Supporting Information

Synthesis of monofluorooxazoles with quaternary C-F centers through photoredox-catalyzed radical addition of methylene-2-oxazolines

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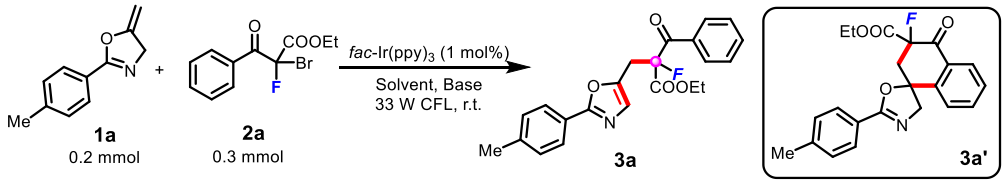
1. General Information

^{1}H and ^{13}C NMR were recorded on a Biotage 400 spectrometer. ^{1}H NMR data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constant (Hz), relative intensity. ^{13}C NMR data are reported as follows: chemical shift in ppm (δ). HPLC-MS analyses were performed on a Shimadzu-2020 LC-MS instrument using the following conditions: Shim-pack VP-ODS C18 column (reverse phase, 50 x 4.6 mm); a linear gradient from 10% water and 90% acetonitrile to 95% acetonitrile and 5% water over 4.0 min; flow rate of 1 mL/min; UV photodiode array detection from 200 to 300 nm. The products were purified by Biotage Isolera™ Spektra Systems and Petroleum Ether/EtOAc solvent systems. All reagents and solvents were obtained from commercial sources and used without further purification. Methylene-2-oxazolines[1] **1a-1o** were prepared according to the literature.

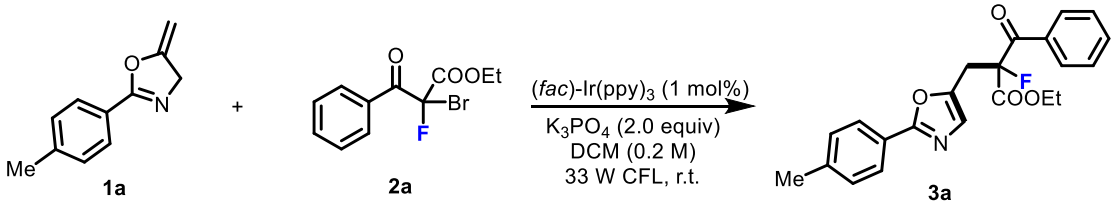
2. Table 1 Optimization of reaction conditions[a]



Entry	Photocatalyst	Solvent	Base	Yield(**3a**)[b]	Yield(**3a'**)[b]
1	*fac*-Ir(ppy)$_3$	CH_2Cl_2	Na_2CO_3	78%	16%
2	*fac*-Ir(ppy)$_3$	$(CH_2)_2Cl_2$	Na_2CO_3	71%	13%
3	*fac*-Ir(ppy)$_3$	DMF	Na_2CO_3	46%	trace
4	*fac*-Ir(ppy)$_3$	DMA	Na_2CO_3	42%	trace
5	*fac*-Ir(ppy)$_3$	THF	Na_2CO_3	75%	<10%
6	*fac*-Ir(ppy)$_3$	MeCN	Na_2CO_3	73%	<10%
7	*fac*-Ir(ppy)$_3$	CH_2Cl_2	K_2CO_3	69%	20%
8	*fac*-Ir(ppy)$_3$	CH_2Cl_2	Cs_2CO_3	47%	17%
9	***fac*-Ir(ppy)$_3$**	**CH_2Cl_2**	**K_3PO_4**	**80%**	**<10%**
10	*fac*-Ir(ppy)$_3$	CH_2Cl_2	KOAc	74%	<10%
11	*fac*-Ir(ppy)$_3$	CH_2Cl_2	$NaBF_4$	48%	trace
12[c]	*fac*-Ir(ppy)$_3$	CH_2Cl_2	K_3PO_4	trace	\
13	\	CH_2Cl_2	K_3PO_4	trace	\
14	*fac*-Ir(ppy)$_3$	CH_2Cl_2	\	<20%	\
15	$[Ru(bpy)_3]PF_6$	CH_2Cl_2	K_3PO_4	trace	\
16	$[IrdF(CF_3)(ppy)_2(dtbbpy)]PF_6$	CH_2Cl_2	K_3PO_4	<10%	\
17	Eosin Y	CH_2Cl_2	K_3PO_4	trace	\
18[d]	*fac*-Ir(ppy)$_3$	CH_2Cl_2	K_3PO_4	69%	trace
19[e]	*fac*-Ir(ppy)$_3$	CH_2Cl_2	K_3PO_4	77%	<10%
20[f]	*fac*-Ir(ppy)$_3$	CH_2Cl_2	K_3PO_4	72%	<10%

[a]Unless otherwise noted, all reactions were performed with **1a** (0.2 mmol), **2a** (0.3 mmol), base (0.4 mmol) and photocatalyst (1.0 mol%) in solvent (1.0 mL) under 33W fluorescent light bulb at room temperature for 12 h. [b]Isolated yield based on **1a**. [c]In the dark. [d]With blue LEDs. [e]In solvent (2.0 mL). [f]In solvent (0.5 mL).

3. General Procedure for Synthesis of Monofluorinated Oxazoles



Methylene-2-oxazoline [1] **1a** (34 mg, 0.2 mmol, 1 eq.), monofluorobromoacetophenone[2] **2a** (87 mg, 0.3 mmol, 1.5 eq), *fac*-Ir(ppy)$_3$ (1.3 mg), K_3PO_4 (84 mg, 0.4 mmol, 2 eq.) were added to a flame-dried Schlenk flask containing a stirring bar and purged by evacuating the flask and backfilling with argon three times. In the absence of light, anhydrous DCM (1 mL, 0.2 M) was added and the flask was sealed. The mixture was then stirred under irradiation from 33 W CFL and the distance between the reaction vessel and the CFL lamp was about 5 cm (Figure 1). After 14 h, the crude products were purified by column chromatography over silica gel using petroleum / EtOAc = 9/1 as eluent to yield **3a** (76 mg, 80%).

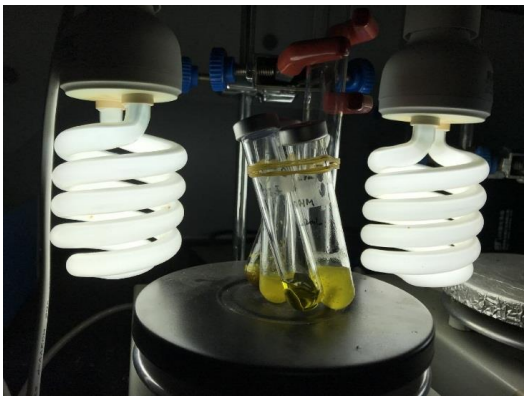
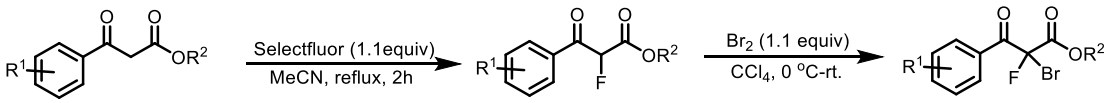


Figure 1 The reaction setup

4. General procedure for the preparation of monofluorobromoacyl arenes[2]



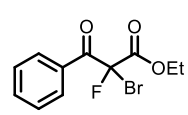
The requisite 2-fluoro-3-oxo-3-phenylpropanoates were prepared according to the previous report.[2a]

To a solution of methyl 3-oxo-3-phenylpropanoates (3 mmol) in MeCN (20 mL) was added Selectfluor (1.1 g, 3.3 mmol) at room temperature. The reaction solution was heated to reflux, keeping stirred for 2 h, then the solvent was removed under reduced pressure. The resulting mixture was diluted by H_2O (15 mL) and extracted with EtOAc (3 × 15 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by flash column chromatography (SiO_2; gradient eluent: petroleum ether to 10% EtOAc in petroleum ether) to provide the methyl 2-fluoro-3-oxo-3-phenylpropanoates.

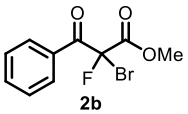
The requisite monofluorobromoacyl arenes were prepared according to the previous report.[2b]

The solution of 2-fluoro-3-oxo-3-phenylpropanoates (3 mmol) in CCl_4 was stirred under the ice bath. To the mixture was added Br_2 (3.3 mL, Br_2 in DCM, 1.0 M) dropwise *via* constant pressure dropping

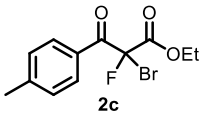
funnel. Then the reaction solution was added by H_2O (15 mL) and washed by EtOAc (15 mL× 2). The combined organic layers were dried over anhydrous Na_2SO_4, and the solvent was removed. Flash chromatography (SiO_2; gradient eluent: petroleum ether to 10% EtOAc in petroleum ether) afforded compound **2a-2i**.



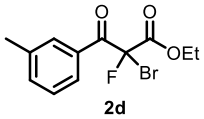
2a



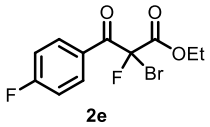
2b



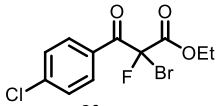
2c



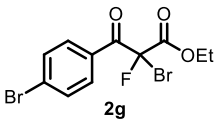
2d



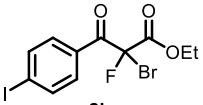
2e



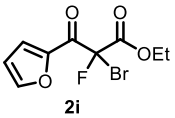
2f



2g



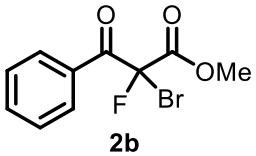
2h



2i

The ^{1}H-NMR, ^{19}F NMR and ^{13}C NMR of **2a** were reported by the reference *J. Org. Chem.* **1992**, *57*, 2199.

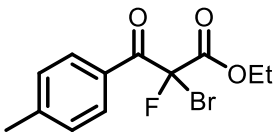
methyl 2-bromo-2-fluoro-3-oxo-3-phenylpropanoate (2b)



2b

colorless oil, 63% yield for two steps, purified by flash column chromatography over 10% EtOAc in petroleum ether, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.7 Hz, 2H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 2H), 3.92 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.9 (d, *J* = 25.3 Hz), 164.0 (d, *J* = 26.8 Hz), 134.8, 130.8 (d, *J* = 3.7 Hz), 130.3, 130.3, 128.9 (s), 97.2 (d, *J* = 275.1 Hz), 54.6 (s) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ = -118.6 (s) ppm.

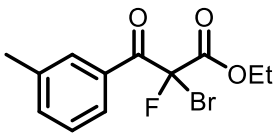
ethyl 2-bromo-2-fluoro-3-oxo-3-(p-tolyl)propanoate (2c)



2c

colorless oil, 66% yield for two steps, purified by flash column chromatography over 10% EtOAc in petroleum ether, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.5 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 4.37 (qd, *J* = 7.2, 2.8 Hz, 2H), 2.44 (s, 3H), 1.29 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.4 (d, *J* = 24.9 Hz), 163.7 (d, *J* = 26.4 Hz), 146.0, 130.4, 130.3, 129.6, 128.3 (d, *J* = 3.3 Hz), 97.8 (d, *J* = 274.7 Hz), 64.2, 21.9, 13.8 ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ = -117.9 (s) ppm.

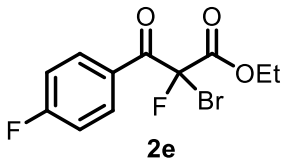
ethyl 2-bromo-2-fluoro-3-oxo-3-(m-tolyl)propanoate (2d)



2d

colorless oil, 60% yield for two steps, purified by flash column chromatography over 10% EtOAc in petroleum ether, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87-7.85 (m, 2H), 7.46 (d, *J* = 7.3 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 4.38-7.36 (m, 2H), 2.42 (s, 3H), 1.28 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.0 (d, *J* = 24.9 Hz), 163. 6 (d, *J* = 26.4 Hz), 138.8, 135.5, 130.9 (d, *J* = 3.3 Hz), 130.6, 130.6, 128.7, 127.4, 127.4, 97.7 (d, *J* = 274.7 Hz), 64.19, 21.4, 13.7 ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ = -118.0 (s) ppm.

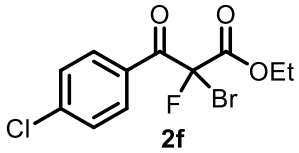
ethyl 2-bromo-2-fluoro-3-(4-fluorophenyl)-3-oxopropanoate (2e)



2e

colorless oil, 67% yield for two steps, purified by flash column chromatography over 10% EtOAc in petroleum ether, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 7.3, 5.4 Hz, 2H), 7.18 (t, *J* = 8.6 Hz, 2H), 4.39 (qd, *J* = 7.2, 1.6 Hz, 2H), 1.30 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.5 (d, *J* = 25.3 Hz), 167.8, 165.2, 163.3 (d, *J* = 26.4 Hz), 133.2 (dd, *J* = 9.7, 4.6 Hz), 127.2 (t, *J* = 3.3 Hz), 116.3, 116.1, 97.3 (d, *J* = 274.4 Hz), 64.3, 13.8 ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ = -99.12–-102.27 (m), -118.49 (s). ppm.

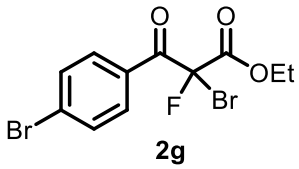
ethyl 2-bromo-3-(4-chlorophenyl)-2-fluoro-3-oxopropanoate (2f)



2f

colorless oil, 63% yield for two steps, purified by flash column chromatography over 10% EtOAc in petroleum ether, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.3 Hz, 2H), 7.48 (d, *J* = 8.7 Hz, 2H), 4.39 (tt, *J* = 7.0, 3.7 Hz, 2H), 1.31 (t, *J* = 7.2 Hz, 3H). ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.9 (d, *J* = 25.7 Hz), 163.2 (d, *J* = 26.4 Hz), 141.5, 131.7, 131.6, 129.3, 129.2 (d, *J* = 3.3 Hz), 97.1 (d, *J* = 274.4 Hz), 64.4, 13.8 ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ = -118.9 (s). ppm.

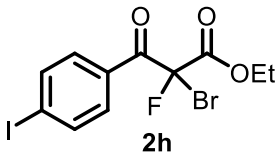
ethyl 2-bromo-3-(4-bromophenyl)-2-fluoro-3-oxopropanoate (2g)



2g

colorless oil, 65% yield for two steps, purified by flash column chromatography over 10% EtOAc in petroleum ether, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.5 Hz, 2H), 7.65 (d, *J* = 8.7 Hz, 2H), 4.38 (qd, *J* = 7.1, 2.1 Hz, 2H), 1.31 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.2 (d, *J* = 25.7 Hz), 163.2 (d, *J* = 26.4 Hz), 132.3, 131.7, 131.6, 130.4, 129.6 (d, *J* = 3.3 Hz), 97.1 (d, *J* = 274.4 Hz), 64.4, 13.8 ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ = -118.9 (s) ppm.

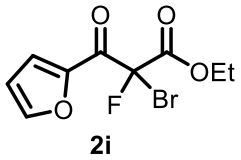
ethyl 2-bromo-2-fluoro-3-(4-iodophenyl)-3-oxopropanoate (2h)



2h

colorless oil, 69% yield for two steps, purified by flash column chromatography over 10% EtOAc in petroleum ether, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.6 Hz, 2H), 7.77 (d, *J* = 8.4 Hz, 2H), 4.38 (dt, *J* = 12.6, 4.3 Hz, 2H), 1.30 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5 (d, *J* = 25.3 Hz), 163.2 (d, *J* = 26.4 Hz), 138.3 (s), 131.3 (d, *J* = 4.4 Hz), 130.2 (d, *J* = 3.3 Hz), 103.5, 97.1 (d, *J* = 274.7 Hz), 64.4, 13.8 ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ = -119.0 (s) ppm.

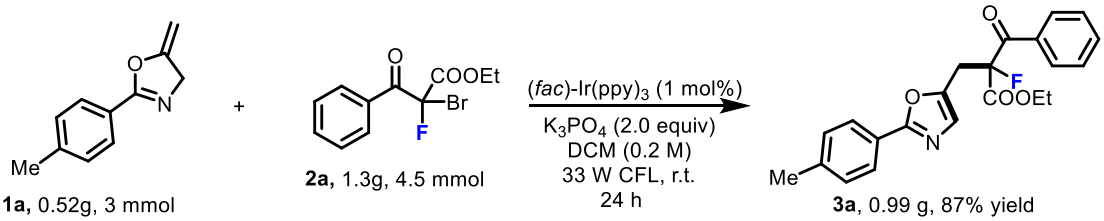
ethyl 2-bromo-2-fluoro-3-(furan-2-yl)-3-oxopropanoate (2i)



2i

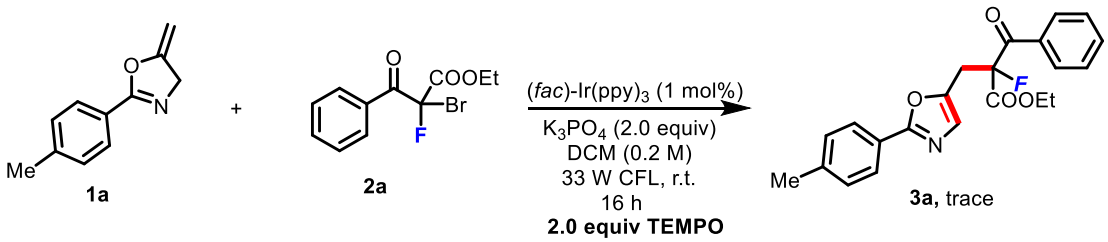
colorless oil, 51% yield for two steps, purified by flash column chromatography over 10% EtOAc in petroleum ether, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.51 (d, *J* = 2.6 Hz, 1H), 6.64 (dd, *J* = 2.2, 1.3 Hz, 1H), 4.38 (qd, *J* = 6.9, 3.4 Hz, 2H), 1.38–1.20 (m, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3 (d, *J* = 26.0 Hz), 162.9 (d, *J* = 26.8 Hz), 148.9, 146.9, 123.0 (d, *J* = 6.2 Hz), 113.0, 96.3 (d, *J* = 271.8 Hz), 64.3, 13.8 ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ = -120.8 (s) ppm.

5. Gram Scale-up Experiment



Methylene-2-oxazoline [1] **1a** (0.52 g, 3 mmol, 1 eq.), monofluorobromoacetophenone[2] **2a** (1.3 g, 4.5 mmol, 1.5 eq.), *fac*-Ir(ppy)$_3$ (20 mg), K_3PO_4 (1.27 g, 6 mmol, 2 eq.) were added to a flame-dried Schlenk flask containing a stirring bar and purged by evacuating the flask and backfilling with argon three times. In the absence of light, anhydrous DCM (15 ml, 0.2 M) was added and the flask was sealed. The mixture was then stirred under irradiation from 33 W CFL and the distance between the reaction vessel and the CFL lamp was about 5 cm. After 24 h, the crude products were purified by column chromatography over silica gel using petroleum / EtOAc = 9/1 as eluent to yield **3a** (0.99 g, 87% yield) .

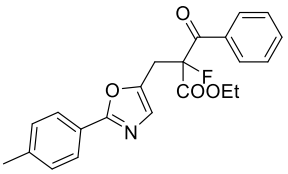
6. Control experiments in the presence of radical scavengers



Procedure: To a flame-dried Schlenk tubes equipped with a magnetic stir bar were added **1a** (34 mg, 0.2 mmol), **2a** (87 mg, 0.3 mmol), *fac*-Ir(ppy)$_3$ (1.3 mg, 2.5 μmol, 1 mol%), K_3PO_4 (84 mg, 0.4 mmol, 2 eq.) and 2,2,6,6-Tetramethylpiperidine 1-oxyl (TEMPO, 134 mg, 0.4 mmol). The tube was evacuated and backfilled with Ar for three times, and then solvent (DCM, 1.0 mL) was added via syringe. The mixture was then stirred under irradiation from 33 W CFL for 16 h. The reaction was totally inhibited.

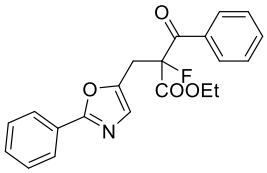
7. Characterization data of compounds

ethyl 2-fluoro-3-oxo-3-phenyl-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propanoate (3a)



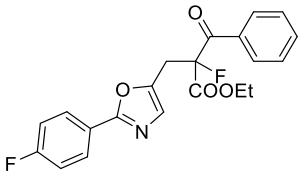
colorless oil, 61 mg, 80% yield, Rf = 0.2 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 – 8.03 (m, 2H), 7.85 (d, *J* = 8.2 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.02 (s, 1H), 4.33 – 4.19 (m, 2H), 3.89 – 3.67 (m, 2H), 2.38 (s, 3H), 1.19 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.8 (d, *J* = 25.1 Hz), 166.4 (d, *J* = 25.6 Hz), 162.0, 144.8, 140.6, 134.3, 133.3 (d, *J* = 3.5 Hz), 129.9 (d, *J* = 5.7 Hz), 129.4 (d, *J* = 5.3 Hz), 128.7, 127.4, 126.1 (d, *J* = 5.3 Hz), 124.7, 97.9 (d, *J* = 203.3 Hz), 63.1, 31.3 (d, *J* = 22.2 Hz), 21.5, 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.72 (dd, *J* = 27.2, 19.0 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{22}H_{21}FNO_4^+$ $(M+H)^+$ 382.14491, found *m/z* 382.14426.

ethyl 2-fluoro-3-oxo-3-phenyl-2-((2-phenyloxazol-5-yl)methyl)propanoate (3b)



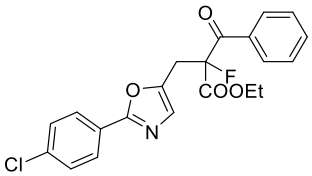
colorless oil, 52 mg, 71% yield, Rf = 0.3 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 – 8.04 (m, 2H), 7.99 – 7.95 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.47 (d, *J* = 7.9 Hz, 2H), 7.44 – 7.42 (m, 3H), 7.05 (s, 1H), 4.33 – 4.20 (m, 2H), 3.88 – 3.68 (m, 2H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.7 (d, *J* = 25.0 Hz), 166.4 (d, *J* = 25.3 Hz), 161.8, 145.2, 134.3, 133.3 (d, *J* = 3.2 Hz), 130.3, 129.9 (d, *J* = 5.6 Hz), 128.7 (d, *J* = 2.9 Hz), 126.2, 97.9 (d, *J* = 203.5 Hz), 63.1, 31.3 (d, *J* = 22.2 Hz), 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.72 (dd, *J* = 26.2, 19.5 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{21}H_{19}FNO_4^+$ $(M+H)^+$ 368.12926, found *m/z* 368.12930.

ethyl 2-fluoro-2-((2-(4-fluorophenyl)oxazol-5-yl)methyl)-3-oxo-3-phenylpropano-ate (3c)



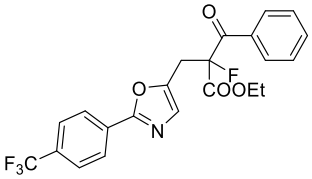
slight yellow oil, 64 mg, 83% yield, Rf = 0.4 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.08 – 8.04 (m, 2H), 7.98 – 7.92 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.12 (t, *J* = 8.7 Hz, 2H), 7.03 (s, 1H), 4.33 – 4.20 (m, 2H), 3.89 – 3.67 (m, 2H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.7 (d, *J* = 25.0 Hz), 166.4 (d, *J* = 25.5 Hz), 165.3, 162.8, 161.0, 145.3, 134.3, 133.3 (d, *J* = 3.6 Hz), 129.9 (d, *J* = 5.7 Hz), 128.7, 128.3 (d, *J* = 8.6 Hz), 127.5, 123.7 (d, *J* = 3.3 Hz), 115.9 (d, *J* = 22.1 Hz), 97.9 (d, *J* = 203.5 Hz), 63.1, 31.3 (d, *J* = 22.2 Hz), 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -109.55 (ddd, *J* = 8.4, 5.4, 3.1 Hz, 1F), -158.76 (dd, *J* = 26.7, 19.4 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{21}H_{18}F_2NO_4^+$ (M+H) $^+$ 386.11984, found *m/z* 386.11987.

ethyl 2-((2-(4-chlorophenyl)oxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenylpropano-ate (3d)



colorless oil, 62 mg, 77% yield, Rf = 0.4 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.1 Hz, 2H), 7.82 (d, *J* = 8.6 Hz, 2H), 7.52 (dd, *J* = 10.7, 4.1 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 6.97 (s, 1H), 4.25 – 4.11 (m, 2H), 3.82 – 3.61 (m, 2H), 1.12 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.7 (d, *J* = 25.0 Hz), 166.4 (d, *J* = 25.5 Hz), 160.9, 145.6, 136.4, 134.3, 133.3 (d, *J* = 3.6 Hz), 129.9 (d, *J* = 5.7 Hz), 129.1, 128.7, 127.6, 127.5, 125.8, 97.9 (d, *J* = 203.5 Hz), 63.1, 31.3 (d, *J* = 22.1 Hz), 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.73 (dd, *J* = 26.5, 19.6 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{21}H_{18}ClFNO_4^+$ (M+H) $^+$ 402.09029, found *m/z* 402.09033.

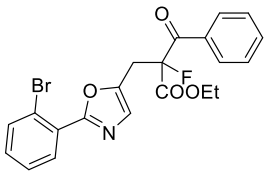
ethyl 2-fluoro-3-oxo-3-phenyl-2-((2-(4-(trifluoromethyl)phenyl)oxazol-5-yl)meth-yl) propanoate (3e)



colorless oil, 69 mg, 79% yield, Rf = 0.4 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 11.0, 4.4 Hz, 4H), 7.70 (d, *J* = 8.3 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.10 (s, 1H), 4.34 – 4.21 (m, 2H), 3.92 – 3.70 (m, 2H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.6 (d, *J* = 24.9 Hz), 166.4 (d, *J* = 25.6 Hz), 160.4, 146.3, 134.4, 133.2 (d, *J* = 3.5 Hz), 131.9 (q, *J* = 32.7 Hz), 130.4 (d, *J* = 1.4 Hz), 129.9 (d, *J* = 5.7 Hz), 128.8, 127.9, 126.4, 125.8 (q, *J* = 3.8 Hz), 125.2, 122.5, 97.8 (d, *J* = 203.6 Hz), 63.2, 31.3 (d, *J* = 22.2 Hz), 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.90 (s, 3F), -158.71 (dd, *J* = 26.0, 19.8 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd

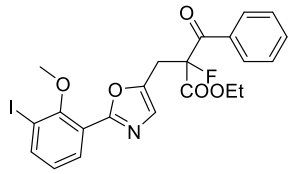
for $C_{22}H_{18}F_4NO_4^+$ (M+H) $^+$ 436.11665, found *m/z* 436.11636.

ethyl 2-((2-(2-bromophenyl)oxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenylpropano-ate (3f)



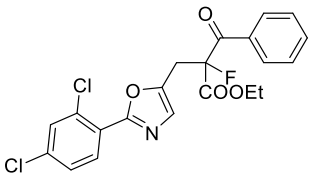
colorless oil, 68 mg, 76% yield, Rf = 0.3 (ethyl acetate/hexane = 15%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.0 Hz, 2H), 7.89 – 7.83 (m, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.30 – 7.25 (m, 1H), 7.14 (s, 1H), 4.34 – 4.20 (m, 2H), 3.91 – 3.69 (m, 2H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.7 (d, *J* = 25.0 Hz), 166.4 (d, *J* = 25.6 Hz), 160.2, 145.7, 134.5, 134.3, 133.3 (d, *J* = 3.5 Hz), 131.1, 129.9 (d, *J* = 5.7 Hz), 128.7, 128.2, 127.4 (d, *J* = 7.9 Hz), 121.0, 97.8 (d, *J* = 203.6 Hz), 63.2, 31.3 (d, *J* = 22.1 Hz), 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.76 (dd, *J* = 26.9, 19.0 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{21}H_{18}BrFNO_4^+$ (M+H) $^+$ 446.03978, found *m/z* 446.03989.

ethyl 2-fluoro-2-((2-(3-iodo-2-methoxyphenyl)oxazol-5-yl)methyl)-3-oxo-3-phen-ylpropanoate (3g)



colorless oil, 71 mg, 68% yield, Rf = 0.3 (ethyl acetate/hexane = 20%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 1.8 Hz, 1H), 8.06 (d, *J* = 7.9 Hz, 2H), 7.93 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.01 (s, 1H), 6.85 (d, *J* = 8.6 Hz, 1H), 4.35 – 4.20 (m, 2H), 3.93 (s, 3H), 3.89 – 3.67 (m, 2H), 1.22 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.8 (d, *J* = 25.1 Hz), 166.4 (d, *J* = 25.5 Hz), 160.3, 159.7, 145.1, 137.4, 134.3, 133.3 (d, *J* = 3.5 Hz), 129.9 (d, *J* = 5.7 Hz), 128.7, 127.8, 127.4, 122.0, 110.6, 97.9 (d, *J* = 203.4 Hz), 86.0, 63.1, 56.5, 31.3 (d, *J* = 22.2 Hz), 14.0 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.78 (dd, *J* = 26.7, 19.3 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{22}H_{20}FINO_5^+$ (M+H) $^+$ 524.03647, found *m/z* 524.03638.

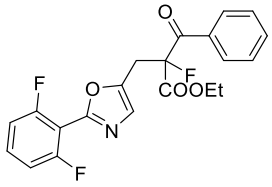
ethyl 2-((2-(2,4-dichlorophenyl)oxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenylpro-panoate (3h)



slight yellow oil, 62 mg, 71% yield, Rf = 0.2 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.2 Hz, 2H), 7.87 (d, *J* = 8.5 Hz, 1H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.51 (d, *J* = 1.7 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.32 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.13 (s, 1H), 4.33 – 4.20 (m, 2H), 3.90 – 3.71 (m, 2H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.6 (d, *J* = 25.0 Hz), 166.3 (d, *J* = 25.6 Hz), 158.8, 146.0, 136.4, 134.3, 133.2 (d, *J* = 3.5 Hz), 133.1, 131.4, 131.0, 129.9 (d,

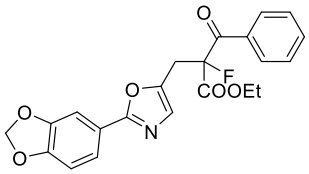
J = 5.7 Hz), 128.7, 127.6, 127.3, 124.7, 97.8 (d, *J* = 203.6 Hz), 63.2, 31.2 (d, *J* = 22.2 Hz), 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.79 (dd, *J* = 26.4, 19.2 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{21}H_{17}Cl_2FNO_4^+$ (M+H) $^+$ 436.05132, found *m/z* 436.05237.

ethyl 2-((2-(2,6-difluorophenyl)oxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenylpro-panoate (3i)



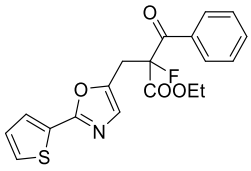
slight yellow oil, 49 mg, 61% yield, Rf = 0.2 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.4 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.39 (dd, *J* = 14.5, 6.3 Hz, 1H), 7.19 (s, 1H), 7.02 (t, *J* = 8.5 Hz, 2H), 4.34 – 4.20 (m, 2H), 3.95 – 3.69 (m, 2H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.6 (d, *J* = 25.0 Hz), 166.3 (d, *J* = 25.6 Hz), 162.0 (d, *J* = 5.7 Hz), 159.4 (d, *J* = 5.6 Hz), 153.3, 146.2, 134.3, 133.2 (d, *J* = 3.5 Hz), 131.8 (t, *J* = 10.6 Hz), 129.9 (d, *J* = 5.6 Hz), 128.7, 127.7, 112.3 – 112.1 (m), 106.4 (t, *J* = 15.9 Hz), 97.7 (d, *J* = 203.4 Hz), 63.1, 31.2 (d, *J* = 22.2 Hz), 13.8 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -109.56 (dd, *J* = 8.3, 6.2 Hz, 2F), -158.81 (dd, *J* = 28.0, 17.8 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{21}H_{17}F_3NO_4^+$ (M+H) $^+$ 404.11042, found *m/z* 404.11047.

ethyl 2-((2-(benzo[*d*][1,3]dioxol-5-yl)oxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenyl-propanoate (3j)



colorless oil, 57 mg, 69% yield, Rf = 0.5 (ethyl acetate/hexane = 20%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 5.6, 4.1 Hz, 2H), 7.62 – 7.57 (m, 1H), 7.50 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.41 (d, *J* = 1.6 Hz, 1H), 6.99 (s, 1H), 6.85 (d, *J* = 8.2 Hz, 1H), 6.01 (s, 2H), 4.33 – 4.19 (m, 2H), 3.88 – 3.65 (m, 2H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.8 (d, *J* = 25.1 Hz), 166.4 (d, *J* = 25.6 Hz), 161.6, 149.5, 148.0, 144.7, 134.3, 133.3 (d, *J* = 3.5 Hz), 129.9 (d, *J* = 5.7 Hz), 128.7, 127.3, 121.6, 121.0, 108.6, 106.6, 101.5, 97.9 (d, *J* = 203.3 Hz), 63.1, 31.3 (d, *J* = 22.2 Hz), 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.64 – -158.99 (m, 1F)ppm; **HRMS (ESI)** m/z calcd for $C_{22}H_{19}FNO_6^+$ (M+H) $^+$ 412.11909, found *m/z* 412.11917.

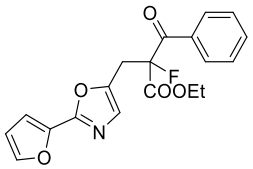
ethyl 2-fluoro-3-oxo-3-phenyl-2-((2-(thiophen-2-yl)oxazol-5-yl)methyl)propano-ate (3k)



slight yellow oil, 47 mg, 63% yield, Rf = 0.5 (ethyl acetate/hexane = 20%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.0 Hz, 2H), 7.64 – 7.56 (m, 2H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.40 (d, *J* = 5.0 Hz, 1H), 7.12 – 7.06 (m, 1H), 7.00 (s, 1H), 4.36 – 4.20 (m, 2H), 3.89 – 3.65 (m, 2H), 1.22 (t, *J* = 7.1 Hz,

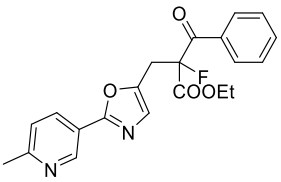
3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.7 (d, *J* = 25.1 Hz), 166.4 (d, *J* = 25.6 Hz), 158.0, 144.8, 134.3, 133.3 (d, *J* = 3.2 Hz), 129.9 (d, *J* = 5.5 Hz), 128.7, 128.2, 127.9, 127.6, 127.4, 97.8 (d, *J* = 203.4 Hz), 63.2, 31.2 (d, *J* = 22.2 Hz), 14.0 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.80 (dd, *J* = 26.4, 19.5 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{19}H_{17}FNO_4S^+$ $(M+H)^+$ 374.08568, found *m/z* 374.08597.

ethyl 2-fluoro-2-((2-(furan-2-yl)oxazol-5-yl)methyl)-3-oxo-3-phenylpropanoate (3l)



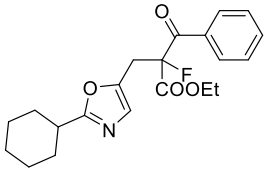
colorless oil, 48 mg, 67% yield, Rf = 0.5 (ethyl acetate/hexane = 20%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 – 8.03 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.53 (d, *J* = 1.1 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.03 (s, 1H), 6.95 (d, *J* = 3.4 Hz, 1H), 6.51 (dd, *J* = 3.4, 1.8 Hz, 1H), 4.36 – 4.19 (m, 2H), 3.88 – 3.65 (m, 2H), 1.22 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.6 (d, *J* = 25.1 Hz), 166.3 (d, *J* = 25.6 Hz), 154.6 (s), 144.8, 144.3, 142.8, 134.3, 133.3 (d, *J* = 3.5 Hz), 129.9 (d, *J* = 5.6 Hz), 128.7, 127.3, 111.5 (d, *J* = 47.3 Hz), 97.8 (d, *J* = 203.4 Hz), 63.2, 31.2 (d, *J* = 22.2 Hz), 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.76 (dd, *J* = 27.4, 18.5 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{19}H_{17}FNO_5^+$ $(M+H)^+$ 358.10853, found *m/z* 358.10809.

ethyl 2-fluoro-2-((2-(6-methylpyridin-3-yl)oxazol-5-yl)methyl)-3-oxo-3-phenyl-propanoate (3m)



colorless oil, 47 mg, 62% yield, Rf = 0.2 (ethyl acetate/hexane = 20%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.08 (s, 1H), 8.12 (dd, *J* = 8.1, 2.0 Hz, 1H), 8.06 (d, *J* = 8.0 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.24 (d, *J* = 8.1 Hz, 1H), 7.07 (s, 1H), 4.35 – 4.21 (m, 2H), 3.92 – 3.70 (m, 2H), 2.61 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.6 (d, *J* = 25.0 Hz), 166.4 (d, *J* = 25.6 Hz), 160.3, 159.8, 146.9, 145.7, 134.3, 133.8, 133.3 (d, *J* = 3.5 Hz), 129.9 (d, *J* = 5.7 Hz), 128.7, 127.6, 123.2, 120.9, 97.8 (d, *J* = 203.4 Hz), 63.2, 31.3 (d, *J* = 22.1 Hz), 24.5, 14.0 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.80 (dd, *J* = 26.6, 19.1 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{21}H_{20}FN_2O_4^+$ $(M+H)^+$ 383.14016, found *m/z* 383.14059.

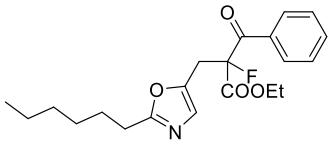
ethyl 2-((2-cyclohexyloxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenylpropanoate (3n)



colorless oil, 63 mg, 84% yield, Rf = 0.2 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.1 Hz, 2H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 6.80 (s, 1H), 4.32 – 4.17 (m, 2H), 3.80 – 3.53 (m, 2H), 2.72 (tt, *J* = 11.2, 3.5 Hz, 1H), 2.00 – 1.98 (m, 2H), 1.79 – 1.76 (m, 2H), 1.69

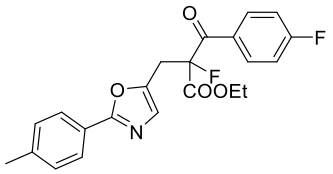
– 1.66 (m, 2H), 1.55 – 1.46 (m, 2H), 1.39 – 1.32 (m, 2H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.9 (d, *J* = 25.2 Hz), 168.3, 166.4 (d, *J* = 25.7 Hz), 144.1, 134.2, 133.4 (d, *J* = 3.5 Hz), 129.8 (d, *J* = 5.8 Hz), 128.7, 125.7, 97.9 (d, *J* = 202.9 Hz), 63.0, 37.4, 31.2 (d, *J* = 22.1 Hz), 30.4 (d, *J* = 3.1 Hz), 25.8, 25.5, 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.94 (dd, *J* = 27.9, 18.9 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{21}H_{25}FNO_4^+$ (M+H) $^+$ 374.17621, found *m/z* 374.17624.

ethyl 2-fluoro-2-((2-hexyloxazol-5-yl)methyl)-3-oxo-3-phenylpropanoate (3o)



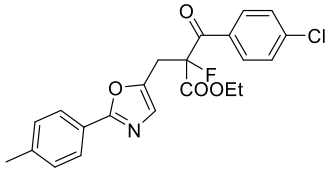
colorless oil, 64 mg, 85% yield, Rf = 0.3 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.07 – 8.01 (m, 2H), 7.63 – 7.57 (m, 1H), 7.45 (dd, *J* = 10.7, 4.9 Hz, 2H), 6.80 (s, 1H), 4.33 – 4.17 (m, 2H), 3.78 – 3.56 (m, 2H), 2.69 (t, *J* = 7.6 Hz, 2H), 1.72 – 1.66 (m, 2H), 1.35 – 1.26 (m, 6H), 1.22 (t, *J* = 7.1 Hz, 3H), 0.88 (t, *J* = 6.8 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.9 (d, *J* = 25.1 Hz), 166.4 (d, *J* = 25.7 Hz), 165.2, 144.5, 134.2, 133.4 (d, *J* = 3.5 Hz), 129.8 (d, *J* = 5.7 Hz), 128.7, 125.9, 97.9 (d, *J* = 202.9 Hz), 63.0, 31.4, 31.2 (d, *J* = 22.1 Hz), 28.7, 28.1, 26.8, 22.5, 14.0 (d, *J* = 8.9 Hz) ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -159.00 (dd, *J* = 27.7, 18.9 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{21}H_{27}FNO_4^+$ (M+H) $^+$ 376.19186, found *m/z* 376.19351.

ethyl 2-fluoro-3-(4-fluorophenyl)-3-oxo-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propan-oate (4a)



yellow oil, 62 mg, 78% yield, Rf = 0.2 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 7.4, 5.6 Hz, 2H), 7.85 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.13 (t, *J* = 8.6 Hz, 2H), 7.02 (s, 1H), 4.34 – 4.19 (m, 2H), 4.34 – 4.20 (m, 2H), 2.39 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.3 (d, *J* = 25.3 Hz), 167.6, 166.31 (d, *J* = 25.7 Hz), 165.1, 162.0, 144.7, 140.6, 132.9 (dd, *J* = 9.4, 6.4 Hz), 129.8 – 129.6 (m), 129.5, 127.4, 126.2, 124.7, 116.0 (d, *J* = 22.0 Hz), 98.0 (d, *J* = 202.9 Hz), 63.2, 31.2 (d, *J* = 21.9 Hz), 21.5, 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -102.11 – -102.62 (m, 1F), -158.49 (dd, *J* = 26.7, 19.3 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{22}H_{20}F_2NO_4^+$ (M+H) $^+$ 400.13549, found *m/z* 400.13583.

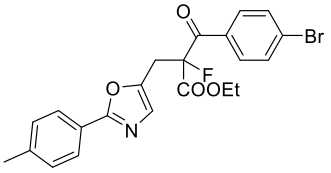
ethyl 3-(4-chlorophenyl)-2-fluoro-3-oxo-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propan-oate (4b)



slight yellow oil, 55 mg, 66% yield, Rf = 0.5 (ethyl acetate/hexane = 20%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.04 – 7.99 (m, 2H), 7.85 (d, *J* = 8.1 Hz, 2H), 7.43 (d, *J* = 8.6 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.02 (s, 1H), 4.34 – 4.19 (m, 2H), 3.88 – 3.66 (m, 2H), 2.39 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H) ppm;

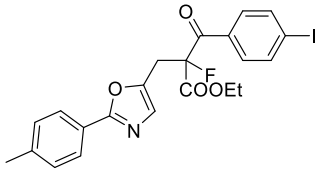
^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8 (d, *J* = 25.3 Hz), 166.2 (d, *J* = 25.5 Hz), 162.1, 144.6, 141.0, 140.6, 131.6 (d, *J* = 3.7 Hz), 131.3 (d, *J* = 6.1 Hz), 129.5, 129.1, 127.4, 126.2, 124.6, 98.0 (d, *J* = 203.1 Hz), 63.2, 31.2 (d, *J* = 22.1 Hz), 21.5, 14.0 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.74 (dd, *J* = 27.1, 19.4 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{22}H_{20}ClFNO_4^+$ $(M+H)^+$416.10594, found *m/z* 416.10580.

ethyl 3-(4-bromophenyl)-2-fluoro-3-oxo-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propan-oate (4c)



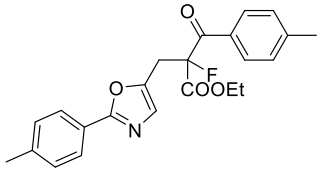
slight yellow oil, 67 mg, 73% yield, Rf = 0.2 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 – 7.91 (m, 2H), 7.85 (d, *J* = 8.1 Hz, 2H), 7.60 (d, *J* = 8.6 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.01 (s, 1H), 4.34 – 4.19 (m, 2H), 3.88 – 3.66 (m, 2H), 2.39 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.0 (d, *J* = 25.4 Hz), 166.2 (d, *J* = 25.5 Hz), 162.1, 144.6, 140.6, 132.1, 132.0 (d, *J* = 3.6 Hz), 131.3 (d, *J* = 6.0 Hz), 129.9, 129.5, 127.4, 126.2, 124.6, 98.0 (d, *J* = 203.1 Hz), 63.2, 31.2 (d, *J* = 22.1 Hz), 21.5, 14.0 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.77 (dd, *J* = 27.0, 19.4 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{22}H_{20}BrFNO_4^+$ $(M+H)^+$ 460.05543, found *m/z* 460.05533.

ethyl 2-fluoro-3-(4-iodophenyl)-3-oxo-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propano-ate (4d)



slight yellow oil, 82 mg, 81% yield, Rf = 0.5 (ethyl acetate/hexane = 20%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 – 7.81 (m, 4H), 7.76 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.01 (s, 1H), 4.34 – 4.17 (m, 2H), 3.88 – 3.65 (m, 2H), 2.39 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.3 (d, *J* = 25.4 Hz), 166.2 (d, *J* = 25.8 Hz), 162.1, 144.6, 140.6, 138.1, 132.6 (d, *J* = 3.6 Hz), 131.1 (d, *J* = 5.9 Hz), 129.5, 127.4, 126.2, 124.6, 103.0, 98.0 (d, *J* = 203.2 Hz), 63.2, 31.2 (d, *J* = 22.1 Hz), 21.5, 14.0 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.84 (dd, *J* = 27.0, 19.4 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{22}H_{20}FINO_4^+$ $(M+H)^+$ 508.04156, found *m/z* 508.04181.

