

Supporting Information

Electrochemical synthesis of oxazoles via phosphine-mediated deoxygenative [3 + 2] cycloaddition of carboxylic acids

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1. General information

All commercially available reagents were directly used as received without further purification. All organic solvents applied in the reactions were pre-dried by distillation over appropriate drying reagents unless otherwise noted. The electrochemical reactions were performed on a DJS-292B potentiostat (made in China) in constant current mode. All yields of products refer to the isolated yields after chromatography.

^1H NMR (400 MHz), ^{13}C NMR (101 MHz) and ^{19}F NMR (376 MHz) spectra were recorded on a Bruker AV-400 spectrometer or a Quantum-I Plus 400 in Chloroform-*d* or DMSO-*d*₆. For ^1H NMR, Chloroform-*d* (δ = 7.26 ppm), DMSO-*d*₆ (δ = 2.50 ppm) or tetramethylsilane (TMS, δ = 0 ppm) serves as the internal standard; for ^{13}C NMR, Chloroform-*d* (δ = 77.16 ppm) or DMSO-*d*₆ (δ = 39.52 ppm) serves as the internal standard. Data are reported as follows: chemical shift (in ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, hept = heptet, m = multiplet, br = broad), coupling constant (in Hz), and integration.

GC analysis was performed on a 7890B/Agilent, while GC-MS analysis was performed on a 7890A-5975C/Agilent. HR-MS spectra were recorded on a Waters Xevo G2QTOF/UPLC mass spectrometer using electrospray ionization. The cyclic voltammogram was collected with a CHI 760E Potentiostat.

Unless otherwise noted, the substrates were directly obtained from commercial sources.

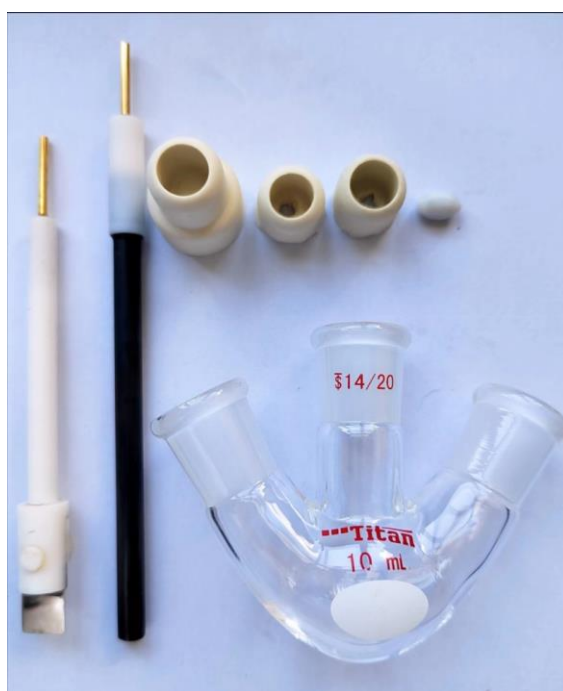


Figure S1. Reaction vessel and electrode materials



Figure S2. The potentiostat

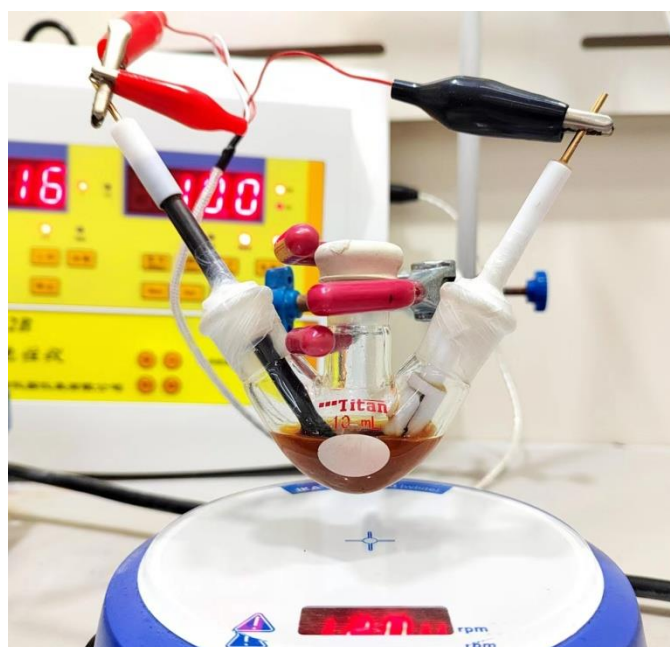
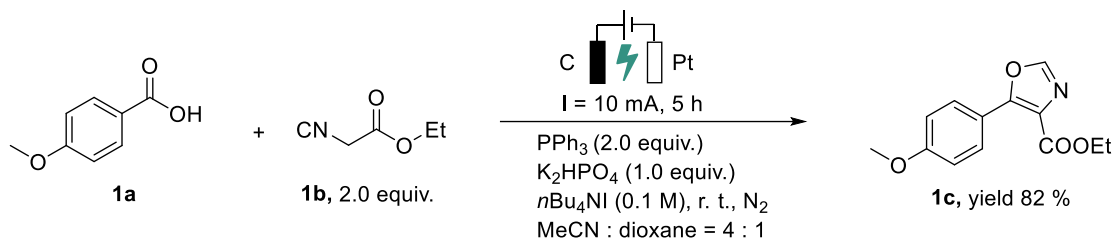


Figure S3. Reaction for standard condition

2. Experimental Procedures and Characterization Data

2.1 Conditions optimizing



Standard conditions: graphite rod anode ($\varphi = 6 \text{ mm}$), Pt plate cathode ($10 \times 10 \times 0.2, \text{ mm}$), **1a** (0.4 mmol), **2a** (0.8 mmol), PPh_3 (0.8 mmol), K_2HPO_4 (0.4 mmol), $n\text{Bu}_4\text{NI}$ (0.1 M) in anhydrous MeCN : dioxane (4 : 1, 4.0 mL), undivided cell, constant current = 10 mA under N_2 at room temperature for 5 h (4.7 F/mol). ^b Isolated yield. NR: no reaction.

Table S1. Control experiments

Entry	Electrolyte	Yield of 3a (%) ^a
1	No current	NR
2	No PPh_3	NR
3	No base	trace

^aIsolated yield, NR= no reaction;

Table S2. Solvent screening

Entry	Electrode	Electrolyte	Solvent	Yield of 3a (%) ^a
1	C/Pt	$n\text{Bu}_4\text{NI}$	MeCN	76
2	C/Pt	$n\text{Bu}_4\text{NI}$	DMF	NR
3	C/Pt	$n\text{Bu}_4\text{NI}$	THF	NR
4	C/Pt	$n\text{Bu}_4\text{NI}$	DMSO	NR
5	C/Pt	$n\text{Bu}_4\text{NI}$	DCE	NR
6	C/Pt	$n\text{Bu}_4\text{NI}$	MTBE	NR
7	C/Pt	$n\text{Bu}_4\text{NI}$	Me_2CO	55
8	C/Pt	$n\text{Bu}_4\text{NI}$	MeCN: HFIP = 4:1	NR
9	C/Pt	$n\text{Bu}_4\text{NI}$	MeCN: AcOH = 4:1	NR
10	C/Pt	$n\text{Bu}_4\text{NI}$	MeCN: MeOH = 4:1	NR
11	C/Pt	$n\text{Bu}_4\text{NI}$	MeCN: H_2O = 4:1	NR
12	C/Pt	$n\text{Bu}_4\text{NI}$	MeCN: dioxane = 4:1	80

^aIsolated yield;

Table S3. Electrolytes screening

Entry	Electrode	Electrolyte	Solvent	Yield of 3a (%) ^a
1	C/Pt	$n\text{Bu}_4\text{NI}$	MeCN: dioxane = 4:1	80
2	C/Pt	NH_4I	MeCN: dioxane = 4:1	Trace
3	C/Pt	$n\text{Bu}_4\text{NBr}$	MeCN: dioxane = 4:1	26

4	C/Pt	<i>n</i> Bu ₄ NCl	MeCN: dioxane = 4:1	67
5	C/Pt	<i>n</i> Bu ₄ NBF ₄	MeCN: dioxane = 4:1	NR
6	C/Pt	<i>n</i> Bu ₄ NClO ₄	MeCN: dioxane = 4:1	NR
7	C/Pt	<i>n</i> Bu ₄ NPF ₆	MeCN: dioxane = 4:1	NR
8	C/Pt	KI	MeCN: dioxane = 4:1	36
9	C/Pt	<i>n</i> Bu ₄ NI (20 %)	MeCN: dioxane = 4:1	33

^aIsolated yield;

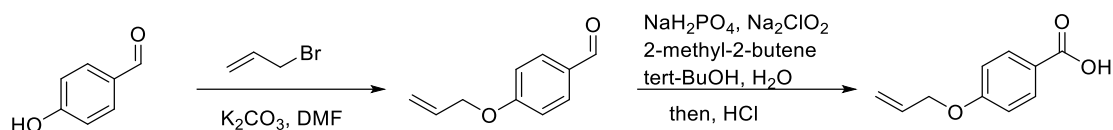
Table S4 . Electrode screening

Entry	Electrode	Electrolyte	Solvent	Yield of 3a (%) ^a
1	C/Pt	<i>n</i> Bu ₄ NI	MeCN: dioxane = 4:1	80
2	C/C	<i>n</i> Bu ₄ NI	MeCN: dioxane = 4:1	46
3	C/Fe	<i>n</i> Bu ₄ NI	MeCN: dioxane = 4:1	33
4	Pt/Pt	<i>n</i> Bu ₄ NI	MeCN: dioxane = 4:1	56
5	Pt/C	<i>n</i> Bu ₄ NI	MeCN: dioxane = 4:1	49
6	RVC/Pt	<i>n</i> Bu ₄ NI	MeCN: dioxane = 4:1	Trace

Table S5 . Base screening

Entry	Electrode	Electrolyte	Base	Yield of 3a (%) ^a
1	C/Pt	<i>n</i> Bu ₄ NI	K ₂ HPO ₄	80
2	C/Pt	<i>n</i> Bu ₄ NI	KH ₂ PO ₄	39
3	C/Pt	<i>n</i> Bu ₄ NI	DABCO	30
4	C/Pt	<i>n</i> Bu ₄ NI	Et ₃ N	Trace
5	C/Pt	<i>n</i> Bu ₄ NI	Collidine	Trace
6	C/Pt	<i>n</i> Bu ₄ NI	K ₂ CO ₃	66
7	C/Pt	<i>n</i> Bu ₄ NI	KAcO	46
8	C/Pt	<i>n</i> Bu ₄ NI	Cs ₂ CO ₃	58
9	C/Pt	<i>n</i> Bu ₄ NI	NaHCO ₃	50

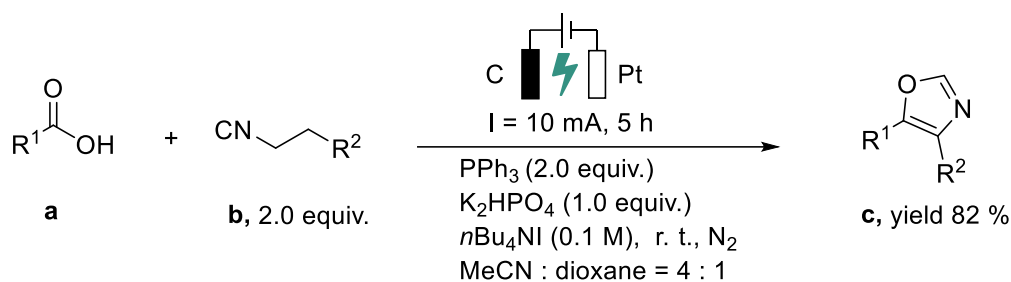
2.2 Substrates preparation



Following the modified procedure of reported literature, a 50 mL oven-dried Schlenk-tube was charged with potassium carbonate (1.25 g, 9.0 mmol), methyl 4-hydroxybenzaldehyde (3.0 mmol, 1.0 equiv.) and the flask was purged and filled with argon. DMF (15 mL, 0.2 M) was added by syringe and the mixture was stirred. The 3-bromoprop-1-ene (3.3 mmol, 1.25 equiv.) was added by syringe and the reaction mixture was stirred under argon at room temperature for 24 h. The mixture was diluted with EtOAc and water, shaken, and separated. The combined organic extracts washed with brine (100 mL), dried (Na_2SO_4), filtered and concentrated in vacuo. Purification by flash chromatography (petroleum ether/EtOAc, 40:1), afforded the corresponding ether products.

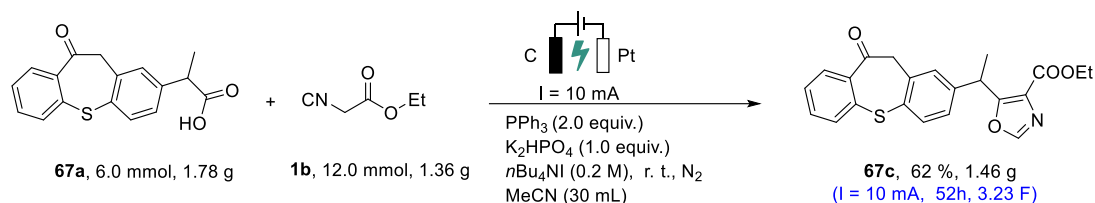
Following the general procedure of reported literature, to a solution of 4-(allyloxy)benzaldehyde (0.20 g, 1.2 mmol), NaH_2PO_4 (144 mg, 1.2 mmol), 2-methyl-2-butene (0.6 mL, 5.3 mmol) in $tert$ -BuOH (8 mL) and water (2 mL) was added $NaClO_2$ (370 mg, 4.1 mmol) and the mixture was stirred for 50 min at room temperature. The reaction mixture was adjusted to pH of 4 by addition of 1 M HCl. The aqueous layer was extracted with CH_2Cl_2 . The organic layers were combined, washed with brine, dried over anhydrous Na_2SO_4 . Purification by flash chromatography, afforded the corresponding 1, 4-(allyloxy)benzoic acid **34a**.

2.3 General procedure for electrocatalysis for oxazoles

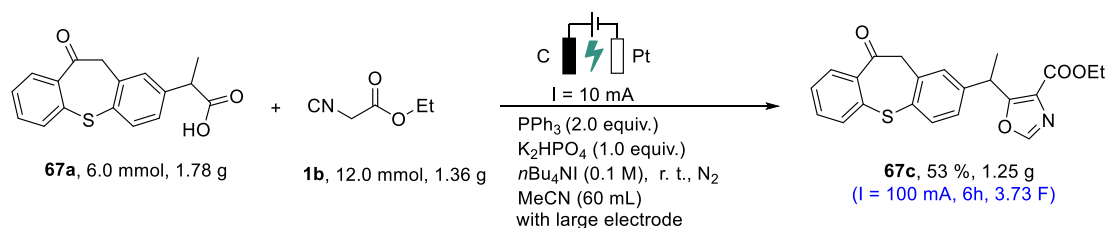


To a 25 mL three-necked flask with a magnetic stir bar was added the substrate carboxylic acid **a** (1 equiv., 0.4 mmol), PPh_3 (2 equiv., 0.4 mmol, 210 mg), K_2HPO_4 (1.0 equiv., 0.4 mmol, 70 mg) and electrolyte $n\text{-Bu}_4\text{NI}$ (0.4 mmol, 148 mg, 0.1 M), followed by 4.0 mL anhydrous MeCN and isocyanide **b** (2.0 equiv, 0.8 mmol). Subsequently, the flask was equipped with a graphite rod (anode, $d = 0.6$ mm, length below the liquid surface = 10 mm) and a platinum plate (cathode, $10 \times 10 \times 0.2$ mm), the distance between which was approximately 1.0 cm. All operations are performed in a glove box and the flask was filled with Ar. The constant current (10 mA) electrolysis was then performed at room temperature (Sealed tube) with vigorous stirring for the indicated time as monitored by TLC or GC-MS analysis. Upon completion, the solvent in reaction mixture was removed under vacuo. The resulting mixture was purified by column chromatography on silica gel (eluted with EtOAc/PE) to afford the desired products **c**.

2.4 Procedure for the gram-scale reactions (6.0 mmol scale)



To a 50 mL flask with a magnetic stir bar was added the substrate carboxylic acid **67a** (1.0 equiv., 6 mmol, 1.78 g), PPh_3 (2.0 equiv., 2.4 mmol, 3.15 g), K_2HPO_4 (1.0 equiv., 6 mmol, 1.05 g) and electrolyte $n\text{-Bu}_4\text{NI}$ (6 mmol, 2.21 g, 0.2 M), followed by 30 mL anhydrous MeCN and isocyanide **1b** (2.0 equiv., 12 mmol, 1.36 g). Subsequently, the flask was equipped with a graphite rod (anode, $d = 0.6$ mm, length below the liquid surface = 10 mm) and a platinum plate (cathode, $10 \times 10 \times 0.2$ mm), the distance between which was approximately 1.0 cm. The constant current (10 mA) electrolysis was then performed at room temperature (sealed tube, under air) with vigorous stirring for the indicated time as monitored by TLC or GC-MS analysis. Upon completion, the solvent in reaction mixture was removed under vacuo. The resulting mixture was purified by column chromatography on silica gel (eluted with EtOAc/PE) to afford the desired products **67c**.

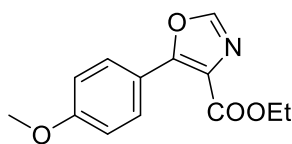


To a 50 mL flask with a magnetic stir bar was added the substrate carboxylic acid **67a** (1 equiv., 6 mmol, 1.78 g), PPh_3 (2 equiv., 2.4 mmol, 3.15 g), K_2HPO_4 (1.0 equiv., 6 mmol, 1.05 g) and electrolyte $n\text{-Bu}_4\text{NI}$ (6 mmol, 2.21 g, 0.1 M), followed by 60 mL anhydrous MeCN and isocyanide **1b** (2.0 equiv., 12 mmol, 1.36 g). Subsequently, the flask was equipped with a graphite plate (anode, $20 \times 20 \times 5$ mm) and a platinum plate (cathode, $10 \times 10 \times 0.2$ mm), the distance between which was approximately 1.0 cm. The constant current (100 mA) electrolysis was then performed at room temperature (sealed tube, under air) with vigorous stirring for the indicated time as monitored by TLC or GC-MS analysis. Upon completion, the solvent in reaction mixture was removed under vacuo. The resulting mixture was purified by column chromatography on silica gel (eluted with EtOAc/PE) to afford the desired products **67c**.



Figure S4. Gram-scale reactions for standard condition

2.5 Characterization data



1c: ethyl 5-(4-methoxyphenyl)oxazole-4-carboxylate

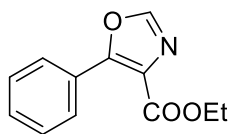
Brown yellow solid.

80.9 mg, 82% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.04 (d, J = 8.9 Hz, 2H), 7.83 (s, 1H), 6.95 (d, J = 9.0 Hz, 2H), 4.38 (q, J = 7.1 Hz, 2H), 3.83 (s, 3H), 1.38 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.24, 161.31, 155.85, 148.48, 130.23, 125.35, 119.27, 113.90, 77.50, 77.18, 76.86, 61.36, 55.43, 14.34.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{14}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 264.1236, found 264.1238.



2c: ethyl 5-phenyloxazole-4-carboxylate

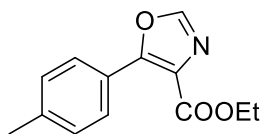
Light yellow oil.

72.3 mg, 83% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.09 – 8.03 (m, 2H), 7.90 (s, 1H), 7.49 – 7.43 (m, 3H), 4.41 (q, J = 7.1 Hz, 2H), 1.39 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.02, 155.60, 149.08, 130.56, 128.55, 128.49, 126.77, 126.69, 77.45, 77.14, 76.82, 61.50, 14.30.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{12}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 218.0817, found 218.0814.



3c: ethyl 5-(p-tolyl)oxazole-4-carboxylate

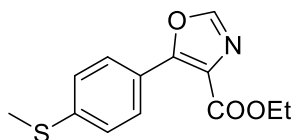
Yellow solid.

73.6 mg, 79% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, J = 8.2 Hz, 2H), 7.88 (s, 1H), 7.28 (d, J = 8.0 Hz, 2H), 4.41 (q, J = 7.1 Hz, 2H), 2.41 (s, 3H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.11, 155.91, 148.82, 140.96, 129.21, 128.47, 126.12, 123.95, 77.48, 77.16, 76.84, 61.43, 21.59, 14.33.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{14}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 232.0974, found 232.0971.



4c: ethyl 5-(4-(methylthio)phenyl)oxazole-4-carboxylate

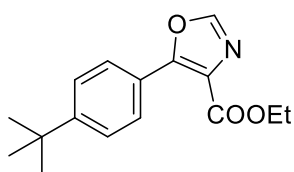
Yellow solid.

69.7 mg, 66% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.02 (d, J = 8.5 Hz, 2H), 7.87 (s, 1H), 7.30 (d, J = 8.6 Hz, 2H), 4.41 (q, J = 7.1 Hz, 2H), 2.51 (s, 3H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.12, 155.42, 148.76, 142.41, 128.72, 126.22, 125.47, 123.02, 77.43, 77.12, 76.80, 61.49, 15.09, 14.34.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{14}\text{NO}_3\text{S}^+$ m/z $[\text{M}+\text{H}]^+$: 264.0694, found 264.0692.



5c: ethyl 5-(4-(tert-butyl)phenyl)oxazole-4-carboxylate

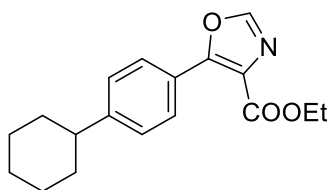
Yellow solid.

92.9 mg, 85% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.00 (d, J = 8.6 Hz, 2H), 7.88 (s, 1H), 7.49 (d, J = 8.6 Hz, 2H), 4.41 (q, J = 7.1 Hz, 2H), 1.41 (t, J = 7.1 Hz, 3H), 1.34 (s, 9H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.13, 155.91, 154.00, 148.86, 128.33, 126.21, 125.50, 123.92, 77.44, 77.12, 76.81, 61.43, 34.99, 31.19, 14.34

HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{20}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 274.1443, found 274.1440.



6c: ethyl 5-(4-cyclohexylphenyl)oxazole-4-carboxylate

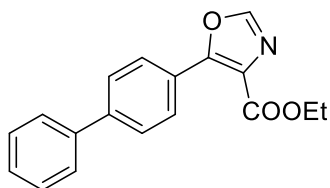
Yellow solid.

91.6 mg, 75% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, J = 8.4 Hz, 2H), 7.87 (s, 1H), 7.31 (d, J = 8.5 Hz, 2H), 4.41 (q, J = 7.2 Hz, 2H), 2.61 – 2.49 (m, 1H), 1.92 – 1.81 (m, 4H), 1.78 – 1.73 (m, 1H), 1.41 (m, 7H), 1.30 – 1.24 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.14, 155.98, 150.96, 148.81, 128.56, 127.02, 126.12, 124.27, 77.44, 77.12, 76.80, 61.42, 44.62, 34.23, 26.83, 26.12, 14.33.

HRMS (ESI) calcd for $C_{18}H_{22}NO_3^+$ m/z $[M+H]^+$: 300.1600, found 300.1600.



7c: ethyl 5-([1,1'-biphenyl]-4-yl)oxazole-4-carboxylate

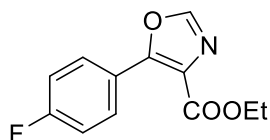
Brown solid.

60.7 mg, 52% yield

1H NMR (400 MHz, Chloroform-*d*) δ 8.17 (d, J = 6.6 Hz, 2H), 7.92 (s, 1H), 7.71 (d, J = 8.5 Hz, 2H), 7.64 (d, J = 6.9 Hz, 2H), 7.50 – 7.44 (m, 2H), 7.41 – 7.36 (m, 1H), 4.45 (q, J = 7.1 Hz, 2H), 1.43 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.12, 155.47, 149.06, 143.24, 140.14, 129.01, 128.97, 128.04, 127.21, 127.16, 126.72, 125.61, 77.46, 77.14, 76.82, 61.57, 14.36.

HRMS (ESI) calcd for $C_{18}H_{16}NO_3^+$ m/z $[M+H]^+$: 294.1130, found 294.1128.



8c: ethyl 5-(4-fluorophenyl)oxazole-4-carboxylate

Yellow solid.

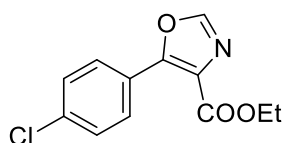
72.0 mg, 77% yield

1H NMR (400 MHz, Chloroform-*d*) δ 8.13 – 8.05 (m, 2H), 7.88 (s, 1H), 7.18 – 7.10 (m, 2H), 4.40 (q, J = 7.1 Hz, 2H), 1.39 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.90 (d, J = 253.5 Hz), 162.02, 154.76, 148.95, 130.80 (d, J = 9.1 Hz), 126.46, 123.00 (d, J = 3.0 Hz), 115.70 (d, J = 21.2 Hz), 77.45, 77.14, 76.82, 61.57, 14.29.

^{19}F NMR (376 MHz, $CDCl_3$) δ -108.77.

HRMS (ESI) calcd for $C_{12}H_{11}FNO_3^+$ m/z $[M+H]^+$: 236.0723, found 236.0724.



9c: ethyl 5-(4-chlorophenyl)oxazole-4-carboxylate

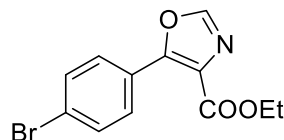
Light yellow solid.

67.1 mg, 67% yield

1H NMR (400 MHz, Chloroform-*d*) δ 8.05 (d, J = 8.7 Hz, 2H), 7.91 (s, 1H), 7.44 (d, J = 8.7 Hz, 2H), 4.41 (q, J = 7.1 Hz, 2H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.96, 154.55, 149.14, 136.70, 129.84, 128.85, 128.51, 125.20, 77.44, 77.12, 76.81, 61.68, 14.31.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{11}\text{ClNO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 252.0427, found 254.0422.



10c: ethyl 5-(4-bromophenyl)oxazole-4-carboxylate

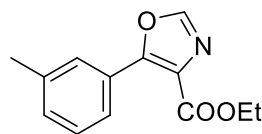
Light yellow solid.

67.7 mg, 58% yield

^1H NMR (400 MHz, $\text{Chloroform-}d$) δ 7.97 (d, $J = 8.7$ Hz, 2H), 7.91 (s, 1H), 7.60 (d, $J = 8.7$ Hz, 2H), 4.41 (q, $J = 7.1$ Hz, 2H), 1.40 (t, $J = 7.2$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.92, 154.55, 149.57, 131.79, 129.98, 127.07, 125.63, 125.11, 77.43, 77.11, 76.79, 61.66, 14.29.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{11}\text{BrNO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 295.9922, found 295.9926.



11c: ethyl 5-(m-tolyl)oxazole-4-carboxylate

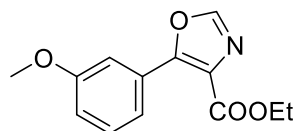
Colorless oil.

66.8 mg, 72% yield

^1H NMR (400 MHz, $\text{Chloroform-}d$) δ 7.89 (s, 1H), 7.88 – 7.83 (m, 2H), 7.39 – 7.33 (m, 1H), 7.27 (d, $J = 7.7$ Hz, 1H), 4.41 (q, $J = 7.1$ Hz, 2H), 2.42 (s, 3H), 1.40 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.02, 155.78, 149.01, 138.19, 131.36, 129.06, 128.40, 126.69, 126.56, 125.78, 77.44, 77.12, 76.80, 61.45, 21.52, 14.31.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{14}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 232.0974, found 232.0974.



12c: ethyl 5-(3-methoxyphenyl)oxazole-4-carboxylate

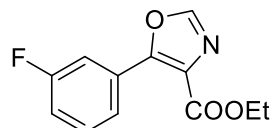
Yellow solid.

79.3 mg, 80% yield

^1H NMR (400 MHz, $\text{Chloroform-}d$) δ 7.90 (s, 1H), 7.72 (s, 1H), 7.64 (d, $J = 7.7$ Hz, 1H), 7.38 (m, 1H), 7.00 (dd, $J = 8.3, 1.7$ Hz, 1H), 4.41 (q, $J = 7.1$ Hz, 2H), 3.86 (s, 3H), 1.40 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.01, 159.55, 155.35, 148.98, 129.59, 127.87, 126.83, 120.85, 116.68, 113.72, 77.43, 77.11, 76.79, 61.54, 55.48, 14.32.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{14}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 248.0923, found 248.0919.



13c: ethyl 5-(3-fluorophenyl)oxazole-4-carboxylate

Yellow solid.

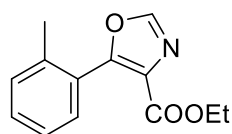
56.6 mg, 60% yield

^1H NMR (400 MHz, Chloroform- d) δ 7.92 (s, 1H), 7.90 – 7.84 (m, 2H), 7.46 – 7.40 (m, 1H), 7.18 – 7.11 (m, 1H), 4.42 (q, J = 7.1 Hz, 2H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.56 (d, J = 45.5 Hz), 161.82, 154.10 (d, J = 3.0 Hz), 149.25, 130.07 (d, J = 8.1 Hz), 130.13, 128.60 (d, J = 9.1 Hz), 127.39, 124.16 (d, J = 6.1 Hz), 117.51 (d, J = 21.2 Hz), 115.51 (d, J = 25.3 Hz), 77.44, 77.12, 76.81, 61.70, 11.64.

^{19}F NMR (376 MHz, CDCl_3) δ -112.02.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{11}\text{FNO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 236.2723, found 236.2720.



14c: ethyl 5-(o-tolyl)oxazole-4-carboxylate

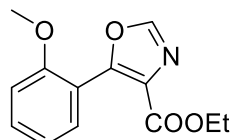
Light yellow oil.

69.3 mg, 75% yield

^1H NMR (400 MHz, Chloroform- d) δ 7.96 (s, 1H), 7.44 (d, J = 7.1 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.32 – 7.26 (m, 2H), 4.31 (q, J = 7.1 Hz, 2H), 2.28 (s, 3H), 1.28 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.48, 156.25, 149.90, 138.05, 130.96, 130.60, 130.45, 128.37, 126.65, 125.49, 77.43, 77.12, 76.80, 61.23, 20.55, 14.15.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{14}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 232.0974, found 232.0974.



15c: ethyl 5-(2-methoxyphenyl)oxazole-4-carboxylate

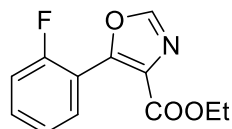
Colorless solid.

75.3 mg, 76% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.93 (s, 1H), 7.50 – 7.42 (m, 2H), 7.07 – 7.01 (m, 1H), 6.98 (d, J = 8.3 Hz, 1H), 4.30 (q, J = 7.1 Hz, 2H), 3.80 (s, 3H), 1.27 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.81, 157.54, 152.98, 149.87, 132.13, 131.52, 128.75, 120.29, 116.24, 111.21, 77.45, 77.13, 76.81, 61.06, 55.64, 14.20.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{14}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 248.0923, found 248.0921.



16c: ethyl 5-(2-fluorophenyl)oxazole-4-carboxylate

Brown solid.

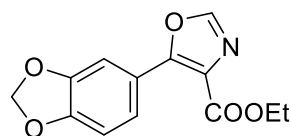
58.2 mg, 62% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.02 (s, 1H), 7.71 – 7.65 (m, 1H), 7.56 – 7.47 (m, 1H), 7.32 – 7.26 (m, 1H), 7.25 – 7.19 (m, 1H), 4.38 (q, J = 7.1 Hz, 2H), 1.34 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.35, 160.20 (d, J = 211.1 Hz), 150.40, 132.60 (d, J = 8.1 Hz), 131.35, 129.24, 124.02 (d, J = 4.0 Hz), 116.16 (d, J = 22.2 Hz), 115.56 (d, J = 14.1 Hz), 77.45, 77.13, 76.82, 61.43, 14.13.

^{19}F NMR (376 MHz, CDCl_3) δ -110.94.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{10}\text{FNO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 236.0723, found 236.0724.



17c: ethyl 5-(benzo[d][1,3]dioxol-5-yl)oxazole-4-carboxylate

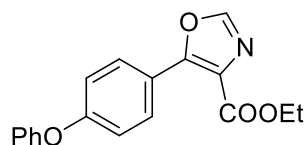
Yellow solid.

76.2 mg, 73% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.84 (s, 1H), 7.68 – 7.65 (m, 1H), 7.61 (d, J = 1.8 Hz, 1H), 6.89 (d, J = 8.3 Hz, 1H), 6.02 (s, 2H), 4.40 (q, J = 7.1 Hz, 2H), 1.40 (t, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.16, 155.49, 149.53, 148.46, 147.81, 125.14, 123.59, 119.29, 108.78, 108.42, 101.69, 77.45, 77.13, 76.82, 61.48, 14.34.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{12}\text{NO}_5^+$ m/z $[\text{M}+\text{H}]^+$: 262.0715, found 262.0718.



18c: ethyl 5-(4-phenoxyphenyl)oxazole-4-carboxylate

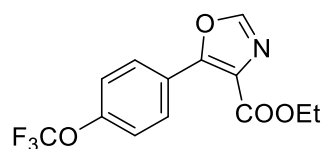
Yellow solid.

83.1 mg, 67% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.07 (d, J = 8.9 Hz, 2H), 7.87 (s, 1H), 7.40 – 7.35 (m, 2H), 7.18 (d, J = 7.4 Hz, 1H), 7.09 – 7.03 (m, 4H), 4.41 (q, J = 7.1 Hz, 2H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.17, 159.63, 155.95, 155.45, 148.74, 130.39, 130.05, 125.91, 124.35, 121.26, 119.94, 117.87, 77.46, 77.15, 76.83, 64.44, 13.48.

HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{16}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 310.1079, found 310.1075.



19c: ethyl 5-(4-(trifluoromethoxy)phenyl)oxazole-4-carboxylate

Yellow solid.

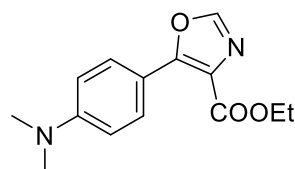
84.4 mg, 70% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.14 (d, J = 8.9 Hz, 2H), 7.91 (s, 1H), 7.29 (d, J = 8.5 Hz, 2H), 4.40 (q, J = 7.1 Hz, 2H), 1.39 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.91, 154.23, 150.54, 149.23, 130.29, 127.09, 125.28, 120.65, 77.45, 77.13, 76.81, 61.66, 14.23.

^{19}F NMR (376 MHz, CDCl_3) δ -57.73.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{11}\text{F}_3\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 302.0640, found 302.0636.



20c: ethyl 5-(4-(dimethylamino)phenyl)oxazole-4-carboxylate

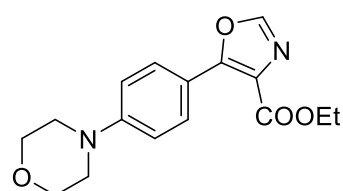
Yellow solid.

69.9 mg, 67% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.04 (d, J = 9.1 Hz, 2H), 7.79 (s, 1H), 6.73 (d, J = 9.1 Hz, 2H), 4.41 (q, J = 7.1 Hz, 2H), 3.03 (s, 6H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.54, 156.96, 151.58, 147.76, 129.78, 123.88, 113.65, 111.31, 77.44, 77.12, 76.80, 61.14, 40.15, 14.43.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{17}\text{N}_2\text{O}_3^+$ m/z $[\text{M}+\text{H}]^+$: 261.1239, found 261.1235.



21c: ethyl 5-(4-morpholinophenyl)oxazole-4-carboxylate

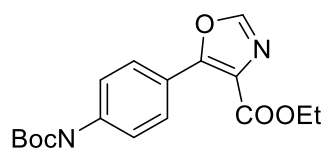
Brown yellow solid.

64.5 mg, 53% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.04 (d, J = 8.9 Hz, 2H), 7.82 (s, 1H), 6.94 (d, J = 9.0 Hz, 2H), 4.40 (q, J = 7.1 Hz, 2H), 3.89 – 3.82 (m, 4H), 3.30 – 3.22 (m, 4H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.37, 156.18, 152.40, 148.19, 129.79, 124.87, 117.40, 114.19, 77.44, 77.12, 76.81, 66.72, 61.29, 48.05, 14.39.

HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{19}\text{N}_2\text{O}_4^+$ m/z $[\text{M}+\text{H}]^+$: 303.1345, found 303.1346.

**22c: ethyl 5-(4-((tert-butoxycarbonyl)-l2-azanyl)phenyl)oxazole-4-carboxylate**

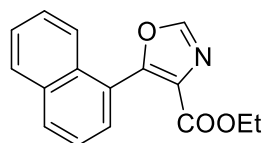
Yellow solid.

79.3 mg, 66% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.03 (d, J = 8.8 Hz, 2H), 7.85 (s, 1H), 7.47 (d, J = 8.7 Hz, 2H), 6.88 (s, 1H), 4.39 (q, J = 7.1 Hz, 2H), 1.50 (s, 6H), 1.38 (t, J = 7.1 Hz, 2H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.21, 155.57, 152.46, 148.62, 140.63, 129.50, 125.74, 121.08, 117.81, 81.07, 77.46, 77.14, 76.82, 61.41, 28.34, 14.32.

HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{20}\text{N}_2\text{O}_5^+$ m/z $[\text{M}+\text{H}]^+$: 232.1372, found 232.1374.

**23c: ethyl 5-(naphthalen-1-yl)oxazole-4-carboxylate**

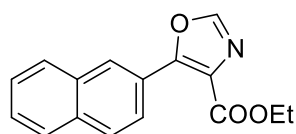
Yellow solid.

44.6 mg, 42% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.07 (s, 1H), 8.01 (d, J = 8.3 Hz, 1H), 7.92 (d, J = 6.4 Hz, 1H), 7.74 – 7.67 (m, 2H), 7.59 – 7.48 (m, 2H), 4.22 (q, J = 7.1 Hz, 2H), 1.10 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.40, 155.23, 150.33, 133.48, 131.53, 131.24, 129.81, 129.37, 128.63, 127.09, 126.41, 125.09, 124.82, 124.44, 77.45, 77.13, 76.81, 61.20, 13.94.

HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{14}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 268.0974, found 268.0974.

**24c: ethyl 5-(naphthalen-2-yl)oxazole-4-carboxylate**

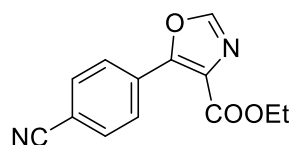
Light yellow solid.

70.7 mg, 66% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.66 (s, 1H), 8.08 (dd, J = 8.6, 1.8 Hz, 1H), 7.95 – 7.88 (m, 3H), 7.87 – 7.82 (m, 1H), 7.56 – 7.49 (m, 2H), 4.44 (q, J = 7.1 Hz, 2H), 1.42 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.09, 155.65, 149.17, 134.02, 132.80, 129.12, 129.01, 128.16, 127.77, 127.68, 126.90, 126.76, 124.95, 124.06, 77.49, 77.18, 76.86, 61.55, 14.36.

HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{14}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 268.0974, found 268.0971.



25c: ethyl 5-(4-cyanophenyl)oxazole-4-carboxylate

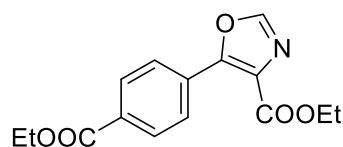
Light yellow solid.

61.2 mg, 63% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.26 (d, J = 8.6 Hz, 2H), 7.99 (s, 1H), 7.76 (d, J = 8.6 Hz, 2H), 4.44 (d, J = 7.1 Hz, 2H), 1.42 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.70, 153.24, 149.87, 132.30, 130.77, 128.92, 128.71, 118.31, 113.83, 77.43, 77.11, 76.80, 61.99, 14.28.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{11}\text{N}_2\text{O}_3^+$ m/z $[\text{M}+\text{H}]^+$: 243.0770, found 243.0772.



26c: ethyl 5-(4-(ethoxycarbonyl)phenyl)oxazole-4-carboxylate

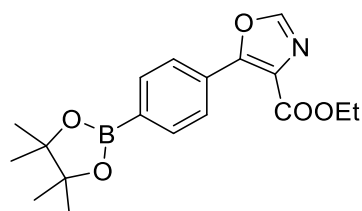
Brown yellow solid.

66.9 mg, 58% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.20 – 8.10 (m, 4H), 7.96 (s, 1H), 4.43 (q, J = 7.1 Hz, 2H), 3.94 (s, 3H), 1.41 (t, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 166.43, 161.81, 154.28, 150.02, 131.56, 130.74, 129.69, 128.42, 128.00, 77.43, 77.11, 76.79, 61.78, 52.46, 14.29.

HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{16}\text{NO}_5^+$ m/z $[\text{M}+\text{H}]^+$: 290.1028, found 290.1026.



27c: ethyl 5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)oxazole-4-carboxylate

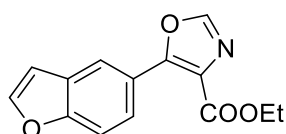
White solid.

53.9 mg, 39% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.04 (d, J = 8.3 Hz, 2H), 7.91 (s, 1H), 7.89 (d, J = 8.3 Hz, 2H), 4.40 (q, J = 7.2 Hz, 2H), 1.39 (t, J = 7.1 Hz, 3H), 1.35 (s, 12H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.88, 155.33, 149.27, 134.76, 129.09, 127.61, 127.19, 84.15, 77.44, 77.12, 76.80, 61.52, 24.92, 14.30.

HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{23}\text{BNO}_5^+$ m/z $[\text{M}+\text{H}]^+$: 344.1669, found 344.1667.



28c: ethyl 5-(benzofuran-5-yl)oxazole-4-carboxylate

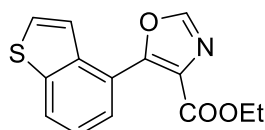
Yellow oil.

70.3 mg, 68% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.40 (d, J = 1.8 Hz, 1H), 7.98 (d, J = 8.7 Hz, 1H), 7.90 (s, 1H), 7.67 (d, J = 2.2 Hz, 1H), 7.58 (d, J = 7.8 Hz, 1H), 6.85 (s, 1H), 4.42 (q, J = 7.1 Hz, 2H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.21, 156.24, 155.87, 148.80, 146.16, 127.16, 125.99, 125.05, 122.38, 121.68, 111.56, 106.43, 77.45, 77.13, 76.81, 61.46, 14.33.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{12}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 258.0766, found 258.0767.



29c: ethyl 5-(benzo[b]thiophen-4-yl)oxazole-4-carboxylate

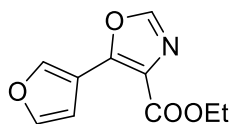
Yellow solid.

57.2 mg, 52% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.03 (s, 1H), 8.00 (d, J = 7.9 Hz, 2H), 7.82 (d, J = 7.4 Hz, 1H), 7.54 (d, J = 5.5 Hz, 1H), 7.47 – 7.41 (m, 1H), 7.37 (d, J = 5.6 Hz, 1H), 4.31 (q, J = 7.1 Hz, 2H), 1.25 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.56, 155.33, 149.78, 140.54, 137.73, 128.10, 128.02, 127.09, 125.07, 123.64, 123.07, 121.37, 77.46, 77.14, 76.82, 61.39, 14.58.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{12}\text{NO}_3\text{S}^+$ m/z $[\text{M}+\text{H}]^+$: 274.0538, found 274.0535.



30c: ethyl 5-(furan-3-yl)oxazole-4-carboxylate

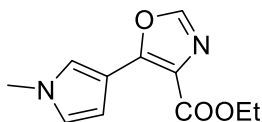
Brown oil.

61.1 mg, 74% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.51 (s, 1H), 7.81 (s, 1H), 7.50 – 7.48 (m, 1H), 6.97 (d, J = 2.4 Hz, 1H), 4.42 (q, J = 7.2 Hz, 2H), 1.42 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.02, 151.06, 148.40, 145.12, 143.48, 126.12, 113.75, 109.03, 77.44, 77.12, 76.80, 61.37, 14.38.

HRMS (ESI) calcd for $\text{C}_{10}\text{H}_{10}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 208.0610, found 208.0615.



31c: ethyl 5-(1-methyl-1H-pyrrol-3-yl)oxazole-4-carboxylate

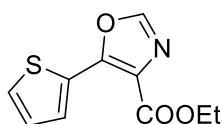
Brown yellow solid.

43.3 mg, 49% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.85 (s, 1H), 7.70 (s, 1H), 6.73 – 6.70 (m, 1H), 6.65 – 6.62 (m, 1H), 4.41 (q, J = 7.1 Hz, 2H), 3.71 (s, 3H), 1.43 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.72, 154.20, 147.03, 125.37, 122.79, 122.21, 111.03, 108.54, 77.43, 77.11, 76.79, 60.93, 36.67, 14.49.

HRMS (ESI) calcd for $\text{C}_{11}\text{H}_{13}\text{N}_2\text{O}_3^+$ m/z $[\text{M}+\text{H}]^+$: 221.0926, found 221.0927.



32c: ethyl 5-(thiophen-2-yl)oxazole-4-carboxylate

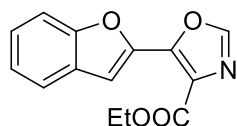
Brown yellow oil.

49.3 mg, 55% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.08 (dd, J = 3.8, 1.2 Hz, 1H), 7.80 (s, 1H), 7.53 (dd, J = 5.0, 1.2 Hz, 1H), 7.16 – 7.13 (m, 1H), 4.45 (q, J = 7.1 Hz, 2H), 1.43 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.97, 151.50, 148.17, 130.55, 129.93, 128.19, 127.84, 124.67, 77.44, 77.13, 76.81, 61.52, 14.41.

HRMS (ESI) calcd for $\text{C}_{10}\text{H}_{10}\text{NO}_3\text{S}^+$ m/z $[\text{M}+\text{H}]^+$: 224.0381, found 224.0376.



33c: ethyl 5-(benzofuran-2-yl)oxazole-4-carboxylate

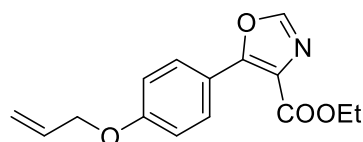
White solid.

46.6 mg, 46% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.11 (s, 1H), 7.96 (s, 1H), 7.69 (d, $J = 5.8$ Hz, 1H), 7.57 (d, $J = 7.4$ Hz, 1H), 7.43 – 7.38 (m, 1H), 7.33 – 7.27 (m, 1H), 4.49 (q, $J = 7.1$ Hz, 2H), 1.47 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.43, 155.20, 149.24, 147.25, 143.07, 128.10, 127.43, 126.69, 123.80, 122.49, 111.97, 111.64, 77.42, 77.10, 76.78, 61.74, 14.40.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{12}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 258.0766, found 258.0764.



34c: ethyl 5-(4-(allyloxy)phenyl)oxazole-4-carboxylate

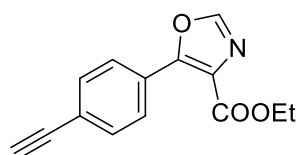
Yellow solid.

72.6 mg, 66% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.05 (d, $J = 9.0$ Hz, 2H), 7.85 (s, 1H), 6.99 (d, $J = 9.0$ Hz, 2H), 6.11 – 5.99 (m, 1H), 5.42 (dd, $J = 17.3, 1.6$ Hz, 1H), 5.31 (dd, $J = 10.5, 1.4$ Hz, 1H), 4.59 (d, $J = 5.4$ Hz, 2H), 4.41 (q, $J = 7.1$ Hz, 2H), 1.40 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.26, 160.34, 155.84, 149.48, 134.11, 130.22, 125.42, 120.09, 117.64, 113.70, 77.43, 77.12, 76.80, 68.90, 60.82, 14.35.

HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{16}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 274.1079, found 274.1082.



35c: ethyl 5-(4-ethynylphenyl)oxazole-4-carboxylate

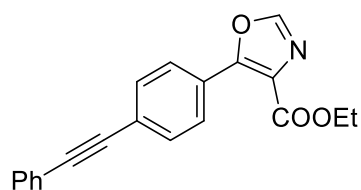
Light yellow solid.

48.3 mg, 50% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, $J = 8.5$ Hz, 2H), 7.91 (s, 1H), 7.57 (d, $J = 8.5$ Hz, 2H), 4.41 (q, $J = 7.2$ Hz, 2H), 3.20 (s, 1H), 1.40 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.91, 154.64, 149.26, 132.18, 128.31, 127.29, 126.88, 124.26, 83.07, 79.46, 77.45, 77.13, 76.81, 61.65, 14.30.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{12}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 242.0817, found 242.0821.



36c: ethyl 5-(4-(phenylethynyl)phenyl)oxazole-4-carboxylate

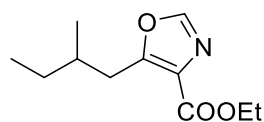
Yellow solid.

76.3 mg, 60% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.11 (d, J = 8.5 Hz, 2H), 7.91 (s, 1H), 7.62 (d, J = 8.5 Hz, 2H), 7.55 (dd, J = 6.7, 3.0 Hz, 2H), 7.39 – 7.33 (m, 3H), 4.42 (q, J = 7.2 Hz, 2H), 1.42 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.99, 154.86, 149.17, 131.79, 131.64, 128.72, 128.49, 128.36, 127.13, 126.26, 125.53, 122.90, 91.77, 88.95, 77.45, 77.14, 76.82, 61.64, 14.33.

HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{16}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 318.1130, found 318.1132.



37c: ethyl 5-(2-methylbutyl)oxazole-4-carboxylate

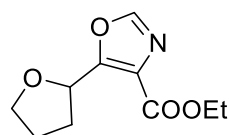
Colorless solid.

58.4 mg, 69% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.74 (s, 1H), 4.35 (q, J = 7.1 Hz, 2H), 3.05 – 2.83 (m, 2H), 1.89 – 1.77 (m, 1H), 1.41 – 1.33 (m, 2H), 1.26 – 1.18 (m, 0H), 0.91 – 0.86 (m, 5H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.19, 159.75, 149.00, 127.68, 77.43, 77.11, 76.79, 60.98, 34.42, 32.66, 29.29, 19.03, 14.82, 11.30.

HRMS (ESI) calcd for $\text{C}_{11}\text{H}_{18}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 212.1287, found 212.1289.



38c: ethyl 5-(tetrahydrofuran-2-yl)oxazole-4-carboxylate

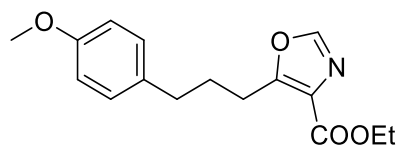
Yellow oil.

43.4 mg, 51% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.80 (s, 1H), 5.65 (t, J = 8.0 Hz, 1H), 4.42 – 4.34 (m, 2H), 4.11 – 4.04 (m, 1H), 3.97 – 3.91 (m, 1H), 2.38 – 2.27 (m, 1H), 2.21 – 1.99 (m, 3H), 1.38 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.62, 158.49, 149.64, 128.01, 77.43, 77.11, 76.79, 71.22, 69.33, 61.39, 30.55, 26.75, 14.32.

HRMS (ESI) calcd for $C_{10}H_{14}NO_4^+$ m/z $[M+H]^+$: 212.0923, found 212.0927.



39c: ethyl 5-(3-(4-methoxyphenyl)propyl)oxazole-4-carboxylate

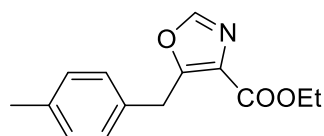
Light yellow oil.

76.6 mg, 66% yield

1H NMR (400 MHz, Chloroform-*d*) δ 7.75 (s, 1H), 7.08 (d, J = 8.6 Hz, 2H), 6.82 (d, J = 8.6 Hz, 2H), 4.35 (q, J = 7.1 Hz, 2H), 3.77 (s, J = 7.6 Hz, 3H), 3.06 (t, J = 7.6 Hz, 2H), 2.61 (t, J = 7.7 Hz, 3H), 2.03 – 1.93 (m, 2H), 1.36 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.12, 159.94, 157.99, 149.00, 133.32, 129.35, 127.14, 113.88, 77.45, 77.13, 76.81, 61.03, 55.31, 34.40, 29.47, 25.50, 14.34.

HRMS (ESI) calcd for $C_{16}H_{20}NO_4^+$ m/z $[M+H]^+$: 290.1392, found 290.1389.



40c: ethyl 5-(4-methylbenzyl)oxazole-4-carboxylate

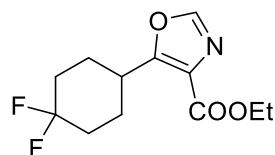
Light yellow oil.

55.5 mg, 56% yield

1H NMR (400 MHz, Chloroform-*d*) δ 7.73 (s, 1H), 7.19 – 7.09 (m, 4H), 4.41 (q, J = 7.2 Hz, 2H), 4.36 (s, 2H), 2.31 (s, 3H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.11, 158.17, 149.39, 136.87, 132.94, 129.51, 128.74, 127.16, 77.46, 77.14, 76.82, 61.21, 31.61, 21.11, 14.39.

HRMS (ESI) calcd for $C_{14}H_{16}NO_3^+$ m/z $[M+H]^+$: 246.1130, found 246.1127.



41c: ethyl 5-(4,4-difluorocyclohexyl)oxazole-4-carboxylate

White solid.

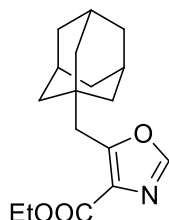
57.1 mg, 55% yield

1H NMR (400 MHz, Chloroform-*d*) δ 7.76 (s, 1H), 4.37 (q, J = 7.1 Hz, 2H), 3.61 – 3.52 (m, 1H), 2.23 – 2.14 (m, 2H), 1.97 – 1.76 (m, 6H), 1.38 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.09, 161.49, 161.46, 149.00, 126.44, 125.40, 122.49, 122.47, 120.67, 77.43, 77.12, 76.80, 61.23, 33.55, 33.42, 33.31, 33.29, 33.06, 26.81 (d, J = 11.1 Hz), 14.32.

^{19}F NMR (376 MHz, Chloroform- d) δ -92.33 (d, J = 237.7 Hz), -102.14 (d, J = 238.1 Hz).

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{16}\text{F}_2\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 260.1098, found 260.1095.



42c: ethyl 5-(((3r,5r,7r)-adamantan-1-yl)methyl)oxazole-4-carboxylate

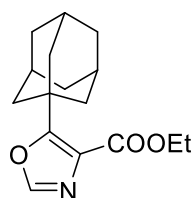
White solid.

101.9 mg, 88% yield

^1H NMR (400 MHz, Chloroform- d) δ 7.76 (s, 1H), 4.35 (q, J = 7.1 Hz, 2H), 2.83 (s, 2H), 1.93 (s, 3H), 1.69 – 1.52 (m, 13H), 1.38 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.29, 158.53, 149.77, 128.65, 77.43, 77.11, 76.79, 60.96, 42.45, 39.74, 36.71, 35.03, 28.66, 14.36.

HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{24}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 290.1756, found 290.1752.



43c: ethyl 5-((3r,5r,7r)-adamantan-1-yl)oxazole-4-carboxylate

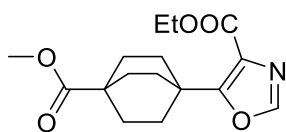
White solid.

93.6 mg, 85% yield

^1H NMR (400 MHz, Chloroform- d) δ 7.68 (s, 1H), 4.36 (q, J = 7.1 Hz, 2H), 2.16 – 2.11 (m, 6H), 2.05 (s, 3H), 1.82 – 1.70 (m, 6H), 1.39 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 165.86, 162.25, 147.41, 126.05, 77.44, 77.13, 76.81, 61.17, 38.92, 37.06, 35.50, 28.18, 14.37.

HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{22}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 276.1600, found 276.1598.



44c: ethyl 5-(4-(methoxycarbonyl)bicyclo[2.2.2]octan-1-yl)oxazole-4-carboxylate

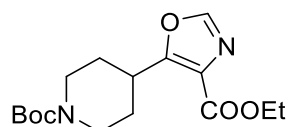
Brown solid.

75.2 mg, 61% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.68 (s, 1H), 4.34 (q, J = 7.1 Hz, 2H), 3.63 (s, 3H), 2.09 – 2.02 (m, 6H), 1.89 – 1.83 (m, 6H), 1.37 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 178.35, 164.65, 162.15, 147.74, 126.64, 77.45, 77.14, 76.82, 61.25, 51.82, 38.52, 33.25, 28.05, 27.92, 14.30.

HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{22}\text{NO}_5^+$ m/z $[\text{M}+\text{H}]^+$: 308.1498, found 308.1495.



45c: ethyl 5-(1-(tert-butoxycarbonyl)piperidin-4-yl)oxazole-4-carboxylate

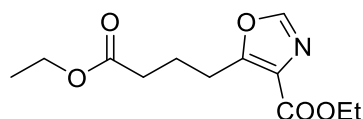
Yellow solid.

85.6 mg, 66% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.74 (s, 1H), 4.36 (q, J = 7.2 Hz, 2H), 4.18 (s, 2H), 3.66 – 3.57 (m, 1H), 2.81 (t, J = 12.5 Hz, 2H), 1.84 – 1.66 (m, 4H), 1.44 (s, 9H), 1.37 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.10, 161.86, 154.25, 149.00, 126.21, 79.75, 77.45, 77.13, 76.81, 61.17, 33.85, 29.58, 28.47, 14.32.

HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{25}\text{N}_2\text{O}_5^+$ m/z $[\text{M}+\text{H}]^+$: 325.1763, found 325.1762.



46c: ethyl 5-(4-ethoxy-4-oxobutyl)oxazole-4-carboxylate

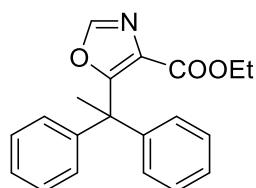
Light yellow solid.

79.8 mg, 78% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.74 (s, 1H), 4.33 (q, J = 7.1 Hz, 2H), 4.07 (q, J = 7.1 Hz, 2H), 3.08 (t, J = 7.4 Hz, 2H), 2.31 (t, J = 7.4 Hz, 2H), 2.03 – 1.94 (m, 2H), 1.35 (t, J = 7.1 Hz, 3H), 1.20 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 172.30, 161.97, 159.00, 149.19, 127.46, 77.47, 77.15, 76.84, 61.07, 60.51, 33.26, 25.15, 22.86, 14.30, 14.21.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{18}\text{NO}_5^+$ m/z $[\text{M}+\text{H}]^+$: 256.1185, found 256.1182.



47c: ethyl 5-(1,1-diphenylethyl)oxazole-4-carboxylate

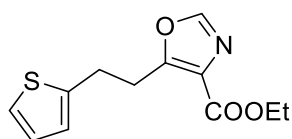
Colorless solid.

87.6 mg, 68% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.75 (s, 1H), 7.32 – 7.22 (m, 6H), 7.21 – 7.17 (m, 4H), 3.99 (q, J = 7.1 Hz, 2H), 2.21 (s, 3H), 1.10 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.69, 161.53, 148.73, 145.67, 128.58, 128.24, 127.80, 126.96, 77.52, 77.20, 76.88, 61.31, 49.95, 28.43, 13.94.

HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{20}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 322.1443, found 322.1446.

**48c: ethyl 5-(2-(thiophen-2-yl)ethyl)oxazole-4-carboxylate**

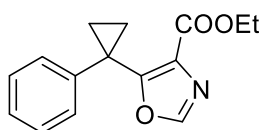
Brown oil.

68.3 mg, 68% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.76 (s, 1H), 7.12 (d, J = 6.3 Hz, 1H), 6.90 – 6.87 (m, 1H), 6.78 (d, J = 3.6 Hz, 1H), 4.36 (q, J = 7.1 Hz, 2H), 3.41 (t, J = 7.6 Hz, 2H), 3.23 (t, J = 7.6 Hz, 2H), 1.38 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.93, 158.94, 149.17, 142.35, 127.73, 126.94, 124.92, 123.81, 77.45, 77.13, 76.81, 61.15, 28.23, 27.85, 14.36.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{14}\text{NO}_3\text{S}^+$ m/z $[\text{M}+\text{H}]^+$: 252.0694, found 252.0699.

**49c: ethyl 5-(1-phenylcyclobutyl)oxazole-4-carboxylate**

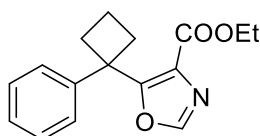
Yellow solid.

80.8 mg, 79% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.76 (s, 1H), 7.35 (d, J = 8.2 Hz, 2H), 7.27 (t, J = 7.4 Hz, 2H), 7.22 – 7.17 (m, 2H), 4.37 (q, J = 7.1 Hz, 3H), 1.46 (s, 4H), 1.36 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.40, 160.77, 149.12, 141.63, 128.54, 128.27, 127.88, 126.97, 77.48, 77.16, 76.85, 61.14, 21.51, 15.79, 14.34.

HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{16}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 258.1130, found 258.127.



50c: ethyl 5-(1-phenylcyclobutyl)oxazole-4-carboxylate

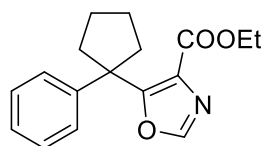
Light yellow solid.

66.3 mg, 61% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.72 (s, 1H), 7.43 (d, J = 8.1 Hz, 2H), 7.31 – 7.23 (m, 2H), 7.20 – 7.15 (m, 1H), 4.28 (q, J = 7.1 Hz, 2H), 2.95 – 2.72 (m, 4H), 2.04 – 1.82 (m, 2H), 1.31 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 164.09, 161.50, 148.16, 144.57, 128.44, 126.67, 126.28, 125.92, 77.50, 77.18, 76.86, 61.07, 46.09, 33.70, 17.20, 14.32.

HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{18}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 272.1287, found 272.1286.

**51c: ethyl 5-(1-phenylcyclopentyl)oxazole-4-carboxylate**

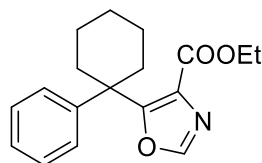
Colorless solid.

73.9 mg, 65% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.77 (s, 1H), 7.34 – 7.30 (m, 2H), 7.29 – 7.24 (m, 2H), 7.20 – 7.15 (m, 1H), 4.22 (q, J = 7.1 Hz, 2H), 2.64 – 2.56 (m, 2H), 2.44 – 2.36 (m, 2H), 1.79 – 1.65 (m, 4H), 1.25 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 164.06, 161.50, 147.93, 144.56, 128.16, 126.57, 126.51, 77.49, 77.17, 76.86, 61.04, 52.44, 37.91, 23.34, 14.19.

HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{20}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 286.1443, found 286.1445.

**52c: ethyl 5-(1-phenylcyclohexyl)oxazole-4-carboxylate**

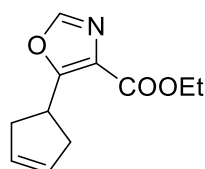
Brown yellow solid.

87.1 mg, 73% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.81 (s, 1H), 7.33 (d, J = 7.5 Hz, 2H), 7.30 – 7.25 (m, 2H), 7.21 – 7.15 (m, 1H), 4.26 (q, J = 7.2 Hz, 2H), 2.86 (d, J = 13.4 Hz, 2H), 2.00 (t, J = 12.1 Hz, 2H), 1.70 (t, J = 5.0 Hz, 2H), 1.64 – 1.56 (m, 1H), 1.45 – 1.33 (m, 3H), 1.30 (t, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.80, 161.77, 148.28, 145.99, 128.31, 127.70, 126.51, 126.23, 77.44, 77.12, 76.81, 61.24, 45.16, 35.70, 25.72, 23.43, 14.20.

HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{22}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 300.1600, found 300.1604.



53c: ethyl 5-(cyclopent-3-en-1-yl)oxazole-4-carboxylate

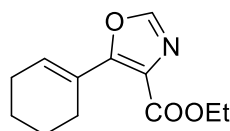
Brown yellow oil.

54.6 mg, 66% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.72 (s, 1H), 5.75 – 5.71 (m, 2H), 4.35 (q, J = 7.1 Hz, 2H), 4.30 – 4.22 (m, 1H), 2.77 (dd, J = 14.5, 9.4 Hz, 2H), 2.54 (dd, J = 13.8, 6.7 Hz, 2H), 1.36 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 163.29, 162.26, 148.73, 129.33, 126.39, 77.51, 77.19, 76.88, 61.08, 38.15, 33.89, 14.40.

HRMS (ESI) calcd for $\text{C}_{11}\text{H}_{14}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 208.0974, found 208.0976.



54c: ethyl 5-(cyclohex-1-en-1-yl)oxazole-4-carboxylate

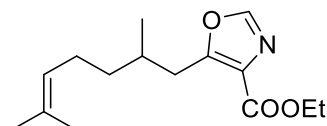
Brown yellow oil.

34.6 mg, 39% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.72 (s, 1H), 6.92 – 6.87 (m, 1H), 4.36 (q, J = 7.1 Hz, 2H), 2.46 – 2.39 (m, 2H), 2.31 – 2.24 (m, 2H), 1.77 – 1.71 (m, 2H), 1.70 – 1.63 (m, 2H), 1.39 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.30, 157.65, 147.87, 135.48, 125.45, 125.15, 77.41, 77.09, 76.77, 61.19, 25.95, 25.80, 22.28, 21.52, 14.34.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{16}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 222.1130, found 222.1130.



55c: ethyl 5-(2,6-dimethylhept-5-en-1-yl)oxazole-4-carboxylate

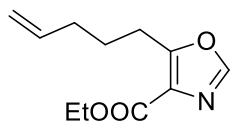
Light yellow oil.

92.8 mg, 88% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.73 (s, 1H), 5.05 – 4.99 (m, 1H), 4.33 (q, J = 7.1 Hz, 2H), 3.03 – 2.84 (m, 2H), 2.03 – 1.87 (m, 3H), 1.63 (s, 3H), 1.55 (s, 3H), 1.35 (t, J = 7.2 Hz, 3H), 1.33 – 1.15 (m, 2H), 0.87 (d, J = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.13, 159.55, 149.02, 131.61, 127.75, 124.21, 77.47, 77.15, 76.83, 60.95, 36.71, 32.94, 32.44, 25.72, 25.41, 19.37, 17.66, 14.32.

HRMS (ESI) calcd for $C_{15}H_{24}NO_3^+$ m/z $[M+H]^+$: 266.1756, found 266.1752.



56c: ethyl 5-(pent-4-en-1-yl)oxazole-4-carboxylate

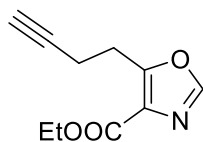
Colorless oil.

46.6 mg, 56% yield

1H NMR (400 MHz, Chloroform-*d*) δ 7.78 (s, 1H), 5.87 – 5.74 (m, 1H), 5.09 – 4.97 (m, 2H), 4.39 (q, J = 7.1 Hz, 2H), 3.08 (t, J = 7.8 Hz, 2H), 2.17 – 2.08 (m, 2H), 1.81 (p, J = 7.5 Hz, 2H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.62, 159.52, 149.55, 137.51, 127.10, 115.50, 77.45, 77.13, 76.81, 61.02, 33.09, 26.85, 25.32, 14.34.

