Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

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1. General information

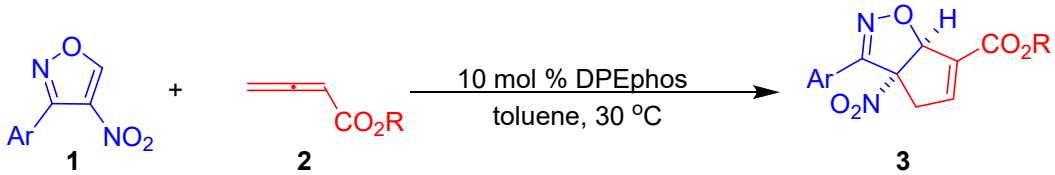
All experiments were carried out under an atmosphere of air. Flash column chromatography was performed over silica gel 48-75 μm. ^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded on Bruker-AV (500 MHz, 471 MHZ and 126 MHz, respectively) instrument internally referenced to $SiMe_4$ or chloroform signals. HRMS was recorded using waters G2-Xs qtof mass spectrometer. The new compounds were characterized by ^{1}H NMR, ^{19}F NMR, ^{13}C NMR, MS and HRMS. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{19}F NMR, ^{13}C NMR data and MS data with those of literature. The Substrates **1**[1], **2**[2]and **4**[3] was synthesized according to the reported methods.

Trichloromethane ($CHCl_3$), dichloromethane, dichloroethane and ethyl acetate were freshly distilled from CaH_2; tetrahydrofuran (THF), toluene and ether were dried with sodium benzophenone and distilled before use.

Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed on silica gel 60 (particle size 300-400 mesh ASTM, purchased from Yantai, China) and eluted with petroleum ether/ethyl acetate. All reagents and solvents were used as received from commercial sources (*Energy Chemical, J&K®, Adamas-beta®, Bidepharm*) without further purification.

2. Experimental procedure

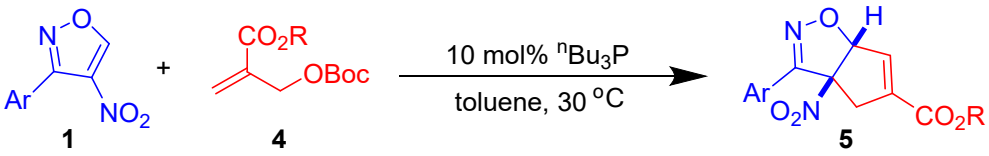
2.1 Phosphine-Catalyzed Dearomative [3+2] Cycloaddition of 4-Nitroisoxazoles with Allenoates



In a 10 mL of sealed tube, a mixture of 4-nitroisoxazoles **1** (0.2 mmol), allenoates **2** (0.24 mmol), DPEphos (0.02 mmol) and toluene (2 mL) was stirred at 30 °C for 12 h. After completion of the reaction (detected by TLC), the reaction mixture was

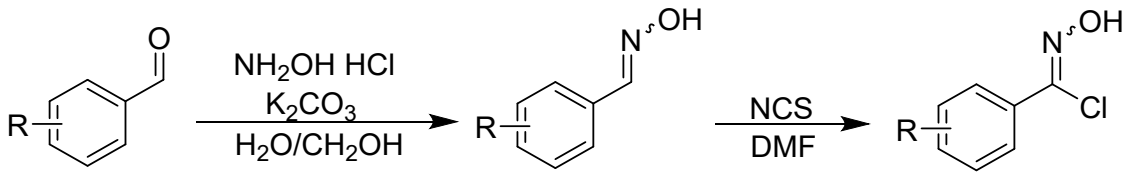
concentrated under reduced pressure. The residue was separated by column chromatography on silica gel with ethyl acetate/petroleum ether as the eluent to afford **3**.

2.2 Phosphine-Catalyzed Dearomative [3+2] Cycloaddition of 4-Nitroisoxazoles with Morita−Baylis−Hillman Carbonates



In a 10 mL of sealed tube, a mixture of 4-nitroisoxazoles **1** (0.2 mmol), MBH carbonates **4** (0.24 mmol), $^{n}Bu_3P$ (0.02 mmol) and toluene (2 mL) was stirred at 30 °C. After completion of the reaction (detected by TLC), the reaction mixture was concentrated under reduced pressure. The residue was separated by column chromatography on silica gel with ethyl acetate/petroleum ether as the eluent to afford **5**.

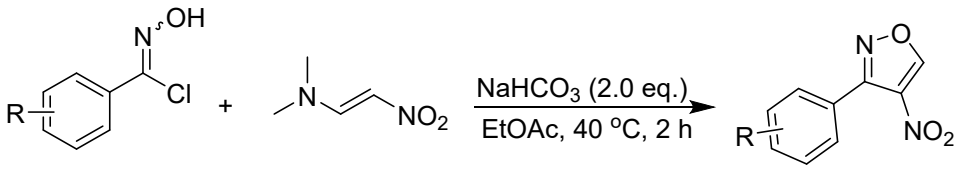
2.2 Representative procedure for the synthesis of 4-nitoroisoxazoles.



The oxime chloride were prepared according to the reference

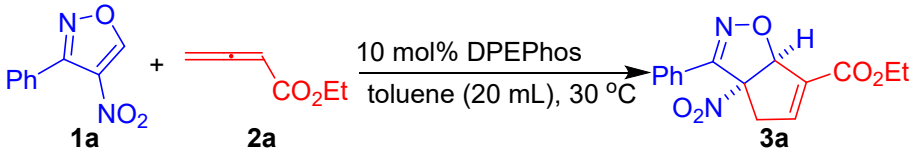
A 50 mL round-bottomed flask was charged with aldehyde (1.0 equiv), hydroxylamine hydrochloride (1.2 equiv), H_2O and methanol. Then, K_2CO_3 (1.5 equiv) was slowly added to the solution. The reaction was stirred at room temperature for overnight. Upon completion, methanol was removed, aqueous layers was extracted with ethyl acetate thrice. The combine organic layers were dried over anhydrous Na_2SO_4. After removal of the solvent, the crude aldoxime was used in the next step. A 50 mL round-bottomed flask was charged with the crude aldoxime

of the first step and *N*,*N*-dimethylformamide. Then, *N*-chlorosuccinimide (1.1 equiv) in *N*,*N*-dimethylformamide was added dropwise over a period of 10 minutes to the solution. The reaction was stirred for 4 hours at room temperature. Upon completion, the reaction mixture was poured into water, extracted with ethyl acetate thrice, the combine organic layers were washed with water and brine and dried over anhydrous Na_2SO_4. After removal of the solvent, the residue purified onsilica gel (petroleum ether: ethyl acetate = 30:1-5:1) to afford desired oxime chloride. Oxime chloride, which were not stable enough, were directly used in the next step without purification by column chromatography.



To a mixture of oxime chloride (1.0 equiv.), (*E*)-*N*,*N*-dimethyl-2-nitroethen-1-amine (1.2 equiv.) and sodium bicarbonate (2.0 equiv.), ethyl acetate (5 mL/mmol of oxime chloride) was added under an argon atmosphere. After being stirred for 2 h at 40 °C, the reaction mixture was filtered through a silica pad, the filtrate was concentrated and purified by silica gel column chromatography with *n*-hexane : diethyl ether (95 : 5) to afford 4-nitoroisoxazoles.

2.3 Scaled-Up version of **3a** and **5a**.



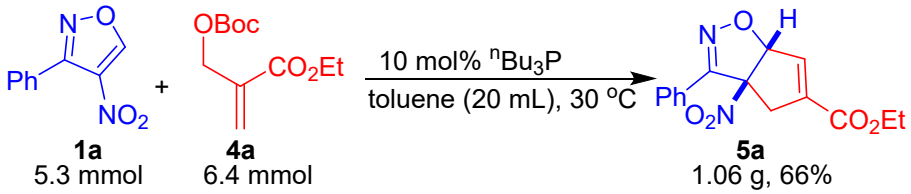
1a 5.0 mmol

2a 6.0 mmol

3a 1.39 g, 92 %

In a 10 mL of sealed tube, a mixture of 4-nitroisoxazoles **1a** (5.0 mmol), allenoates **2a** (6.0 mmol), DPEphos (0.5 mmol) and toluene (20 mL) was stirred at 30 °C for 12 h. After completion of the reaction (detected by TLC), the reaction mixture was concentrated under reduced pressure. The residue was separated by column

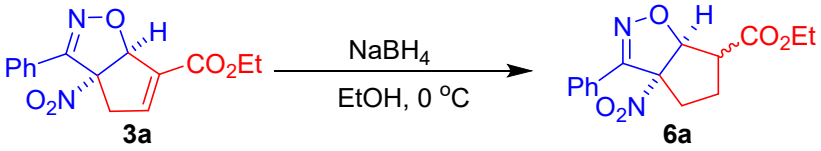
chromatography on silica gel with ethyl acetate/petroleum ether as the eluent to afford **3** in 1.39 g, 92% yield.



1a 5.3 mmol **4a** 6.4 mmol **5a** 1.06 g, 66%

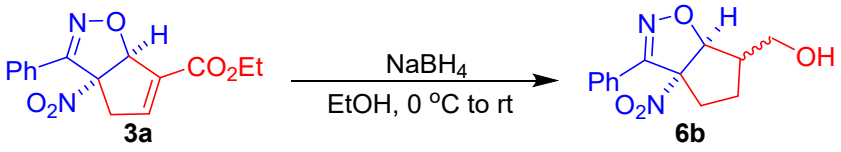
In a 10 mL of sealed tube, a mixture of 4-nitroisoxazoles **1** (5.3 mmol), MBH carbonates **4** (6.4 mmol), $^{n}Bu_3P$ (0.53 mmol) and toluene (20 mL) was stirred at 30 °C. After completion of the reaction (detected by TLC), the reaction mixture was concentrated under reduced pressure. The residue was separated by column chromatography on silica gel with ethyl acetate/petroleum ether as the eluent to afford **5a** in 1.06 g, 66% yield.

2.4 The transformation of the Product **3a.**



3a **6a**

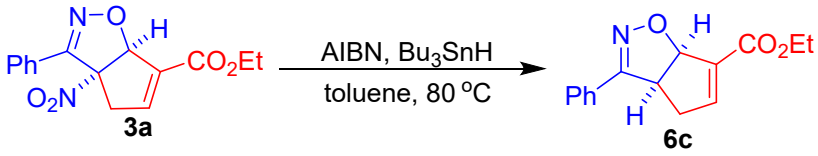
To compound **3a** (60.5 mg, 0.2 mmol) in 3 mL ethanol was added $NaBH_4$ (75.6 mg, 2.0 mmol) at 0 °C. Then the reaction was stirred for 1 h at 0 °C, and quenched with 20 mL saturated NH_4Cl solution. The aqueous solution was extracted with DCM three times. The combined organic layers were dried over Na_2SO_4. After evaporation of the solvent, the resulting crude mixture was purified by flash chromatography on silica gel to afford compound **6a** in 58% yield, 1:1 dr.



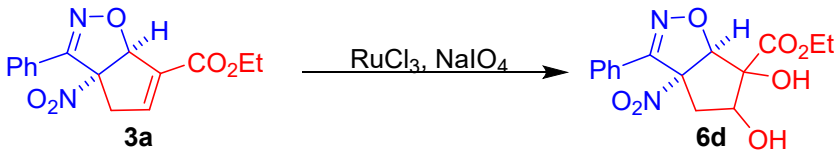
3a **6b**

To compound **3a** (60.5 mg, 0.2 mmol) in 3 mL ethanol was added $NaBH_4$ (75.6 mg, 2.0 mmol) at 0 °C. After the reaction was stirred for 1 h at 0 °C, the resulting mixture was warmed to room temperature and stirred for 3 h. The resulting mixture was then

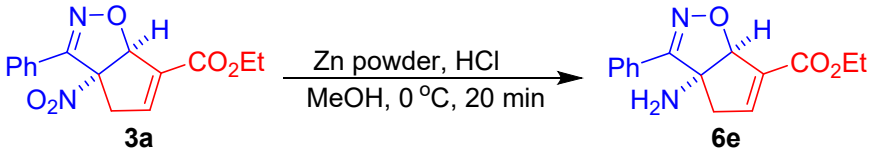
quenched with 20 mL saturated NH_4Cl solution and extracted with DCM three times. The combined organic layers were dried over Na_2SO_4. After evaporation of solvent, the resulting crude mixture was purified by flash chromatography on silica gel to afford compound **6b** in 65% yield, >20:1 dr.



To a stirred solution of **3a** (60.5 mg, 0.2 mmol) and tributyltin hydride (107.6 µl, 0.4 mmol) in PhMe (2.0 mL), AIBN (39.4 mg, 0.24 mmol) were added at rt. After being stirred at 80 ºC for 30 min, the reaction mixture was cooled to rt and 400 µl CCl4 were added. After being stirred at rt for 20 min, sat. KF aq. solution (40 ml) was added to the reaction mixture and the organic layer was extracted with AcOEt. The combined organic layers were dried over anhydrous Na_2SO_4. After removal of Na_2SO_4 by a filtration, the solution was concentrated under reduced pressure. The resulting crude mixture was purified by silica gel column chromatographyto afford **6c** in 60% yield.

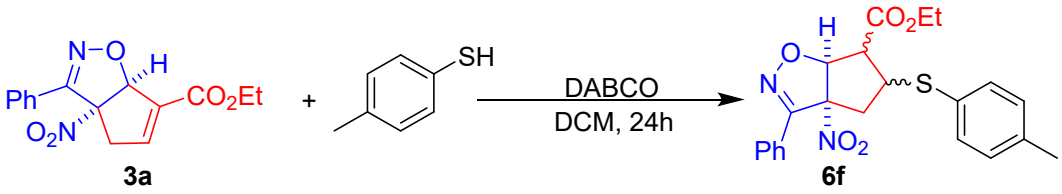


The reaction was carried out under following conditions: $NaIO_4$ (0.4 mmol) was dissolved in 0.2 mL distilled water, cooled with ice bath, then 4 drops of 2M H_2SO_4 and $RuCl_3{\cdot}3H_2O$ were subsequently added. After 5 min stirring, 0.4 mL MeCN was added. The solution was stirred for additional 5 min, **3a** (0.2 mmol, 60.5 mg) in 0.4 mL ethyl acetate was then added in one portion. The mixture was further stirred 60 min in ice bath, and then it was transferred into a solution of 10% $NaHCO_3$ (1.2 mL) and saturated Na_2SO_3 (2.0 mL), which was stirred for 60 min. After extraction with dichloromethane, dried over $MgSO_4$, it was subjected to chromatographic purification on silica gel, afforded **6d** in 75% yield.



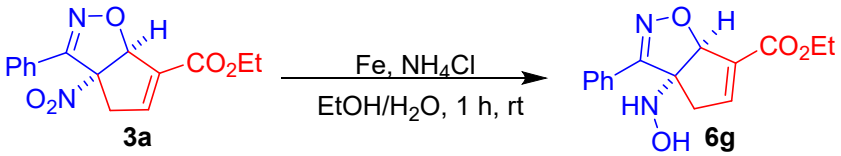
3a **6e**

Zinc powder (65.41 mg, 1.0 mmol, 10.0 equiv) was slowly added to a solution of **3a** (30.21 mg, 0.1 mmol,) and HCl(0.2 mL) in methanol at 0°C. After stirring the reaction suspension at 0°C for 20 min, the suspension was filtered and washed with dichloromethane. Then the filtrate was washed with saturated $NaHCO_3$, extracted with dichloromethane. The combined organic fractions were dried over Na_2SO_4, filtered and concentrated by rotary evaporation. Then the residue was purified by silica gel column chromatography to afford the desired product **6e** in 65% yield.



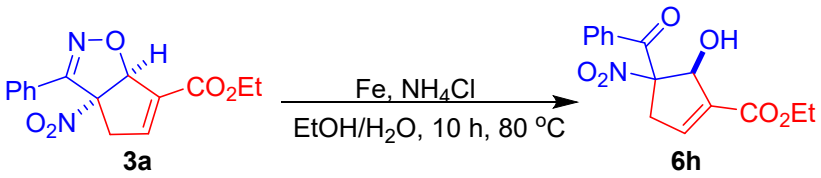
3a **6f**

A stirred solution of **3a** (0.2 mmol, 60.5 mg) in DCM (2 mL) was added p-toluenethiol (0.40 mmol), DABCO (0.20 mmol). The mixture was stirred at r.t. for 12 h. After completion of the reaction, the reaction mixture was directly applied to a silica gel chromatography column to afford the desired **6f** in 99% yield.



3a **6g**

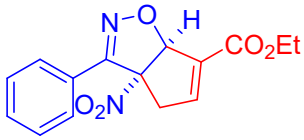
A sealed tube was charged with 3a (0.2 mmol, 60.5 mg), Fe powder (107.52 mg, 1.92 mmol, 9.6 equiv.) and NH_4Cl (107.0 mg, 2.0 mmol, 10 equiv.), followed by the addition of ethanol / water (1 : 1.4).The reaction mixture was stirred for 1 h at room temperature. The reaction mixture was filtered through a silica pad. The filtratewas concentrated in vacuo. The residue was purified by silica gel chromatography column to afford a desire product **6g** in 43.8 mg, 76% yield.



Fe powder (2.0 mmol, 112 mg) was added to isoxazoline **3a** (0.2 mmol, 60.5 mg) and NH_4Cl (2.0 mmol, 107 mg) in ethanol and water (1:1, 4 mL). The mixture was stirred in an 80 °C oil bath for 10 hours. After the reaction was completed by TLC monitoring, the reaction mixture was cooled to room temperature, diluted with ethyl acetate, and filtered through a silica pad. The filtrate was washed with brine and the organic layer was separated, dried over Na_2SO_4, and evaporated in vacuo. The residue was then purified by flash chromatography on silica gel to give product **6h** in 45 mg, 78% yield.

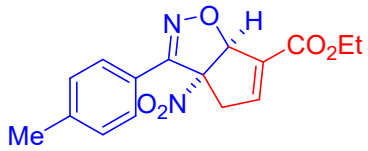
3. Characterization data of the products

Ethyl (3aR,6aS)-3a-nitro-3-phenyl-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3a)



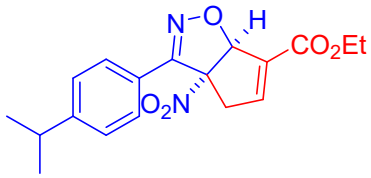
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3a** as a yellow solid (62 mg, 99% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 – 7.58 (m, 2H), 7.46 – 7.41 (m, 3H), 6.86 (s, 1H), 6.34 (s, 1H), 4.30 (q, J = 7.1 Hz, 2H), 4.12 (dd, J = 19.8, 2.1 Hz, 1H), 3.37 (dd, J = 19.8, 1.4 Hz, 1H), 1.35 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.82, 152.88, 142.31, 133.36, 130.97, 129.28, 126.72, 125.82, 104.49, 96.24, 61.46, 40.15, 14.17; HRMS (ESI) m/z calcd. for $C_{15}H_{15}N_2O_5^+$ $[M+H]^+$ = 303.0975, found 303.0970.

Ethyl (3aR,6aS)-3a-nitro-3-(p-tolyl)-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3b)



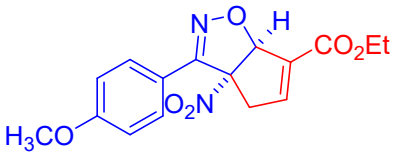
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3b** as a colorless viscous liquid (63.2 mg, 99% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.3 Hz, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 6.85 (t, *J* = 2.4 Hz, 1H), 6.31 (s, 1H), 4.32 – 4.27 (m, 2H), 4.13 – 4.08 (m, 1H), 3.38-3.33 (m, 1H), 2.38 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.88, 152.87, 142.34, 141.50, 133.32, 129.98, 126.64, 122.88, 104.61, 96.02, 61.45, 40.17, 21.46, 14.19; HRMS (ESI) m/z calcd. for $C_{16}H_{17}N_2O_5^+$ $[M+H]^+$ = 317.1132, found 317.1137.

Ethyl (3aR,6aS)-3-(4-isopropylphenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3c)



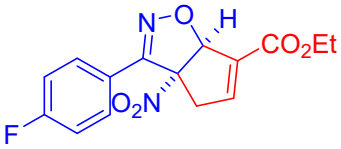
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3c** as a yellow solid (52.0 mg, 76% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 6.85 (s, 1H), 6.31 (s, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 4.11 (dd, *J* = 19.8, 2.1 Hz, 1H), 3.37 (dd, *J* = 19.8, 1.3 Hz, 1H), 2.97 – 2.88 (m, 1H), 1.34 (t, *J* = 7.1 Hz, 3H), 1.25 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.89, 152.86, 152.29, 142.33, 133.34, 127.42, 126.79, 123.20, 104.63, 96.02, 61.45, 40.15, 34.10, 23.68, 14.19; HRMS (ESI) m/z calcd. for $C_{18}H_{21}N_2O_5^+$ $[M+H]^+$ = 345.1445, found 345.1440.

Ethyl (3aR,6aS)-3-(4-methoxyphenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3d)



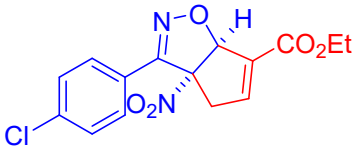
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3d** as a white powder (50.7 mg, 78% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.52 (m, 2H), 6.94 – 6.91 (m, 2H), 6.85 (t, *J* = 2.3 Hz, 1H), 6.30 (s, 1H), 4.30 (tt, *J* = 7.2, 3.6 Hz, 2H), 4.10 (dd, *J* = 19.8, 2.3 Hz, 1H), 3.84 (s, 3H), 3.38 – 3.34 (m, 1H), 1.34 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.90, 161.64, 152.51, 142.17, 133.40, 128.37, 118.05, 114.75, 104.76, 95.86, 61.46, 55.45, 40.14, 14.20; HRMS (ESI) m/z calcd. for $C_{16}H_{16}N_2NaO_6^+$ $[M+Na]^+$ =355.0901, found 355.0897.

Ethyl (3aR,6aS)-3-(4-fluorophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3e)



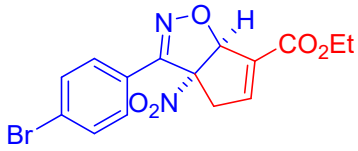
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3e** as a white powder (48.5 mg, 76% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 8.6, 5.2 Hz, 2H), 7.13 (t, *J* = 8.5 Hz, 2H), 6.86 (s, 1H), 6.35 (s, 1H), 4.31 (q, *J* = 7.0 Hz, 2H), 4.10 (d, *J* = 19.4 Hz, 1H), 3.34 (dd, *J* = 19.8, 0.9 Hz, 1H), 1.35 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.11 (d, *J* = 253.2 Hz), 161.77, 151.96, 142.21, 133.34, 128.89 (d, *J* = 8.6 Hz), 122.06, 116.60 (d, *J* = 22.1 Hz), 104.42, 96.30, 61.52, 40.10, 14.17; ^{19}F NMR (471 MHz, $CDCl_3$) δ -107.83; HRMS (ESI) m/z calcd. for $C_{15}H_{13}FN_2NaO_5^+$ $[M+Na]^+$ = 343.0701, found 343.0706.

Ethyl (3aR,6aS)-3-(4-chlorophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3f)



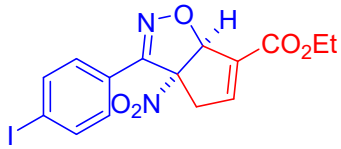
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3f** as a white solid(46.6 mg, 71% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.6 Hz, 2H), 7.40 (d, *J* = 8.7 Hz, 2H), 6.86 (s, 1H), 6.36 (s, 1H), 4.38 – 4.28 (m, 2H), 4.09 (dd, *J* = 19.8, 2.2 Hz, 1H), 3.36 – 3.31 (m, 1H), 1.34 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.74, 152.04, 142.30, 137.16, 133.29, 129.61, 127.97, 124.30, 104.24, 96.47, 61.53, 40.15, 14.18; HRMS (ESI) m/z calcd. for $C_{15}H_{13}ClN_2NaO_5^+$ $[M+Na]^+$ = 359.0405, found 359.0408.

Ethyl (3aR,6aS)-3-(4-bromophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3g)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3g** as a white powder (57.2 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.6 Hz, 2H), 7.46 (d, *J* = 8.6 Hz, 2H), 6.86 (s, 1H), 6.36 (s, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 4.09 (dd, *J* = 19.8, 2.2 Hz, 1H), 3.33 (dd, *J* = 19.7, 1.5 Hz, 1H), 1.34 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.73, 152.15, 142.30, 133.30, 132.58, 128.12, 125.54, 124.75, 104.19, 96.49, 61.55, 40.15, 14.19; HRMS (ESI) m/z calcd. for $C_{15}H_{13}BrN_2NaO_5^+$ $[M+Na]^+$ =402.9900, found 402.9904.

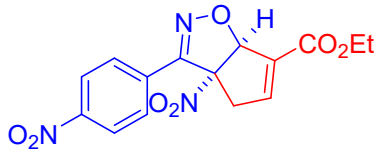
Ethyl (3aR,6aS)-3-(4-iodophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3h)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3h** as a yellow solid

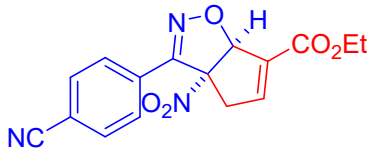
(71.0 mg, 71% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 – 7.76 (m, 2H), 7.33 – 7.30 (m, 2H), 6.86 (t, *J* = 2.2 Hz, 1H), 6.35 (s, 1H), 4.32 – 4.28 (m, 2H), 4.09 (dd, *J* = 19.8, 2.3 Hz, 1H), 3.35 – 3.30 (m, 1H), 1.34 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.72, 152.31, 142.28, 138.52, 133.33, 128.08, 125.29, 104.14, 97.58, 96.50, 61.56, 40.16, 14.20; HRMS (ESI) m/z calcd. for $C_{15}H_{14}IN_2O_5^+$ $[M+H]^+$ =428.9942, found 428.9936.

Ethyl (3aR,6aS)-3a-nitro-3-(4-nitrophenyl)-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3i)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3i** as a white solid (43.4 mg, 68% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 – 8.28 (m, 2H), 7.81 (d, *J* = 9.0 Hz, 2H), 6.90 (s, 1H), 6.45 (s, 1H), 4.32 (q, *J* = 7.0 Hz, 2H), 4.13 (dd, *J* = 19.7, 2.3 Hz, 1H), 3.38 – 3.34 (m, 1H), 1.36 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.54, 151.46, 148.87, 142.28, 133.36, 131.93, 127.60, 124.48, 103.68, 97.30, 61.70, 40.32, 14.19; HRMS (ESI) m/z calcd. for $C_{15}H_{14}N_3O_7^+$ $[M+H]^+$ =348.0826, found 348.0821.

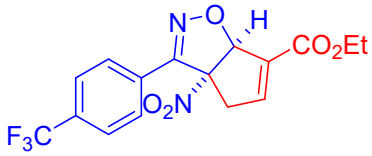
Ethyl (3aR,6aS)-3-(4-cyanophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3j)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3j** as a white solid (53.0 mg, 81% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (s, 4H), 6.89 (s, 1H), 6.43

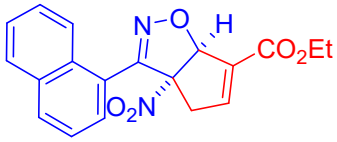
(s, 1H), 4.31 (q, J = 7.1 Hz, 2H), 4.11 (dd, J = 19.7, 1.7 Hz, 1H), 3.34 (d, J = 19.7 Hz, 1H), 1.35 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.57, 151.67, 142.31, 133.31, 132.97, 130.19, 127.20, 117.86, 114.41, 103.70, 97.16, 61.66, 40.26, 14.19; HRMS (ESI) m/z calcd. for $C_{16}H_{13}N_3NaO_5^+$ $[M+Na]^+$ =350.0747, found 350.0742.

Ethyl (3aR,6aS)-3a-nitro-3-(4-(trifluoromethyl)phenyl)-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3k)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3k** as a white solid (62.7 mg, 85% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, J = 8.5 Hz, 2H), 7.69 (d, J = 8.6 Hz, 2H), 6.88 (t, J = 2.3 Hz, 1H), 6.40 (s, 1H), 4.31 (q, J = 7.1 Hz, 2H), 4.12 (dd, J = 19.7, 2.3 Hz, 1H), 3.37 – 3.33 (m, 1H), 1.35 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.65, 151.91, 142.30, 133.34, 132.60 (q, J = 33.0 Hz), 129.35, 127.05, 126.27 (q, J = 3.7 Hz), 123.51 (d, J = 272.4 Hz), 103.98, 96.84, 61.60, 40.19, 14.17; HRMS (ESI) m/z calcd. for $C_{16}H_{14}F_3N_2O_5^+$ $[M+H]^+$ =371.0849, found 371.0845.

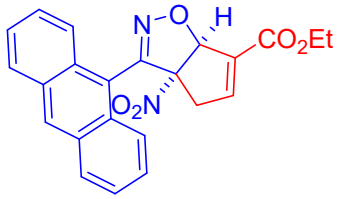
Ethyl (3aR,6aS)-3-(naphthalen-1-yl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3l)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3l** as a white liquid(72.8 mg, 99% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (dd, J = 7.9, 6.5 Hz, 1H), 7.94 (d, J = 8.2 Hz, 1H), 7.89 – 7.87 (m, 1H), 7.58 – 7.44 (m, 2H), 7.46 (t, J =

7.8 Hz, 1H), 7.30 (d, J = 7.2 Hz, 1H), 6.88 (t, J = 2.3 Hz, 1H), 6.41 (s, 1H), 4.33 (q, J = 7.1 Hz, 2H), 3.87 (dd, J = 20.0, 2.2 Hz, 1H), 3.19 – 3.14 (m, 1H), 1.37 (t, J = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.96, 152.52, 142.42, 134.05, 133.37, 131.82, 131.65, 128.78, 128.03, 127.16, 126.79, 125.40, 124.86, 122.63, 106.52, 94.41, 61.53, 39.51, 14.22; HRMS (ESI) m/z calcd. for $C_{19}H_{16}N_2NaO_5^+$ $[M+Na]^+$ =375.0951, found 375.0959.

Ethyl (3aR,6aS)-3-(anthracen-9-yl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3m)



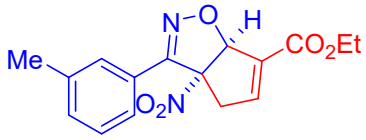
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3m** as a white powder (77.7 mg, 97% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (s, 1H), 7.96 (d, J = 5.8 Hz, 2H), 7.56 – 7.41 (m, 6H), 6.80 (d, J = 48.6 Hz, 2H), 4.33 (q, J = 7.0 Hz, 2H), 3.14 (s, 1H), 1.37 (dd, J = 7.1, 6.7 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.16, 150.75, 141.55, 134.84, 131.85, 131.12, 130.51, 128.87, 127.58, 125.75, 123.82, 118.59, 106.99, 92.43, 61.66, 39.42, 14.27; HRMS (ESI) m/z calcd. for $C_{22}H_{18}N_2O_5^+$ $[M+H]^+$ =390.1210, found 390.1214.

Ethyl (3aR,6aS)-3a-nitro-3-(o-tolyl)-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3n)

The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3n** as a red solid (37.7 mg, 60% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.31 (m, 2H), 7.23 (dd, J =

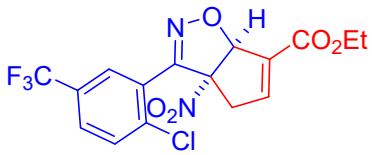
10.5, 4.1 Hz, 1H), 7.03 (d, J = 7.8 Hz, 1H), 6.88 (d, J = 2.0 Hz, 1H), 6.31 (s, 1H), 4.33 – 4.29 (m, 2H), 3.95 (dd, J = 19.9, 2.0 Hz, 1H), 3.21 – 3.17 (m, 1H), 2.43 (s, 3H), 1.35 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.92, 153.04, 142.19, 139.47, 133.34, 132.16, 130.36, 127.79, 126.20, 124.74, 16.04, 94.43, 61.50, 39.60, 22.31, 14.19; HRMS (ESI) m/z calcd. for $C_{16}H_{16}N_2NaO_5^+$ $[M+Na]^+$ =339.0951, found 339.0966.

Ethyl (3aR,6aS)-3a-nitro-3-(m-tolyl)-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3o)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3o** as a yellow solid (62.8 mg, 99% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.24 – 7.17 (m, 3H), 6.77 (d, J = 2.3 Hz, 1H), 6.23 (s, 1H), 4.21 (q, J = 7.1 Hz, 2H), 4.05 – 4.01 (m, 1H), 3.27 (dd, J = 19.8, 1.4 Hz, 1H), 2.28 (s, 3H), 1.26 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.84, 153.01, 142.34, 139.20, 133.34, 131.82, 129.11, 127.31, 125.68, 123.77, 104.54, 96.16, 61.44, 40.19, 21.40, 14.17; HRMS (ESI) m/z calcd. for $C_{16}H_{16}N_2NaO_5^+$ $[M+Na]^+$ =339.0951, found 339.0957.

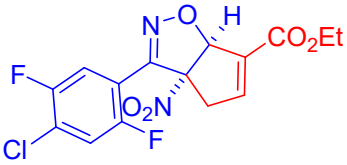
Ethyl (3aR,6aS)-3-(2-chloro-5-(trifluoromethyl)phenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3p)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3p** as a white solid (69.3 mg, 88% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, J = 1.6 Hz, 1H), 7.71 (dd, J = 8.5, 1.9 Hz, 1H), 7.65 (d, J = 8.5 Hz, 1H), 6.93 (t, J = 2.1 Hz, 1H), 6.48 (s,

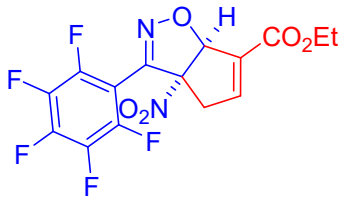
1H), 4.33 (q, J = 7.1 Hz, 2H), 3.72 (dd, J = 19.7, 2.1 Hz, 1H), 3.27 – 3.22 (m, 1H), 1.37 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.73, 150.08, 142.33, 137.92, 133.22, 131.36, 130.08 (q, J = 33.8 Hz), 128.77, 128.73 (t, J = 3.5 Hz), 126.46, 123.04 (d, J = 272.7 Hz), 104.94, 95.02, 61.63, 39.71, 14.19; HRMS (ESI) m/z calcd. for $C_{16}H_{13}ClF_3N_2O_5^+$ $[M+H]^+$ =405.0460, found 405.0454.

Ethyl (3aR,6aS)-3-(4-chloro-2,5-difluorophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3q)



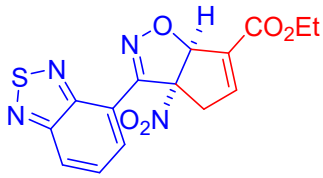
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3q** as a white powder (63.6 mg, 84% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (dd, J = 9.3, 6.3 Hz, 1H), 7.25 (dd, J = 10.6, 5.9 Hz, 1H), 6.94 (dd, J = 2.4, 1.9 Hz, 1H), 6.27 (s, 1H), 4.33 – 4.28 (m, 2H), 4.05 (d, J = 20.2 Hz, 1H), 3.18 – 3.13 (m, 1H), 1.35 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.64, 155.66 (dd, J = 85.8, 2.6 Hz), 153.68 (dd, J = 86.7, 2.5 Hz), 148.37 (t, J = 2.4 Hz), 143.37 (d, J = 2.3 Hz), 132.90, 125.27 (dd, J = 20.6, 11.7 Hz), 118.99 (d, J = 28.6 Hz), 115.99 (dd, J = 25.9, 4.4 Hz), 114.14 (dd, J = 13.8, 7.4 Hz), 103.47, 97.18, 61.58, 41.30 (d, J = 7.6 Hz), 14.18; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.82; HRMS (ESI) m/z calcd. for $C_{15}H_{11}ClF_2N_2NaO_5^+$ $[M+Na]^+$ =395.0217, found 395.0214.

(4-(perfluoroethyl)-1,2-diphenyl-4,5-dihydro-1H-imidazol-5-yl)(phenyl)methanone (3ra)



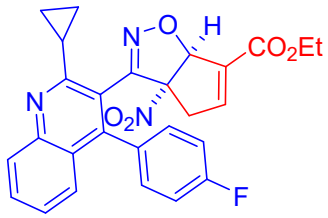
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3r** as a Colorless viscous liquid (61.3 mg, 99% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.93 (d, *J* = 2.1 Hz, 1H), 6.43 (s, 1H), 4.32 (d, *J* = 7.1 Hz, 2H), 3.83 (dd, *J* = 20.0, 1.8 Hz, 1H), 3.19 (d, *J* = 19.9 Hz, 1H), 1.36 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.50, 146.29 (t, *J* = 13.6 Hz), 142.48, 141.63 (t, *J* = 13.4 Hz), 139.16 (t, *J* = 17.4 Hz), 137.14 (t, *J* = 16.9 Hz), 133.02, 104.17, 102.44 (dd, *J* = 17.3, 13.1 Hz), 95.33, 61.66, 40.69, 14.13; ^{19}F NMR (471 MHz, $CDCl_3$) δ -134.93 – 135.02, -144.12 – -151.36, -159.11 – -159.24; HRMS (ESI) m/z calcd. for $C_{15}H_9F_5N_2NaO_5^+$ $[M+Na]^+$ =415.0324, found 415.0327.

Ethyl (3aR,6aS)-3-(benzo[c][1,2,5]thiadiazol-4-yl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3s)



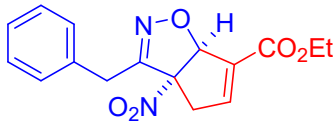
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3s** as a white solid (64.7 mg, 90% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (d, *J* = 7.0 Hz, 1H), 8.14 (d, *J* = 8.7 Hz, 1H), 7.72 (t, *J* = 7.8 Hz, 1H), 6.94 (s, 1H), 6.34 (s, 1H), 4.34 – 4.31 (m, 2H), 4.26 (s, 1H), 3.22 (d, *J* = 20.4 Hz, 1H), 1.36 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.94, 155.09, 151.00, 144.02, 132.87, 129.55, 124.10, 119.62, 104.16, 96.93, 61.48, 42.47, 14.22; HRMS (ESI) m/z calcd. for $C_{15}H_{12}N_4NaO_5S^+$ $[M+Na]^+$ =383.0421, found 383.0423.

Ethyl (3aR,6aS)-3-(2-cyclopropyl-4-(4-fluorophenyl)quinolin-3-yl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3t)



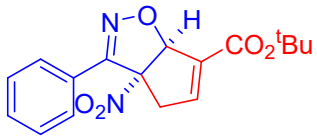
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3t** as a white powder (94 mg, 96% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.3 Hz, 1H), 7.71 – 7.68 (m, 1H), 7.55 (d, *J* = 8.3 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.31 (s, 1H), 7.17 (t, *J* = 6.9 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 6.44 (s, 1H), 4.32 – 4.27 (m, 2H), 1.80 (dd, *J* = 10.0, 6.0 Hz, 1H), 1.42 (s, 2H), 1.35 (t, *J* = 7.1 H z, 3H), 1.03 (dd, *J* = 11.8, 4.6 Hz, 2H), 0.89 – 0.78 (m, 1H); ^{13}C NMR (126 MHz, DMSO) δ 162.7 (d, *J* = 246.9 Hz), 162.0, 161.8, 161.0, 151.2, 148.9, 148.2, 134.1 (d, *J* = 8.3 Hz), 131.7, 129.1, 127.2, 126.8, 126.7, 124.92, 118.1, 116.1, 115.8, 115.4 (d, *J* = 21.5 Hz), 105.6, 105.6, 92.2, 92.0, 61.1, 14.4; ^{19}F NMR (471 MHz, $CDCl_3$) δ -111.99; HRMS (ESI) m/z calcd. for $C_{24}H_{20}FN_3NaO_3^+$ $[M+Na]^+$ =440.1381, found 440.1377.

Ethyl (3aR,6aS)-3-benzyl-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3u)



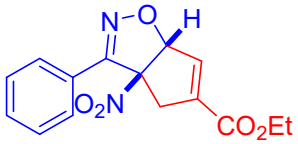
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3u** as a white solid(36.5 mg, 58% yield,dr > 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 – 7.24 (m, 1H), 6.61 (t, *J* = 2.2 Hz, 5H), 6.31 (s, 1H), 4.27 (q, *J* = 7.1 Hz, 1H), 4.04 (d, *J* = 15.6 Hz, 1H), 3.71 (d, *J* = 15.6 Hz, 1H), 3.34 (dd, *J* = 19.8, 2.2 Hz, 1H), 2.80 – 2.75 (m, 1H), 1.33 (t, *J* = 7.1 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.96, 152.08, 141.42, 134.19, 133.76, 129.08, 128.88, 127.75, 105.36, 93.25, 61.42, 39.95, 31.46, 14.16; HRMS (ESI) m/z calcd. for $C_{16}H_{17}N_2O_5^+$ $[M+H]^+$ =317.1132, found 317.1136.

tert-Butyl (3aR,6aS)-3a-nitro-3-phenyl-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (3v)



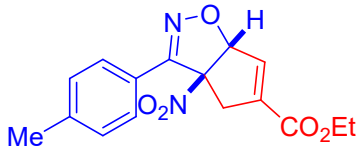
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:5) to afford **3v** as a white powder(53.7 mg, 82% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 – 7.58 (m, 2H), 7.46 – 7.42 (m, 3H), 6.76 (d, *J* = 2.4 Hz, 1H), 6.28 (s, 1H), 4.09 (dd, *J* = 19.7, 2.3 Hz, 1H), 3.35 – 3.31 (m, 1H), 1.58 (s, 1H), 1.54 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.06, 152.82, 141.28, 134.84, 130.93, 129.28, 126.70, 125.88, 104.47, 96.48, 82.48, 39.99, 28.09; HRMS (ESI) m/z calcd. for $C_{16}H_{13}N_2O_5^+$ $[M+H]^+$ =331.1288, found 331.1288.

Ethyl (3aS,6aR)-3a-nitro-3-phenyl-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5a)



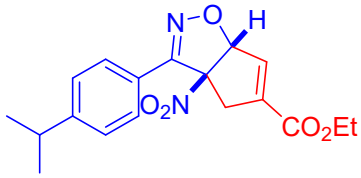
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:15) to afford **5a** as a yellow oil 3gf(51.4 mg, 85% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (t, *J* = 11.0 Hz, 2H), 7.52 – 7.38 (m, 3H), 6.61 (d, *J* = 2.6 Hz, 1H), 6.19 (s, 1H), 4.27 – 4.21 (m, 2H), 4.15 (d, *J* = 18.3 Hz, 1H), 3.50 (d, *J* = 18.3 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.61, 153.16, 137.56, 134.05, 131.08, 129.31, 126.84, 125.71, 104.07, 97.09, 61.64, 39.40, 14.13; HRMS calcd. for: $C_{15}H_{15}N_2O_5^+$ $[M+H]^+$ = 303.0975, found 303.0973.