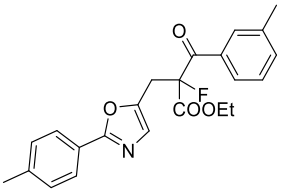
ethyl 2-fluoro-3-oxo-3-(p-tolyl)-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propanoate (4e)



slight yellow oil, 60 mg, 76% yield, Rf = 0.2 (ethyl acetate/hexane = 10%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.0 Hz, 2H), 7.86 (d, *J* = 8.1 Hz, 2H), 7.27 – 7.22 (m, 4H), 7.02 (s, 1H), 4.34 – 4.17 (m, 2H), 3.91 – 3.64 (m, 2H), 2.40 (s, 3H), 2.39 (s, 3H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR**

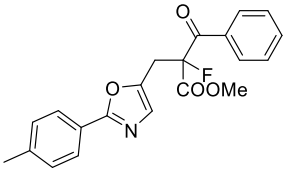
(100 MHz, $CDCl_3$) δ 190.2 (d, *J* = 24.8 Hz), 166.6 (d, *J* = 25.6 Hz), 162.0, 145.4, 145.0, 140.5, 130.8 (d, *J* = 3.6 Hz), 130.0 (d, *J* = 5.7 Hz), 129.4, 127.3, 126.2, 124.7, 97.9 (d, *J* = 203.3 Hz), 63.0, 31.3 (d, *J* = 22.2 Hz), 21.6 (d, *J* = 28.9 Hz), 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.51 (dd, *J* = 27.7, 18.6 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{23}H_{23}FNO_4^+$ (M+H) $^+$ 396.16056, found *m/z* 396.16150.

ethyl 2-fluoro-3-oxo-3-(m-tolyl)-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propanoate (4f)



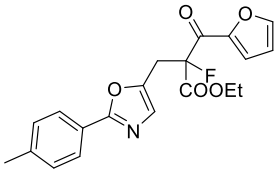
colorless oil, 57 mg, 72% yield, Rf = 0.5 (ethyl acetate/hexane = 20%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 – 7.83 (m, 4H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.02 (s, 1H), 4.34 – 4.18 (m, 2H), 3.88 – 3.67 (m, 2H), 2.39 (s, 6H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.0 (d, *J* = 25.0 Hz), 166.5 (d, *J* = 25.5 Hz), 162.0, 144.9, 140.5, 138.6, 135.1, 133.4 (d, *J* = 3.5 Hz), 130.2 (d, *J* = 4.8 Hz), 129.4, 128.6, 127.3, 127.1 (d, *J* = 6.4 Hz), 126.2, 124.7, 97.9 (d, *J* = 203.6 Hz), 63.0, 31.4 (d, *J* = 22.2 Hz), 21.4 (d, *J* = 15.9 Hz), 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.61 (dd, *J* = 27.1, 19.0 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{23}H_{23}FNO_4^+$ (M+H) $^+$ 396.16056, found *m/z* 396.16095.

methyl 2-fluoro-3-oxo-3-phenyl-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propanoate (4g)



slight yellow oil, 56 mg, 77% yield, Rf = 0.4 (ethyl acetate/hexane = 20%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.9 Hz, 2H), 7.77 (d, *J* = 8.1 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 6.94 (s, 1H), 3.82 – 3.60 (m, 2H), 3.74 (s, 3H), 2.31 (s, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.7 (d, *J* = 25.1 Hz), 165.9 (d, *J* = 25.8 Hz), 161.0, 143.7, 139.6, 133.3, 132.3 (d, *J* = 3.5 Hz), 128.8 (t, *J* = 4.8 Hz), 128.4, 127.7, 126.7, 126.3, 125.1, 123.6, 97.1 (d, *J* = 203.6 Hz), 52.6, 30.4 (d, *J* = 22.1 Hz), 20.5 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -158.89 (dd, *J* = 26.9, 19.2 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{21}H_{19}FNO_4^+$ (M+H) $^+$ 368.12926, found *m/z* 368.12926.

ethyl 2-fluoro-3-(furan-2-yl)-3-oxo-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propanoate (4h)



colorless oil, 47 mg, 64% yield, Rf = 0.3 (ethyl acetate/hexane = 20%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.1 Hz, 2H), 7.70 (s, 1H), 7.52 (t, *J* = 3.6 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.01 (s, 1H), 6.56 (dd, *J* = 3.5, 1.4 Hz, 1H), 4.34 – 4.20 (m, 2H), 3.88 – 3.66 (m, 2H), 2.39 (s, 3H), 1.23 (t, *J* = 7.1

Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 178.7 (d, *J* = 25.8 Hz), 165.7 (d, *J* = 26.0 Hz), 162.0, 148.6 (d, *J* = 3.5 Hz), 144.5, 140.6, 129.4, 127.4, 126.2, 124.6, 123.1 (d, *J* = 11.3 Hz), 112.8 (d, *J* = 2.0 Hz), 97.2 (d, *J* = 202.6 Hz), 63.2, 30.7 (d, *J* = 21.5 Hz), 21.5, 14.0 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -162.07 (ddd, *J* = 26.1, 20.6, 3.7 Hz, 1F) ppm; **HRMS (ESI)** m/z calcd for $C_{20}H_{19}FNO_5^+$ $(M+H)^+$ 372.12418, found *m/z* 372.12439.

8. Reference:

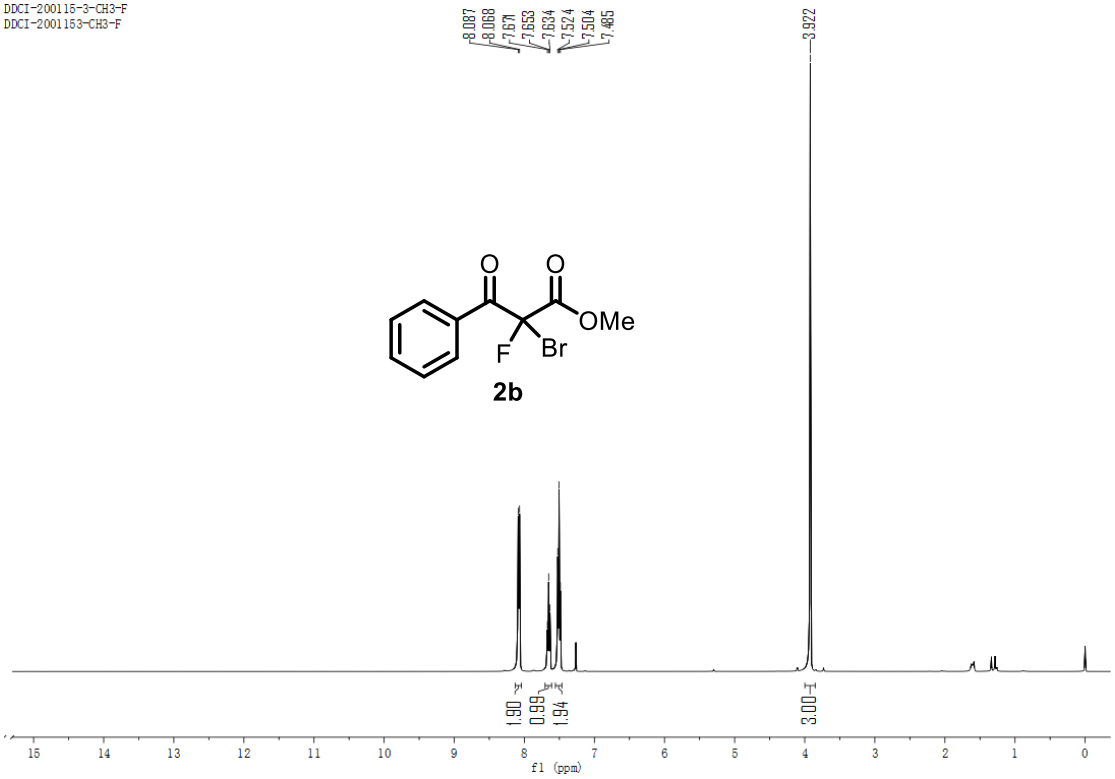
1. G. C. Senadi, W. P. Hu, J. S. Hsiao, J. K. Vandavasi, *Org. Lett.* **2012**, *14*, 4478.

2. (a) Y. Takeuchi, H. Ogura, A. Kanada, T. Koizumi, *J. Org. Chem.* **1992**, *57*, 2196; (b) J. Evenäs, F. Edfeldt, M. Lepistö, N. Svitacheva, A. Synnergren, B. Lundquist, M. Gränse, A. Rönnholm, M. Varga, J. Wright, M. Wei, S. Yue, J. Wang, C. Li, X. Li, G. Chen, Y. Liao, G. Lv, A. Tjörnebo, F. Narjes, *Bioorg. Med. Chem. Lett.* **2014**, *24*, 1315.

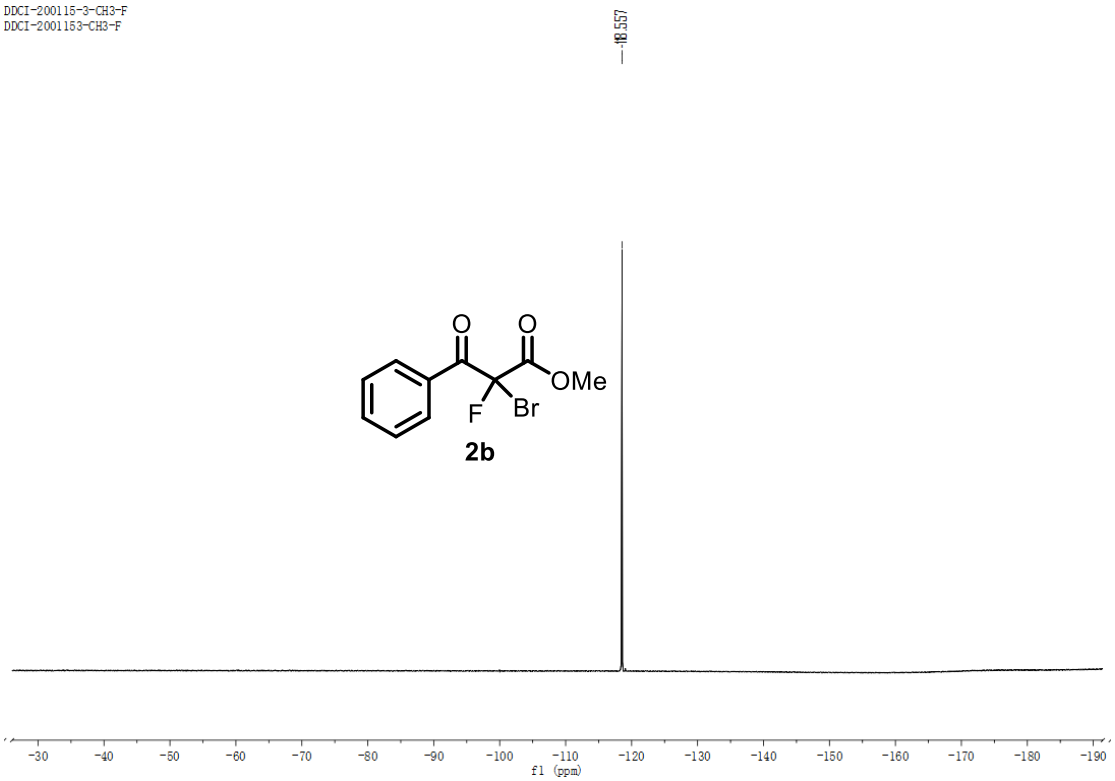
9. Copies ^{1}H NMR, ^{13}C NMR, ^{19}F NMR

methyl 2-bromo-2-fluoro-3-oxo-3-phenylpropanoate (2b)

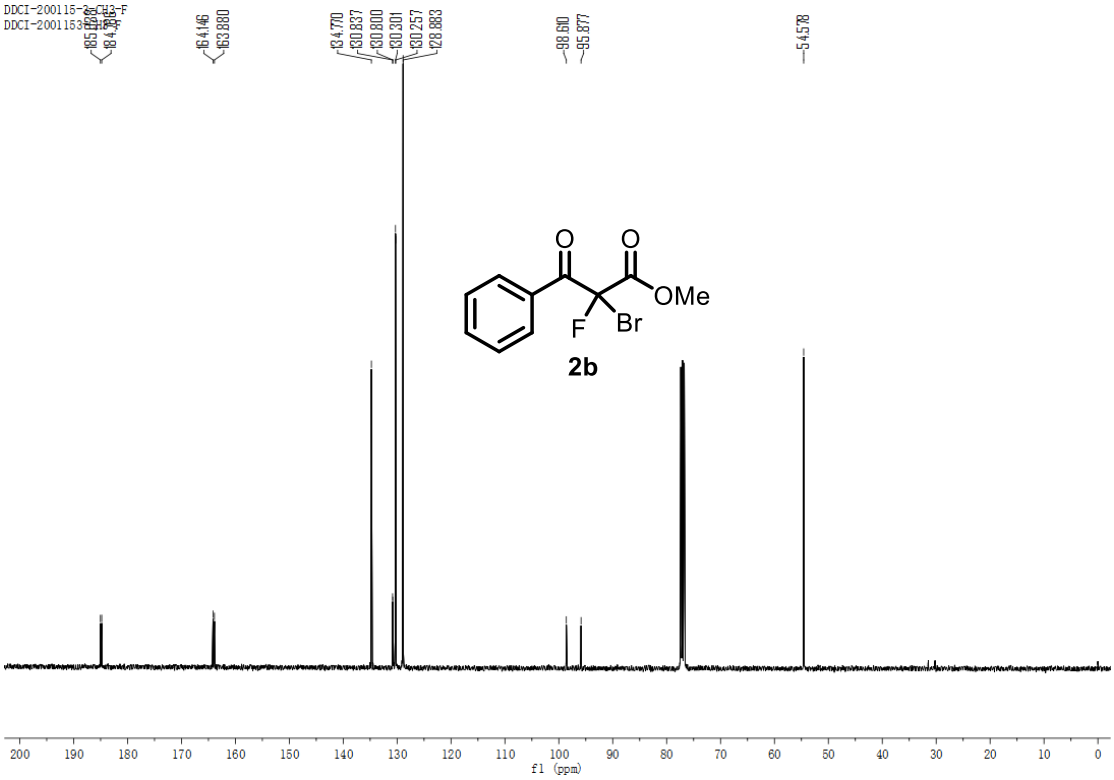
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

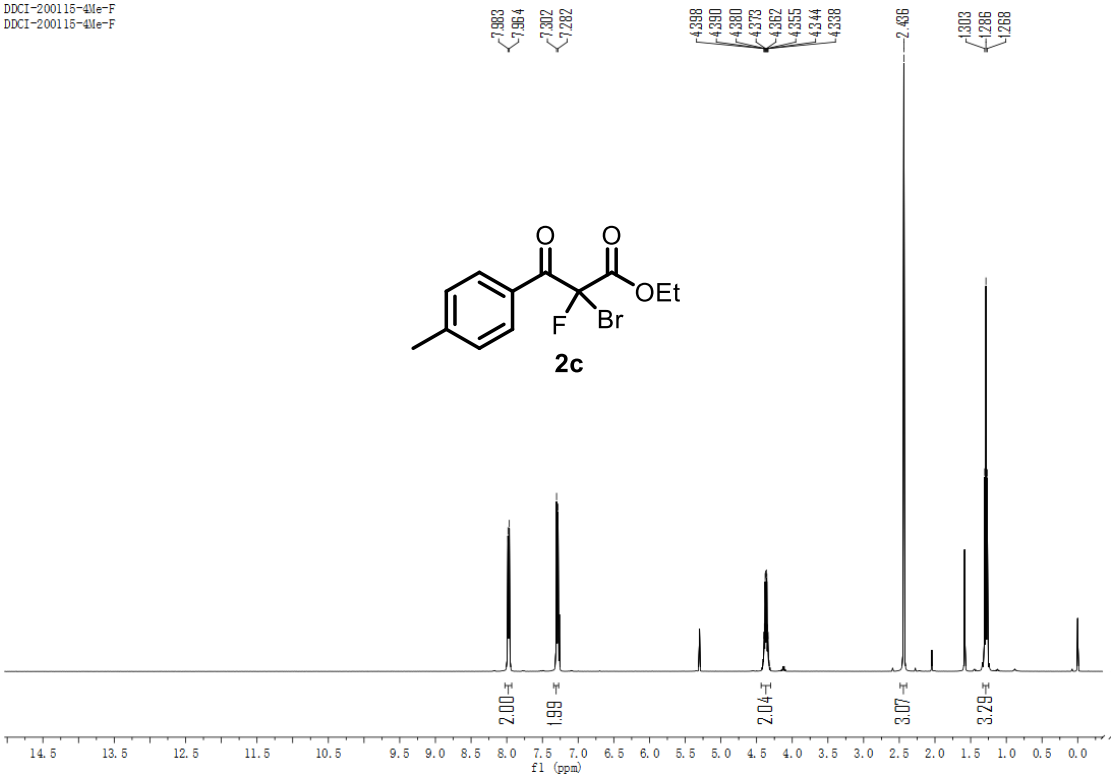


^{13}C NMR (100 MHz, $CDCl_3$):

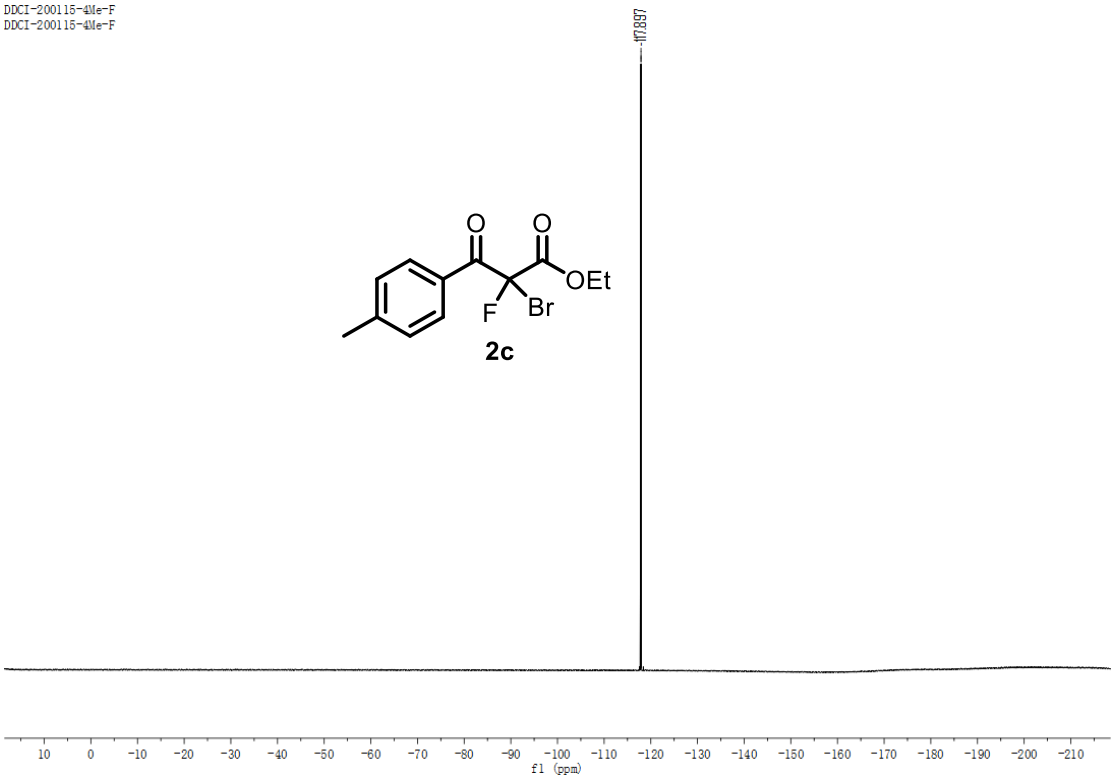


ethyl 2-bromo-2-fluoro-3-oxo-3-(p-tolyl)propanoate (2c)

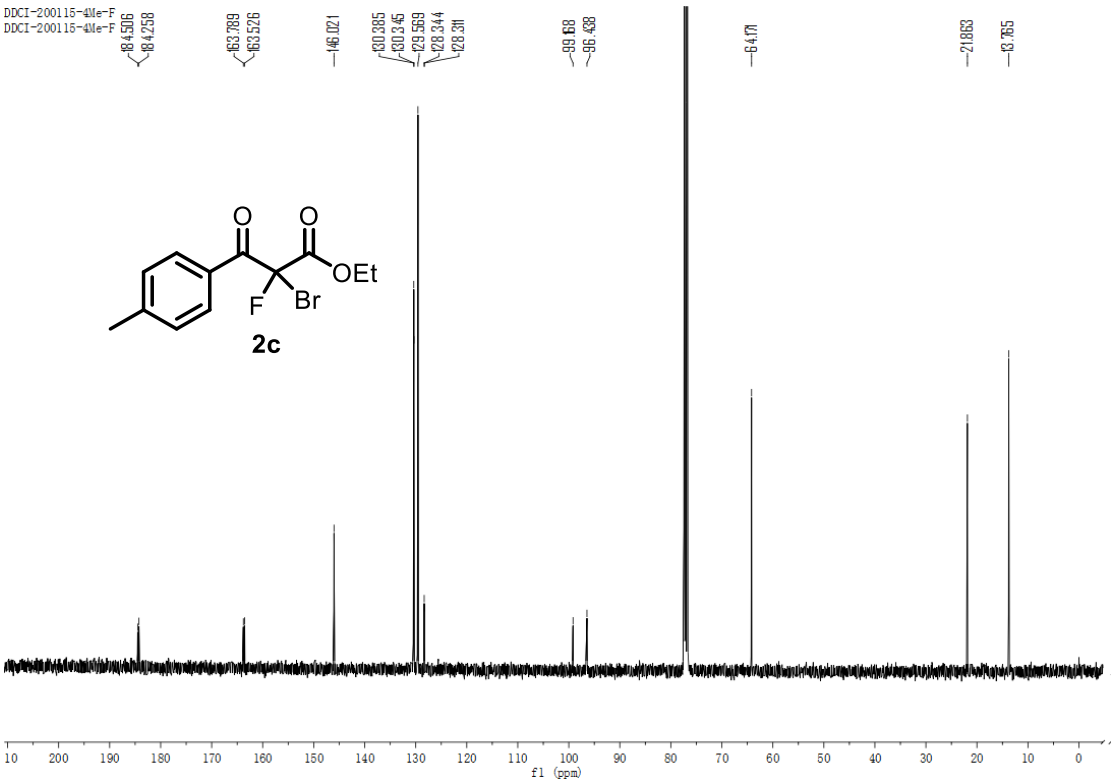
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

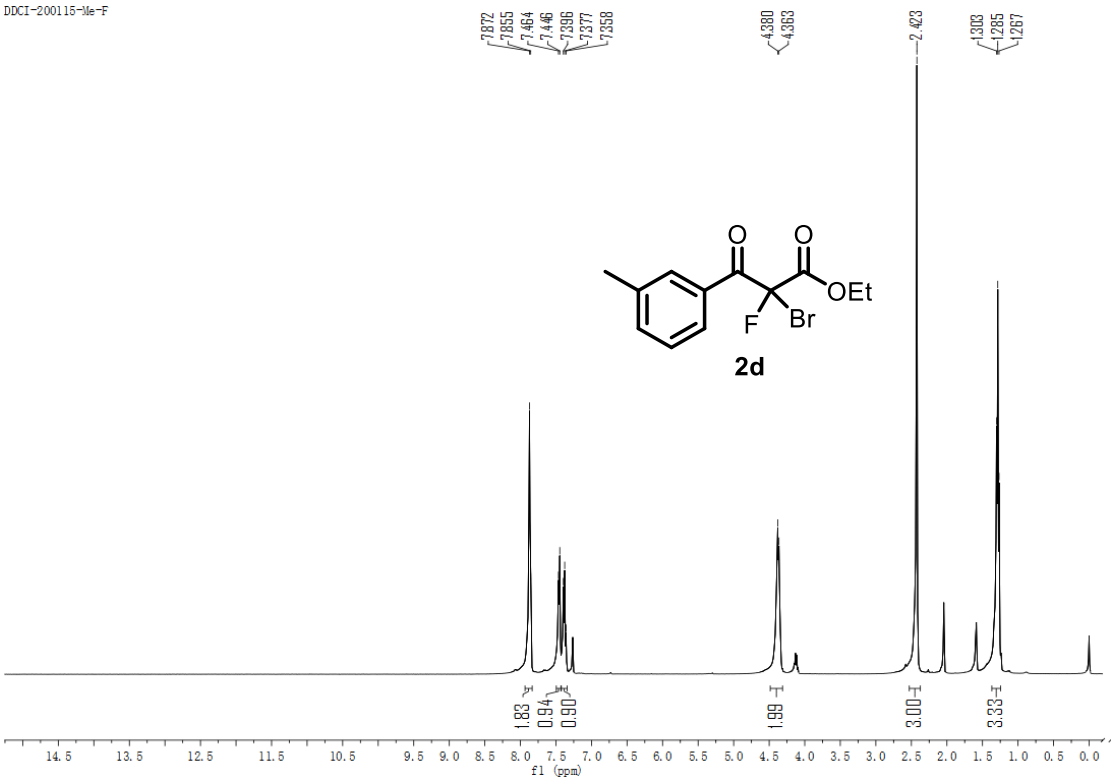


^{13}C NMR (100 MHz, $CDCl_3$):

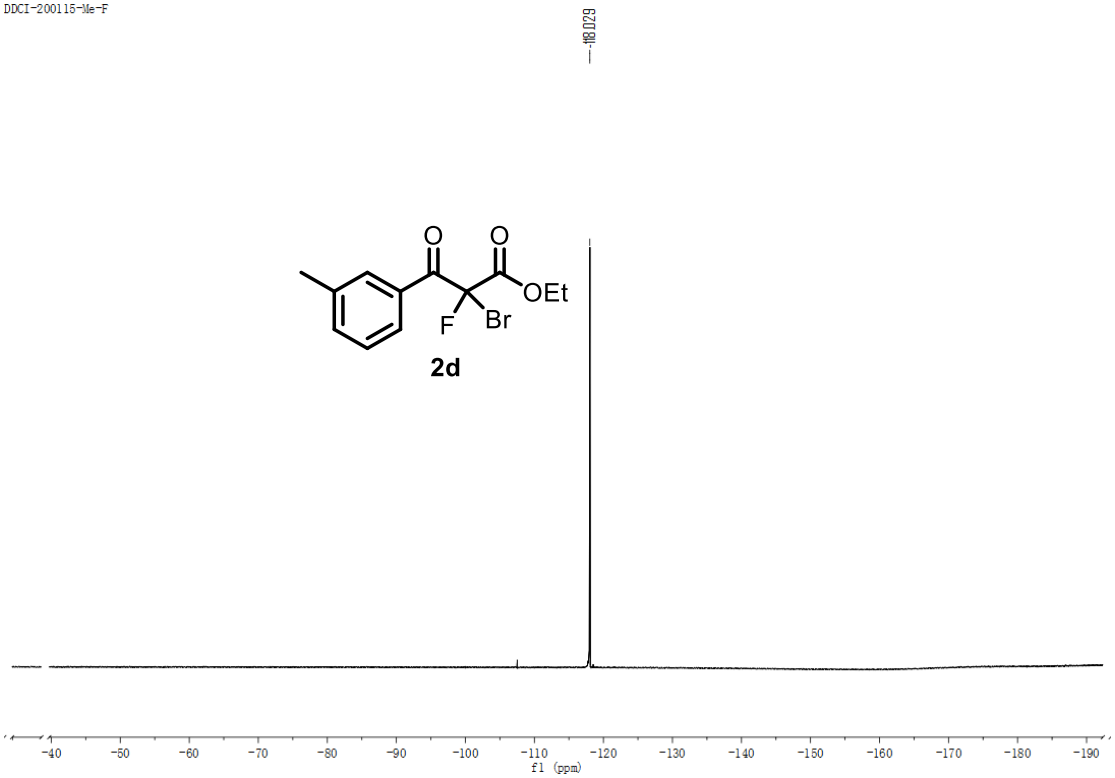


ethyl 2-bromo-2-fluoro-3-oxo-3-(m-tolyl)propanoate (2d)

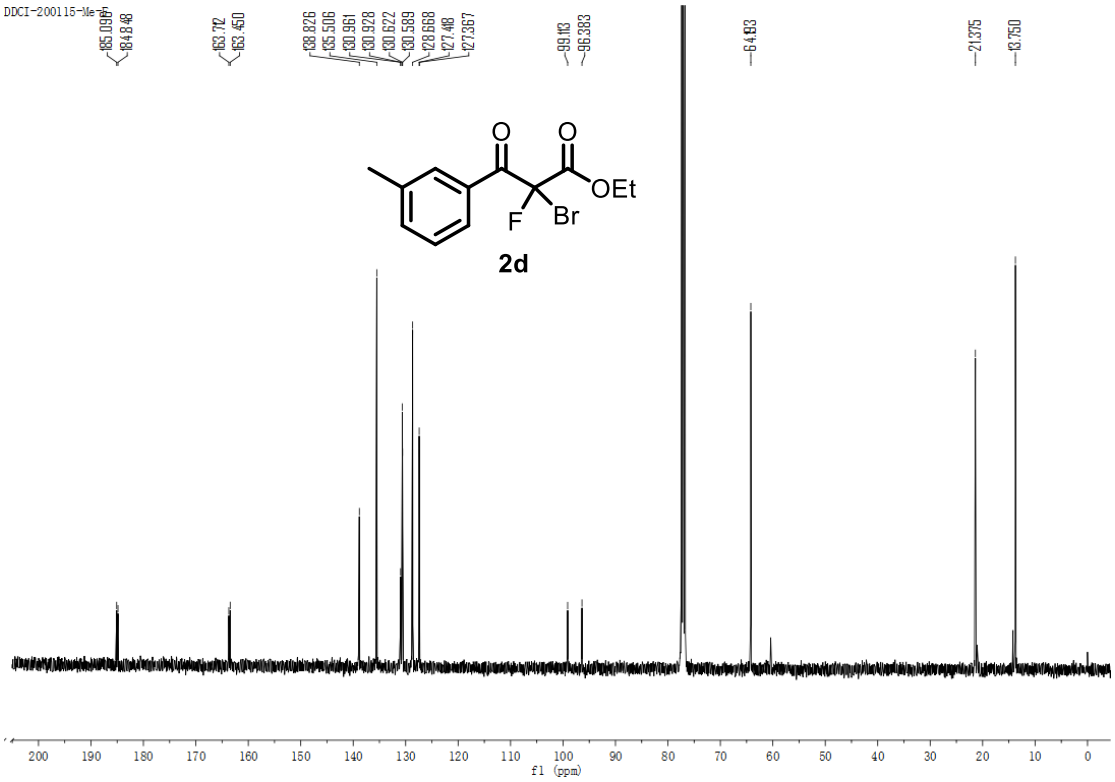
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

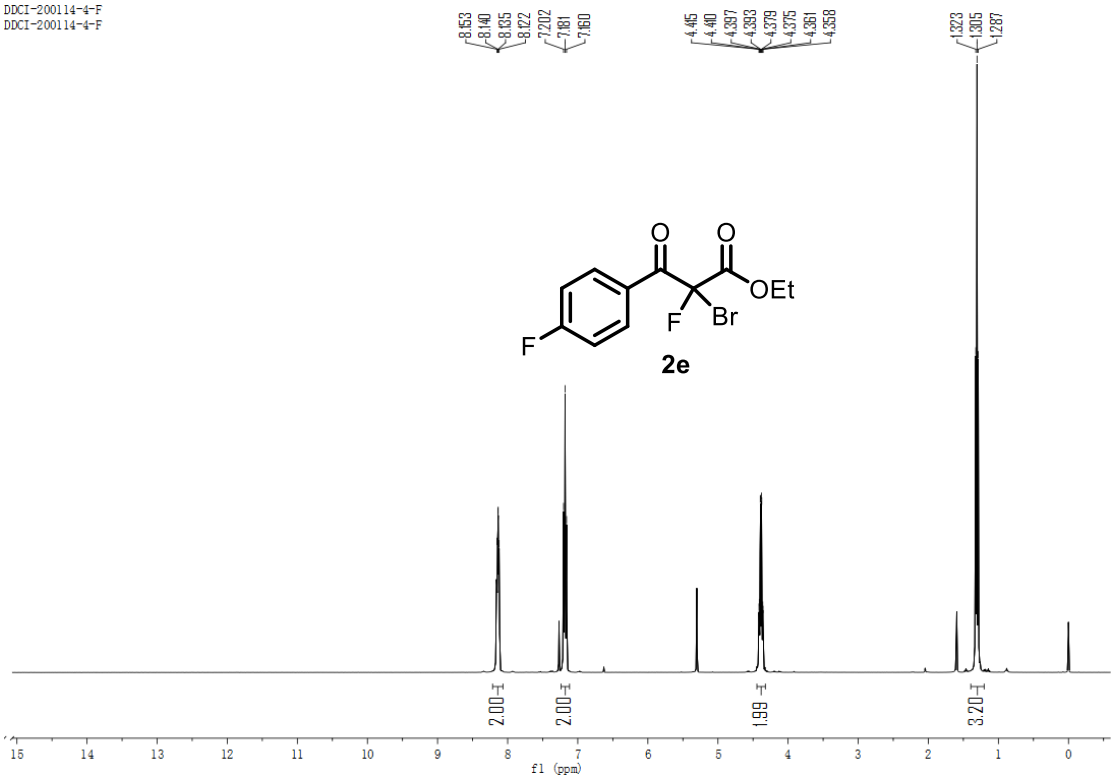


^{13}C NMR (100 MHz, $CDCl_3$):

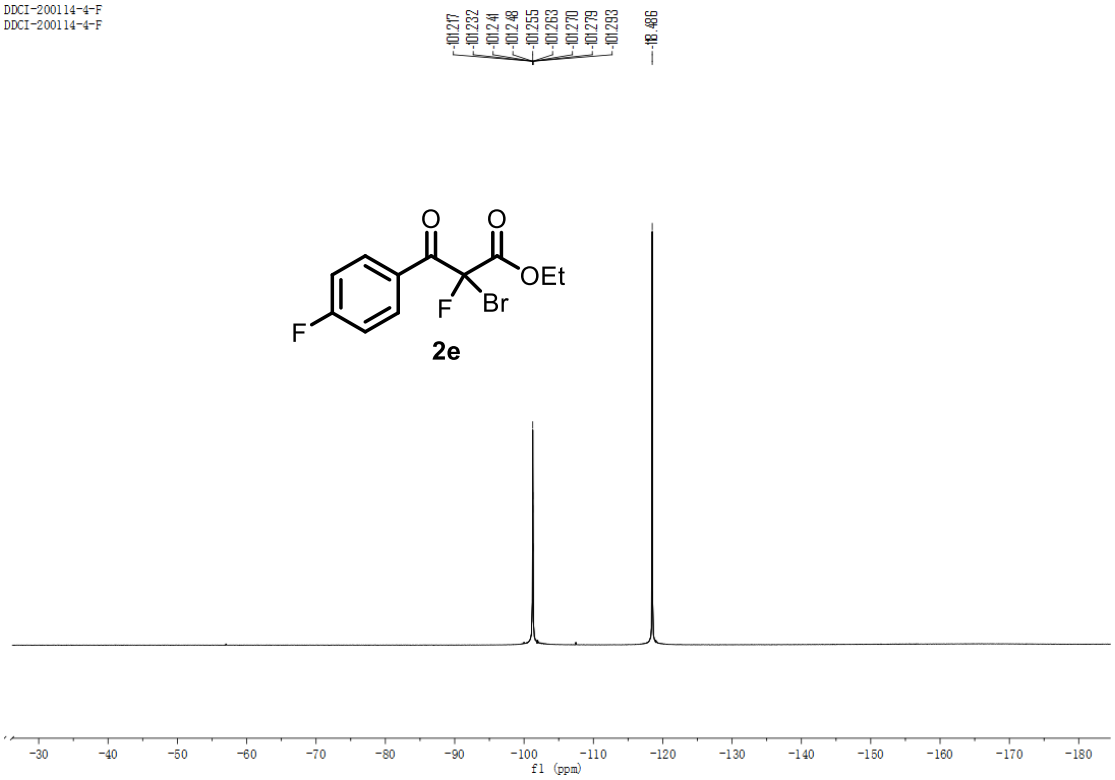


ethyl 2-bromo-2-fluoro-3-(4-fluorophenyl)-3-oxopropanoate (2e)

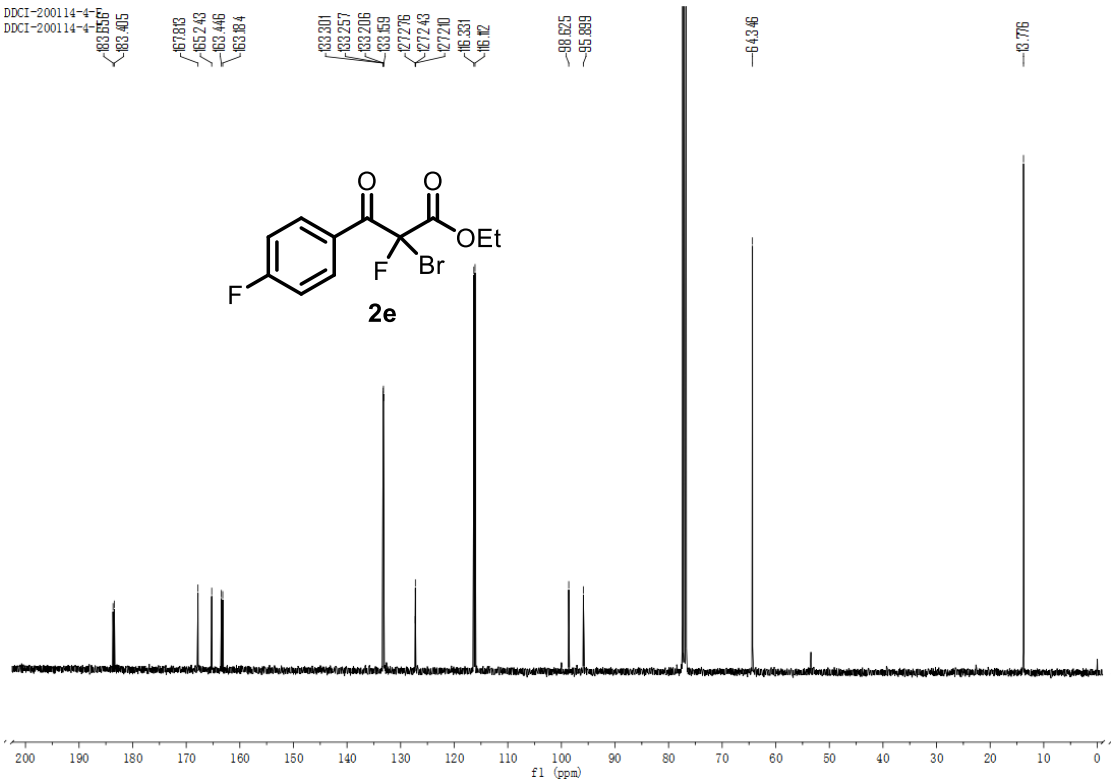
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

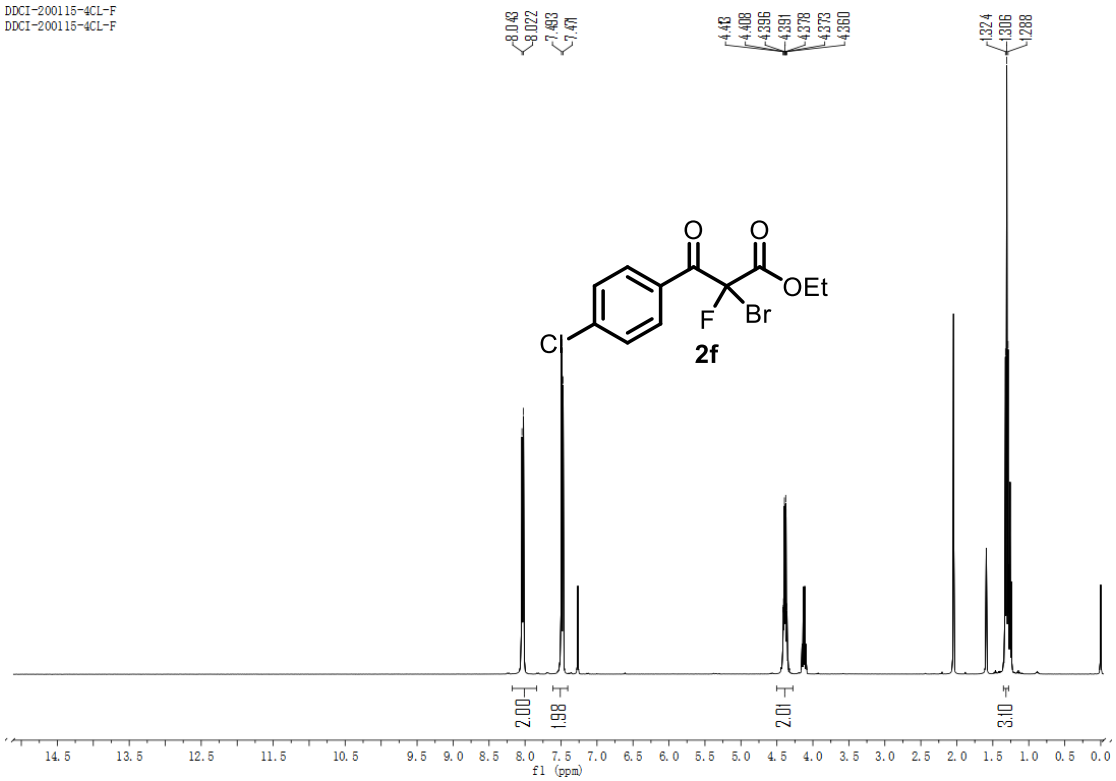


^{13}C NMR (100 MHz, $CDCl_3$):

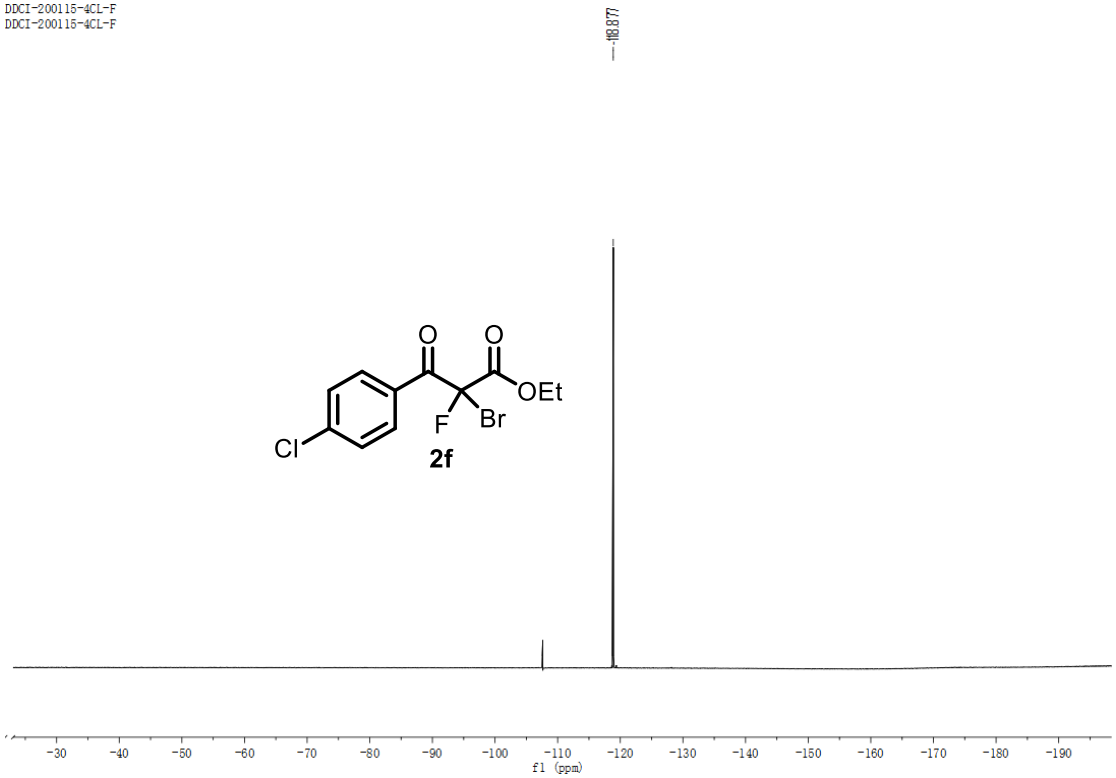


ethyl 2-bromo-3-(4-chlorophenyl)-2-fluoro-3-oxopropanoate (2f)

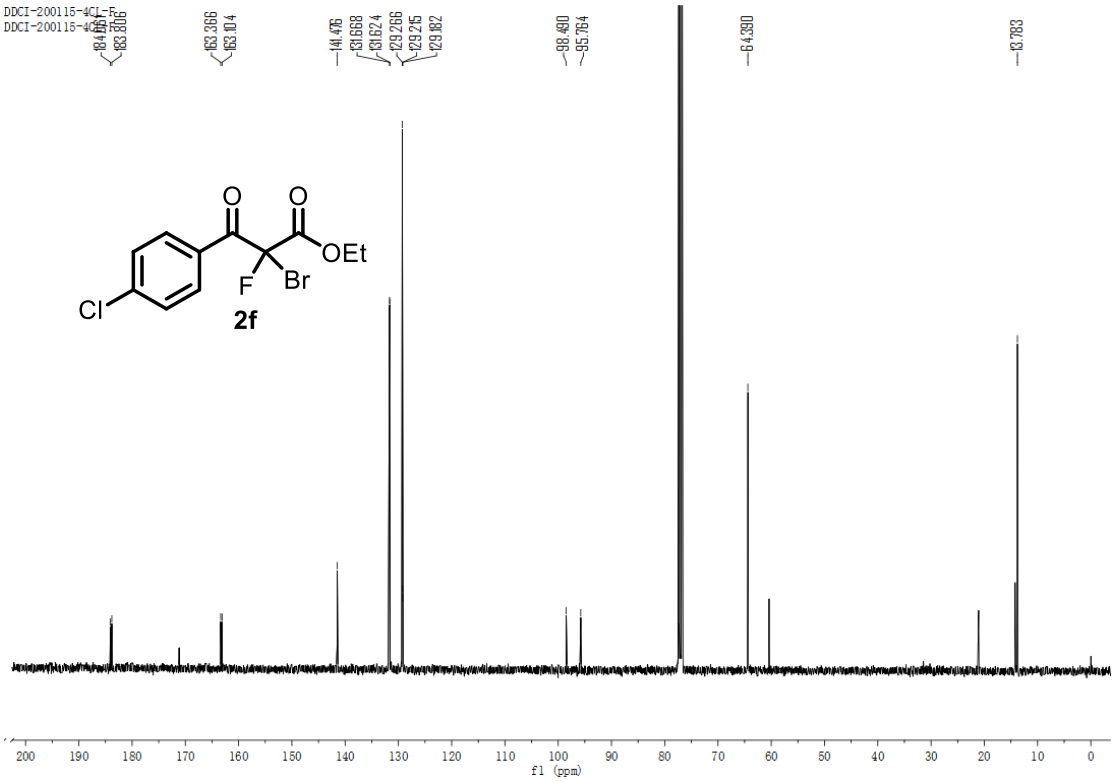
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