HRMS (ESI) calcd for $C_{11}H_{16}NO_3^+$ m/z $[M+H]^+$: 210.1130, found 210.1128.



57c: ethyl 5-(but-3-yn-1-yl)oxazole-4-carboxylate

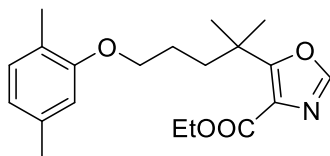
Yellow solid.

45.2 mg, 59% yield

1H NMR (400 MHz, Chloroform-*d*) δ 7.77 (s, 1H), 4.37 (q, J = 7.2 Hz, 2H), 3.28 (t, J = 7.3 Hz, 2H), 2.59 (td, J = 7.3, 2.7 Hz, 2H), 1.96 (t, J = 2.7 Hz, 1H), 1.38 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.93, 158.29, 150.10, 127.88, 81.84, 77.43, 77.11, 76.80, 69.77, 61.19, 25.31, 17.13, 14.33.

HRMS (ESI) calcd for $C_{10}H_{12}NO_3^+$ m/z $[M+H]^+$: 194.0817, found 194.0822.



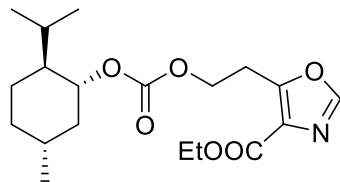
58c: ethyl 5-(5-(2,5-dimethylphenoxy)-2-methylpentan-2-yl)oxazole-4-carboxylate

Colorless oil.

80.2 mg, 58% yield

1H NMR (400 MHz, Chloroform-*d*) δ 7.72 (s, 1H), 6.98 (d, J = 7.4 Hz, 1H), 6.64 (d, J = 7.4 Hz, 1H), 6.56 (s, 1H), 4.37 (q, J = 7.1 Hz, 2H), 3.87 (t, J = 6.3 Hz, 2H), 2.29 (s, 3H), 2.15 (s, 3H), 2.09 – 2.01 (m, 2H), 1.67 – 1.57 (m, 2H), 1.48 (s, 6H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 165.04, 162.10, 156.95, 147.70, 136.49, 130.34, 126.67, 123.58, 120.73, 111.92, 77.47, 77.15, 76.83, 67.84, 61.26, 37.26, 36.76, 26.22, 25.29, 21.46, 15.81, 14.33.
HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{28}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 346.2018, found 346.2014.



59c: **ethyl** **5-(2-((((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)carbonyl)oxy)ethyl)oxazole-4-carboxylate**

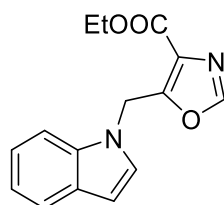
Colorless oil.

111.7 mg, 76% yield

^1H NMR (400 MHz, $\text{Chloroform-}d$) δ 7.73 (s, 1H), 4.71 – 4.61 (m, 1H), 4.36 (q, $J = 7.1$ Hz, 2H), 3.36 (td, $J = 7.4, 1.7$ Hz, 2H), 2.69 (t, $J = 7.5$ Hz, 2H), 1.97 – 1.88 (m, 1H), 1.78 – 1.69 (m, 1H), 1.69 – 1.59 (m, 2H), 1.50 – 1.40 (m, 1H), 1.37 (t, $J = 7.1$ Hz, 3H), 1.34 – 1.26 (m, 1H), 1.07 – 0.89 (m, 2H), 0.88 – 0.83 (m, 6H), 0.80 (s, 1H), 0.71 (d, $J = 6.9$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.23, 161.37, 158.16, 148.37, 127.47, 77.44, 77.13, 76.81, 74.76, 61.16, 46.97, 40.84, 34.21, 32.68, 31.39, 26.29, 23.41, 22.03, 21.70, 20.77, 16.31, 14.32.

HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{30}\text{NO}_6^+$ m/z $[\text{M}+\text{H}]^+$: 368.2073, found 368.2074.



60c: ethyl 5-((1H-indol-1-yl)methyl)oxazole-4-carboxylate

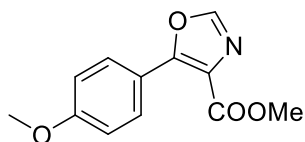
Brown solid.

71.1 mg, 66% yield

^1H NMR (400 MHz, $\text{Chloroform-}d$) δ 7.74 (s, 1H), 7.63 (d, $J = 6.9$ Hz, 1H), 7.52 (d, $J = 7.4$ Hz, 1H), 7.27 – 7.22 (m, 2H), 7.16 – 7.10 (m, 1H), 6.55 (d, $J = 3.3$ Hz, 1H), 5.71 (s, 2H), 4.50 (q, $J = 7.1$ Hz, 2H), 1.47 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.74, 153.76, 150.17, 136.12, 128.74, 128.66, 128.14, 122.23, 121.16, 120.07, 109.49, 102.71, 77.46, 77.14, 76.82, 61.79, 40.30, 14.39.

HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{15}\text{N}_2\text{O}_3^+$ m/z $[\text{M}+\text{H}]^+$: 271.1083, found 271.1084.



61c: methyl 5-(4-methoxyphenyl)oxazole-4-carboxylate

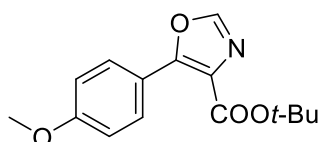
Yellow solid.

76.1 mg, 82% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, J = 9.0 Hz, 2H), 7.84 (s, 1H), 6.98 (d, J = 9.0 Hz, 2H), 3.93 (s, 2H), 3.85 (s, 2H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.67, 161.40, 156.02, 148.02, 130.19, 125.08, 119.18, 113.98, 77.45, 77.13, 76.81, 54.93, 52.30.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{12}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 234.0766, found 234.0768.



62c: tert-butyl 5-(4-methoxyphenyl)oxazole-4-carboxylate

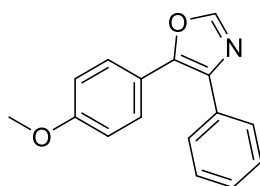
White solid.

82.5 mg, 75% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, J = 8.9 Hz, 2H), 7.82 (s, 1H), 6.97 (d, J = 8.9 Hz, 2H), 3.84 (s, 3H), 1.59 (s, 9H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.44, 161.12, 155.12, 148.46, 130.31, 126.71, 119.63, 113.82, 82.22, 77.45, 77.13, 76.81, 55.41, 28.28.

HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{18}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 276.1236, found 276.1235.



63c: 5-(4-methoxyphenyl)-4-phenyloxazole

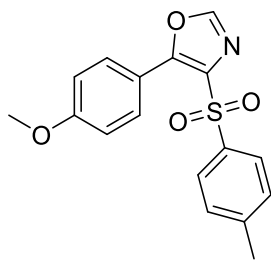
Brown yellow solid.

46.5 mg, 46% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.92 (s, 1H), 7.66 (d, J = 6.7 Hz, 2H), 7.54 (d, J = 8.9 Hz, 2H), 7.40 – 7.29 (m, 3H), 6.91 (d, J = 8.9 Hz, 2H), 3.84 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 160.08, 149.44, 145.97, 133.60, 132.39, 128.64, 128.47, 128.05, 127.80, 121.32, 114.25, 77.41, 77.09, 76.77, 55.39.

HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{14}\text{NO}_2^+$ m/z $[\text{M}+\text{H}]^+$: 252.1025, found 252.1028.



64c: 5-(4-methoxyphenyl)-4-tosyloxazole

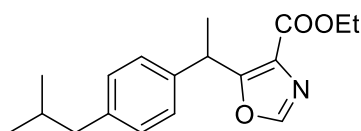
White solid.

73.0 mg, 55% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, J = 9.0 Hz, 2H), 7.89 (d, J = 8.4 Hz, 2H), 7.80 (s, 1H), 7.31 (d, J = 8.0 Hz, 2H), 7.01 (d, J = 8.9 Hz, 2H), 3.88 (s, 3H), 2.41 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.73, 152.99, 148.76, 144.94, 137.41, 134.24, 130.78, 129.86, 128.23, 118.00, 114.15, 77.43, 77.11, 76.79, 55.50, 21.74.

HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{16}\text{NO}_4\text{S}^+$ m/z $[\text{M}+\text{H}]^+$: 330.0800, found 330.0795.



65c: ethyl 5-(1-(4-isobutylphenyl)ethyl)oxazole-4-carboxylate

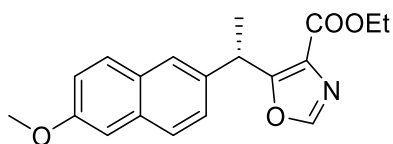
Yellow solid.

97.7 mg, 81% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.76 (s, 1H), 7.25 (d, J = 8.1 Hz, 2H), 7.08 (d, J = 8.2 Hz, 2H), 5.05 (d, J = 7.3 Hz, 1H), 4.46 – 4.33 (m, 2H), 2.43 (d, J = 7.2 Hz, 2H), 1.90 – 1.76 (m, 1H), 1.66 (d, J = 7.3 Hz, 3H), 1.40 (t, J = 7.2 Hz, 3H), 0.88 (d, J = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.14, 161.93, 149.11, 140.61, 138.84, 129.44, 127.14, 125.92, 77.47, 77.16, 76.84, 61.12, 45.06, 35.93, 30.23, 22.43, 19.22, 13.85.

HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{24}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 302.1756, found 302.1756.



66c: ethyl (S)-5-(1-(6-methoxynaphthalen-2-yl)ethyl)oxazole-4-carboxylate

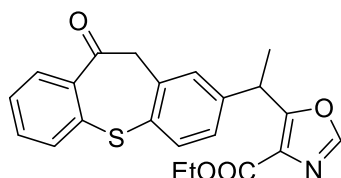
Light yellow solid.

102.1 mg, 79% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.77 (s, 1H), 7.72 – 7.66 (m, 3H), 7.44 (dd, J = 8.6, 1.8 Hz, 1H), 7.14 (dd, J = 9.0, 2.5 Hz, 1H), 7.09 (d, J = 2.5 Hz, 1H), 5.21 (q, J = 7.3 Hz, 1H), 4.47 – 4.34 (m, 2H), 3.90 (s, 3H), 1.75 (d, J = 7.3 Hz, 3H), 1.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.16, 161.84, 157.75, 149.19, 136.73, 133.67, 129.35, 128.96, 127.28, 126.33, 126.09, 125.67, 119.14, 105.64, 77.44, 77.12, 76.80, 61.20, 55.37, 36.25, 19.16, 14.40.

HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{20}\text{NO}_4^+$ m/z $[\text{M}+\text{H}]^+$: 326.1392, found 326.1392.



67c: ethyl 5-(1-(10-oxo-10,11-dihydrodibenzo[b,f]thiepin-2-yl)ethyl)oxazole-4-carboxylate

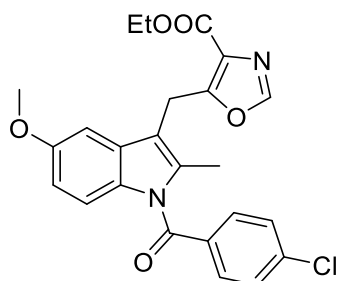
Brown yellow solid.

118.8 mg, 76% yield

^1H NMR (400 MHz, Chloroform- d) δ 8.18 (dd, $J = 7.9, 1.7$ Hz, 1H), 7.77 (s, 1H), 7.57 (d, $J = 7.9$ Hz, 2H), 7.43 – 7.37 (m, 2H), 7.32 – 7.26 (m, 1H), 7.18 (dd, $J = 8.0, 2.0$ Hz, 1H), 5.06 (q, $J = 7.3$ Hz, 1H), 4.41 – 4.35 (m, 2H), 4.34 (s, 2H), 1.64 (d, $J = 7.3$ Hz, 3H), 1.39 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 191.38, 161.96, 160.74, 149.33, 144.24, 140.20, 138.10, 136.14, 133.34, 132.62, 131.61, 131.59, 130.95, 128.33, 126.95, 126.47, 126.36, 77.45, 77.13, 76.81, 61.72, 52.15, 36.75, 19.71, 15.37.

HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{20}\text{NO}_4\text{S}^+$ m/z $[\text{M}+\text{H}]^+$: 394.1113, found 394.1117.



68c: ethyl 5-((1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)methyl)oxazole-4-carboxylate

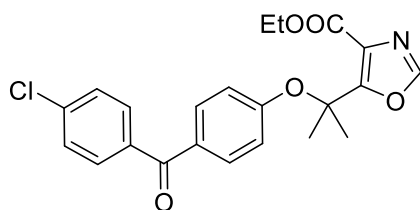
Brown solid.

69.7 mg, 39% yield

^1H NMR (400 MHz, Chloroform- d) δ 7.72 (s, 1H), 7.65 (d, $J = 8.5$ Hz, 2H), 7.46 (d, $J = 8.5$ Hz, 2H), 7.12 (d, $J = 2.6$ Hz, 1H), 6.81 (d, $J = 9.0$ Hz, 1H), 6.66 (d, $J = 2.6$ Hz, 1H), 4.49 – 4.43 (m, 4H), 3.81 (s, 3H), 2.48 (s, 3H), 1.44 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 168.39, 162.35, 157.26, 156.11, 149.36, 139.42, 135.58, 133.86, 131.25, 130.78, 130.47, 129.21, 127.08, 114.97, 114.06, 111.84, 101.45, 77.44, 77.12, 76.81, 61.40, 56.45, 20.94, 14.43, 13.36.

HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{22}\text{ClN}_2\text{O}_5^+$ m/z $[\text{M}+\text{H}]^+$: 453.1217, found 453.1217.



69c: ethyl 5-(2-(4-(4-chlorobenzoyl)phenoxy)propan-2-yl)oxazole-4-carboxylate

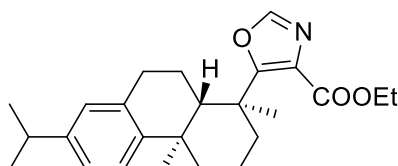
Light yellow solid.

81.2 mg, 49% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.85 (s, 1H), 7.68 – 7.62 (m, 4H), 7.41 (d, J = 8.5 Hz, 2H), 6.70 (d, J = 8.8 Hz, 2H), 4.33 (q, J = 7.2 Hz, 2H), 1.92 (s, 6H), 1.35 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 194.38, 161.03, 159.39, 158.24, 148.80, 138.52, 136.27, 132.81, 132.01, 130.70, 128.61, 118.24, 115.48, 77.45, 77.14, 76.82, 76.74, 61.72, 27.09, 14.19.

HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{22}\text{ClNO}_5^+$ m/z $[\text{M}+\text{H}]^+$: 414.1108, found 414.112.



70c: 4-((ethylperoxy)-12-methyl)-5-((1S,4aR,10aS)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-yl)oxazole

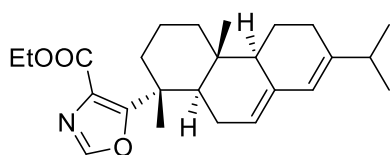
Brown oil.

103.6 mg, 66% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.74 (s, 1H), 7.18 (d, J = 8.2 Hz, 1H), 6.99 (d, J = 8.2 Hz, 1H), 6.83 (s, 1H), 4.37 – 4.19 (m, 3H), 2.85 – 2.75 (m, 2H), 2.74 – 2.63 (m, 1H), 2.60 – 2.54 (m, 1H), 2.43 – 2.29 (m, 2H), 1.91 – 1.66 (m, 5H), 1.52 (s, 3H), 1.34 (t, J = 7.1 Hz, 3H), 1.28 (s, 3H), 1.21 (d, J = 6.9 Hz, 6H).

^{13}C NMR (101 MHz, CDCl_3) δ 166.59, 162.35, 147.58, 146.91, 145.65, 134.55, 126.88, 126.53, 124.28, 124.02, 77.45, 77.14, 76.82, 61.34, 45.57, 42.07, 37.83, 37.37, 35.84, 33.50, 30.26, 25.67, 24.03, 21.39, 18.80, 17.85, 14.91.

HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{34}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 396.2539, found 396.2540.



71c: ethyl 5-((1R,4aR,4bR,10aR)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,10,10a-decahydrophenanthren-1-yl)oxazole-4-carboxylate

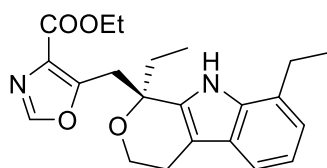
Yellow oil.

79.7 mg, 50% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 7.70 (s, 1H), 5.72 (s, 1H), 5.27 (t, J = 2.4, 1H), 4.39 – 4.31 (m, 2H), 2.48 (td, J = 13.0, 4.3 Hz, 2H), 2.23 – 2.15 (m, 1H), 2.14 – 1.96 (m, 5H), 1.90 – 1.80 (m, 2H), 1.71 – 1.56 (m, 3H), 1.48 (s, 3H), 1.42 – 1.36 (m, 5H), 1.01 – 0.97 (m, 6H), 0.87 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 167.07, 162.33, 147.41, 145.56, 135.77, 125.97, 122.36, 120.62, 77.43, 77.11, 76.79, 61.30, 50.63, 45.66, 40.96, 37.55, 35.97, 35.20, 34.93, 27.44, 25.63, 22.48, 21.44, 20.87, 18.30, 18.17, 14.37, 14.29.

HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{36}\text{NO}_3^+$ m/z $[\text{M}+\text{H}]^+$: 398.2695, found 398.2694.



72c: ethyl (S)-5-((1,8-diethyl-1,3,4,9-tetrahydropyrano[3,4-b]indol-1-yl)methyl)oxazole-4-carboxylate

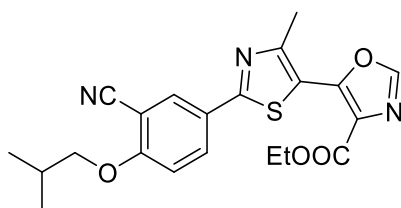
Yellow solid.

67.2 mg, 44% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.33 (s, 1H), 7.76 (s, 1H), 7.31 (d, J = 7.7 Hz, 1H), 7.08 – 6.97 (m, 2H), 4.42 – 4.27 (m, 2H), 4.08 (t, J = 6.4 Hz, 2H), 3.83 (d, J = 14.8 Hz, 1H), 3.56 (d, J = 14.7 Hz, 1H), 2.91 – 2.67 (m, 4H), 2.11 – 2.01 (m, 1H), 1.92 – 1.81 (m, 1H), 1.38 – 1.32 (m, 6H), 0.88 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.98, 156.69, 149.71, 134.87, 134.85, 128.73, 126.59, 126.43, 120.46, 119.79, 115.92, 109.47, 77.43, 77.34, 77.11, 76.80, 61.33, 60.93, 34.56, 32.26, 23.85, 22.14, 14.17, 13.84, 7.82.

HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{27}\text{N}_2\text{O}_4^+$ m/z $[\text{M}+\text{H}]^+$: 383.1971, found 383.1967.



73c: ethyl 5-(2-(3-cyano-4-isobutoxyphenyl)-4-methylthiazol-5-yl)oxazole-4-carboxylate

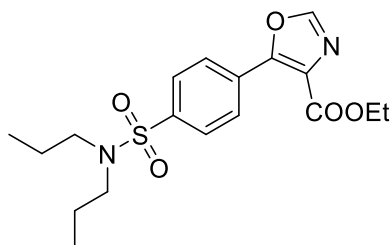
Yellow solid.

70.1 mg, 43% yield

^1H NMR (400 MHz, Chloroform-*d*) δ 8.19 (d, J = 2.3 Hz, 1H), 8.09 (d, J = 8.8 Hz, 1H), 7.96 (s, 1H), 7.00 (d, J = 8.9 Hz, 1H), 4.43 (q, J = 7.1 Hz, 2H), 3.89 (d, J = 6.5 Hz, 2H), 2.64 (s, 3H), 2.26 – 2.12 (m, 1H), 1.41 (t, J = 7.1 Hz, 3H), 1.08 (d, J = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, CDCl_3) δ 166.69, 162.32, 161.58, 156.71, 149.47, 148.79, 132.46, 131.96, 127.73, 126.08, 116.51, 115.53, 112.64, 102.98, 77.43, 77.12, 76.80, 75.71, 61.76, 28.22, 19.12, 17.98, 14.36.

HRMS (ESI) calcd for $\text{C}_{21}\text{H}_{22}\text{N}_3\text{O}_4\text{S}^+$ m/z $[\text{M}+\text{H}]^+$: 412.1331, found 412.1335.



74c: ethyl 5-(4-(N,N-dipropylsulfamoyl)phenyl)oxazole-4-carboxylate

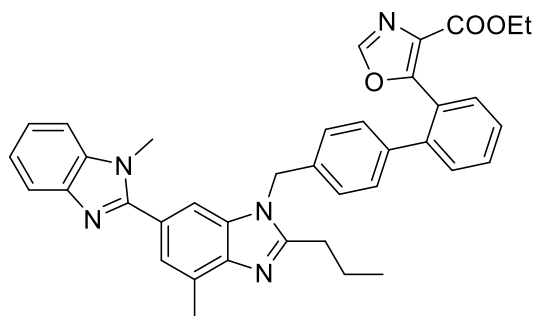
Light yellow solid.

90.3 mg, 60% yield

^1H NMR (400 MHz, Chloroform-d) δ 8.24 (d, J = 8.6 Hz, 1H), 7.97 (s, 1H), 7.88 (d, J = 8.5 Hz, 2H), 4.42 (q, J = 7.1 Hz, 2H), 3.09 (t, J = 8.0 Hz, 4H), 1.60 – 1.48 (m, 4H), 1.40 (t, J = 7.1 Hz, 3H), 0.86 (t, J = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.80, 153.64, 149.74, 141.65, 130.22, 128.94, 128.25, 127.15, 77.46, 77.14, 76.82, 61.86, 50.13, 22.11, 14.27, 11.22.

HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{25}\text{N}_2\text{O}_5\text{S}^+$ m/z $[\text{M}+\text{H}]^+$: 381.1484, found 381.1480.



75c: ethyl 5-(4'-((1,7'-dimethyl-2'-propyl-1H,3'H-[2,5'-bibenzo[d]imidazol]-3'-yl)methyl)-[1,1'-biphenyl]-2-yl)oxazole-4-carboxylate

Yellow solid.

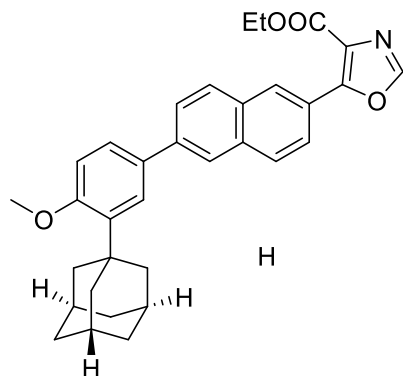
195.3 mg, 80% yield

^1H NMR (400 MHz, Chloroform-d) δ 7.80 – 7.75 (m, 1H), 7.68 (s, 1H), 7.58 – 7.49 (m, 2H), 7.45 – 7.37 (m, 4H), 7.37 – 7.33 (m, 1H), 7.29 – 7.27 (m, 1H), 7.08 (d, J = 8.1 Hz, 2H), 6.95 (d, J = 8.0 Hz, 2H), 5.36 (s, 2H), 4.17 (q, J = 7.1 Hz, 2H), 3.80 (s, 2H), 2.87 (t, J = 8.0 Hz, 2H), 2.75 (s, 3H), 1.88 – 1.76 (m, 2H), 1.18 (t, J = 7.1 Hz, 2H), 1.01 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.18, 156.52, 155.87, 154.71, 149.82, 143.13, 142.82, 141.76, 140.25, 136.70, 135.12, 134.97, 131.59, 130.85, 130.05, 129.46, 129.21, 128.54, 127.26, 126.17,

125.72, 123.96, 123.85, 122.64, 122.45, 119.52, 109.66, 109.01, 77.48, 77.16, 76.84, 61.13, 46.97, 31.93, 29.83, 21.86, 17.00, 14.14, 14.10.

HRMS (ESI) calcd for $C_{38}H_{36}N_5O_3^+$ m/z $[M+H]^+$: 610.2818, found 610.2822.



76c: ethyl 5-(6-(3-((3r,5r,7r)-adamantan-1-yl)-4-methoxyphenyl)naphthalen-2-yl)oxazole-4-carboxylate

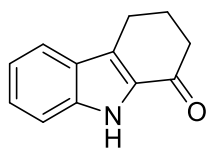
White solid.

117.9 mg, 58% yield

1H NMR (400 MHz, Chloroform- d) δ 8.70 (s, 1H), 8.12 (d, J = 8.7 Hz, 1H), 8.02 – 7.94 (m, 4H), 7.80 (d, J = 8.5 Hz, 1H), 7.61 (d, J = 2.3 Hz, 1H), 7.56 (d, J = 8.3 Hz, 1H), 7.00 (d, J = 8.4 Hz, 1H), 4.47 (q, J = 7.1 Hz, 2H), 3.91 (s, 3H), 2.19 (s, 6H), 2.11 (s, 3H), 1.81 (s, 6H), 1.44 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.18, 158.93, 155.83, 149.06, 140.81, 139.06, 134.46, 132.69, 131.59, 129.40, 128.87, 128.28, 126.76, 126.58, 125.98, 125.75, 125.25, 124.75, 123.61, 112.17, 77.41, 77.09, 76.77, 61.56, 55.24, 40.66, 37.27, 37.19, 29.17, 14.38.

HRMS (ESI) calcd for $C_{33}H_{34}NO_4^+$ m/z $[M+H]^+$: 508.2488, found 508.2489.



f: 2,3,4,9-tetrahydro-1H-carbazol-1-one

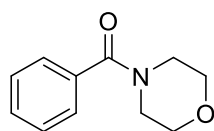
Light yellow solid.

26.7 mg, 36% yield.

1H NMR (400 MHz, Chloroform- d) δ 9.46 (s, 1H), 7.66 (d, J = 8.1 Hz, 1H), 7.46 (d, J = 8.3 Hz, 1H), 7.40 – 7.34 (m, 1H), 7.18 – 7.12 (m, 1H), 3.02 (t, J = 6.1 Hz, 2H), 2.72 – 2.65 (m, 2H), 2.32 – 2.24 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 191.73, 138.10, 131.31, 129.75, 127.11, 125.91, 121.42, 120.42, 112.75, 77.43, 77.12, 76.80, 38.34, 25.07, 21.49.

HRMS (ESI) calcd for $C_{12}H_{12}NO^+$ m/z $[M+H]^+$: 186.0919, found 186.0923.



h: morpholino(phenyl)methanone

Colorless oil.

63.7 mg, 87% yield.

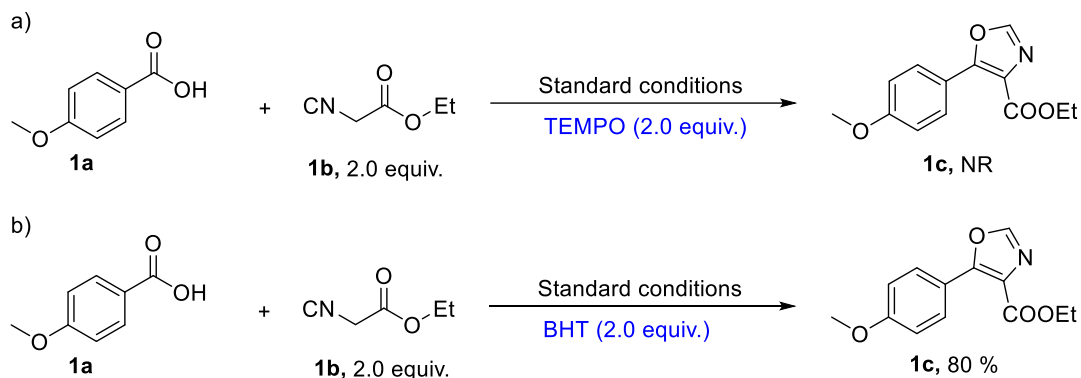
^1H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.34 (m, 7H), 3.82 – 3.35 (m, 8H).

^{13}C NMR (101 MHz, CDCl_3) δ 170.52, 135.34, 129.95, 128.63, 127.14, 77.48, 77.16, 76.85, 66.94.

HRMS (ESI) calcd for $\text{C}_{11}\text{H}_{14}\text{NO}_2^+$ m/z $[\text{M}+\text{H}]^+$: 192.1025, found 192.1021.

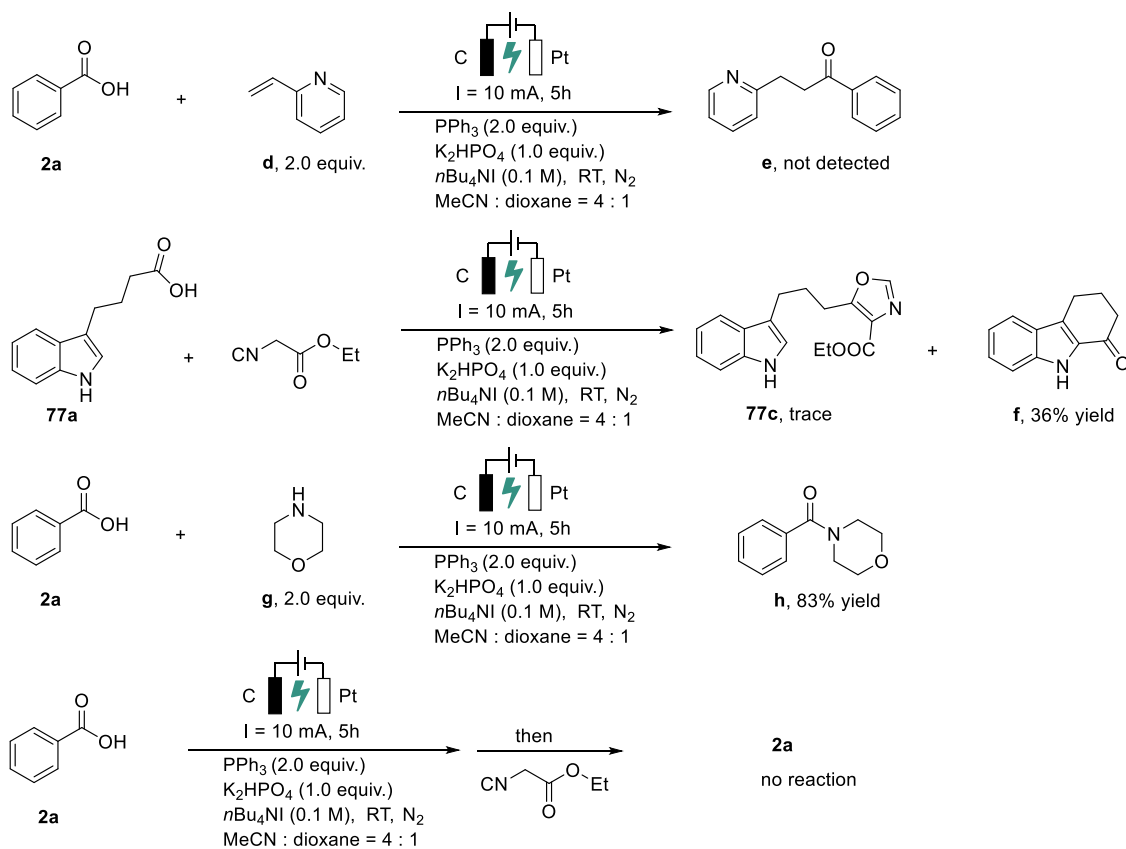
3. Mechanism Study Experiments

3.1 Radical quenching experiments



Under standard reaction conditions, **1a** (1.0 equiv., 0.4 mmol) was selected as the substrate for validation. For reaction **a**), TEMPO (2.0 equiv., 0.8 mmol) was added as an additive, no target product was detected (monitored by TLC or GC-MS analysis) after 5 hours. For reaction **b**), BHT (2.0 equiv., 0.8 mmol) was added as an additive, the substrate was transformed completely and the **1c** was separated in 80% yield after 6 hours.

3.2 Control experiments



According to Zhu's work, 2-vinylpyridine was found to be the acceptors of acyl radical. So, 2-vinylpyridine was added without isocyanides presence. Unfortunately, the ketone was not observed under standard conditions. The intramolecular acyl addition reaction of 4-(1H-indol-3-yl)butanoic acid happened, while the intermolecular cycloaddition was completely inhibited. Furthermore, when morpholine, a common nucleophile, was added, the corresponding amide product was obtained in a 83% yield, indicating that the key intermediates are not acyl radicals but are more likely the cationic species. Furthermore, the "step-by-step" experiment demonstrated that the electrochemical single electron transfer oxidation to generate the electrophilic intermediates and the following two-electron process with the nucleophilic site of isocyanides are simultaneous in this reaction system.

3.3 Cyclic voltammetry studies

The cyclic voltammogram was collected with a CHI 760E Potentiostat. The potential ($E_{1/2p}$) of each compound was obtained using Origin.

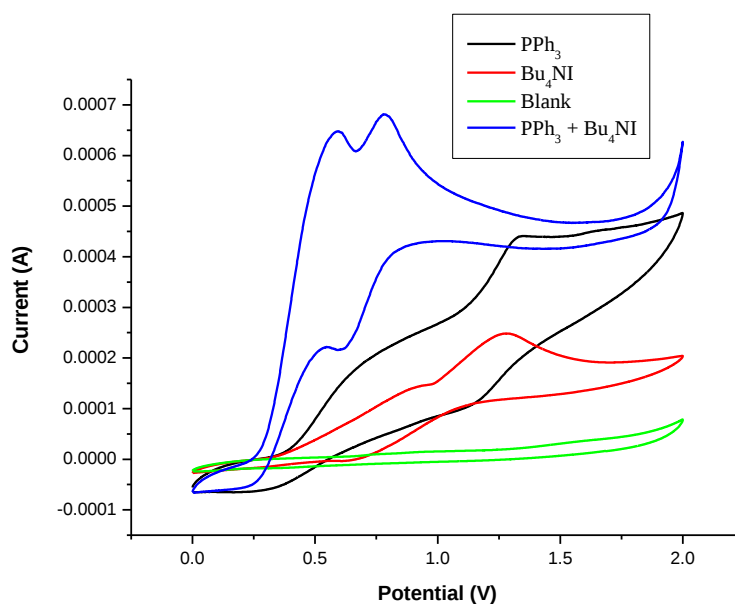


Figure 5. Cyclic voltammograms of PPh_3 and $n-Bu_4NI$ in 0.1 M $n-Bu_4NBF_4$ (CH_3CN), using a glassy carbon working electrode and platinum sheet and saturated calomel electrode (SCE) as counter electrode and reference electrodes at a 100 mV s^{-1} scan rate. The sample was prepared with 0.1 mmol of target molecule.

The $E_{1/2}$ vs SCE of PPh_3 in MeCN is 0.84 V and the $E_{1/2}$ vs SCE of $n-Bu_4NI$ in MeCN is 0.65 V and 0.83 V, suggesting that $n-Bu_4NI$ are more susceptible to oxidation when compared with PPh_3 . Treatment $n-Bu_4NI$ with same amount of PPh_3 (0.1 M) results in a dramatic increase of anodic peak of $n-Bu_4NI$. This result suggests that the active species I^+ arising from the oxidation of I can be readily intercepted by PPh_3 to form an intermediate $Ph_3P \cdot I^+$. The in-situ generated $Ph_3P \cdot I^+$ is regarded as the active species in the activation process of carboxylic acid.

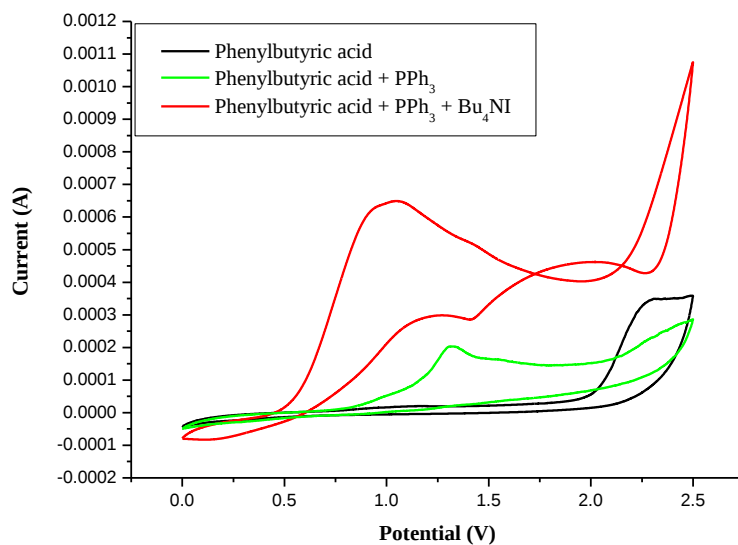
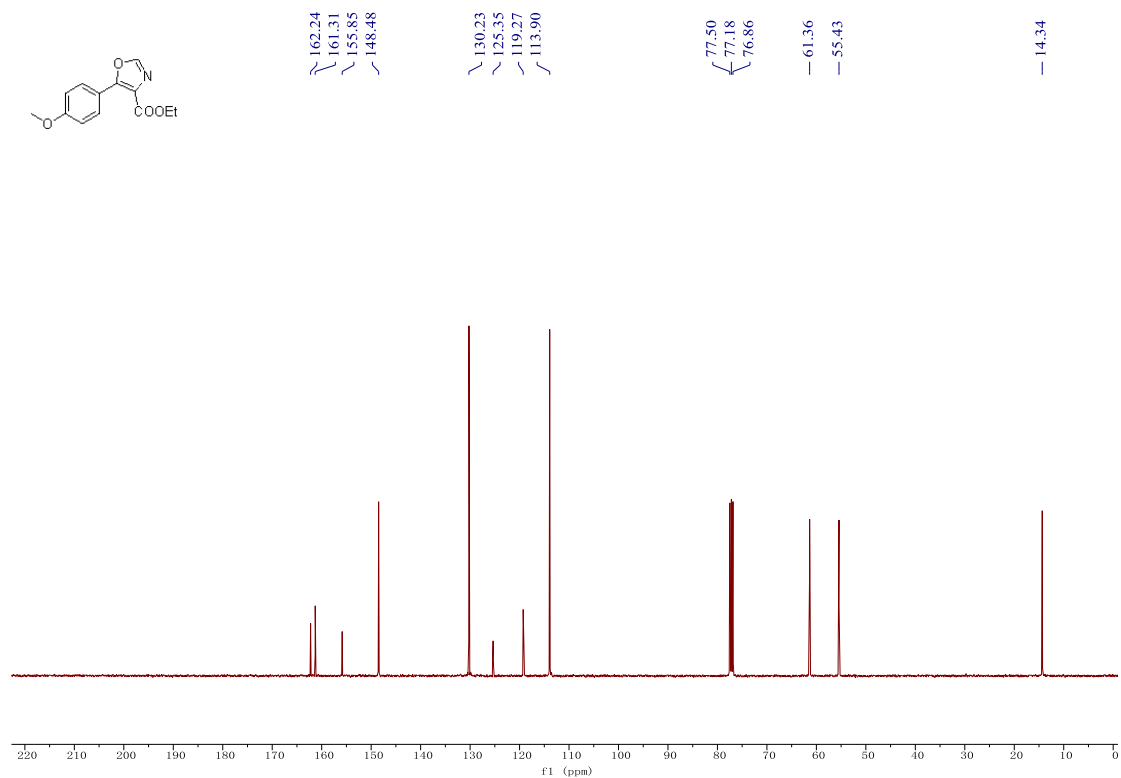
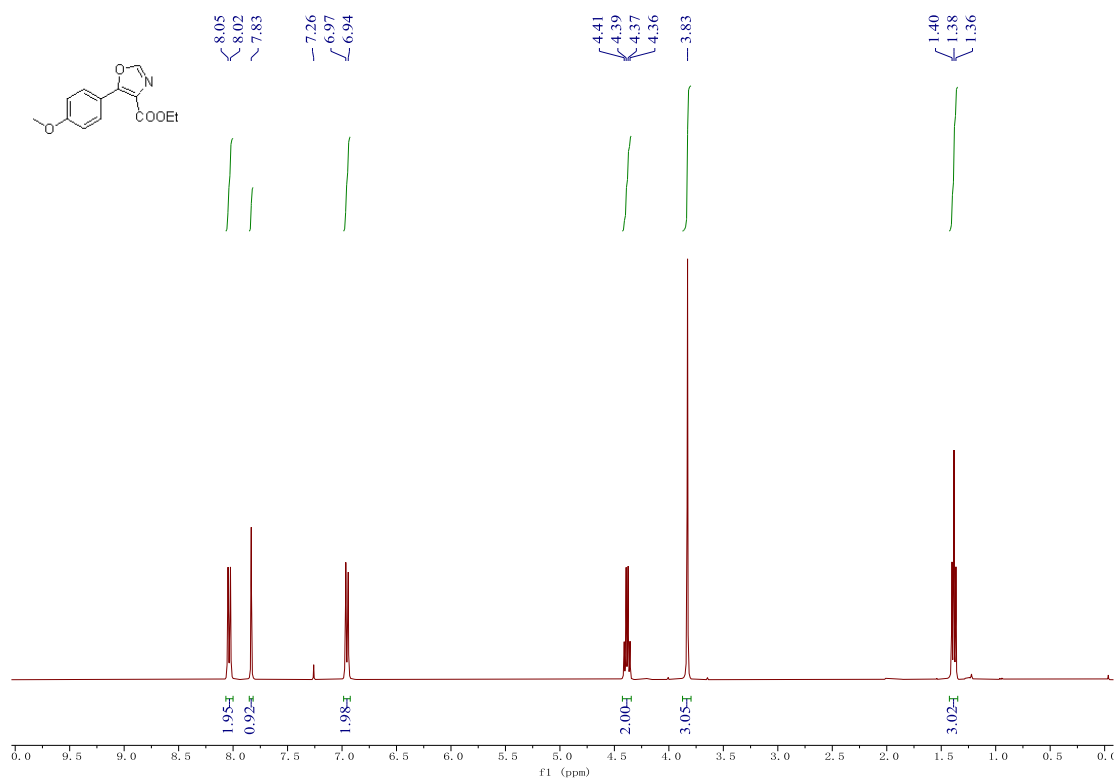


Figure 6. Cyclic voltammograms of PPh₃ and *n*-Bu₄N⁺I⁻ in 0.1 M *n*-Bu₄NBF₄ (CH₃CN), using a glassy carbon working electrode and platinum sheet and saturated calomel electrode (SCE) as counter electrode and reference electrodes at a 100 mV s⁻¹ scan rate. The sample for carboxylic acids was prepared with 0.05 mmol and others were prepared with 0.1 mmol.

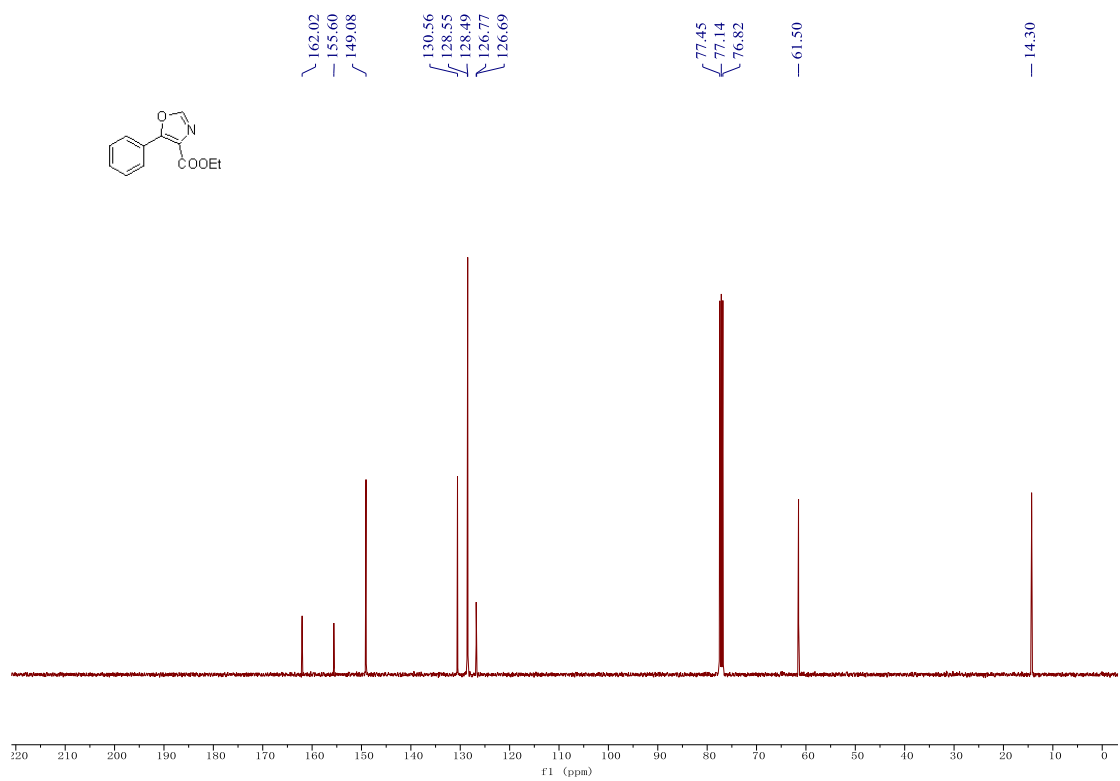
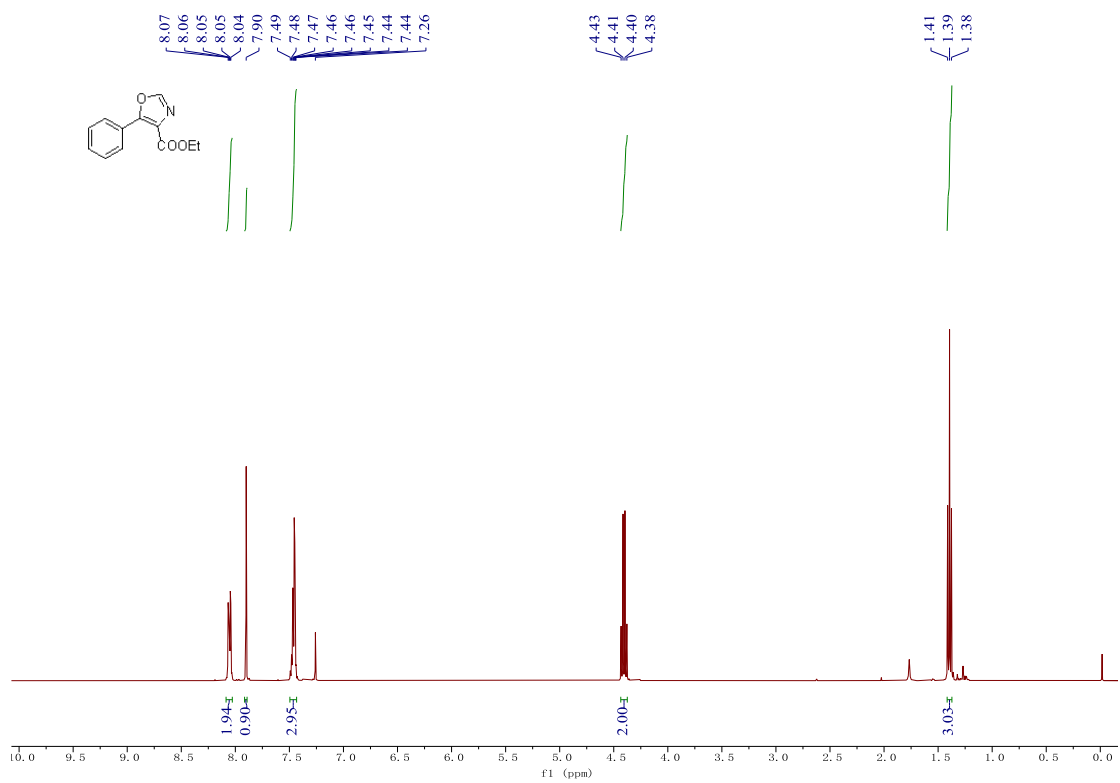
The $E_{1/2}$ vs SCE of phenylbutyric acid in MeCN is 2.10 V, suggesting that the corresponding carboxylic acids are more harder to oxidation than both *n*-Bu₄N⁺I⁻ and PPh₃.

4. NMR Spectra

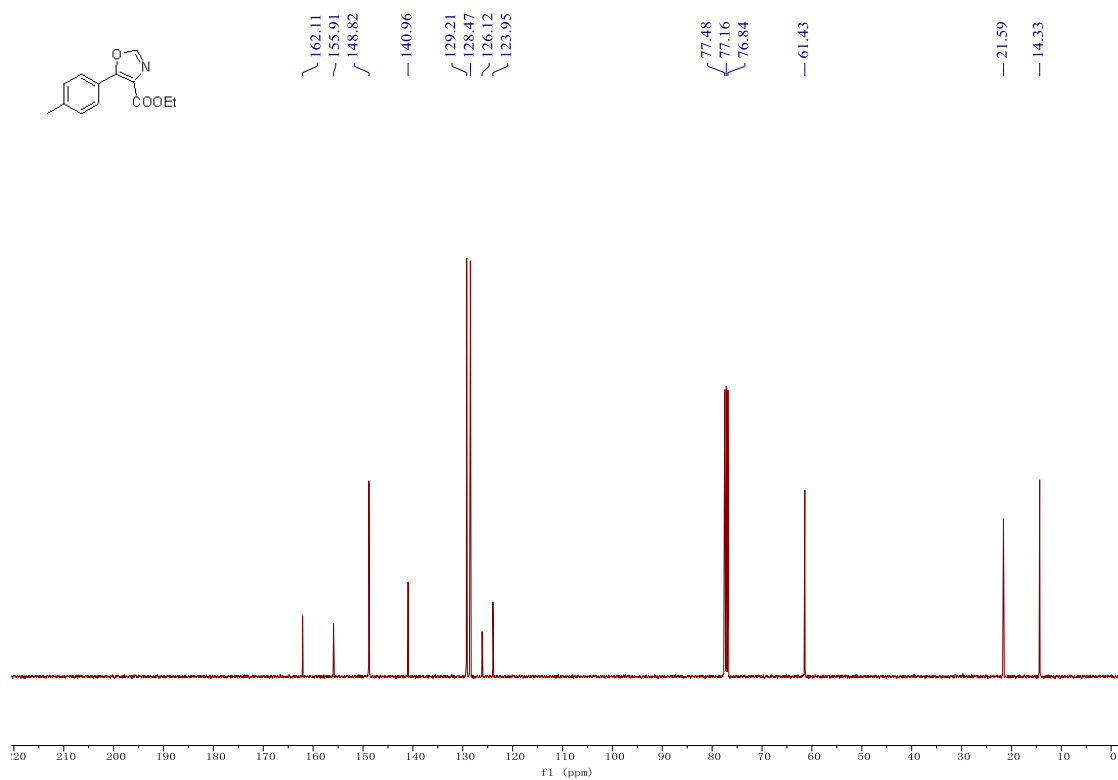
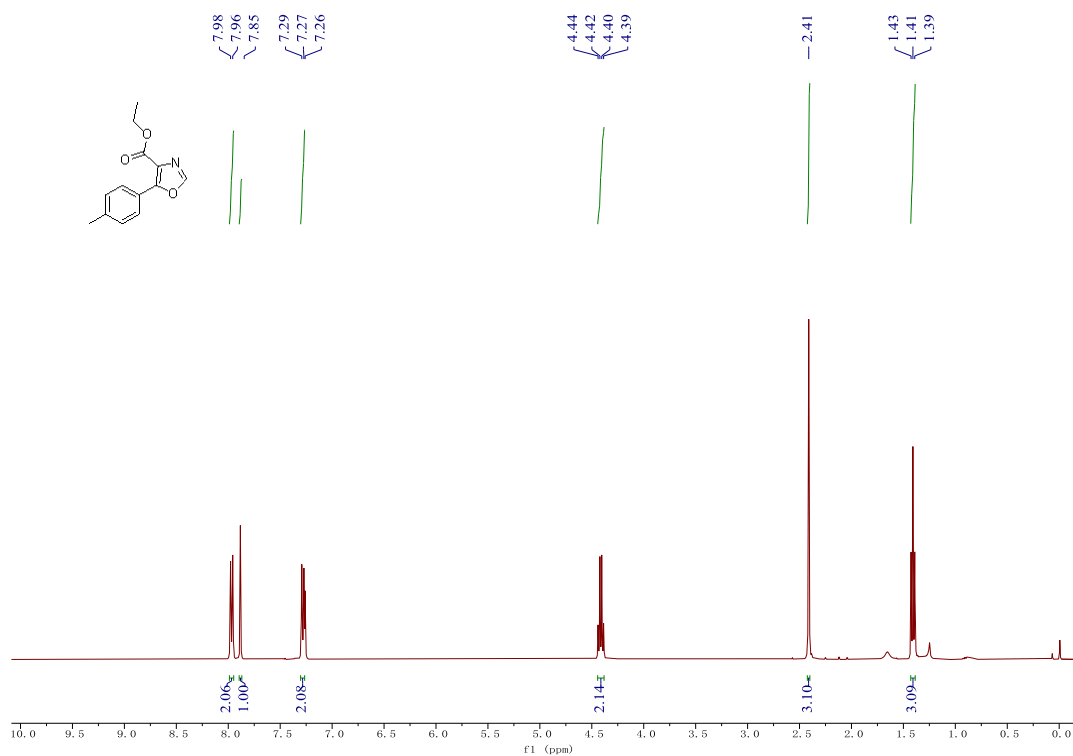
1c ^1H NMR and ^{13}C NMR



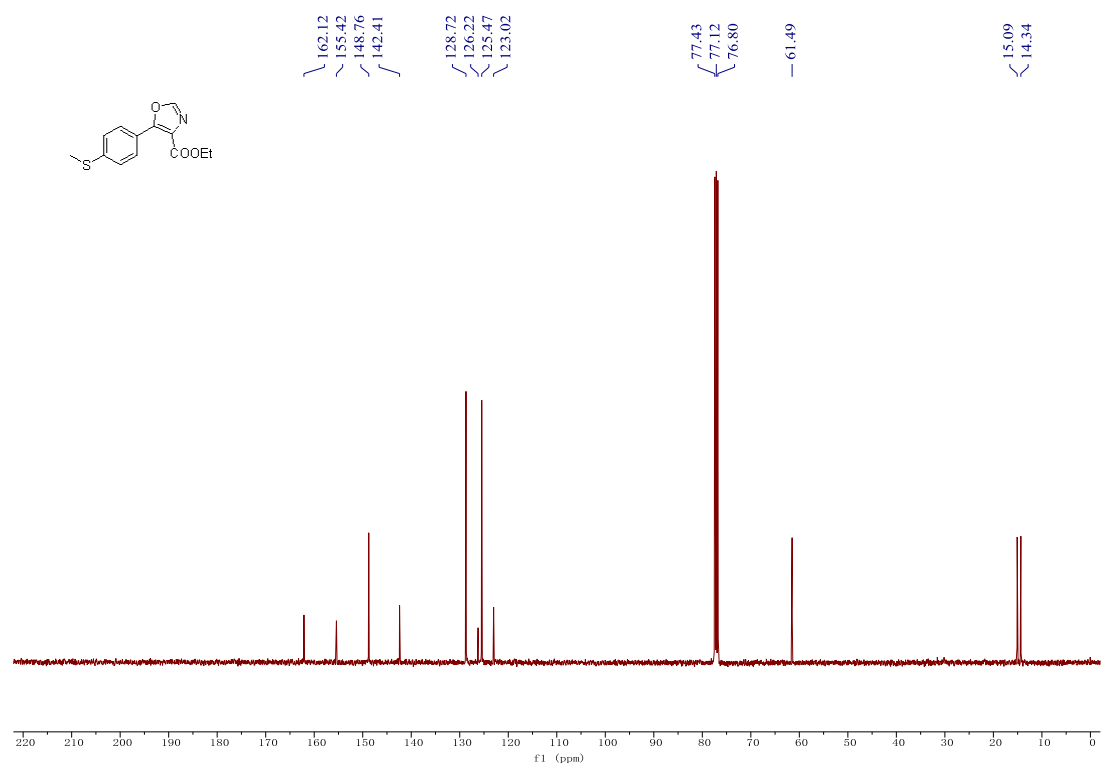
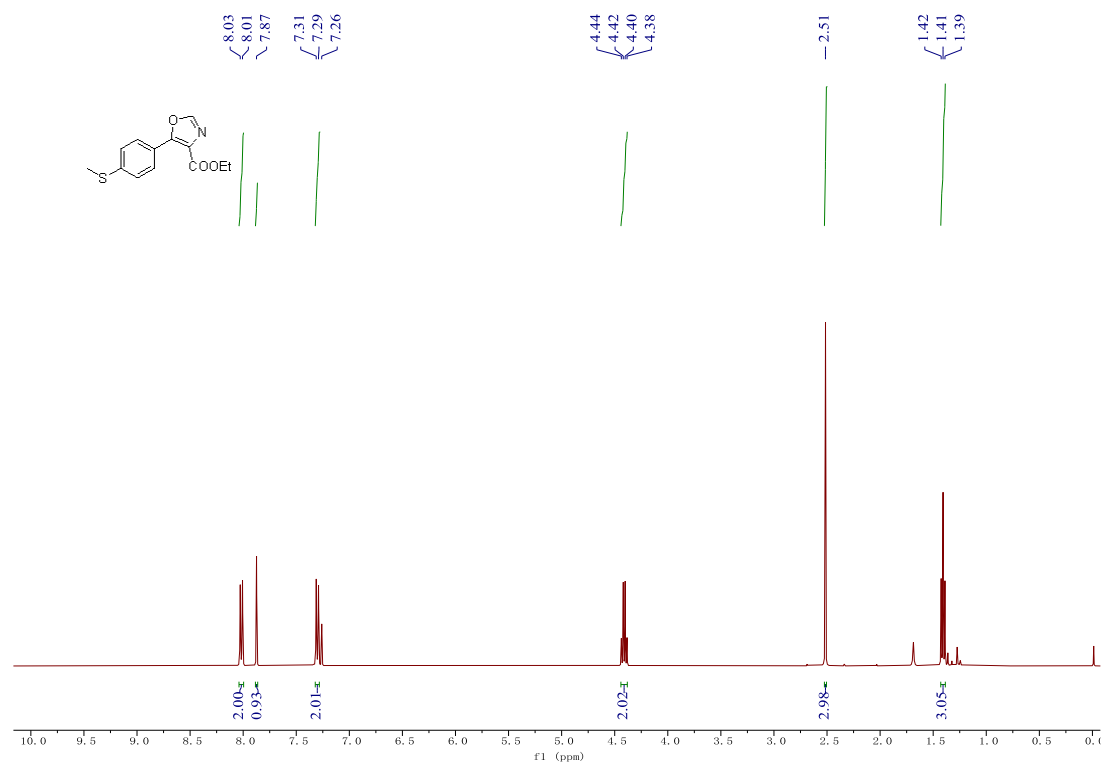
2c ^1H NMR and ^{13}C NMR



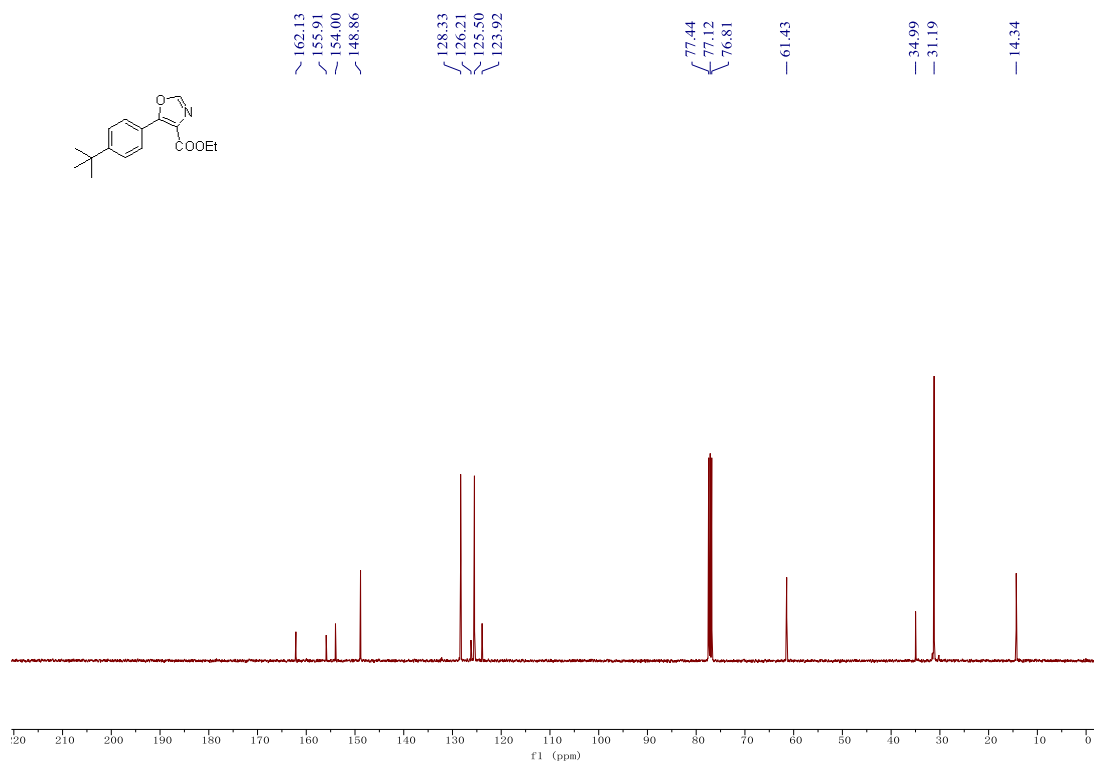
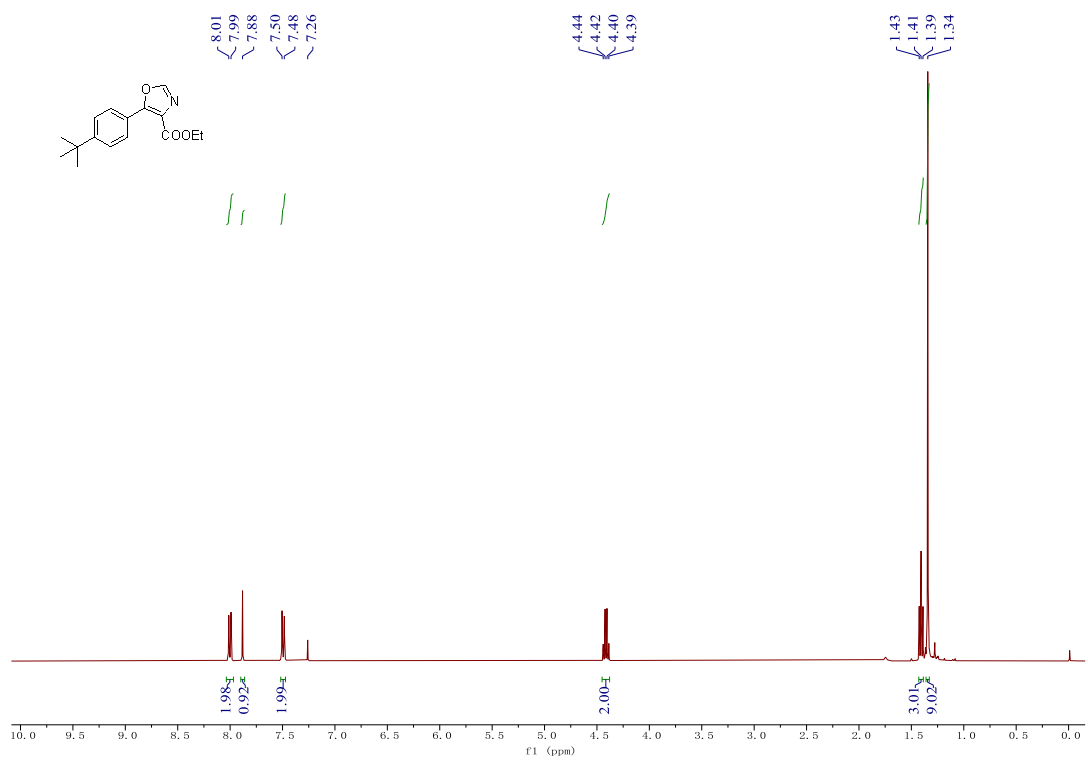
3c ^1H NMR and ^{13}C NMR



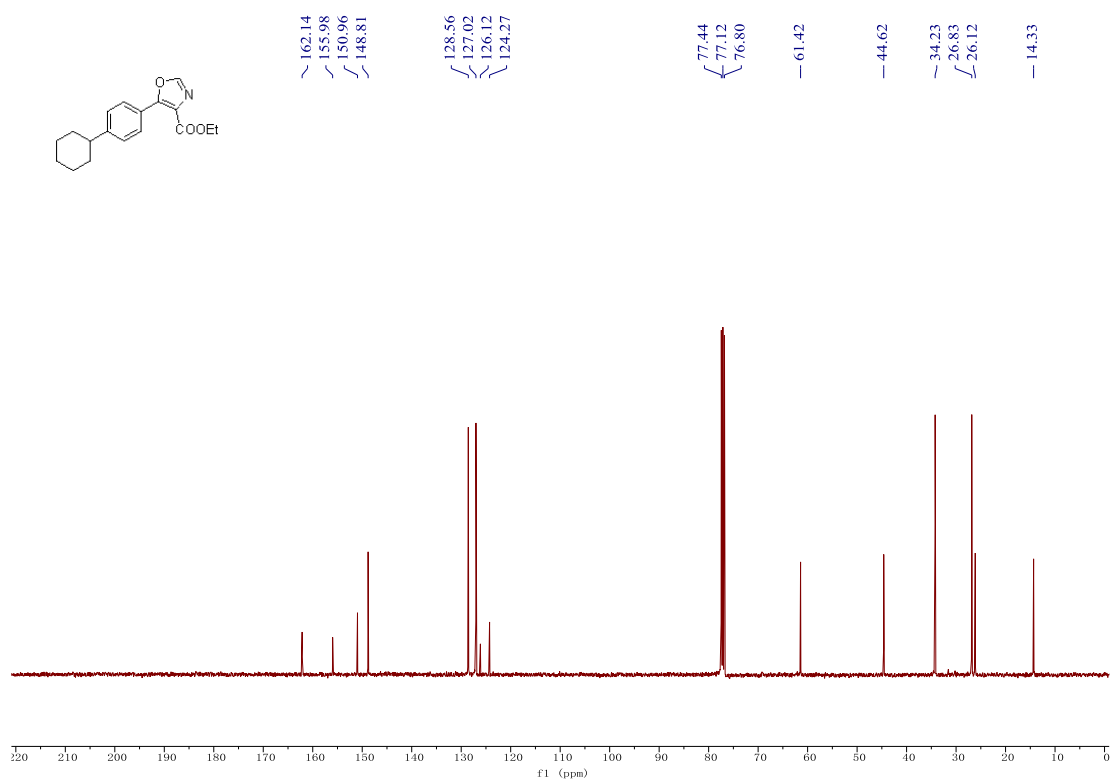
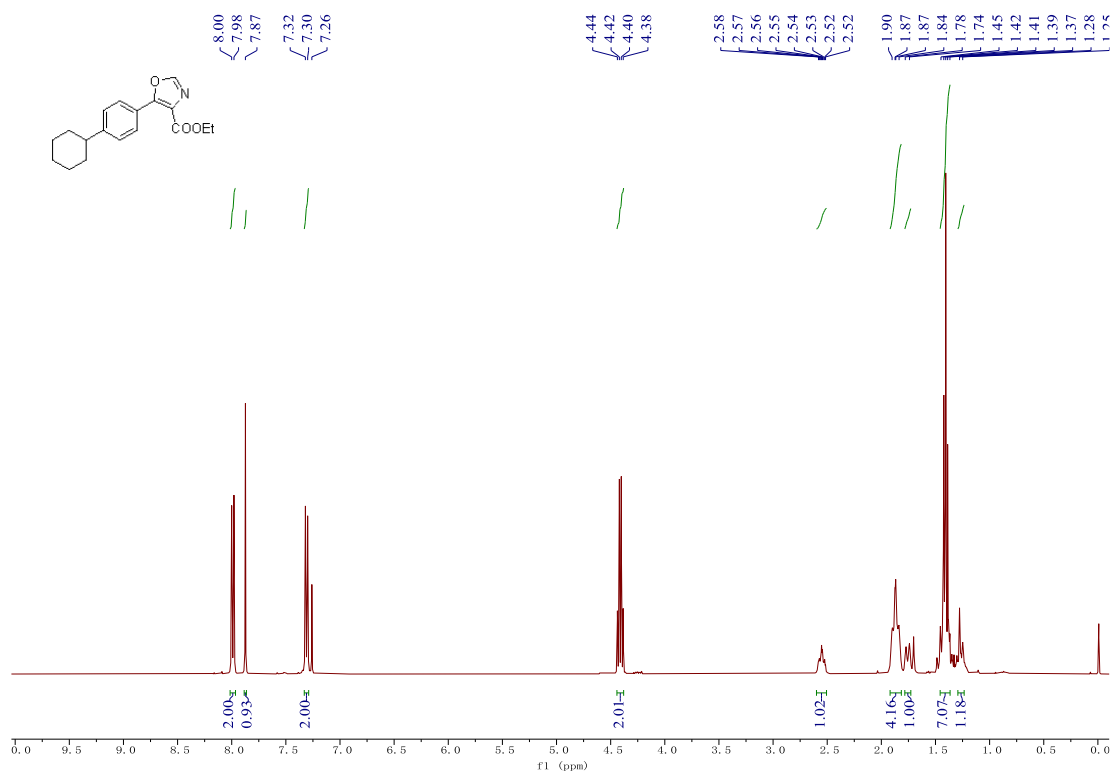
4c ^1H NMR and ^{13}C NMR



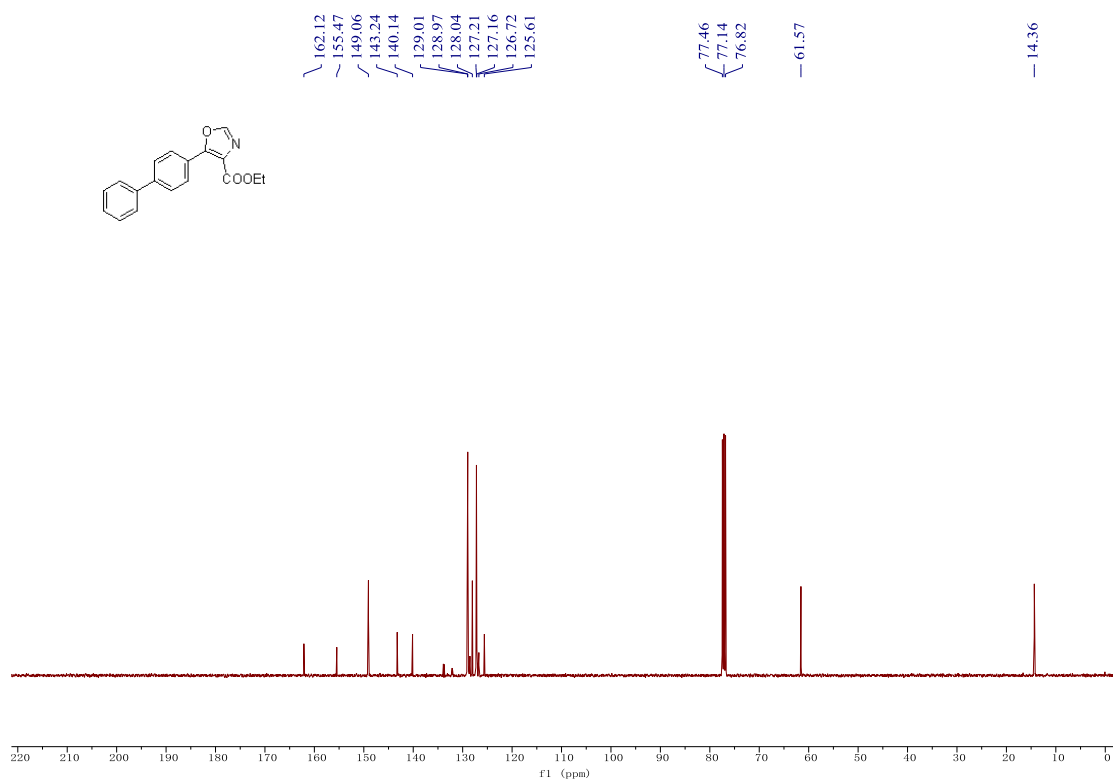
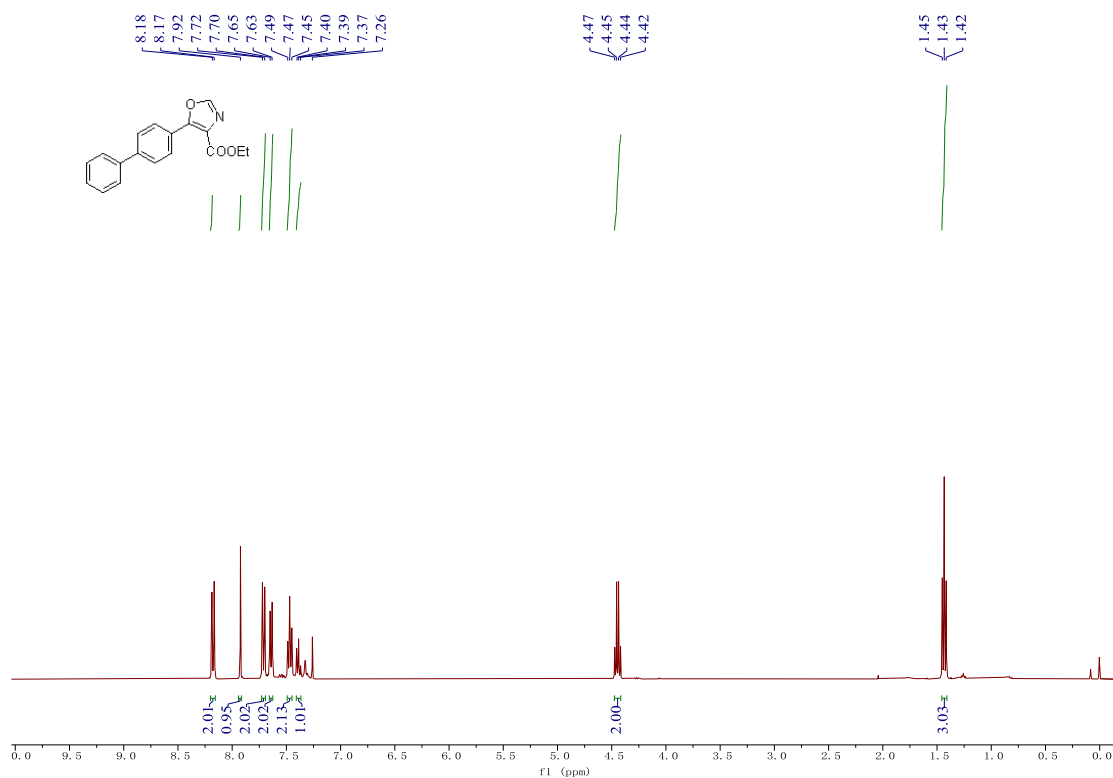
5c ^1H NMR and ^{13}C NMR



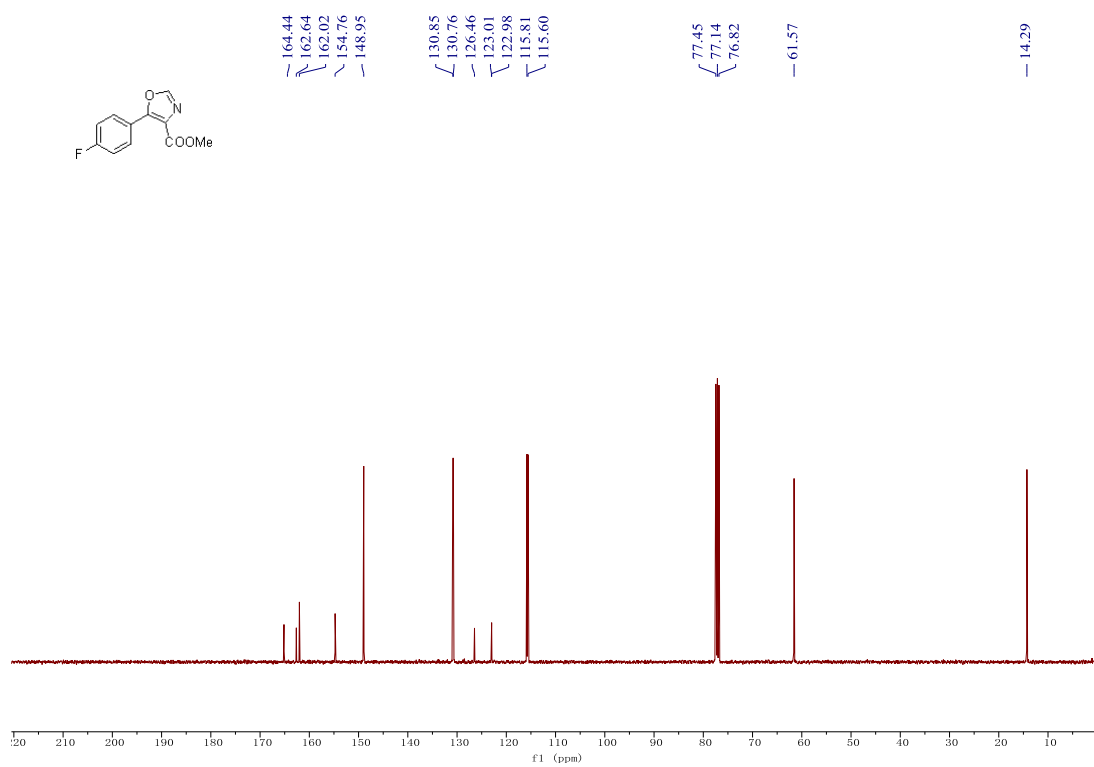
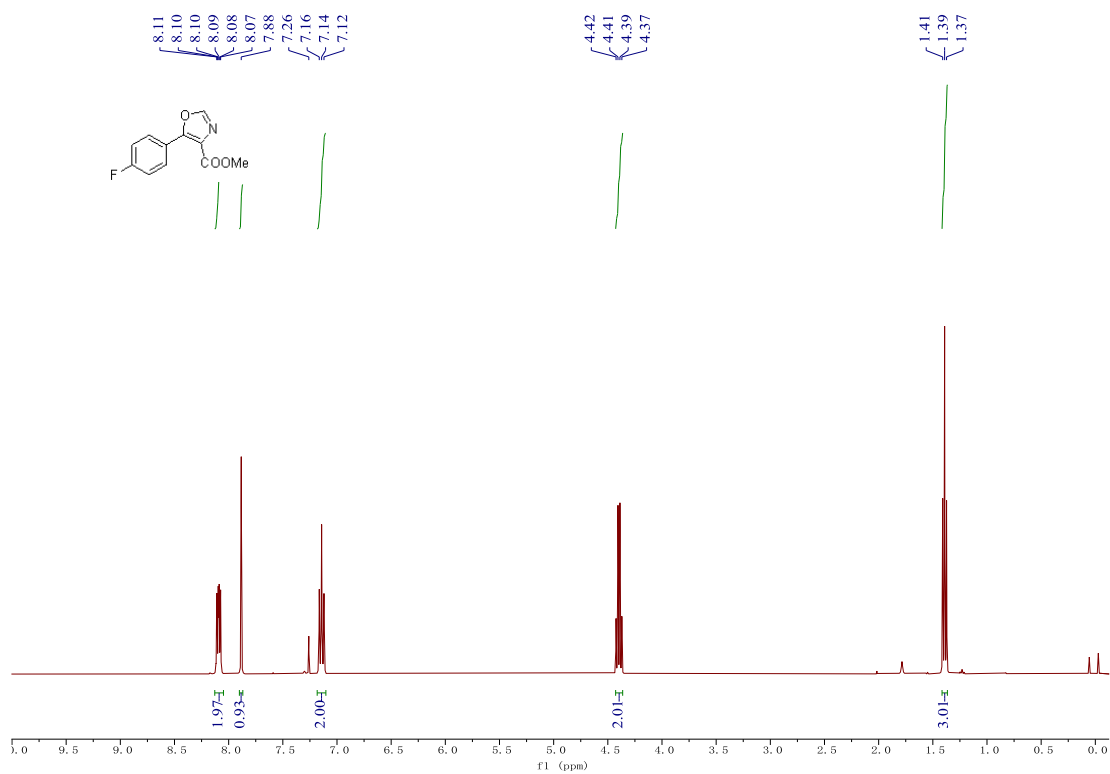
6c ^1H NMR and ^{13}C NMR

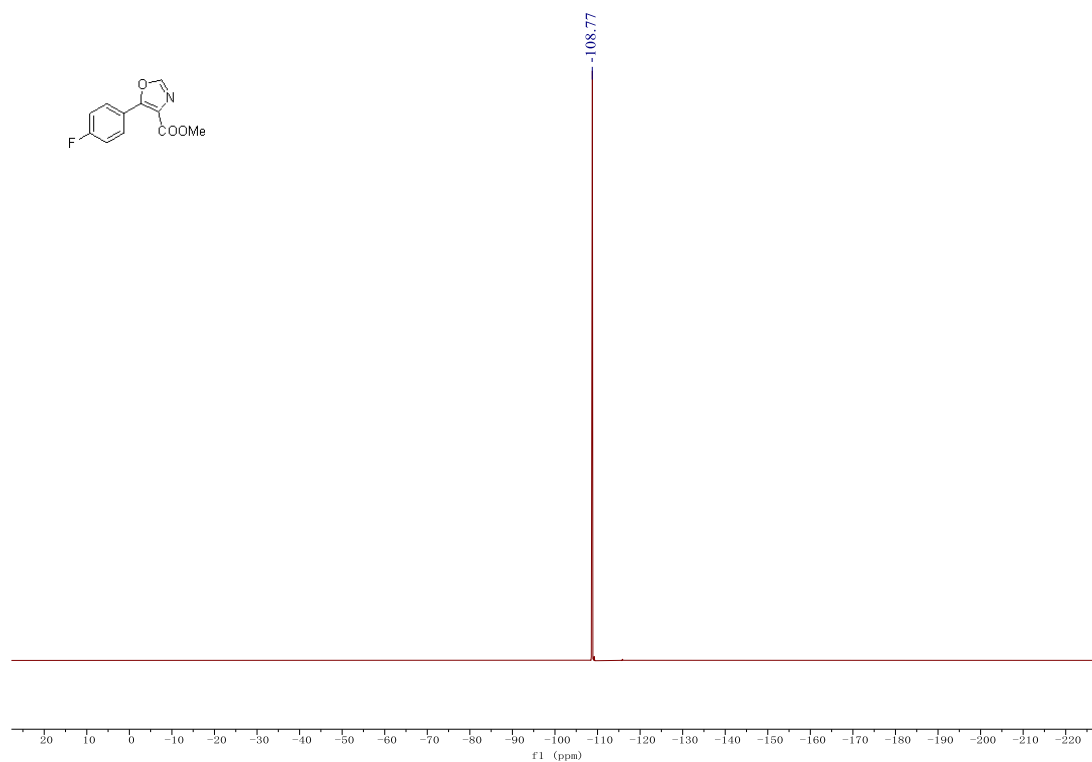


7c¹H NMR and ¹³C NMR

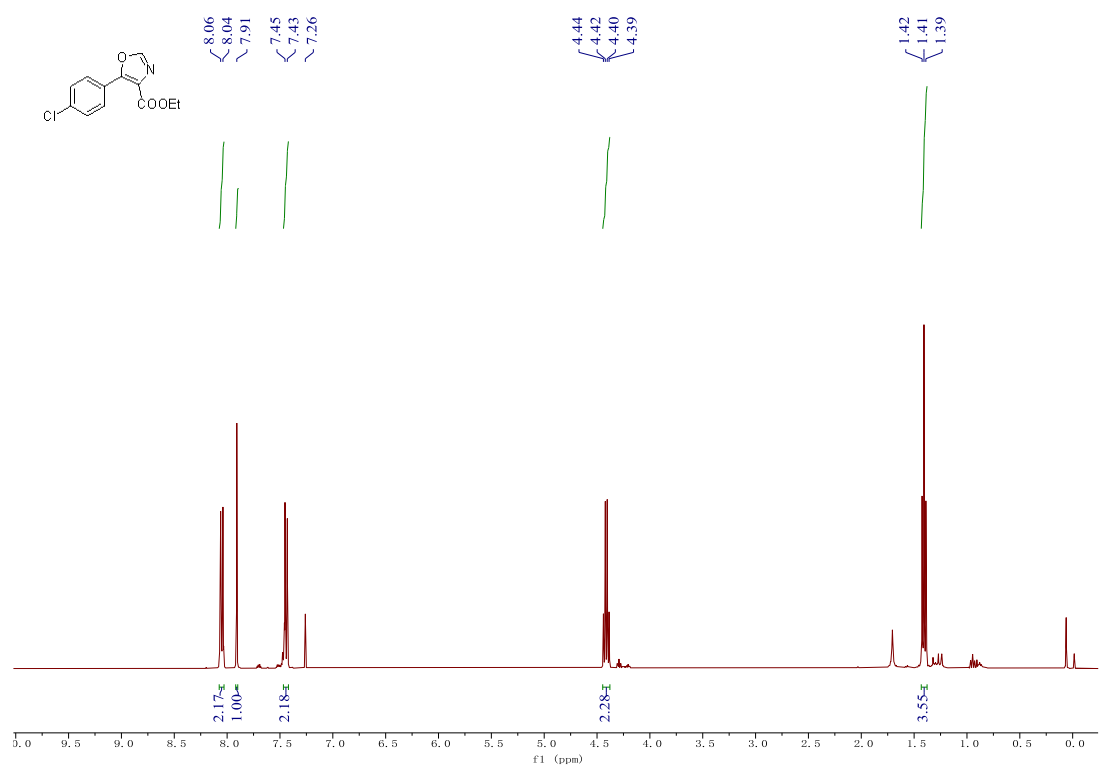
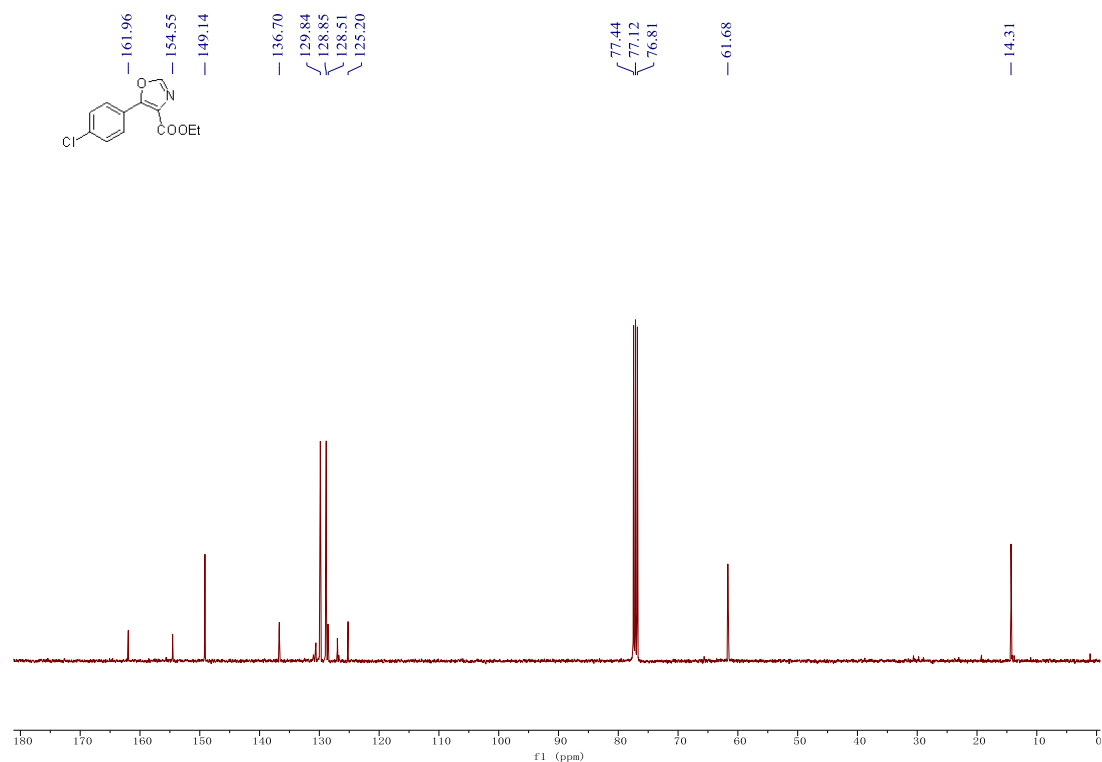


8c ^1H NMR, ^{13}C NMR and ^{19}F NMR

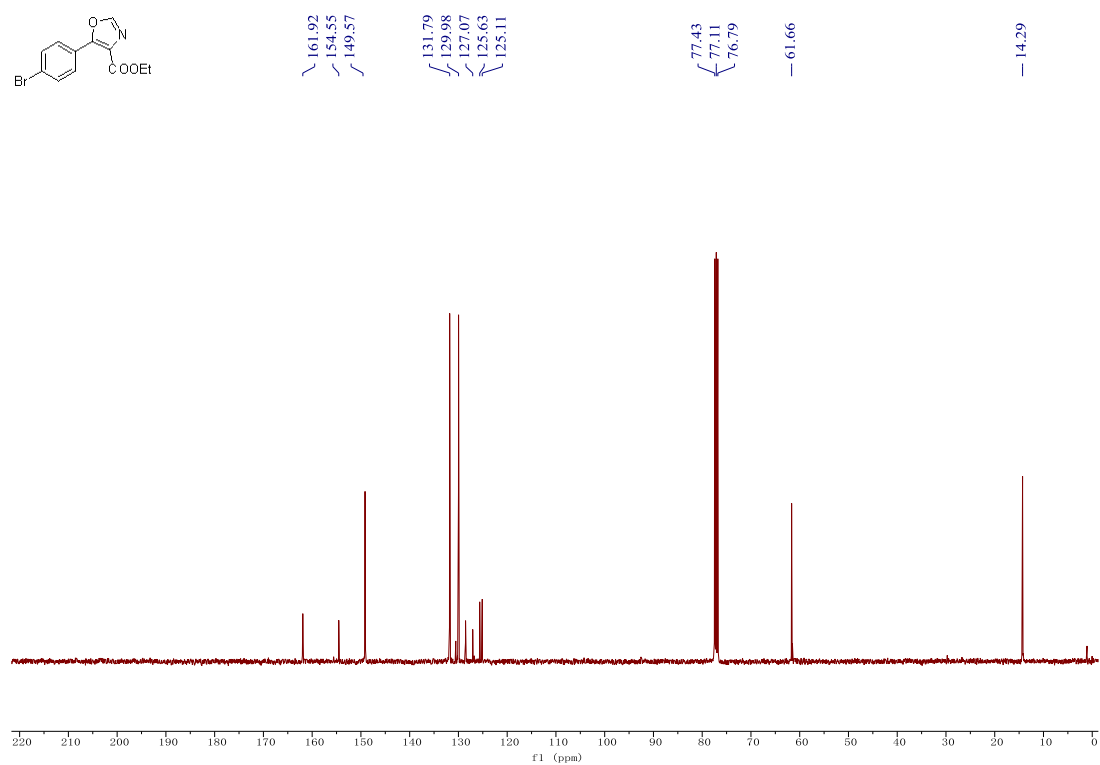
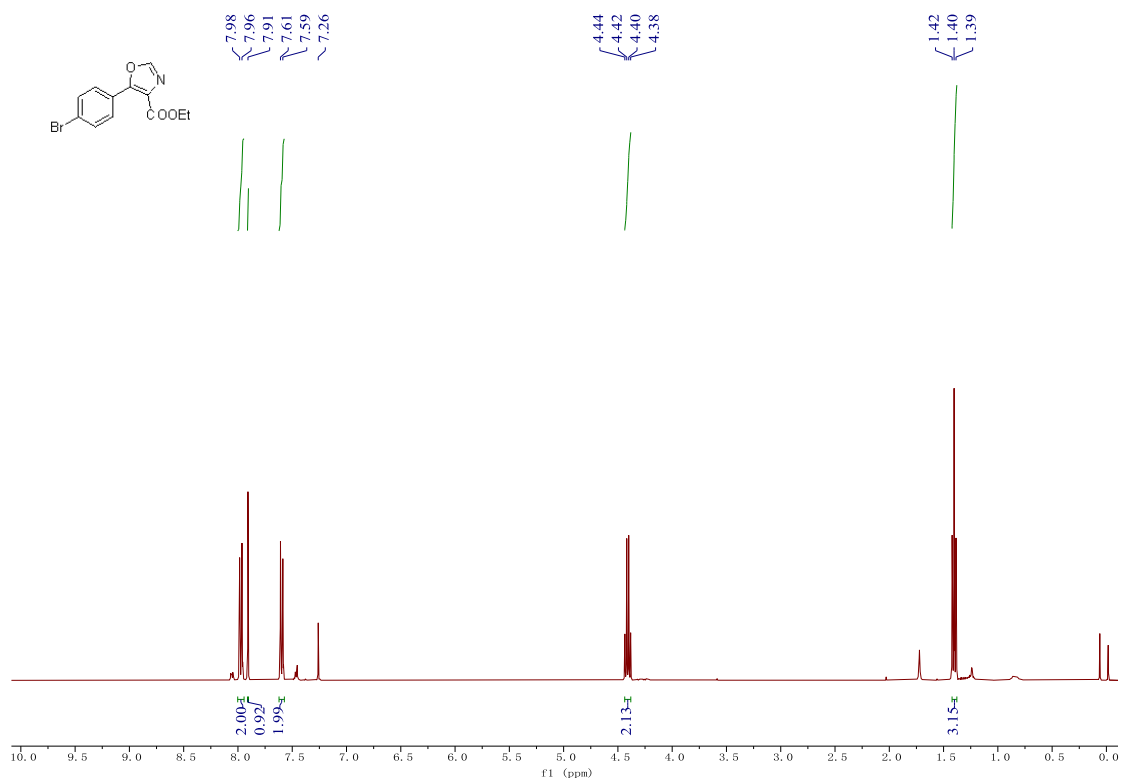




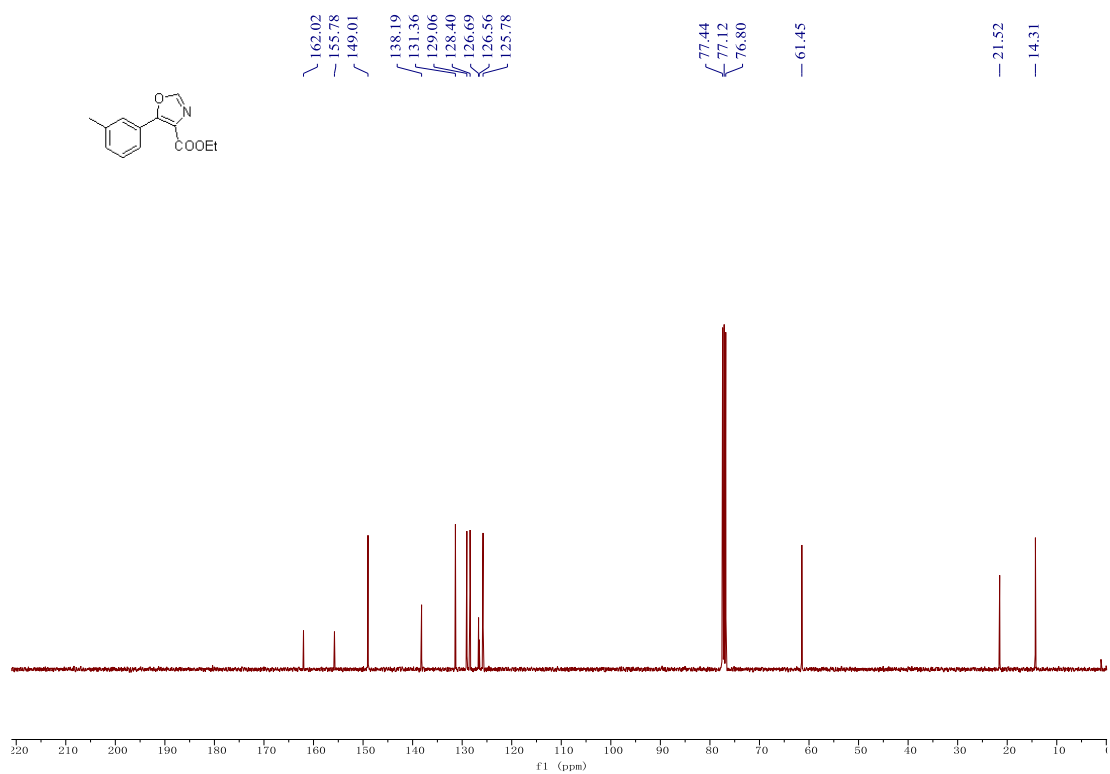
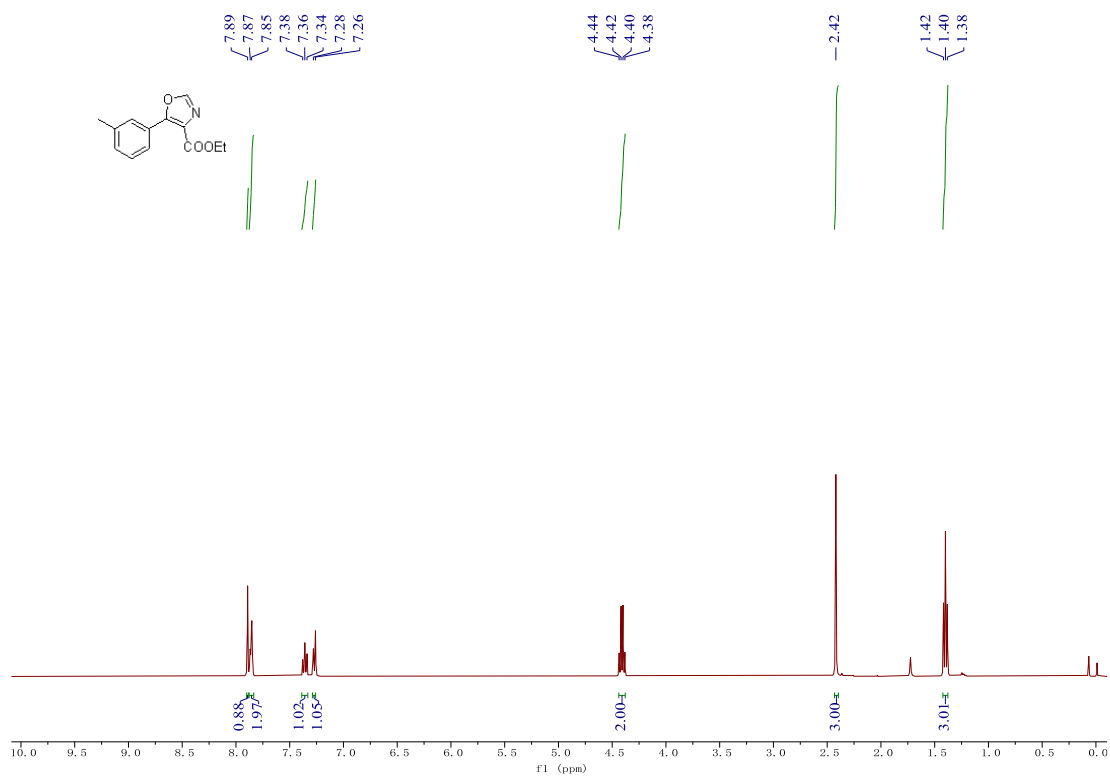
9c ^1H NMR and ^{13}C NMR



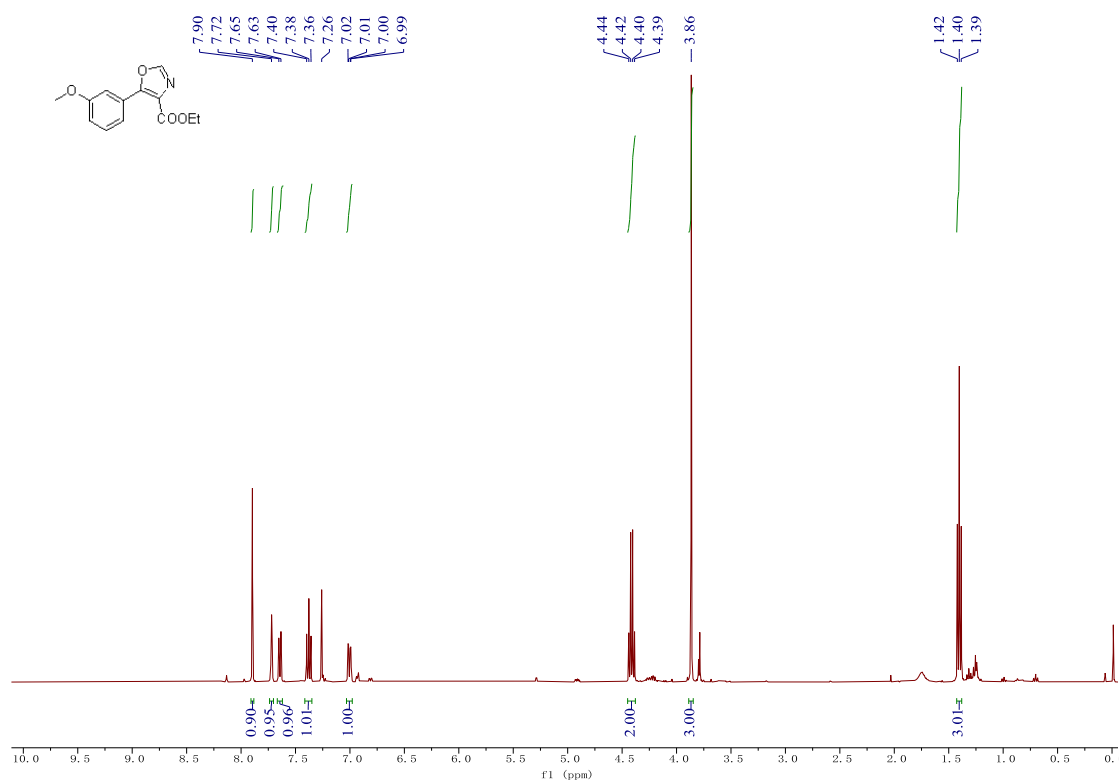
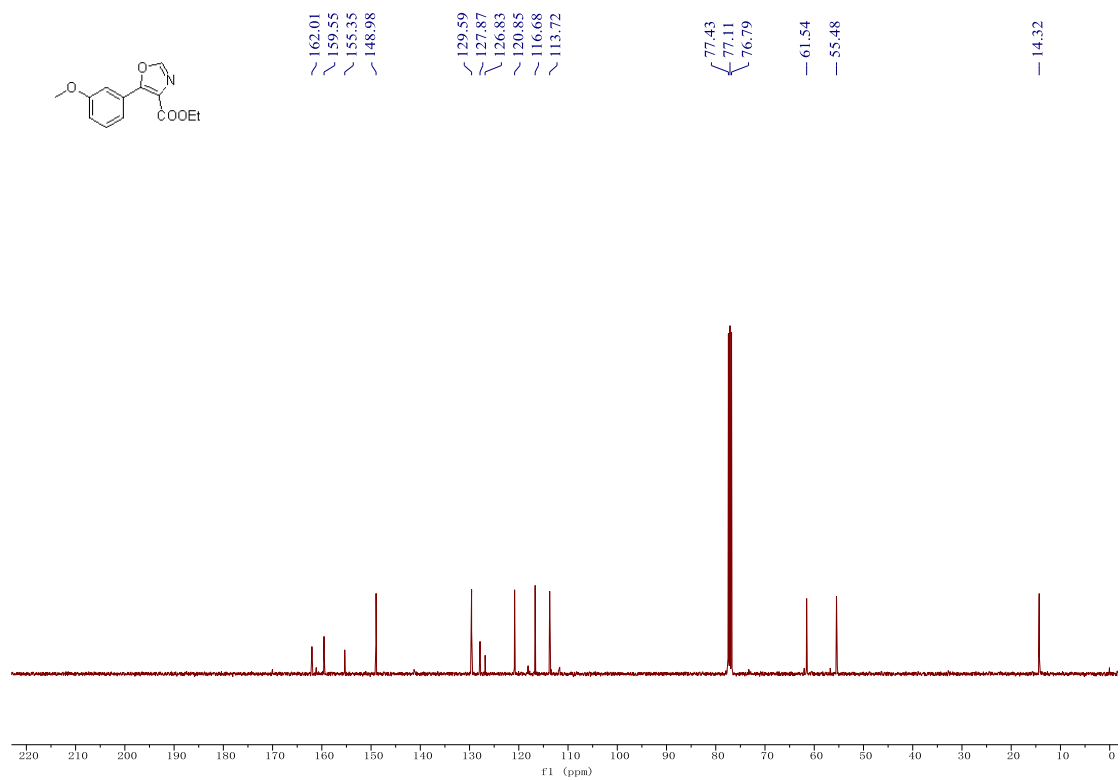
10c ^1H NMR and ^{13}C NMR



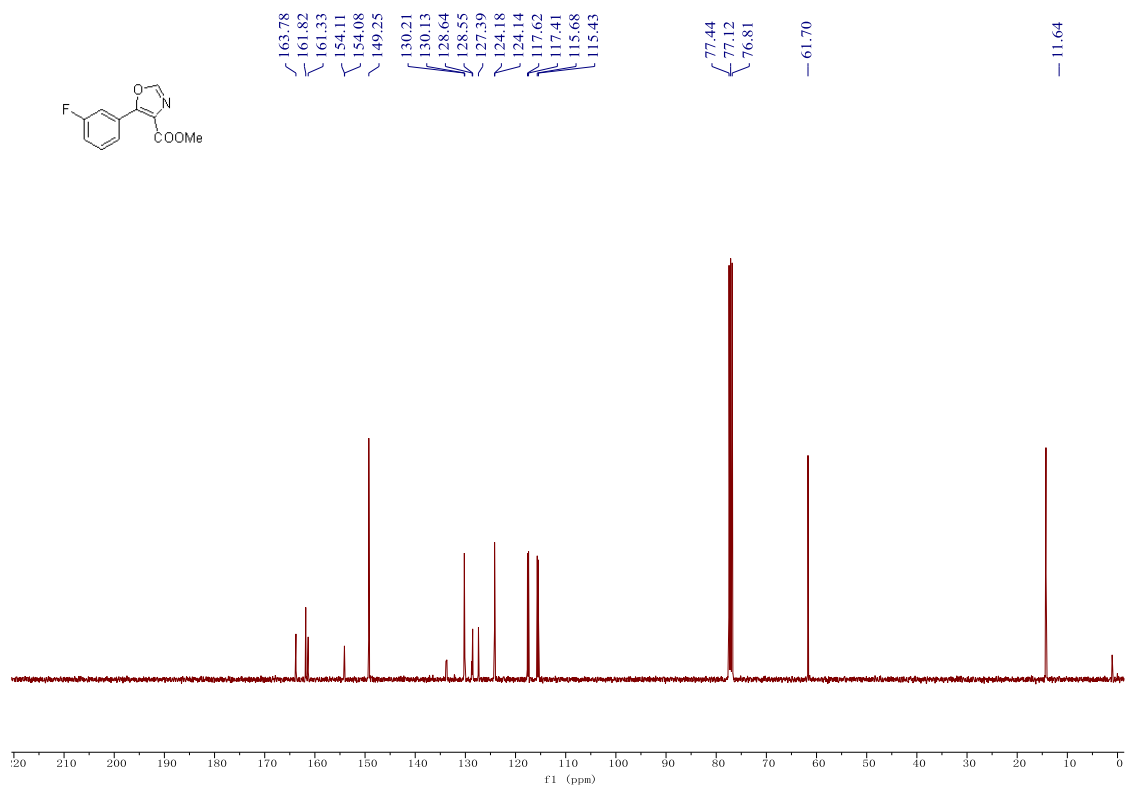
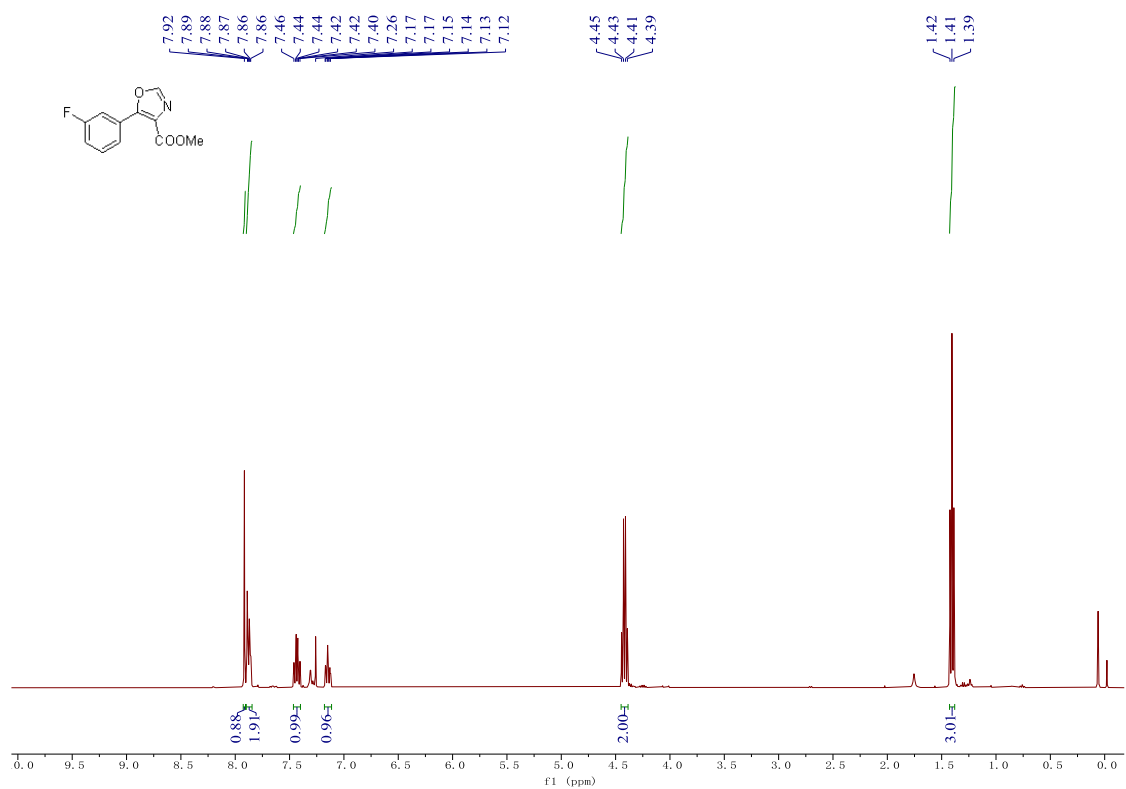
11c ^1H NMR and ^{13}C NMR

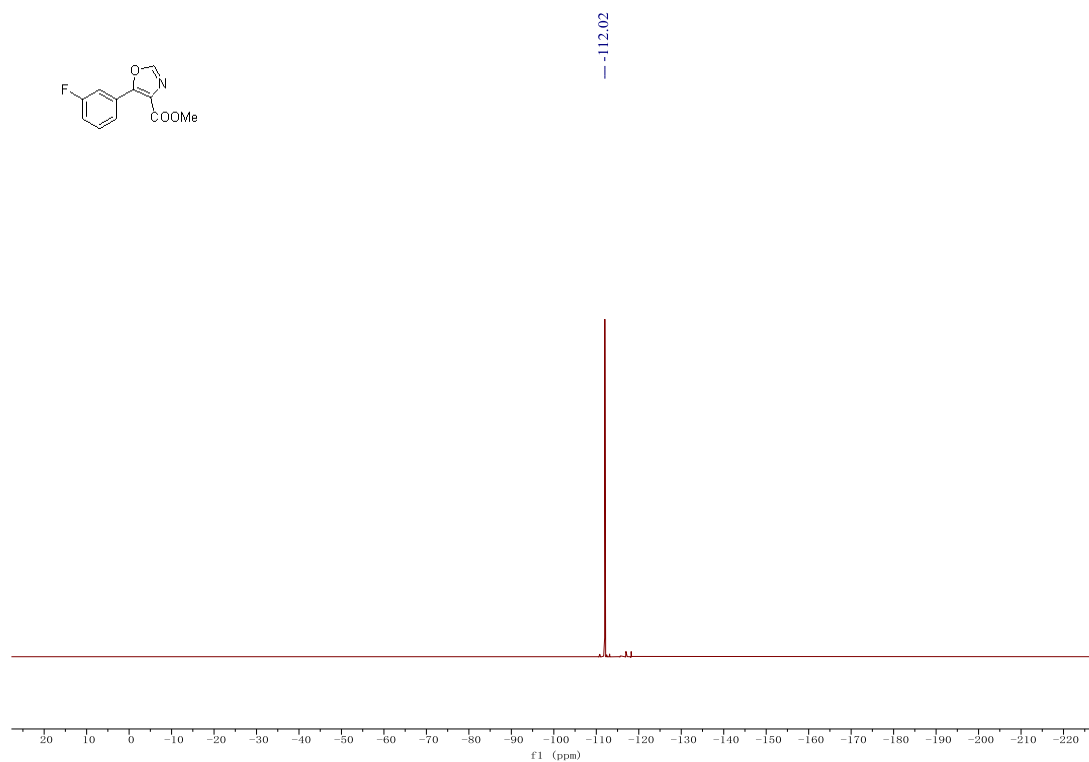


12c ^1H NMR and ^{13}C NMR

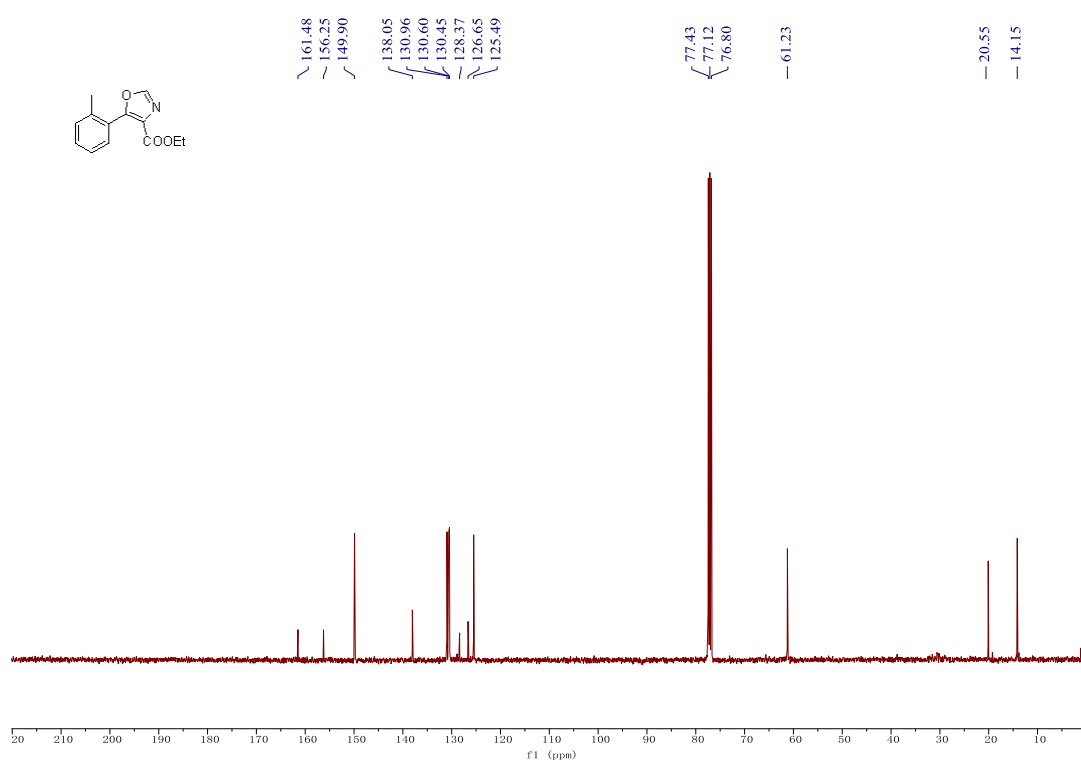
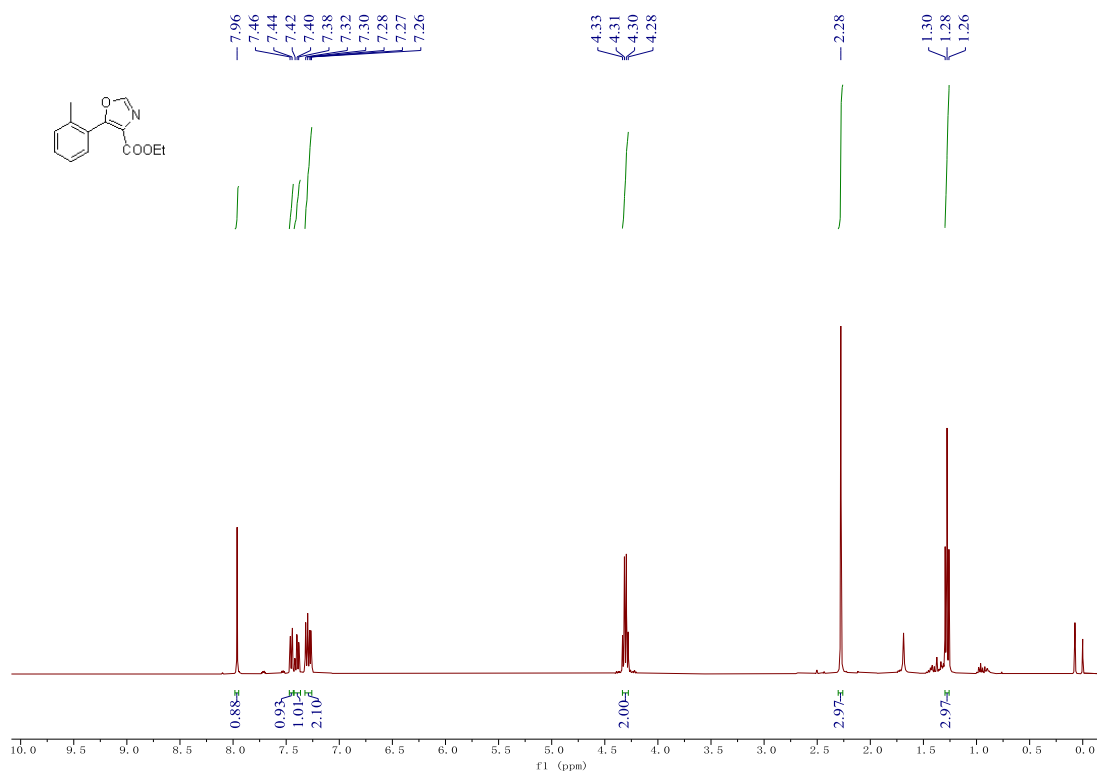


13c ¹H NMR, ¹³C NMR and ¹⁹F NMR

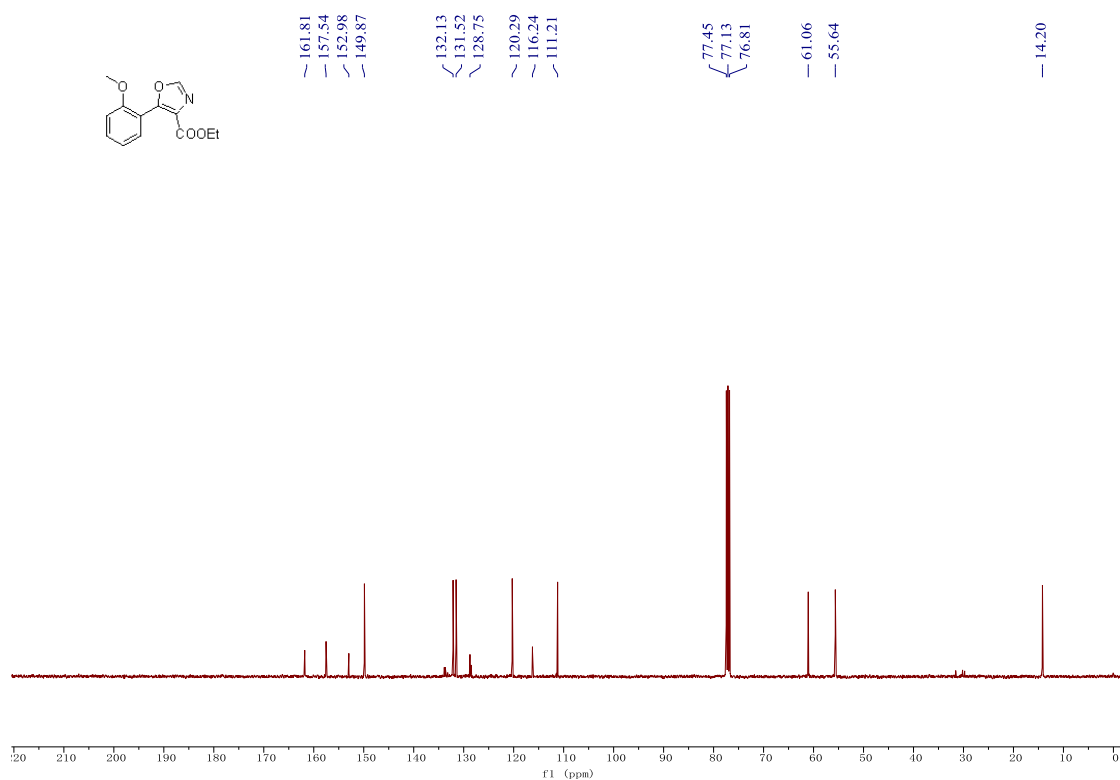
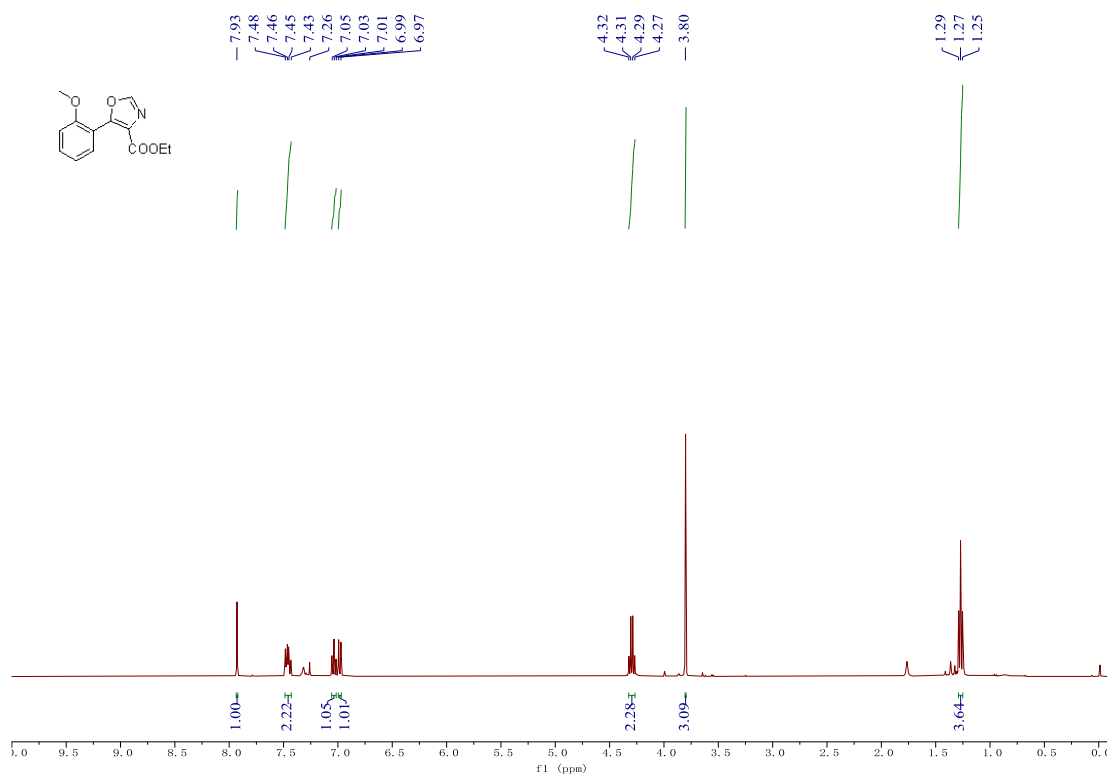




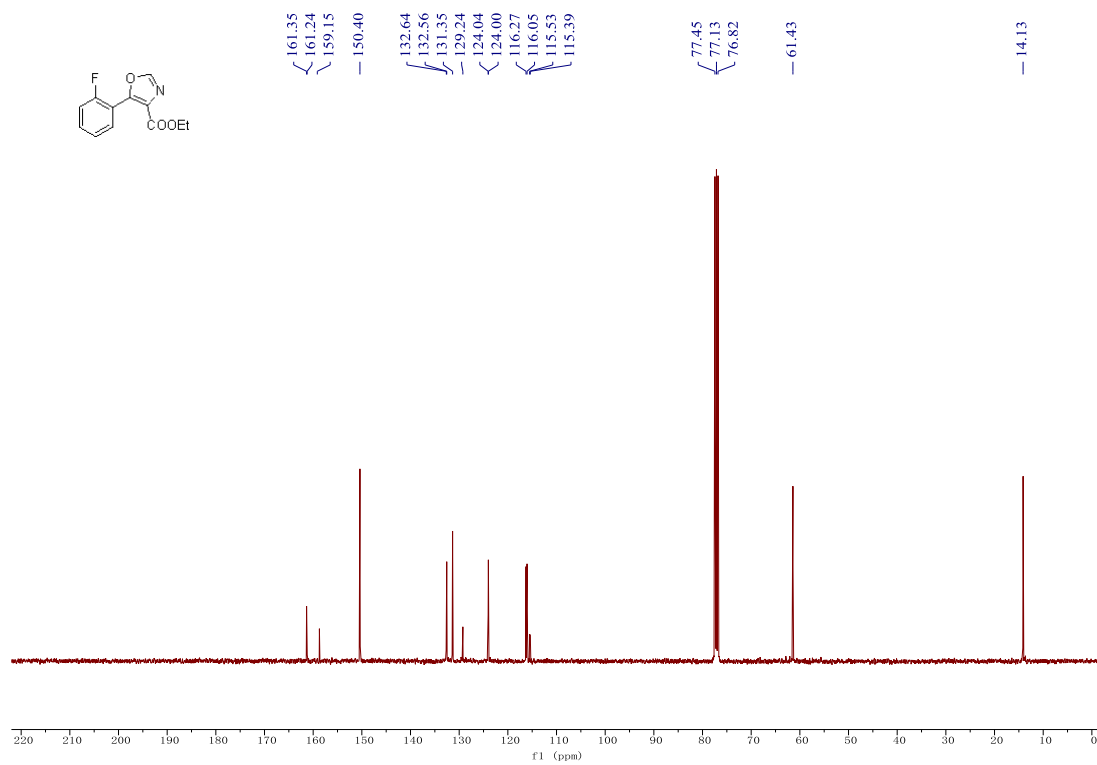
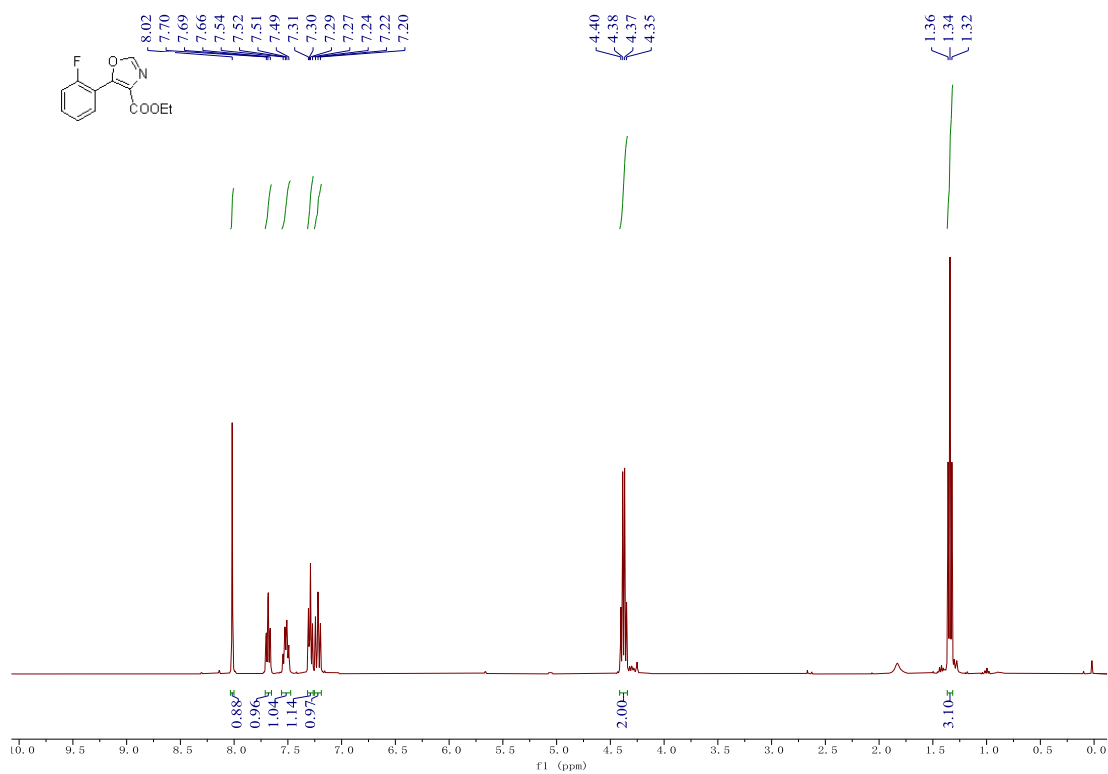
14c ^1H NMR and ^{13}C NMR

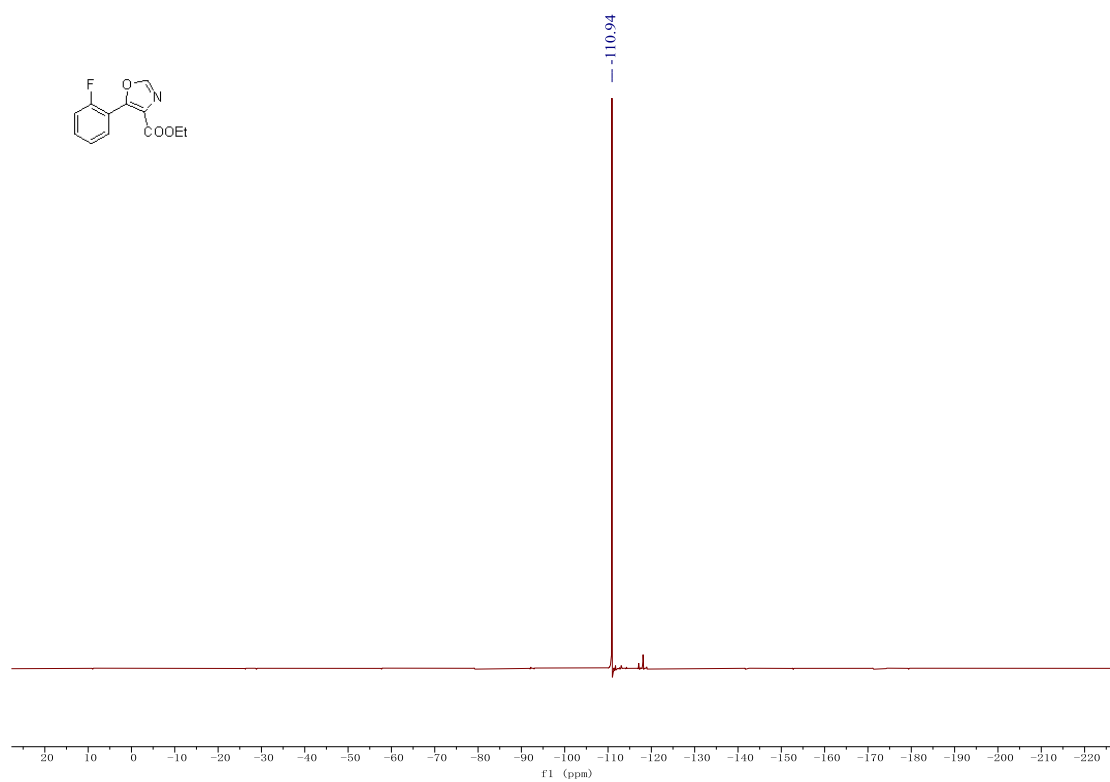


15c ^1H NMR and ^{13}C NMR

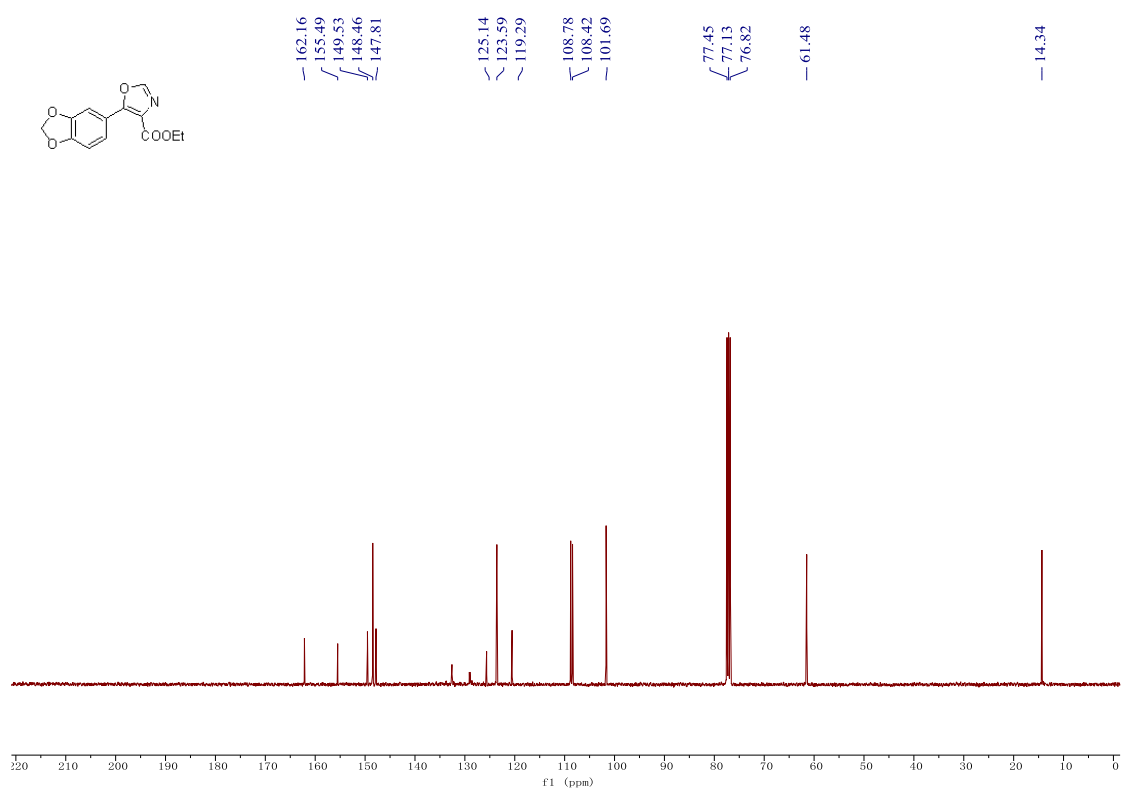
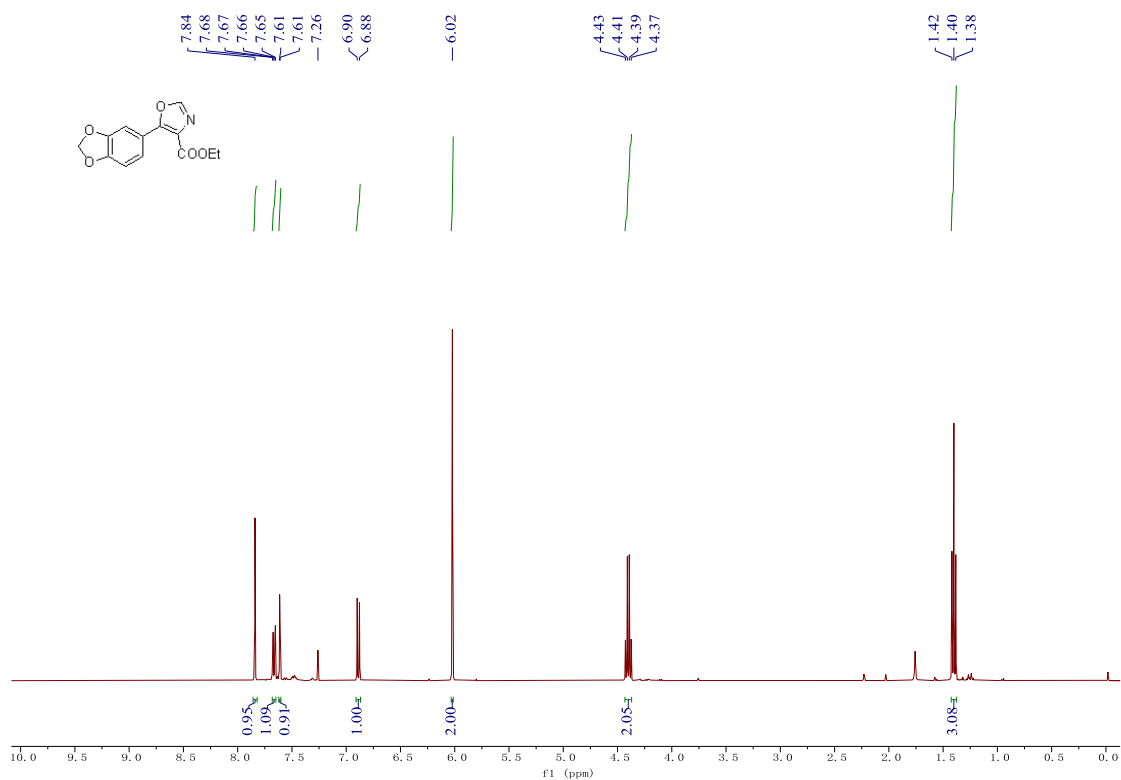


16c ^1H NMR, ^{13}C NMR and ^{19}F NMR

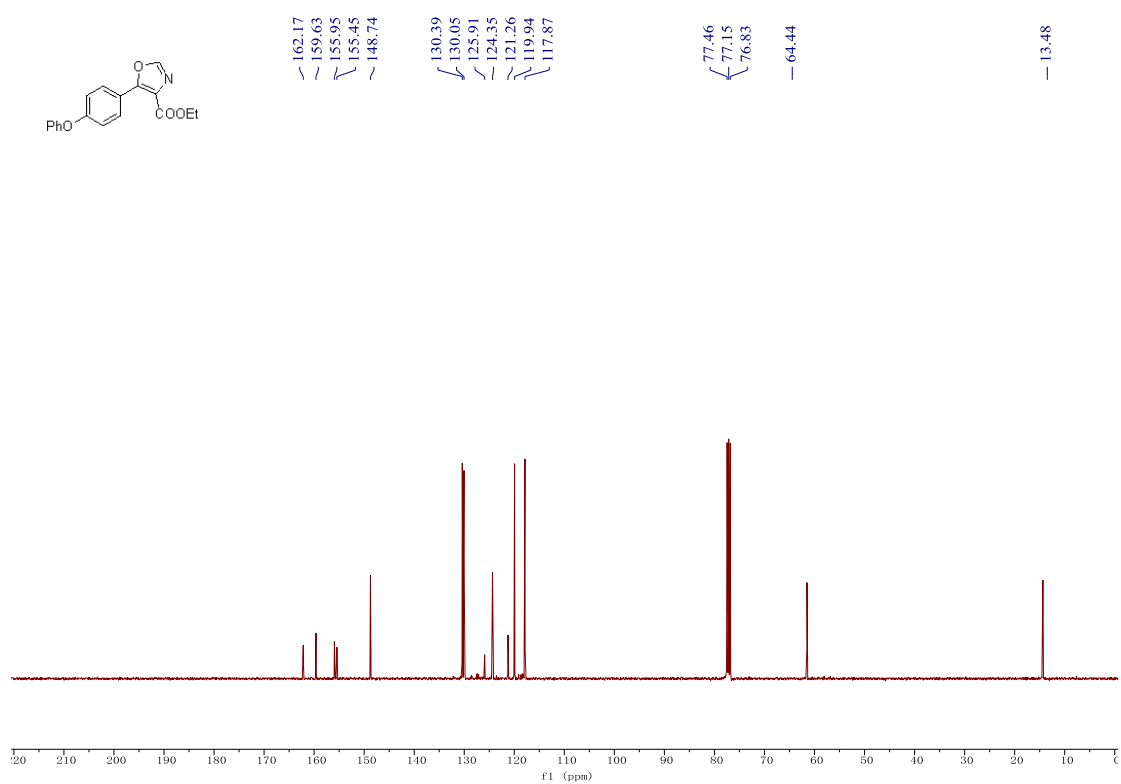
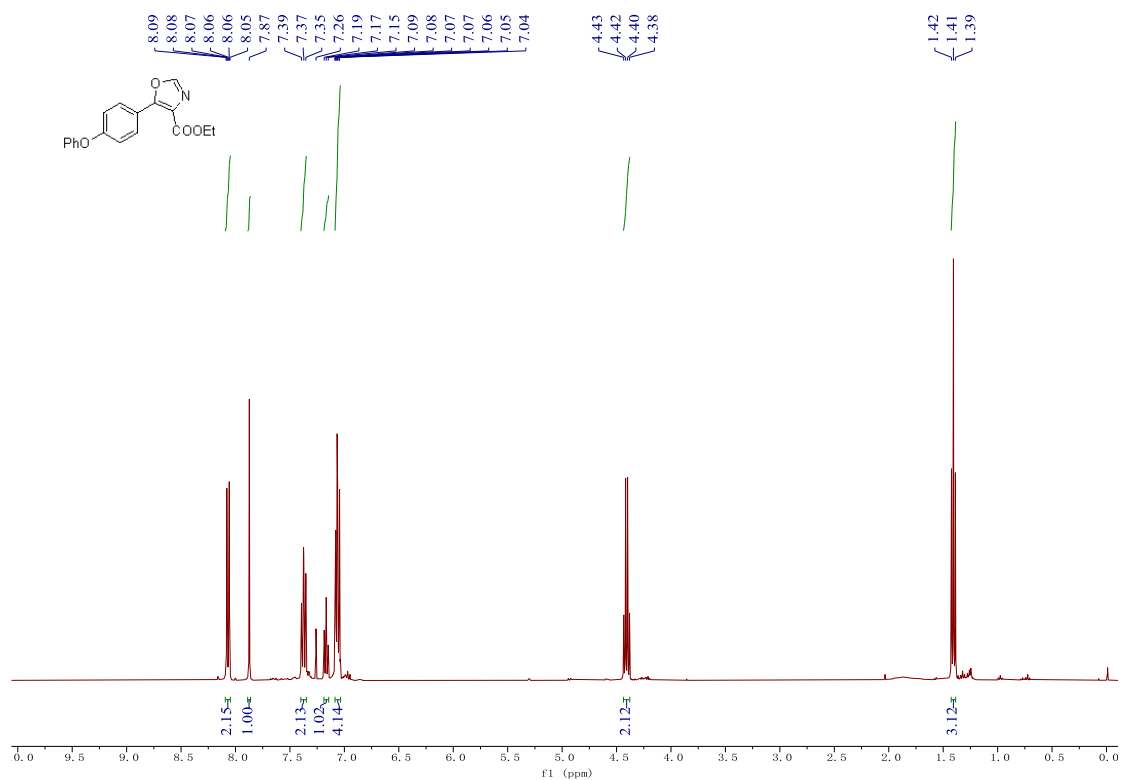




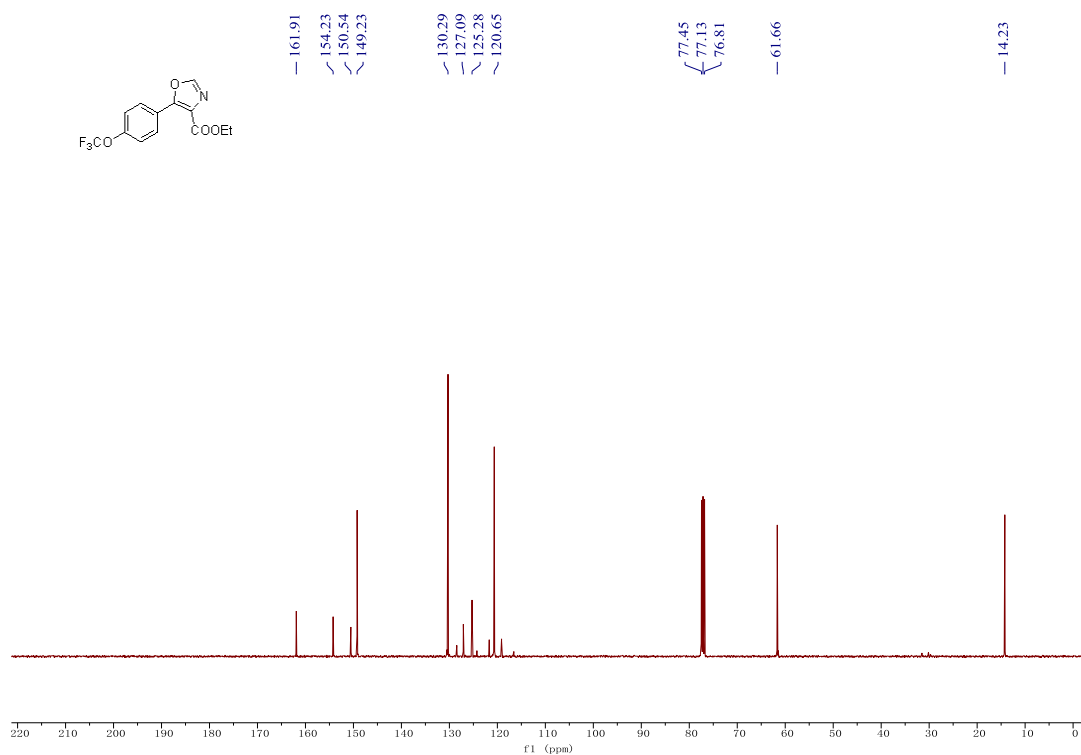
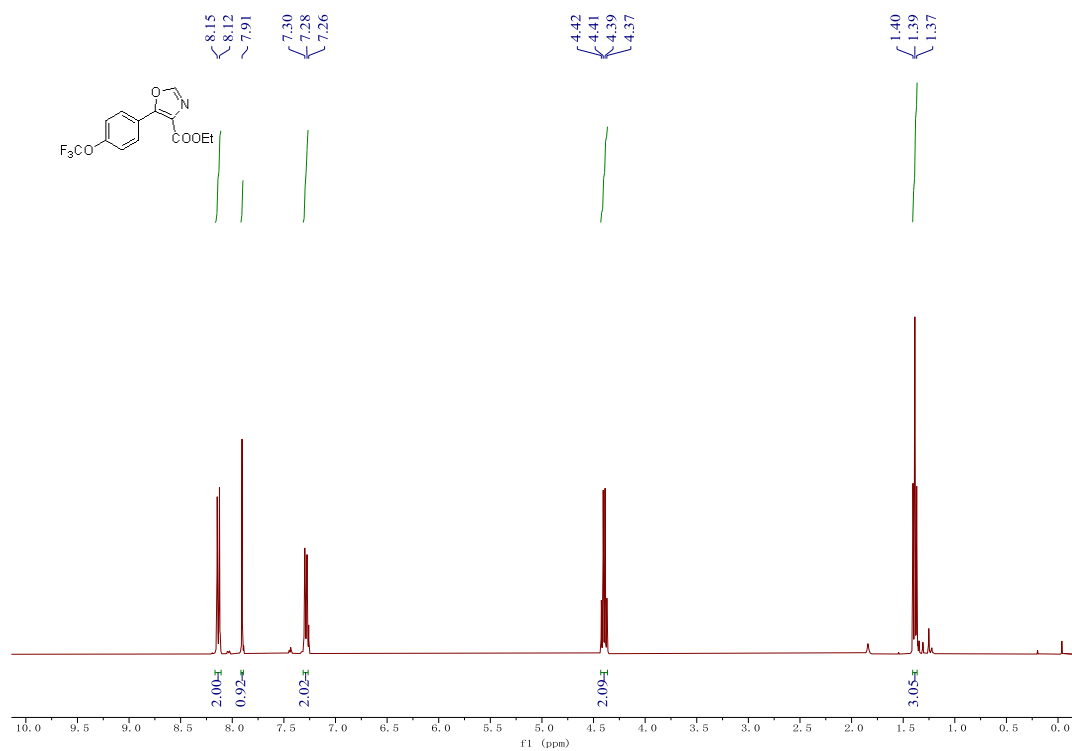
17c ^1H NMR and ^{13}C NMR

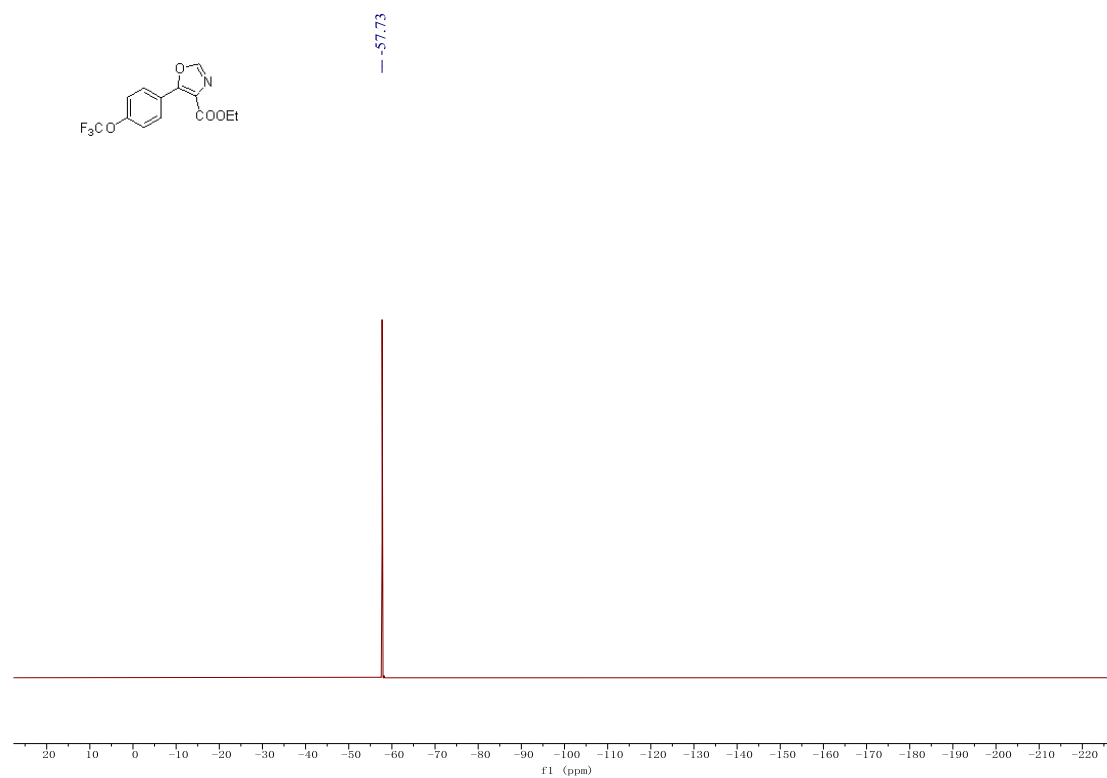


18c ^1H NMR and ^{13}C NMR

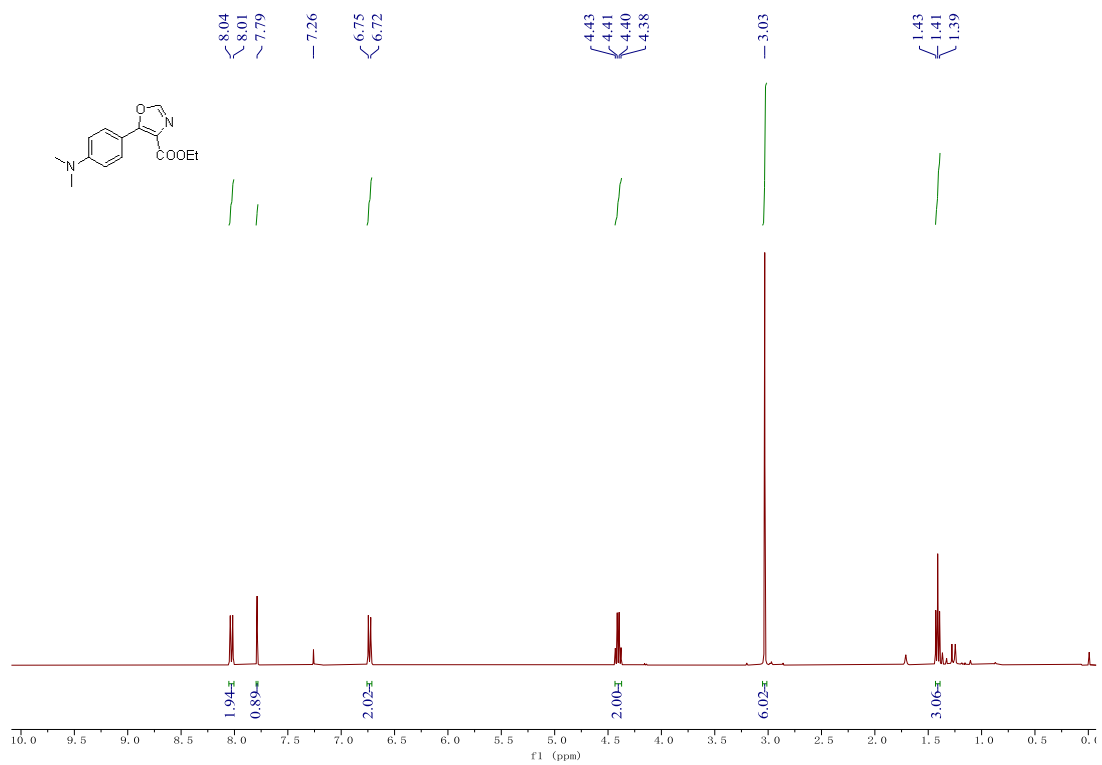
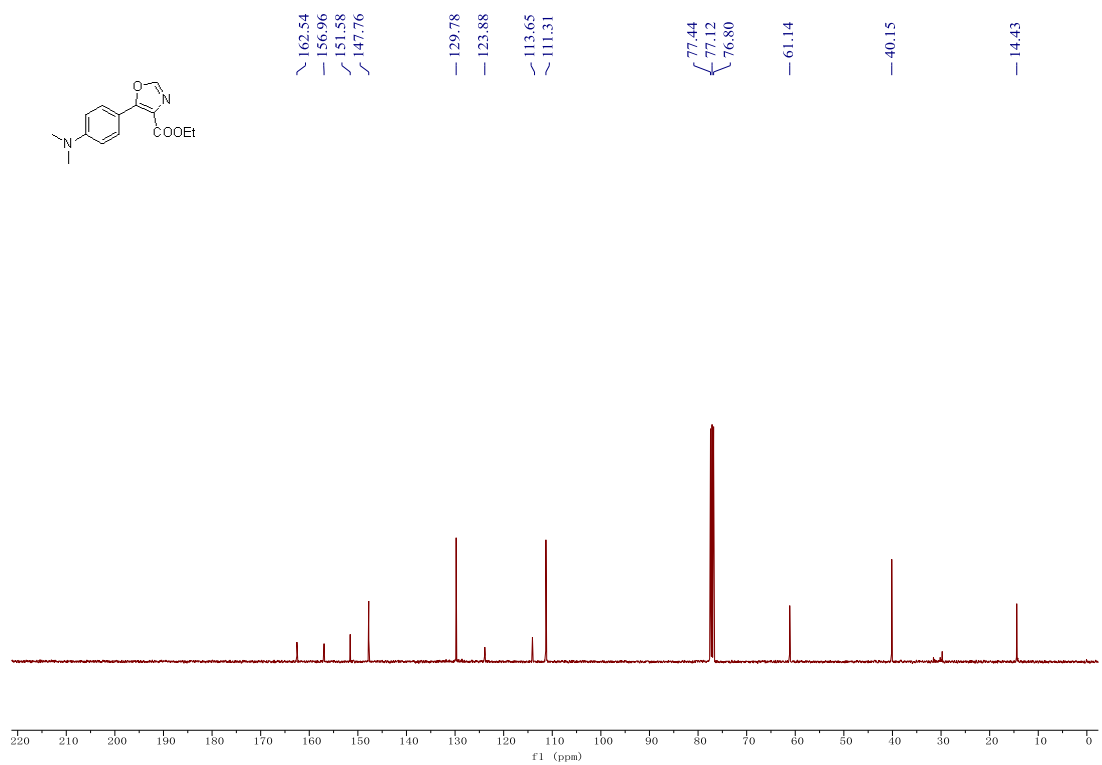


19c ^1H NMR, ^{13}C NMR and ^{19}F NMR

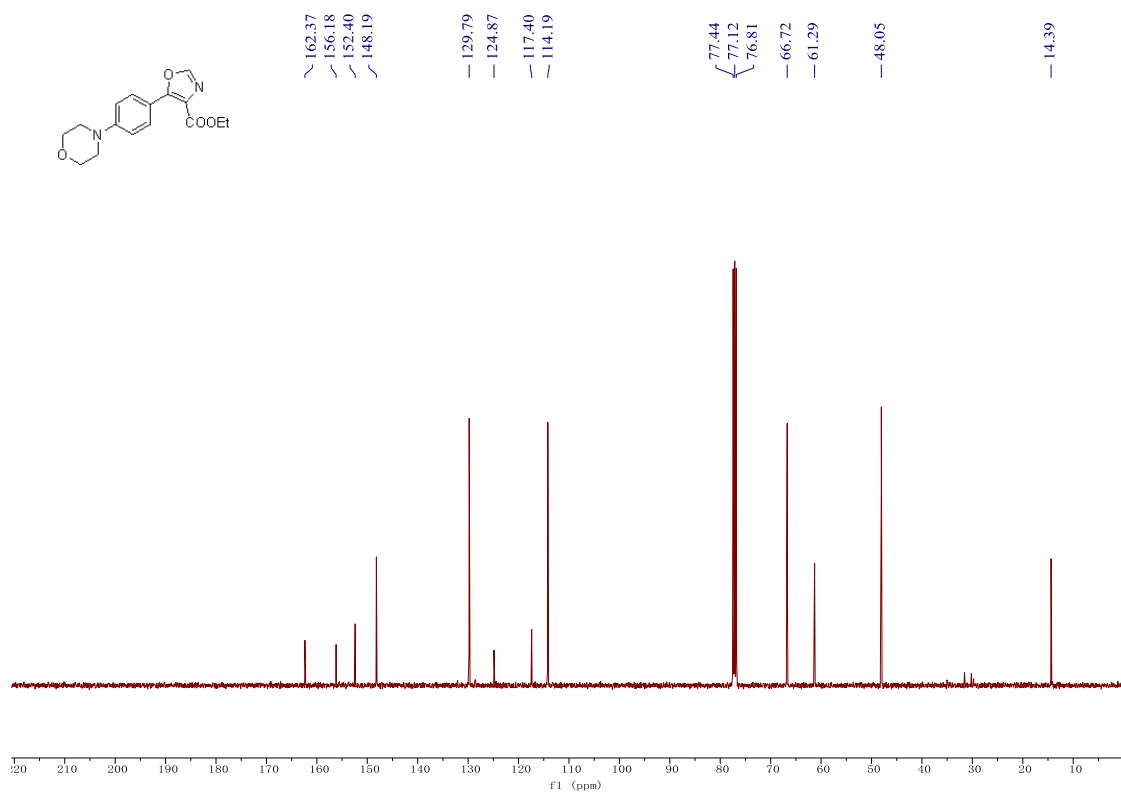
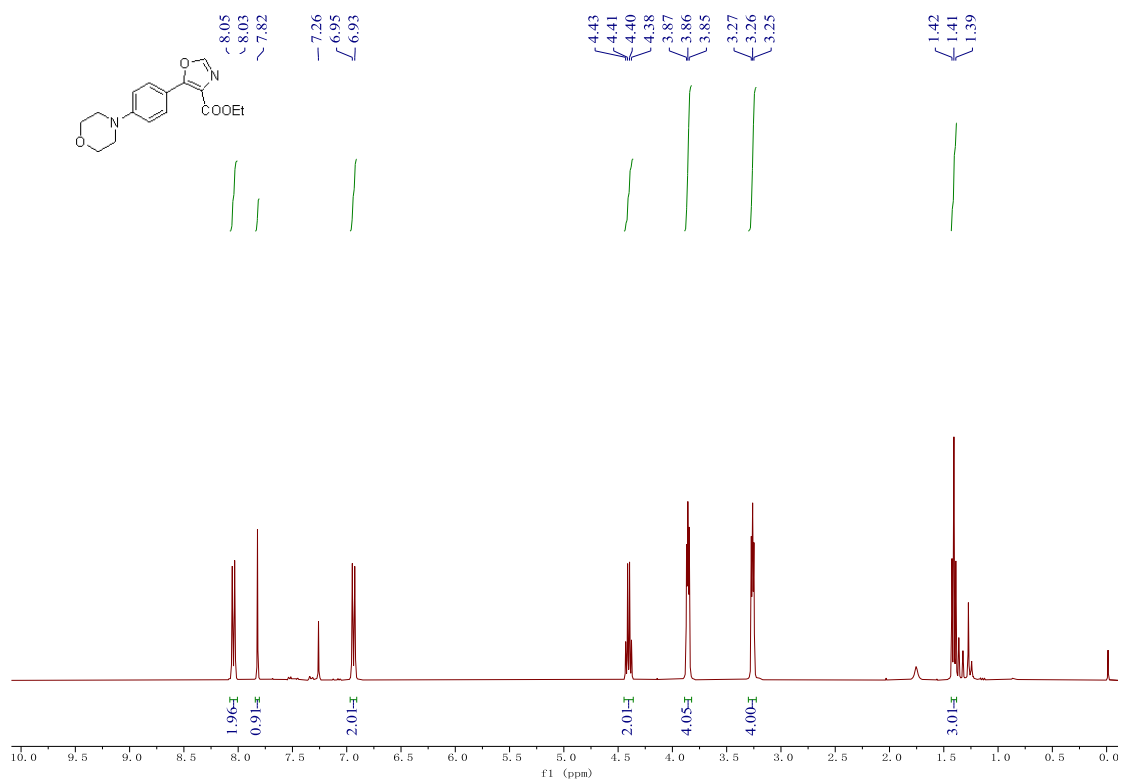




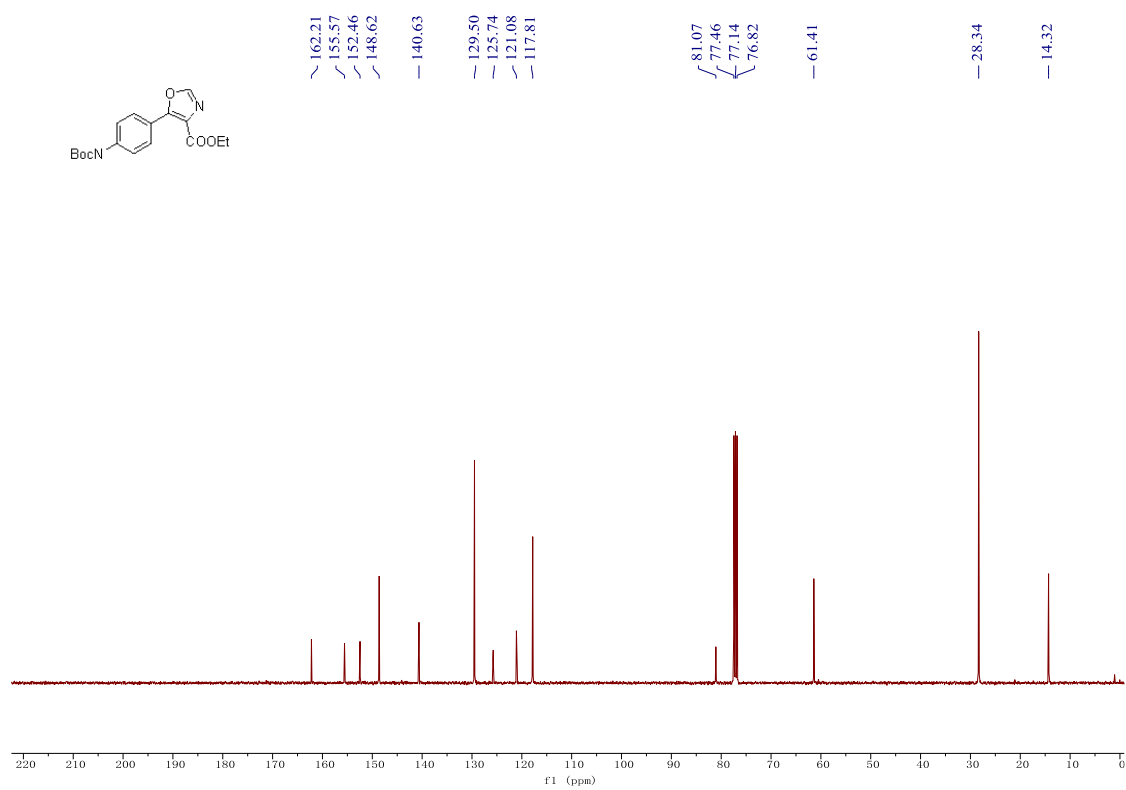
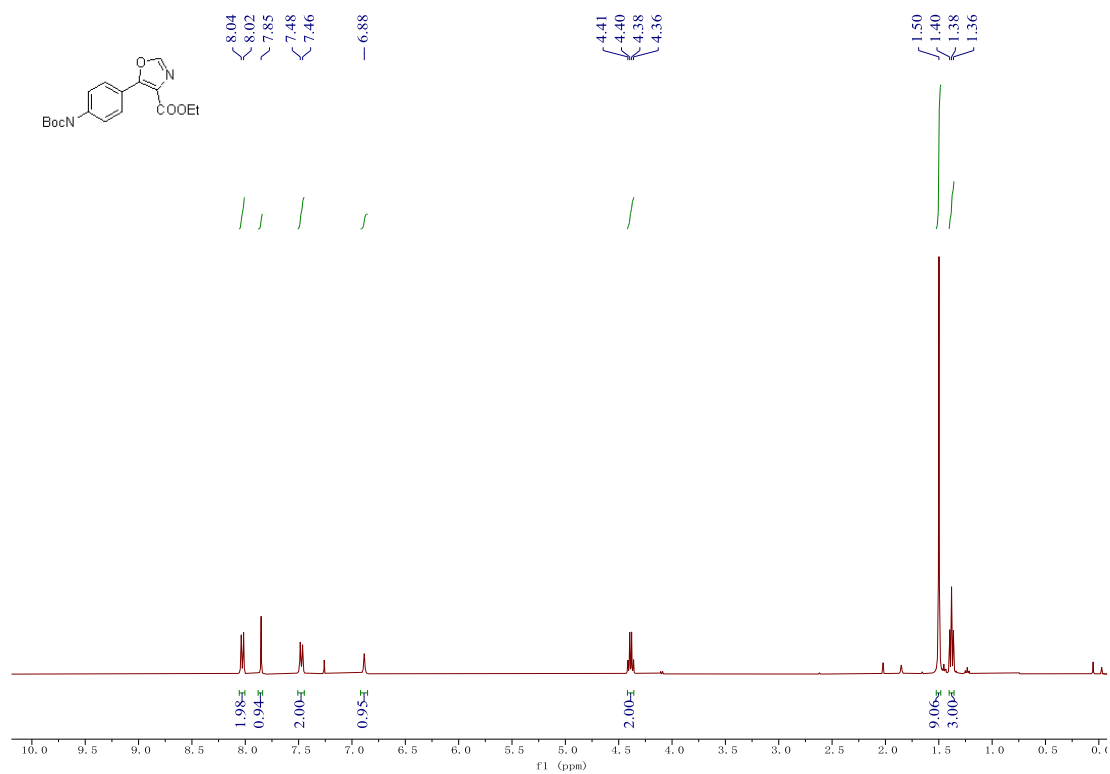
20c ^1H NMR and ^{13}C NMR



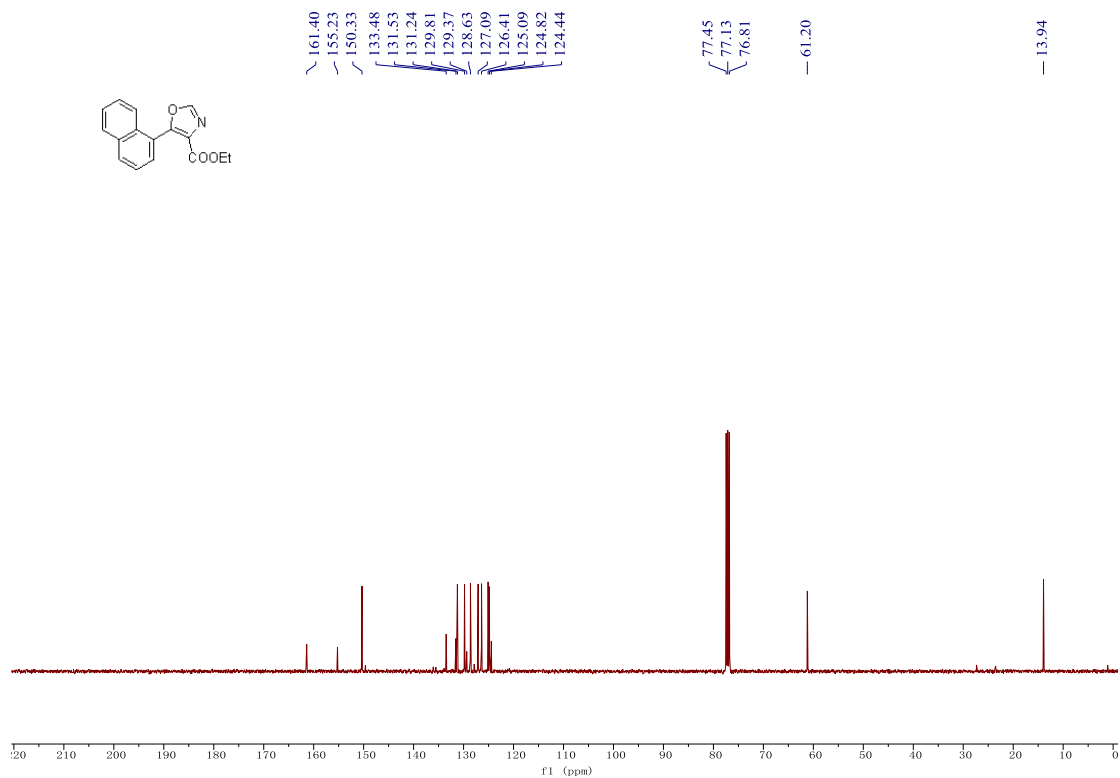
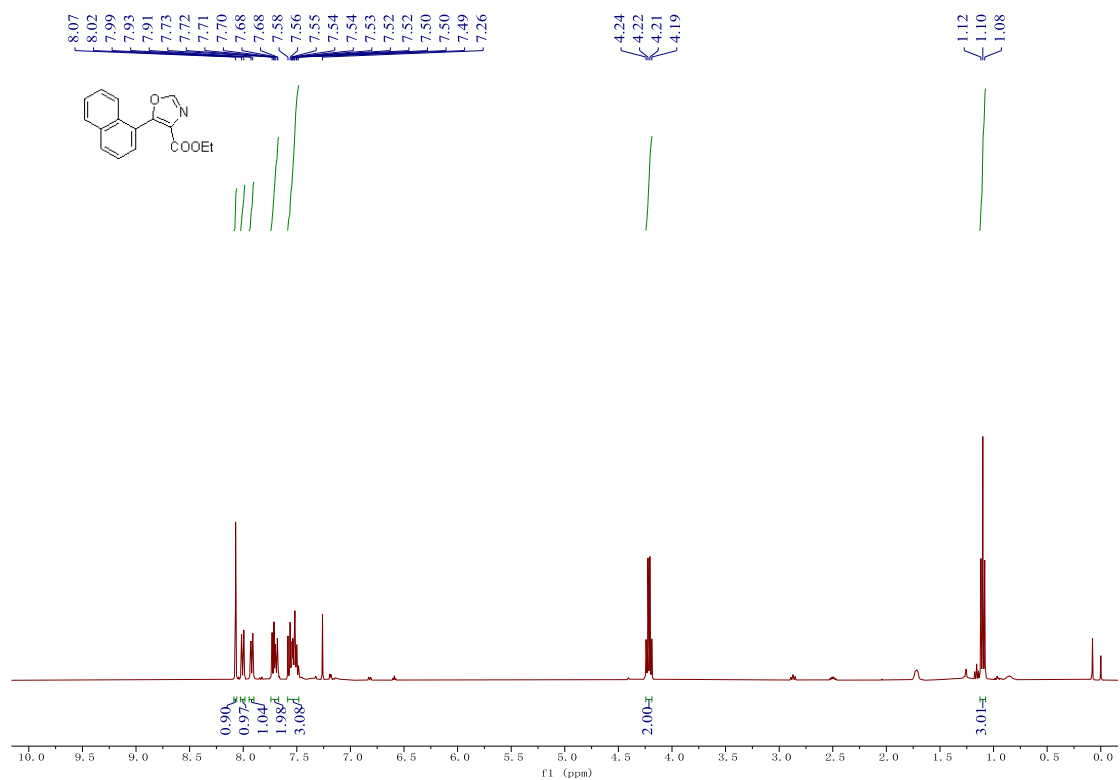
21c ^1H NMR and ^{13}C NMR



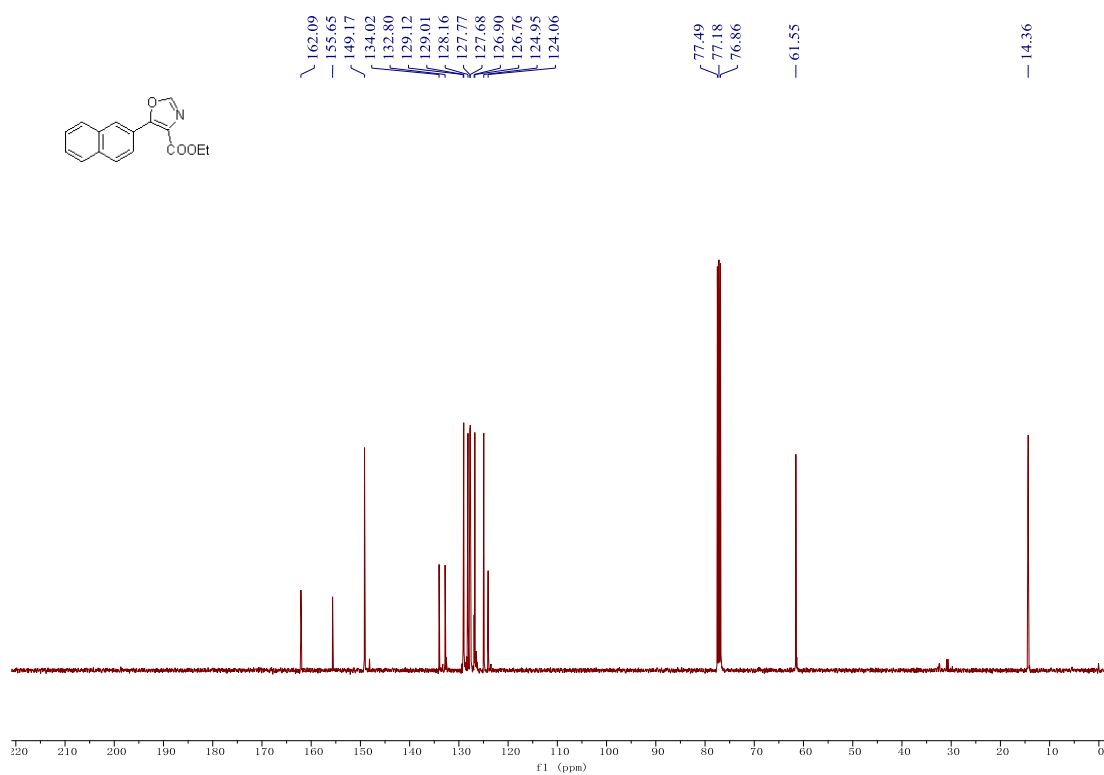
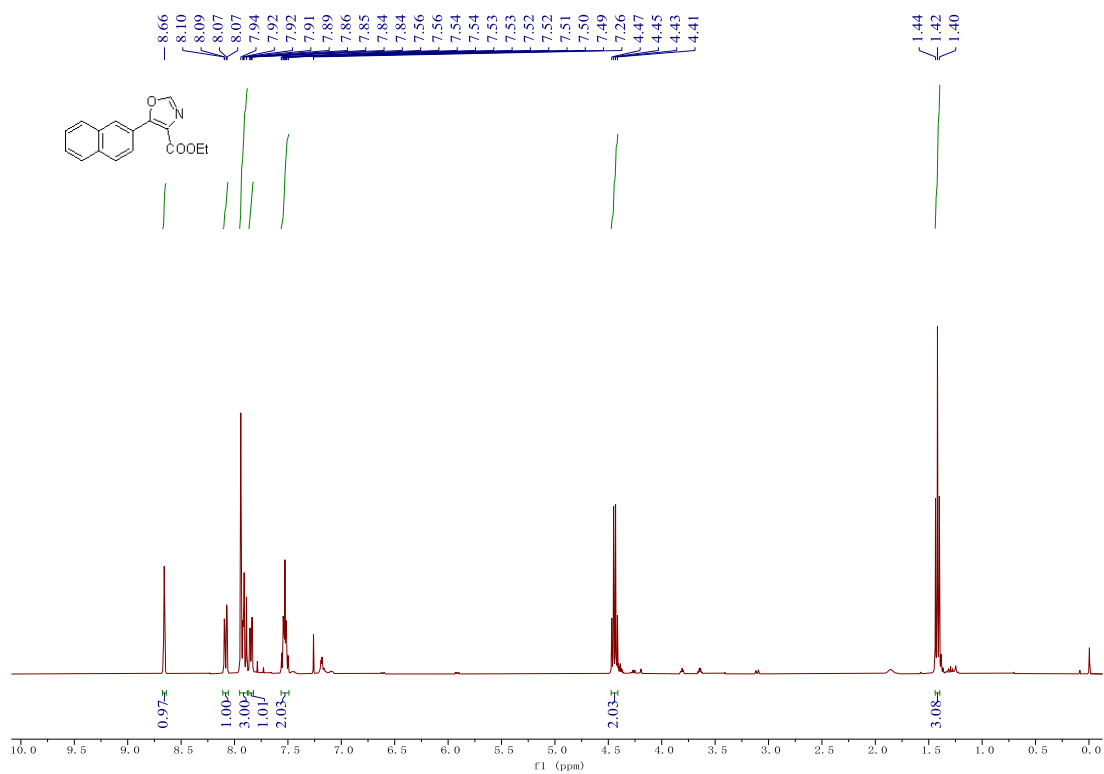
22c ¹H NMR and ¹³C NMR



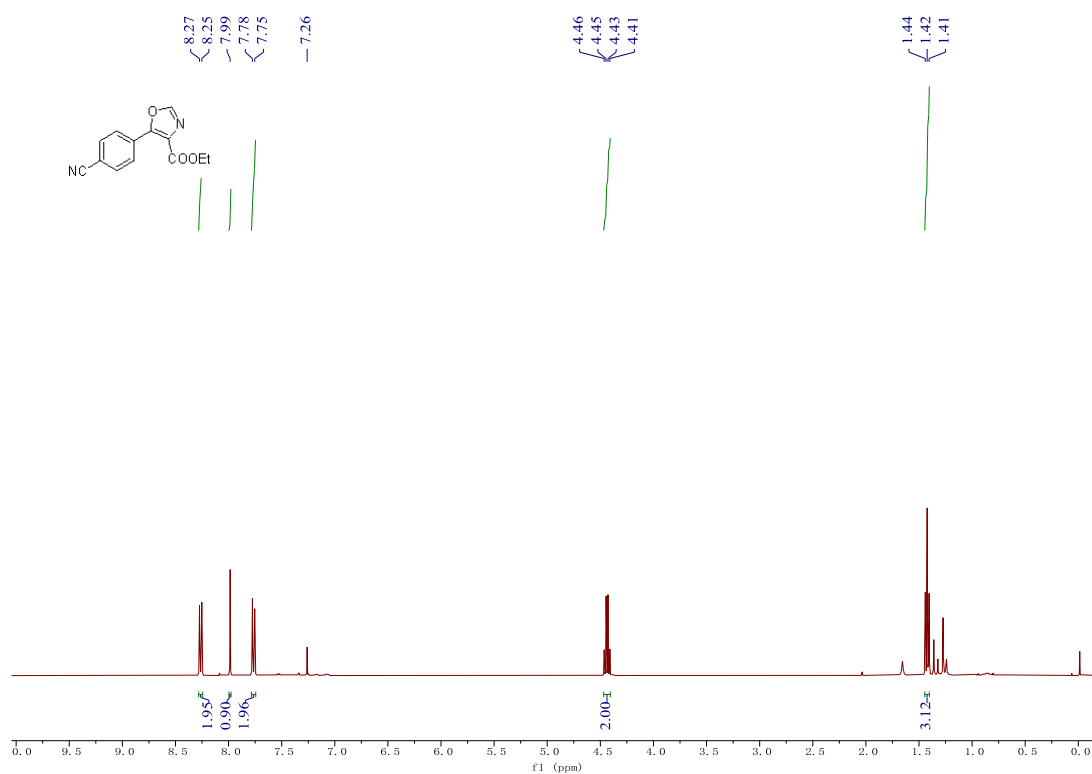
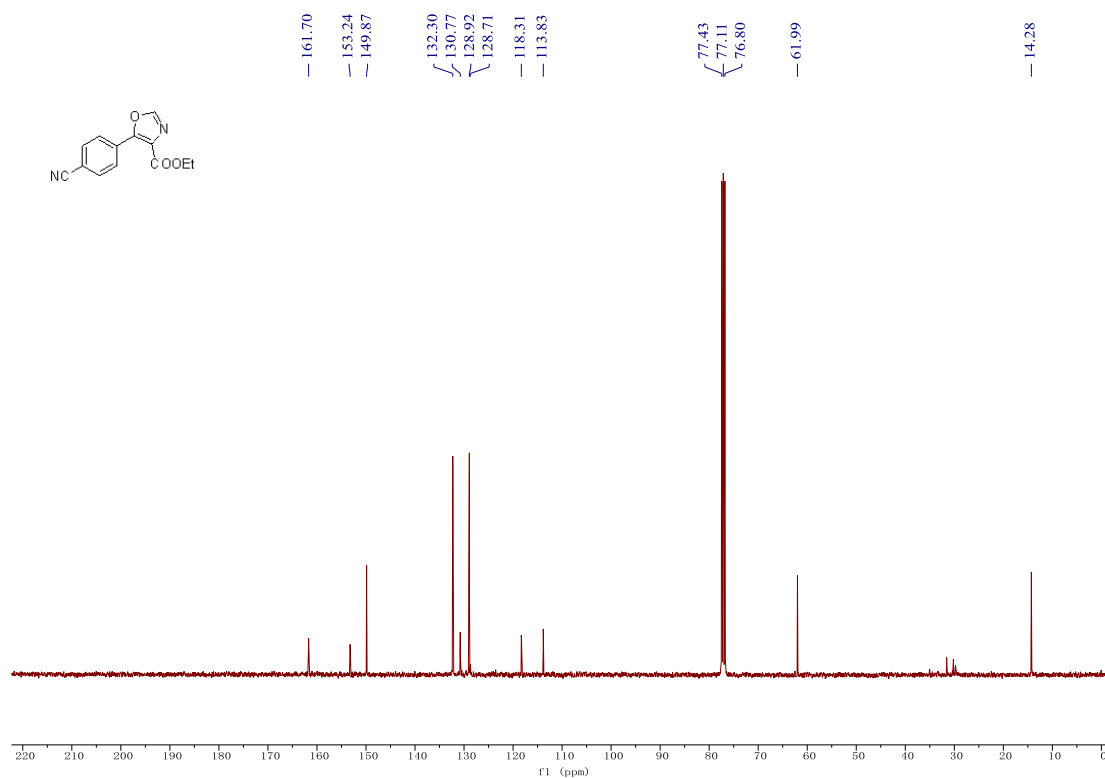
23c ^1H NMR and ^{13}C NMR



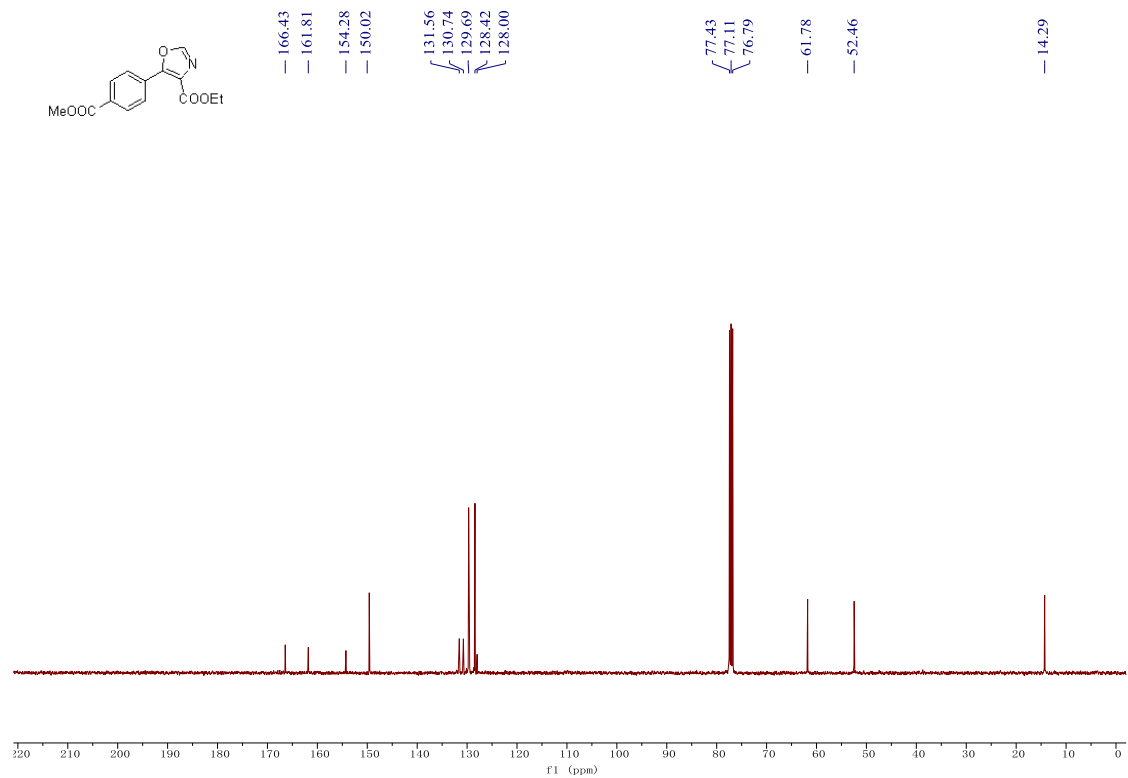
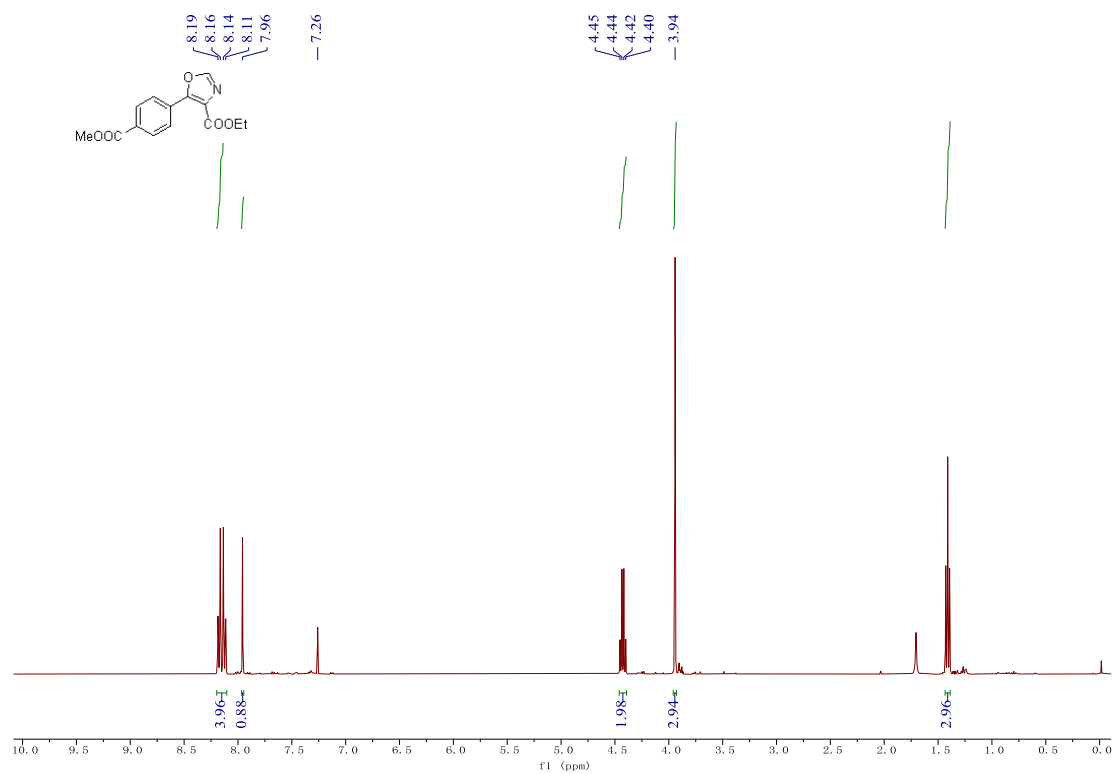
24c ^1H NMR and ^{13}C NMR



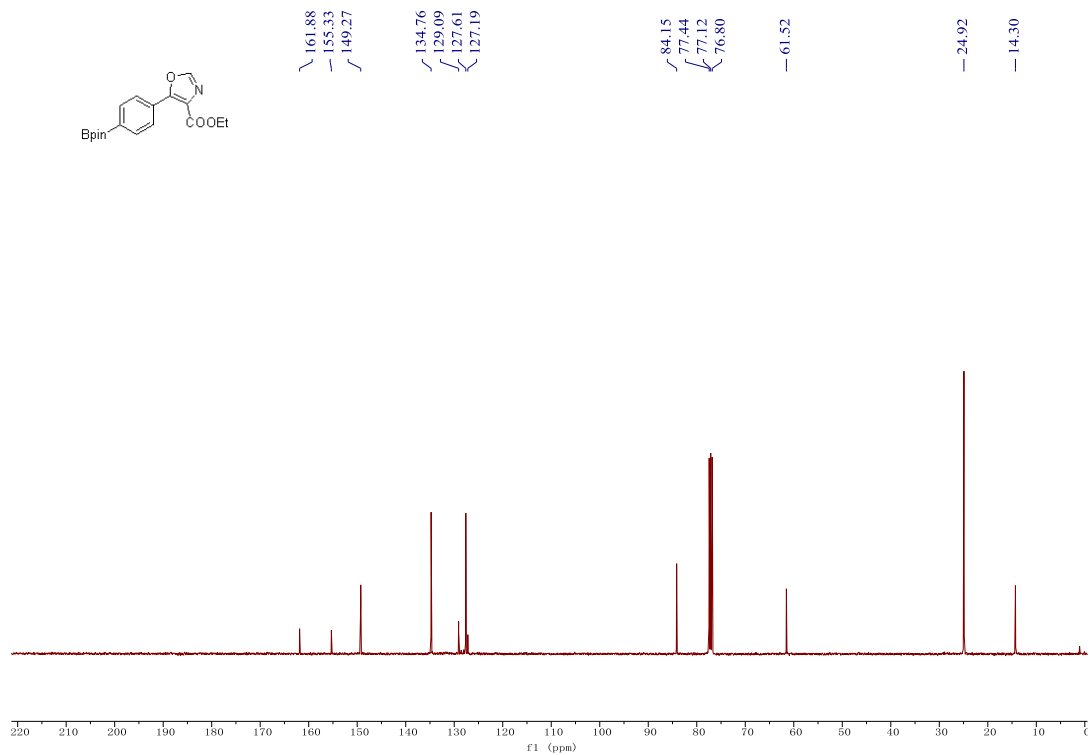
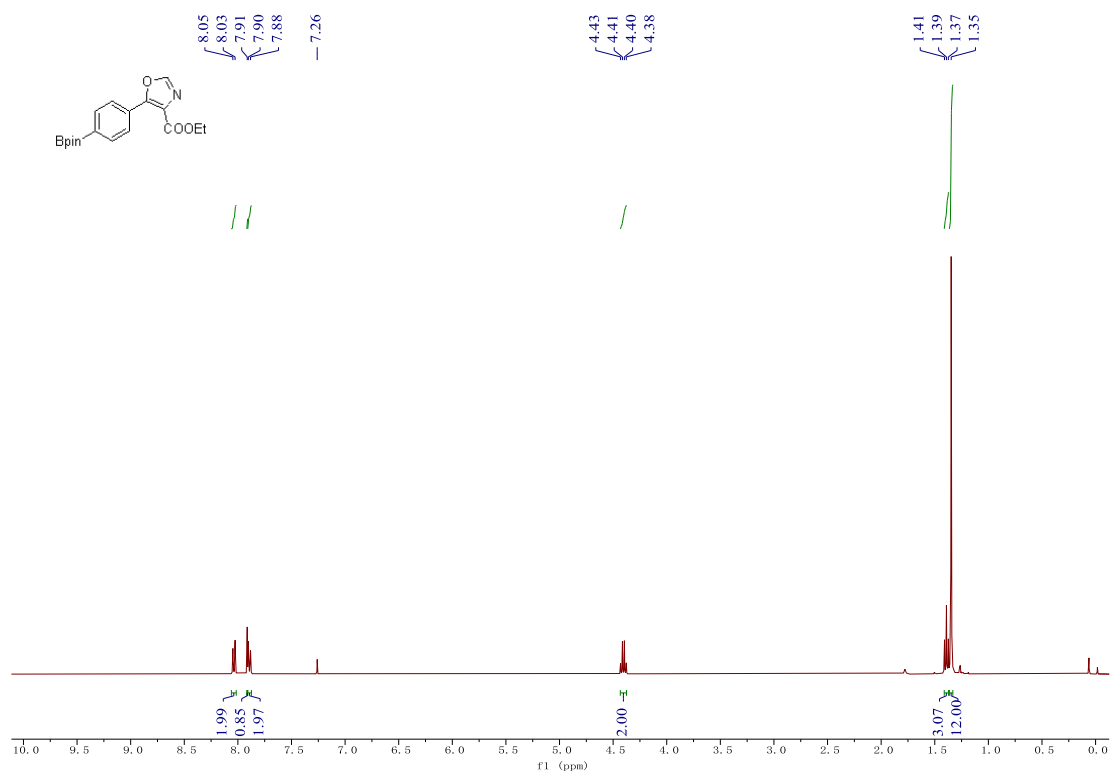
25c ¹H NMR and ¹³C NMR



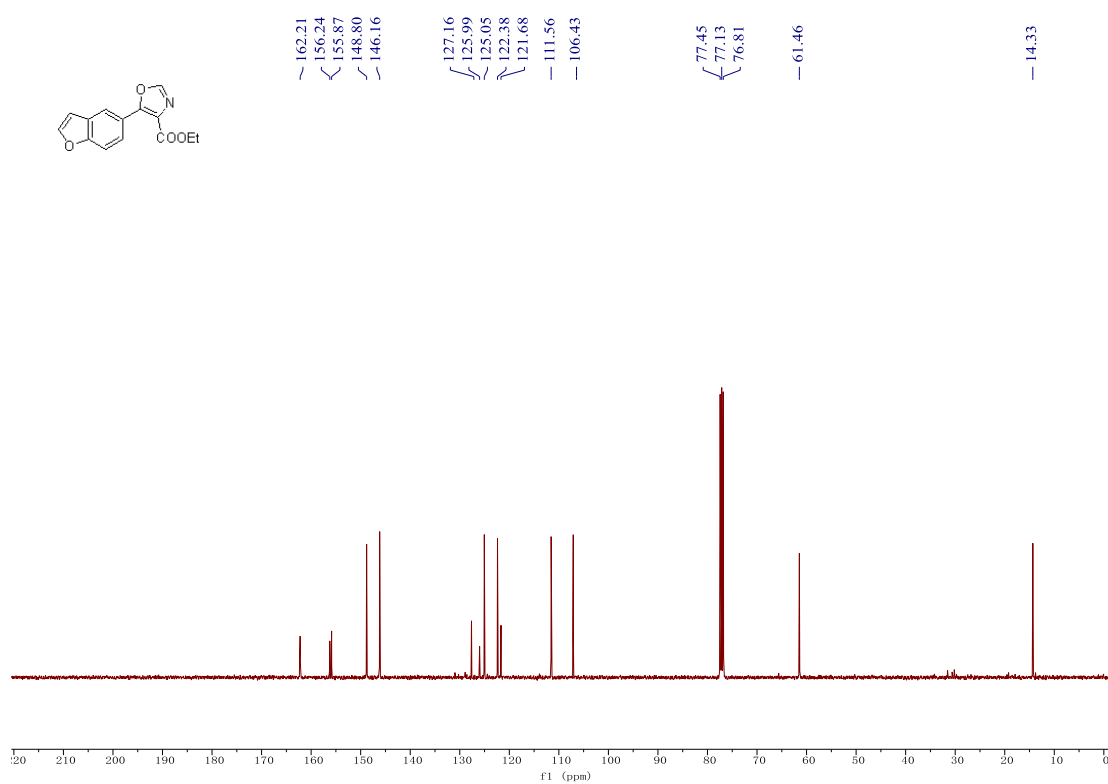
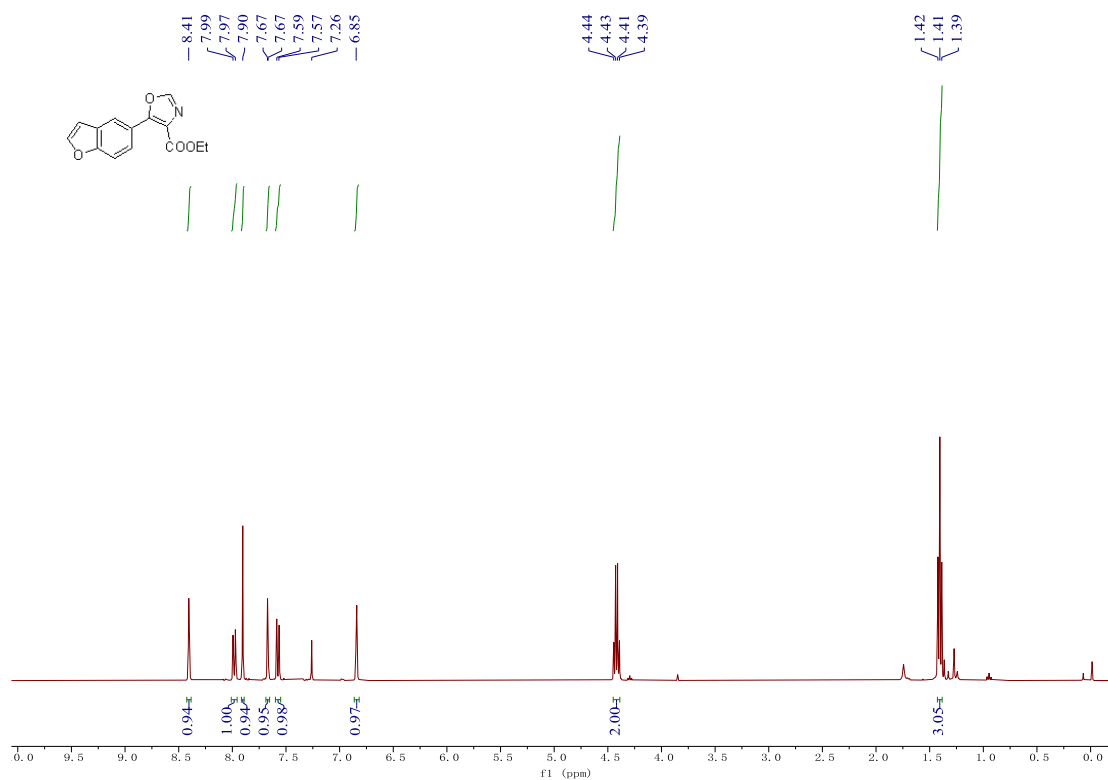
26c ^1H NMR and ^{13}C NMR