Ethyl (3aS,6aR)-3a-nitro-3-(p-tolyl)-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5b)



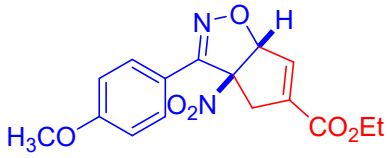
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5b** as a yellow solid (51.2 mg, 81% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 – 7.50 (m, 2H), 7.23 (d, *J* = 8.1 Hz, 2H), 6.60 (d, *J* = 2.1 Hz, 1H), 6.17 (t, *J* = 1.9 Hz, 1H), 4.24 – 4.21 (m, 2H), 4.14 (dd, *J* = 18.3, 2.3 Hz, 1H), 3.49 (d, *J* = 18.3 Hz, 1H), 2.38 (s, 3H), 1.29 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.64, 153.15, 141.60, 137.47, 134.13, 130.00, 126.77, 122.81, 104.21, 96.88, 61.60, 39.41, 21.49, 14.13; HRMS calcd. for: $C_{16}H_{17}N_2O_5^+$ $[M+H]^+$ = 317.1132, found 317.1136.

Ethyl (3aS,6aR)-3-(4-isopropylphenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5c)



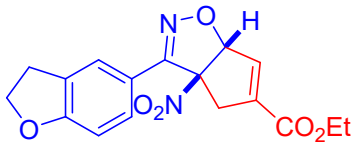
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5c** as a colorless oil (54.4 mg, 79% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.3 Hz, 2H), 6.60 (dd, *J* = 4.1, 2.0 Hz, 1H), 6.17 (s, 1H), 4.26 – 4.12 (m, 2H), 4.14 (dd, *J* = 18.3, 2.0 Hz, 1H), 2.96 – 2.91 (m, 1H), 2.93 (dt, *J* = 13.8, 6.9 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H), 1.25 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.65, 153.14, 152.39, 137.46, 134.12, 127.43, 126.91, 123.13, 104.21, 96.87, 61.61, 39.39, 34.12, 23.69, 14.14; HRMS calcd. for: $C_{18}H_{21}N_2O_5^+$ $[M+H]^+$ = 345.1445, found 345.1449.

Ethyl (3aS,6aR)-3-(4-methoxyphenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5d)



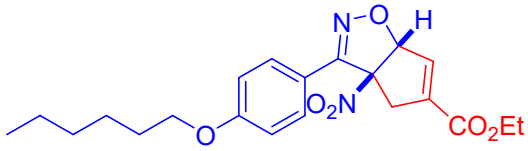
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5d** as a yellow oil (36.8 mg, 52% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 – 7.56 (m, 2H), 6.95 – 6.93 (m, 2H), 6.60 (d, *J* = 2.1 Hz, 1H), 6.16 (d, *J* = 1.7 Hz, 1H), 4.31 – 4.19 (m, 2H), 4.13 (dd, *J* = 18.2, 1.8 Hz, 1H), 3.84 (s, 3H), 3.51 – 3.47 (m, 1H), 1.34 – 1.28 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.66, 161.72, 152.79, 137.34, 134.21, 128.50, 117.97, 114.76, 104.35, 96.72, 61.60, 55.46, 39.40, 14.13; HRMS calcd. for: $C_{16}H_{16}N_2NaO_6^+$ $[M+Na]^+$ = 355.0901, found 355.0900.

Ethyl (3aS,6aR)-3-(2,3-dihydrobenzofuran-5-yl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5e)



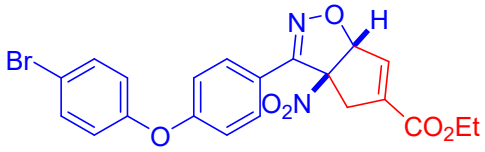
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5e** as a colorless oil (51.6 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.34 (d, *J* = 8.4 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 6.60 (d, *J* = 2.0 Hz, 1H), 6.14 (s, 1H), 4.63 (t, *J* = 8.8 Hz, 2H), 4.28 – 4.20 (m, 2H), 4.13 (dd, *J* = 18.2, 2.0 Hz, 1H), 3.49 (d, *J* = 18.2 Hz, 1H), 3.24 (t, *J* = 8.6 Hz, 2H), 1.34 – 1.26 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.70, 162.58, 153.09, 137.30, 134.22, 128.74, 127.60, 123.77, 117.82, 109.99, 104.42, 96.69, 71.96, 61.60, 39.41, 29.29, 14.14; HRMS calcd. for: $C_{17}H_{17}N_2O_6^+$ $[M+H]^+$ =345.1081, found 345.1084.

Ethyl (3aS,6aR)-3-(4-(hexyloxy)phenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5f)



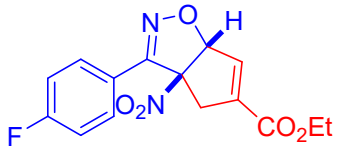
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:30) to afford **5f** as a yellow solid (73.2 mg, 91% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.54 (m, 2H), 6.93 – 6.91 (m, 2H), 6.60 (q, *J* = 2.0 Hz, 1H), 6.16 (d, *J* = 1.5 Hz, 1H), 4.26 – 4.20 (m, 2H), 4.13 (dd, *J* = 18.2, 2.1 Hz, 1H), 3.98 (t, *J* = 6.6 Hz, 2H), 3.49 (d, *J* = 18.2 Hz, 1H), 1.81 – 1.76 (m, 2H), 1.48 – 1.42 (m, 2H), 1.36 – 1.32 (m, 4H), 1.30 (t, *J* = 7.1 Hz, 3H), 0.91 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.65, 161.31, 152.82, 137.30, 134.21, 128.45, 117.65, 115.22, 104.37, 96.68, 68.23, 61.57, 39.39, 31.53, 29.03, 25.65, 22.59, 14.13, 14.04; HRMS calcd. for: $C_{21}H_{27}N_2O_6^+$ $[M+H]^+$ = 403.1864, found 403.1866.

Ethyl (3aS,6aR)-3-(4-(4-bromophenoxy)phenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5g)



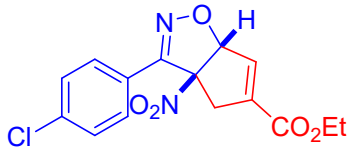
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5g** as a yellow solid (78.3 mg, 83% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.7 Hz, 2H), 7.48 (d, *J* = 8.6 Hz, 2H), 7.01 (d, *J* = 8.7 Hz, 2H), 6.94 (d, *J* = 8.6 Hz, 2H), 6.61 (d, *J* = 1.8 Hz, 1H), 6.19 (s, 1H), 4.27 – 4.21 (m, 2H), 4.14 – 4.10 (m, 1H), 3.49 (d, *J* = 18.2 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.58, 159.49, 154.95, 152.48, 137.38, 134.09, 133.03, 128.71, 121.53, 120.56, 118.72, 117.07, 104.13, 97.00, 61.63, 39.41, 14.13; HRMS calcd. for: $C_{21}H_{18}BrN_2O_6^+$ $[M+H]^+$ = 473.0343, found 473.0346.

Ethyl (3aS,6aR)-3-(4-fluorophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5h)



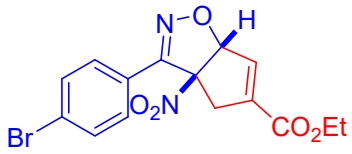
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5h** as a colorless oil (52.5 mg, 82% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 – 7.63 (m, 2H), 7.16 – 7.11 (m, 2H), 6.62 (dd, *J* = 4.2, 2.1 Hz, 1H), 6.22 – 6.21 (m, 1H), 4.27 – 4.21 (m, 2H), 4.12 (dd, *J* = 18.2, 1.8 Hz, 1H), 3.49 – 3.44 (m, 1H), 1.30 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.16 (d, *J* = 253.1 Hz), 162.55, 152.23, 137.44, 134.04, 129.01 (d, *J* = 8.6 Hz), 121.97 (d, *J* = 3.5 Hz), 116.60 (d, *J* = 22.2 Hz) 104.01, 97.15, 61.68, 39.37, 14.11; ^{19}F NMR (471 MHz, $CDCl_3$) δ -107.71; HRMS calcd. for: $C_{15}H_{13}FKN_2O_5^+$ $[M+K]^+$ = 359.0446, found 359.0442.

Ethyl (3aS,6aR)-3-(4-chlorophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5i)



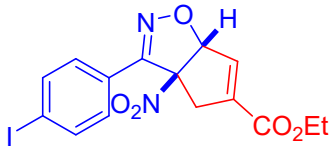
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5i** as a white solid (36.9 mg, 55% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 – 7.56 (m, 2H), 7.43 – 7.40 (m, 2H), 6.62 (dd, *J* = 4.2, 2.1 Hz, 1H), 6.22 (s, 1H), 4.28 – 4.20 (m, 2H), 4.12 (dd, *J* = 18.2, 2.2 Hz, 1H), 3.48 – 3.43 (m, 1H), 1.30 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.49, 152.30, 137.51, 137.27, 133.97, 129.62, 128.08, 124.22, 103.84, 97.30, 61.70, 39.42, 14.12; HRMS calcd. for: $C_{15}H_{14}ClN_2O_5^+$ $[M+H]^+$ = 337.0586, found 337.0590.

Ethyl (3aS,6aR)-3-(4-bromophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5j)



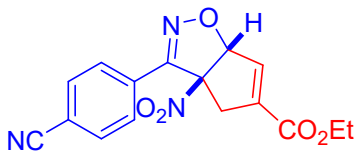
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5j** as a yellow solid (52.4 mg, 69% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.6 Hz, 2H), 7.50 (d, *J* = 8.6 Hz, 2H), 6.62 (dd, *J* = 4.0, 2.0 Hz, 1H), 6.22 (s, 1H), 4.26 – 4.21 (m, 2H), 4.11 (dd, *J* = 18.2, 2.1 Hz, 1H), 3.47 – 3.43 (m, 1H), 1.30 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.47, 152.41, 137.53, 133.95, 132.57, 128.23, 125.64, 124.67, 103.77, 97.32, 61.70, 39.42, 14.13; HRMS calcd. for: $C_{15}H_{13}BrKN_2O_5^+$ $[M+K]^+$ = 418.9639, found 418.9635.

Ethyl (3aS,6aR)-3-(4-iodophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5k)



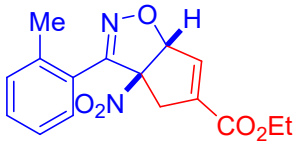
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5k** as a yellow solid (55.6 mg, 65% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 – 7.78 (m, 2H), 7.36 – 7.27 (m, 2H), 6.61 (q, *J* = 2.0 Hz, 1H), 6.21 (s, 1H), 4.27 – 4.09 (m, 2H), 4.11 (dd, *J* = 18.3, 2.1 Hz, 1H), 3.47 – 3.42 (m, 1H), 1.30 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, CD_3CN) δ 157.16, 147.27, 133.20, 132.24, 128.64, 122.88, 119.90, 98.41, 92.39, 92.01, 56.41, 34.11, 8.83; HRMS calcd. for: $C_{15}H_{13}IN_2NaO_5^+$ $[M+Na]^+$ = 450.9761, found 450.9760.

Ethyl (3aS,6aR)-3-(4-cyanophenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5l)



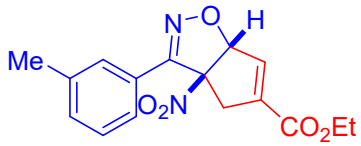
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:20) to afford **5l** as a yellow oil (22.9 mg, 35% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 – 7.73 (m, 4H), 6.64 (d, *J* = 2.1 Hz, 1H), 6.29 (t, *J* = 2.0 Hz, 1H), 4.28 – 4.22 (m, 2H), 4.13 (dd, *J* = 18.2, 2.1 Hz, 1H), 3.47 – 3.43 (m, 1H), 1.31 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.34, 151.91, 137.70, 133.75, 132.95, 130.12, 127.32, 117.86, 114.50, 103.29, 97.97, 61.82, 39.56, 14.12; HRMS calcd. for: $C_{16}H_{14}N_3O_5^+$ $[M+H]^+$ = 328.0928, found 328.0926.

Ethyl (3aS,6aR)-3a-nitro-3-(o-tolyl)-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5m)



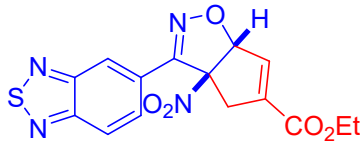
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5m** as a yellow oil (48.0 mg, 76% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.32 (m, 2H), 7.26 – 7.23 (m, 1H), 7.07 (d, *J* = 7.8 Hz, 1H), 6.62 (dd, *J* = 4.0, 2.0 Hz, 1H), 6.17 (s, 1H), 4.25 (q, *J* = 7.1 Hz, 2H), 3.97 (dd, *J* = 18.3, 2.1 Hz, 1H), 3.35 – 3.31 (m, 1H), 2.42 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.64, 153.41, 139.43, 137.35, 134.27, 132.13, 130.40, 128.02, 126.24, 124.69, 105.62, 95.20, 61.64, 38.82, 22.21, 14.14; HRMS calcd. for: $C_{13}H_{16}N_2NaO_5^+$ $[M+Na]^+$ = 339.0951, found 339.0953.

Ethyl (3aS,6aR)-3a-nitro-3-(m-tolyl)-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5n)



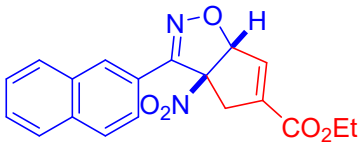
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5n** as a yellow oil (47.4 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (s, 1H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 8.1 Hz, 1H), 6.61 (dd, *J* = 4.2, 2.1 Hz, 1H), 6.18 – 6.17 (m, 1H), 4.27 – 4.20 (m, 2H), 4.15 (dd, *J* = 18.2, 1.9 Hz, 1H), 3.51 – 3.47 (m, 1H), 2.38 (s, 3H), 1.30 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.64, 153.29, 139.21, 137.55, 134.06, 131.94, 129.15, 127.38, 125.58, 123.92, 104.11, 97.02, 61.63, 39.40, 21.45, 14.14; HRMS calcd. for: $C_{16}H_{17}N_2O_5^+$ $[M+H]^+$ = 317.1132, found 317.1133.

Ethyl (3aS,6aR)-3-(benzo[c][1,2,5]thiadiazol-5-yl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5o)



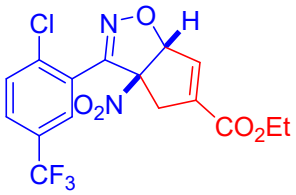
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5o** as a yellow solid (46.8 mg, 65% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (dd, *J* = 7.2, 0.8 Hz, 1H), 8.16 (dd, *J* = 8.7, 0.8 Hz, 1H), 7.71 (dd, *J* = 8.7, 7.2 Hz, 1H), 6.64 (q, *J* = 2.0 Hz, 1H), 6.21 (d, *J* = 1.4 Hz, 1H), 4.31 (dd, *J* = 18.8, 2.0 Hz, 1H), 4.24 – 4.19 (m, 2H), 3.31 – 3.30 (m, 1H), 1.27 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.79, 155.08, 151.42, 151.00, 138.71, 133.61, 129.57, 129.42, 124.25, 119.50, 103.80, 97.70, 61.58, 41.35, 14.13; HRMS calcd. for: $C_{15}H_{13}N_4O_5S^+$ $[M+H]^+$ = 361.0601, found 361.0598.

Ethyl (3aS,6aR)-3-(naphthalen-2-yl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5p)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5p** as a yellow solid (61.9 mg, 88% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 – 8.35 (m, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.91 – 7.89 (m, 1H), 7.56 (dd, *J* = 9.5, 5.0 Hz, 2H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.35 (dd, *J* = 7.2, 0.6 Hz, 1H), 6.69 (d, *J* = 1.9 Hz, 1H), 6.26 (s, 1H), 4.23 (q, *J* = 7.1 Hz, 2H), 3.96 (dd, *J* = 18.4, 1.5 Hz, 1H), 3.35 (d, *J* = 18.4 Hz, 1H), 1.28 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.54, 153.00, 137.60, 134.31, 134.07, 131.76, 128.81, 127.98, 127.38, 126.78, 125.48, 124.87, 122.53, 106.04, 95.21, 61.62, 38.84, 14.13; HRMS calcd. for: $C_{19}H_{17}N_2O_5^+$ $[M+H]^+$ = 353.1132, found 353.1137.

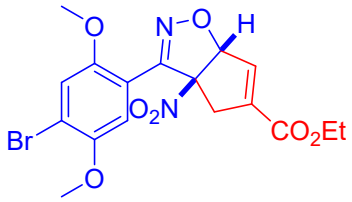
Ethyl (3aS,6aR)-3-(2-chloro-5-(trifluoromethyl)phenyl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5q)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5q** as a yellow oil (28.2 mg, 35% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 1.7 Hz, 1H), 7.71 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.65 (d, *J* = 8.5 Hz, 1H), 6.65 (dd, *J* = 3.9, 2.0 Hz, 1H), 6.34 (s, 1H), 4.30 – 4.24 (m, 2H), 3.79 – 3.68 (m, 1H), 3.37 – 3.33 (m, 1H), 1.32 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.36, 149.58, 136.98, 136.66, 132.88, 130.35, 129.00 (q, *J* = 33.7 Hz), 127.67 (q, *J* = 3.0 Hz), 125.34, 122.01 (q, *J* = 272.6 Hz), 103.39, 94.70, 60.68, 37.89, 25.88, 13.08; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.79; HRMS calcd. for: $C_{16}H_{13}ClF_3N_2O_5^+$ $[M+H]^+$ = 405.0460, found 405.0463.

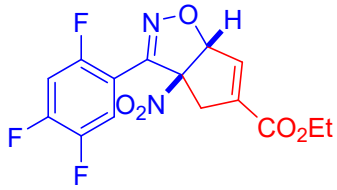
Ethyl (3aS,6aR)-3-(4-bromo-2,5-dimethoxyphenyl)-3a-nitro-3a,6a-dihydro-4H-

cyclopenta[d]isoxazole-5-carboxylate (5r)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5r** as a colorless oil (66.0 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.17 (s, 1H), 6.54 (d, *J* = 2.0 Hz, 1H), 6.02 (s, 1H), 4.23 (qd, *J* = 7.1, 1.7 Hz, 2H), 4.10 (dd, *J* = 18.7, 1.9 Hz, 1H), 3.89 (s, 3H), 3.71 (s, 3H), 3.13 – 3.09 (m, 1H), 1.30 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.88, 151.90, 150.73, 150.10, 138.31, 133.56, 117.60, 116.19, 114.31, 111.75, 103.81, 96.76, 61.54, 56.77, 55.54, 39.78, 14.15; HRMS calcd. for: $C_{17}H_{17}BrN_2NaO_7^+$ $[M+Na]^+$ = 4663.0111, found 463.0108.

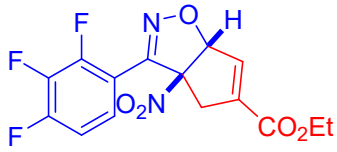
Ethyl (3aS,6aR)-3a-nitro-3-(2,4,5-trifluorophenyl)-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5s)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5s** as a yellow solid (39.8 mg, 56% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 – 7.87 m, 1H), 7.06 – 7.01 (m, 1H), 6.59 (d, *J* = 2.0 Hz, 1H), 6.13 – 6.12 (m, 1H), 4.28 – 4.23 (m, 2H), 4.11 – 4.07 (m, 1H), 3.27 – 3.22 (m, 1H), 1.31 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.54, 155.60 (d, *J* = 6.9 Hz), 153.63 (d, *J* = 9.5 Hz), 153.19 (d, *J* = 13.4 Hz), 151.13 (d, *J* = 13.4 Hz), 146.61 (dd, *J* = 13.0, 3.1 Hz), 138.35 (d, *J* = 2.2 Hz), 133.40, 117.03 (dd, *J* = 22.2, 4.2 Hz), 106.85 (dd, *J* = 29.3, 21.3 Hz), 103.22, 97.81, 61.71, 40.31 (d, *J* = 7.3 Hz), 14.11; ^{19}F NMR (471 MHz, $CDCl_3$) δ -112.86 (dd, *J* =

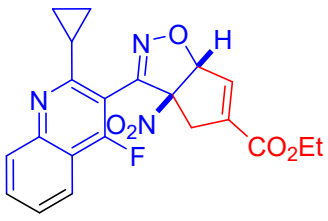
14.6, 6.0 Hz), -126.59 (dd, J = 21.6, 6.1 Hz), -139.12 (dd, J = 21.6, 14.5 Hz); HRMS calcd. for: $C_{15}H_{12}F_3N_2O_5^+$ $[M+H]^+$ = 357.0693, found 357.0692.

Ethyl (3aS,6aR)-3a-nitro-3-(2,3,4-trifluorophenyl)-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5t)



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5t** as a yellow solid (39.2 mg, 55% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 – 7.79 (m, 1H), 6.99 – 6.93 (m, 1H), 6.52 (d, J = 1.9 Hz, 1H), 6.05 (d, J = 1.5 Hz, 1H), 4.21 – 4.15 (m, 2H), 4.04 – 4.00 (m, 1H), 3.20 – 3.15 (m, 1H), 1.24 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.52, 155.61 (d, J = 9.5 Hz), 153.18 (d, J = 13.4 Hz), 148.65 (d, J = 2.4 Hz), 148.52 (d, J = 3.1 Hz), 146.60 (dd, J = 13.0, 3.1 Hz), 138.35 (d, J = 2.2 Hz), 133.39, 117.03 (dd, J = 21.1, 4.1 Hz), 106.85 (dd, J = 29.2, 21.4 Hz), 103.21, 97.81, 61.71, 40.30 (d, J = 7.3 Hz), 14.11; ^{19}F NMR (471 MHz, $CDCl_3$) δ -112.86 (dd, J = 14.4, 6.0 Hz), -126.60 (dd, J = 21.6, 6.0 Hz), -139.14 (dd, J = 21.6, 14.5 Hz); HRMS calcd. for: $C_{15}H_{12}F_3N_2O_5^+$ $[M+H]^+$ = 357.0693, found 357.0698.

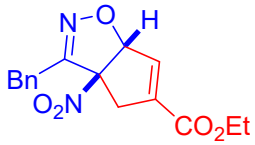
Ethyl (3aS,6aR)-3-(2-cyclopropyl-4-fluoroquinolin-3-yl)-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5u)



The general procedure was followed and then purified by silica column chromatograkphy (ethyl acetate/petroleum ether = 1:10) to afford **5u** as a white solid (32.9 mg, 40% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, J = 8.4 Hz, 1H), 7.73 –

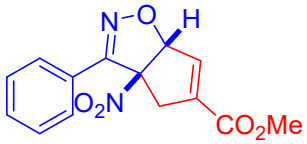
7.70 (m, 1H), 7.53 (d, J = 8.4 Hz, 1H), 7.47 – 7.37 (m, 2H), 7.32 (s, 1H), 7.10 (s, 2H), 6.33 (d, J = 3.8 Hz, 1H), 4.22 (dd, J = 13.2, 6.4 Hz, 2H), 1.78 (s, 1H), 1.62 (d, J = 4.1 Hz, 1H), 1.32 (t, J = 7.1 Hz, 3H), 1.03 (s, 1H), 0.91 – 0.83 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.26, 150.80, 148.65, 133.75 (d, J = 26.4 Hz), 130.75, 129.26, 126.39, 126.17, 124.85, 117.53, 115.22 (d, J = 21.7 Hz), 105.57, 92.92, 61.54, 38.31, 35.44, 26.93, 14.86, 14.06; ^{19}F NMR (471 MHz, $CDCl_3$) δ -112.29; HRMS calcd. for: $C_{21}H_{19}FN_3O_5^+$ $[M+H]^+$ = 412.1303, found 412.1302.

Ethyl (3aS,6aR)-3-benzyl-3a-nitro-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5v）



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5v** as a white solid (44.3 mg, 70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.24 (m, 5H), 6.54 (d, J = 1.8 Hz, 1H), 6.17 (s, 1H), 4.16 (q, J = 7.1 Hz, 2H), 4.00 (d, J = 15.8 Hz, 1H), 3.77 (d, J = 15.8 Hz, 1H), 3.42 (dd, J = 18.0, 1.8 Hz, 1H), 3.03 (d, J = 18.0 Hz, 1H), 1.25 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.33, 152.76, 136.63, 134.76, 134.05, 128.96, 128.83, 127.70, 104.44, 93.65, 61.45, 38.85, 31.53, 14.10; HRMS calcd. for: $C_{16}H_{17}N_2O_5^+$ $[M+H]^+$ = 317.1132, found 317.1133.

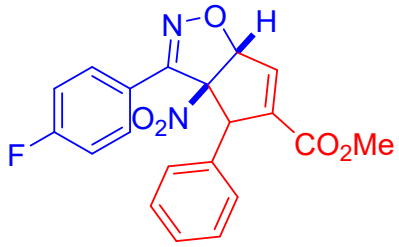
Methyl (3aS,6aR)-3a-nitro-3-phenyl-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate（5w）



The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford **5w** as a colorless oil (51.8 mg, 90% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, J = 7.3 Hz, 2H), 7.48 –

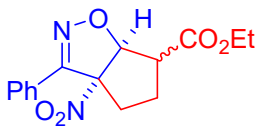
7.42 (m, 3H), 6.62 (d, J = 1.7 Hz, 1H), 6.20 (s, 1H), 4.15 (dd, J = 18.2, 1.7 Hz, 1H), 3.78 (s, 3H), 3.50 (d, J = 18.3 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.00, 153.14, 137.15, 134.34, 131.09, 129.30, 126.83, 125.66, 104.02, 97.02, 52.47, 39.39; HRMS calcd. for: $C_{14}H_{12}N_2NaO_5^+$ $[M+Na]^+$ = 311.0638, found 311.0636.

Methyl (3aS,6aR)-3-(4-fluorophenyl)-3a-nitro-4-phenyl-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-5-carboxylate (5x)



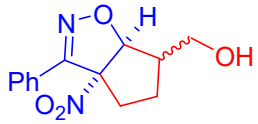
The general procedure was followed and then purified by silica column chromatography (ethyl acetate/petroleum ether = 1:10) to afford mixture **5x** as a colorless oil (30.6 mg, 40% yield, 3:1 dr), and the diastereoisomers cannot be separated. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 – 8.08 (m, 1H), 7.39 – 7.34 (m, 2H), 7.25 – 7.20 (m, 3H), 7.04 – 7.01 (m, 7H), 6.91 – 6.90 (m, 1H), 6.80 – 6.79 (m, 1H), 6.74 – 6.69 (m, 3H), 6.20 (d, J = 2.5 Hz, 1H), 5.71 (d, J = 1.7 Hz, 1H), 5.02 (s, 0.35H), 3.63 (s, 3H), 3.62 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.26, 163.39 (d, J = 210.3 Hz), 163.24, 162.24 (d, J = 1.8 Hz), 152.56, 151.73, 141.43, 139.23, 134.75, 134.63, 133.82, 133.28, 130.89 (d, J = 8.5 Hz), 129.16, 128.71 (d, J = 8.9 Hz), 128.48, 122.46 (d, J = 3.6 Hz), 122.21 (d, J = 3.2 Hz), 116.31 (d, J = 22.0 Hz), 115.19 (d, J = 22.1 Hz), 110.40, 107.59, 97.98, 92.75, 56.85, 56.24, 52.42, 52.33; ^{19}F NMR (471 MHz, $CDCl_3$) δ -108.12, -109.39; HRMS calcd. for: $C_{20}H_{16}FN_2O_5^+$ $[M+H]^+$ = 383.1038, found 383.1047.

Ethyl (3aR,6aS)-3a-nitro-3-phenyl-3a,5,6,6a-tetrahydro-4H-cyclopenta[d]isoxazole-6-carboxylate (6a)



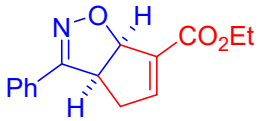
6a, a colorless oil (38.1 mg, 58% yield, dr = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 5.3, 3.3 Hz, 2H), 7.45 – 7.39 (m, 3H), 5.79 (d, *J* = 3.8 Hz, 1H), 4.23 (dd, *J* = 7.2, 4.1 Hz, 2H), 3.29 – 3.23 (m, 1H), 3.19 – 3.15 (m, 1H), 2.52 – 2.46 (m, 1H), 2.35 – 2.28 (m, 1H), 2.20 – 2.13 (m, 1H), 1.30 (t, *J* = 7.1 Hz, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.55, 152.88, 130.91, 129.15, 126.71, 125.76, 106.90, 93.23, 61.44, 50.85, 33.28, 25.93, 14.16; HRMS calcd. for: $C_{15}H_{17}N_2O_5^+$ $[M+H]^+$ = 305.1132, found 305.1143.

((3aR,6aS)-3a-Nitro-3-phenyl-3a,5,6,6a-tetrahydro-4H-cyclopenta[d]isoxazol-6-yl)methanol (6b)



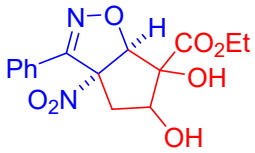
6b, a colorless oil (33.6 mg, 65% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 – 7.60 (m, 2H), 7.45 – 7.39 (m, 3H), 5.38 (d, *J* = 5.6 Hz, 1H), 3.86 (dd, *J* = 10.8, 5.5 Hz, 1H), 3.78 (dd, *J* = 10.8, 5.9 Hz, 1H), 3.30 – 3.25 (m, 1H), 2.41 – 2.35 (m, 2H), 2.01 – 1.96 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.60, 130.77, 129.14, 126.72, 126.12, 107.90, 96.44, 62.47, 50.49, 34.56, 27.97; HRMS calcd. for: $C_{13}H_{15}N_2O4^+$ $[M+H]^+$ = 263.1026, found 263.1031.

Ethyl (3aS,6aR)-3-phenyl-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (6c)



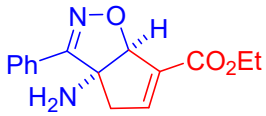
6c, a red solid (30.3 mg, 60% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 5.1, 2.7 Hz, 2H), 7.40 (d, *J* = 2.1 Hz, 3H), 6.89 (s, 1H), 6.02 (d, *J* = 9.5 Hz, 1H), 4.45 – 4.41 (m, 1H), 4.31 – 4.25 (m, 2H), 3.06 – 3.00 (m, 1H), 2.75 (dd, *J* = 19.3, 2.1 Hz, 1H), 1.35 – 1.32 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.43, 158.09, 144.27, 136.09, 129.99, 128.87, 128.80, 127.01, 89.07, 60.82, 49.61, 37.44, 14.27; HRMS calcd. for: $C_{15}H_{15}NNaO_3^+$ $[M+Na]^+$ = 28.0944, found 280.0949.

Ethyl (3aR,6aR)-5,6-dihydroxy-3a-nitro-3-phenyl-3a,5,6,6a-tetrahydro-4H-cyclopenta[d]isoxazole-6-carboxylate (6d)



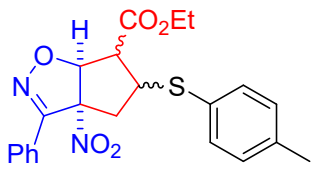
6d, a colorless oil (30.3 mg, 60% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 6.9 Hz, 2H), 7.45 – 7.41 (m, 3H), 6.85 (t, *J* = 2.0 Hz, 1H), 6.33 (s, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 4.11 (dd, *J* = 19.8, 2.1 Hz, 1H), 3.36 (d, *J* = 19.8 Hz, 1H), 1.34 (t, *J* = 7.1 Hz, 3H), 0.89 – 0.83 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.82, 152.89, 142.36, 133.31, 130.97, 129.28, 126.71, 125.80, 104.49, 96.24, 61.45, 40.15, 14.17; HRMS calcd. for: $C_{15}H_{17}NNaO_5^+$ $[M+Na]^+$ = 314.0999, found 314.1000.

Ethyl (3aR,6aS)-3a-amino-3-phenyl-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (6e)



6e, a colorless oil (35.4 mg, 65% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 7.1, 2.3 Hz, 2H), 7.39 (dd, *J* = 5.2, 1.5 Hz, 3H), 6.81 (s, 1H), 6.01 (s, 1H), 5.35 (s, 1H), 5.10 (s, 1H), 4.30 – 4.26 (m, 2H), 3.07 (d, *J* = 19.4 Hz, 1H), 2.77 (dd, *J* = 19.5, 1.9 Hz, 1H), 1.33 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.36, 155.69, 143.07, 135.21, 130.04, 128.79, 128.10, 127.22, 90.39, 85.50, 60.96, 39.90, 14.22; HRMS calcd. for: $C_{15}H_{16}N_2NaO_3^+$ $[M+Na]^+$ = 295.1053, found 295.1053.

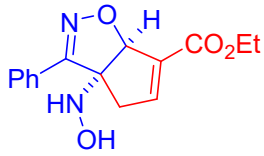
ethyl (3aR,6aS)-3a-nitro-3-phenyl-5-(p-tolylthio)-3a,5,6,6a-tetrahydro-4H-cyclopenta[d]isoxazole-6-carboxylate (6f)



6f, a white solid (84.4 mg, 99% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 – 7.52 (m, 2H), 7.44 (d, *J* = 7.2 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.27 (t, *J* = 8.2 Hz, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 5.67 (d, *J* = 6.9 Hz, 1H), 4.20 (dd, *J* = 7.1, 1.7 Hz, 2H), 3.95 (dd, *J* = 10.3, 3.4 Hz, 1H), 3.58 (dd, *J* = 14.9, 6.8 Hz, 1H), 2.94 (dd, *J* = 10.4, 6.9 Hz, 1H),

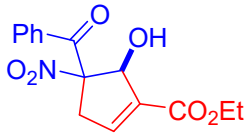
2.33 – 2.33 (m, 1H), 2.31 (s, 3H), 1.30 (t, J = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.04, 153.84, 139.04, 134.21, 131.13, 130.12, 129.27, 127.26, 126.77, 125.42, 105.58, 95.15, 62.11, 57.77, 49.54, 41.29, 21.17, 14.13; HRMS calcd. for: $C_{22}H_{23}N_2O_5^+$ $[M+H]^+$ = 427.1322, found 427.1324.

Ethyl (3aR,6aS)-3a-(hydroxyamino)-3-phenyl-3a,6a-dihydro-4H-cyclopenta[d]isoxazole-6-carboxylate (6g)



6g, a yellow liquid (43.8 mg, 76% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (dd, J = 6.6, 3.1 Hz, 2H), 7.41 – 7.38 (m, 3H), 6.80 (t, J = 2.4 Hz, 1H), 5.52 (s, 1H), 4.29 – 4.23 (m, 2H), 3.29 – 3.24 (m, 1H), 2.80 – 2.76 (m, 1H), 1.94 (s, 2H), 1.32 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.35, 159.05, 143.67, 134.62, 129.96, 128.77, 127.95, 127.39, 96.50, 76.88, 60.86, 44.80, 14.24; HRMS calcd. for: $C_{15}H_{17}N_2O_4^+$ $[M+H]^+$ = 289.1183, found 289.1177.

Ethyl (5S)-4-benzoyl-5-hydroxy-4-nitrocyclopent-1-ene-1-carboxylate (6h)

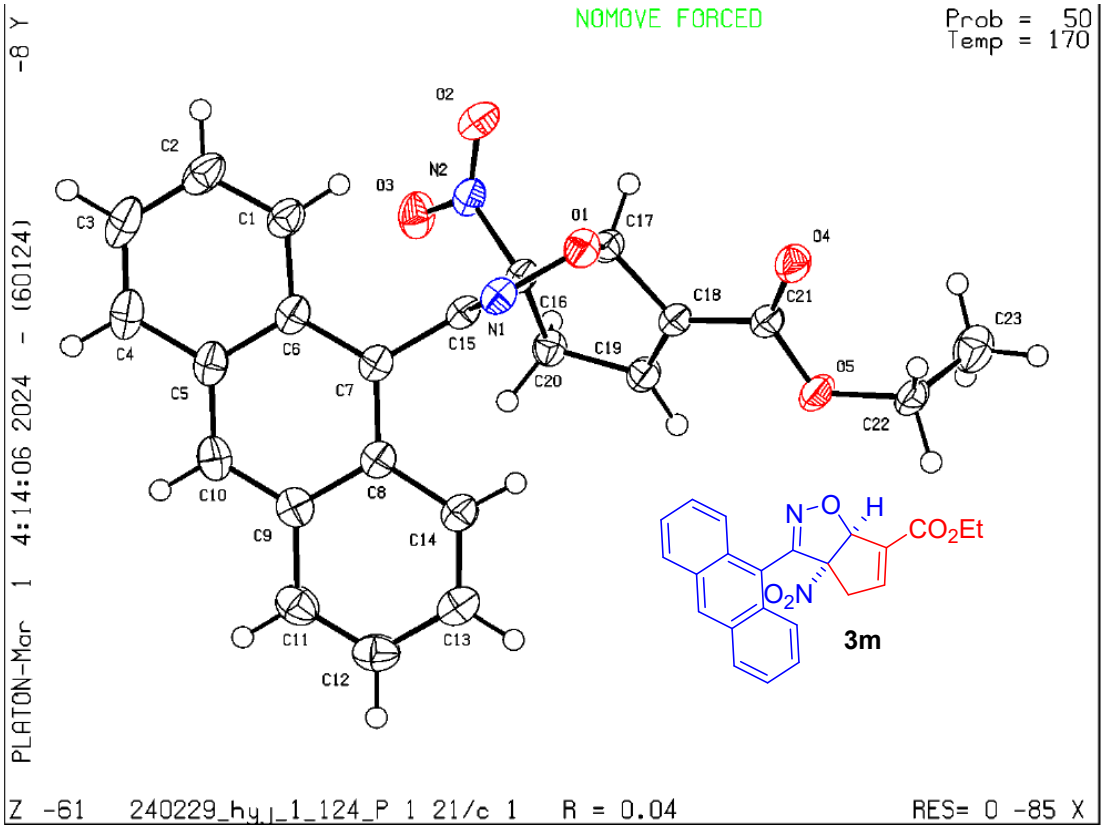


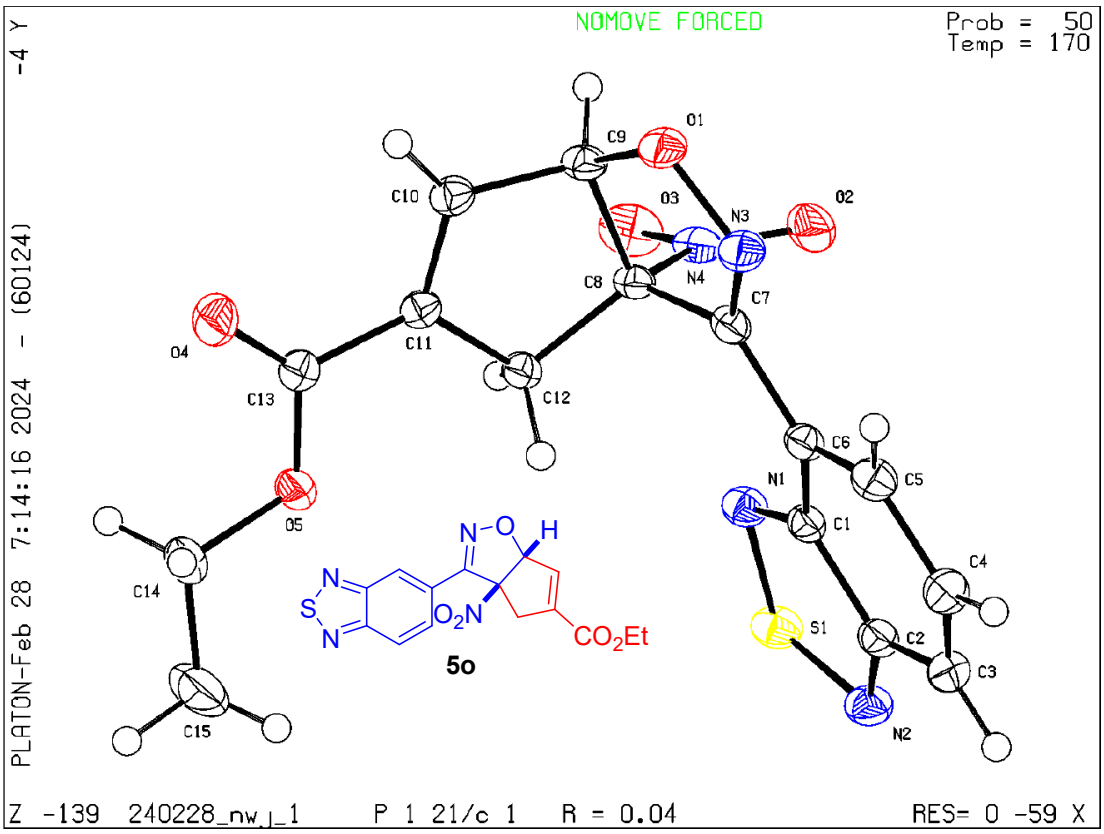
6h, a yellow liquid (45 mg, 78% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 – 7.91 (m, 2H), 7.41 – 7.40 (m, 3H), 6.81 (t, J = 2.4 Hz, 1H), 5.52 (d, J = 0.7 Hz, 1H), 4.30 – 4.25 (m, 2H), 3.28 (d, J = 19.4 Hz, 1H), 2.80 (d, J = 2.2 Hz, 1H), 1.83 (s, 1H), 1.33 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.33, 159.02, 143.63, 134.65, 129.96, 128.77, 127.93, 127.38, 96.52, 7.68, 60.87, 44.79, 14.24; HRMS calcd. for: $C_{15}H_{16}NO_5^+$ $[M+H]^+$ = 306.0972, found 306.0969.

4. X-ray Crystal Structure for 3m and 5o

Suitable crystals of compound **3m** and **5o** were obtained by slowly evaporating a mixture of dichloromethane and hexane solution at ambient temperature. A colorless crystal of **3m** and **5o** was mounted on a glass fiber at a random orientation.

A Single colourless needle-shaped crystals of **3m** and **5o** were used as supplied. A suitable crystal with dimensions 0.40 × 0.15 × 0.05 mm3 was selected and mounted on a Bruker D8 Venture diffractometer. The crystal was kept at a steady T = 170.00 K during data collection. The structure was solved with the ShelXT 2018/2 (Sheldrick, 2018) solution program using dual methods and by using Olex2 1.5 (Dolomanov et al., 2009) as the graphical interface. The model was refined with ShelXL 2019/2 (Sheldrick, 2015) using full matrix least squares minimisation on F2. The ellipsoids are shown at 30% probability levels. Crystallographic data for the structure reported in this paper have been deposited at the Cambridge Crystallographic Data Center and allocated with the deposition numbers: CCDC 2345876 for compound **3m,** CCDC 2345879 for compound **5o**.