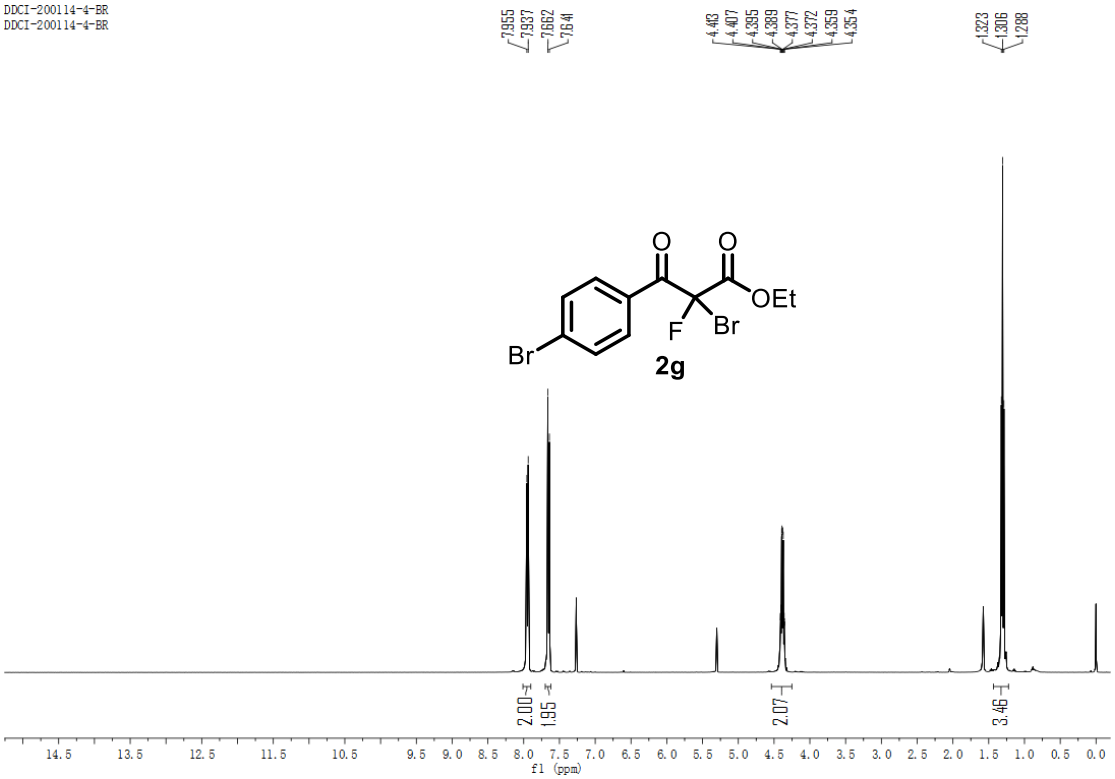


^{13}C NMR (100 MHz, $CDCl_3$):

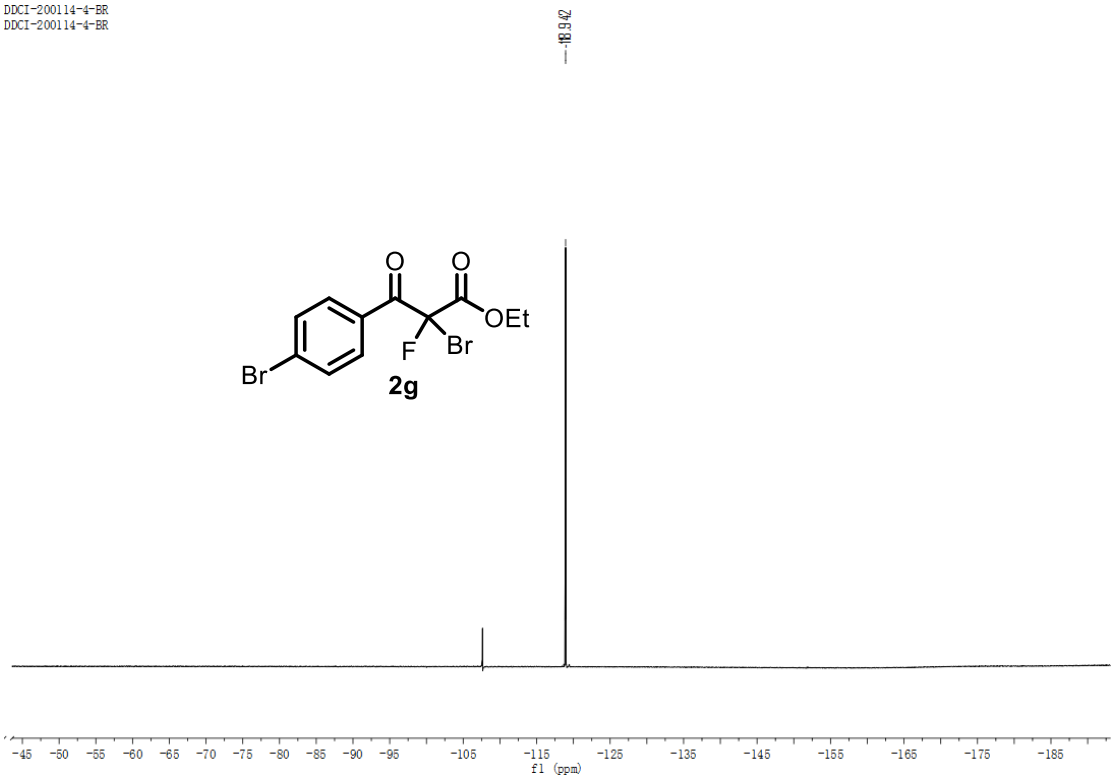


ethyl 2-bromo-3-(4-bromophenyl)-2-fluoro-3-oxopropanoate (2g)

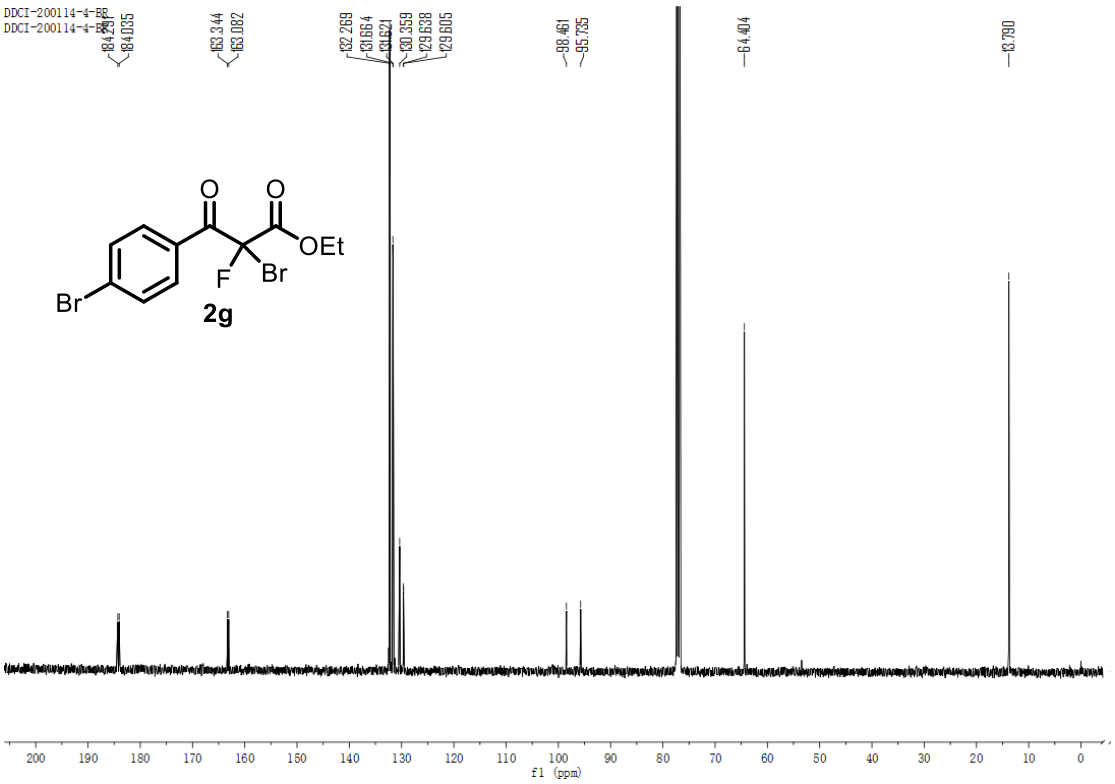
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

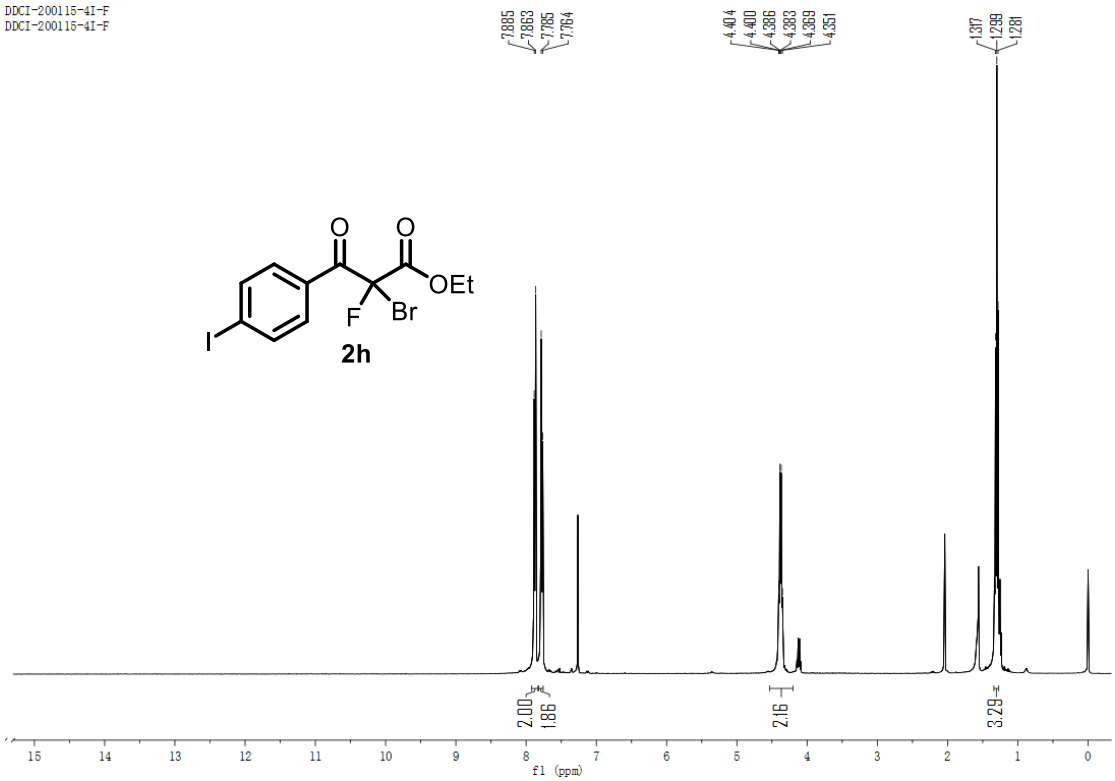


^{13}C NMR (100 MHz, $CDCl_3$):

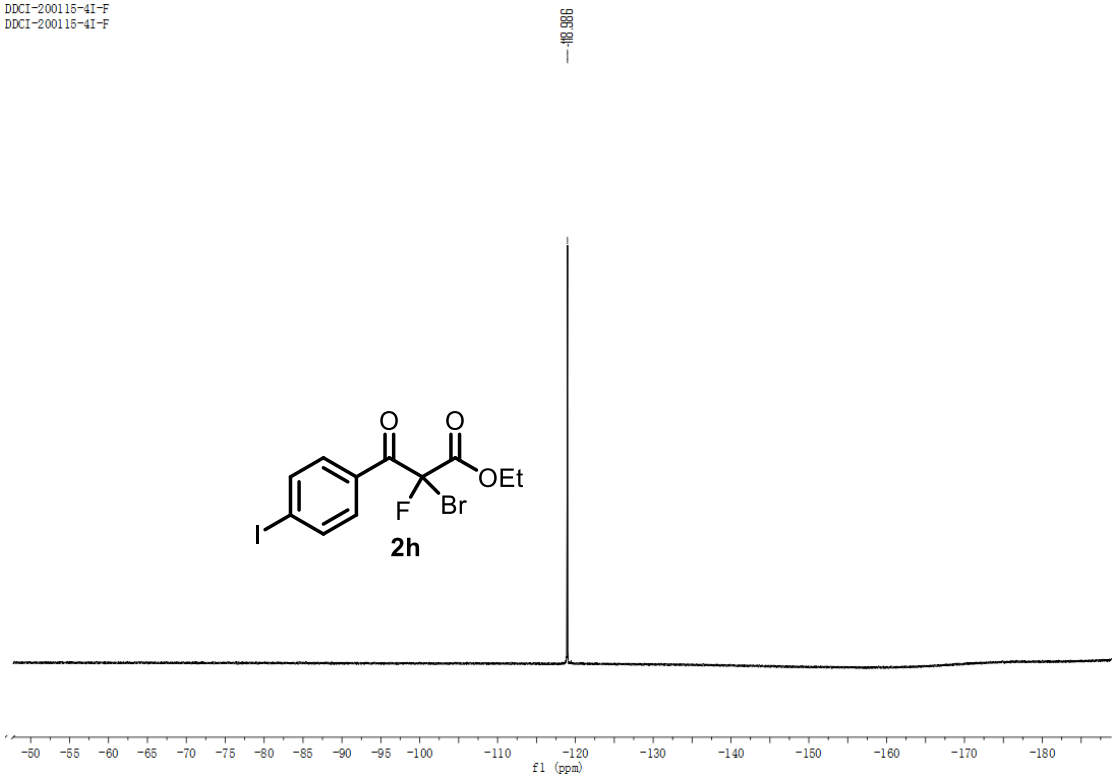


ethyl 2-bromo-2-fluoro-3-(4-iodophenyl)-3-oxopropanoate (2h)

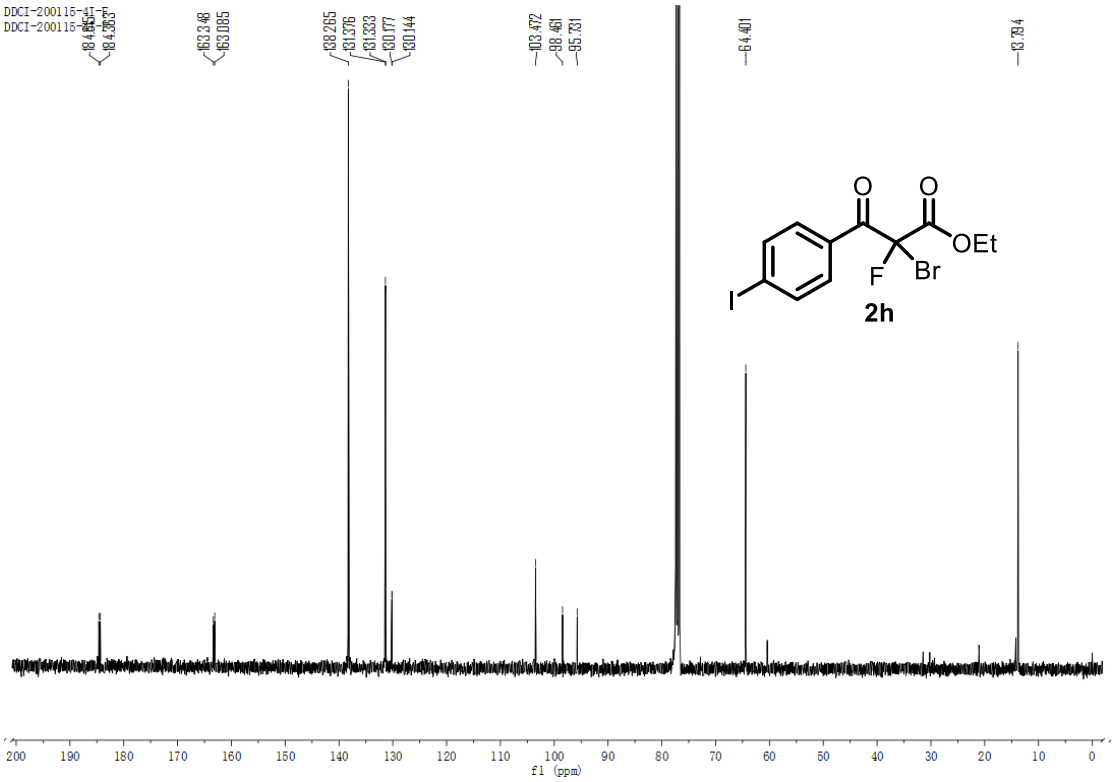
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

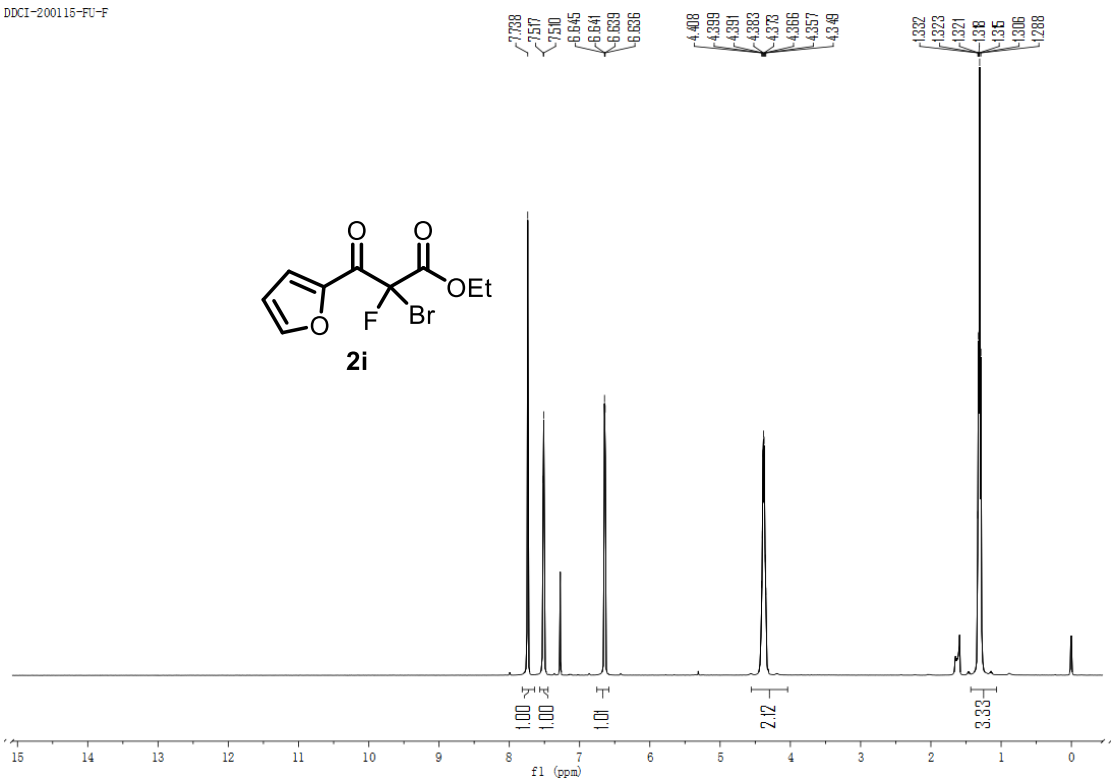


^{13}C NMR (100 MHz, $CDCl_3$):

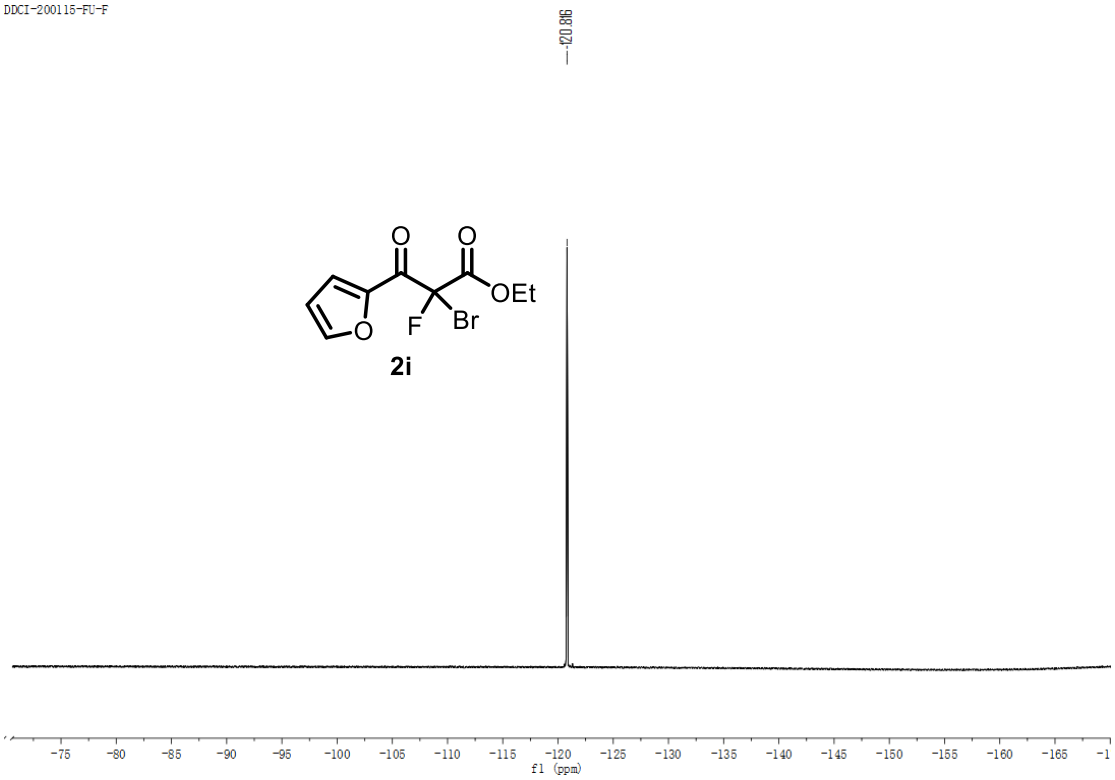


ethyl 2-bromo-2-fluoro-3-(furan-2-yl)-3-oxopropanoate (2i)

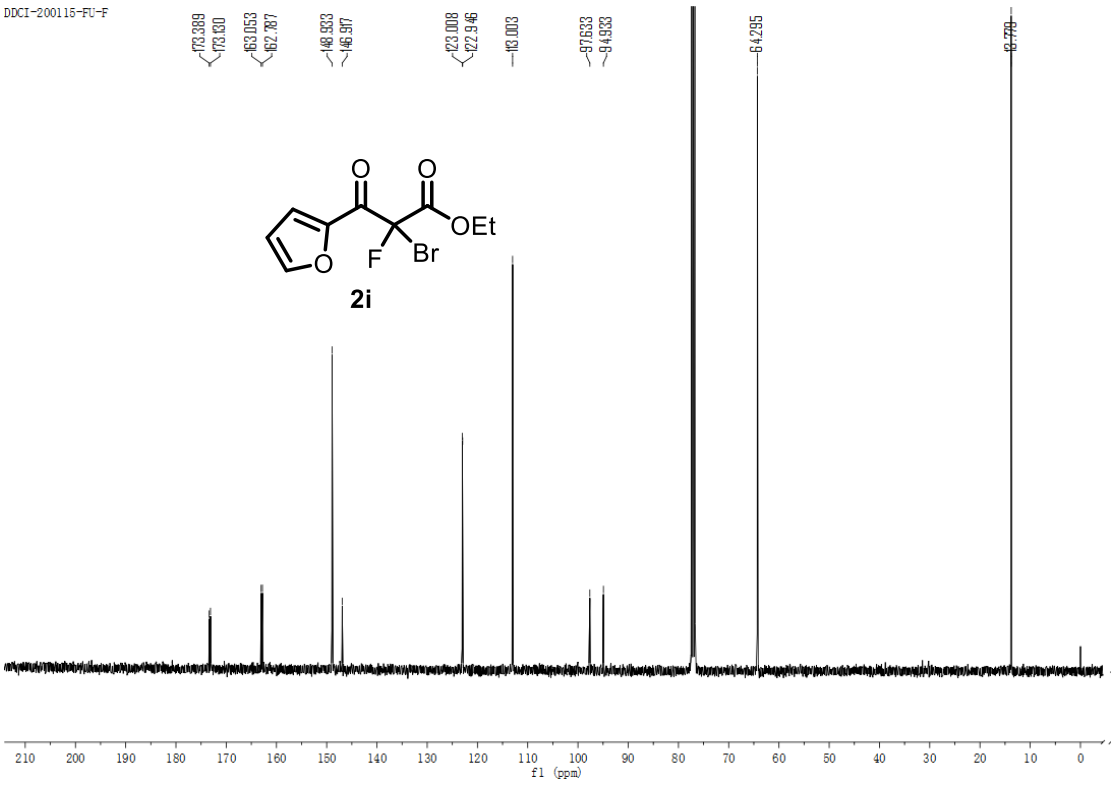
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

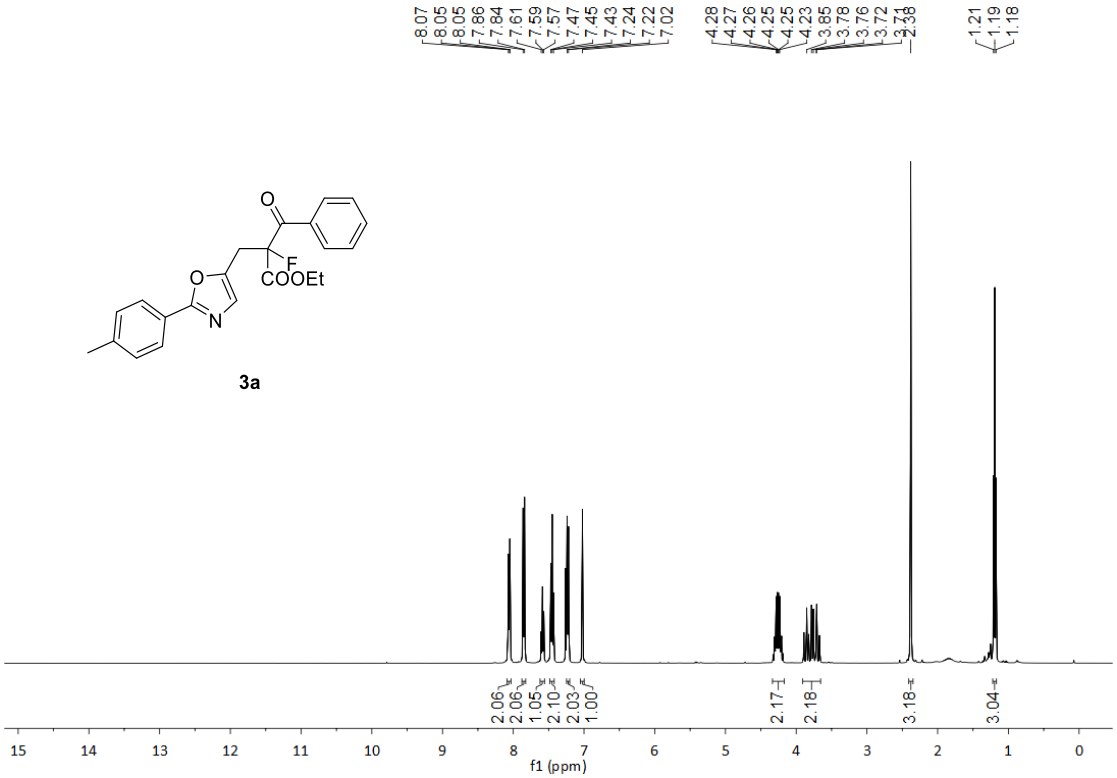


^{13}C NMR (100 MHz, $CDCl_3$):



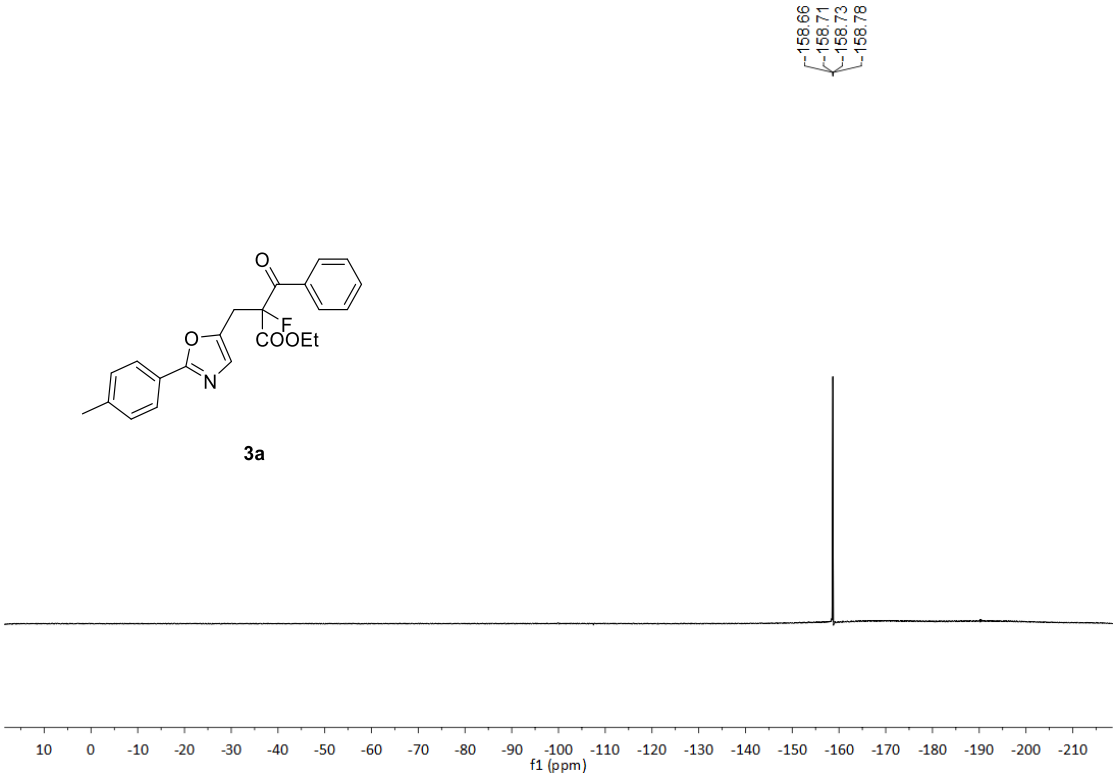
ethyl 2-fluoro-3-oxo-3-phenyl-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propanoate (3a)

^{1}H NMR (400 MHz, $CDCl_3$)：



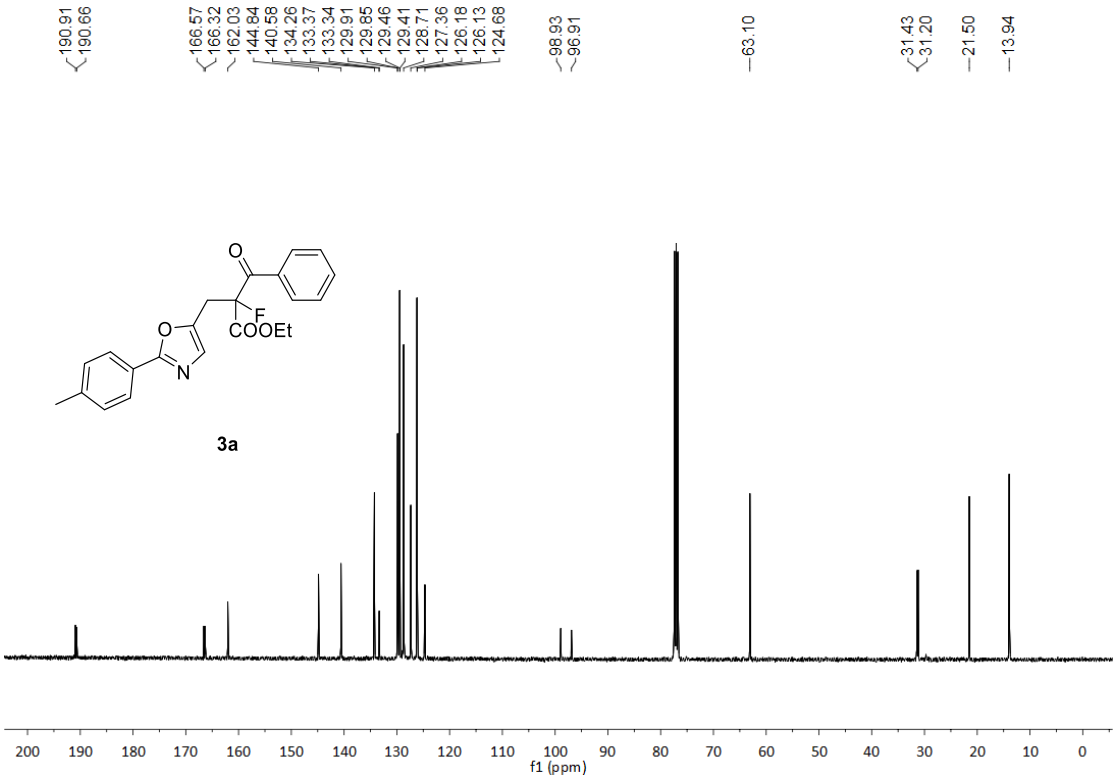
3a

^{19}F NMR (376 MHz, $CDCl_3$):



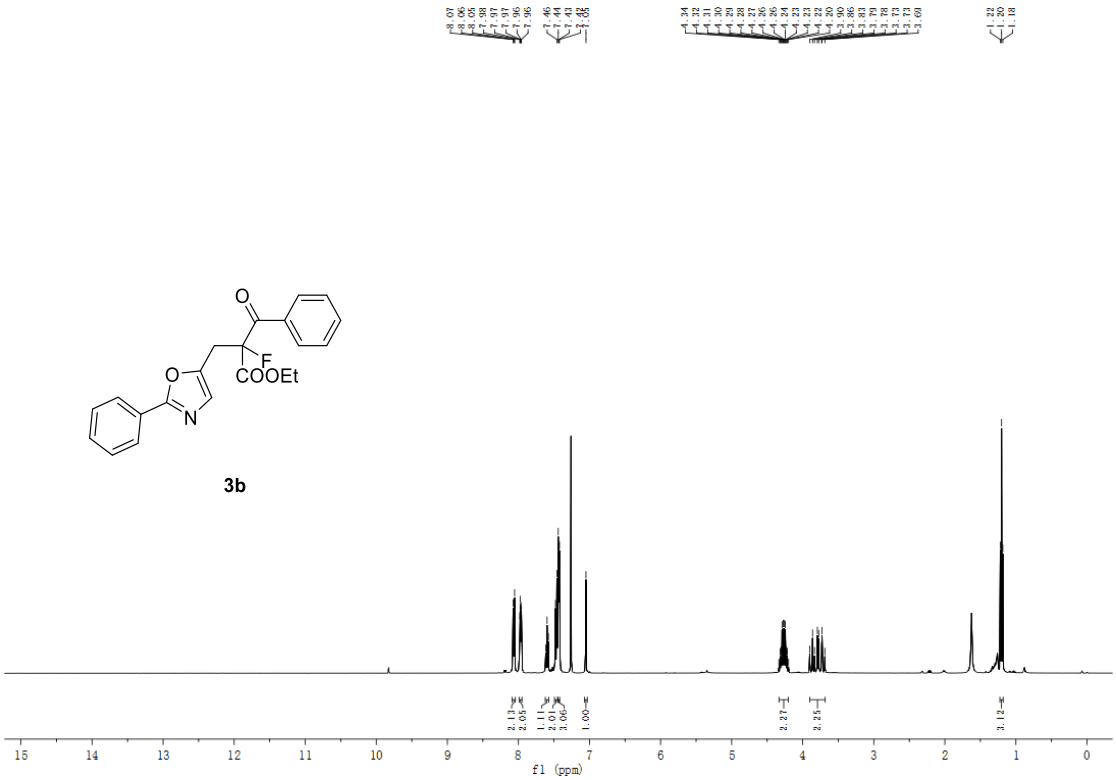
3a

^{13}C NMR (100 MHz, $CDCl_3$):

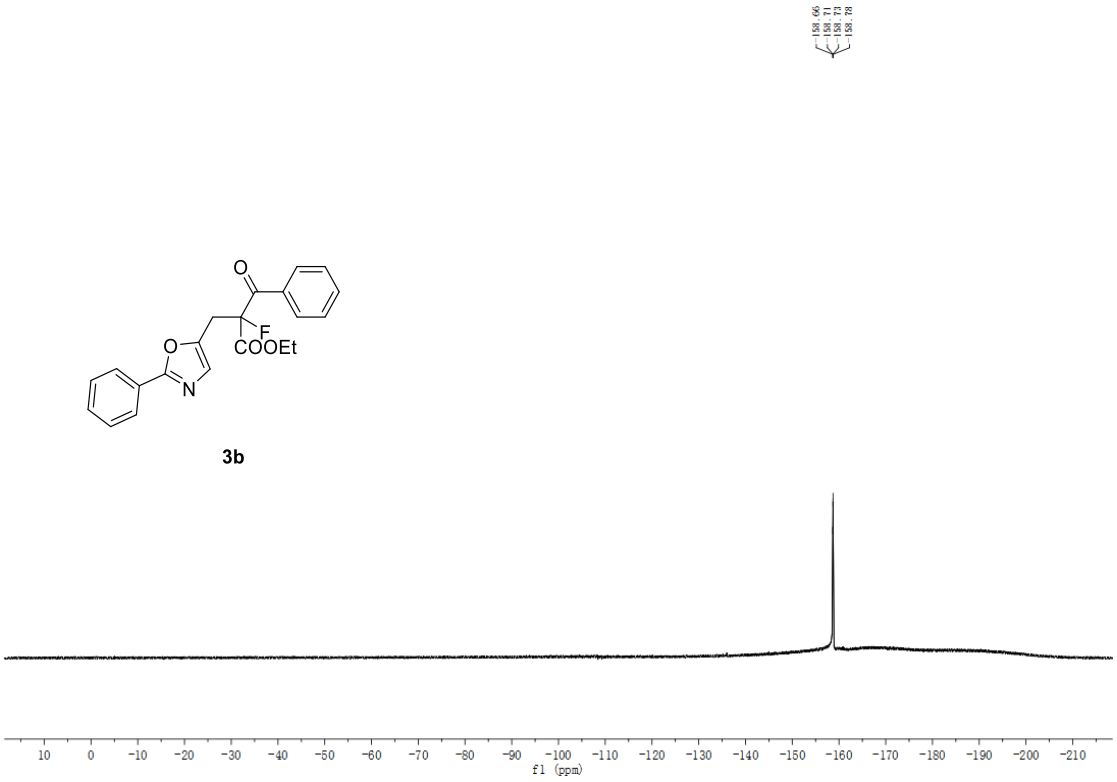


ethyl 2-fluoro-3-oxo-3-phenyl-2-((2-phenyloxazol-5-yl)methyl)propanoate (3b)

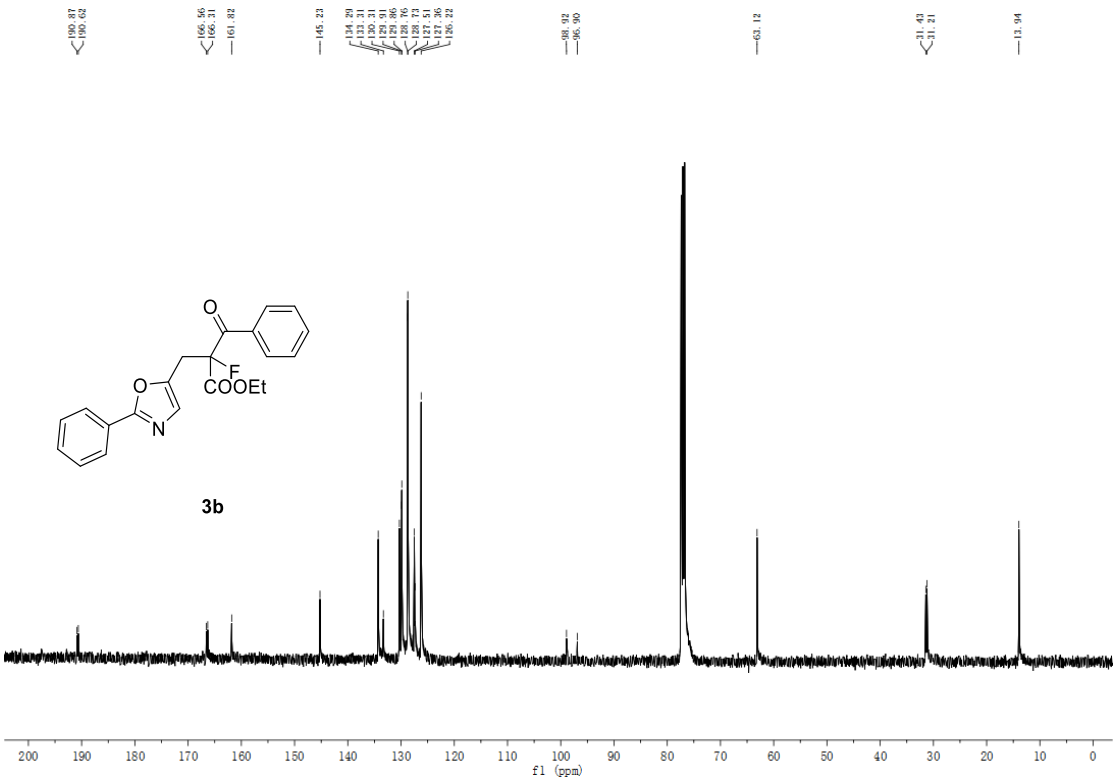
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

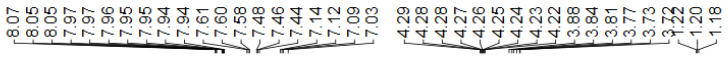


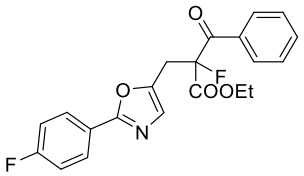
^{13}C NMR (100 MHz, $CDCl_3$):



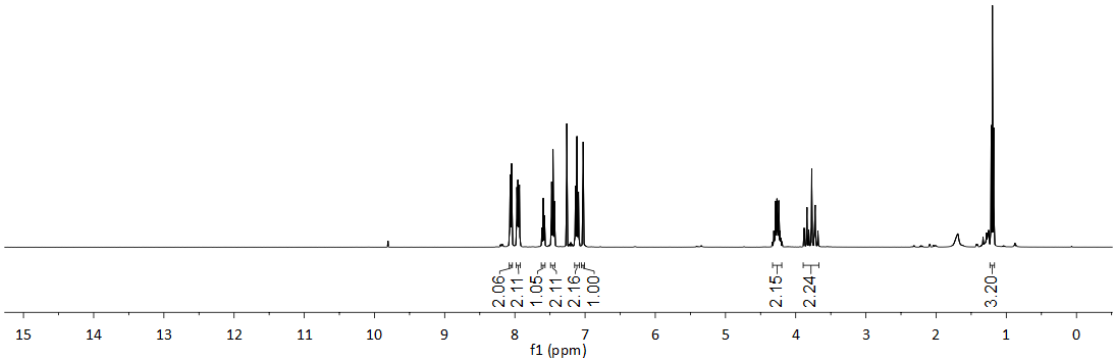
ethyl 2-fluoro-2-((2-(4-fluorophenyl)oxazol-5-yl)methyl)-3-oxo-3-phenylpropano-ate (3c)

^{1}H NMR (400 MHz, $CDCl_3$)：

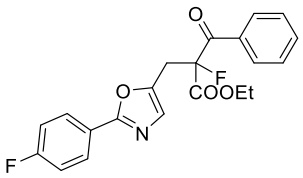




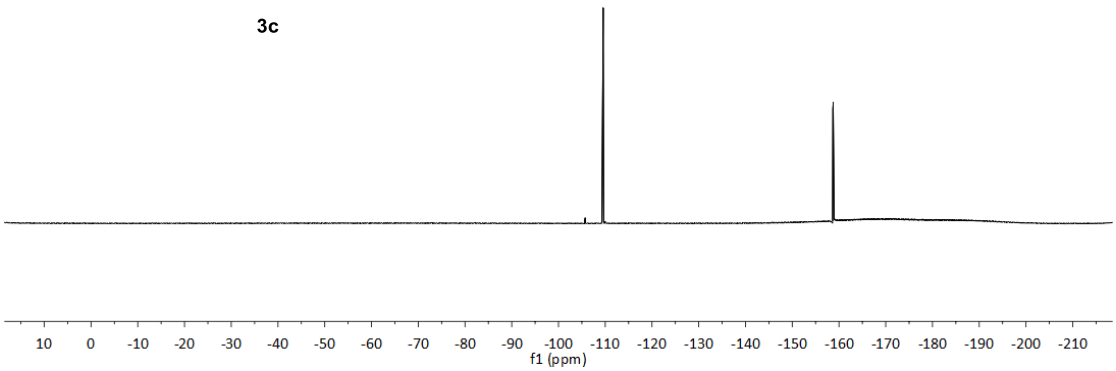
3c



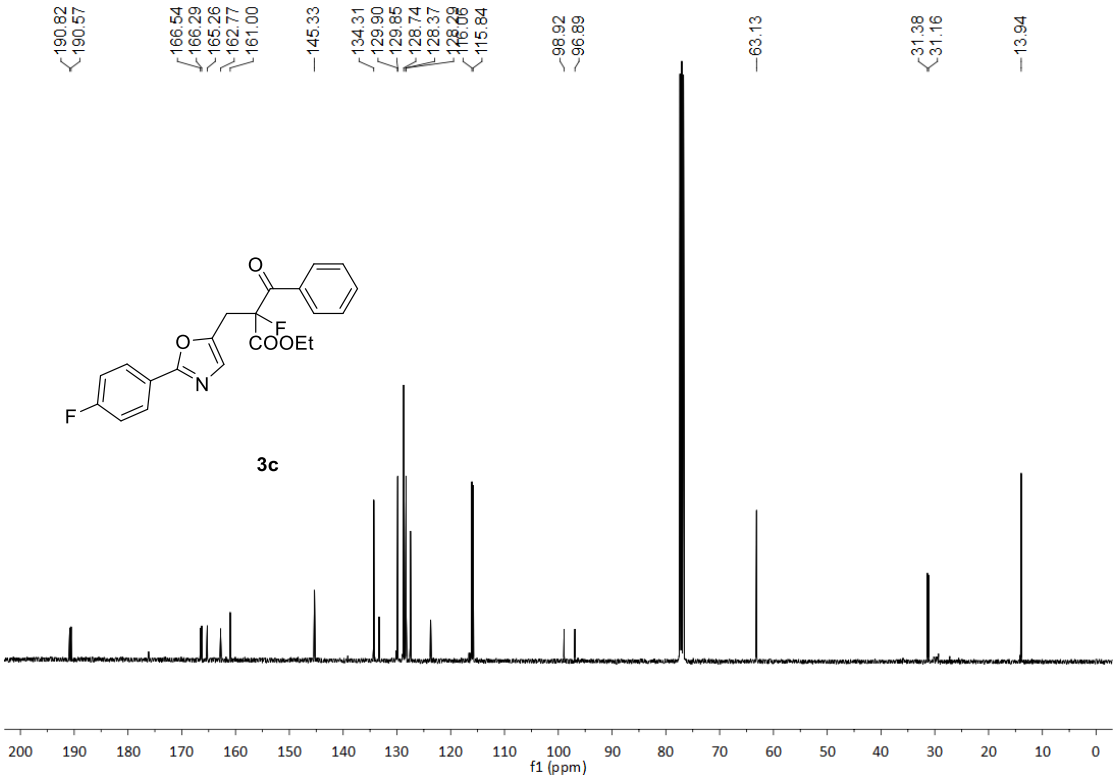
^{19}F NMR (376 MHz, $CDCl_3$):



3c

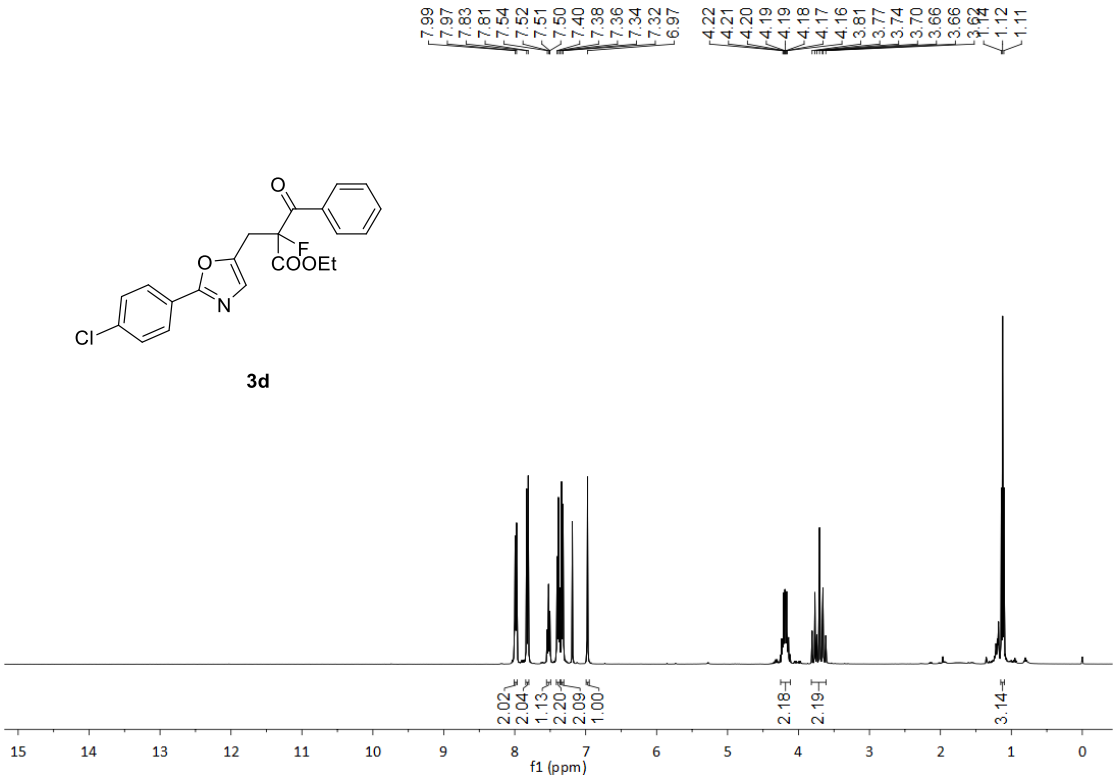


^{13}C NMR (100 MHz, $CDCl_3$):

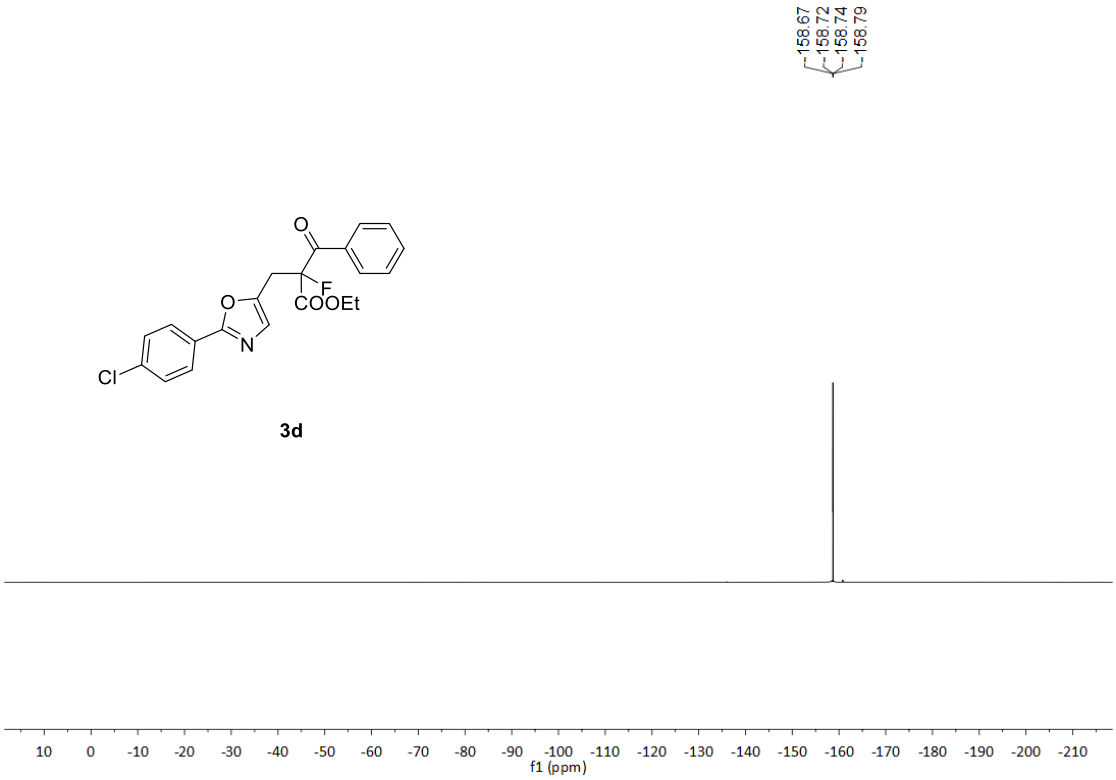


ethyl 2-((2-(4-chlorophenyl)oxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenylpropano-ate (3d)

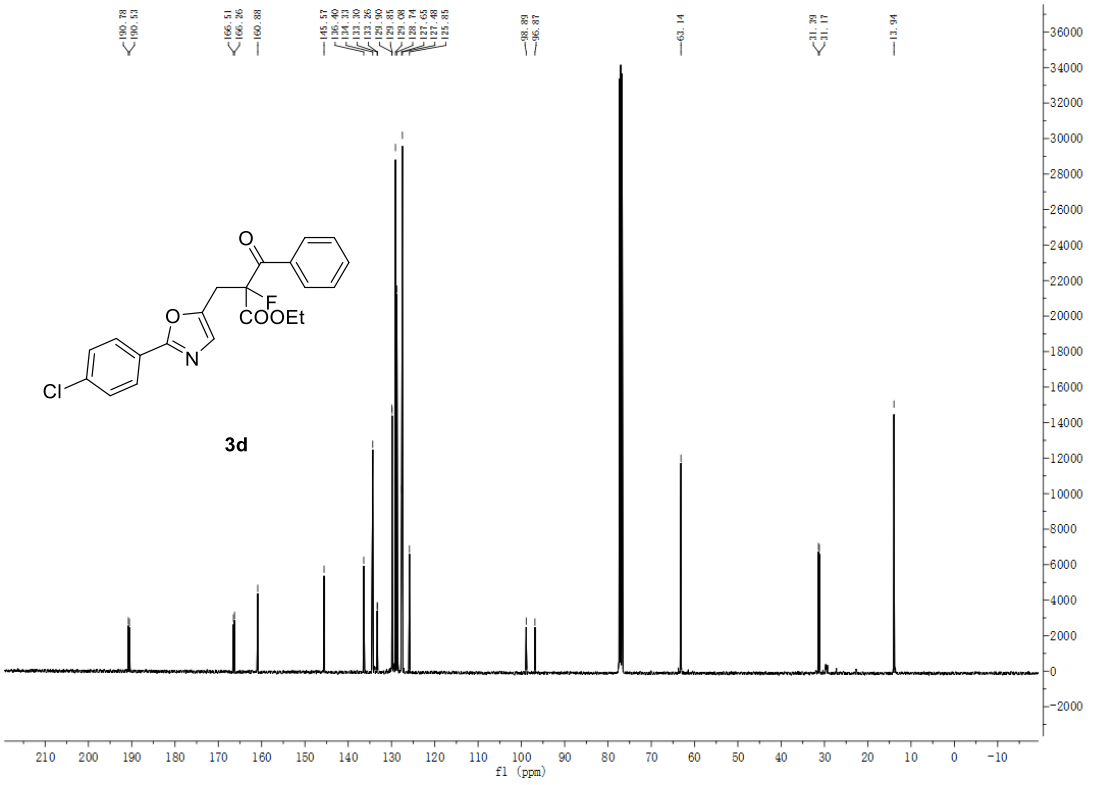
^{1}H NMR (400 MHz, $CDCl_3$):



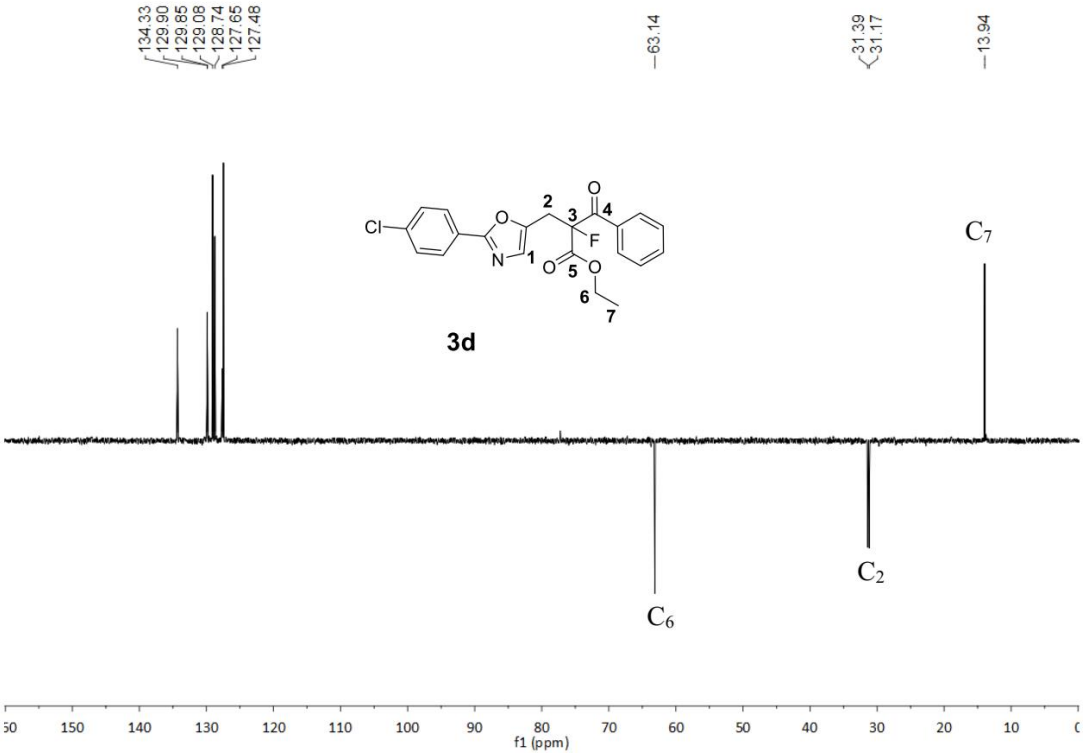
^{19}F NMR (376 MHz, $CDCl_3$):



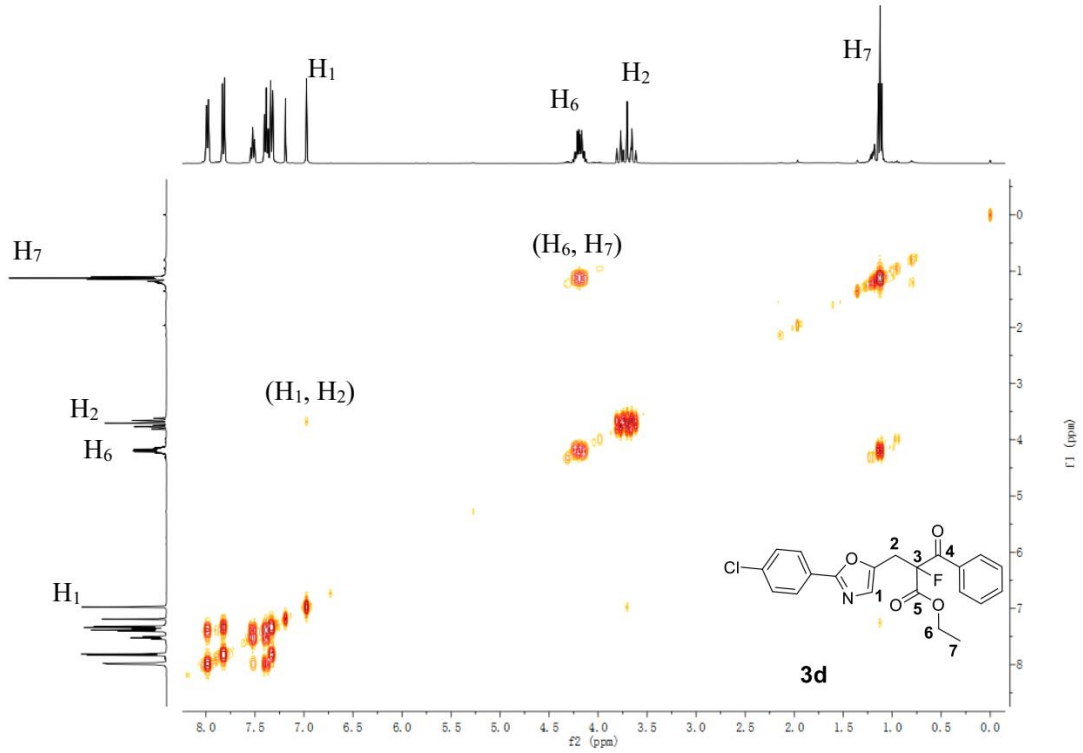
^{13}C NMR (100 MHz, $CDCl_3$):



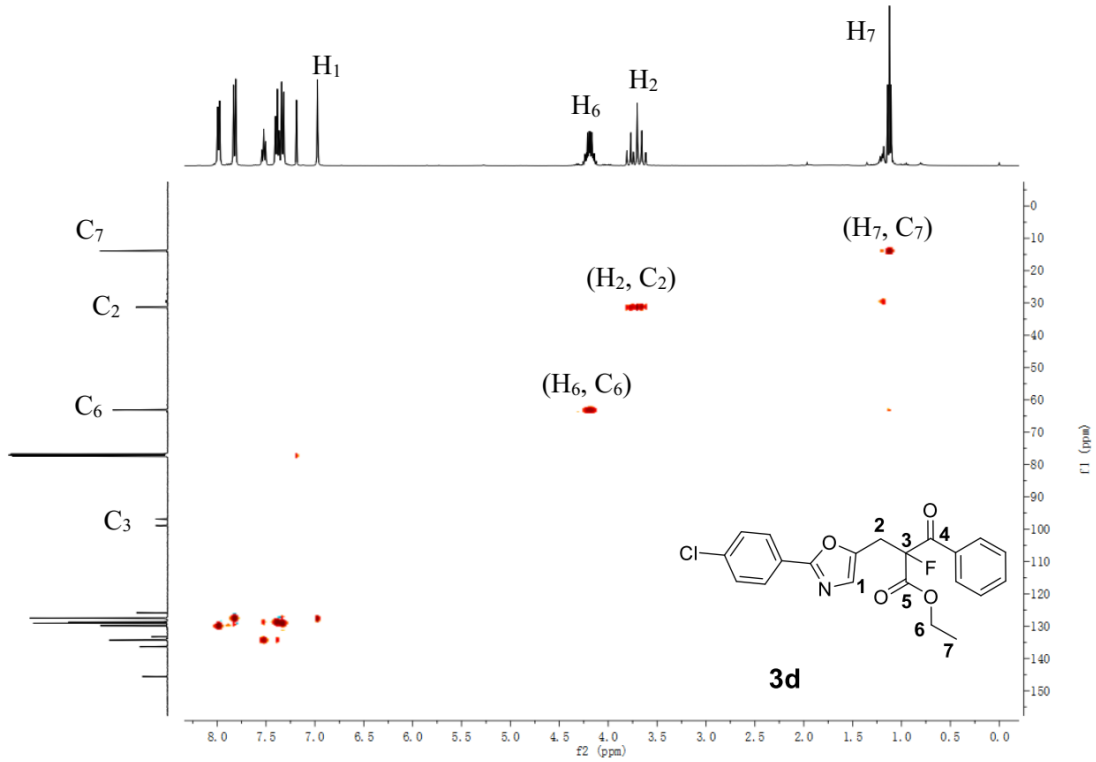
DEPT 135:



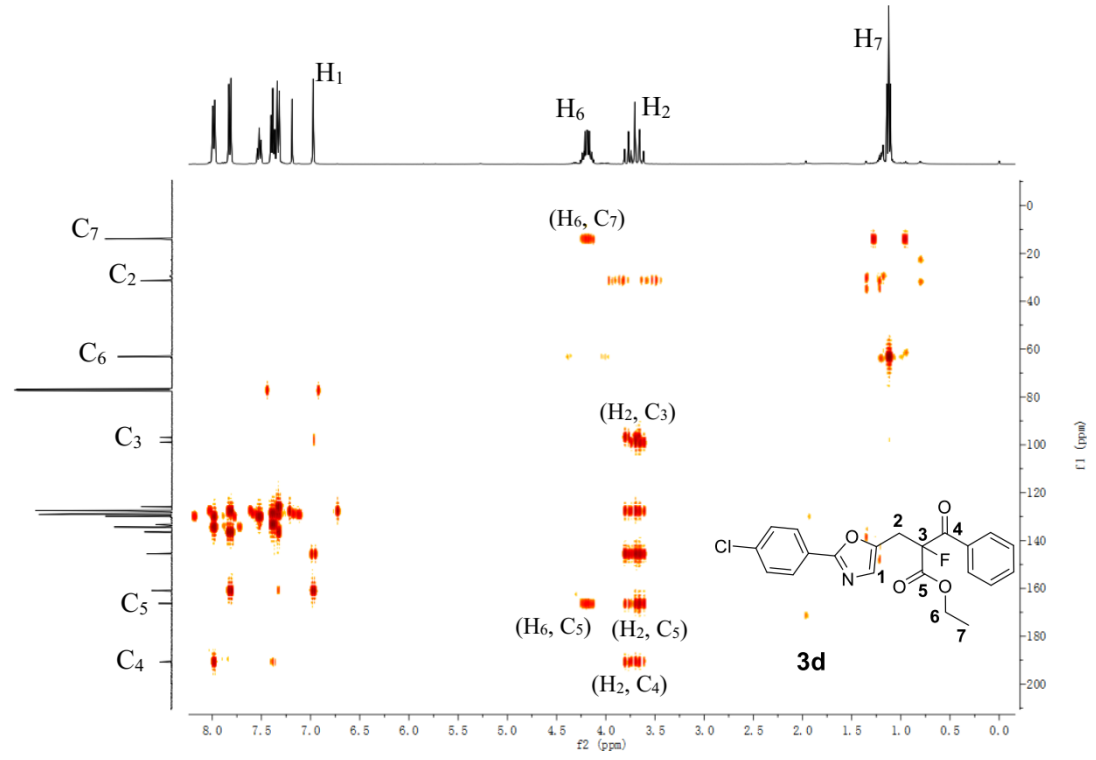
NOESY:



HSQC:

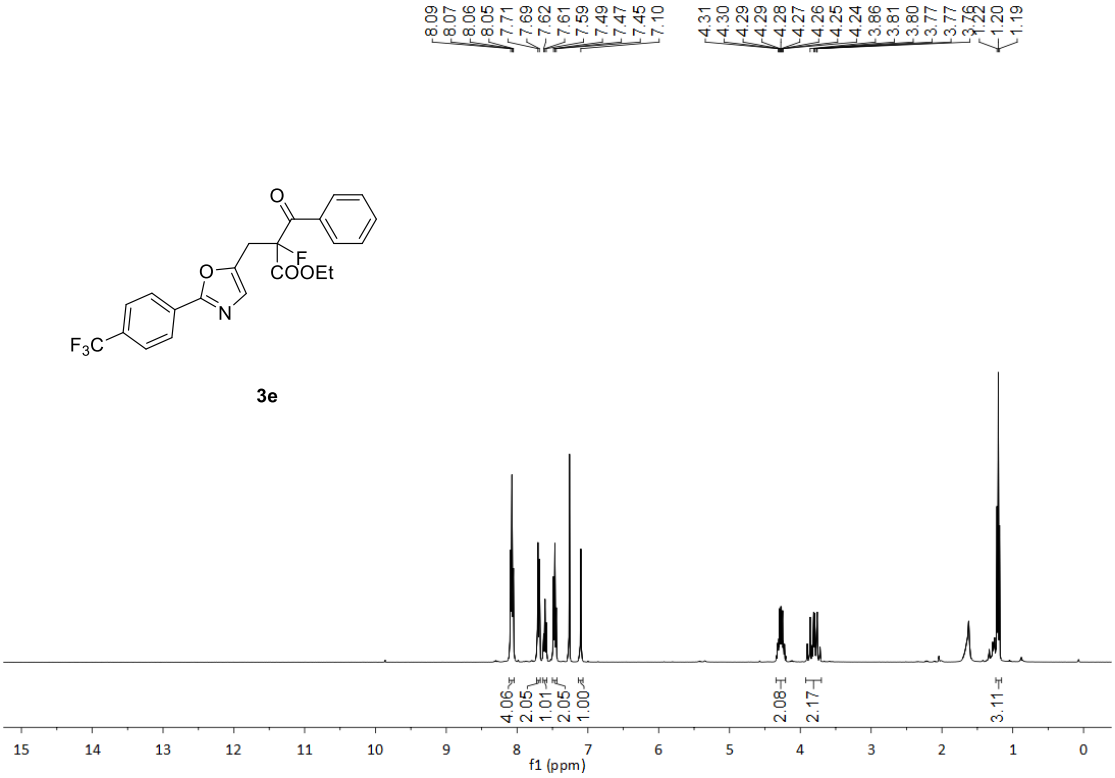

H1
H6
H2
H7
C7
C2
C6
C3
(H7, C7)
(H2, C2)
(H6, C6)
Cl
O
N
F
1
2
3
4
5
6
7
3d
f2 (ppm)
f1 (ppm)

HMBC:

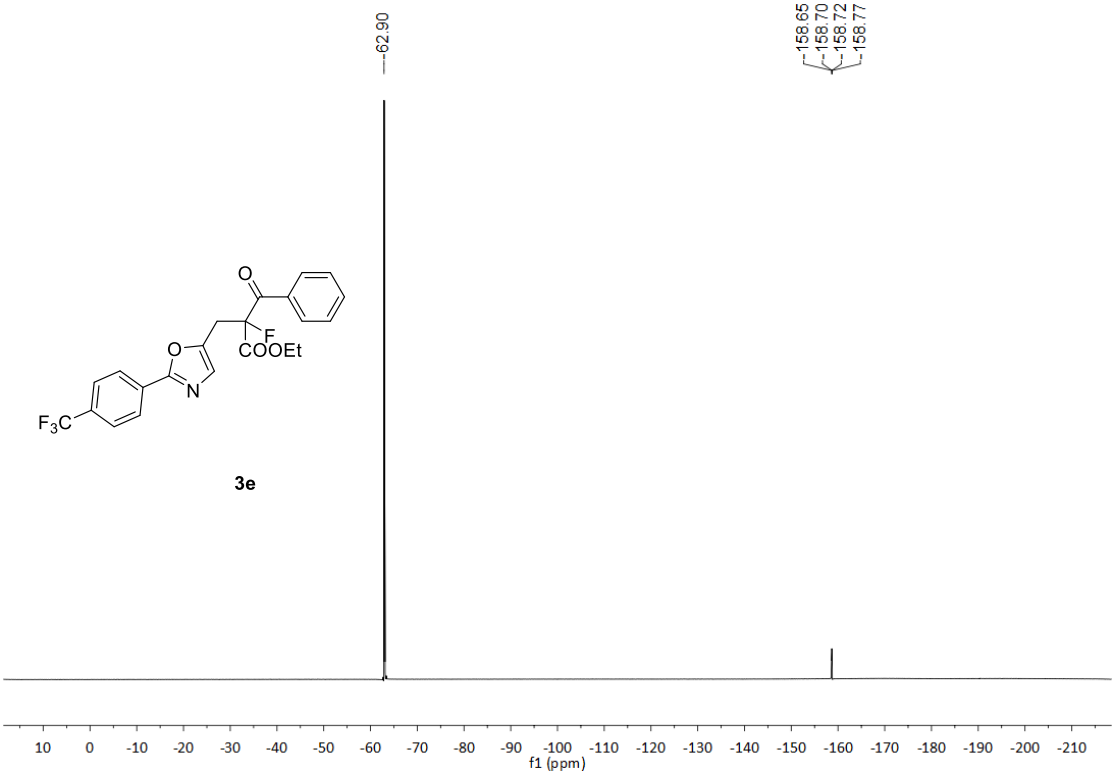

H1
H6
H2
H7
C7
C2
C6
C3
C5
C4
(H6, C7)
(H2, C3)
(H6, C5)
(H2, C5)
(H2, C4)
Cl
O
N
F
1
2
3
4
5
6
7
3d
f2 (ppm)
f1 (ppm)

ethyl 2-fluoro-3-oxo-3-phenyl-2-((2-(4-(trifluoromethyl)phenyl)oxazol-5-yl)meth-yl) propanoate (3e)

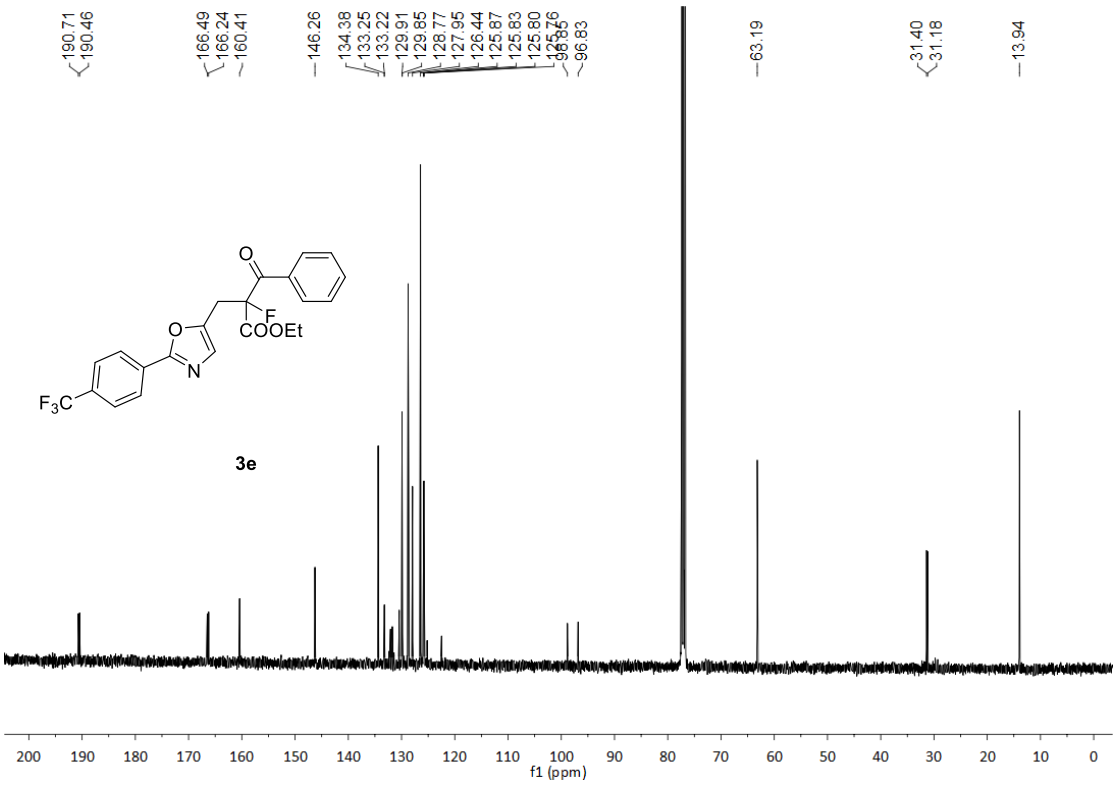
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

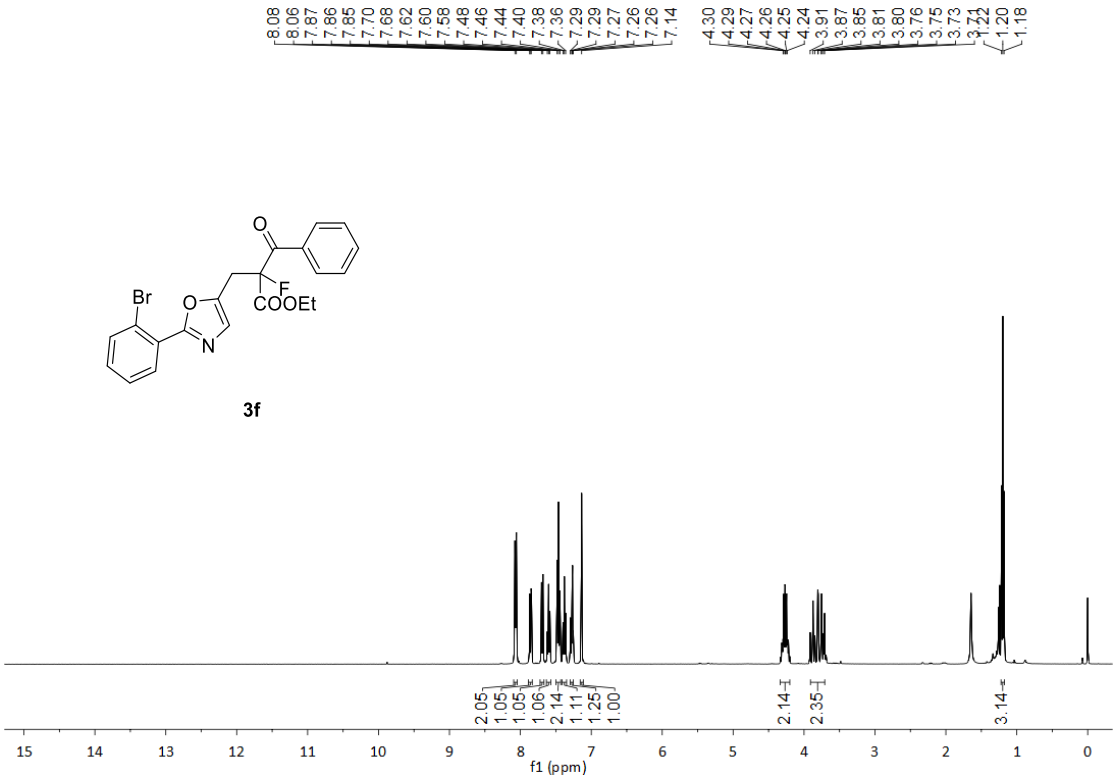


^{13}C NMR (100 MHz, $CDCl_3$):

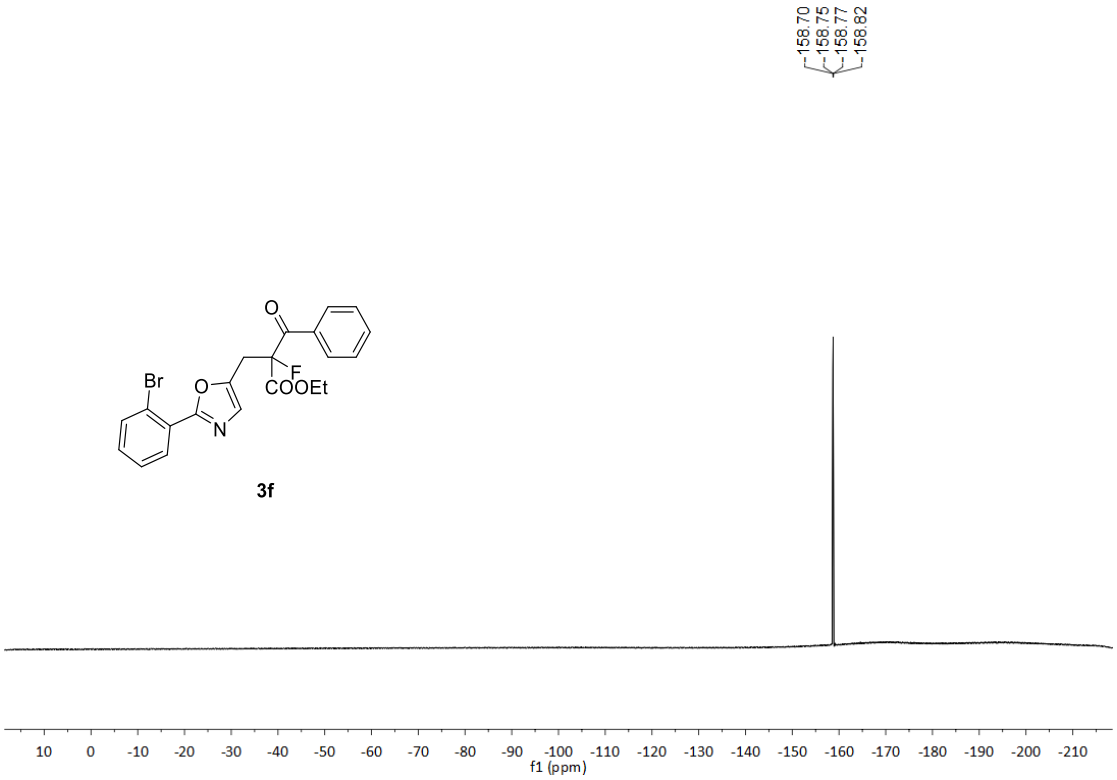


ethyl 2-((2-(2-bromophenyl)oxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenylpropano-ate (3f)

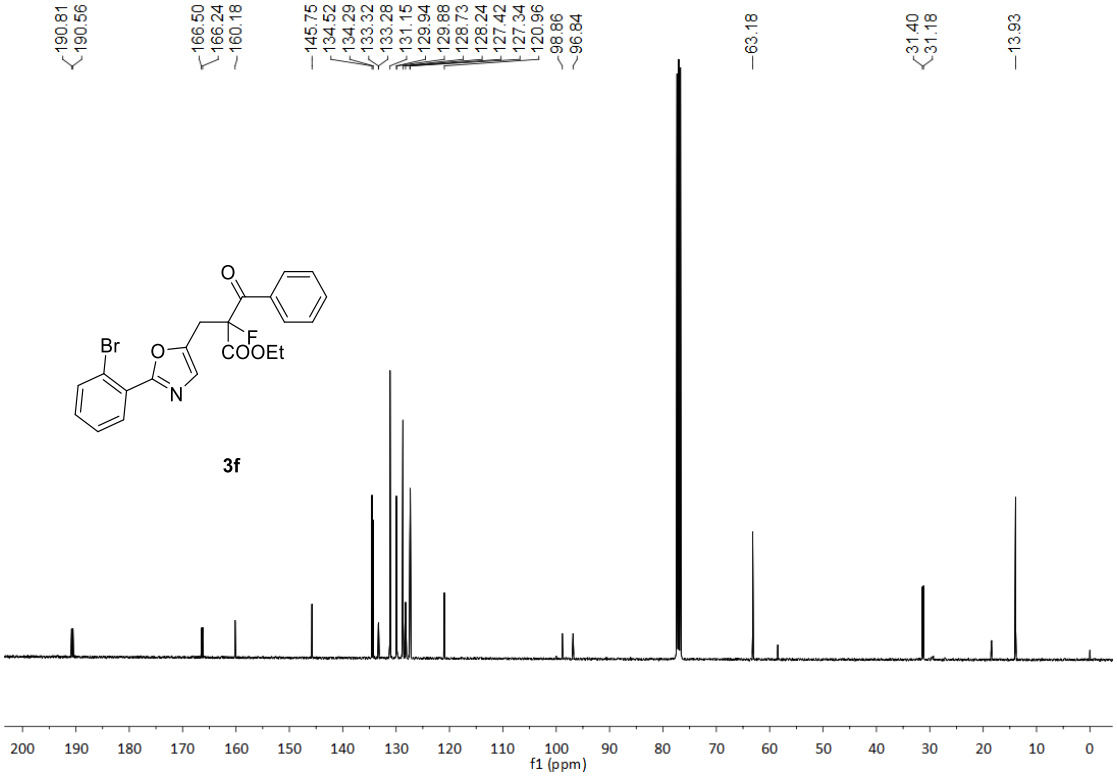
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

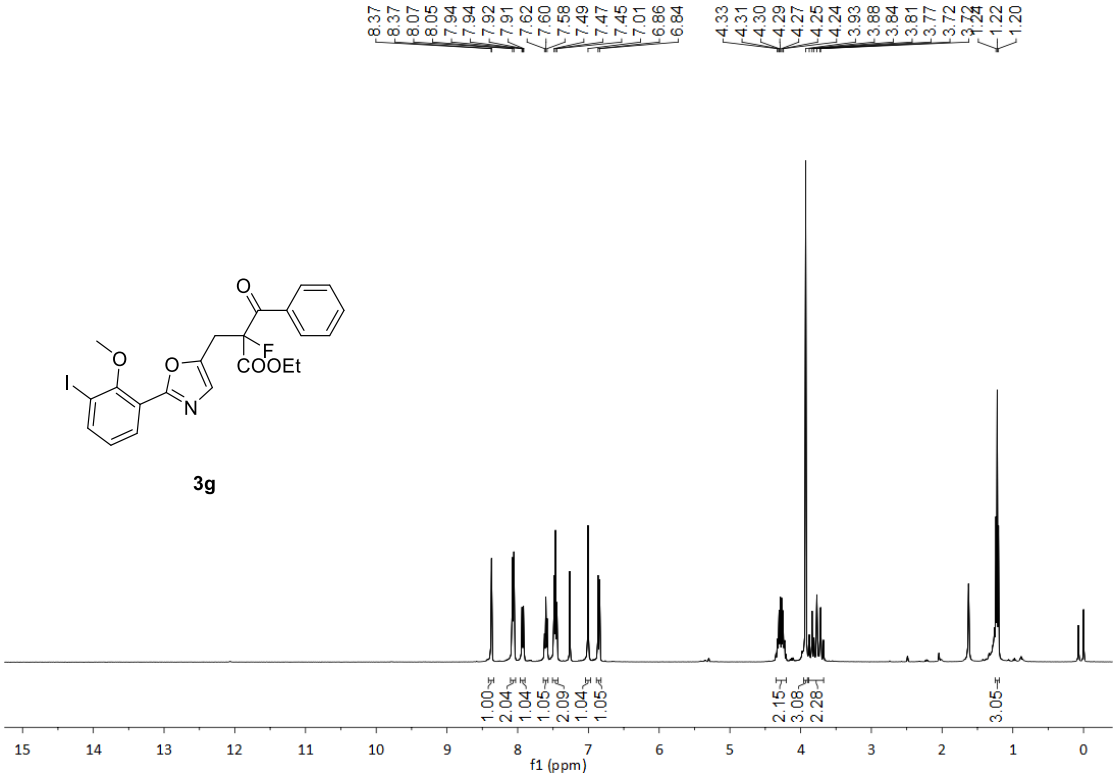


^{13}C NMR (100 MHz, $CDCl_3$):

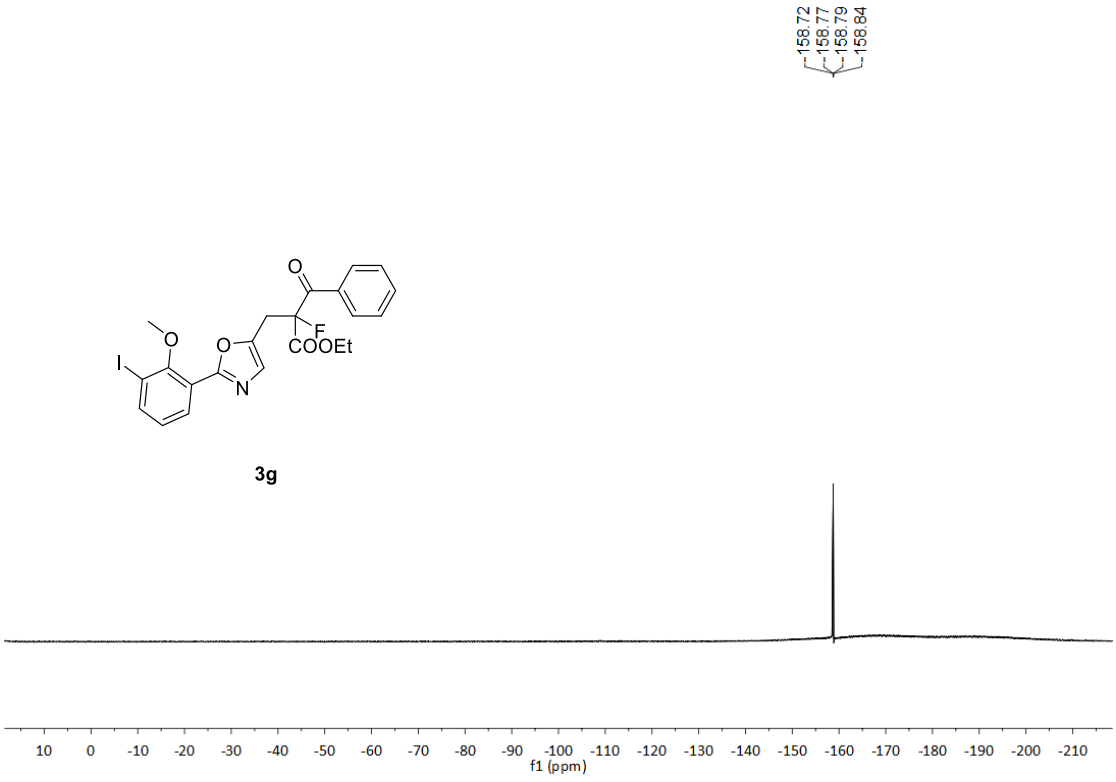


ethyl 2-fluoro-2-((2-(3-iodo-2-methoxyphenyl)oxazol-5-yl)methyl)-3-oxo-3-phen-ylpropanoate (3g)

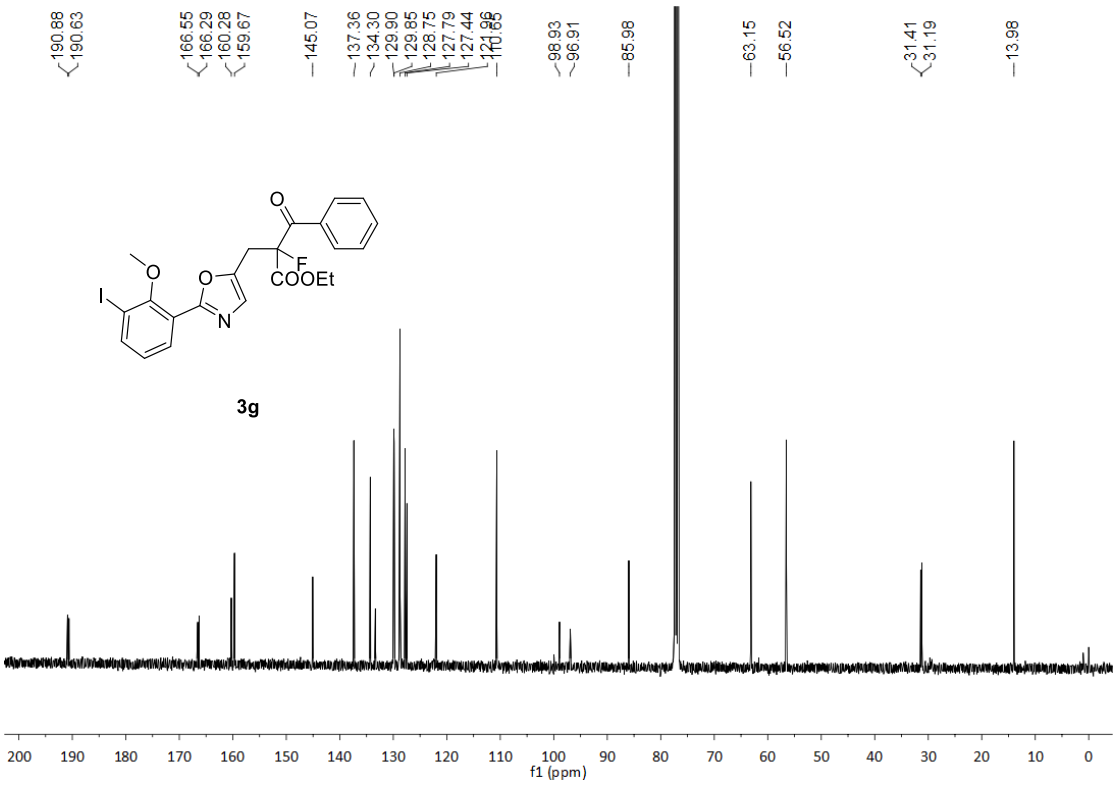
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

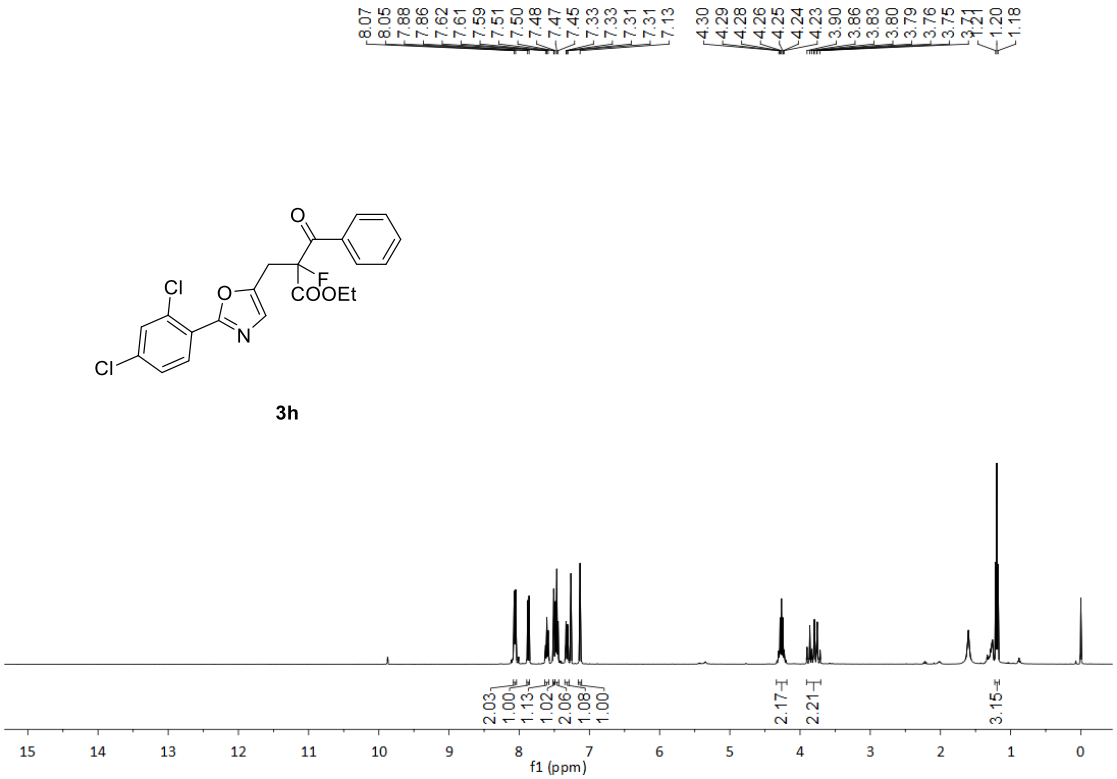


^{13}C NMR (100 MHz, $CDCl_3$):