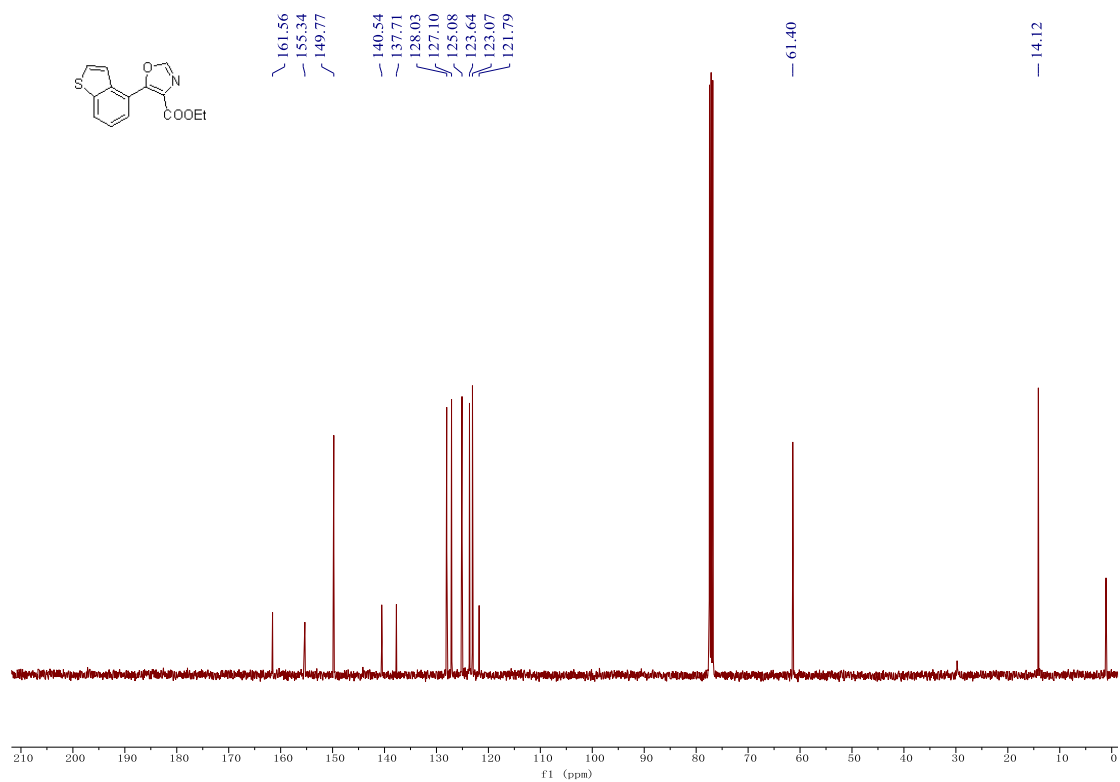
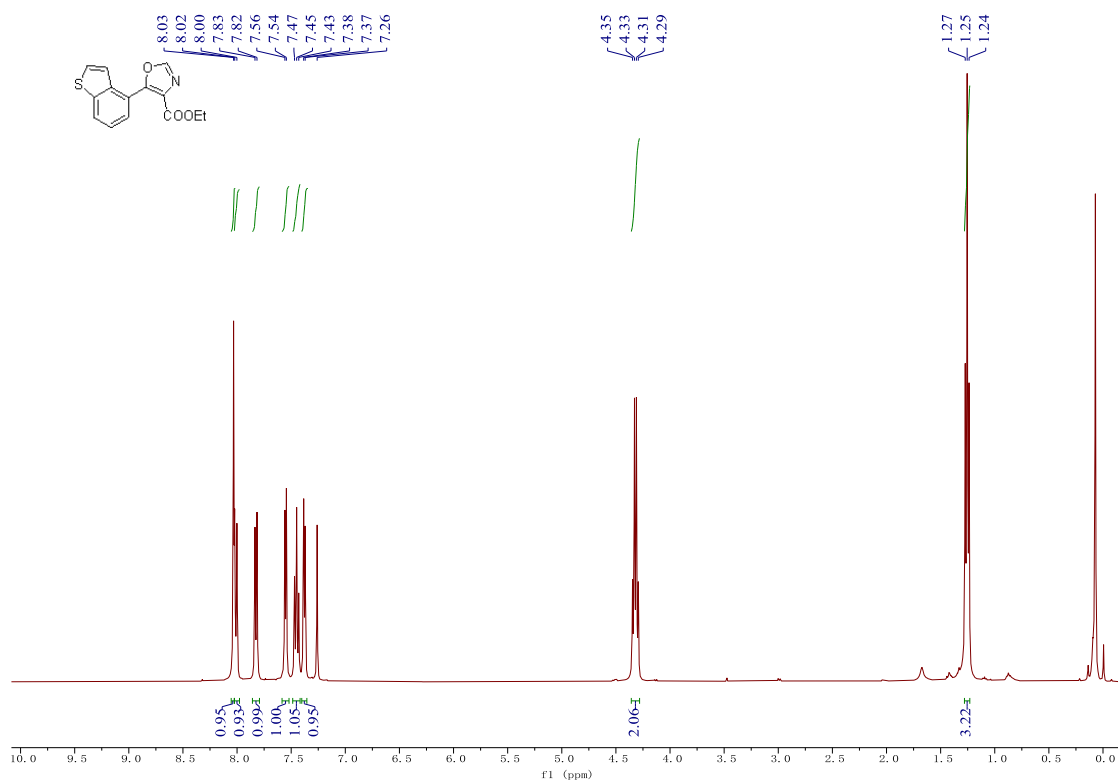
27c ¹H NMR and ¹³C NMR



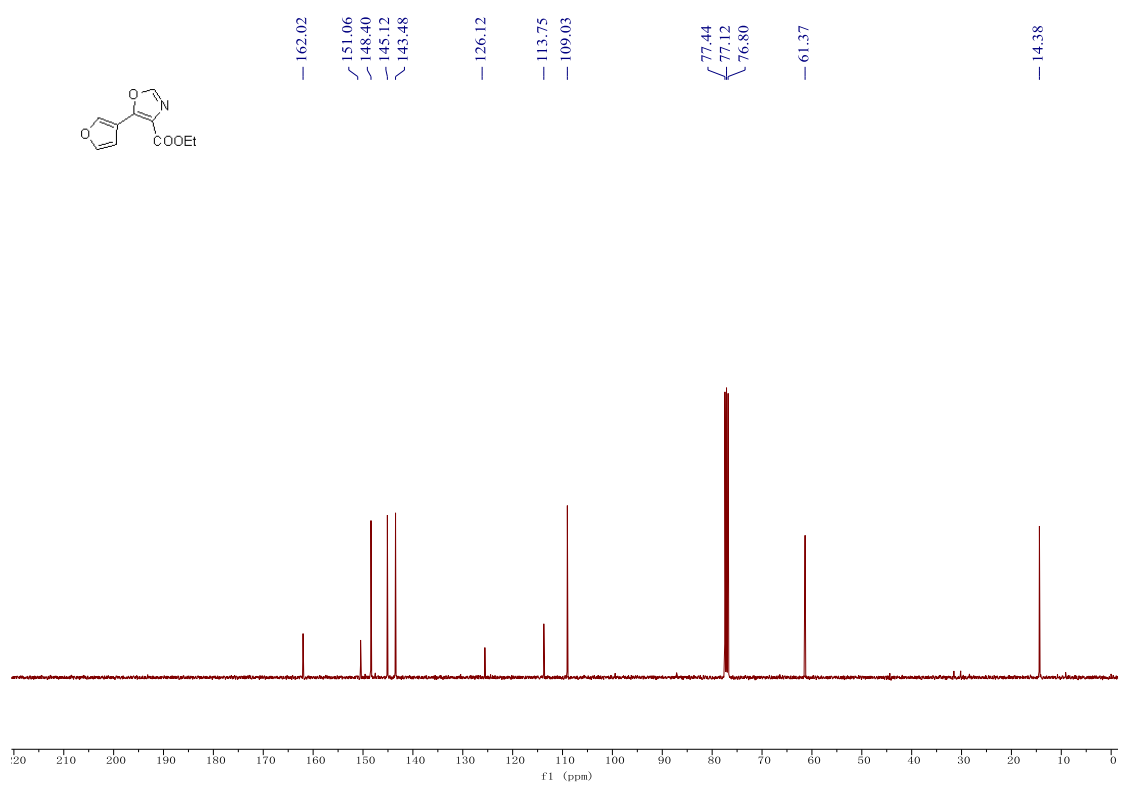
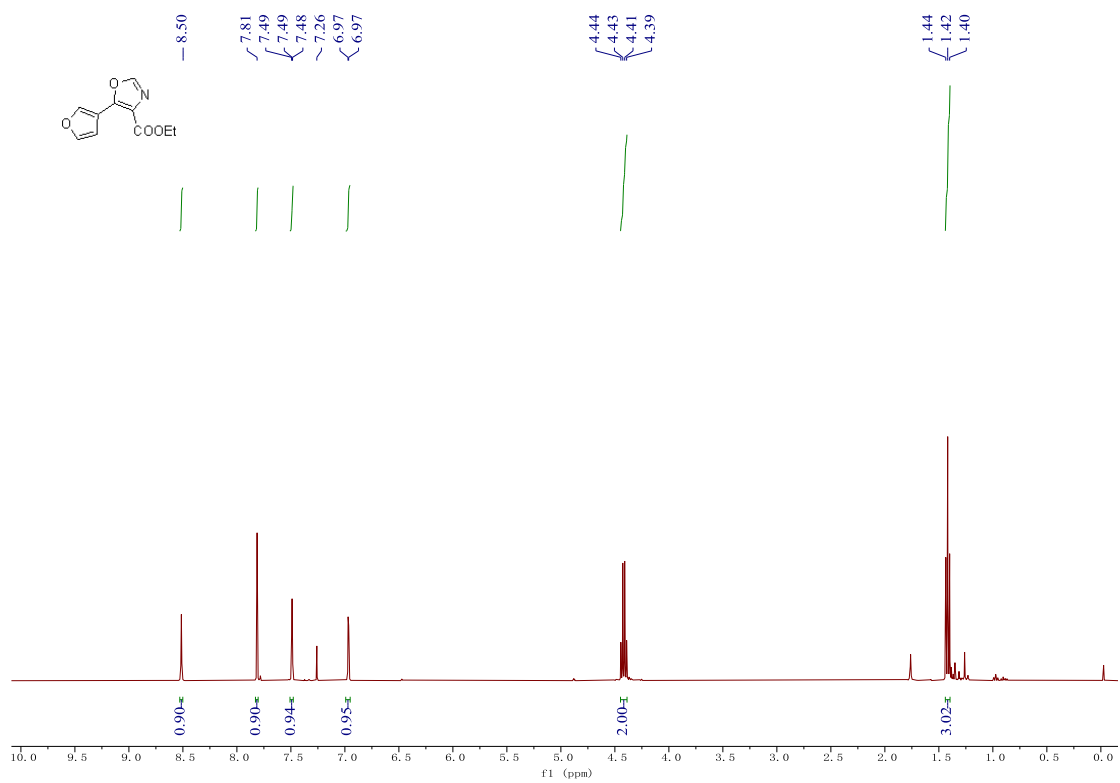
28c ^1H NMR and ^{13}C NMR



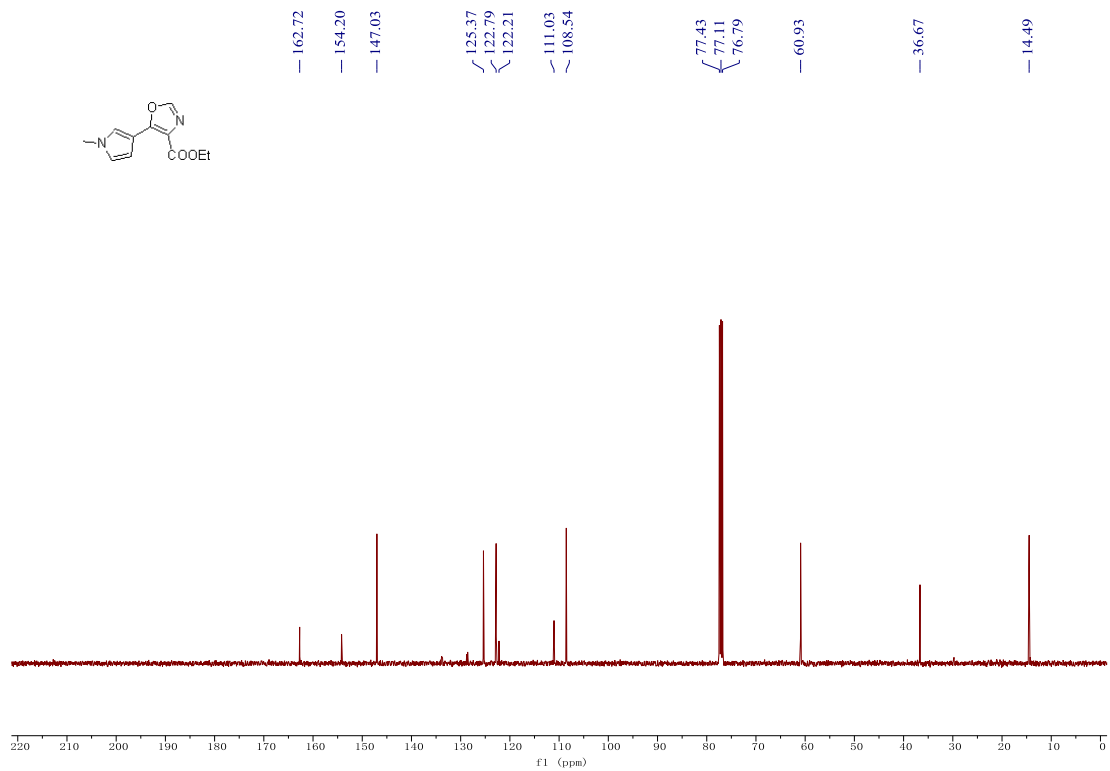
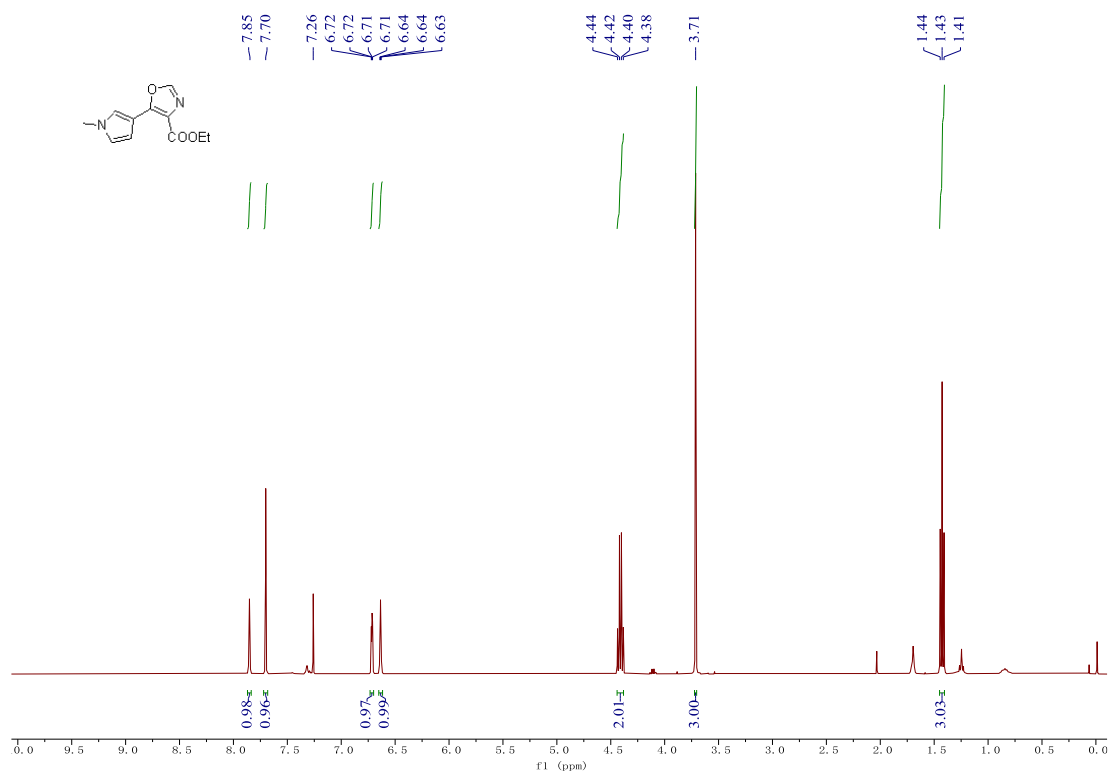
29c ^1H NMR and ^{13}C NMR



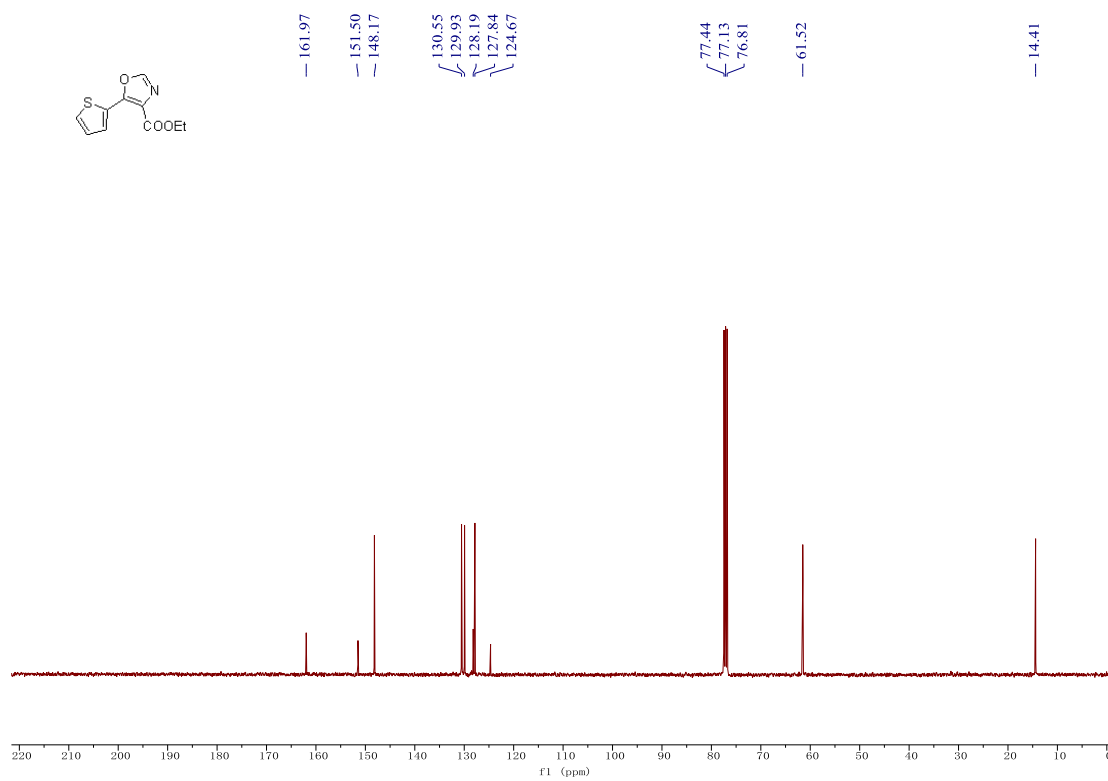
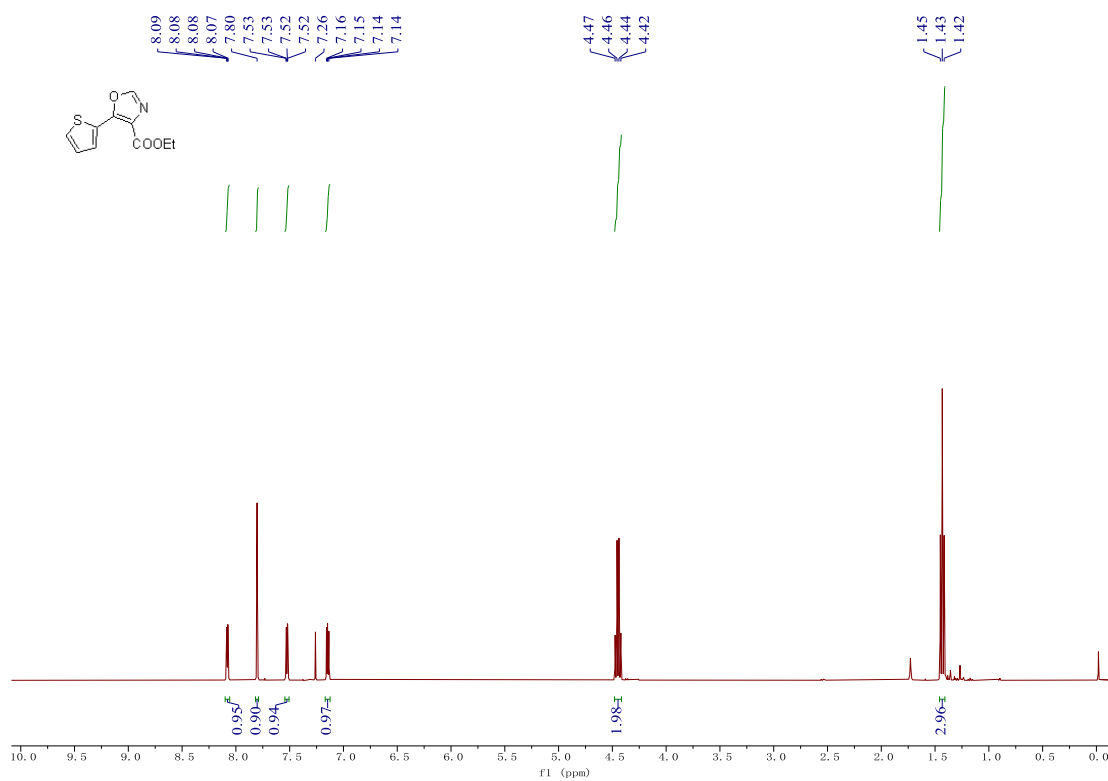
30c ^1H NMR and ^{13}C NMR



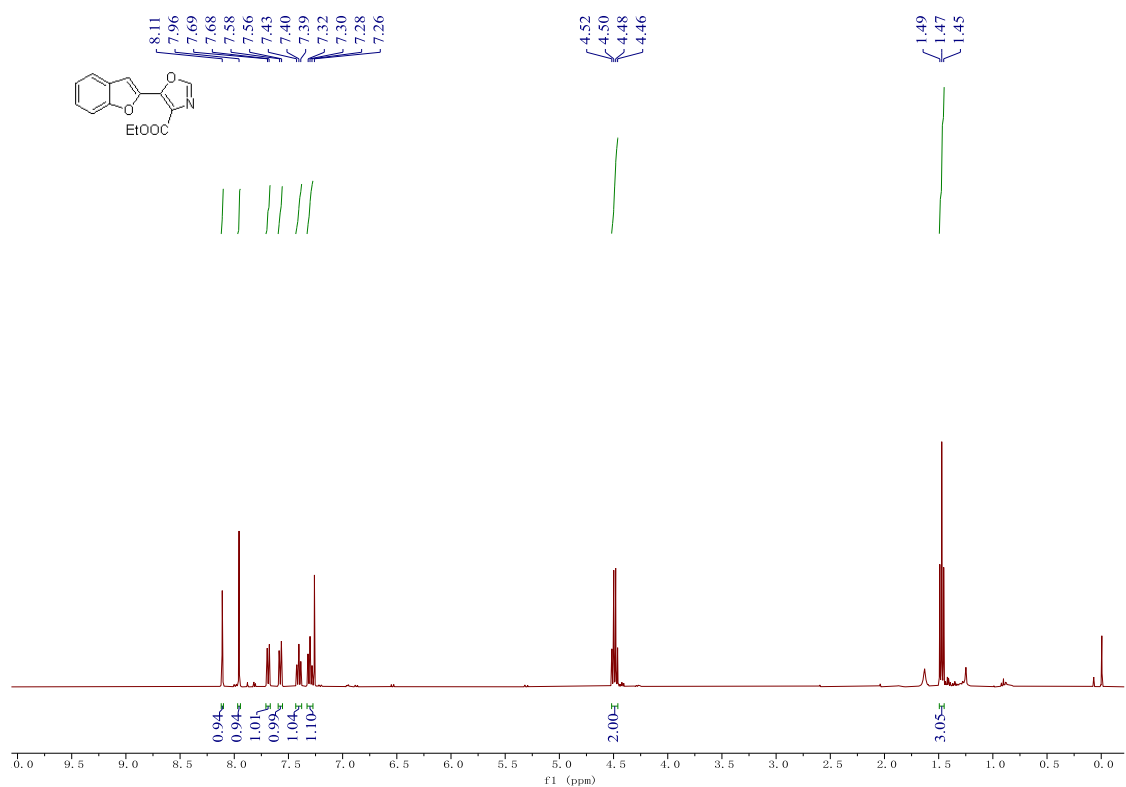
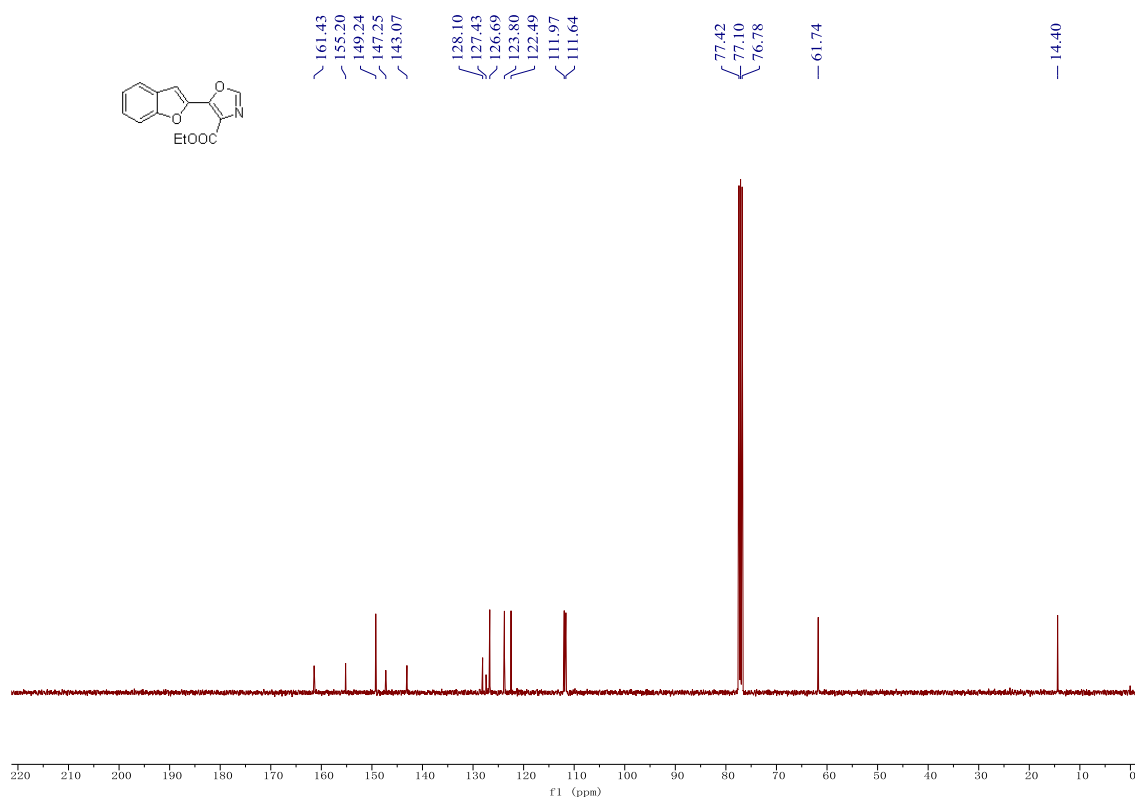
31c ^1H NMR and ^{13}C NMR



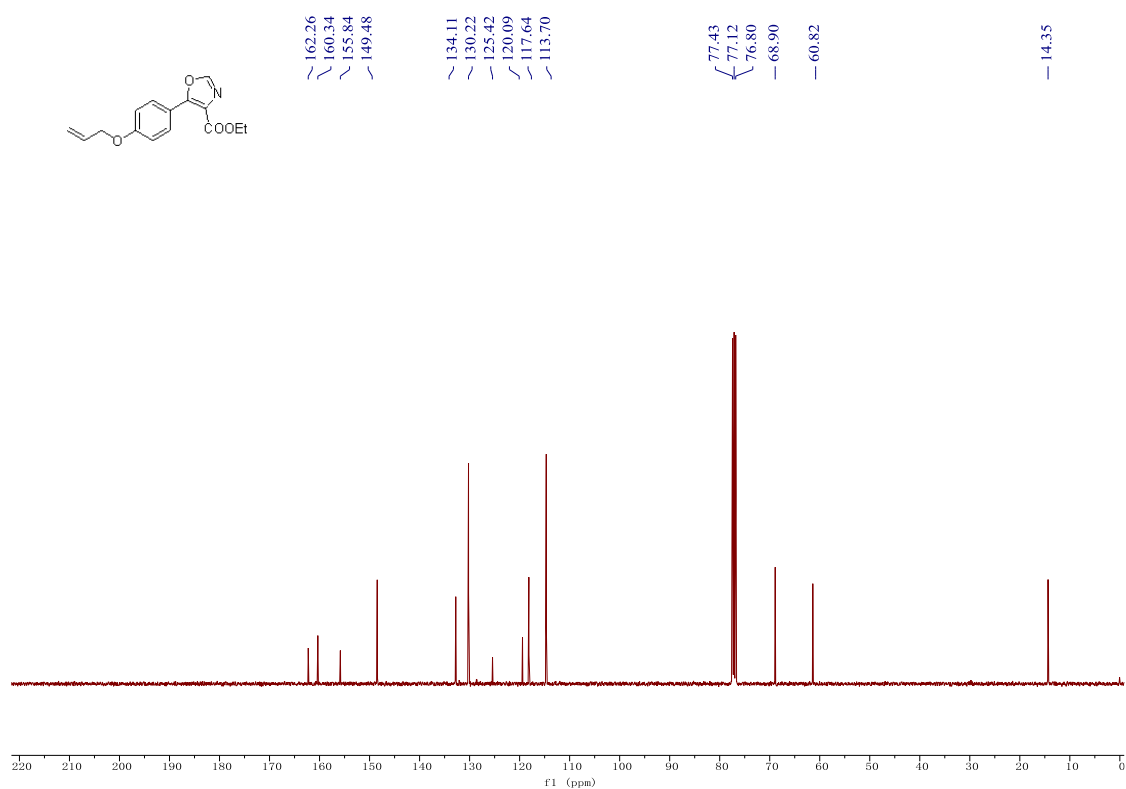
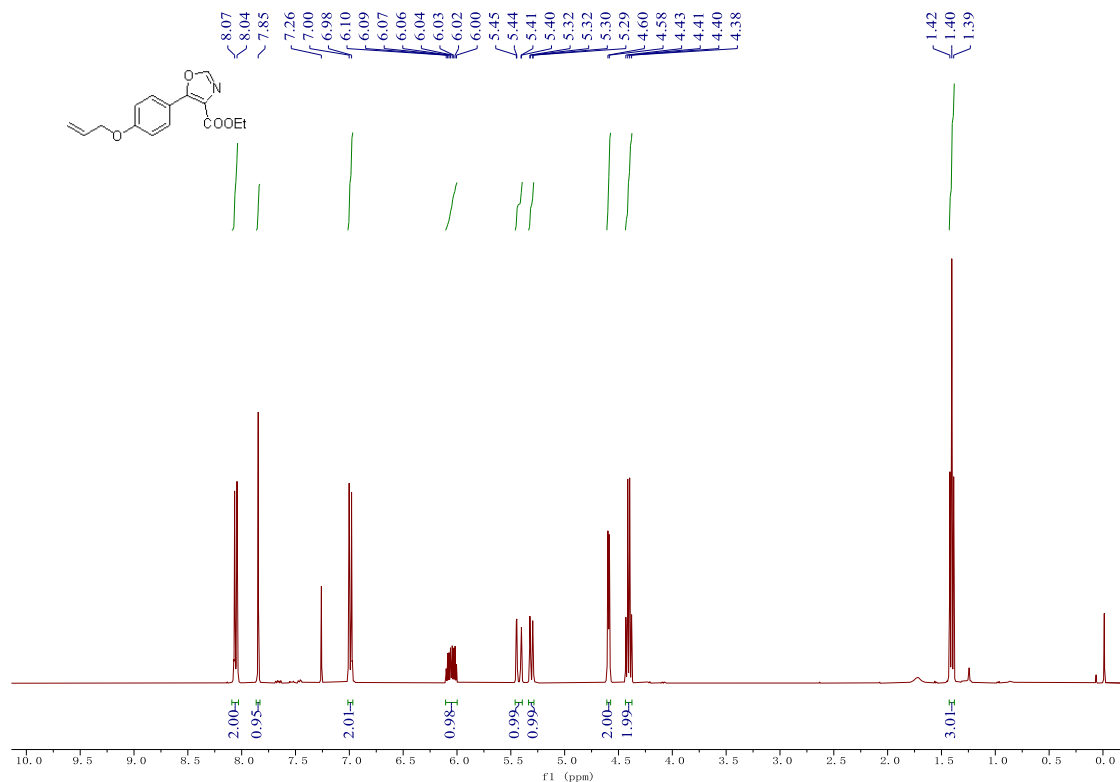
32c ^1H NMR and ^{13}C NMR



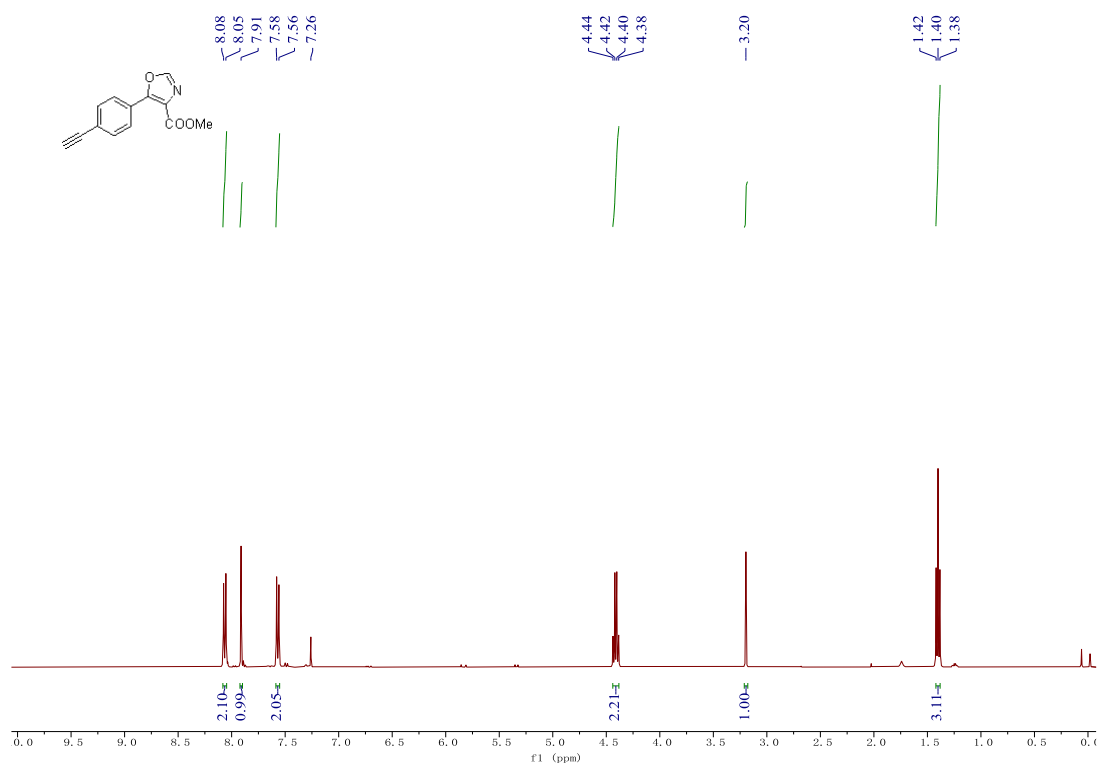
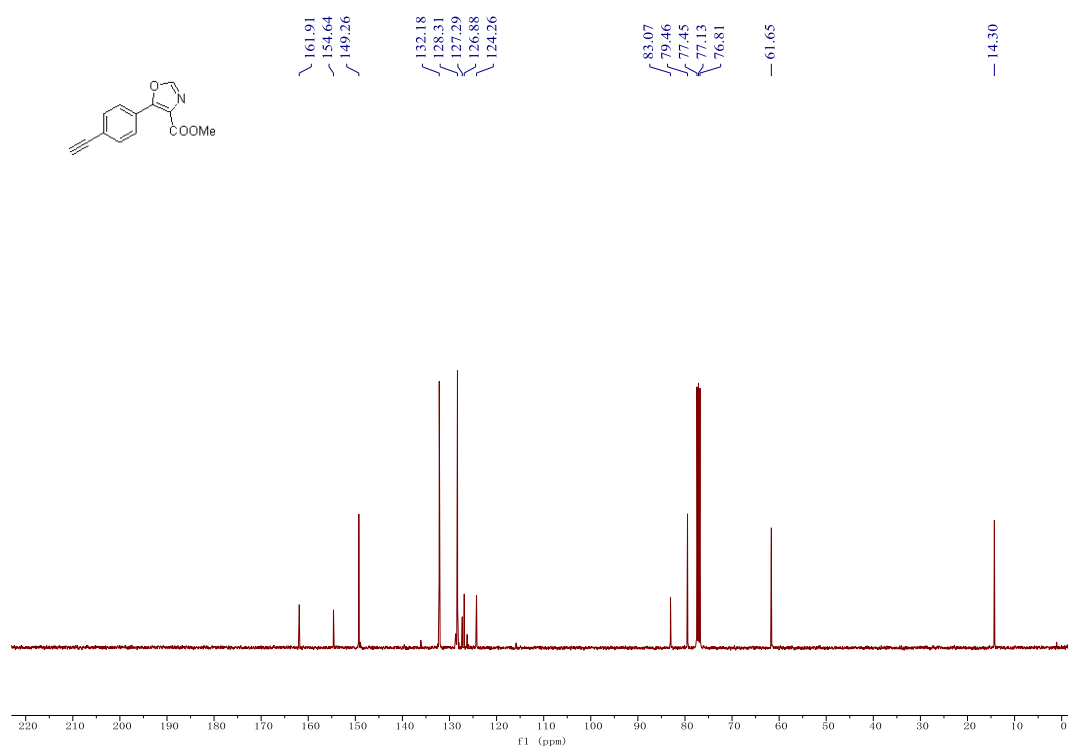
33c ^1H NMR and ^{13}C NMR



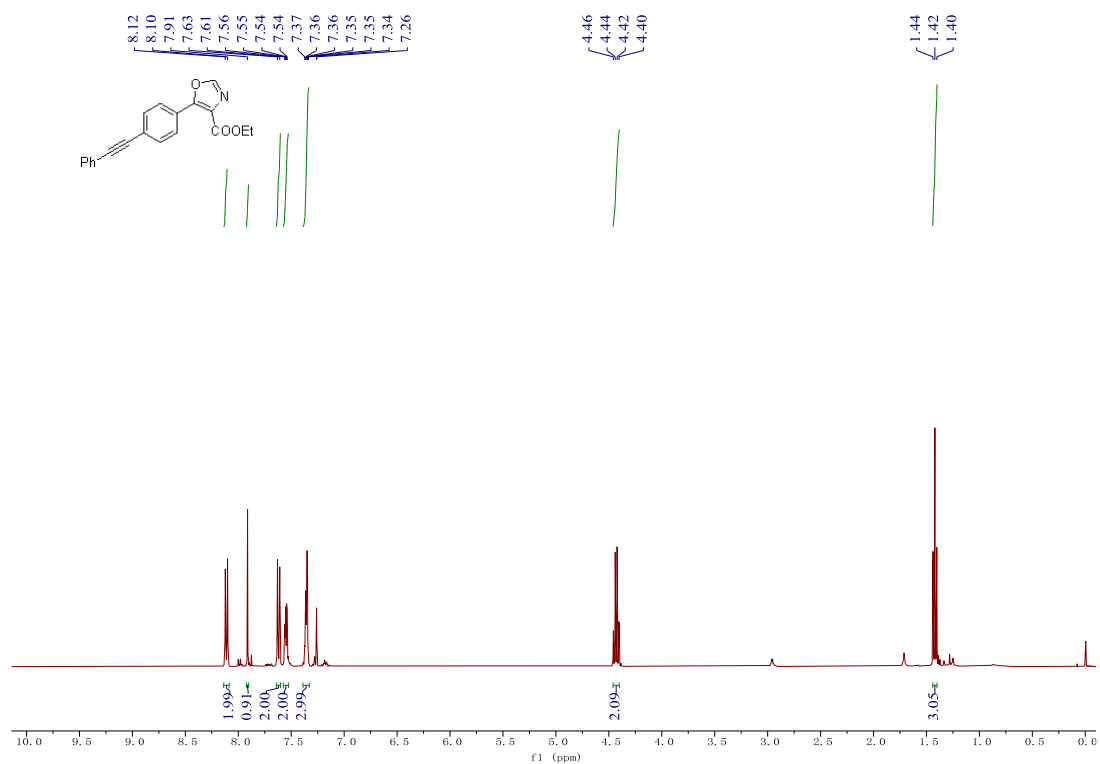
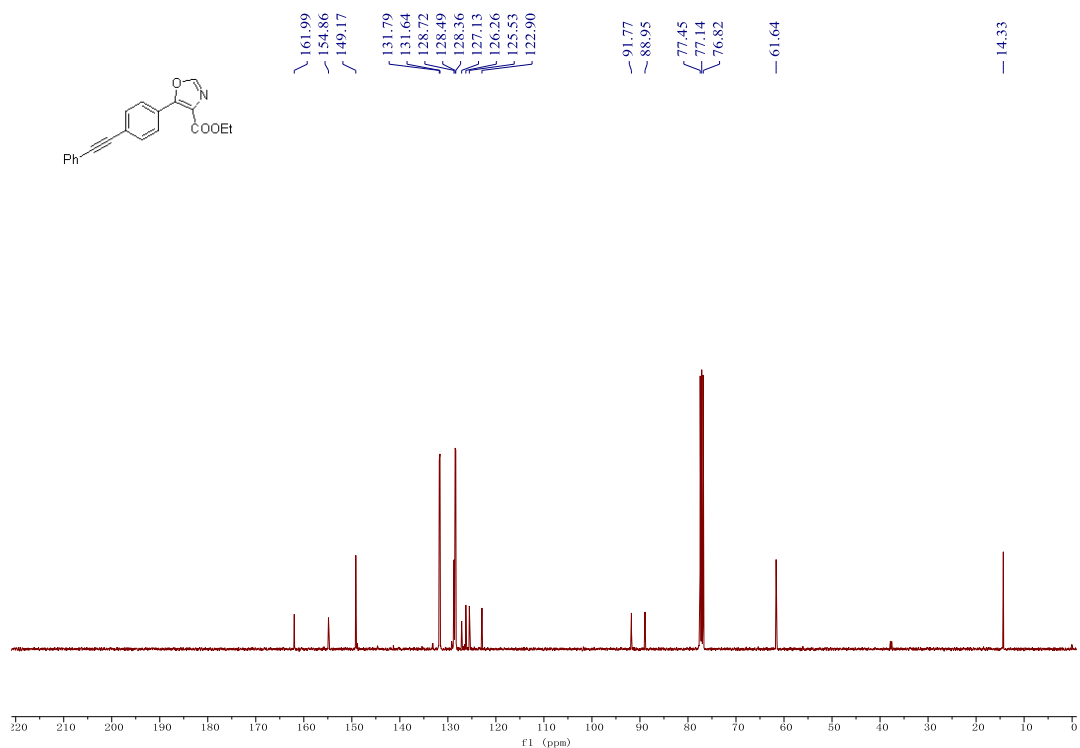
34c ^1H NMR and ^{13}C NMR



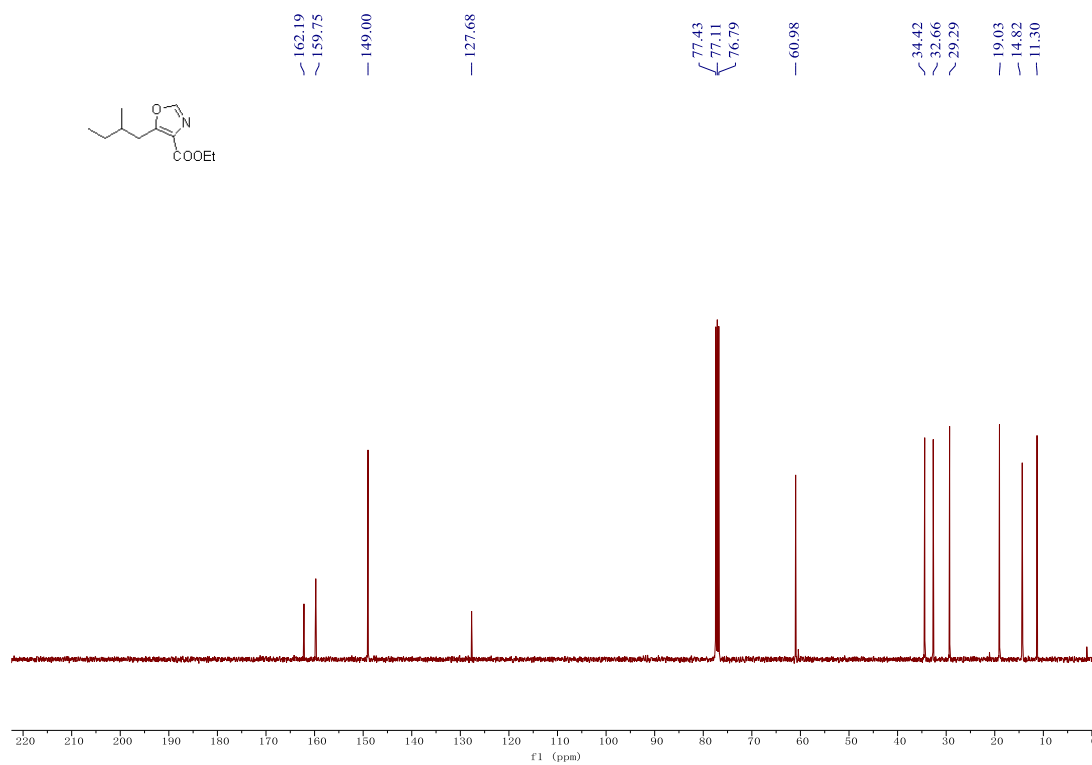
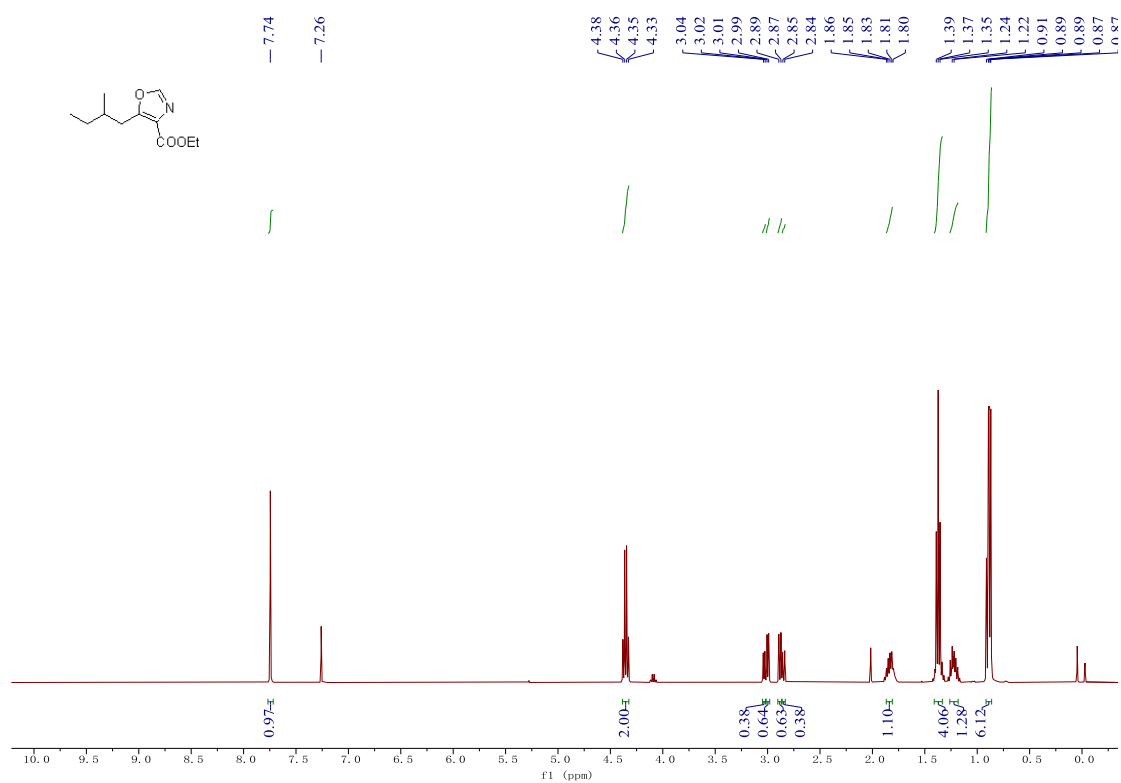
35c ^1H NMR and ^{13}C NMR



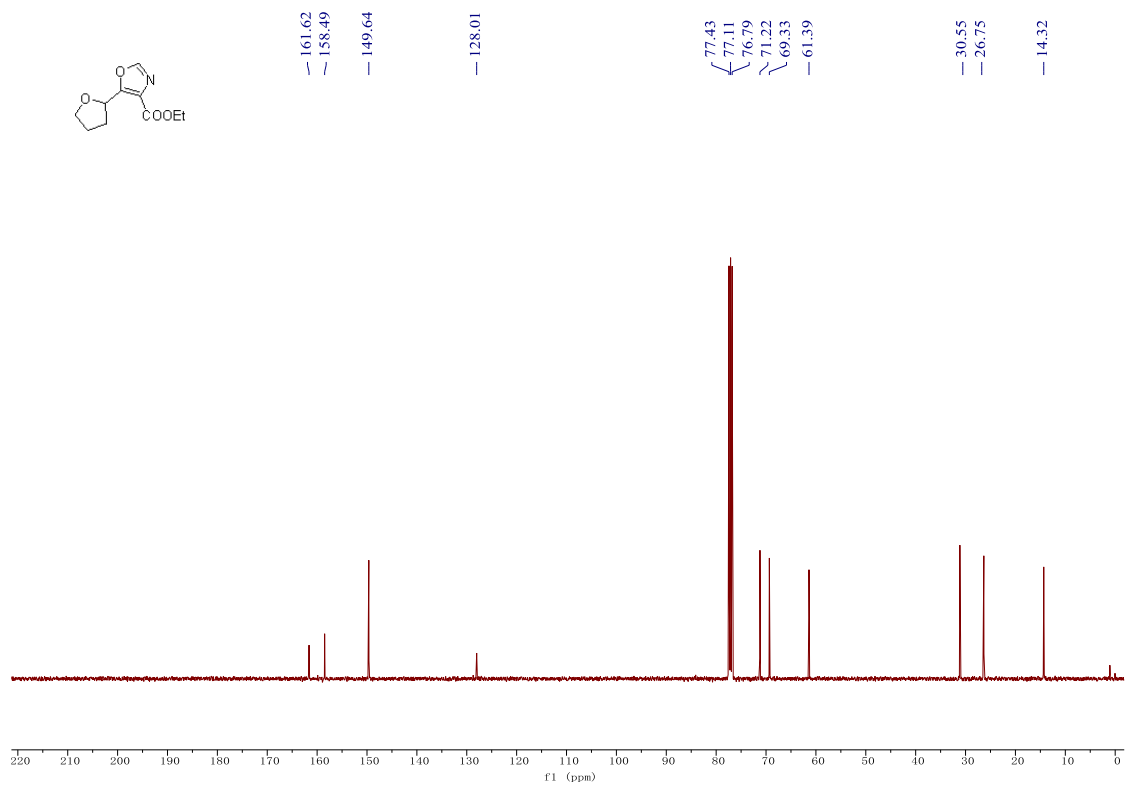
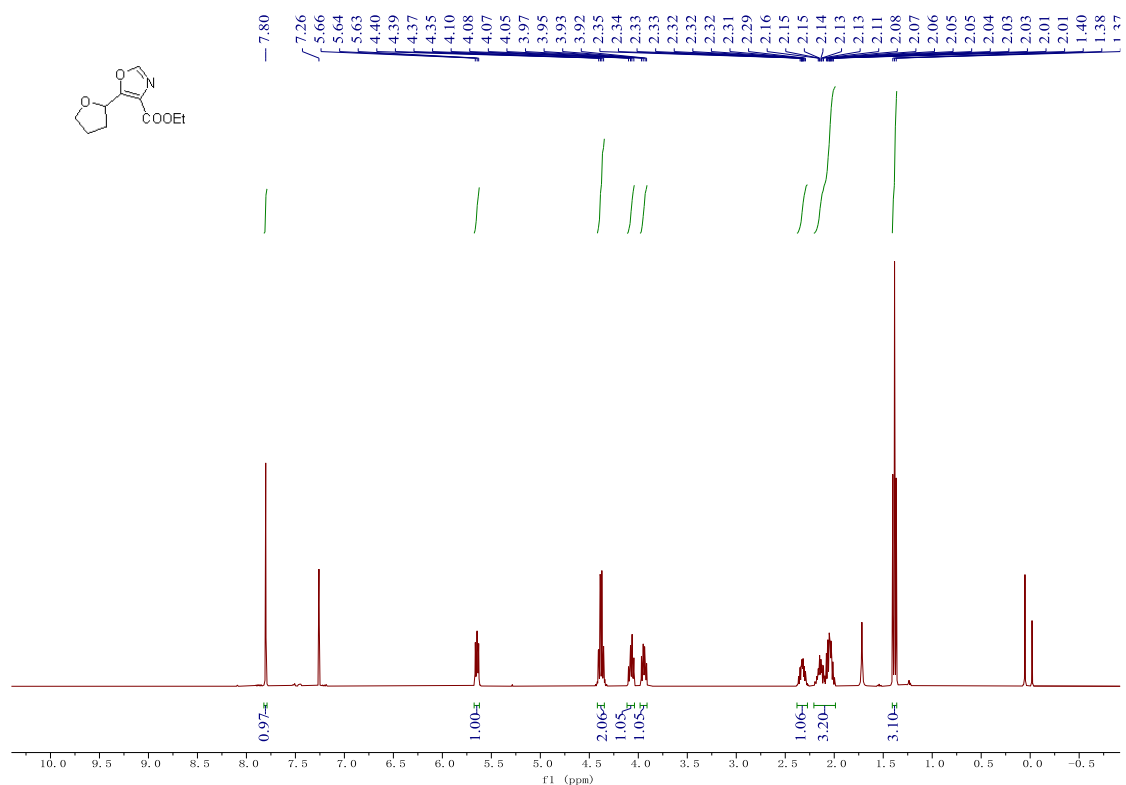
36c ^1H NMR and ^{13}C NMR



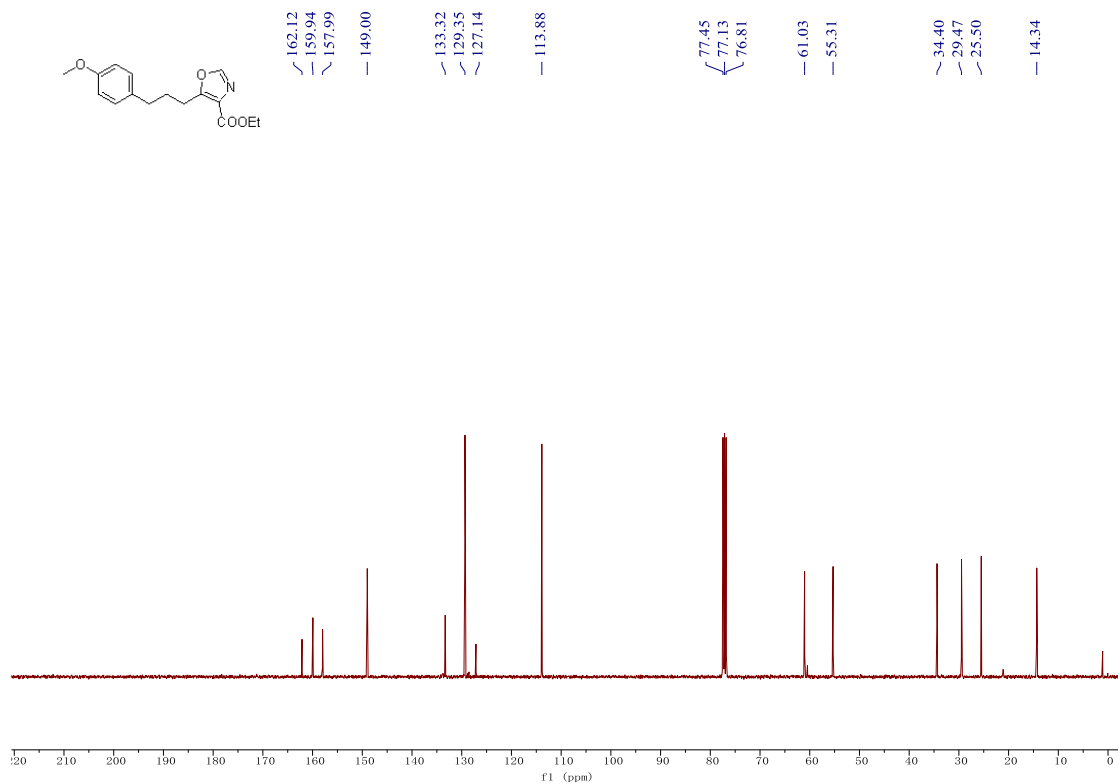
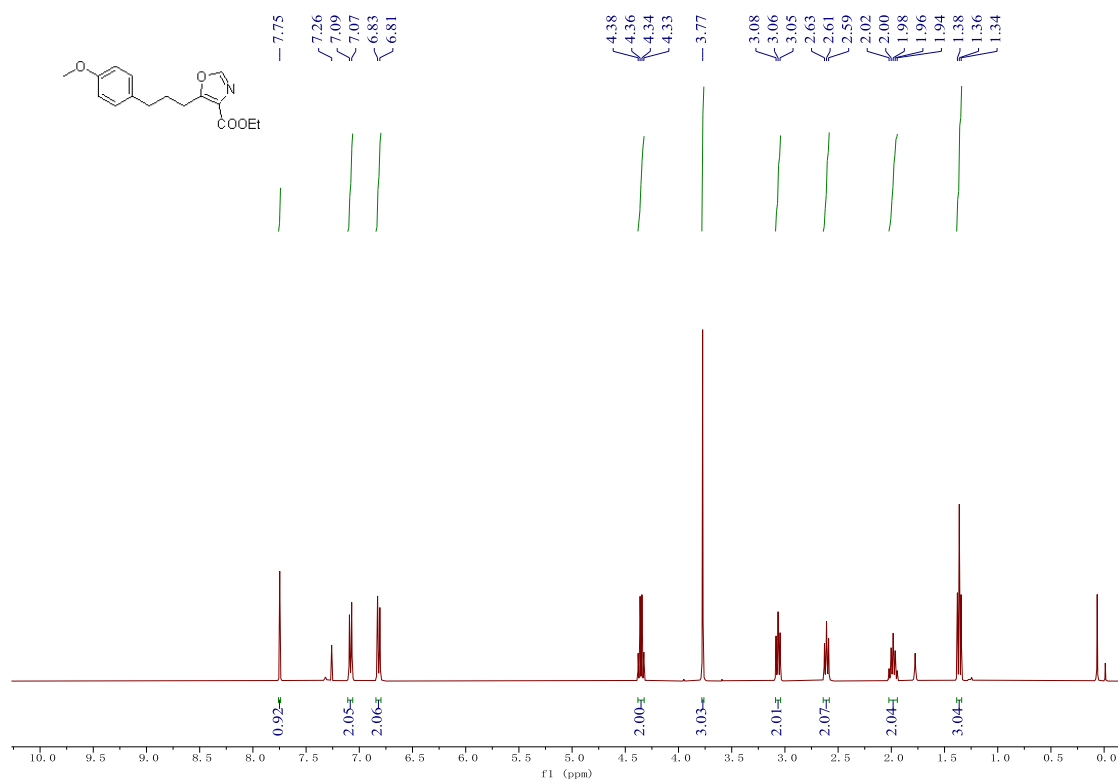
37c ¹H NMR and ¹³C NMR



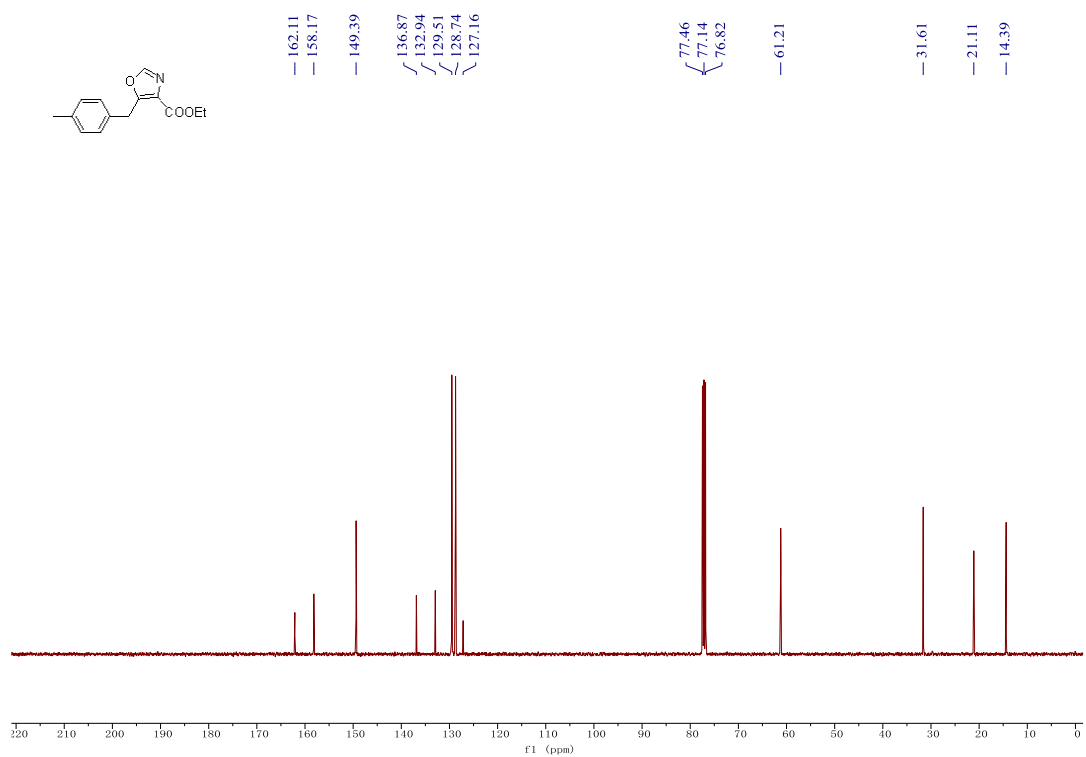
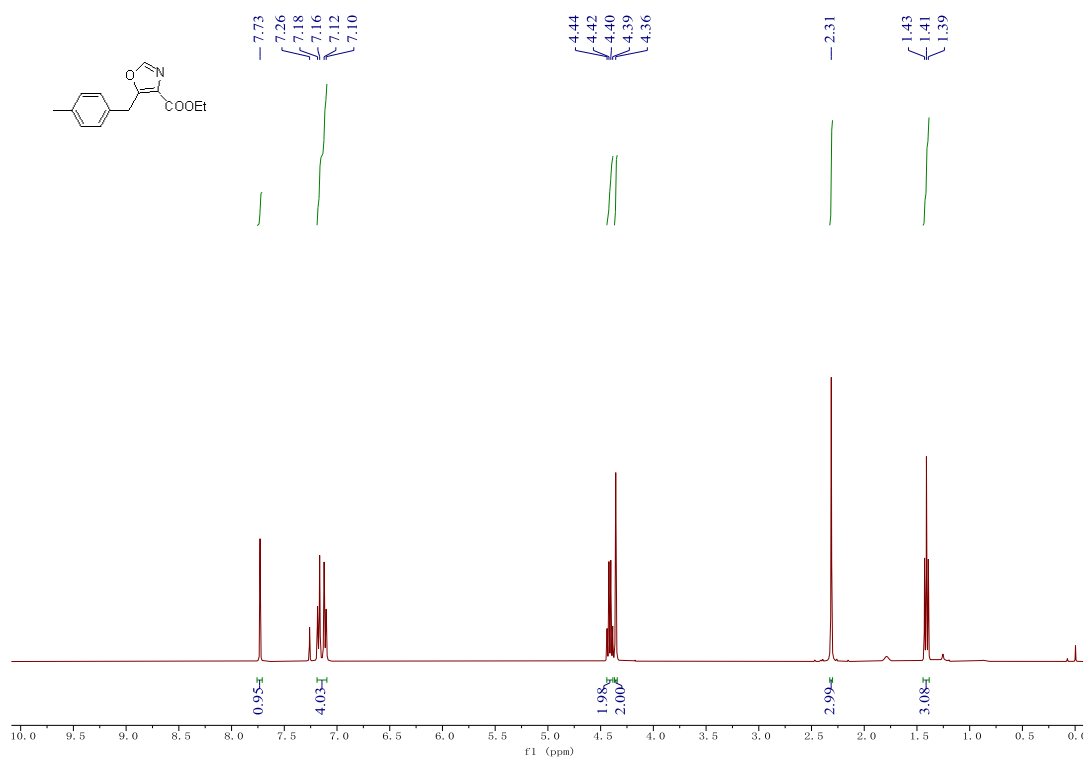
38c ^1H NMR and ^{13}C NMR



