Supplementary Information

EDA complex-directed streamlined synthesis of isoxazolidines from nitroarenes

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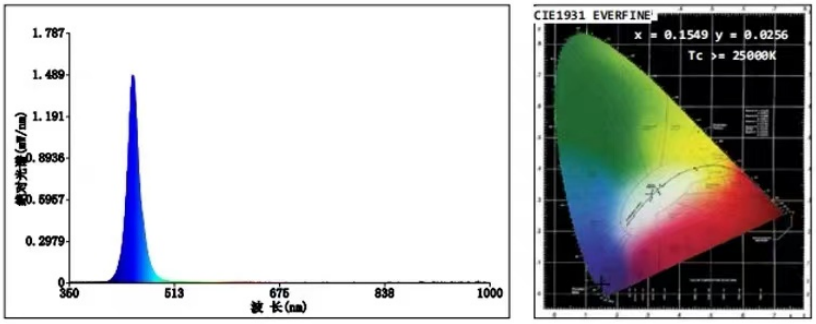
1. General information

The reagents and solvents were purchased from commercial suppliers and used without further purification unless noted. All reactions were monitored by TLC with silica gel-coated plates. Product purification was accomplished by flash chromatography using 200-300 mesh silica gel. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker AV 600 or AV 400 NMR spectrometer at ambient temperature. Chemical shifts were reported in parts per million (ppm) and calibrated using residual undeuterated solvent as an internal reference ($CDCl_3$: 7.26 ppm ^{1}H NMR, 77.0 ppm ^{13}C NMR; DMSO-d_6: 2.50 ppm ^{1}H NMR, 39.6 ppm ^{13}C NMR). Abbreviations used in the description of NMR data are listed as follows: s = singlet, d = doublet, dd = doublet of doublet, t = triplet, m = multiplet. Mass spectra were measured with a HRMS-APCI instrument using ESI ionization. UV/vis absorption spectra experiments were conducted on a HitachiF-7000 FL Spectrophotometer. Photo-induced reactions were performed under 450-460 nm light irradiation using a 25 W LED lamp (purchased from Xuzhou Ai Jia Electronic Technology Co., Ltd. in Taobao.com) (Figure S1). The distance from the light source to the irradiation vessel was approximately 1.5 cm, and no filter was used in our study. A fan was employed to ensure reactions remained at or near room temperature when using LED.



颜色参数:

色品坐标(2度):x=0.1549 y=0.0256/u'=0.2067 v'=0.0767 duv=-2.164e-001
相关色温:Tc=100000K 主波长:λd=453.8nm 色纯度: Purity=98.7%
色比:R=0.9% G=12.6% B=86.5% 峰值波长:λp=448.4nm 半宽度:Δλd=18.0nm
显色指数:Ra=-59.2

R1 =-6.69	R2 =-48.04	R3 =-160.84	R4 =-103.25	R5 =7.64
R6 =-55.65	R7 =-60.46	R8 =-45.98	R9 =-258.25	R10=-235.20
R11=-128.87	R12=-123.53	R13=-25.53	R14=-37.58	R15=9.69

TM30 参数: Rf = 0.0, Rg:16.6

光度参数:

光通量 Φ = 1.209 lm 光效 : 19.59 lm/W Φe = 35.07 mW
光量子=1.322e-001umol/s 荧光蓝光比=0.017 荧光效能=9.460e-003

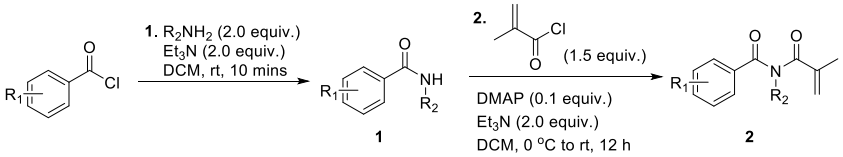
电参数:

正向电压 VF = 3.089 V 正向电流 IF = 19.98 mA 功率 P = 61.75 mW
反向电流 IR = 0 uA (反向电压 VR=5.010V)
分级:**[OUT] 白光分类:OUT

Figure S1. The spectrum of our lamp.

2. Preparation of substrates

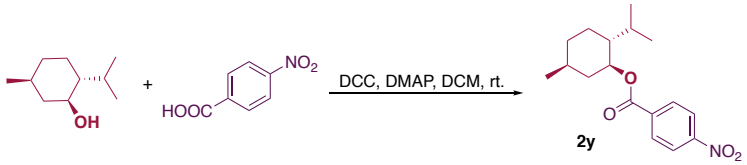
2.1 General Procedure for the synthesis of *N*-methacryloyl-*N*-methylbenzamide substrates[1-4]



STEP 1: A dried round-bottom flask was charged with a magnetic stirring bar, aniline (10 mmol), triethylamine (10 mmol) and DCM (30 mL). Benzoyl chloride (5 mmol) dissolved in DCM (10 mL) was added slowly for 5 mins at room temperature, and the mixture was stirred for 30 mins. The reaction was monitored by TLC. After completion, the reaction was quenched with saturated NaCl solution (100 mL) and extracted with DCM (30 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The reaction mixture was purified *via* column chromatography to give **1** (98% yield).

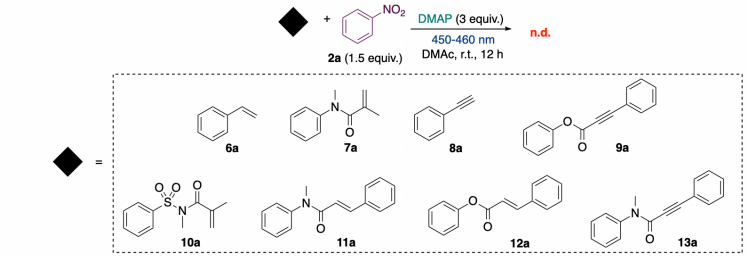
STEP 2: A dried round-bottom flask was charged with a magnetic stirring bar, benzamide **1** (5 mmol), triethylamine (10 mmol), DMAP (0.5 mmol) and DCM (30 mL). Methacryloyl chloride (10 mmol) dissolved in DCM (10 mL) was added slowly for 5 mins at 0 °C, and the mixture was stirred for 12 h at room temperature. The reaction was monitored by TLC. After completion, the reaction was quenched with saturated NaCl solution (100 mL) and extracted with DCM (30 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The reaction mixture was purified *via* column chromatography to give **2** (91% yield).

2.2 Procedure for the synthesis of substrate 2v-2y (2y as an example)[5]



A dried round-bottom flask was charged with a magnetic stirring bar, menthol (10 mmol), 4-nitrobenzoic acid (10 mmol), DCC (20 mmol), DMAP (10 mmol) and DCM (30 mL). The mixture was stirred for 1 h at room temperature. The reaction was monitored by TLC. After completion, the reaction was quenched with saturated NaCl solution (100 mL) and extracted with DCM (30 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The reaction mixture was purified *via* column chromatography to give **2y** (92% yield).

2.3 Unsuccessful olefin or alkyne derivatives

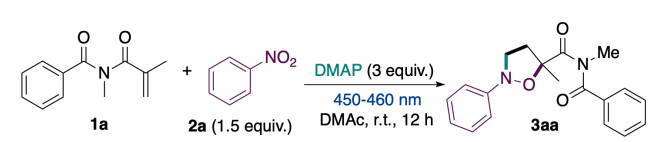


Standard conditions: derivatives **6a**-**13a** (0.3 mmol), **2a** (0.45 mmol) and DMAP (0.9 mmol) in DMAc (2 mL) under air atmosphere and stirred under 450-460 nm light-irradiation (LEDs) at room temperature for 12 h.

Other olefin or alkyne derivatives including styrene (**6a**), *N*-methyl-*N*-acryloylphenylamine (**7a**), ethynylbenzene **(8a**), phenyl phenylpropiolate (**9a**), *N*-methyl-*N*-(phenylsulfonyl)methacrylamide (**10a**), *N*-methyl-*N*-phenylcinnamamide (**11a**), phenyl cinnamate (**12a**) and *N*-methyl-*N*-diphenylpropiolamide (**13a**) react with nitrobenzene (**2a**) under standard conditions. Unfortunately, no expected products were detected, indicating that these olefin or alkyne derivatives may not be suitable for this visible light-driven EDA-complex-mediated reduction/cycloaddition reaction.

3. Optimization studies

Table 1. Optimization of the reaction conditions



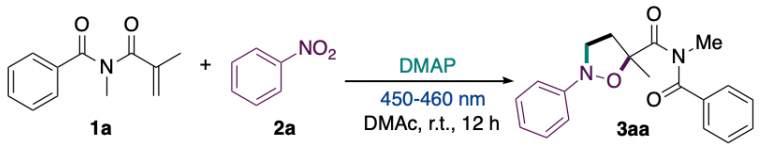
Entry	Changes from standard conditions [a]	Yield [b] (%)
1	None	82
2	EA, MeCN, DMSO, DMPU, Acetone, DCE	42, 52, 70, 72,57, 61
	H_2O, DMAc/H_2O as solvent	n.d., 37
3	TMEDA, DIPEA, PMDETA, Et_3N, DABCO as amines	65, 59, 46, n.d., n.d.
4	1 equiv. or 2 equiv. of $PhNO_2$	59, 86
5	1.5 equiv. or 4 equiv. of DMAP	48, 89
6	6h, 24h of reaction time	43, 81
7	50 °C of reaction temperature	80
8	Using 390-400 nm LEDs	59
9	Using 480-490 nm LEDs	45
10	Using sunlight irradiation	n.d.
11	No PMDETA	n.d.
12	No light	n.d.
13	K_2CO_3 or Cs_2CO_3 instead of DMAP	n.d., n.d.
14	N_2 or O_2 atmosphere	75, 78

[a] Reaction condition: **1a** (0.3 mmol), **2a** (0.45 mmol) and DMAP (0.9 mmol) in DMAc (2 mL) under air atmosphere and stirred under 450-460 nm light-irradiation (LEDs) at room temperature for 12 h. [b] Isolated yields based on **1a**.

N-methacryloyl-*N*-methylbenzamide **1a** and nitrobenzene **2a** were employed as the model substrates to optimize the reaction conditions. When 3 equivalents (equiv.) of DMAP were used as the electron donor (Table 1, entry 1), the title product **3aa** of **1a** with exclusive regioselectivity was obtained in 82% yield at room temperature in DMAc. When other solvents, such as EA, MeCN, DMSO, DMPU, acetone, DCE, H_2O and mixtures of DMAc and H_2O, were tested, none led to a better yield than DMAc (entries 2). Studies on amines demonstrated that TEMED, DIPEA and PMDETA were inferior to DMAP, and Et_3N and DABCO were ineffective (entry 3). Changing the equivalents of **2a** and DMAP did not significantly affect the final yield (entries 4 and 5). Shortening the reaction time could lead to incomplete conversion, while prolonging the reaction time or increasing the reaction temperature would not further increase the conversion (entries 6 and 7). Further, research on the wavelengths of the light source revealed that 450-460 nm exerted a noteworthy influence on the efficiency of the reaction (entries 8 and 9). Besides, no desired product **3aa** was detected under sunlight irradiation (entry 10). Moreover, this reaction was unable to

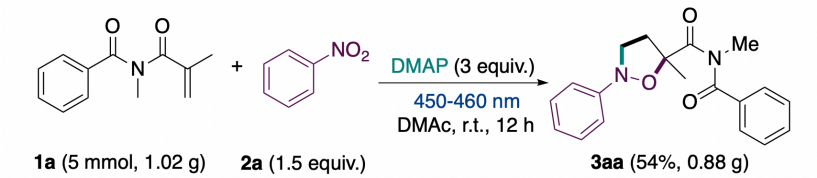
proceed when either light or amines were absent (entries 11 and 12). The reaction would not proceed when inorganic bases such as K_2CO_3 or Cs_2CO_3 were used instead of DMAP (entries 13). Finally, no notable decrease in yield was observed under nitrogen or oxygen atmospheres, showing that oxygen had almost no impact on the transformation process (entry 14).

4. General procedure for the synthesis of products (3aa as an example)



A Schlenk-tube was charged with **1a** (0.3 mmol), **2a** (0.45 mmol), DMAP (0.9 mmol) and DMAc (2 mL). The mixture was stirred under 450-460 nm light-irradiation (LEDs) at room temperature with air atmosphere for 12 hours. After completion, the reaction was quenched with saturated NaCl solution (10 mL) and extracted with EtOAc (4 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by chromatography on silica gel column (PE/EtOAc = 15/1-5/1) to afford **3aa (**82%) as a yellow oil.

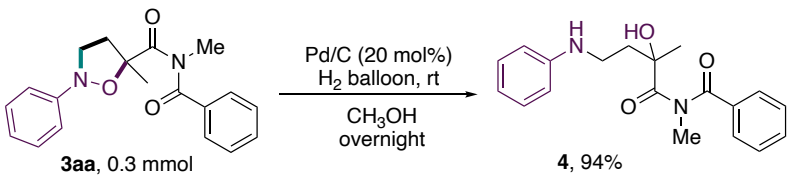
5. Gram-scale experiments



A 250 mL dried round-bottom flask was charged with a magnetic stirring bar, **1a** (5 mmol), **2a** (7.5 mmol), DMAP (15 mmol) and DMAc (15 mL). The resulting mixture was stirred under 450-460 nm light-irradiation (LEDs) at room temperature with air atmosphere for 12 hours. After completion, the reaction was quenched with saturated NaCl solution (30 mL) and extracted with EtOAc (10 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography. Compound **3aa** was isolated in 54% yield (0.88 g) as a yellow oil.

6. Synthetic transformations of production 3aa

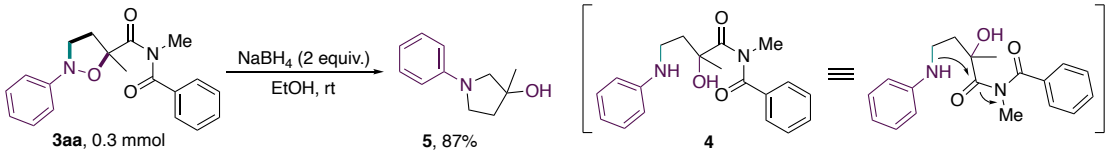
6.1 The synthesis of 1,3-amino alcohol derivatives[6]



A Schlenk-tube was charged with **3aa** (0.3 mmol), Pd/C (20 mol%) and CH_3OH (2 mL). The mixture was stirred overnight at room temperature under a hydrogen atmosphere. After completion, the reaction was quenched with saturated NaCl solution (10 mL) and extracted with EtOAc (4 mL).

The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by chromatography on silica gel column (PE/EtOAc = 15/1-5/1) to afford **4 (**94%) as a white oil.

6.2 The synthesis of phenylpyrrolidin derivatives



A Schlenk-tube was charged with **3aa** (0.3 mmol), $NaBH_4$ (0.6 mmol) and EtOH (2 mL). The mixture was stirred at room temperature for 5 min. After completion, the reaction was quenched with saturated NaCl solution (10 mL) and extracted with EtOAc (4 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by chromatography on silica gel column (PE/EtOAc = 15/1-5/1) to afford **5 (**87%) as a white oil. Based on previous works[5,7], the treatment of the compound **3aa** with $NaBH_4$ resulted in the cleavage of N-O bond, producing 1,3-aminoalcohol **4**. Subsequently, the amino group underwent spontaneous cyclization *via* deamidation and a carbonyl reduction process, ultimately generating the pyrrolidine derivative **5**.

7. "On/off" LED irradiation experiment

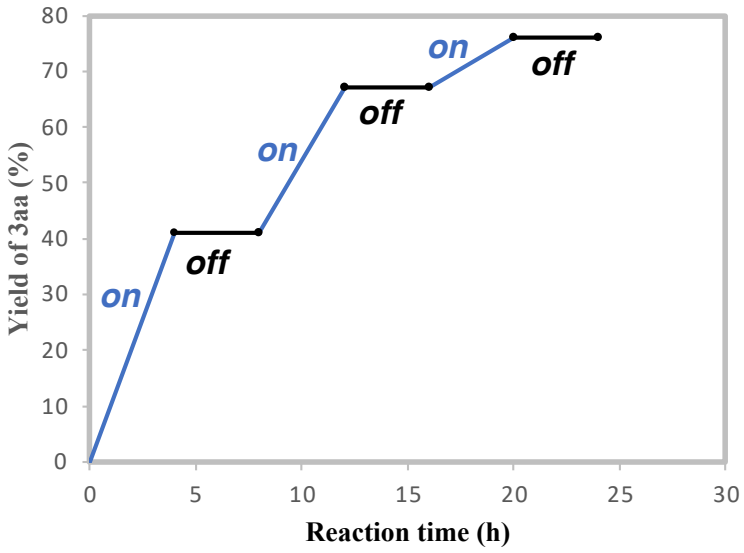


Figure S2. "On/off" LED irradiation experiment for the synthesis of **3aa**

"On/off" LED irradiation experiment was used to explore the essential role of visible light in this transformation, as descripted in Figure S2. The model reaction of **1a** and **2a** was designed to be irradiated under successive on/off LED irradiation conditions at every 4 h interval for a total of 24 h. The yield of **3aa** was isolated based on **1a** every 4 h. As can be seen, obvious increases in yield were observed once the reaction was irradiated with blue light. In contrast, almost no increase in

yield was observed when the reaction was conducted in dark, demonstrating an essential role of the visible-light irradiation in this transformation.

8. UV-vis absorbance experiment

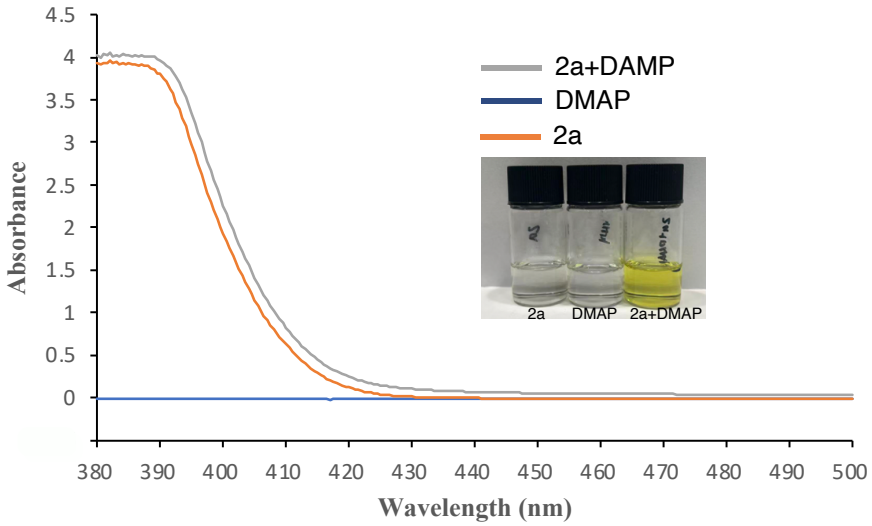


Figure S3. UV/vis absorbance spectra of a variety of solutions of **2a**, DMAP and **2a** + DMAP. All spectra were measured in DMAc with a concentration of 0.2 M.

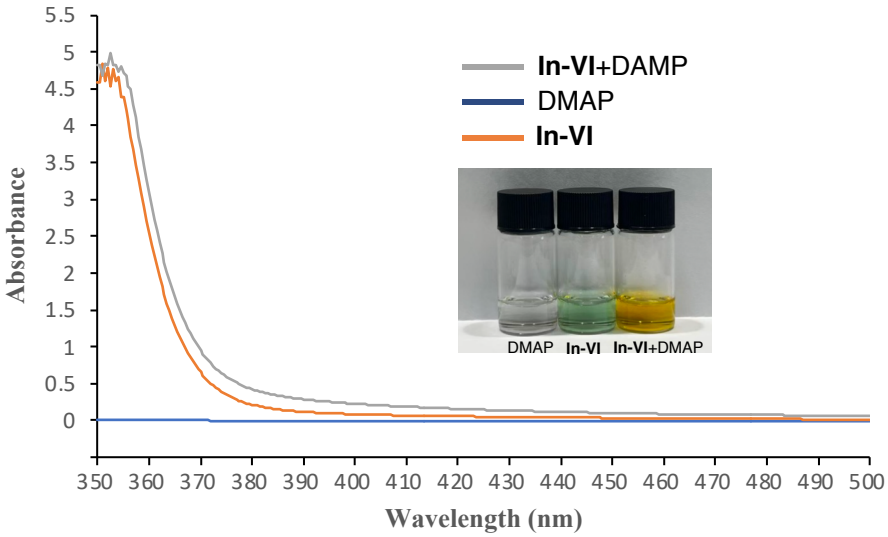


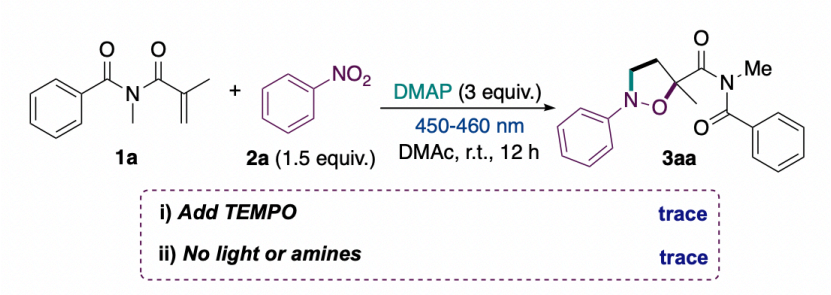
Figure S4. UV/vis absorbance spectra of a variety of solutions of **Int-VI**, DMAP and **Int-VI** + DMAP. All spectra were measured in DMAc with a concentration of 0.2 M.

As illustrated in Figure S3, a UV-vis absorbance experiment has been carried out to confirm the formation of the EDA complex. The blue UV absorbance line represents the DMAP solution, the orange one represents the nitrobenzene **2a** solution, and the gray one represents the mixed solution of **2a** and DMAP. UV-vis spectra revealed that upon mixing **2a** with DMAP, an obvious bathochromic shift of the UV-vis absorbance was observed. Besides, as shown in Figure S4, when nitrosobenzene **Int-VI** was mixed with DMAP, a similar bathochromic phenomenon occurred. This

strongly suggests that two separate EDA complexes are formed, one is the $PhNO_2$ – DMAP complex and another one is the PhNO – DMAP complex.

9. Mechanistic studies

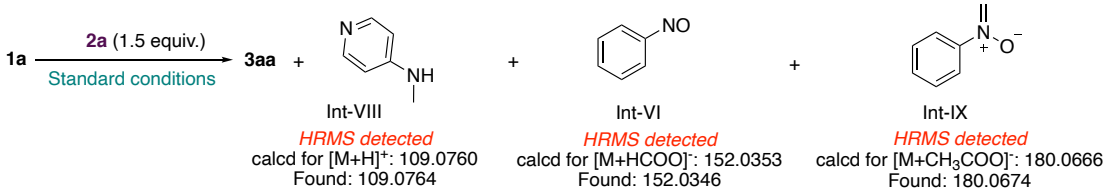
9.1 Control experiments



Standard conditions: 1a (0.3 mmol), **2a** (0.45 mmol) and DMAP (0.9 mmol) in DMAc (2 mL) under air atmosphere and stirred under 450-460 nm light-irradiation (LEDs) at room temperature for 12 h.

No desired product **3aa** was detected when TEMPO was employed as the radical scavenger, indicating that the reaction was completely inhibited and a radical pathway was involved in this transformation. Moreover, this reaction was unable to proceed when either light or amines were absent.

9.2 HRMS analysis for proposed intermediates



A Schlenk-tube was charged with **1a** (0.3 mmol), **2a** (0.45 mmol), DMAP (0.9 mmol) and DMAc (2 mL). The mixture was stirred under 450-460 nm light-irradiation (LEDs) at room temperature with air atmosphere for 12 hours. After completion, the reaction mixture was detected *via* HRMS. Evidently, the proposed intermediates were detected by HRMS.

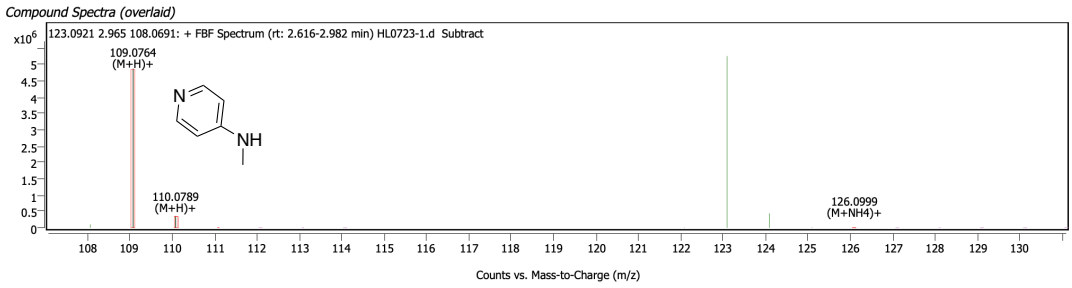


Figure S5. HRMS date of Int-VIII

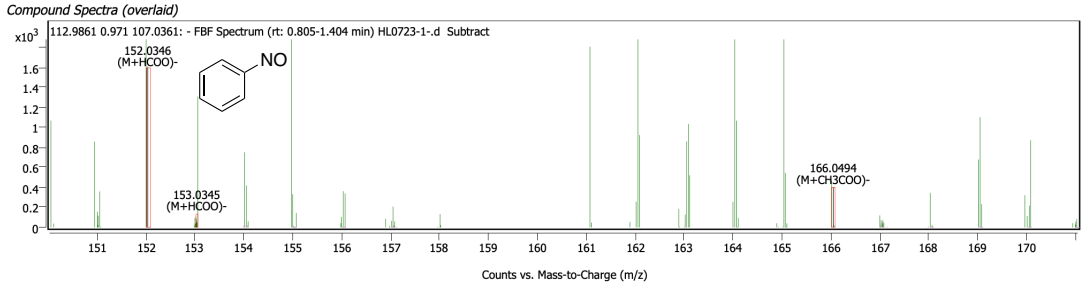


Figure S6. HRMS date of Int-VI

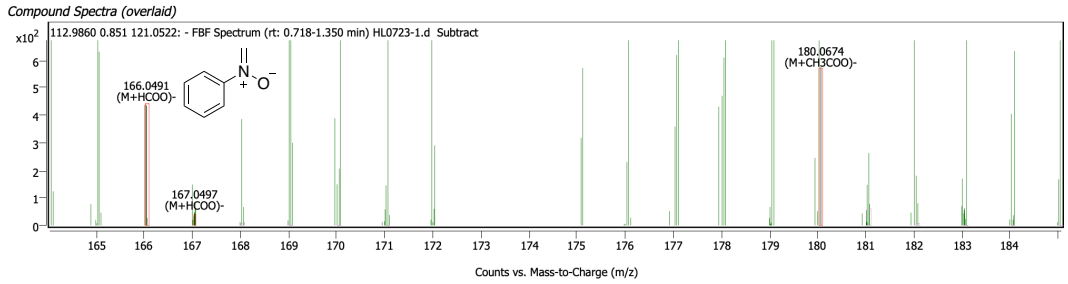


Figure S7. HRMS date of Int-IX

9.3 Quantum yield experiment

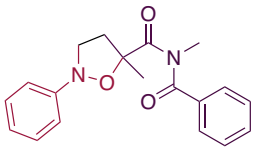
Based on the report by Yoon et al.,[8] the photon flux of the LED (λ_{max} = 458 nm) was determined using the standard ferrous oxalate spectrophotometric method. The photon flux of the LED with a wavelength range of 450-460nm (λmax = 458 nm) was determined by the Li group,[9] and the photon flux is calculated to be 5.54 × 10^{-9} einstein s^{-1}. To calculate the quantum yield, nitrobenzene (0.45 mmol), DMAP (0.9 mmol) and methacryloyl benzamide (0.3 mmol) were tested at λmax = 458 nm. Under the irradiation of an LED lamp, the reaction lasted for 12000 seconds, and the nuclear magnetic resonance yield was calculated using 1,3,5-trimethoxybenzene as the internal standard. The yield of 3aa was 19% (0.057×10^{-3} mol). Finally, according to formula (9-1), the quantum yield of the reaction can be obtained.

$$\textbf{Quantum Yield (}\Phi\textbf{) = moles of product formed / (flux × f × t)} \text{ ---- (9-1)}$$

$$\textbf{Quantum Yield = 0.057×10}^{-3}\textbf{/ (5.54 × 10}^{-9}\textbf{ × 0.999 × 12000) = 0.86}$$

(Where **Φ** is the quantum yield, **f** is the fraction of absorbed light at λ = 458 nm (**f = 1 – $10^{-A458\ nm}$ = 0.999**, and **t** is the exposure time (12000 s))

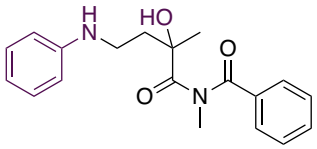
10. Characterization date



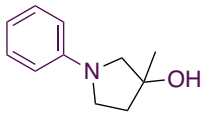
***N*-benzoyl-*N*,5-dimethyl-2-phenylisoxazolidine-5-carboxamide (3aa)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Colorless oil, yield 82%.

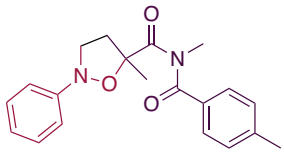
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 – 7.64 (m, 2H), 7.59 – 7.49 (m, 1H), 7.40 – 7.36 (m, 2H), 7.08 – 6.98 (m, 2H), 6.87 – 6.75 (m, 1H), 6.72 – 6.59 (m, 2H), 3.76 – 3.81 (m, 1H), 3.12 (s, 3H), 3.07 – 2.90 (m, 2H), 2.32 – 2.26 (m, 1H), 1.62 (s, 3H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 179.37, 174.20, 150.45, 133.76, 133.46, 129.99, 129.02, 128.63, 121.97, 115.55, 84.85, 52.93, 41.31, 34.42, 25.40.
HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{19}H_{20}N_2O_3$: 325.1547. Found: 325.1551.



***N*-(2-hydroxy-2-methyl-4-(phenylamino)butanoyl)-*N*-methylbenzamide (4)**
The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 94%.
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 – 7.96 (m, 2H), 7.66 – 7.62 (m, 1H), 7.51 – 7.48 (m, 2H), 7.17 – 7.14 (m, 2H), 6.71 – 6.69 (m, 1H), 6.57 – 6.55 (m, 2H), 6.38 – 6.36 (m, 1H), 3.24 (t, J = 7.1 Hz, 2H), 2.90 (d, J = 4.9 Hz, 3H), 2.67 – 2.63 (m, 1H), 2.53 – 2.49 (m, 1H), 1.87 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$) δ 173.06, 164.88, 147.89, 133.48, 130.29, 129.54, 129.25, 128.68, 117.40, 112.73, 84.33, 84.32, 39.17, 36.48, 26.58, 23.23.
HRMS (ESI) m/z: $[M + NH_4]^+$ Calcd for $C_{19}H_{22}N_2O_3$: 344.1969. Found: 344.1974.

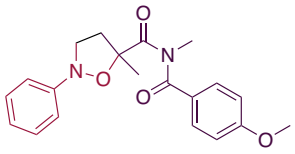


3-methyl-1-phenylpyrrolidin-3-ol (5)
The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Colorless oil, yield 87%.
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 – 7.27 (m, 2H), 7.09 – 7.04 (m, 2H), 7.00 – 6.98 (m, 1H), 3.71 – 3.56 (m, 3H), 3.46 – 3.42 (m, 1H), 2.51 – 2.47 (m, 1H), 2.14 – 2.10 (m, 1H), 1.39 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$) δ 150.95, 128.78, 121.93, 115.43, 82.90, 68.75, 53.90, 36.60, 22.69.
HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{11}H_{15}NO$: 178.1226. Found: 178.1221.



***N*,5-dimethyl-*N*-(4-methylbenzoyl)-2-phenylisoxazolidine-5-carboxamide (3ba)**
The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Colorless oil, yield 78%.
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.62 – 7.57 (m, 2H), 7.19 – 7.17 (m, 2H), 7.07 – 7.00 (m, 2H), 6.84 – 6.78 (m, 1H), 6.67 – 6.60 (m, 2H), 3.79 – 3.74 (m, 1H), 3.09 (s, 3H), 3.05 – 2.90 (m, 2H), 2.29 (s, 3H), 2.28 – 2.23 (m, 1H), 1.61 (s, 3H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 179.07, 174.05, 150.45, 144.01, 130.88, 130.24, 129.59, 128.57, 121.86, 115.53, 84.84, 52.94, 41.25, 34.44, 25.47, 21.56.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{20}H_{22}N_2O_3$: 339.1703. Found: 339.1704.



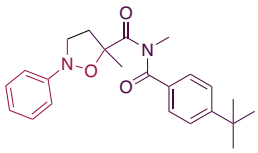
***N*-(4-methoxybenzoyl)-*N*,5-dimethyl-2-phenylisoxazolidine-5-carboxamide (3ca)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Orange oil, yield 79%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74 – 7.65 (m, 2H), 7.04 – 6.95 (m, 2H), 6.90 – 6.83 (m, 2H), 6.80 – 6.77 (m, 1H), 6.60 – 6.54 (m, 2H), 3.78 – 3.76 (m, 0.6H), 3.75 (s, 3H), 3.73 – 3.72 (m, 0.4H), 3.06 (s, 3H), 3.03 – 2.92 (m, 2H), 2.31 – 2.22 (m, 1H), 1.62 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 178.56, 173.41, 163.78, 150.41, 132.74, 128.47, 125.37, 121.75, 115.46, 114.38, 84.71, 55.97, 53.01, 41.15, 34.51, 25.60.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{20}H_{22}N_2O_4$: 355.1652. Found: 355.1657.



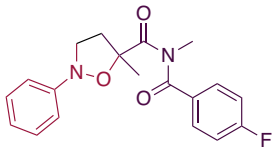
***N*-(4-(*tert*-butyl)benzoyl)-*N*,5-dimethyl-2-phenylisoxazolidine-5-carboxamide (3da)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 71%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.69 – 7.62 (m, 2H), 7.38 – 7.32 (m, 2H), 6.99 – 6.92 (m, 2H), 6.79 – 6.72 (m, 1H), 6.55 – 6.48 (m, 2H), 3.79 – 3.75 (m, 1H), 3.08 (s, 3H), 3.02 – 2.91 (m, 2H), 2.34 – 2.21 (m, 1H), 1.63 (s, 3H), 1.22 (s, 9H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 178.79, 173.89, 156.92, 150.28, 130.39, 130.35, 128.43, 125.85, 121.75, 115.44, 84.71, 52.97, 41.14, 35.25, 34.35, 31.20, 25.56.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{23}H_{28}N_2O_3$: 381.2173. Found: 381.2170.



***N*-(4-fluorobenzoyl)-*N*,5-dimethyl-2-phenylisoxazolidine-5-carboxamide (3ea)**

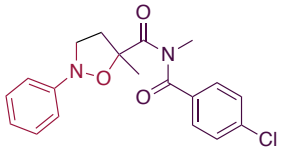
The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 80%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.81 – 7.74 (m, 2H), 7.21 – 7.14 (m, 2H), 7.08 – 7.00 (m, 2H), 6.86 – 6.79 (m, 1H), 6.64 – 6.59 (m, 2H), 3.85 – 3.74 (m, 1H), 3.10 (s, 3H), 3.04 – 2.94 (m, 2H), 2.36 – 2.23 (m, 1H), 1.64 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.01, 173.04, 165.34 (d, J = 251.9 Hz), 150.32, 133.11 (d, J = 9.7 Hz), 130.02 (d, J = 2.9 Hz), 128.59, 121.97, 116.11 (d, J = 22.2 Hz), 115.46, 84.74, 53.05, 41.18, 34.29, 25.35.