NOMOVE FORCED
Prob = 50
Temp = 170
PLATON-Mar 1 4:14:06 2024 - (60124)
-8 Y
O2
N2
O3
C2
C3
C1
O1
C17
O4
C18
C21
C16
N1
C15
C4
C6
C19
C23
C5
C7
C20
O5
C22
C10
C8
C9
C14
C11
C13
C12
N-O
H
CO2Et
O2N
3m
Z -61 240229_hyj_1_124_P 1 21/c 1 R = 0.04
RES= 0 -85 X


NOMOVE FORCED
Prob = 50
Temp = 170
PLATON-Feb 28 7:14:16 2024 - (60124)
-4 Y
O1
C9
C10
O3
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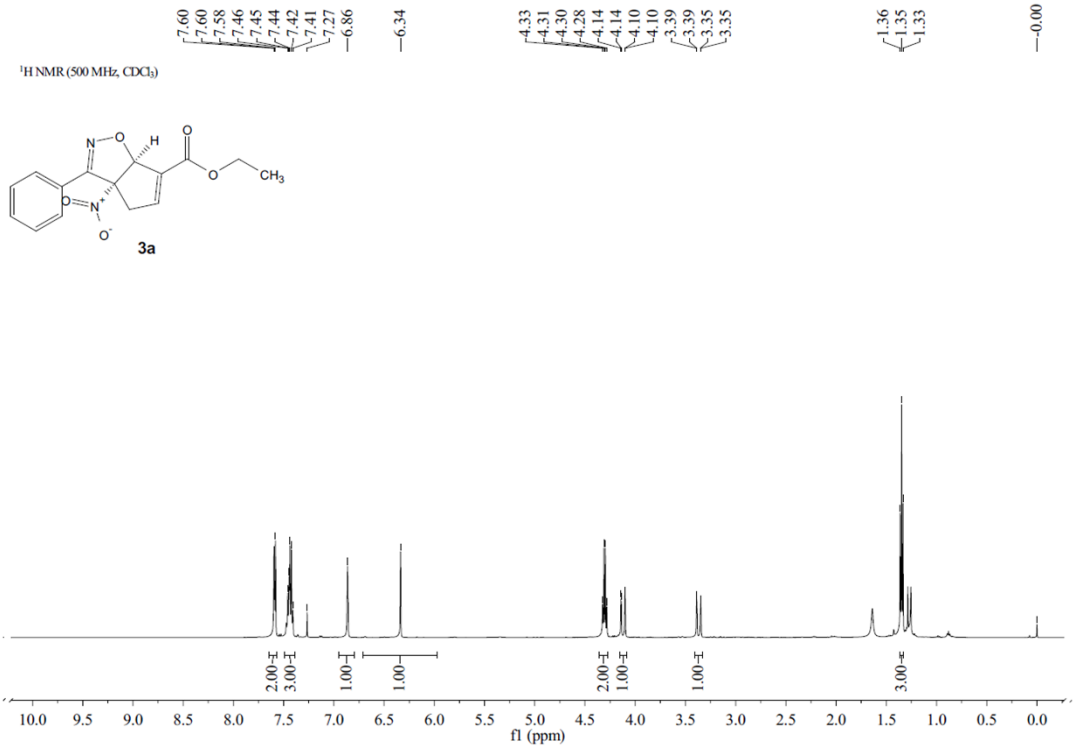
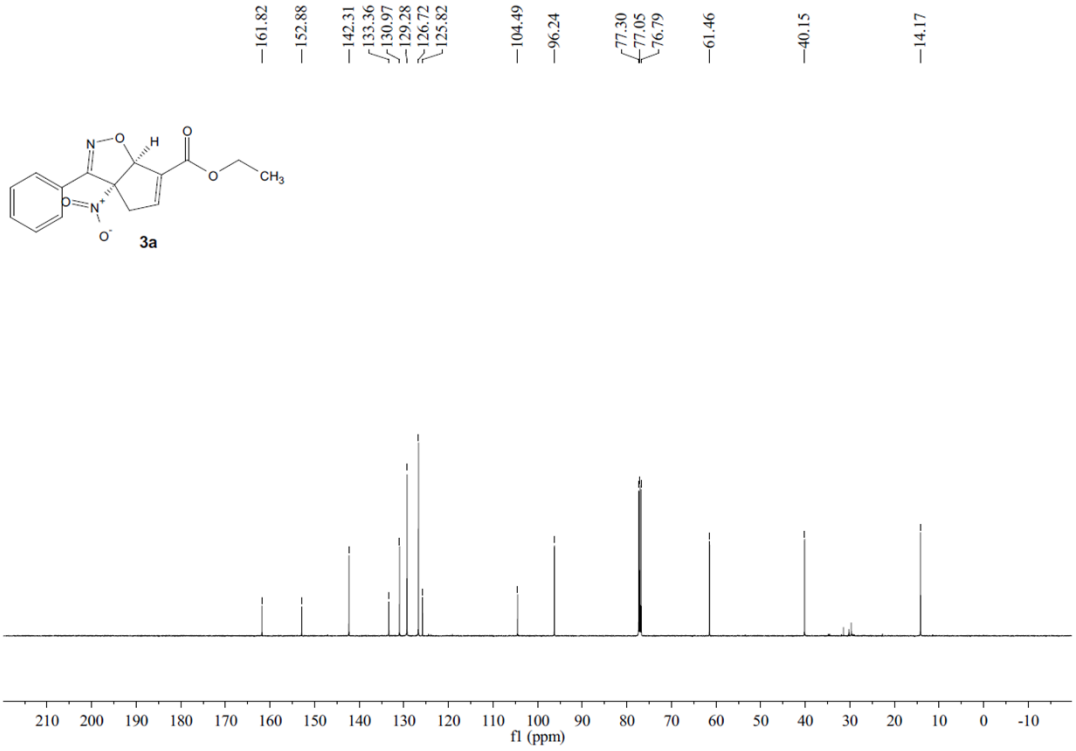
C7
O4
C11
C13
C12
C6
N1
C5
O5
C1
C4
N-O
H
N
S
N
O2N
CO2Et
S1
C2
C14
C3
5o
C15
N2
Z -139 240228_nwj_1 P 1 21/c 1 R = 0.04
RES= 0 -59 X

5. Reference

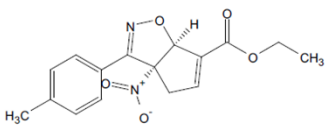
1. T. Morita, N. Ito and H. Nakamura, Asymmetric Synthesis of Bicyclic Isoxazolines via Dearomative Cycloaddition of 4-Nitroisoxazoles with Zwitterionic π-Allyl Palladium Species. *Org. Lett.,* 2023, **25**, 26, 4787–4791.
2. Z. Huang, X. Yang, F. Yang, T. Lu and Q. Zhou, Phosphine-Catalyzed Domino β/γ-Additions of Benzofuranones with Allenoates: A Method for Unsymmetrical 3,3-Disubstituted Benzofuranones. *Org. Lett.,* 2017, **19**, 3524–3527.
3. J. Jia, A. Yu, S. Ma, Y. Zhang, K. Li and X. Meng, Solvent-Controlled Switchable Domino Reactions of MBH Carbonate: Synthesis of Benzothiophene Fused α-Pyran, 2,3-Dihydrooxepine, and Oxatricyclodecene Derivatives. *Org. Lett.,* 2017, **19**, 6084–6087.

6. ^{1}H, ^{13}C, ^{19}F NMR spectra of compounds.

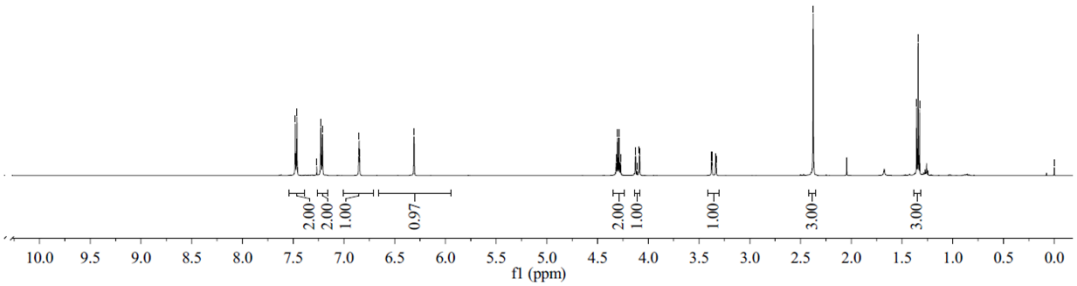




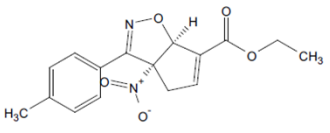
^{1}H NMR (500 MHz, $CDCl_3$)



3b

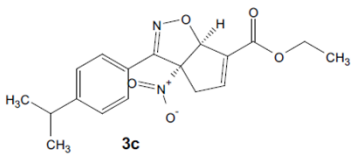


^{13}C NMR (126 MHz, $CDCl_3$)

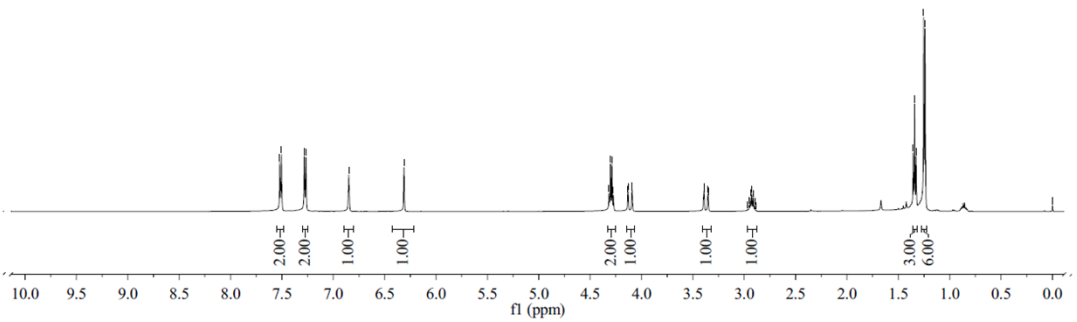


3b

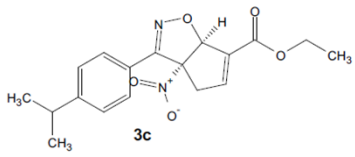
^{1}H NMR (500 MHz, $CDCl_3$)



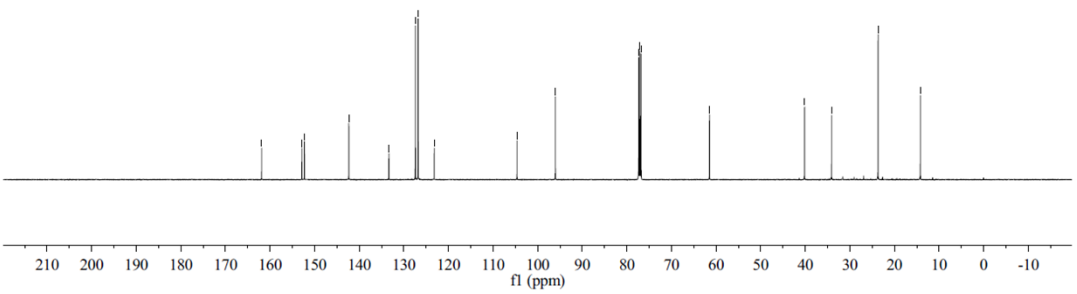
3c

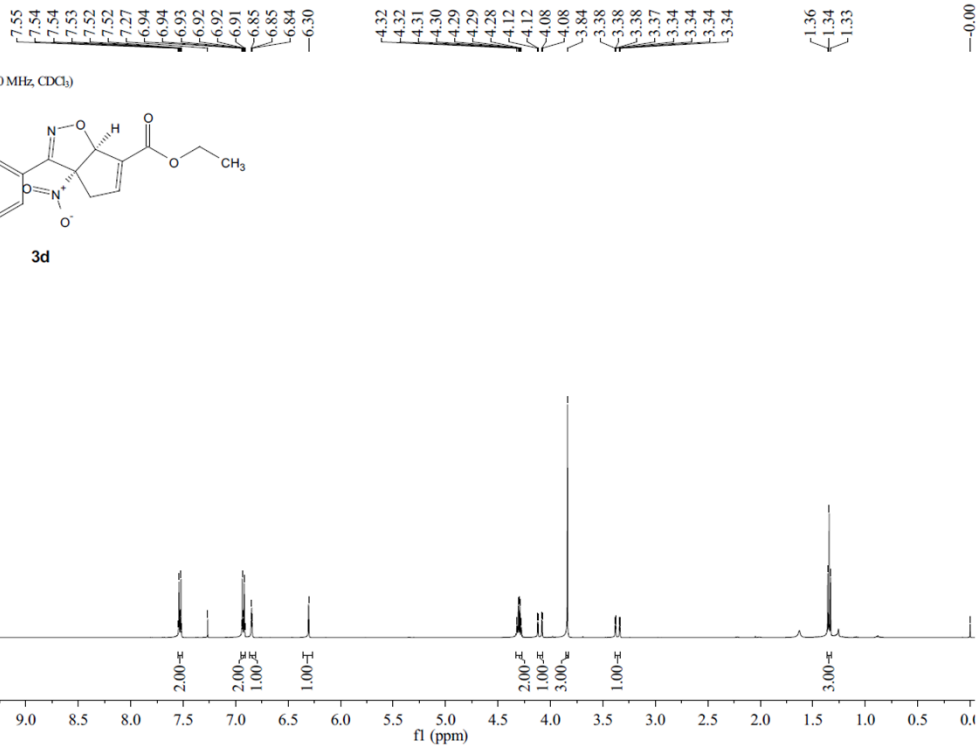


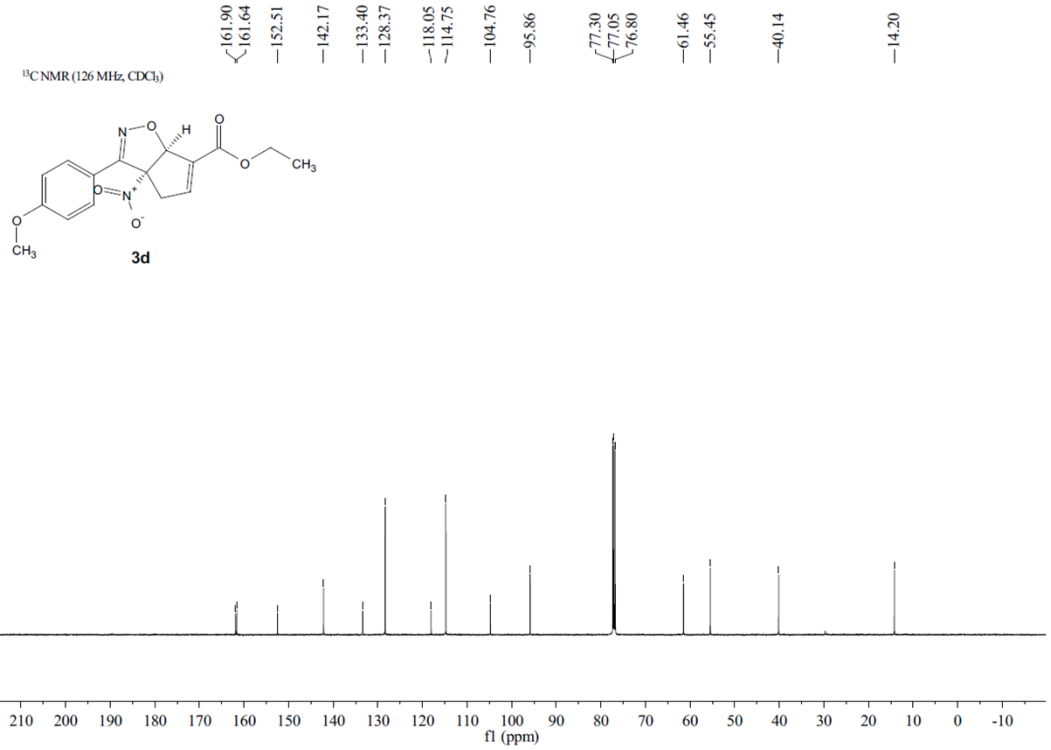
^{13}C NMR (126 MHz, $CDCl_3$)



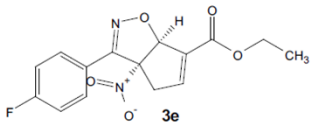
3c



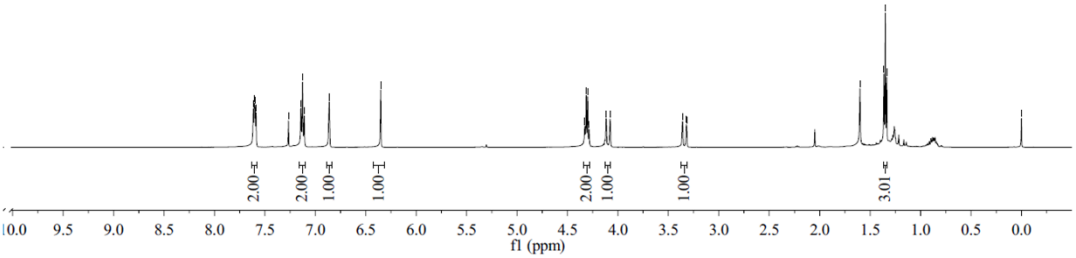

7.55
7.54
7.54
7.53
7.52
7.52
7.27
6.94
6.94
6.93
6.92
6.92
6.91
6.85
6.84
6.30
4.32
4.32
4.31
4.30
4.29
4.29
4.28
4.12
4.12
4.08
4.08
3.84
3.38
3.38
3.38
3.37
3.34
3.34
3.34
3.34
1.36
1.34
1.33
0.00
1H NMR (500 MHz, CDCl3)
3d
2.00
2.00
1.00
1.00
2.00
1.00
3.00
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


161.90
161.64
152.51
142.17
133.40
128.37
118.05
114.75
104.76
95.86
77.30
77.05
76.80
61.46
55.45
40.14
14.20
13C NMR (126 MHz, CDCl3)
3d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

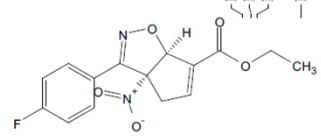
^{1}H NMR (500 MHz, $CDCl_3$)



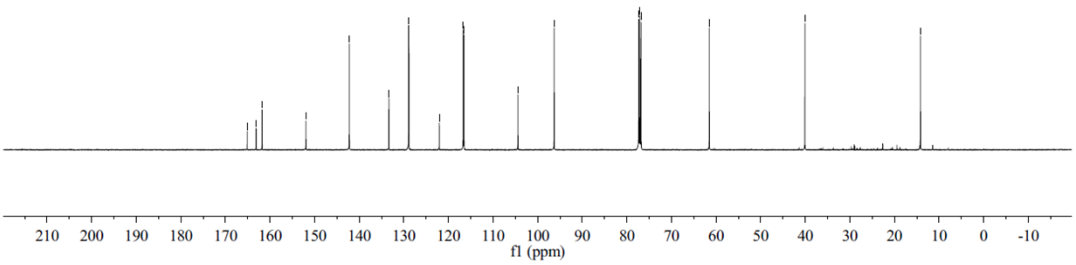
7.61, 7.60, 7.60, 7.59, 7.27, 7.14, 7.13, 7.11, 6.86, 6.35, 4.33, 4.31, 4.30, 4.29, 4.12, 4.08, 3.36, 3.36, 3.32, 3.32, 1.60, 1.36, 1.35, 1.34, 0.00



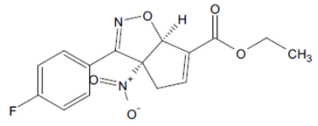
^{13}C NMR (126 MHz, $CDCl_3$)



165.12, 163.11, 161.77, 151.96, 142.21, 133.34, 128.92, 128.85, 122.06, 116.69, 116.51, 104.42, 96.30, 77.33, 77.07, 76.82, 61.52, 40.10, 14.17

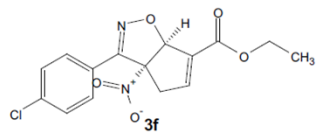


^{19}F NMR (471 MHz, $CDCl_3$)



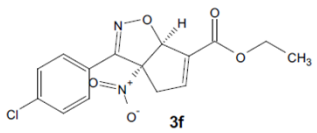
3e

^{1}H NMR (500 MHz, $CDCl_3$)



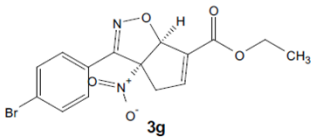
3f

^{13}C NMR (126 MHz, $CDCl_3$)

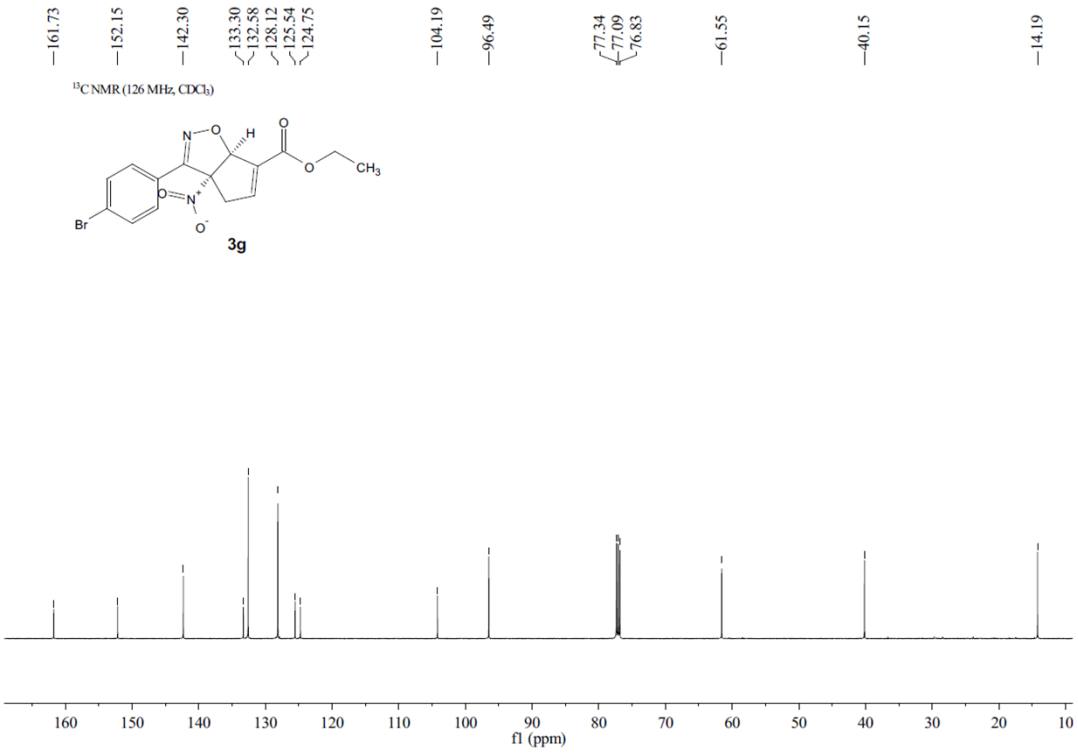


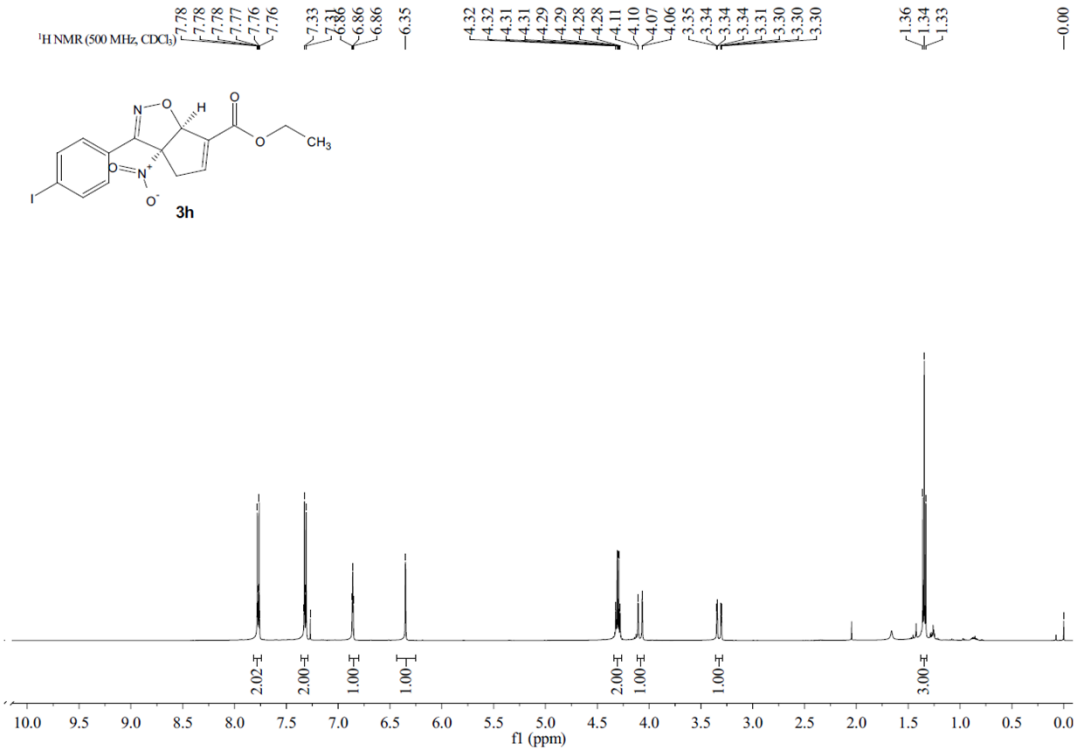
3f

^{1}H NMR (500 MHz, $CDCl_3$)

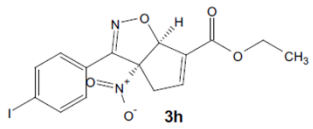


3g


161.73
152.15
142.30
133.30
132.58
128.12
125.54
124.75
104.19
96.49
77.34
77.09
76.83
61.55
40.15
14.19
13C NMR (126 MHz, CDCl3)
Br
3g
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

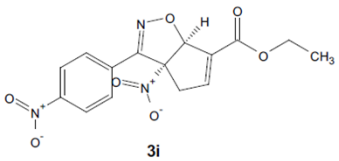

7.78
7.78
7.78
7.77
7.76
7.76
7.33
7.31
6.86
6.86
6.86
6.35
4.32
4.32
4.31
4.31
4.29
4.29
4.28
4.28
4.11
4.10
4.07
4.06
3.35
3.34
3.34
3.34
3.31
3.30
3.30
3.30
1.36
1.34
1.33
0.00
1H NMR (500 MHz, CDCl3)
I
3h
2.02
2.00
1.00
1.00
2.00
1.00
1.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

^{13}C NMR (126 MHz, $CDCl_3$)



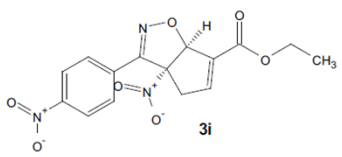
3h

^{1}H NMR (500 MHz, $CDCl_3$)

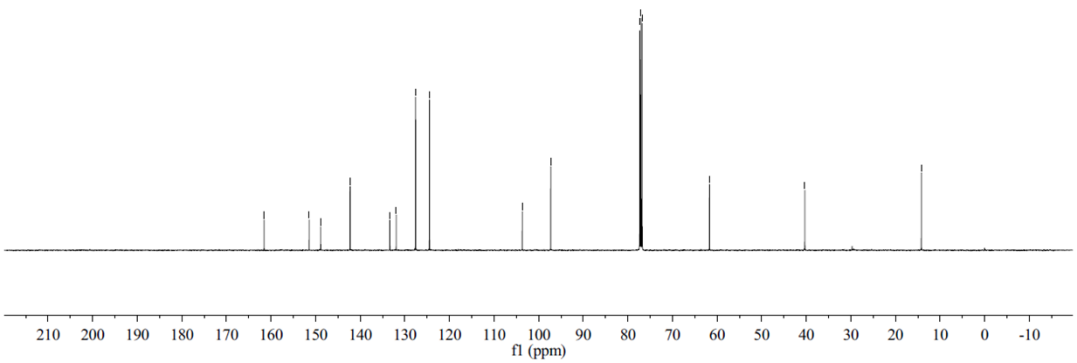


3i

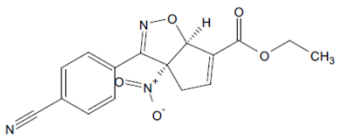
^{13}C NMR (126 MHz, $CDCl_3$)



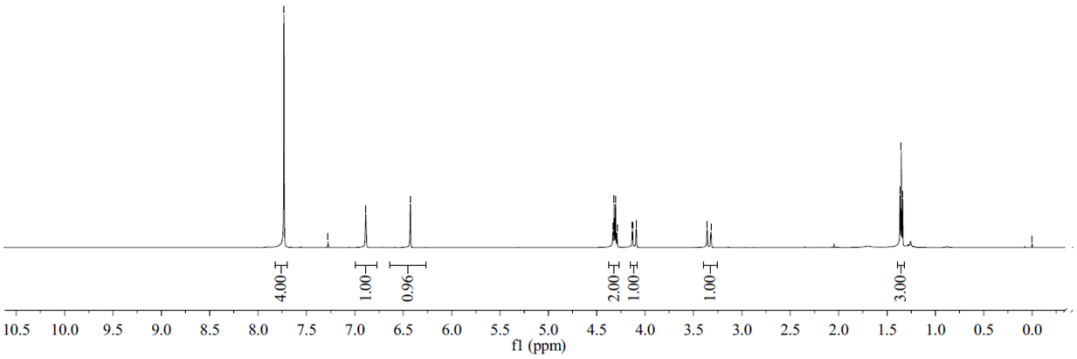
3i



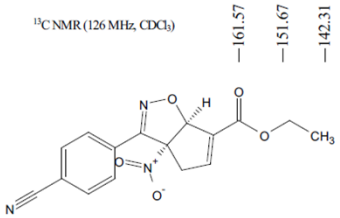
^{1}H NMR (500 MHz, $CDCl_3$)



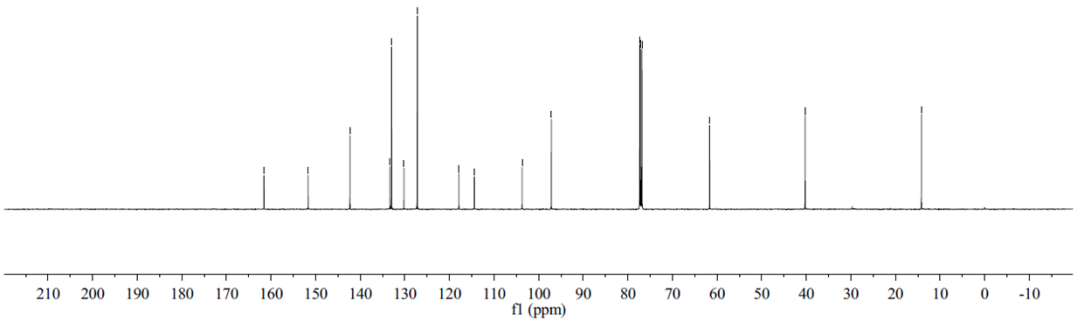
3j



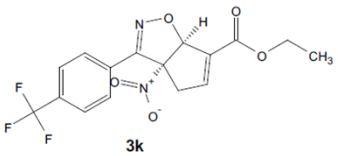
^{13}C NMR (126 MHz, $CDCl_3$)



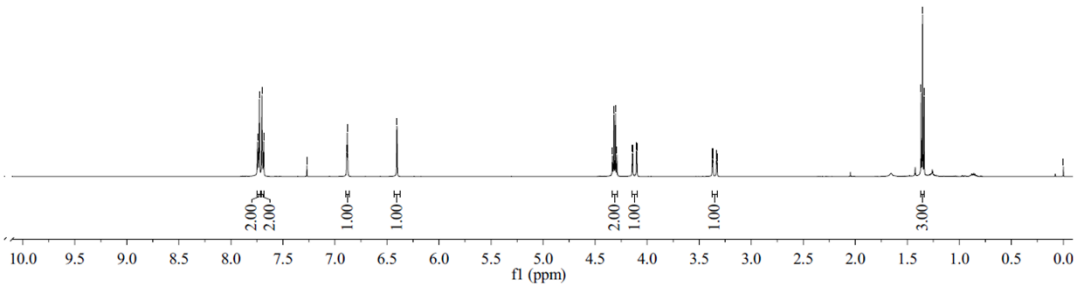
3j



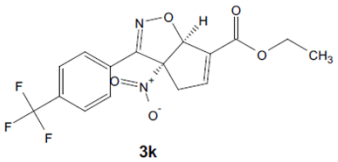
^{1}H NMR (500 MHz, $CDCl_3$)



3k

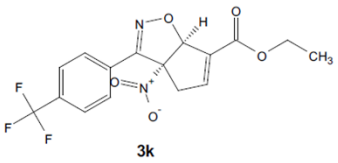


^{13}C NMR (126 MHz, $CDCl_3$)

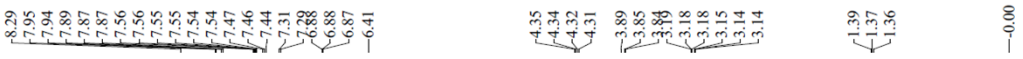


3k

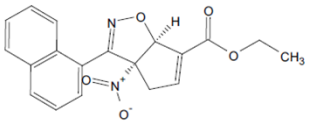
^{19}F NMR (471 MHz, $CDCl_3$)



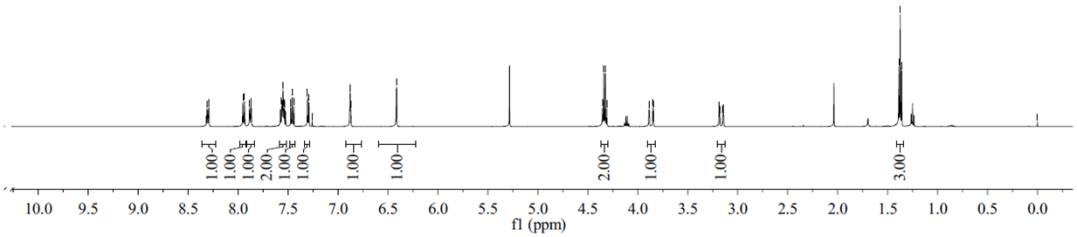
3k

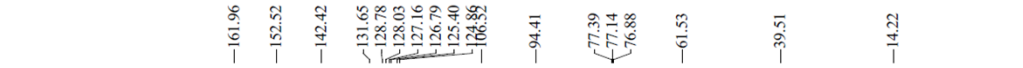


^{1}H NMR (500 MHz, $CDCl_3$)

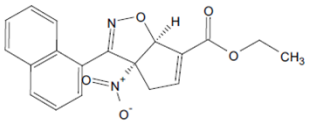


3l

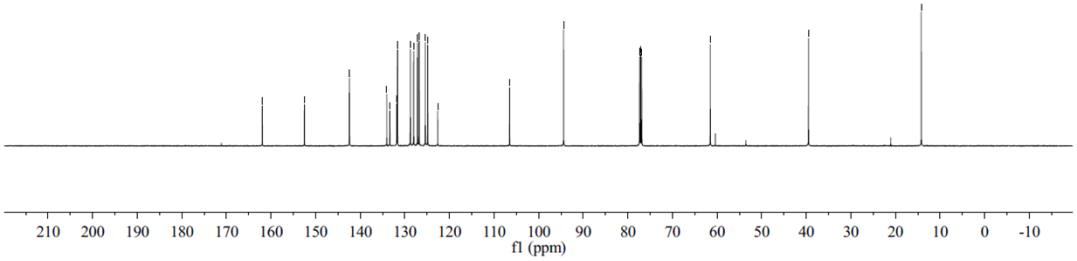


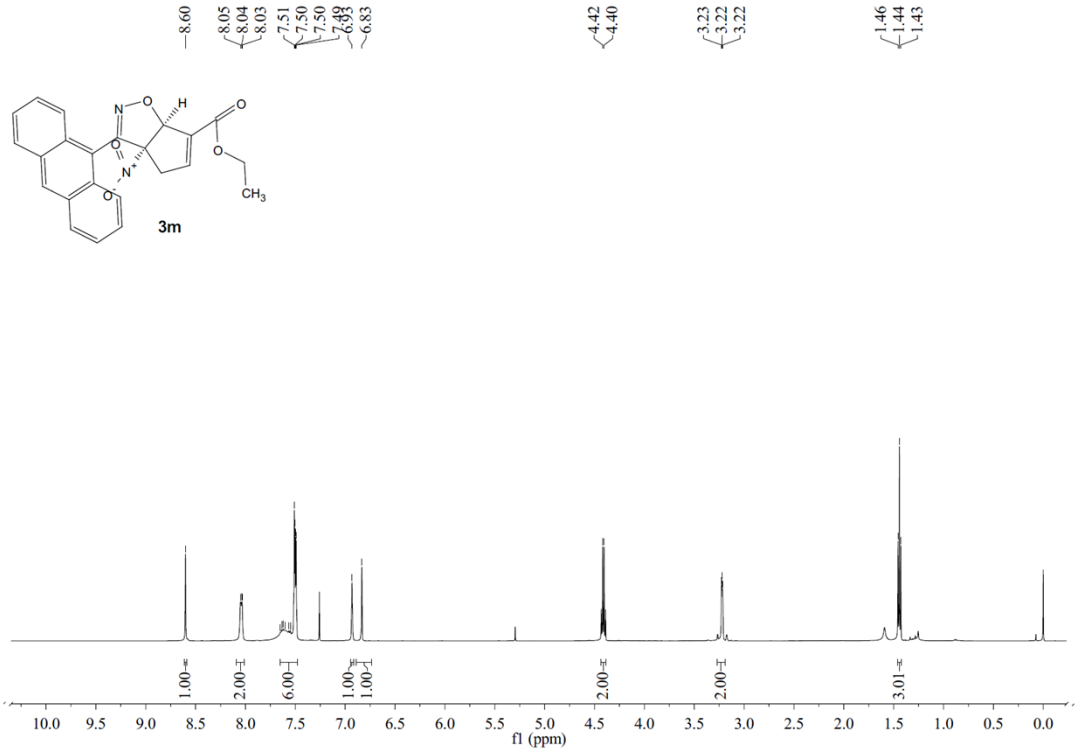


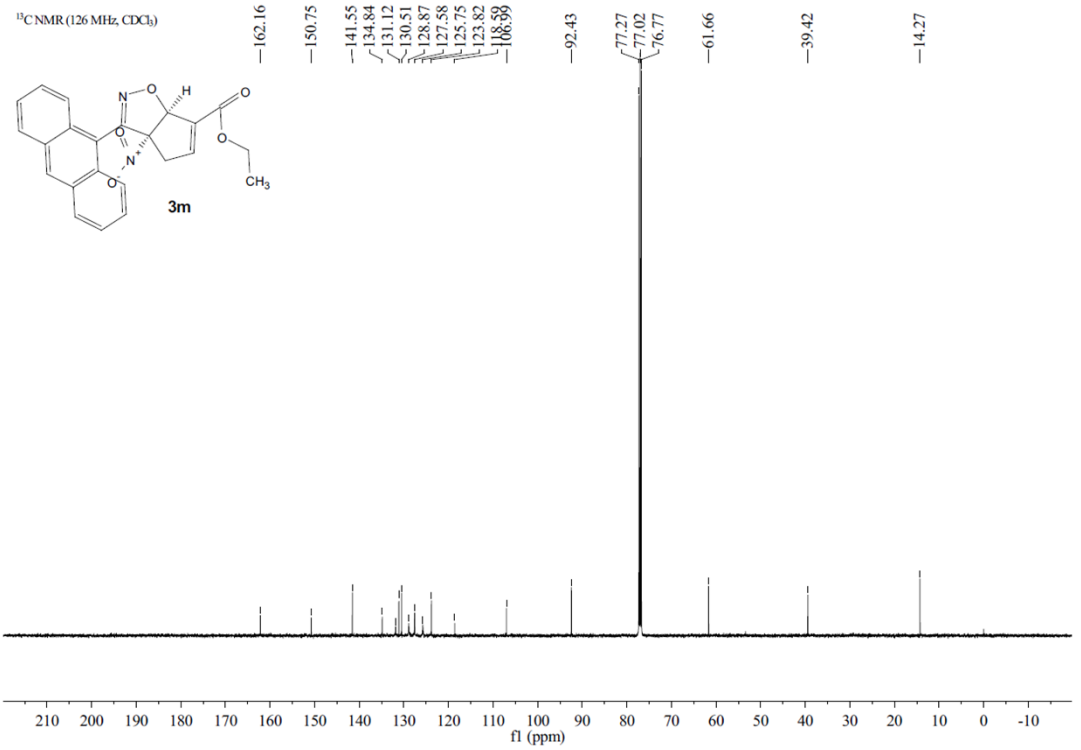
^{13}C NMR (126 MHz, $CDCl_3$)



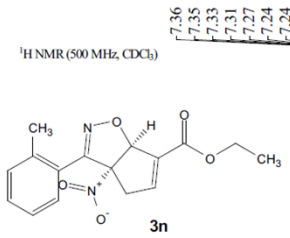
3l



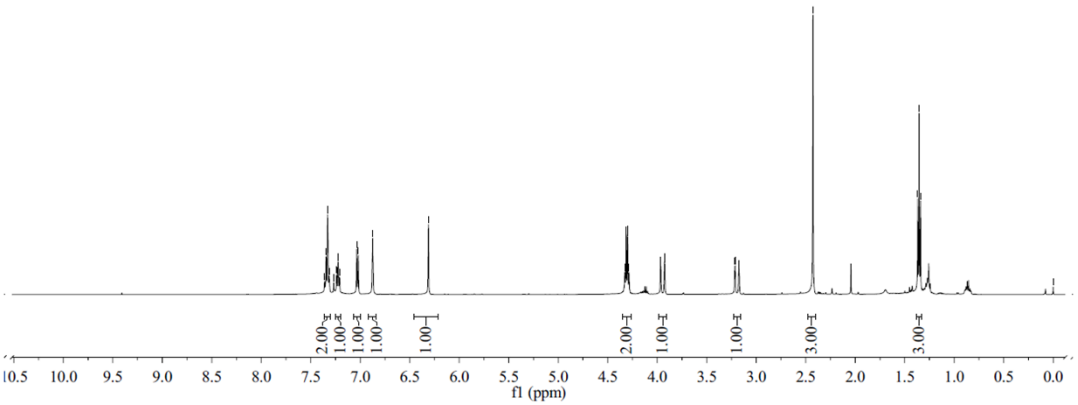

8.60
8.05
8.04
8.03
7.51
7.50
7.50
7.49
6.93
6.83
4.42
4.40
3.23
3.22
3.22
1.46
1.44
1.43
3m
1.00
2.00
6.00
1.00
1.00
2.00
2.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


13C NMR (126 MHz, CDCl3)
162.16
150.75
141.55
134.84
131.12
130.51
128.87
127.58
125.75
123.82
118.59
106.99
92.43
77.27
77.02
76.77
61.66
39.42
14.27
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

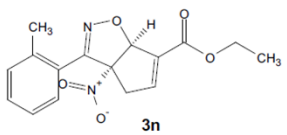
^{1}H NMR (500 MHz, $CDCl_3$)