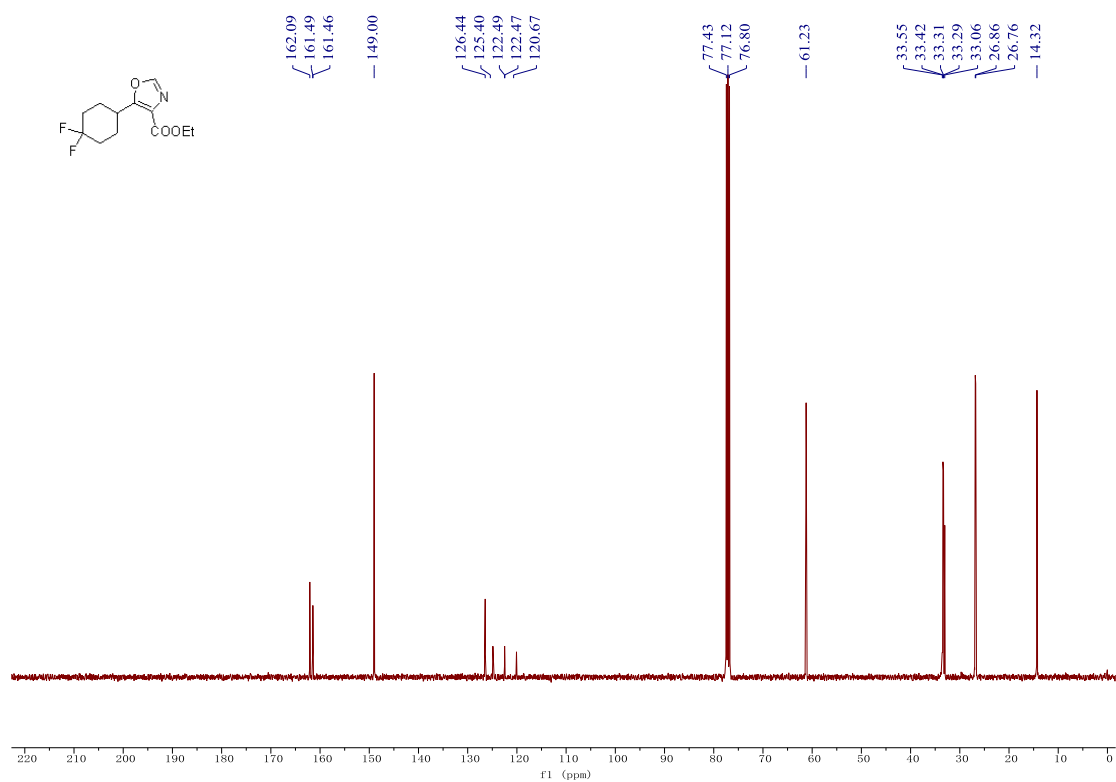
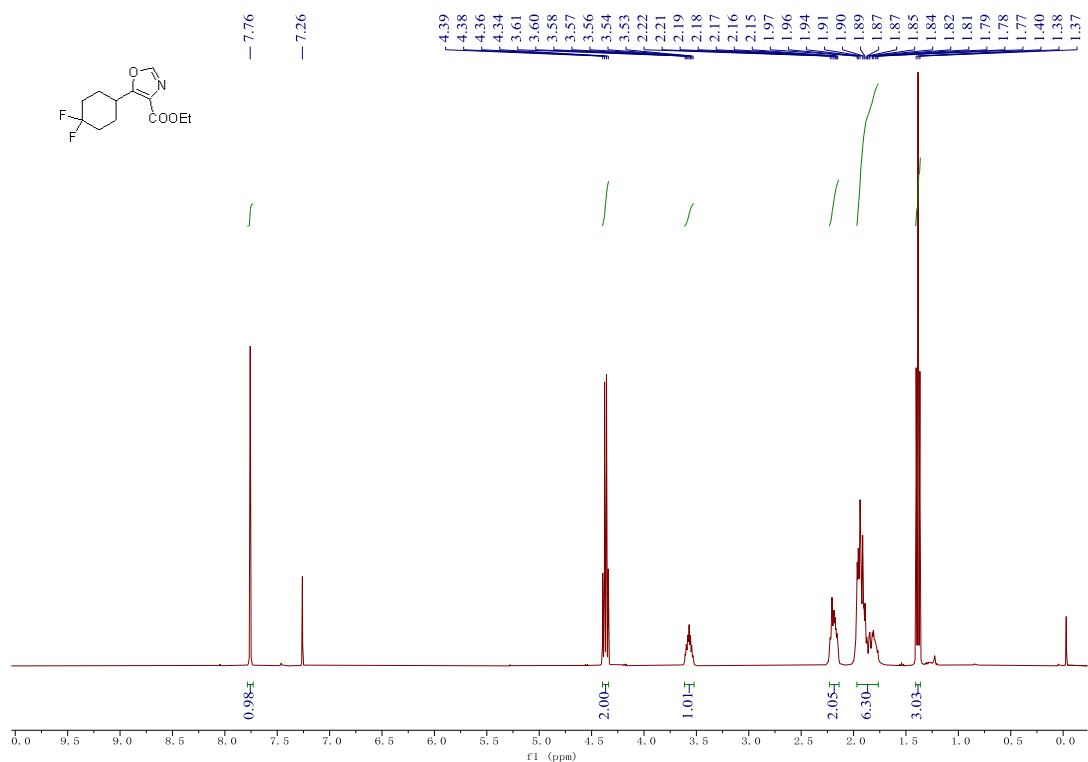
39c ¹H NMR and ¹³C NMR

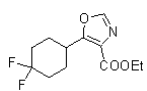


40c ^1H NMR and ^{13}C NMR

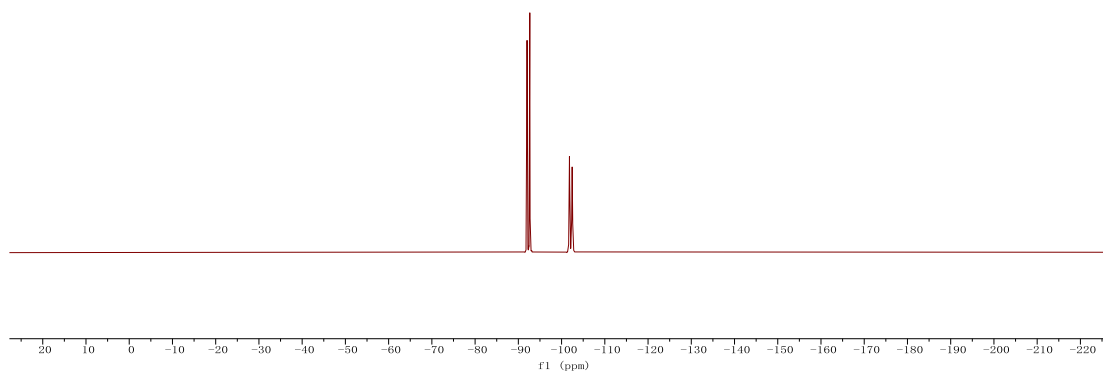


41c ^1H NMR, ^{13}C NMR and ^{19}F NMR

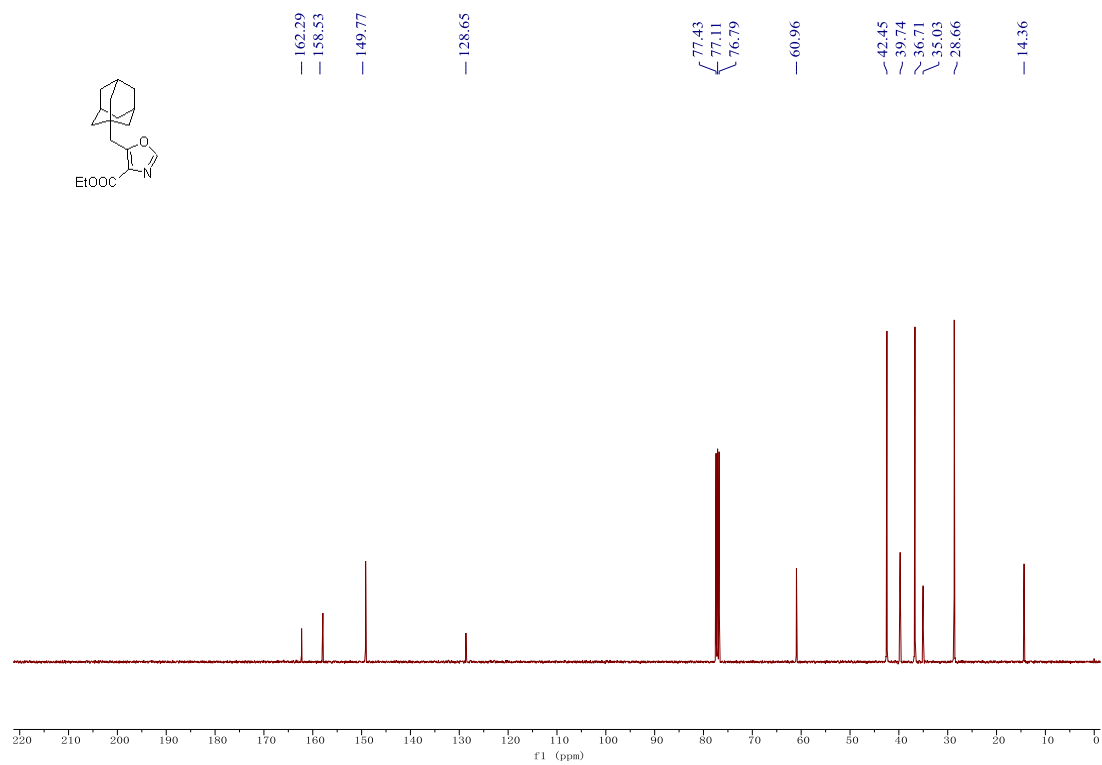
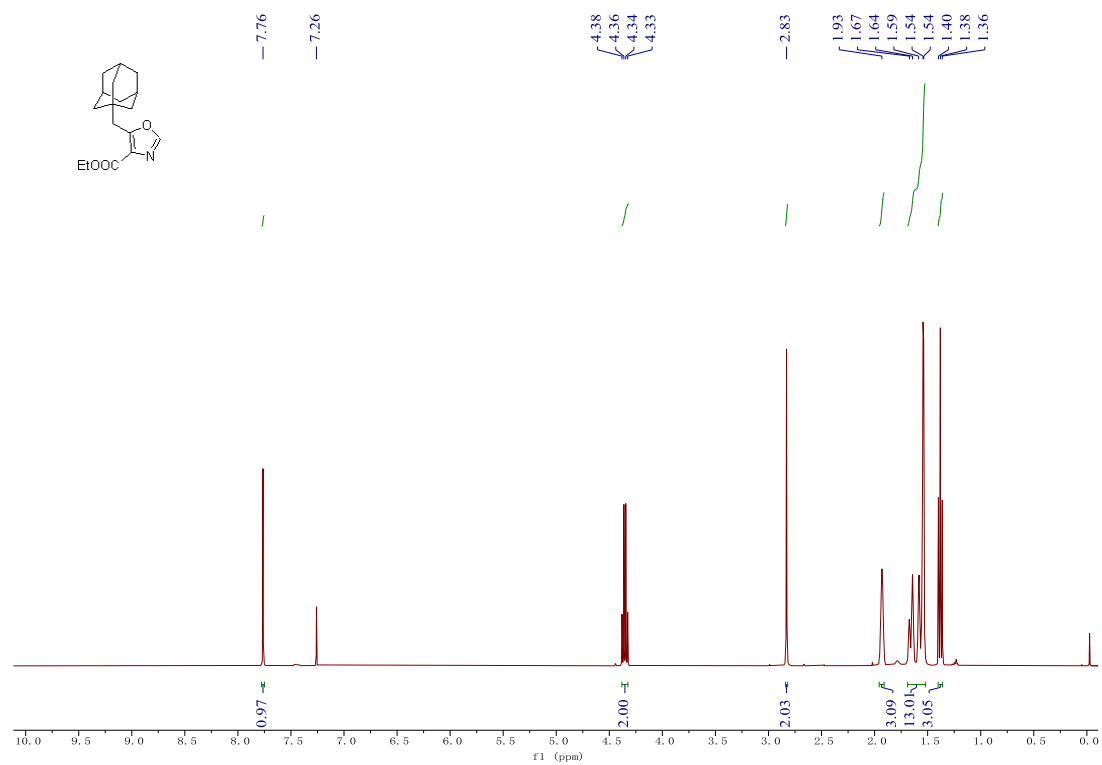




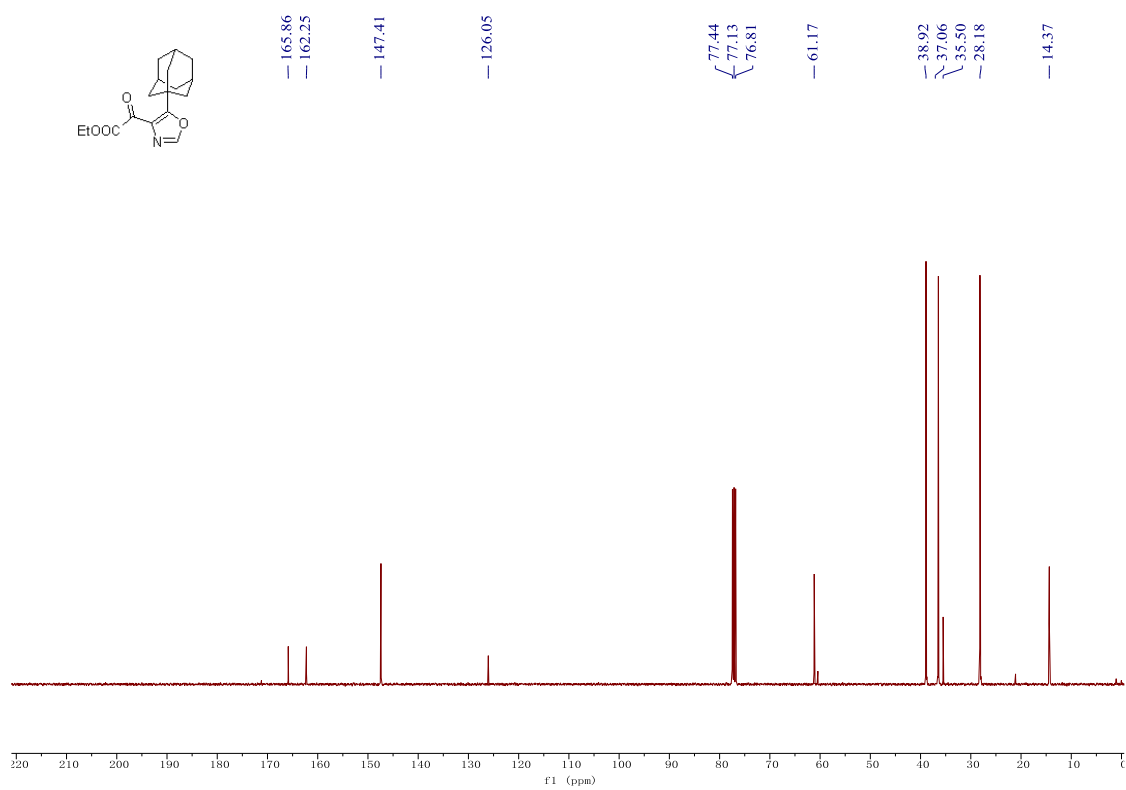
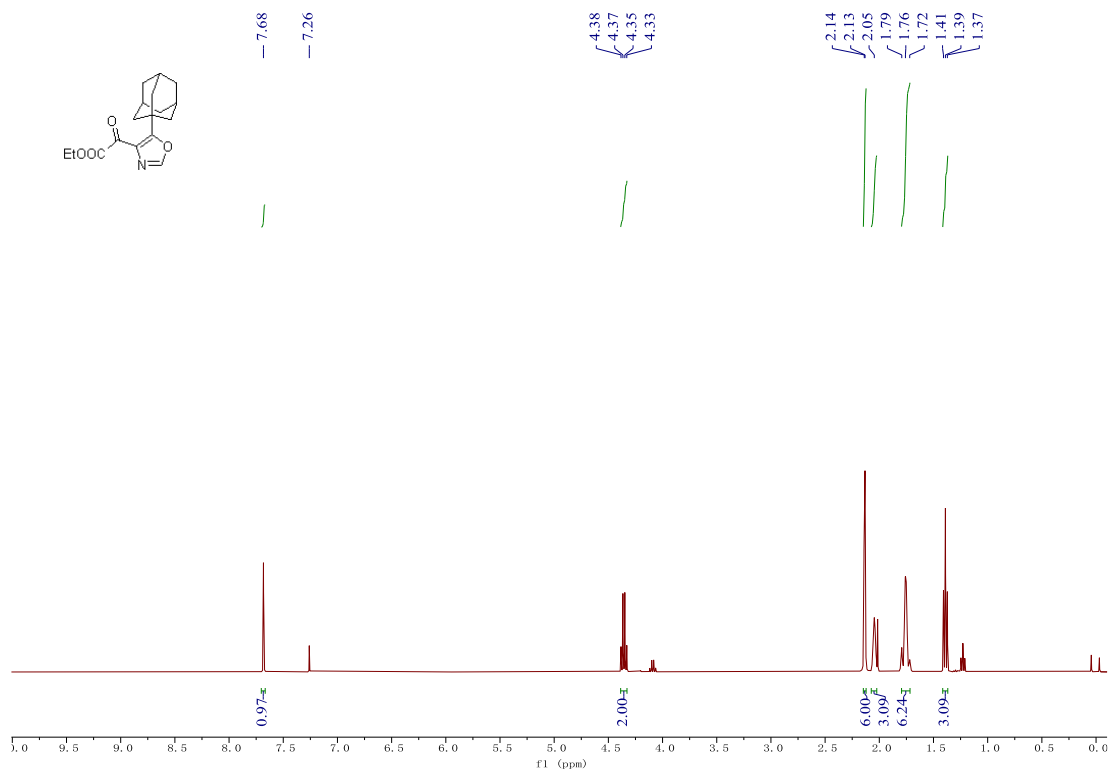
92.02
 92.65
 101.82
 102.45



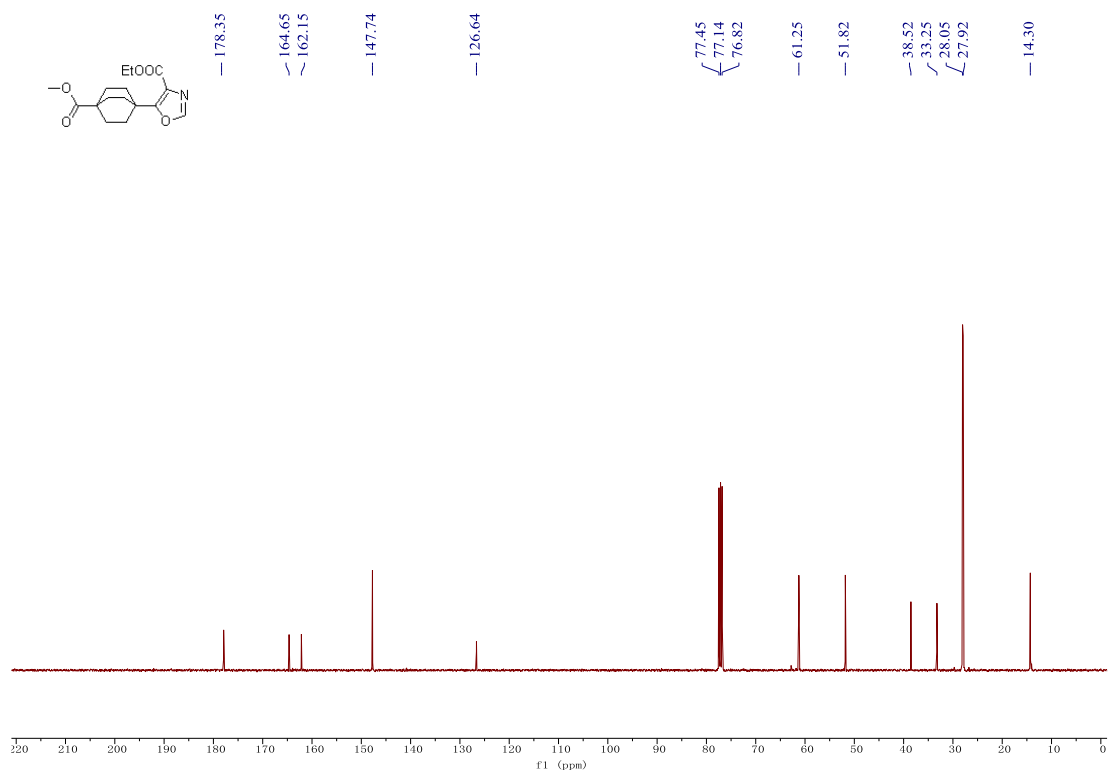
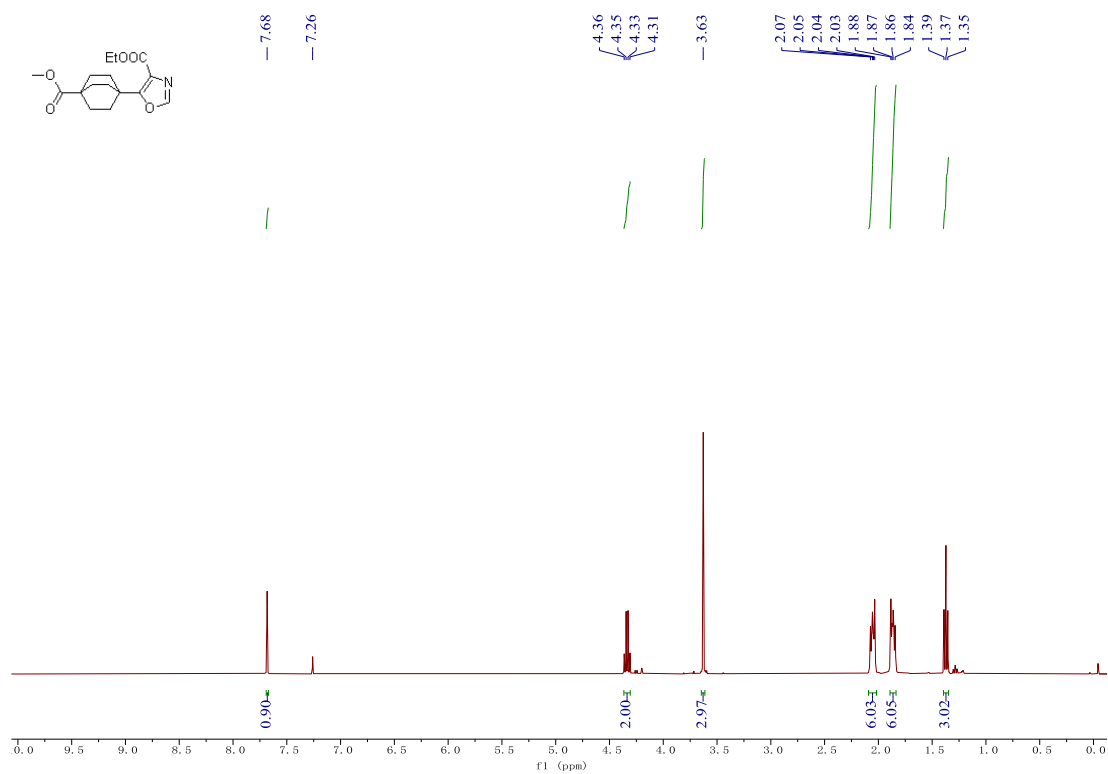
42c ^1H NMR and ^{13}C NMR



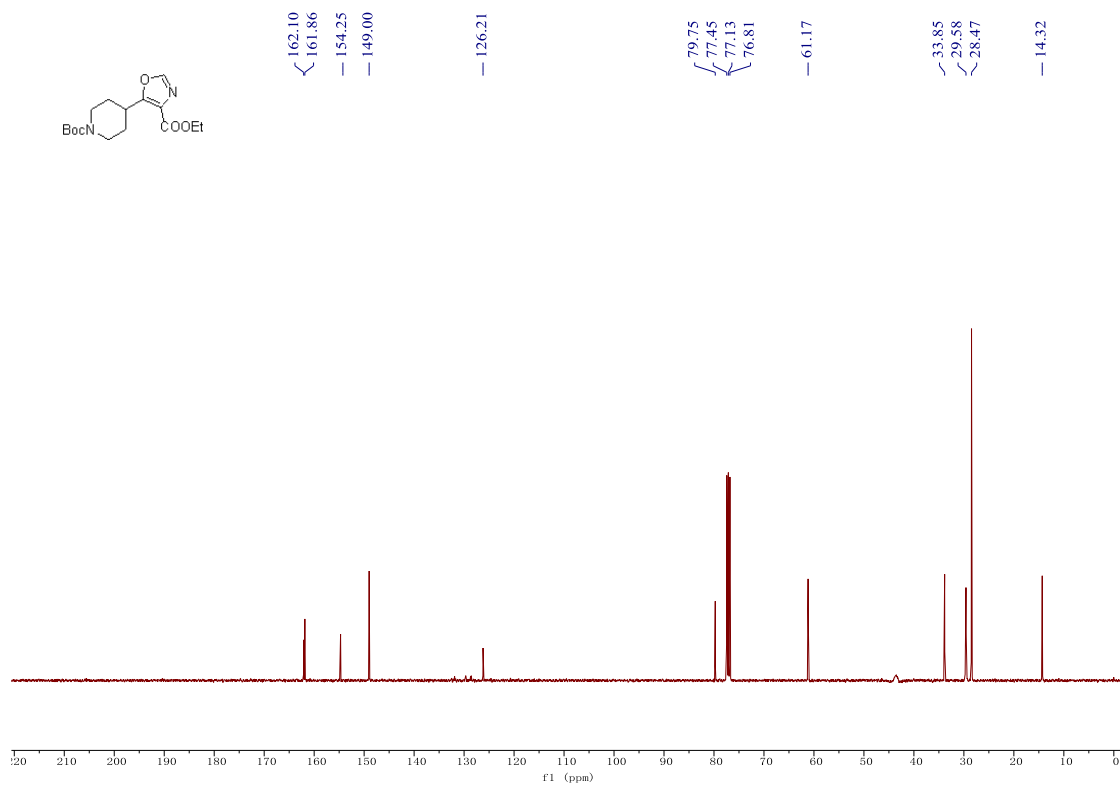
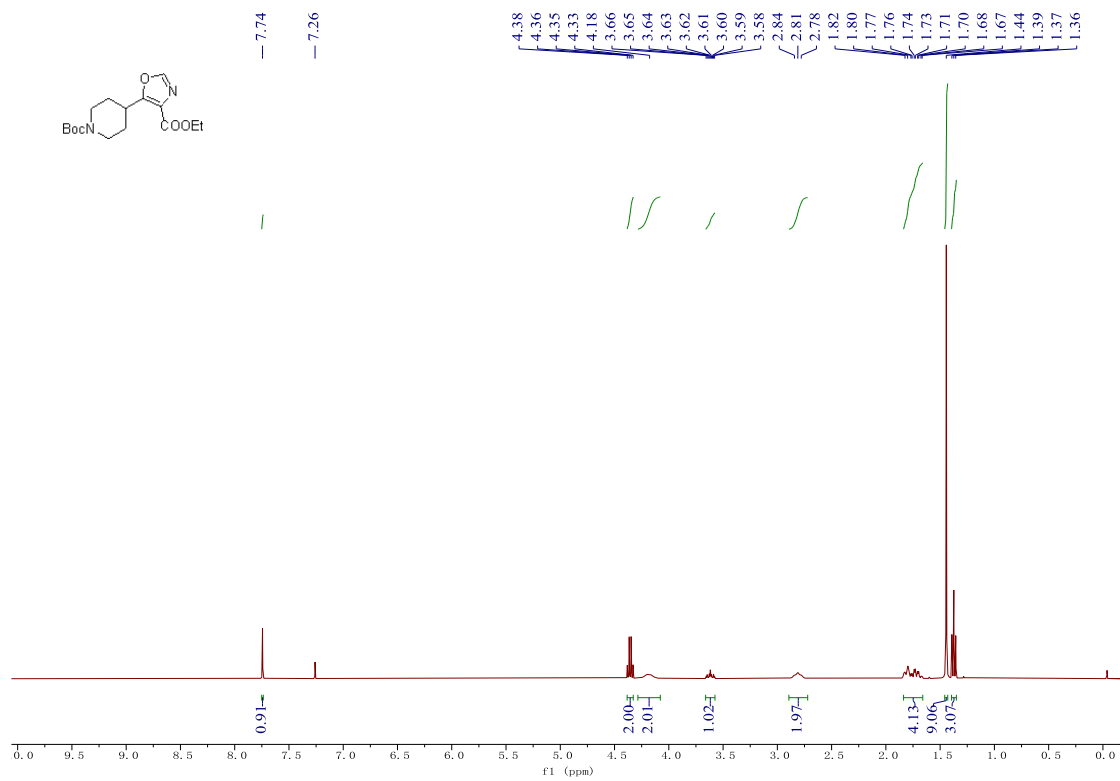
43c ^1H NMR and ^{13}C NMR



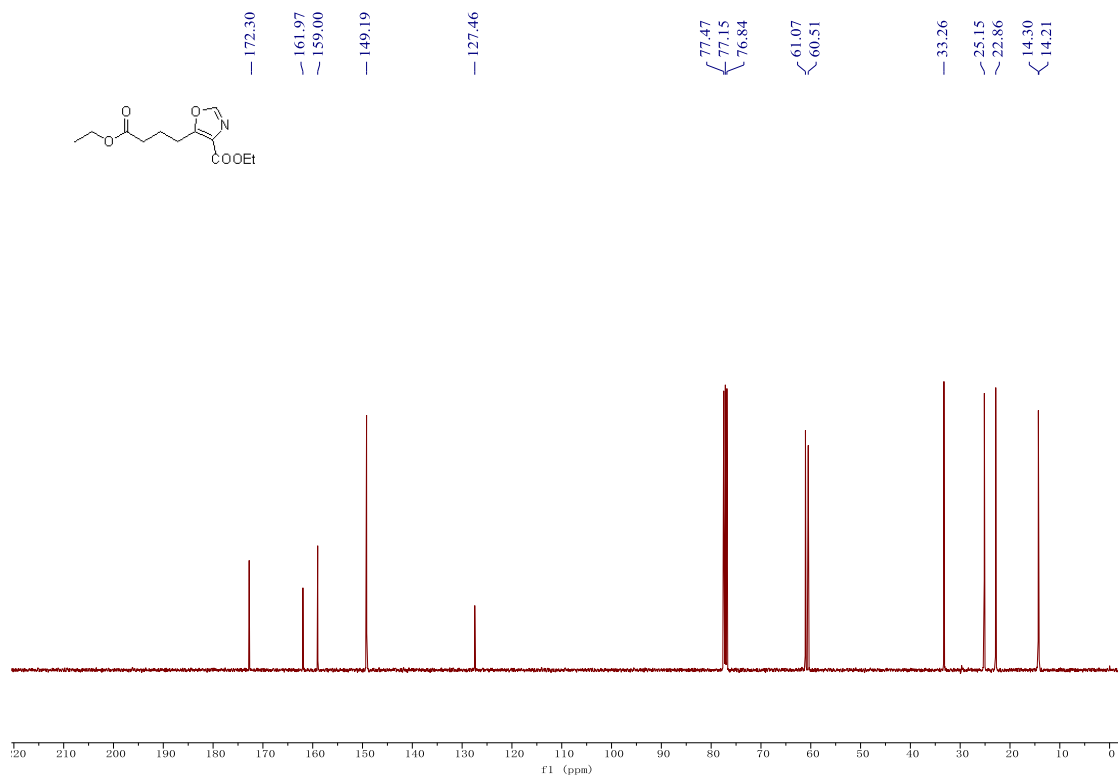
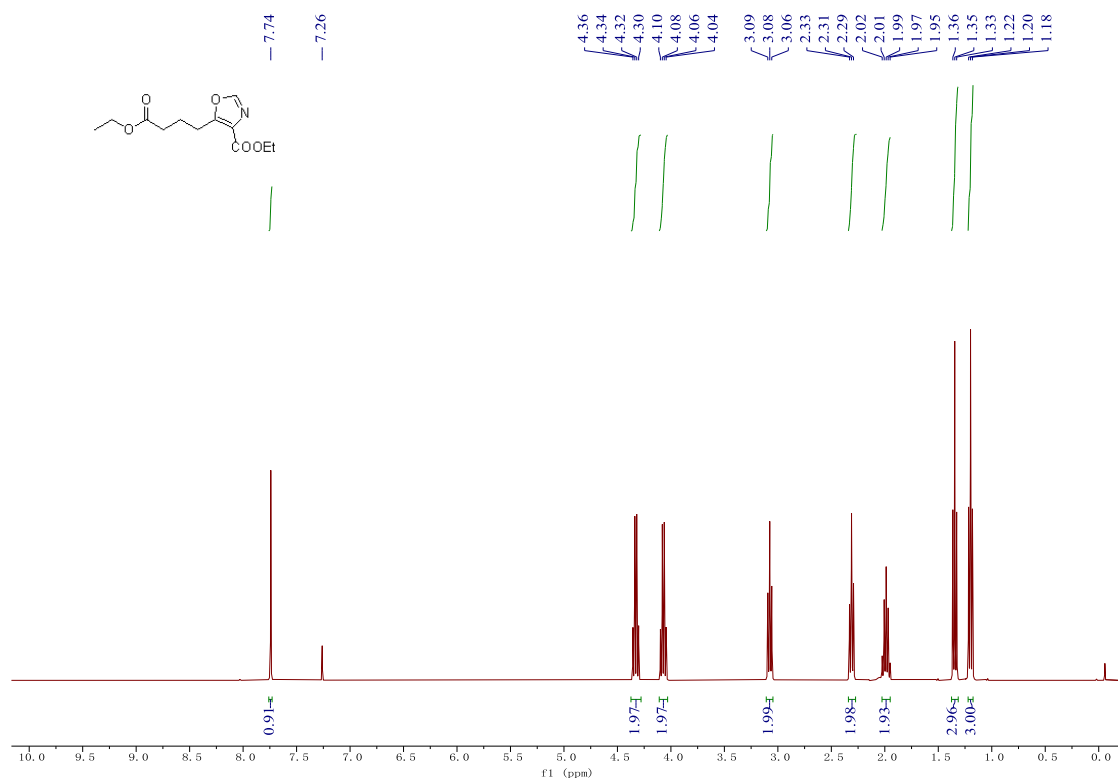
44c ^1H NMR and ^{13}C NMR



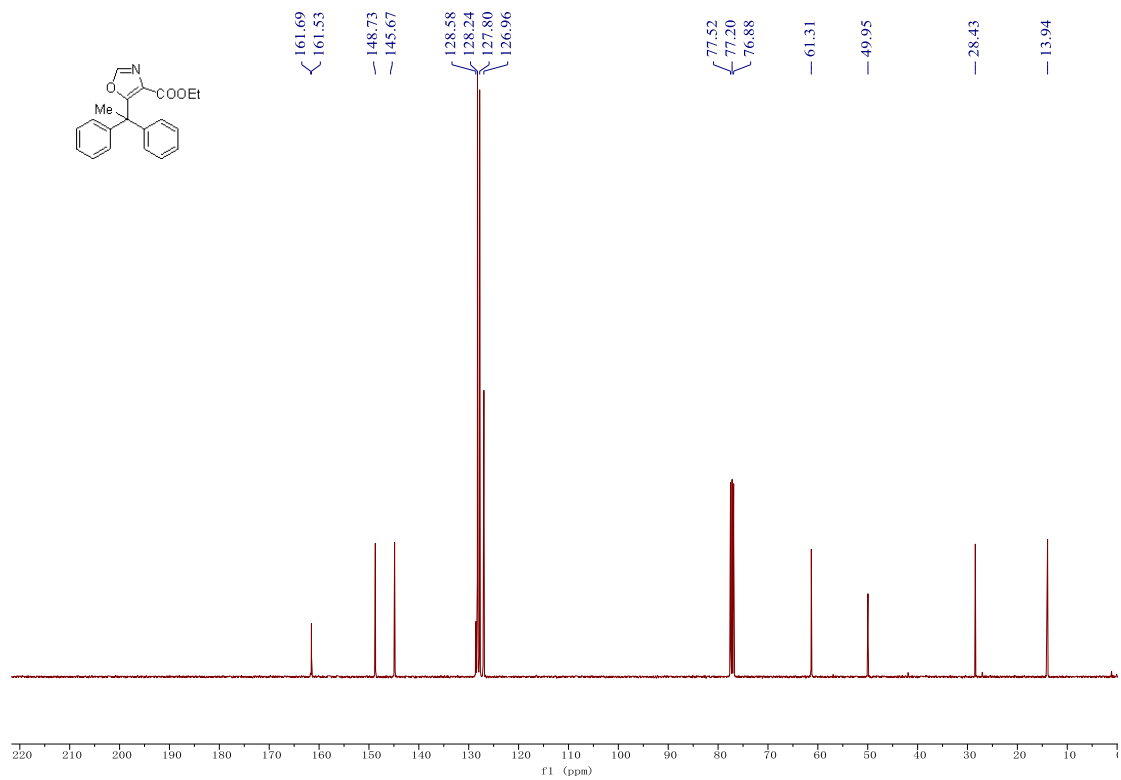
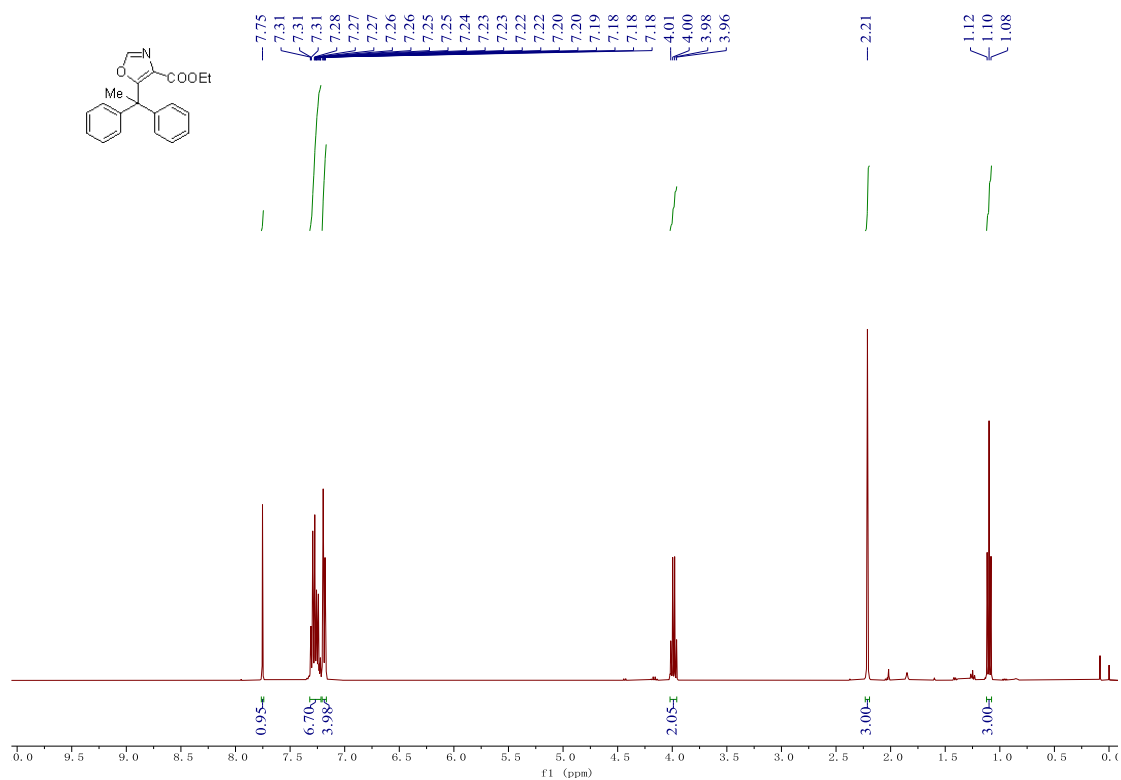
45c ^1H NMR and ^{13}C NMR



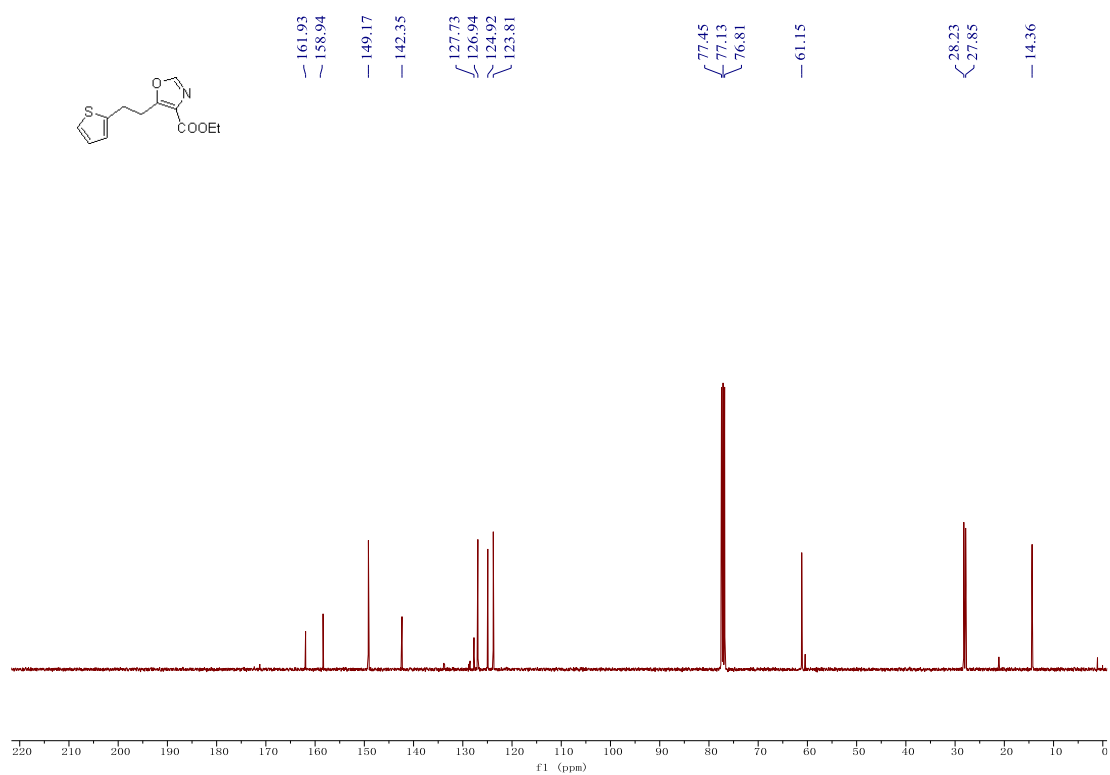
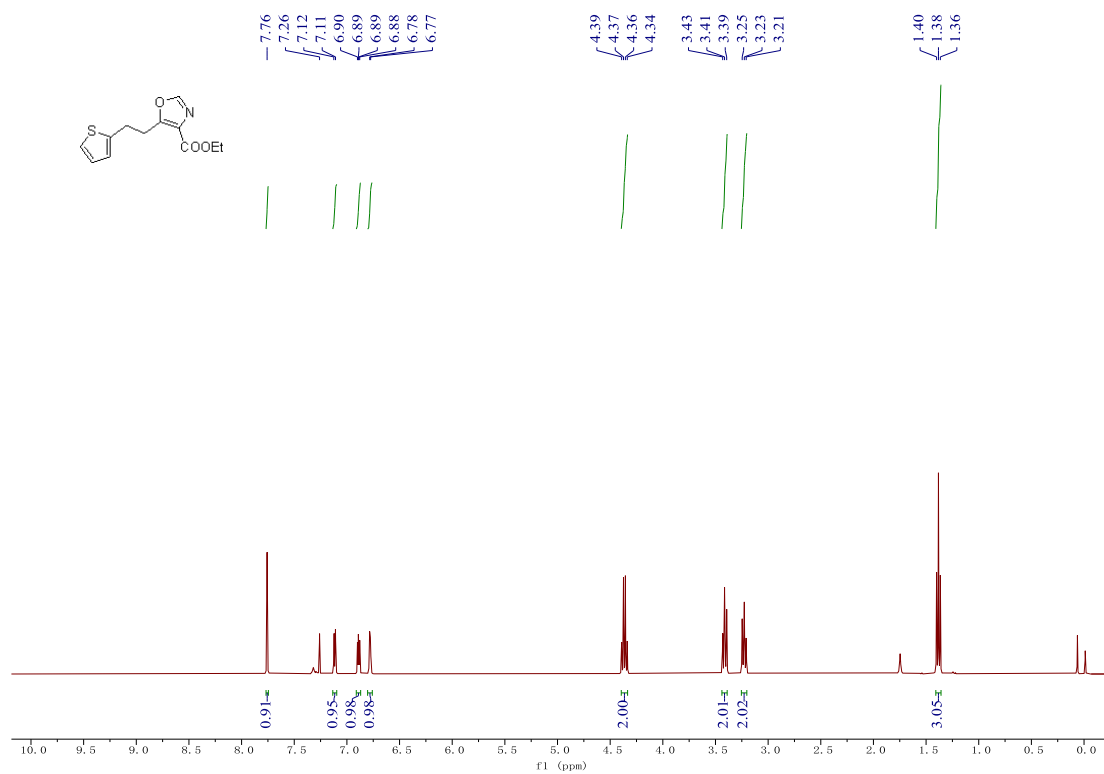
46c ^1H NMR and ^{13}C NMR



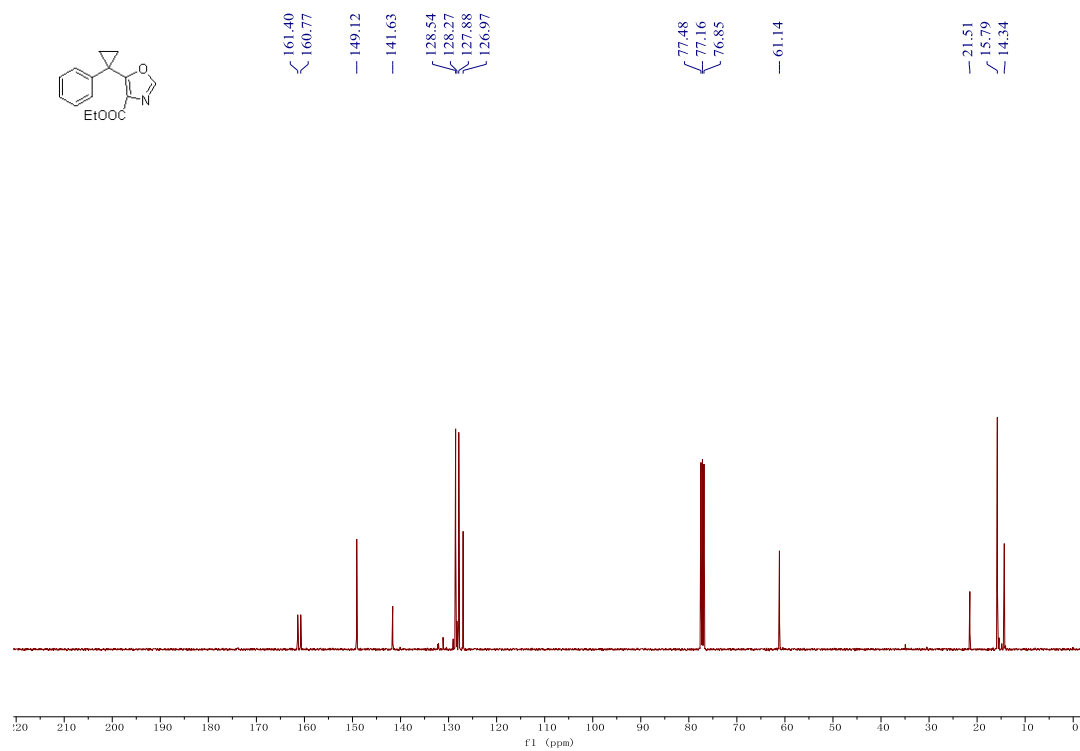
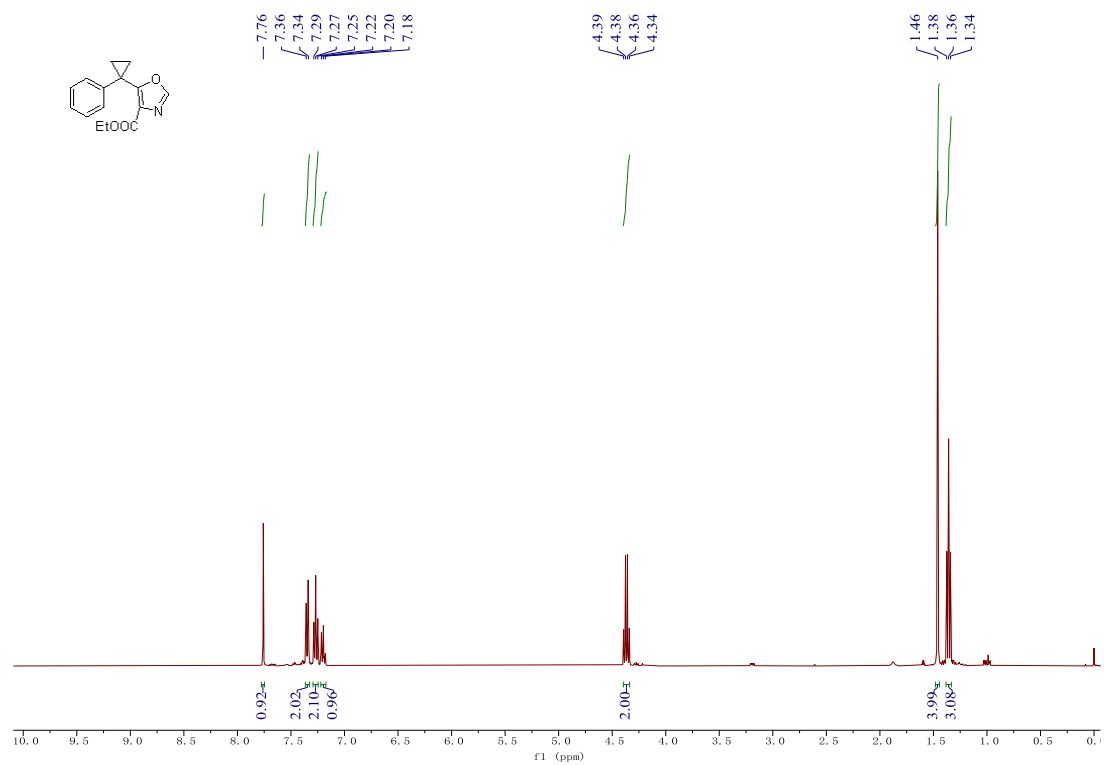
47c ^1H NMR and ^{13}C NMR



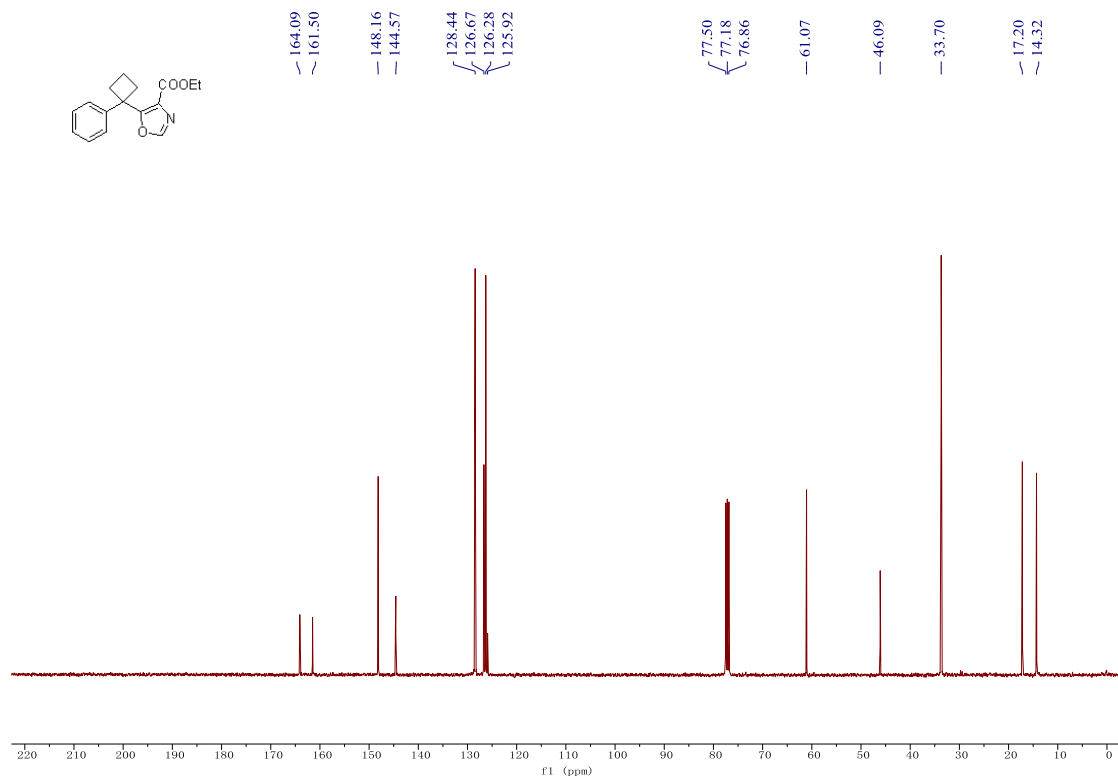
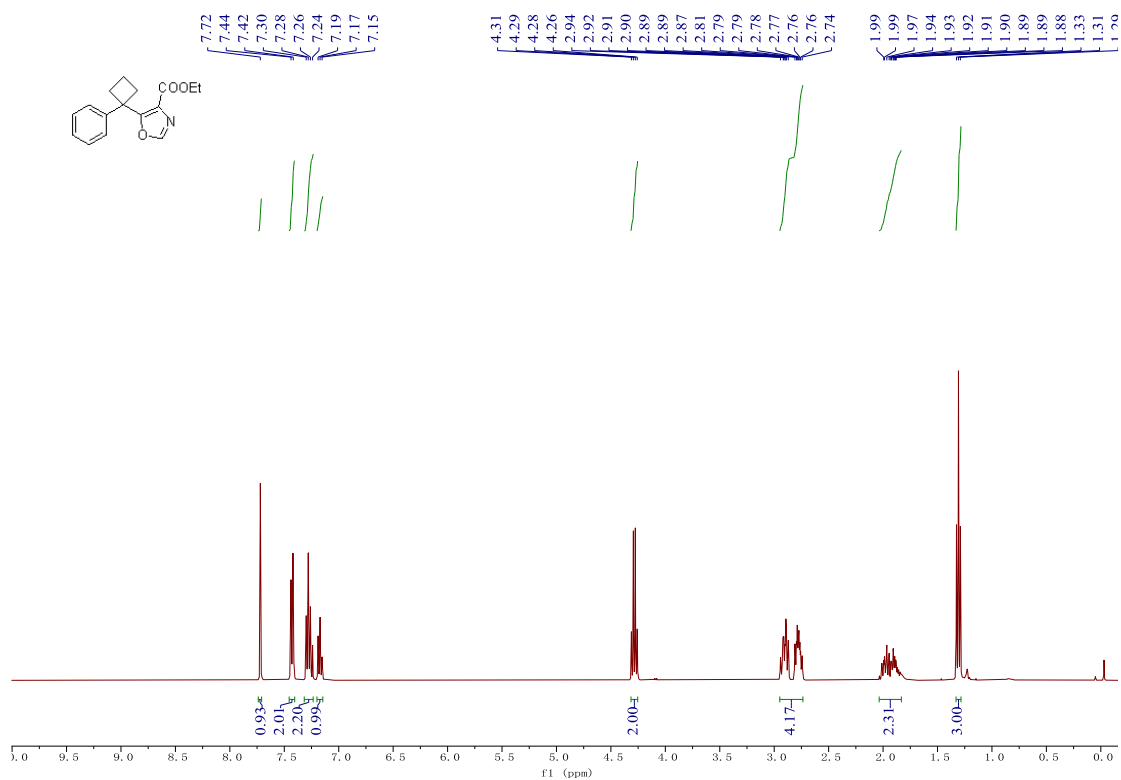
48c ^1H NMR and ^{13}C NMR



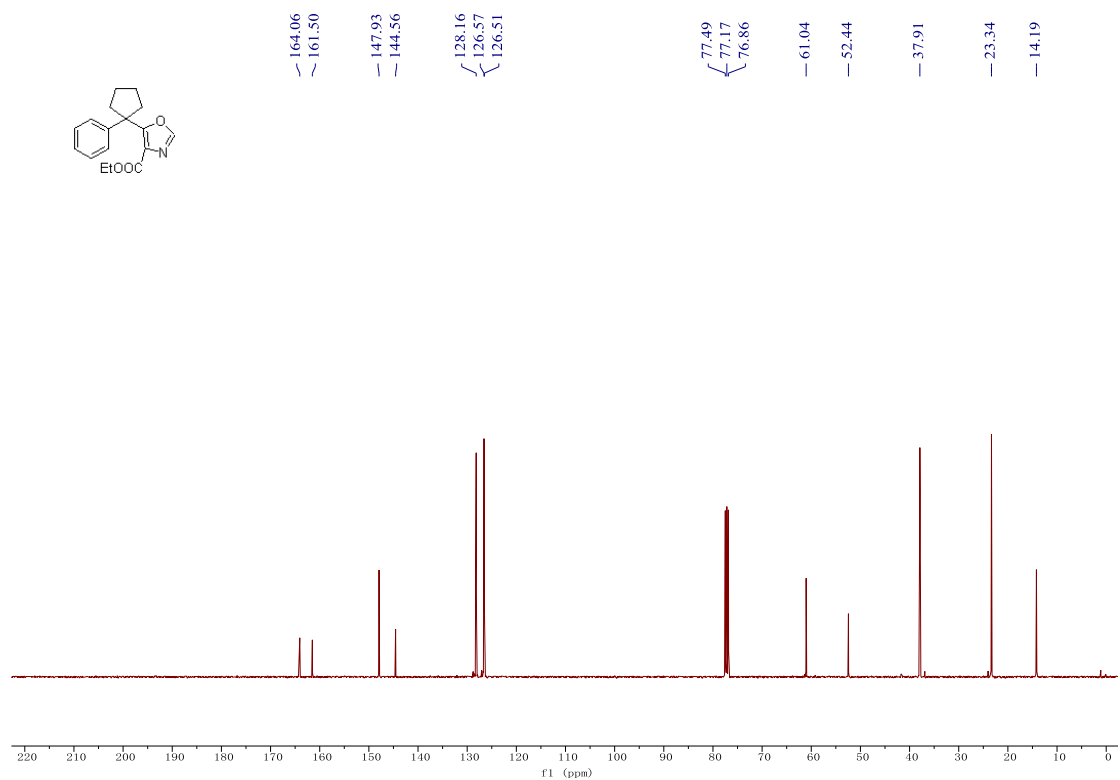
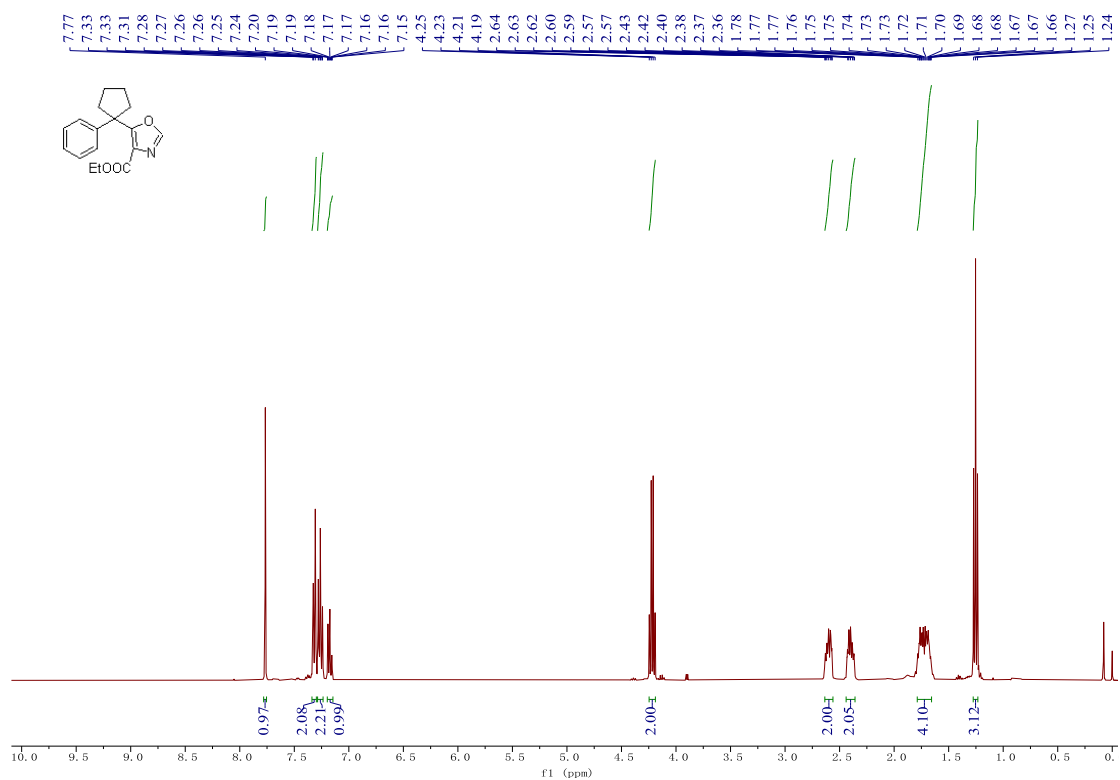
49c ^1H NMR and ^{13}C NMR



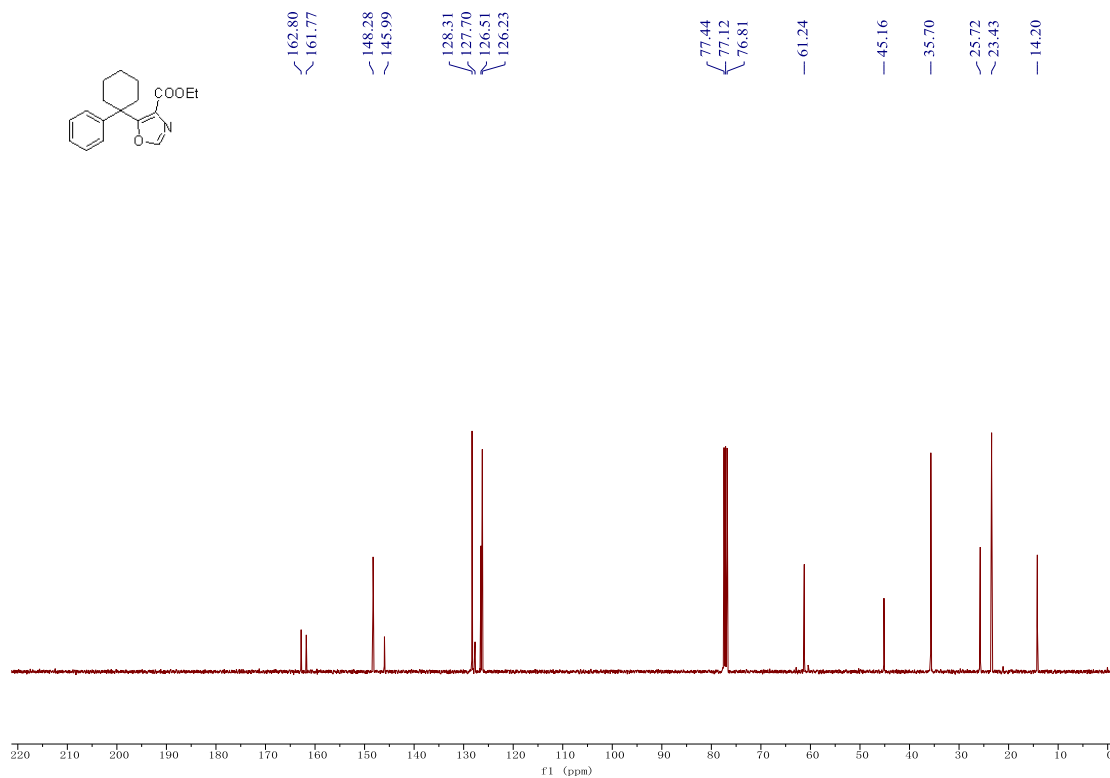
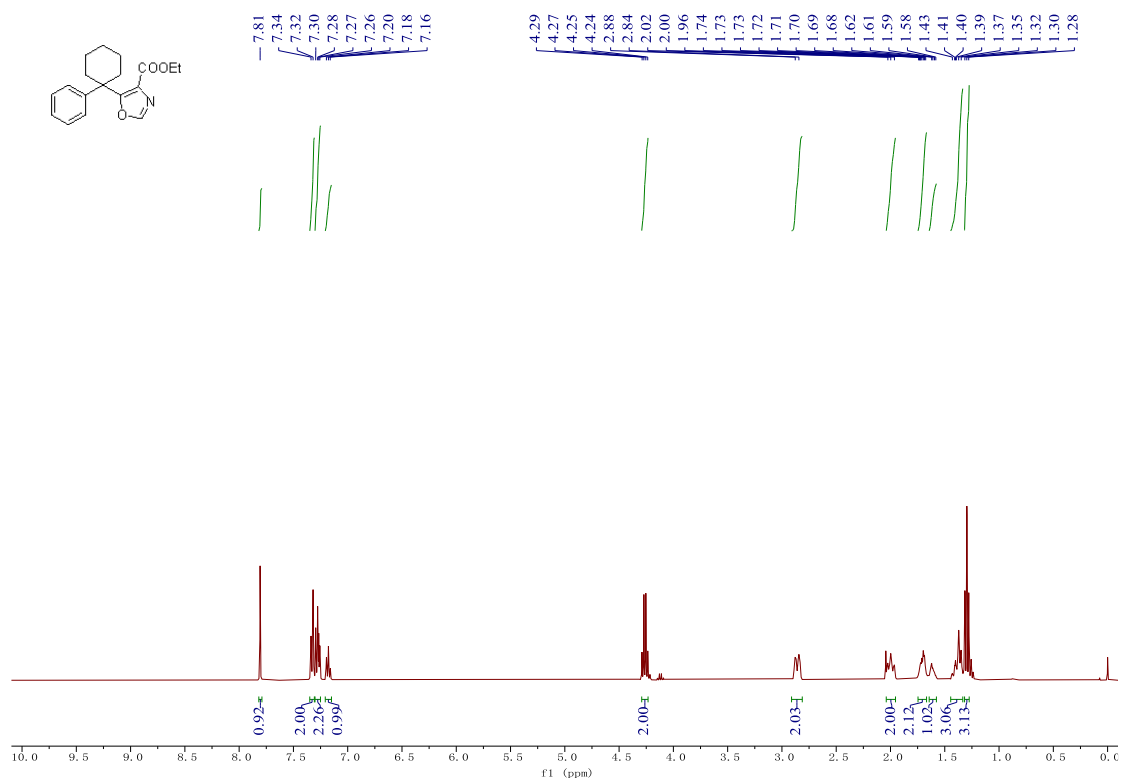
50c ^1H NMR and ^{13}C NMR