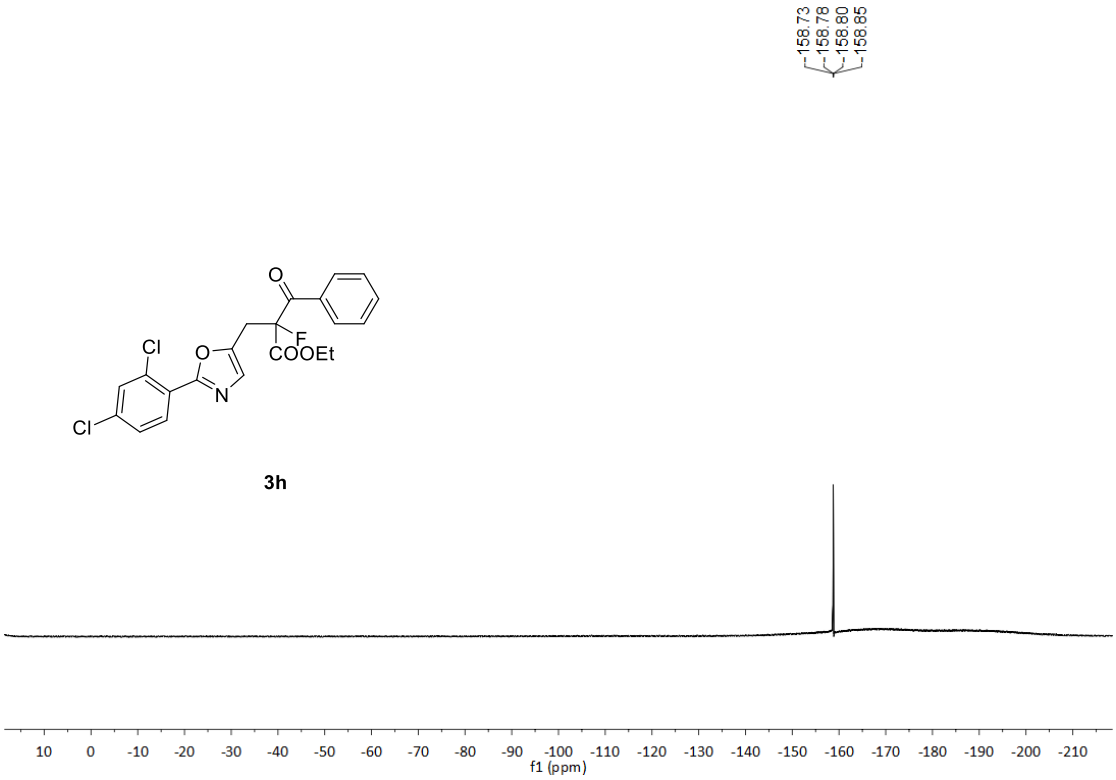


ethyl 2-((2-(2,4-dichlorophenyl)oxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenylpro-panoate (3h)

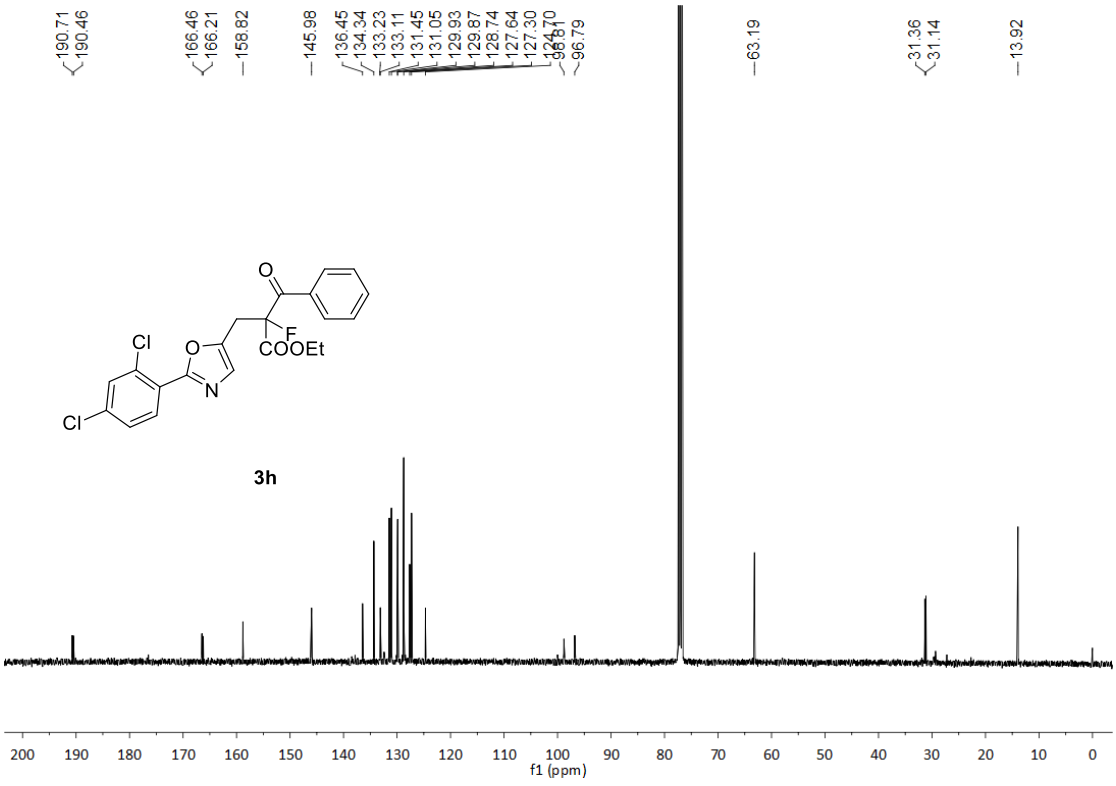
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

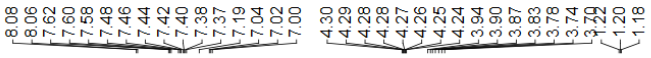


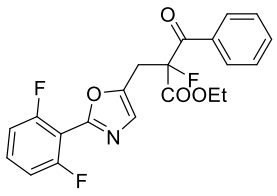
^{13}C NMR (100 MHz, $CDCl_3$):



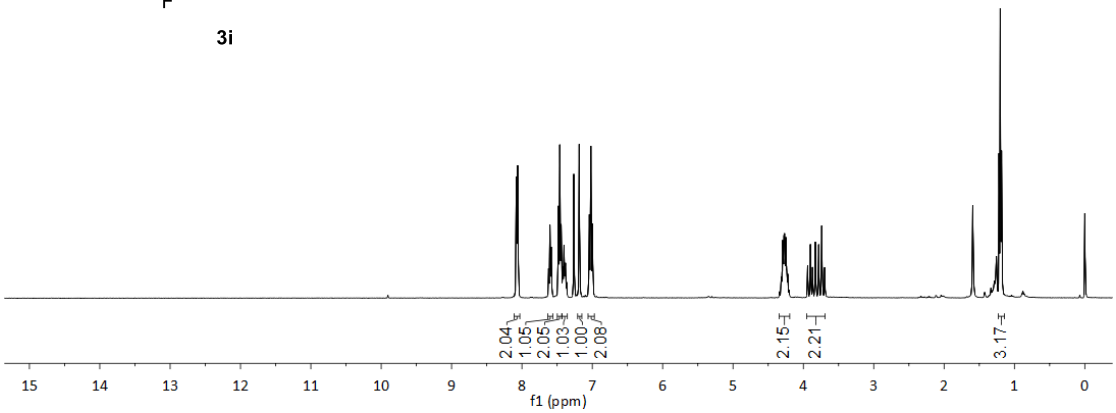
ethyl 2-((2-(2,6-difluorophenyl)oxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenylpro-panoate (3i)

^{1}H NMR (400 MHz, $CDCl_3$)：

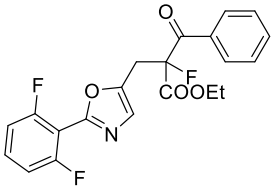




3i



^{19}F NMR (376 MHz, $CDCl_3$):



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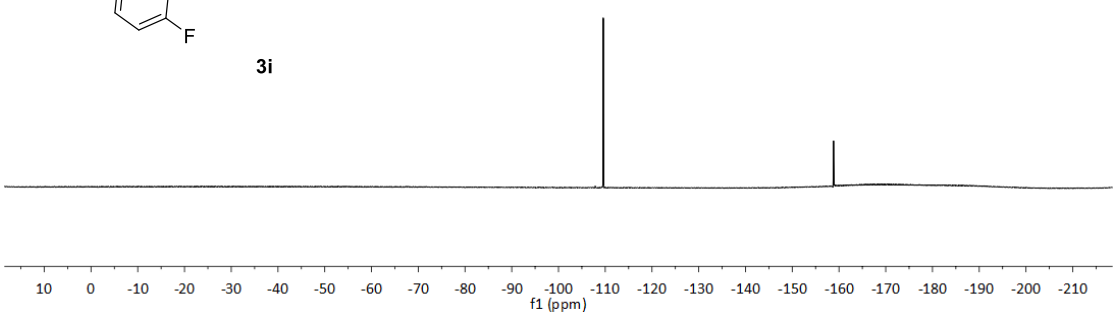
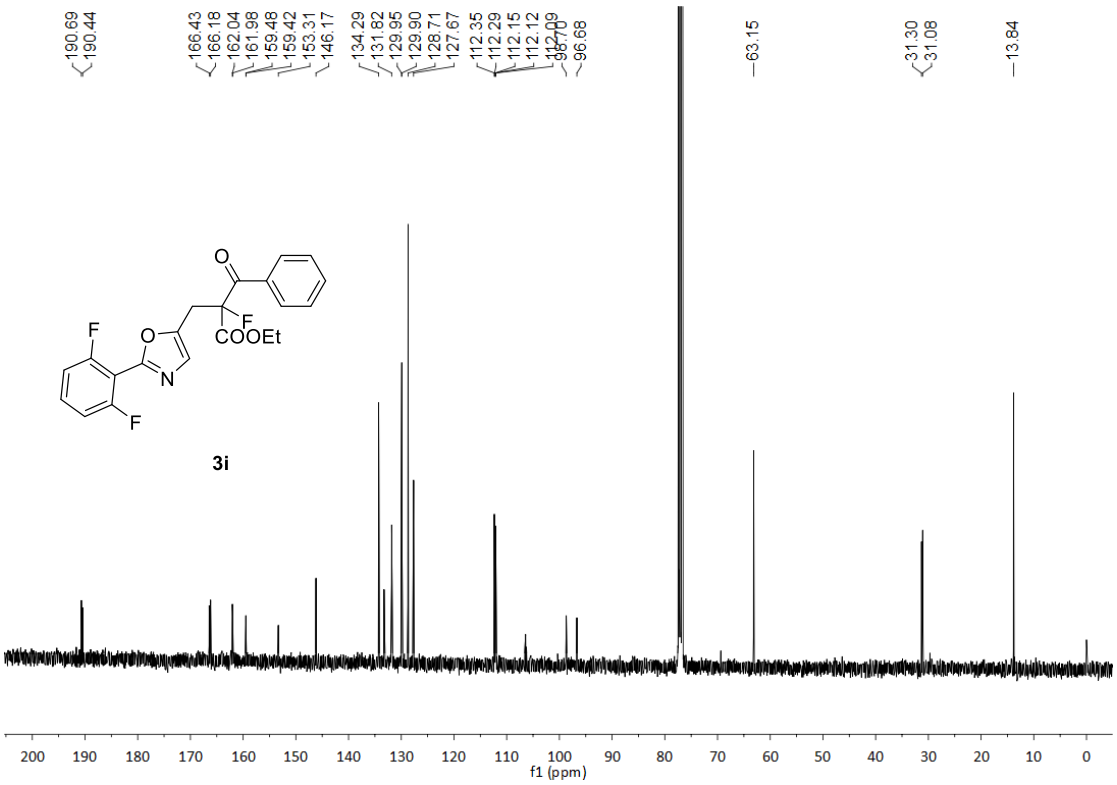


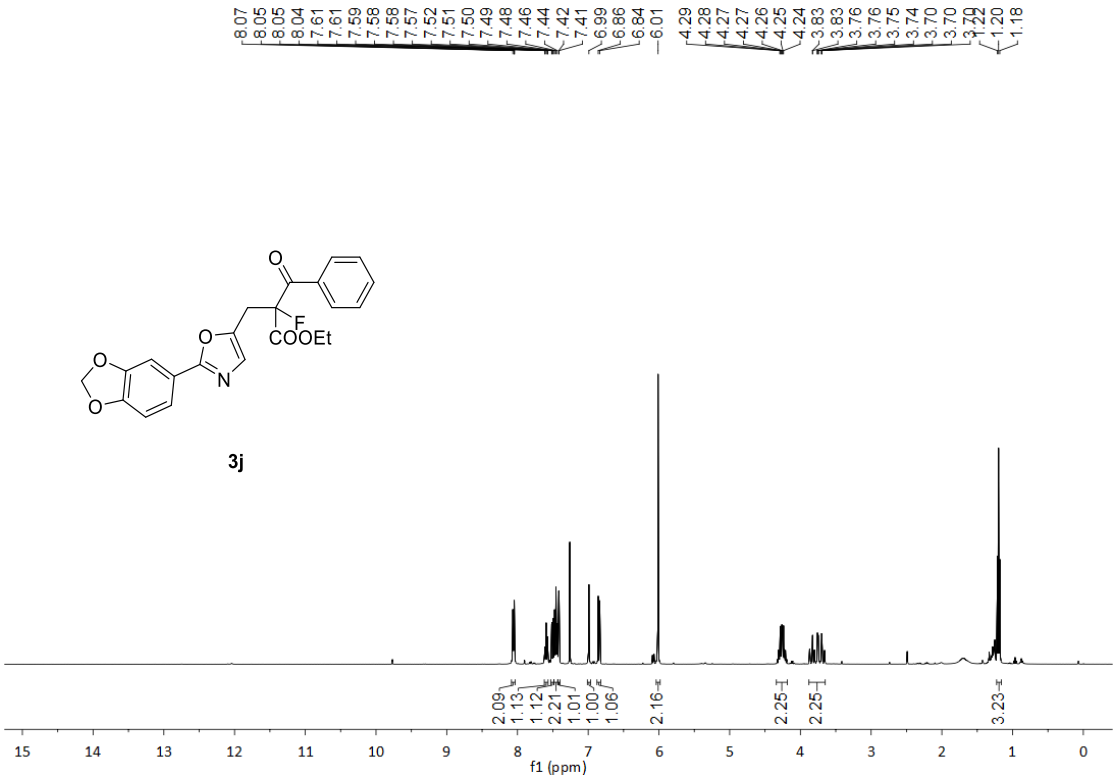
^{13}C NMR (100 MHz, $CDCl_3$):



3i

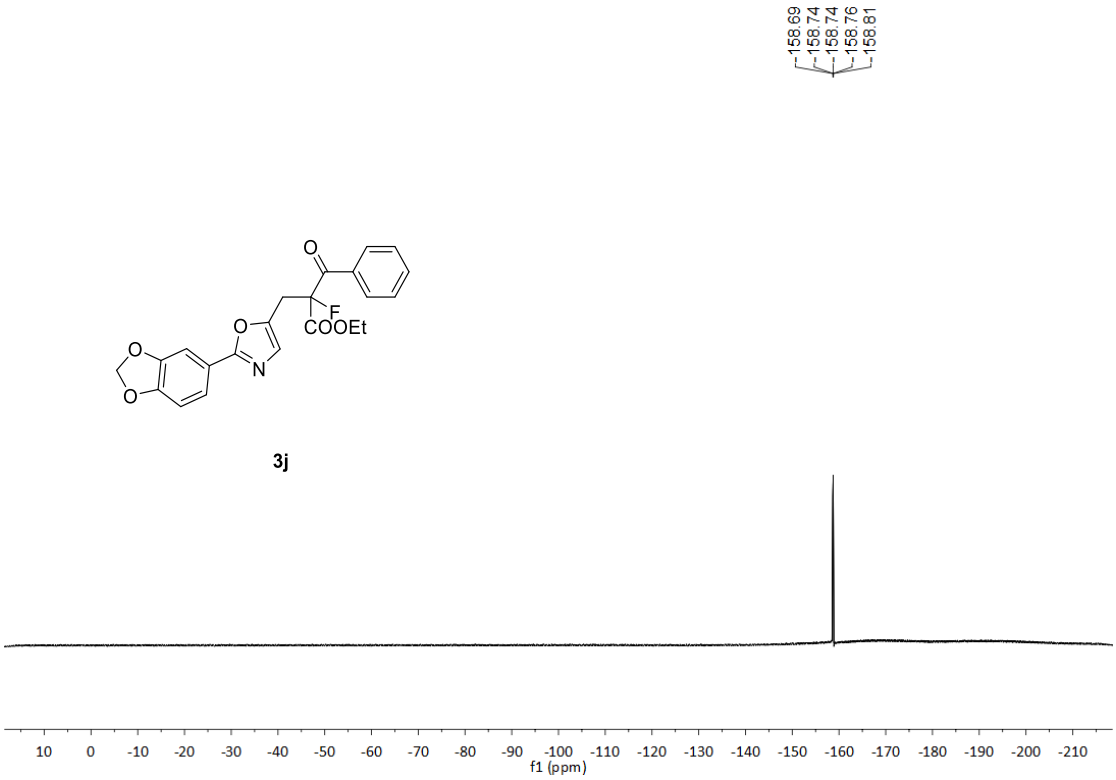
ethyl 2-((2-(benzo[d][1,3]dioxol-5-yl)oxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenyl-propanoate (3j)

^{1}H NMR (400 MHz, $CDCl_3$):

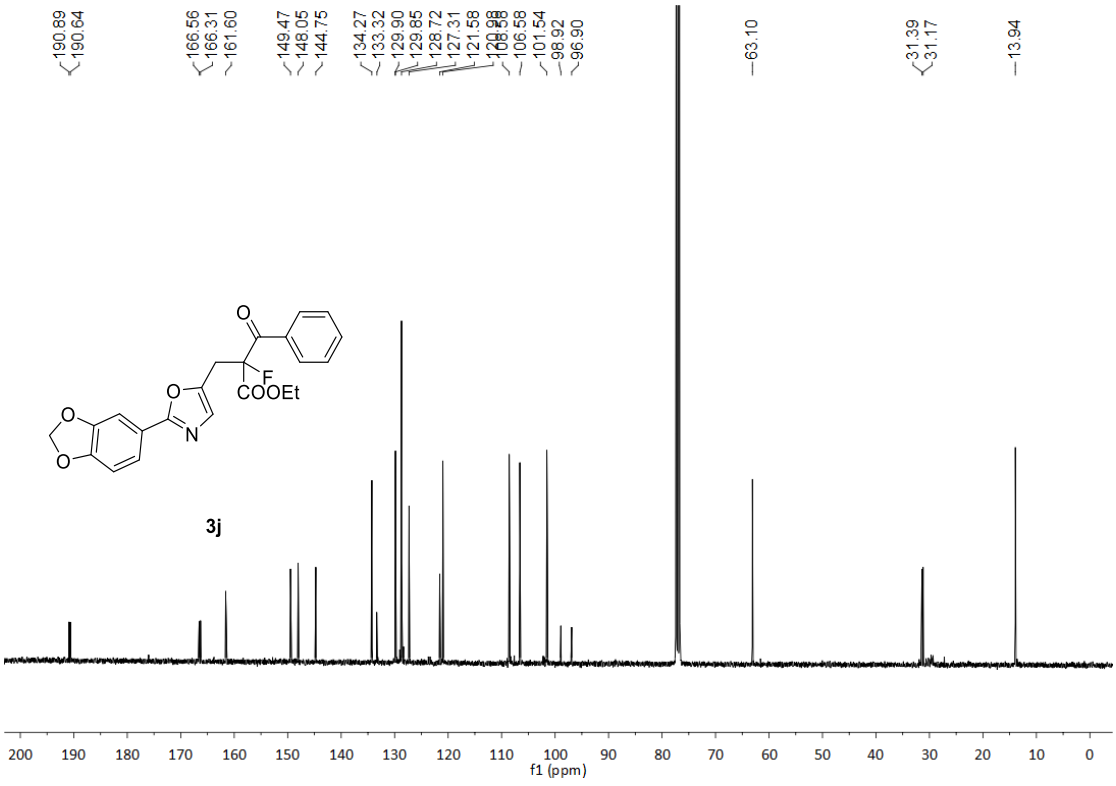


3j

^{19}F NMR (376 MHz, $CDCl_3$):

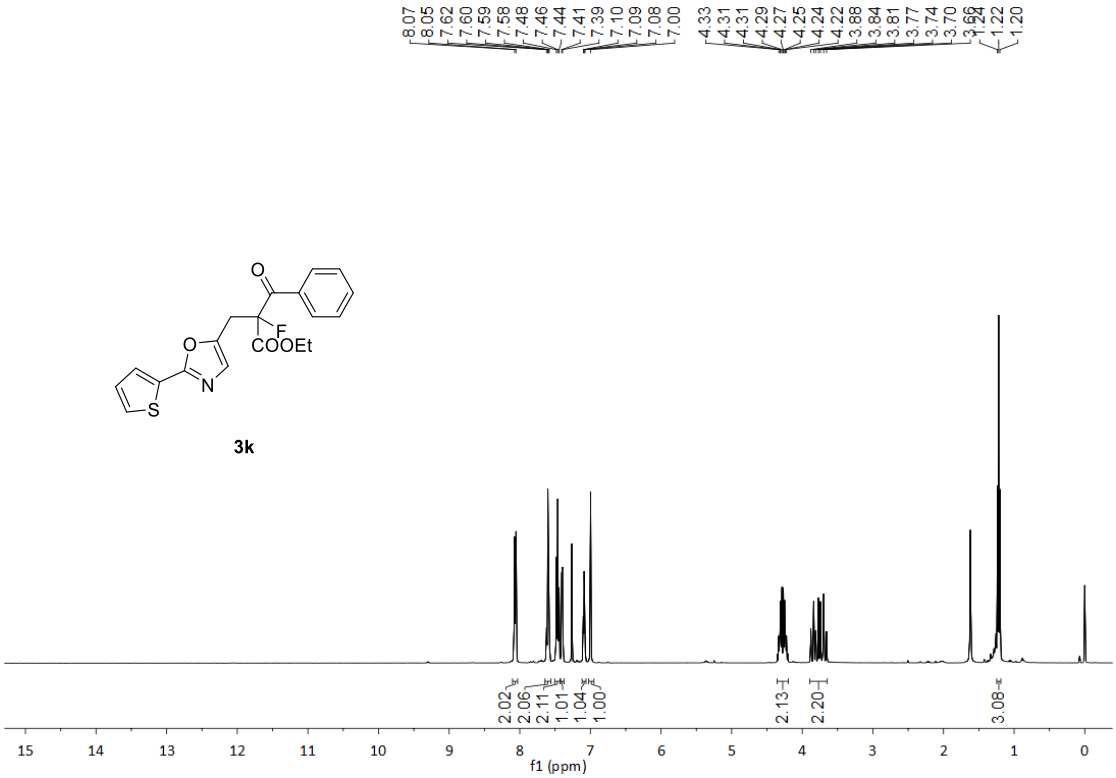


^{13}C NMR (100 MHz, $CDCl_3$):

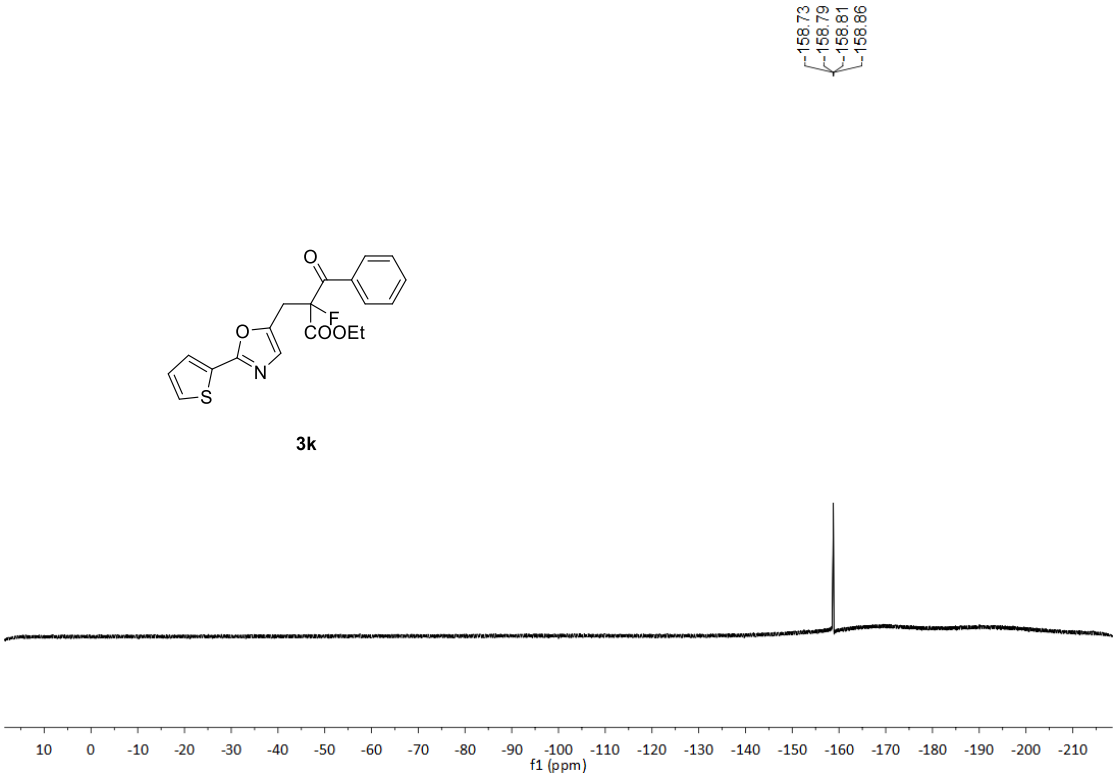


ethyl 2-fluoro-3-oxo-3-phenyl-2-((2-(thiophen-2-yl)oxazol-5-yl)methyl)propano-ate (3k)

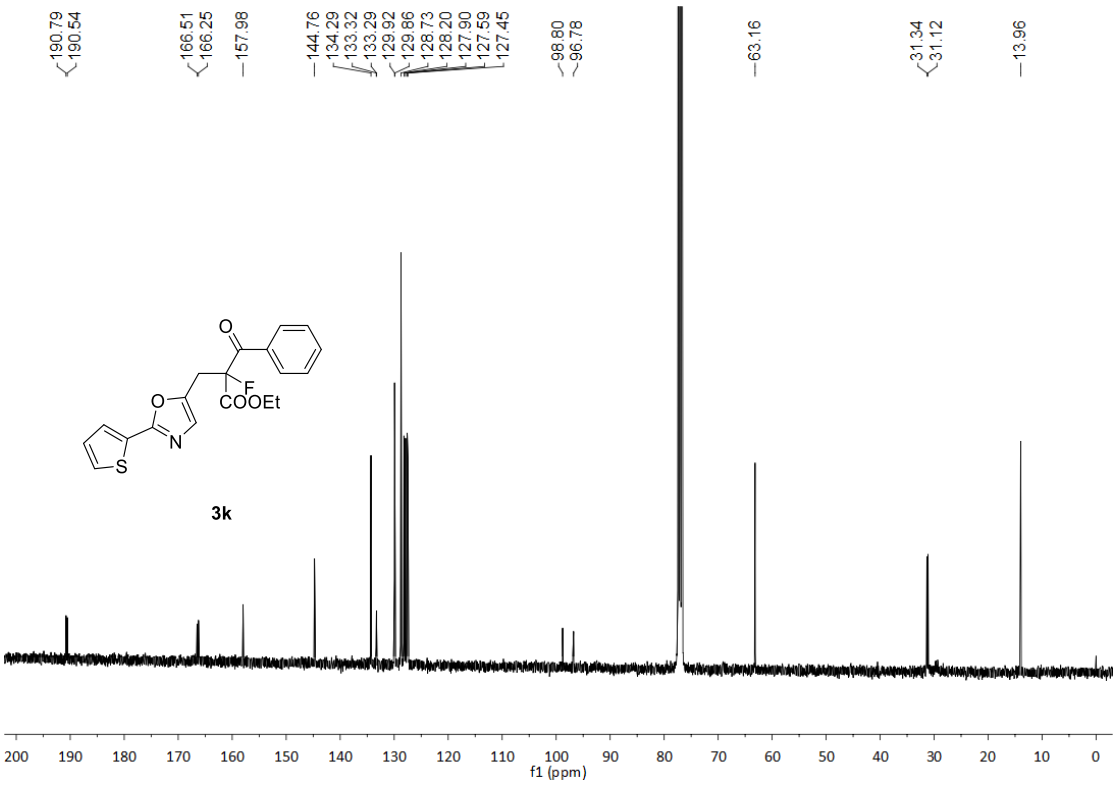
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

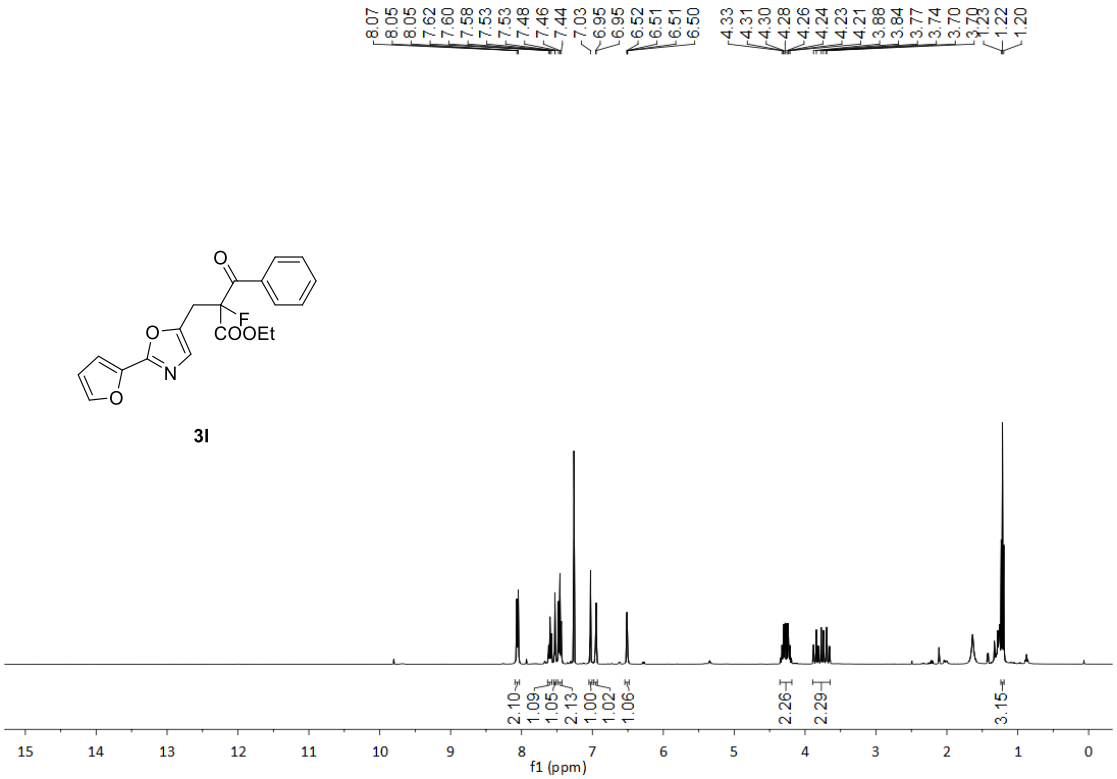


^{13}C NMR (100 MHz, $CDCl_3$):

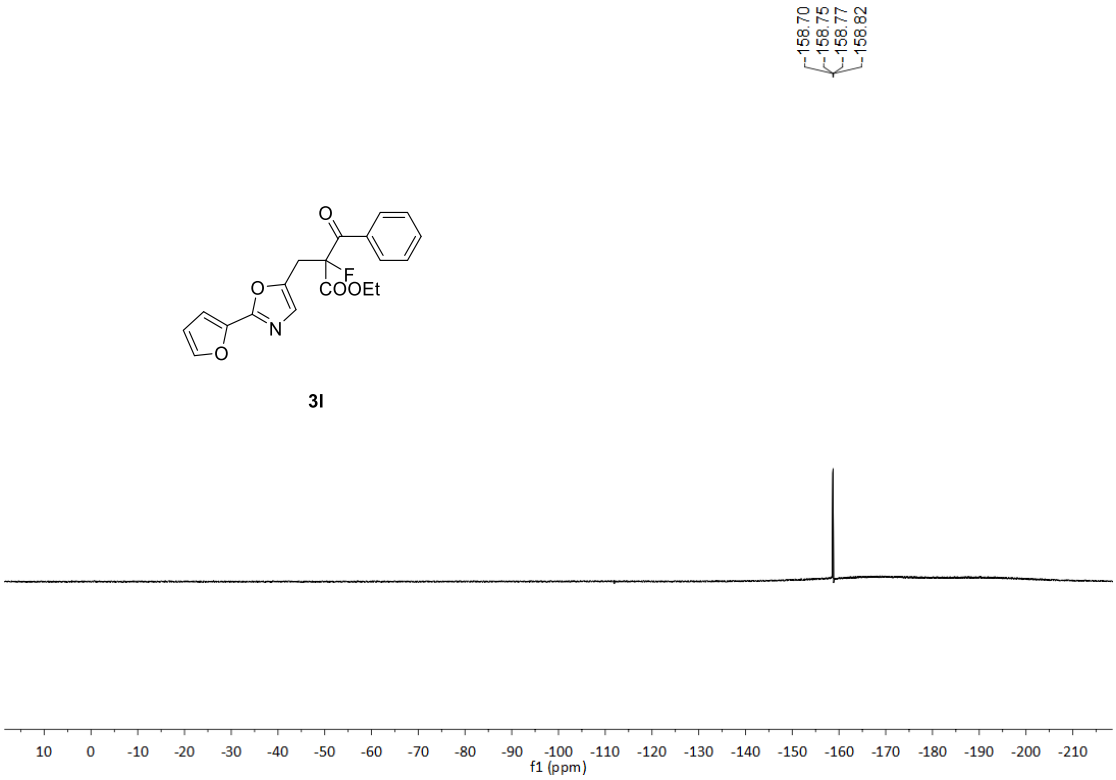


ethyl 2-fluoro-2-((2-(furan-2-yl)oxazol-5-yl)methyl)-3-oxo-3-phenylpropanoate (3l)

^{1}H NMR (400 MHz, $CDCl_3$):

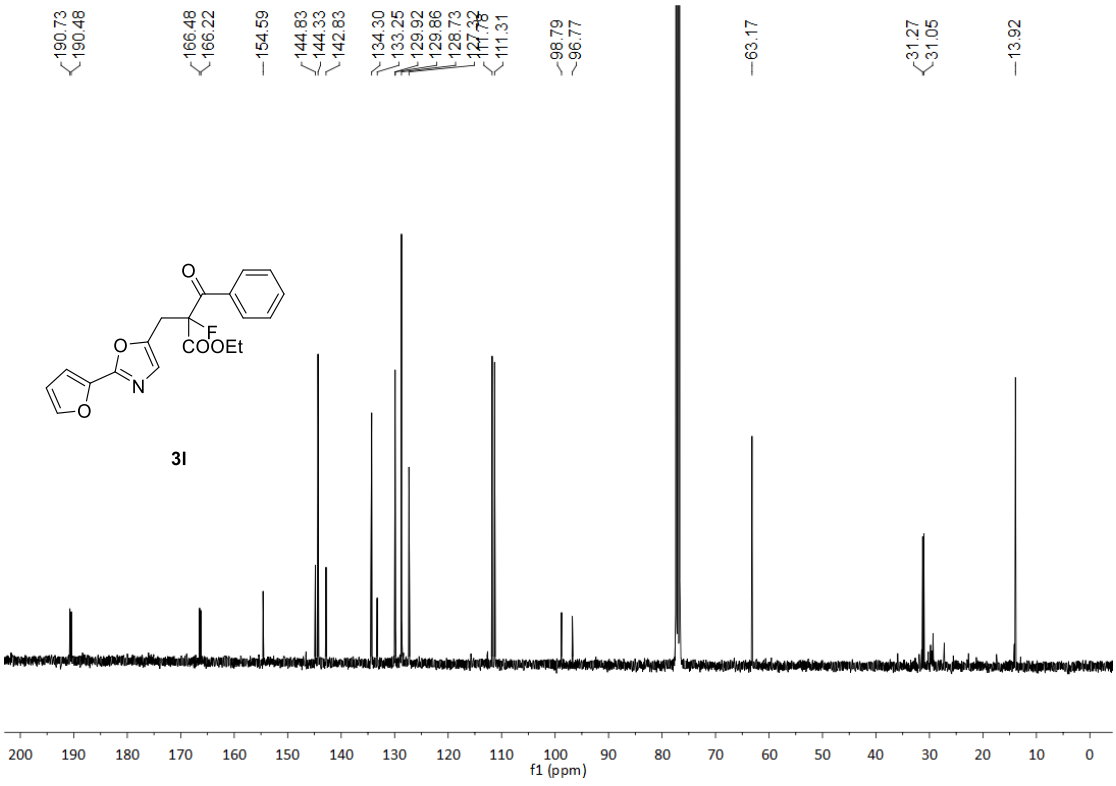


^{19}F NMR (376 MHz, $CDCl_3$):



3l

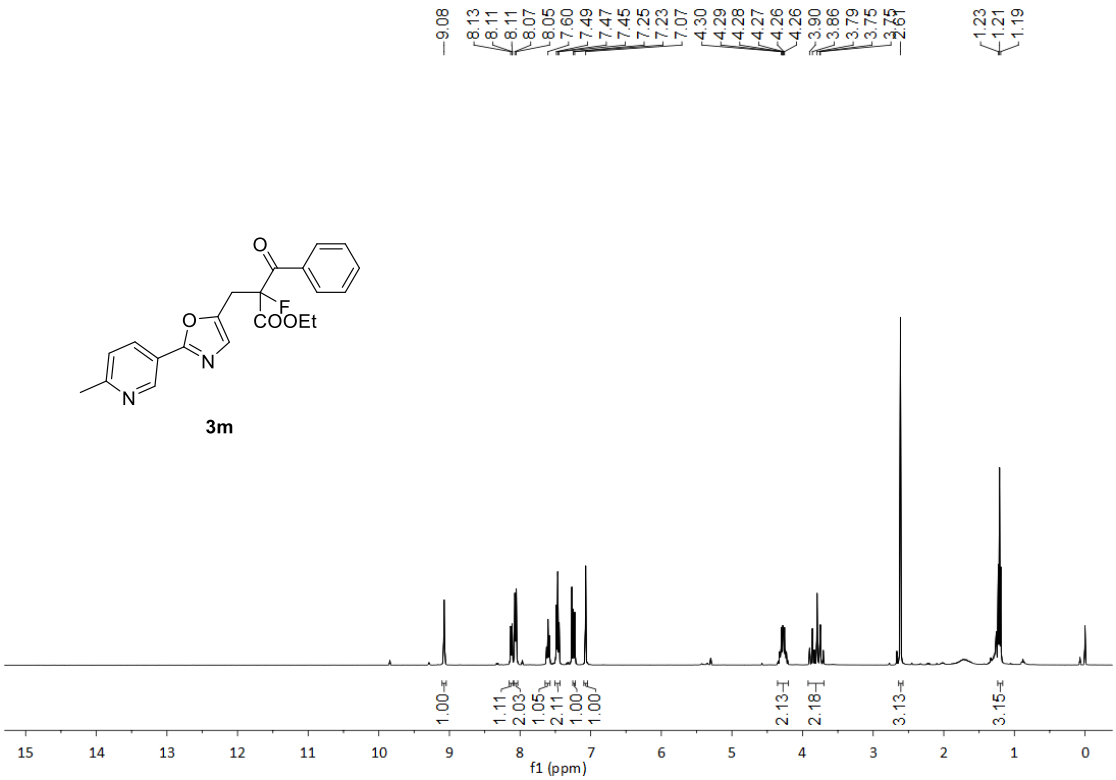
^{13}C NMR (100 MHz, $CDCl_3$):



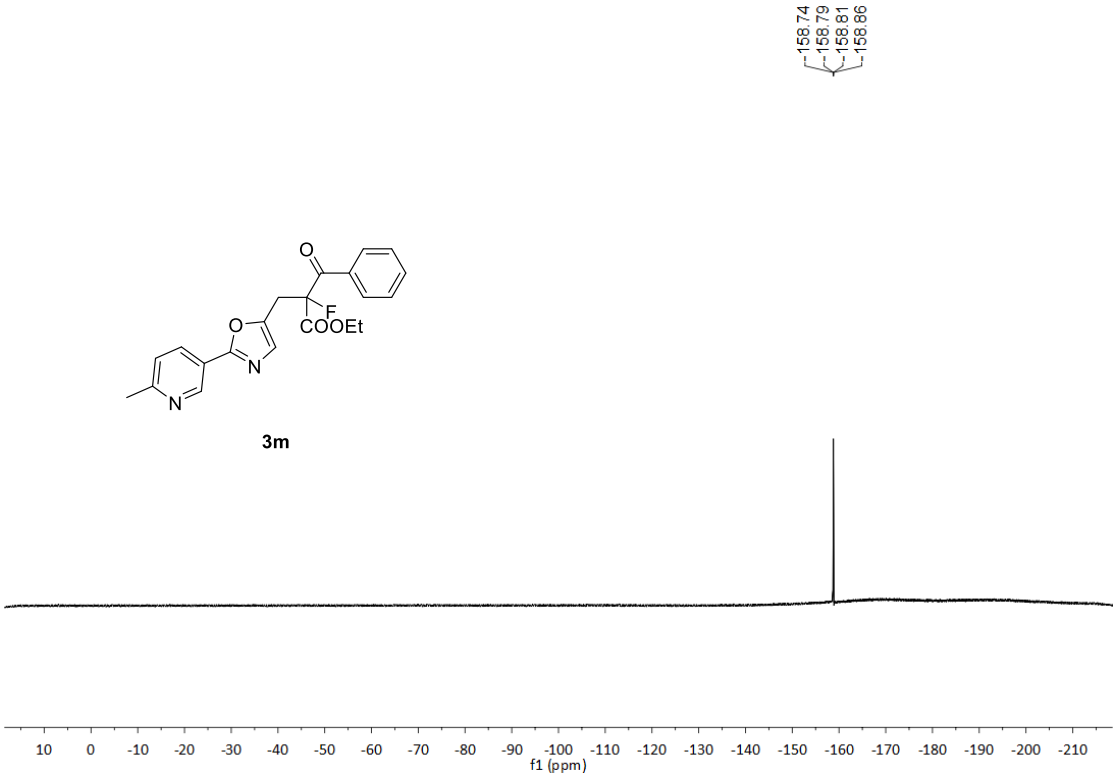
3l

ethyl 2-fluoro-2-((2-(6-methylpyridin-3-yl)oxazol-5-yl)methyl)-3-oxo-3-phenyl-propanoate (3m)

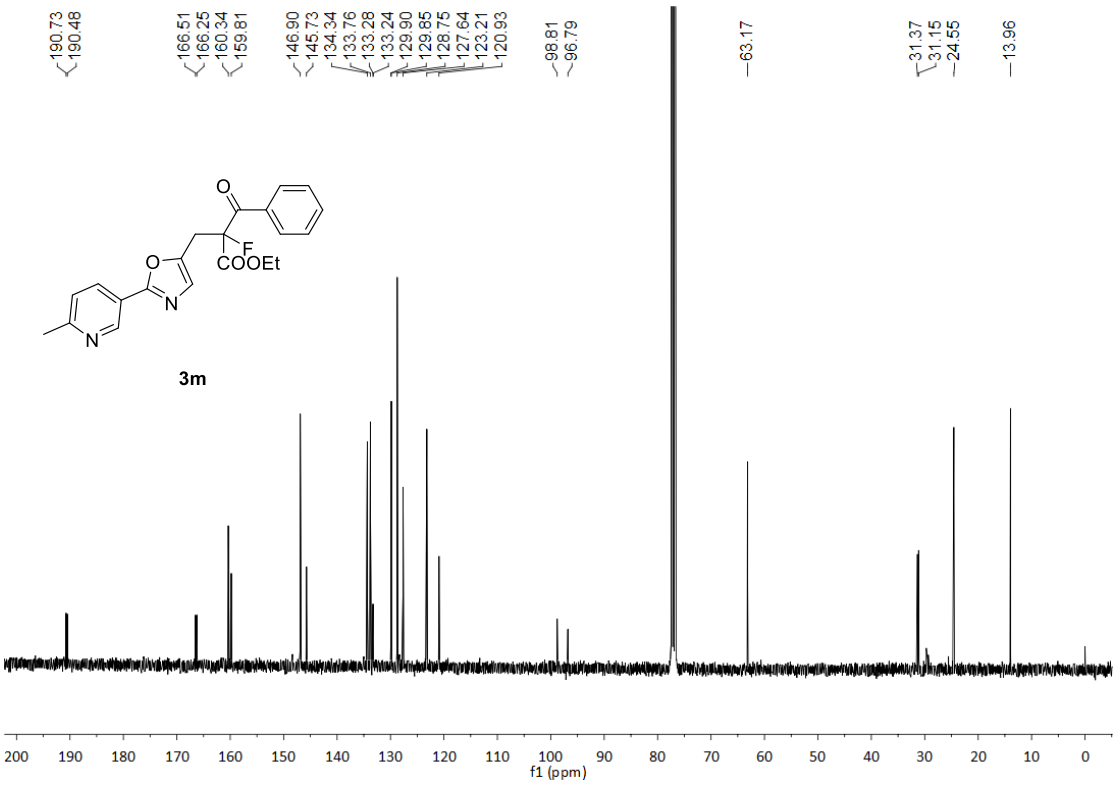
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