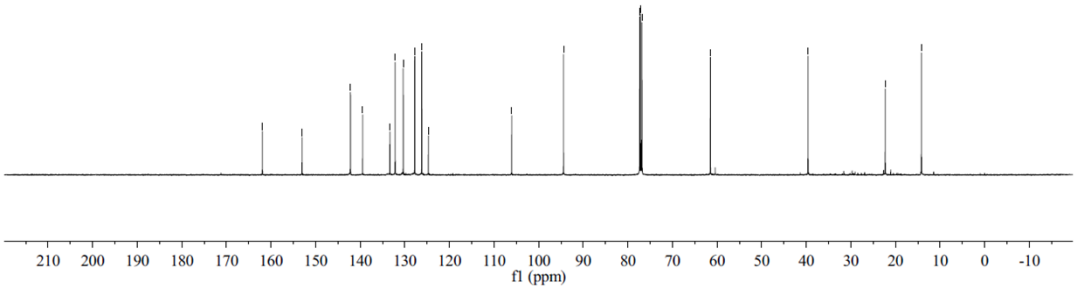
3n

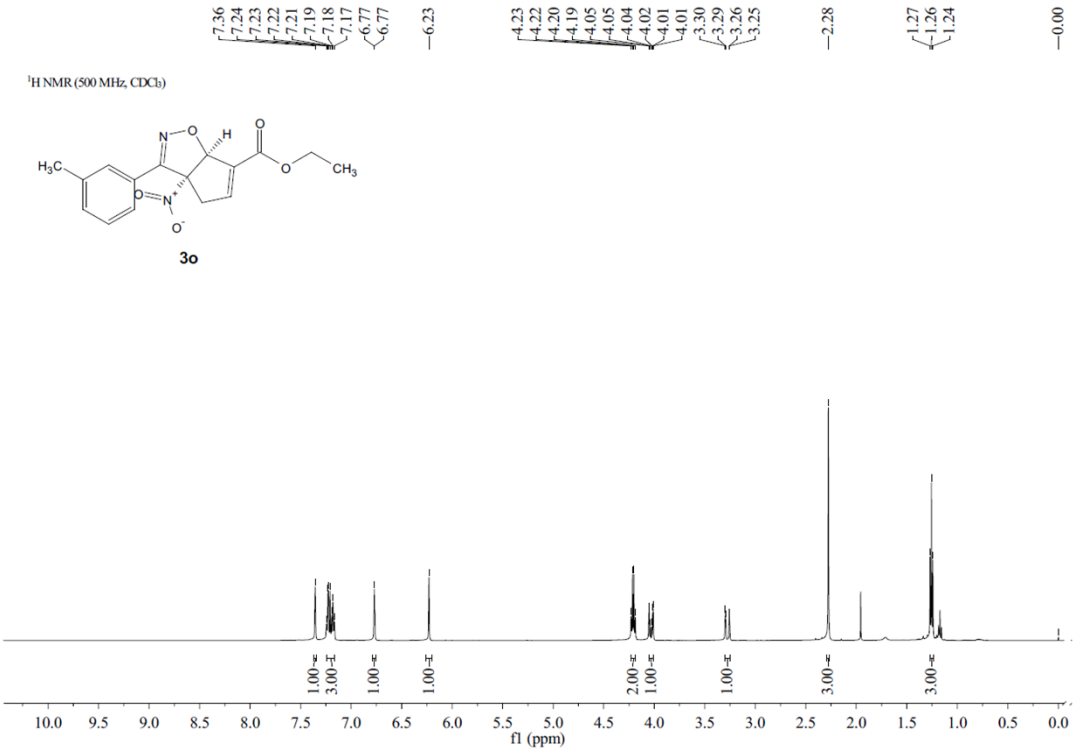


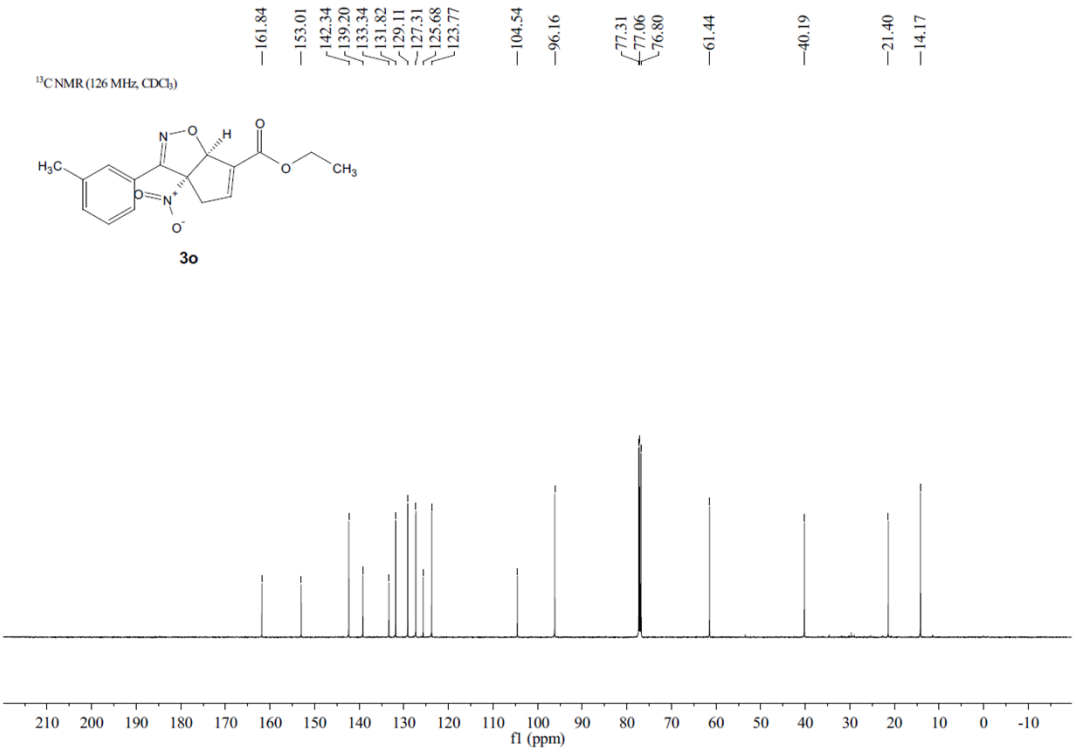
^{13}C NMR (126 MHz, $CDCl_3$)

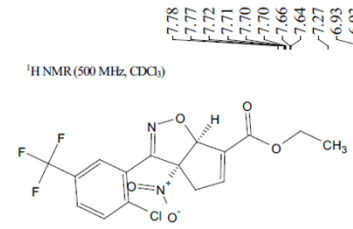


3n

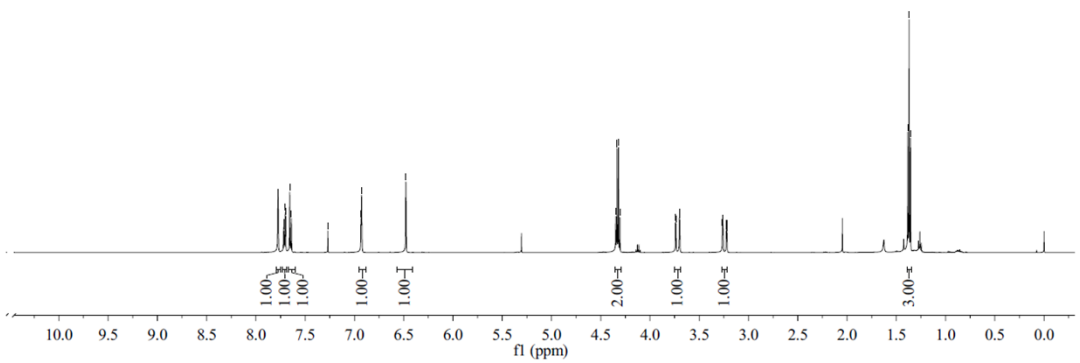


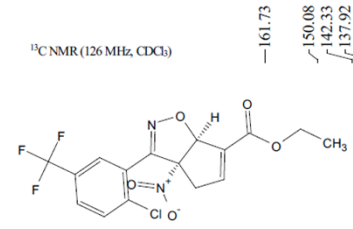

7.36
7.24
7.23
7.22
7.21
7.19
7.18
7.17
6.77
6.77
6.23
4.23
4.22
4.20
4.19
4.05
4.05
4.04
4.02
4.01
4.01
3.30
3.29
3.26
3.25
2.28
1.27
1.26
1.24
0.00
1H NMR (500 MHz, CDCl3)
3o
1.00
3.00
1.00
1.00
2.00
1.00
1.00
3.00
3.00
f1 (ppm)


161.84
153.01
142.34
139.20
133.34
131.82
129.11
127.31
125.68
123.77
104.54
96.16
77.31
77.06
76.80
61.44
40.19
21.40
14.17
13C NMR (126 MHz, CDCl3)
3o
f1 (ppm)

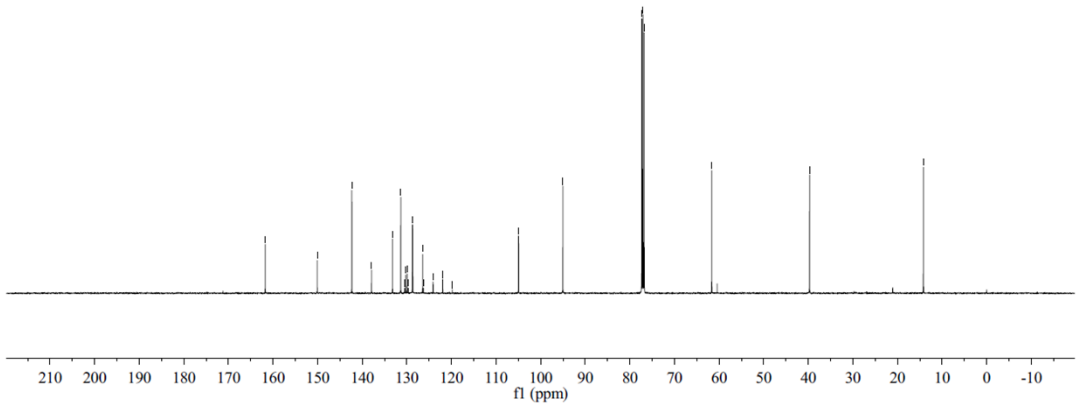


3p

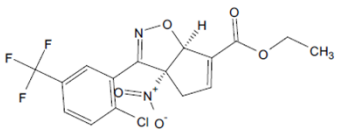




3p

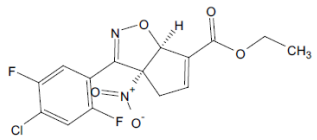


^{19}F NMR (471 MHz, $CDCl_3$)

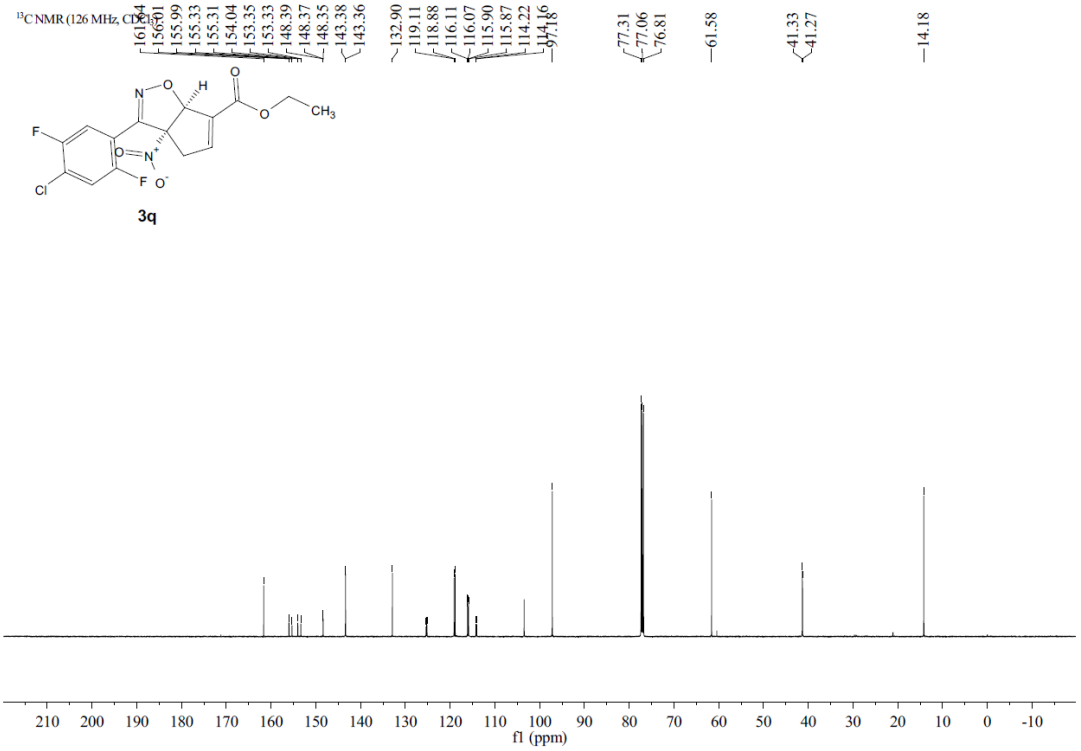


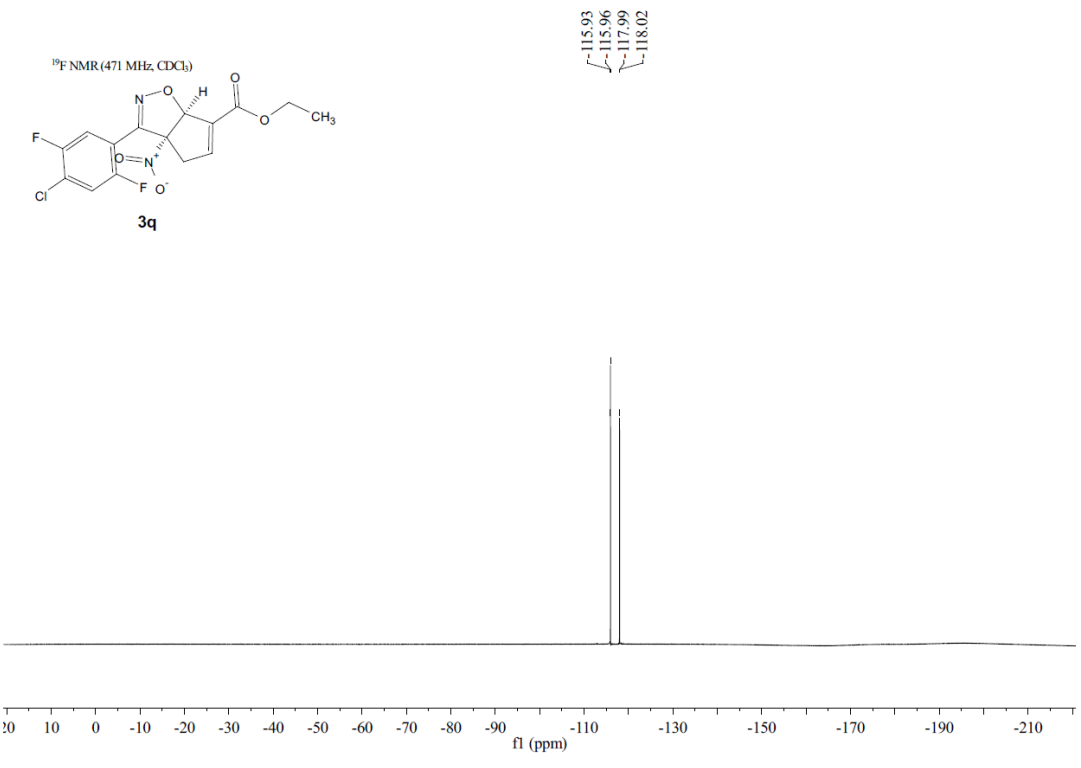
3p

^{1}H NMR (500 MHz, $CDCl_3$)

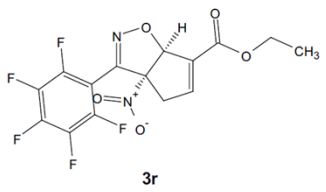


3q

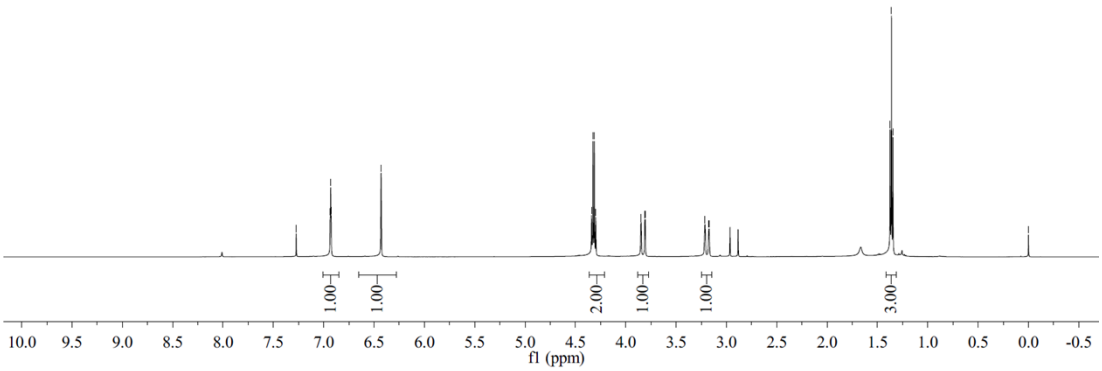

13C NMR (126 MHz, CDCl3)
161.84
156.01
155.99
155.33
155.31
154.04
153.35
153.33
148.39
148.37
148.35
143.38
143.36
132.90
119.11
118.88
116.11
116.07
115.90
115.87
114.22
114.16
97.18
77.31
77.06
76.81
61.58
41.33
41.27
14.18
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


19F NMR (471 MHz, CDCl3)
-115.93
-115.96
-117.99
-118.02
3q
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

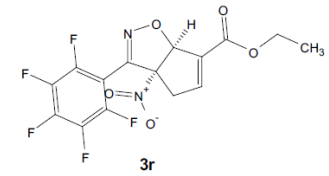
^{1}H NMR (500 MHz, $CDCl_3$)



3r

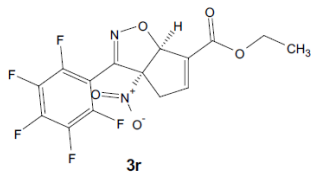


^{13}C NMR (126 MHz, $CDCl_3$)



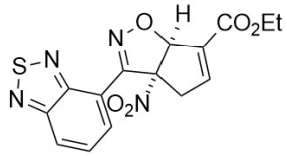
3r

^{19}F NMR (471 MHz, $CDCl_3$)



3r

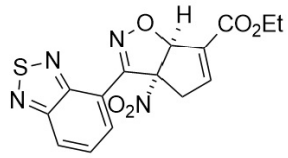
^{1}H NMR (500 MHz, $CDCl_3$)



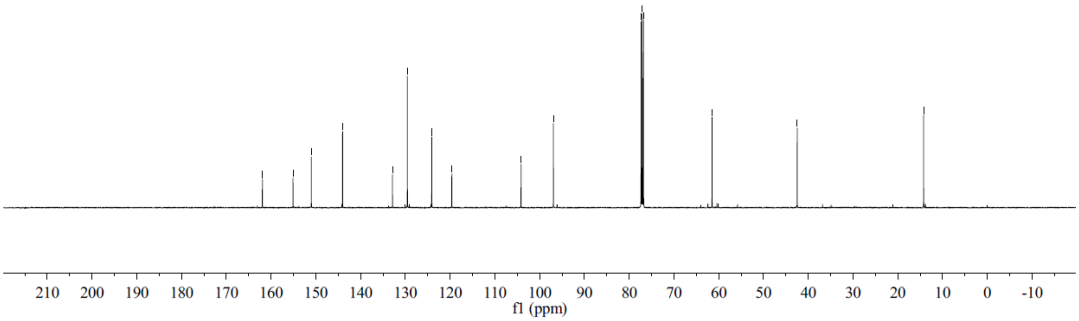
3s

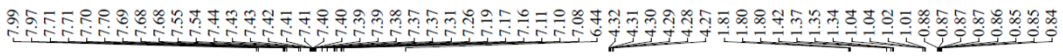
^{13}C NMR (126 MHz, $CDCl_3$)

161.94
155.09
151.00
144.02
132.87
129.55
124.10
119.62
104.16
96.93
77.33
77.07
76.82
61.48
42.47
14.22

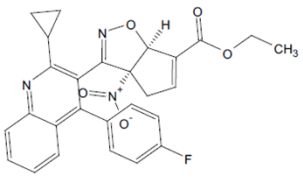


3s

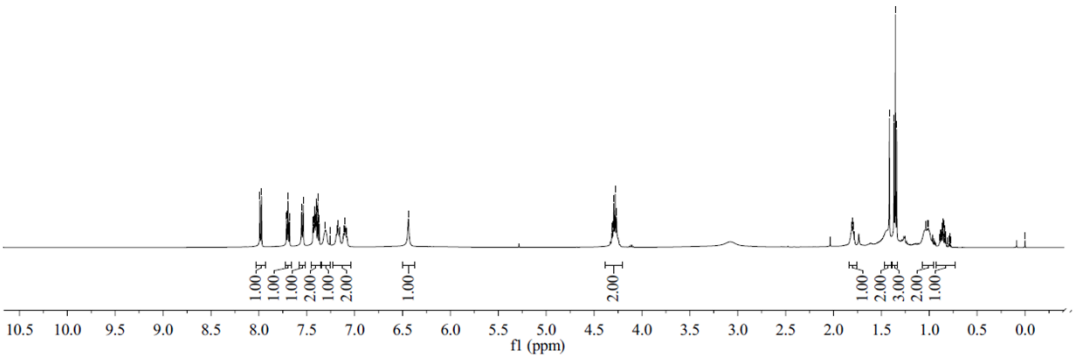


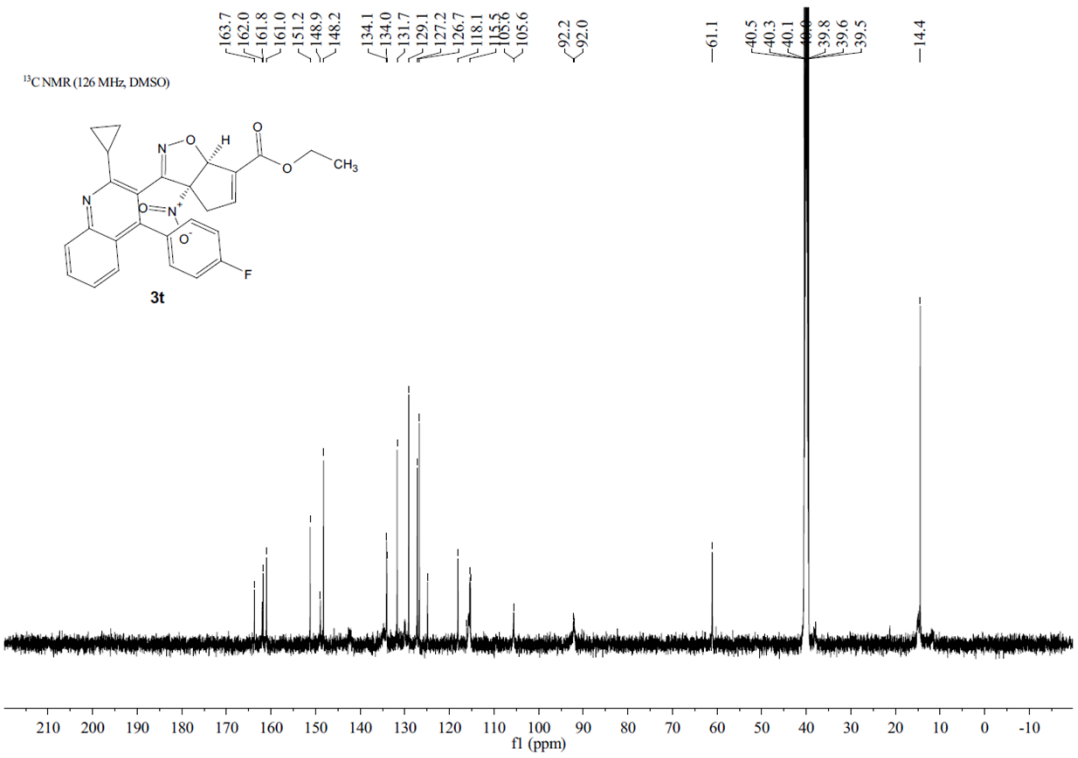


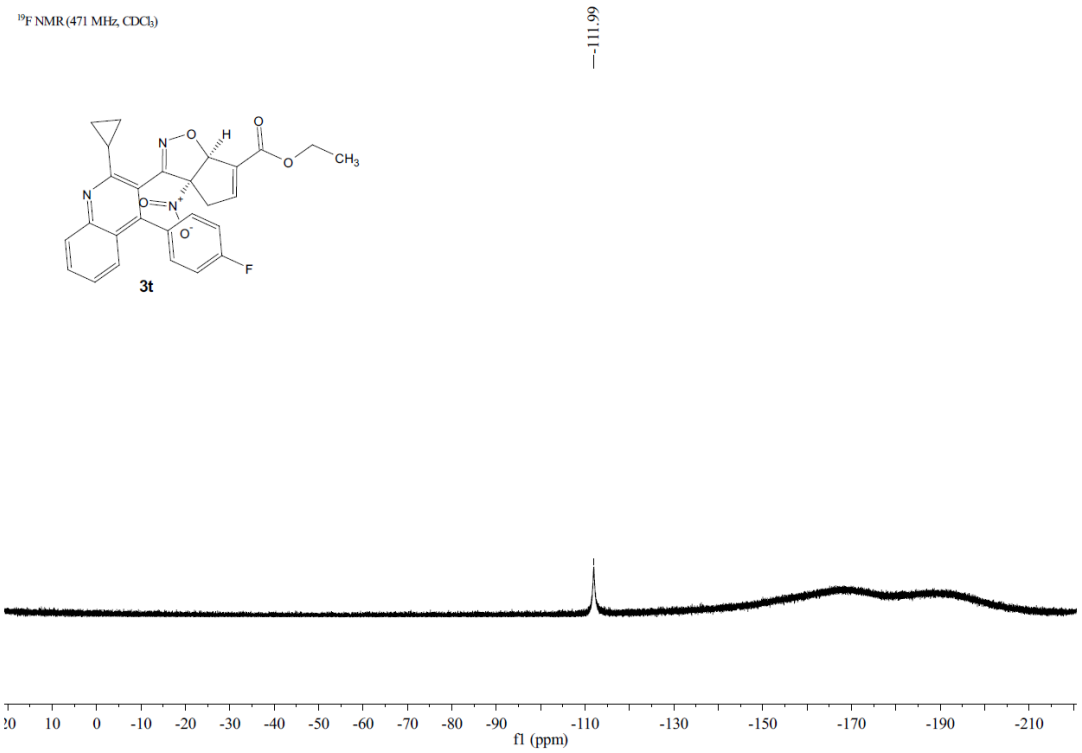
^{1}H NMR (500 MHz, $CDCl_3$)

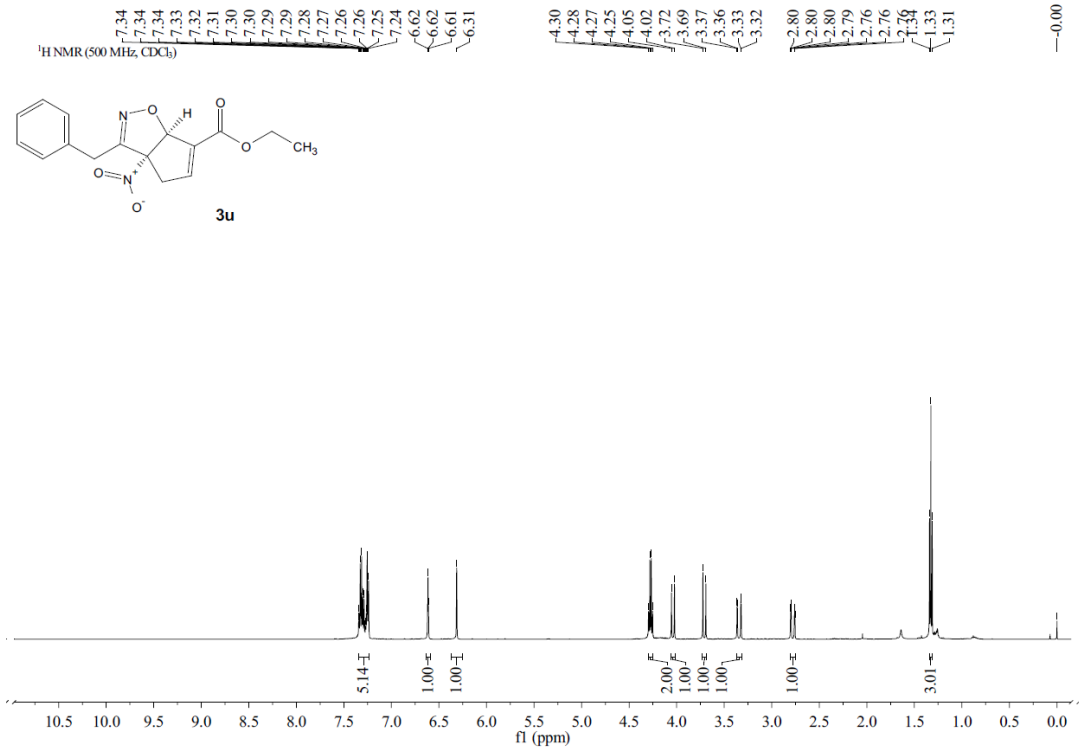


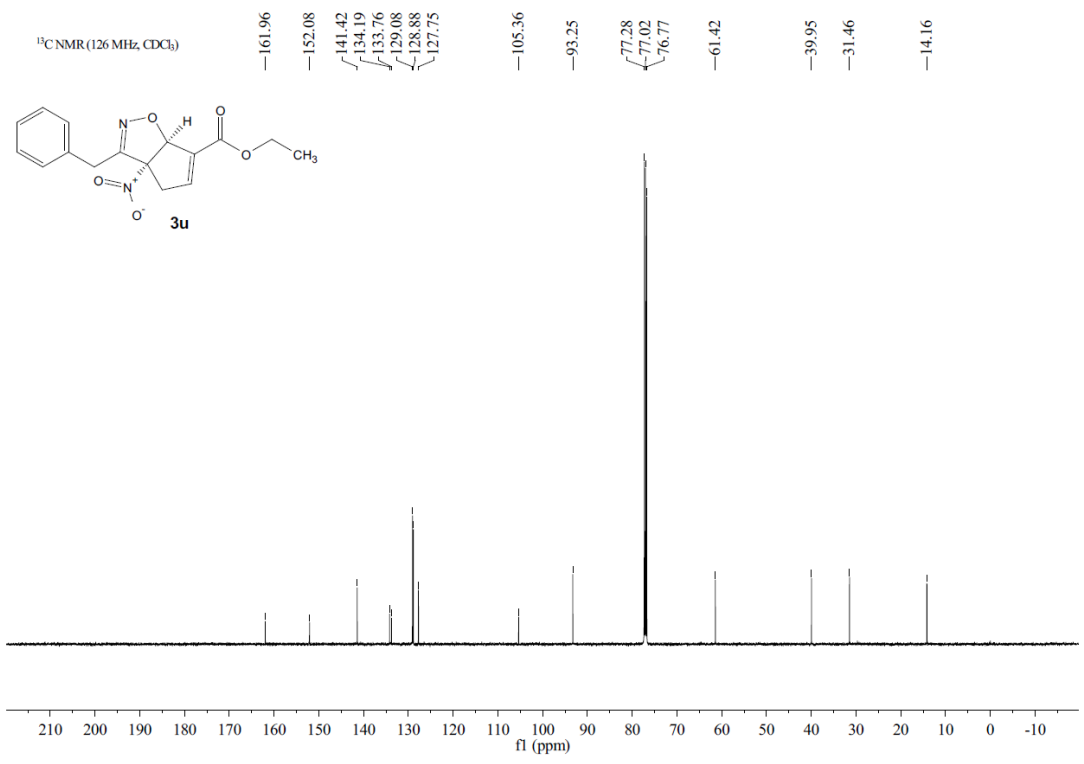
3t

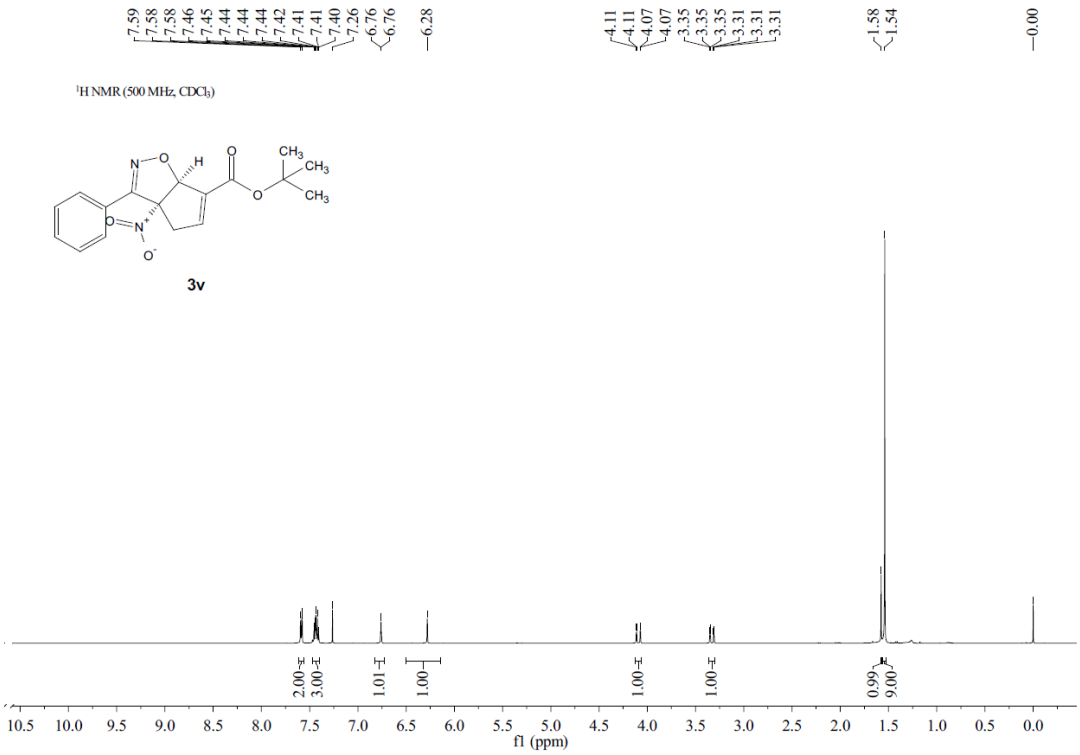



163.7
162.0
161.8
161.0
151.2
148.9
148.2
134.1
134.0
131.7
129.1
127.2
126.7
118.1
115.5
115.6
105.6
92.2
92.0
61.1
40.5
40.3
40.1
39.8
39.6
39.5
14.4
13C NMR (126 MHz, DMSO)
3t
fl (ppm)


-111.99
19F NMR (471 MHz, CDCl3)
3t
fl (ppm)

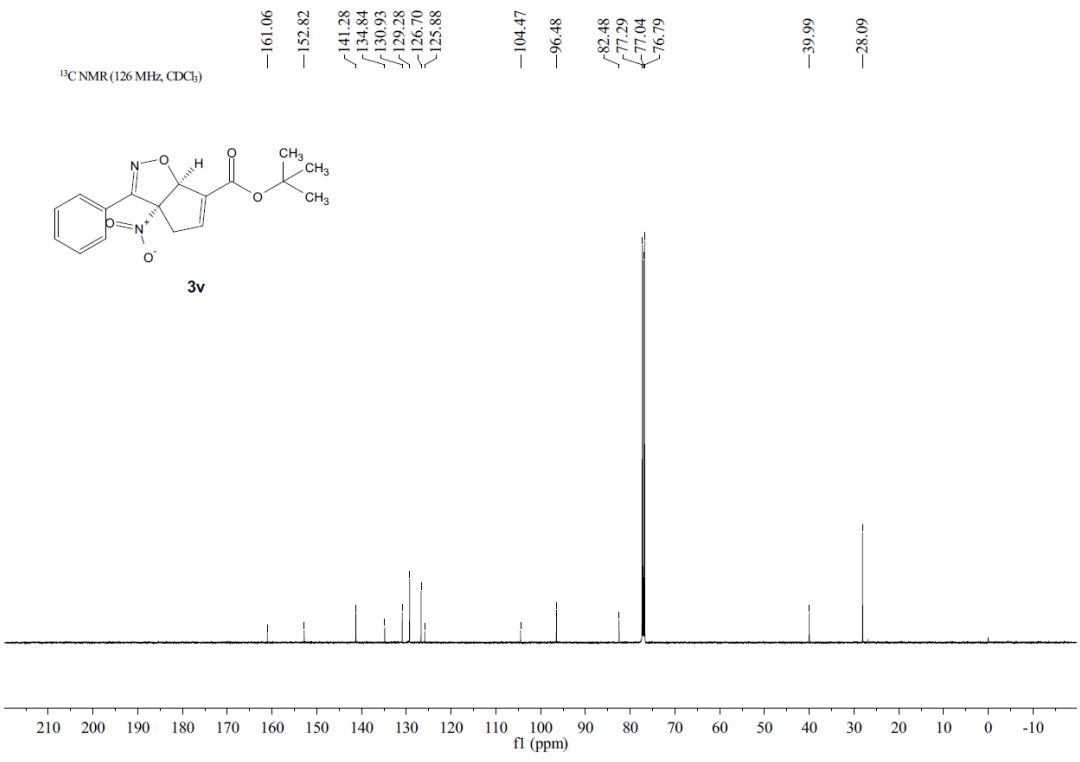

^{1}H NMR (500 MHz, CDCl$_3$)
7.34 7.34 7.34 7.33 7.32 7.31 7.30 7.30 7.29 7.29 7.28 7.27 7.26 7.26 7.25 7.24 6.62 6.62 6.61 6.31
4.30 4.28 4.27 4.25 4.05 4.02 3.72 3.69 3.37 3.36 3.33 3.32
2.80 2.80 2.80 2.79 2.76 2.76 2.76 1.34 1.33 1.31
-0.00
3u
5.14 1.00 1.00 2.00 1.00 1.00 1.00 1.00 3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


^{13}C NMR (126 MHz, CDCl$_3$)
161.96 152.08 141.42 134.19 133.76 129.08 128.88 127.75 105.36 93.25 77.28 77.02 76.77 61.42 39.95 31.46 14.16
3u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



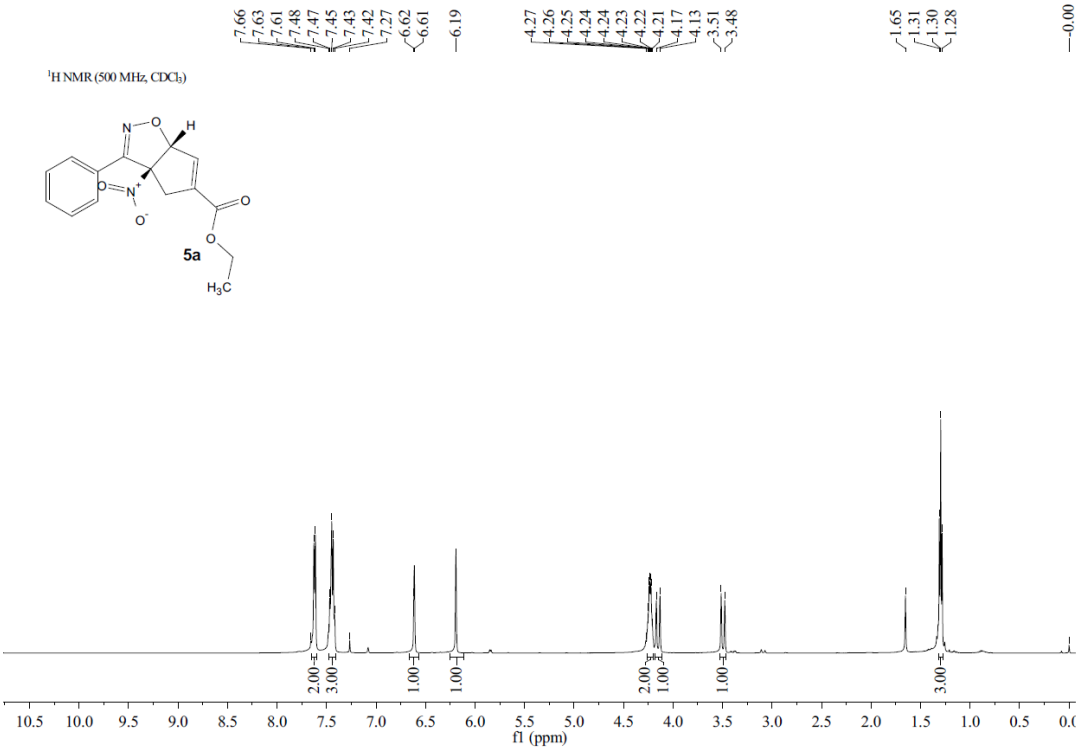
^{1}H NMR (500 MHz, $CDCl_3$)

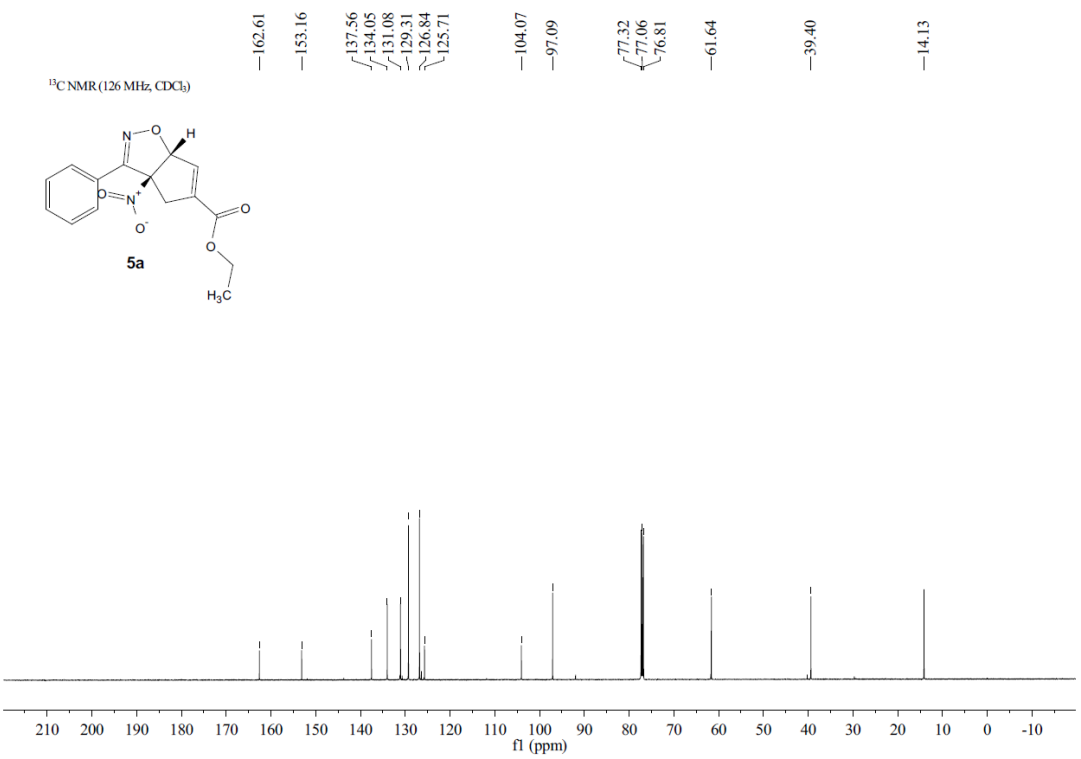
3v



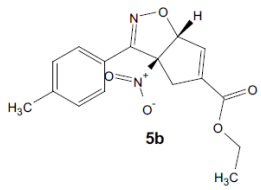
^{13}C NMR (126 MHz, $CDCl_3$)

3v

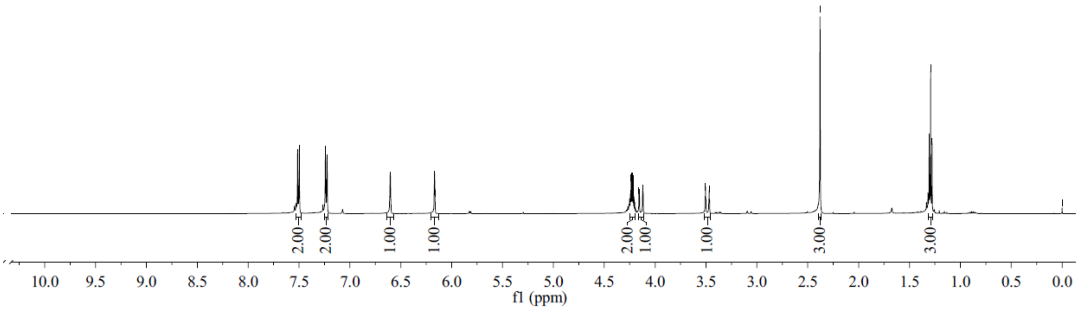

7.66
7.63
7.61
7.48
7.47
7.45
7.43
7.42
7.27
6.62
6.61
6.19
4.27
4.26
4.25
4.24
4.24
4.23
4.22
4.21
4.17
4.13
3.51
3.48
1.65
1.31
1.30
1.28
0.00
1H NMR (500 MHz, CDCl3)
5a
2.00
3.00
1.00
1.00
2.00
1.00
1.00
3.00
f1 (ppm)


162.61
153.16
137.56
134.05
131.08
129.31
126.84
125.71
104.07
97.09
77.32
77.06
76.81
61.64
39.40
14.13
13C NMR (126 MHz, CDCl3)
5a
f1 (ppm)

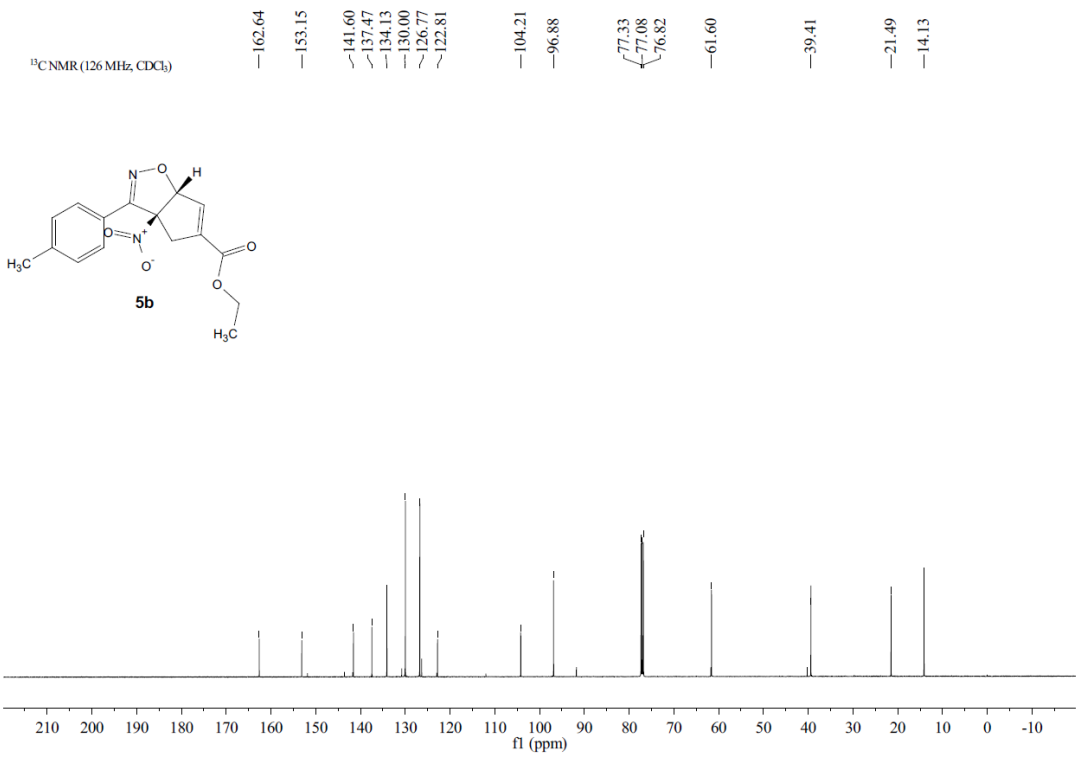
^{1}H NMR (500 MHz, $CDCl_3$)



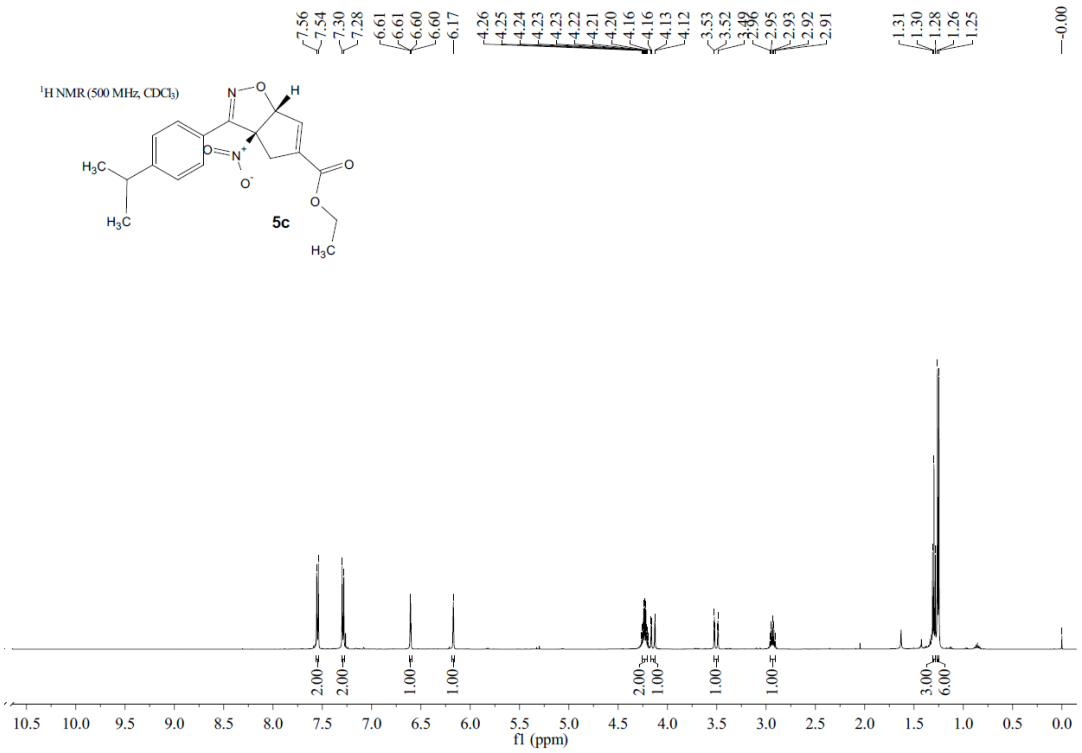
5b

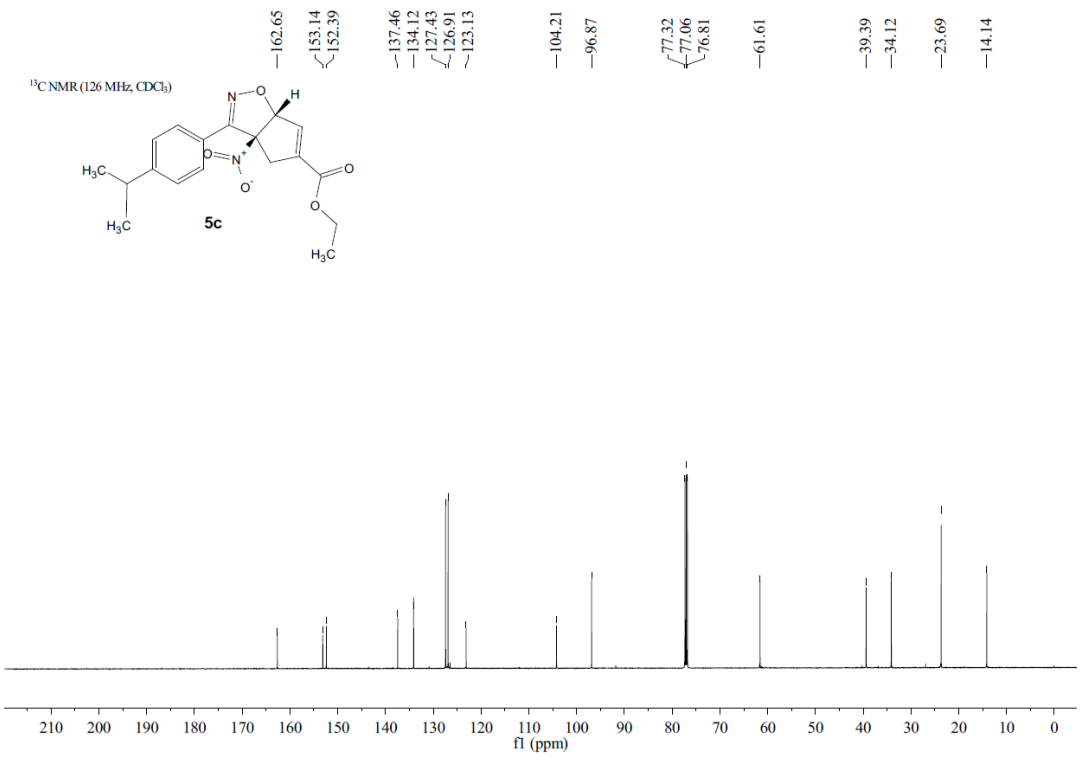


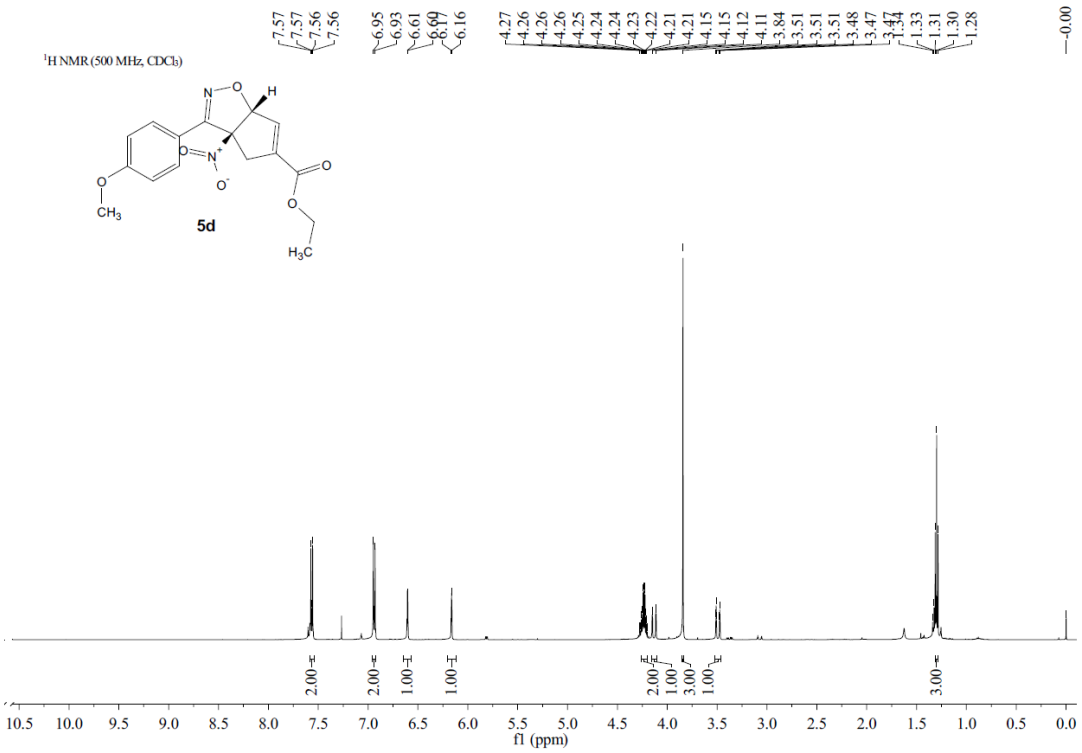
^{13}C NMR (126 MHz, $CDCl_3$)

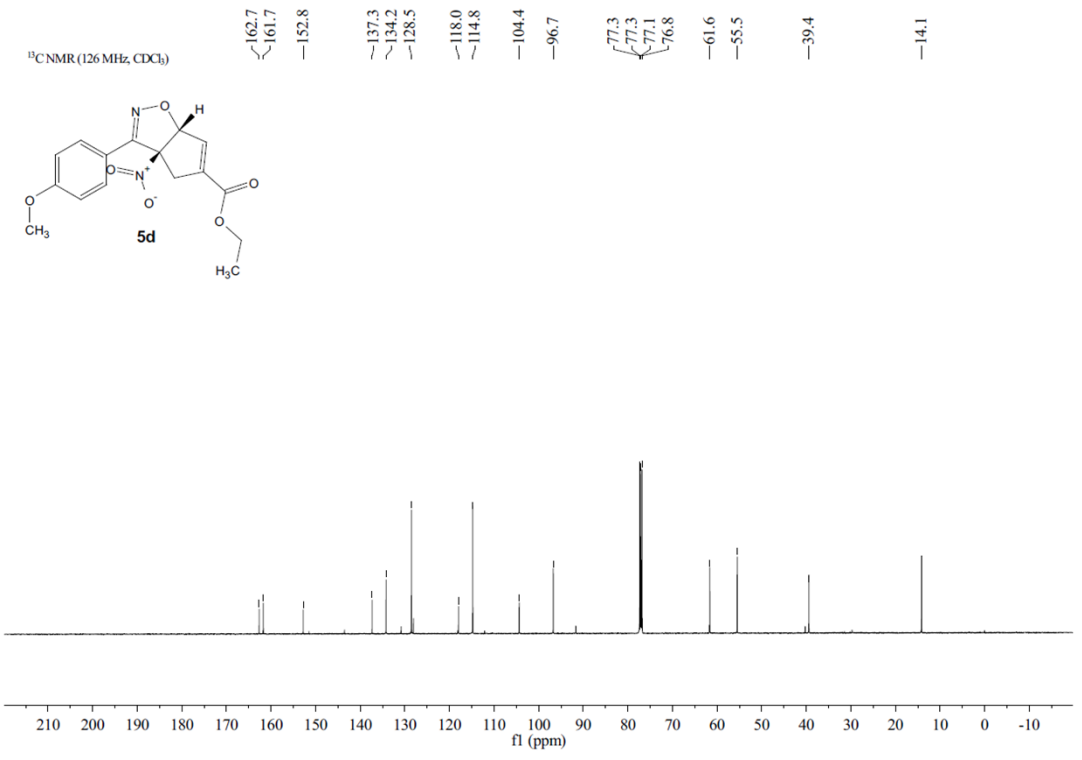


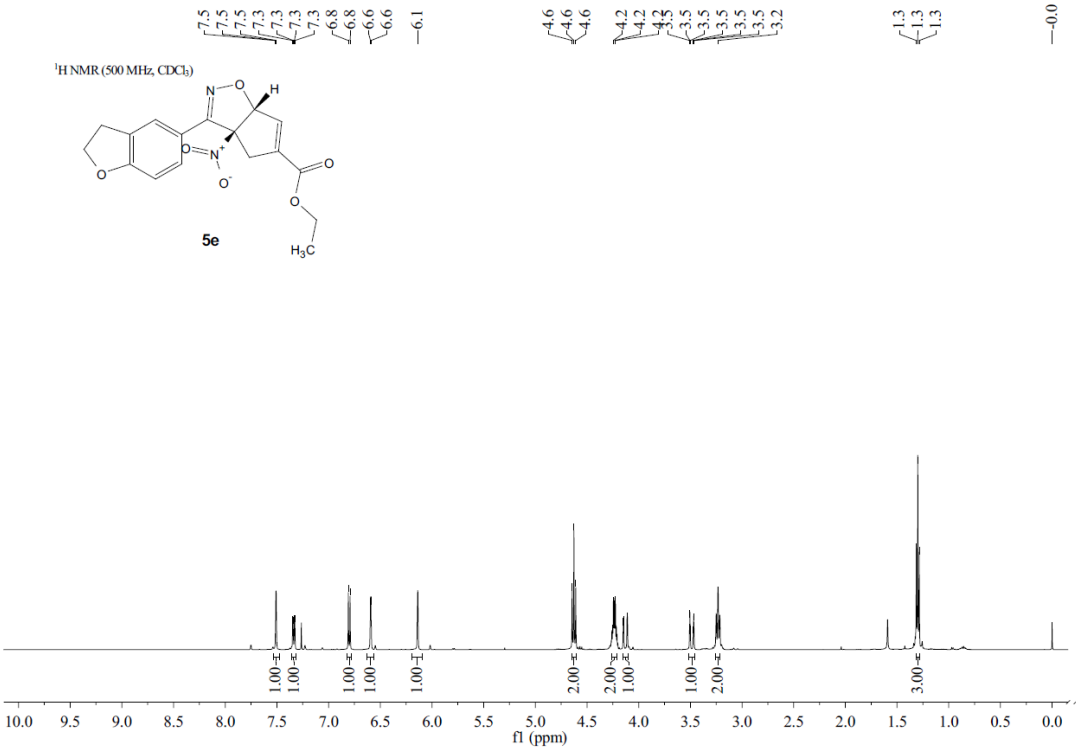
5b

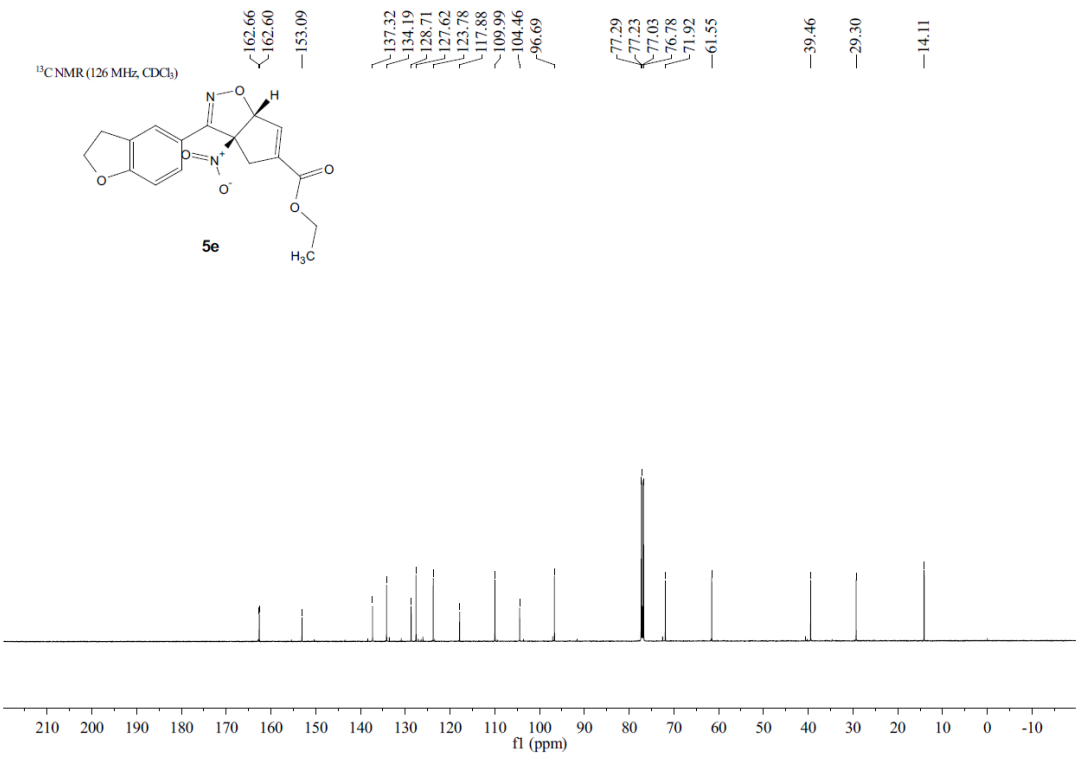

7.56
7.54
7.30
7.28
6.61
6.61
6.60
6.60
6.17
4.26
4.25
4.24
4.23
4.23
4.22
4.21
4.20
4.16
4.16
4.13
4.12
3.53
3.52
2.95
2.93
2.92
2.91
1.31
1.30
1.28
1.26
1.25
0.00
1H NMR (500 MHz, CDCl3)
5c
2.00
2.00
1.00
1.00
2.00
1.00
1.00
1.00
3.00
6.00
f1 (ppm)

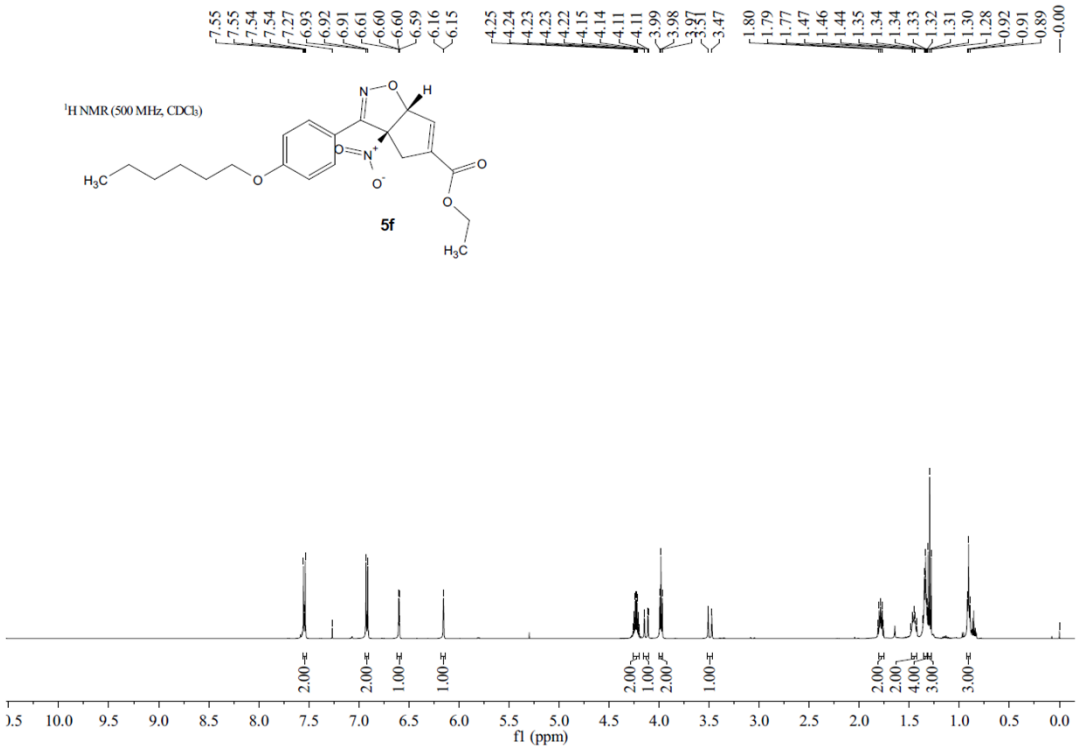

162.65
153.14
152.39
137.46
134.12
127.43
126.91
123.13
104.21
96.87
77.32
77.06
76.81
61.61
39.39
34.12
23.69
14.14
13C NMR (126 MHz, CDCl3)
5c
f1 (ppm)

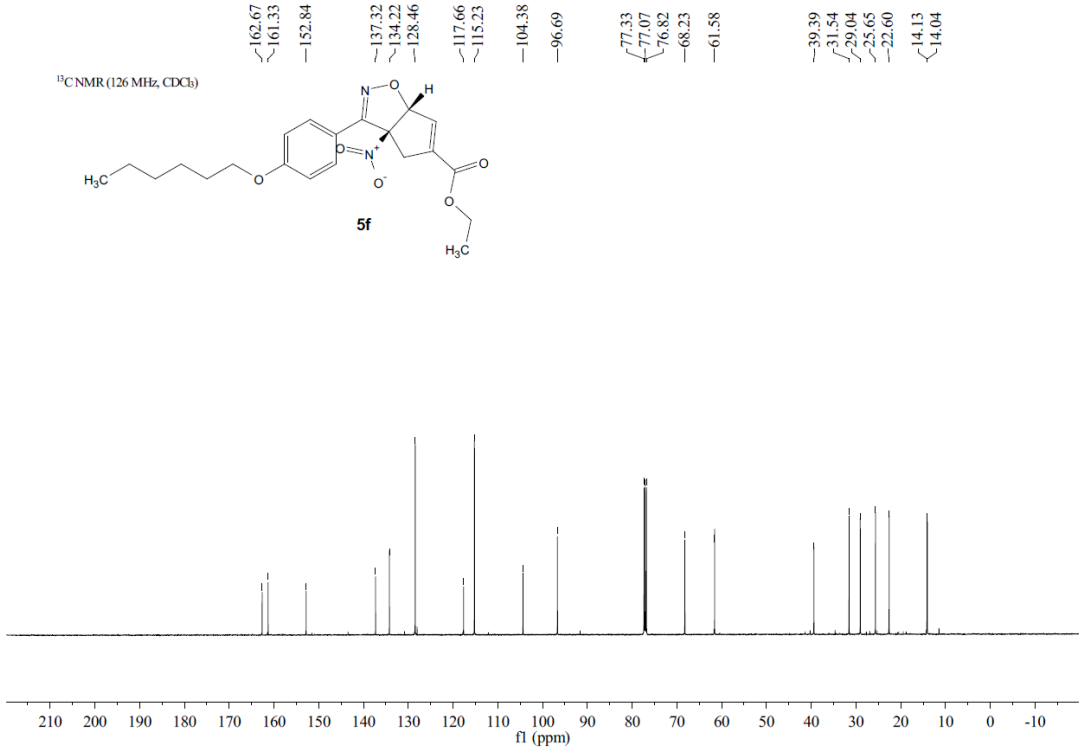

^{1}H NMR (500 MHz, CDCl$_3$)
5d
7.57
7.57
7.56
7.56
6.95
6.93
6.61
6.60
6.16
4.27
4.26
4.26
4.26
4.25
4.24
4.24
4.24
4.23
4.22
4.21
4.21
4.15
4.15
4.12
4.11
3.84
3.51
3.51
3.51
3.48
3.47
3.47
3.34
1.33
1.31
1.30
1.28
0.00
2.00
2.00
1.00
1.00
2.00
1.00
3.00
1.00
3.00
fl (ppm)

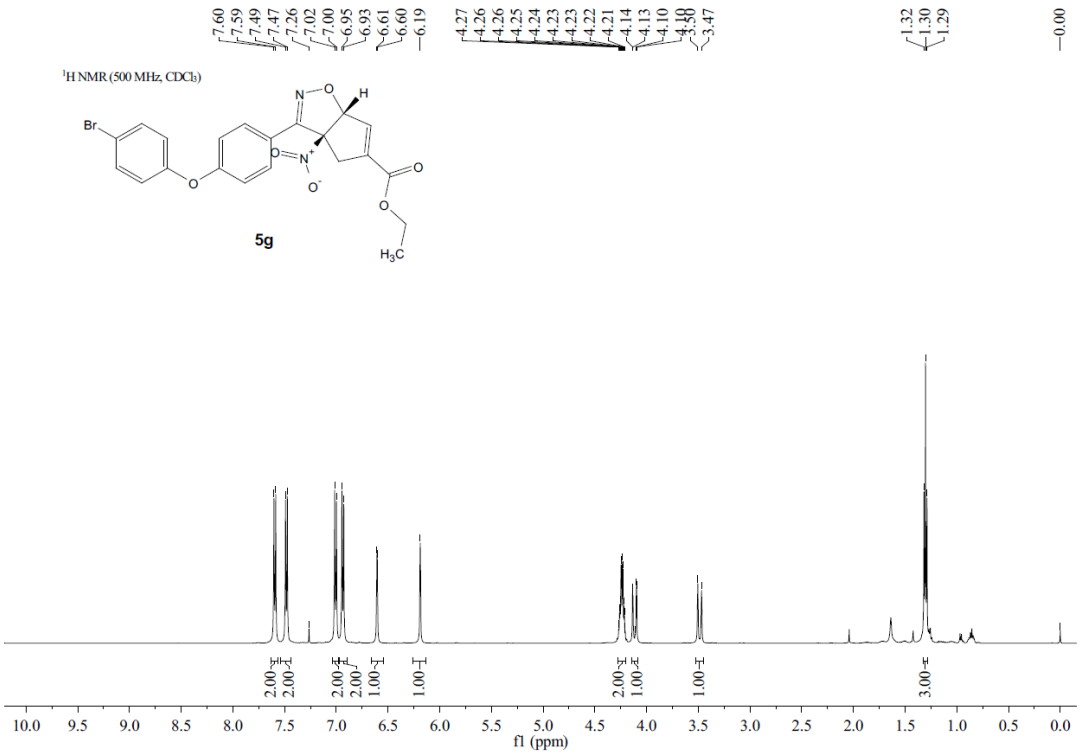

^{13}C NMR (126 MHz, CDCl$_3$)
5d
162.7
161.7
152.8
137.3
134.2
128.5
118.0
114.8
104.4
96.7
77.3
77.3
77.1
76.8
61.6
55.5
39.4
14.1
fl (ppm)

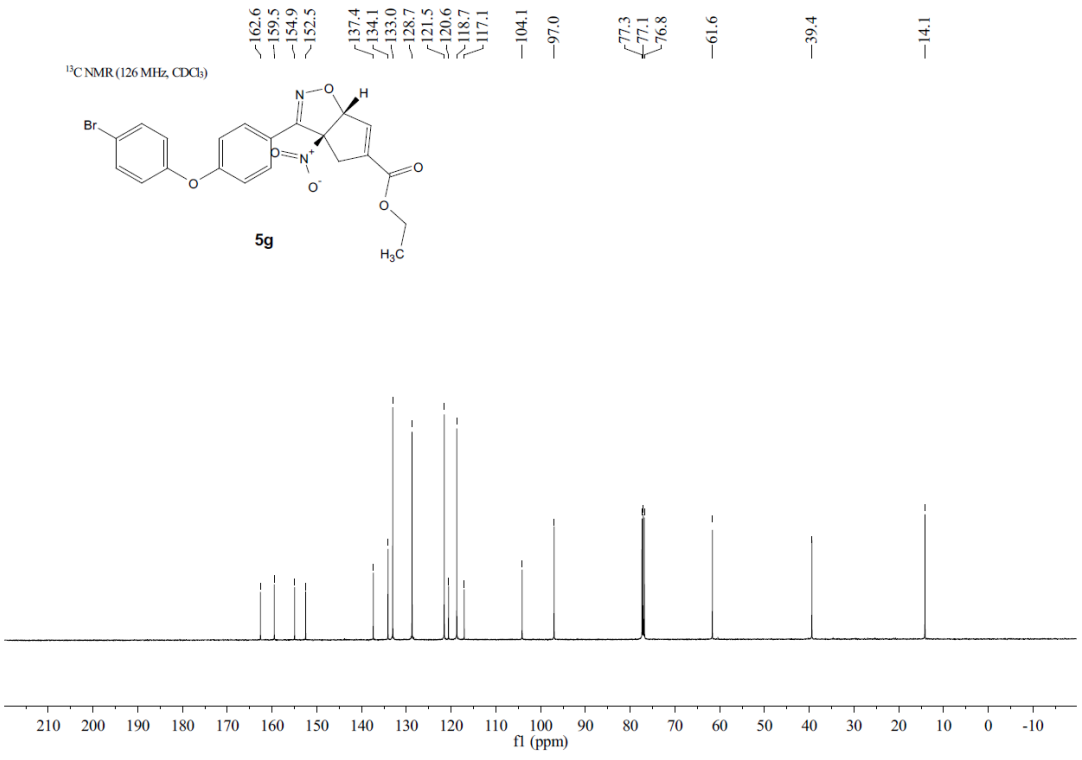

7.5
7.5
7.5
7.3
7.3
7.3
7.3
6.8
6.8
6.6
6.6
6.1
4.6
4.6
4.6
4.2
4.2
4.2
3.5
3.5
3.5
3.5
3.5
3.5
3.2
1.3
1.3
1.3
0.0
1H NMR (500 MHz, CDCl3)
5e
1.00
1.00
1.00
1.00
1.00
2.00
2.00
1.00
1.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

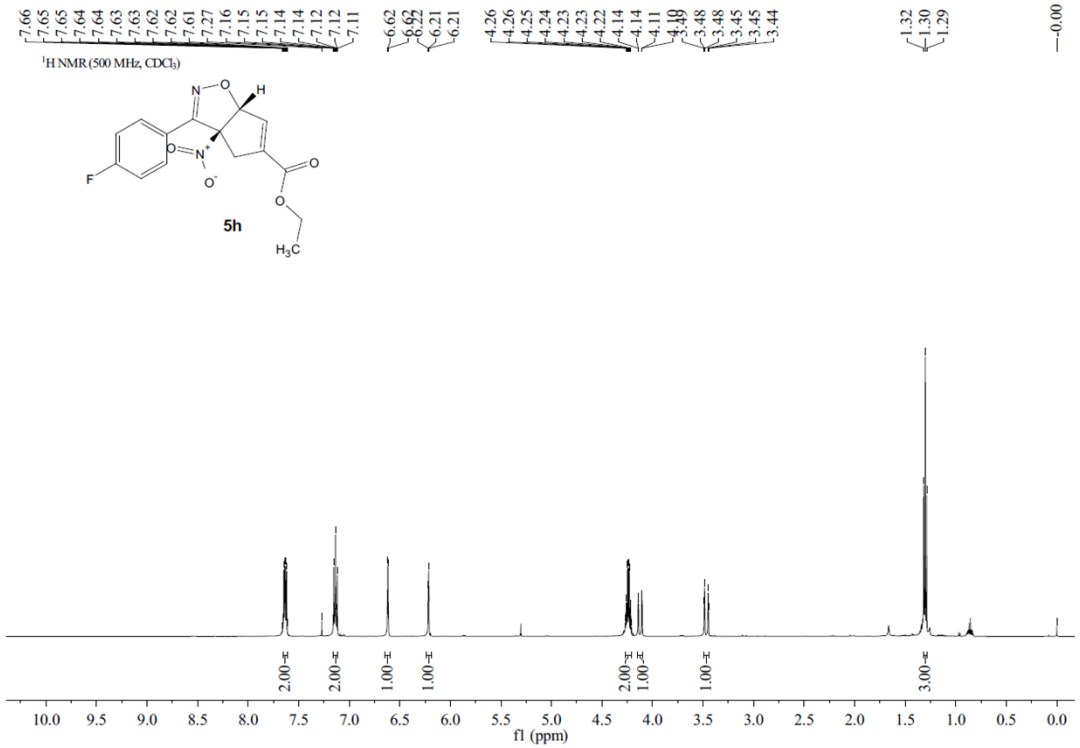

162.66
162.60
153.09
137.32
134.19
128.71
127.62
123.78
117.88
109.99
104.46
96.69
77.29
77.23
77.03
76.78
71.92
61.55
39.46
29.30
14.11
13C NMR (126 MHz, CDCl3)
5e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

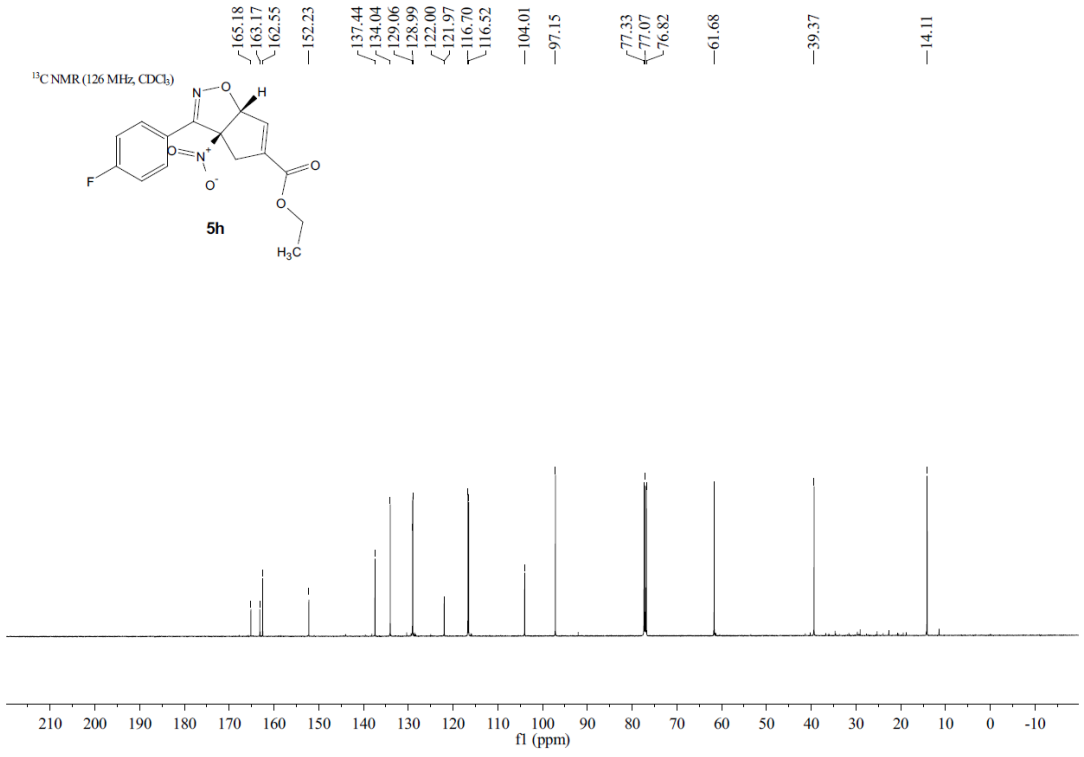

7.55
7.55
7.54
7.54
7.27
6.93
6.92
6.91
6.61
6.60
6.60
6.59
6.16
6.15
4.25
4.24
4.23
4.23
4.22
4.15
4.14
4.11
4.11
3.99
3.98
3.87
3.51
3.47
1.80
1.79
1.77
1.47
1.46
1.44
1.35
1.34
1.34
1.33
1.32
1.31
1.30
1.28
0.92
0.91
0.89
0.00
1H NMR (500 MHz, CDCl3)
5f
2.00
2.00
1.00
1.00
2.00
1.00
2.00
1.00
2.00
2.00
4.00
3.00
3.00
f1 (ppm)


162.67
161.33
152.84
137.32
134.22
128.46
117.66
115.23
104.38
96.69
77.33
77.07
76.82
68.23
61.58
39.39
31.54
29.04
25.65
22.60
14.13
14.04
13C NMR (126 MHz, CDCl3)
5f
f1 (ppm)

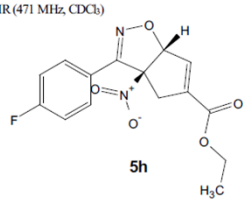

7.60
7.59
7.49
7.47
7.26
7.02
7.00
6.95
6.93
6.61
6.60
6.19
4.27
4.26
4.26
4.25
4.24
4.23
4.23
4.22
4.21
4.14
4.13
4.10
3.58
3.47
1.32
1.30
1.29
0.00
1H NMR (500 MHz, CDCl3)
Br
O
N
O
H
O
N+
O-
O
O
H3C
5g
2.00
2.00
2.00
2.00
1.00
1.00
2.00
1.00
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


162.6
159.5
154.9
152.5
137.4
134.1
133.0
128.7
121.5
120.6
118.7
117.1
104.1
97.0
77.3
77.1
76.8
61.6
39.4
14.1
13C NMR (126 MHz, CDCl3)
Br
O
N
O
H
O
N+
O-
O
O
H3C
5g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.66
7.65
7.65
7.64
7.64
7.63
7.63
7.62
7.62
7.61
7.27
7.16
7.15
7.15
7.14
7.14
7.12
7.12
7.11
6.62
6.62
6.22
6.21
6.21
4.26
4.26
4.25
4.24
4.23
4.23
4.22
4.14
4.14
4.11
3.48
3.48
3.45
3.45
3.44
1.32
1.30
1.29
0.00
1H NMR (500 MHz, CDCl3)
5h
2.00
2.00
1.00
1.00
2.00
1.00
1.00
3.00
fl (ppm)

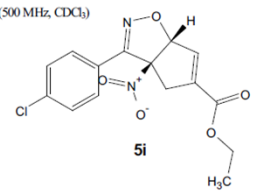

165.18
163.17
162.55
152.23
137.44
134.04
129.06
128.99
122.00
121.97
116.70
116.52
104.01
97.15
77.33
77.07
76.82
61.68
39.37
14.11
13C NMR (126 MHz, CDCl3)
5h
fl (ppm)

^{19}F NMR (471 MHz, $CDCl_3$)

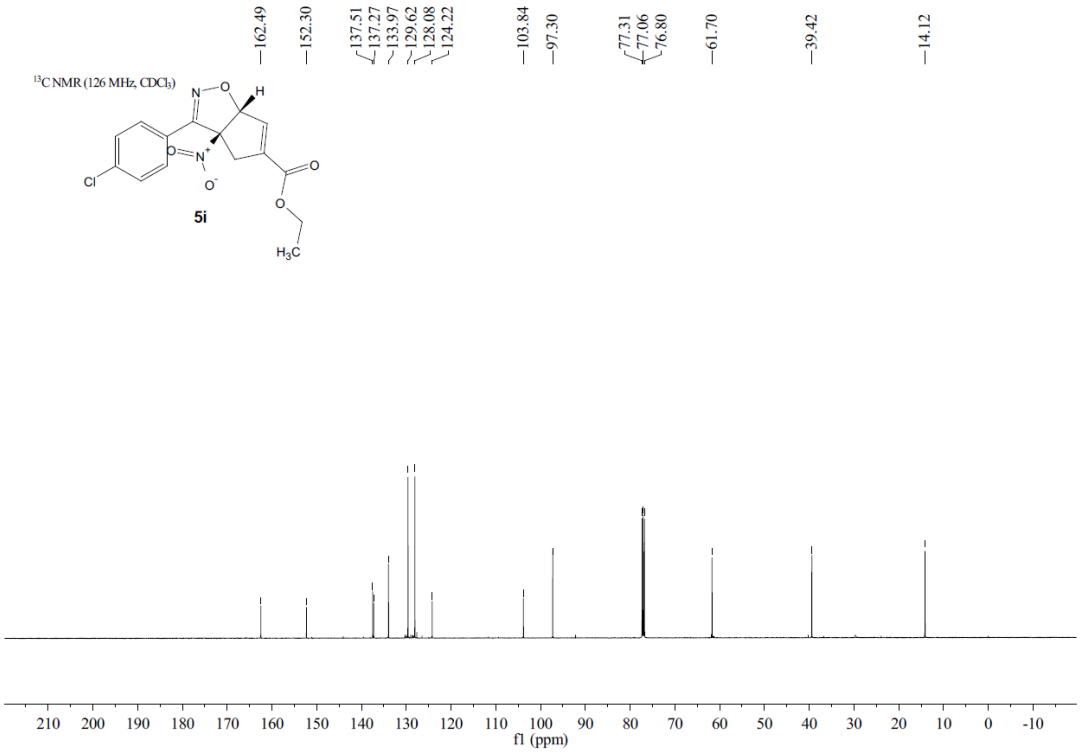


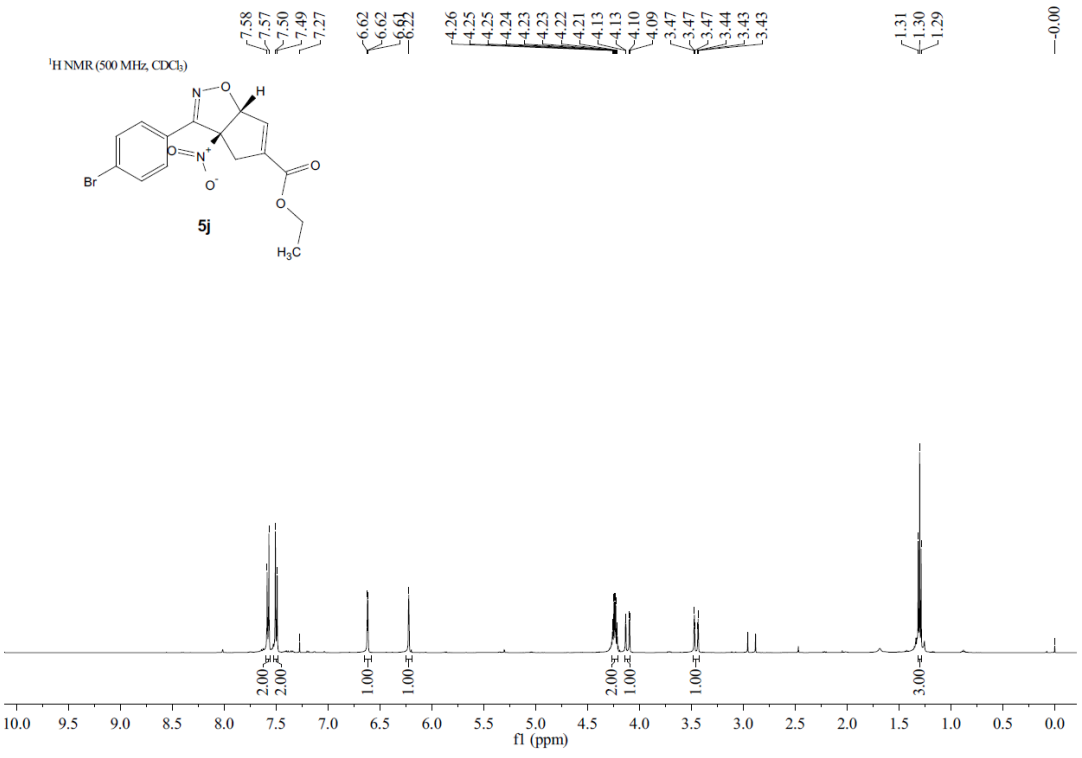
5h

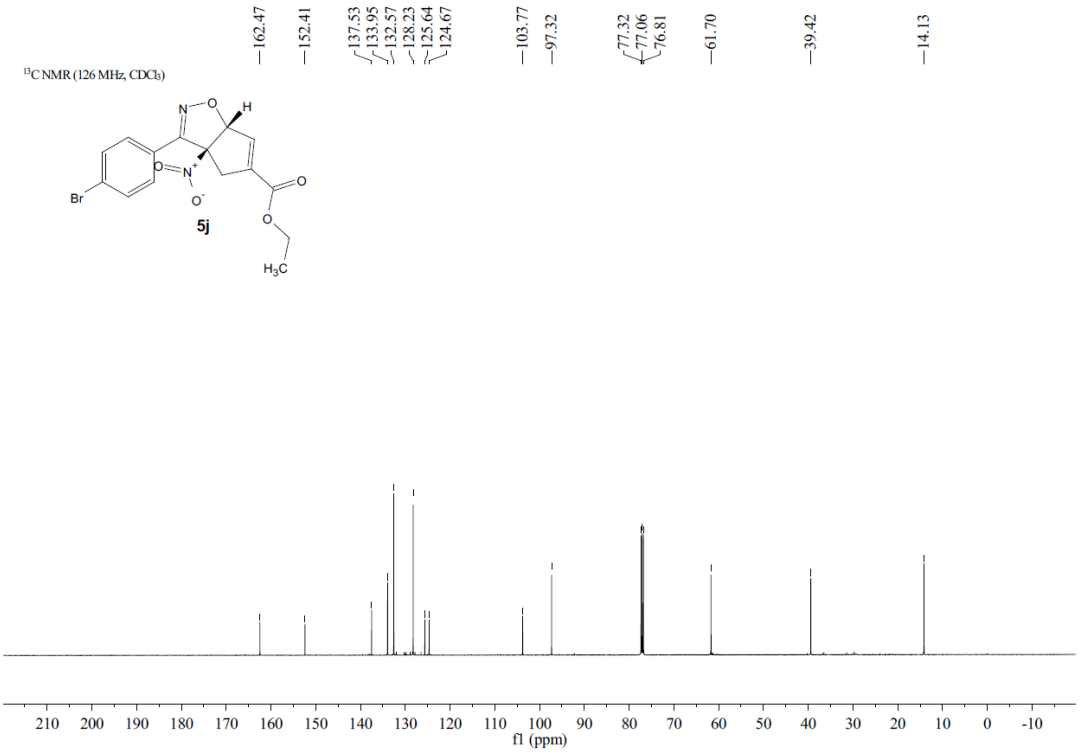
^{1}H NMR (500 MHz, $CDCl_3$)

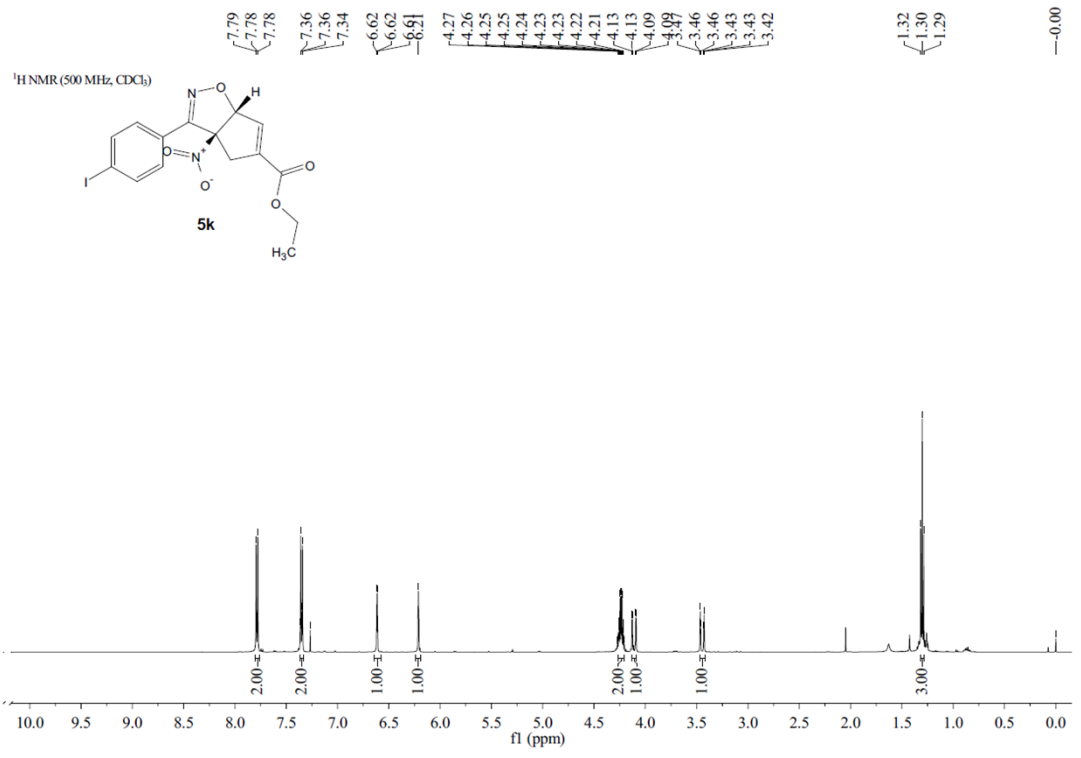


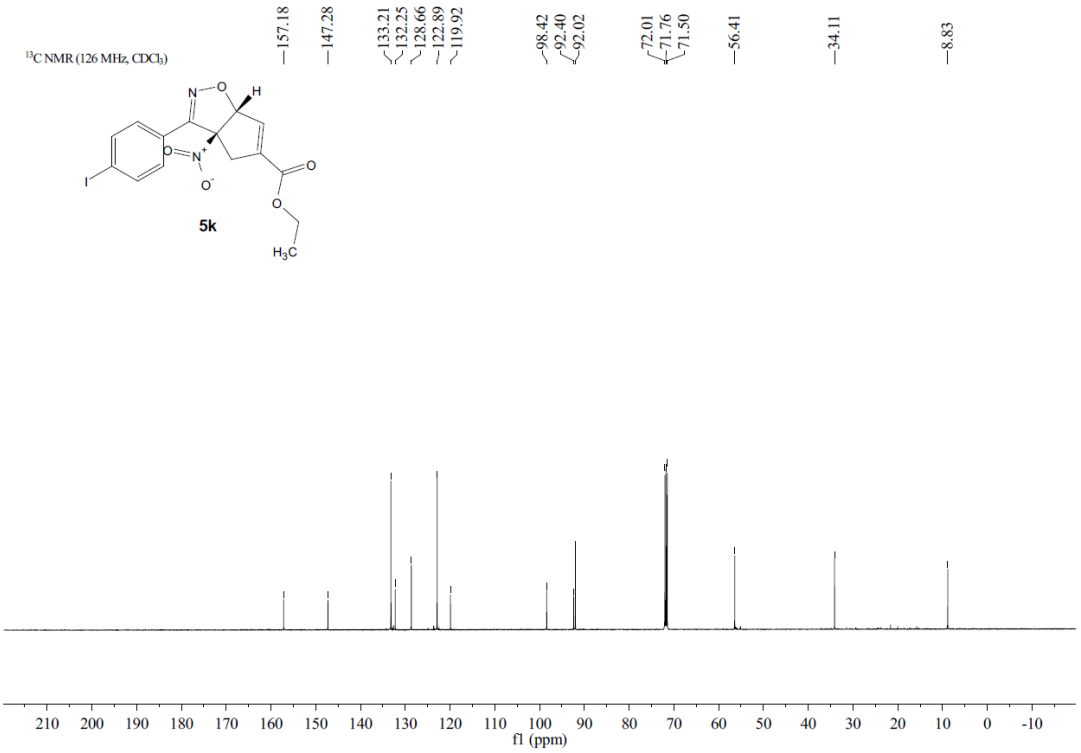
5i

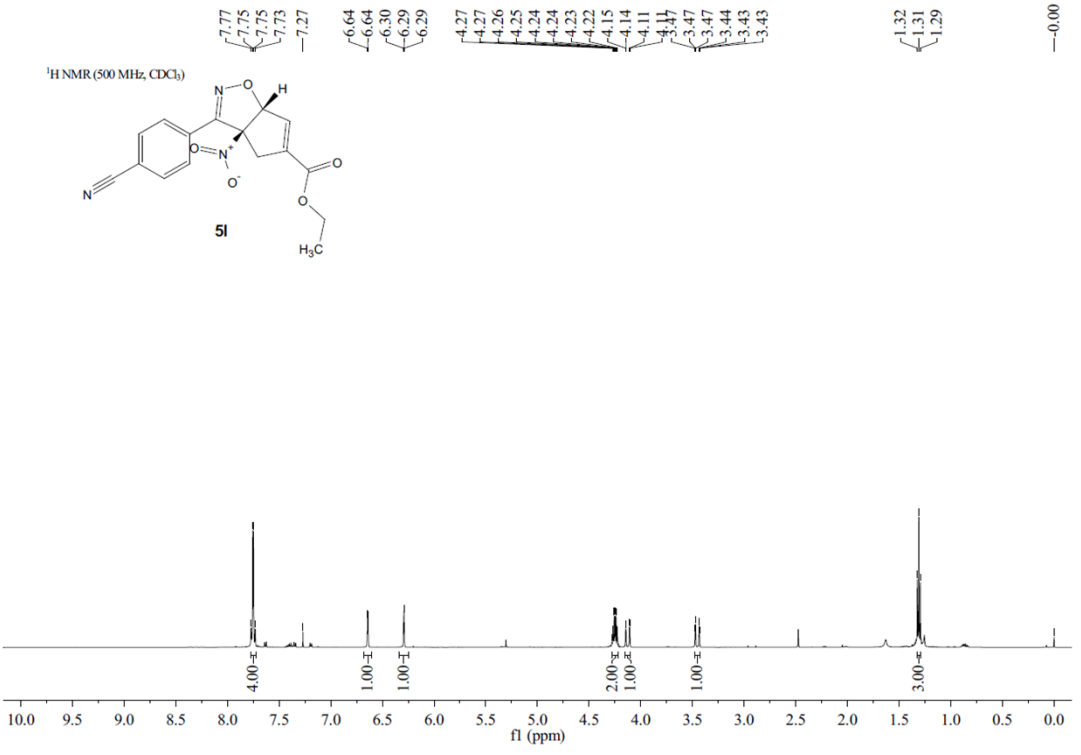

162.49
152.30
137.51
137.27
133.97
129.62
128.08
124.22
103.84
97.30
77.31
77.06
76.80
61.70
39.42
14.12
13C NMR (126 MHz, CDCl3)
5i
f1 (ppm)


7.58
7.57
7.50
7.49
7.27
6.62
6.62
6.61
6.22
4.26
4.25
4.25
4.24
4.23
4.23
4.22
4.21
4.13
4.13
4.10
4.09
3.47
3.47
3.47
3.44
3.43
3.43
1.31
1.30
1.29
0.00
1H NMR (500 MHz, CDCl3)
5j
2.00
2.00
1.00
1.00
2.00
1.00
1.00
3.00
f1 (ppm)


162.47
152.41
137.53
133.95
132.57
128.23
125.64
124.67
103.77
97.32
77.32
77.06
76.81
61.70
39.42
14.13
13C NMR (126 MHz, CDCl3)
5j
f1 (ppm)


7.79
7.78
7.78
7.36
7.36
7.34
6.62
6.62
6.61
6.61
4.27
4.26
4.25
4.25
4.24
4.23
4.23
4.22
4.21
4.13
4.13
4.09
4.09
3.47
3.46
3.46
3.43
3.43
3.42
1.32
1.30
1.29
-0.00
1H NMR (500 MHz, CDCl3)
5k
2.00
2.00
1.00
1.00
2.00
1.00
1.00
3.00
f1 (ppm)


157.18
147.28
133.21
132.25
128.66
122.89
119.92
98.42
92.40
92.02
72.01
71.76
71.50
56.41
34.11
8.83
13C NMR (126 MHz, CDCl3)
5k
fl (ppm)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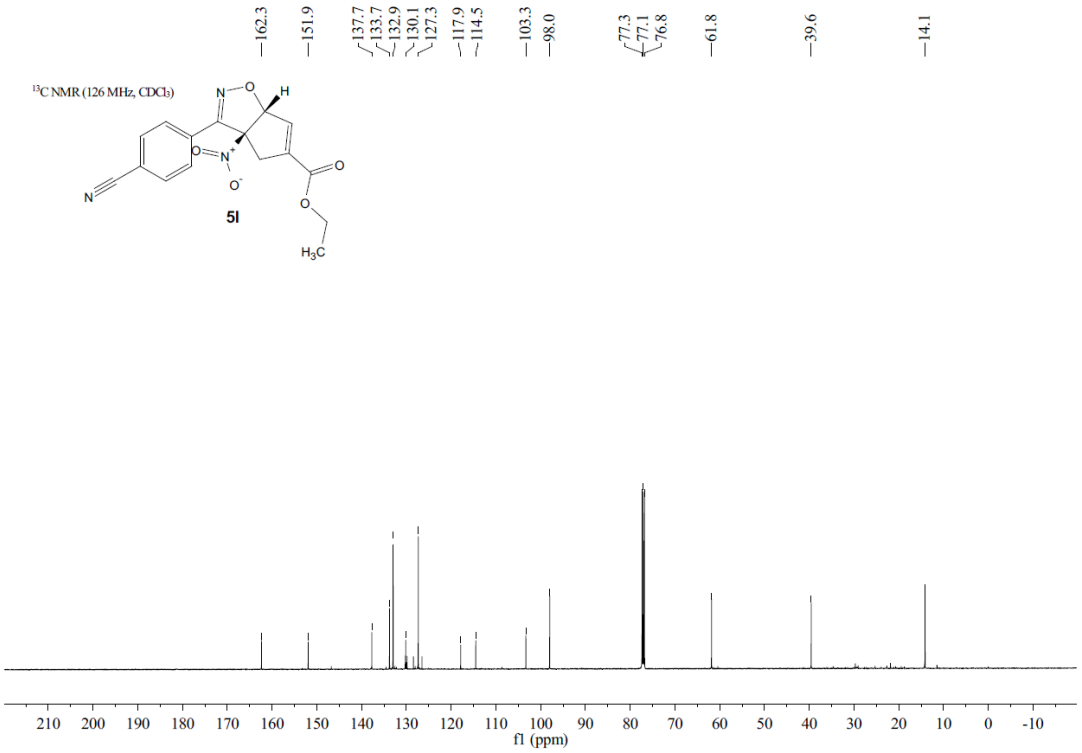
7.73
7.27
6.64
6.64
6.30
6.29
6.29
4.27
4.27
4.26
4.25
4.24
4.24
4.23
4.22
4.15
4.14
4.11
4.11
3.47
3.47
3.47
3.44
3.43
3.43
1.32
1.31
1.29
0.00
1H NMR (500 MHz, CDCl3)
5l
4.00
1.00
1.00
2.00
1.00
1.00
3.00
fl (ppm)


162.3
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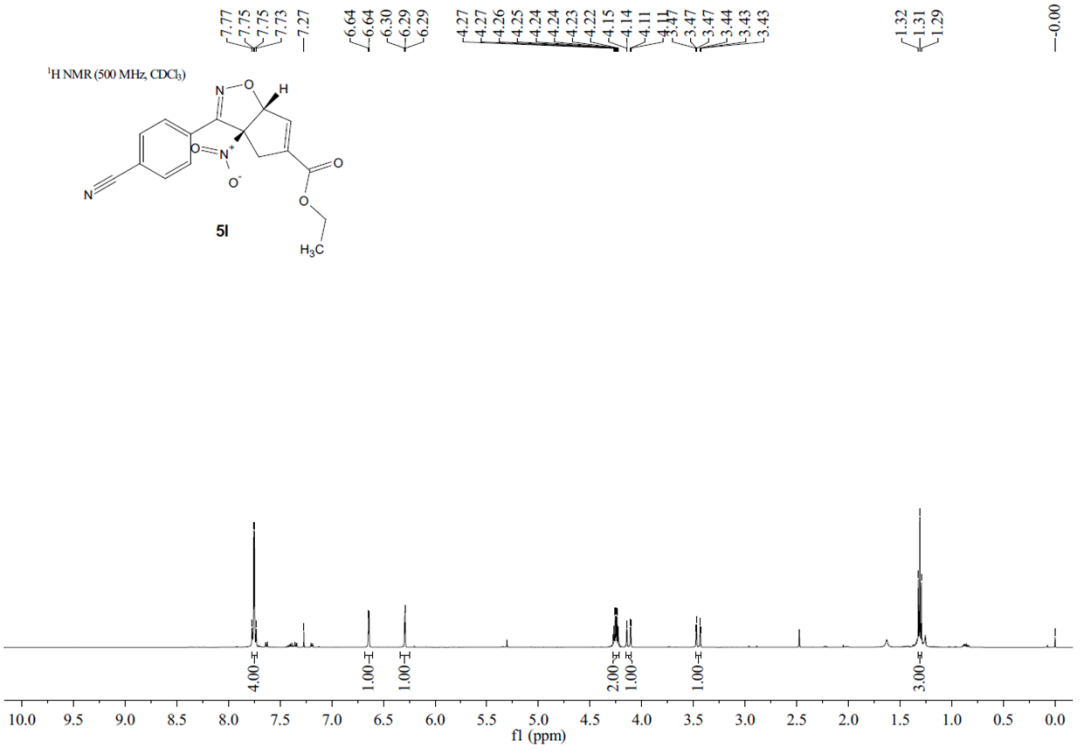
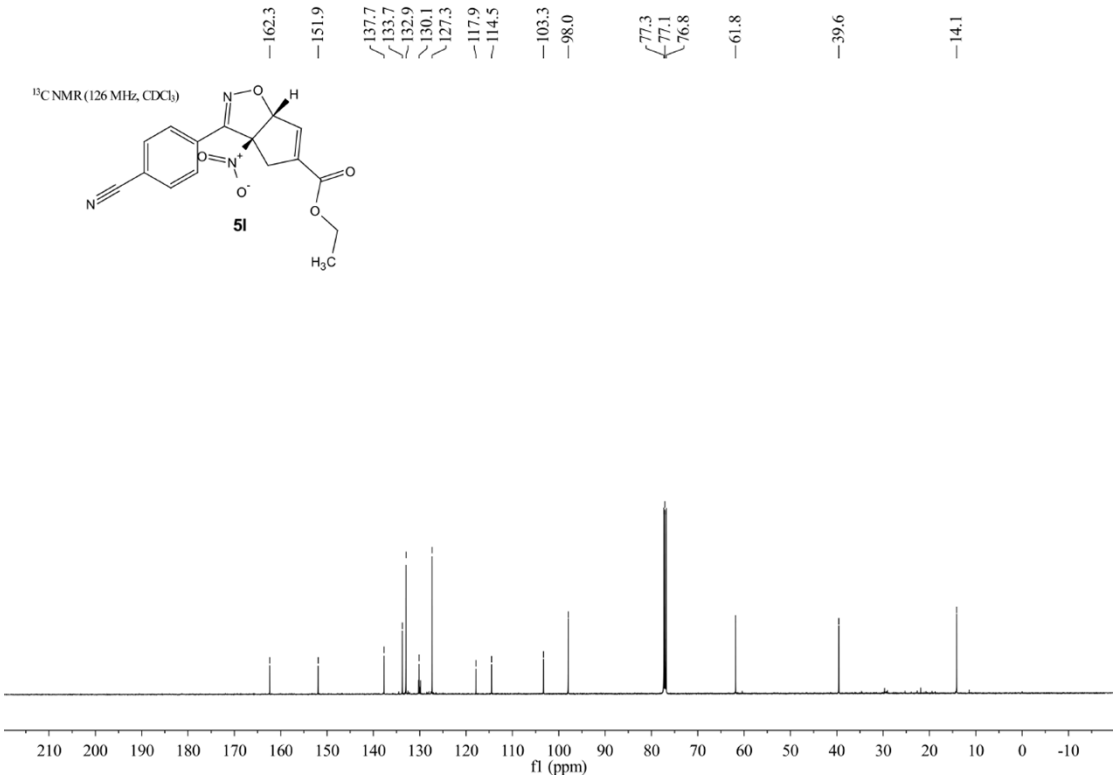
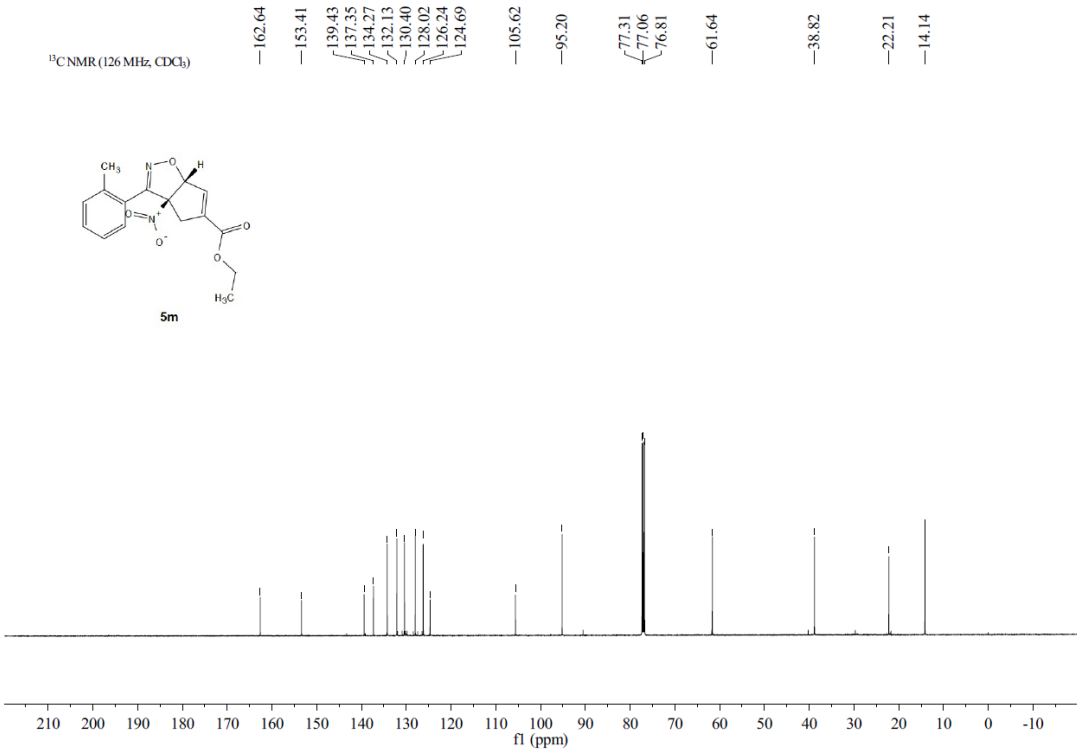
137.7
133.7
132.9
130.1
127.3
117.9
114.5
103.3
98.0
77.3
77.1
76.8
61.8
39.6
14.1
13C NMR (126 MHz, CDCl3)
5l
fl (ppm)

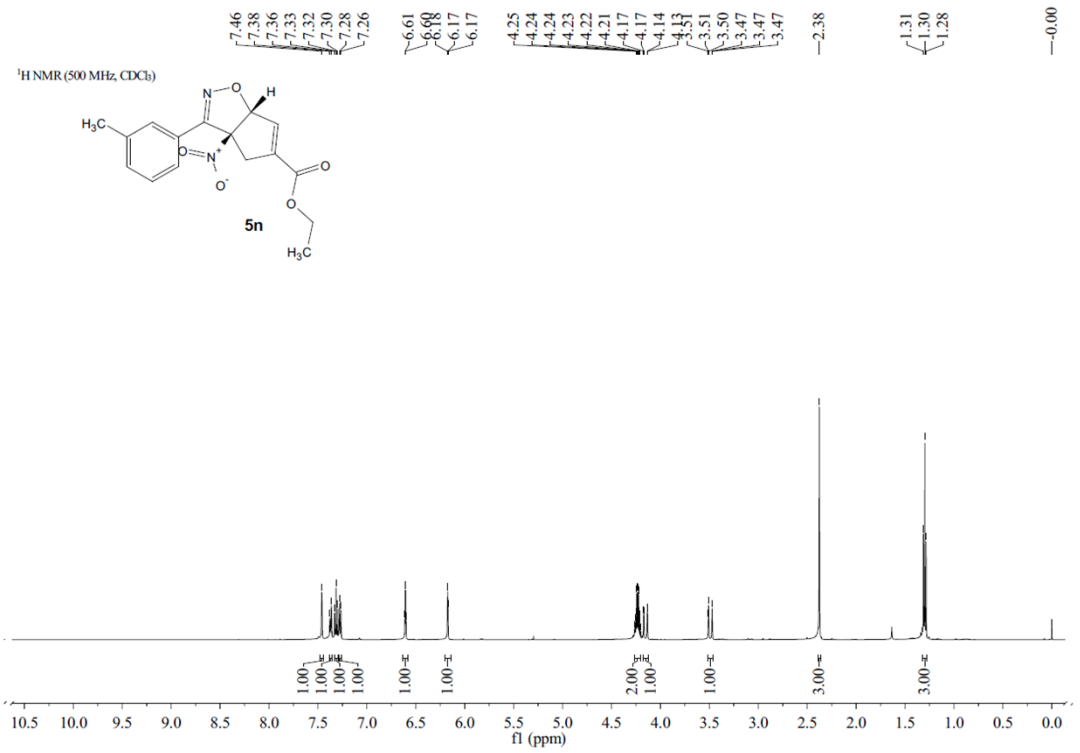

7.77
7.75
7.75
7.73
7.27
6.64
6.64
6.30
6.29
6.29
4.27
4.27
4.26
4.25
4.24
4.24
4.23
4.22
4.15
4.14
4.11
4.11
3.47
3.47
3.44
3.43
3.43
1.32
1.31
1.29
0.00
1H NMR (500 MHz, CDCl3)
5l
4.00
1.00
1.00
2.00
1.00
1.00
3.00
fl (ppm)

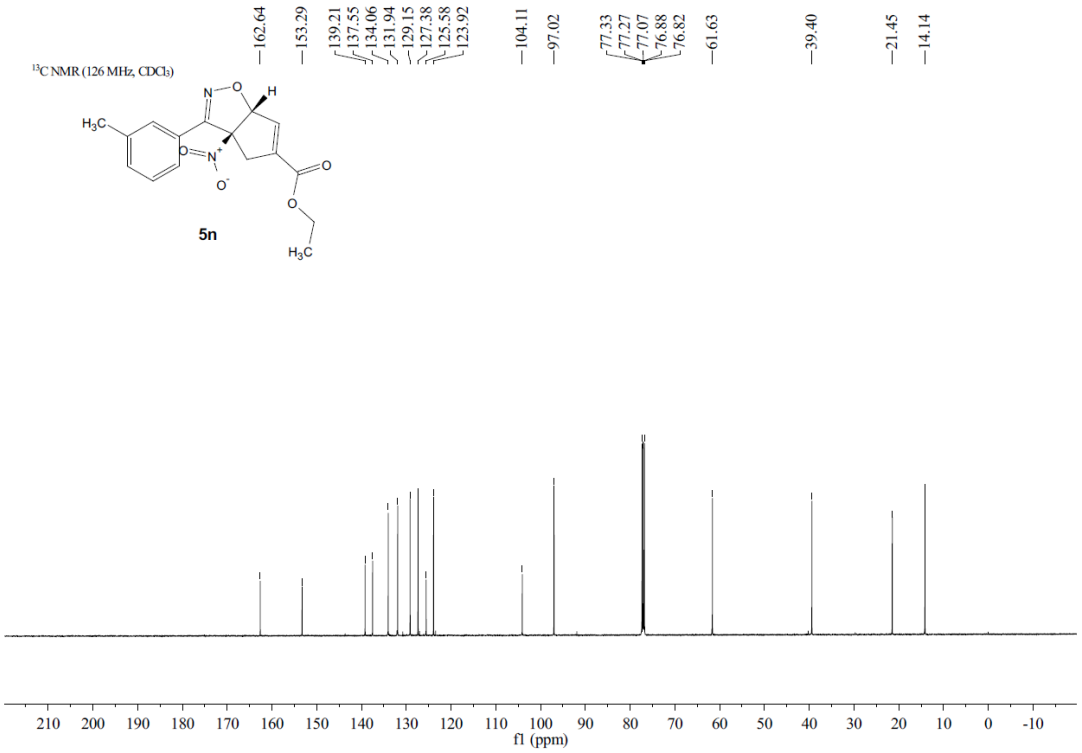

162.3
151.9
137.7
133.7
132.9
130.1
127.3
117.9
114.5
103.3
98.0
77.3
77.1
76.8
61.8
39.6
14.1
13C NMR (126 MHz, CDCl3)
5l
fl (ppm)
7.37
7.37
7.36
7.34
7.34
7.33
7.32
7.26
7.26
7.26
7.25
7.23
7.23
7.08
7.06
6.63
6.62
6.62
6.17
4.27
4.25
4.24
4.22
3.99
3.99
3.96
3.95
3.35
3.35
3.35
3.32
3.31
3.31
2.42
1.32
1.31
1.29
0.00
1H NMR (500 MHz, CDCl3)
5m
2.00
1.00
1.00
1.00
1.00
2.00
1.00
1.00
3.00
3.00
fl (ppm)

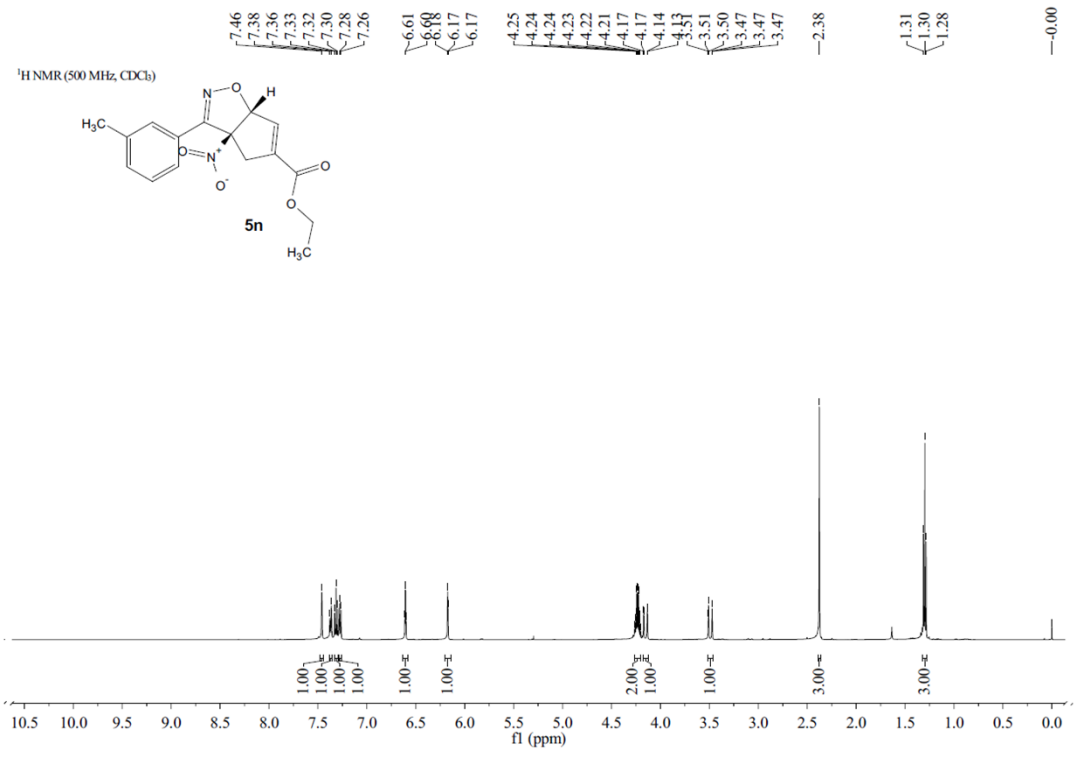
^{13}C NMR (126 MHz, $CDCl_3$)

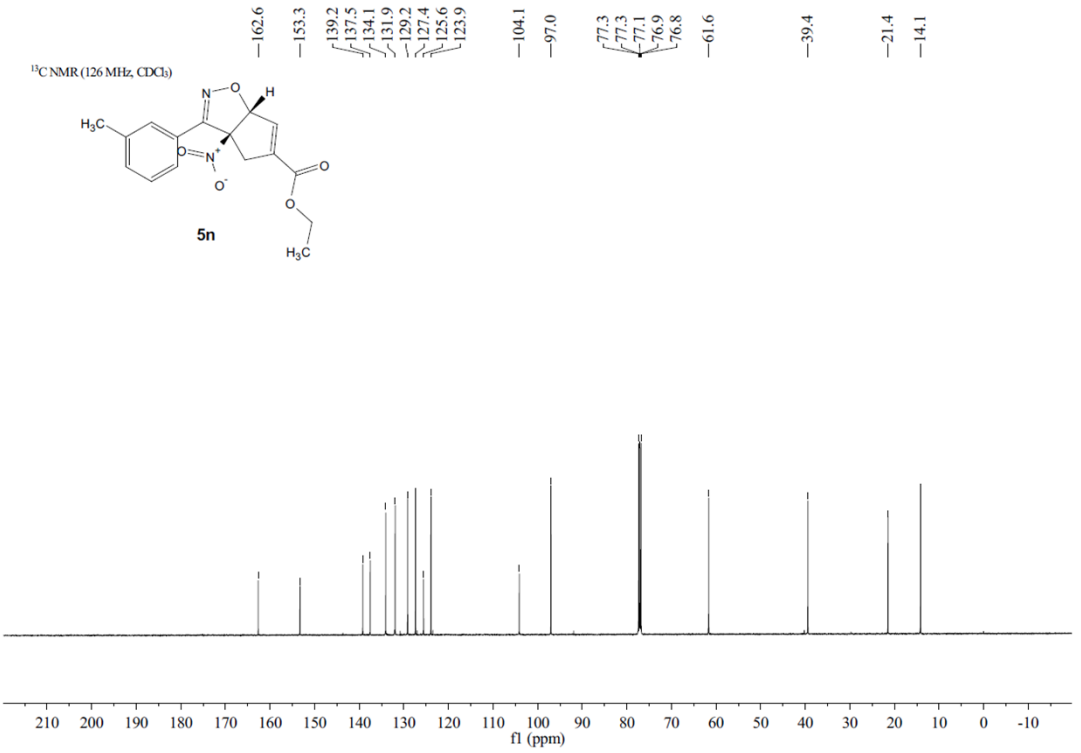


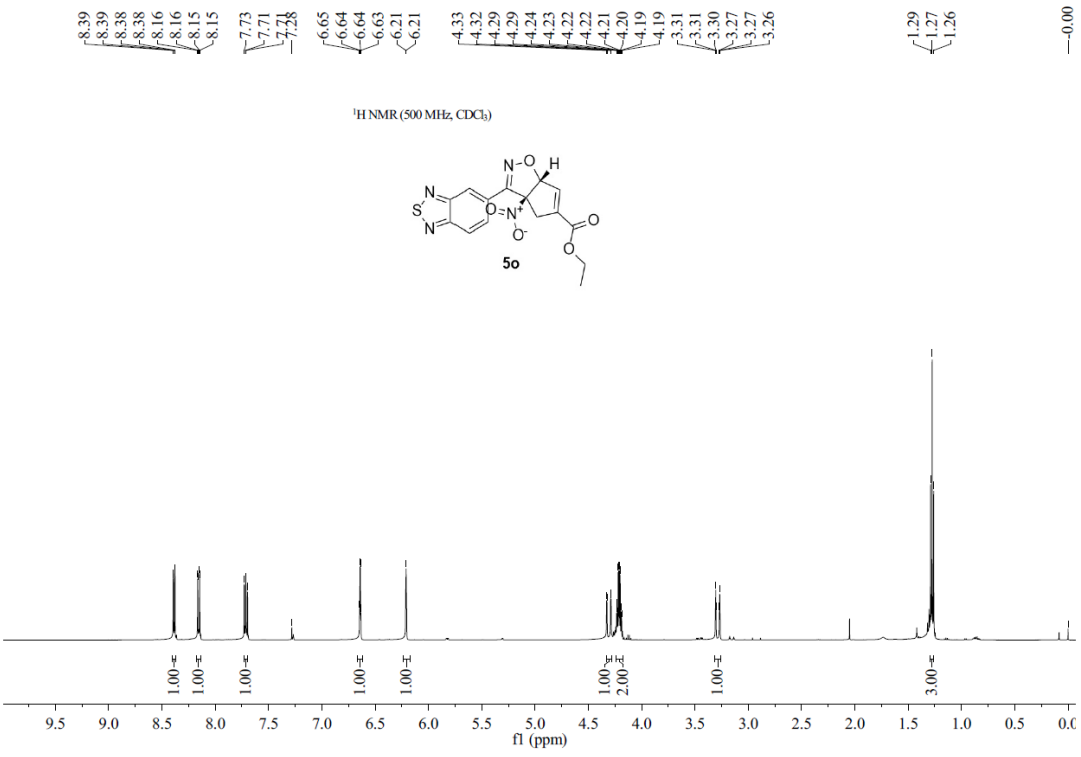
^{1}H NMR (500 MHz, $CDCl_3$)



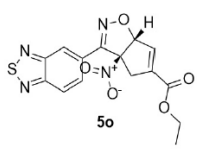

13C NMR (126 MHz, CDCl3)
162.64
153.29
139.21
137.55
134.06
131.94
129.15
127.38
125.58
123.92
104.11
97.02
77.33
77.27
77.07
76.88
76.82
61.63
39.40
21.45
14.14
5n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


1H NMR (500 MHz, CDCl3)
7.46
7.38
7.36
7.33
7.32
7.30
7.28
7.26
6.61
6.60
6.18
6.17
6.17
4.25
4.24
4.24
4.23
4.22
4.21
4.17
4.17
4.14
4.13
3.51
3.51
3.50
3.47
3.47
3.47
2.38
1.31
1.30
1.28
-0.00
5n
1.00
1.00
1.00
1.00
1.00
1.00
2.00
1.00
1.00
3.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


162.6
153.3
139.2
137.5
134.1
131.9
129.2
127.4
125.6
123.9
104.1
97.0
77.3
77.3
77.1
76.9
76.8
61.6
39.4
21.4
14.1
13C NMR (126 MHz, CDCl3)
5n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

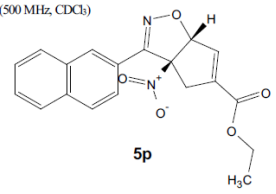

8.39
8.39
8.38
8.38
8.16
8.16
8.15
8.15
7.73
7.71
7.71
7.28
6.65
6.64
6.64
6.63
6.21
6.21
4.33
4.32
4.29
4.29
4.24
4.23
4.22
4.22
4.21
4.20
4.19
4.19
3.31
3.31
3.30
3.27
3.27
3.26
1.29
1.27
1.26
0.00
1H NMR (500 MHz, CDCl3)
5o
1.00
1.00
1.00
1.00
1.00
1.00
2.00
1.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

^{13}C NMR (126 MHz, CDCl$_3$)

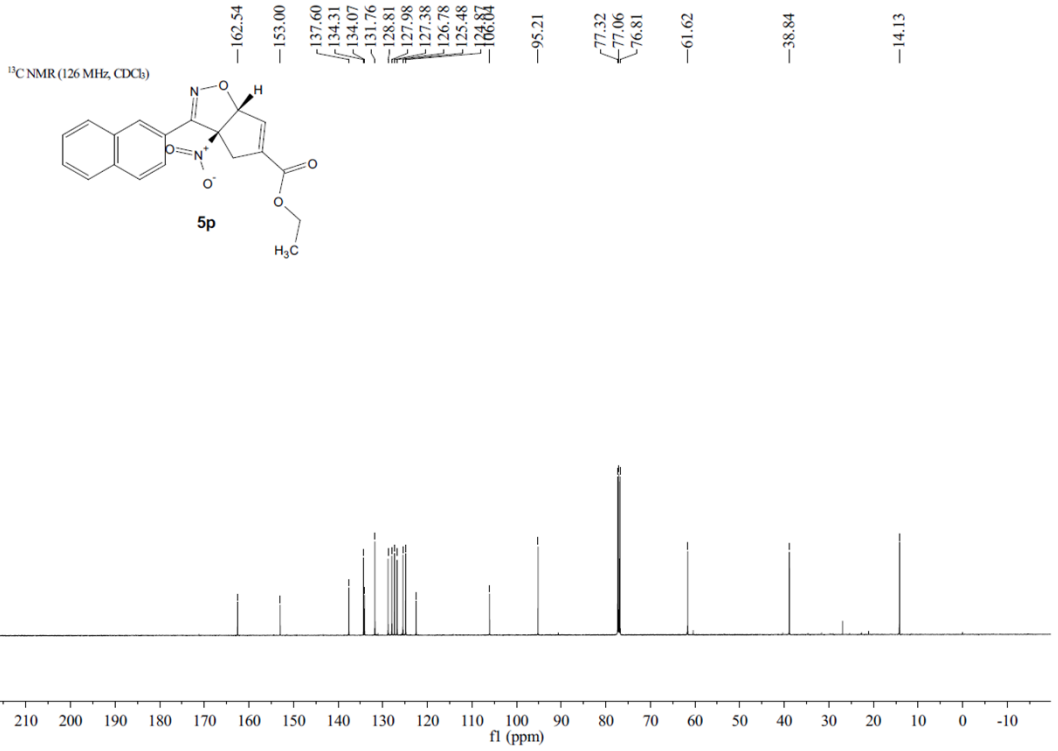


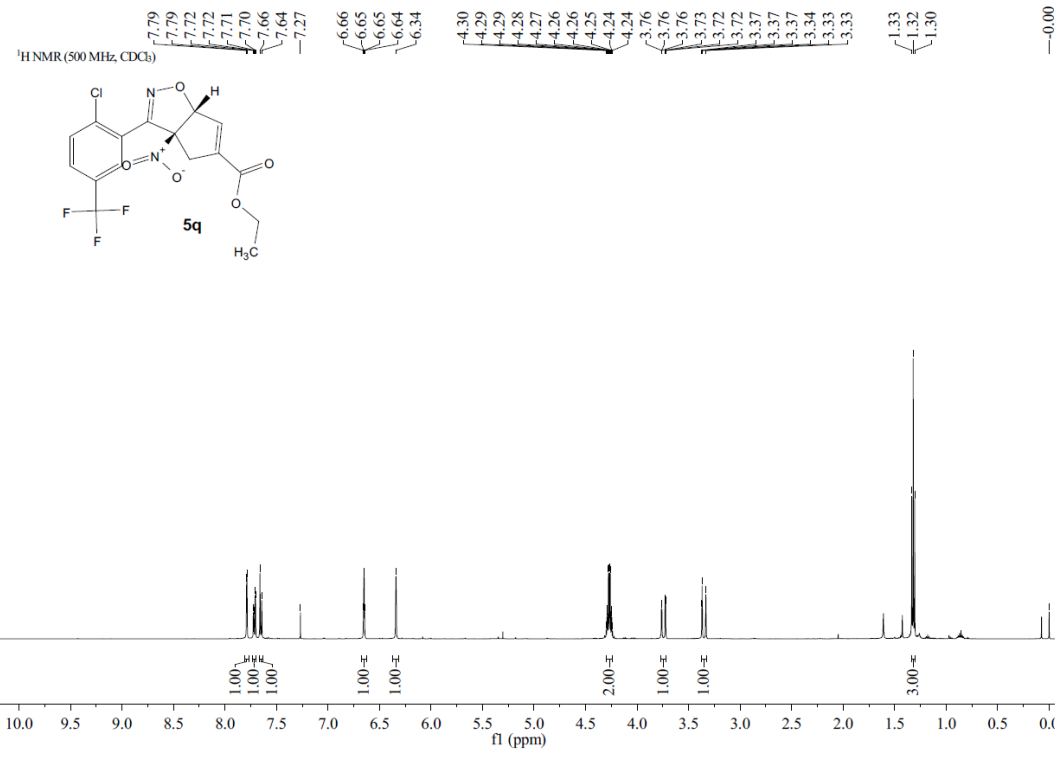
5o

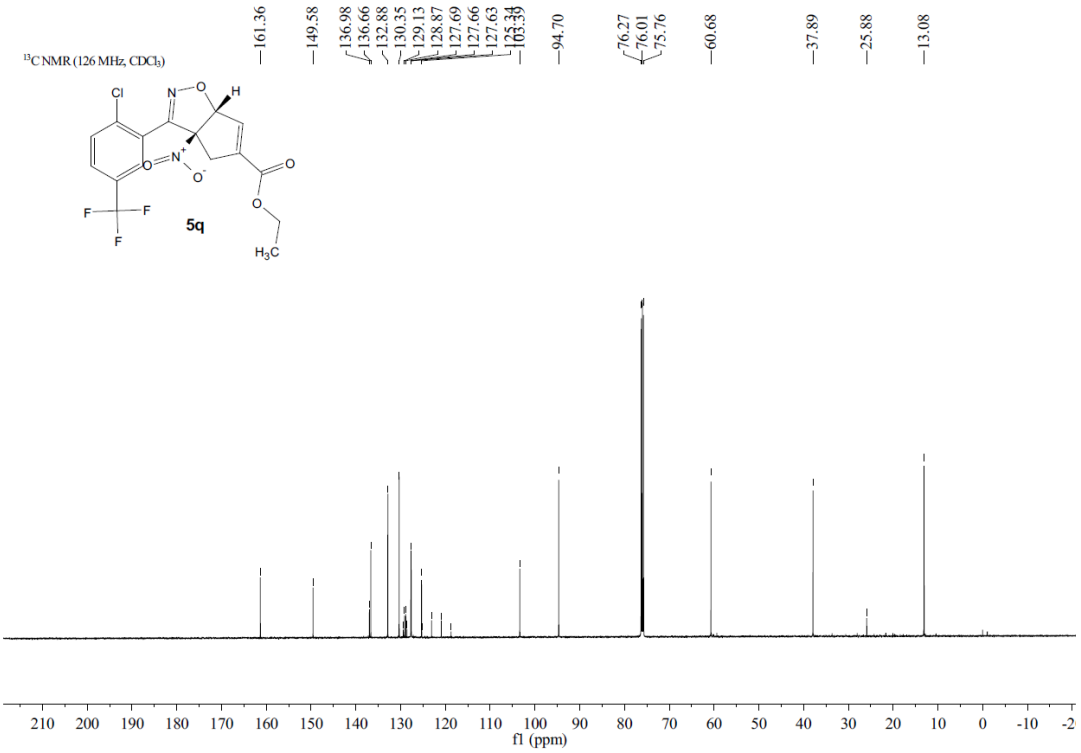
^{1}H NMR (500 MHz, CDCl$_3$)

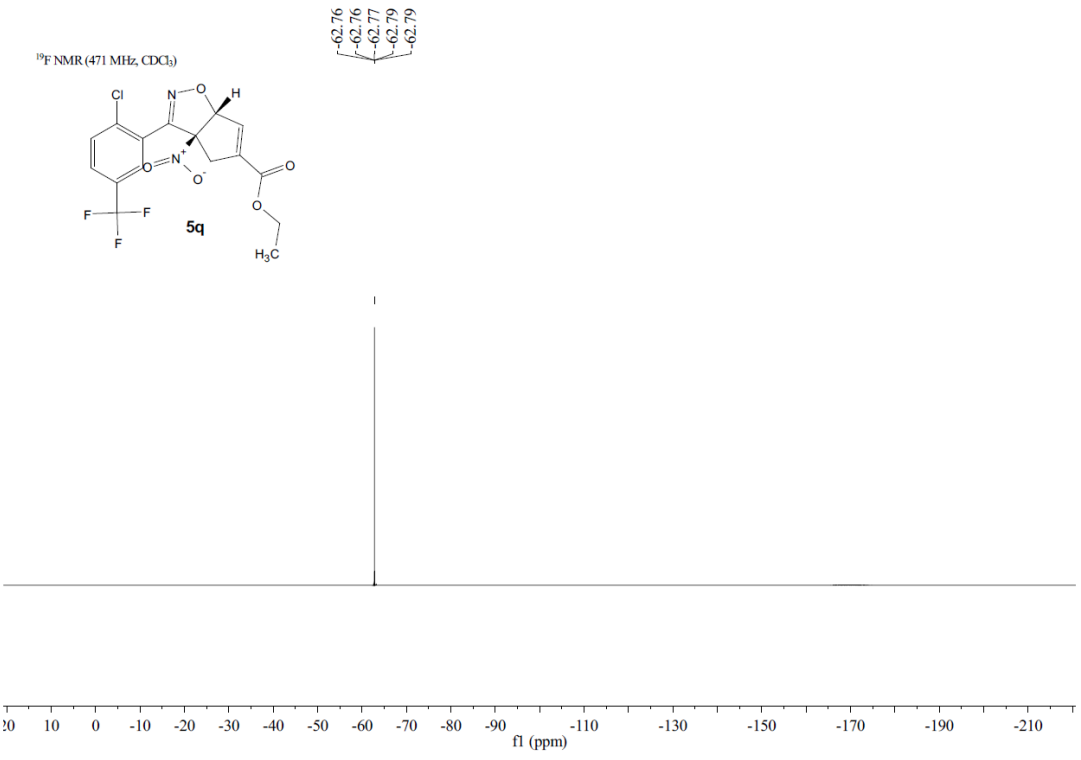


5p

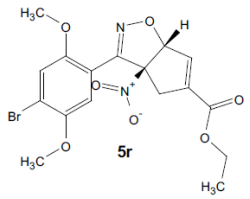

13C NMR (126 MHz, CDCl3)
162.54
153.00
137.60
134.31
134.07
131.76
128.81
127.98
127.38
126.78
125.48
95.21
77.32
77.06
76.81
61.62
38.84
14.13
5p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


1H NMR (500 MHz, CDCl3)
7.79
7.72
7.71
7.70
7.66
7.64
7.27
6.66
6.65
6.64
6.34
4.30
4.29
4.28
4.27
4.26
4.25
4.24
3.76
3.73
3.72
3.37
3.34
3.33
1.33
1.32
1.30
0.00
5q
1.00
1.00
1.00
1.00
1.00
2.00
1.00
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


161.36
149.58
136.98
136.66
132.88
130.35
129.13
128.87
127.69
127.66
127.63
125.34
125.30
94.70
76.27
76.01
75.76
60.68
37.89
25.88
13.08
13C NMR (126 MHz, CDCl3)
Cl
N
O
H
O
N+
O-
O
O
F
F
F
5q
H3C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)

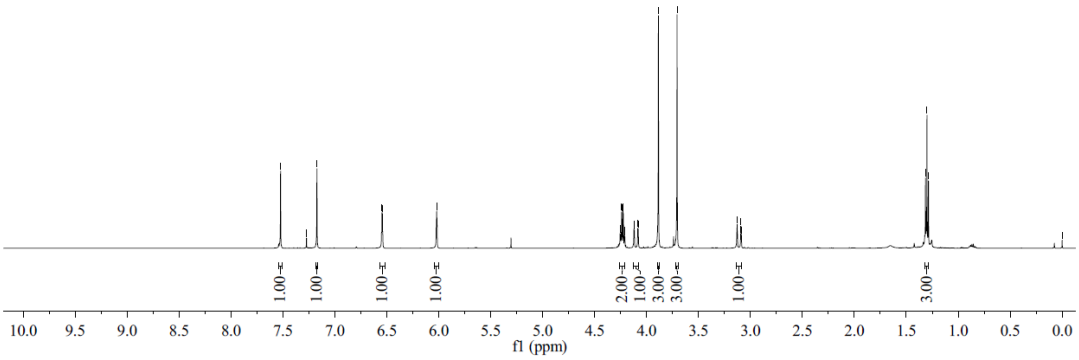

-62.76
-62.76
-62.77
-62.79
-62.79
19F NMR (471 MHz, CDCl3)
Cl
N
O
H
O
N+
O-
O
O
F
F
F
5q
H3C
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

^{1}H NMR (500 MHz, CDCl$_3$)

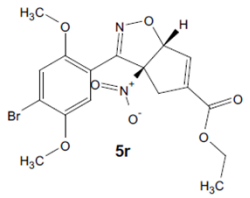


5r

7.52
7.27
7.17
6.55
6.54
6.02
4.25
4.25
4.24
4.24
4.23
4.22
4.21
4.21
4.12
4.12
4.08
4.08
3.89
3.71
3.13
3.13
3.12
3.09
3.09
3.09
1.32
1.30
1.29
0.00

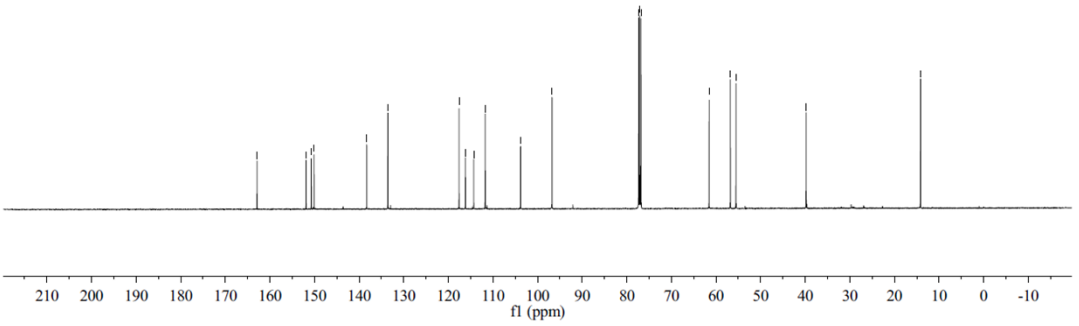


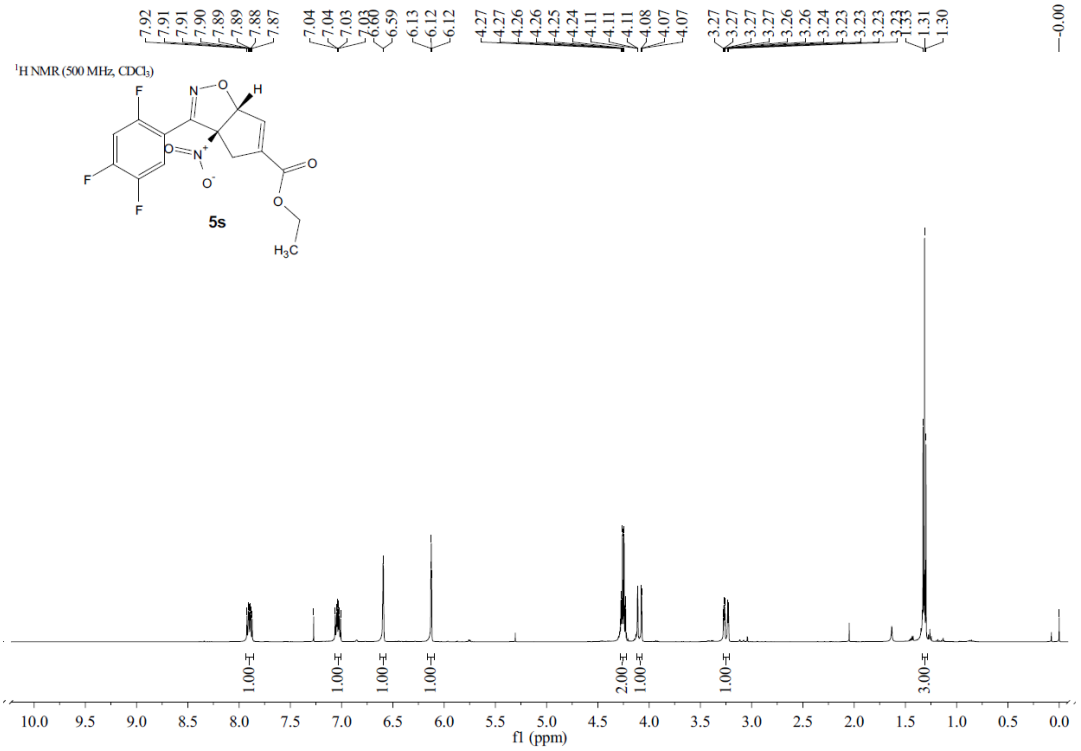
^{13}C NMR (126 MHz, CDCl$_3$)

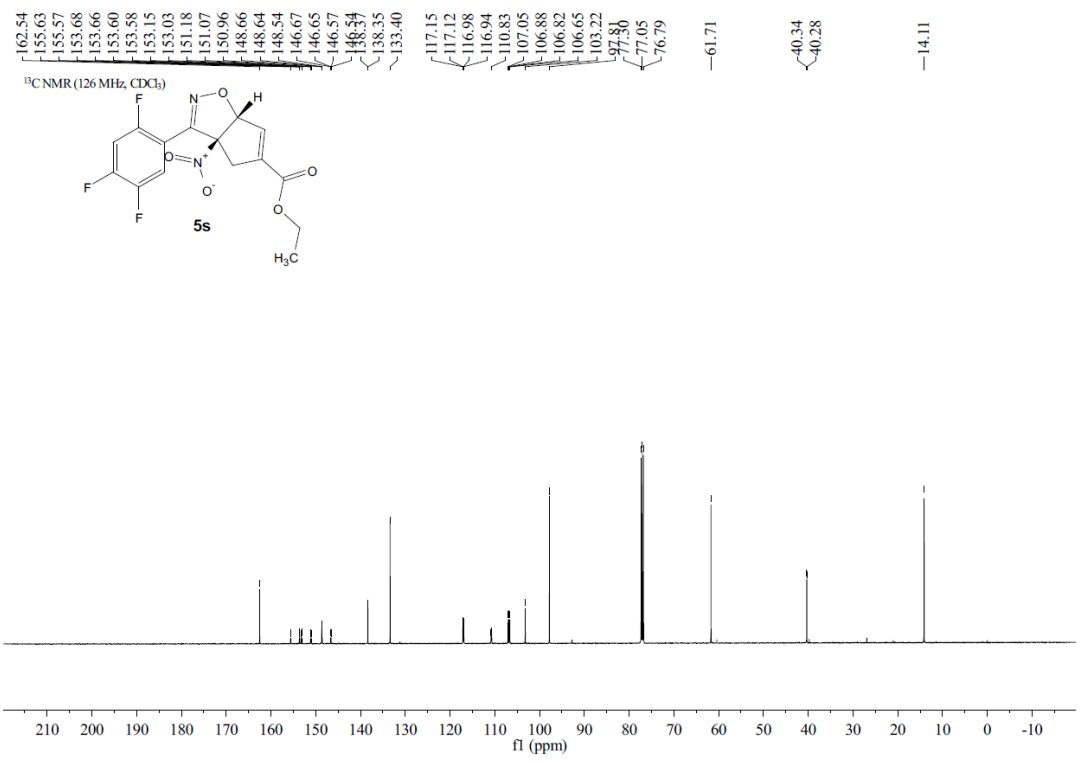


5r

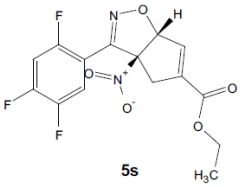
162.88
151.90
150.73
150.10
138.31
133.56
117.60
116.19
114.31
111.75
103.81
96.76
77.32
77.07
76.82
61.54
56.77
55.54
39.78
14.15



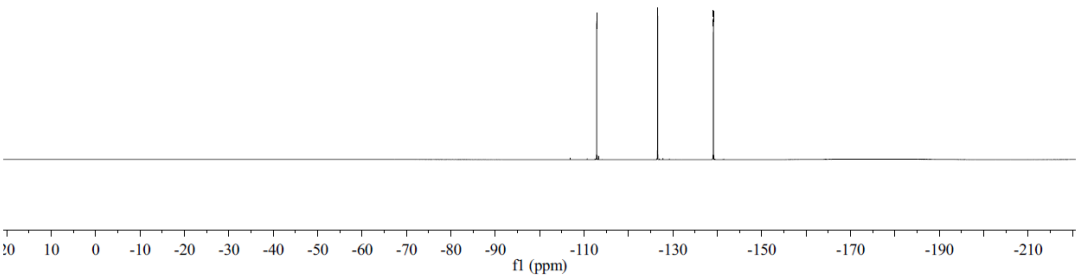

7.92
7.91
7.91
7.90
7.89
7.89
7.88
7.87
7.04
7.04
7.03
7.03
6.60
6.59
6.13
6.12
6.12
4.27
4.27
4.26
4.26
4.25
4.24
4.11
4.11
4.11
4.08
4.07
4.07
3.27
3.27
3.27
3.27
3.26
3.26
3.24
3.23
3.23
3.23
3.23
3.23
1.33
1.31
1.30
-0.00
1H NMR (500 MHz, CDCl3)
5s
1.00
1.00
1.00
1.00
2.00
1.00
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

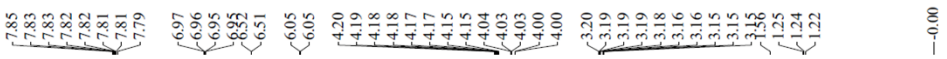

162.54
155.63
155.57
153.68
153.66
153.60
153.58
153.15
153.03
151.18
151.07
150.96
148.66
148.64
148.54
146.67
146.65
146.57
138.35
133.40
117.15
117.12
116.98
116.94
110.83
107.05
106.88
106.82
106.65
103.22
77.05
76.79
61.71
40.34
40.28
14.11
13C NMR (126 MHz, CDCl3)
5s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

^{19}F NMR (471 MHz, $CDCl_3$)

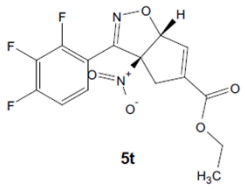


5s

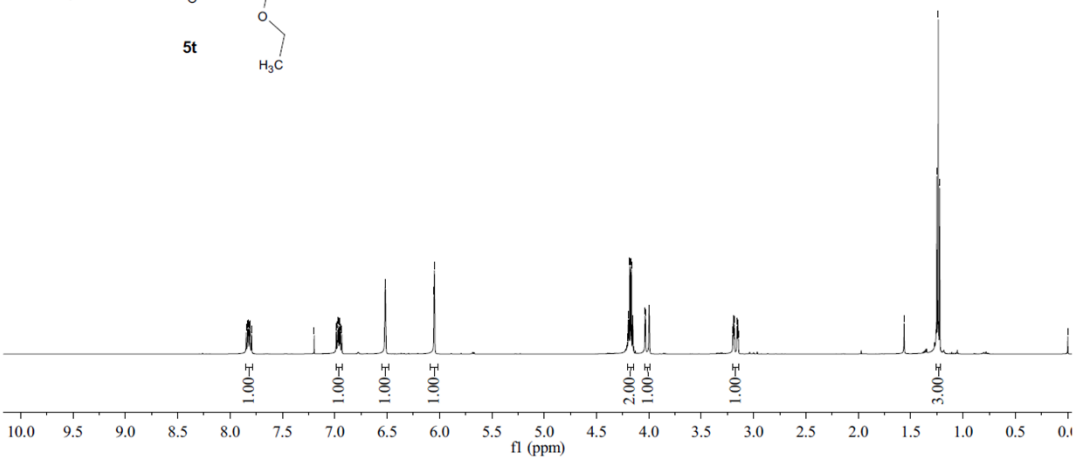


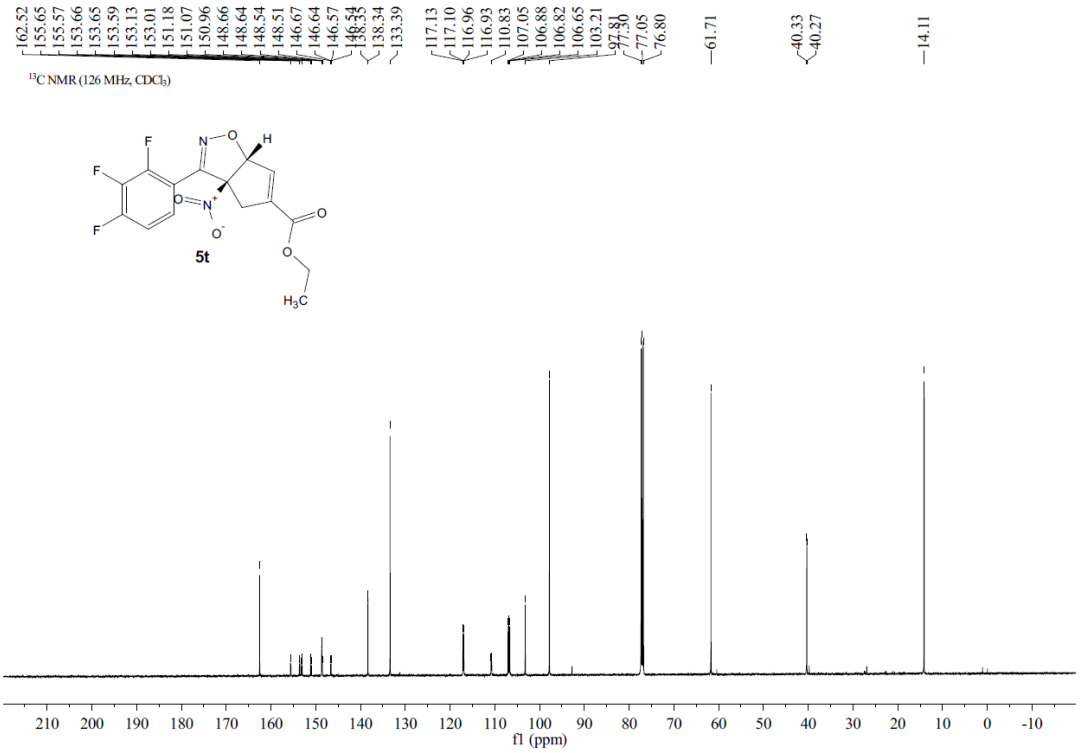


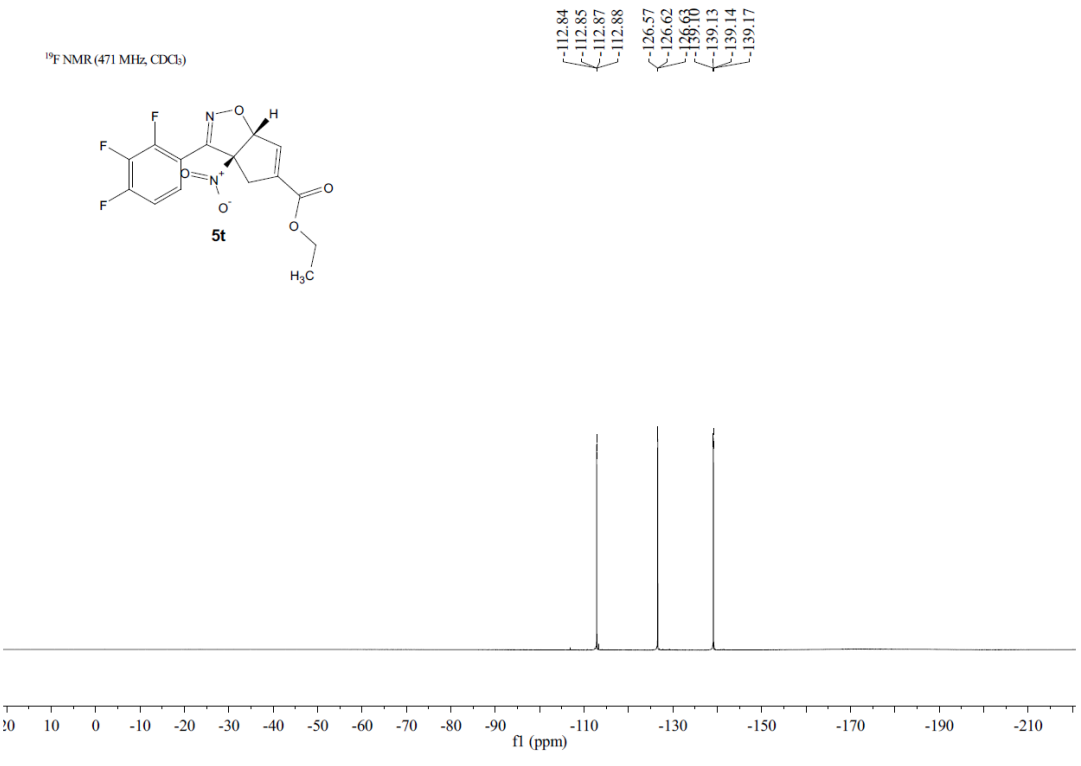
^{1}H NMR (500 MHz, $CDCl_3$)

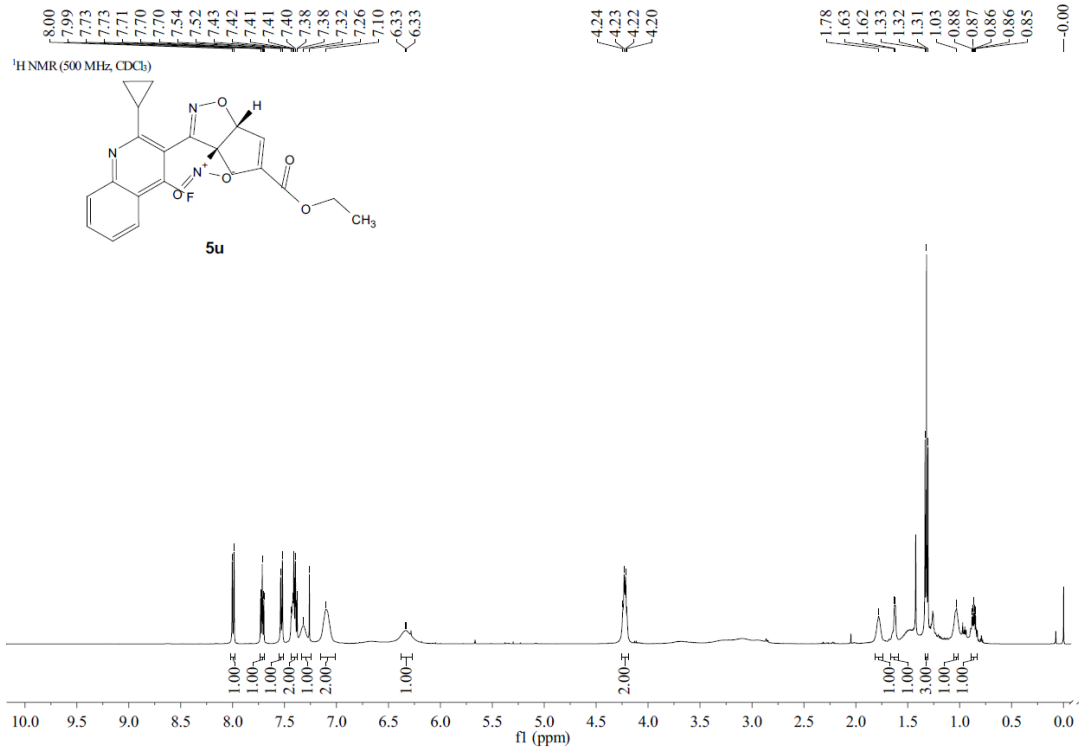


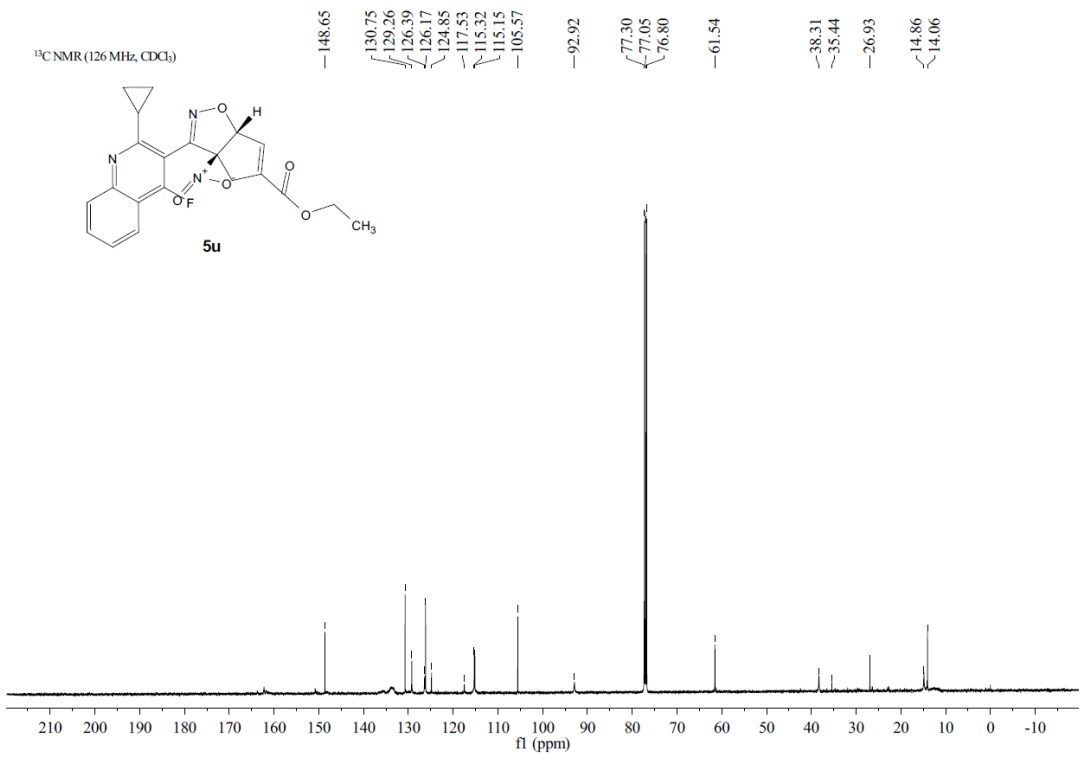
5t



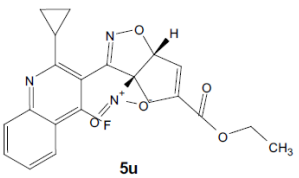

162.52
155.65
155.57
153.66
153.65
153.59
153.13
153.01
151.18
151.07
150.96
148.66
148.64
148.54
148.51
146.67
146.64
146.57
138.34
133.39
117.13
117.10
116.96
116.93
110.83
107.05
106.88
106.82
106.65
103.21
77.05
76.80
61.71
40.33
40.27
14.11
13C NMR (126 MHz, CDCl3)
5t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-112.84
-112.85
-112.87
-112.88
-126.57
-126.62
-139.13
-139.14
-139.17
19F NMR (471 MHz, CDCl3)
5t
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


8.00
7.99
7.73
7.73
7.71
7.70
7.70
7.54
7.52
7.43
7.42
7.41
7.41
7.40
7.38
7.38
7.32
7.26
7.10
6.33
6.33
4.24
4.23
4.22
4.20
1.78
1.63
1.62
1.33
1.32
1.31
1.03
0.88
0.87
0.86
0.86
0.85
0.00
1H NMR (500 MHz, CDCl3)
5u
1.00
1.00
1.00
2.00
1.00
2.00
1.00
2.00
1.00
1.00
3.00
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

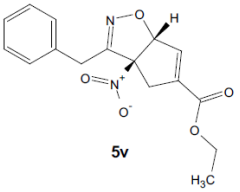

148.65
130.75
129.26
126.39
126.17
124.85
117.53
115.32
115.15
105.57
92.92
77.30
77.05
76.80
61.54
38.31
35.44
26.93
14.86
14.06
13C NMR (126 MHz, CDCl3)
5u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

^{19}F NMR (471 MHz, $CDCl_3$)

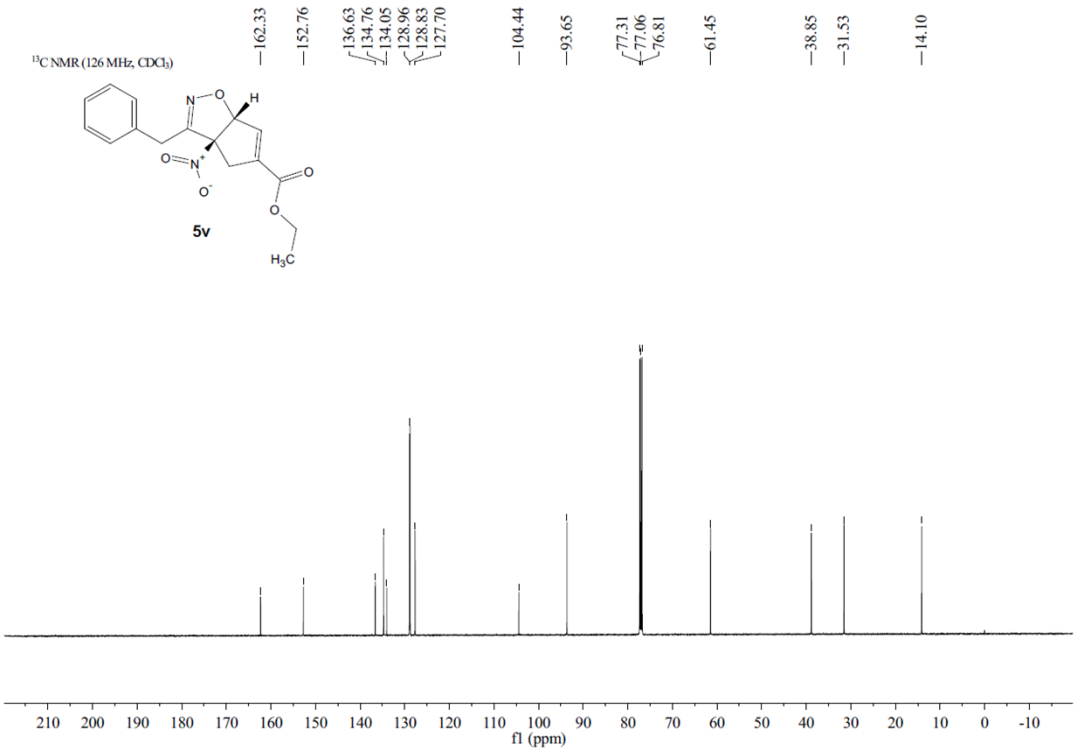


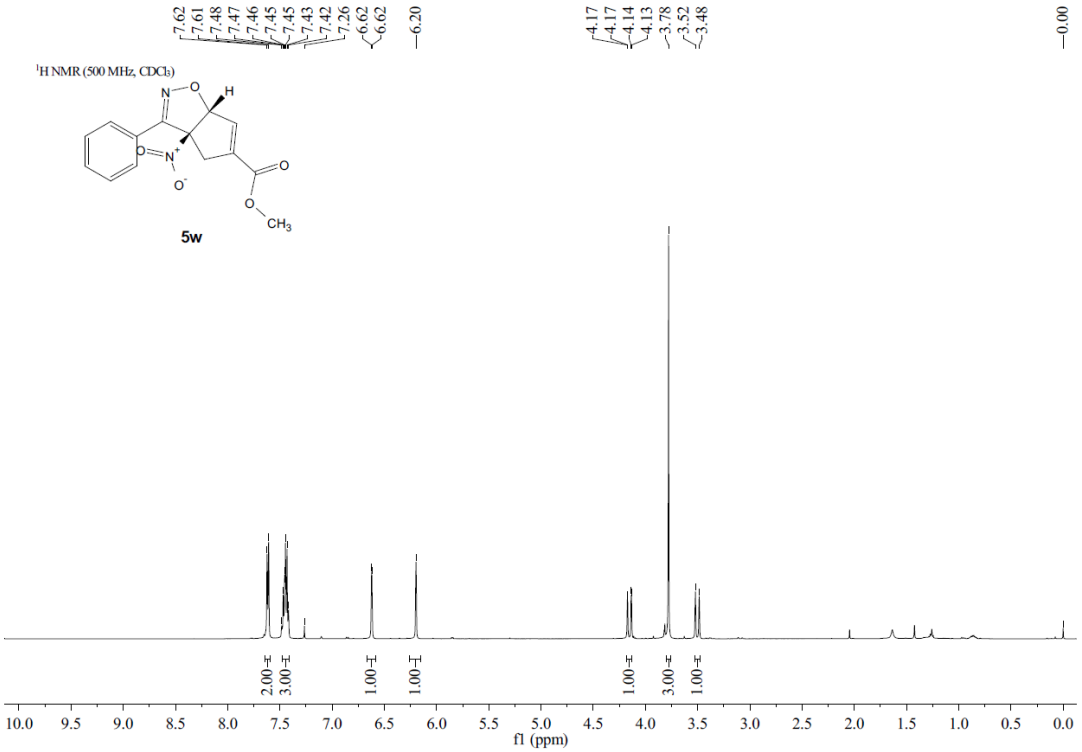
5u

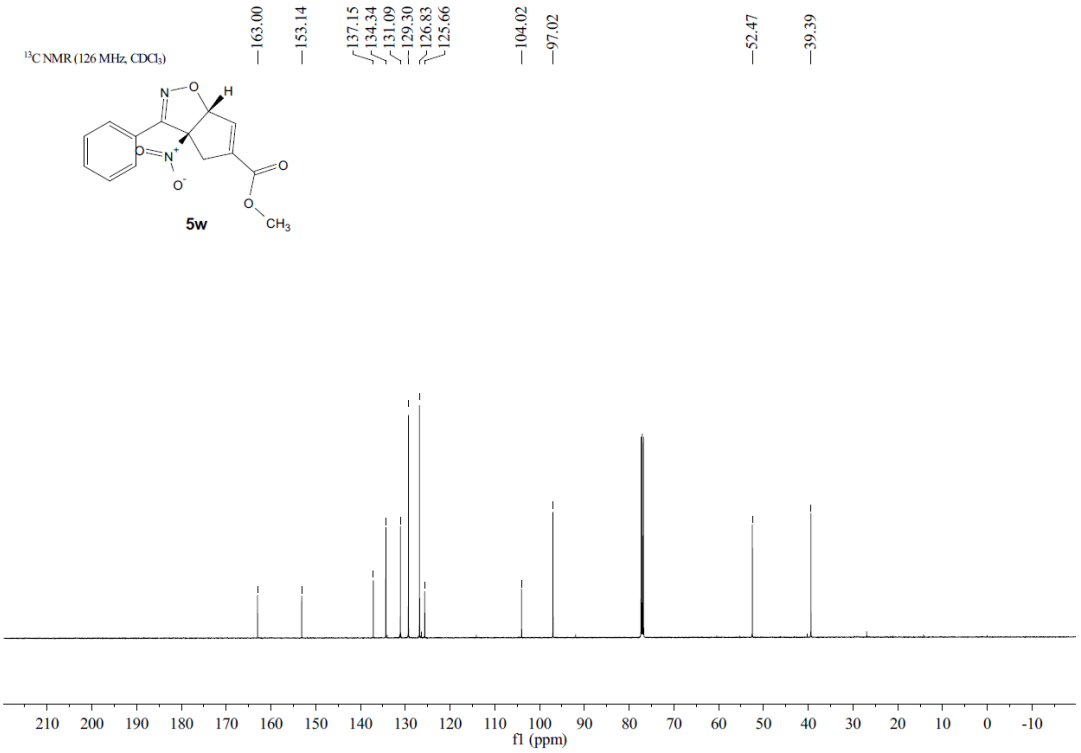
^{1}H NMR (500 MHz, $CDCl_3$)

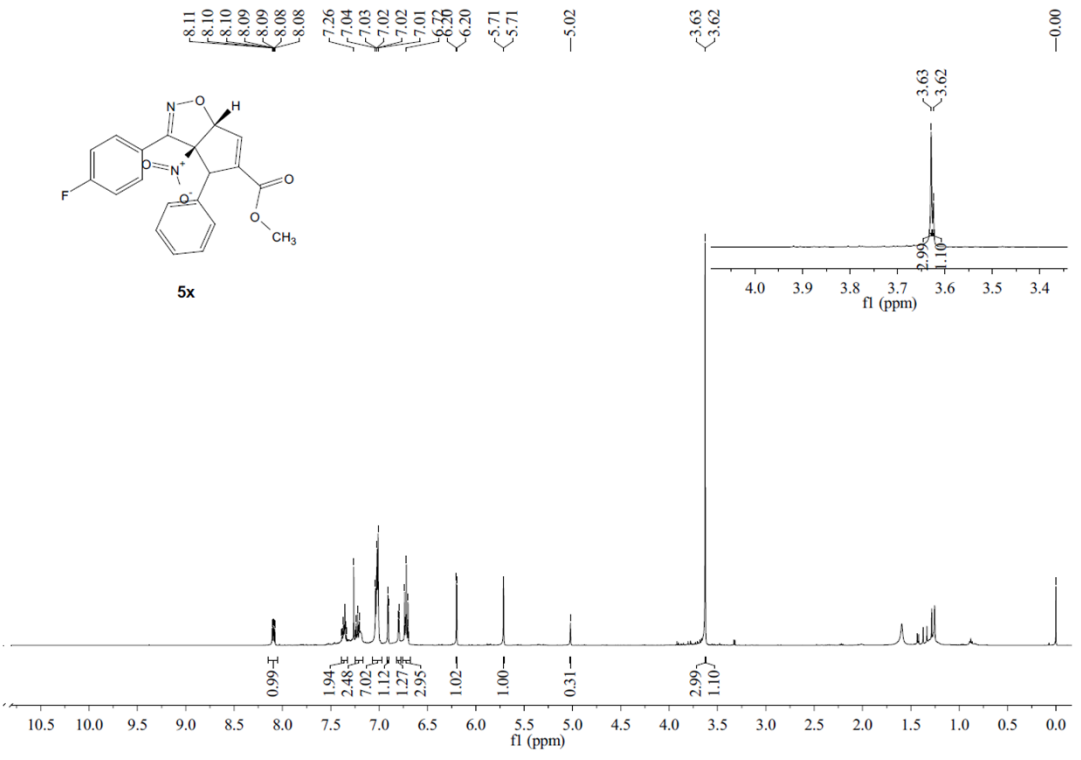


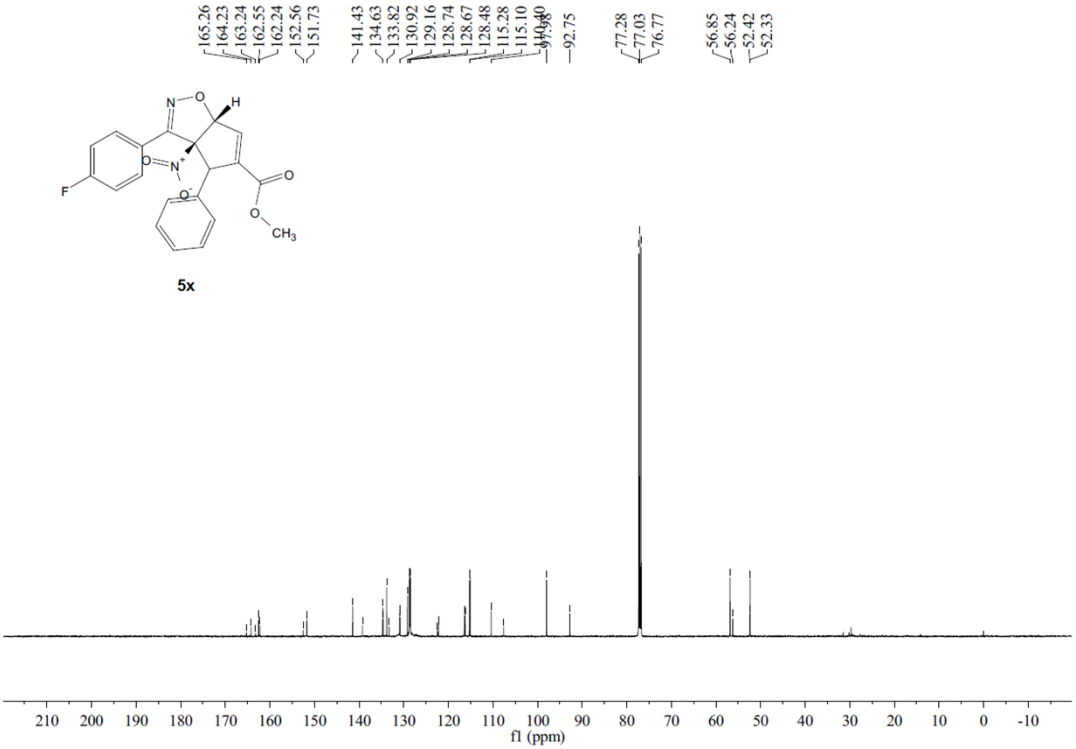
5v

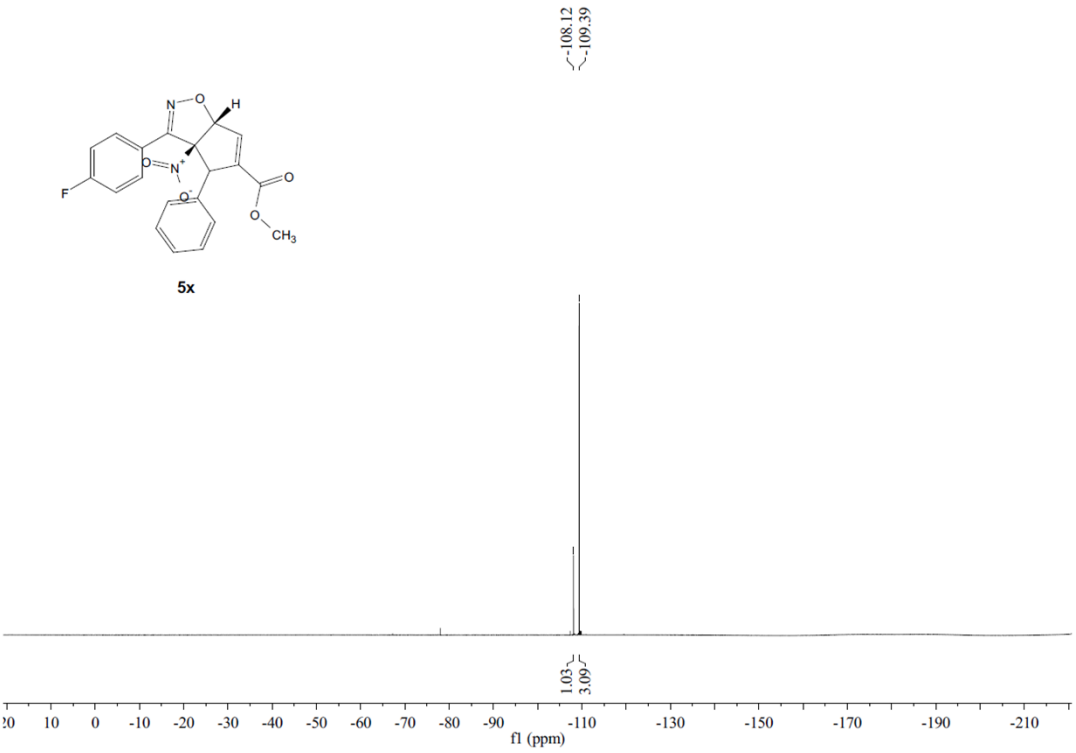

13C NMR (126 MHz, CDCl3)
162.33
152.76
136.63
134.76
134.05
128.96
128.83
127.70
104.44
93.65
77.31
77.06
76.81
61.45
38.85
31.53
14.10
5v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

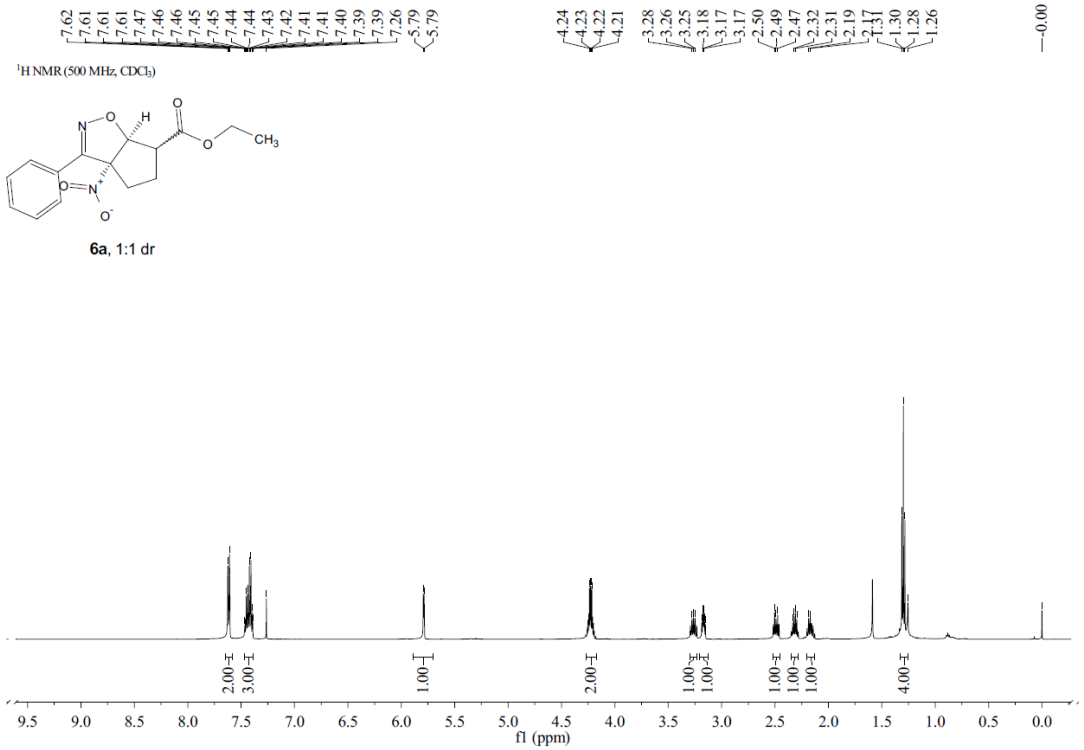

1H NMR (500 MHz, CDCl3)
7.62
7.61
7.48
7.47
7.46
7.45
7.45
7.43
7.42
7.26
6.62
6.62
6.20
4.17
4.17
4.14
4.13
3.78
3.52
3.48
0.00
5w
2.00
3.00
1.00
1.00
1.00
3.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

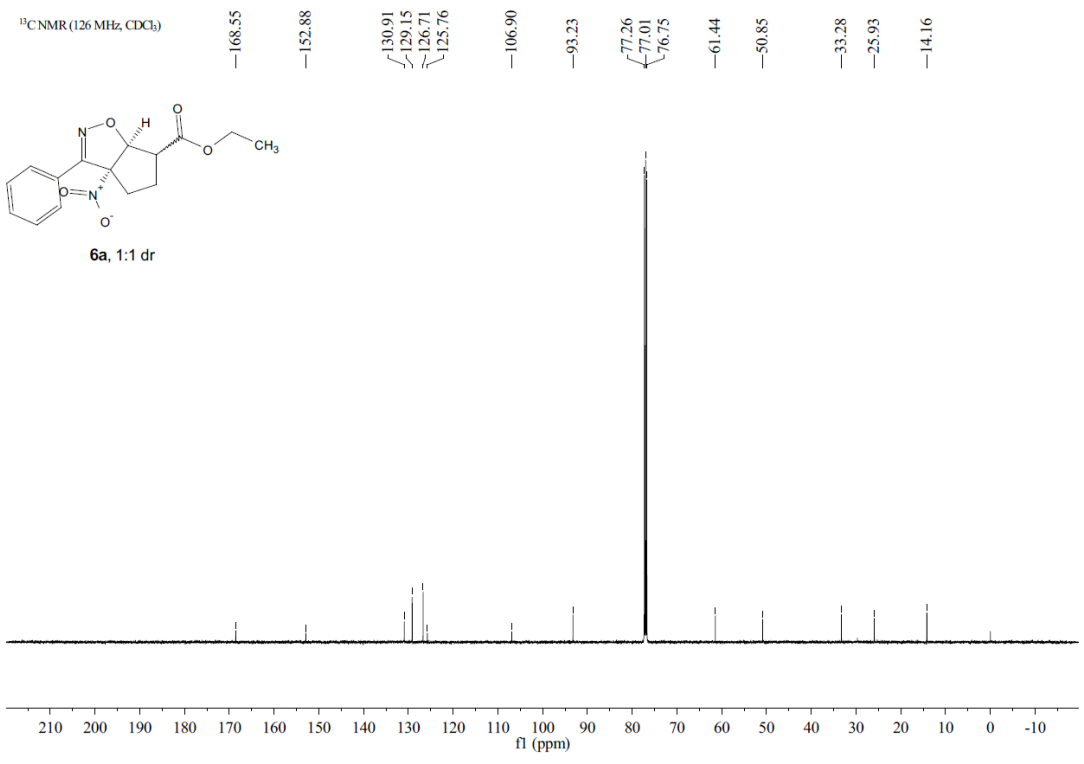

13C NMR (126 MHz, CDCl3)
163.00
153.14
137.15
134.34
131.09
129.30
126.83
125.66
104.02
97.02
52.47
39.39
5w
f1 (ppm)

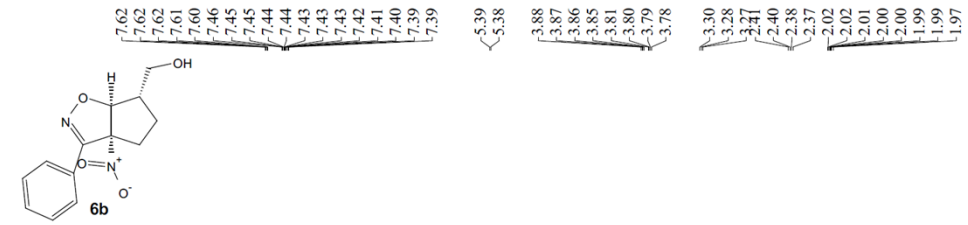

8.11
8.10
8.10
8.09
8.09
8.08
8.08
8.08
7.26
7.04
7.03
7.02
7.02
7.01
6.22
6.20
5.71
5.71
5.02
3.63
3.62
0.00
5x
3.63
3.62
2.99
1.10
f1 (ppm)
0.99
1.94
2.48
7.02
1.12
1.27
2.95
1.02
1.00
0.31
2.99
1.10
f1 (ppm)

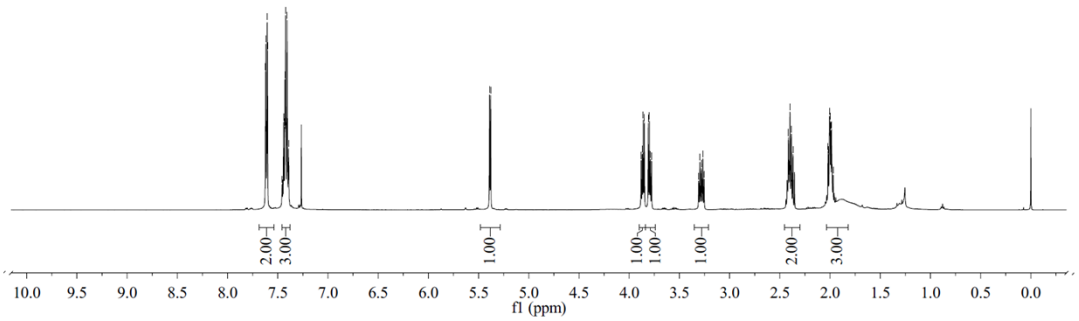

165.26
164.23
163.24
162.55
162.24
152.56
151.73
141.43
134.63
133.82
130.92
129.16
128.74
128.67
128.48
115.28
115.10
110.40
97.98
92.75
77.28
77.03
76.77
56.85
56.24
52.42
52.33
5x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

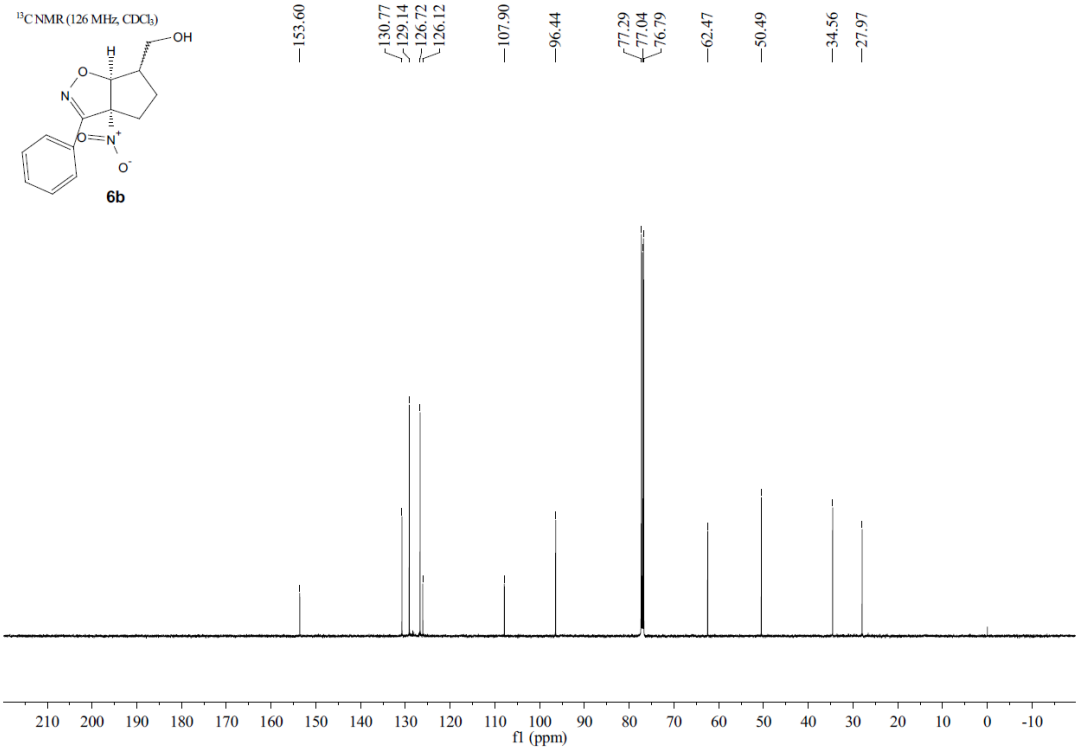

-108.12
-109.39
5x
1.03
3.09
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


7.62
7.61
7.61
7.61
7.47
7.46
7.46
7.45
7.45
7.44
7.44
7.43
7.42
7.41
7.41
7.40
7.39
7.39
7.26
5.79
5.79
4.24
4.23
4.22
4.21
3.28
3.26
3.25
3.18
3.17
3.17
2.50
2.49
2.47
2.32
2.31
2.19
2.17
1.31
1.30
1.28
1.26
0.00
1H NMR (500 MHz, CDCl3)
CH3
6a, 1:1 dr
2.00
3.00
1.00
2.00
1.00
1.00
1.00
1.00
1.00
4.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

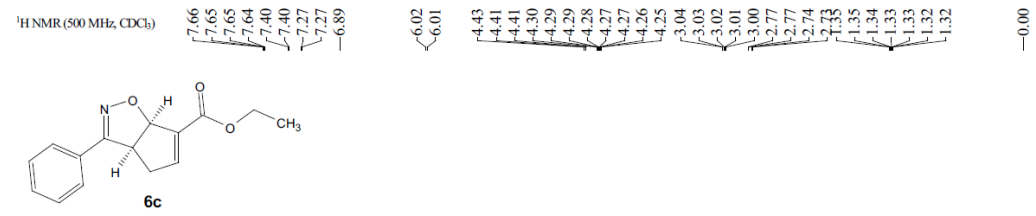

13C NMR (126 MHz, CDCl3)
168.55
152.88
130.91
129.15
126.71
125.76
106.90
93.23
77.26
77.01
76.75
61.44
50.85
33.28
25.93
14.16
CH3
6a, 1:1 dr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.62
7.62
7.62
7.61
7.60
7.46
7.45
7.45
7.44
7.44
7.43
7.43
7.43
7.42
7.41
7.40
7.39
7.39
5.39
5.38
3.88
3.87
3.86
3.85
3.81
3.80
3.79
3.78
3.30
3.28
3.27
2.41
2.40
2.38
2.37
2.02
2.02
2.01
2.00
2.00
1.99
1.99
1.97
OH
H
O
N
O
N+
O-
6b

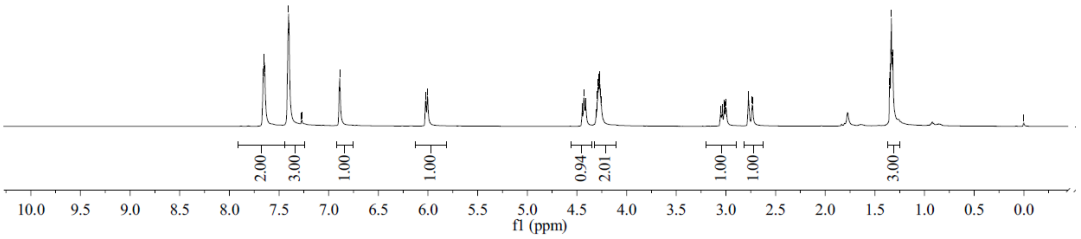

2.00
3.00
1.00
1.00
1.00
1.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


13C NMR (126 MHz, CDCl3)
153.60
130.77
129.14
126.72
126.12
107.90
96.44
77.29
77.04
76.79
62.47
50.49
34.56
27.97
OH
H
O
N
O
N+
O-
6b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

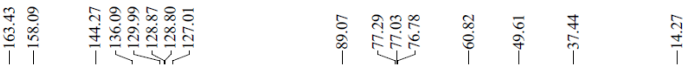
^{1}H NMR (500 MHz, $CDCl_3$)

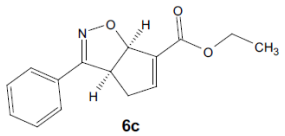


6c

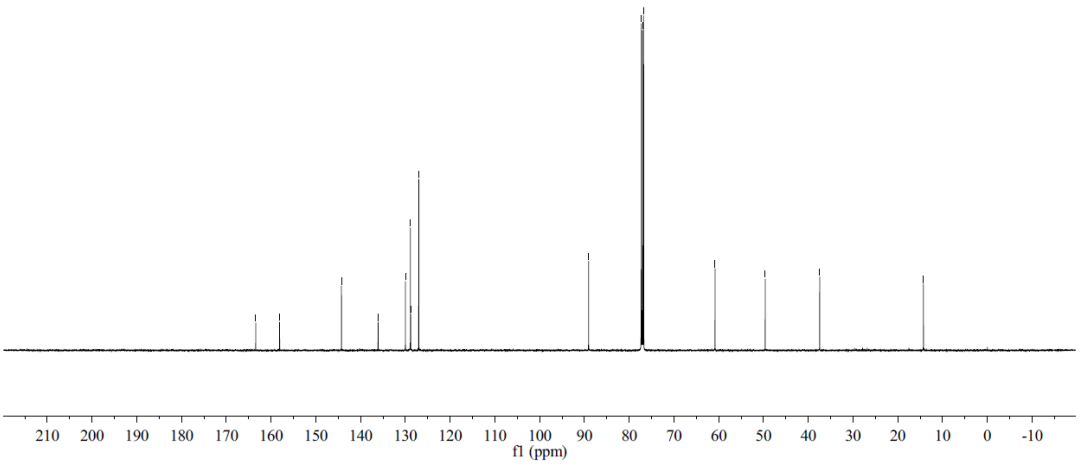


^{13}C NMR (126 MHz, $CDCl_3$)



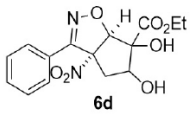


6c

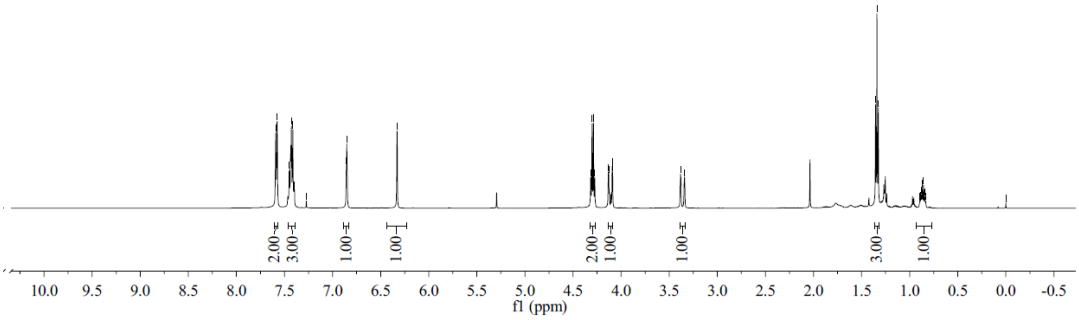


^{1}H NMR (500 MHz, $CDCl_3$)

7.59, 7.58, 7.45, 7.44, 7.43, 7.43, 7.41, 7.27, 6.86, 6.85, 6.85, 6.33, 4.32, 4.30, 4.29, 4.27, 4.13, 4.13, 4.09, 4.09, 3.38, 3.34, 1.35, 1.34, 1.33, 0.88, 0.87, 0.86, 0.85, 0.84, 0.00

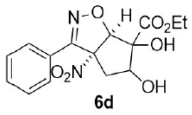


6d

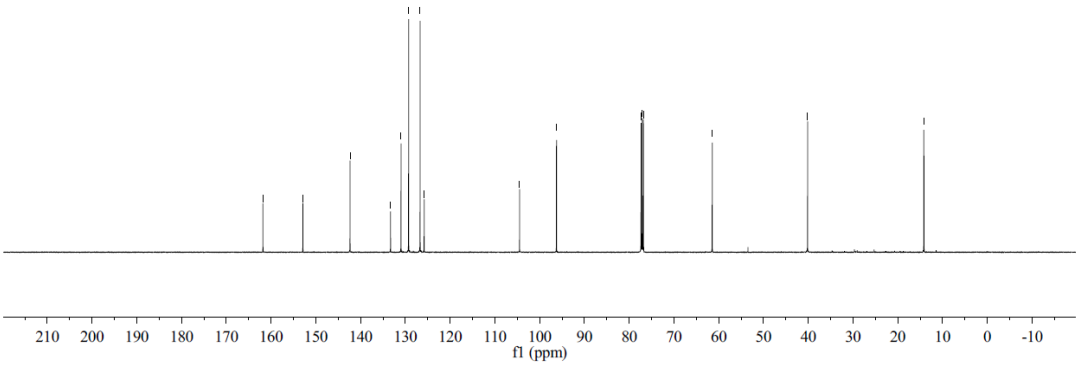


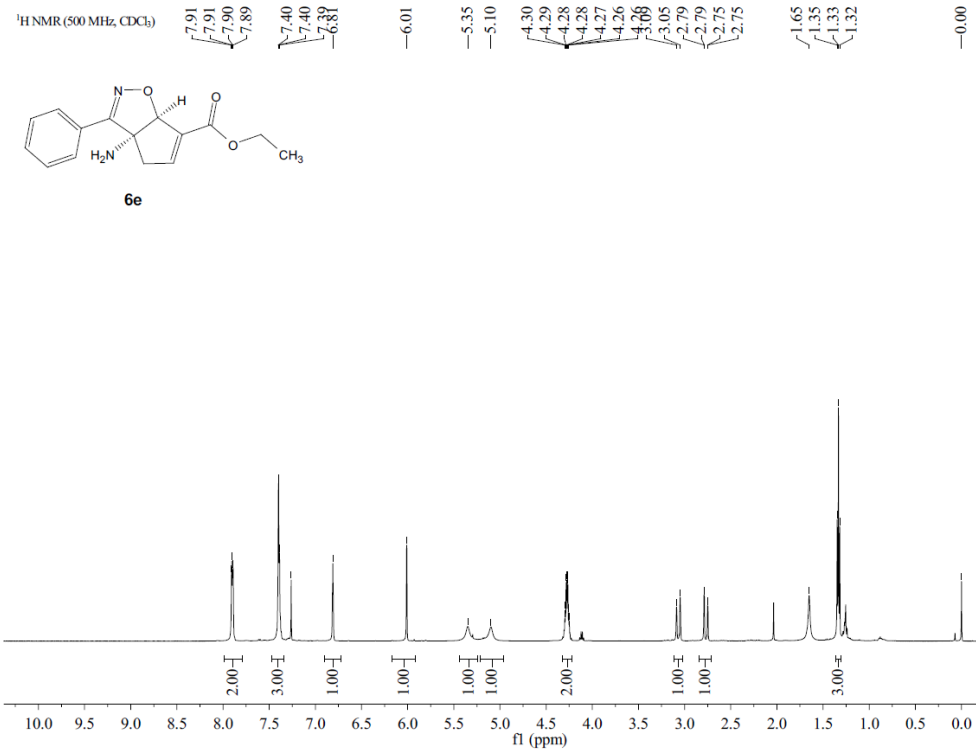
^{13}C NMR (126 MHz, $CDCl_3$)

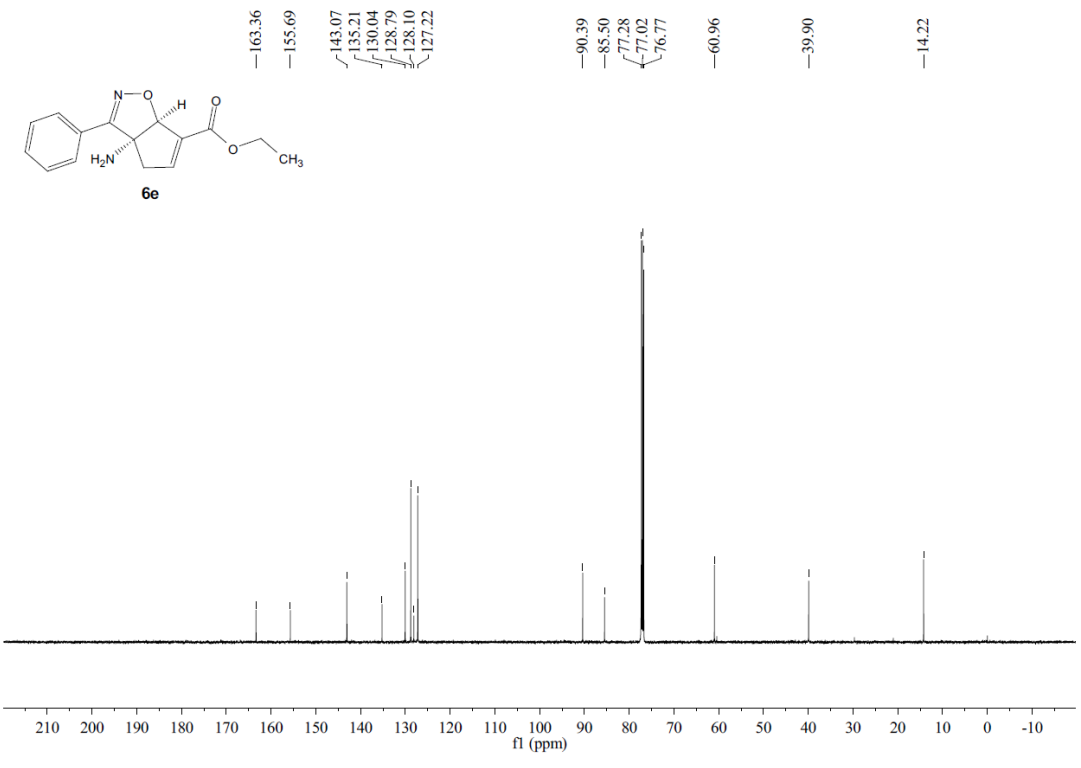
161.82, 152.89, 142.36, 133.31, 130.97, 129.28, 126.71, 125.80, 104.49, 96.24, 77.33, 77.08, 76.82, 61.45, 40.15, 14.17



6d

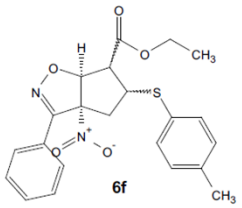


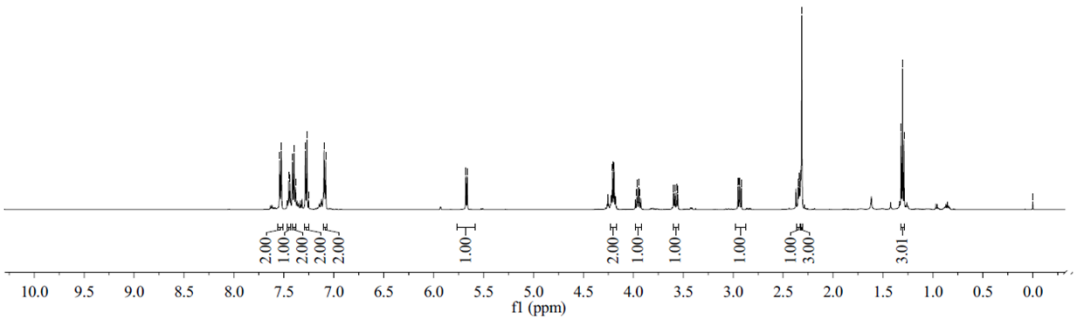

1H NMR (500 MHz, CDCl3)
7.91
7.91
7.90
7.89
7.40
7.40
7.39
6.81
6.01
5.35
5.10
4.30
4.29
4.28
4.28
4.27
4.26
4.26
3.08
3.05
2.79
2.79
2.75
2.75
1.65
1.35
1.33
1.32
0.00
N
O
H
O
H2N
O
CH3
6e
2.00
3.00
1.00
1.00
1.00
1.00
2.00
1.00
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


163.36
155.69
143.07
135.21
130.04
128.79
128.10
127.22
90.39
85.50
77.28
77.02
76.77
60.96
39.90
14.22
N
O
H
O
H2N
O
CH3
6e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

^{1}H NMR (500 MHz, $CDCl_3$)

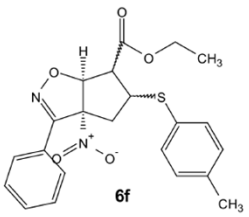
7.54 7.53 7.52 7.45 7.44 7.41 7.40 7.38 7.28 7.27 7.25 7.10 7.08 5.68 5.66 4.21 4.21 4.20 4.19 3.97 3.96 3.95 3.94 3.60 3.58 3.57 3.55 2.95 2.94 2.93 2.34 2.33 2.31 1.32 1.30 1.29 0.00

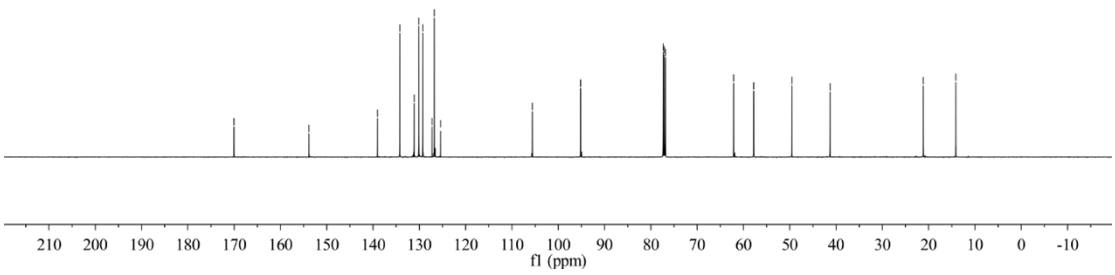




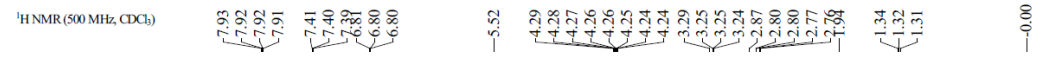
^{13}C NMR (126 MHz, $CDCl_3$)

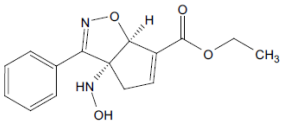
170.04 153.84 139.04 134.21 131.13 130.12 129.27 127.26 126.77 125.42 105.58 95.15 77.34 77.09 76.83 62.11 57.77 49.54 41.29 21.17 14.13



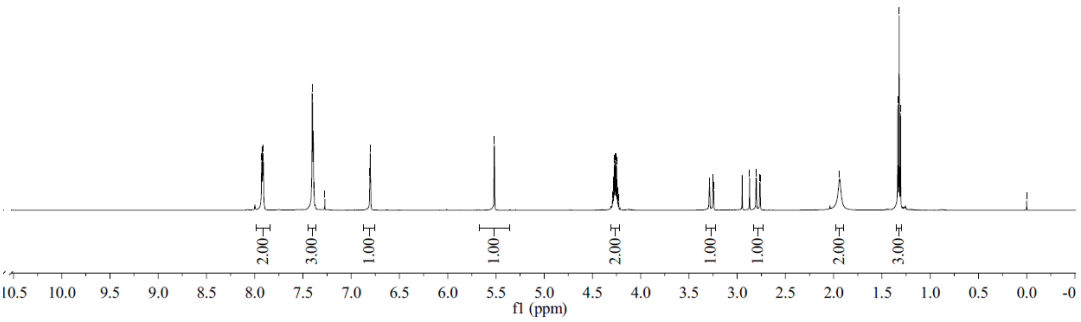


^{1}H NMR (500 MHz, $CDCl_3$)

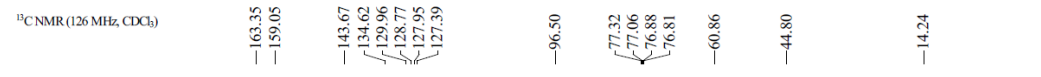


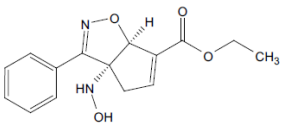


6g

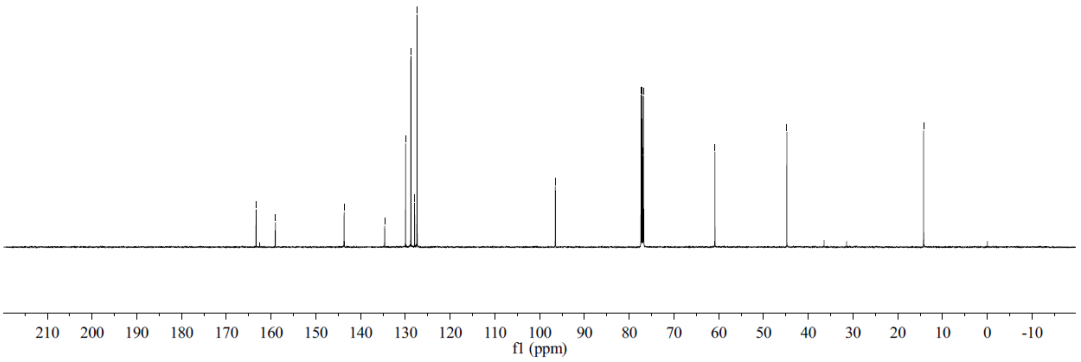


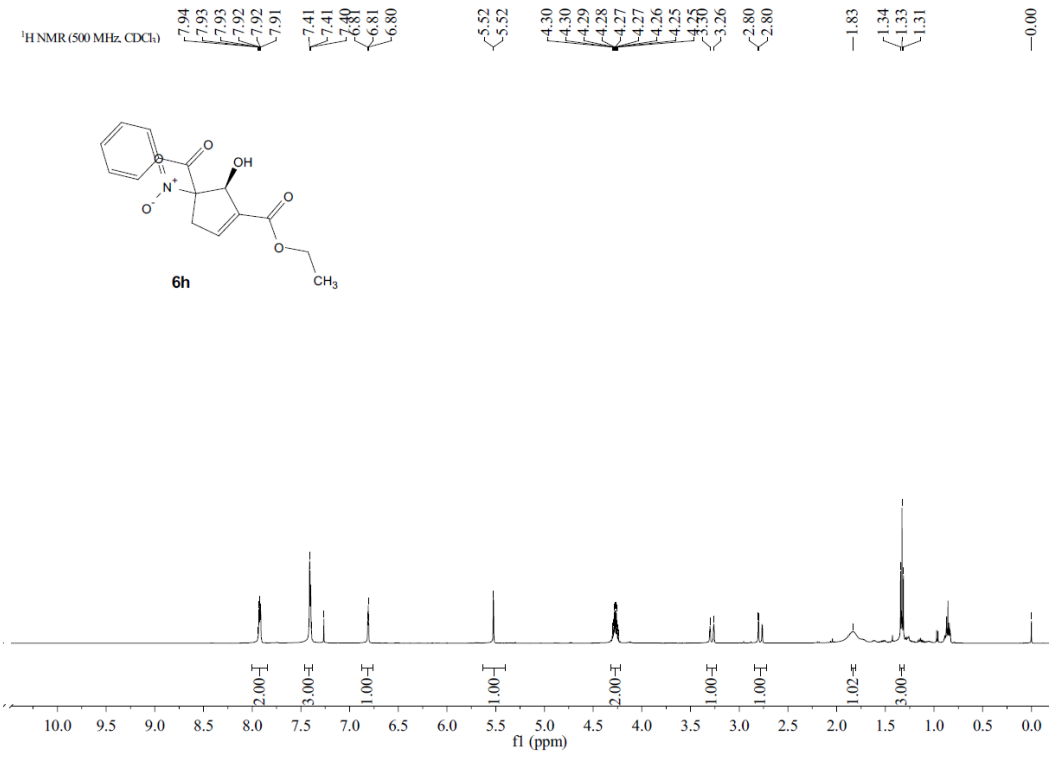
^{13}C NMR (126 MHz, $CDCl_3$)

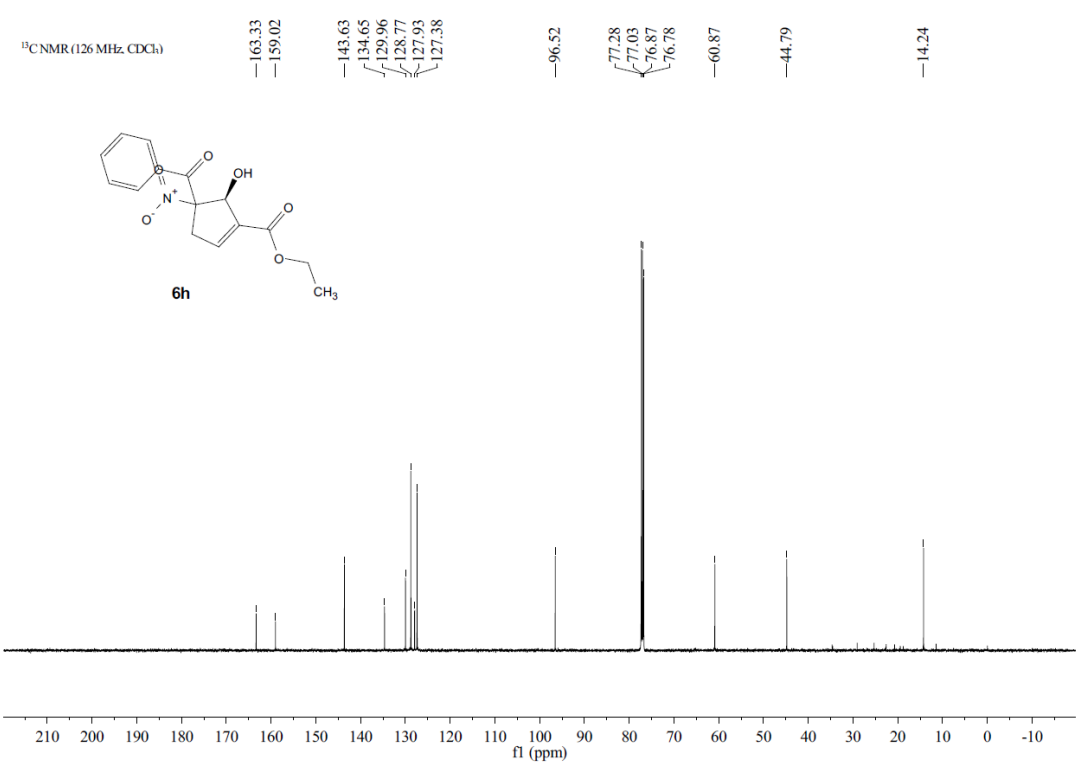




6g




^{1}H NMR (500 MHz, CDCl$_3$)
7.94
7.93
7.93
7.92
7.92
7.91
7.41
7.41
7.40
6.81
6.81
6.80
5.52
5.52
4.30
4.30
4.29
4.28
4.27
4.27
4.26
4.25
4.25
3.30
3.26
2.80
2.80
1.83
1.34
1.33
1.31
0.00
OH
O
N+
O-
O
O
CH3
6h
2.00
3.00
1.00
1.00
2.00
1.00
1.00
1.02
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


^{13}C NMR (126 MHz, CDCl$_3$)
163.33
159.02
143.63
134.65
129.96
128.77
127.93
127.38
96.52
77.28
77.03
76.87
76.78
60.87
44.79
14.24
OH
O
N+
O-
O
O
CH3
6h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)