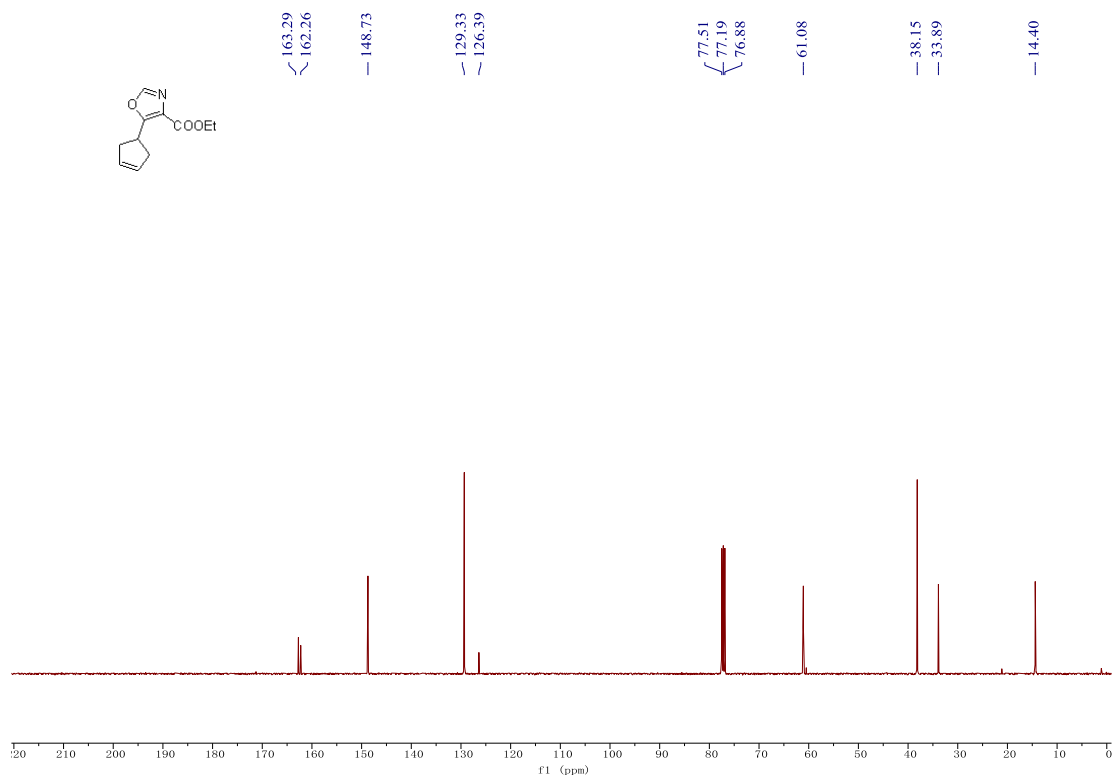
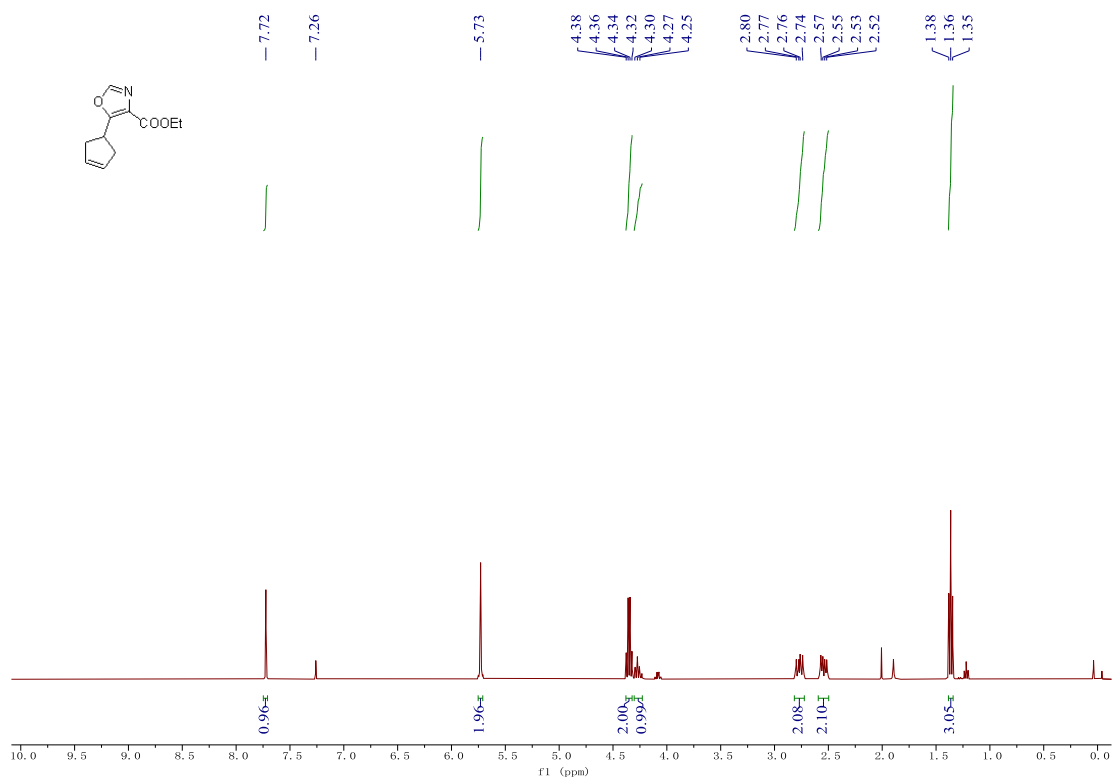
51c ¹H NMR and ¹³C NMR



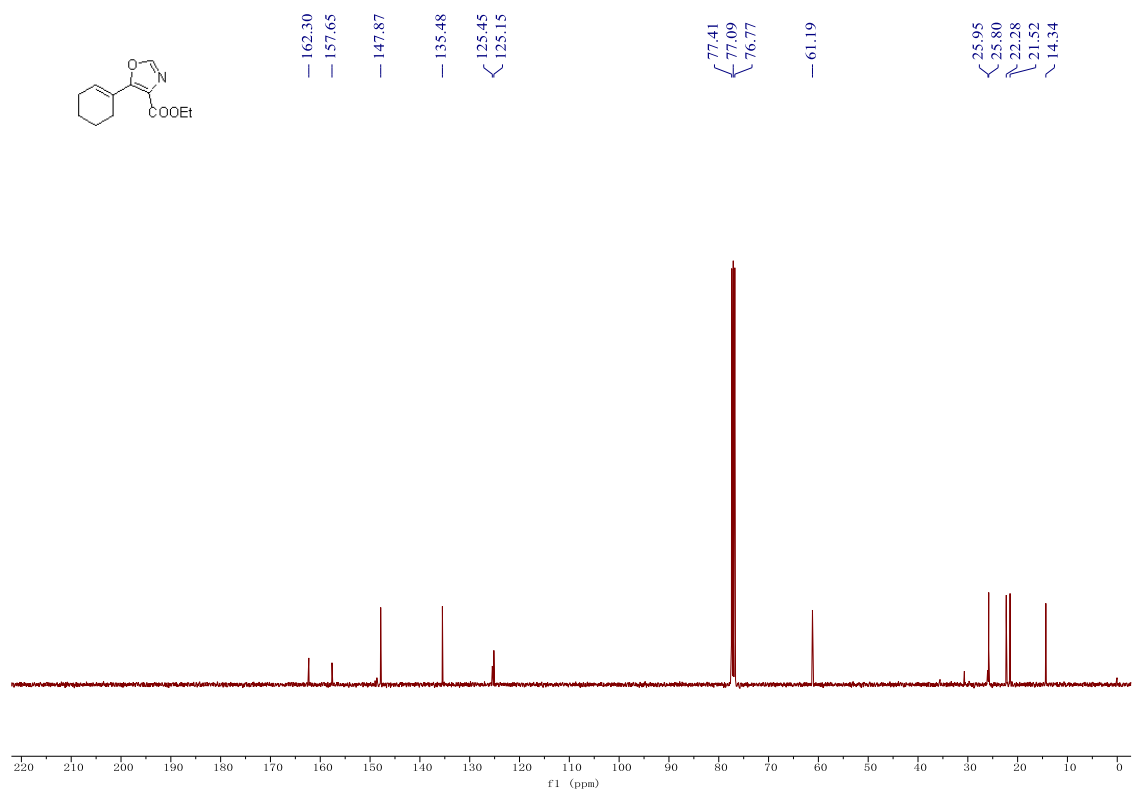
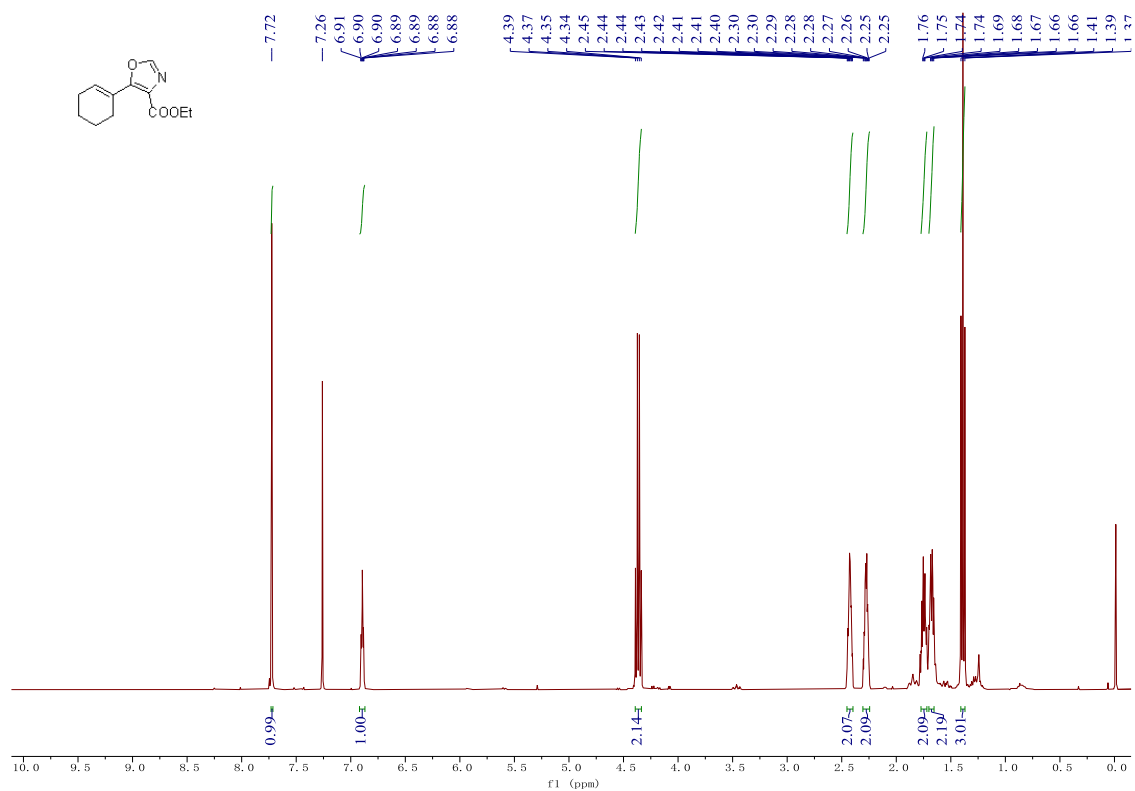
52c ¹H NMR and ¹³C NMR



53c ^1H NMR and ^{13}C NMR



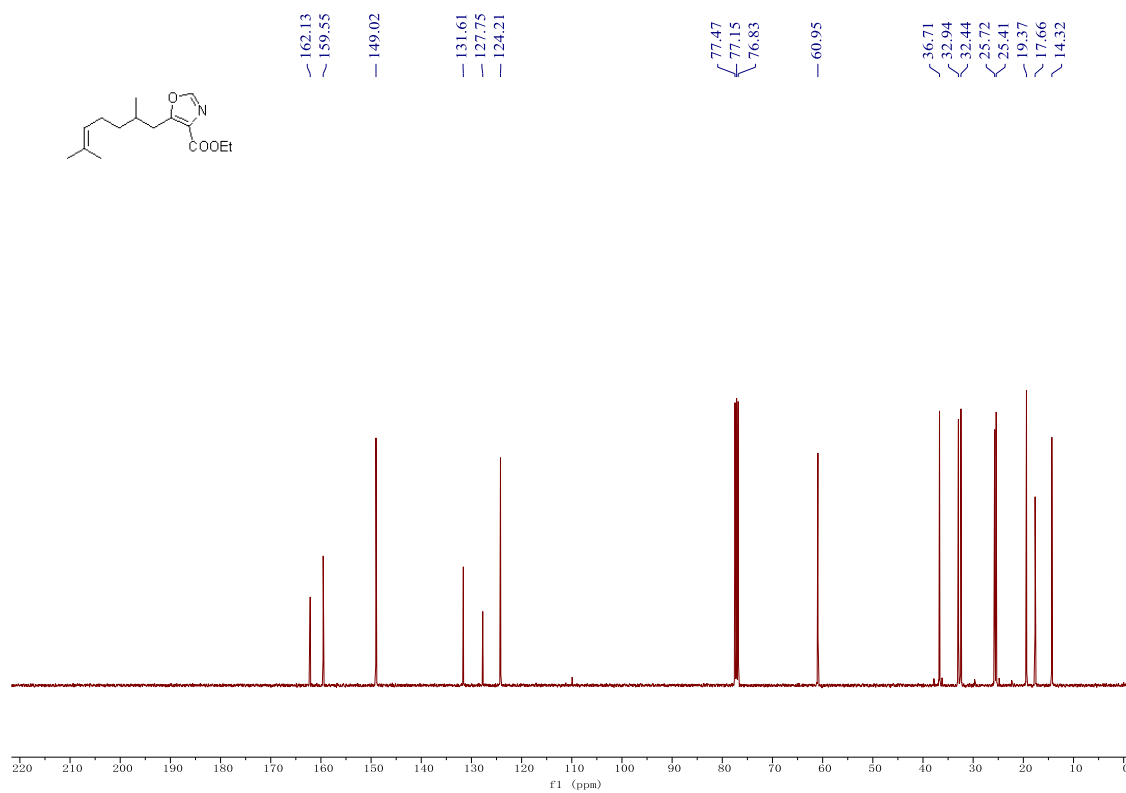
54c ^1H NMR and ^{13}C NMR



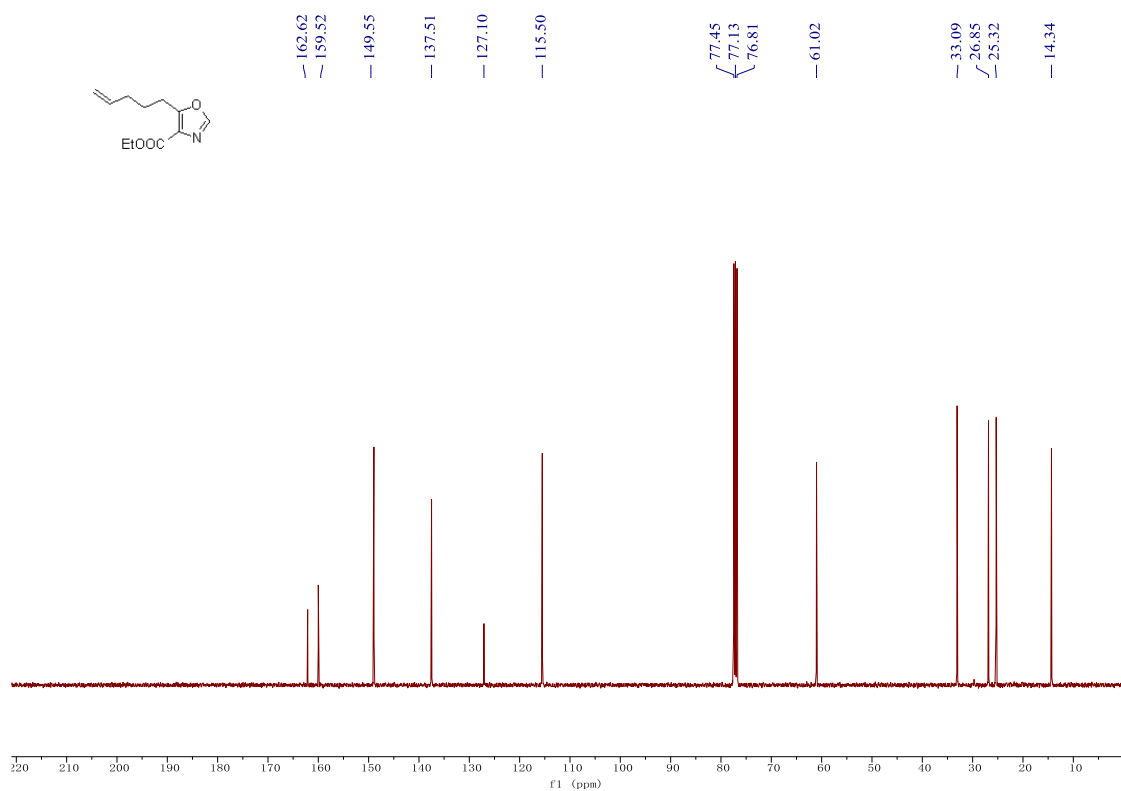
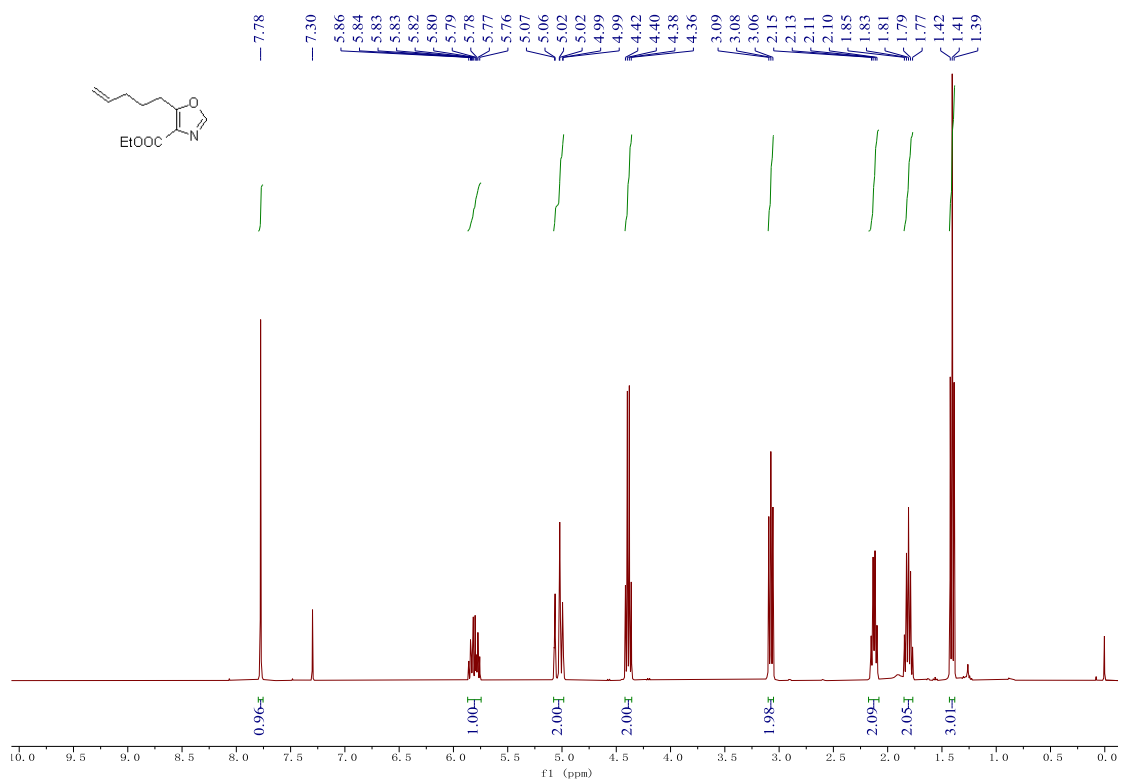
Chemical structure: CC(C)C#CC=Cc1ncoc1C(=O)OCC

¹H NMR spectrum (CDCl₃) showing peaks and integration values:

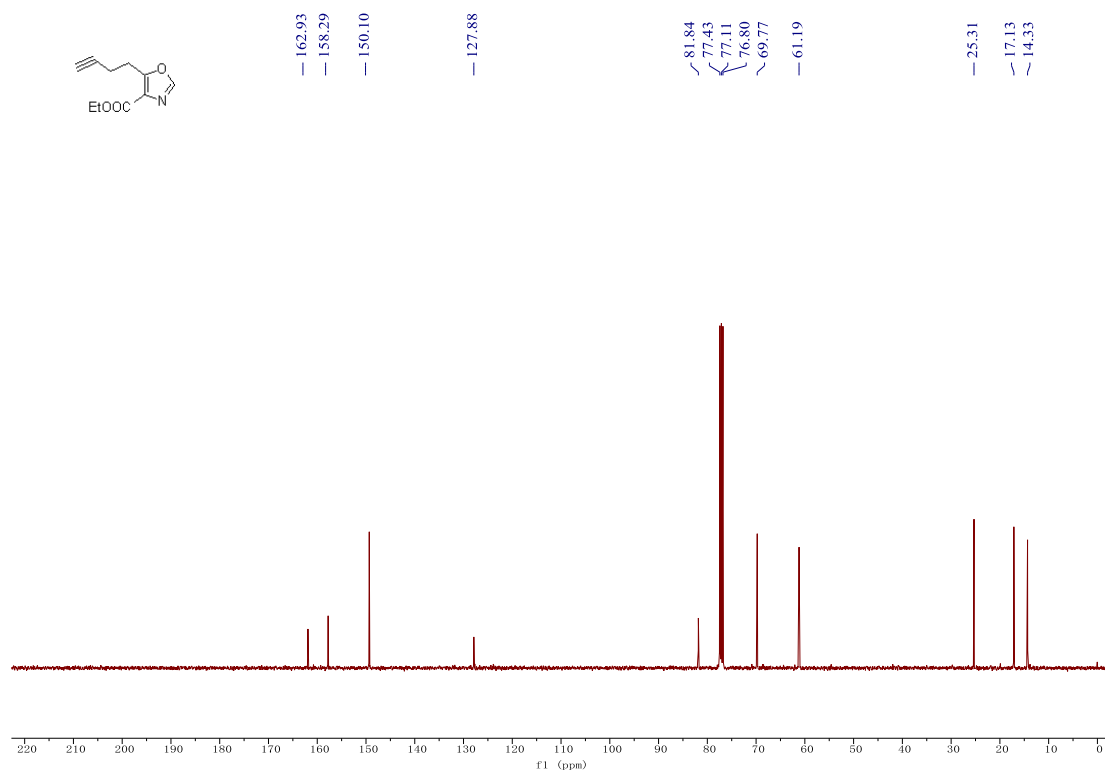
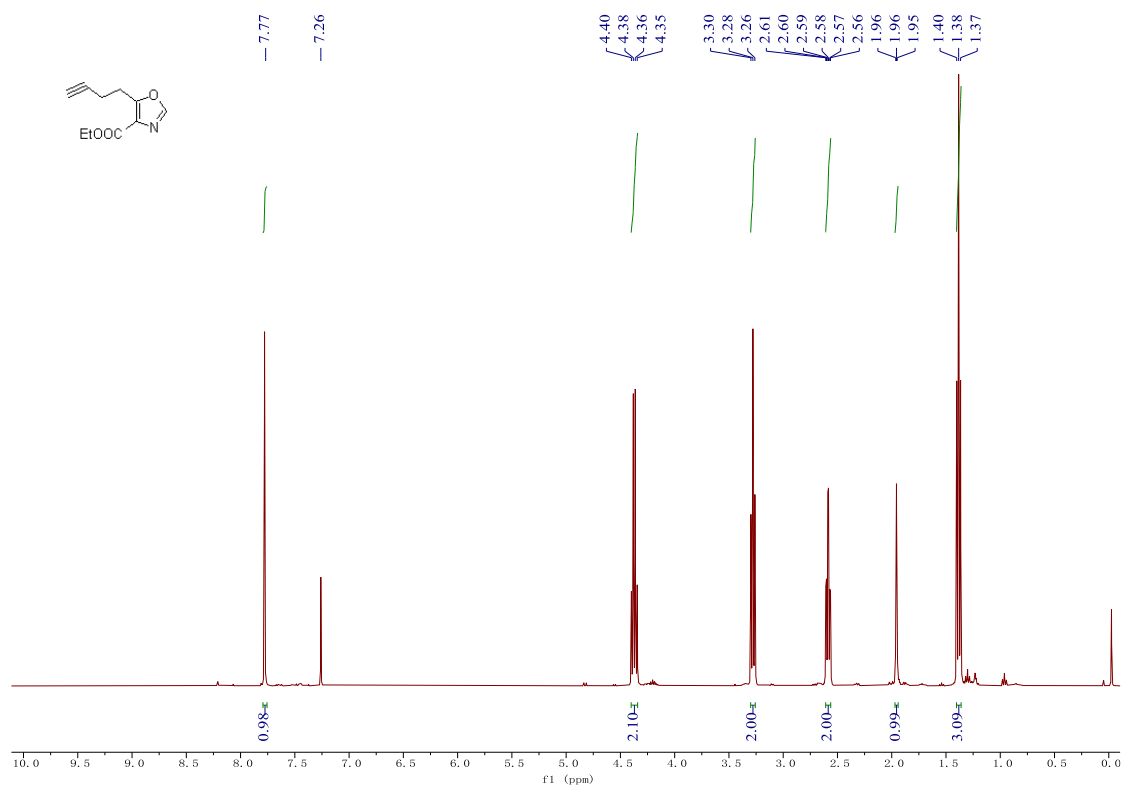
Chemical Shift (ppm)	Integration
7.73	0.94
7.26	
5.04	
5.02	
5.01	
4.36	
4.34	
4.32	
4.31	
3.02	
3.00	
2.98	
2.97	
2.88	
2.86	
2.84	
2.02	
2.00	
1.98	
1.96	
1.94	
1.92	
1.90	
1.89	
1.63	
1.55	
1.37	
1.35	
1.33	
1.30	
1.29	
1.25	
1.24	
1.23	
1.22	
1.21	
1.19	
1.17	
1.16	
0.86	



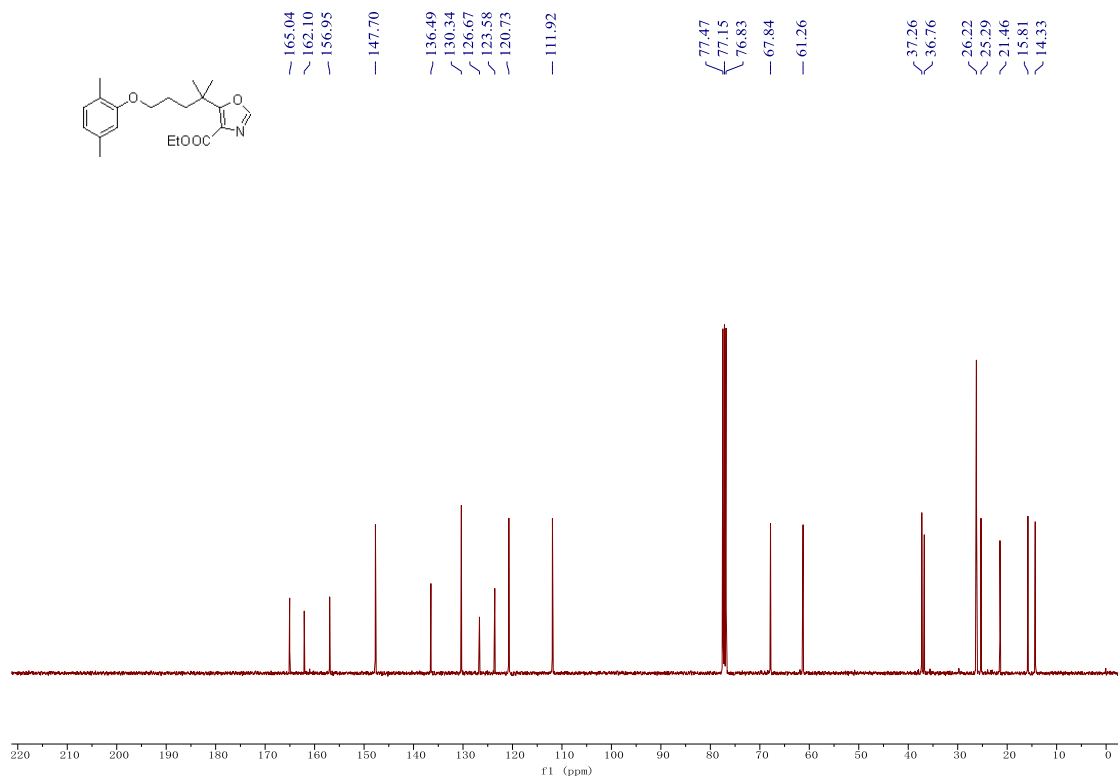
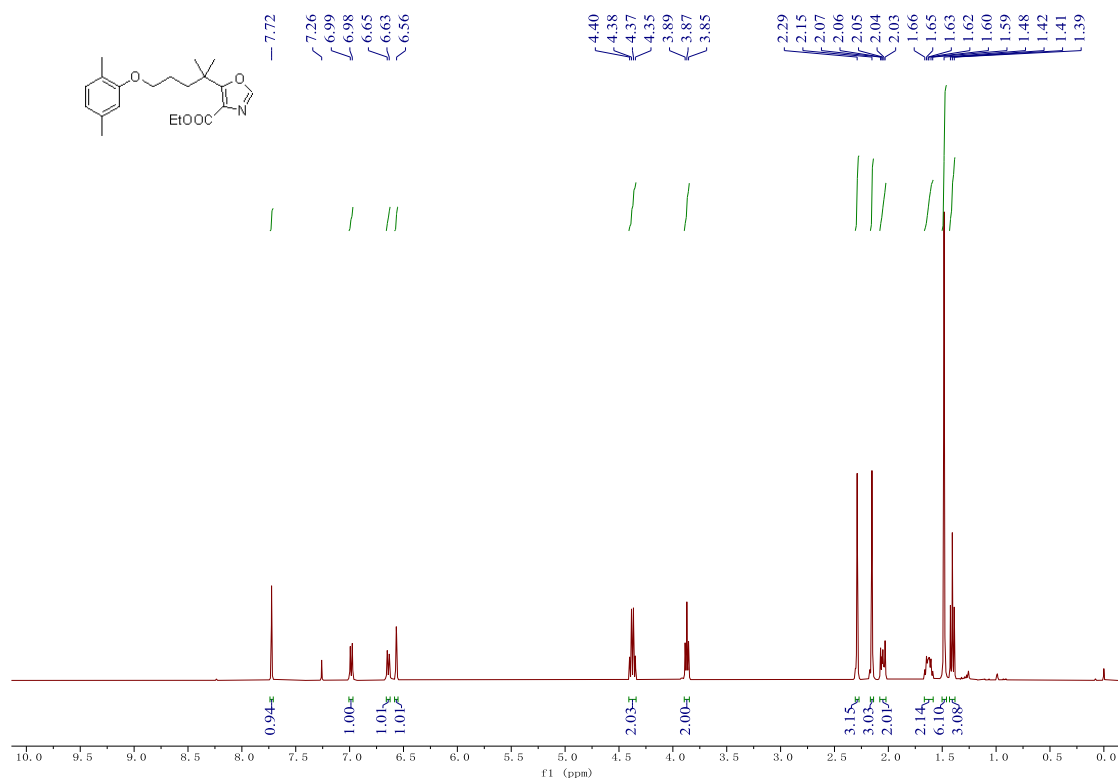
56c ^1H NMR and ^{13}C NMR



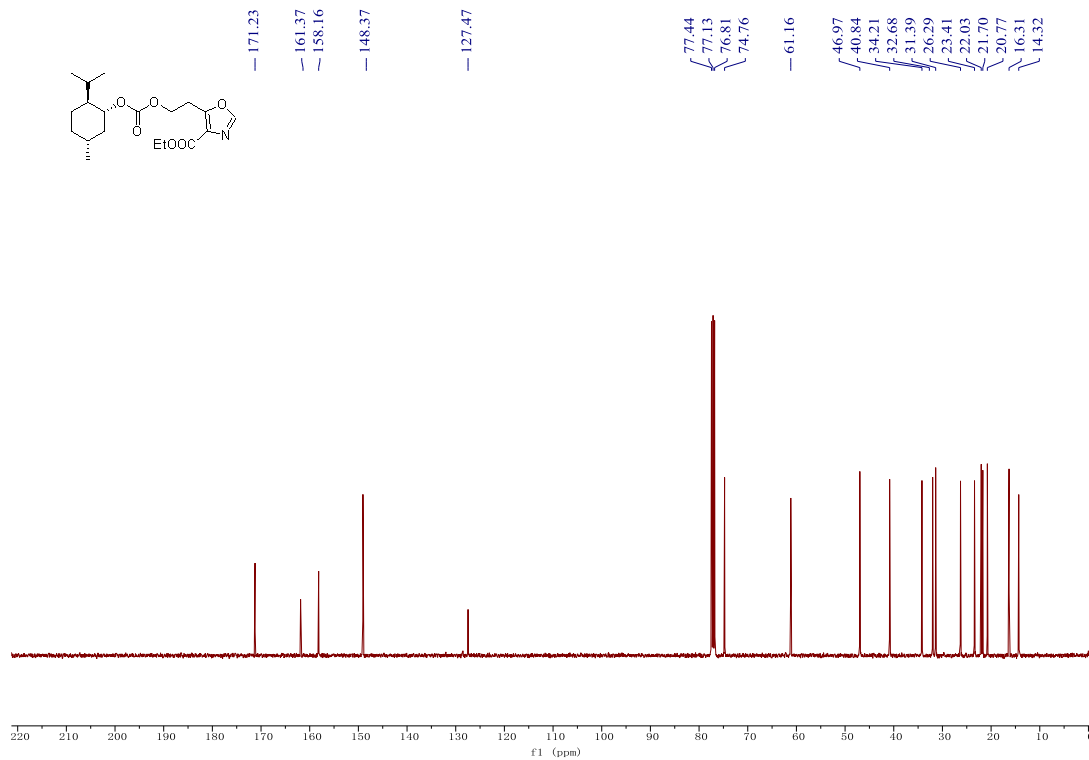
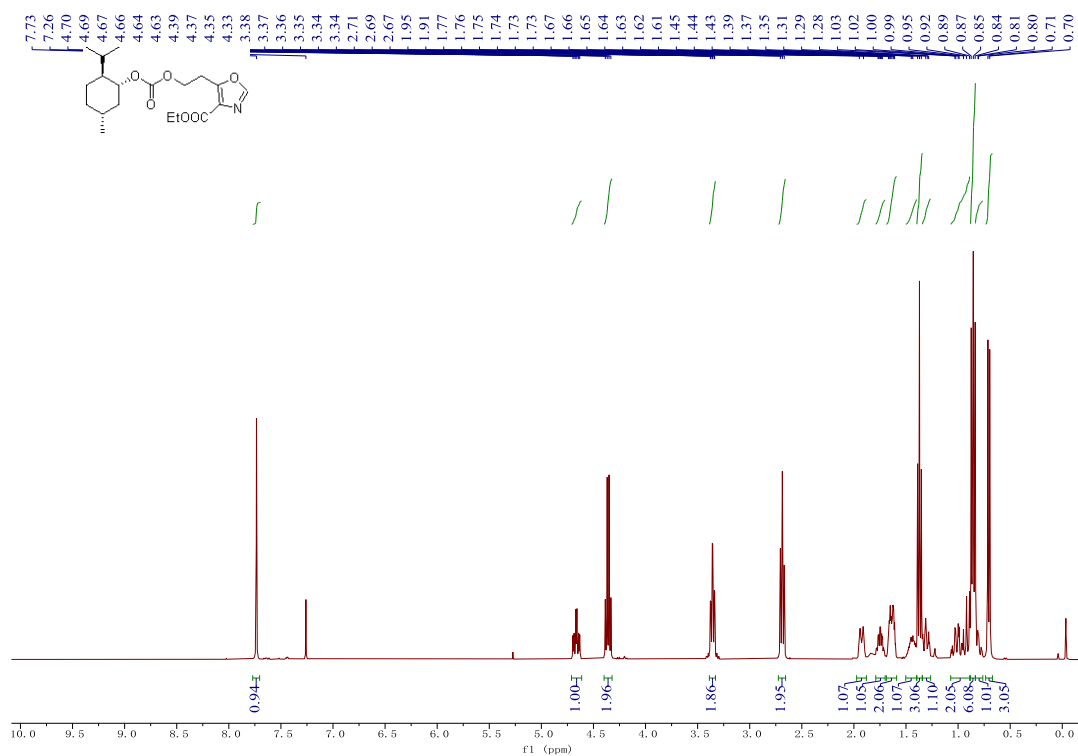
57c ^1H NMR and ^{13}C NMR



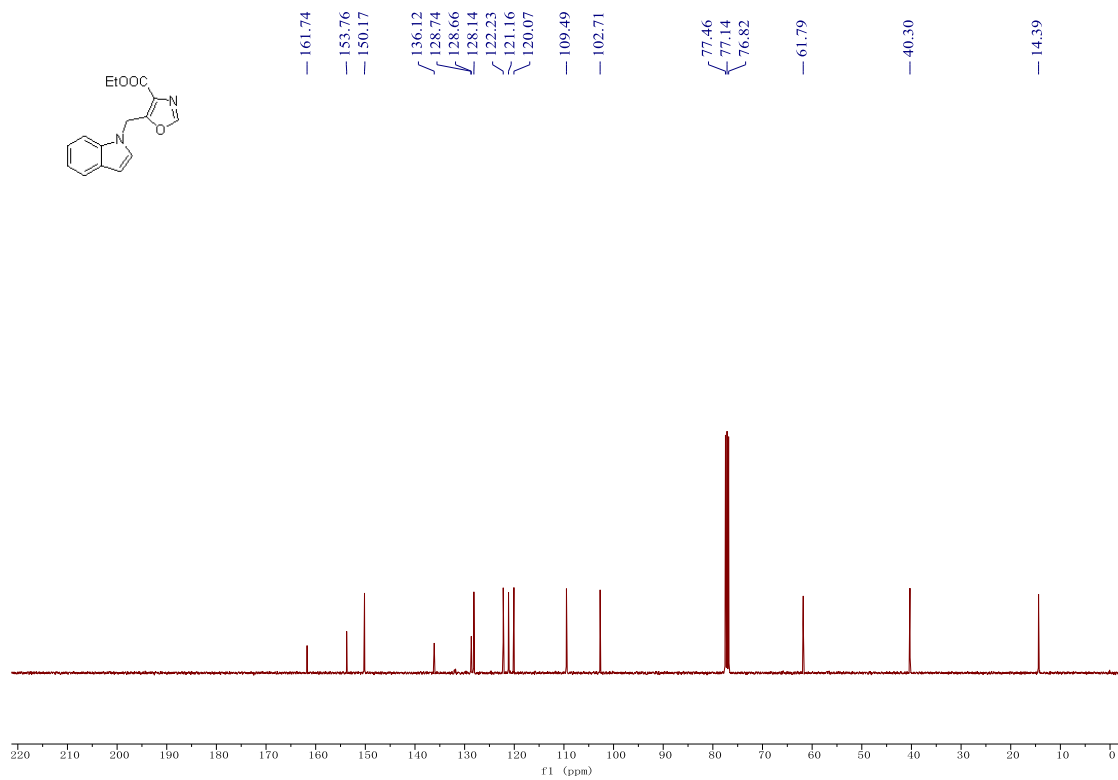
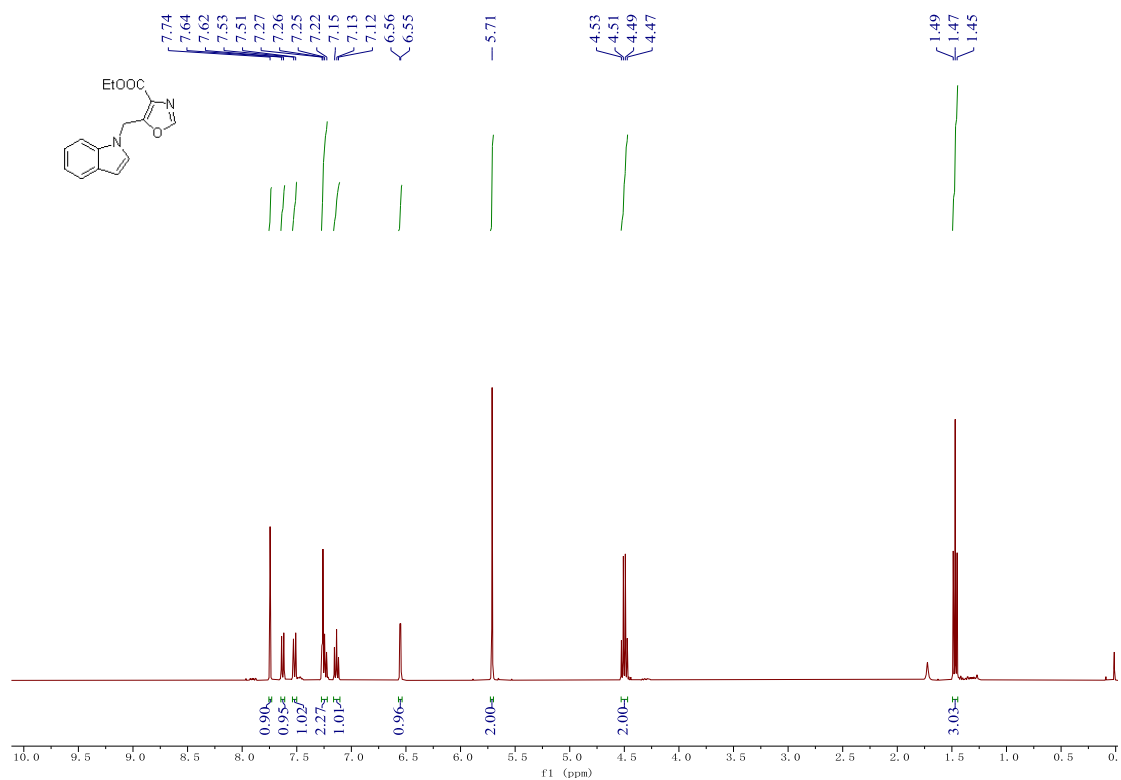
58c ^1H NMR and ^{13}C NMR



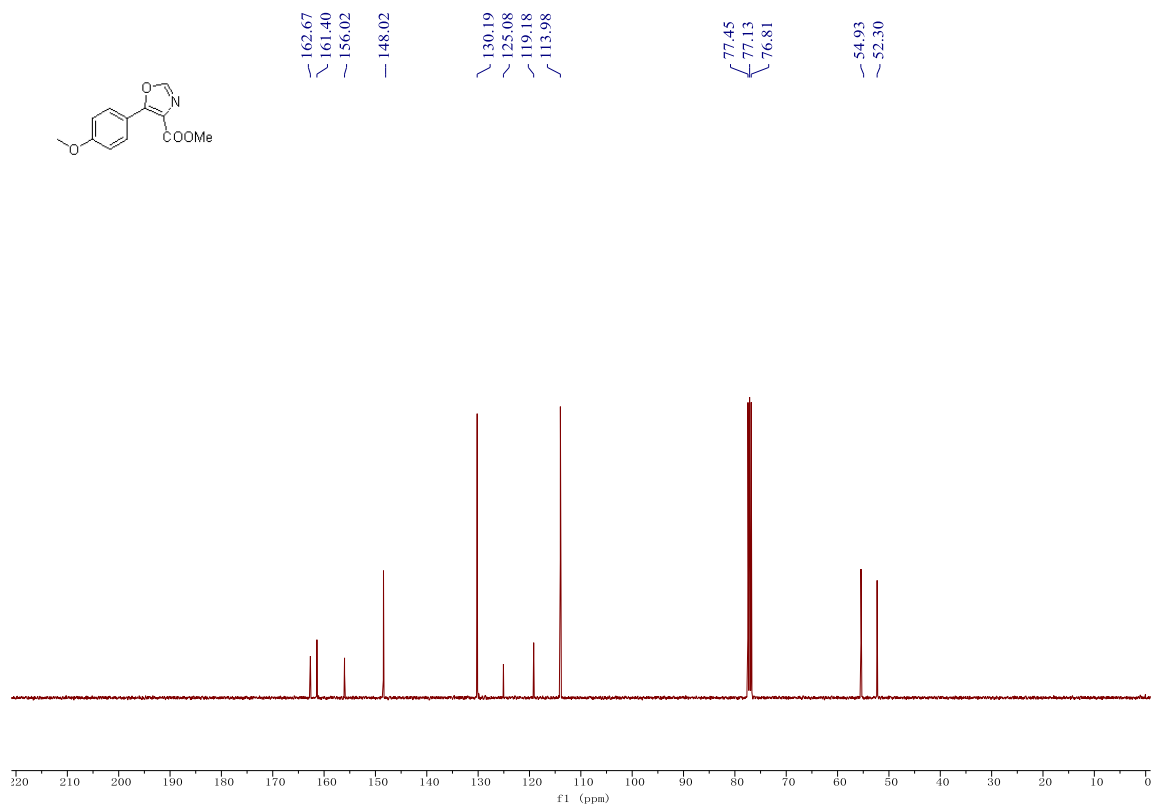
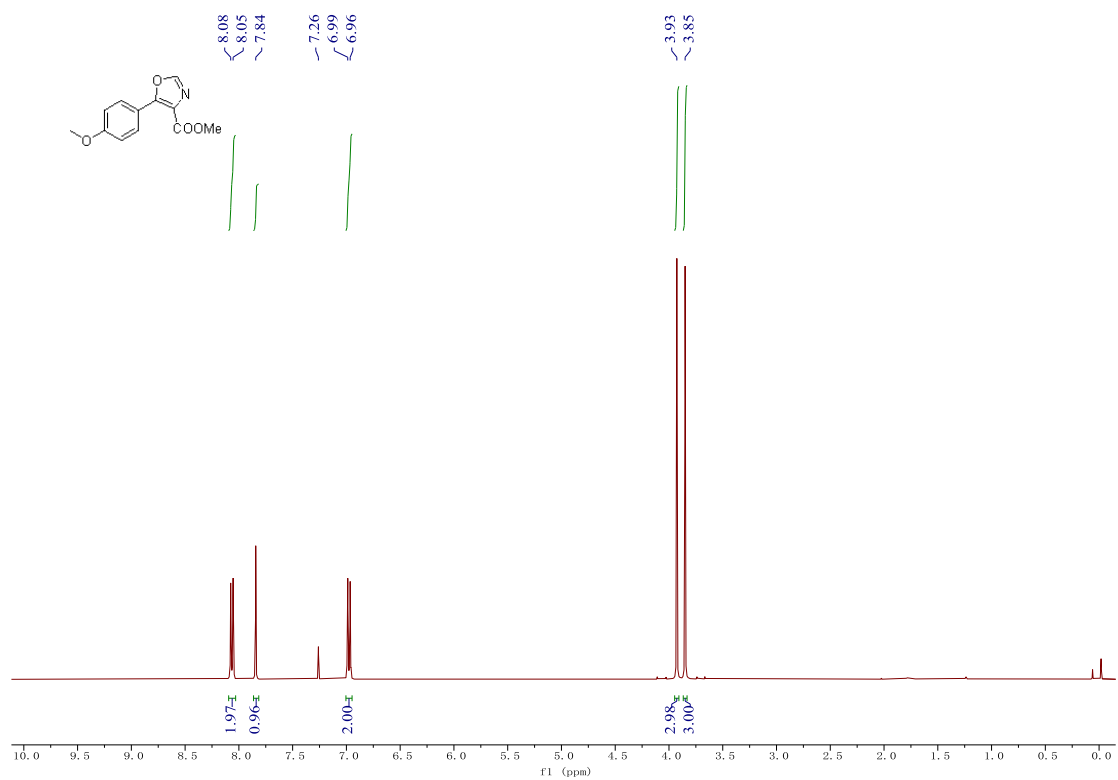
59c ^1H NMR and ^{13}C NMR



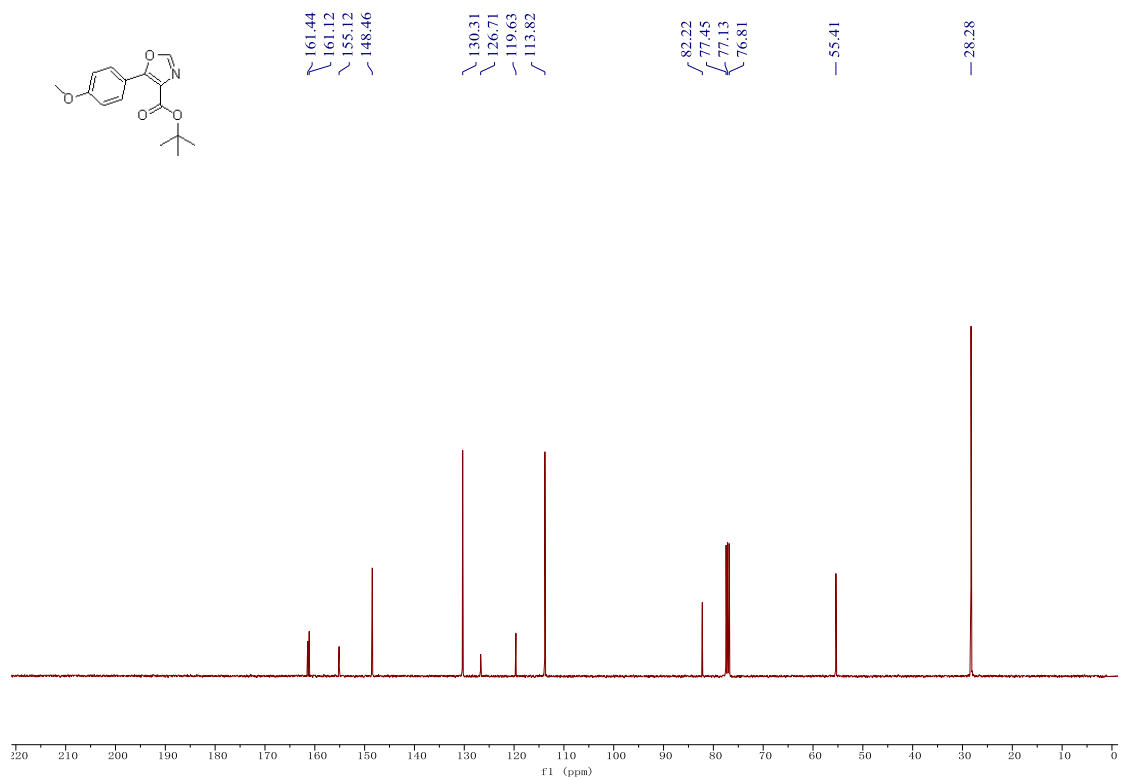
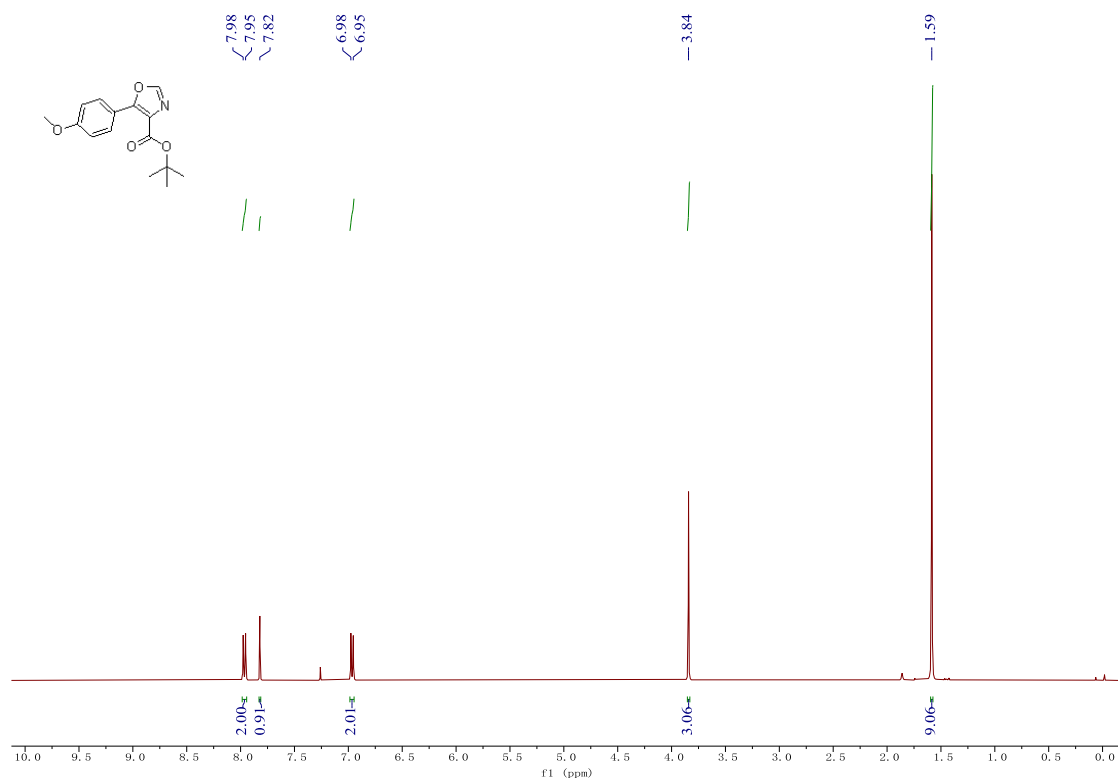
60c ^1H NMR and ^{13}C NMR



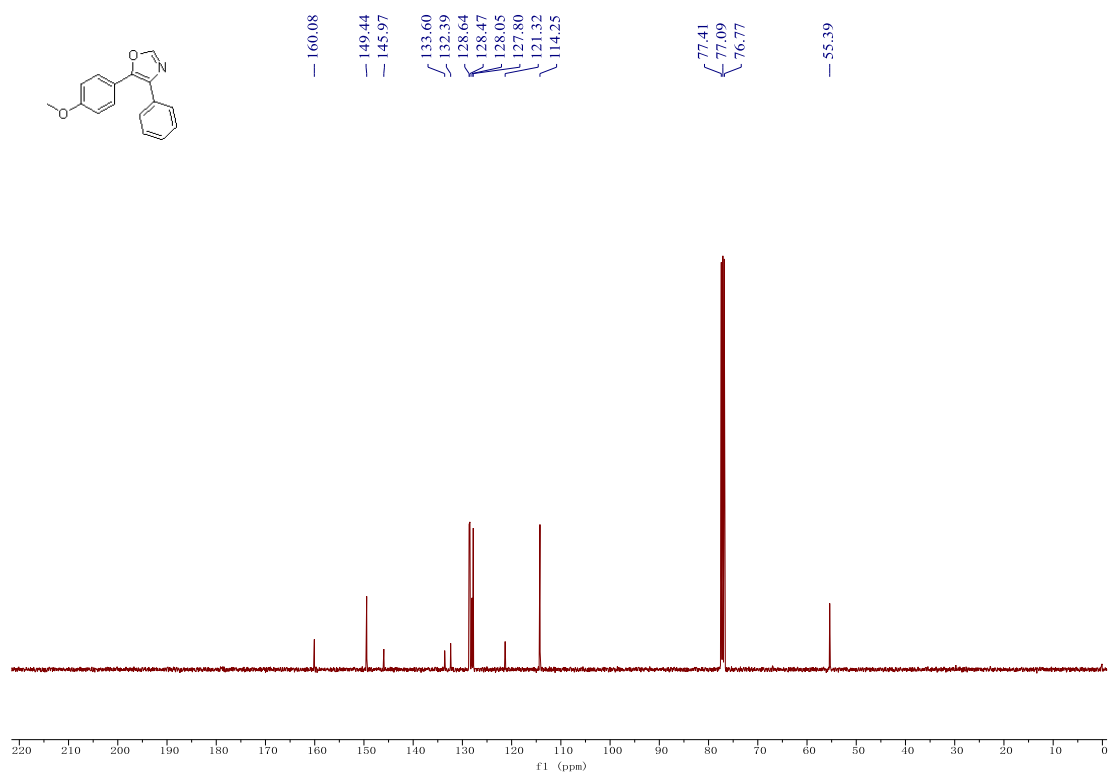
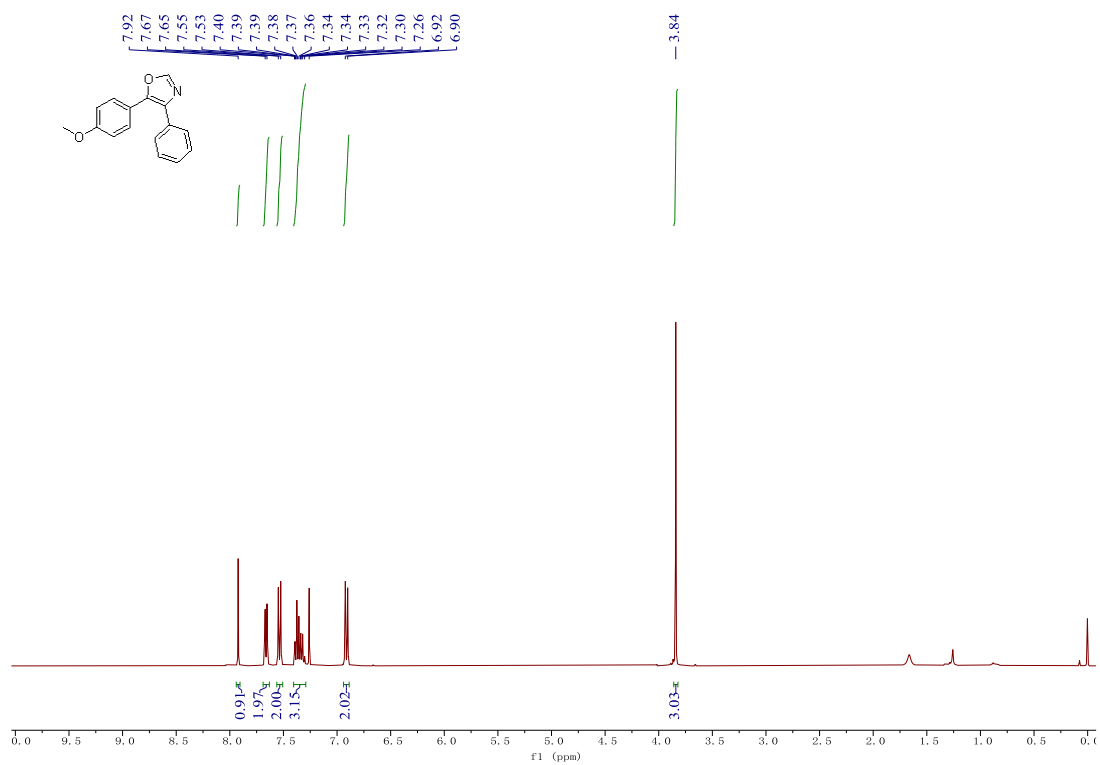
61c ^1H NMR and ^{13}C NMR



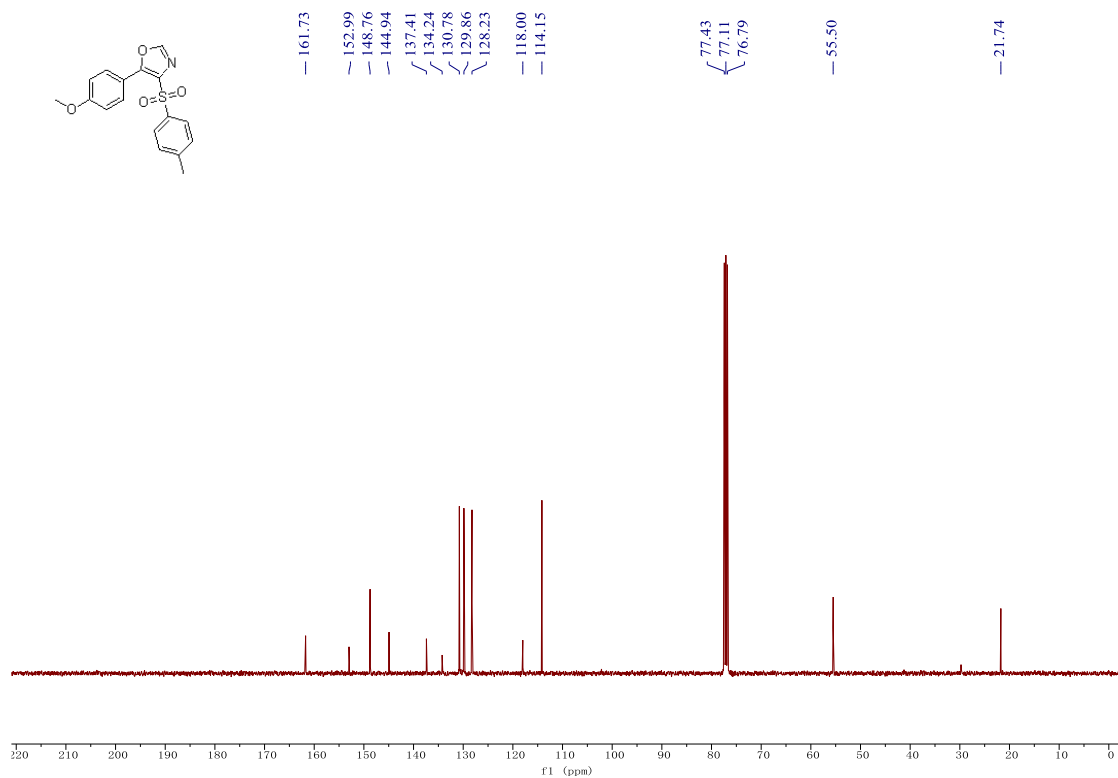
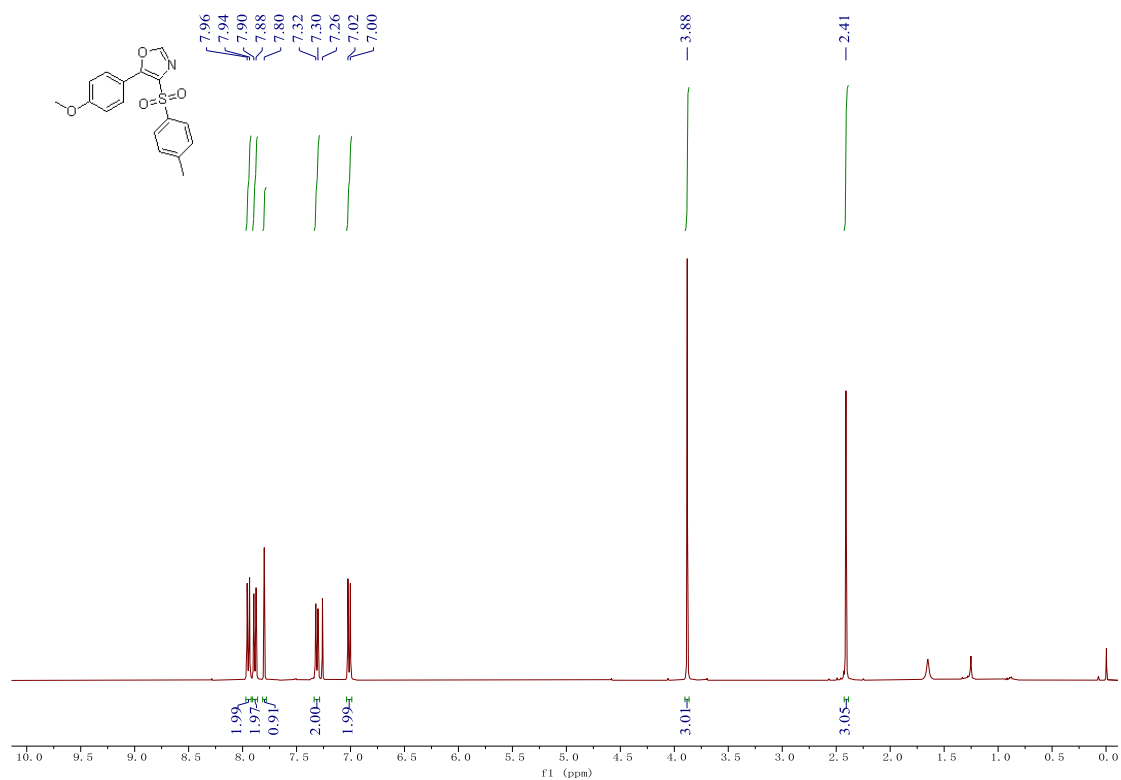
62c ^1H NMR and ^{13}C NMR



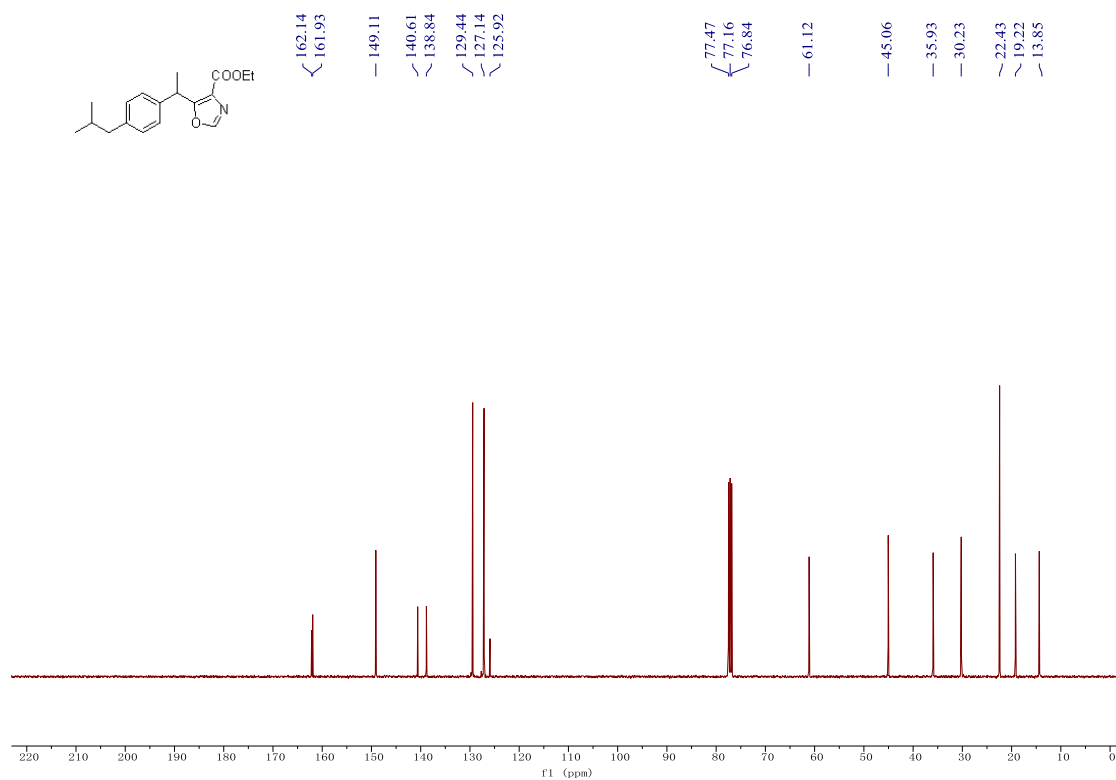
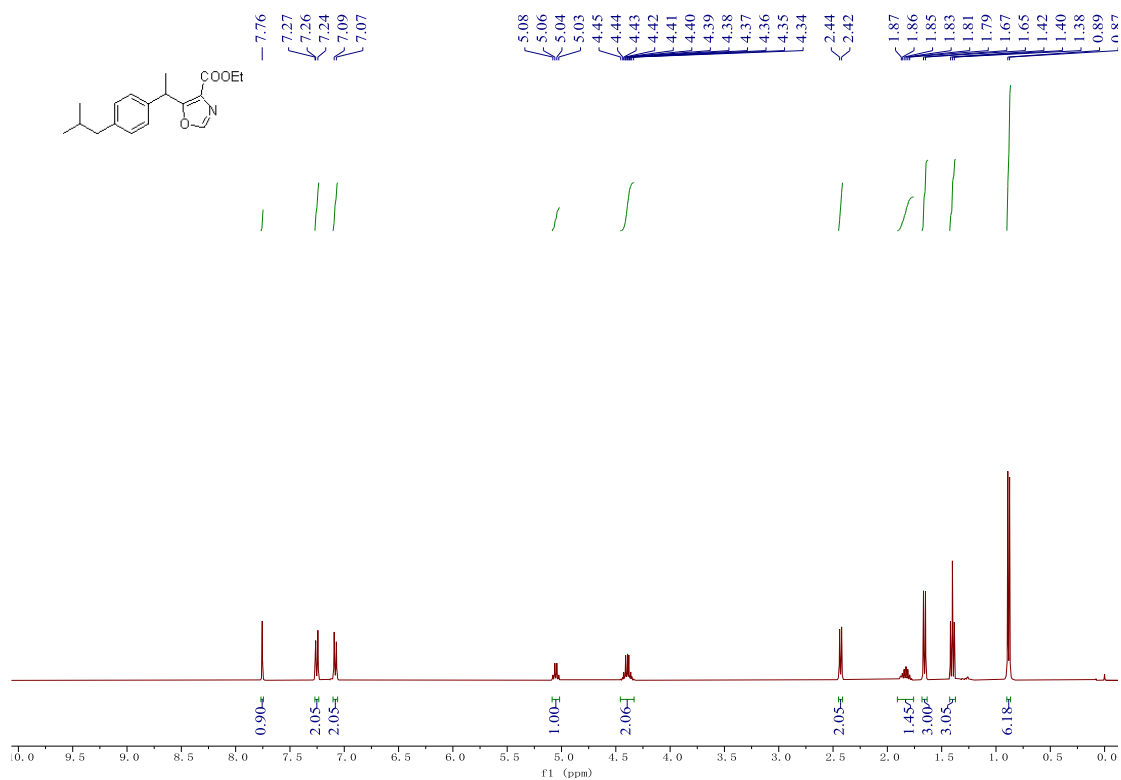
63c ^1H NMR and ^{13}C NMR



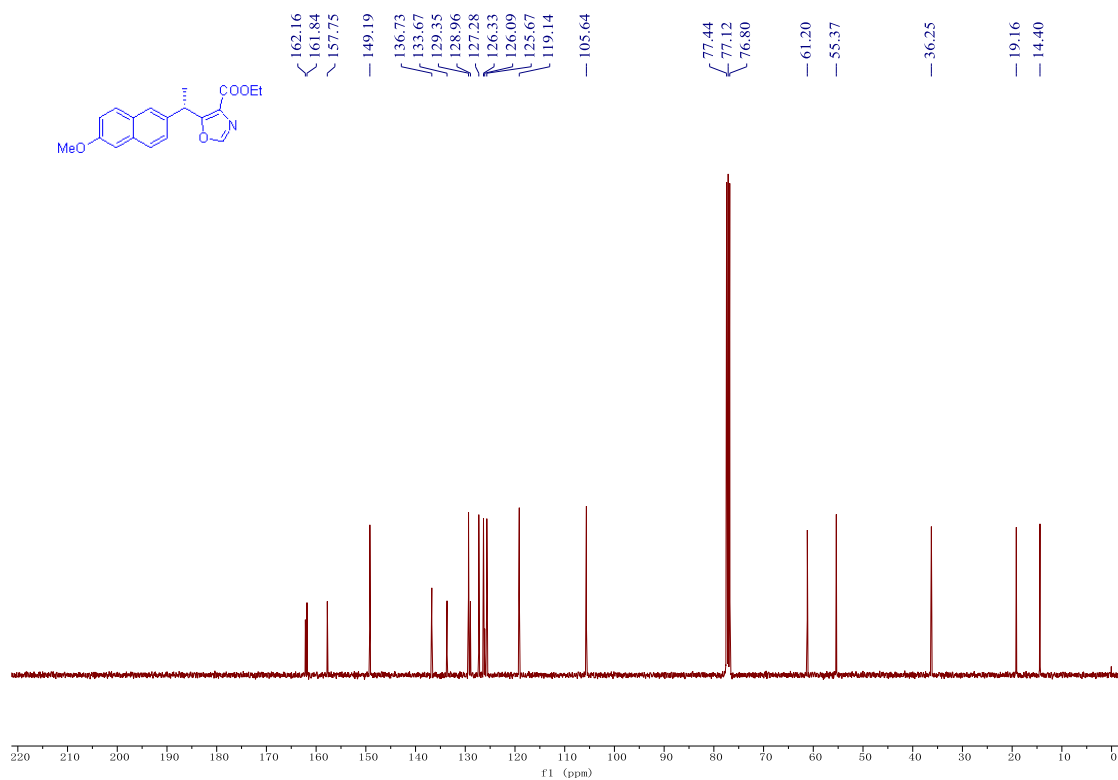
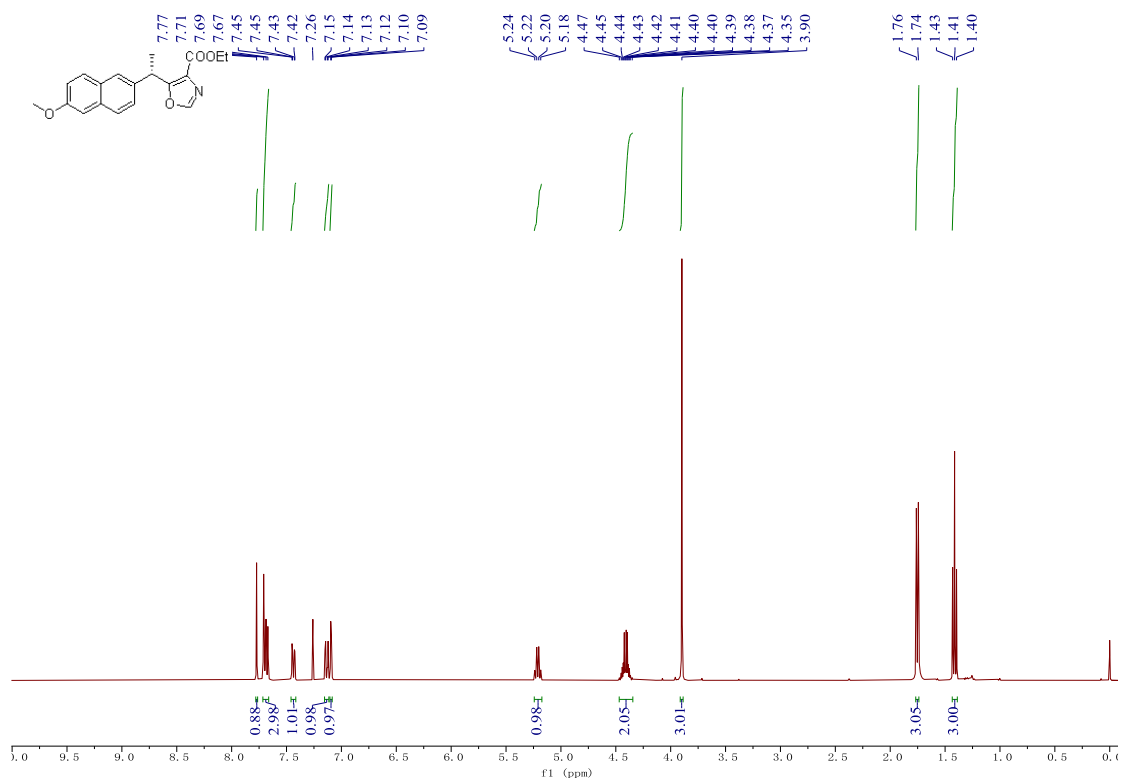
64c ^1H NMR and ^{13}C NMR



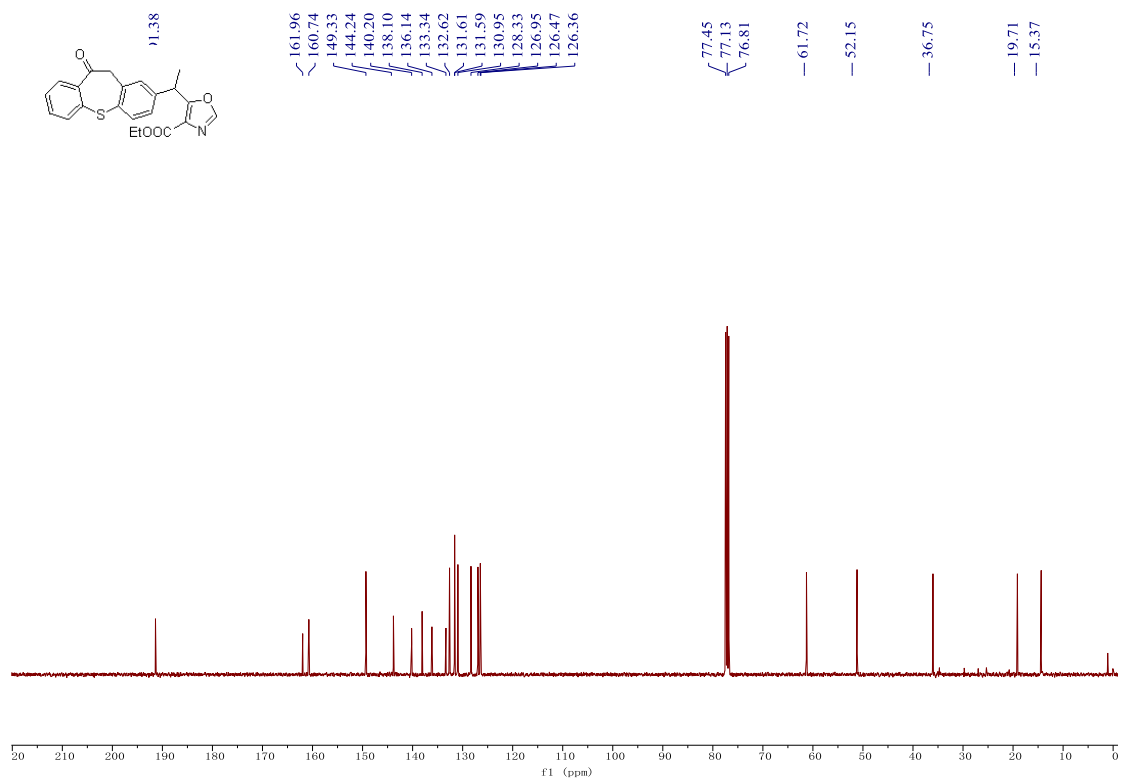
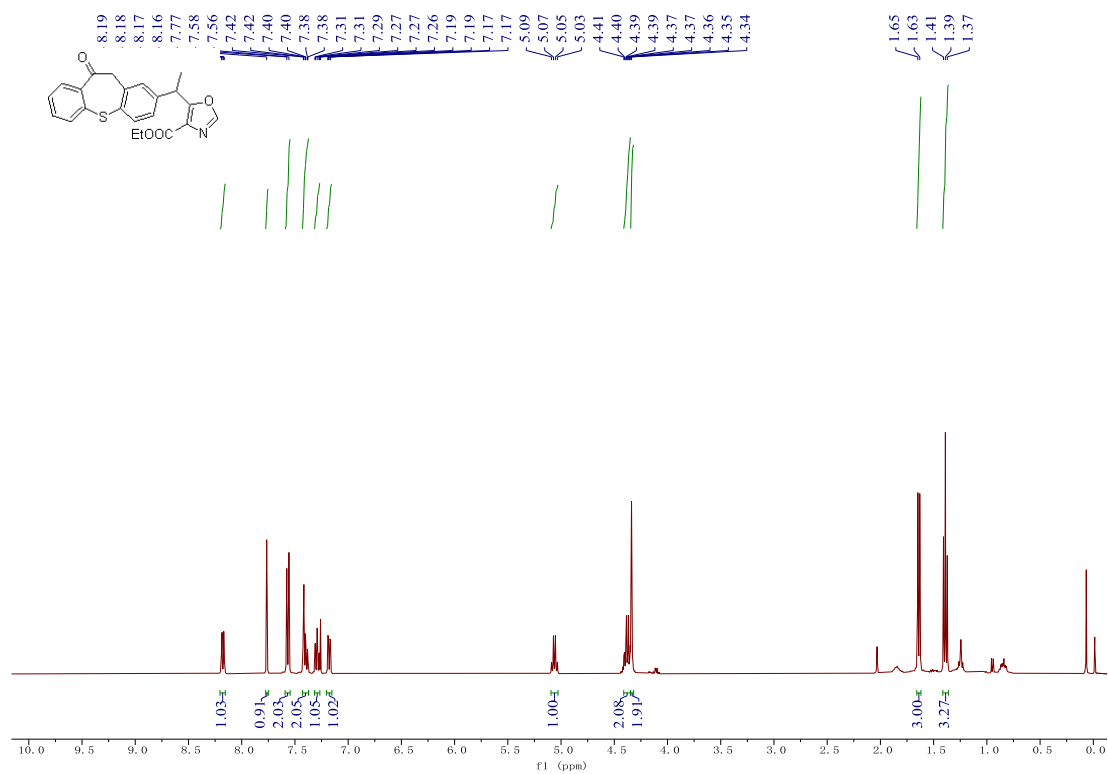
65c ^1H NMR and ^{13}C NMR



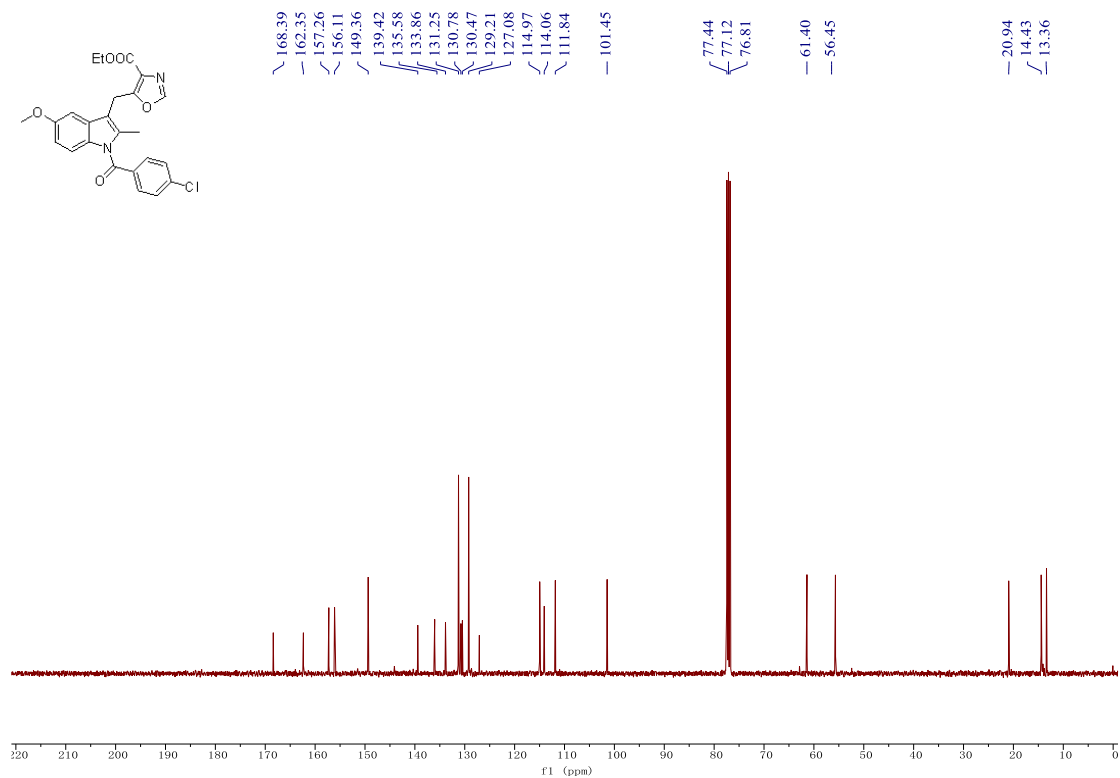
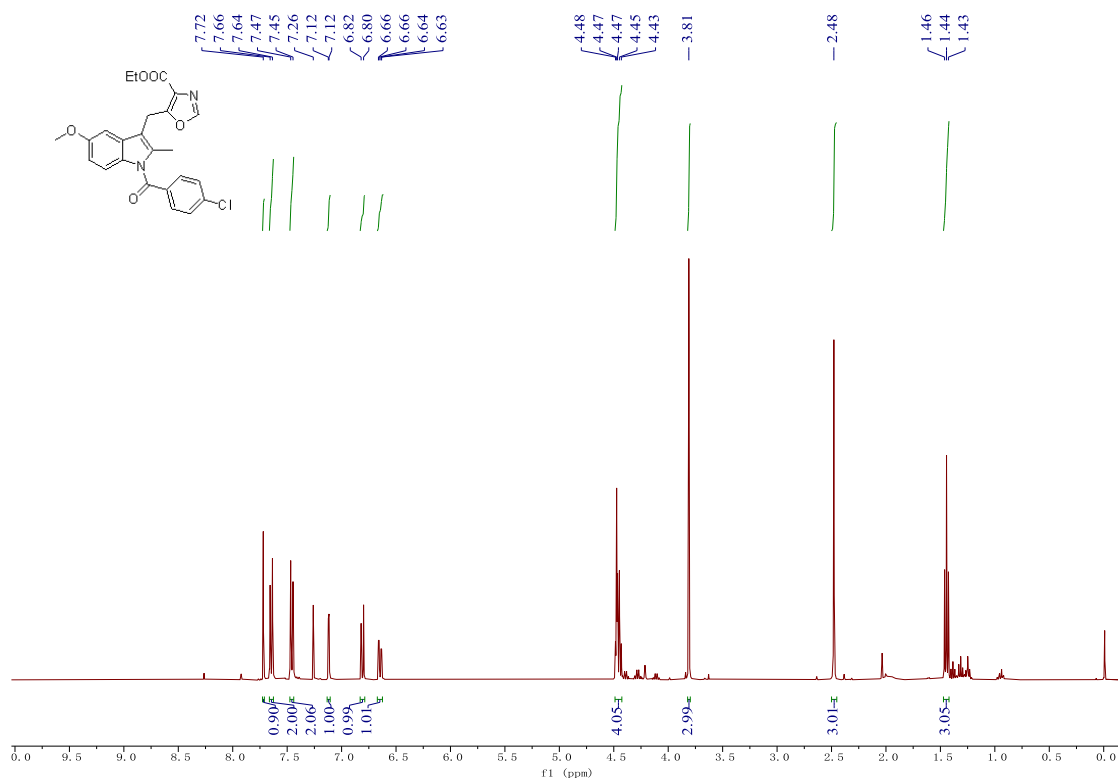
66c ^1H NMR and ^{13}C NMR



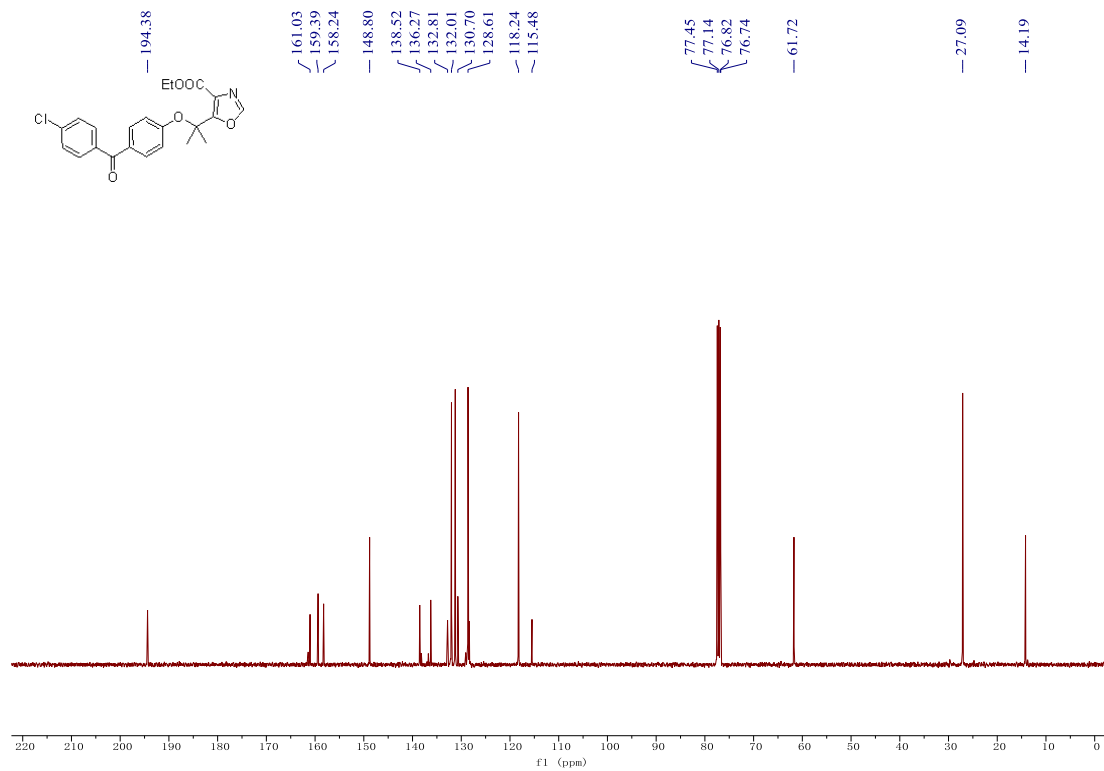
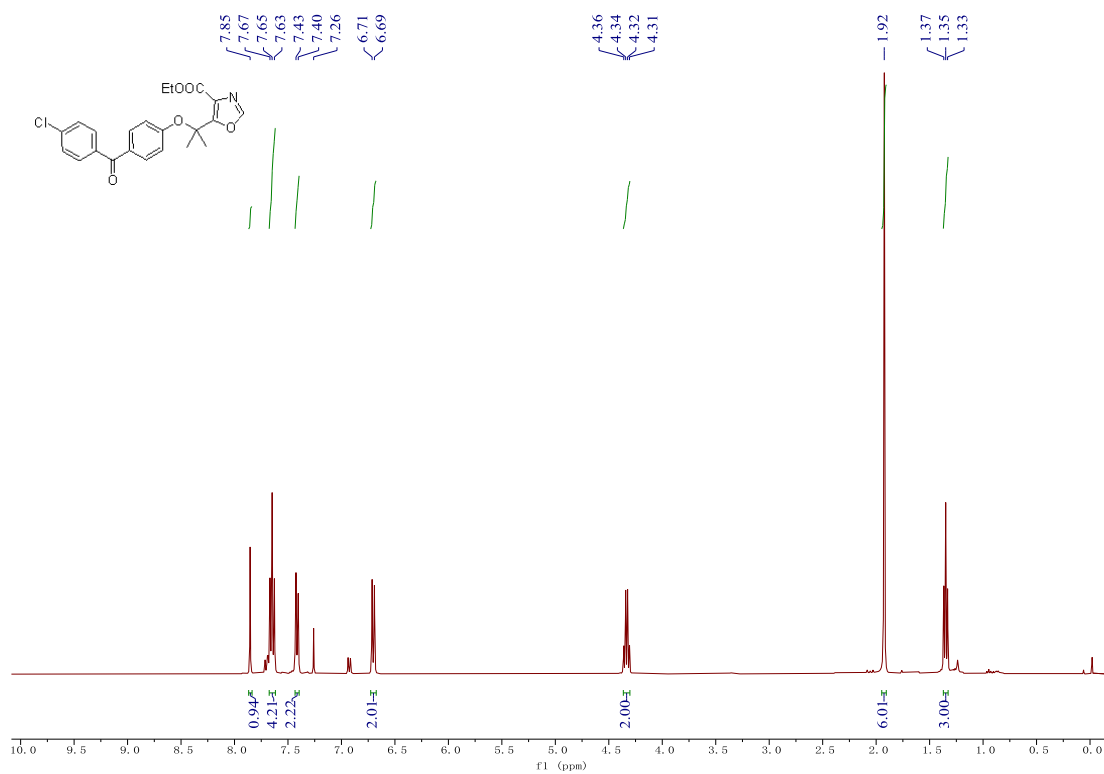
67c ^1H NMR and ^{13}C NMR



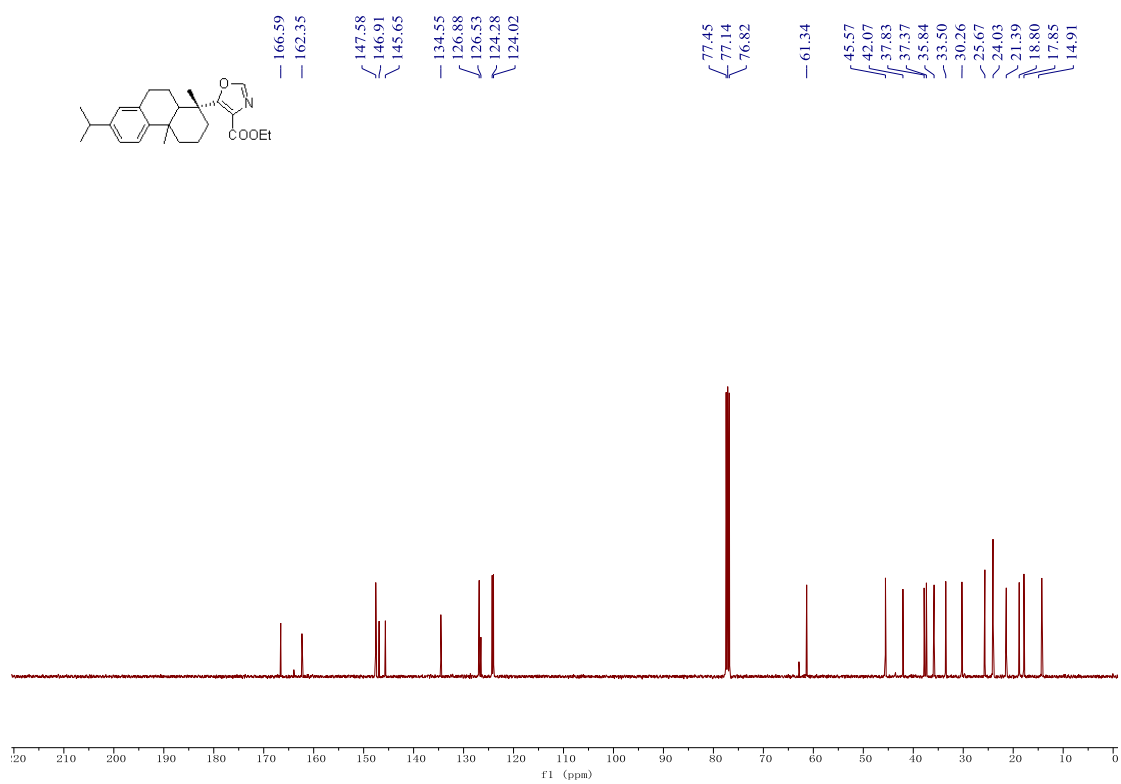
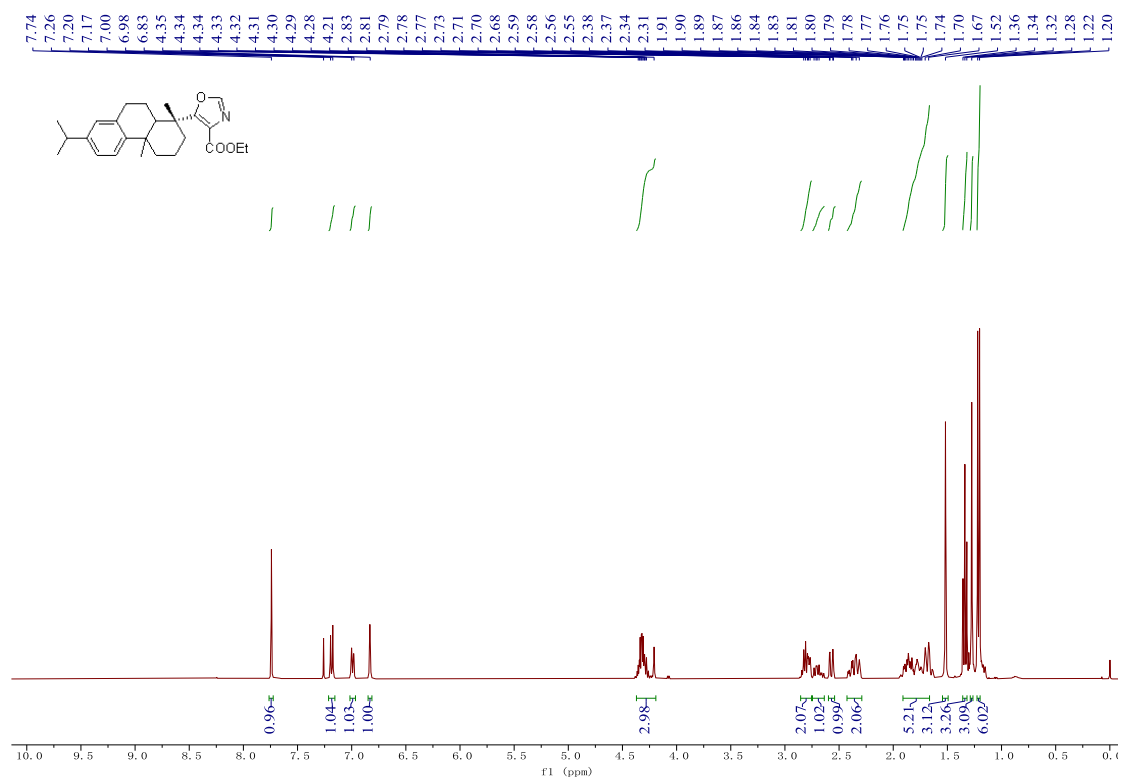
68c ^1H NMR and ^{13}C NMR



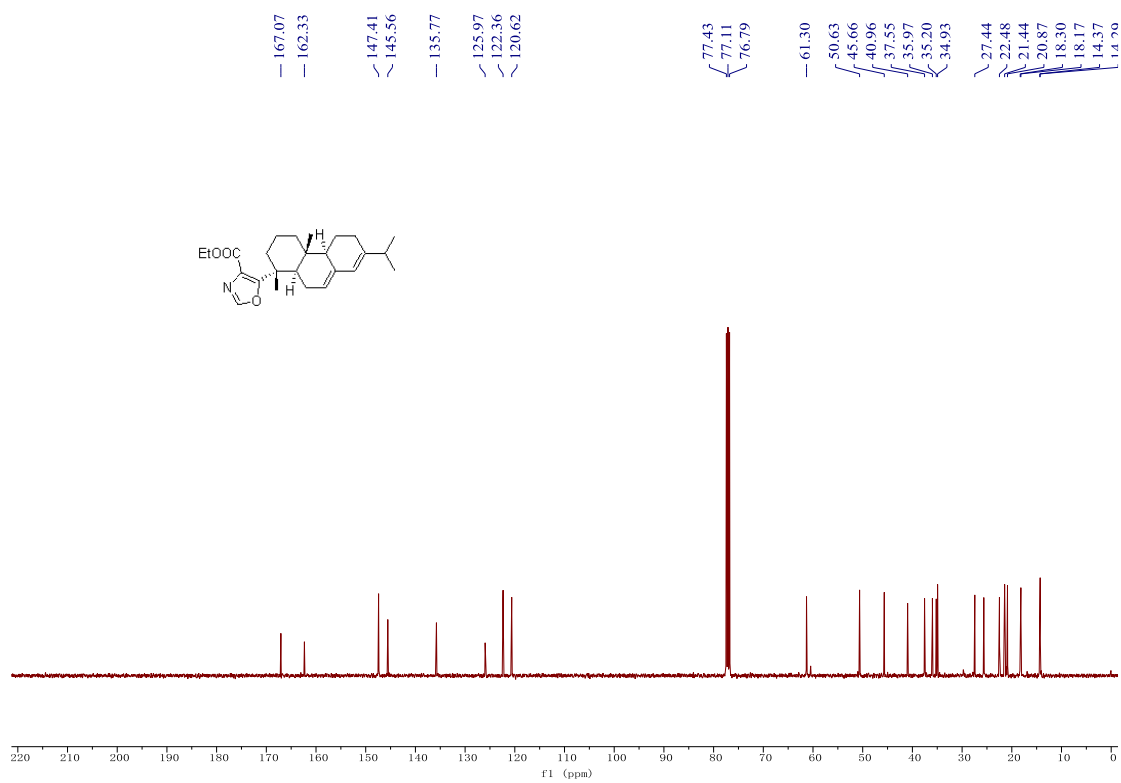
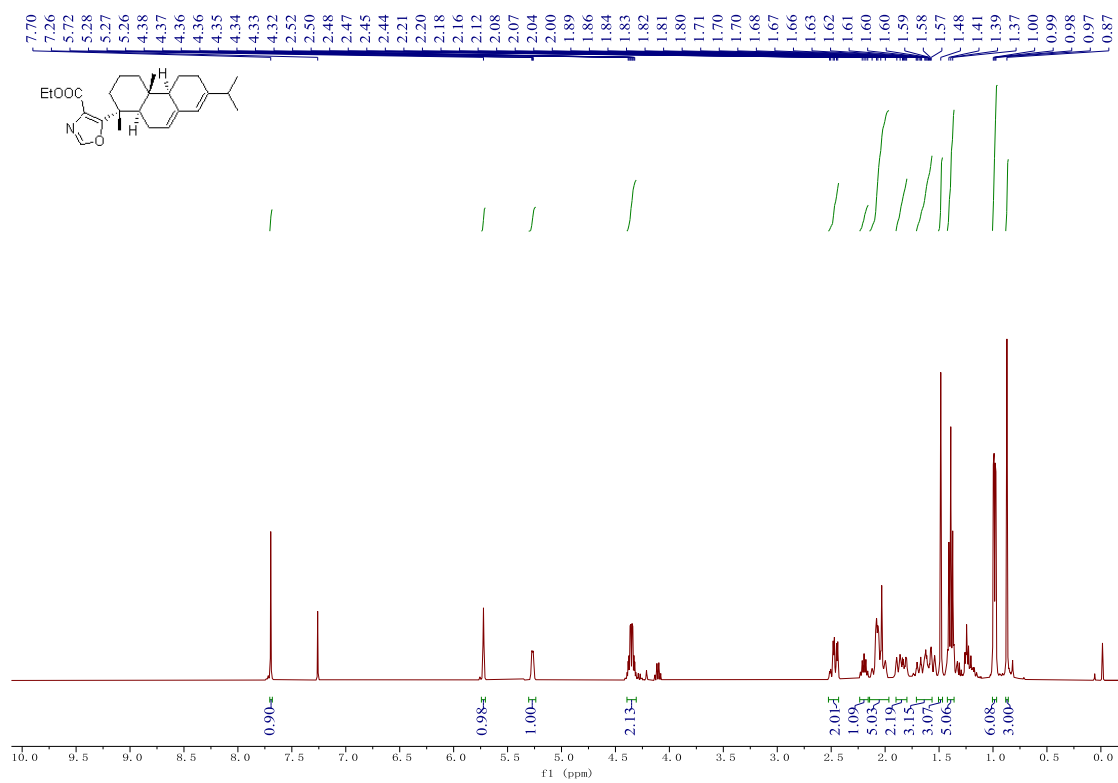
69c ^1H NMR and ^{13}C NMR



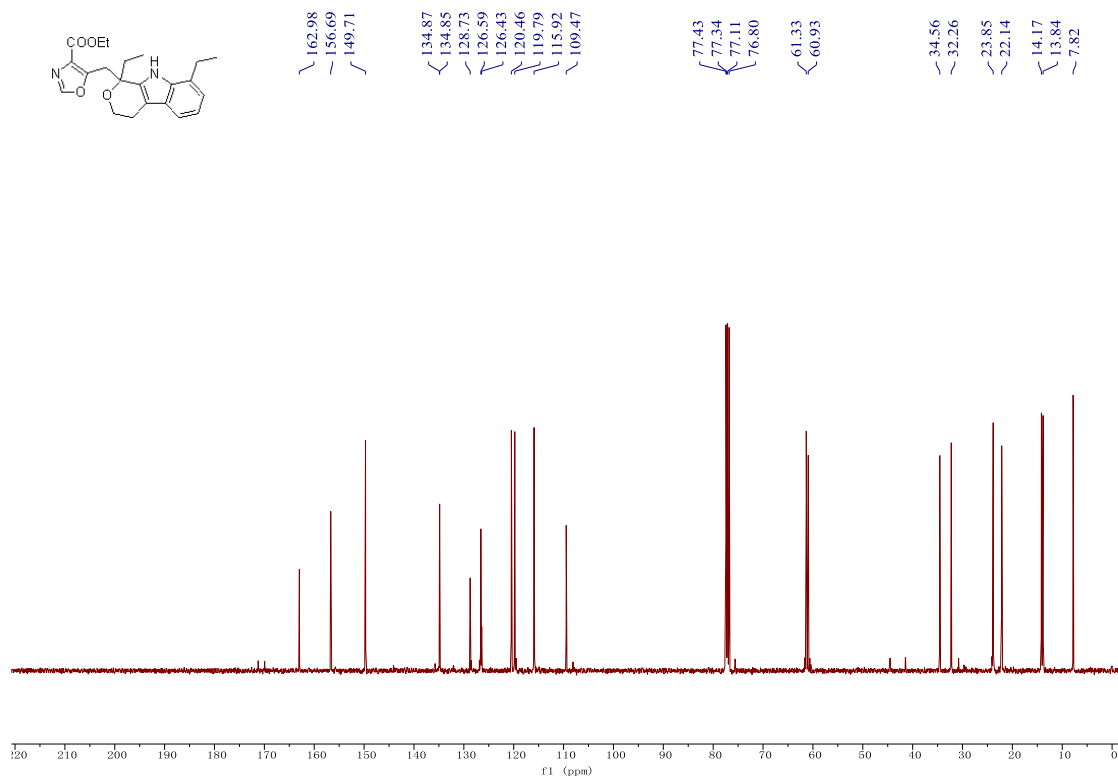
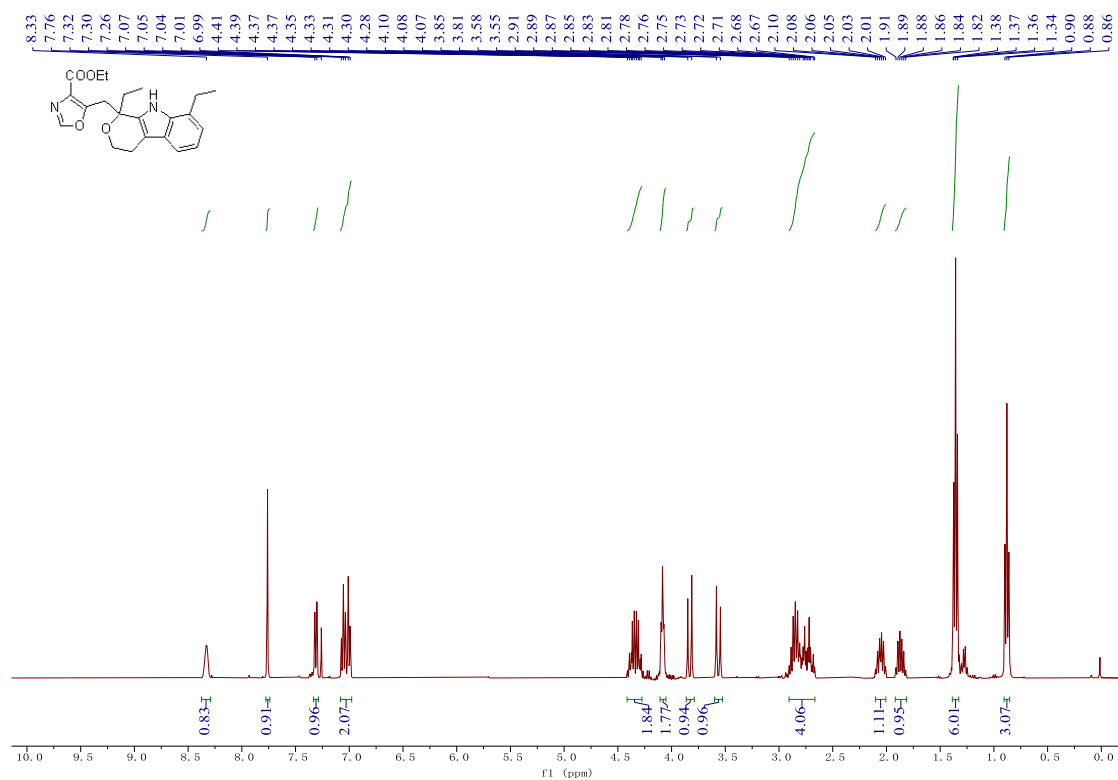
70c ^1H NMR and ^{13}C NMR



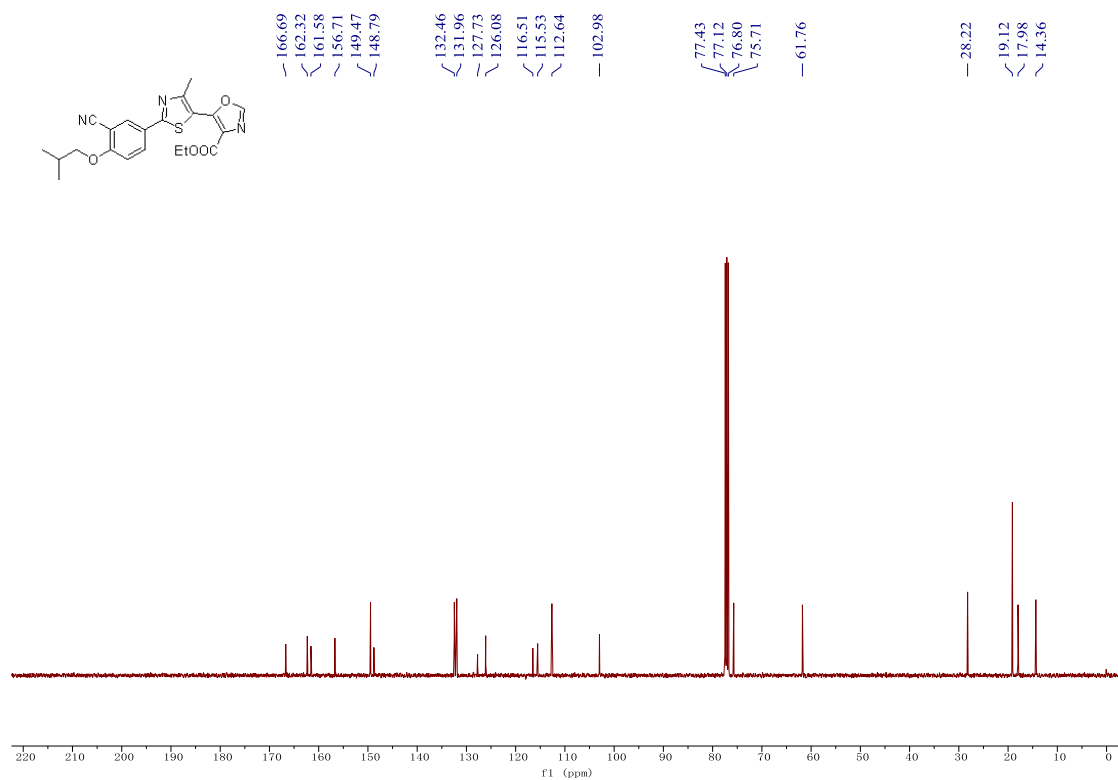
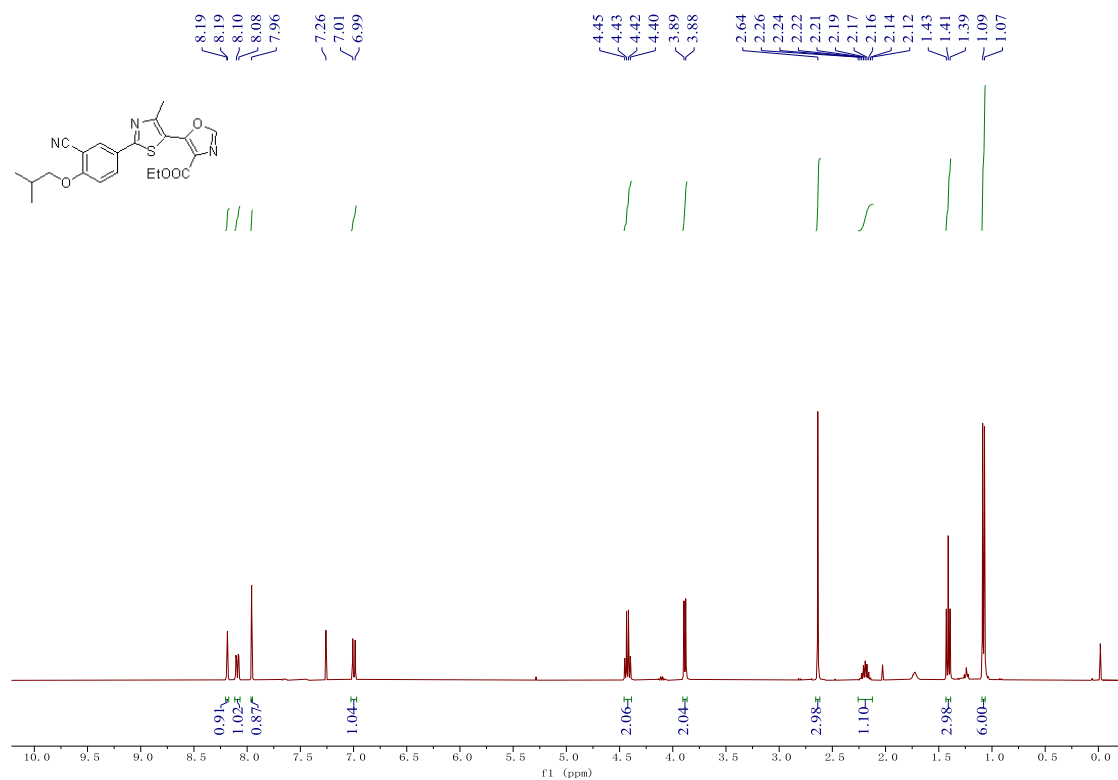
71c ^1H NMR and ^{13}C NMR



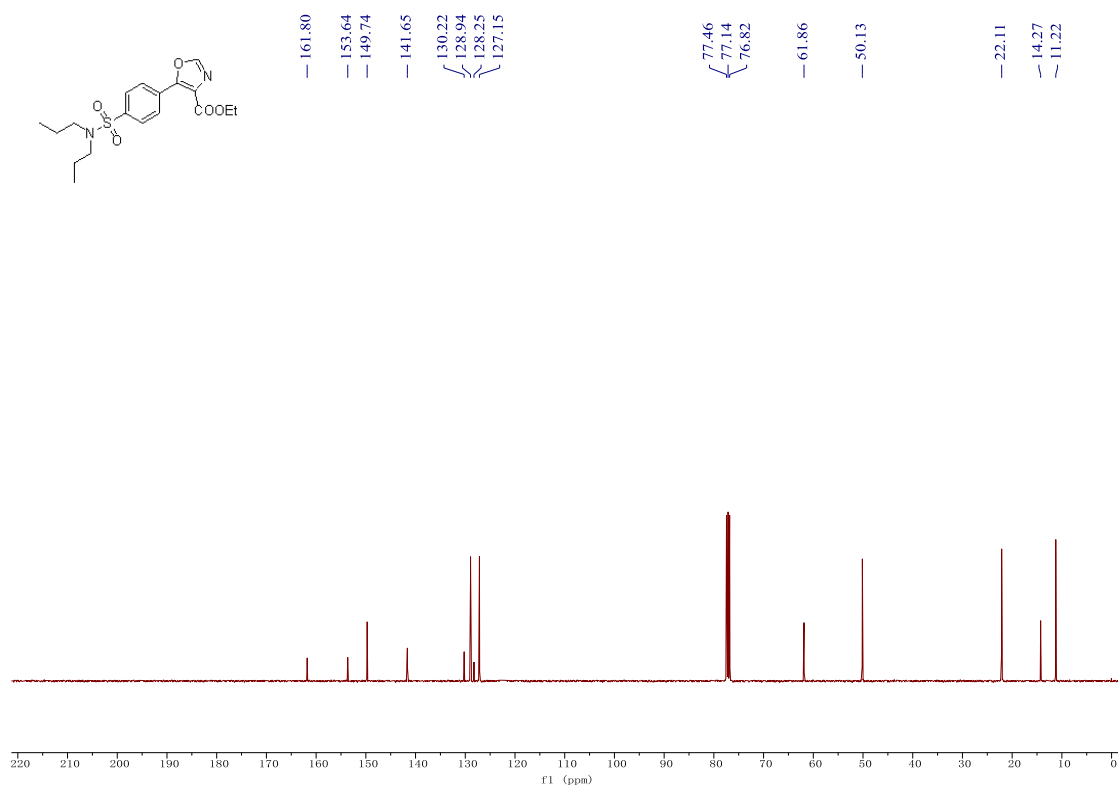
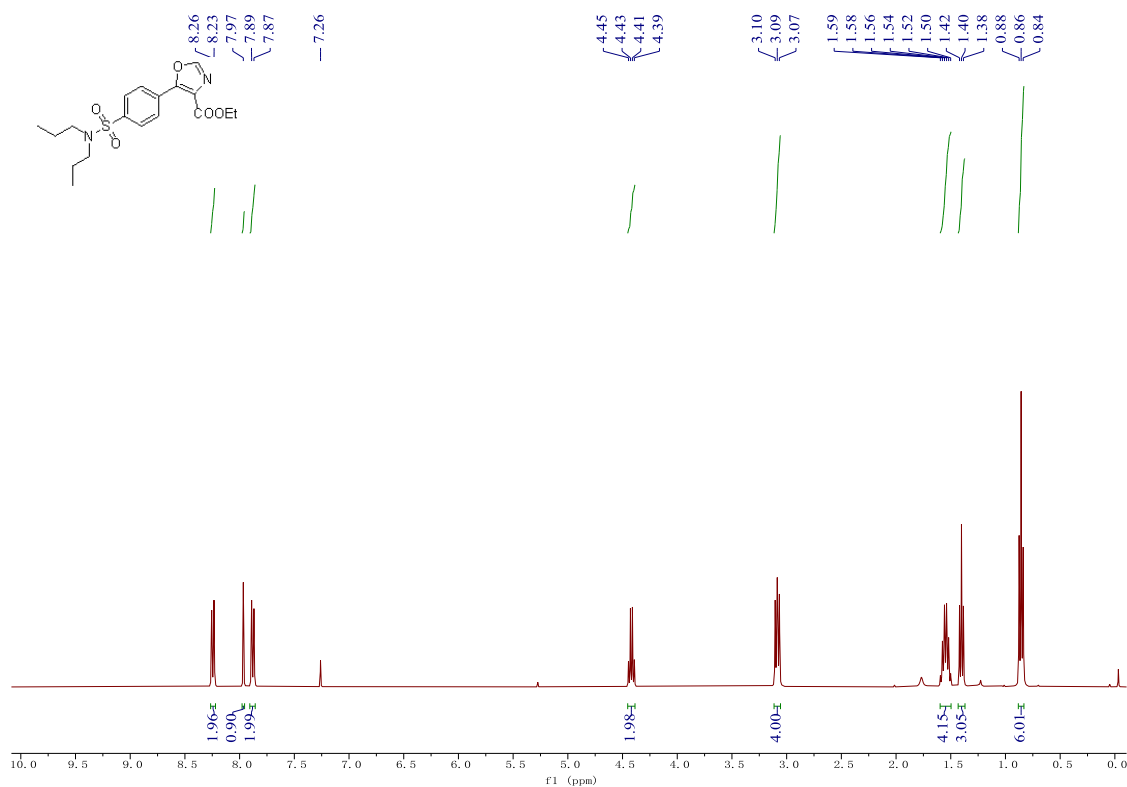
72c ^1H NMR and ^{13}C NMR



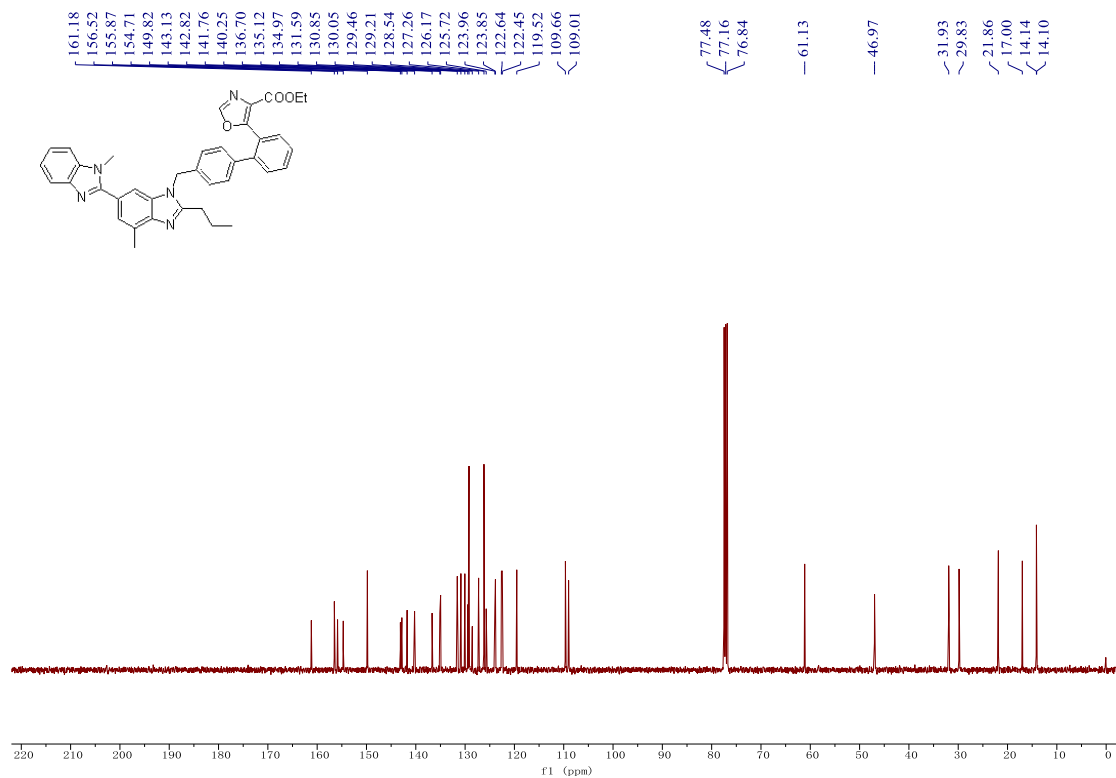
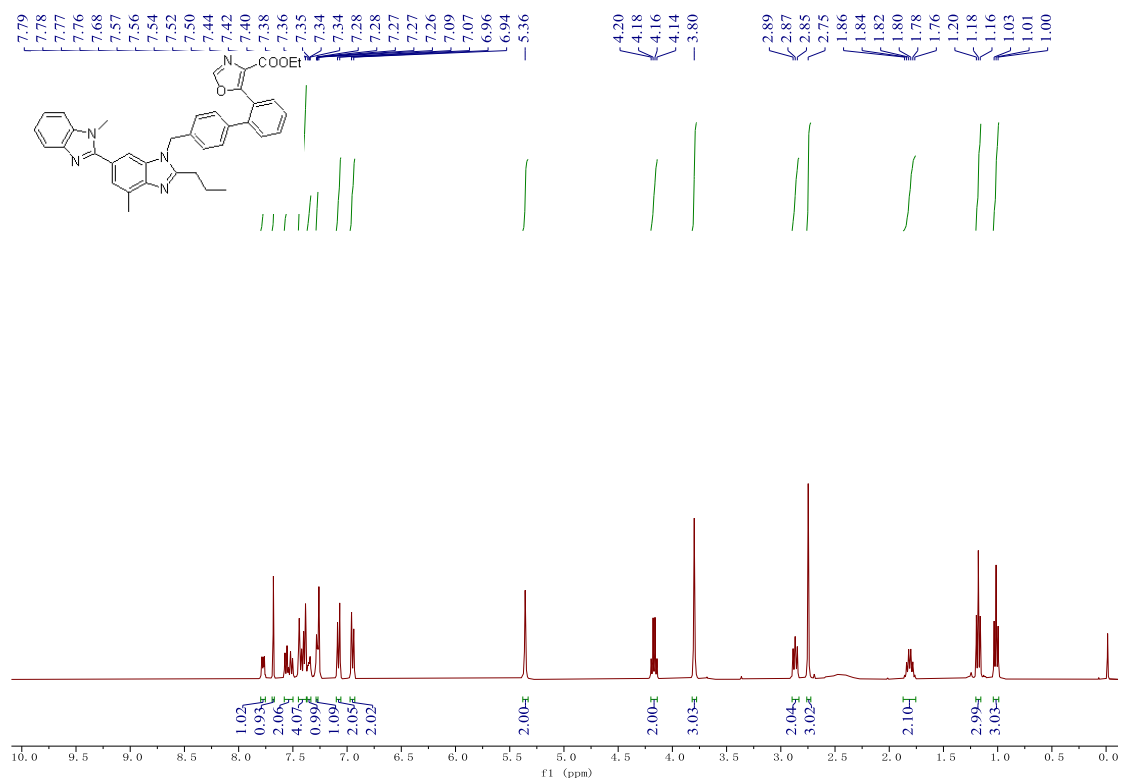
73c ^1H NMR and ^{13}C NMR



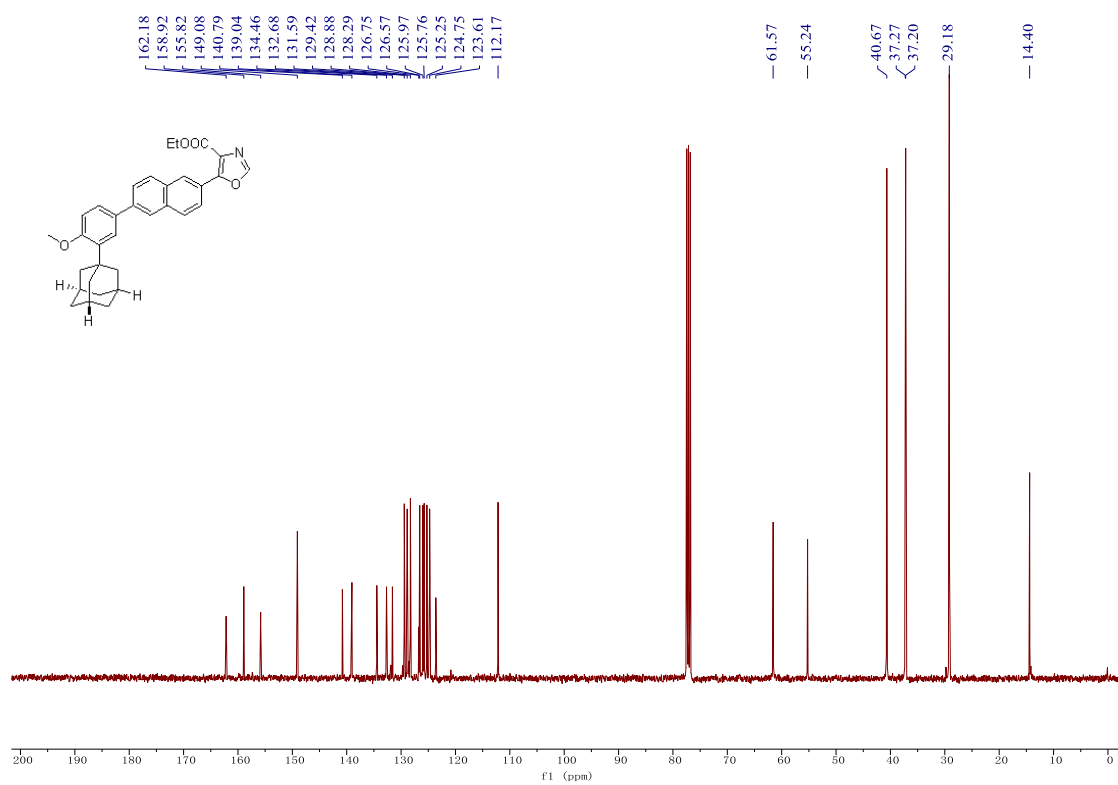
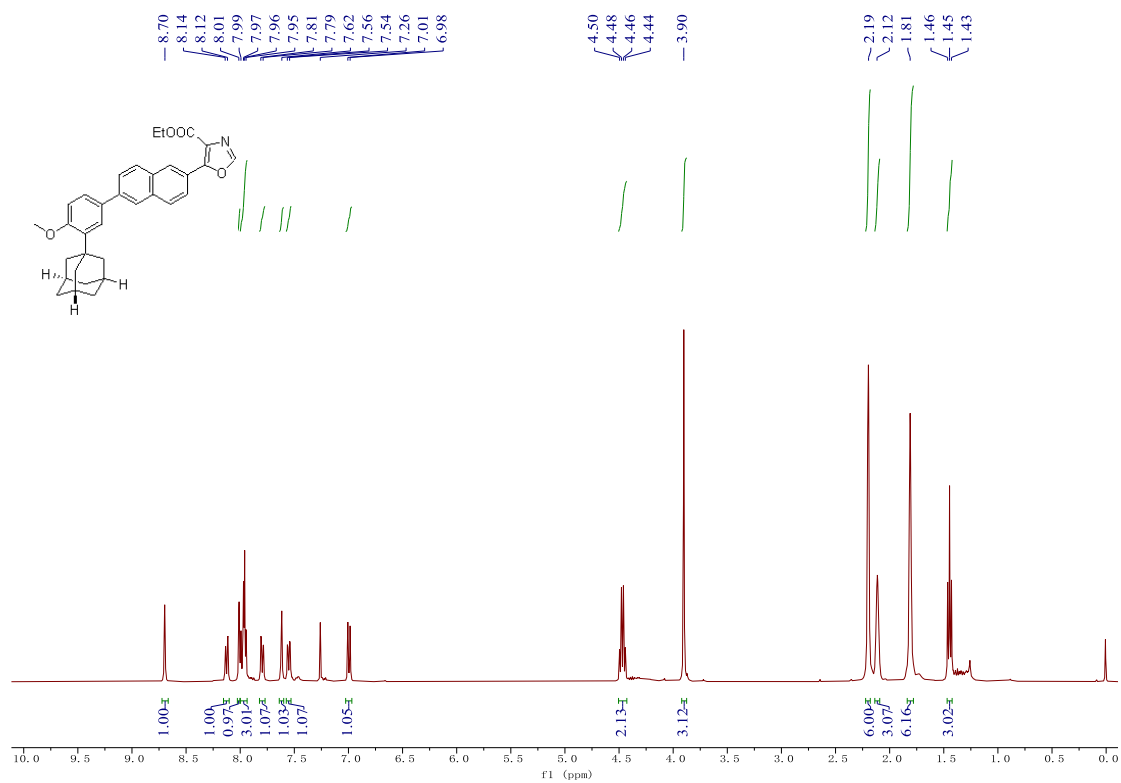
74c ^1H NMR and ^{13}C NMR



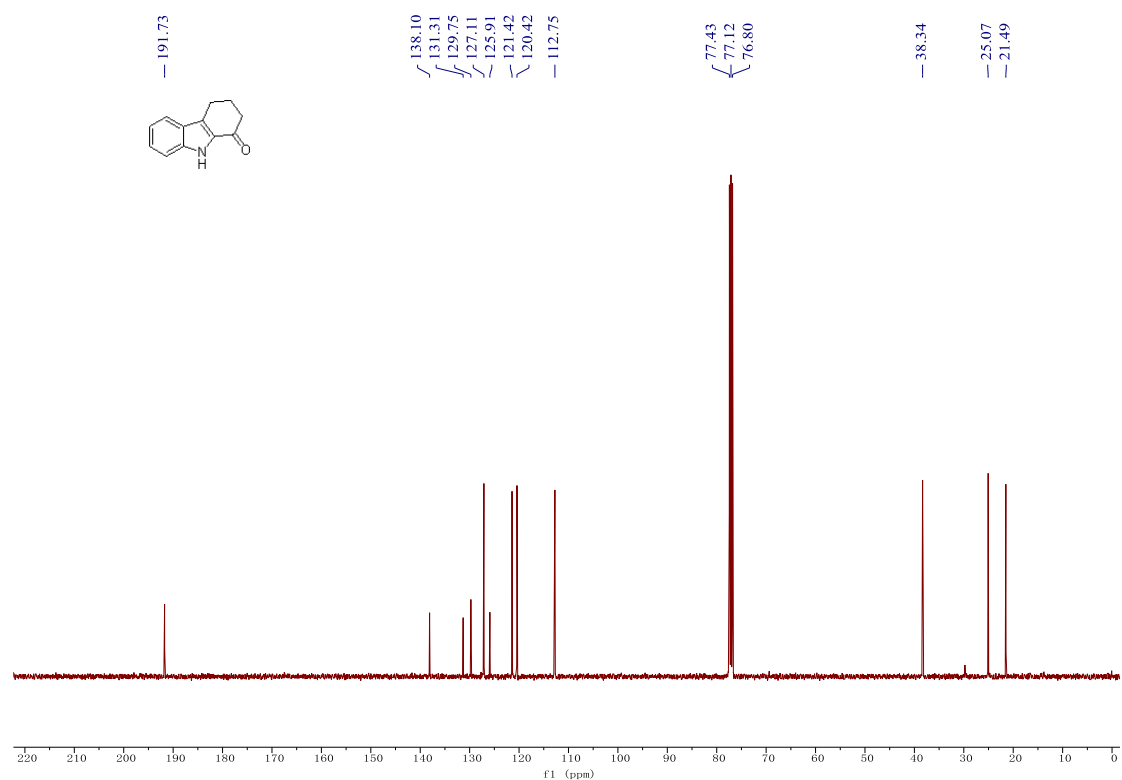
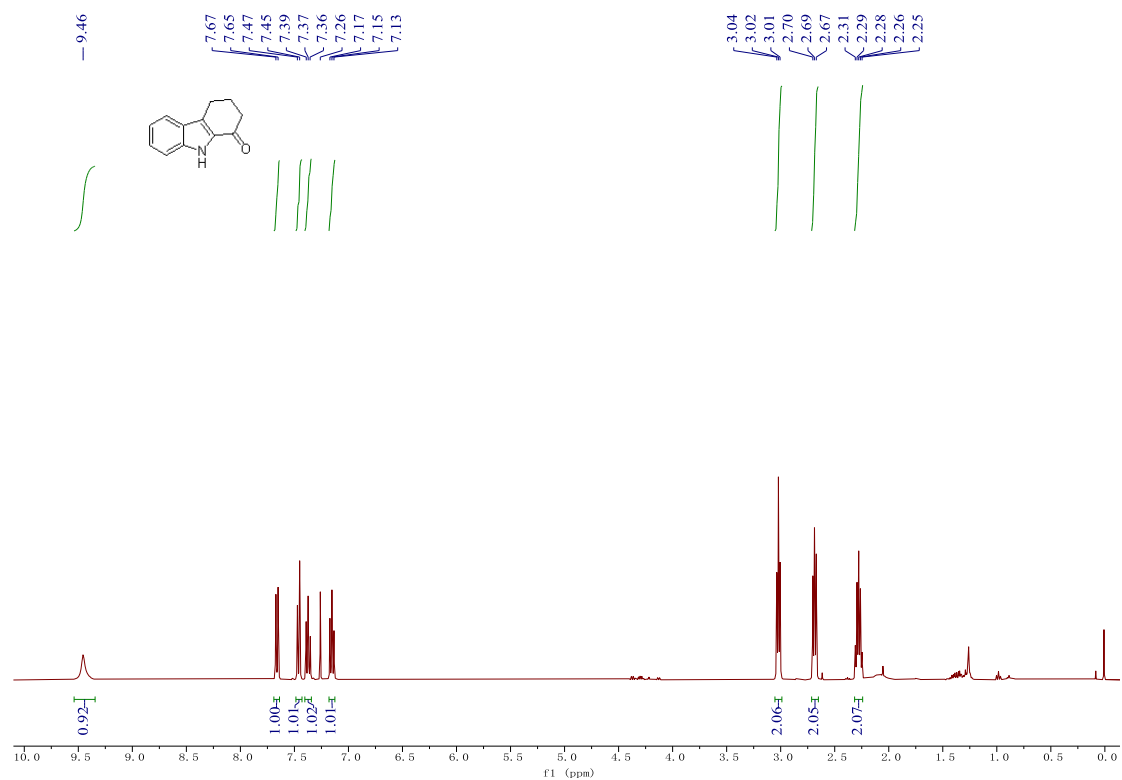
75c ^1H NMR and ^{13}C NMR



76c ^1H NMR and ^{13}C NMR



¹H NMR and ¹³C NMR



h . ^1H NMR and ^{13}C NMR