^{19}F NMR (377 MHz, DMSO-d_6) δ -105.97.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{19}H_{19}FN_2O_3$: 343.1452. Found: 343.1448.



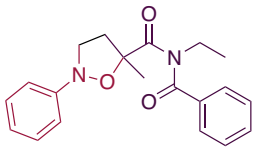
***N*-(4-chlorobenzoyl)-*N*,5-dimethyl-2-phenylisoxazolidine-5-carboxamide (3fa)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 86%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.69 – 7.63 (m, 2H), 7.45 – 7.37 (m, 2H), 7.09 – 7.02 (m, 2H), 6.87 – 6.79 (m, 1H), 6.68 – 6.62 (m, 2H), 3.82 – 3.76 (m, 1H), 3.12 (s, 3H), 3.06 – 2.91 (m, 2H), 2.31 – 2.25 (m, 1H), 1.63 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.17, 173.21, 150.30, 138.33, 132.49, 131.82, 129.13, 128.65, 122.03, 115.51, 84.80, 53.01, 41.16, 34.19, 25.19.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{19}H_{19}ClN_2O_3$: 359.1157. Found: 359.1159.



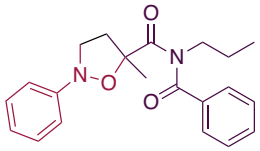
***N*-benzoyl-*N*-ethyl-5-methyl-2-phenylisoxazolidine-5-carboxamide (3ga)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 84%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74 – 7.69 (m, 2H), 7.58 – 7.50 (m, 1H), 7.41 – 7.37 (m, 2H), 7.08 – 7.01 (m, 2H), 6.86 – 6.79 (m, 1H), 6.70 – 6.62 (m, 2H), 3.80 – 3.64 (m, 2H), 3.56 – 3.47 (m, 1H), 3.03 – 2,99 (m, 1H), 2.94 – 2.87 (m, 1H), 2.33 – 2.27 (m, 1H), 1.55 (s, 3H), 1.08 (t, J = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.54, 174.07, 150.54, 134.27, 133.51, 129.94, 129.05, 128.60, 122.00, 115.62, 84.80, 53.15, 42.19, 41.67, 25.74, 14.03.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{20}H_{22}N_2O_3$: 361.1523. Found: 361.1516.



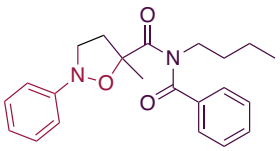
***N*-benzoyl-5-methyl-2-phenyl-*N*-propylisoxazolidine-5-carboxamide (3ha)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 76%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74 – 7.69 (m, 2H), 7.56 – 7.50 (m, 1H), 7.41 – 7.37 (m, 2H), 7.08 – 7.00 (m, 2H), 6.86 – 6.78 (m, 1H), 6.66 – 6.60 (m, 2H), 3.78 – 3.72 (m, 1H), 3.68 – 3.61 (m, 1H), 3.43 – 3.39 (m, 1H), 3.05 – 2.85 (m, 2H), 2.33 – 2.27 (m, 1H), 1.62 – 1.56 (m, 0.7H), 1.54 (s, 3H), 1.52 – 1.43 (m, 1.3H), 0.80 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.47, 174.12, 150.53, 134.22, 133.53, 130.01, 129.05, 128.58, 122.00, 115.62, 84.85, 53.17, 48.76, 41.72, 25.84, 22.08, 11.46.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{21}H_{24}N_2O_3$: 353.1860. Found: 353.1856.



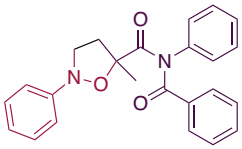
***N*-benzoyl-*N*-butyl-5-methyl-2-phenylisoxazolidine-5-carboxamide (3ia)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 70%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.73 – 7.68 (m, 2H), 7.57 – 7.51 (m, 1H), 7.41 – 7.38 (m, 2H), 7.07 – 6.99 (m, 2H), 6.86 – 6.79 (m, 1H), 6.68 – 6.61 (m, 2H), 3.79 – 3.62 (m, 2H), 2.46 – 3.40 (m, 1H), 3.07 – 2.79 (m, 2H), 2.34 – 2.67 (m, 1H), 1.53 (s, 3H), 1.51 – 1.37 (m, 2H), 1.26 – 1.17 (m, 2H), 0.80 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.43, 174.13, 150.53, 134.23, 133.54, 129.99, 129.06, 128.59, 122.01, 115.62, 84.84, 53.18, 46.92, 41.71, 30.81, 25.81, 19.83, 13.98.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{22}H_{26}N_2O_3$: 389.1836. Found: 389.1841.



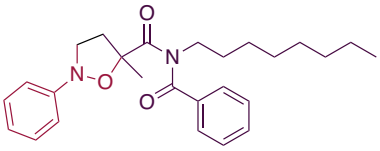
***N*-benzoyl-5-methyl-*N*,2-diphenylisoxazolidine-5-carboxamide (3ja)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 73%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74 – 7.69 (m, 2H), 7.39 – 7.32 (m, 3H), 7.25 – 7.14 (m, 5H), 7.03 – 6.99 (m, 2H), 6.86 – 6.77 (m, 1H), 6.69 – 6.62 (m, 2H), 4.00 – 3.95 (m, 1H), 3.17 – 2.99 (m, 2H), 2.49 – 2.43 (m, 1H), 1.75 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 181.79, 172.14, 150.51, 139.50, 133.41, 133.29, 130.81, 129.87, 128.68, 128.53, 127.86, 127.83, 121.98, 115.65, 85.14, 53.24, 42.24, 26.06.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{24}H_{22}N_2O_3$: 409.1523. Found: 409.1531.



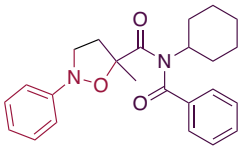
***N*-benzoyl-5-methyl-*N*-octyl-2-phenylisoxazolidine-5-carboxamide (3ka)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Orange oil, yield 64%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.73 – 7.67 (m, 1.5H), 7.55 – 7.50 (m, 1H), 7.40 – 7.36 (m, 1.5H), 7.29 – 7.21 (m, 1H), 7.06 – 7.00 (m, 1.5H), 6.97 – 6.92 (m, 1.3H), 6.83 – 6.80 (m, 0.7H), 6.68 – 6.60 (m, 1.5H), 3.76 – 3.63 (m, 2H), 3.48 – 3.39 (m, 0.7H), 3.35 – 3.28 (m, 0.3H), 3.06 – 2.82 (m, 2H), 2.32 – 2.26 (m, 0.7H), 2.22 – 2.16 (m, 0.3H), 1.55 (d, J = 8.5 Hz, 3H), 1.51 – 1.38 (m, 2H), 1.25 – 1.20 (m, 4H), 1.18 – 1.11 (m, 6H), 0.82 (t, J = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.41 (d, J = 3.4 Hz), 174.11, 150.88 (d, J = 71.4 Hz), 134.26, 133.47, 129.95, 129.02 (d, J = 2.9 Hz), 128.55, 122.07 (d, J = 16.4 Hz), 115.57 (d, J = 10.6 Hz), 85.17 (d, J = 67.3 Hz), 53.27 (d, J = 18.2 Hz), 47.11, 41.70, 31.60, 28.92 (d, J = 3.1 Hz), 28.57, 26.48, 25.77, 25.43, 22.50, 14.37.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{26}H_{34}N_2O_3$: 423.2642. Found: 423.2643.



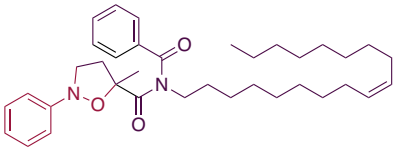
<u>*N*-benzoyl-*N*-cyclohexyl-5-methyl-2-phenylisoxazolidine-5-carboxamide (3la)</u>

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Colorless oil, yield 71%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.78 – 7.72 (m, 2H), 7.58 – 7.53 (m, 1H), 7.45 – 7.41 (m, 2H), 7.14 – 7.07 (m, 2H), 6.88 – 6.84 (m, 1H), 6.69 – 6.67 (m, 2H), 4.07 – 3.99 (m, 1H), 3.69 – 3.64 (m, 1H), 3.04 – 2.98 (m, 1H), 2.80 – 2.73 (m, 1H), 2.30 – 2.24 (m, 1H), 1.83 – 1.66 (m, 5H), 1.64 – 1.50 (m, 2H), 1.30 (s, 3H), 1.24 – 1.12 (m, 2H), 1.05 – 0.94 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.01, 173.36, 150.66, 136.47, 133.48, 130.05, 129.02, 128.68, 122.12, 115.69, 84.81, 57.97, 53.03, 42.05, 31.83, 29.43, 26.19, 26.14, 25.86, 25.39.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{24}H_{28}N_2O_3$: 393.2173. Found: 393.2177.



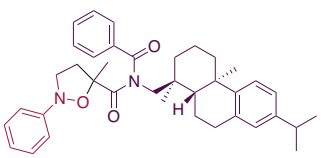
<u>(*Z*)-*N*-benzoyl-5-methyl-*N*-(octadec-9-en-1-yl)-2-phenylisoxazolidine-5-carboxamide (3ma)</u>

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 67%.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 – 7.67 (m, 2H), 7.54 – 7.51 (m, 1H), 7.39 – 7.31 (m, 2H), 7.05 – 7.02 (m, 2H), 6.83 – 6.80 (m, 1H), 6.65 – 6.63 (m, 2H), 5.34 – 5.26 (m, 2H), 3.74 – 3.71 (m, 1H), 3.69 – 3.64 (m, 1H), 3.44 – 3.39 (m, 1H), 3.04 – 2.99 (m, 1H), 2.92 – 2.86 (m, 1H), 2.31 – 2.27 (m, 1H), 2.00 – 1.92 (m, 4H), 1.53 (s, 3H), 1.31 – 1.25 (m, 6H), 1.24 – 1.22 (m, 9H), 1.19 – 1.16 (m, 9H), 0.87 – 0.80 (m, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 179.40, 174.08, 150.53, 134.29, 133.46, 130.07, 130.06, 129.92, 129.00, 128.56, 121.99, 115.62, 84.85, 53.17, 47.09, 41.69, 31.75, 29.56, 29.50, 29.30, 29.15, 29.10, 29.05, 28.91, 28.56, 27.03, 26.46, 25.75, 22.56, 14.38.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{36}H_{52}N_2O_3$: 583.3870. Found: 583.3873.



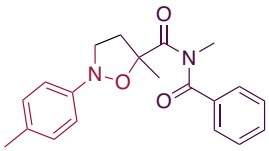
<u>*N*-benzoyl-N-(((1*S*,4a*R*,10a*S*)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-yl)methyl)-5-methyl-2-phenylisoxazolidine-5-carboxamide (3na)</u>

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 72% (dr = 1.4:1).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 – 7.76 (m, 2H), 7.40 – 7.38 (m, 0.5H), 7.34 – 7.31 (m, 0.5H), 7.26 – 7.24 (m, 1H), 7.20 – 7.17 (m, 1.5H), 7.13 – 7.11 (m, 0.5H), 7.03 – 6.92 (m, 3H), 6.89 – 6.87 (m, 1H), 6.80 – 6.75 (m, 1H), 6.54 – 6.49 (m, 2H), 4.30 – 4.27 (m, 0.5H), 3.91 – 3.89 (m, 0.5H), 3.70 – 3.66 (m, 1H), 3.61 – 3.59 (m, 0.5H), 3.36 – 3.25 (m, 1H), 3.17 – 3.15 (m, 0.5H), 3.05 – 2.96 (m, 1H), 2.92 – 2.73 (m, 3H), 2.32 – 2.17 (m, 2H), 1.93 – 1.86 (m, 0.4H), 1.81 – 1.62 (m, 8H), 1.61 – 1.54 (m, 1H), 1.50 – 1.41 (m, 0.7H), 1.33 – 1.31 (m, 1H), 1.28 – 1.17 (m, 9H), 1.06 (s, 1.3H), 0.90 (s, 1.8H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 178.18, 175.12 & 174.95, 150.15 & 150.05, 147.42 & 147.39, 145.55 & 145.46, 134.68 & 134.65, 132.95 & 132.87, 130.52, 128.30 & 128.20, 128.07 & 128.01, 126.79, 124.05, 123.79 & 123.77, 123.67, 121.63 & 121.53, 115.29 & 115.17, 85.13 & 85.09, 58.92 & 58.47, 53.58 & 53.51, 47.37 & 46.15, 41.38 & 41.07, 40.41 & 40.03, 38.19, 38.09 & 37.92, 37.71 & 37.61, 35.54, 33.46, 30.11 & 29.73, 25.93 & 25.75, 25.64 & 25.49, 24.02 & 24.00, 19.37 & 19.30, 18.96 & 18.62, 18.48 & 17.44.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{38}H_{46}N_2O_3$: 579.3581. Found: 579.3586.



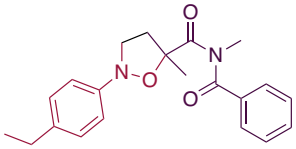
<u>*N*-benzoyl-*N*,5-dimethyl-2-(*p*-tolyl)isoxazolidine-5-carboxamide (3ab)</u>

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 72%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71 – 7.64 (m, 2H), 7.59 – 7.52 (m, 1H), 7.41 – 7.37 (m, 2H), 6.88 – 6.83 (m, 2H), 6.61 – 6.54 (m, 2H), 3.75 – 3.70 (m, 1H), 3.12 (s, 3H), 3.04 – 2.86 (m, 2H), 3.30 – 2.22 (m, 1H), 2.15 (s, 3H), 1.60 (s, 3H)

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.57, 174.20, 148.24, 133.91, 133.38, 130.97, 129.92, 129.08, 129.04, 115.84, 84.82, 53.11, 41.46, 34.41, 25.47, 20.62.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{20}H_{22}N_2O_3$: 339.1703. Found: 339.1705.



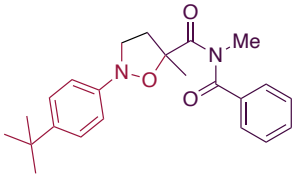
<u>*N*-benzoyl-2-(4-ethylphenyl)-*N*,5-dimethylisoxazolidine-5-carboxamide (3ac)</u>

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Orange oil, yield 75%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71 – 7.63 (m, 2H), 7.57 – 7.49 (m, 1H), 7.40 – 7.36 (m, 2H), 6.92 – 6.85 (m, 2H), 6.63 – 6.57 (m, 2H), 3.76 – 3.70 (m, 1H), 3.13 (s, 3H), 3.05 – 2.87 (m, 2H), 2.48 – 2.42 (m, 2H), 2.30 – 2.24 (m, 1H), 1.08 (t, J = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, DMSO-d_6)δ 179.57, 174.19, 148.42, 137.49, 133.95, 133.33, 129.91, 129.00, 127.91, 115.85, 84.83, 53.10, 41.46, 34.38, 27.83, 25.41, 16.27.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{21}H_{24}N_2O_3$: 353.1860. Found: 353.1864.



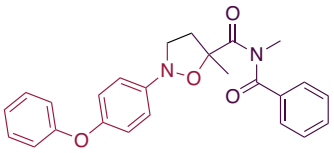
***N*-benzoyl-2-(4-(*tert*-butyl)phenyl)-*N*,5-dimethylisoxazolidine-5-carboxamide (3ad)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 67%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.68 – 7.62 (m, 2H), 7.54 – 7.47 (m, 1H), 7.39 – 7.35 (m, 2H), 7.10 – 7.05 (m, 2H), 6.66 – 6.59 (m, 2H), 3.75 – 3.70 (m, 1H), 3.14 (s, 3H), 3.08 – 2.99 (m, 1H), 2.96 – 2.89 (m, 1H), 2.29 – 2.23 (m, 1H), 1.59 (s, 3H), 1.19 (s, 9H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.57, 174.18, 148.08, 144.35, 134.04, 133.25, 129.88, 128.96, 125.31, 115.46, 84.89, 53.02, 41.45, 34.34, 34.18, 31.66, 25.30.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{23}H_{28}N_2O_3$: 381.2173. Found: 381.2177.



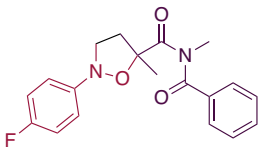
***N*-benzoyl-*N*,5-dimethyl-2-(4-phenoxyphenyl)isoxazolidine-5-carboxamide (3ae)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Red oil, yield 62%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74 – 7.69 (m, 2H), 7.57 – 7.51 (m, 1H), 7.40 – 7.33 (m, 4H), 7.09 – 7.04 (m, 1H), 6.86 – 6.81 (m, 2H), 6.75 – 6.65 (m, 4H), 3.80 – 3.74 (m, 1H), 3.10 (s, 3H), 3.05 – 2.93 (m, 2H), 2.40 – 2.24 (m, 1H), 1.63 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.27, 174.15, 158.24, 150.81, 146.62, 133.53, 133.51, 130.31, 130.19, 129.01, 123.07, 119.89, 117.72, 117.28, 84.83, 53.43, 41.45, 34.38, 25.39.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{25}H_{24}N_2O_4$: 439.1628. Found: 439.1627.



***N*-benzoyl-2-(4-fluorophenyl)-*N*,5-dimethylisoxazolidine-5-carboxamide (3af)**

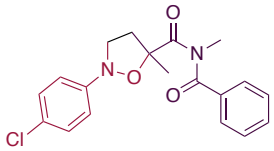
The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 84%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.76 – 7.65 (m, 2H), 7.57 – 7.50 (m, 1H), 7.40 – 7.36 (m, 2H), 6.89 – 6.84 (m, 2H), 6.68 – 6.64 (m, 2H), 3.83 – 3.70 (m, 1H), 3.09 (s, 3H), 3.02 – 2.90 (m, 2H), 2.36 – 2.22 (m, 1H), 1.62 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.24, 174.15, 159.58 – 153.77 (m, 1C), 146.90 (d, J = 2.2 Hz), 133.55 (d, J = 3.1 Hz), 129.56 (d, J = 105.3 Hz), 126.26, 117.31 (d, J = 8.0 Hz), 115.15 (d, J = 22.5 Hz), 111.11, 84.92, 53.51, 41.45, 34.40, 25.44.

^{19}F NMR (377 MHz, DMSO-d_6) δ -122.36.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{19}H_{19}FN_2O_3$: 343.1452. Found: 343.1456.



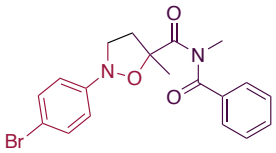
***N*-benzoyl-2-(4-chlorophenyl)-*N*,5-dimethylisoxazolidine-5-carboxamide (3ag)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Colorless oil, yield 80%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.79 – 7.66 (m, 2H), 7.58 – 7.51 (m, 1H), 7.40 – 7.36 (m, 2H), 7.08 – 7.01 (m, 2H), 6.70 – 6.58 (m, 2H), 3.81 – 3.76 (m, 1H), 3.09 (s, 3H), 3.06 – 2.92 (m, 2H), 2.33 – 2.73 (m, 1H), 1.63 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 178.94, 174.11, 149.21, 133.59, 133.45, 130.09, 129.05, 128.38, 125.72, 117.10, 85.07, 52.95, 41.28, 34.43, 25.37.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{19}H_{19}ClN_2O_3$: 381.0976. Found: 381.0982.



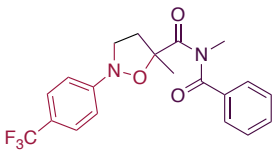
***N*-benzoyl-2-(4-bromophenyl)-*N*,5-dimethylisoxazolidine-5-carboxamide (3ah)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Colorless oil, yield 82%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.79 – 7.65 (m, 2H), 7.60 – 7.49 (m, 1H), 7.41 – 7.37 (m, 2H), 7.24 – 7.13 (m, 2H), 6.66 – 6.52 (m, 2H), 3.80 – 3.75 (m, 1H), 3.09 (s, 3H), 3.06 – 2.90 (m, 2H), 2.34 – 2.23 (m, 1H), 1.62 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 178.93, 174.14, 149.63, 133.61, 133.48, 131.28, 130.09, 129.09, 117.52, 113.59, 85.10, 52.84, 41.25, 34.44, 25.36.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{19}H_{19}BrN_2O_3$: 425.0471. Found: 425.0475.



***N*-benzoyl-*N*,5-dimethyl-2-(4-(trifluoromethyl)phenyl)isoxazolidine-5-carboxamide (3ai)**

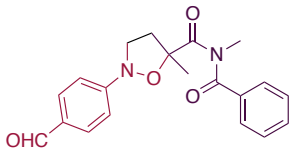
The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Red oil, yield 87%.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 – 7.71 (m, 2H), 7.42 – 7.39 (m, 1H), 7.26 – 7.22 (m, 2H), 7.20 – 7.18 (m, 2H), 6.60 – 6.58 (m, 2H), 3.78 – 3.74 (m, 1H), 3.31 – 3.26 (m, 1H), 3.16 (s, 3H), 3.15 – 3.11 (m, 1H), 2.38 – 2.27 (m, 1H), 1.82 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ178.33, 173.99, 152.29, 133.38, 132.67, 130.19, 128.44, 125.41 – 125.33 (m, 2C), 123.69 – 122.53 (m, 1C), 114.53, 85.20, 52.50, 40.97, 34.33, 24.99.

^{19}F NMR (377 MHz, DMSO-d_6) δ -60.08.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{20}H_{19}F_3N_2O_3$: 393.1421. Found:393.1418.



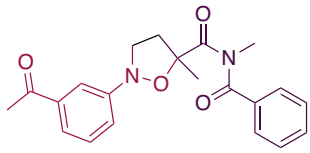
<u>*N*-benzoyl-2-(4-formylphenyl)-*N*,5-dimethylisoxazolidine-5-carboxamide (3aj)</u>

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 79%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.73 (s, 1H), 7.73 – 7.68 (m, 2H), 7.57 – 7.49 (m, 3H), 7.39 – 7.36 (m, 2H), 6.73 – 6.66 (m, 2H), 3.91 – 3.85 (m, 1H), 3.31 – 3.25 (m, 1H), 3.10 (s, 3H), 3.04 – 2.97 (m, 1H), 2.42 – 2.32 (m, 1H), 1.67 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 191.60, 178.25, 174.12, 154.40, 133.75, 133.29, 130.83, 130.15, 129.62, 129.11, 114.36, 85.54, 51.49, 40.79, 34.54, 25.01.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{20}H_{20}N_2O_4$: 353.1496. Found: 353.1501.



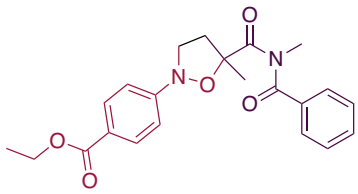
<u>2-(3-acetylphenyl)-*N*-benzoyl-*N*,5-dimethylisoxazolidine-5-carboxamide (3ak)</u>

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Colorless oil, yield 74%.

^{1}H NMR (400 MHz, DMSO-d_6)δ 7.71 – 7.66 (m, 2H), 7.53 – 7.46 (m, 1H), 7.41 – 7.38 (m, 1H), 7.35 – 7.31 (m, 2H), 7.22 – 7.18 (m, 1H), 7.13 – 7.12 (m, 1H), 6.91 – 6.83 (m, 1H), 3.91 – 3.86 (m, 1H), 3.08 (s, 3H), 3.06 – 2.93 (m, 2H), 2.35 (s, 3H), 2.34 – 2.29 (m, 1H), 1.65 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 197.96, 179.11, 174.15, 150.48, 137.31, 133.58, 133.43, 130.13, 129.06, 129.01, 121.73, 119.95, 114.83, 85.05, 52.87, 41.33, 34.51, 27.00, 25.38.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{21}H_{22}N_2O_4$: 367.1652. Found: 367.1656.



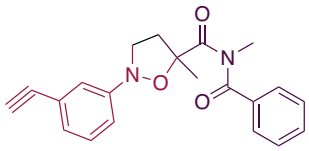
<u>ethyl 4-(5-(benzoyl(methyl)carbamoyl)-5-methylisoxazolidin-2-yl)benzoate (3al)</u>

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 83%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.72 – 7.67 (m, 2H), 7.63 – 7.57 (m, 2H), 7.55 – 7.49 (m, 1H), 7.39 – 7.35 (m, 2H), 6.73 – 6.59 (m, 2H), 4.23 (q, J = 7.1 Hz, 2H), 3.86 – 3.81 (m, 1H), 3.23 – 3.16 (m, 1H), 3.10 (s, 3H), 3.04 – 2.94 (m, 1H), 2.36 – 2.30 (m, 1H), 1.66 (s, 3H), 1.27 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 178.51, 174.12, 165.83, 153.69, 133.62, 133.42, 130.10, 129.06, 122.43, 114.38, 85.37, 60.66, 51.93, 40.93, 34.48, 25.10, 14.66.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{22}H_{24}N_2O_5$: 397.1758. Found: 397.1762.



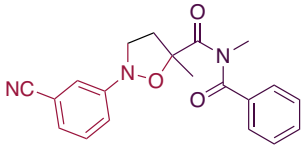
***N*-benzoyl-2-(3-ethynylphenyl)-*N*,5-dimethylisoxazolidine-5-carboxamide (3am)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 82%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74 – 7.66 (m, 2H), 7.57 – 7.49 (m, 1H), 7.39 – 7.36 (m, 2H), 7.07 – 6.99 (m, 1H), 6.92 – 6.89 (m, 1H), 6.71 – 6.63 (m, 2H), 4.06 (s, 1H), 3.84 – 3.79 (m, 1H), 3.39 (s, 3H), 3.05 – 2.91 (m, 2H), 2.33 – 2.78 (m, 1H), 1.63 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 178.94, 174.12, 150.35, 133.67, 133.37, 130.07, 129.09, 128.98, 125.18, 122.09, 118.42, 116.12, 84.95, 83.85, 80.67, 52.76, 41.22, 34.44, 25.44.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{21}H_{20}N_2O_3$: 349.1547. Found: 349.1555.



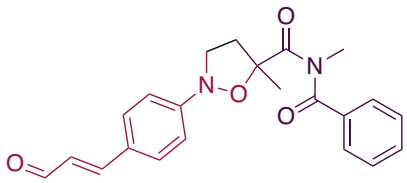
***N*-benzoyl-2-(3-cyanophenyl)-*N*,5-dimethylisoxazolidine-5-carboxamide (3an)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Colorless oil, yield 67%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.76 – 7.69 (m, 2H), 7.58 – 7.50 (m, 1H), 7.39 – 7.35 (m, 2H), 7.23 – 7.21 (m, 2H), 6.94 – 6.91 (m, 1H), 6.80 – 6.76 (m, 1H), 3.90 – 3.85 (m, 1H), 3.11 – 3.09 (m, 0.5H), 3.07 (s, 3H), 3.06 – 2.96 (m, 1.5H), 2.38 – 2.32 (m, 1H), 1.66 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 178.43, 174.06, 150.41, 133.94, 132.93, 130.27, 129.96, 129.16, 125.16, 119.81, 118.97, 117.98, 111.53, 85.15, 52.49, 41.06, 34.43, 25.41.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{20}H_{19}N_3O_3$: 372.1319. Found: 372.1324.



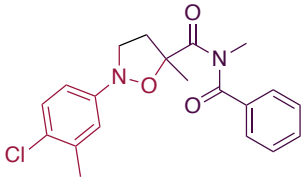
(*E*)-*N*-benzoyl-*N*,5-dimethyl-2-(4-(3-oxoprop-1-en-1-yl)phenyl)isoxazolidine-5-carboxamide (3ao)

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 58%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.57 (d, J = 7.8 Hz, 1H), 7.71 – 7.65 (m, 2H), 7.60 – 7.50 (m, 2H), 7.47 – 7.34 (m, 4H), 6.74 – 6.61 (m, 3H), 3.88 – 3.82 (m, 1H), 3.23 – 3.14 (m, 1H), 3.11 (s, 3H), 3.02 – 2.95 (m, 1H), 2.37 – 2.31 (m, 1H), 1.65 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 194.54, 178.66, 174.16, 153.71, 152.42, 133.63, 133.49, 130.06, 129.80, 129.11, 127.28, 126.57, 115.16, 85.34, 52.02, 41.01, 34.51, 25.18.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{22}H_{22}N_2O_4$: 379.1652. Found: 379.1659.



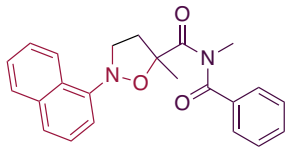
***N*-benzoyl-2-(4-chloro-3-methylphenyl)-*N*,5-dimethylisoxazolidine-5-carboxamide (3ap)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 82%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74 – 7.69 (m, 2H), 7.59 – 7.52 (m, 1H), 7.41 – 7.38 (m, 2H), 7.06 – 7.04 (m, 1H), 6.53 – 6.42 (m, 2H), 3.81 – 3.71 (m, 1H), 3.08 (s, 3H), 3.04 – 2.91 (m, 2H), 2.39 – 2.26 (m, 1H), 2.01 (s, 3H), 1.64 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.06, 174.07, 149.04, 135.42, 133.67, 133.34, 130.22, 129.10, 128.77, 125.99, 118.24, 114.60, 84.94, 52.67, 41.36, 34.44, 25.56, 20.06.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{20}H_{21}ClN_2O_3$: 373.1313. Found: 373.1324.



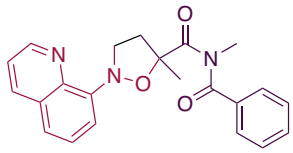
***N*-benzoyl-*N*,5-dimethyl-2-(naphthalen-1-yl)isoxazolidine-5-carboxamide (3aq)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Red oil, yield 73%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.09 – 8.03 (m, 1H), 7.88 – 7.82 (m, 1H), 7.66 – 7.63 (m, 2H), 7.57 – 7.55 (m, 1H), 7.53 – 7.48 (m, 2H), 7.34 – 7.23 (m, 2H), 7.16 – 7.05 (m, 3H), 3.89 – 3.78 (m, 1H), 3.10 (s, 3H), 3.08 – 2.98 (m, 2H), 2.39 – 2.27 (m, 1H), 1.72 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.44, 174.24, 146.31, 133.91, 133.62, 133.07, 129.87, 128.58, 128.33, 126.54, 126.36, 126.07, 125.95, 124.80, 123.45, 113.39, 84.95, 55.98, 41.70, 34.22, 25.12.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{23}H_{22}N_2O_3$: 375.1703. Found: 375.1707.



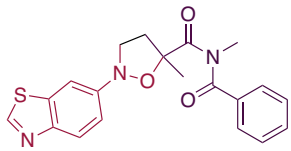
***N*-benzoyl-*N*,5-dimethyl-2-(quinolin-8-yl)isoxazolidine-5-carboxamide (3ar)**

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Red oil, yield 52%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.90 – 8.89 (m, 1H), 8.29 – 8.27 (m, 1H), 7.74 – 7.67 (m, 2H), 7.55 – 7.52 (m, 1H), 7.46 – 7.44 (m, 1H), 7.35 – 7.28 (m, 1H), 7.19 – 7.15 (m, 1H), 7.13 – 7.07 (m, 2H), 7.04 – 7.02 (m, 1H), 4.66 – 4.52 (m, 1H), 3.49 – 3.39 (m, 1H), 3.11 (s, 3H), 3.10 – 3.05 (m, 1H), 2.33 – 2.29 (m, 1H), 1.73 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ179.25, 174.33, 148.93, 146.92, 139.17, 136.57, 133.59, 133.17, 130.05, 128.64, 128.52, 126.62, 122.39, 121.81, 114.07, 84.02, 55.26, 41.76, 34.15, 24.88.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{22}H_{21}N_3O_3$: 498.1475. Found: 498.1478.



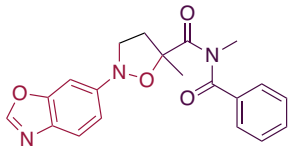
2-(benzo[*d*]thiazol-6-yl)-*N*-benzoyl-*N*,5-dimethylisoxazolidine-5-carboxamide (3as)

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Red oil, yield 66%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.13 (s, 1H), 7.77 – 7.70 (m, 3H), 7.48 – 7.42 (m, 1H), 7.34 – 7.31 (m, 2H), 7.17 – 7.16 (m, 1H), 6.93 – 6.90 (m, 1H), 3.90 – 3.85 (m, 1H), 3.15 – 3.13 (m, 1H), 3.12 (s, 3H), 3.05 – 2.98 (m, 1H), 2.39 – 2.33 (m, 1H), 1.68 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 178.97, 174.16, 154.06, 148.60, 148.11, 134.49, 133.65, 133.34, 130.16, 129.05, 122.87, 115.72, 107.64, 85.08, 53.19, 41.35, 34.41, 25.55.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{20}H_{19}N_3O_3S$: 382.1220. Found: 382.1225.



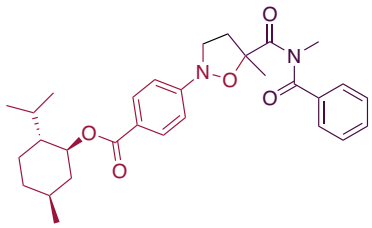
2-(benzo[*d*]oxazol-6-yl)-*N*-benzoyl-*N*,5-dimethylisoxazolidine-5-carboxamide (3at)

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Orange oil, yield 53%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.52 (s, 1H), 7.74 – 7.66 (m, 2H), 7.49 – 7.42 (m, 2H), 7.34 – 7.30 (m, 2H), 6.87 – 6.86 (m, 1H), 6.78 – 6.75 (m, 1H), 3.89 – 3.84 (m, 1H), 3.14 – 3.12 (m, 0.7H), 3.10 (s, 3H), 3.09 – 3.08 (m, 0.3H), 3.04 – 2.97 (m, 1H), 2.38 – 3.32 (m, 1H), 1.66 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 179.01, 174.16, 153.63, 149.93, 148.87, 134.53, 133.52, 133.41, 130.12, 129.01, 119.76, 113.46, 98.00, 85.08, 53.44, 41.37, 34.44, 25.47.

HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{20}H_{19}N_3O_4$: 366.1448. Found: 366.1458.