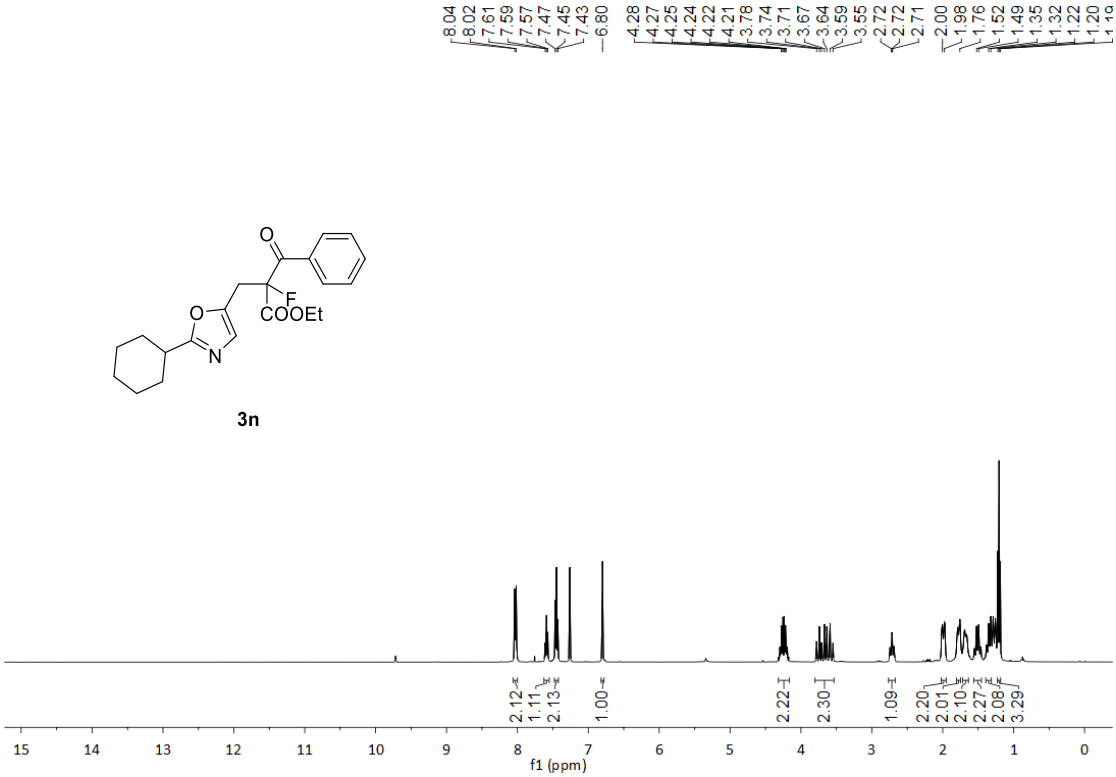


^{13}C NMR (100 MHz, $CDCl_3$):

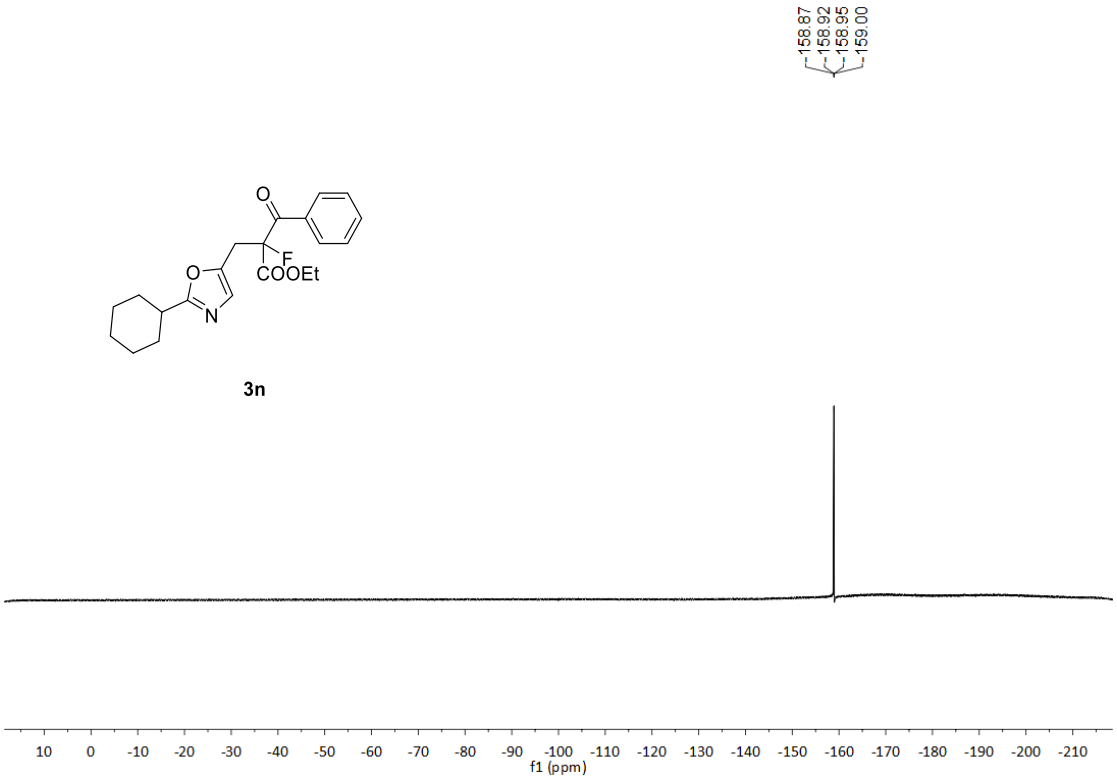


ethyl 2-((2-cyclohexyloxazol-5-yl)methyl)-2-fluoro-3-oxo-3-phenylpropanoate (3n)

^{1}H NMR (400 MHz, $CDCl_3$):

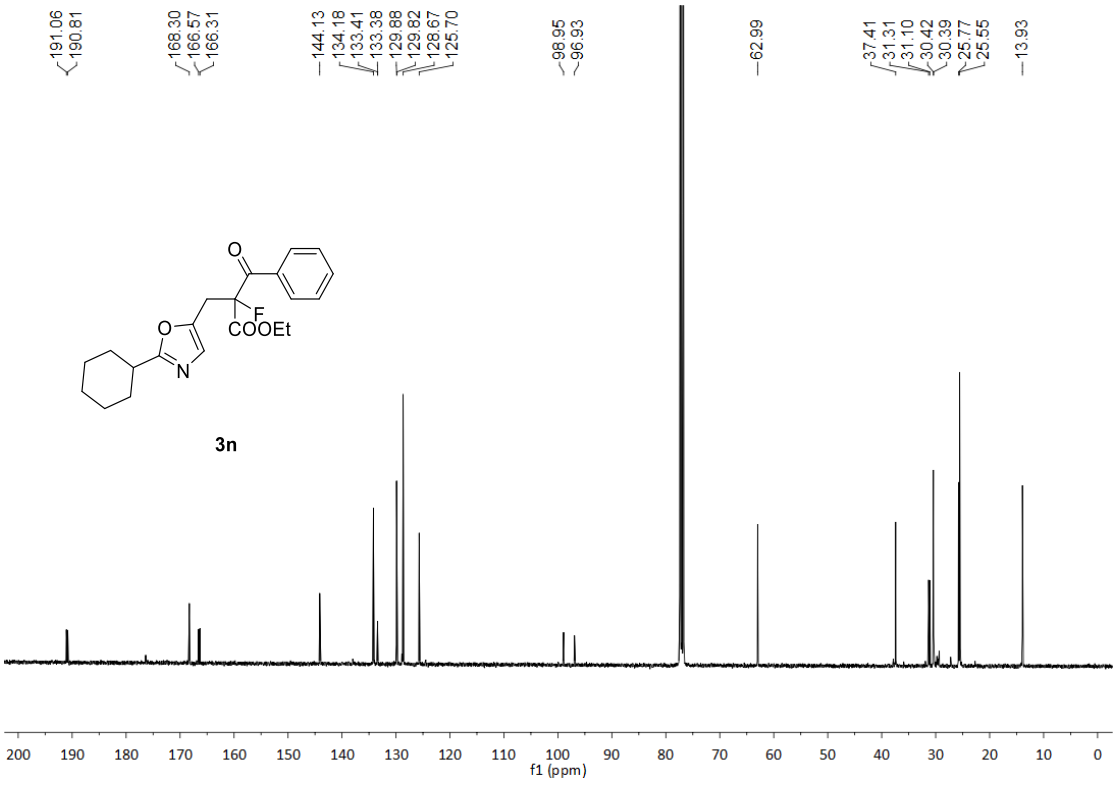


^{19}F NMR (376 MHz, $CDCl_3$):



3n

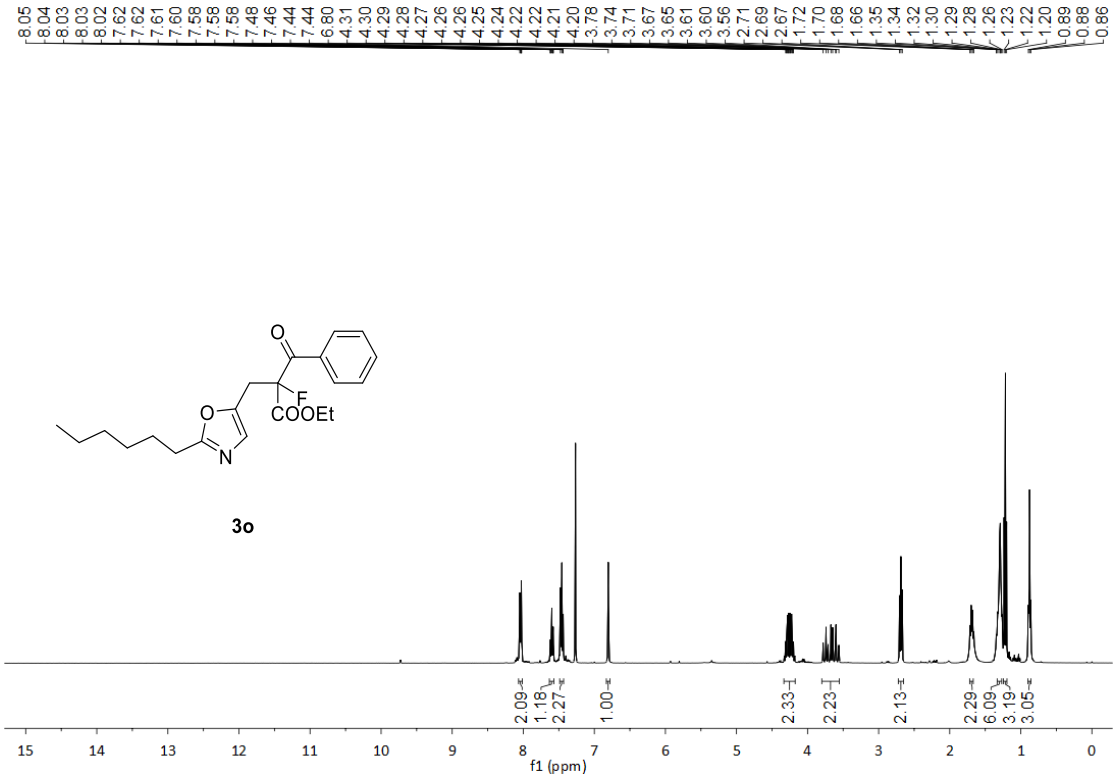
^{13}C NMR (100 MHz, $CDCl_3$):



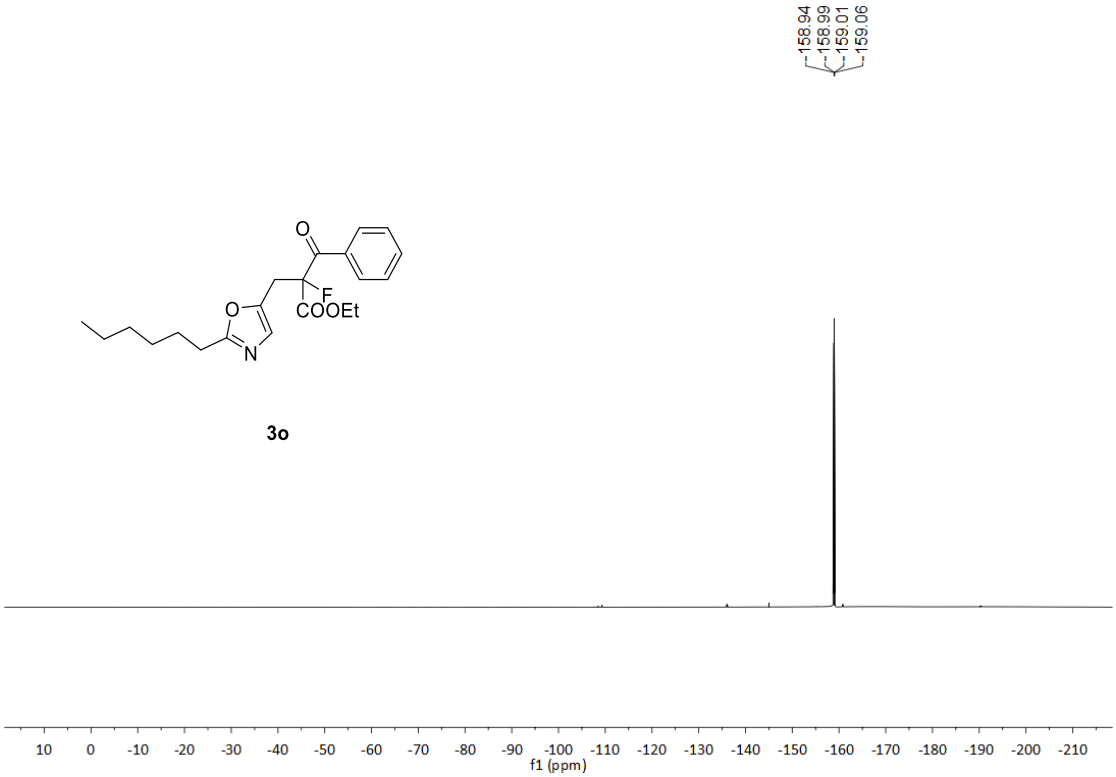
3n

ethyl 2-fluoro-2-((2-hexyloxazol-5-yl)methyl)-3-oxo-3-phenylpropanoate (3o)

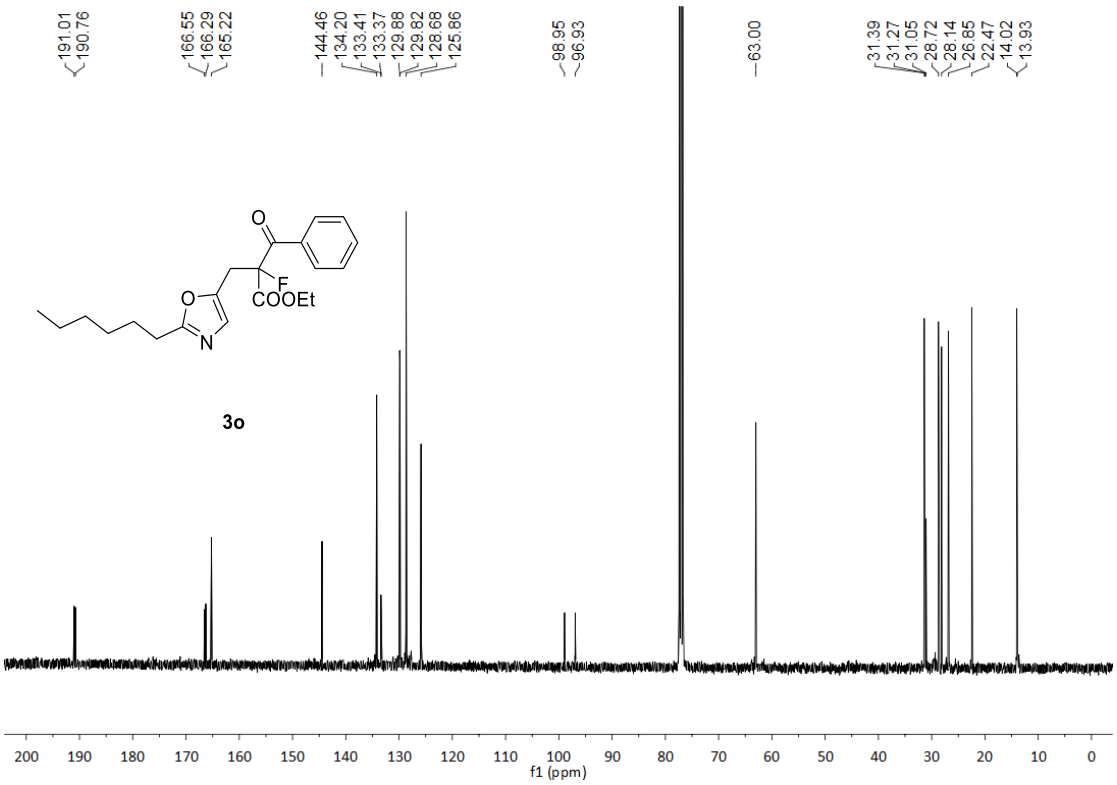
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

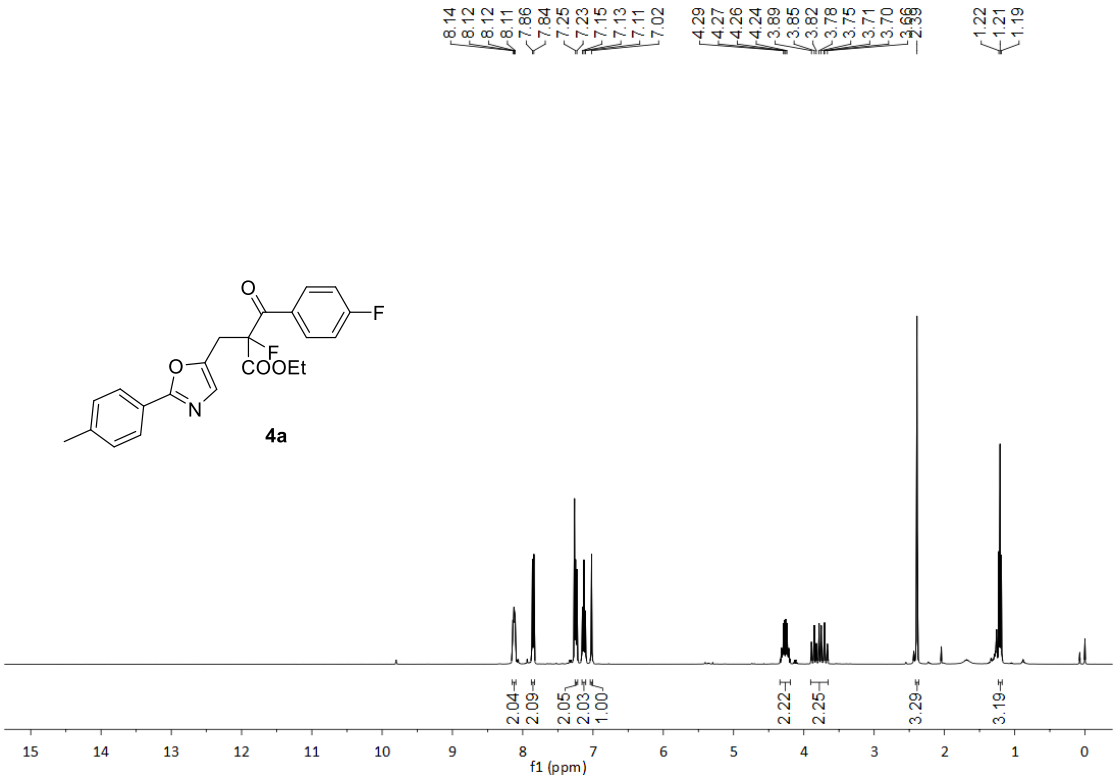


^{13}C NMR (100 MHz, $CDCl_3$):

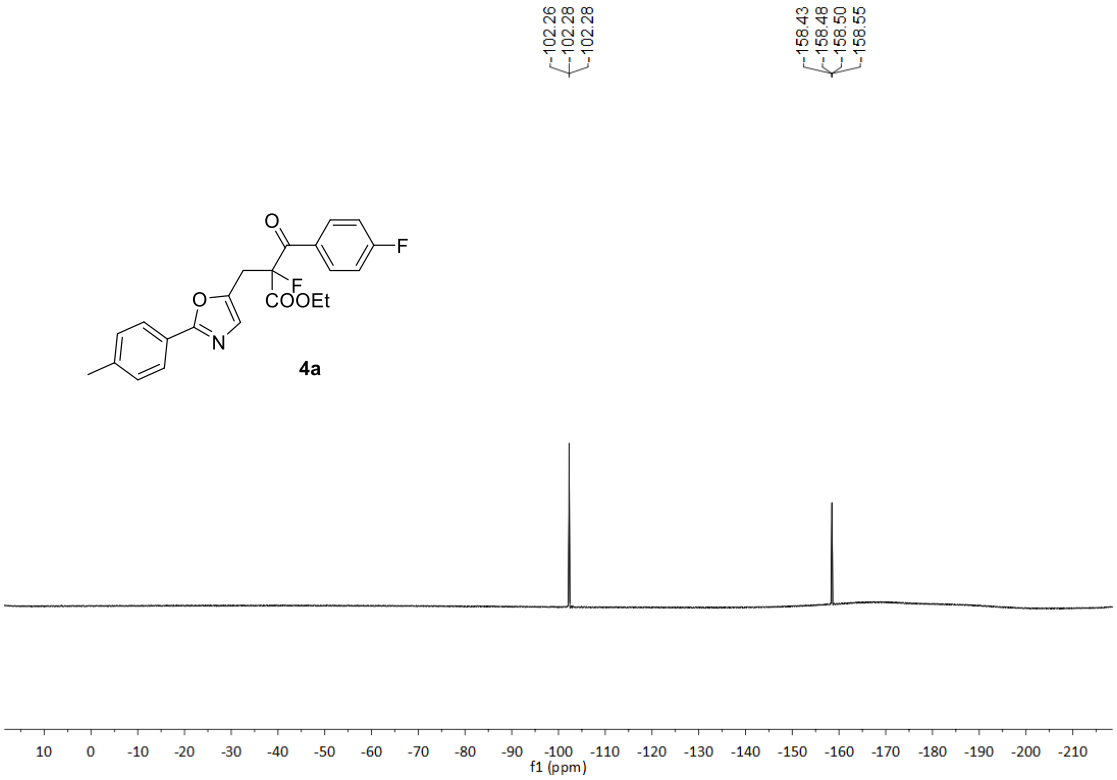


ethyl 2-fluoro-3-(4-fluorophenyl)-3-oxo-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propan-oate (4a)

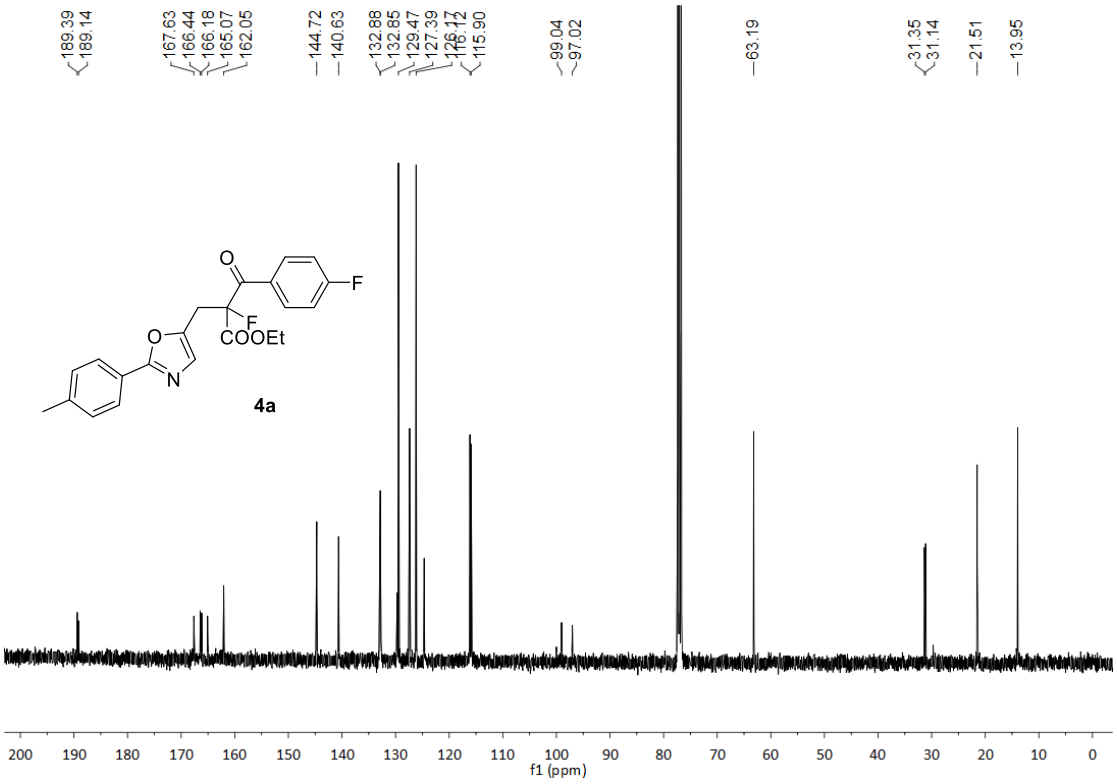
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

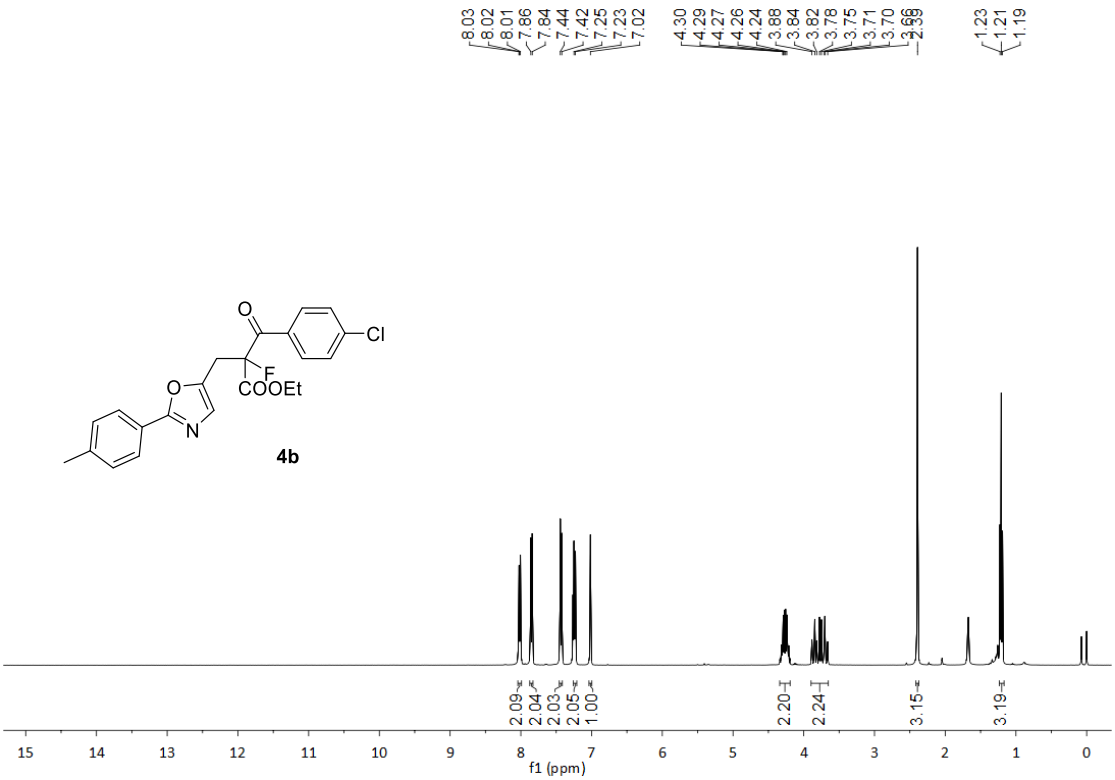


^{13}C NMR (100 MHz, $CDCl_3$):

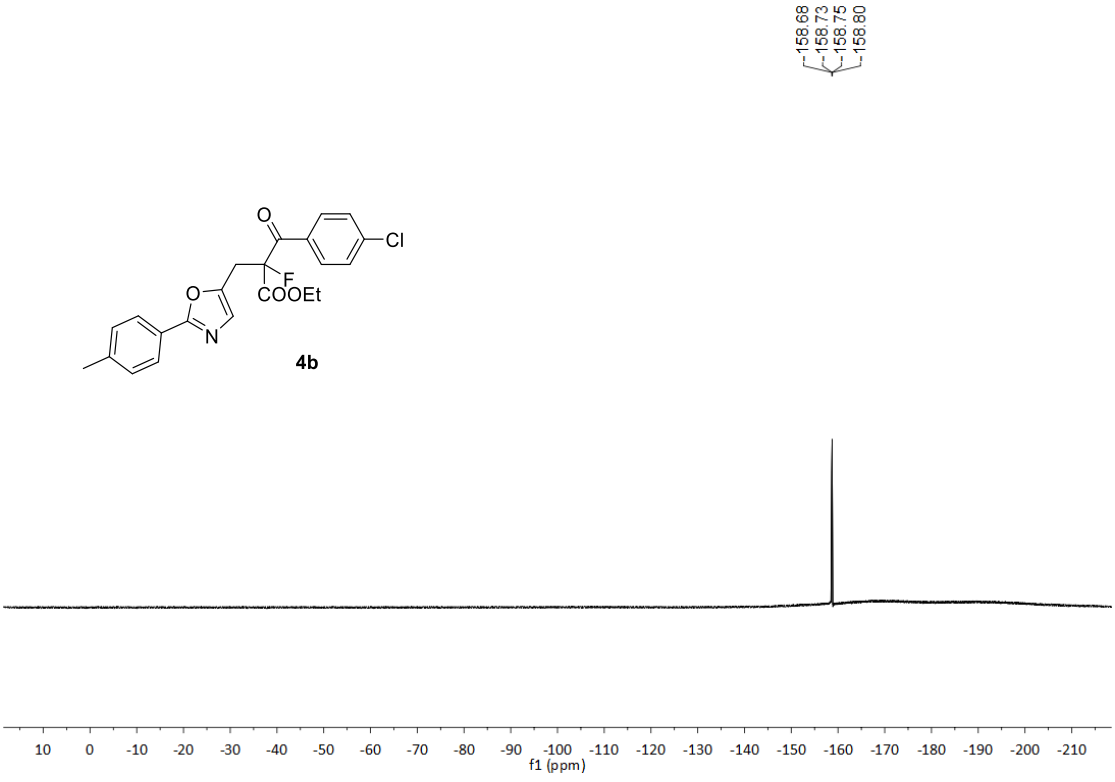


ethyl 3-(4-chlorophenyl)-2-fluoro-3-oxo-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propan-oate (4b)

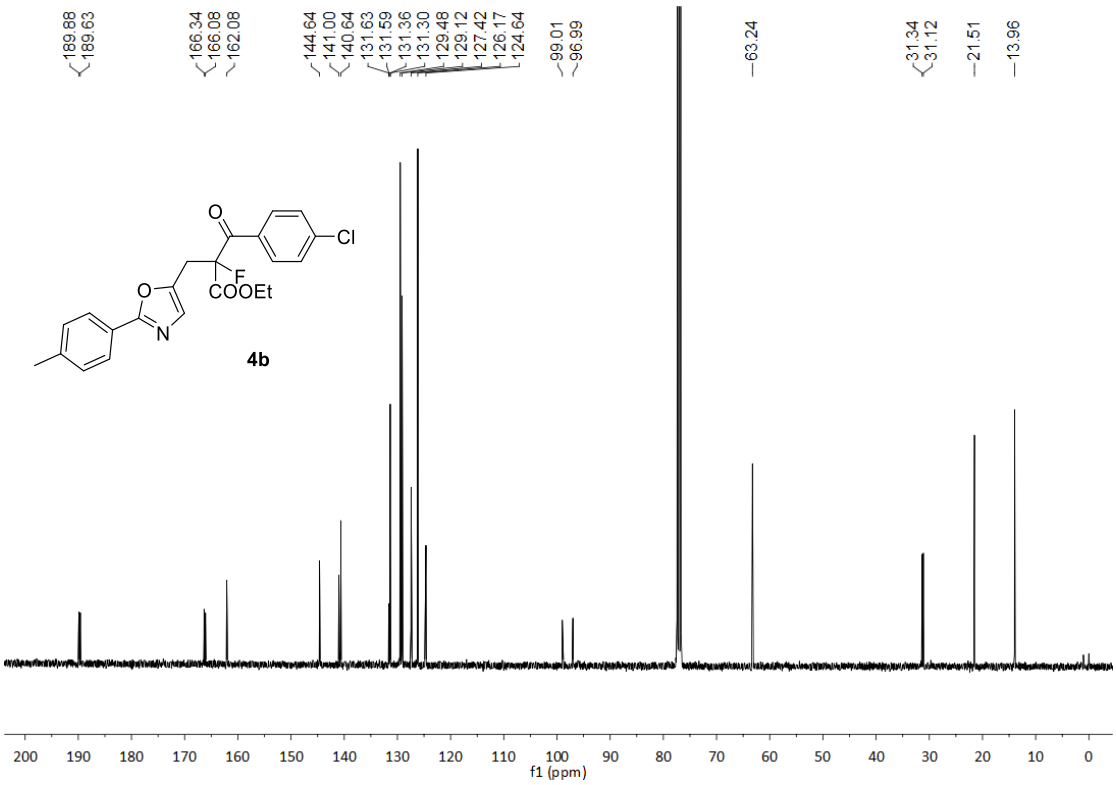
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

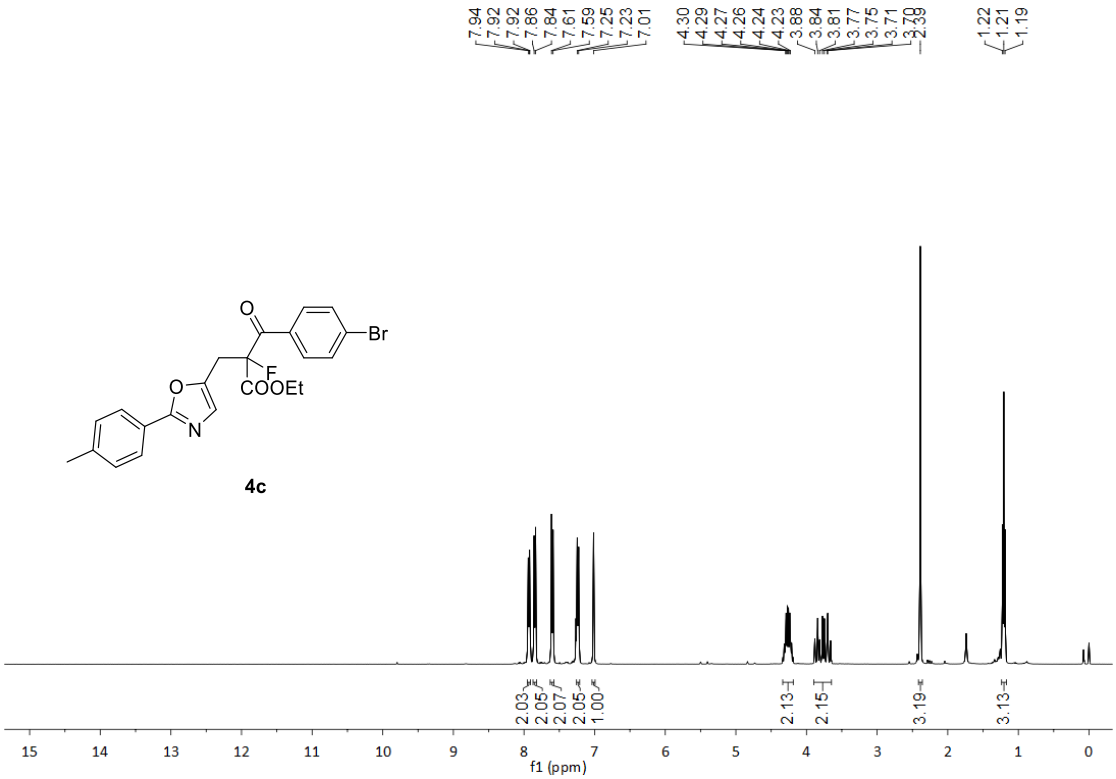


^{13}C NMR (100 MHz, $CDCl_3$):

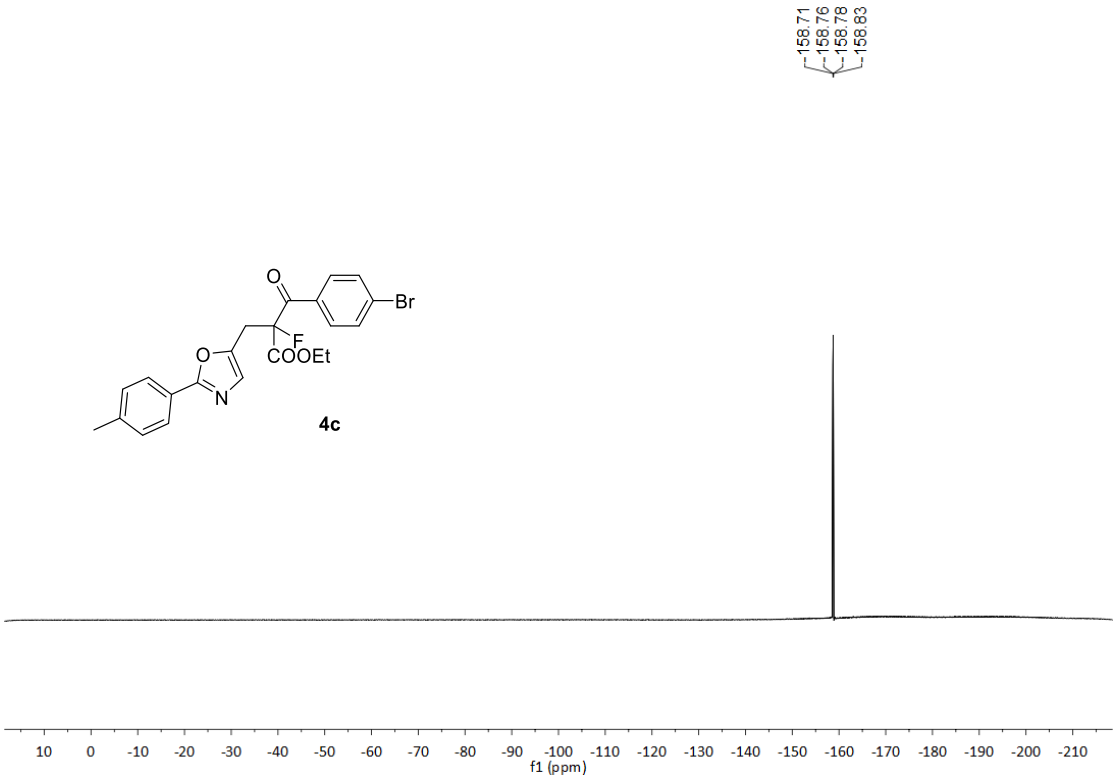


ethyl 3-(4-bromophenyl)-2-fluoro-3-oxo-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propan-oate (4c)

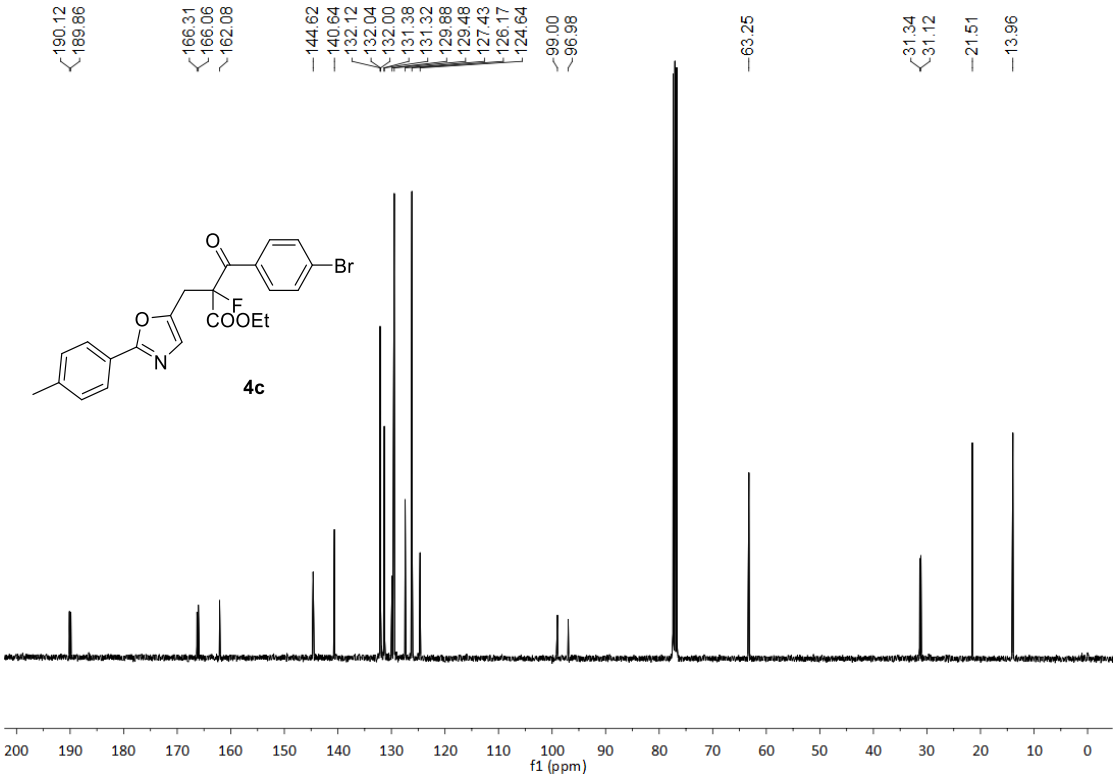
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

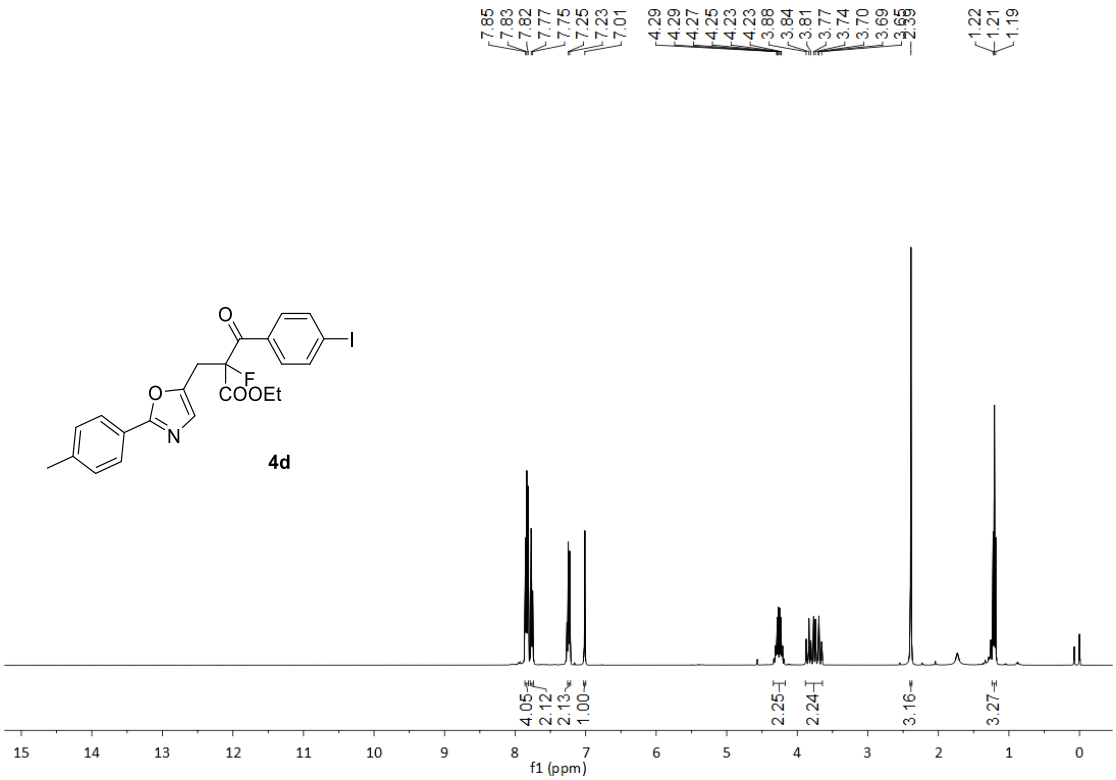


^{13}C NMR (100 MHz, $CDCl_3$):

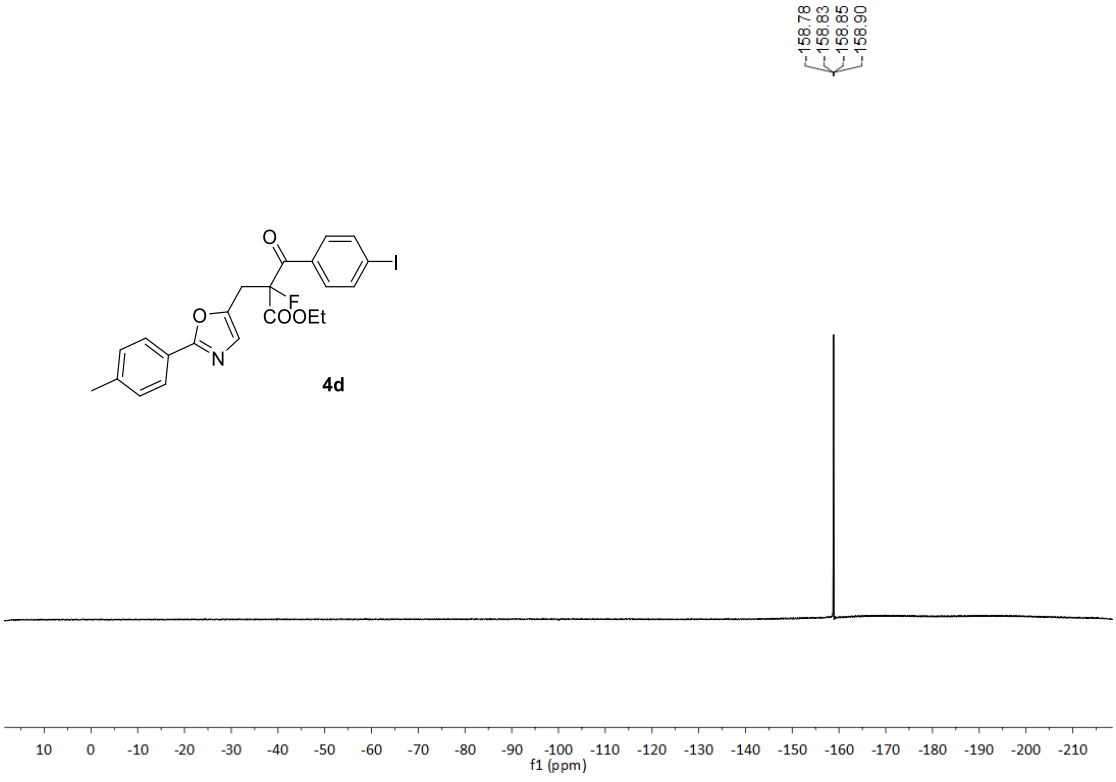


ethyl 2-fluoro-3-(4-iodophenyl)-3-oxo-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propano-ate (4d)

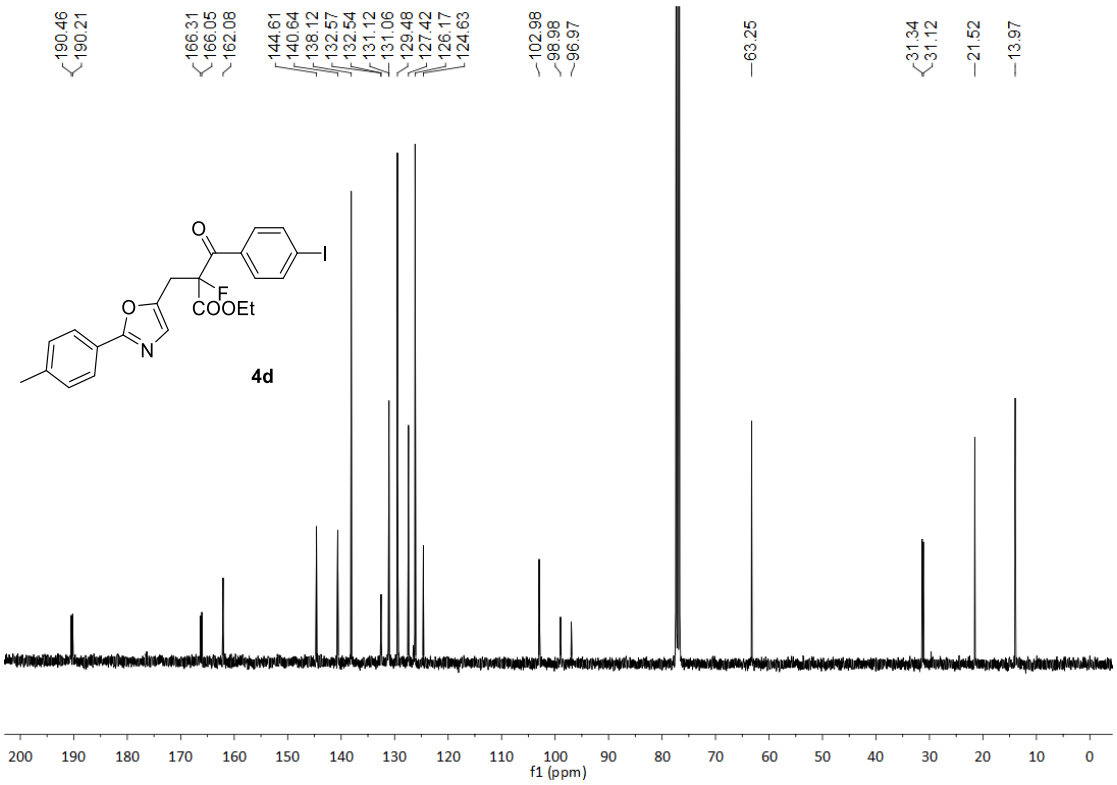
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

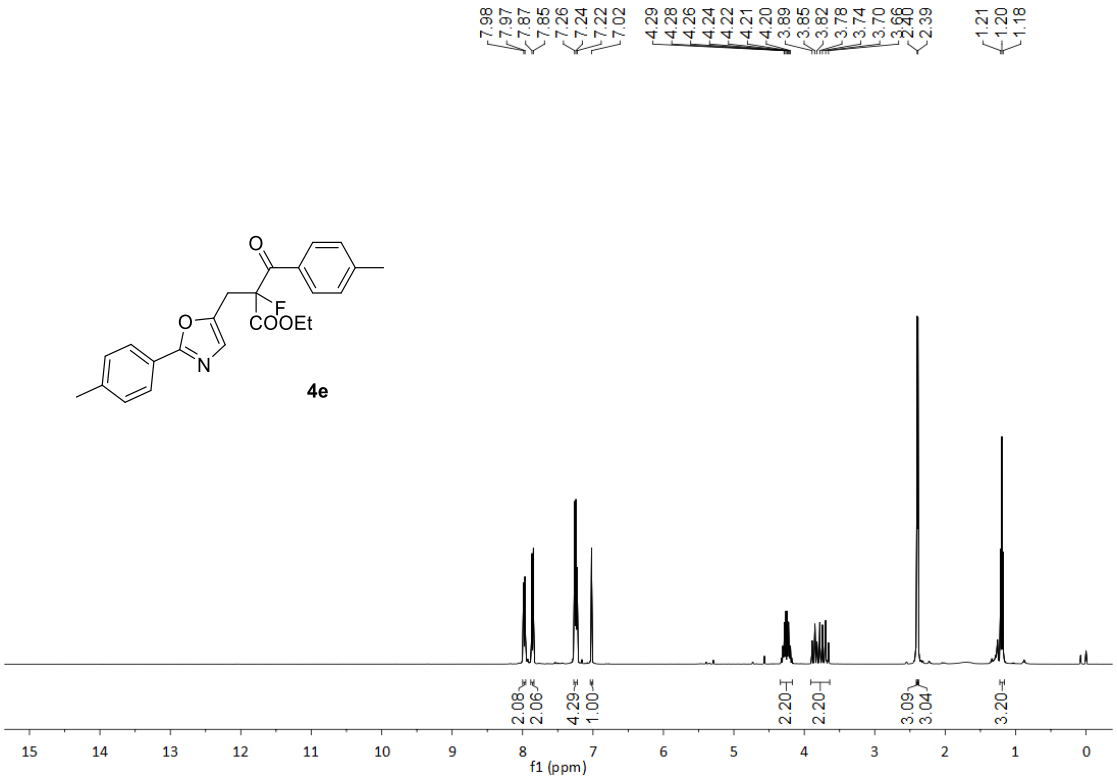


^{13}C NMR (100 MHz, $CDCl_3$):

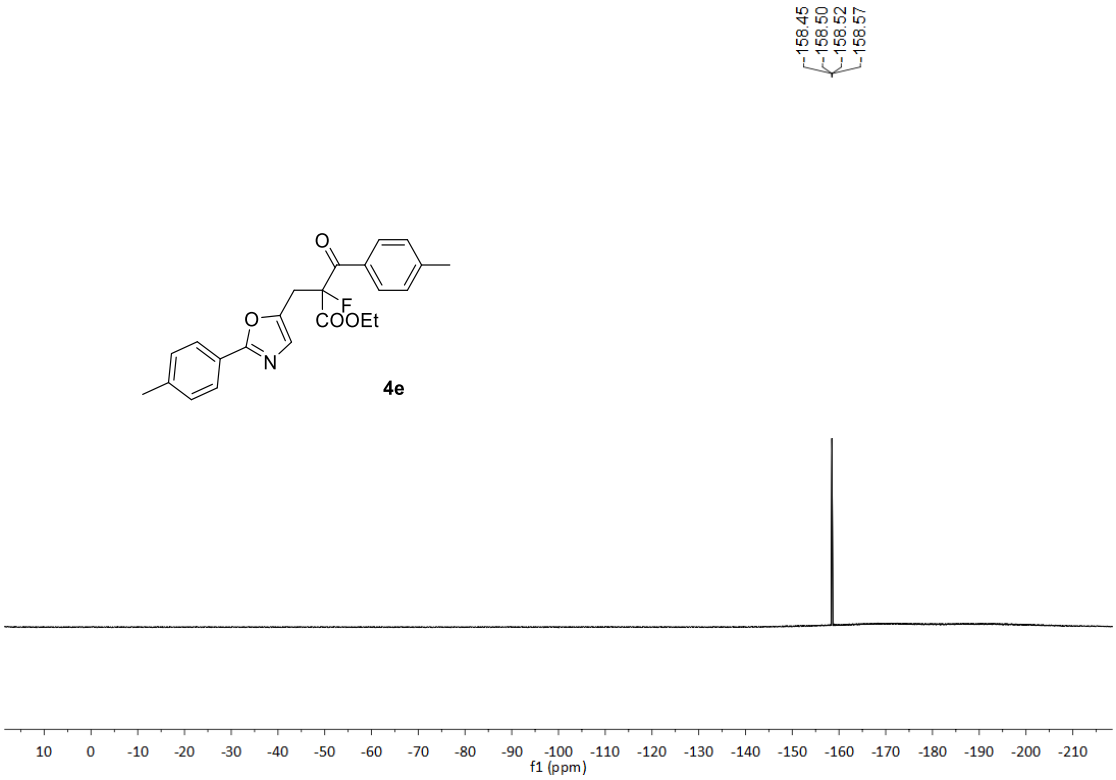


ethyl 2-fluoro-3-oxo-3-(p-tolyl)-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propanoate (4e)

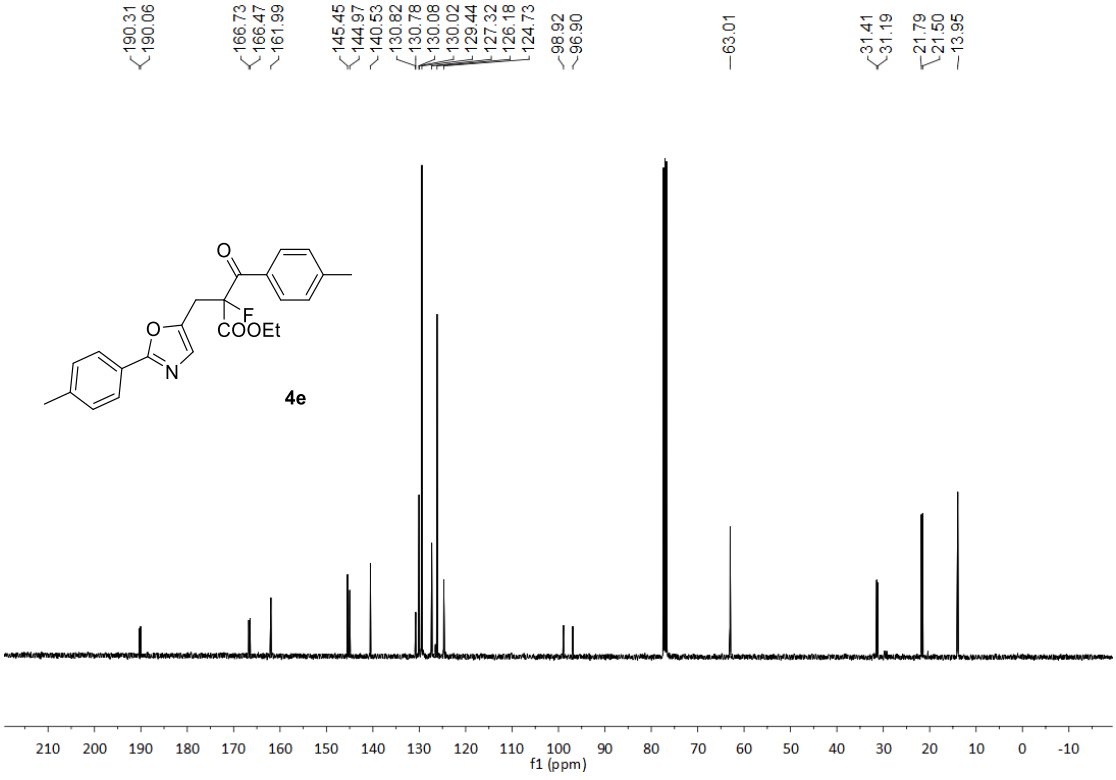
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

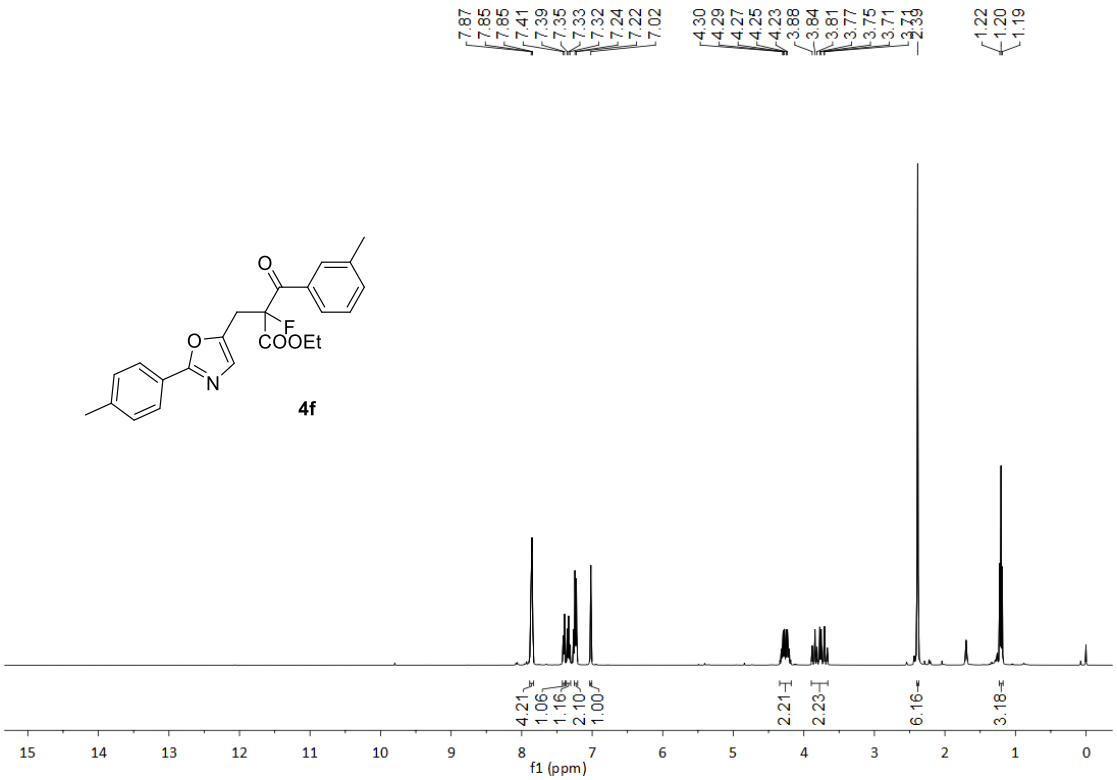


^{13}C NMR (100 MHz, $CDCl_3$):

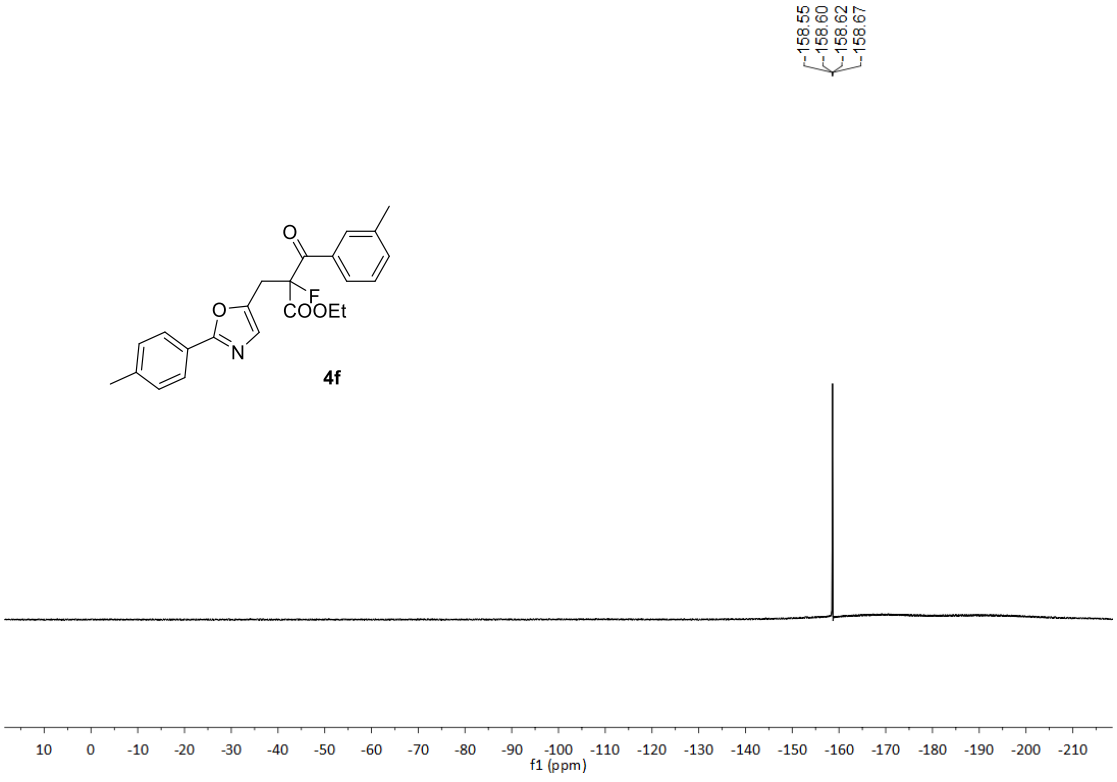


ethyl 2-fluoro-3-oxo-3-(m-tolyl)-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propanoate (4f)

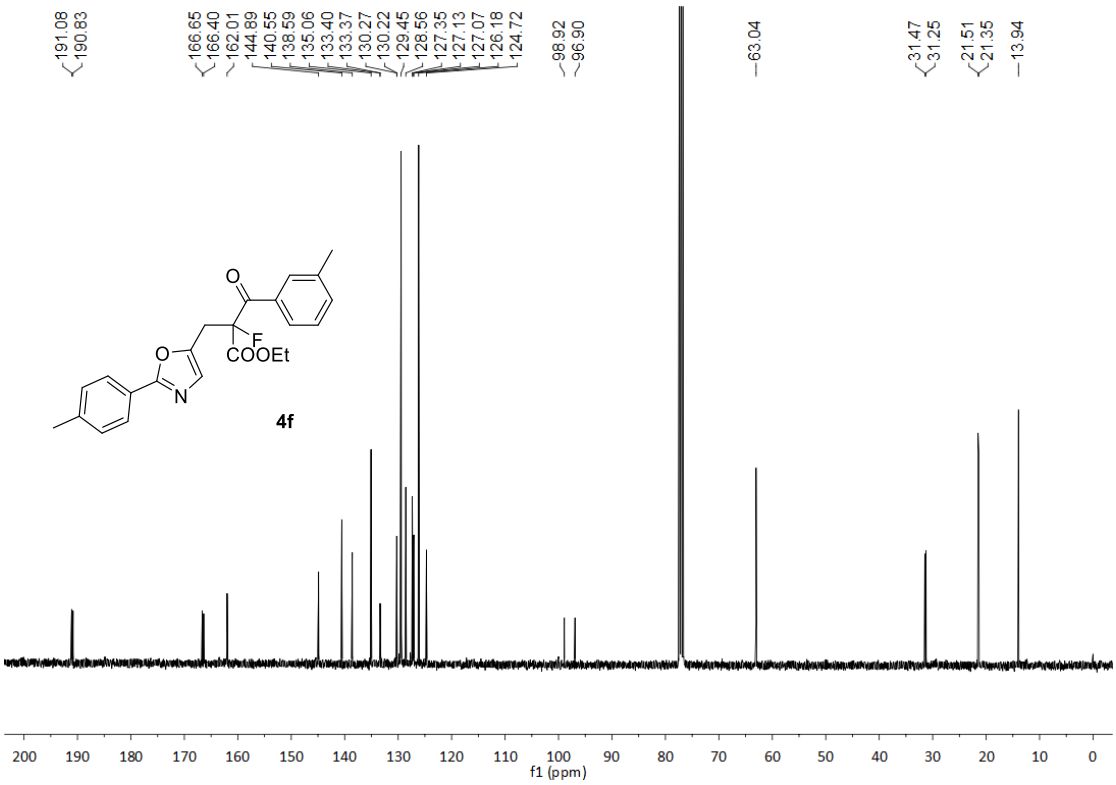
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

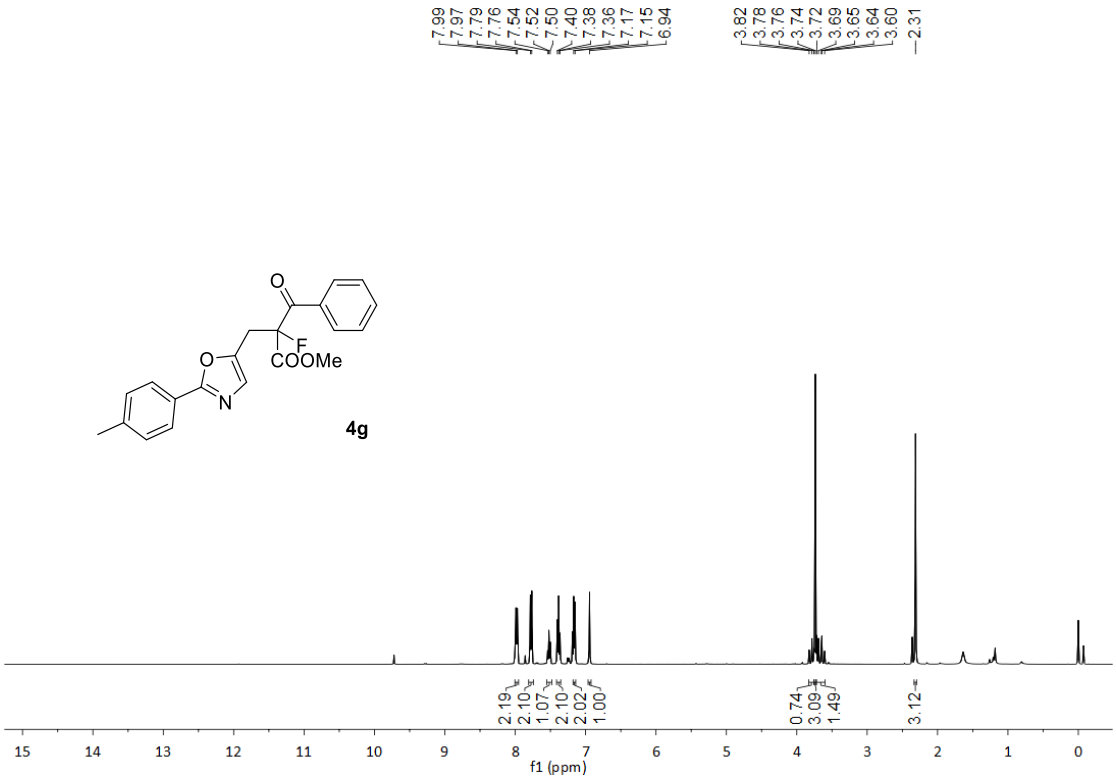


^{13}C NMR (100 MHz, $CDCl_3$):

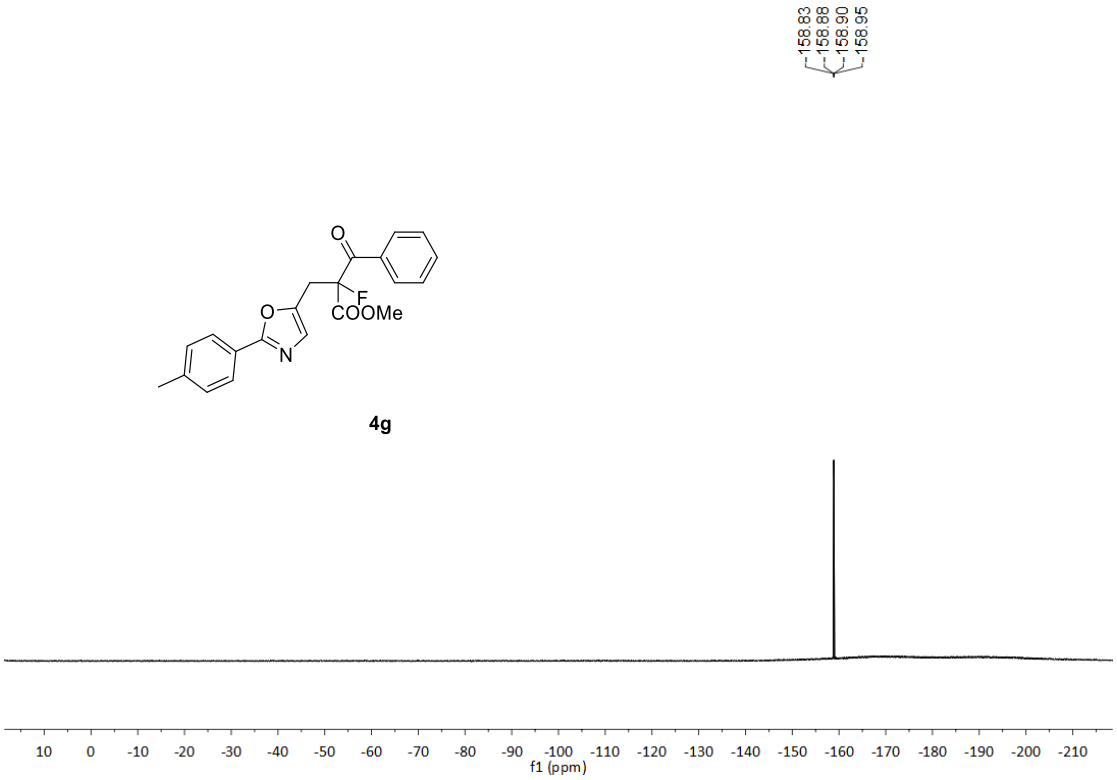


methyl 2-fluoro-3-oxo-3-phenyl-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propanoate (4g)

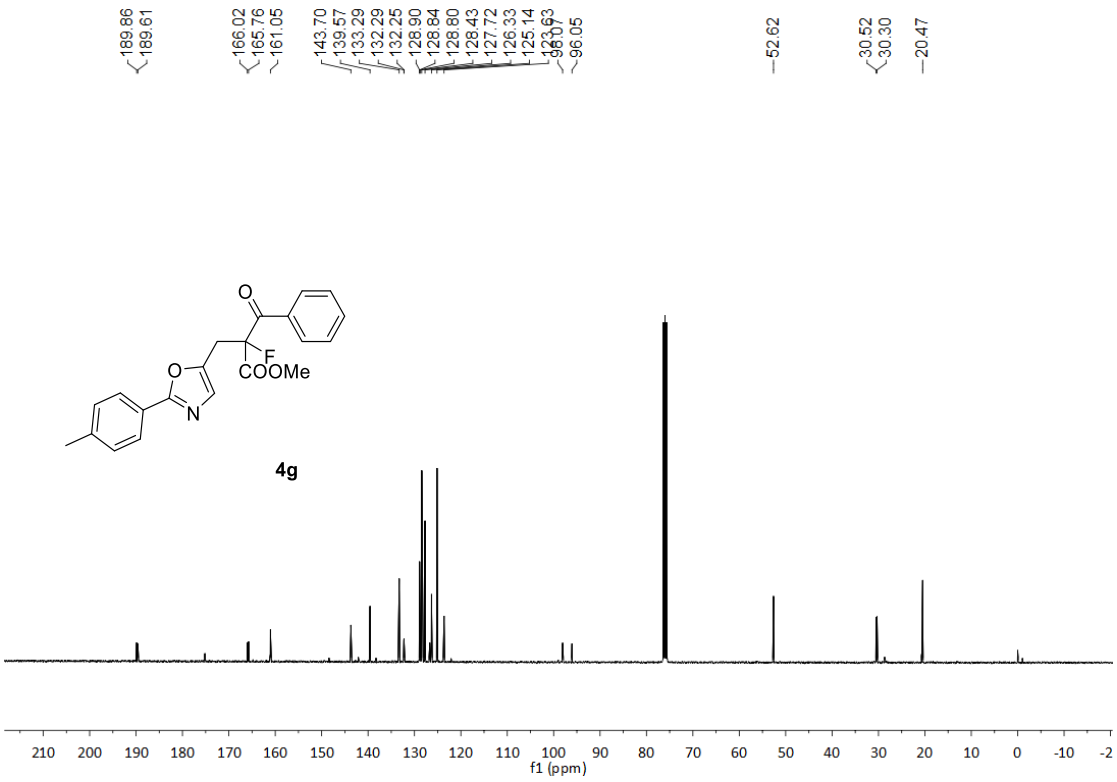
^{1}H NMR (400 MHz, $CDCl_3$):



^{19}F NMR (376 MHz, $CDCl_3$):

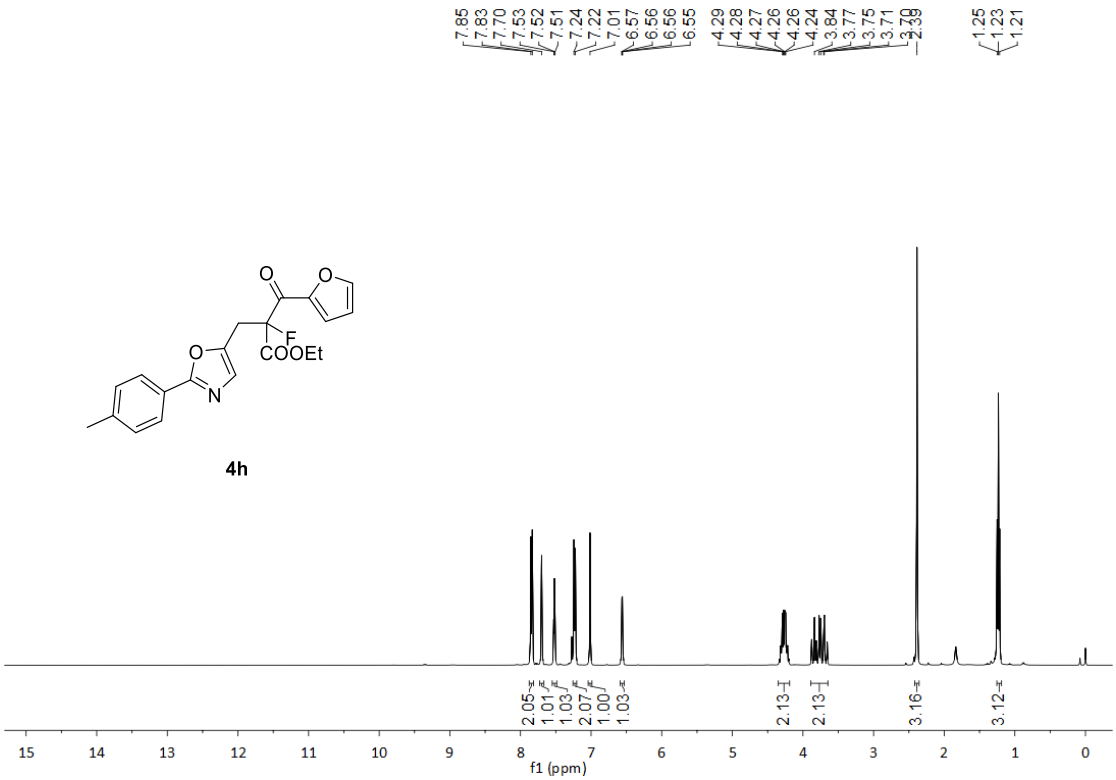


^{13}C NMR (100 MHz, $CDCl_3$):

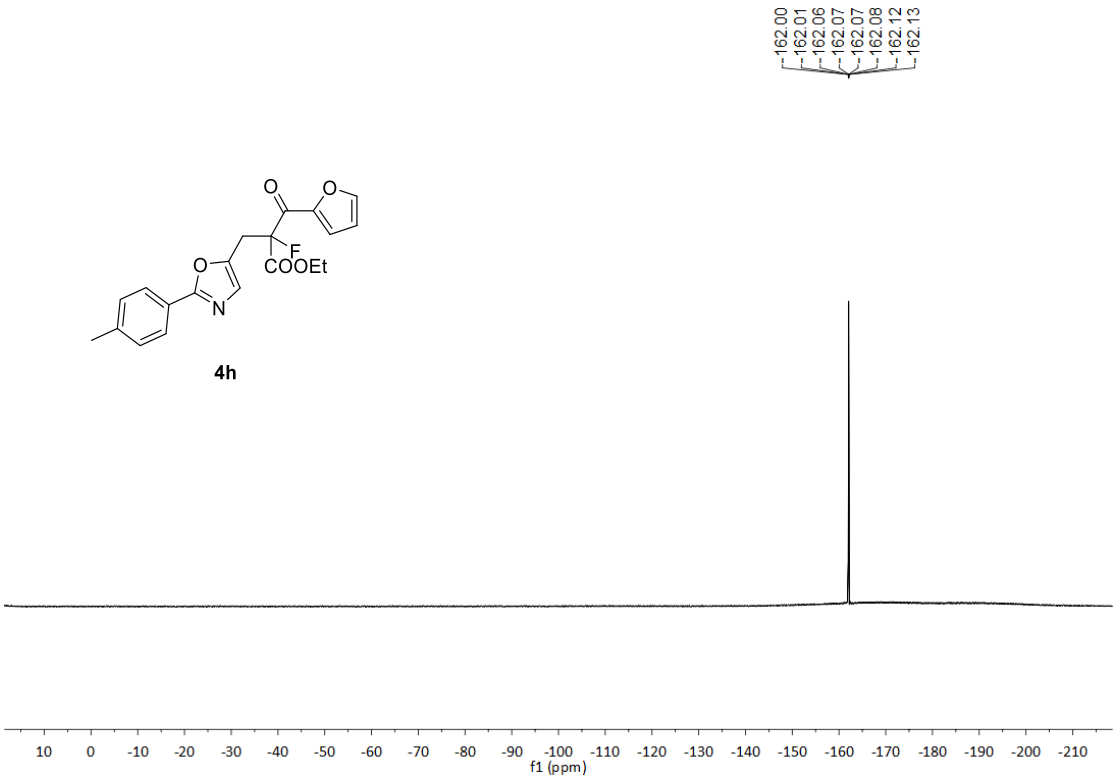


ethyl 2-fluoro-3-(furan-2-yl)-3-oxo-2-((2-(*p*-tolyl)oxazol-5-yl)methyl)propanoate (4h)

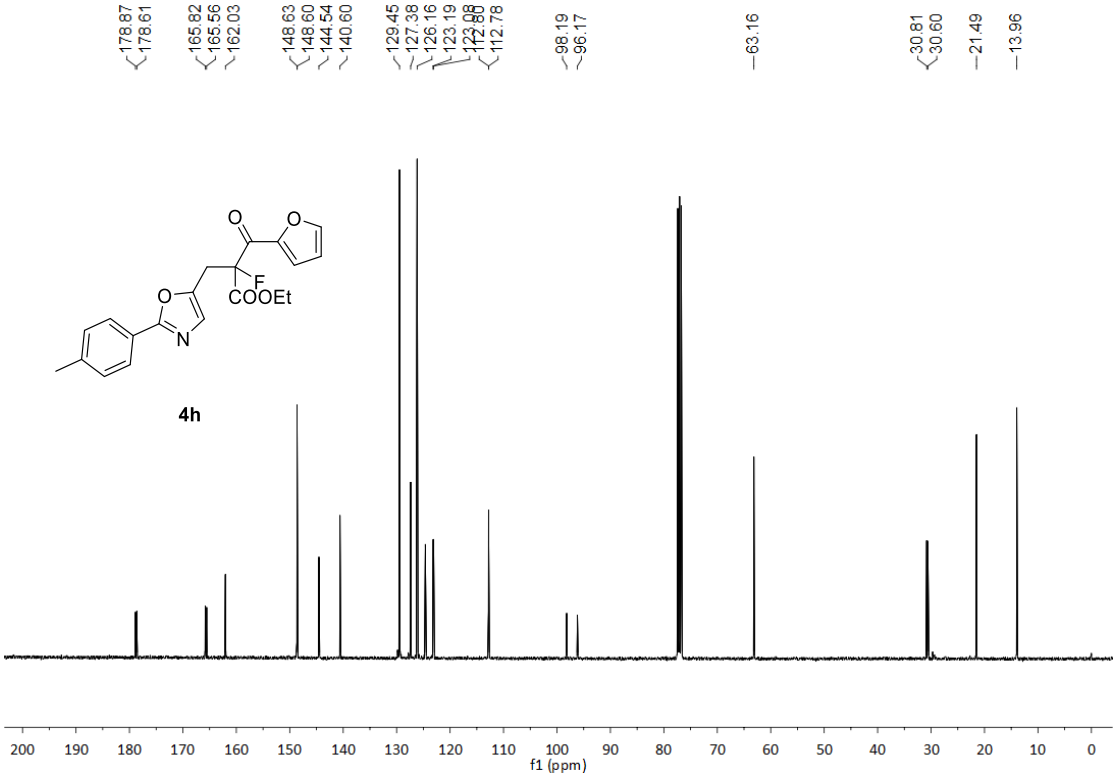
^{1}H NMR (400 MHz, $CDCl_3$)：



^{19}F NMR (376 MHz, $CDCl_3$):

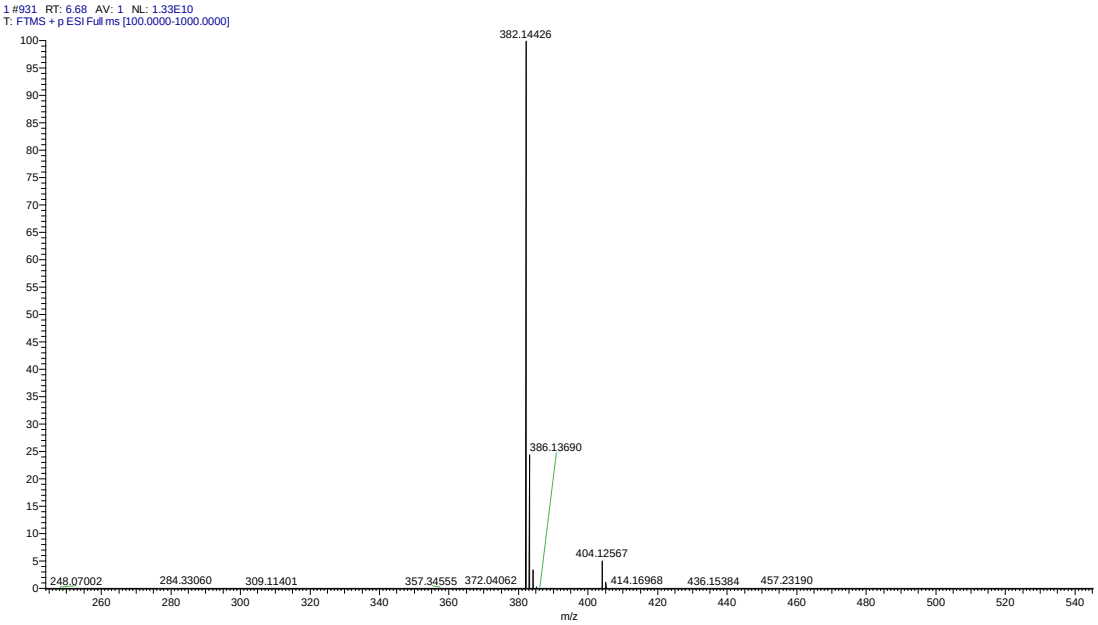


^{13}C NMR (100 MHz, $CDCl_3$):

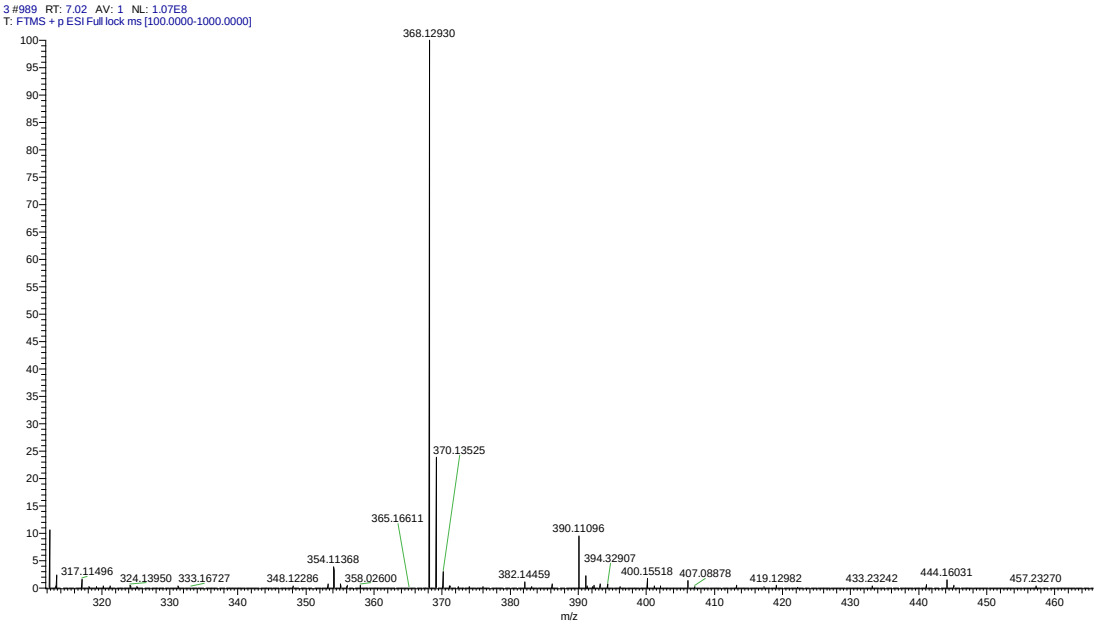


10. Copies HRMS

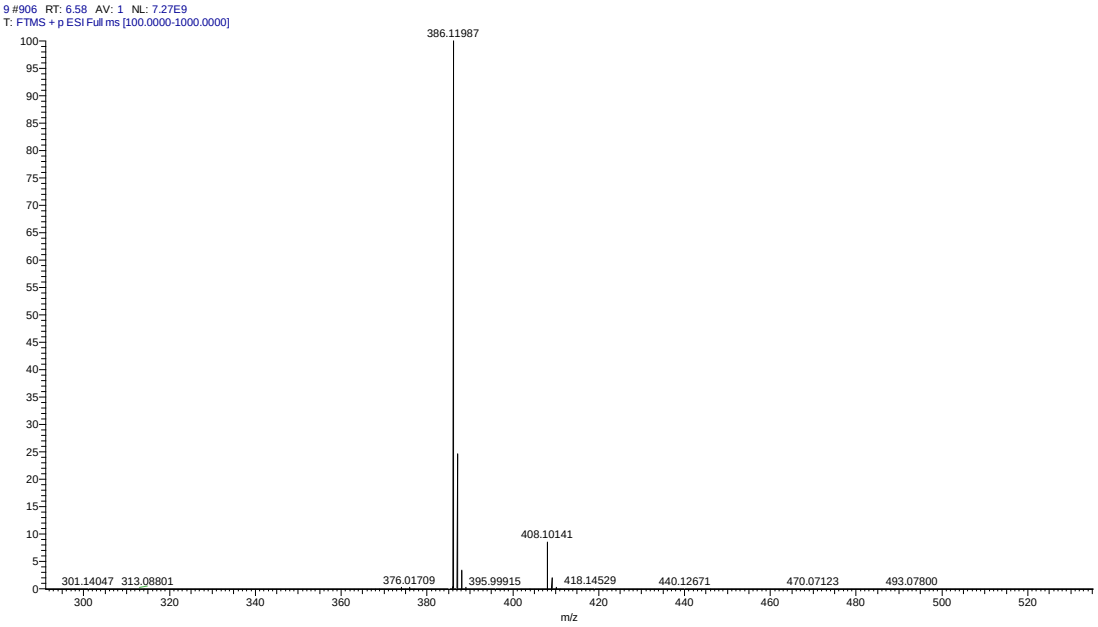
3a



3b



3c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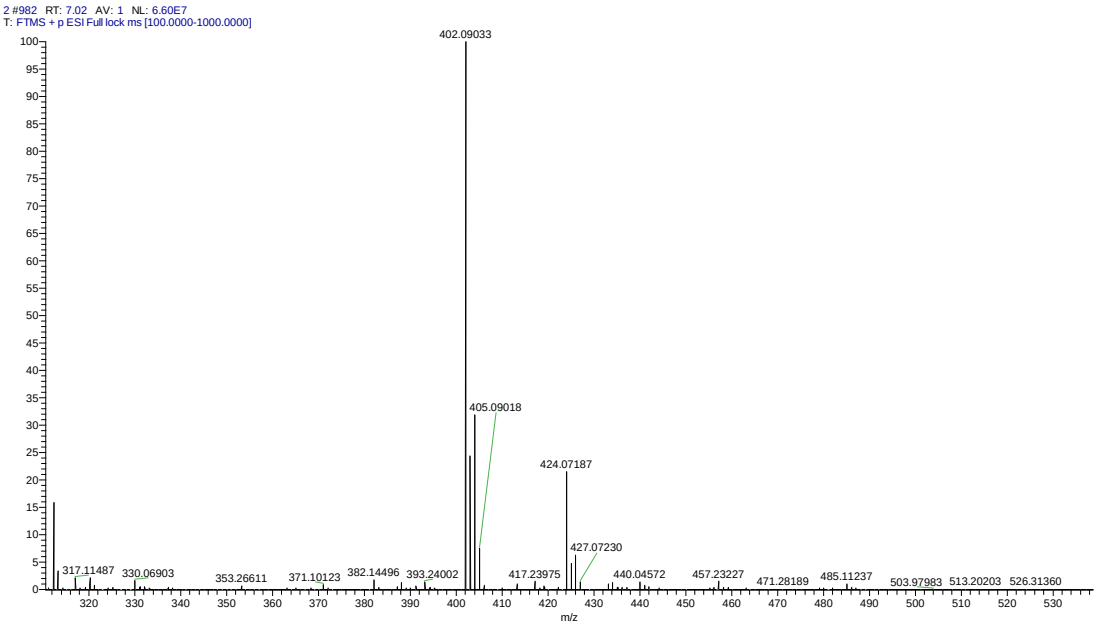
3d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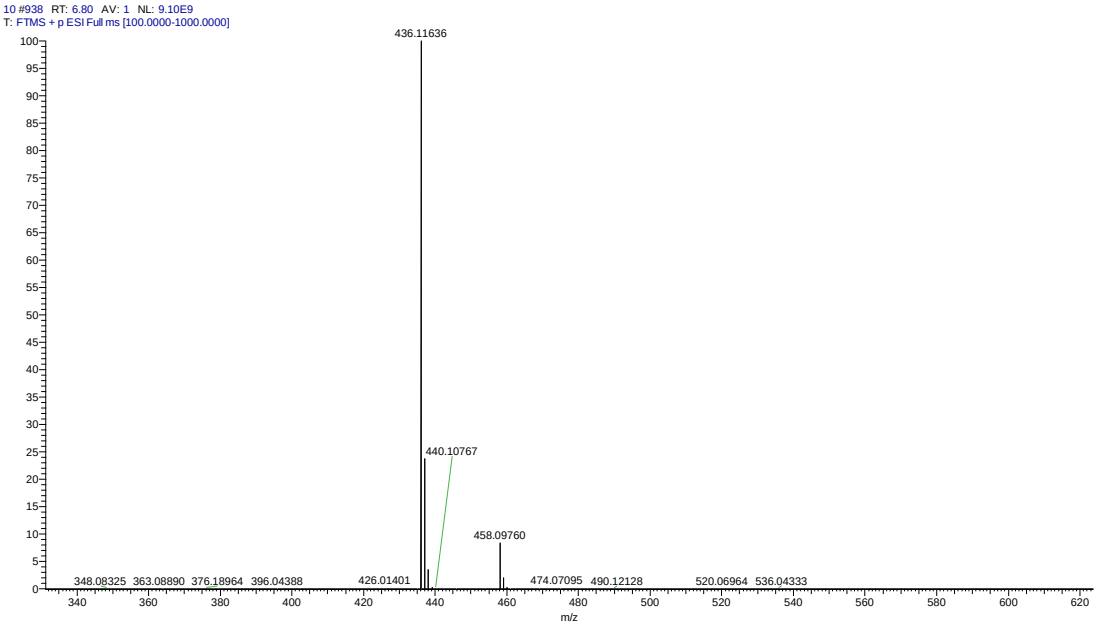
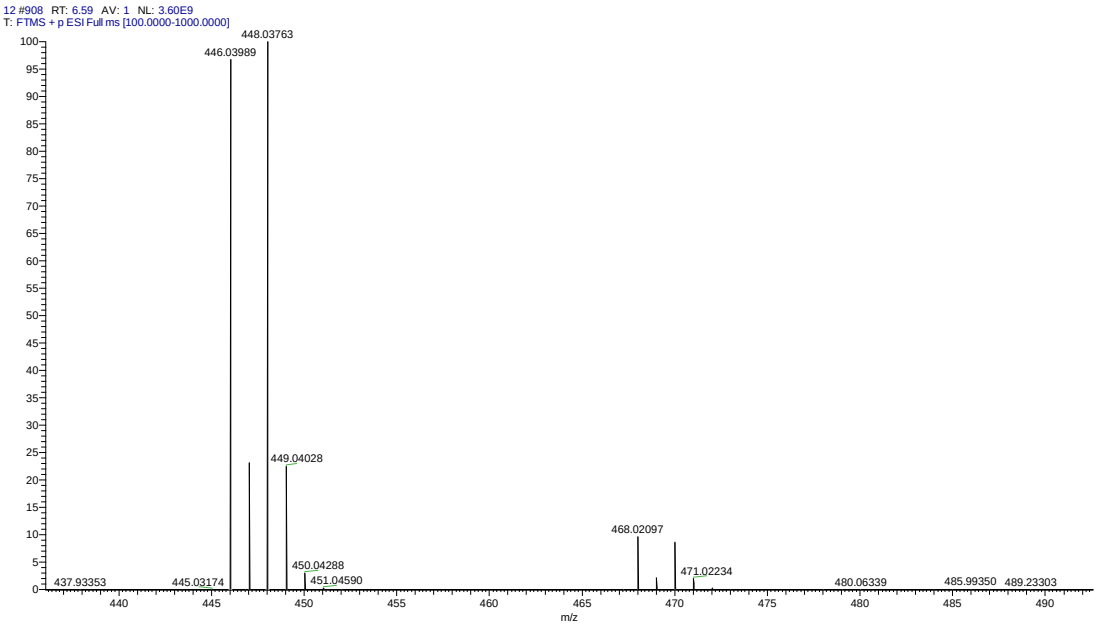
424.07187
427.07230
317.11487
330.06903
353.26611
371.10123
382.14496
393.24002
417.23975
440.04572
457.23227
471.28189
485.11237
503.97983
513.20203
526.31360
m/z

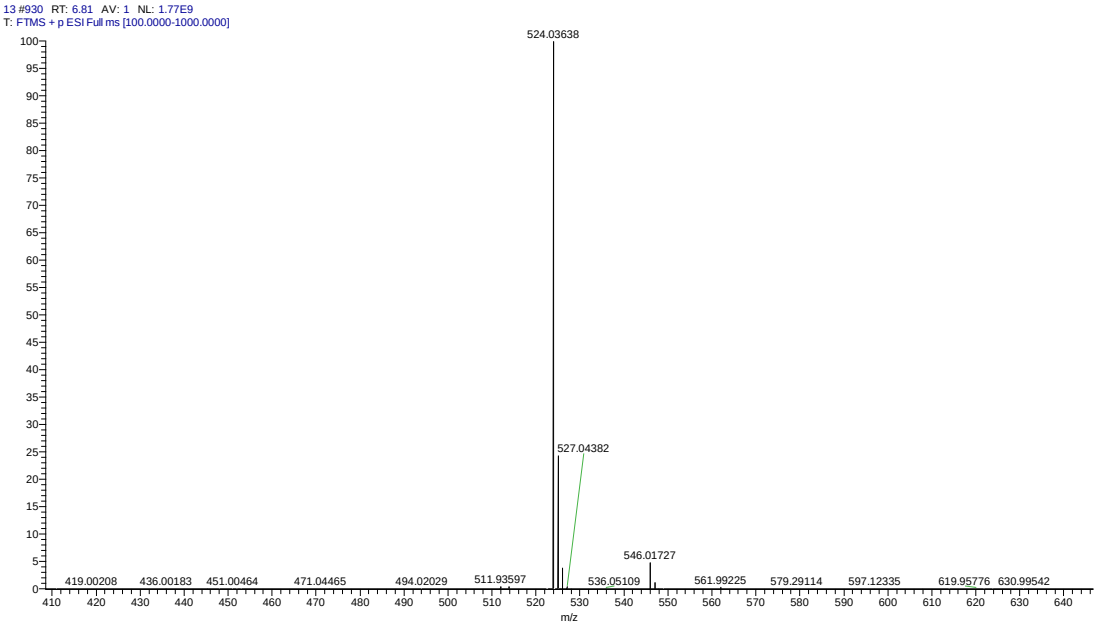
3e


10 #938 RT: 6.80 AV: 1 NL: 9.10E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
436.11636
440.10767
458.09760
348.08325
363.08890
376.18964
396.04388
426.01401
474.07095
490.12128
520.06964
536.04333
m/z

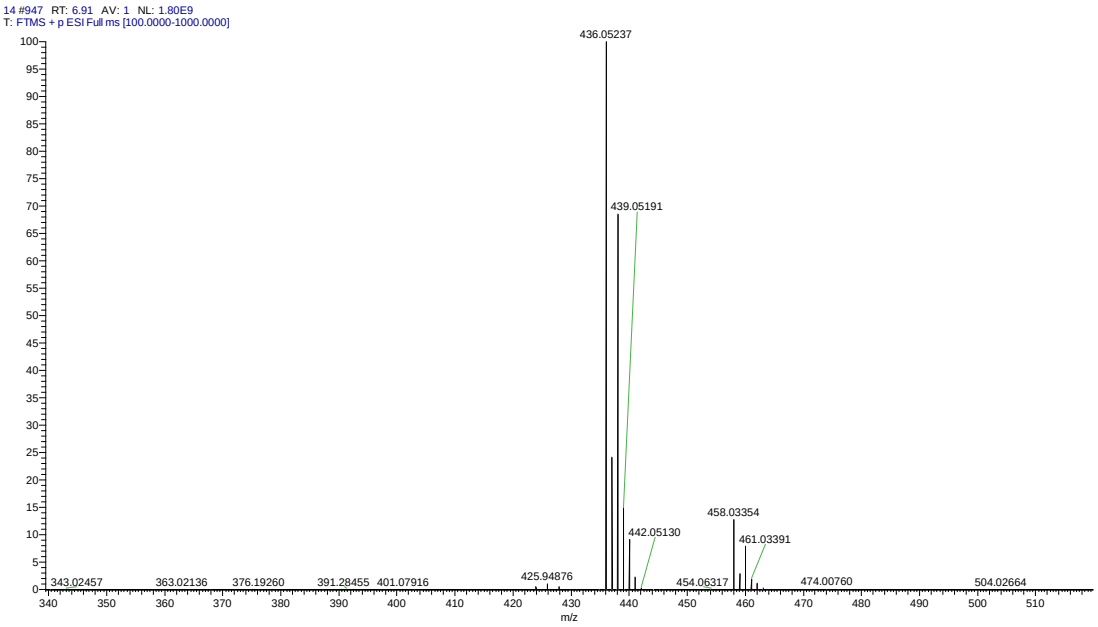
3f


12 #908 RT: 6.59 AV: 1 NL: 3.60E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
448.03763
446.03989
449.04028
468.02097
450.04288
471.02234
451.04590
437.93353
445.03174
480.06339
485.99350
489.23303
m/z

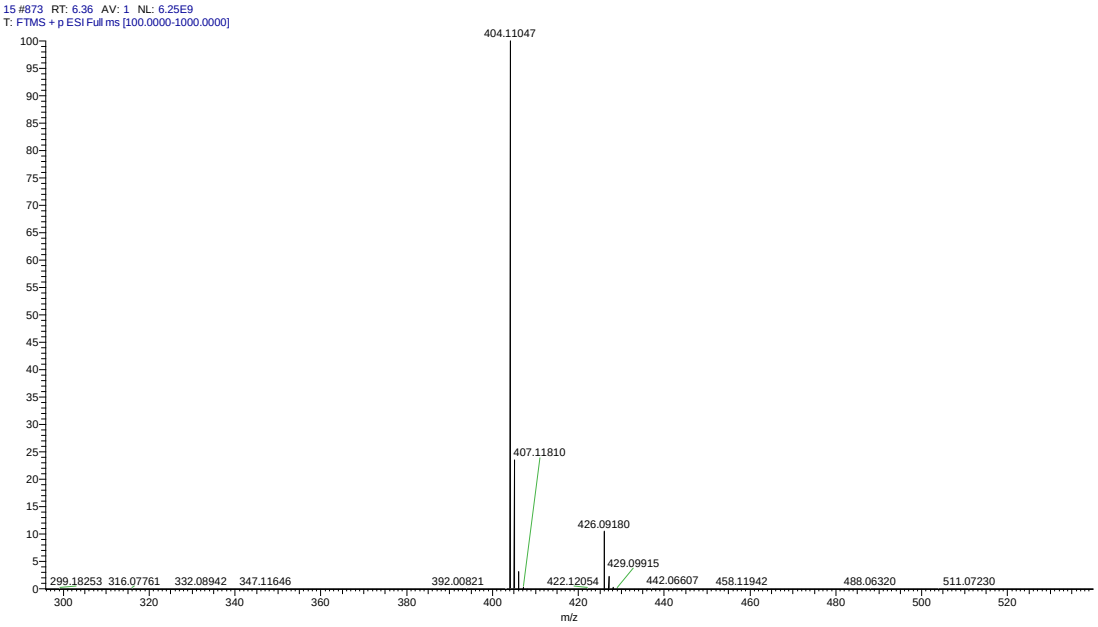
3g


13 #930 RT: 6.81 AV: 1 NL: 1.77E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
524.03638
527.04382
546.01727
419.00208
436.00183
451.00464
471.04465
494.02029
511.93597
536.05109
561.99225
579.29114
597.12335
619.95776
630.99542
m/z

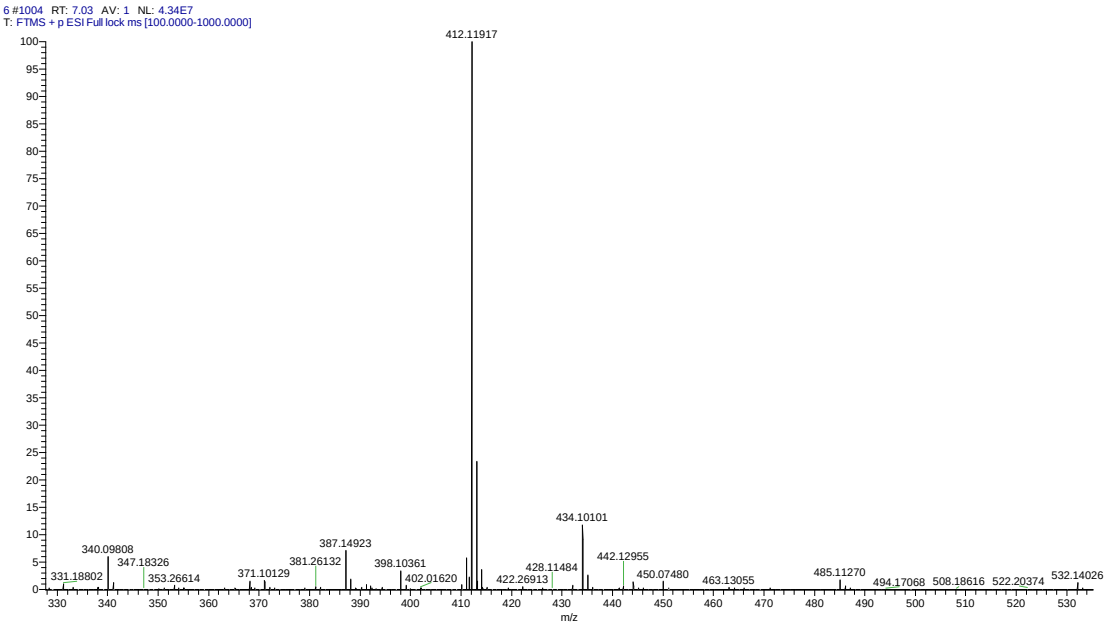
3h


14 #947 RT: 6.91 AV: 1 NL: 1.80E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
436.05237
439.05191
458.03354
442.05130
461.03391
343.02457
363.02136
376.19260
391.28455
401.07916
425.94876
454.06317
474.00760
504.02664
m/z

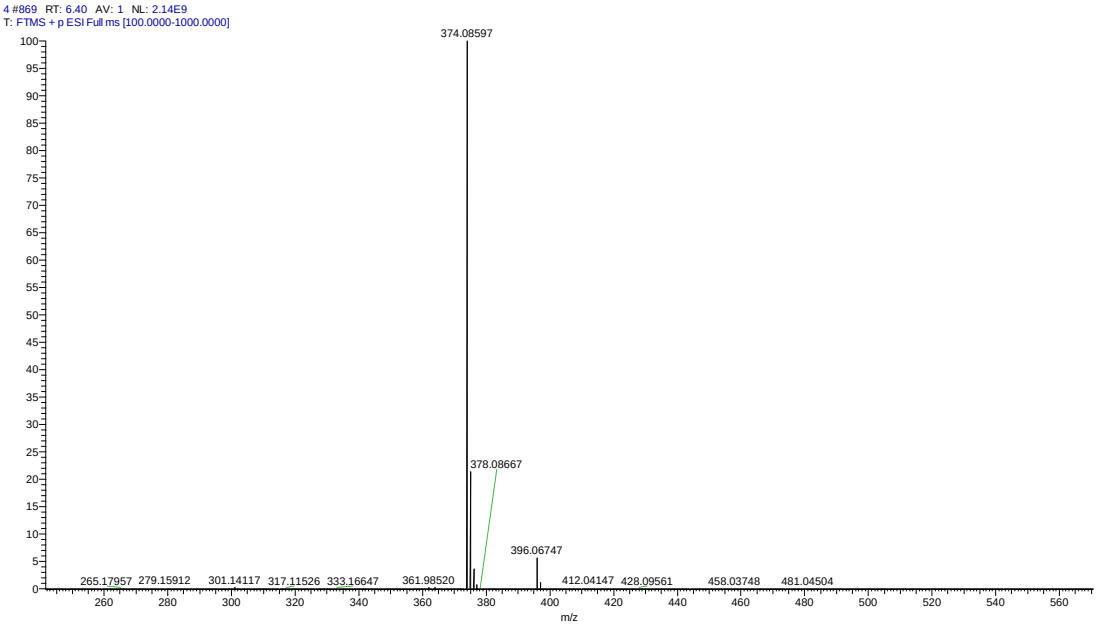
3i


15 #873 RT: 6.36 AV: 1 NL: 6.25E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
404.11047
407.11810
426.09180
429.09915
299.18253
316.07761
332.08942
347.11646
392.00821
422.12054
442.06607
458.11942
488.06320
511.07230
m/z

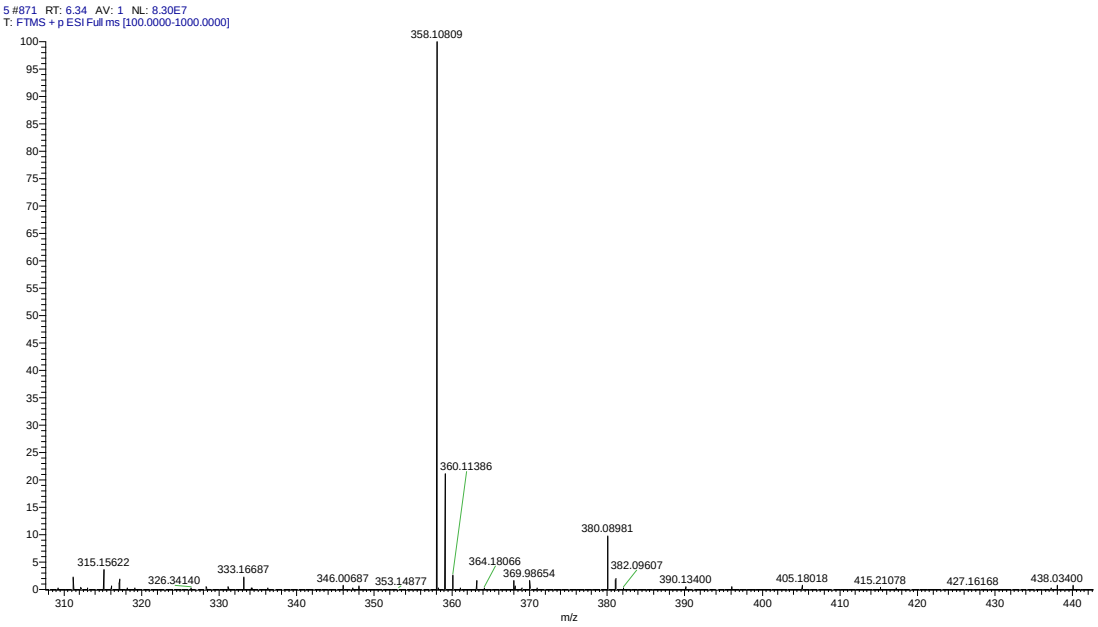
3j


6 #1004 RT: 7.03 AV: 1 NL: 4.34E7
T: FTMS + p ESI Full lock ms [100.0000-1000.0000]
412.11917
434.10101
340.09808
347.18326
387.14923
381.26132
398.10361
442.12955
331.18802
353.26614
371.10129
402.01620
422.26913
428.11484
450.07480
463.13055
485.11270
494.17068
508.18616
522.20374
532.14026
m/z

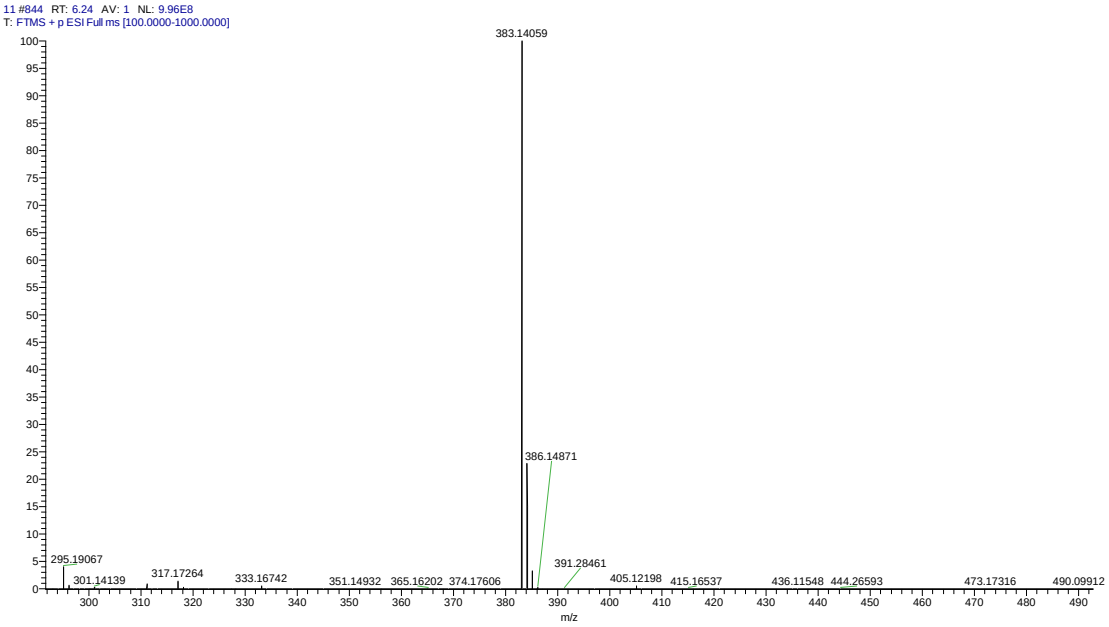
3k


4 #869 RT: 6.40 AV: 1 NL: 2.14E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
374.08597
378.08667
396.06747
265.17957
279.15912
301.14117
317.11526
333.16647
361.98520
412.04147
428.09561
458.03748
481.04504
m/z

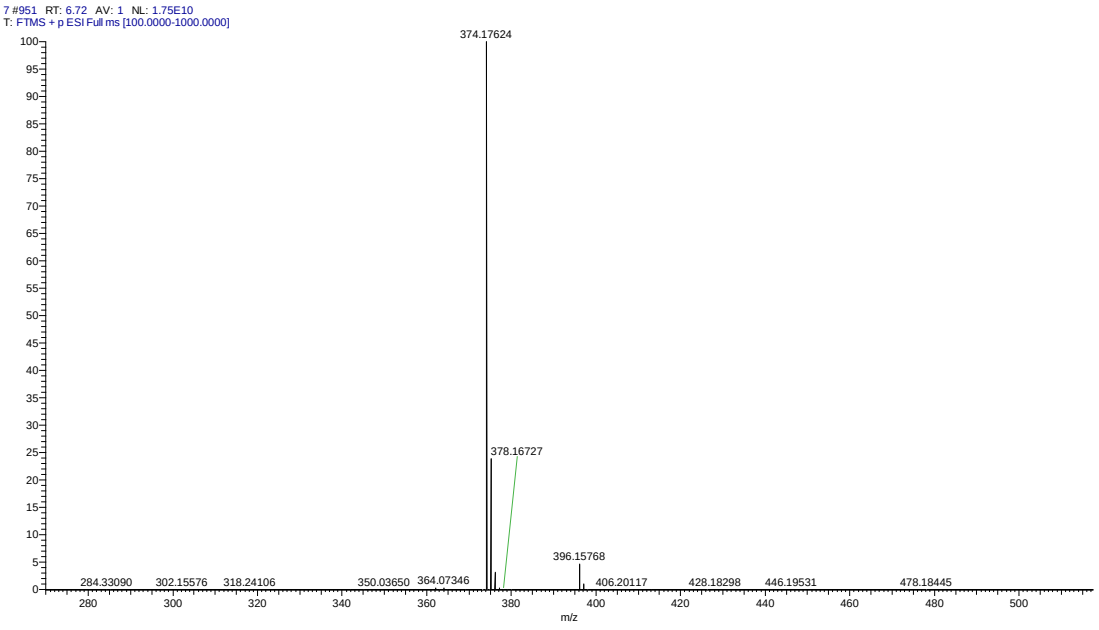
3l


5 #871 RT: 6.34 AV: 1 NL: 8.30E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]
358.10809
360.11386
380.08981
315.15622
326.34140
333.16687
346.00687
353.14877
364.18066
369.98654
382.09607
390.13400
405.18018
415.21078
427.16168
438.03400
m/z

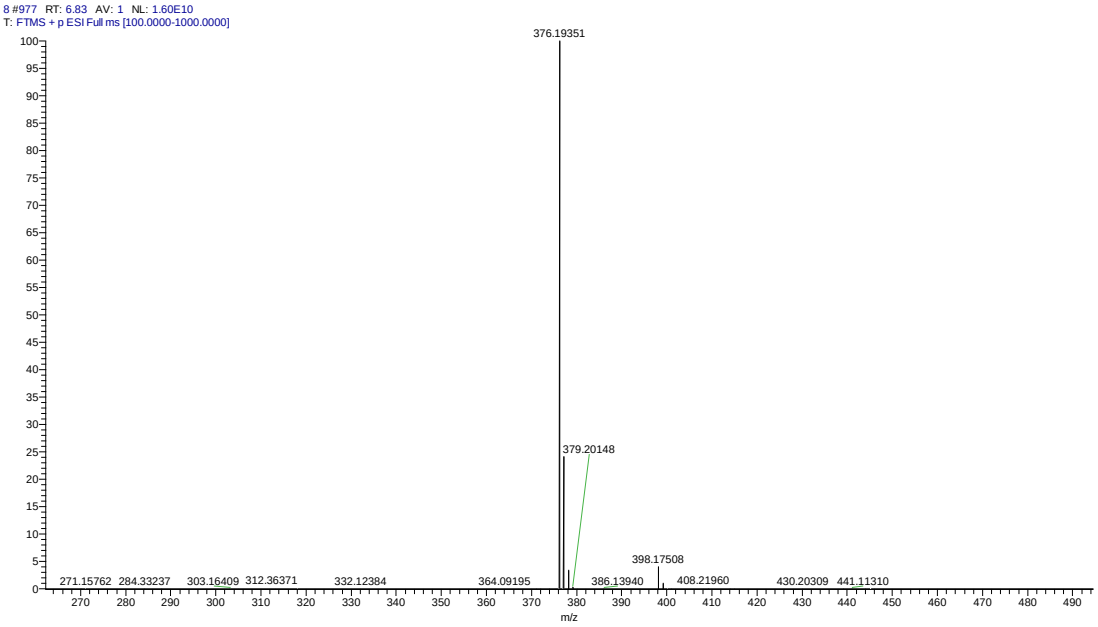
3m


11 #844 RT: 6.24 AV: 1 NL: 9.96E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]
383.14059
386.14871
295.19067
301.14139
317.17264
333.16742
351.14932
365.16202
374.17606
391.28461
405.12198
415.16537
436.11548
444.26593
473.17316
490.09912
m/z

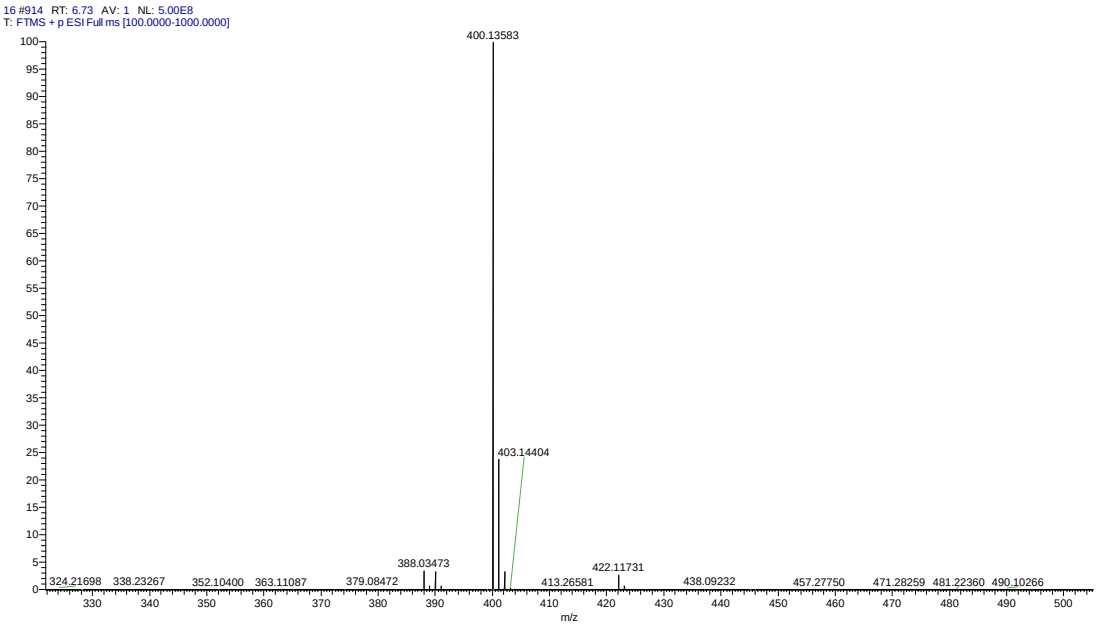
3n


7 #951 RT: 6.72 AV: 1 NL: 1.75E10
T: FTMS + p ESI Full ms [100.0000-1000.0000]
374.17624
378.16727
396.15768
284.33090
302.15576
318.24106
350.03650
364.07346
406.20117
428.18298
446.19531
478.18445
m/z

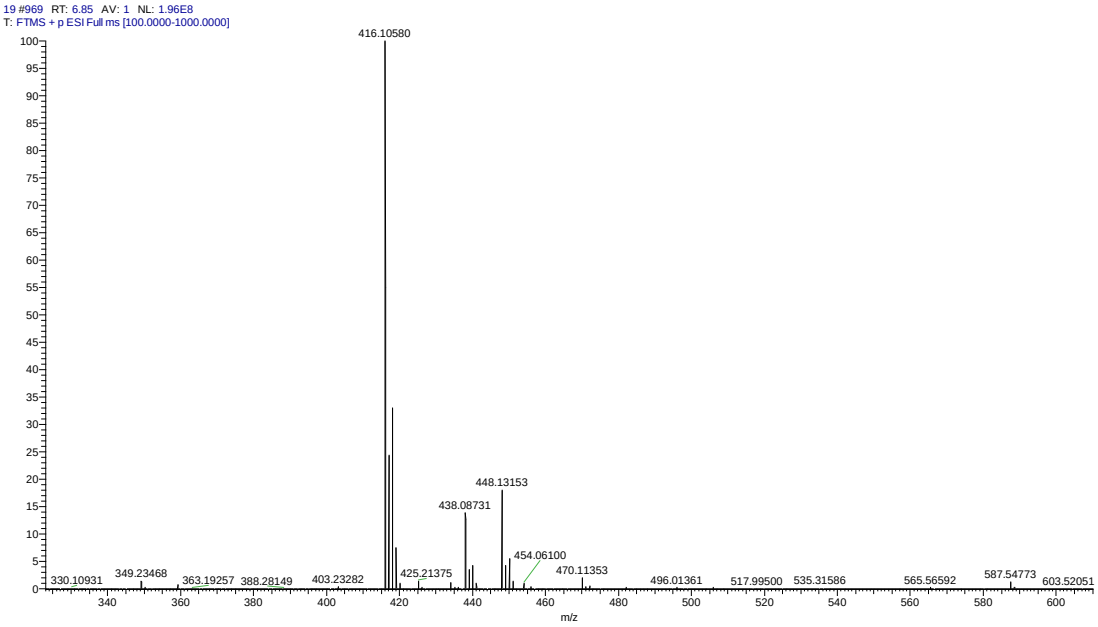
3o


8 #977 RT: 6.83 AV: 1 NL: 1.60E10
T: FTMS + p ESI Full ms [100.0000-1000.0000]
376.19351
379.20148
398.17508
271.15762
284.33237
303.16409
312.36371
332.12384
364.09195
386.13940
408.21960
430.20309
441.11310
m/z

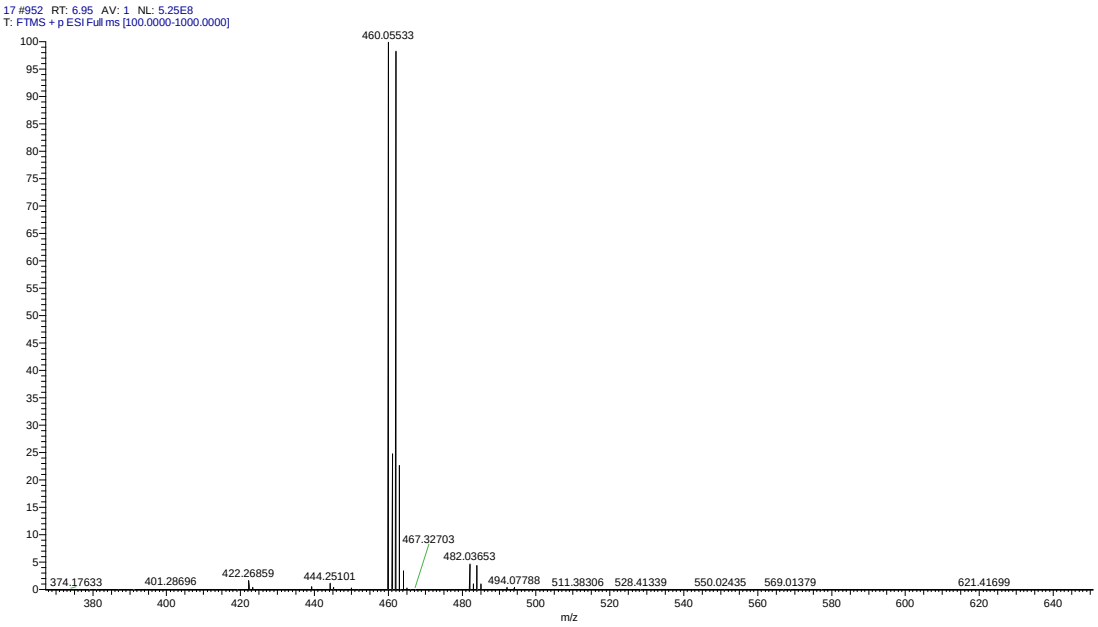
4a


16 #914 RT: 6.73 AV: 1 NL: 5.00E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]
400.13583
403.14404
388.03473
422.11731
324.21698
338.23267
352.10400
363.11087
379.08472
413.26581
438.09232
457.27750
471.28259
481.22360
490.10266
m/z

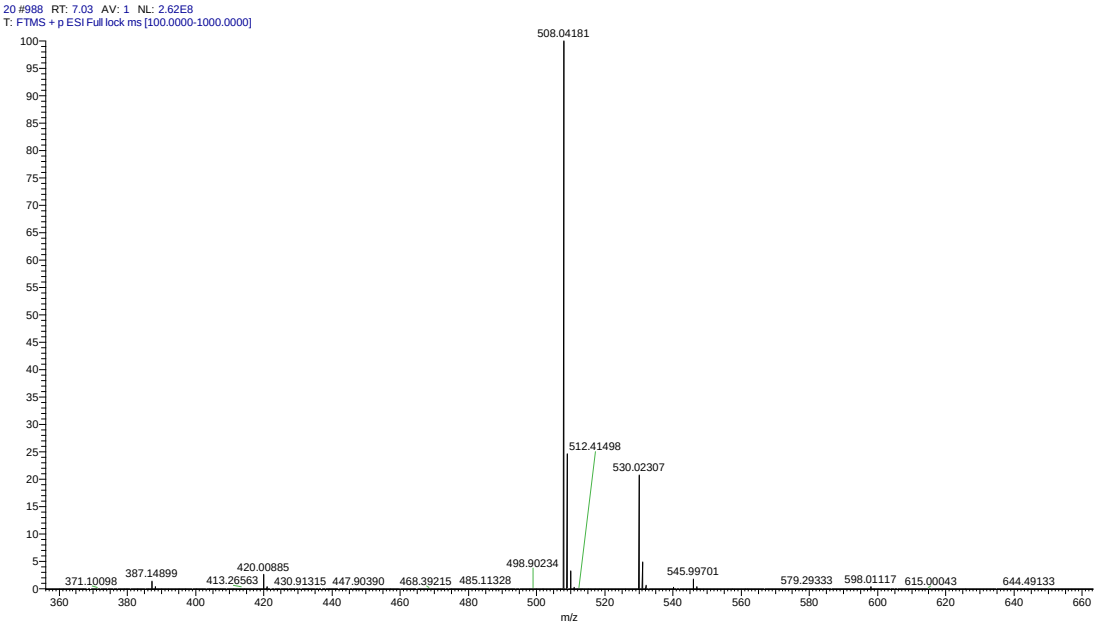
4b


19 #969 RT: 6.85 AV: 1 NL: 1.96E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]
416.10580
448.13153
438.08731
454.06100
470.11353
330.10931
349.23468
363.19257
388.28149
403.23282
425.21375
496.01361
517.99500
535.31586
565.56592
587.54773
603.52051
m/z

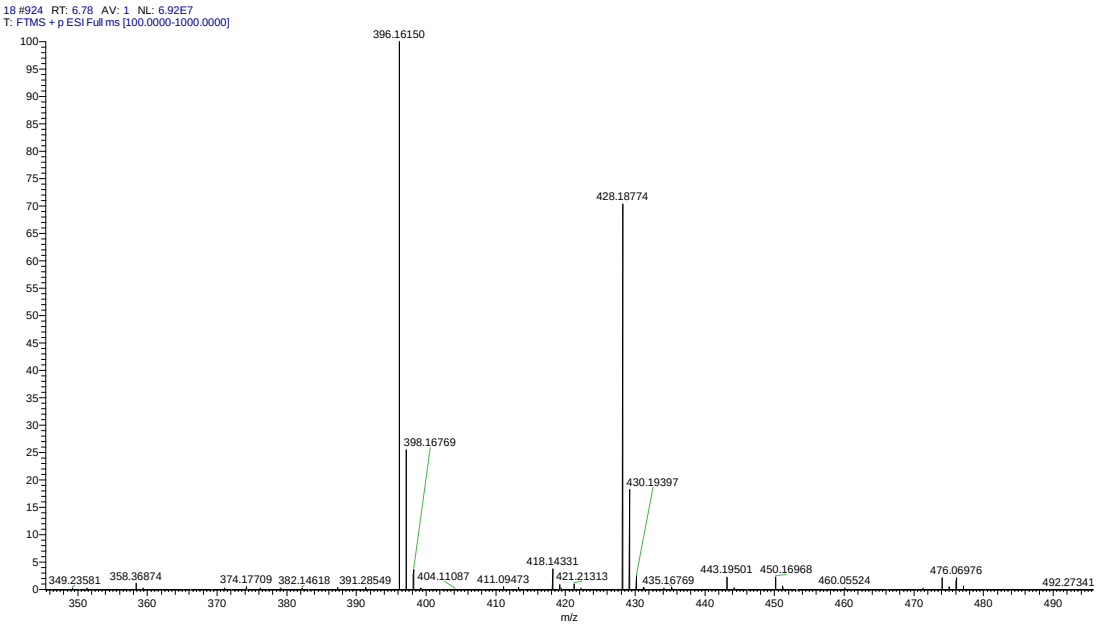
4c


17 #952 RT: 6.95 AV: 1 NL: 5.25E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]
460.05533
467.32703
482.03653
374.17633
401.28696
422.26859
444.25101
494.07788
511.38306
528.41339
550.02435
569.01379
621.41699
m/z

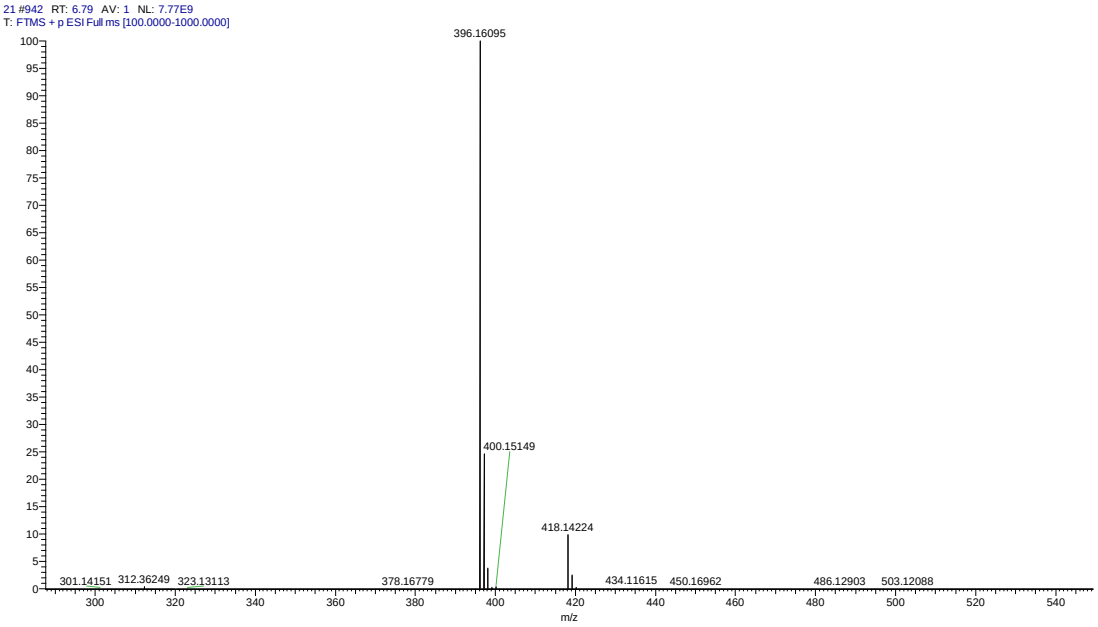
4d


20 #988 RT: 7.03 AV: 1 NL: 2.62E8
T: FTMS + p ESI Full lock ms [100.0000-1000.0000]
508.04181
512.41498
530.02307
498.90234
545.99701
420.00885
387.14899
371.10098
413.26563
430.91315
447.90390
468.39215
485.11328
579.29333
598.01117
615.00043
644.49133
m/z

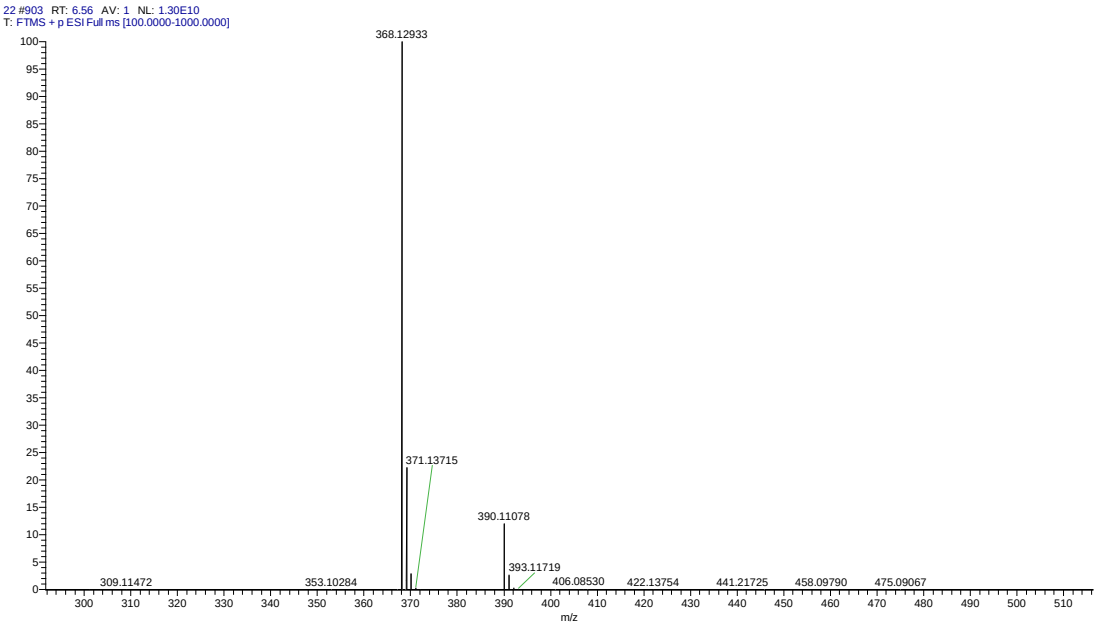
4e


18 #924 RT: 6.78 AV: 1 NL: 6.92E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]
396.16150
428.18774
398.16769
430.19397
418.14331
349.23581
358.36874
374.17709
382.14618
391.28549
404.11087
411.09473
421.21313
435.16769
443.19501
450.16968
460.05524
476.06976
492.27341
m/z

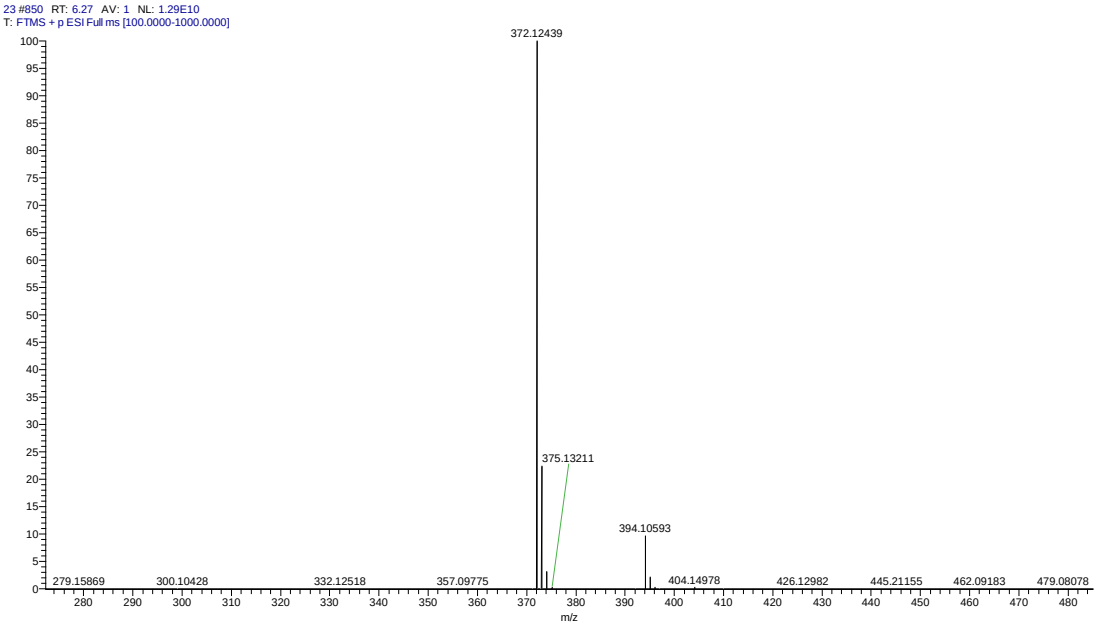
4f


21 #942 RT: 6.79 AV: 1 NL: 7.77E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
396.16095
400.15149
418.14224
301.14151
312.36249
323.13113
378.16779
434.11615
450.16962
486.12903
503.12088
m/z

4g


22 #903 RT: 6.56 AV: 1 NL: 1.30E10
T: FTMS + p ESI Full ms [100.0000-1000.0000]
368.12933
371.13715
390.11078
393.11719
309.11472
353.10284
406.08530
422.13754
441.21725
458.09790
475.09067
m/z

4h


23 #850 RT: 6.27 AV: 1 NL: 1.29E10
T: FTMS + p ESI Full ms [100.0000-1000.0000]
372.12439
375.13211
394.10593
279.15869
300.10428
332.12518
357.09775
404.14978
426.12982
445.21155
462.09183
479.08078
m/z