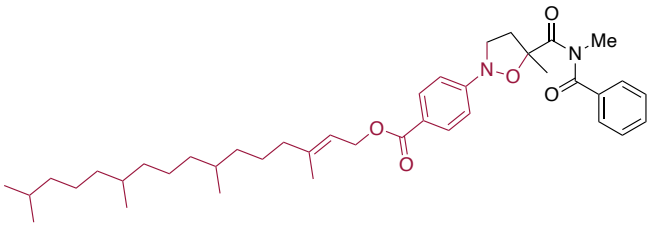


(1*S*,2*R*,5*S*)-2-isopropyl-5-methylcyclohexyl 4-(5-(benzoyl(methyl)carbamoyl)-5-methylisoxazolidin-2-yl)benzoate (3au)

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 83%.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 – 7.72 (m, 2H), 7.67 – 7.63 (m, 2H), 7.44 – 7.34 (m, 1H), 7.28 – 7.22 (m, 2H), 6.57 – 6.52 (m, 2H), 4.88 – 4.83 (m, 1H), 3.77 – 3.73 (m, 1H), 3.29 – 3.22 (m, 1H), 3.19 – 3.16 (m, 0.7H), 3.16 (d, J = 4.2 Hz, 3H), 3.15 – 3.14 (m, 0.3H), 2.32 – 2.28 (m, 1H), 2.12 – 2.06 (m, 1H), 1.93 – 1.88 (m, 1H), 1.79 (d, J = 7.2 Hz, 3H), 1.75 – 1.68 (m, 2H), 1.58 – 1.48 (m, 2H), 1.17 – 1.01 (m, 2H), 0.96 – 0.88 (m, 7H), 0.80 – 0.77 (m, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 178.35 (d, *J* = 9.5 Hz), 174.00 (d, *J* = 3.3 Hz), 165.84 (d, *J* = 4.6 Hz), 153.23 (d, *J* = 26.1 Hz), 133.25 (d, *J* = 3.4 Hz), 132.85 (d, *J* = 20.5 Hz), 130.12 (d, *J* = 12.8 Hz), 130.04 (d, *J* = 2.0 Hz), 128.47 (d, *J* = 11.1 Hz), 123.33 (d, *J* = 25.1 Hz), 114.00 (d, *J* = 13.8 Hz), 85.23 (d, *J* = 6.1 Hz), 74.33, 52.25 (d, *J* = 18.9 Hz), 47.28 (d, *J* = 3.9 Hz), 41.04, 40.92 (d, *J* = 6.6 Hz), 34.36 (d, *J* = 3.7 Hz), 31.42, 26.63 (d, *J* = 16.4 Hz), 24.96 (d, *J* = 4.6 Hz), 23.83 (d, *J* = 15.1 Hz), 22.06 (d, *J* = 2.2 Hz), 20.71, 16.73 (d, *J* = 23.1 Hz).
HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{30}H_{38}N_2O_5$: 507.2853. Found: 507.2857.

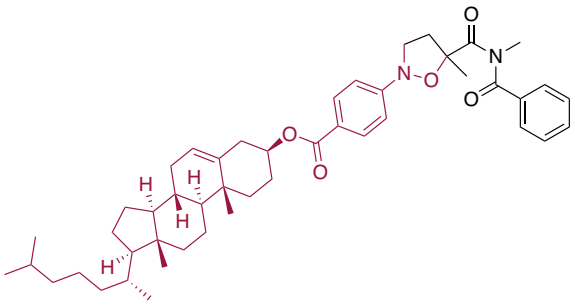


(*E*)-3,7,11,15-tetramethylhexadec-2-en-1-yl 4-(5-(benzoyl(methyl)carbamoyl)-5-methylisoxazolidin-2-yl)benzoate (3av)

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Colorless oil, yield 68%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.70 – 7.66 (m, 2H), 7.60 – 7.56 (m, 2H), 7.53 – 7.47 (m, 1H), 7.37 – 7.34 (m, 2H), 6.67 – 6.61 (m, 2H), 5.40 – 5.35 (m, 1H), 4.70 (d, *J* = 7.0 Hz, 2H), 3.85 – 3.80 (m, 1H), 3.22 – 3.15 (m, 1H), 3.10 (s, 3H), 3.04 – 2.92 (m, 1H), 2.35 – 2.29 (m, 1H), 1.20 – 1.96 (m, 2H), 1.69 – 1.63 (m, 6H), 1.41 – 1.31 (m, 4H), 1.27 – 1.16 (m, 8H), 1.11 – 0.97 (m, 7H), 0.87 – 0.76 (m, 12H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 178.48, 174.08, 165.72, 153.69, 142.18, 133.55, 133.45, 130.11, 130.07, 129.02, 122.40, 119.04, 114.35, 85.36, 61.35, 51.91, 40.93, 39.23, 37.19, 37.16, 37.06, 36.23, 34.46, 32.51, 32.33, 27.83, 25.08, 24.76, 24.60, 24.19, 22.99, 22.90, 20.04, 16.53.
HRMS (ESI) m/z: $[M + H]^+$ Calced for $C_{40}H_{58}N_2O_5$: 647.4418. Found: 647.4423.



(3*S*)-8,10-dimethyl-15-(6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-(5-(benzoyl(methyl)carbamoyl)-5-methylisoxazolidin-2-yl)benzoate (3aw)

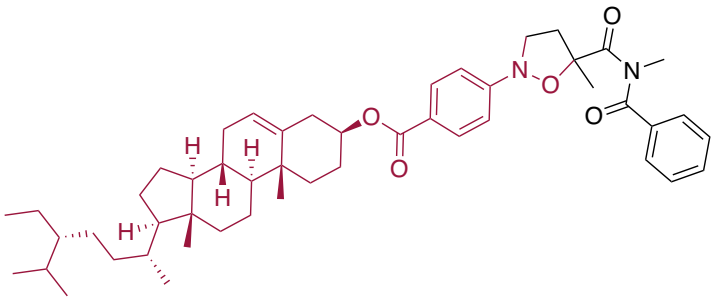
The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Yellow oil, yield 74%.

^{1}H NMR (600 MHz, DMSO-d_6) δ 7.65 – 7.62 (m, 2H), 7.56 – 7.53 (m, 2H), 7.43 – 7.36 (m, 1H), 7.27 – 7.22 (m, 2H), 6.53 – 6.50 (m, 2H), 5.32 – 5.30 (m, 1H), 4.68 – 4.59 (m, 1H), 3.74 – 3.69 (m, 1H), 3.18 – 3.09 (m, 2H), 3.07 (d, *J* = 3.1 Hz, 3H), 2.37 – 2.30 (m, 2H), 2.28 – 2.22 (m, 1H), 1.97

– 1.81 (m, 4H), 1.79 – 1.74 (m, 1H), 1.67 (d, *J* = 3.0 Hz, 3H), 1.64 – 1.60 (m, 1H), 1.55 – 1.37 (m, 6H), 1.36 – 1.18 (m, 5H), 1.16 – 1.03 (m, 7H), 0.99 (d, *J* = 3.0 Hz, 3H), 0.96 – 0.89 (m, 2H), 0.87 – 0.85 (m, 3H), 0.82 – 0.78 (m, 6H), 0.62 (d, *J* = 3.0 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 178.37, 174.06, 165.78, 153.29, 139.79, 133.33, 132.84, 130.09, 130.07, 128.51, 123.38, 122.66, 113.98, 85.26, 74.14, 56.72, 56.16, 52.33, 50.07, 42.34, 40.91, 39.76, 39.53, 38.29, 37.06, 36.67, 36.20, 35.81, 34.40, 31.95, 31.91, 29.70, 28.24, 28.02, 27.94, 24.99, 24.31, 23.85, 22.83, 22.57, 21.07, 19.40, 18.74, 11.88.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{47}H_{64}N_2O_5$: 759.4707. Found: 759.4710.



(3*S*)-17-(5-ethyl-6-methylheptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-*1H*-cyclopenta[a]phenanthren-3-yl 4-(5-(benzoyl(methyl)carbamoyl)-5-methylisoxazolidin-2-yl)benzoate (3ax)

The crude was purified by silica gel column chromatography with petroleum ether/ethyl acetate (15:1-5:1). Colorless oil, yield 76%.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 – 7.71 (m, 2H), 7.67 – 7.63 (m, 2H), 7.43 – 7.40 (m, 1H), 7.28 – 7.25 (m, 2H), 6.56 – 6.54 (m, 2H), 5.48 – 5.33 (m, 1H), 4.89 – 4.71 (m, 1H), 3.78 – 3.74 (m, 1H), 3.29 – 3.24 (m, 1H), 3.19 – 3.17 (m, 0.6H), 3.16 (s, 3H), 3.15 – 3.14 (m, 0.4H), 2.44 – 2.42 (m, 2H), 2.33 – 2.29 (m, 1H), 2.08 – 1.85 (m, 5H), 1.81 (s, 3H), 1.73 – 1.46 (m, 8H), 1.40 – 1.34 (m, 2H), 1.32 – 1.24 (m, 4H), 1.23 – 1.11 (m, 6H), 1.07 (s, 3H), 1.04 – 0.99 (m, 2H), 0.95 – 0.94 (m, 3H), 0.89 – 0.82 (m, 9H), 0.71 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 178.35, 174.03, 165.74, 153.28, 139.77, 133.31, 132.85, 130.08, 130.06, 128.50, 123.37, 122.65, 113.98, 85.25, 74.12, 56.71, 56.06, 52.31, 50.06, 45.85, 42.34, 40.91, 39.75, 38.29, 37.07, 36.66, 36.17, 34.38, 33.96, 31.95, 31.90, 29.18, 28.26, 27.94, 26.11, 24.98, 24.32, 23.09, 21.07, 19.84, 19.40, 19.07, 18.81, 12.01, 11.88.

HRMS (ESI) m/z: $[M + Na]^+$ Calced for $C_{49}H_{68}N_2O_5$: 787.5020. Found: 787.5014.

11. References

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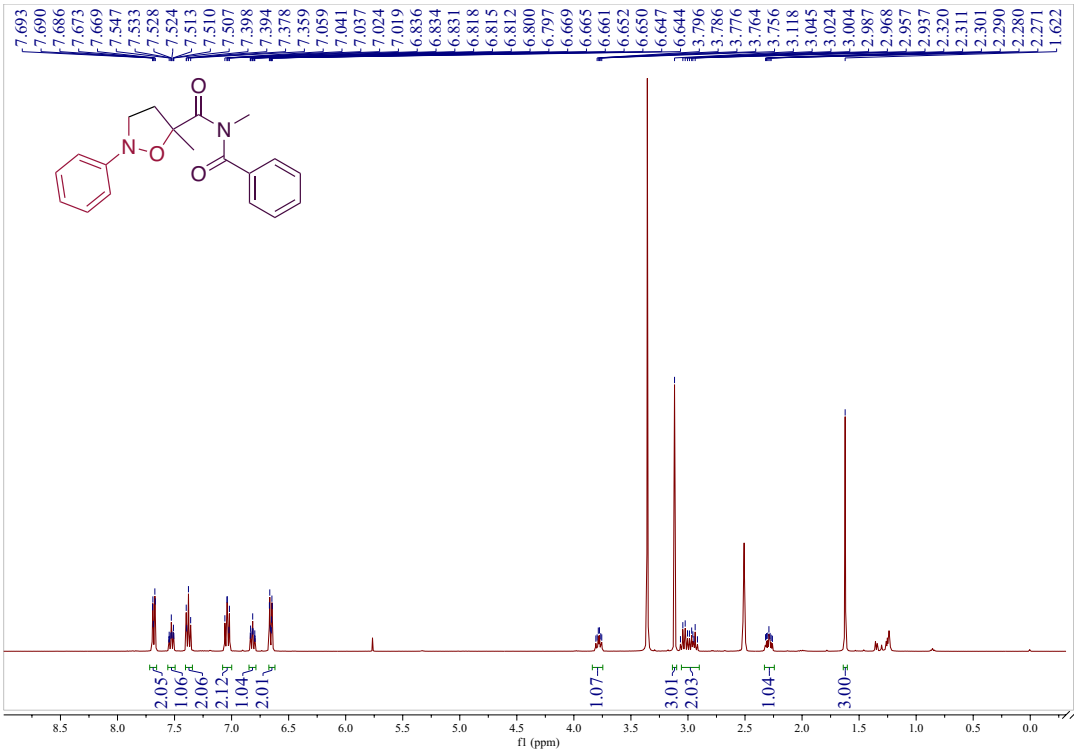
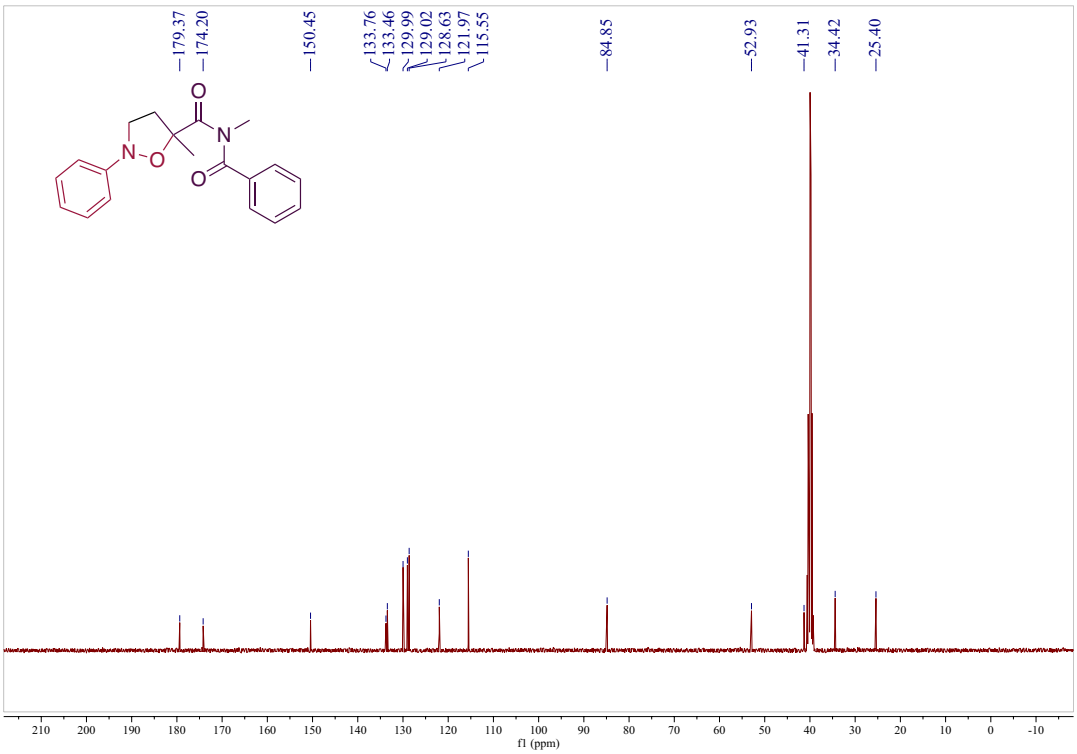
12. Copies of NMR Spectra

^{1}H and ^{13}C NMR spectra of 3aa:





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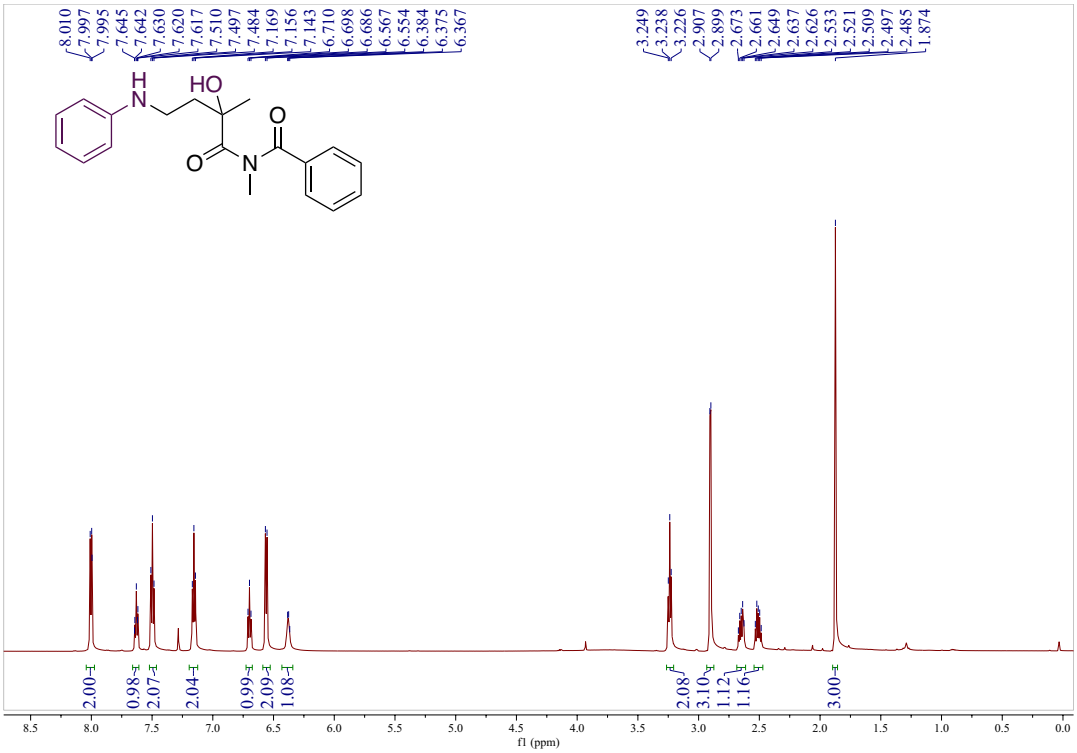
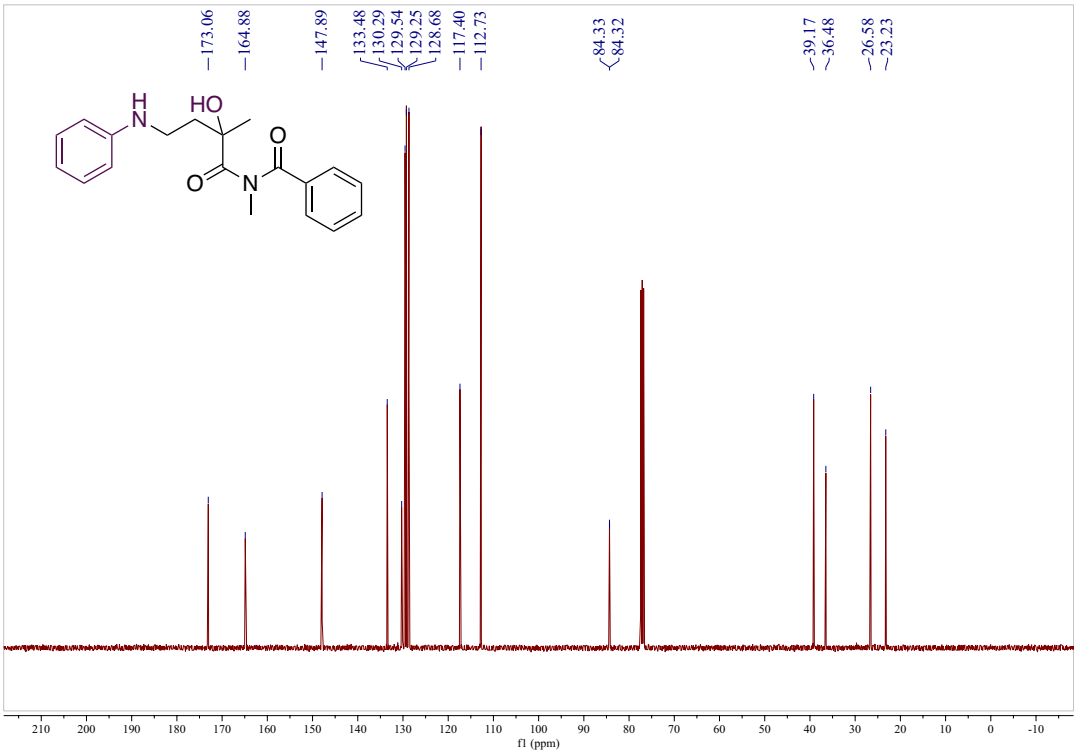
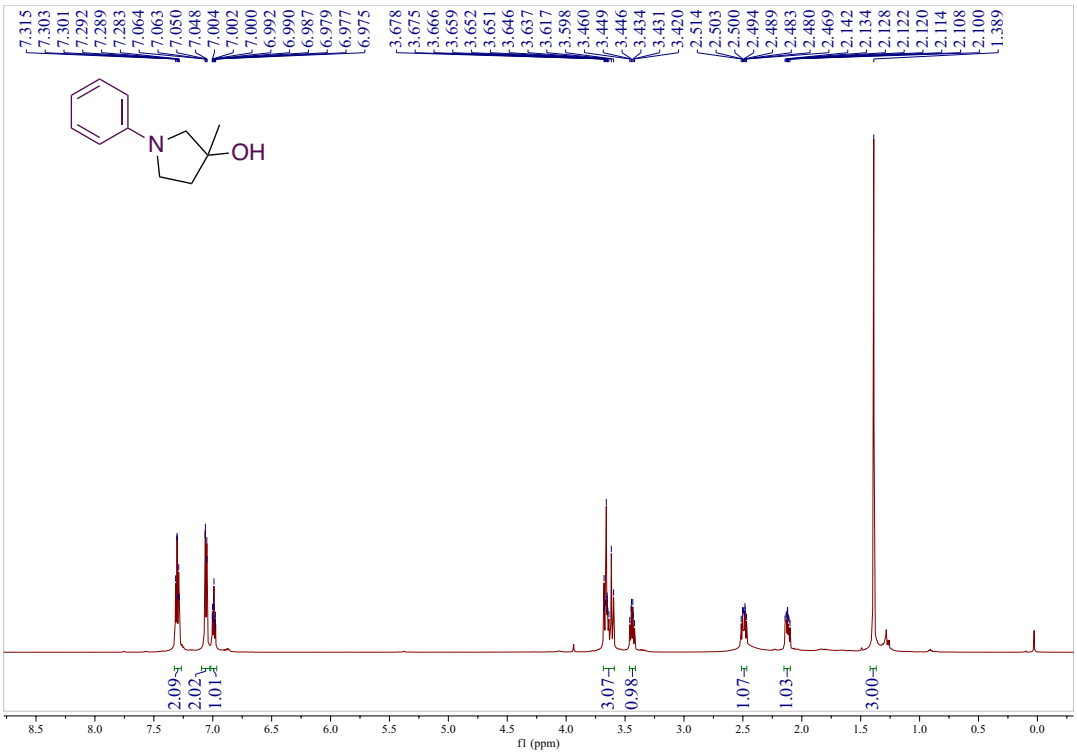
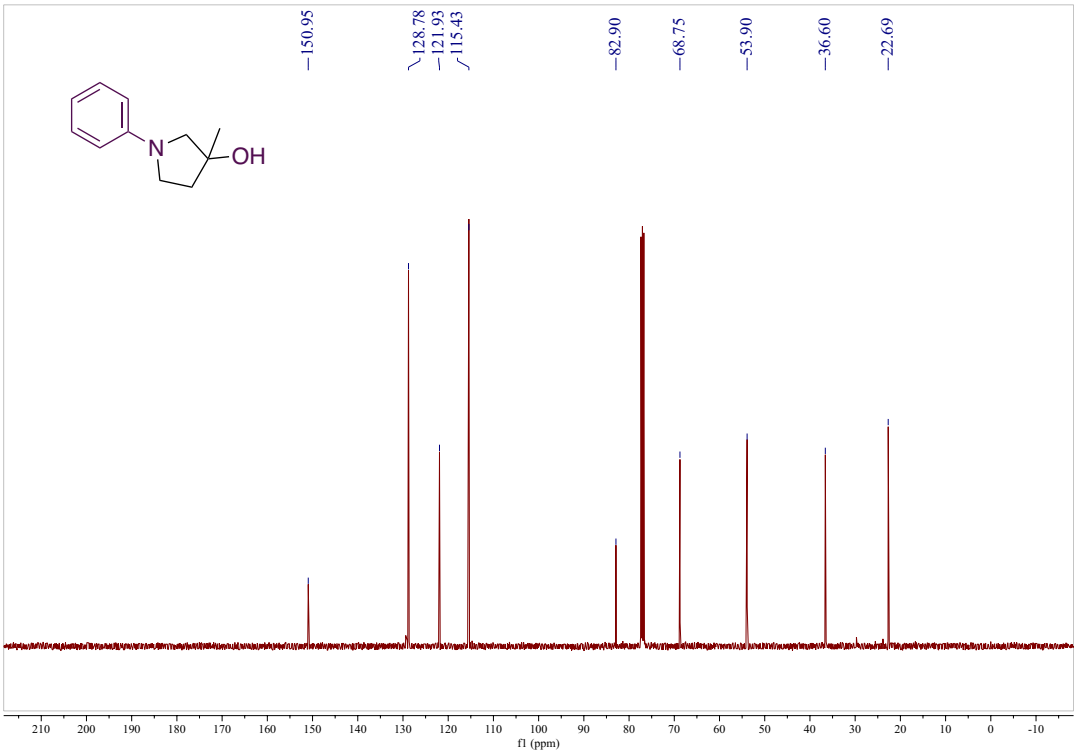


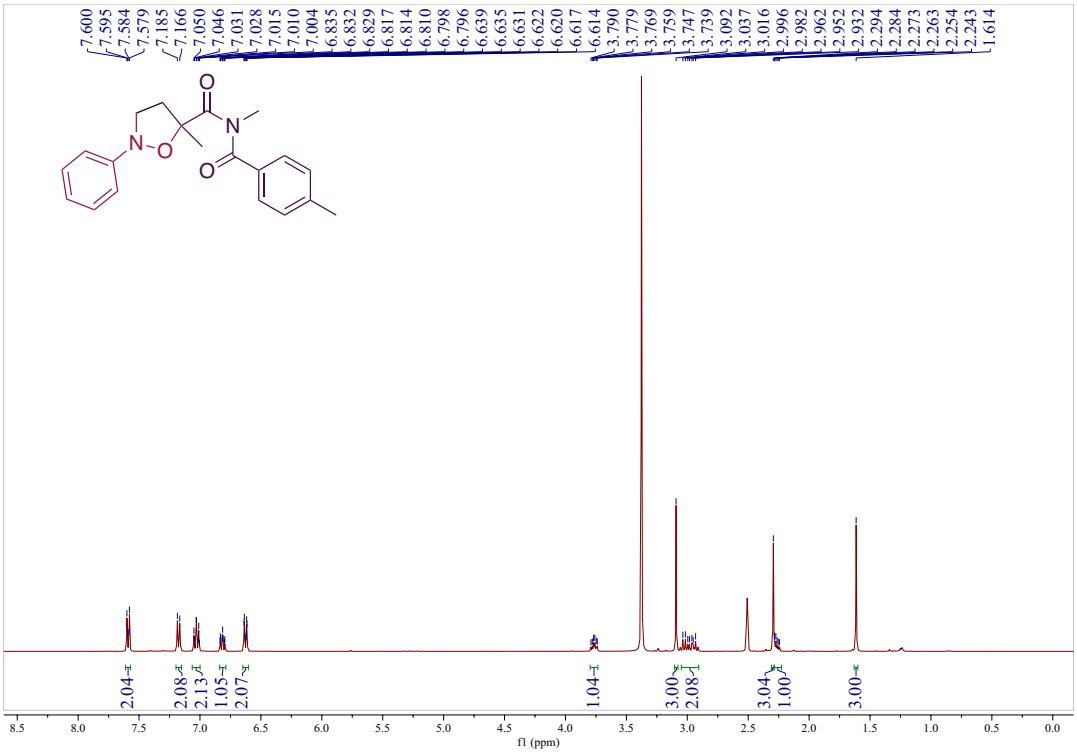


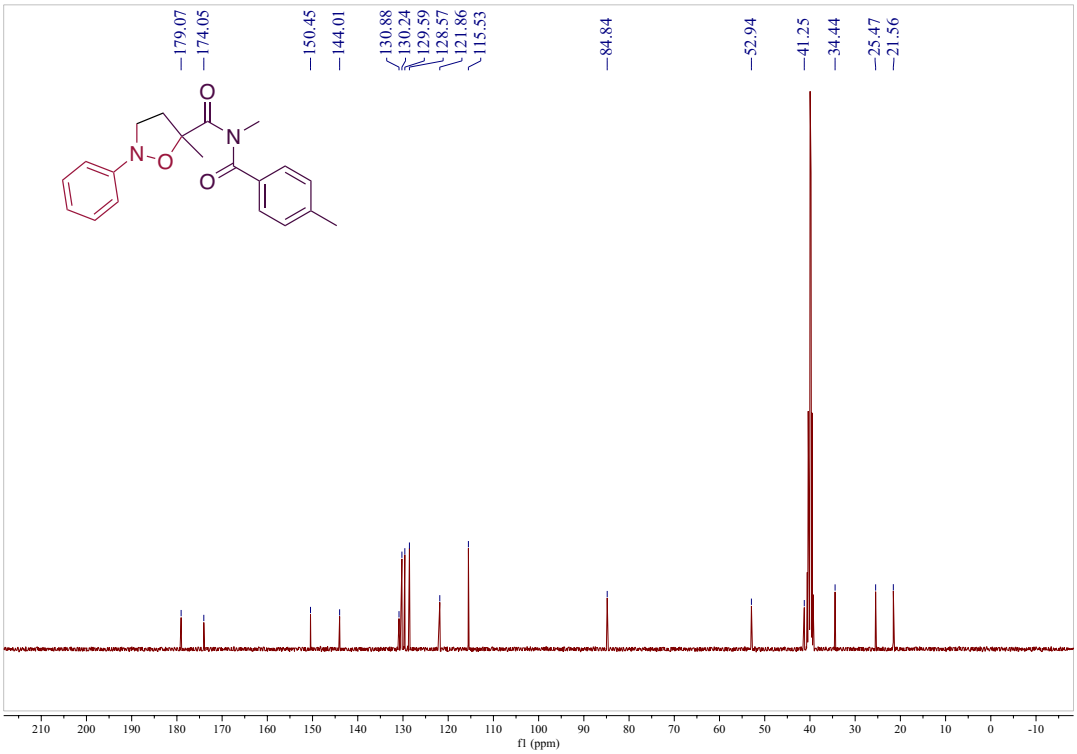
^{1}H and ^{13}C NMR spectra of 5:



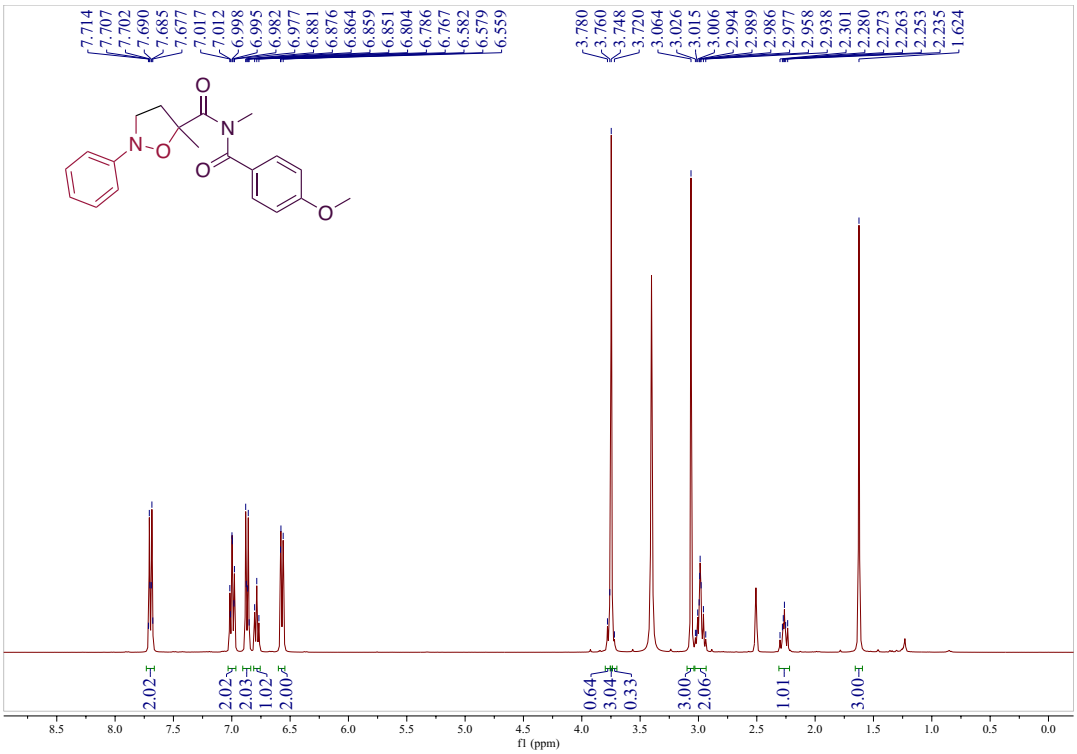


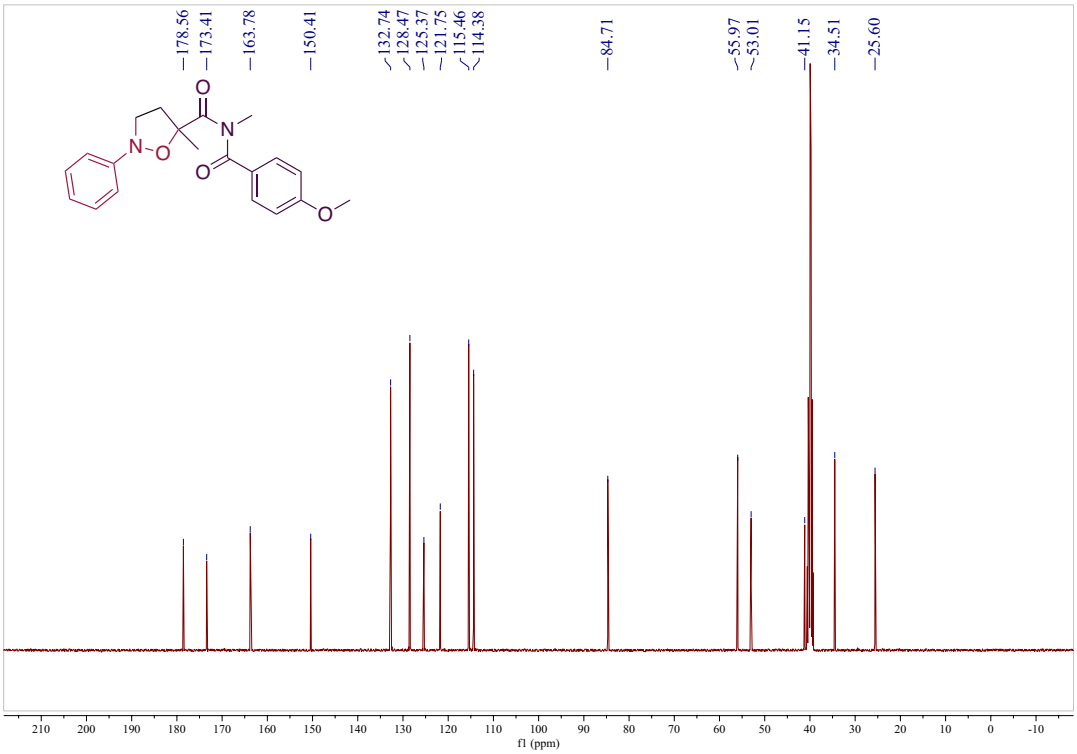
^{1}H and ^{13}C NMR spectra of 3ba:



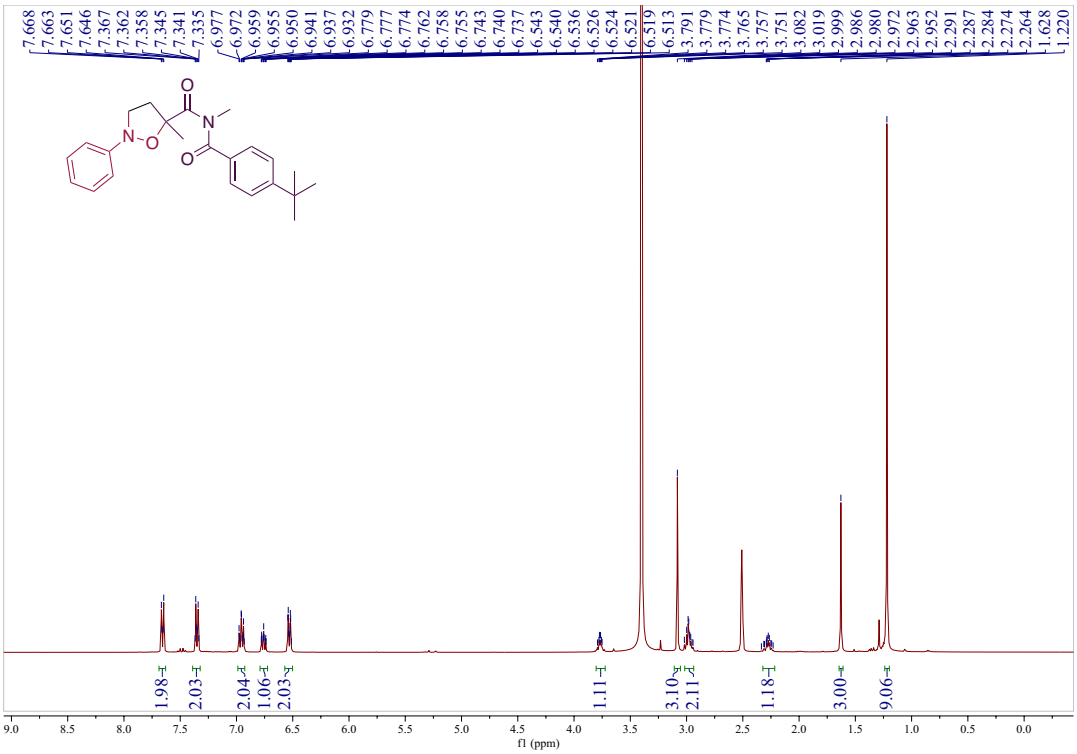


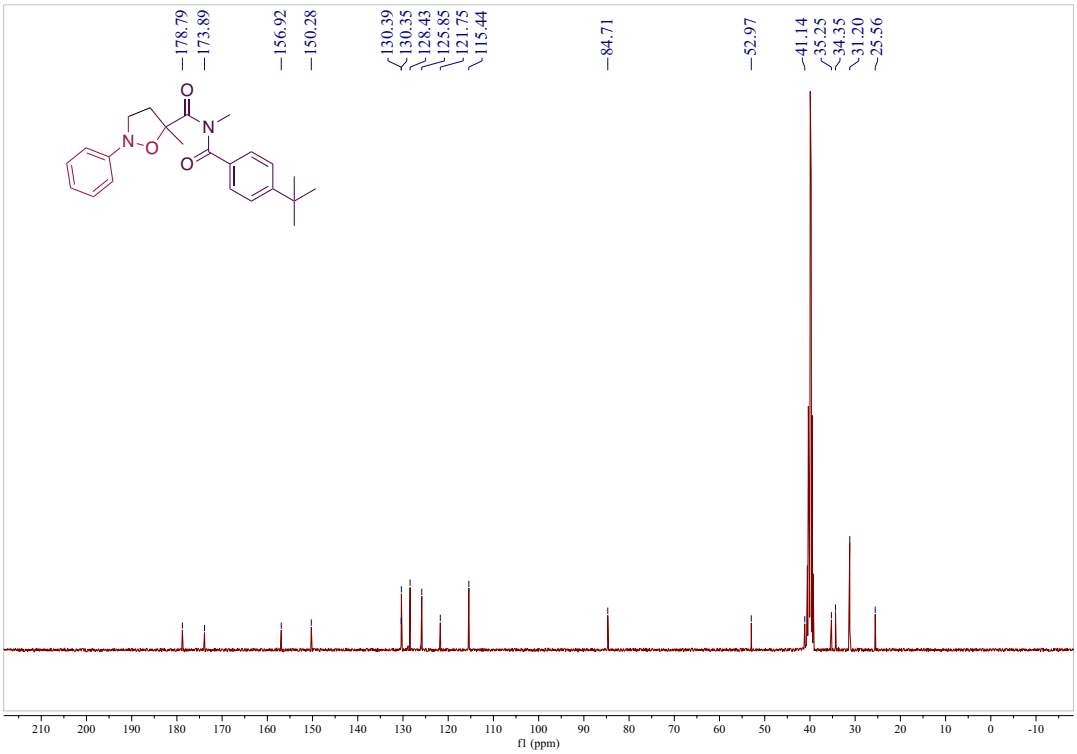
^{1}H and ^{13}C NMR spectra of 3ca:



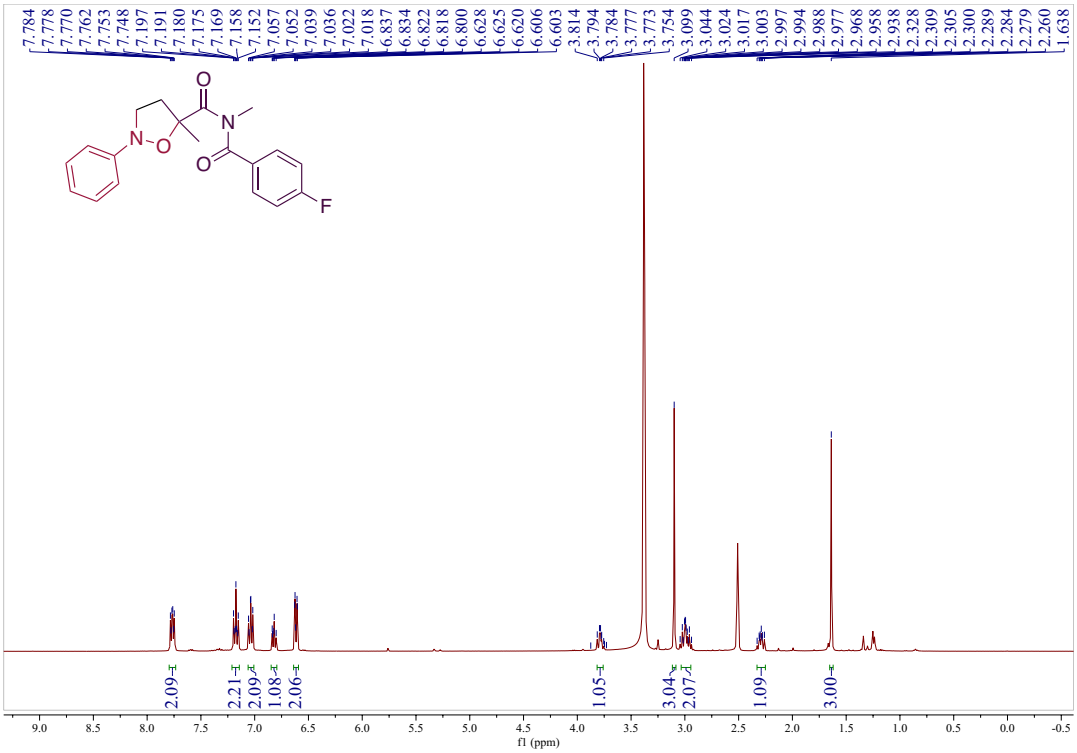


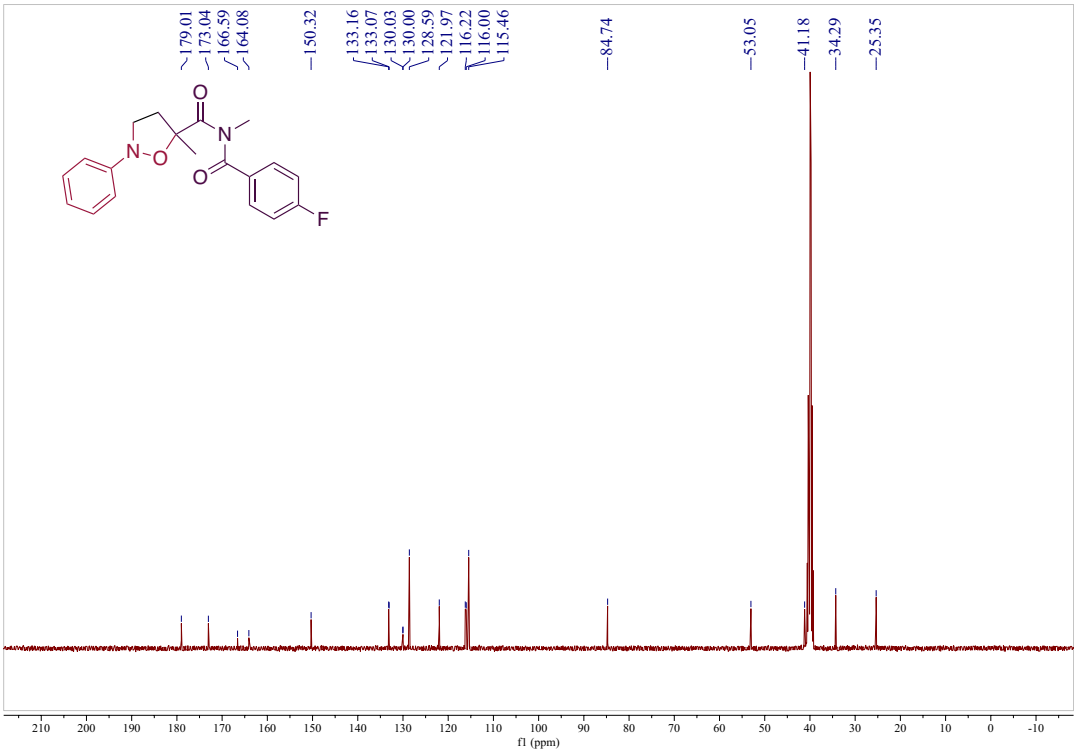
^{1}H and ^{13}C NMR spectra of 3da:





^{1}H ^{19}F and ^{13}C NMR spectra of 3ea:




179.01
173.04
166.59
164.08
150.32
133.16
133.07
130.03
130.00
128.59
121.97
116.22
116.00
115.46
84.74
53.05
41.18
34.29
25.35
O
N
O
N
O
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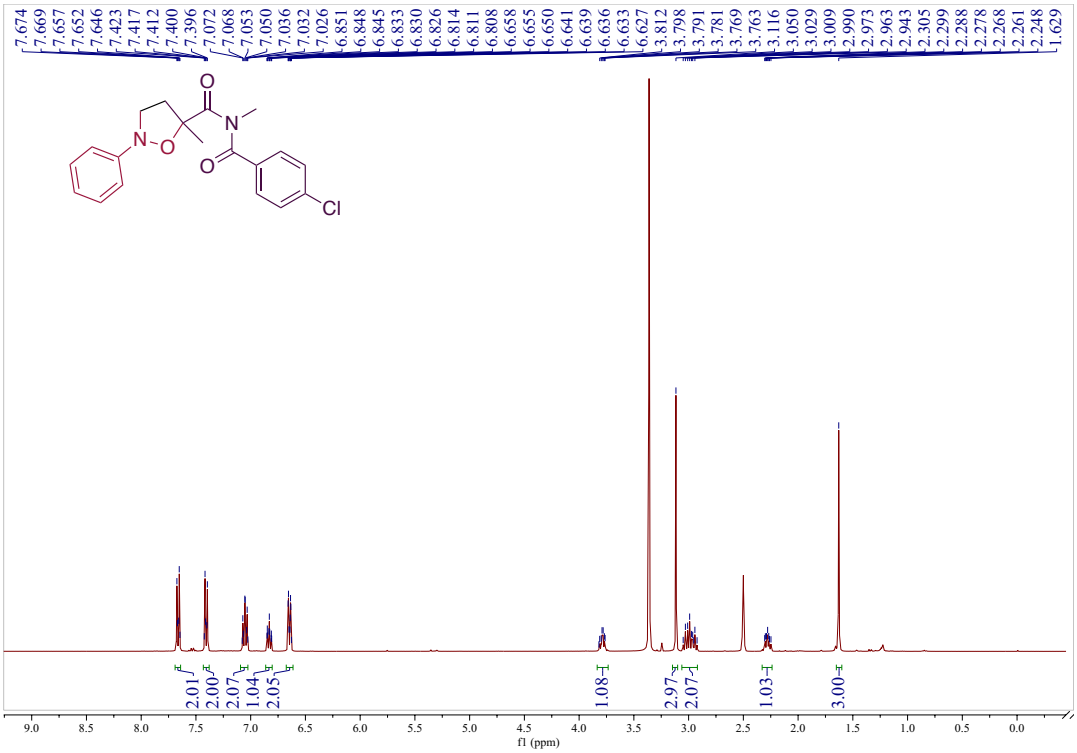
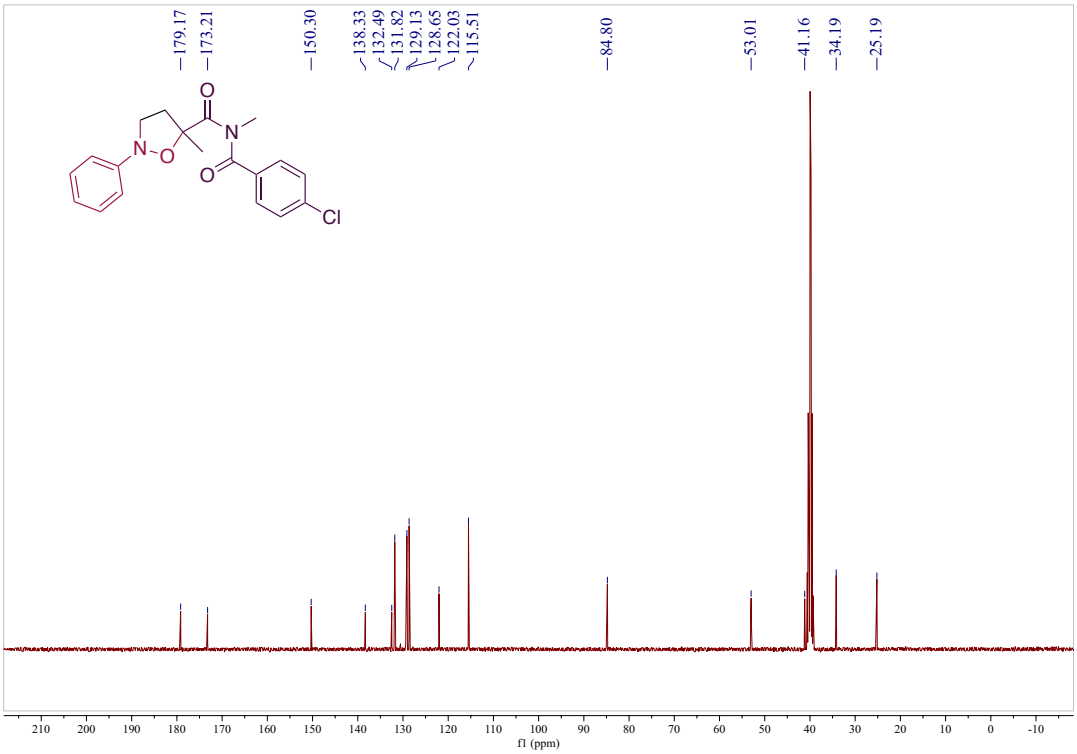
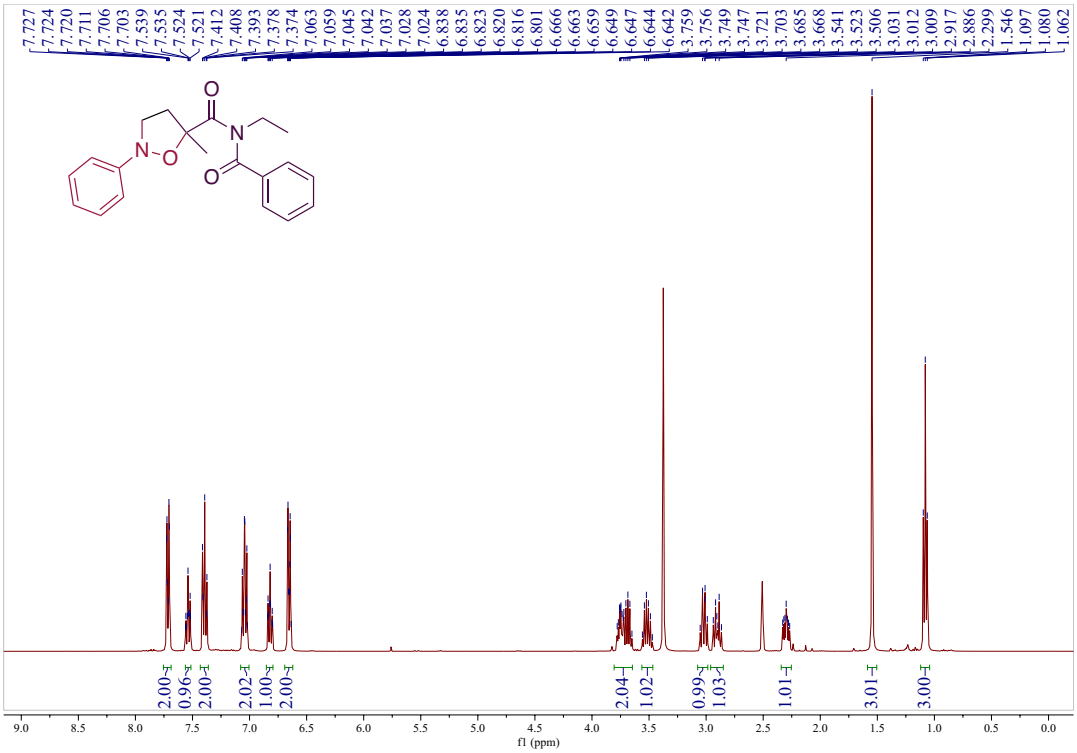
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

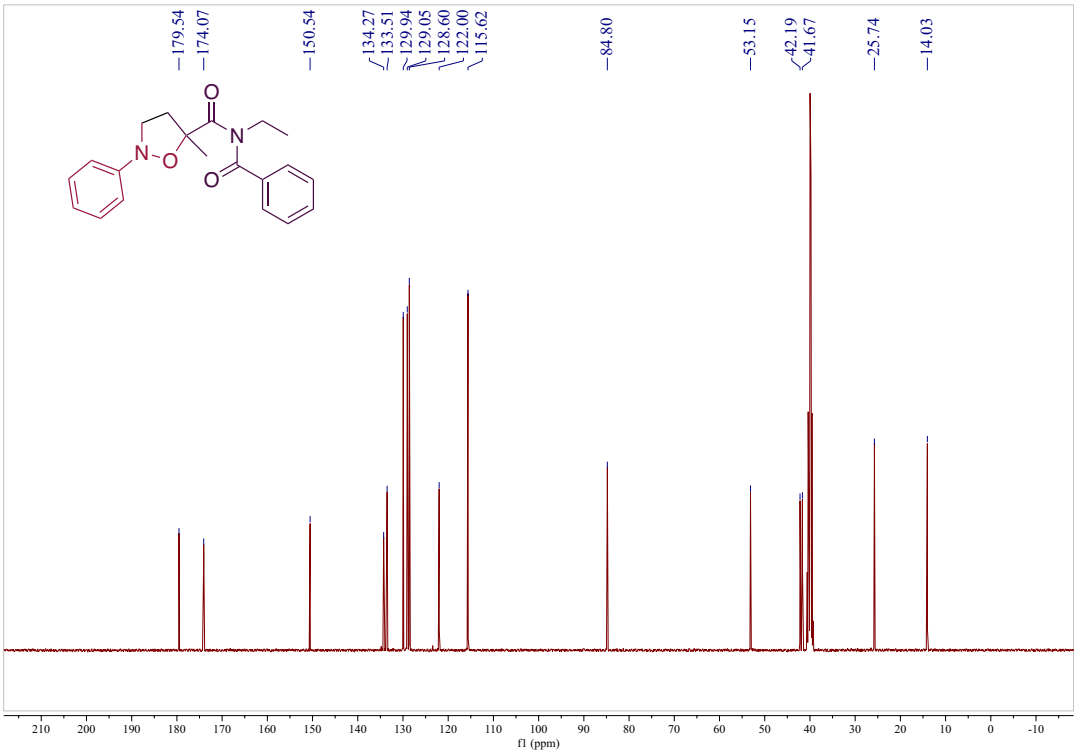
^{1}H and ^{13}C NMR spectra of 3fa:



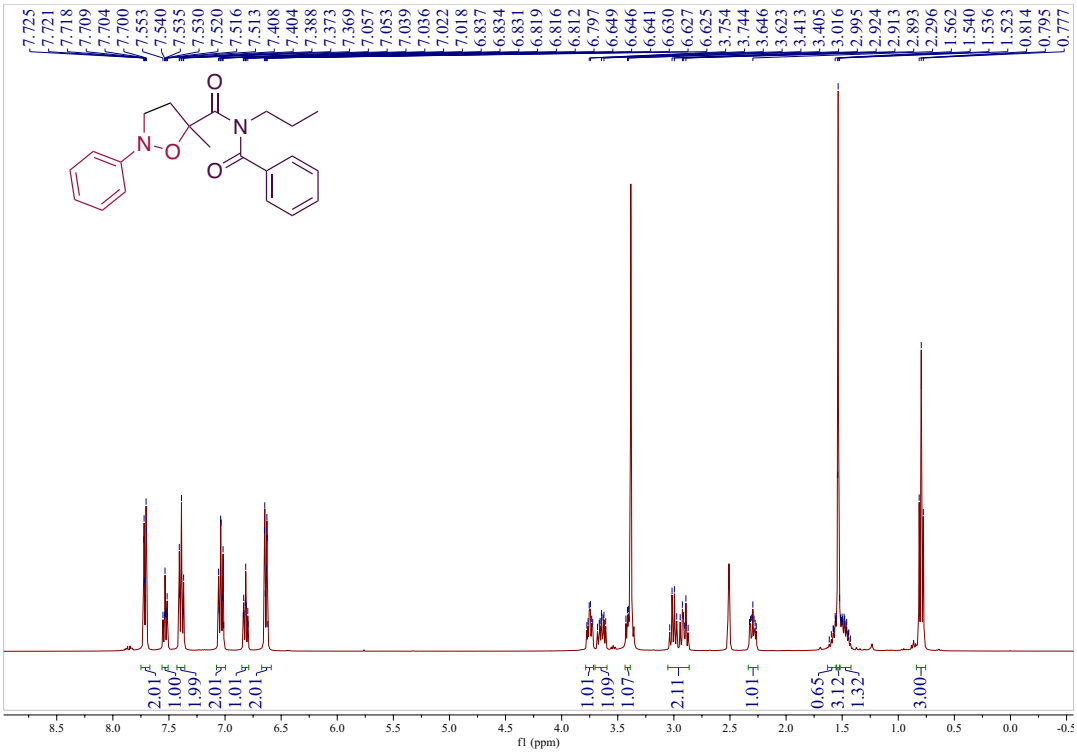


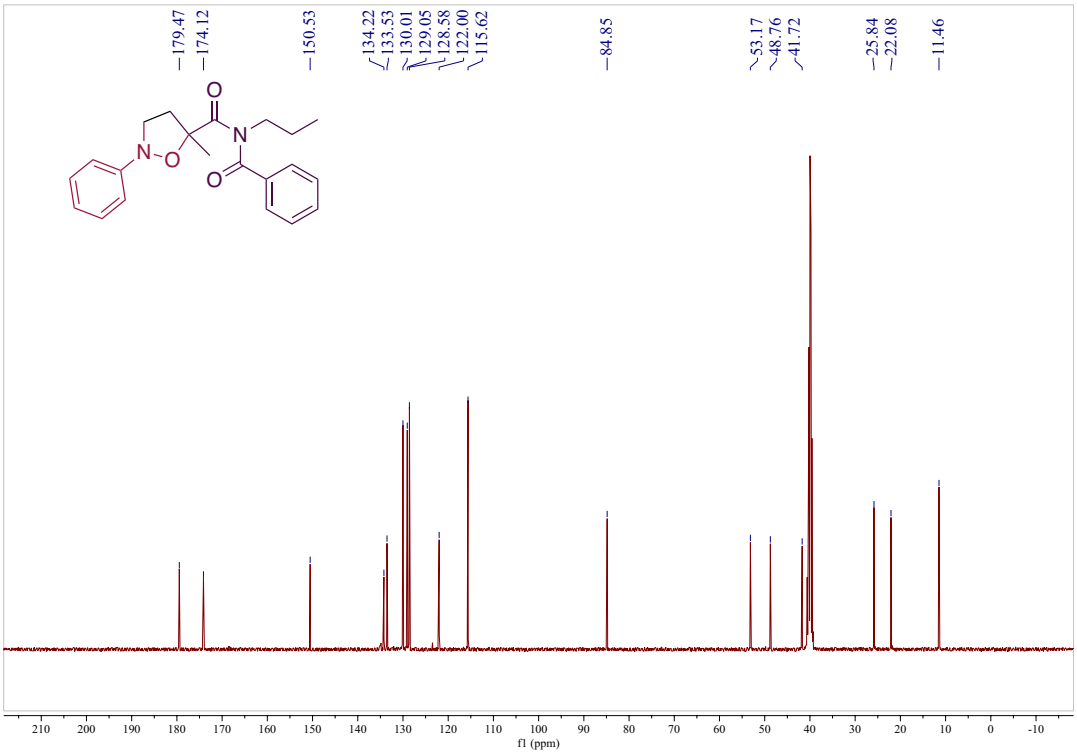
^{1}H and ^{13}C NMR spectra of 3ga:



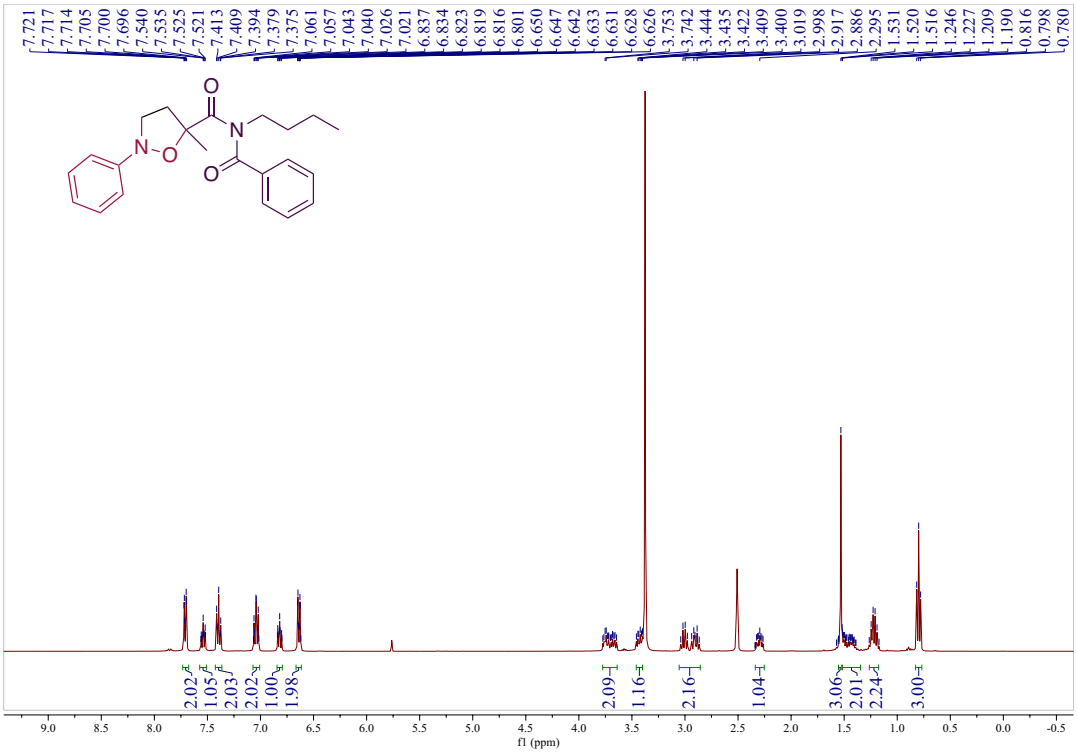


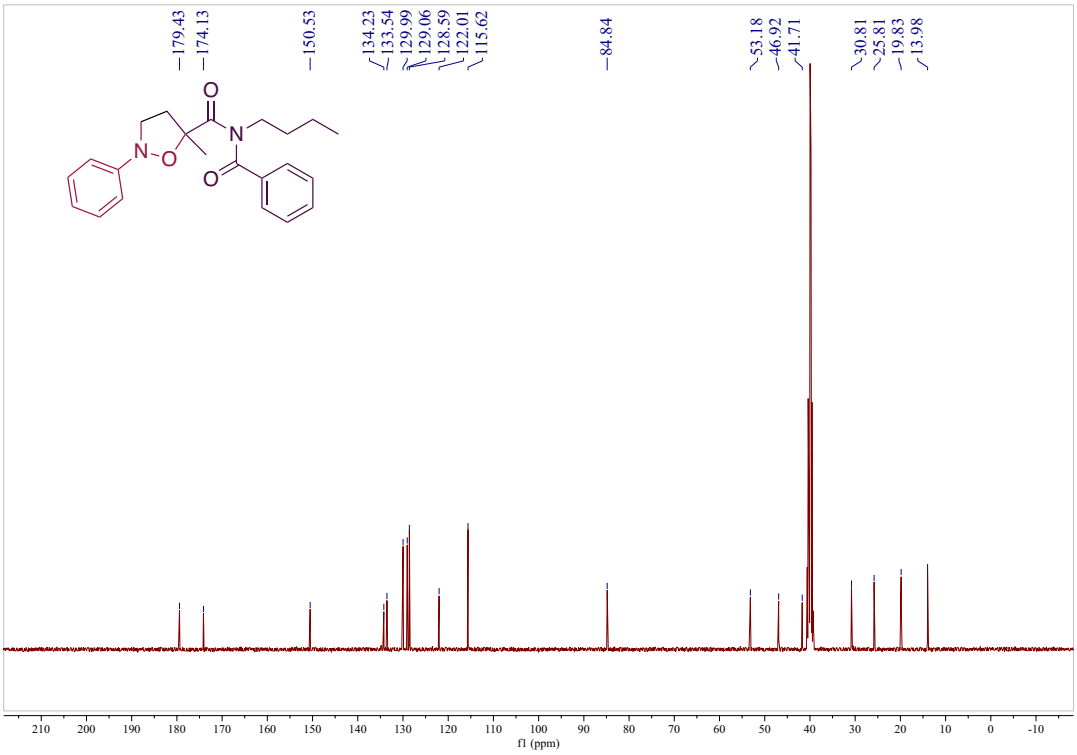
^{1}H and ^{13}C NMR spectra of 3ha:



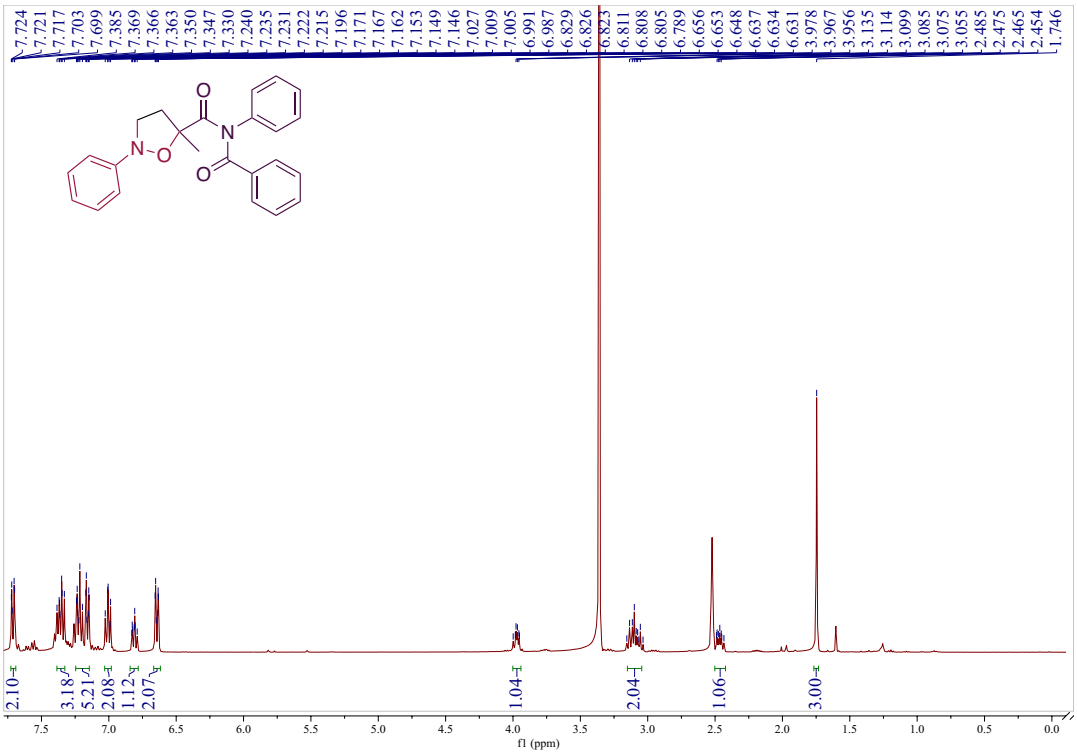


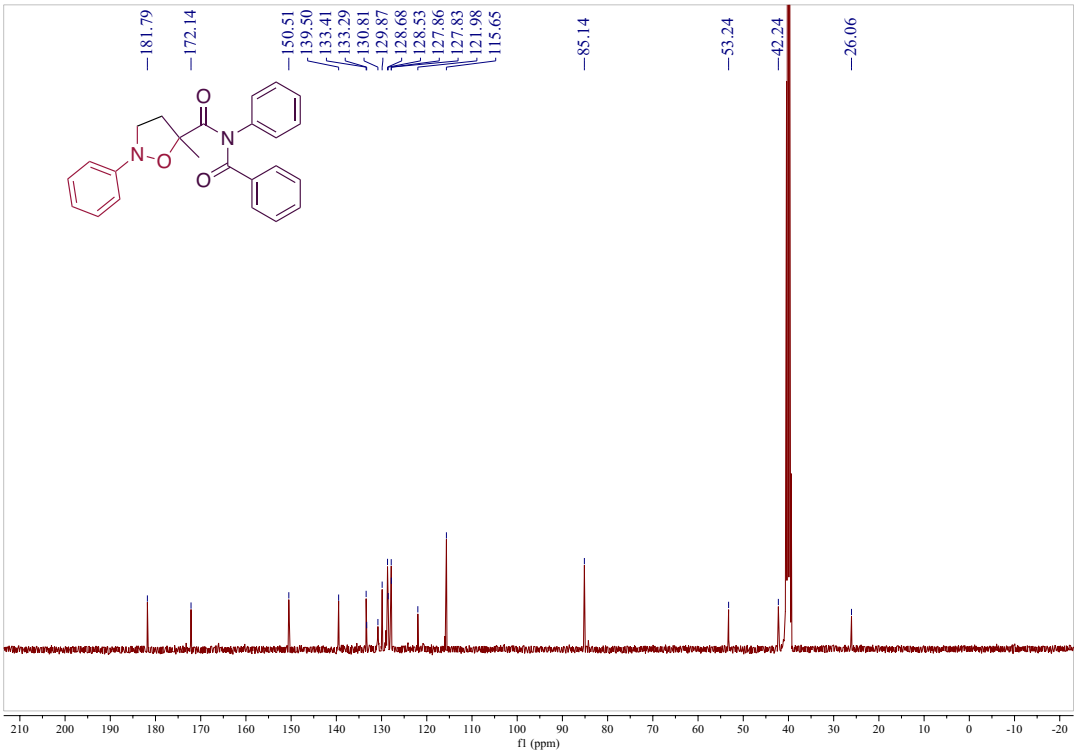
^{1}H and ^{13}C NMR spectra of 3ia:



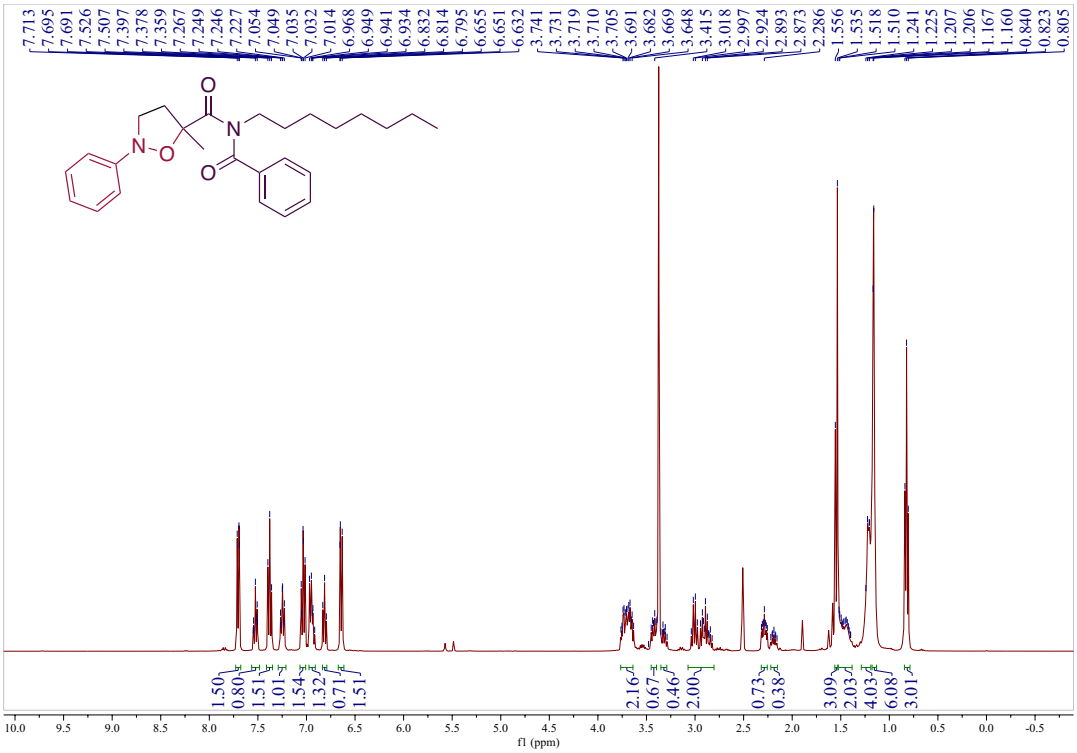


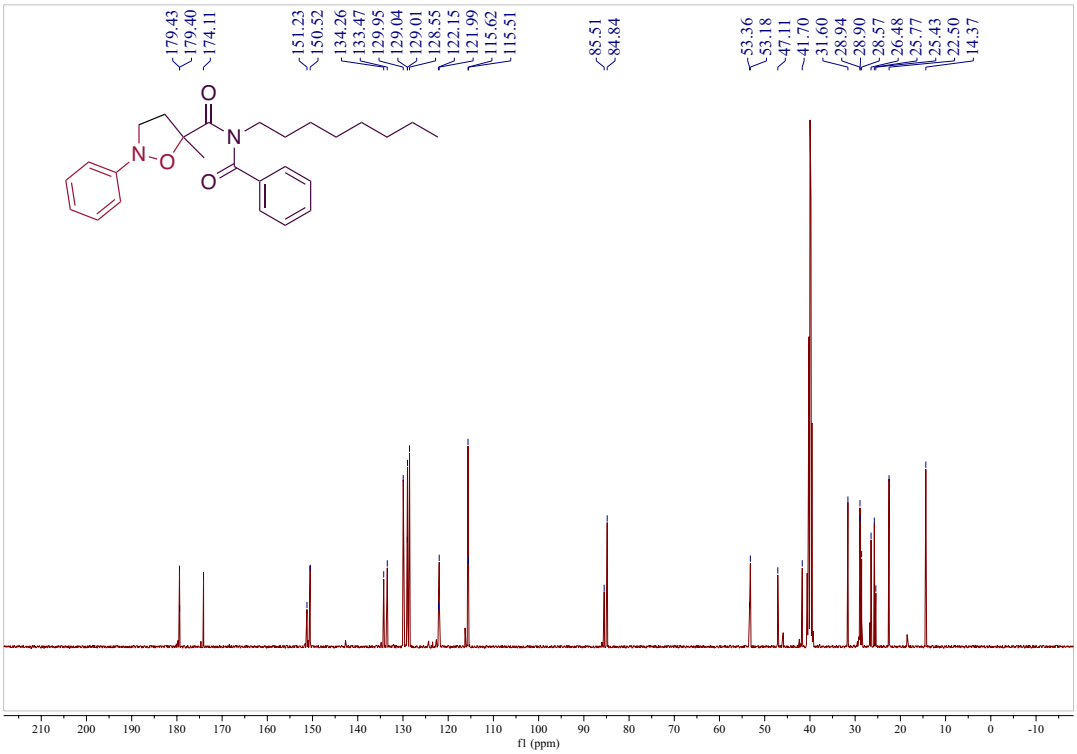
^{1}H and ^{13}C NMR spectra of 3ja:



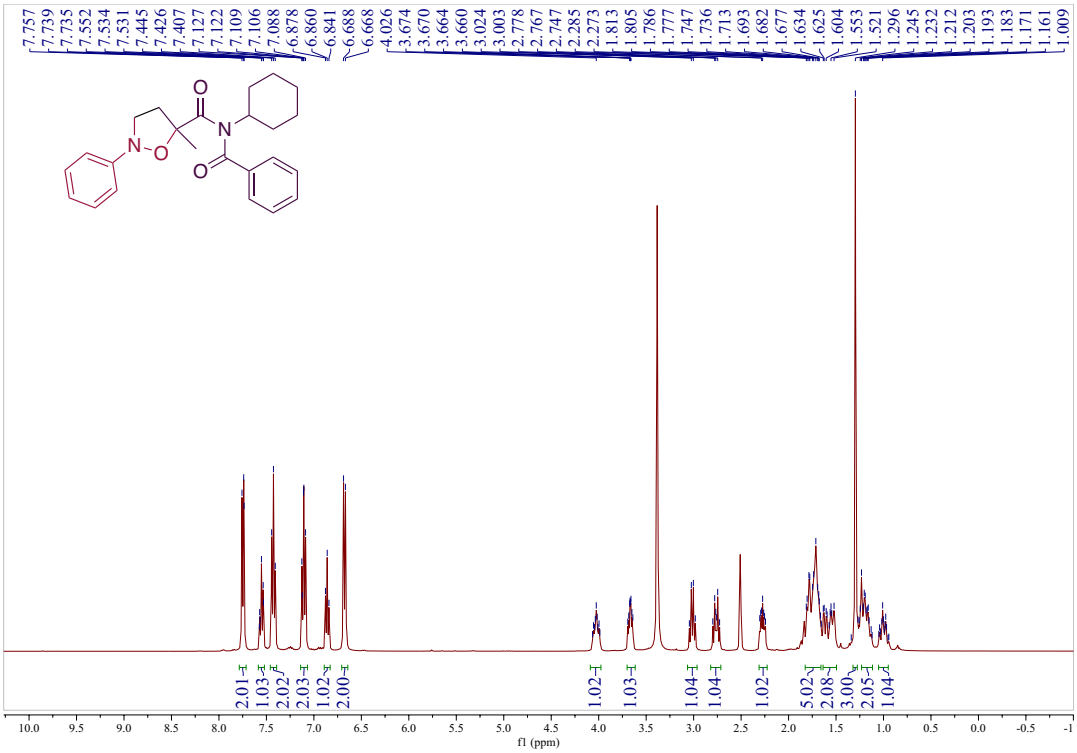


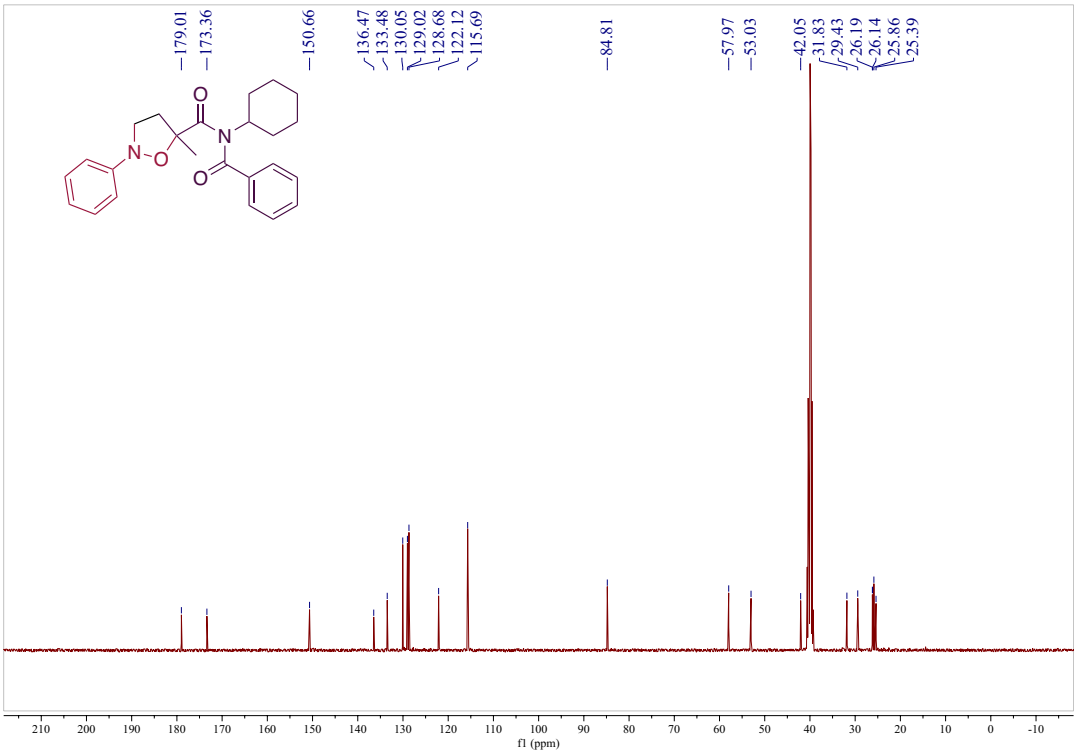
^{1}H and ^{13}C NMR spectra of 3ka:



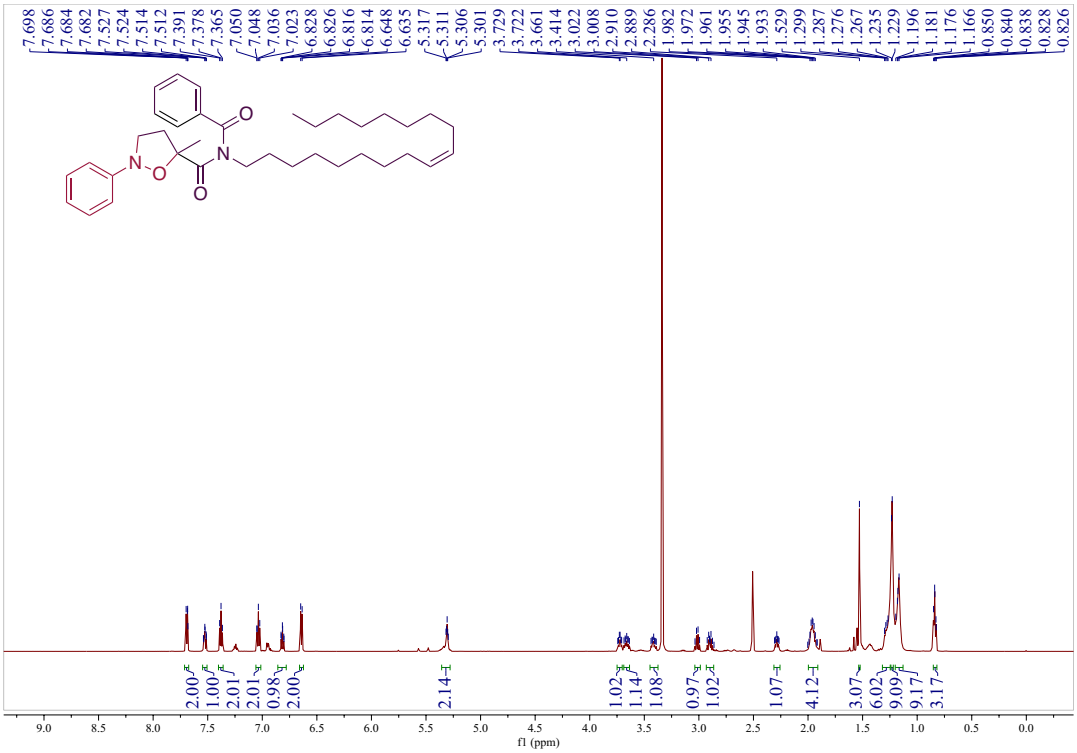


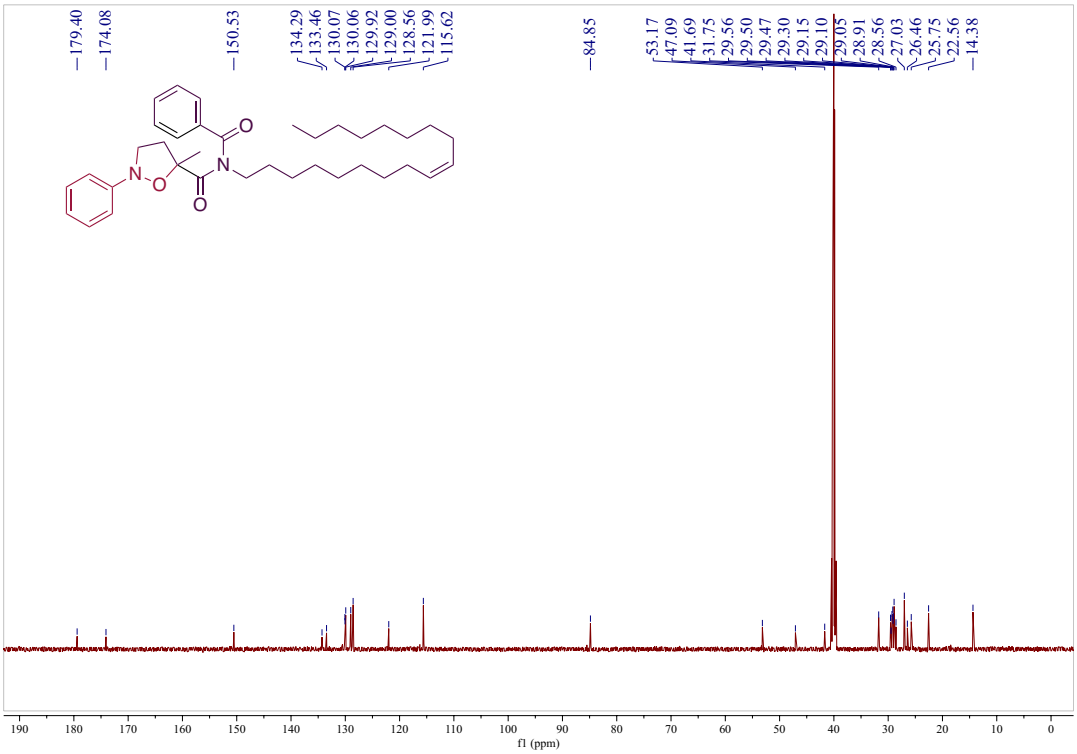
^{1}H and ^{13}C NMR spectra of 3la:



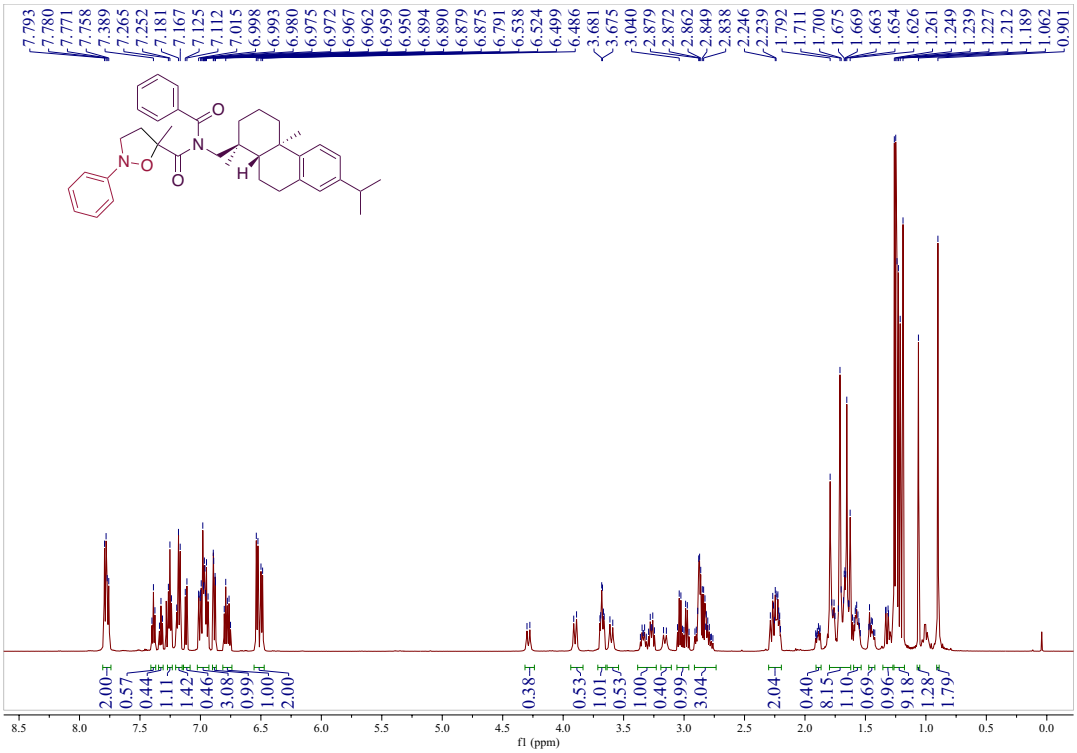


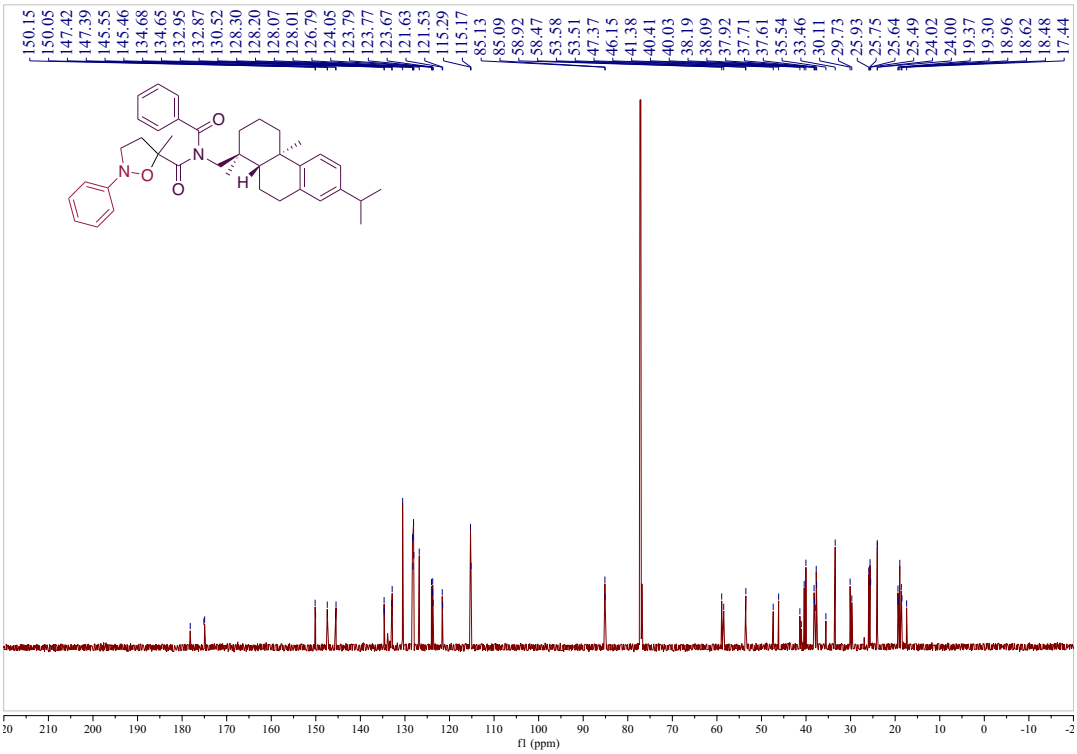
^{1}H and ^{13}C NMR spectra of 3ma:



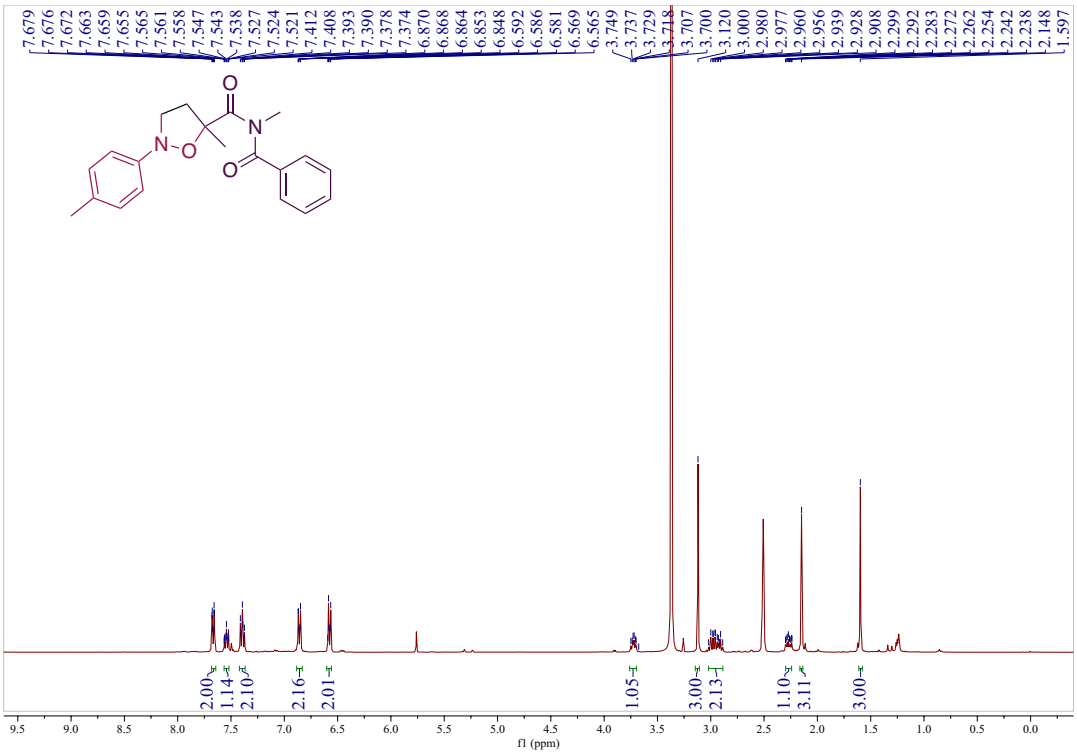


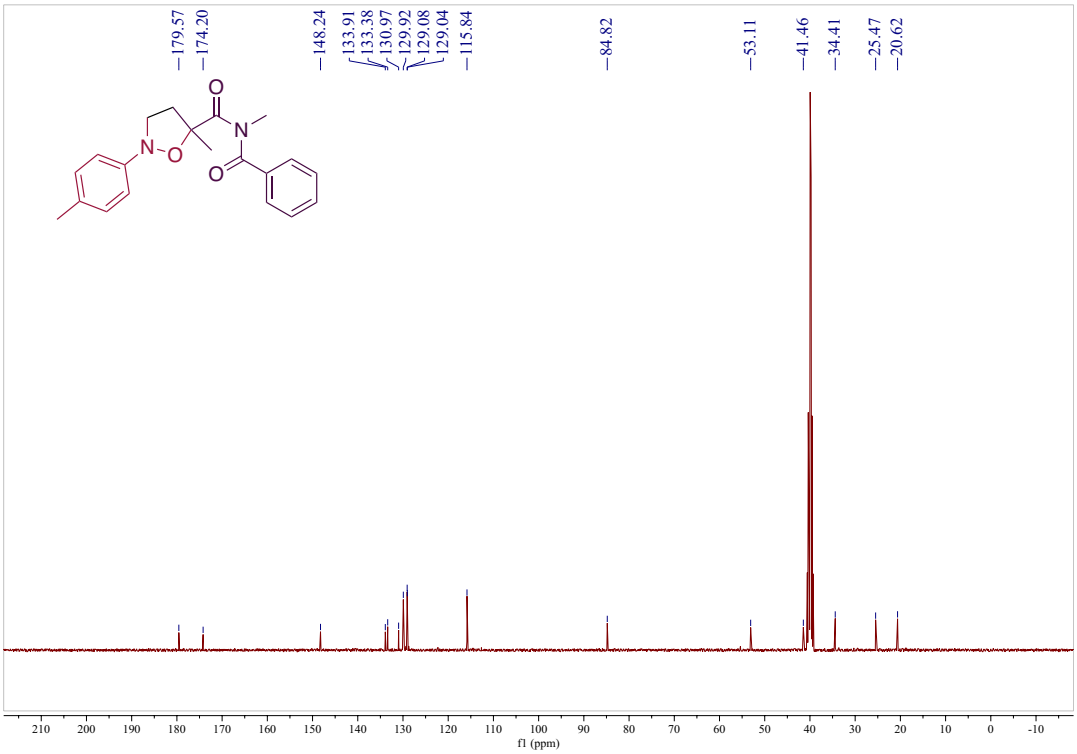
^{1}H and ^{13}C NMR spectra of 3na:



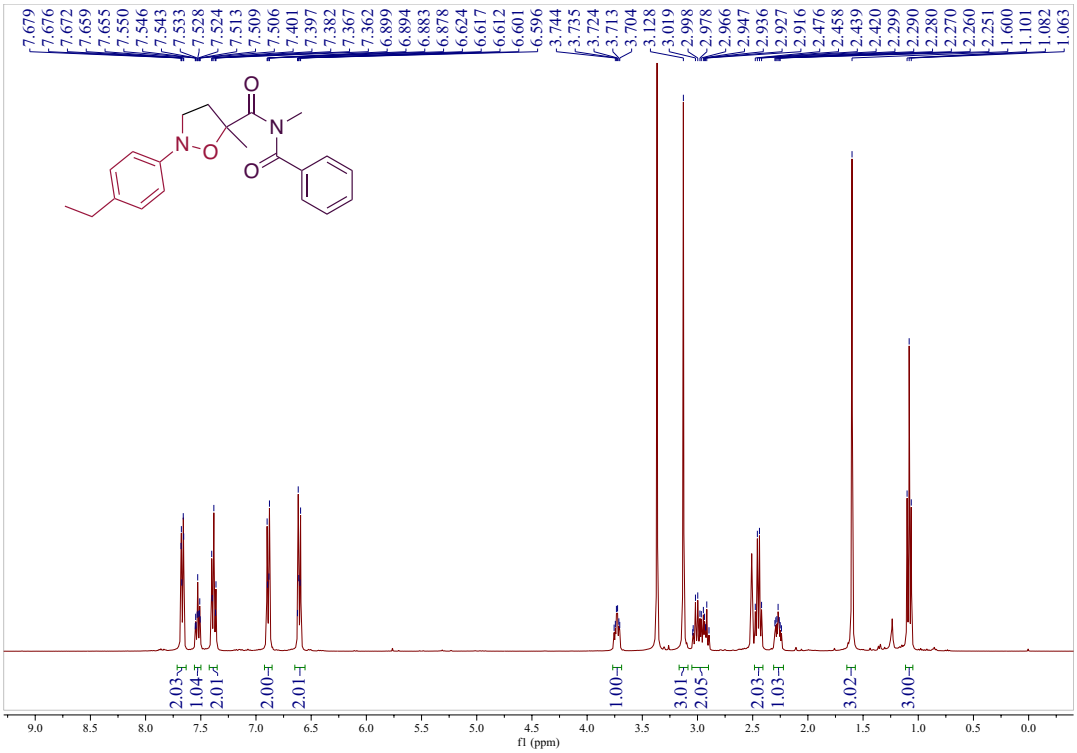


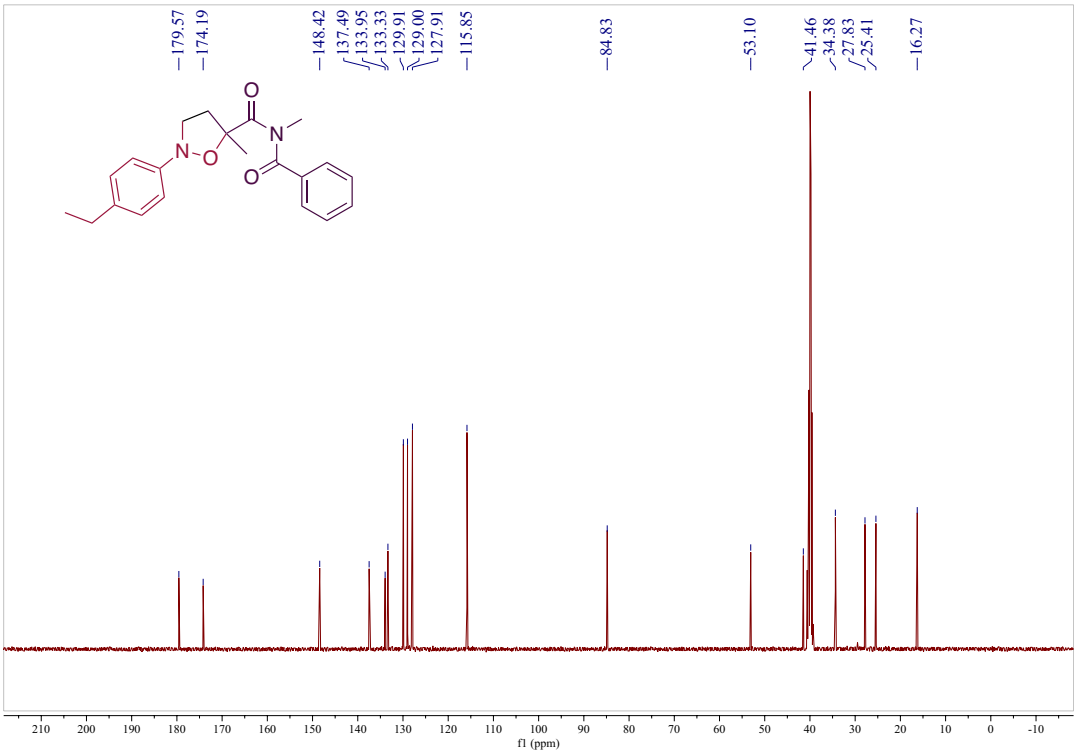
^{1}H and ^{13}C NMR spectra of 3ab:



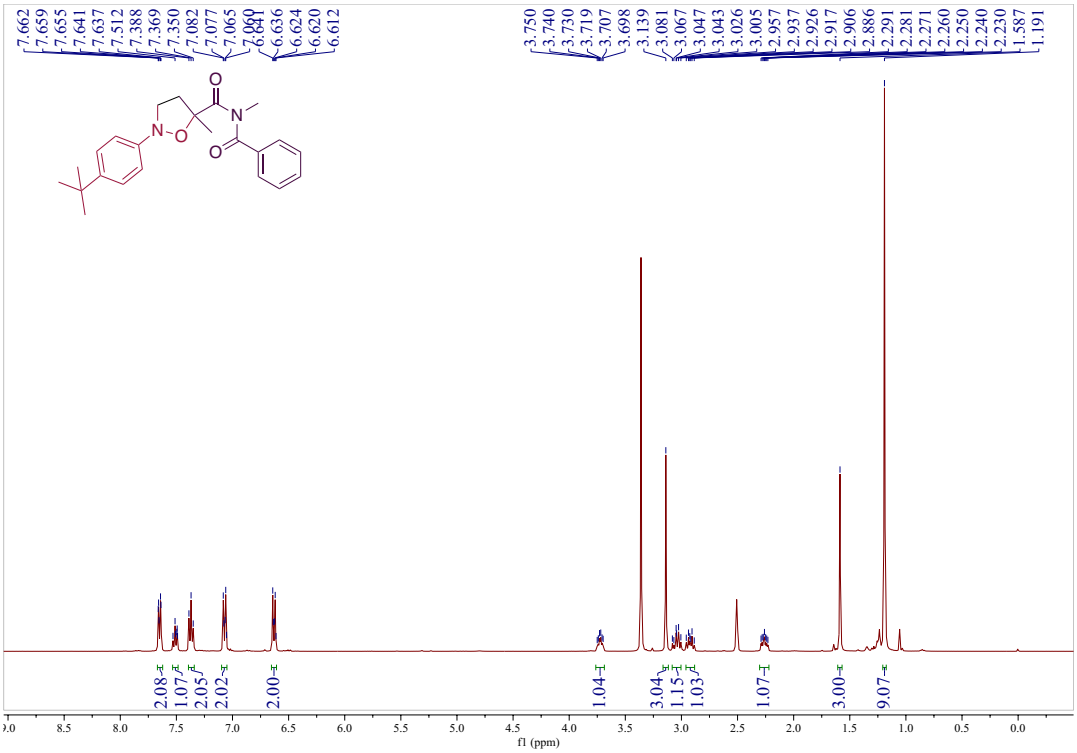


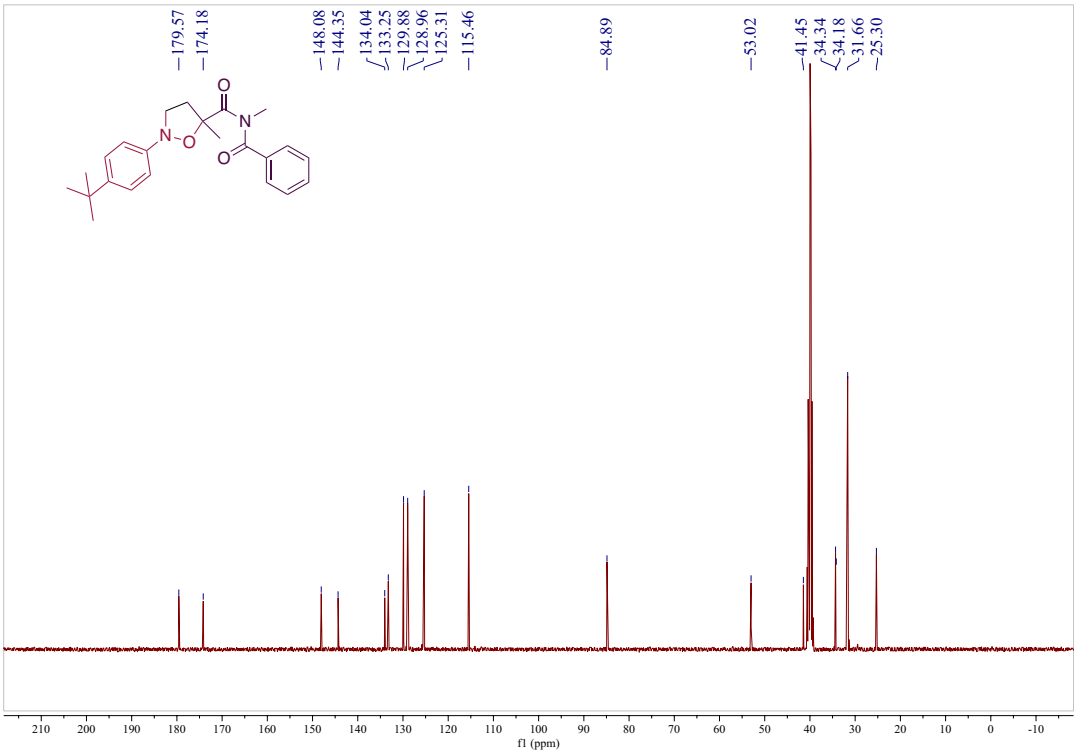
^{1}H and ^{13}C NMR spectra of 3ac:



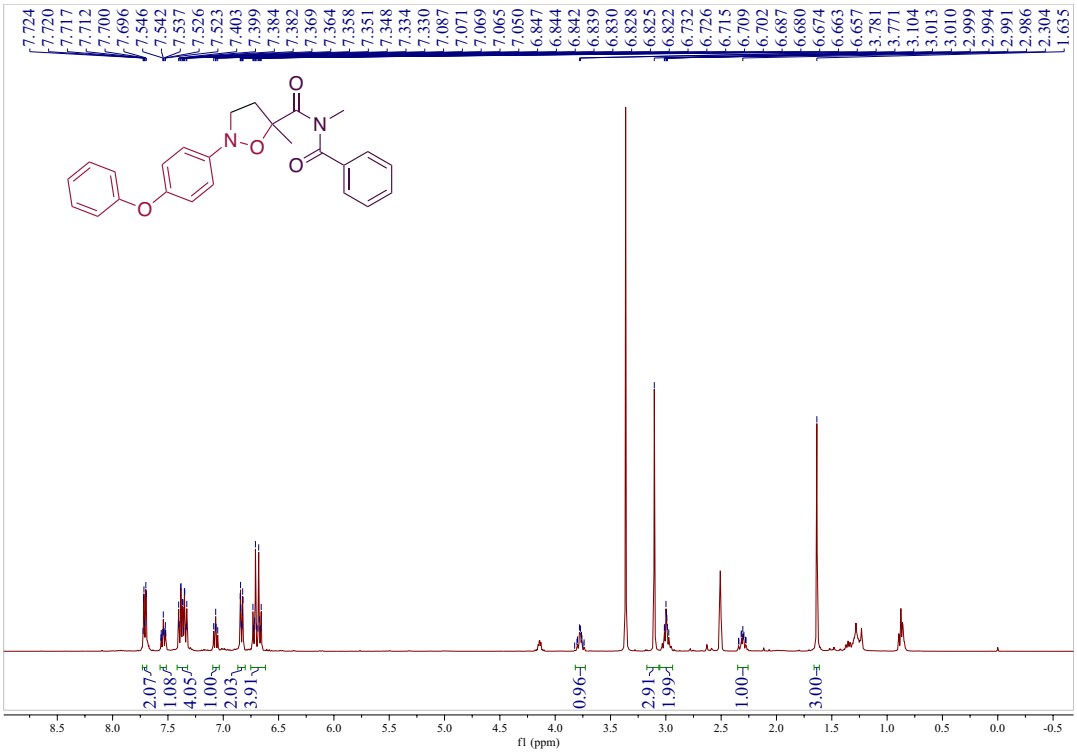


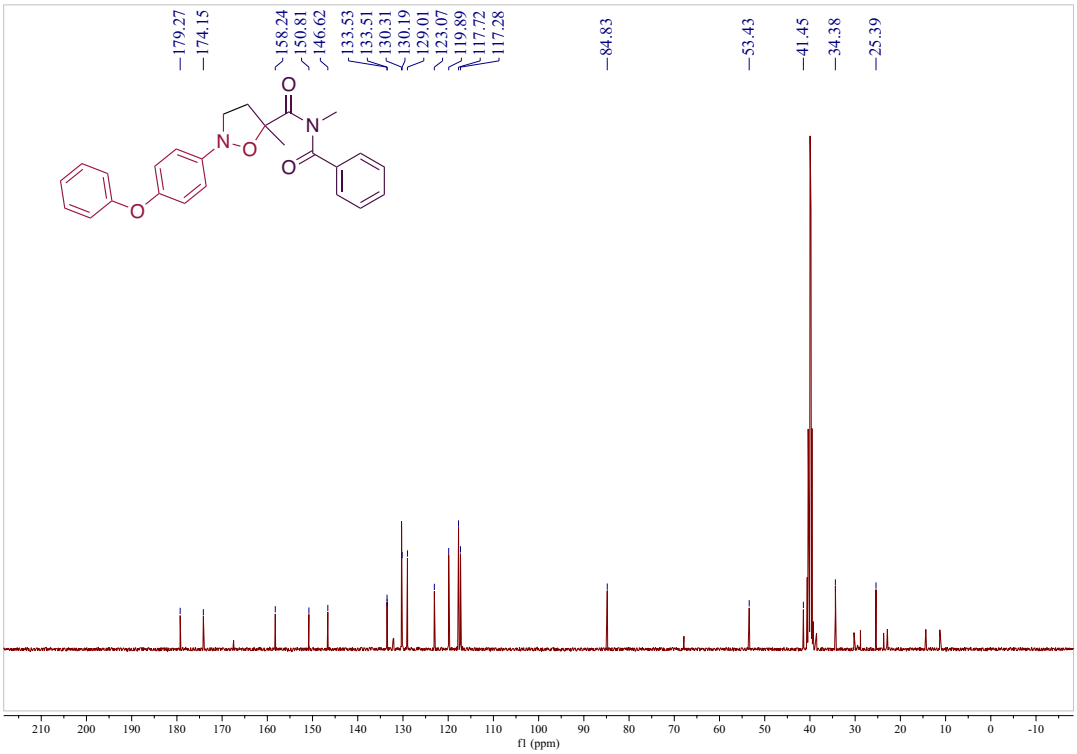
^{1}H and ^{13}C NMR spectra of 3ad:



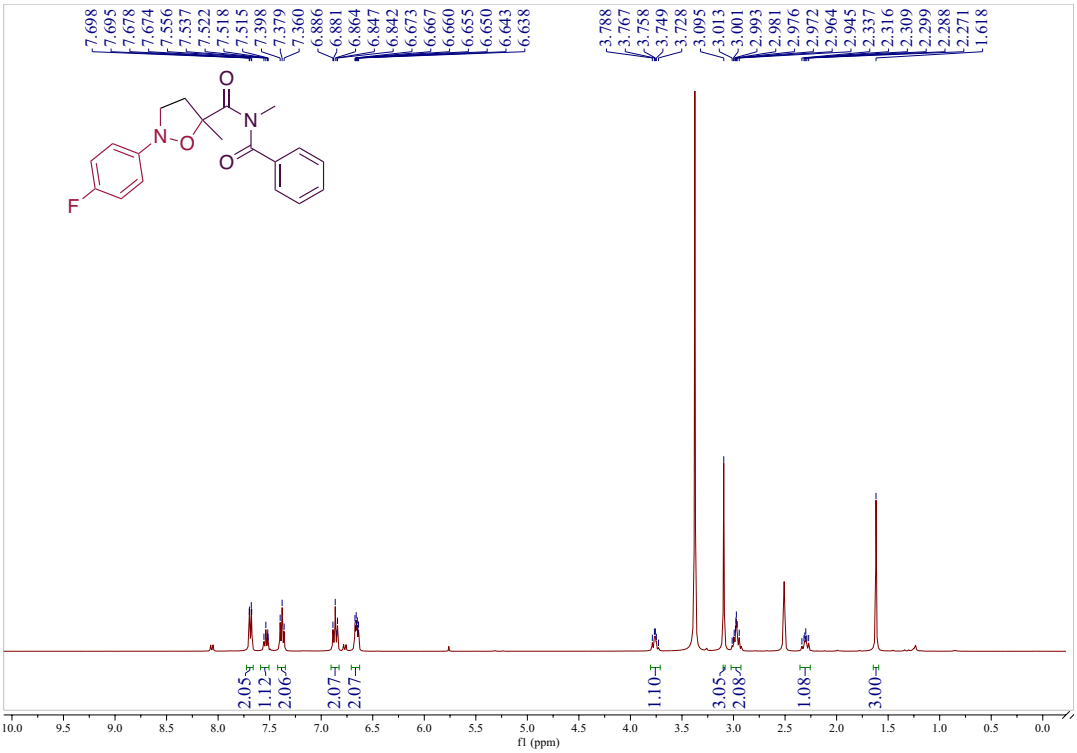


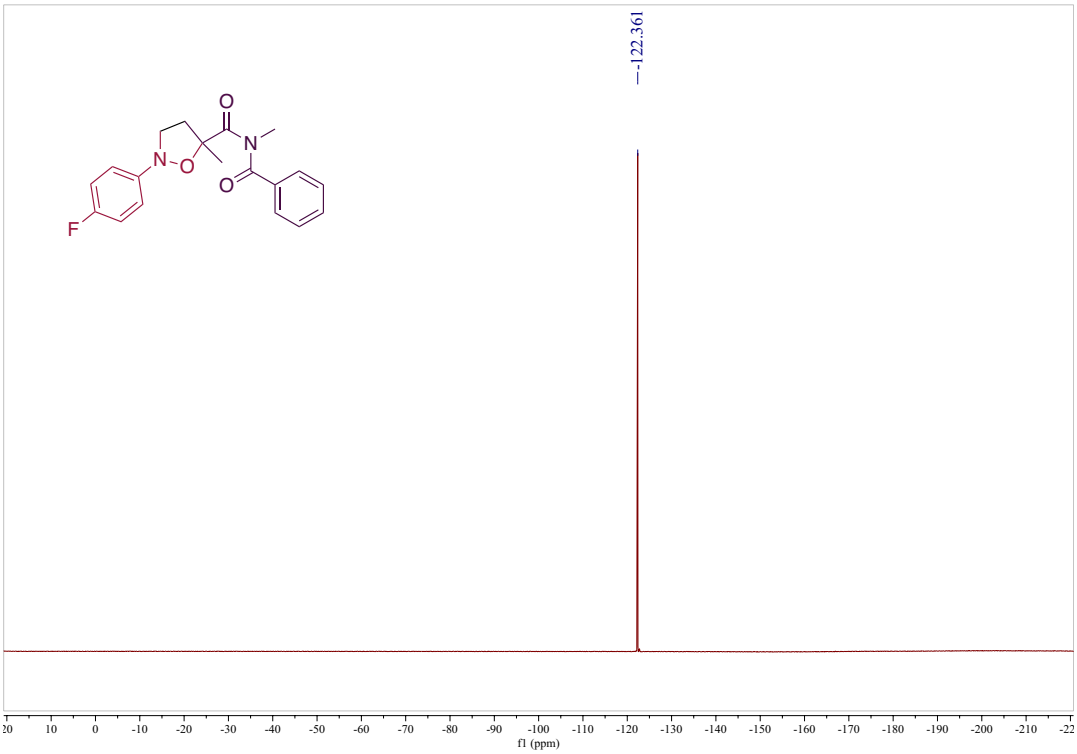
^{1}H and ^{13}C NMR spectra of 3ae:

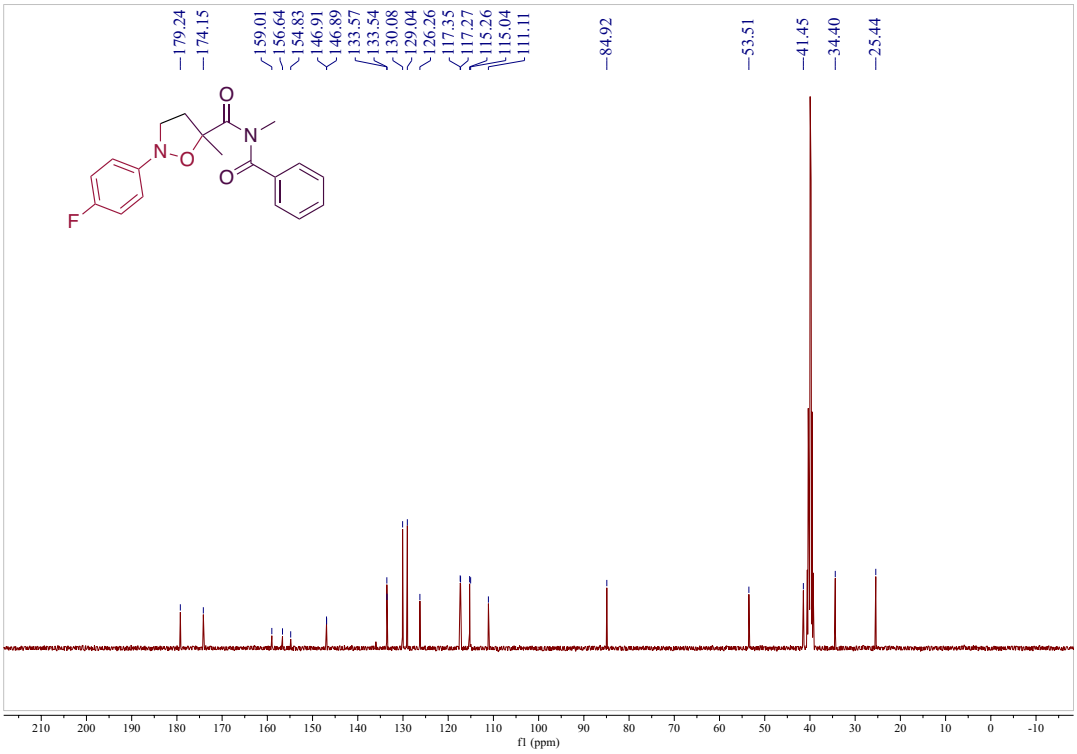




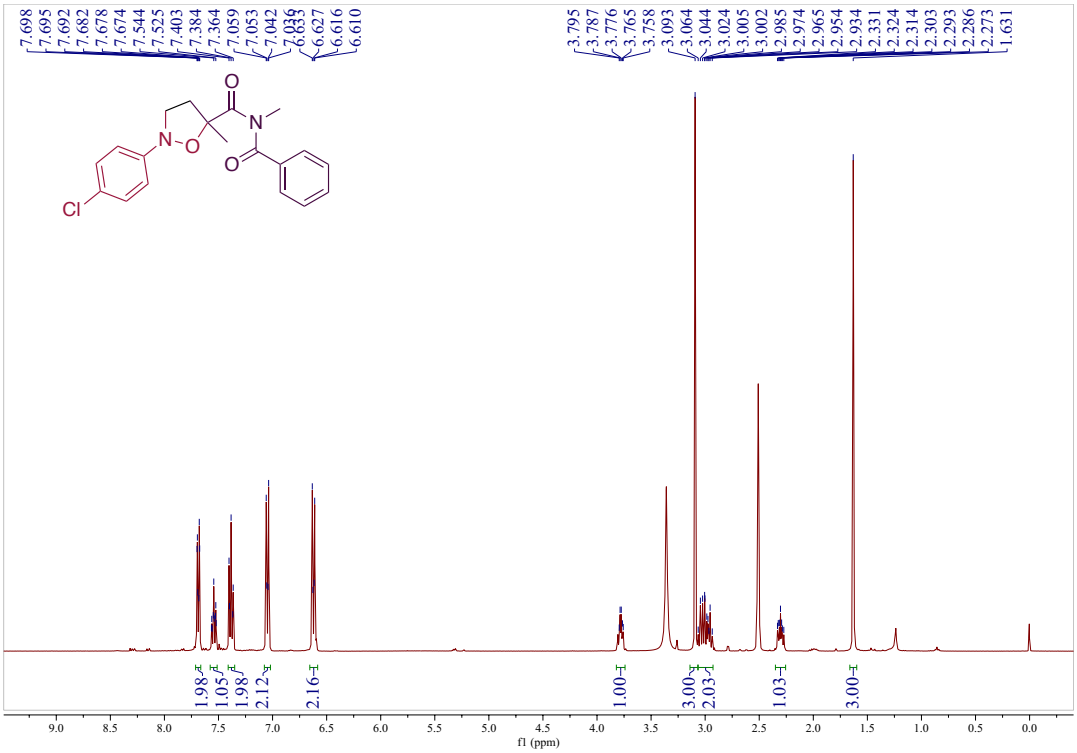
^{1}H ^{19}F and ^{13}C NMR spectra of 3af:

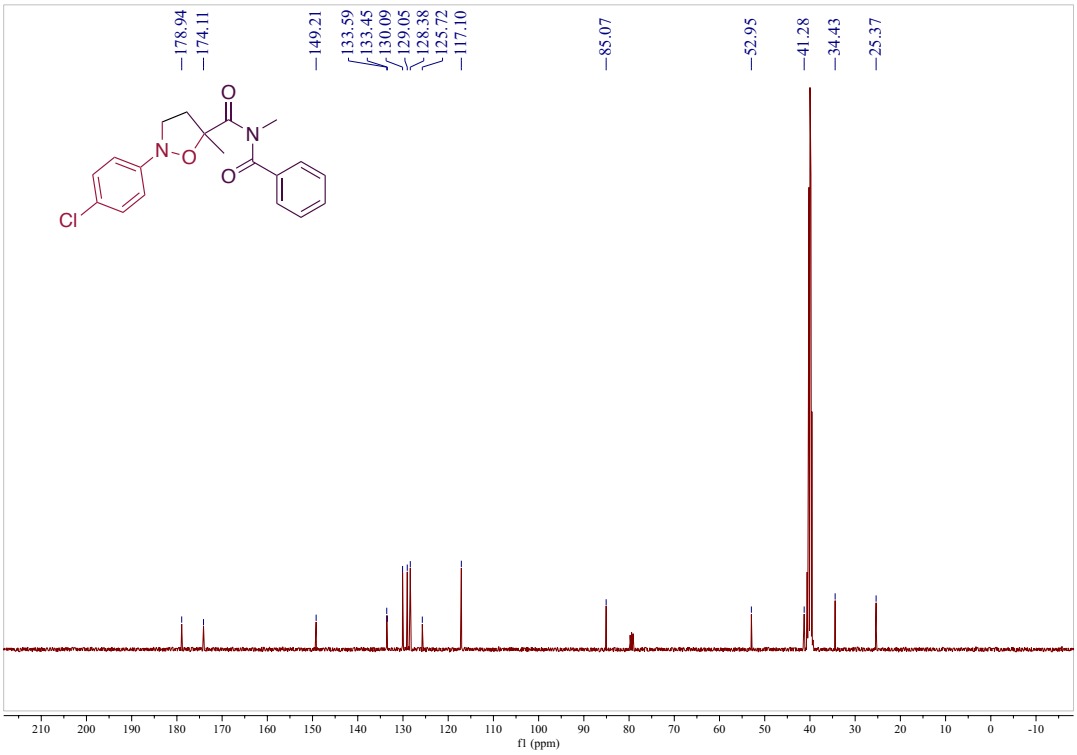




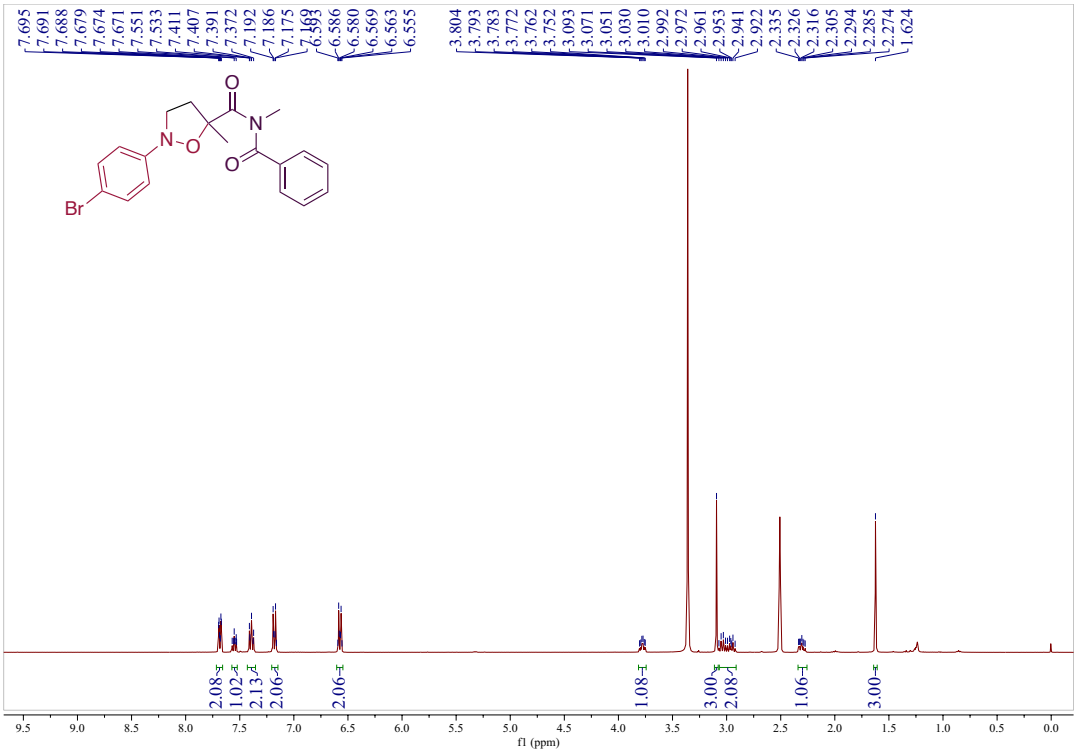

179.24
174.15
159.01
156.64
154.83
146.91
146.89
133.57
133.54
130.08
129.04
126.26
117.35
117.27
115.26
115.04
111.11
84.92
53.51
41.45
34.40
25.44
O
N
O
N
O
F
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

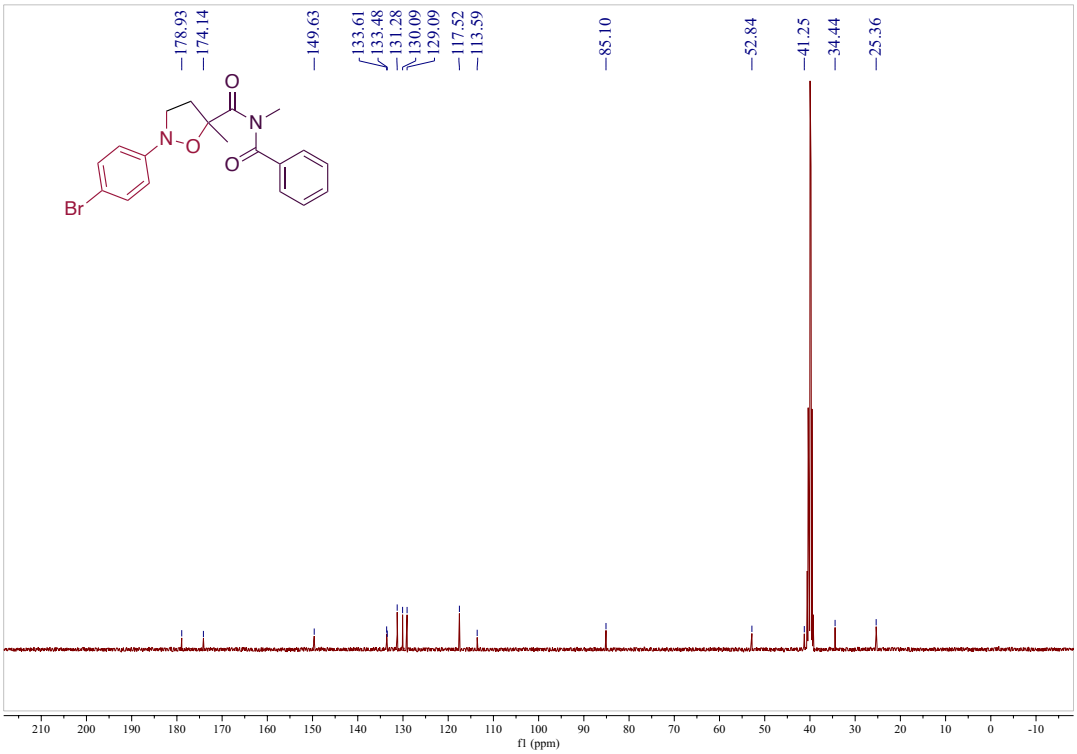
^{1}H and ^{13}C NMR spectra of 3ag:



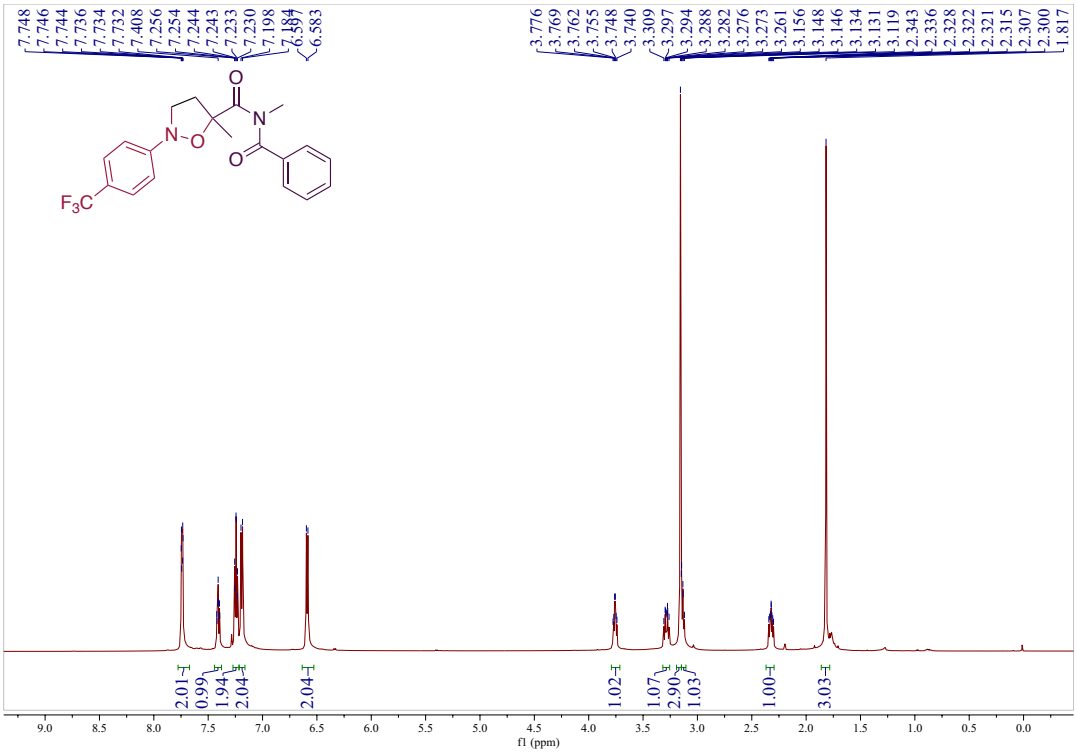


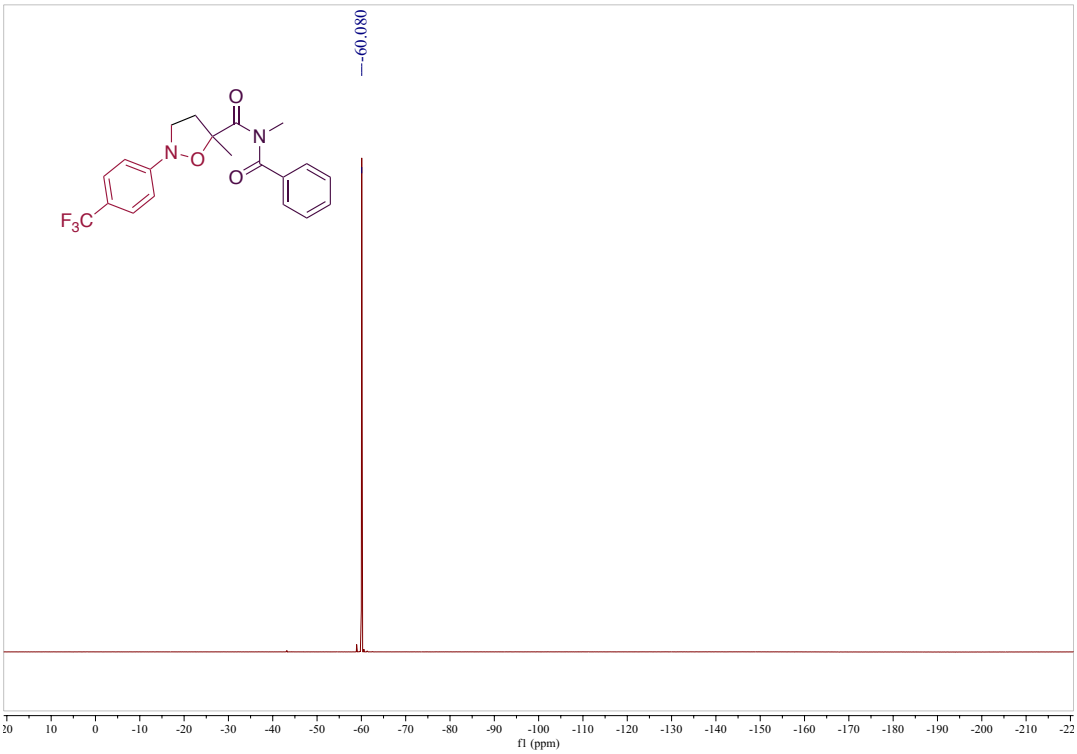
^{1}H and ^{13}C NMR spectra of 3ah:

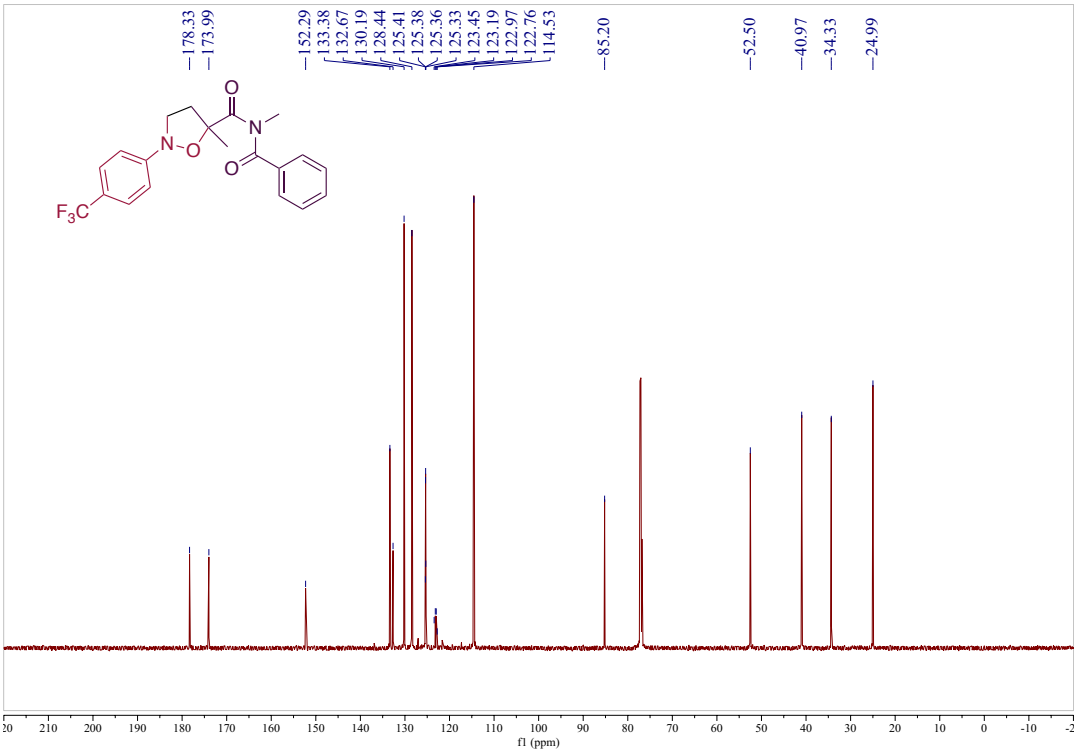




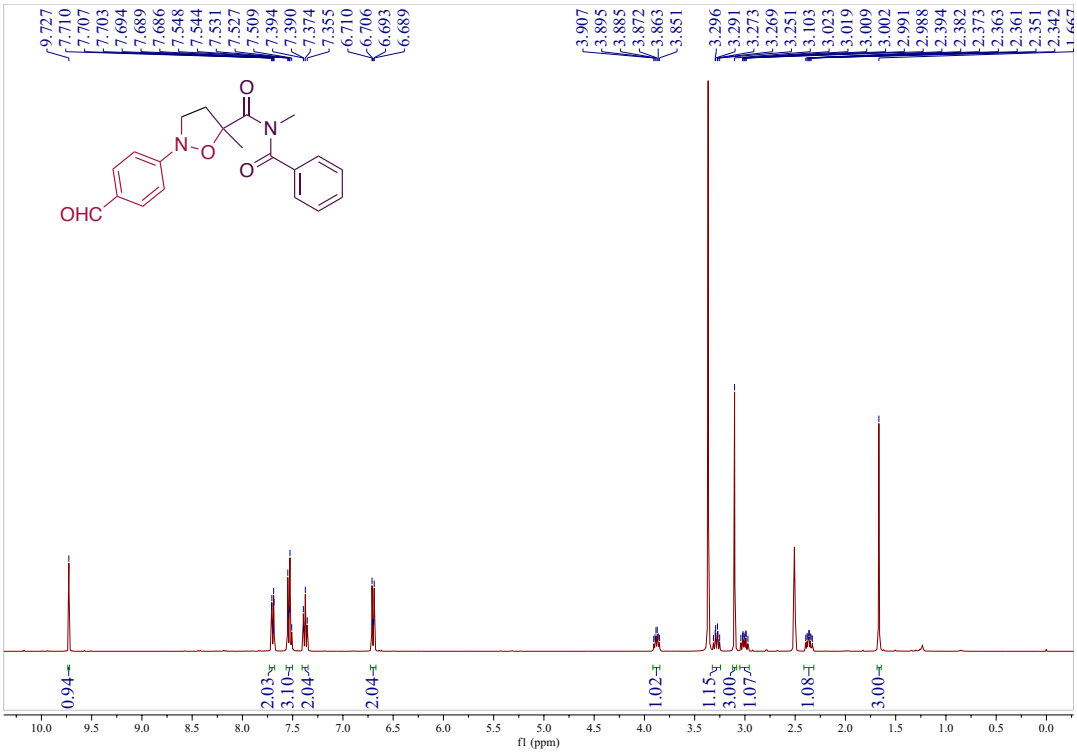
^{1}H ^{19}F and ^{13}C NMR spectra of 3ai:

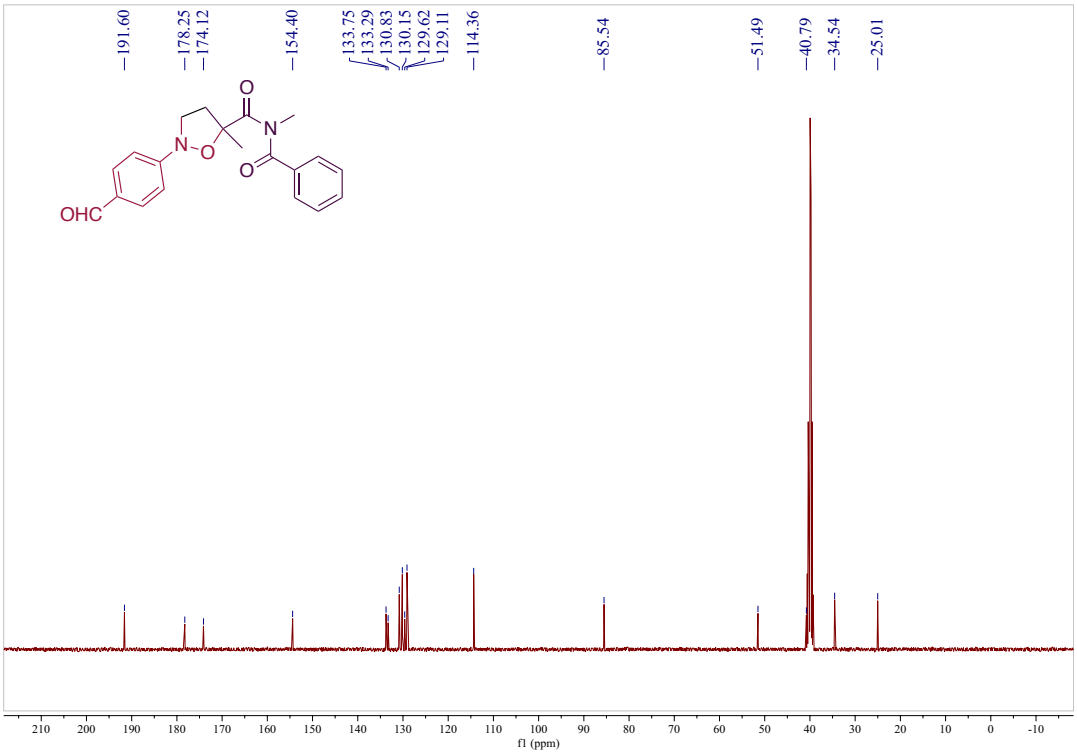




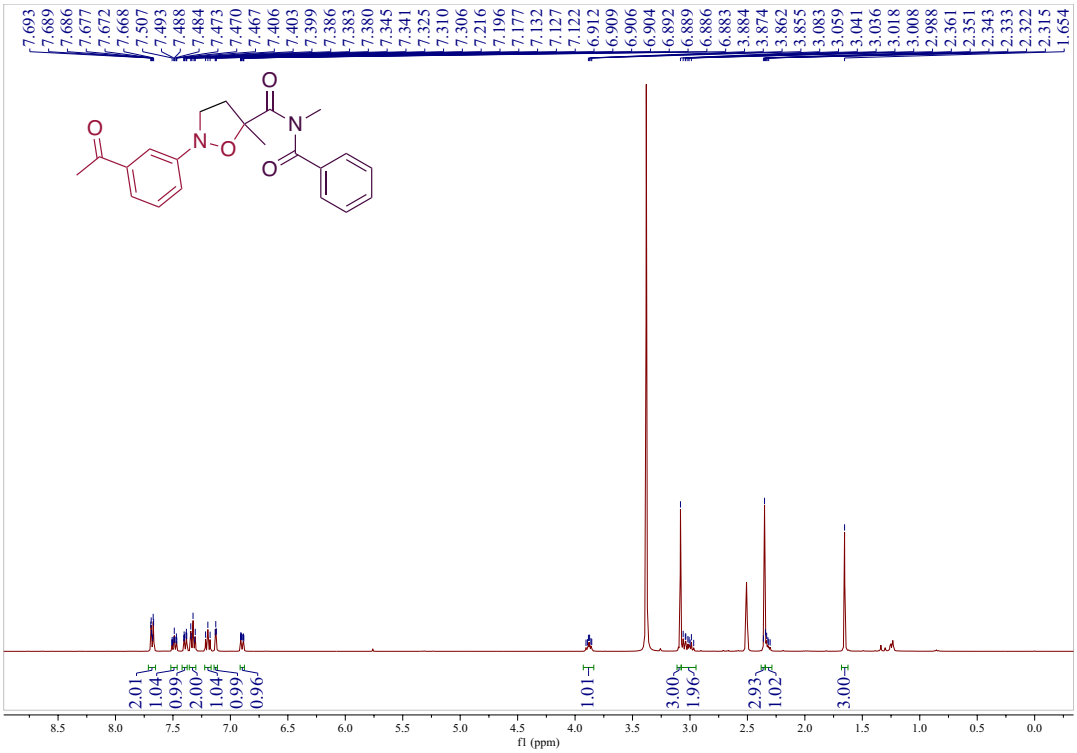

178.33
173.99
152.29
133.38
132.67
130.19
128.44
125.41
125.38
125.36
125.33
123.45
123.19
122.97
122.76
114.53
85.20
52.50
40.97
34.33
24.99
O
N
O
N
O
F3C
f1 (ppm)

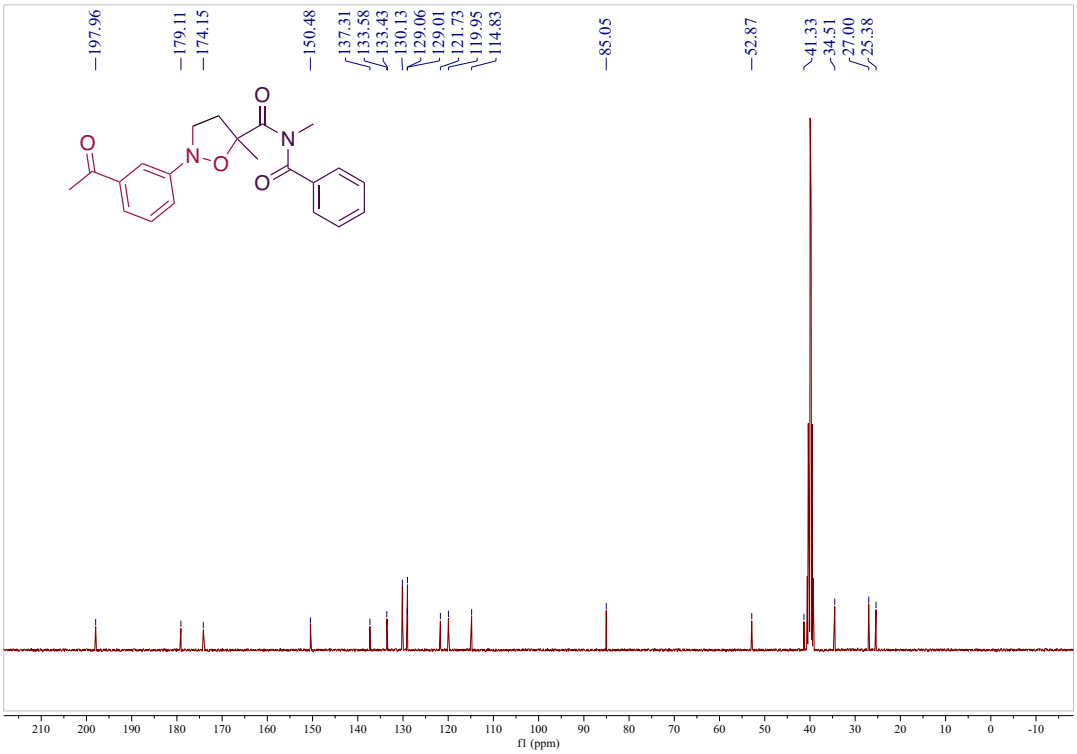
^{1}H and ^{13}C NMR spectra of 3aj:



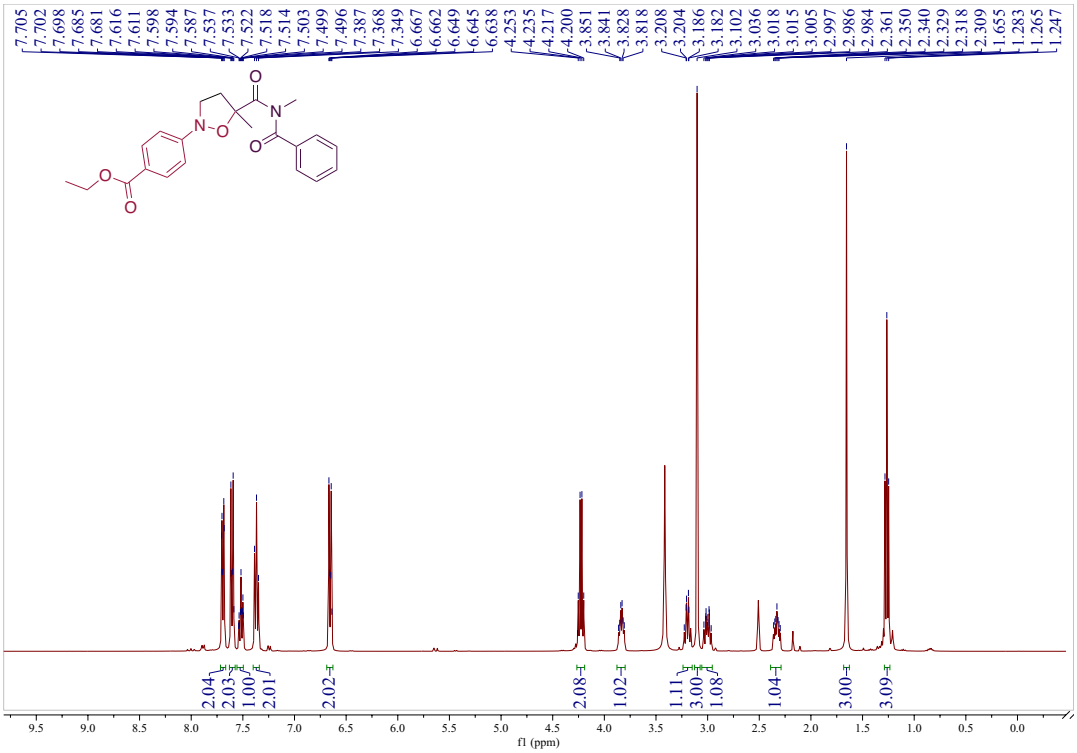


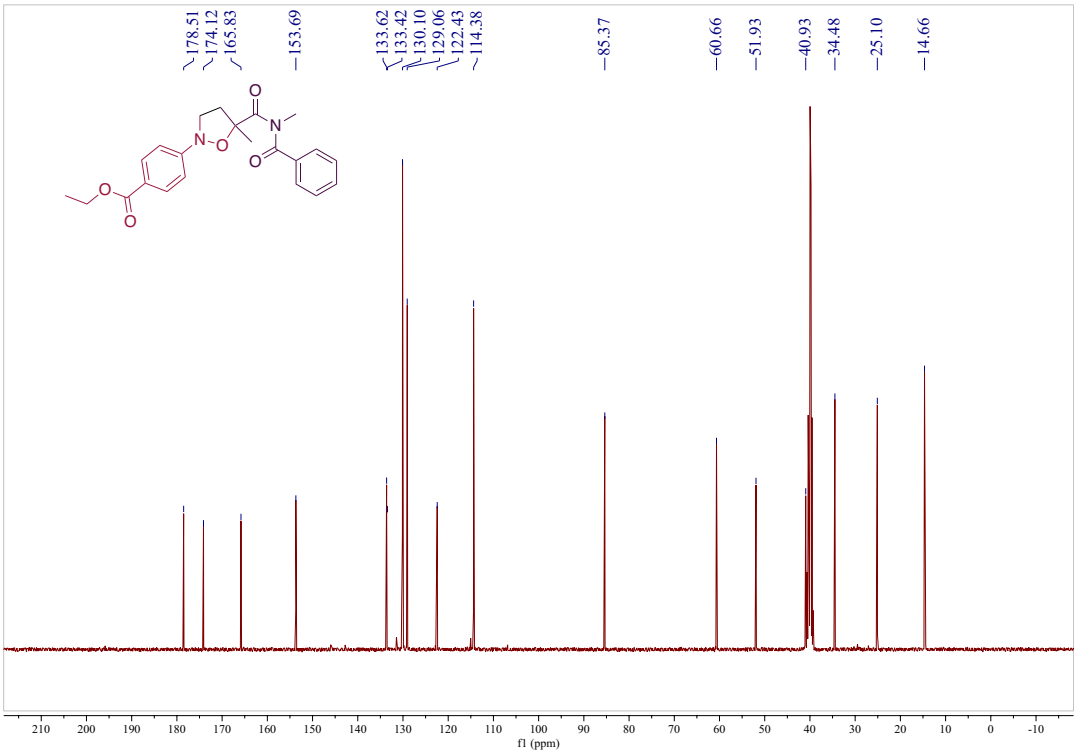
^{1}H and ^{13}C NMR spectra of 3ak:



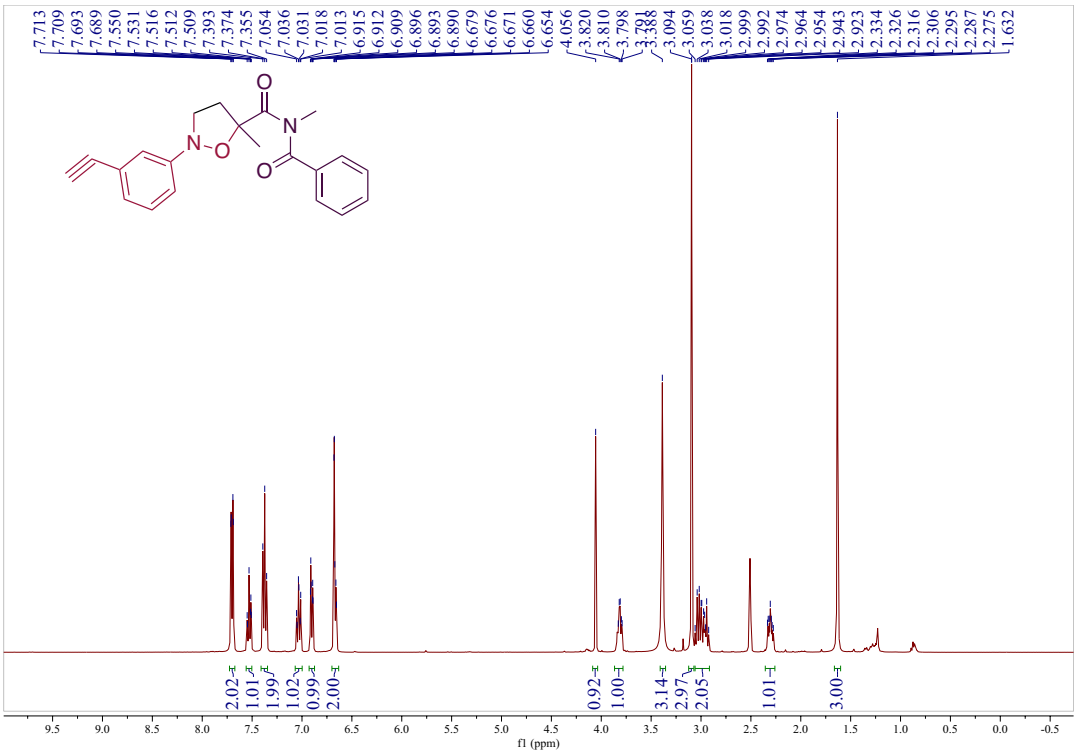


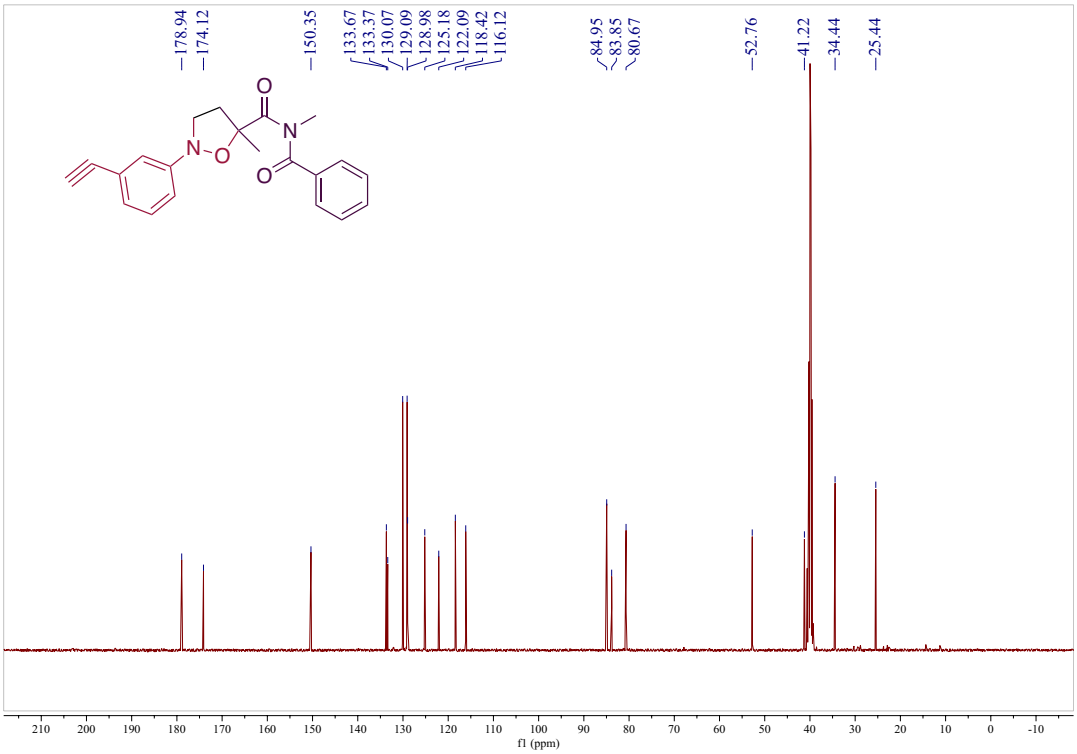
^{1}H and ^{13}C NMR spectra of 3al:



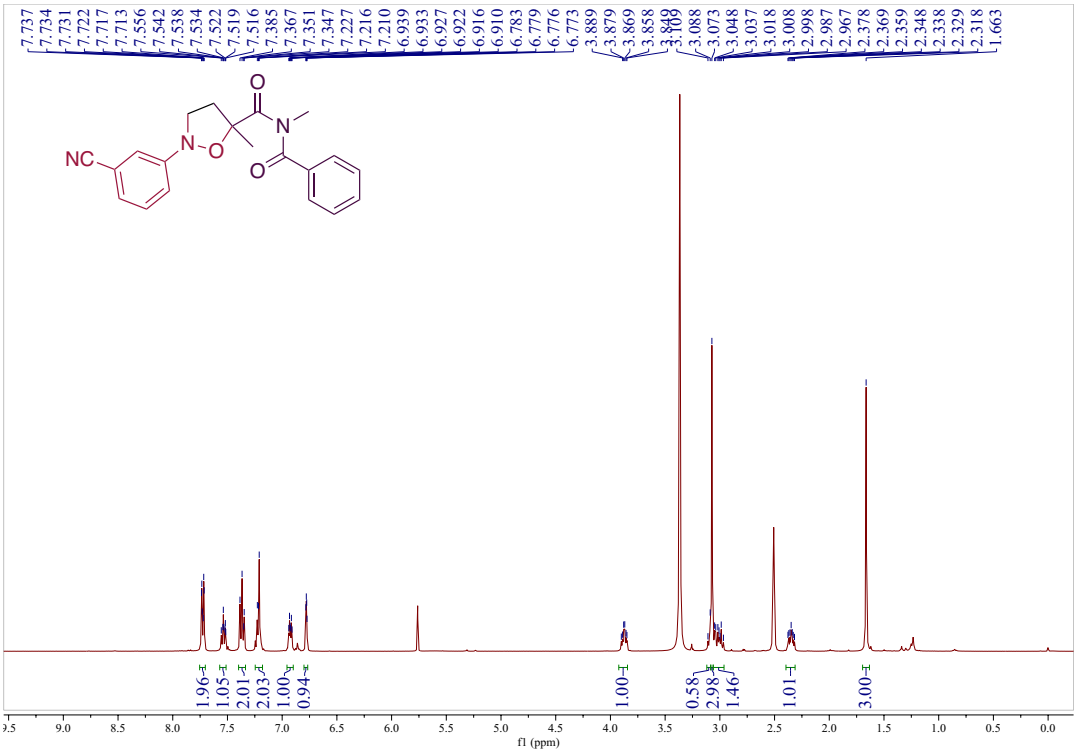


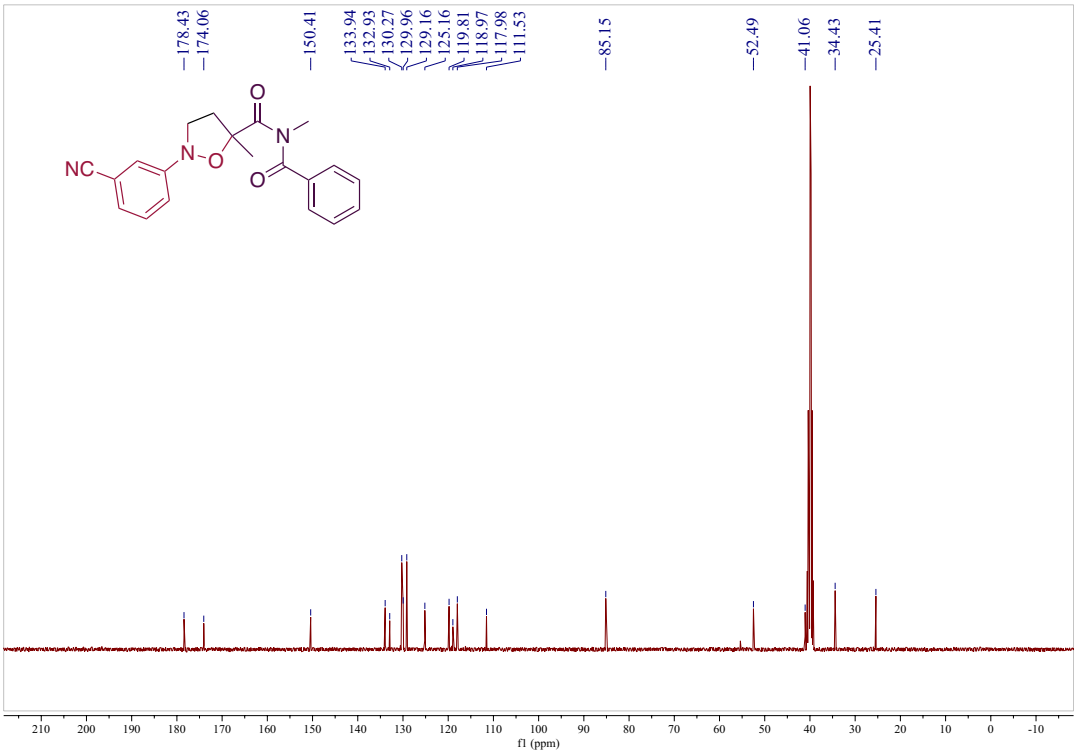
^{1}H and ^{13}C NMR spectra of 3am:



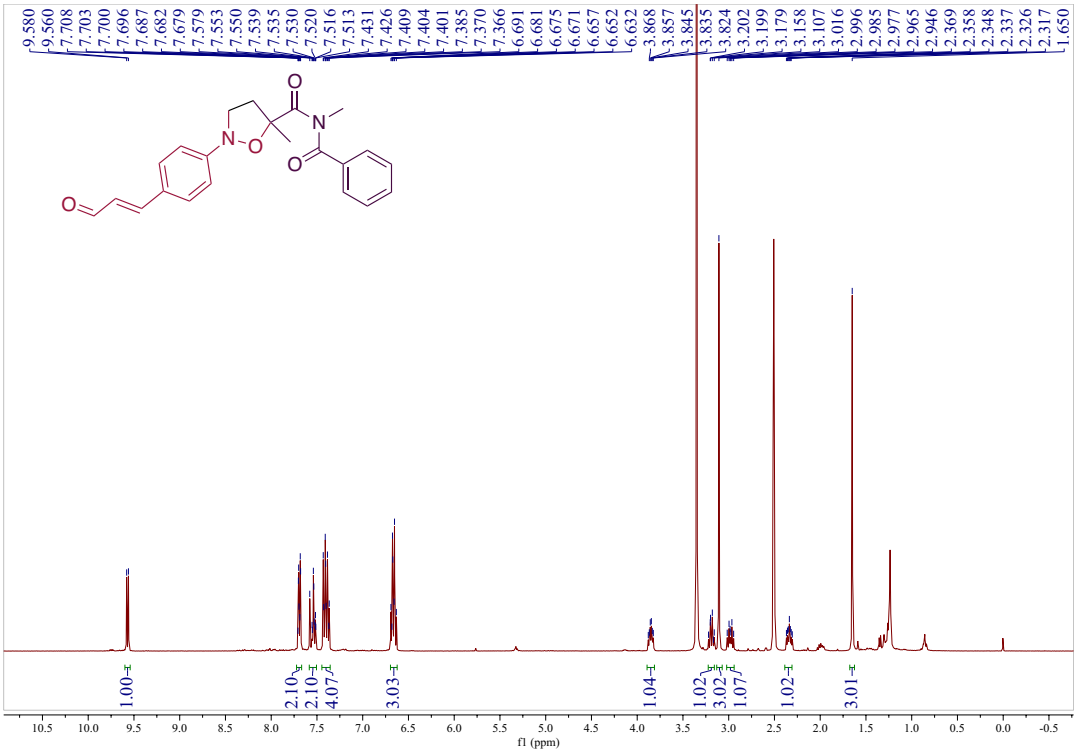


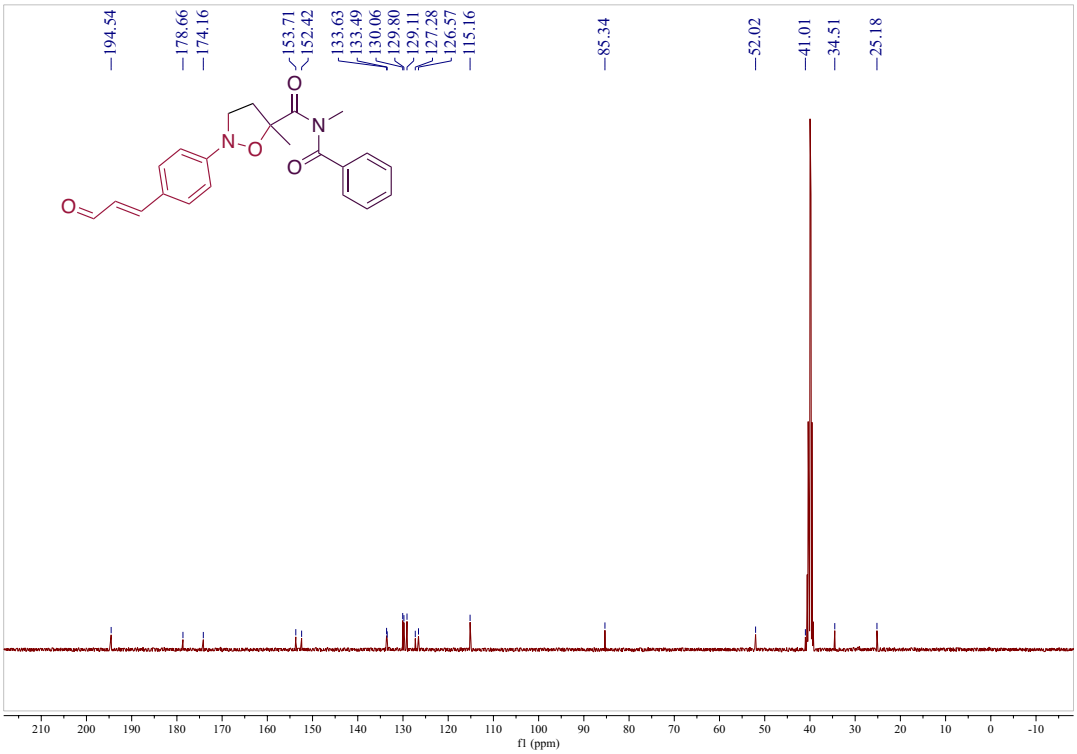
^{1}H and ^{13}C NMR spectra of 3an:



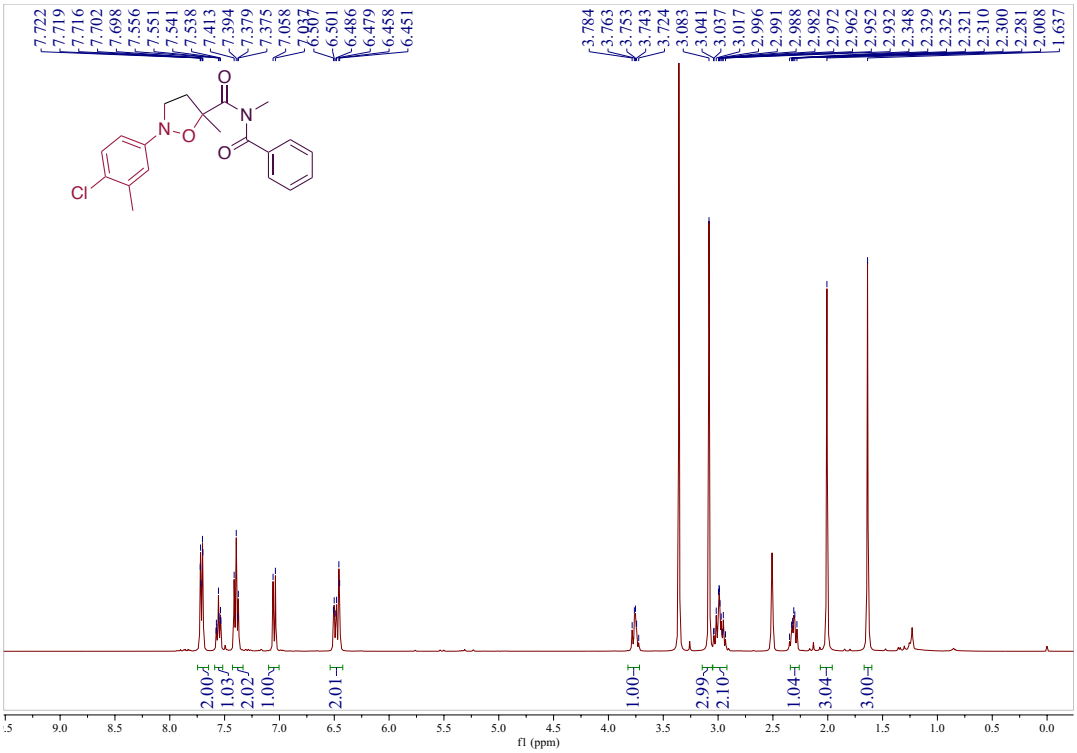


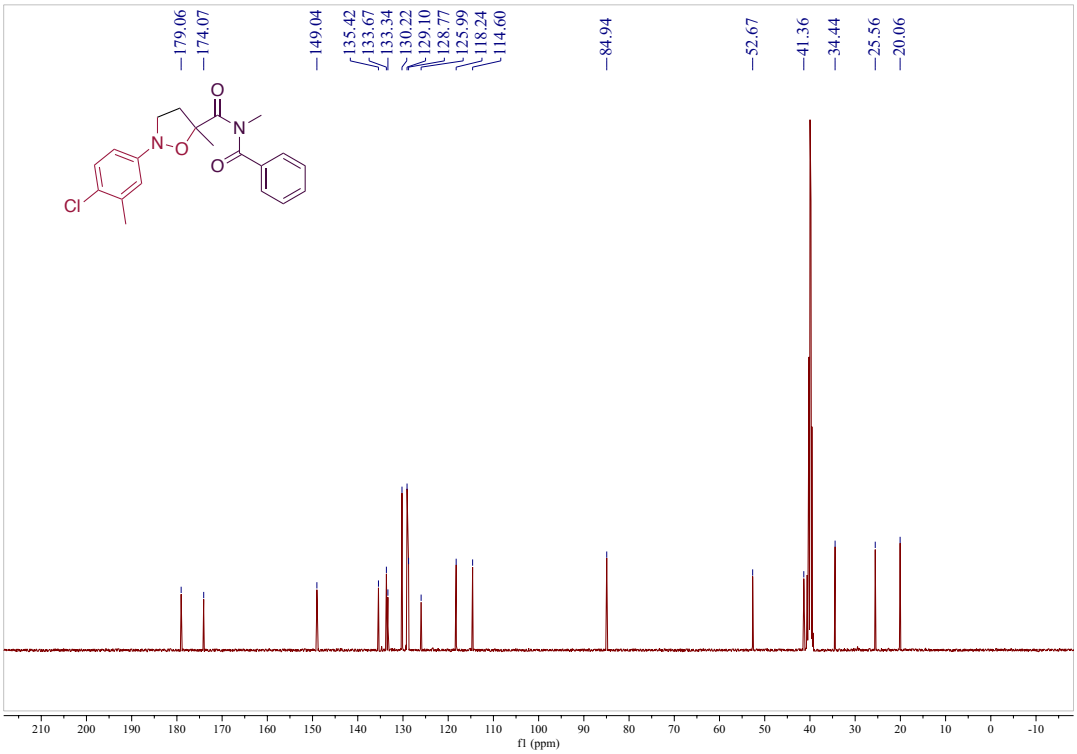
^{1}H and ^{13}C NMR spectra of 3ao:



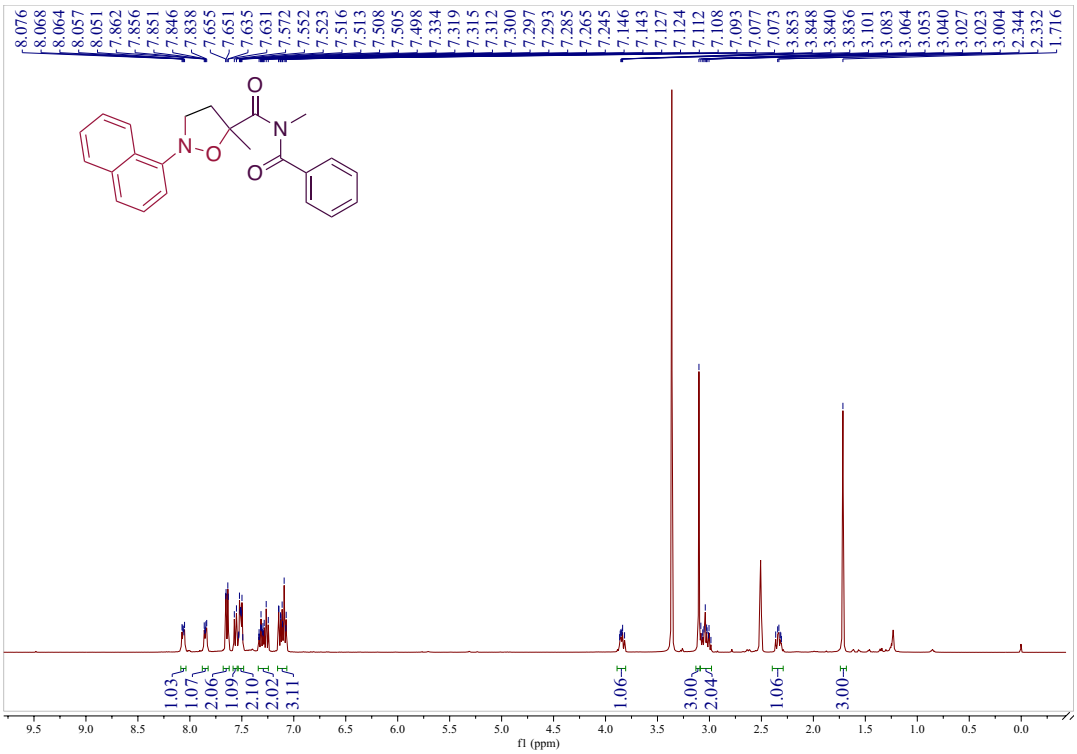


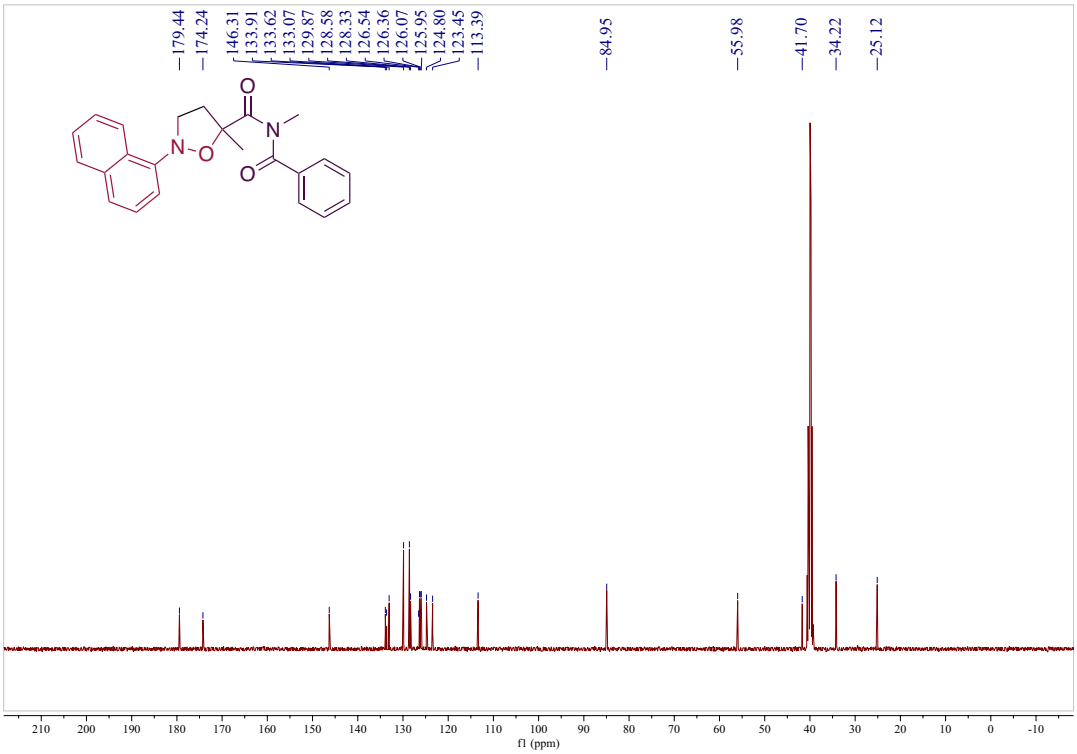
^{1}H and ^{13}C NMR spectra of 3ap:



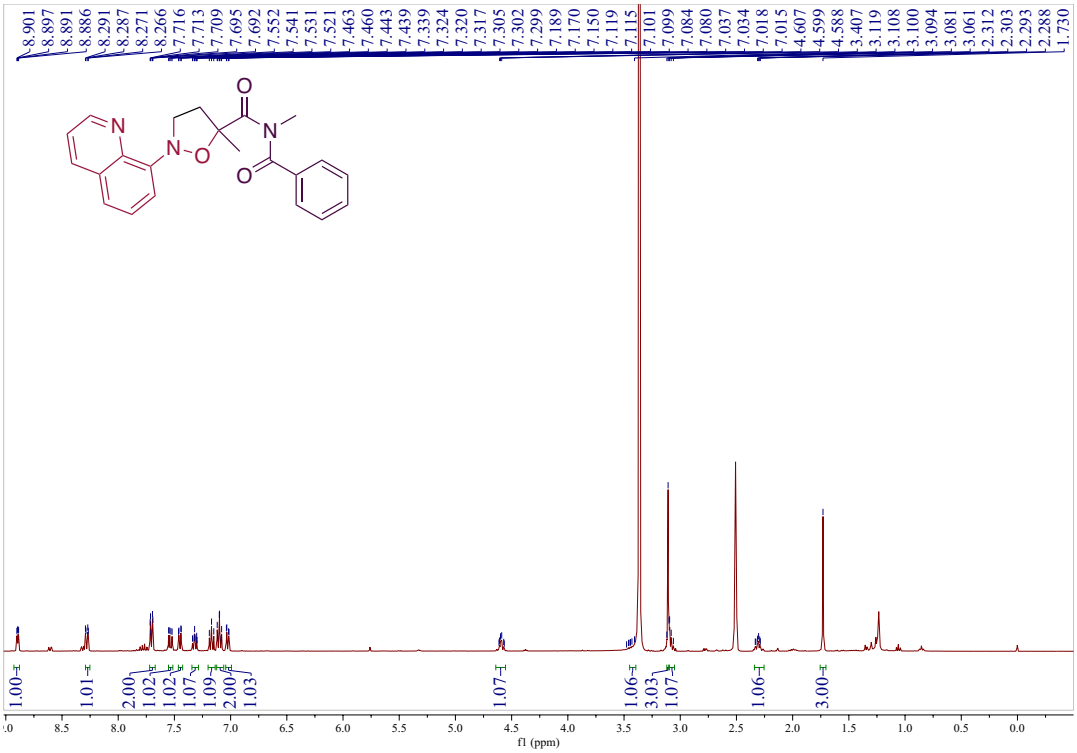


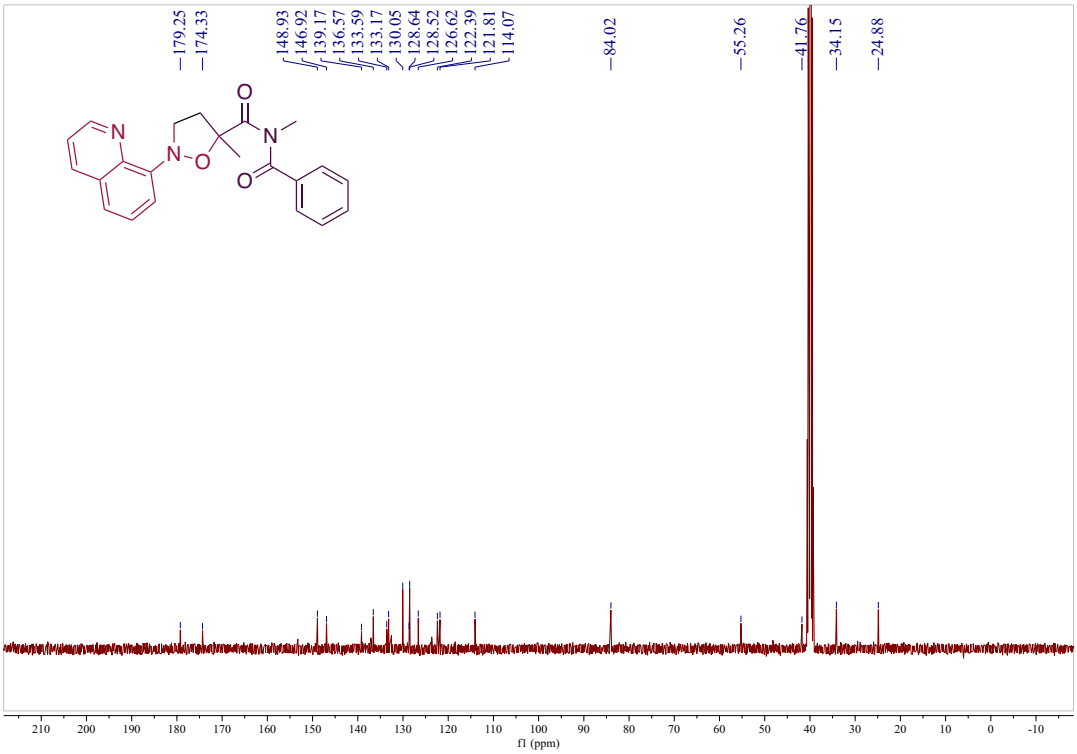
^{1}H and ^{13}C NMR spectra of 3aq:



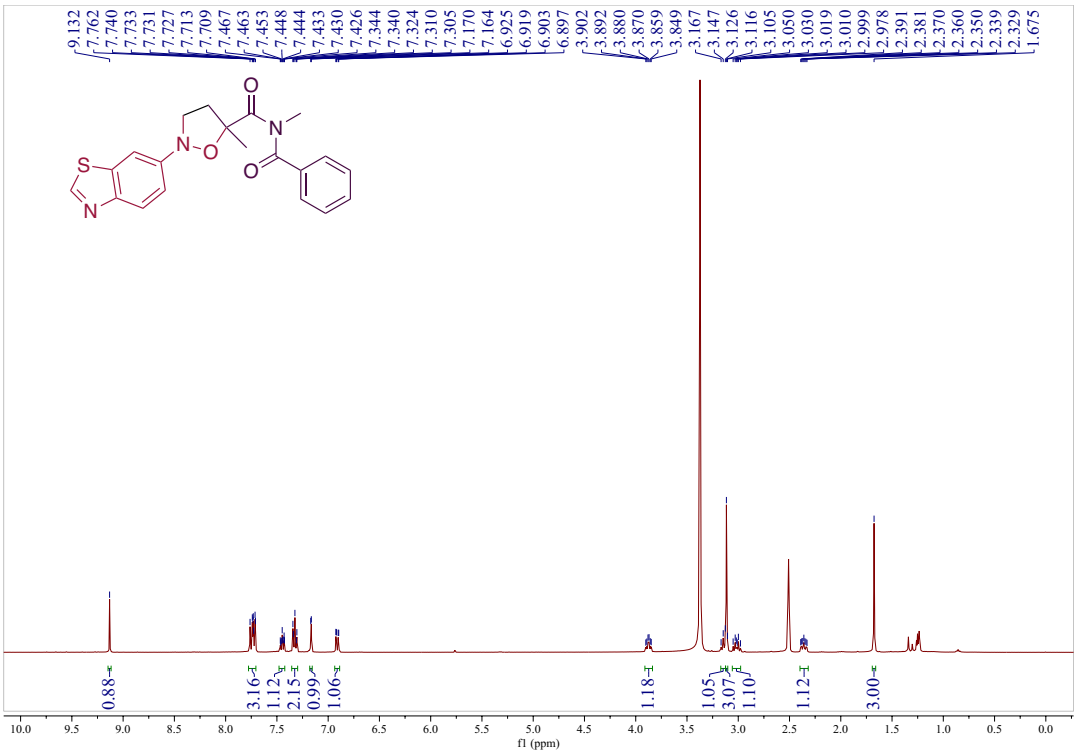


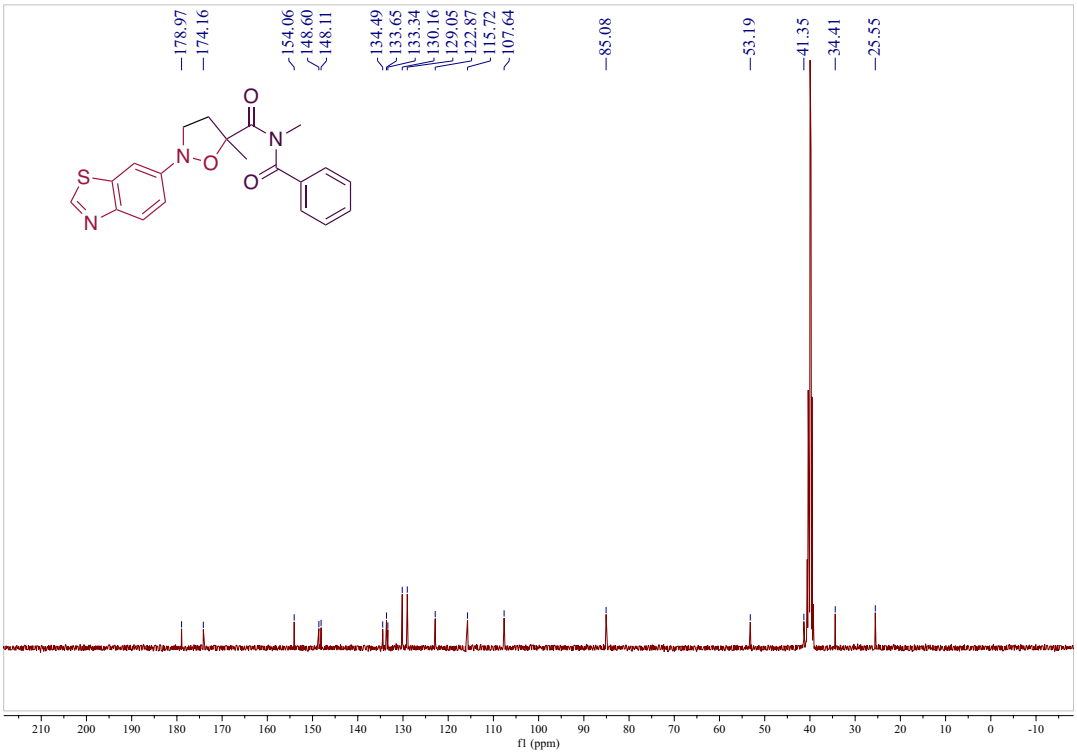
^{1}H and ^{13}C NMR spectra of 3ar:



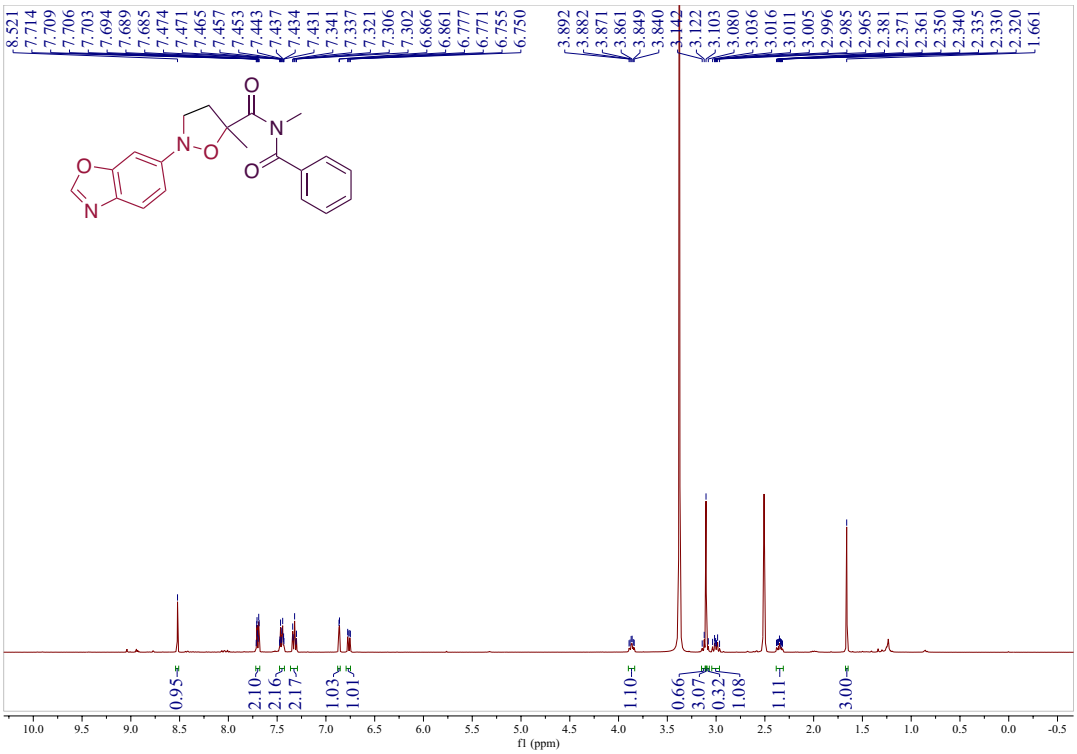


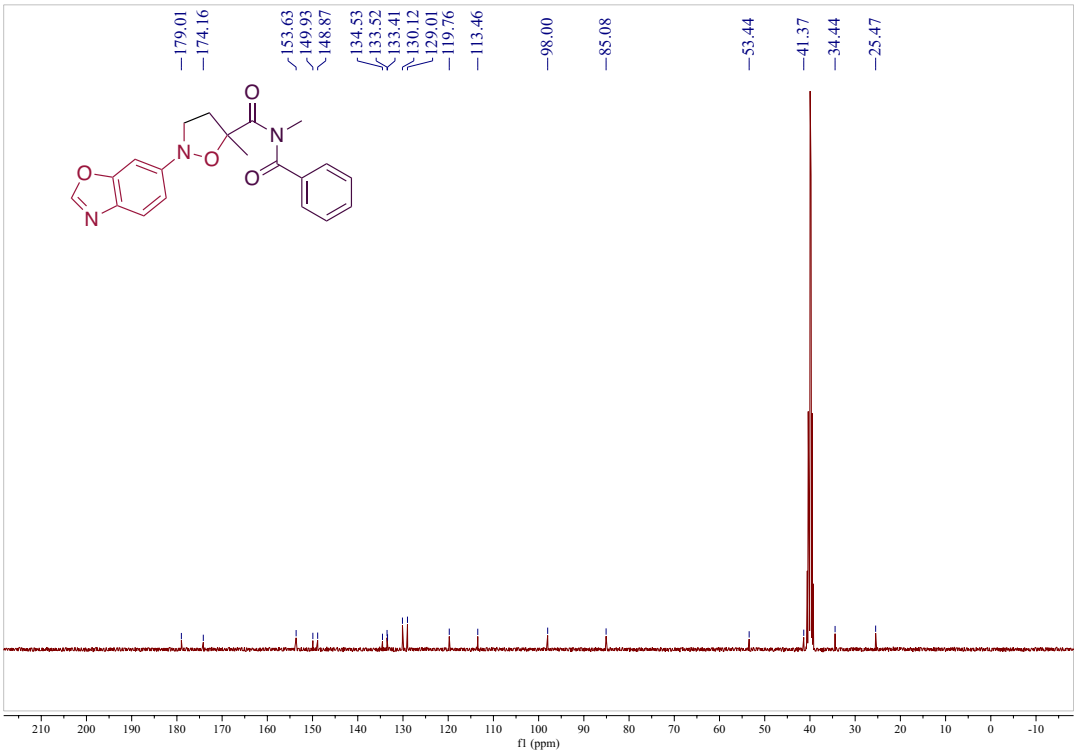
^{1}H and ^{13}C NMR spectra of 3as:



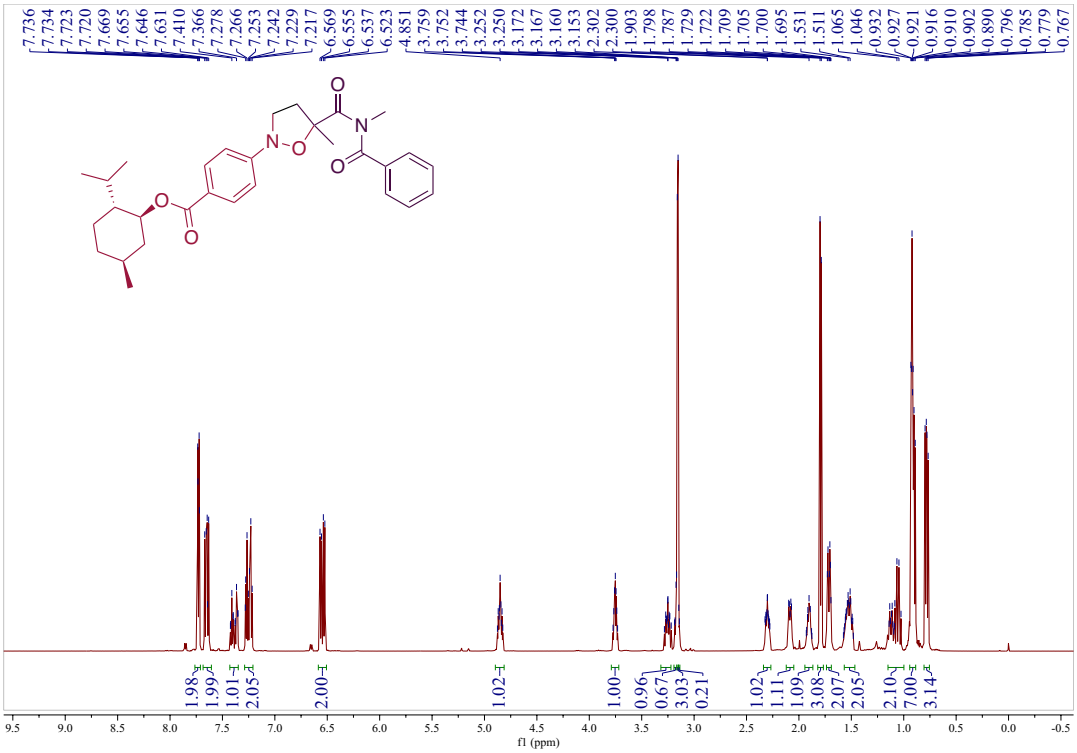


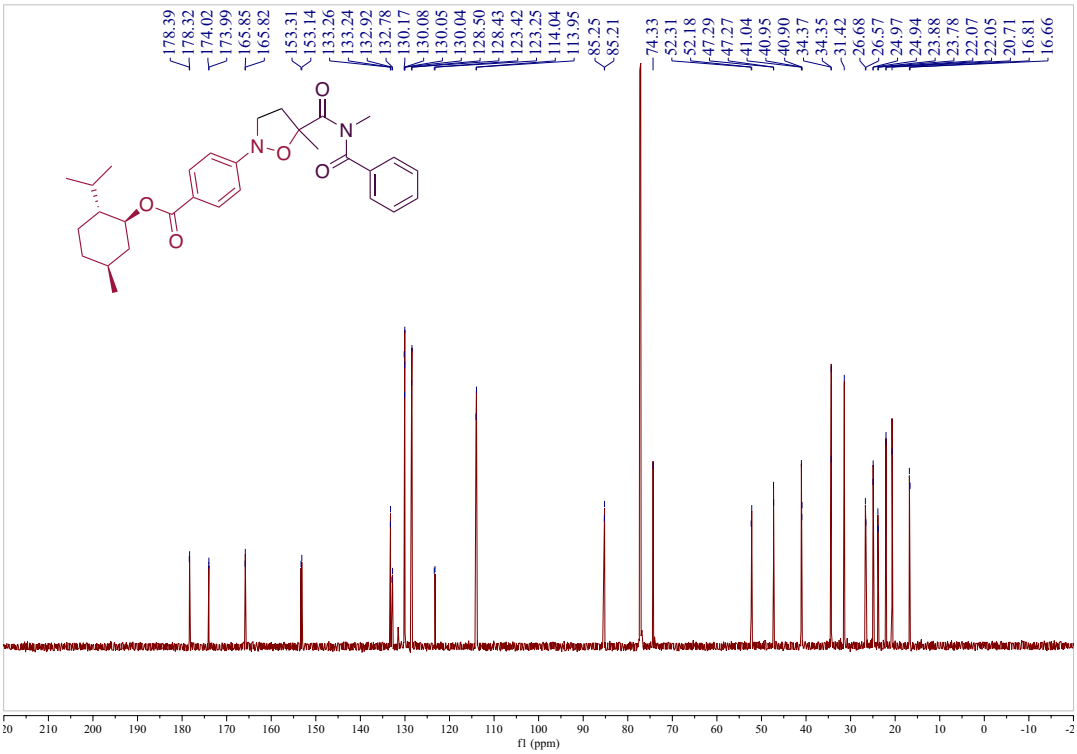
^{1}H and ^{13}C NMR spectra of 3at:



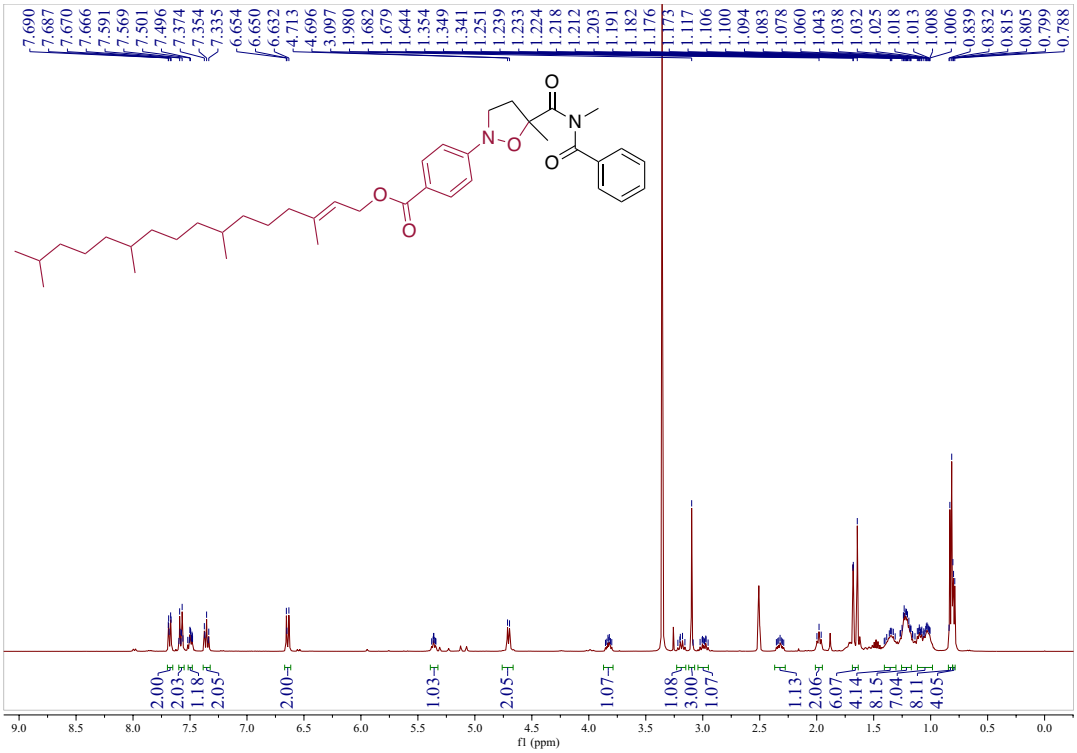


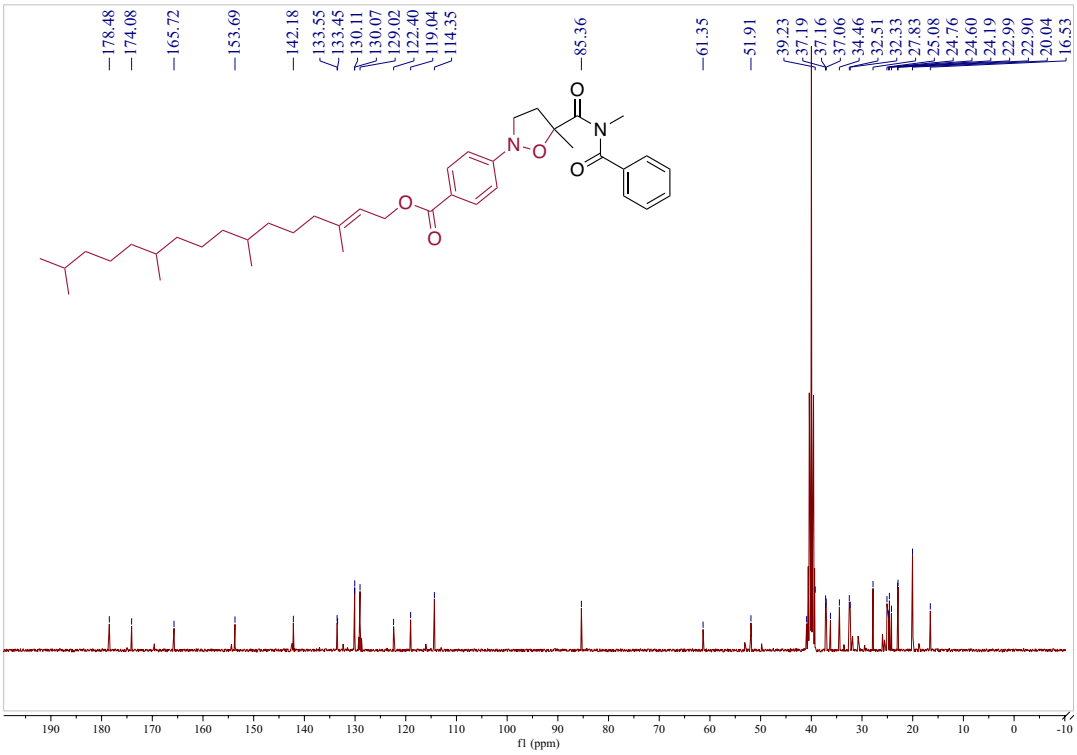
^{1}H and ^{13}C NMR spectra of 3au:



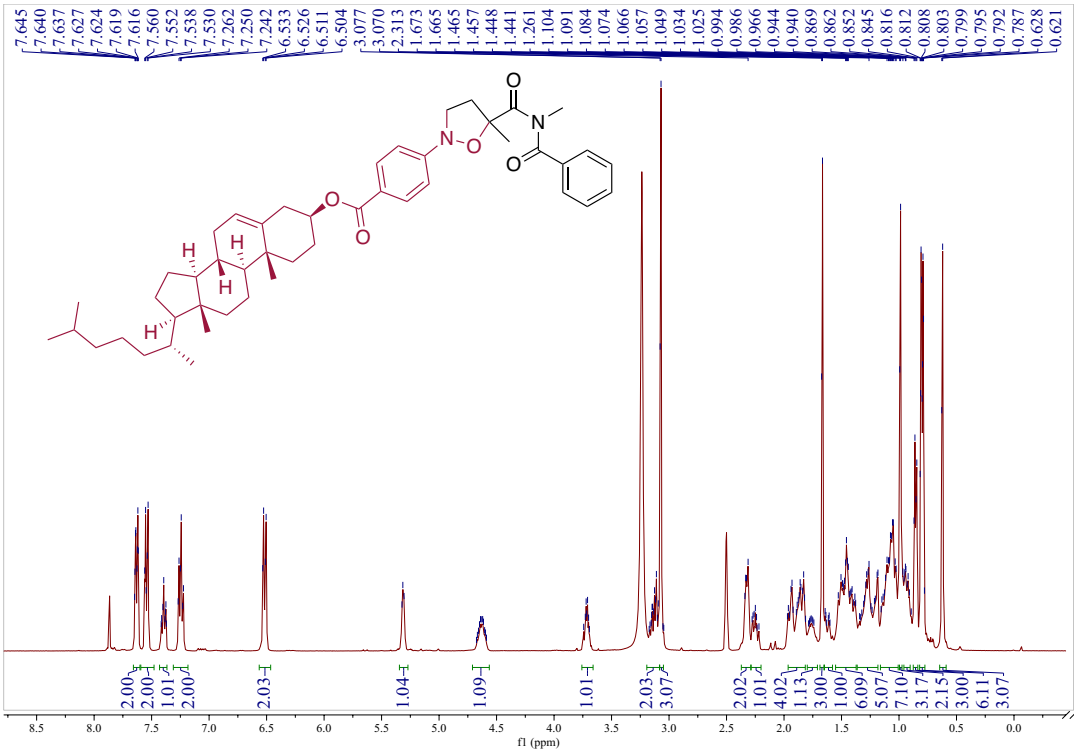


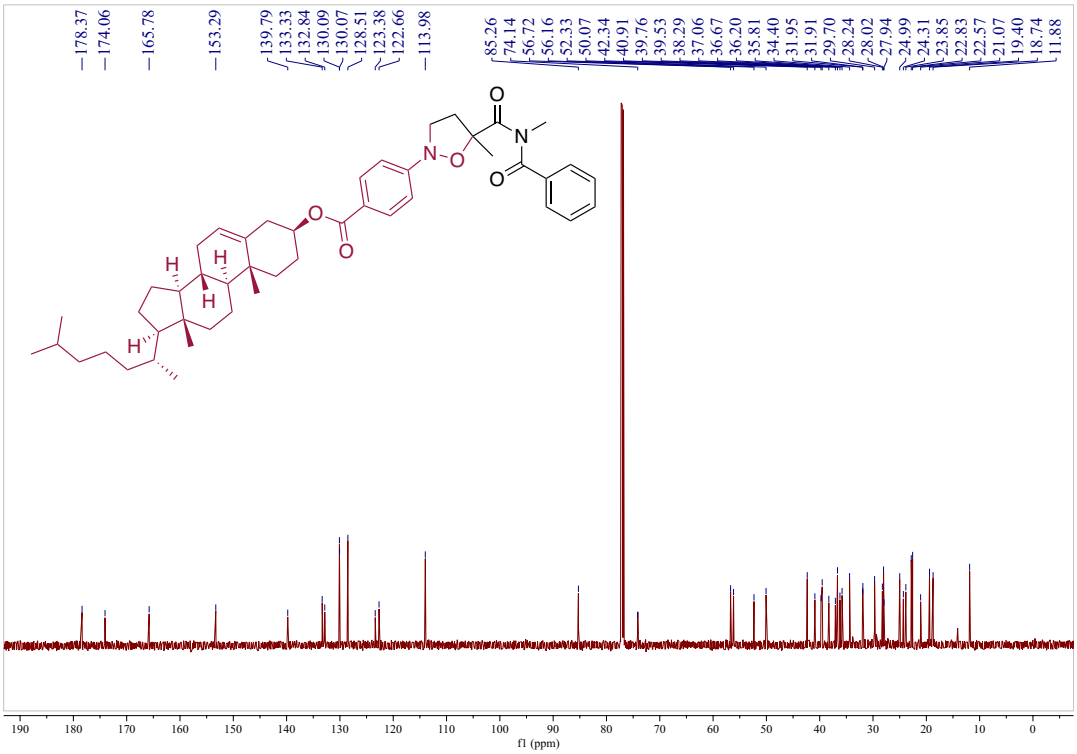
^{1}H and ^{13}C NMR spectra of 3av:





^{1}H and ^{13}C NMR spectra of 3aw:





^{1}H and ^{13}C NMR spectra of 3ax: