Supporting Information

Intramolecular Cascade Cyclization via Photogenerated N-Amidyl Radicals toward Isoindolin-1-one/3,4-Dihydroisoquinolin-1(2H)-one Fused Oxazinane

Yuan-Xiang He, [a, b] Kui Hu, [a, b] Yu Ran, [a, b] Zhen-Yao Lei, [b] Shu Geng, [b] Li-Na Chen, [b] Li Pan, *[b] Jun-Bo Zhong, *[a] and Feng Huang *[b]

[a] College of Chemistry and Environmental Engineering, Sichuan University of Science and Engineering, Zigong, 643000, PR China.

*E-mail: junbozhong@suse.edu.cn;

[b] State Key Laboratory of NBC Protection for Civilian, Beijing 102205, P. R. China.

*E-mail: bk6180b@163.com; john_hf@163.com;

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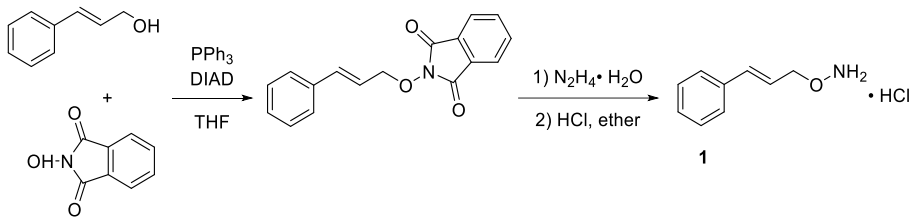
1. General

Unless otherwise noted, reagents obtained from commercial suppliers were used without further purification. All glassware was washed with detergent, rinsed with acetone, and dried in an oven at 125 °C before use. Moisture-sensitive reactions were carried out in the argon atmosphere, and sensitive reagents were added via syringe and cannula techniques. TLC (Thin Layer Chromatography) was performed on precoated silica gel HSGF254 plates, which were visualized by UV light (254 nm), iodine, $KMnO_4$ solution, or alcoholic solution of phosphomolybdic acid. CC (column chromatography) was performed on silica gel 100-200/, 200–300/, and 300–400 mesh obtained from Qingdao Haiyang Chemical. ^{1}H NMR (300 MHz or 600 MHz), ^{13}C NMR (75 MHz or 150 MHz), and ^{19}F NMR (282 MHz) spectra were recorded in $CDCl_3$ (^{1}H NMR: δ 7.26, ^{13}C NMR: δ 77.16) or CD_3OD (^{1}H NMR: δ 3.30, ^{13}C NMR: δ 49.00) on Bruker AVANCE 300 or 600 instruments. The chemical shifts (δ) are reported in ppm using TMS as an internal standard, and coupling constants (*J*) are given in Hz. The high-resolution mass spectrometry (HRMS) spectra were obtained on an Ultimate 3000 UHPLC-Thermo QE Focus MS instrument. IR spectra were obtained on a Bruker Mobile-IR instrument, and the photoreactor is SSSTECH-AF1 from Shanghai 3S Technology Co., Ltd.

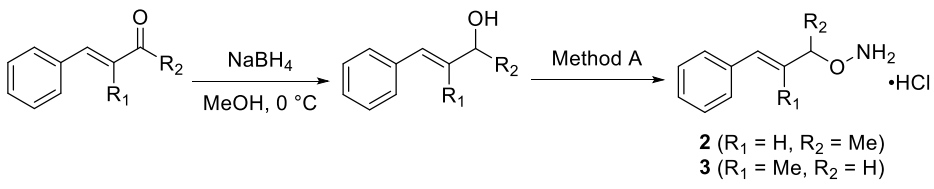
2. Substrates preparation

Procedure for the synthesis of substrate 1 (Method A)[1]:



To a solution of cinnamyl alcohol (22.4 mmol, 1.0 equiv) in dry THF (150 mL) was added triphenylphosphine (24.7 mmol, 1.1 equiv) and N-hydroxylphthalimide (24.7 mmol, 1.1 equiv). After the solution was cooled to 0 °C, the diisopropylazodicarboxylate (24.7 mmol, 1.1 equiv) was added dropwise. The solution was allowed to warm to room temperature and stirred over 3 h. Reaction progress was monitored by TLC. The hydrazine monohydrate (85%, 1.1 equiv) was then added, and the solution was stirred for another 30 min. The resulting reaction mixture was filtered to remove the white precipitate. The filtrate was concentrated, and the resulting product was dissolved in ether and treated with HCl (2 M solution in ether) to afford the HCl salt of the O-cinnamylhydroxylamine (55% overall yield, white power).

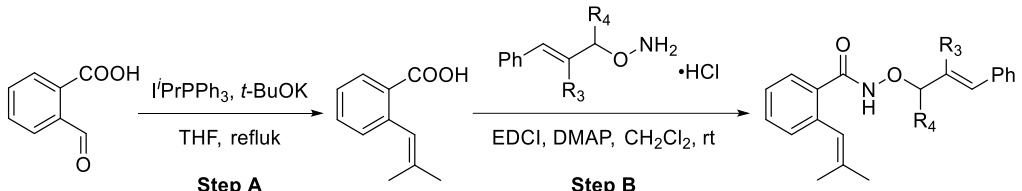
Procedure for the synthesis of substrates 2 and 3 (Method B):



$NaBH_4$ (24.0 mmol, 1.2 equiv) was added to a stirred solution of benzylidene acetone (20.0 mmol,

1.0 equiv) in MeOH (20 mL) at 0 °C, and the mixture was stirred at 0 °C for 30 min. After that, the reaction was quenched by adding saturated aqueous NH_4Cl and extracting with ethyl acetate. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure to obtain secondary allyl alcohol in the form of a yellow liquid in an almost quantitative yield, which was used in the subsequent step without further purification[2]. The corresponding HCl salt of the O-cinnamylhydroxylamine was synthesized by the same **method A**.

Procedure for the synthesis of substrates 1a, 1s and 1t (Method C):

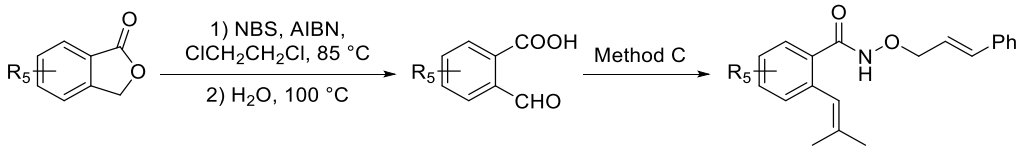


1a, R_3 = H, R_4 = H;
1s, R_3 = H, R_4 = Me;
1t, R_3 = Me, R_4 = H;

Step A. A solution of isopropyltriphenylphosphinium iodide (32.0 mmol, 2.0 equiv) and potassium tertbutoxide (48.0 mmol, 3.0 equiv) in THF (120 mL) was stirred at room temperature for 1.5 h. 2-formylbenzoic acid (16.0 mmol, 1.0 equiv) was added, and the solution was refluxed overnight. Until the reaction was completed, as monitored by TLC, the resulting mixture was quenched with water, basified with aqueous NaOH (3 M), and washed with diethyl ether. The resulting aqueous phase was acidified with aqueous HCl (3 M) until pH = 1-2 and extracted twice with ethyl acetate. The combined organic layers were washed with water, and brine, dried with Na_2SO_4, filtered, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel (gradient eluent of EtOAc/petroleum ether: 2/1 to 5/1) to afford the desired unsaturated benzoic acid derivatives (white solid 95%)[3].

Step B. To a solution of 2-(2-methylprop-1-en-1-yl) benzoic acid (13.0 mmol, 1.0 equiv) in CH_2Cl_2 (90 mL) was added the corresponding HCl salt of the O-cinnamylhydroxylamine (19.5 mmol, 1.5 equiv), EDCI (26.0 mmol, 2.0 equiv) and DMAP (26.0 mmol, 2.0 equiv) successively. The resulting mixture was stirred at room temperature overnight. The reaction was quenched by adding HCl (3 M). The organic layer was separated, and the aqueous layer was extracted with CH_2Cl_2. The combined extracts were washed with brine, dried over Na_2SO_4, and filtrated. The filtrate was concentrated and purified by column chromatography on silica gel (gradient eluent of EtOAc/petroleum ether: 1/3 to 1/2) to yield the product (white solid 91%)[4–6].

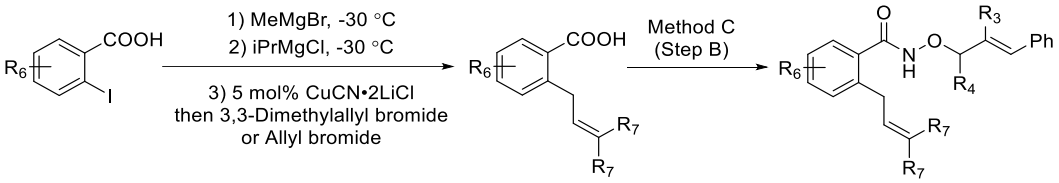
Procedure for the synthesis of substrates 1b-1r (Method D):



To a solution of phthalides (12.0 mmol, 1.0 equiv) in 60 mL 1, 2-dichloroethane was added NBS (13.2 mmol, 1.1 equiv) and AIBN (0.6 mmol, 0.05 equiv) was added at room temperature. Then the mixture was refluxed at 85 °C overnight. It was cooled to room temperature and purified by flash column chromatography on silica gel (gradient eluent of EtOAc/petroleum ether: 1/5 to 1/4). The product was then suspended in 100 mL H_2O and heated to 100 °C. After 1 h, the mixture was cooled

to room temperature and extracted with EtOAc (3×30 mL). The combined extracts were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. To give a corresponding 2-formylbenzoic acid as a solid[7,8]. From the benzoic acid derivative, the corresponding benzamide derivate was synthesized by the same **method C**.

Procedure for the synthesis of substrates 3a-3q (Method E):

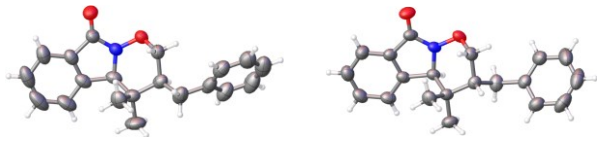


To a stirred solution of 2-iodobenzoic acid (10.0 mmol, 1.0 equiv) and THF (30 mL) at -30 ºC in an oven-dried flask under argon was added MeMgBr (1.0 equiv, 1 M in THF) and stirred for 5 min. ^{i}PrMgCl (1.2 equiv, 2 M in THF) was added slowly, and the reaction was stirred at -30 ºC for 1 h or until the reaction was complete by TLC (an aliquot was quenched with water before analysis). The reaction was then cooled to -40 ºC, and a solution of CuCN·2LiCl in THF (0.09 mL, 0.05 mol) was added slowly and stirred for 10 min while warming to -30 ºC. 3, 3-Dimethylallyl bromide (30.0 mmol, 3.0 equiv) was added at once, and the reaction was allowed to warm to ambient temperature overnight. The reaction was diluted with EtOAc, acidified with 1 M HCl to pH = 3, and extracted with EtOAc. The combined organic layers were washed with brine and dried over Na_2SO_4. The crude mixture was concentrated and purified by column chromatography on silica gel (gradient eluent of EtOAc/petroleum ether: 1/2 to 1/1) to yield 2-(3-methylbut-2-en-1-yl) benzoic acid (white solid 48%)[9]. The corresponding benzamide derivate was synthesized by the same **method C (Step B)**.

3. General experimental procedure

Typical experimental procedure for the cascade annulations:

1a **2a**

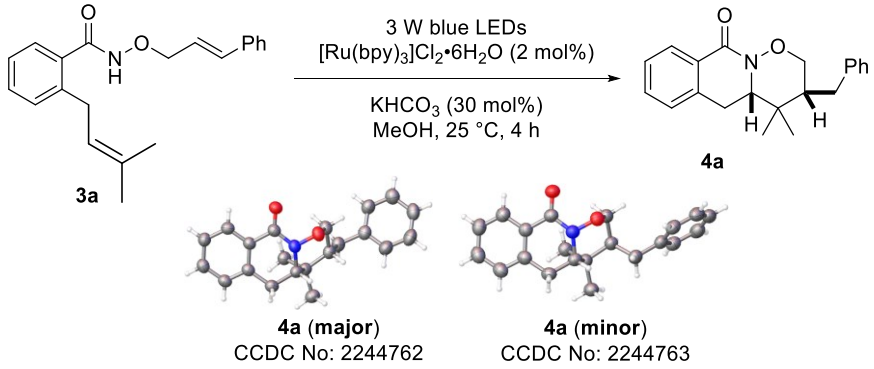


2a (major)
CCDC No: 2243178

2a (minor)
CCDC No: 2244760

To a Schlenk tube were added **1a** (61.4 mg, 0.2 mmol, 1.0 equiv), $[Ru(bpy)_3]Cl_2•6H_2O$ (3.0 mg, 0.004 mmol, 2 mol%), $KHCO_3$ (6.0 mg, 0.06 mmol, 30 mol%). The tube was degassed and refilled with N_2 three times, and anhydrous MeOH (3 mL) was added. The mixture was then placed around the Blue LEDs (450 nm, 100% light intensity) and stirred until the substrate was consumed (monitored by TLC), the solvent was removed by rotary evaporation, and the resulting residue was purified directly by flash column chromatography on silica gel (gradient eluent of EtOAc/petroleum

ether: 1/3 to 1/2) to give the desired product **2a** (52.0 mg, 85% yield, dr = 5.4:1).



To a Schlenk tube were added **3a** (64.3 mg, 0.2 mmol, 1.0 equiv), $[Ru(bpy)_3]Cl_2 \cdot 6H_2O$ (3.0 mg, 0.004 mmol, 2 mol%), $KHCO_3$ (6.0 mg, 0.06 mmol, 30 mol%). The tube was degassed and refilled with N_2 three times, and anhydrous MeOH (3 mL) was added. The mixture was then placed around the Blue LEDs (450 nm, 100% light intensity) and stirred until the substrate was consumed (monitored by TLC), the solvent was removed by rotary evaporation, and the resulting residue was purified directly by flash column chromatography on silica gel (gradient eluent of EtOAc/petroleum ether: 1/3 to 1/2) to give the desired product **4a** (53.0 mg, 83% yield, dr = 4.3:1).

4. Mechanistic Studies

Luminescence quenching experiments

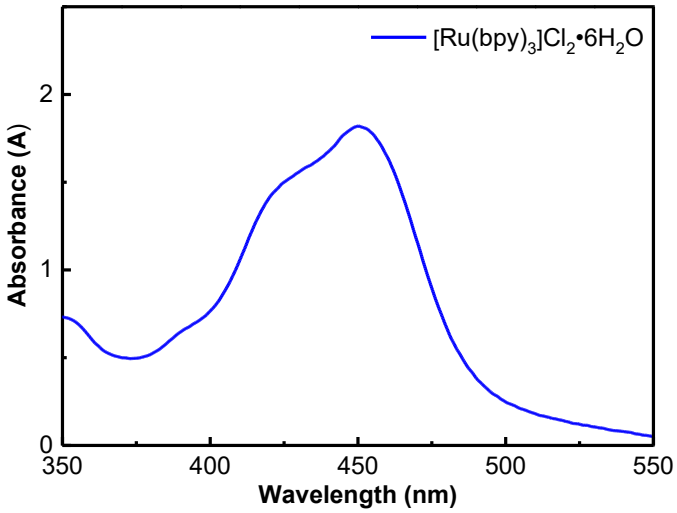


Figure S1. The UV absorption spectra of $[Ru(bpy)_3]Cl_2 \cdot 6H_2O$

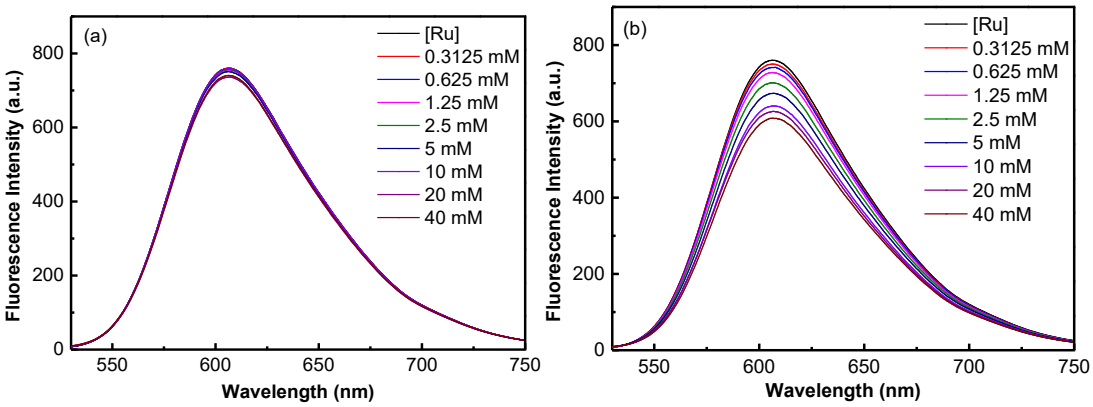
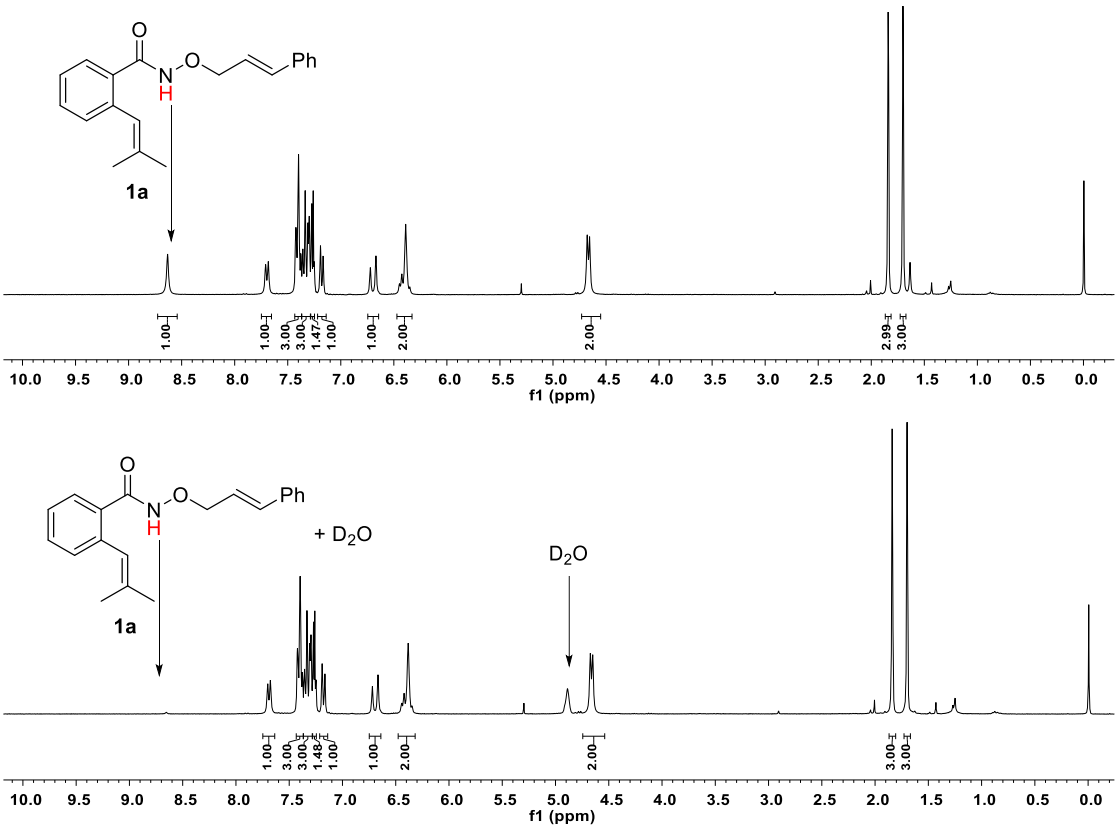


Figure S2. The luminescence spectra under different conditions of $[Ru(bpy)_3]Cl_2 \cdot 6H_2O$

The maximum excitation wavelength of $[Ru(bpy)_3]Cl_2 \cdot 6H_2O$ in solvent MeOH was determined to be 450 nm by UV absorption spectrum (**Figure S1**). Fluorescence spectra were collected on Cary Eclipse Fluorescence Spectrophotometer. The solution of $[Ru(bpy)_3]Cl_2 \cdot 6H_2O$ in MeOH was excited at 450 nm, and the emission intensity at 606 nm was observed. In a typical experiment, the emission spectrum of a 1×10^{-4} M solution of $[Ru(bpy)_3]Cl_2 \cdot 6H_2O$ was collected. The decrease of $Ru(bpy)_3^{2+}$ luminescence couldn't be observed in the presence of substrate **1a** (**Figure S2-(a)**). Under essential conditions ($KHCO_3$, 0.06 mmol), a significant decrease of $Ru(bpy)_3^{2+}$ luminescence was successfully observed in the presence of **1a** (**Figure S2-(b)**).

^{1}H NMR Study on the effect of the base with 1a



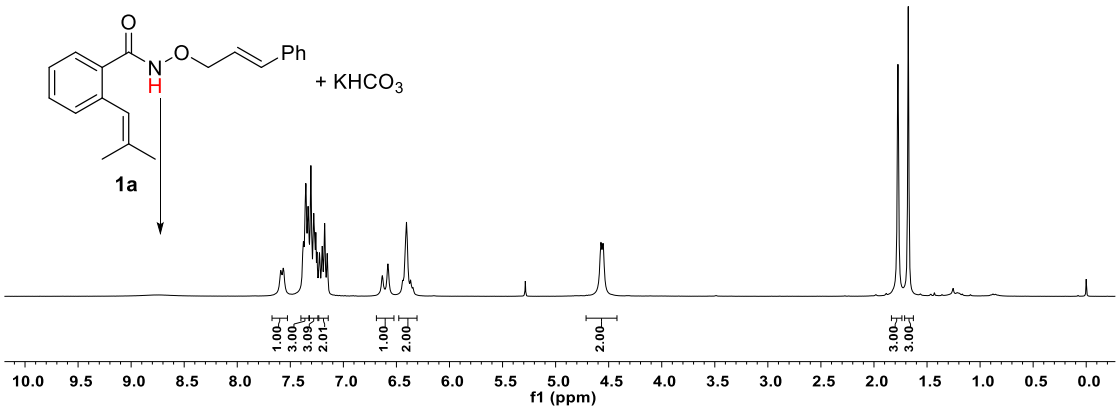
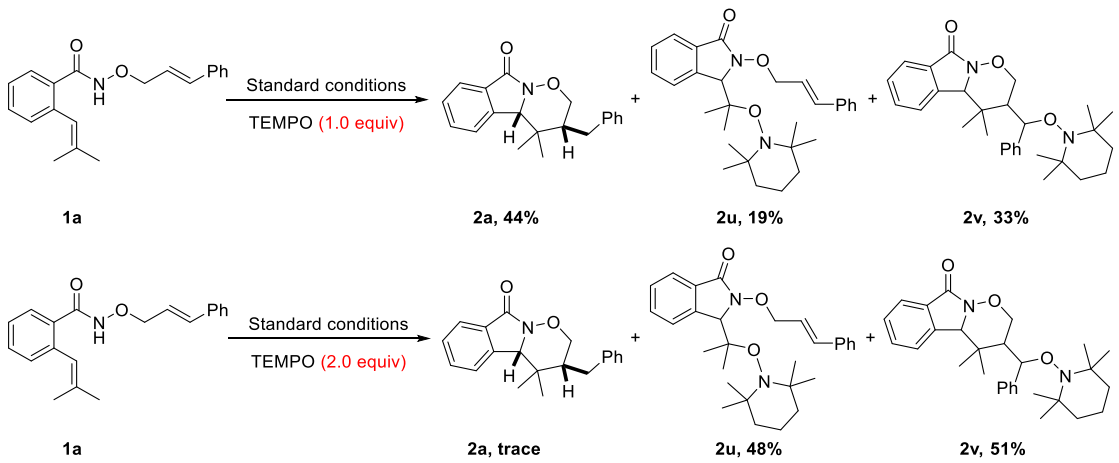


Figure S3. The ^{1}H NMR spectra of substrate **1a** under different conditions

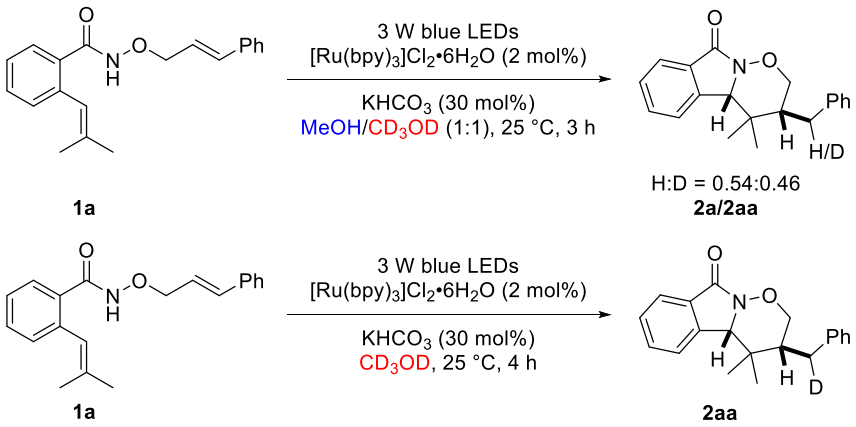
Under the essential condition ($KHCO_3$ in MeOH), the signal of N-H disappeared in proton nuclear magnetic resonance (^{1}H NMR) spectra after stirring at room temperature for 2 h. These results suggested that the $KHCO_3$ can abstract the proton of the N-H bond of **1a** to generate the corresponding nitrogen anion intermediate (**Figure S3**).

Radical trapping experiments

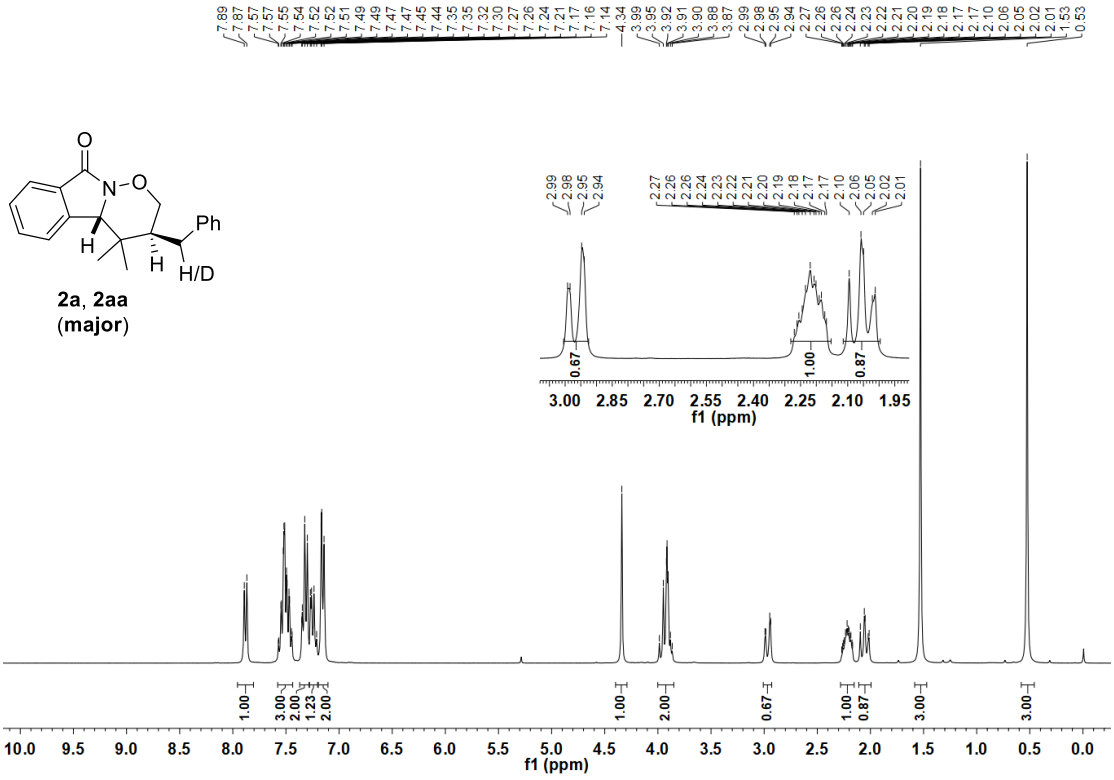


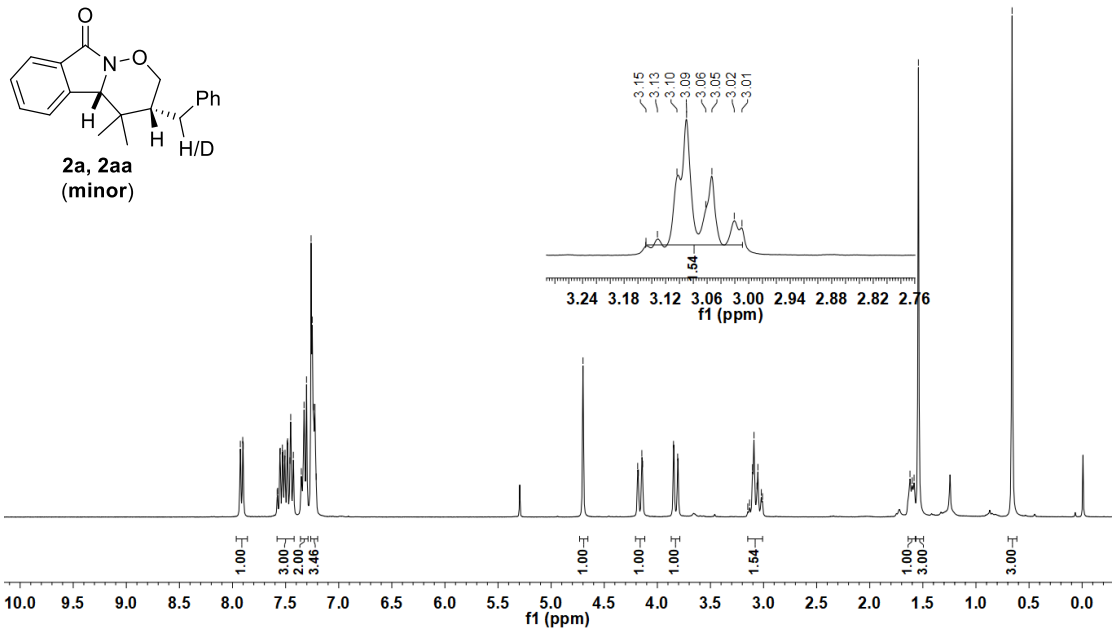
To a Schlenk tube were added **1a** (61.4 mg, 0.2 mmol, 1.0 equiv), $[Ru(bpy)_3]Cl_2 \cdot 6H_2O$ (3.0 mg, 0.004 mmol, 2 mol%), $KHCO_3$ (6.0 mg, 0.06 mmol, 30 mol%) and TEMPO (32.6 mg, 0.2 mmol, 1.0 equiv.). The tube was degassed and refilled with N_2 three times, and anhydrous MeOH (3 mL) was added. The mixture was then placed around the Blue LEDs (450 nm, 100% light intensity) and stirred until the substrate was consumed (monitored by TLC), the solvent was removed by rotary evaporation, and the resulting residue was purified directly by flash column chromatography on silica gel (gradient eluent of EtOAc/petroleum ether: 1/5 to 1/2) to give the product **2a** (27.0 mg, 44% yield) and the desired products **2u** (17.0 mg, 19% yield) and **2v** (30.0 mg, 33% yield) as white solids. When the amount of TEMPO is increased to 2.0 equivalents, almost no product **2a** is generated. However, the yields of **2u** and **2v** increased from 19% to 48% and 33% to 51%, respectively, which indicates that the reaction is likely to involve a free radical process.

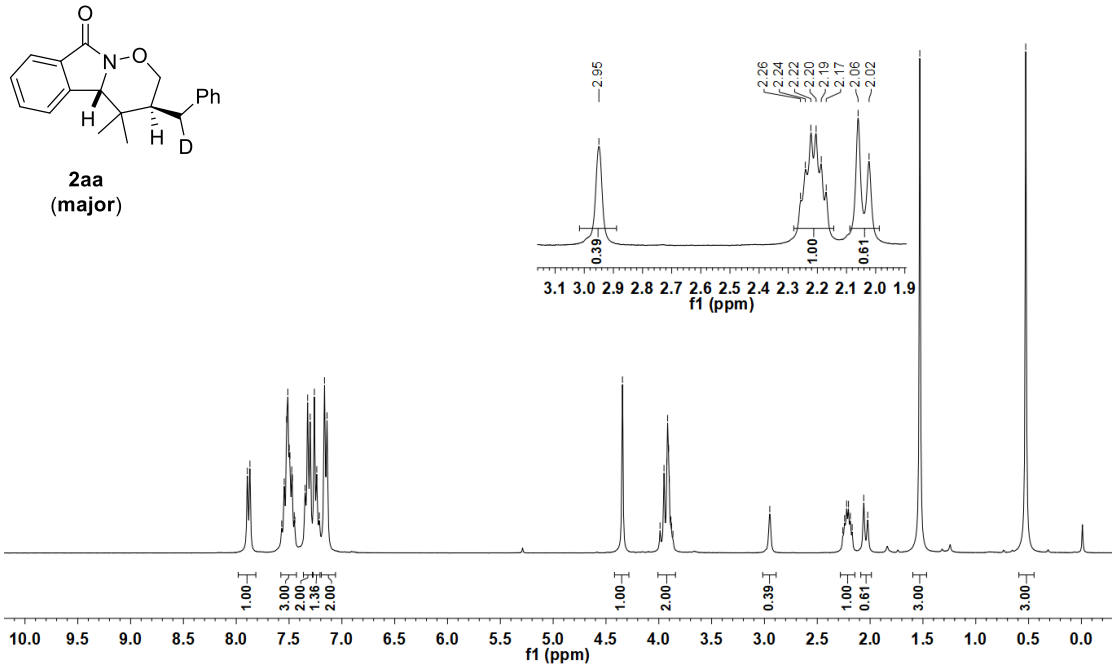
H/D exchange experiments



To a Schlenk tube were added **1a** (61.4 mg, 0.2 mmol, 1.0 equiv), $[Ru(bpy)_3]Cl_2 \cdot 6H_2O$ (3.0 mg, 0.004 mmol, 2 mol%), $KHCO_3$ (6.0 mg, 0.06 mmol, 30 mol%). The tube was degassed and refilled with N_2 three times, and anhydrous CD_3OD/MeOH (1:1) (3 mL) was added. The mixture was then placed around the Blue LEDs (450 nm, 100% light intensity) and stirred until the substrate was consumed (monitored by TLC), the solvent was removed by rotary evaporation, and the resulting residue was purified directly by flash column chromatography on silica gel (gradient eluent of EtOAc/petroleum ether: 1/3 to 1/2) to give the mixture of **2a** and **2aa** (47.0 mg, 77% yield) as white solids. When the solvent becomes anhydrous CD_3OD, only **2aa** (39.0 mg, 62% yield) is detected in the mixture. The products were analyzed by ^1H NMR spectroscopy (**Figure S4**).




2a, 2aa
(minor)
f1 (ppm)


2aa
(major)
f1 (ppm)

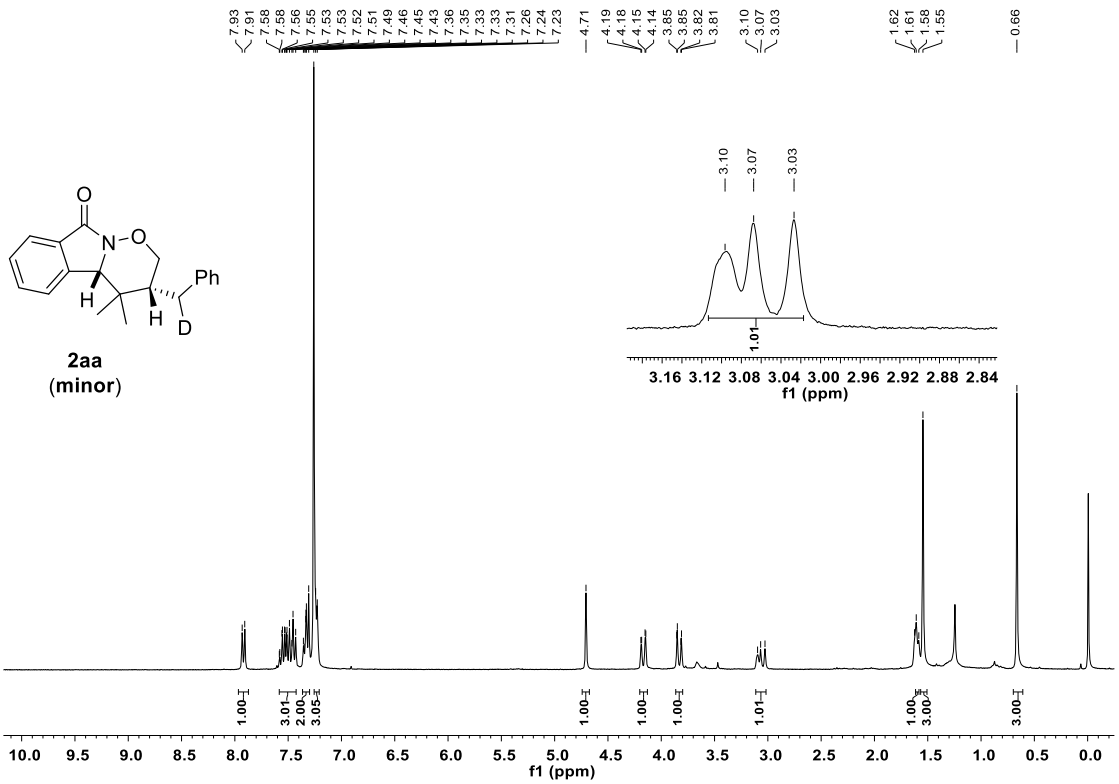


Figure S4. The ^{1}H NMR spectrum of the H/D exchange experiments

5. Density functional theory (DFT) calculation

Investigation of regioselectivity for N-amidyl radical by DFT calculation:

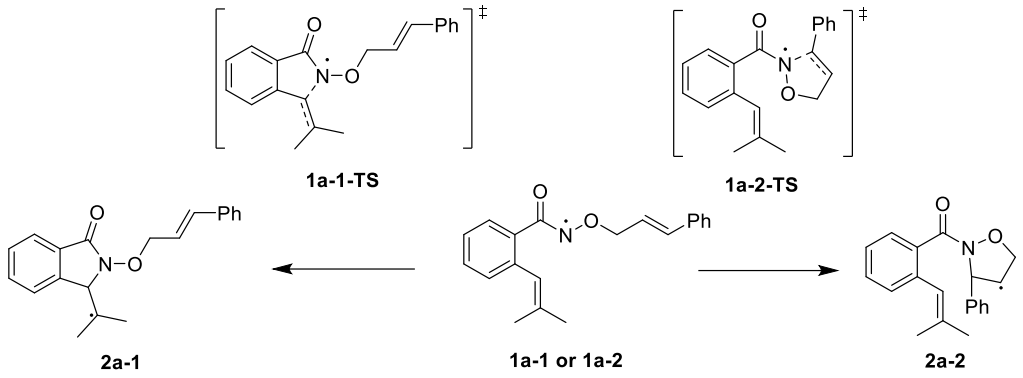


Figure S5. 2D Structures of all stationary points

All calculations were carried out with the density functional theory (DFT) at the M06-2X level[10] theory using the Gaussian 16 series of programs[11]. The def2-TZVP basis set was used for all the atoms. The gas-phase geometries of all intermediates and transition states were fully optimized without any symmetry restriction, following harmonic frequency calculations to ensure that the local minima had zero imaginary frequencies and the transition state one and to derive the thermal corrections for Gibbs free energies. The transition states were verified by intrinsic reaction coordinate (IRC) calculation and imaginary vibration modes, which linked reactants and products. Double hybrid functional (B2PLYPD3 method)[12], which could give more accurate energetic

information, was used to calculate single point energies with a jul-cc-pvtz basis set. Gibbs free energies of all stationary points were obtained by the thermal correction to Gibbs free energy in the gas phase and single point energy in the gas phase.

Table S1. Gibbs free energies of all stationary points

Geometry[a]	$E_{(gas\text{-}B2PLYP)}$[b] (Hartree)	$G_{(corr\text{-}M062X)}$ [c] (Hartree)	IF[d]	ΔG[e] (kcal/mol)
1a-1	-978.81942166381	0.299178	-	0.0
1a-1-TS	-978.81031403032	0.298789	-396.72	5.47
2a-1	-978.83651361468	0.299116	-	-10.76
1a-2	-978.81444949752	0.302333	-	0.0
1a-2-TS	-978.77796202461	0.300163	-513.42	21.52
2a-2	-978.82394077394	0.302330	-	-5.95

[a] **1a-1** and **1a-2** have the same 2D structures and different 3D geometries. [b] The electronic energy calculated by B2PLYPD3 in the gas phase. [c] The thermal correction to Gibbs free energy calculated by M062X in the gas phase. [d] The M062X calculated imaginary frequencies for the transition states. [e] $\Delta G = [G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYPD3)}]$ (Sum of electronic and thermal free energies for transition state) - $[G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYP\ D3)}]$ (Sum of electronic and thermal free energies for reactant) or $\Delta G = [G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYP\ D3)}]$ (Sum of electronic and thermal free energies for the product) - $[G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYP\ D3)}]$ (Sum of electronic and thermal free energies for reactant)

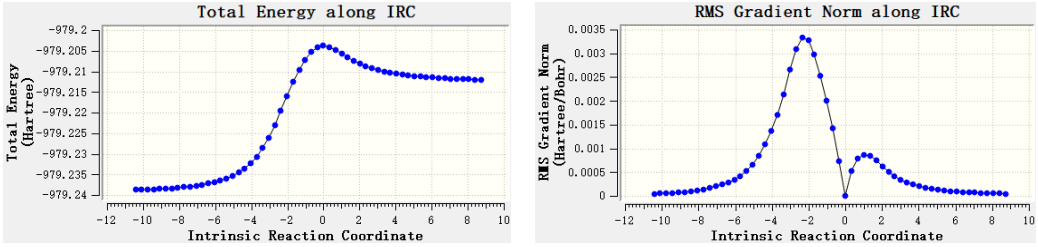


Figure S6. Plots of total energy and root-mean-squared (RMS) gradient norm along IRC for **1a-1-TS**

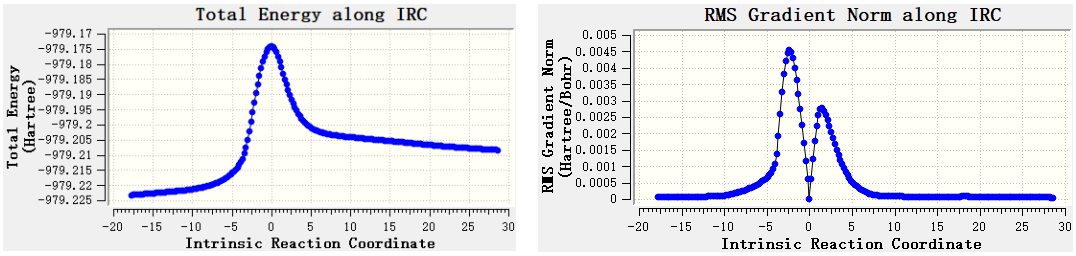


Figure S7. Plots of total energy and root-mean-squared (RMS) gradient norm along IRC for **1a-2-TS**

Investigation of diastereoselectivity for target product 2a by DFT calculation:

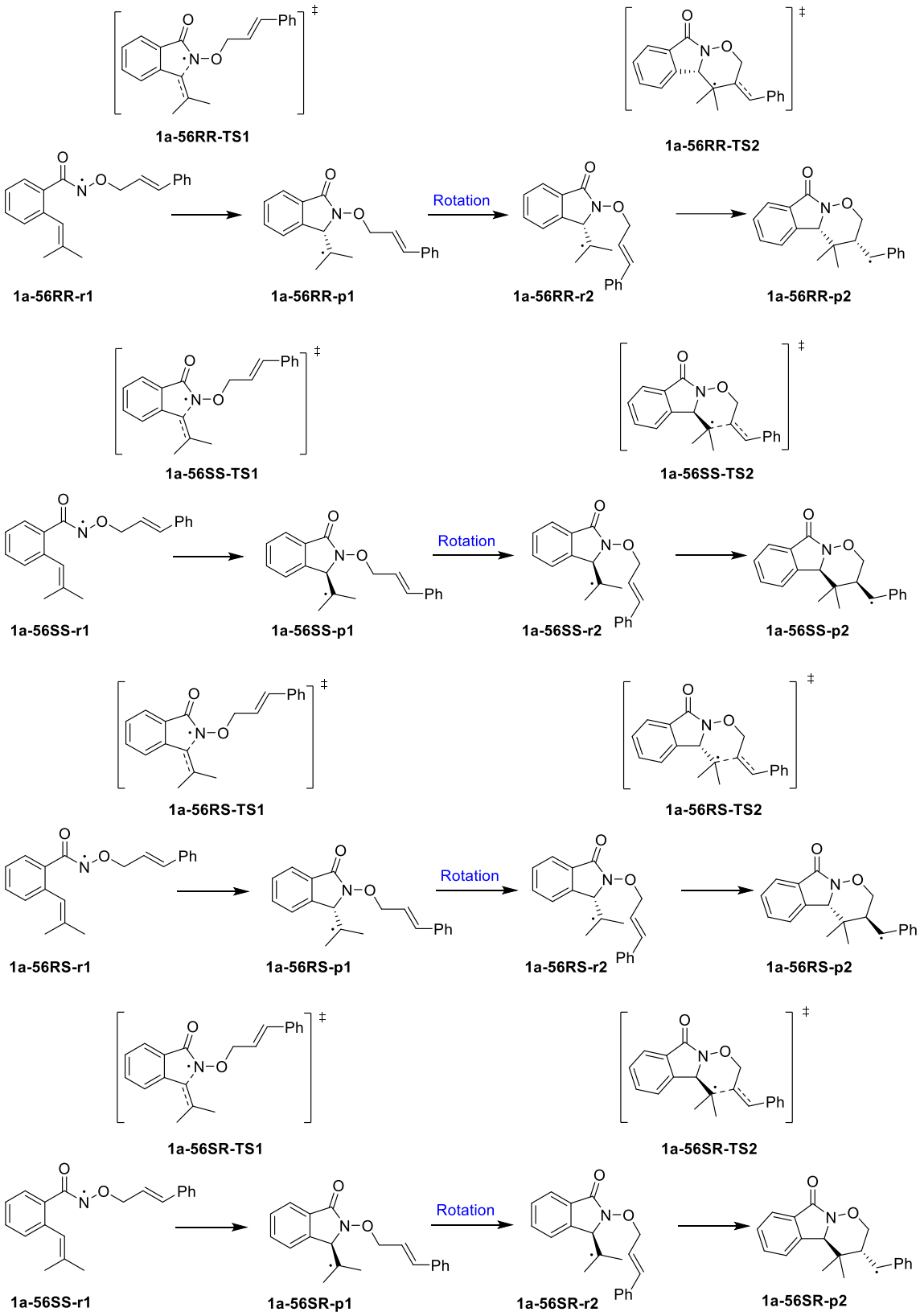


Figure S8. 2D Structures of all stationary points

DFT calculations to determine the barrier to rotation around the C-O bond to be -2.66 kcal/mol, 0.47 kcal/mol, 45.51 kcal/mol, and 1.65 kcal/mol, which correspond to **1a-56RR-p1**/**1a-56RR-r2**, **1a-**

56SS-p1/**1a-56SS-r2**, **1a-56RS-p1**/**1a-56RS-r2**, **1a-56SR-p1**/**1a-56SR-r2** (**Figure S8** and **Table S2**). The free energy changes for **1a-56RR-p2 vs. 1a-56RR-r1**, **1a-56SS-p2 vs. 1a-56SS-r1**, **1a-56RS-p2 vs. 1a-56RS-r1**, **1a-56SR-p2 vs. 1a-56SR-r1** are -26.24 kcal/mol, -21.92 kcal/mol, 19.26 kcal/mol, -14.83 kcal/mol, respectively (**Table S2**). Rotational barrier and free energy changes for the major product (**1a-56RR-p2** and **1a-56SS-p2**, red numbers in **Table S2**) are lower than the minor product (**1a-56RS-p2** and **1a-56SR-p2**, green numbers in **Table S2**).

Table S2. Gibbs free energies of all stationary points

Geometry[a]	ΔG[b] (kcal/mol)	IF[c]	Barrier of Rotation[d] (kcal/mol)
1a-56RR-r1	0.00	-	-
1a-56RR-TS1	5.47	396.72	-
1a-56RR-p1	-10.76	-	-
1a-56RR-r2	-13.42	-	**-2.66**
1a-56RR-TS2	-3.02	489.25	-
1a-56RR-p2	**-26.24**	-	-
1a-56SS-r1	0.00	-	-
1a-56SS-TS1	4.35	420.24	-
1a-56SS-p1	-12.87	-	-
1a-56SS-r2	-12.40	-	**0.47**
1a-56SS-TS2	0.20	514.97	-
1a-56SS-p2	**-21.92**	-	-
1a-56RS-r1	0.00	-	-
1a-56RS-TS1	2.92	387.06	-
1a-56RS-p1	-12.37	-	-
1a-56RS-r2	33.14	-	**45.51**
1a-56RS-TS2	43.67	493.60	-
1a-56RS-p2	**19.26**	-	-
1a-56SR-r1	0.00	-	-
1a-56SR-TS1	7.39	438.25	-
1a-56SR-p1	-7.49	-	-
1a-56SR-r2	-5.84	-	**1.65**

1a-56SR-TS2	5.65	497.56	-
1a-56SR-p2	**-14.83**	-	-

[a] **1a-56RR-p1** and **1a-56RR-r2**, **1a-56SS-p1** and **1a-56SS-r2**, **1a-56RS-p1** and **1a-56RS-r2**, **1a-56SR-p1** and **1a-56SR-r2**, have the same 2D structures and different 3D geometries. [b] $G_{(corr\text{-}M062X)}$ is the thermal correction to Gibbs free energy calculated by M062X in gas phase. $E_{(gas\text{-}B2PLYPD3)}$ is the electronic energy calculated by B2PLYPD3 in the gas phase. $\Delta G = [G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYPD3)}]$ (Sum of electronic and thermal free energies for **1a-56RR-TS1**/**1a-56RR-p1**/**1a-56RR-r2**/**1a-56RR-TS2**/**1a-56RR-p1**) - $[G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYP\ D3)}]$ (Sum of electronic and thermal free energies for **1a-56RR-r1**). Similarly, ΔG for **1a-56SS/1a-56RS/1a-56SR** can be obtained. [c] The M062X calculated imaginary frequencies for the transition states. [d] Barrier of Rotation = $[G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYPD3)}]$ (Sum of electronic and thermal free energies for **1a-56RR-r2/1a-56SS-r2/1a-56RS-r2/1a-56SR-r2**) - $[G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYP\ D3)}]$ (Sum of electronic and thermal free energies for **1a-56RR-p1/1a-56SS-p1/1a-56RS-p1/1a-56SR-p1**).

Optimized Geometries for All the Compounds and Transition State

1a-1

C	-4.53750900	1.56128100	-0.55694400
C	-5.74570800	1.03308100	-0.12951400
C	-5.80085700	-0.25158500	0.40089700
C	-4.64343600	-1.00537800	0.48081800
C	-3.43191200	-0.48336100	0.02909300
C	-3.35620100	0.82273800	-0.47083100
H	-4.49650100	2.57139200	-0.94729000
H	-6.64739800	1.62869400	-0.20129200
H	-6.74254800	-0.66359000	0.74003100
H	-4.66812900	-2.01458200	0.87317500
C	-2.24252000	-1.37402200	0.08262700
O	-2.07647400	-2.21294200	0.95255200
N	-1.43830100	-1.27938800	-1.05651800
O	-0.21855400	-1.75932500	-0.99627600
C	0.53137600	-1.83286500	0.26147100
H	0.12835800	-1.11136200	0.96794700
H	0.40275300	-2.84390100	0.64750200
C	-1.05105300	1.73293800	-0.07381600
C	-1.03581500	1.47742400	1.40425600
H	-0.11781300	0.95937700	1.69393200
H	-1.02725900	2.43515200	1.93417000
H	-1.89156200	0.90370000	1.75698400
C	0.18684700	2.38973800	-0.60734700
H	1.05040400	1.73188300	-0.46528400
H	0.10013700	2.62351200	-1.66804300
H	0.39967800	3.31113400	-0.05781600
C	4.01420400	-0.16402800	0.26302500

C	4.90407100	-0.96587100	-0.45860300
C	4.47588400	1.04895900	0.77828000
C	6.21055800	-0.55523400	-0.66734800
H	4.57807100	-1.92132200	-0.85073000
C	5.78460500	1.46147400	0.56769600
H	3.79596900	1.67392400	1.34668100
C	6.65602500	0.66069100	-0.15748600
H	6.88870100	-1.18837200	-1.22618400
H	6.12339500	2.40717400	0.97232200
H	7.67877000	0.97670500	-0.32109600
C	1.94697900	-1.53397200	-0.08430500
H	2.41086600	-2.17786700	-0.82487200
C	2.61243800	-0.53919700	0.49815400
H	2.08374400	0.08090700	1.21890400
C	-2.07903100	1.45083500	-0.88016500
H	-2.01497100	1.74942500	-1.92337900

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C	-4.62933600	-1.38956400	0.44454300
C	-5.79824400	-0.90404100	-0.12835300
C	-5.84323900	0.37352300	-0.68048700
C	-4.71548900	1.17914200	-0.65466500
C	-3.55289900	0.69398900	-0.07102600
C	-3.49238100	-0.59061700	0.46621200
H	-4.59601600	-2.39000600	0.85889800
H	-6.68151300	-1.53028400	-0.15188800
H	-6.75982500	0.73728900	-1.12686100
H	-4.73006600	2.17764800	-1.07456200
C	-2.30535800	1.48788200	0.01677500
O	-2.07125300	2.50148400	-0.63604200
N	-1.50194000	0.97052500	0.99486400
O	-0.18917200	1.27715900	0.99720400
C	0.50186600	1.21191000	-0.27592500
H	0.15181300	0.33406200	-0.82337700
H	0.26487000	2.10986200	-0.84732800
C	-1.25513100	-1.71819000	0.27952800
C	-1.37087800	-1.90871700	-1.19685300
H	-0.39538700	-1.80424800	-1.67727800
H	-1.71514600	-2.92814400	-1.40438900
H	-2.07416600	-1.21639700	-1.65902500
C	-0.02742600	-2.25474900	0.93027400
H	0.84561500	-1.68067600	0.59746700
H	-0.08171100	-2.20326900	2.01681700
H	0.14735100	-3.29068700	0.62515600

C	4.20218100	0.07416400	-0.29664000
C	4.95977600	1.01547400	0.40816300
C	4.85466600	-1.03858300	-0.83122000
C	6.32331900	0.83937000	0.57679200
H	4.48362100	1.89449600	0.82453400
C	6.22157100	-1.21544900	-0.66288700
H	4.27872900	-1.77290200	-1.38315200
C	6.96086400	-0.27693800	0.04317200
H	6.89502800	1.57835200	1.12474100
H	6.70776000	-2.08646100	-1.08470100
H	8.02734000	-0.40967600	0.17612000
C	1.95736000	1.13636100	0.02437800
H	2.34639100	1.91552200	0.67300400
C	2.75014800	0.20167300	-0.49387400
H	2.30384900	-0.55851700	-1.13143100
C	-2.19177800	-1.04731100	1.02084900
H	-2.11911900	-1.11474900	2.10137000

2a-1

C	4.76330800	1.01181200	0.52179000
C	5.94413200	0.35116600	0.19683100
C	5.94109200	-0.98815800	-0.19370900
C	4.75048600	-1.69860700	-0.27312400
C	3.58206200	-1.03127700	0.05303500
C	3.58054900	0.29861400	0.45348100
H	4.77093500	2.05397600	0.81884900
H	6.88420500	0.88653800	0.24605700
H	6.87636900	-1.47397600	-0.44091700
H	4.72946600	-2.73664100	-0.58167200
C	2.18761500	-1.53221600	0.04448700
O	1.76686900	-2.65226100	-0.22052100
N	1.44091600	-0.46453000	0.39811300
O	0.10105900	-0.56189800	0.61896800
C	-0.65071500	-0.34109300	-0.60032200
H	-0.52941200	0.69657900	-0.91721600
H	-0.24780000	-1.00904600	-1.36640200
C	1.72443700	1.95675900	-0.03906500
C	1.96182000	1.99516700	-1.50972900
H	1.06294200	2.31945100	-2.04316100
H	2.75354000	2.70932800	-1.76870700
H	2.25905600	1.02035500	-1.90428200
C	0.84463400	2.97774600	0.58734000
H	-0.21522900	2.77849300	0.36870400
H	0.95580500	3.00084000	1.67241200

H	1.05826400	3.97544000	0.19274300
C	-4.47824200	0.02034700	-0.17278700
C	-5.02253000	-1.24673200	0.06083900
C	-5.33455600	1.12332900	-0.17368400
C	-6.37896600	-1.39794300	0.29765700
H	-4.38502700	-2.12211100	0.04960400
C	-6.69400900	0.97240800	0.06425900
H	-4.92438500	2.10945500	-0.36001200
C	-7.22061100	-0.28942900	0.30247700
H	-6.78514600	-2.38620200	0.47505100
H	-7.34106300	1.84090100	0.06190800
H	-8.28067600	-0.41244500	0.48637000
C	-2.07144200	-0.65887300	-0.29540200
H	-2.27359600	-1.67700600	0.02276800
C	-3.04477100	0.24126300	-0.41501300
H	-2.77888000	1.25174400	-0.71684100
C	2.17229100	0.76693300	0.74336100
H	2.04129900	0.95200900	1.81404700

1a-2

C	1.91538200	-2.33775000	-0.12904000
C	1.59594000	-3.02724700	-1.28662100
C	1.03200600	-2.35391700	-2.36476000
C	0.76264800	-1.00196100	-2.25159100
C	1.05187100	-0.31096100	-1.07180500
C	1.67846700	-0.96502400	0.00151000
H	2.38019500	-2.86199800	0.69795400
H	1.79679500	-4.08942400	-1.35271100
H	0.78824000	-2.88218800	-3.27751800
H	0.28837600	-0.46890300	-3.06663800
C	0.53812000	1.08567500	-1.03883700
O	0.64070100	1.85871200	-1.97387400
C	2.81447300	0.82151700	1.37344500
C	3.25616500	1.69080100	0.23423400
H	2.64004300	2.59507300	0.18470100
H	4.28412900	2.02120500	0.40208400
H	3.21032400	1.19109500	-0.73253100
C	3.20139800	1.33192300	2.72948000
H	2.79021400	2.33478800	2.88208600
H	2.84198000	0.68380600	3.52816200
H	4.28811200	1.42361400	2.81008200
C	2.12610600	-0.31630000	1.24768700
H	1.91331300	-0.88390500	2.15005600
C	-1.89079000	2.50482100	-1.06083400

H	-2.76942000	2.98953100	-0.63413300
H	-1.38852500	3.21078500	-1.71727200
N	-0.08262200	1.43144600	0.16732700
O	-1.05383600	2.31333900	0.12238200
C	-2.43679100	0.02091300	-1.35884600
H	-2.60737300	-0.74997900	-2.10538000
C	-2.24648700	1.25967000	-1.81321900
H	-2.31138000	1.41582800	-2.88479300
C	-2.38968900	-0.46220400	0.03318100
C	-2.94755100	0.25832700	1.09005600
C	-1.77132900	-1.68498500	0.30372800
C	-2.86552500	-0.22012900	2.38939700
H	-3.45278000	1.19653800	0.89206300
C	-1.67520200	-2.15656400	1.60530400
H	-1.34786200	-2.25870900	-0.51443900
C	-2.22035700	-1.42340900	2.65239300
H	-3.30593100	0.34731300	3.19997500
H	-1.17711100	-3.09844000	1.80129700
H	-2.15105400	-1.79174400	3.66843100

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C	-2.79602300	1.02323800	-1.75836700
C	-3.53537900	0.02136200	-2.36337200
C	-3.51563500	-1.26709900	-1.84182300
C	-2.73543400	-1.53476700	-0.73073300
C	-1.97060500	-0.53221600	-0.13129800
C	-2.01309000	0.78248000	-0.62269100
H	-2.83020700	2.03063000	-2.15710100
H	-4.13268600	0.24660000	-3.23824900
H	-4.09293400	-2.05732900	-2.30437900
H	-2.68946000	-2.53859900	-0.32519800
C	-1.08995600	-0.99871900	0.98463900
O	-1.50172700	-1.73624100	1.87062500
C	-1.26365400	2.30463800	1.25153100
C	-1.92224400	1.56592000	2.37748000
H	-1.17484500	1.01777400	2.96132400
H	-2.39347900	2.27840500	3.05901400
H	-2.68033500	0.85937100	2.04170200
C	-0.50296100	3.52777100	1.67000700
H	0.26675100	3.25706400	2.39965000
H	-0.02212500	4.01905700	0.82447200
H	-1.16592200	4.24318400	2.16459300
C	-1.31108100	1.94022600	-0.03227300
H	-0.83631600	2.59322300	-0.76032600

C	1.28963600	-2.53610200	1.44374300
H	2.29280900	-2.79907100	1.78618400
H	0.56794900	-3.17300500	1.95676700
N	0.21044000	-0.55308400	0.88122200
O	1.06827300	-1.15954700	1.78745600
C	1.17831800	-1.51815200	-0.82602900
H	0.55944600	-1.51551800	-1.72050100
C	1.07304000	-2.64423600	-0.03335700
H	0.53073700	-3.50449100	-0.40481900
C	2.24527200	-0.50654700	-0.84503400
C	3.40589900	-0.61387500	-0.07841700
C	2.09703600	0.58474000	-1.70517400
C	4.38335300	0.36834200	-0.15095600
H	3.56044300	-1.47220400	0.56186900
C	3.07112500	1.56702100	-1.77207600
H	1.20579300	0.65725500	-2.31854000
C	4.21638300	1.46297100	-0.98993900
H	5.28183800	0.27493700	0.44612500
H	2.94131300	2.41148200	-2.43729100
H	4.98178500	2.22715700	-1.04366500

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C	1.85172500	-2.32444400	-0.68430800
C	2.93456700	-2.17585800	-1.53395500
C	3.53439000	-0.93064700	-1.68569100
C	3.02303100	0.15654200	-0.99873700
C	1.91672100	0.01202400	-0.16135400
C	1.32891000	-1.24544300	0.03832500
H	1.39853400	-3.30067400	-0.55503100
H	3.31707700	-3.03339900	-2.07349600
H	4.38577500	-0.80659600	-2.34246600
H	3.46445800	1.13850600	-1.12168700
C	1.41219800	1.27868500	0.45961800
O	2.10980000	1.97011900	1.19169800
C	0.07365000	-1.16717200	2.23273200
C	1.10694000	-0.42700200	3.02752100
H	0.76913200	0.59168300	3.24240100
H	1.24610800	-0.92269900	3.99179500
H	2.07179500	-0.37020400	2.52668100
C	-1.17008700	-1.51742200	2.99564400
H	-1.67022900	-0.60446700	3.33565000
H	-1.87156100	-2.09036300	2.38933600
H	-0.92433700	-2.09332300	3.89215100
C	0.19534200	-1.51392700	0.94916200

H	-0.60293000	-2.10706700	0.50862600
C	-0.70028400	3.61592700	-0.42342000
H	-1.48258100	4.29571100	-0.08449100
H	0.17802200	4.19956900	-0.73247300
N	0.13243800	1.59836000	0.15151600
O	-0.35057300	2.78531400	0.69633500
C	-0.56359400	1.29932000	-1.11761900
H	0.18129500	0.97746800	-1.84997900
C	-1.12751700	2.64318500	-1.45493300
H	-1.52957500	2.89147200	-2.42351900
C	-1.61628100	0.21835900	-0.98723700
C	-2.56983800	0.28485900	0.02510800
C	-1.62178500	-0.85283400	-1.86955300
C	-3.50788000	-0.72614400	0.16437800
H	-2.56237000	1.12244300	0.71530700
C	-2.56847600	-1.86346800	-1.73667200
H	-0.87201500	-0.90635200	-2.65177800
C	-3.50744400	-1.80467900	-0.71631500
H	-4.23924400	-0.67762300	0.96194200
H	-2.56436100	-2.70023900	-2.42436900
H	-4.23960000	-2.59499200	-0.60563300

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C	-4.53750900	1.56128100	-0.55694400
C	-5.74570800	1.03308100	-0.12951400
C	-5.80085700	-0.25158500	0.40089700
C	-4.64343600	-1.00537800	0.48081800
C	-3.43191200	-0.48336100	0.02909300
C	-3.35620100	0.82273800	-0.47083100
H	-4.49650100	2.57139200	-0.94729000
H	-6.64739800	1.62869400	-0.20129200
H	-6.74254800	-0.66359000	0.74003100
H	-4.66812900	-2.01458200	0.87317500
C	-2.24252000	-1.37402200	0.08262700
O	-2.07647400	-2.21294200	0.95255200
N	-1.43830100	-1.27938800	-1.05651800
O	-0.21855400	-1.75932500	-0.99627600
C	0.53137600	-1.83286500	0.26147100
H	0.12835800	-1.11136200	0.96794700
H	0.40275300	-2.84390100	0.64750200
C	-1.05105300	1.73293800	-0.07381600
C	-1.03581500	1.47742400	1.40425600
H	-0.11781300	0.95937700	1.69393200
H	-1.02725900	2.43515200	1.93417000

H	-1.89156200	0.90370000	1.75698400
C	0.18684700	2.38973800	-0.60734700
H	1.05040400	1.73188300	-0.46528400
H	0.10013700	2.62351200	-1.66804300
H	0.39967800	3.31113400	-0.05781600
C	4.01420400	-0.16402800	0.26302500
C	4.90407100	-0.96587100	-0.45860300
C	4.47588400	1.04895900	0.77828000
C	6.21055800	-0.55523400	-0.66734800
H	4.57807100	-1.92132200	-0.85073000
C	5.78460500	1.46147400	0.56769600
H	3.79596900	1.67392400	1.34668100
C	6.65602500	0.66069100	-0.15748600
H	6.88870100	-1.18837200	-1.22618400
H	6.12339500	2.40717400	0.97232200
H	7.67877000	0.97670500	-0.32109600
C	1.94697900	-1.53397200	-0.08430500
H	2.41086600	-2.17786700	-0.82487200
C	2.61243800	-0.53919700	0.49815400
H	2.08374400	0.08090700	1.21890400
C	-2.07903100	1.45083500	-0.88016500
H	-2.01497100	1.74942500	-1.92337900

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C	-4.62933600	-1.38956400	0.44454300
C	-5.79824400	-0.90404100	-0.12835300
C	-5.84323900	0.37352300	-0.68048700
C	-4.71548900	1.17914200	-0.65466500
C	-3.55289900	0.69398900	-0.07102600
C	-3.49238100	-0.59061700	0.46621200
H	-4.59601600	-2.39000600	0.85889800
H	-6.68151300	-1.53028400	-0.15188800
H	-6.75982500	0.73728900	-1.12686100
H	-4.73006600	2.17764800	-1.07456200
C	-2.30535800	1.48788200	0.01677500
O	-2.07125300	2.50148400	-0.63604200
N	-1.50194000	0.97052500	0.99486400
O	-0.18917200	1.27715900	0.99720400
C	0.50186600	1.21191000	-0.27592500
H	0.15181300	0.33406200	-0.82337700
H	0.26487000	2.10986200	-0.84732800
C	-1.25513100	-1.71819000	0.27952800
C	-1.37087800	-1.90871700	-1.19685300
H	-0.39538700	-1.80424800	-1.67727800

H	-1.71514600	-2.92814400	-1.40438900
H	-2.07416600	-1.21639700	-1.65902500
C	-0.02742600	-2.25474900	0.93027400
H	0.84561500	-1.68067600	0.59746700
H	-0.08171100	-2.20326900	2.01681700
H	0.14735100	-3.29068700	0.62515600
C	4.20218100	0.07416400	-0.29664000
C	4.95977600	1.01547400	0.40816300
C	4.85466600	-1.03858300	-0.83122000
C	6.32331900	0.83937000	0.57679200
H	4.48362100	1.89449600	0.82453400
C	6.22157100	-1.21544900	-0.66288700
H	4.27872900	-1.77290200	-1.38315200
C	6.96086400	-0.27693800	0.04317200
H	6.89502800	1.57835200	1.12474100
H	6.70776000	-2.08646100	-1.08470100
H	8.02734000	-0.40967600	0.17612000
C	1.95736000	1.13636100	0.02437800
H	2.34639100	1.91552200	0.67300400
C	2.75014800	0.20167300	-0.49387400
H	2.30384900	-0.55851700	-1.13143100
C	-2.19177800	-1.04731100	1.02084900
H	-2.11911900	-1.11474900	2.10137000

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C	4.76330800	1.01181200	0.52179000
C	5.94413200	0.35116600	0.19683100
C	5.94109200	-0.98815800	-0.19370900
C	4.75048600	-1.69860700	-0.27312400
C	3.58206200	-1.03127700	0.05303500
C	3.58054900	0.29861400	0.45348100
H	4.77093500	2.05397600	0.81884900
H	6.88420500	0.88653800	0.24605700
H	6.87636900	-1.47397600	-0.44091700
H	4.72946600	-2.73664100	-0.58167200
C	2.18761500	-1.53221600	0.04448700
O	1.76686900	-2.65226100	-0.22052100
N	1.44091600	-0.46453000	0.39811300
O	0.10105900	-0.56189800	0.61896800
C	-0.65071500	-0.34109300	-0.60032200
H	-0.52941200	0.69657900	-0.91721600
H	-0.24780000	-1.00904600	-1.36640200
C	1.72443700	1.95675900	-0.03906500
C	1.96182000	1.99516700	-1.50972900

H	1.06294200	2.31945100	-2.04316100
H	2.75354000	2.70932800	-1.76870700
H	2.25905600	1.02035500	-1.90428200
C	0.84463400	2.97774600	0.58734000
H	-0.21522900	2.77849300	0.36870400
H	0.95580500	3.00084000	1.67241200
H	1.05826400	3.97544000	0.19274300
C	-4.47824200	0.02034700	-0.17278700
C	-5.02253000	-1.24673200	0.06083900
C	-5.33455600	1.12332900	-0.17368400
C	-6.37896600	-1.39794300	0.29765700
H	-4.38502700	-2.12211100	0.04960400
C	-6.69400900	0.97240800	0.06425900
H	-4.92438500	2.10945500	-0.36001200
C	-7.22061100	-0.28942900	0.30247700
H	-6.78514600	-2.38620200	0.47505100
H	-7.34106300	1.84090100	0.06190800
H	-8.28067600	-0.41244500	0.48637000
C	-2.07144200	-0.65887300	-0.29540200
H	-2.27359600	-1.67700600	0.02276800
C	-3.04477100	0.24126300	-0.41501300
H	-2.77888000	1.25174400	-0.71684100
C	2.17229100	0.76693300	0.74336100
H	2.04129900	0.95200900	1.81404700

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C	3.10806400	-2.03108300	-0.53779000
C	4.18224300	-2.40862400	0.26068000
C	4.76212700	-1.51809700	1.16616400
C	4.27515200	-0.22502200	1.29456100
C	3.20554400	0.14015800	0.49298600
C	2.63391700	-0.73640100	-0.41875300
H	2.65953100	-2.72938300	-1.23469200
H	4.57756400	-3.41366400	0.18011900
H	5.59618700	-1.84386600	1.77442200
H	4.70953300	0.47735200	1.99544500
C	2.50500400	1.43834900	0.40153600
O	2.78198000	2.50621300	0.92754300
N	1.44839300	1.21496200	-0.42852100
O	0.84606500	2.28805900	-1.03137900
C	-0.32426500	2.73215400	-0.31620500
H	-0.06803300	2.89381600	0.73225400
H	-0.54232600	3.69477000	-0.78319100
C	1.48628200	-0.07308500	-1.14921500

H	1.76417300	0.13524600	-2.18726900
C	0.19637800	-0.82675900	-1.09942900
C	-0.22440100	-1.43605700	0.19116600
H	-1.31193500	-1.52531700	0.24490800
H	0.18598500	-2.44894500	0.30870800
H	0.11578600	-0.84807600	1.04809800
C	-0.48293600	-1.23048400	-2.35859300
H	-1.56781900	-1.26381200	-2.22049400
H	-0.25617700	-0.54654200	-3.17862900
H	-0.17990700	-2.23812100	-2.67922600
C	-3.30199600	0.40654300	0.52417600
C	-3.76156300	-0.15881100	1.71564400
C	-3.94518700	0.06019900	-0.66896200
C	-4.82265100	-1.05417800	1.71961300
H	-3.27252500	0.10486300	2.64684100
C	-5.00390100	-0.83386300	-0.66553400
H	-3.62404000	0.49675100	-1.60666900
C	-5.44654400	-1.39670800	0.52779400
H	-5.16174500	-1.48347400	2.65432800
H	-5.49185600	-1.09022100	-1.59798900
H	-6.27567900	-2.09328500	0.52614600
C	-1.47008900	1.79206800	-0.46724600
H	-1.73684900	1.53274100	-1.48807700
C	-2.14817500	1.31575300	0.57433600
H	-1.82099600	1.59394600	1.57373200

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C	2.85314700	-2.16893400	-0.44297100
C	4.10493900	-2.57481800	0.01002400
C	5.03765100	-1.65474800	0.48848600
C	4.73818700	-0.29919800	0.52258200
C	3.49134400	0.09465700	0.06837800
C	2.55870000	-0.81710200	-0.41232400
H	2.13762500	-2.89233500	-0.81344000
H	4.36114600	-3.62683500	-0.01062600
H	6.00225600	-2.00327100	0.83461200
H	5.45040900	0.42973700	0.88959500
C	2.92205800	1.46069500	-0.01635500
O	3.43776600	2.53412500	0.26957000
N	1.67947900	1.27474600	-0.50820800
O	0.88701200	2.31876500	-0.87005600
C	-0.28896500	2.40760600	-0.04998300
H	-0.00053200	2.43654800	1.00362600
H	-0.70628300	3.37755200	-0.32718500

C	1.28307800	-0.09659300	-0.79649000
H	1.06727300	-0.19546900	-1.86462500
C	0.08531800	-0.51614800	0.02074100
C	0.24765100	-0.51408300	1.50529500
H	-0.72875900	-0.51414000	1.99472800
H	0.77442300	-1.41964400	1.83304300
H	0.81681400	0.34680400	1.86274700
C	-0.73386700	-1.62248800	-0.55142000
H	-1.68335200	-1.71321900	-0.02019300
H	-0.93380500	-1.47566200	-1.61487800
H	-0.21271100	-2.58325400	-0.43984100
C	-3.52799600	0.35396300	0.25764300
C	-4.41449100	0.09277600	1.31234400
C	-3.85733500	-0.14159400	-1.01419900
C	-5.57319600	-0.64206000	1.11161800
H	-4.17969500	0.47268000	2.30052200
C	-5.01422000	-0.87527900	-1.21233800
H	-3.20337600	0.05379800	-1.85522000
C	-5.87919700	-1.13305600	-0.15164300
H	-6.23954300	-0.83229900	1.94427400
H	-5.24834100	-1.24728400	-2.20252500
H	-6.78363700	-1.70635300	-0.31185800
C	-1.28339800	1.31894100	-0.33458900
H	-1.36608100	1.03032200	-1.37895000
C	-2.32198200	1.12335500	0.52112400
H	-2.24297100	1.54063800	1.52201500

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C	2.90433100	-2.11958200	-0.39515600
C	4.17580400	-2.45820900	0.05957100
C	5.07630900	-1.48629500	0.49262600
C	4.72621900	-0.14280800	0.46767800
C	3.46031200	0.18297600	0.01420400
C	2.54713700	-0.78182100	-0.40245500
H	2.22546000	-2.88839900	-0.73993100
H	4.47275200	-3.49953100	0.07333400
H	6.05739800	-1.78317900	0.84059700
H	5.41622600	0.62935700	0.78537400
C	2.85141400	1.52629000	-0.13720200
O	3.30819400	2.62438900	0.15527700
N	1.65516900	1.27961300	-0.71123900
O	0.74953700	2.26420700	-0.97606700
C	-0.37618400	2.13590200	-0.09127600
H	-0.05401400	2.35186700	0.93074300

H	-1.07060000	2.90649400	-0.42185200
C	1.25522400	-0.11723400	-0.80367500
H	0.97542800	-0.34755300	-1.83598800
C	0.03445300	-0.37583100	0.12233200
C	0.44744200	-0.34418100	1.59377700
H	-0.43217300	-0.42568800	2.23379400
H	1.10082400	-1.18776300	1.82165400
H	0.97707700	0.57219700	1.86383300
C	-0.56477000	-1.73646700	-0.21386600
H	-1.45846100	-1.91490500	0.38723900
H	-0.84193600	-1.79702500	-1.26881300
H	0.14369100	-2.53709600	0.00396300
C	-3.48330200	0.18586300	0.30327200
C	-4.54947600	0.27217200	1.23355000
C	-3.75545300	-0.43505800	-0.93974800
C	-5.80163900	-0.22552100	0.93812100
H	-4.36386300	0.74284500	2.19241600
C	-5.01400400	-0.93052000	-1.22444600
H	-2.97100700	-0.52896900	-1.67933400
C	-6.04655200	-0.83186400	-0.29403700
H	-6.59769300	-0.14404300	1.66837000
H	-5.19658000	-1.40178800	-2.18274900
H	-7.02919000	-1.22284600	-0.52512900
C	-1.00290100	0.74823500	-0.21009400
H	-1.28442500	0.61435400	-1.25882700
C	-2.21606400	0.70839600	0.65565800
H	-2.12675600	1.14896500	1.64330300

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C	3.67088000	1.74352200	-0.63780200
C	5.03174300	1.47736800	-0.63670600
C	5.50000000	0.19818500	-0.35830400
C	4.59339700	-0.80905400	-0.07695400
C	3.22804900	-0.53549300	-0.05027800
C	2.73769000	0.74856300	-0.33723700
H	3.31832900	2.73181600	-0.90500100
H	5.73096700	2.27035800	-0.87183100
H	6.56191000	-0.01071400	-0.36519400
H	4.93316800	-1.81353800	0.14398200
C	2.30944400	-1.64889800	0.28695600
O	2.50345800	-2.81024400	-0.02621600
N	1.26806300	-1.27670500	1.14852000
O	0.18662300	-2.02478000	1.13331300
C	-0.33268100	-2.55079600	-0.11154000

H	0.34046800	-2.31692700	-0.93525200
H	-0.37587200	-3.63557400	0.00032500
C	0.63152900	2.07189100	0.05491700
C	1.25317500	3.15247200	0.88834200
H	1.33874400	4.07832600	0.31150800
H	0.60398800	3.37308100	1.73957000
H	2.24012500	2.88826400	1.26337000
C	-0.83943600	2.23720100	-0.18477200
H	-1.04028800	3.21952200	-0.62314300
H	-1.23615100	1.46972800	-0.84921600
H	-1.38532000	2.20085500	0.76263200
C	-3.55271800	-0.37186700	0.06779600
C	-4.34821100	-0.70924600	-1.03204600
C	-4.02926900	0.59039100	0.96055300
C	-5.58070500	-0.10615800	-1.22371300
H	-4.00265300	-1.44487000	-1.74788700
C	-5.26459100	1.19525300	0.76938900
H	-3.42152900	0.86122900	1.81662100
C	-6.04556300	0.84860900	-0.32420000
H	-6.18261200	-0.37895500	-2.08192600
H	-5.61555300	1.93764500	1.47560100
H	-7.00872700	1.31881000	-0.47871200
C	-1.68551700	-1.97271100	-0.36429000
H	-2.20150600	-2.43700800	-1.19904800
C	-2.23418300	-0.97487400	0.32227500
H	-1.68706300	-0.54625300	1.15714000
C	1.28726400	1.01261100	-0.43387100
H	0.71071600	0.26951800	-0.98103500

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C	3.81056900	1.55938000	-0.94652400
C	5.15315700	1.22395300	-1.05600200
C	5.60611600	-0.03992200	-0.68245000
C	4.71467700	-0.97478000	-0.18171300
C	3.37532800	-0.62837300	-0.05918200
C	2.90544100	0.62310400	-0.45594000
H	3.46180600	2.53694600	-1.25764900
H	5.85500100	1.95112000	-1.44522100
H	6.65563000	-0.28721800	-0.77803800
H	5.04700700	-1.95843000	0.12734400
C	2.35149400	-1.53121800	0.50228800
O	2.43822300	-2.75433900	0.56602700
N	1.30385300	-0.79724900	0.99899400
O	0.13620900	-1.45375900	1.17056700

C	-0.36688500	-2.18899200	0.04347400
H	0.28573900	-2.03562600	-0.81925200
H	-0.34114900	-3.25346400	0.29173400
C	0.86373000	1.93092000	0.24690500
C	1.60940700	2.82444700	1.17704000
H	1.69054100	3.82856800	0.74782800
H	1.04971300	2.93140700	2.11067700
H	2.61034600	2.46183000	1.40311000
C	-0.59274500	2.20169800	0.09901700
H	-0.75481100	3.25145100	-0.16467300
H	-1.05825800	1.56703500	-0.65373400
H	-1.09771700	2.04403700	1.05834200
C	-3.78019500	-0.31698100	0.02218300
C	-4.59612500	-0.91517000	-0.94385200
C	-4.27534400	0.79171300	0.71254300
C	-5.86047800	-0.41464900	-1.20901400
H	-4.24497000	-1.78145200	-1.49089000
C	-5.54211400	1.29492000	0.44655000
H	-3.65515600	1.26125800	1.46811100
C	-6.33987700	0.69350400	-0.51653400
H	-6.47882000	-0.89227000	-1.95925600
H	-5.90502500	2.15627900	0.99381700
H	-7.32908300	1.08075100	-0.72661800
C	-1.75771800	-1.75658300	-0.28497000
H	-2.19964700	-2.30405400	-1.11236900
C	-2.42422900	-0.79139100	0.34129700
H	-1.93965200	-0.27318400	1.16221900
C	1.44378700	0.85593800	-0.37886600
H	0.83810500	0.31144200	-1.09869300

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C	-2.64898000	-2.08530300	-0.83927900
C	-3.94169200	-2.26553100	-1.32032400
C	-4.84018700	-1.20088500	-1.40644200
C	-4.46252000	0.07517200	-1.01199600
C	-3.17343700	0.24374600	-0.53390200
C	-2.27658700	-0.81214300	-0.44360700
H	-1.95807100	-2.91725800	-0.77672800
H	-4.25888900	-3.25226900	-1.63445600
H	-5.83907200	-1.37515800	-1.78537900
H	-5.14586000	0.91331900	-1.07388700
C	-2.51375000	1.47076800	-0.03836400
O	-2.97831400	2.59083500	0.11885000
N	-1.23135600	1.10187800	0.21722900

O	-0.43894700	1.93119600	0.96111000
C	0.40768000	2.74018400	0.13427800
H	-0.16325800	3.08495200	-0.73056400
H	0.63913100	3.61412900	0.74856400
C	-0.65930900	-0.93842200	1.48515900
C	-1.57329900	-0.65111700	2.62394400
H	-2.41052200	-1.36362600	2.64964000
H	-1.04635700	-0.75013300	3.57577500
H	-2.00074700	0.35267300	2.57174100
C	0.18762300	-2.15995000	1.52609500
H	-0.42102000	-3.07254100	1.44678600
H	0.91230400	-2.17770200	0.70928400
H	0.72545000	-2.22983900	2.47564000
C	3.37824800	0.24054900	-0.14149900
C	4.10728600	0.56351200	-1.29073100
C	3.85153300	-0.78749700	0.67716300
C	5.27743700	-0.11195600	-1.59780700
H	3.75413200	1.34133700	-1.95670100
C	5.02464200	-1.46433300	0.37039500
H	3.29184800	-1.05053800	1.56808300
C	5.74331400	-1.12767100	-0.76832700
H	5.82813100	0.15023600	-2.49298300
H	5.37551700	-2.25568600	1.02140600
H	6.65693500	-1.65484200	-1.01337400
C	1.66609000	2.05462800	-0.29327500
H	2.20990700	2.57214000	-1.07815000
C	2.13677500	0.93171500	0.24133000
H	1.58160900	0.46427600	1.05108400
C	-0.96323900	-0.34042500	0.14556000
H	-0.13935300	-0.53310700	-0.54630400

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C	-2.56434700	-2.24932400	-0.22866800
C	-3.87568600	-2.62779800	-0.49632900
C	-4.87391200	-1.67864700	-0.72288600
C	-4.58001400	-0.32276700	-0.68674100
C	-3.27127400	0.04335000	-0.41746600
C	-2.27572000	-0.89607600	-0.18770200
H	-1.79547900	-2.99225700	-0.05404700
H	-4.12923800	-3.68021500	-0.52843200
H	-5.88485000	-2.00655000	-0.92828300
H	-5.34174700	0.42726800	-0.86126600
C	-2.68634600	1.39607100	-0.29893100
O	-3.24380100	2.48338400	-0.33401300

N	-1.35207800	1.19269700	-0.12713900
O	-0.59687500	2.21185500	0.38198100
C	0.38829400	2.68673400	-0.56434500
H	-0.13332700	3.03894000	-1.45546200
H	0.84032400	3.53121400	-0.04534800
C	-0.42831200	-0.43267700	1.48391200
C	-1.24146000	0.01909900	2.64523900
H	-1.92742000	-0.77200400	2.98039600
H	-0.60030700	0.26120000	3.49637800
H	-1.84669400	0.89798300	2.41173100
C	0.61593600	-1.47105400	1.68775500
H	0.17228900	-2.44404400	1.94430600
H	1.22661700	-1.61329000	0.79368200
H	1.27348300	-1.20348500	2.52015800
C	-0.95798500	-0.20910100	0.10327700
H	-0.20688500	-0.50982800	-0.63172900
C	2.47745000	1.44354400	-0.11928400
H	2.63176300	2.11119500	0.72606500
C	1.40663000	1.63760500	-0.88741500
H	1.21272100	1.00977000	-1.75083700
C	3.49731500	0.39692500	-0.27959600
C	3.39287800	-0.62240900	-1.23231000
C	4.60805400	0.40644800	0.56649800
C	4.37585000	-1.59271600	-1.33690800
H	2.53606100	-0.66244200	-1.89366900
C	5.59387000	-0.56597300	0.46199700
H	4.69547700	1.18790300	1.31308100
C	5.48096600	-1.56874200	-0.49079100
H	4.27960500	-2.37594000	-2.07881900
H	6.44834300	-0.54066200	1.12695700
H	6.24610400	-2.33050200	-0.57446500

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C	-3.00017200	-2.06585800	-0.52648700
C	-4.23440400	-2.44397500	-0.00726500
C	-5.06262800	-1.52642100	0.64005000
C	-4.67470300	-0.20083900	0.77958100
C	-3.44239300	0.16426600	0.26416200
C	-2.60823500	-0.74722200	-0.37016300
H	-2.37002700	-2.78434300	-1.03553800
H	-4.56034500	-3.47173100	-0.10865900
H	-6.01753400	-1.85348600	1.03107300
H	-5.30906700	0.52724200	1.27015500
C	-2.78161800	1.48712500	0.27671500

O	-3.12478600	2.51755100	0.84156700
N	-1.66712700	1.32972300	-0.48021200
O	-0.67127800	2.26882800	-0.33349200
C	0.32772300	2.13061300	-1.35257200
H	-0.16385200	2.00599700	-2.31823100
H	0.83108200	3.09646800	-1.33994400
C	-0.08871800	-0.50868800	-0.09173100
C	-0.00222800	-0.24951900	1.37599400
H	-0.57248900	-1.00702000	1.92972400
H	1.03626500	-0.32257000	1.70904300
H	-0.38364400	0.73293700	1.65806800
C	0.48738000	-1.80310600	-0.56114200
H	-0.09665900	-2.64565300	-0.16686600
H	0.49235100	-1.88172600	-1.65028300
H	1.50700800	-1.92486000	-0.19084800
C	-1.33263200	-0.06216400	-0.80677300
H	-1.19178600	-0.17438000	-1.88640600
C	2.32272800	1.21896000	-0.18445000
H	2.23503200	2.06794000	0.48984000
C	1.31710800	1.01554600	-1.08191600
H	1.42763700	0.27686500	-1.86785400
C	3.48316000	0.36917100	0.02993900
C	3.83934600	-0.67500200	-0.83885400
C	4.30496800	0.60566800	1.14209800
C	4.96018900	-1.45034900	-0.59461800
H	3.23817700	-0.87729400	-1.71679500
C	5.42547800	-0.17323900	1.38580300
H	4.04947800	1.41253000	1.81997000
C	5.75873000	-1.20791300	0.51978600
H	5.21716500	-2.24932900	-1.27953300
H	6.04119500	0.02824700	2.25396400
H	6.63393900	-1.81726000	0.70706800

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C	-2.96952600	-2.08600200	-0.41067200
C	-4.21767200	-2.43726700	0.09289500
C	-5.08347500	-1.48072800	0.62443100
C	-4.72053800	-0.14187900	0.65556000
C	-3.47384600	0.19651500	0.15595500
C	-2.59550600	-0.75300400	-0.35397400
H	-2.31480400	-2.83779100	-0.83233300
H	-4.52534900	-3.47529000	0.07005800
H	-6.04844900	-1.78820800	1.00658300
H	-5.38432700	0.61708700	1.05111400

C	-2.83621800	1.52705300	0.07293700
O	-3.19828600	2.59346900	0.55226800
N	-1.71003900	1.32934400	-0.66033200
O	-0.70542800	2.27394500	-0.52998900
C	0.42980600	1.85284800	-1.28812100
H	0.12357300	1.71981600	-2.32808500
H	1.11946100	2.69247600	-1.23030700
C	-0.03320600	-0.33541000	-0.02742100
C	-0.23135200	0.01904900	1.44758300
H	-1.05744400	-0.56202500	1.86347600
H	0.66579500	-0.23264700	2.01516900
H	-0.44050100	1.07862900	1.60291200
C	0.37492700	-1.79931900	-0.13973500
H	-0.31381500	-2.43937300	0.41453000
H	0.39916900	-2.12898800	-1.18114800
H	1.37114900	-1.93650800	0.28640600
C	-1.33209700	-0.08322900	-0.81835300
H	-1.14908500	-0.30633200	-1.87369800
C	2.20791200	0.86389200	0.16820000
H	2.05814800	1.65258700	0.89876600
C	1.05683100	0.55859800	-0.72689100
H	1.40222100	-0.00788800	-1.59375400
C	3.47584300	0.23712100	0.15451600
C	3.82350300	-0.81298100	-0.73139300
C	4.47054500	0.66793900	1.06948200
C	5.08204900	-1.38295800	-0.69756900
H	3.09799100	-1.18227500	-1.44464500
C	5.72290300	0.09032400	1.09422400
H	4.22879400	1.46983900	1.75792900
C	6.04226600	-0.94082100	0.21043900
H	5.32158200	-2.18450800	-1.38600400
H	6.46156000	0.44154800	1.80461900
H	7.02543500	-1.39331000	0.22992600

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C	-4.05687700	1.93850000	-0.27922500
C	-5.37016100	1.51377900	-0.16099400
C	-5.65750600	0.16152300	-0.00592900
C	-4.62220100	-0.75477700	0.00712000
C	-3.30025000	-0.33064500	-0.13454900
C	-2.99429900	1.03168700	-0.24919500
H	-3.83787500	2.99528800	-0.37764000
H	-6.17331300	2.24010200	-0.18195400
H	-6.68205200	-0.17363800	0.09122300

H	-4.82522500	-1.81415100	0.10281800
C	-2.26145700	-1.39019700	-0.19799400
O	-2.36930200	-2.46726400	0.36459900
N	-1.24985000	-1.11975000	-1.12497800
O	-0.15192700	-1.83894100	-1.05196000
C	0.39951700	-2.27841600	0.21221800
H	-0.22573900	-1.95003500	1.03895600
H	0.39612100	-3.36994900	0.19309700
C	-0.68056900	1.47870700	0.63751000
C	-0.85245100	0.75805000	1.94055700
H	-0.04380400	0.03517500	2.08072900
H	-0.76885300	1.47463900	2.76360200
H	-1.80770100	0.24336800	2.03392900
C	0.63375000	2.18674900	0.48811500
H	1.46444700	1.50211800	0.67721800
H	0.75228300	2.62331300	-0.50343900
H	0.71251400	2.98547400	1.23225400
C	3.67506300	-0.23605400	-0.26785000
C	4.64125100	-0.77798100	0.58557500
C	4.00202800	0.90647200	-1.00146900
C	5.88787500	-0.18534500	0.70662300
H	4.42298100	-1.67469900	1.15253800
C	5.25063400	1.50155200	-0.87965900
H	3.26307700	1.33082200	-1.67214300
C	6.19809900	0.95832300	-0.02304000
H	6.62529600	-0.61990300	1.37042200
H	5.48294400	2.38868500	-1.45595200
H	7.17408200	1.41736700	0.07347400
C	1.78340600	-1.73969800	0.35461300
H	2.32624500	-2.16311200	1.19438900
C	2.32781900	-0.80774000	-0.42196200
H	1.74294200	-0.39366900	-1.23833300
C	-1.61682400	1.57049400	-0.31299200
H	-1.40065700	2.18079200	-1.18629700

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C	4.47847400	-1.54273800	-0.38627700
C	5.73149000	-0.97033300	-0.20506700
C	5.86815400	0.40434100	-0.02995600
C	4.74694900	1.21957100	-0.04497800
C	3.49843100	0.64459500	-0.23914300
C	3.34933500	-0.73283000	-0.39308500
H	4.37683000	-2.61473800	-0.50544600
H	6.61054700	-1.60277900	-0.19192600

H	6.85054900	0.83538100	0.11453900
H	4.83142800	2.29184000	0.08417900
C	2.24562600	1.43291400	-0.29373200
O	2.11600000	2.58102000	0.12080500
N	1.28569300	0.71284800	-0.95162000
O	-0.00642000	1.07095800	-0.80322800
C	-0.45977500	1.36495900	0.52611500
H	0.11053000	0.76030100	1.23937400
H	-0.26883600	2.41526400	0.75554300
C	1.20820400	-1.64582700	0.54719900
C	1.62916600	-1.42241700	1.96217300
H	0.77766400	-1.11573100	2.57370200
H	1.99383300	-2.36611400	2.38325700
H	2.42446100	-0.68373000	2.05704400
C	-0.12243100	-2.28214700	0.34150200
H	-0.90802300	-1.63460000	0.74698400
H	-0.33136300	-2.47074900	-0.71094300
H	-0.18300800	-3.22449300	0.89514100
C	-4.10024600	0.20213400	-0.20169600
C	-4.91549800	0.73470900	0.80231100
C	-4.68148100	-0.64604700	-1.14682600
C	-6.26189700	0.41326300	0.86427900
H	-4.49884000	1.41582200	1.53421000
C	-6.03040700	-0.96961000	-1.08491100
H	-4.06260100	-1.05726500	-1.93645900
C	-6.82596300	-0.44260200	-0.07694000
H	-6.87835400	0.83754900	1.64741400
H	-6.45942800	-1.63239400	-1.82641800
H	-7.87911300	-0.68948100	-0.02647800
C	-1.91757600	1.07383700	0.63304400
H	-2.35122700	1.38058700	1.58031100
C	-2.66147100	0.49486800	-0.30525500
H	-2.19146300	0.18008200	-1.23164800
C	1.96803700	-1.26358400	-0.52805300
H	1.67718800	-1.63283600	-1.50588000

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C	-4.59642800	0.91757000	-0.84534000
C	-5.79257200	0.22093900	-0.70325500
C	-5.81169900	-1.10487800	-0.26946500
C	-4.62949500	-1.76504800	0.03883700
C	-3.44547600	-1.06208600	-0.10602800
C	-3.41977700	0.25399800	-0.54976400
H	-4.58764500	1.94895000	-1.17781100

H	-6.72764100	0.71699300	-0.93224500
H	-6.75872800	-1.61937200	-0.16827300
H	-4.62723400	-2.79153500	0.38442800
C	-2.05749100	-1.50767800	0.15924000
O	-1.64856500	-2.60672800	0.51212200
N	-1.30044700	-0.41174500	-0.07070800
O	0.05982900	-0.46660700	-0.10153600
C	0.61296900	-0.20999600	1.19675600
H	0.22224100	0.74105900	1.57348800
H	0.29566900	-1.00232700	1.88209600
C	-1.72635400	2.01813700	0.14860900
C	-2.25751500	2.16640500	1.53341100
H	-1.46561000	2.47009000	2.22589200
H	-3.02856100	2.94502500	1.58347700
H	-2.70042000	1.24077100	1.90746900
C	-0.68362900	2.96141600	-0.33434500
H	0.30014200	2.71994400	0.09653800
H	-0.57889100	2.93188600	-1.42020200
H	-0.91143000	3.98724000	-0.03180200
C	4.26647200	-0.21739800	-0.13328200
C	5.11827200	-0.17453500	0.97558800
C	4.83829100	-0.21137900	-1.40744100
C	6.49258100	-0.11846200	0.80940100
H	4.70837300	-0.19191900	1.97797400
C	6.21556300	-0.15446800	-1.57506200
H	4.18999200	-0.24968900	-2.27561300
C	7.04882200	-0.10658500	-0.46633000
H	7.13618400	-0.08799800	1.68014800
H	6.63623200	-0.14898600	-2.57314300
H	8.12356500	-0.06417200	-0.59170400
C	2.09701000	-0.15987500	1.10334900
H	2.58635600	-0.01389500	2.06113500
C	2.79933200	-0.27005600	-0.02107300
H	2.27342400	-0.40398000	-0.96102300
C	-2.00004800	0.76592000	-0.61596700
H	-1.68598200	0.88917100	-1.65759000

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C	3.29675000	-2.08200000	-0.20837200
C	4.66236800	-2.16832900	0.04309900
C	5.44626300	-1.02358600	0.19186300
C	4.87796700	0.23949500	0.09446200
C	3.51857700	0.31369900	-0.15865900
C	2.73558800	-0.82221700	-0.31719800

H	2.69320000	-2.97533900	-0.31668200
H	5.12721000	-3.14285000	0.12706900
H	6.50585900	-1.12465600	0.38893900
H	5.47057800	1.13843300	0.21287400
C	2.65980800	1.51035400	-0.30848500
O	2.96540100	2.69606200	-0.27612300
N	1.41529300	1.01828700	-0.49410700
O	0.38074300	1.83769300	-0.82302500
C	-0.32553600	2.35175800	0.31975100
H	0.27506800	2.18512400	1.21709600
H	-0.39981300	3.43232700	0.16990600
C	1.28754800	-0.44274700	-0.55611000
H	0.97217000	-0.72829800	-1.56428000
C	0.33721600	-0.99117400	0.45906400
C	0.56682300	-0.70012300	1.90026900
H	-0.36727100	-0.40881100	2.39351200
H	0.93547500	-1.58823200	2.43049400
H	1.29453200	0.10043200	2.04866100
C	-0.61918000	-2.06479600	0.08380600
H	-1.55829500	-1.95758700	0.63659100
H	-0.84343300	-2.05659400	-0.98439000
H	-0.22654300	-3.06113600	0.33211000
C	-3.55652400	0.24505000	-0.20564200
C	-4.40933800	0.49605000	0.87462600
C	-3.99012500	-0.63460000	-1.20025000
C	-5.65431000	-0.10754400	0.94760800
H	-4.09819600	1.16340100	1.66891900
C	-5.23776400	-1.24006500	-1.12800000
H	-3.33695800	-0.84176200	-2.04071000
C	-6.07599600	-0.97780400	-0.05331600
H	-6.30043200	0.09886300	1.79217200
H	-5.55359000	-1.91736800	-1.91199600
H	-7.04917500	-1.44856900	0.00857400
C	-1.68844500	1.76147800	0.47324000
H	-2.24071200	2.15639300	1.32122500
C	-2.22166800	0.85061200	-0.33499300
H	-1.63601900	0.49712000	-1.17874300

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C	-2.57679700	2.21471000	-0.39281400
C	-3.91032600	2.61217200	-0.37488000
C	-4.94631300	1.67893000	-0.34235800
C	-4.66950800	0.31822500	-0.33165200
C	-3.34031600	-0.06707800	-0.35208400

C	-2.30281900	0.85783100	-0.38341500
H	-1.78177200	2.94919400	-0.42156400
H	-4.14901600	3.66842700	-0.38823300
H	-5.97308200	2.02121100	-0.32766600
H	-5.46094700	-0.42104400	-0.30945800
C	-2.77009500	-1.43480600	-0.35757500
O	-3.34696000	-2.51544000	-0.34832500
N	-1.43506300	-1.24180400	-0.39687200
O	-0.56910300	-2.28742400	-0.49077900
C	0.22903600	-2.41075000	0.70046700
H	-0.42540300	-2.39441400	1.57200600
H	0.66910200	-3.40536300	0.61452000
C	-0.97033600	0.14066400	-0.35418200
H	-0.36880700	0.35276600	-1.24328500
C	-0.16836400	0.43272900	0.89231200
C	-0.84792000	0.22821700	2.20909300
H	-0.12199100	-0.01811300	2.98864900
H	-1.34796100	1.15416700	2.52187200
H	-1.60343100	-0.55836400	2.17991100
C	0.75287400	1.60126400	0.80346900
H	1.44278000	1.61628100	1.65002000
H	1.33065200	1.59445300	-0.12242800
H	0.18429100	2.54033000	0.83651900
C	3.34375300	-0.33807100	-0.28330700
C	3.90961500	0.20118000	0.88304600
C	4.00334600	-0.10476800	-1.49863000
C	5.07626900	0.94454500	0.82780000
H	3.43562900	0.03519500	1.84256700
C	5.17147200	0.64040600	-1.55208800
H	3.58382400	-0.51734200	-2.40943500
C	5.71441000	1.17193000	-0.38878200
H	5.49520600	1.34997400	1.74092200
H	5.65946100	0.80672400	-2.50482700
H	6.62633000	1.75445000	-0.42627200
C	1.30103500	-1.35500600	0.77513000
H	1.60591800	-1.07584400	1.77786800
C	2.12327400	-1.13073200	-0.28497100
H	1.83941500	-1.54669500	-1.24822900

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C	2.65208100	-2.12378000	-0.57004900
C	3.99449000	-2.48414500	-0.49670800
C	4.99524600	-1.52989100	-0.31785000
C	4.67318400	-0.18294700	-0.21979600

C	3.33564600	0.16484400	-0.29301600
C	2.32831400	-0.78239400	-0.45271200
H	1.89045300	-2.87740400	-0.72268900
H	4.26770500	-3.52841400	-0.58446800
H	6.02989100	-1.84359700	-0.26492200
H	5.43665200	0.57533400	-0.09544100
C	2.72799300	1.51551800	-0.23946600
O	3.26296400	2.60167300	-0.05543600
N	1.41511500	1.29521700	-0.47007500
O	0.48830600	2.29650000	-0.41401200
C	-0.31366900	2.14908300	0.77316900
H	0.32112700	2.29669400	1.64856400
H	-1.04014500	2.95767100	0.71224900
C	0.98651700	-0.09918300	-0.46807600
H	0.43041900	-0.31333900	-1.38523800
C	0.07411100	-0.35891700	0.76047200
C	0.88122100	-0.33209300	2.06048100
H	0.20130800	-0.33286900	2.91501500
H	1.51401900	-1.21798500	2.13377300
H	1.52604200	0.54416800	2.14674100
C	-0.59730700	-1.72072900	0.62371100
H	-1.31433900	-1.86355200	1.43519100
H	-1.12942100	-1.82015700	-0.32400100
H	0.14155700	-2.52058800	0.69115600
C	-3.28945300	0.18680100	-0.28197100
C	-3.84857800	-0.38812900	0.88478000
C	-4.10531900	0.22570700	-1.44055700
C	-5.13873800	-0.88517400	0.88288900
H	-3.26409500	-0.44401900	1.79392400
C	-5.39107700	-0.27423100	-1.43111000
H	-3.69845900	0.66094200	-2.34637300
C	-5.92100400	-0.83469700	-0.26880000
H	-5.54324900	-1.31958000	1.78921900
H	-5.99085200	-0.23014700	-2.33216900
H	-6.93005600	-1.22659400	-0.26144400
C	-0.99892000	0.78286000	0.78282600
H	-1.52109000	0.69783900	1.73851500
C	-1.97554300	0.71067500	-0.34526900
H	-1.65860000	1.11862500	-1.29917700

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C	-2.84855900	-2.44334100	-0.38541200
C	-4.18534400	-2.51349400	-0.73908200
C	-4.96007000	-1.35846600	-0.78114600

C	-4.37605900	-0.13888600	-0.49094400
C	-3.02226800	-0.06287000	-0.16122700
C	-2.24148600	-1.22450700	-0.06568700
H	-2.25646500	-3.34946400	-0.33085000
H	-4.62901500	-3.47301000	-0.97453900
H	-6.00682400	-1.40986300	-1.05167100
H	-4.95490600	0.77517800	-0.54287700
C	-2.46138800	1.29777600	0.04274000
O	-3.05683700	2.18633600	0.62499200
N	-1.22556400	1.48703400	-0.59322600
O	-0.71517400	2.63780200	-0.21714300
C	0.53019400	2.91536100	-0.91354600
H	0.35735400	2.75929400	-1.97766900
H	0.70302600	3.97105300	-0.70991700
C	-0.32515800	-0.66472900	1.47609800
C	-1.10223600	0.15695100	2.46092100
H	-0.81686300	-0.12596300	3.47696700
H	-0.85327400	1.21884300	2.35106900
H	-2.18096300	0.04298400	2.36375800
C	1.12658200	-0.82307000	1.81486000
H	1.23592500	-1.32536500	2.78064000
H	1.66659500	-1.39194900	1.05794500
H	1.59919300	0.15882900	1.91735100
C	3.27881000	0.21088400	-0.71883700
C	4.09442300	0.47920400	0.38416000
C	3.47568900	-0.97719400	-1.42501100
C	5.05958500	-0.43150700	0.78306600
H	3.97880500	1.40897100	0.92822100
C	4.44001200	-1.89159600	-1.02336400
H	2.85473700	-1.18783100	-2.28850800
C	5.23182000	-1.62325200	0.08520500
H	5.68537300	-0.21030600	1.63896600
H	4.57331200	-2.81286500	-1.57686900
H	5.98683700	-2.33274400	0.40020900
C	2.19829300	1.11207800	-1.14088900
H	1.82515500	0.95674100	-2.15061800
C	-0.83613000	-1.24515900	0.38320100
H	-0.17569000	-1.86989600	-0.21337600
C	1.62822200	2.05403000	-0.39242400
H	1.93314700	2.22575400	0.63545600

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C	-2.43462400	-2.44988000	0.20191300
C	-3.67953600	-2.90178200	-0.21763900

C	-4.62067600	-2.01941700	-0.74460600
C	-4.31761700	-0.67233900	-0.87020700
C	-3.06632100	-0.23079200	-0.46420700
C	-2.13167900	-1.09833100	0.09216700
H	-1.71452800	-3.13764700	0.62854800
H	-3.92441800	-3.95270800	-0.12578300
H	-5.58714100	-2.38944600	-1.06215600
H	-5.03088900	0.02795800	-1.28769900
C	-2.58906200	1.16319000	-0.57789000
O	-3.30458900	2.15799100	-0.64317000
N	-1.21886700	1.15965600	-0.63688100
O	-0.69988700	2.37708900	-0.32646200
C	0.51537000	2.61838800	-1.06046000
H	0.34164600	2.37644300	-2.10984200
H	0.67104800	3.69279800	-0.95490300
C	-0.74314700	0.11136300	1.80773300
C	-1.92085900	0.61212300	2.57002900
H	-1.75477900	0.50984600	3.64407200
H	-2.04193300	1.68571000	2.37058000
H	-2.85129200	0.11312100	2.30323700
C	0.59649400	0.44283200	2.36387200
H	0.69444300	0.02258500	3.36982700
H	1.40774700	0.06732600	1.74135100
H	0.70125800	1.52874400	2.47248900
C	3.38000400	0.04009600	-0.67719600
C	4.06572000	0.32071200	0.50976900
C	3.77181200	-1.07247900	-1.42463500
C	5.10247400	-0.49393400	0.93476900
H	3.79511000	1.18682400	1.10126400
C	4.81039900	-1.88969000	-0.99869000
H	3.25071500	-1.29648400	-2.34860700
C	5.47853100	-1.60365000	0.18376800
H	5.62470000	-0.26115100	1.85469100
H	5.09741800	-2.74913500	-1.59192700
H	6.29058900	-2.23700000	0.51857600
C	2.25921600	0.85973100	-1.16137800
H	1.88637500	0.59886100	-2.14951600
C	-0.86124400	-0.49535300	0.57169600
H	0.05170300	-0.86444500	0.11444100
C	1.66376400	1.84977200	-0.50028000
H	1.98598400	2.13620600	0.49540000

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C	2.30723900	1.94774000	1.35047600

C	3.25044400	2.88555800	0.94253900
C	3.90804200	2.76693200	-0.28255100
C	3.63652900	1.70110600	-1.12979200
C	2.69495700	0.77452800	-0.71380700
C	2.03706900	0.88815800	0.50340200
H	1.80436700	2.04212200	2.30566600
H	3.48194700	3.72330900	1.58862500
H	4.63757900	3.51289900	-0.57076100
H	4.14130200	1.59091700	-2.08180100
C	2.23789300	-0.46028500	-1.39044400
O	2.63502100	-0.96367800	-2.43307100
N	1.25351000	-0.94689400	-0.59631900
O	0.79327500	-2.21979000	-0.77356300
C	-0.43327900	-2.23677600	-1.53969100
H	-0.26352500	-1.73184300	-2.49239900
H	-0.59778500	-3.30084100	-1.71571300
C	1.40713100	-1.16406700	1.85644200
C	2.73341300	-1.83948100	1.86590000
H	3.05041400	-2.06761000	2.88615300
H	2.68565100	-2.79656100	1.32655000
H	3.50863300	-1.23585600	1.38883200
C	0.30016600	-1.74564600	2.66123700
H	0.62345600	-1.94627200	3.68614200
H	-0.57014800	-1.08778200	2.69232800
H	-0.02659600	-2.70951200	2.24292900
C	-3.35299900	0.11136700	-0.55901600
C	-3.82290000	-0.26761900	0.70307000
C	-3.96955800	1.18601800	-1.20294000
C	-4.87605400	0.40919000	1.29573200
H	-3.36469600	-1.09671700	1.22808400
C	-5.02646100	1.86381100	-0.61003700
H	-3.61305500	1.49034200	-2.18053700
C	-5.48329800	1.47752100	0.64209700
H	-5.22709800	0.10331000	2.27364500
H	-5.49162500	2.69403500	-1.12697200
H	-6.30670300	2.00348300	1.10894000
C	-2.23312400	-0.56591200	-1.23004800
H	-1.94265900	-0.14015200	-2.18797500
C	1.08262300	-0.26634600	0.70396900
H	0.05394700	0.09403200	0.78636600
C	-1.56106300	-1.62450100	-0.78274700
H	-1.80497500	-2.09307700	0.16644100

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C	-2.39611100	-2.30327600	-0.13295600
C	-3.63376900	-2.78573800	-0.54505200
C	-4.64099600	-1.92310100	-0.98107900
C	-4.43110600	-0.55164600	-1.01291900
C	-3.19583300	-0.08168100	-0.59732600
C	-2.19184400	-0.93442500	-0.16118000
H	-1.61960600	-2.97927700	0.20440000
H	-3.82191800	-3.85210700	-0.52633900
H	-5.59292300	-2.33087600	-1.29618000
H	-5.20101400	0.13202900	-1.34918200
C	-2.71188100	1.31237800	-0.50520300
O	-3.32349200	2.35309100	-0.70074400
N	-1.40780000	1.21210400	-0.13394000
O	-0.80212200	2.32211600	0.38678500
C	0.39216200	2.68474700	-0.33271000
H	0.18791400	2.66616900	-1.40457700
H	0.56908300	3.71432800	-0.01586600
C	-0.59733700	-0.24241900	1.68874500
C	-1.58572900	0.19039800	2.71307200
H	-2.21874700	-0.64945400	3.03307400
H	-1.08037300	0.56243300	3.60781400
H	-2.24878900	0.97554200	2.34257600
C	0.52546900	-1.13251700	2.08437800
H	0.16924700	-2.13730400	2.35396900
H	1.25334100	-1.24741000	1.27826600
H	1.04000200	-0.74176600	2.96739800
C	3.42204000	0.27943300	-0.60634800
C	3.93711200	0.06675100	0.67736500
C	4.03113200	-0.36935800	-1.68241400
C	5.02347300	-0.77035400	0.87143500
H	3.48885300	0.55851600	1.53196700
C	5.12104800	-1.20775300	-1.48858100
H	3.64122400	-0.21169900	-2.68171000
C	5.62083900	-1.41154700	-0.21015000
H	5.40957700	-0.92377100	1.87171200
H	5.57881300	-1.70086700	-2.33724300
H	6.47058700	-2.06427400	-0.05368700
C	2.26302500	1.14582500	-0.86952500
H	1.97753100	1.22877200	-1.91607400
C	-0.96541700	-0.14477800	0.24371100
H	-0.11322100	-0.43686300	-0.37375800
C	1.54597200	1.81097400	0.03321200
H	1.77643700	1.76000600	1.09385200

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C	-2.53583600	-2.21821600	-0.49507800
C	-3.80997500	-2.74875100	-0.31848100
C	-4.90341700	-1.93263400	-0.02684500
C	-4.74689500	-0.55832900	0.09052700
C	-3.47409000	-0.04090000	-0.08161500
C	-2.37904200	-0.84921800	-0.35901500
H	-1.69709500	-2.86073300	-0.73168800
H	-3.95706900	-3.81767400	-0.41108300
H	-5.88162000	-2.37760000	0.10300900
H	-5.58593500	0.09190500	0.30594300
C	-3.02356300	1.36560200	-0.01014400
O	-3.65083100	2.36227900	0.32475900
N	-1.72343600	1.33648500	-0.39272700
O	-0.94789800	2.42671800	-0.06896800
C	0.31461900	2.38457900	-0.73980700
H	0.16360600	2.14404500	-1.79513100
H	0.67237600	3.41281500	-0.66472800
C	-0.09965500	-0.21971100	0.59558500
C	-0.46846000	0.15750300	1.99462800
H	-1.14700000	-0.59304400	2.42319200
H	0.42113100	0.18197000	2.62777500
H	-0.96305500	1.12761500	2.05700600
C	0.71314000	-1.46058300	0.44117600
H	0.13119700	-2.33603400	0.75693100
H	1.02494300	-1.61860200	-0.59332900
H	1.60348000	-1.42325300	1.07153800
C	3.47030400	0.21573700	-0.41404100
C	3.87555500	0.21063600	0.93021500
C	4.28321100	-0.44487300	-1.34640200
C	5.03792700	-0.43379300	1.31848000
H	3.27650800	0.71577900	1.67807200
C	5.44698500	-1.08913200	-0.95564000
H	3.98723000	-0.44937100	-2.38954100
C	5.83074300	-1.08903900	0.38002200
H	5.33103700	-0.42521600	2.36133400
H	6.05611600	-1.59381400	-1.69571500
H	6.73887500	-1.59160700	0.68840300
C	2.25496200	0.86792300	-0.87354300
H	2.08426700	0.83744300	-1.94698400
C	-1.13096700	-0.00363700	-0.47744500
H	-0.66505700	-0.14904400	-1.45745500
C	1.30476300	1.45519100	-0.09299900
H	1.49808500	1.64693000	0.95773900

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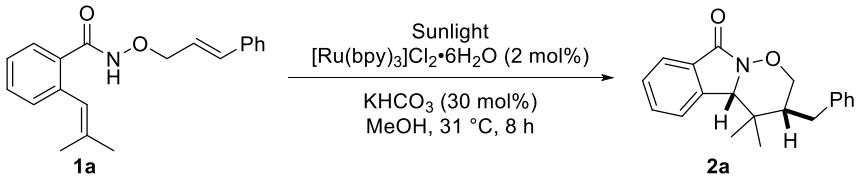
C	-2.57994400	-2.17169300	-0.51576400
C	-3.84943700	-2.68555300	-0.27214600
C	-4.91659200	-1.85563700	0.07325000
C	-4.73762900	-0.48338800	0.17348100
C	-3.46877500	0.01735900	-0.06678600
C	-2.39411200	-0.80448300	-0.38769300
H	-1.76580900	-2.82760000	-0.79582500
H	-4.01395700	-3.75276200	-0.35452300
H	-5.89222000	-2.28816000	0.25459200
H	-5.55675900	0.17891400	0.42533100
C	-3.00001700	1.41808700	-0.02619300
O	-3.58099000	2.42132300	0.36711000
N	-1.73543700	1.37688300	-0.51834100
O	-0.90889600	2.44356200	-0.20561200
C	0.40656600	2.16879500	-0.68813000
H	0.34998000	1.97829900	-1.76342500
H	0.96010300	3.09055300	-0.52313200
C	-0.02657700	-0.08677400	0.45425900
C	-0.55166700	0.22813100	1.85561300
H	-1.35662900	-0.45665700	2.13219500
H	0.25715400	0.10347800	2.57859900
H	-0.91972800	1.25185000	1.94151900
C	0.54500400	-1.50036300	0.44707900
H	-0.17688300	-2.20094000	0.86973000
H	0.80487600	-1.83361000	-0.55983000
H	1.44683200	-1.54104700	1.06089800
C	3.43589600	0.05354700	-0.37549800
C	3.83125000	0.05926300	0.98367000
C	4.38300600	-0.40104200	-1.32603400
C	5.09515400	-0.35811800	1.35679500
H	3.13628200	0.38760700	1.74602500
C	5.64180900	-0.81594000	-0.94221100
H	4.10147100	-0.41700700	-2.37287200
C	6.01066500	-0.79725400	0.40277100
H	5.37320800	-0.34479300	2.40376900
H	6.34594900	-1.15795500	-1.69103000
H	6.99844900	-1.12265000	0.70325200
C	2.15460500	0.46690600	-0.81485600
H	1.94871500	0.37977900	-1.87742100
C	-1.15698700	0.02664200	-0.58860700
H	-0.73608900	-0.14928600	-1.58312700
C	1.05874800	0.98839900	0.04974700

H 1.47641400 1.36342000 0.98518700

6. Sunlight-catalyzed reaction

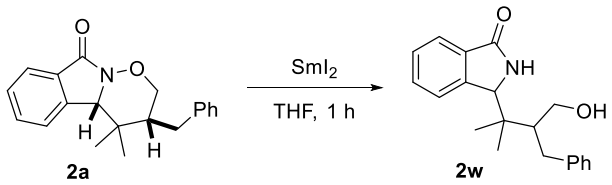
Sunlight-catalyzed reaction:



To a Schlenk tube were added **1a** (61.4 mg, 0.2 mmol, 1.0 equiv), $[Ru(bpy)_3]Cl_2•6H_2O$ (3.0 mg, 0.004 mmol, 2 mol%), $KHCO_3$ (6.0 mg, 0.06 mmol, 30 mol%). The tube was degassed and refilled with N_2 three times, and anhydrous MeOH (3 mL) was added. The mixture was placed in the sunlight and stirred until the substrate was consumed (monitored by TLC), the solvent was removed by rotary evaporation, and the resulting residue was purified directly by flash column chromatography on silica gel (gradient eluent of EtOAc/petroleum ether: 1/3 to 1/2) to give the desired product **2a** (42.0 mg, 68% yield, dr = 5.5:1).

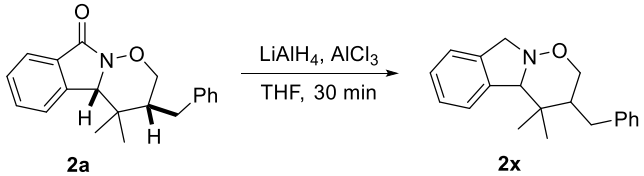
7. Procedure for the follow-up transformations of 2a

Procedure for the transformation of 2a to product 2w[1]:



A round-bottom flask was charged with the mixture of **2a** (61.4 mg, 0.2 mmol, 1.0 equiv). The flask was degassed and refilled with N_2 three times. Then SmI_2 (0.1 M in THF, 8 mL, 0.8 mmol, 4.0 equiv) was added dropwise under N_2. The resulting mixture was stirred at room temperature for 1 h, and then the reaction was quenched by the addition of a saturated aqueous solution of $Na_2S_2O_3$. The organic layer was separated, and the aqueous layer was extracted with EtOAc. The combined organic solvent was dried over Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure. Purification by column chromatography on silica gel (gradient eluent of EtOAc/petroleum ether: 1/1 to 2/1) to give the desired product **2w** as a white solid (61.3 mg, 99 % yield).

Procedure for the transformation of 2a to product 2x[13]:



A round-bottom flask was charged **2a** (61.4 mg, 0.2 mmol, 1.0 equiv). The flask was degassed and refilled with N_2 three times, and anhydrous dry THF (5 mL) and $LiAlH_4$ (0.2 mmol, 1.0 equiv) were

added. After 10 min, $AlCl_3$ (0.4 mmol, 2.0 equiv) was added. The mixture was stirred for 30 min until TLC analysis of the reaction mixture showed complete conversion of the precursor to the corresponding amine. The reaction mixture was hydrolyzed with saturated Na_2CO_3 solution (4 mL), and the aqueous phase was extracted with ether (3 x 5 mL). The combined organic phase was washed with brine and dried with Na_2SO_4. The solvent was removed by rotary evaporation, and the resulting residue was purified directly by flash column chromatography on silica gel (gradient eluent of EtOAc/petroleum ether: 1/15 to 1/10) to give the desired product **2x** (53.1 mg, 91% yield).

8. References

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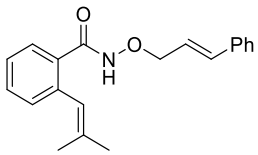
9. Analytical data for substrates

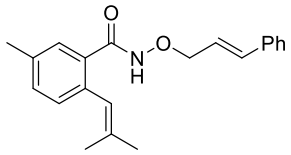
N-(cinnamyloxy)-2-(2-methylprop-1-en-1-yl)benzamide



1a

White solid; R_f = 0.63 (2:1 petroleum ether/ethyl acetate); 2763.0 mg, 90% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (s, 1H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.44 – 7.24 (m, 7H), 7.18 (d, *J* = 7.7 Hz, 1H), 6.69 (d, *J* = 15.9 Hz, 1H), 6.41 (d, *J* = 9.5 Hz, 2H), 4.66 (d, *J* = 6.8 Hz, 2H), 1.84 (d, *J* = 1.4 Hz, 3H), 1.70 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.1, 138.5, 136.5, 136.2, 136.1, 131.9, 130.5, 130.5, 128.8, 128.7, 128.3, 126.8, 126.7, 123.1, 26.2, 19.5. HRMS (ESI) m/z calcd for $C_{20}H_{21}NO_2$ $[M+H]^+$: 308.1645, found: 308.1644. IR (neat): ν_{max} 3178, 2972, 2931, 1648, 1596, 1494, 1471, 1444, 1374, 1302, 1097, 1017, 967, 910, 831, 743, 693, 645 cm^{-1}

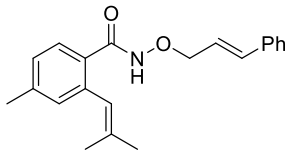
N-(cinnamyloxy)-5-methyl-2-(2-methylprop-1-en-1-yl)benzamide



1b

White solid; R_f = 0.65 (2:1 petroleum ether/ethyl acetate); 453.0 mg, 94% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (s, 1H), 7.53 (s, 1H), 7.44 – 7.38 (m, 2H), 7.36 – 7.26 (m, 3H), 7.20 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.06 (d, *J* = 7.8 Hz, 1H), 6.69 (d, *J* = 15.9 Hz, 1H), 6.38 (d, *J* = 22.5 Hz, 2H), 4.66 (d, *J* = 6.8 Hz, 2H), 2.33 (s, 3H), 1.83 (d, *J* = 1.5 Hz, 3H), 1.68 (d, *J* = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.3, 138.3, 136.6, 136.3, 136.1, 133.5, 131.7, 131.4, 130.5, 129.5, 128.8, 128.4, 126.8, 123.1, 123.1, 26.2, 21.0, 19.5. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1802. IR (neat): ν_{max} 3174, 3024, 2970, 2923, 2856, 1646, 1607, 1493, 1446, 1375, 1304, 1022, 967, 859, 745, 693 cm^{-1}

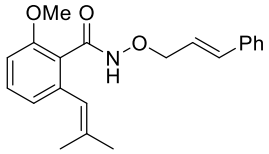
N-(cinnamyloxy)-4-methyl-2-(2-methylprop-1-en-1-yl)benzamide



1c

White solid; R_f = 0.78 (2:1 petroleum ether/ethyl acetate); 193.0 mg, 49% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.67 (s, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.38 (m, 2H), 7.36 – 7.26 (m, 3H), 7.09 (dd, *J* = 8.0, 1.7 Hz, 1H), 6.97 (d, *J* = 1.7 Hz, 1H), 6.68 (d, *J* = 15.9 Hz, 1H), 6.39 (d, *J* = 15.0 Hz, 2H), 4.65 (d, *J* = 6.8 Hz, 2H), 2.34 (s, 3H), 1.83 (d, *J* = 1.5 Hz, 3H), 1.68 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.2, 141.0, 138.5, 136.5, 136.3, 136.2, 131.1, 129.2, 129.0, 128.8, 128.4, 127.6, 126.8, 123.5, 123.2, 26.1, 21.5, 19.5. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1797. IR (neat): ν_{max} 3186, 3026, 2972, 2924, 2858, 1647, 1495, 1447, 1373, 1300, 1156, 1105, 1017, 966, 881, 826, 780, 743, 692, 649, 606 cm^{-1}

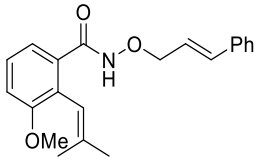
N-(cinnamyloxy)-2-methoxy-6-(2-methylprop-1-en-1-yl)benzamide



1d

Colorless oil; R_f = 0.51 (2:1 petroleum ether/ethyl acetate); 429.0 mg, 85% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.41 (d, *J* = 7.5 Hz, 2H), 7.35 – 7.25 (m, 4H), 6.85 (d, *J* = 7.7 Hz, 1H), 6.81 – 6.57 (m, 2H), 6.40 (dt, *J* = 15.2, 6.8 Hz, 1H), 6.29 (s, 1H), 4.68 (d, *J* = 6.8 Hz, 2H), 3.78 (s, 3H), 1.84 (d, *J* = 1.5 Hz, 3H), 1.80 – 1.69 (m, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.9, 156.8, 139.0, 138.0, 136.2, 136.2, 130.4, 128.7, 128.3, 126.8, 123.2, 122.4, 122.2, 121.8, 108.8, 55.9, 26.6, 19.8. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_3$ $[M+H]^+$: 338.1751, found: 338.1751. IR (neat): ν_{max} 3190, 2967, 2933, 1653, 1594, 1573, 1489, 1467, 1435, 1374, 1271, 1196, 1149, 1089, 1048, 1016, 966, 934, 888, 834, 795, 742, 692, 608 cm^{-1}

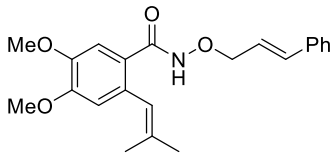
N-(cinnamyloxy)-3-methoxy-2-(2-methylprop-1-en-1-yl)benzamide



1e

Colorless oil; R_f = 0.56 (2:1 petroleum ether/ethyl acetate); 274.0 mg, 54% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (s, 1H), 7.42 – 7.37 (m, 2H), 7.36 – 7.23 (m, 5H), 6.99 – 6.92 (m, 1H), 6.67 (d, *J* = 15.9 Hz, 1H), 6.37 (dt, *J* = 15.1, 6.7 Hz, 1H), 6.16 (p, *J* = 1.4 Hz, 1H), 4.62 (d, *J* = 6.7 Hz, 2H), 3.79 (s, 3H), 1.90 (d, *J* = 1.5 Hz, 3H), 1.54 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.6, 157.2, 140.4, 136.2, 136.1, 133.9, 128.8, 128.3, 128.2, 126.8, 125.4, 123.2, 121.1, 118.1, 113.0, 55.9, 25.9, 19.9. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_3$ $[M+H]^+$: 338.1751, found: 338.1749. IR (neat): ν_{max} 3190, 2965, 2934, 2911, 1648, 1591, 1572, 1493, 1460, 1435, 1374, 1305, 1256, 1203, 1181, 1071, 1051, 1020, 966, 944, 911, 861, 823, 783, 731, 693, 645, 609, 531 cm^{-1}

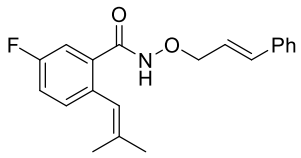
N-(cinnamyloxy)-4,5-dimethoxy-2-(2-methylprop-1-en-1-yl)benzamide



1f

Colorless oil; R_f = 0.33 (2:1 petroleum ether/ethyl acetate); 536.0 mg, 97% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.83 (s, 1H), 7.43 – 7.38 (m, 3H), 7.36 – 7.26 (m, 3H), 6.68 (d, J = 15.9 Hz, 1H), 6.57 (s, 1H), 6.45 – 6.32 (m, 2H), 4.64 (dd, J = 6.8, 1.2 Hz, 2H), 3.88 (s, 3H), 3.87 (s, 3H), 1.81 (d, J = 1.5 Hz, 3H), 1.66 (d, J = 1.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.6, 150.6, 147.7, 138.9, 136.2, 136.1, 129.8, 128.7, 128.4, 126.8, 123.8, 123.6, 123.2, 113.0, 112.0, 77.1, 56.0, 25.9, 19.5. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_4$ $[M+H]^+$: 368.1856, found: 368.1855. IR (neat): ν_{max} 3178, 2963, 2934, 2910, 2849, 1645, 1600, 1569, 1507, 1463, 1443, 1349, 1333, 1263, 1216, 1174, 1102, 1070, 1054, 1022, 988, 967, 911, 876, 831, 803, 769, 731, 693, 646, 608, 576 cm^{-1}

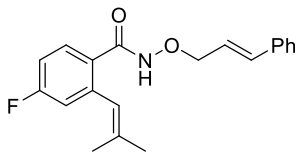
N-(cinnamyloxy)-5-fluoro-2-(2-methylprop-1-en-1-yl)benzamide



1g

White solid; R_f = 0.71 (2:1 petroleum ether/ethyl acetate); 363.0 mg, 74% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.82 (s, 1H), 7.40 (ddd, *J* = 7.9, 4.2, 1.9 Hz, 3H), 7.36 – 7.26 (m, 3H), 7.11 (qd, *J* = 8.5, 5.7 Hz, 2H), 6.68 (d, *J* = 15.9 Hz, 1H), 6.48 – 6.26 (m, 2H), 4.63 (d, *J* = 6.8 Hz, 2H), 1.82 (d, *J* = 1.4 Hz, 3H), 1.66 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.7, 161.2 (d, *J* = 247.4 Hz), 139.1, 136.4, 136.0, 133.7 (d, *J* = 6.6 Hz), 132.5 (d, *J* = 3.6 Hz), 132.4 (d, *J* = 7.3 Hz), 128.8, 128.4, 126.8, 122.9, 122.2, 117.6 (d, *J* = 21.0 Hz), 115.8 (d, *J* = 23.4 Hz), 77.2, 26.0, 19.4. ^{19}F NMR (282 MHz, $CDCl_3$) δ -114.8 (q, *J* = 7.8 Hz). HRMS (ESI) m/z calcd for $C_{20}H_{20}FNO_2$ $[M+H]^+$: 326.1551, found: 326.1541. IR (neat): ν_{max} 3177, 2975, 2930, 2911, 1648, 1604, 1578, 1483, 1447, 1409, 1375, 1304, 1269, 1230, 1203, 1175, 1138, 1090, 1070, 1055, 1020, 964, 921, 862, 845, 815, 800, 744, 692, 675, 608, 569 cm^{-1}

N-(cinnamyloxy)-4-fluoro-2-(2-methylprop-1-en-1-yl)benzamide

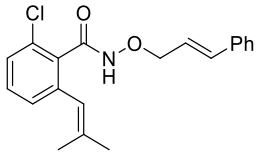


1h

White solid; R_f = 0.71 (2:1 petroleum ether/ethyl acetate); 321.0 mg, 66% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.67 (s, 1H), 7.69 (dd, *J* = 8.6, 5.9 Hz, 1H), 7.44 – 7.37 (m, 2H), 7.37 – 7.27 (m, 3H), 7.00 – 6.84 (m, 2H), 6.68 (d, *J* = 15.9 Hz, 1H), 6.37 (d, *J* = 17.6 Hz, 2H), 4.64 (d, *J* = 6.8 Hz, 2H), 1.83 (d, *J* = 1.4 Hz, 3H), 1.71 (d, *J* = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.3, 163.8 (d, *J* = 251.4 Hz), 139.9, 139.3 (d, *J* = 8.6 Hz), 136.4, 136.1, 131.3 (d, *J* = 9.5 Hz), 128.8, 128.5, 128.2 (d), 126.9, 123.0, 122.4 (d, *J* = 1.7 Hz), 117.3 (d, *J* = 21.7 Hz), 113.9 (d, *J* = 21.7 Hz), 77.3, 26.2, 19.6. ^{19}F NMR (282 MHz, $CDCl_3$)

δ -109.3 (d, J = 9.6 Hz). HRMS (ESI) m/z calcd for $C_{20}H_{20}FNO_2$ $[M+H]^+$: 326.1551, found: 326.1544. IR (neat): ν_{max} 3170, 3026, 2974, 2932, 1645, 1601, 1577, 1477, 1447, 1413, 1375, 1304, 1270, 1233, 1161, 1095, 1054, 1017, 967, 884, 829, 783, 745, 692, 647, 608 cm^{-1}

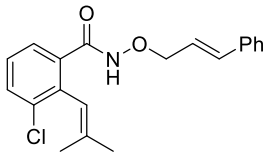
2-chloro-N-(cinnamyloxy)-6-(2-methylprop-1-en-1-yl)benzamide



1i

White solid; R_f = 0.70 (2:1 petroleum ether/ethyl acetate); 284.0 mg, 56% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.21 (s, 1H), 7.46 – 7.37 (m, 2H), 7.36 – 7.27 (m, 4H), 7.26 – 7.19 (m, 2H), 7.14 (dd, J = 7.5, 1.5 Hz, 1H), 6.73 (d, J = 15.9 Hz, 1H), 6.39 (dt, J = 15.9, 6.9 Hz, 1H), 6.26 (d, J = 2.0 Hz, 1H), 4.71 (dd, J = 6.9, 1.1 Hz, 2H), 1.86 (d, J = 1.5 Hz, 3H), 1.75 (d, J = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.7, 139.6, 139.1, 136.8, 136.1, 131.8, 130.4, 128.8, 128.5, 128.3, 127.3, 126.9, 122.8, 121.0, 26.6, 19.8. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1260. IR (neat): ν_{max} 3151, 3024, 2973, 2931, 2855, 1651, 1588, 1558, 1494, 1447, 1375, 1292, 1196, 1175, 1131, 1070, 1017, 965, 910, 897, 833, 781, 743, 719, 692, 674 cm^{-1}

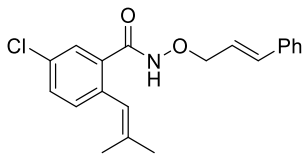
3-chloro-N-(cinnamyloxy)-2-(2-methylprop-1-en-1-yl)benzamide



1j

White solid; R_f = 0.40(2:1 petroleum ether/ethyl acetate); 645.0 mg, 63% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.87 (s, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.47 (dd, J = 8.0, 1.3 Hz, 1H), 7.41 – 7.36 (m, 2H), 7.36 – 7.27 (m, 3H), 7.24 – 7.18 (m, 1H), 6.66 (d, J = 15.9 Hz, 1H), 6.36 (dt, J = 15.0, 6.7 Hz, 1H), 6.17 (t, J = 1.6 Hz, 1H), 4.60 (d, J = 6.9 Hz, 2H), 1.89 (d, J = 1.5 Hz, 3H), 1.50 (d, J = 1.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.4, 140.9, 136.0, 136.0, 135.0, 134.7, 131.7, 128.7, 128.3, 128.1, 127.3, 126.8, 123.0, 120.0, 77.6, 77.2, 76.7, 25.4, 19.7. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1259. IR (neat): ν_{max} 3182, 2974, 2934, 1652, 1583, 1494, 1441, 1376, 1300, 1127, 1025, 967, 910, 815, 794, 735, 693, 647 cm^{-1}

5-chloro-N-(cinnamyloxy)-2-(2-methylprop-1-en-1-yl)benzamide

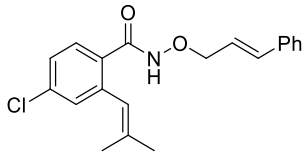


1k

White solid; R_f = 0.76 (2:1 petroleum ether/ethyl acetate); 220.0 mg, 43% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.79 (s, 1H), 7.70 – 7.56 (m, 1H), 7.43 – 7.37 (m, 2H), 7.37 – 7.26 (m, 4H), 7.10 (d, J = 8.3 Hz, 1H), 6.68 (d, J = 15.9 Hz, 1H), 6.35 (d, J = 25.6 Hz, 2H), 4.63 (d, J = 6.8 Hz, 2H), 1.82 (d, J = 1.5 Hz, 3H), 1.67 (d, J = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.7, 139.5, 136.5, 136.0, 135.0, 133.4,

132.6, 131.9, 130.6, 128.8, 128.5, 126.8, 122.9, 122.0, 26.2, 19.5. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1259. IR (neat): ν_{max} 3173, 2973, 2932, 1648, 1589, 1494, 1469, 1446, 1375, 1295, 1202, 1159, 1110, 1069, 1017, 965, 918, 859, 808, 740, 692, 664, 594, 532 cm^{-1}

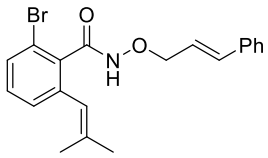
4-chloro-N-(cinnamyloxy)-2-(2-methylprop-1-en-1-yl)benzamide



1l

White solid; R_f = 0.75 (2:1 petroleum ether/ethyl acetate); 236.0 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.74 (s, 1H), 7.61 (d, *J* = 8.3 Hz, 1H), 7.43 – 7.37 (m, 2H), 7.36 – 7.26 (m, 3H), 7.23 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.16 (d, *J* = 2.1 Hz, 1H), 6.67 (d, *J* = 15.9 Hz, 1H), 6.47 – 6.27 (m, 2H), 4.63 (d, *J* = 6.8 Hz, 2H), 1.82 (d, *J* = 1.5 Hz, 3H), 1.70 (d, *J* = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.2, 140.1, 138.3, 136.7, 136.5, 136.0, 130.4, 128.8, 128.5, 126.9, 126.9, 123.0, 122.1, 26.2, 19.6. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1260. IR (neat): ν_{max} 3177, 2973, 2933, 1645, 1587, 1555, 1494, 1446, 1374, 1299, 1210, 1156, 1087, 1016, 965, 913, 892, 825, 742, 692, 584, 537, 505 cm^{-1}

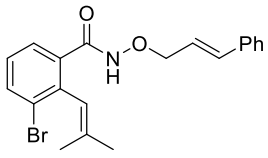
2-bromo-N-(cinnamyloxy)-6-(2-methylprop-1-en-1-yl)benzamide



1m

White solid; R_f = 0.74 (2:1 petroleum ether/ethyl acetate); 217.0 mg, 37% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.42 – 7.35 (m, 3H), 7.34 – 7.26 (m, 3H), 7.26 – 7.20 (m, 1H), 7.20 – 7.09 (m, 2H), 6.71 (d, *J* = 15.9 Hz, 1H), 6.38 (dt, *J* = 15.9, 6.8 Hz, 1H), 6.25 (p, *J* = 1.4 Hz, 1H), 4.68 (dd, *J* = 6.8, 1.2 Hz, 2H), 1.84 (d, *J* = 1.5 Hz, 3H), 1.73 (d, *J* = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.4, 139.5, 139.2, 136.5, 136.1, 130.5, 130.3, 128.7, 128.7, 128.3, 126.8, 122.9, 121.1, 120.6, 26.5, 19.7. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0750. IR (neat): ν_{max} 3154, 2975, 2931, 1654, 1584, 1552, 1494, 1445, 1376, 1282, 1122, 1018, 966, 909, 776, 735, 695 cm^{-1}

3-bromo-N-(cinnamyloxy)-2-(2-methylprop-1-en-1-yl)benzamide

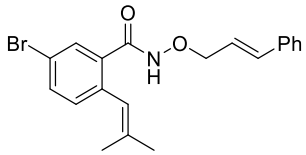


1n

White solid; R_f = 0.73 (2:1 petroleum ether/ethyl acetate); 452.0 mg, 78% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.67 (s, 1H), 7.73 – 7.58 (m, 2H), 7.40 (d, *J* = 6.7 Hz, 2H), 7.36 – 7.27 (m, 3H), 7.16 (t, *J* = 7.9 Hz, 1H), 6.68 (d, *J* = 15.9 Hz, 1H), 6.37 (dt, *J* = 15.9, 7.1 Hz, 1H), 6.17 (s, 1H), 4.61 (d, *J* = 6.9 Hz, 2H), 1.90 (d, *J* = 1.5 Hz, 3H), 1.51 (d, *J* = 1.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.5, 140.8, 136.8,

136.2, 136.1, 135.1, 134.8, 128.8, 128.5, 128.1, 126.8, 123.0, 122.4, 77.3, 25.4, 19.7. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0749. IR (neat): ν_{max} 3172, 2973, 2933, 1646, 1494, 1441, 1373, 1299, 1206, 1159, 1112, 1021, 965, 910, 792, 731, 692, 646 cm^{-1}

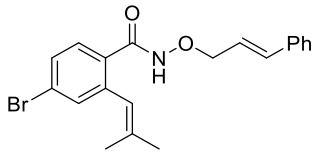
5-bromo-N-(cinnamyloxy)-2-(2-methylprop-1-en-1-yl)benzamide



1o

White solid; R_f = 0.46 (4:1 petroleum ether/ethyl acetate); 204.0 mg, 36% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (s, 1H), 7.81 (d, *J* = 2.1 Hz, 1H), 7.50 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.43 – 7.37 (m, 2H), 7.37 – 7.27 (m, 3H), 7.05 (d, *J* = 8.3 Hz, 1H), 6.69 (d, *J* = 15.9 Hz, 1H), 6.45 – 6.26 (m, 2H), 4.64 (d, *J* = 6.8 Hz, 2H), 1.82 (d, *J* = 1.4 Hz, 3H), 1.68 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.6, 139.4, 136.5, 136.0, 135.5, 133.7, 133.5, 132.1, 131.6, 128.8, 128.4, 126.8, 122.9, 122.1, 120.4, 26.2, 19.5. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0748. IR (neat): ν_{max} 3154, 2970, 2932, 1648, 1581, 1554, 1494, 1467, 1448, 1377, 1295, 1203, 1159, 1104, 1053, 1021, 966, 909, 859, 806, 732, 692, 647, 522 cm^{-1}

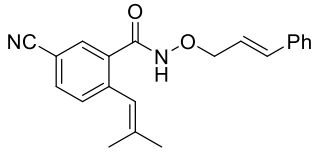
4-bromo-N-(cinnamyloxy)-2-(2-methylprop-1-en-1-yl)benzamide



1p

White solid; R_f = 0.37 (4:1 petroleum ether/ethyl acetate); 188.0 mg, 32% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.81 (s, 1H), 7.51 (d, *J* = 8.3 Hz, 1H), 7.42 – 7.24 (m, 7H), 6.67 (d, *J* = 15.8 Hz, 1H), 6.34 (d, *J* = 27.8 Hz, 2H), 4.62 (d, *J* = 6.8 Hz, 2H), 1.82 (d, *J* = 1.5 Hz, 3H), 1.69 (d, *J* = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.2, 139.7, 138.5, 136.2, 136.0, 133.1, 130.9, 130.2, 129.6, 128.7, 128.4, 126.8, 124.9, 123.0, 121.9, 26.2, 19.5. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0746. IR (neat): ν_{max} 3175, 2972, 2932, 1651, 1582, 1552, 1495, 1447, 1377, 1299, 1208, 1079, 1018, 967, 906, 826, 734, 693 cm^{-1}

N-(cinnamyloxy)-5-cyano-2-(2-methylprop-1-en-1-yl)benzamide

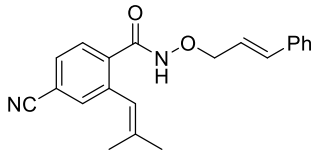


1q

White solid; R_f = 0.67 (2:1 petroleum ether/ethyl acetate); 453.0 mg, 91% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.83 (s, 1H), 7.86 (s, 1H), 7.62 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.40 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.36 – 7.26 (m, 4H), 6.69 (d, *J* = 15.9 Hz, 1H), 6.39 (d, *J* = 10.2 Hz, 2H), 4.65 (d, *J* = 6.9 Hz, 2H), 1.85 (d, *J* = 1.4 Hz, 3H), 1.72 (d, *J* = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.1, 141.7, 141.4, 136.7, 135.9, 133.6, 133.3, 132.5, 131.3, 128.8, 128.6, 126.8, 122.7, 121.7, 118.1, 110.4, 26.6, 19.8. HRMS (ESI) m/z

calcd for $C_{21}H_{20}N_2O_2$ [M+H]$^+$: 333.1598, found: 333.1599. IR (neat): ν_{max} 3185, 2977, 2935, 2229, 1651, 1599, 1482, 1447, 1376, 1303, 1203, 1102, 1055, 1019, 967, 909, 864, 817, 731, 692, 647, 612, 558 cm^{-1}

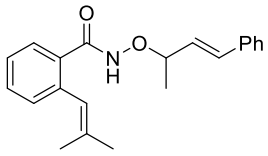
N-(cinnamyloxy)-4-cyano-2-(2-methylprop-1-en-1-yl)benzamide



1r

White solid; R_f = 0.55 (2:1 petroleum ether/ethyl acetate); 327.0 mg, 64% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.62 (s, 1H), 7.74 (d, J = 8.0 Hz, 1H), 7.56 – 7.45 (m, 2H), 7.45 – 7.27 (m, 5H), 6.69 (d, J = 15.9 Hz, 1H), 6.49 – 6.22 (m, 2H), 4.66 (d, J = 6.9 Hz, 2H), 1.85 (d, J = 1.4 Hz, 3H), 1.71 (d, J = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.3, 141.2, 137.7, 136.7, 136.2, 135.8, 134.0, 123.0, 129.5, 128.8, 128.6, 126.8, 122.7, 121.0, 114.2, 77.4, 26.3, 19.6. HRMS (ESI) m/z calcd for $C_{21}H_{20}N_2O_2$ [M+H]$^+$: 333.1598, found: 333.1598. IR (neat): ν_{max} 3179, 2975, 2934, 2231, 1652, 1599, 1554, 1495, 1448, 1376, 1295, 1206, 1185, 1104, 1057, 1016, 967, 909, 835, 731, 693, 648, 610, 560 cm^{-1}

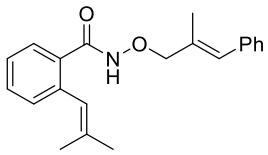
(E)-2-(2-methylprop-1-en-1-yl)-N-((4-phenylbut-3-en-2-yl)oxy)benzamide



1s

White solid; R_f = 0.61 (2:1 petroleum ether/ethyl acetate); 206.0 mg, 43% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.65 (d, J = 7.7 Hz, 1H), 7.40 – 7.21 (m, 7H), 7.16 (d, J = 7.7 Hz, 1H), 6.61 (d, J = 15.9 Hz, 1H), 6.38 (s, 1H), 6.23 (dd, J = 16.0, 8.2 Hz, 1H), 4.72 (d, J = 10.4 Hz, 1H), 1.80 (d, J = 1.5 Hz, 3H), 1.67 (d, J = 1.4 Hz, 3H), 1.49 (d, J = 6.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.8, 138.5, 136.5, 136.0, 134.3, 130.6, 128.8, 128.3, 126.8, 123.2, 83.0, 26.2, 19.5, 19.5. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ [M+H]$^+$: 322.1802, found: 322.1802. IR (neat): ν_{max} 3178, 2976, 2930, 1644, 1595, 1494, 1442, 1374, 1301, 1151, 1045, 1015, 966, 903, 821, 786, 746, 693, 634, 515 cm^{-1}

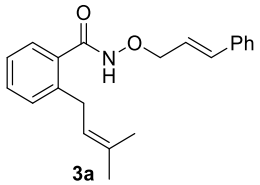
(E)-N-((2-methyl-3-phenylallyl)oxy)-2-(2-methylprop-1-en-1-yl)benzamide



1t

Colorless oil; R_f = 0.59 (2:1 petroleum ether/ethyl acetate); 780.0 mg, 97% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.66 (s, 1H), 7.69 (d, J = 7.7 Hz, 1H), 7.43 – 7.15 (m, 8H), 6.55 (s, 1H), 6.41 (s, 1H), 4.55 (s, 2H), 2.02 (s, 3H), 1.84 (s, 3H), 1.70 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.0, 138.6, 136.9, 136.5, 132.9, 130.9, 130.6, 130.6, 129.0, 128.9, 128.3, 127.1, 126.8, 123.2, 83.0, 26.3, 19.5, 15.9. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ [M+H]$^+$: 322.1802, found: 322.1797. IR (neat): ν_{max} 3175, 2968, 2911, 1645, 1596, 1491, 1442, 1376, 1302, 1015, 982, 918, 894, 855, 746, 699, 518 cm^{-1}

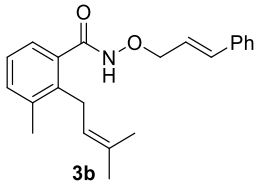
N-(cinnamyloxy)-2-(3-methylbut-2-en-1-yl)benzamide



3a

White solid; R_f = 0.65 (2:1 petroleum ether/ethyl acetate); 1648.0 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.44 – 7.14 (m, 9H), 6.70 (d, *J* = 15.9 Hz, 1H), 6.40 (dt, *J* = 15.6, 6.9 Hz, 1H), 5.23 (ddt, *J* = 8.7, 7.1, 1.5 Hz, 1H), 4.68 (d, *J* = 6.9 Hz, 2H), 3.49 (d, *J* = 7.2 Hz, 2H), 1.77 – 1.64 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.9, 140.5, 136.5, 136.0, 133.4, 132.7, 130.8, 130.1, 128.7, 128.4, 127.6, 126.9, 126.0, 123.0, 122.8, 31.8, 25.9, 18.1. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1802. IR (neat): ν_{max} 3153, 3024, 2965, 2925, 2855, 1644, 1598, 1496, 1447, 1374, 1302, 1280, 1017, 967, 928, 892, 745, 693, 668 cm^{-1}

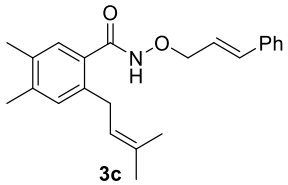
N-(cinnamyloxy)-3-methyl-2-(3-methylbut-2-en-1-yl)benzamide



3b

White solid; R_f = 0.67 (2:1 petroleum ether/ethyl acetate); 215.0 mg, 65% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.47 – 7.03 (m, 9H), 6.70 (d, *J* = 15.8 Hz, 1H), 6.39 (dt, *J* = 16.0, 6.7 Hz, 1H), 5.04 (s, 1H), 4.67 (d, *J* = 7.0 Hz, 2H), 3.43 (d, *J* = 6.4 Hz, 2H), 2.28 (s, 3H), 1.69 (d, *J* = 15.7 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.5, 138.3, 138.0, 136.4, 136.1, 133.6, 132.8, 132.6, 128.8, 128.4, 126.9, 126.1, 125.5, 123.1, 122.5, 29.5, 25.8, 19.8, 18.2. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_2$ $[M+H]^+$: 336.1958, found: 336.1960. IR (neat): ν_{max} 3171, 2965, 2918, 2855, 1644, 1589, 1495, 1448, 1375, 1304, 1100, 1041, 1001, 966, 908, 826, 782, 739, 693, 645 cm^{-1}

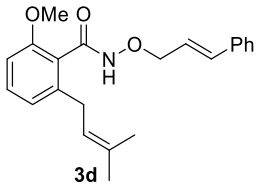
N-(cinnamyloxy)-4,5-dimethyl-2-(3-methylbut-2-en-1-yl)benzamide



3c

White solid; R_f = 0 27 (4:1 petroleum ether/ethyl acetate); 205.0 mg, 39% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.46 – 7.37 (m, 2H), 7.36 – 7.26 (m, 3H), 7.11 (s, 1H), 6.98 (s, 1H), 6.69 (d, *J* = 15.9 Hz, 1H), 6.38 (dt, *J* = 15.1, 7.0 Hz, 1H), 5.22 (ddt, *J* = 8.6, 7.2, 1.4 Hz, 1H), 4.66 (d, *J* = 6.8 Hz, 2H), 3.43 (d, *J* = 7.1 Hz, 2H), 2.23 (s, 3H), 2.18 (s, 3H), 1.70 (d, *J* = 1.4 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.7, 137.9, 136.5, 136.1, 134.3, 133.0, 131.5, 130.0, 128.9, 128.8, 128.4, 126.9, 123.4, 123.0, 31.6, 25.9, 19.9, 19.2, 18.1. HRMS (ESI) m/z calcd for $C_{23}H_{27}NO_2$ $[M+H]^+$: 350.2115, found: 350.2113. IR (neat): ν_{max} 3185, 2970, 2920, 2857, 1642, 1494, 1448, 1373, 1305, 1274, 1238, 1205, 1142, 1100, 1068, 965, 910, 882, 844, 798, 733, 692, 645, 606, 581 cm^{-1}

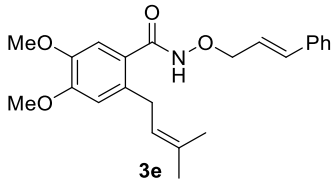
N-(cinnamyloxy)-2-methoxy-6-(3-methylbut-2-en-1-yl)benzamide



3d

White solid; R_f = 0.41 (2:1 petroleum ether/ethyl acetate); 336.0 mg, 34% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.40 (d, *J* = 7.5 Hz, 2H), 7.29 (dt, *J* = 18.7, 7.6 Hz, 4H), 6.82 (d, *J* = 7.8 Hz, 1H), 6.77 – 6.61 (m, 2H), 6.41 (dt, *J* = 15.2, 6.9 Hz, 1H), 5.29 – 5.15 (m, 1H), 4.68 (d, *J* = 6.7 Hz, 2H), 3.76 (s, 3H), 3.37 (d, *J* = 7.2 Hz, 2H), 1.68 (d, *J* = 11.9 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.3, 156.7, 142.3, 136.3, 136.1, 133.1, 131.0, 128.7, 128.3, 126.9, 123.2, 122.5, 121.8, 108.4, 55.8, 31.5, 25.9, 18.0. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_3$ $[M+H]^+$: 352.1907, found: 352.1917. IR (neat): ν_{max} 3179, 2965, 2925, 2855, 1649, 1596, 1581, 1494, 1468, 1450, 1436, 1374, 1263, 1151, 1104, 1069, 1016, 966, 938, 908, 889, 845, 790, 743, 693, 647, 525 cm^{-1}

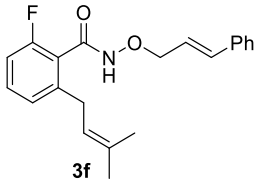
N-(cinnamyloxy)-4,5-dimethoxy-2-(3-methylbut-2-en-1-yl)benzamide



3e

White solid; R_f = 0.21 (2:1 petroleum ether/ethyl acetate); 153.0 mg, 40% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.30 (dt, *J* = 23.5, 7.8 Hz, 5H), 6.84 (s, 1H), 6.74 – 6.54 (m, 2H), 6.36 (dt, *J* = 15.1, 7.0 Hz, 1H), 5.32 – 5.02 (m, 1H), 4.62 (d, *J* = 6.8 Hz, 2H), 3.82 (d, *J* = 2.0 Hz, 3H), 3.69 (s, 3H), 3.39 (d, *J* = 6.9 Hz, 2H), 1.67 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.7, 146.9, 136.5, 136.0, 133.5, 133.5, 128.7, 128.4, 126.8, 124.4, 123.3, 123.0, 112.7, 111.0, 56.0, 31.8, 25.8, 18.1. HRMS (ESI) m/z calcd for $C_{23}H_{27}NO_4$ $[M+H]^+$: 382.2013, found: 382.2018. IR (neat): ν_{max} 3171, 2962, 2933, 2850, 1641, 1603, 1579, 1511, 1463, 1448, 1345, 1303, 1261, 1208, 1187, 1086, 1019, 966, 913, 864, 805, 781, 731, 692, 646, 603 cm^{-1}

N-(cinnamyloxy)-4,5-dimethoxy-2-(3-methylbut-2-en-1-yl)benzamide

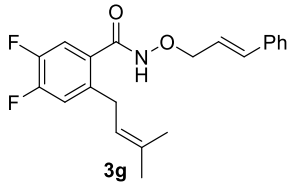


3f

White solid; R_f = 0.37 (4:1 petroleum ether/ethyl acetate); 231.0 mg, 35% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.48 – 7.37 (m, 2H), 7.37 – 7.27 (m, 4H), 7.02 (d, *J* = 7.7 Hz, 1H), 6.91 (t, *J* = 8.8 Hz, 1H), 6.73 (d, *J* = 15.9 Hz, 1H), 6.39 (dt, *J* = 15.8, 6.9 Hz, 1H), 5.21 (td, *J* = 6.9, 3.4 Hz, 1H), 4.82 – 4.55 (m, 2H), 3.42 (d, *J* = 7.3 Hz, 2H), 1.71 (d, *J* = 1.5 Hz, 3H), 1.67 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.0, 159.6 (d, *J* = 247.4 Hz), 143.3, 137.0, 136.1, 133.9, 131.5 (d, *J* = 8.8 Hz), 128.8, 128.4, 126.9, 125.3 (d, *J* = 3.0 Hz), 122.6, 121.9, 121.2 (d, *J* = 17.3 Hz), 113.2 (d, *J* = 21.9 Hz), 31.5, 31.5, 25.9, 18.0. ^{19}F NMR (282 MHz, $CDCl_3$) δ -115.7 (dd, *J* = 9.3, 5.8 Hz). HRMS (ESI) m/z calcd for $C_{21}H_{22}FNO_2$ $[M+H]^+$: 340.1707, found: 340.1713. IR (neat): ν_{max} 3152, 2967, 2919, 2856, 1651, 1614,

1577, 1495, 1459, 1375, 1297, 1247, 1148, 1104, 1069, 1019, 967, 927, 892, 847, 790, 769, 745, 693, 639 cm^{-1}

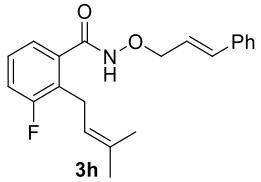
N-(cinnamyloxy)-4,5-difluoro-2-(3-methylbut-2-en-1-yl)benzamide



3g

White solid; R_f = 0.57 (2:1 petroleum ether/ethyl acetate); 251.0 mg, 36% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.45 (s, 1H), 7.44 – 7.27 (m, 5H), 7.16 (dd, *J* = 10.1, 7.8 Hz, 1H), 7.02 (dd, *J* = 11.4, 7.7 Hz, 1H), 6.69 (d, *J* = 15.9 Hz, 1H), 6.49 – 6.23 (m, 1H), 5.16 (tdt, *J* = 7.2, 2.9, 1.4 Hz, 1H), 4.65 (d, *J* = 6.6 Hz, 2H), 3.41 (d, *J* = 7.2 Hz, 2H), 1.72 (d, *J* = 1.4 Hz, 3H), 1.66 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.9, 153.1 (d, *J* = 12.4 Hz), 149.8 (d, *J* = 4.9 Hz), 149.7 (d, *J* = 5.5 Hz), 146.4 (d, *J* = 13.0 Hz), 138.3 (q), 136.8, 135.9, 134.8, 128.8, 128.6, 126.9, 122.7, 121.6, 118.9 (d, *J* = 17.6 Hz), 117.0 (d, *J* = 18.3 Hz), 77.6, 77.2, 76.7, 31.1, 25.8, 18.0. ^{19}F NMR (282 MHz, $CDCl_3$) δ -133.7 (d, *J* = 19.5 Hz), -138.1 – -145.8 (m). HRMS (ESI) m/z calcd for $C_{21}H_{21}F_2NO_2$ $[M+H]^+$: 358.1613, found: 358.1610. IR (neat): ν_{max} 3167, 3028, 2970, 2927, 2856, 1647, 1604, 1498, 1449, 1407, 1375, 1357, 1320, 1188, 1155, 1074, 1010, 967, 933, 883, 831, 808, 781, 745, 692, 622 cm^{-1}

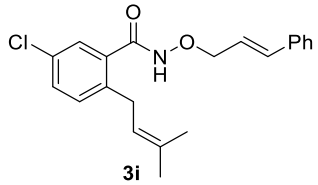
N-(cinnamyloxy)-3-fluoro-2-(3-methylbut-2-en-1-yl)benzamide



3h

White solid; R_f = 0.72 (2:1 petroleum ether/ethyl acetate); 504.0 mg, 74% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.35 (dt, *J* = 24.4, 8.2 Hz, 5H), 7.22 – 7.07 (m, 3H), 6.70 (d, *J* = 15.8 Hz, 1H), 6.47 – 6.32 (m, 1H), 5.23 – 5.10 (m, 1H), 4.68 (d, *J* = 6.8 Hz, 2H), 3.49 (d, *J* = 7.0 Hz, 2H), 1.74 (s, 3H), 1.67 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.6, 161.2 (d, *J* = 246.9 Hz), 136.4, 136.0, 134.8 (d, *J* = 4.2 Hz), 133.2, 128.7, 128.4, 127.5 (d, *J* = 8.7 Hz), 126.8, 123.4 (d, *J* = 3.6 Hz), 122.9, 121.8, 117.7 (d, *J* = 22.9 Hz), 25.8, 25.2, 17.9. ^{19}F NMR (282 MHz, $CDCl_3$) δ -115.2 (d, *J* = 8.7 Hz). HRMS (ESI) m/z calcd for $C_{21}H_{22}FNO_2$ $[M+H]^+$: 340.1707, found: 340.1710. IR (neat): ν_{max} 3167, 3028, 2970, 2927, 2856, 1647, 1604, 1498, 1449, 1407, 1375, 1357, 1320, 1188, 1155, 1074, 1010, 967, 933, 883, 831, 808, 781, 745, 692, 622 cm^{-1}

5-chloro-N-(cinnamyloxy)-2-(3-methylbut-2-en-1-yl)benzamide

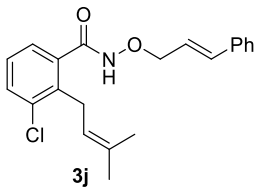


3i

White solid; R_f = 0.62 (2:1 petroleum ether/ethyl acetate); 396.0 mg, 58% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.74 (s, 1H), 7.39 (d, *J* = 7.5 Hz, 2H), 7.35 – 7.21 (m, 5H), 7.13 (d, *J* = 8.2 Hz, 1H), 6.67 (d, *J*

= 15.8 Hz, 1H), 6.36 (dt, *J* = 15.0, 6.9 Hz, 1H), 5.15 (t, *J* = 7.4 Hz, 1H), 4.63 (d, *J* = 6.8 Hz, 2H), 3.39 (d, *J* = 7.1 Hz, 2H), 1.69 (s, 3H), 1.64 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.5, 139.0, 136.7, 135.9, 134.1, 134.0, 131.6, 131.5, 130.7, 128.8, 128.5, 127.5, 126.9, 122.8, 122.2, 31.2, 25.9, 18.0. HRMS (ESI) m/z calcd for $C_{21}H_{22}ClNO_2$ $[M+H]^+$: 356.1412, found: 356.1411. IR (neat): ν_{max} 3153, 2967, 2926, 1645, 1593, 1565, 1495, 1447, 1375, 1303, 1160, 1110, 1018, 966, 933, 856, 820, 744, 692, 651 cm^{-1}

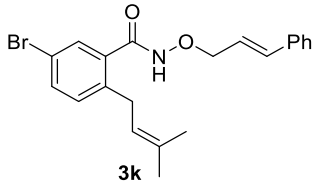
3-chloro-N-(cinnamyloxy)-2-(3-methylbut-2-en-1-yl)benzamide



3j

White solid; R_f = 0.52 (2:1 petroleum ether/ethyl acetate); 205.0 mg, 58% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.42 (td, *J* = 8.3, 1.6 Hz, 3H), 7.36 – 7.27 (m, 3H), 7.23 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.14 (t, *J* = 7.7 Hz, 1H), 6.70 (d, *J* = 15.8 Hz, 1H), 6.38 (dt, *J* = 15.2, 6.8 Hz, 1H), 5.16 – 5.06 (m, 1H), 4.67 (d, *J* = 6.8 Hz, 2H), 3.59 (d, *J* = 6.6 Hz, 2H), 1.74 (d, *J* = 1.3 Hz, 3H), 1.68 (d, *J* = 1.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.0, 137.8, 136.6, 136.0, 135.6, 133.7, 131.9, 128.8, 128.5, 127.3, 126.9, 126.5, 122.8, 121.3, 30.0, 25.9, 18.3. HRMS (ESI) m/z calcd for $C_{21}H_{22}ClNO_2$ $[M+H]^+$: 356.1412, found: 356.1418. IR (neat): ν_{max} 3158, 2966, 2926, 2856, 1644, 1588, 1495, 1436, 1374, 1279, 1206, 1158, 1119, 1100, 1070, 1019, 966, 944, 922, 858, 832, 799, 779, 734, 692, 549 cm^{-1}

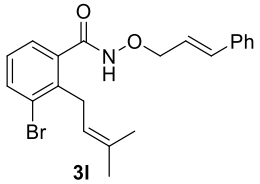
5-bromo-N-(cinnamyloxy)-2-(3-methylbut-2-en-1-yl)benzamide



3k

White solid; R_f = 0.71 (2:1 petroleum ether/ethyl acetate); 223.0 mg, 58% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.48 – 7.38 (m, 4H), 7.37 – 7.27 (m, 3H), 7.13 – 7.07 (m, 1H), 6.71 (d, *J* = 15.9 Hz, 1H), 6.39 (dd, *J* = 15.2, 8.0 Hz, 1H), 5.22 – 5.13 (m, 1H), 4.67 (d, *J* = 6.9 Hz, 2H), 3.41 (d, *J* = 7.1 Hz, 2H), 1.72 – 1.65 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.4, 139.6, 136.8, 135.9, 134.4, 134.1, 133.7, 131.8, 130.4, 128.8, 128.5, 126.9, 122.7, 122.0, 119.4, 31.3, 25.9, 18.0. HRMS (ESI) m/z calcd for $C_{21}H_{22}BrNO_2$ $[M+H]^+$: 400.0907, found: 400.0892. IR (neat): ν_{max} 3149, 2965, 2922, 2854, 1646, 1588, 1562, 1495, 1476, 1447, 1375, 1302, 1159, 1100, 1018, 967, 929, 909, 856, 818, 744, 692 cm^{-1}

3-bromo-N-(cinnamyloxy)-2-(3-methylbut-2-en-1-yl)benzamide

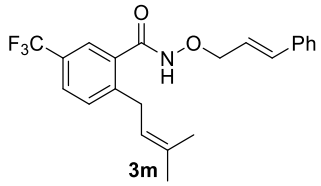


3l

White solid; R_f = 0.61 (2:1 petroleum ether/ethyl acetate); 231.0 mg, 60% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.63 (d, *J* = 8.1 Hz, 1H), 7.35 (dt, *J* = 22.3, 7.2 Hz, 6H), 7.06 (t, *J* = 7.8 Hz, 1H), 6.70 (d, *J* = 15.9 Hz, 1H), 6.38 (dt, *J* = 15.7, 6.9 Hz, 1H), 5.11 (d, *J* = 7.7 Hz, 1H), 4.66 (d, *J* = 6.8 Hz,

2H), 3.61 (d, J = 6.5 Hz, 2H), 1.72 (d, J = 18.7 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.0, 139.4, 136.5, 136.0, 135.3, 135.2, 133.7, 128.8, 128.5, 127.5, 127.1, 126.9, 126.2, 122.9, 121.4, 32.6, 25.9, 18.4. HRMS (ESI) m/z calcd for $C_{21}H_{22}BrNO_2$ $[M+H]^+$: 400.0907, found: 400.0892. IR (neat): ν_{max} 3151, 2924, 2854, 1644, 1586, 1495, 1434, 1374, 1301, 1105, 1017, 966, 937, 778, 742, 707, 693 cm^{-1}

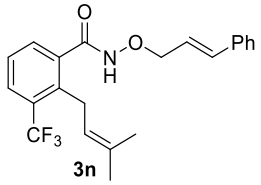
N-(cinnamyloxy)-2-(3-methylbut-2-en-1-yl)-5-(trifluoromethyl)benzamide



3m

White solid; R_f = 0.78 (2:1 petroleum ether/ethyl acetate); 368.0 mg, 36% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.51 (s, 1H), 7.59 (dd, J = 10.3, 2.5 Hz, 2H), 7.45 – 7.27 (m, 6H), 6.71 (d, J = 15.9 Hz, 1H), 6.40 (dd, J = 15.5, 7.8 Hz, 1H), 5.19 (tdd, J = 7.3, 3.0, 1.5 Hz, 1H), 4.83 – 4.50 (m, 2H), 3.51 (d, J = 7.2 Hz, 2H), 1.72 (d, J = 1.4 Hz, 3H), 1.68 (d, J = 1.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.6, 144.9, 137.0, 135.9, 134.7, 133.4, 130.7, 128.8, 128.6, 127.4, 126.9, 124.6, 122.6, 121.6, 31.8, 25.9, 18.1. ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.5. HRMS (ESI) m/z calcd for $C_{22}H_{22}F_3NO_2$ $[M+H]^+$: 390.1675, found: 390.1675. IR (neat): ν_{max} 3151, 2972, 2926, 1650, 1618, 1581, 1494, 1449, 1414, 1335, 1305, 1272, 1154, 1125, 1077, 1021, 967, 935, 906, 859, 833, 745, 692, 632 cm^{-1}

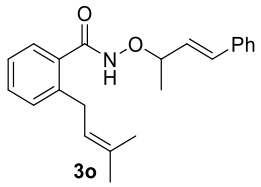
N-(cinnamyloxy)-2-(3-methylbut-2-en-1-yl)-3-(trifluoromethyl)benzamide



3n

White solid; R_f = 0.47 (2:1 petroleum ether/ethyl acetate); 362.0 mg, 46% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.43 (s, 1H), 7.71 (dd, J = 8.0, 1.4 Hz, 1H), 7.47 (dd, J = 7.6, 1.4 Hz, 1H), 7.41 (d, J = 6.9 Hz, 2H), 7.32 (dt, J = 9.9, 6.7 Hz, 4H), 6.70 (d, J = 15.9 Hz, 1H), 6.38 (dt, J = 15.9, 6.8 Hz, 1H), 5.11 – 5.01 (m, 1H), 4.64 (d, J = 6.8 Hz, 2H), 3.67 (d, J = 6.3 Hz, 2H), 1.73 (s, 3H), 1.68 (d, J = 1.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.1, 139.4, 136.5, 136.1, 136.0, 133.7, 131.7, 128.8, 128.5, 128.3, 126.9, 126.4, 122.8, 122.6, 28.7, 25.9, 18.2. ^{19}F NMR (282 MHz, $CDCl_3$) δ -59.3. HRMS (ESI) m/z calcd for $C_{22}H_{22}F_3NO_2$ $[M+H]^+$: 390.1675, found: 390.1677. IR (neat): ν_{max} 3162, 2968, 2930, 1647, 1591, 1495, 1448, 1375, 1321, 1282, 1246, 1177, 1151, 1120, 1099, 1020, 965, 856, 813, 784, 742, 689, 579, 545 cm^{-1}

(E)-2-(3-methylbut-2-en-1-yl)-N-((4-phenylbut-3-en-2-yl)oxy)benzamide

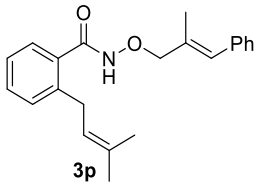


3o

White solid; R_f = 0.58 (2:1 petroleum ether/ethyl acetate); 151.0 mg, 31% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.47 – 7.09 (m, 9H), 6.63 (d, J = 15.9 Hz, 1H), 6.24 (dd, J = 15.9, 8.4 Hz, 1H),

5.22 (t, J = 7.4 Hz, 1H), 4.75 (q, J = 7.0 Hz, 1H), 3.46 (d, J = 7.2 Hz, 2H), 1.68 (d, J = 9.0 Hz, 6H), 1.51 (d, J = 6.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.7, 140.5, 136.0, 134.5, 133.4, 132.9, 130.7, 130.0, 128.8, 128.3, 127.5, 126.8, 126.0, 122.8, 83.2, 31.7, 25.9, 19.5, 18.0. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_2$ $[M+H]^+$: 336.1958, found: 336.1956. IR (neat): ν_{max} 3171, 3059, 3025, 2974, 2928, 1642, 1598, 1576, 1495, 1445, 1374, 1301, 1152, 1102, 1045, 1015, 966, 923, 899, 854, 820, 777, 747, 692, 671, 602, 545 cm^{-1}

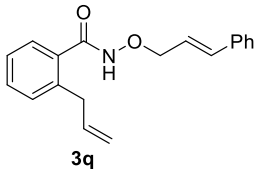
(E)-N-((2-methyl-3-phenylallyl)oxy)-2-(3-methylbut-2-en-1-yl)benzamide



3p

White solid; R_f = 0.63 (2:1 petroleum ether/ethyl acetate); 784.0 mg, 93% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.26 (ddt, J = 28.5, 21.3, 7.7 Hz, 9H), 6.58 (s, 1H), 5.25 (t, J = 7.4 Hz, 1H), 4.58 (s, 2H), 3.51 (d, J = 7.1 Hz, 2H), 2.03 (s, 3H), 1.71 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.9, 140.5, 136.9, 133.5, 132.8, 131.2, 130.8, 130.1, 129.1, 128.3, 127.7, 127.1, 126.0, 122.9, 83.3, 31.9, 25.9, 18.1, 16.0. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_2$ $[M+H]^+$: 336.1958, found: 336.1963. IR (neat): ν_{max} 3167, 3023, 2965, 2916, 2856, 1643, 1599, 1493, 1444, 1376, 1344, 1304, 1015, 983, 919, 890, 851, 747, 699, 668 cm^{-1}

2-allyl-N-(cinnamyloxy)benzamide

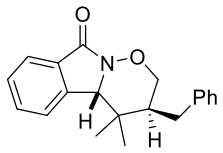


3q

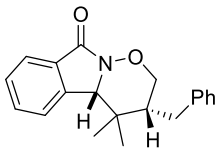
White solid; R_f = 0.66 (2:1 petroleum ether/ethyl acetate); 169.0 mg, 58% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.45 – 7.26 (m, 7H), 7.22 (dd, J = 9.4, 6.5 Hz, 2H), 6.71 (d, J = 15.9 Hz, 1H), 6.40 (dd, J = 15.1, 7.9 Hz, 1H), 5.97 (ddt, J = 16.6, 10.1, 6.3 Hz, 1H), 5.13 – 4.90 (m, 2H), 4.68 (d, J = 6.8 Hz, 2H), 3.55 (d, J = 6.3 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.7, 138.5, 137.5, 136.6, 136.1, 132.9, 130.9, 130.7, 128.8, 128.5, 127.8, 126.9, 126.5, 123.0, 116.4, 37.4. HRMS (ESI) m/z calcd for $C_{19}H_{19}NO_2$ $[M+H]^+$: 294.1489, found: 294.1491. IR (neat): ν_{max} 3167, 3024, 2975, 2930, 1642, 1598, 1496, 1445, 1303, 1016, 967, 915, 747, 693 cm^{-1}

10. Analytical data for products

3-benzyl-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2a (major)



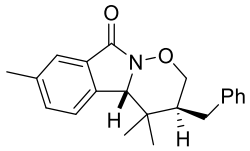
2a (minor)

White solid; 52.0 mg, 85% yield, dr = 5.4:1;

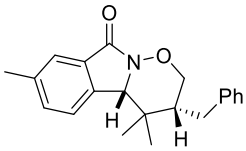
2a (major): R_f = 0.57 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 (dt, *J* = 7.2, 1.2 Hz, 1H), 7.51 (dtd, *J* = 14.0, 6.9, 3.3 Hz, 3H), 7.33 (dd, *J* = 8.0, 6.4 Hz, 2H), 7.27 – 7.22 (m, 1H), 7.20 – 7.08 (m, 2H), 4.35 (s, 1H), 4.01 – 3.86 (m, 2H), 2.97 (dd, *J* = 13.6, 2.4 Hz, 1H), 2.23 (tdd, *J* = 10.5, 5.1, 2.4 Hz, 1H), 2.07 (dd, *J* = 13.7, 11.2 Hz, 1H), 1.54 (s, 3H), 0.54 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.6, 139.4, 131.4, 131.3, 128.9, 128.9, 128.6, 126.7, 124.3, 123.1, 72.8, 65.8, 47.1, 37.8, 31.7, 24.8, 13.5. HRMS (ESI) m/z calcd for $C_{20}H_{21}NO_2$ $[M+H]^+$: 308.1645, found: 308.1650. IR (neat): ν_{max} 3025, 2969, 2930, 2874, 1707, 1616, 1495, 1469, 1390, 1372, 1299, 1258, 1199, 1169, 1089, 1030, 998, 925, 789, 769, 749, 725, 701, 684, 652, 618, 586, 533 cm^{-1}

2a (minor): R_f = 0.58 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 – 7.86 (m, 1H), 7.60 – 7.42 (m, 3H), 7.38 – 7.29 (m, 2H), 7.25 (dd, *J* = 7.3, 3.1 Hz, 3H), 4.71 (s, 1H), 4.17 (dt, *J* = 11.7, 1.7 Hz, 1H), 3.84 (dd, *J* = 11.7, 1.5 Hz, 1H), 3.17 – 3.00 (m, 2H), 1.65 – 1.59 (m, 1H), 1.55 (s, 3H), 0.67 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.3, 140.3, 140.0, 131.4, 129.5, 128.8, 128.6, 126.6, 124.3, 123.0, 70.3, 61.9, 47.2, 36.8, 32.0, 25.6, 21.8. HRMS (ESI) m/z calcd for $C_{20}H_{21}NO_2$ $[M+H]^+$: 308.1645, found: 308.1642. IR (neat): ν_{max} 3025, 2970, 2882, 1704, 1618, 1493, 1468, 1371, 1297, 1204, 1088, 1049, 992, 951, 911, 825, 803, 774, 727, 699, 683, 645, 592, 554, 510 cm^{-1}

3-benzyl-4,4,7-trimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2b (major)



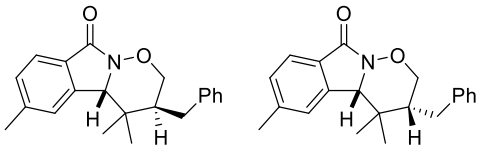
2b (minor)

White solid; 55.0 mg, 86% yield, dr = 5.3:1;

2b (major): R_f = 0.58 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.41 – 7.27 (m, 4H), 7.27 – 7.19 (m, 1H), 7.19 – 7.08 (m, 2H), 4.29 (s, 1H), 4.00 – 3.81 (m, 2H), 2.96 (dd, *J* = 13.7, 2.4 Hz, 1H), 2.42 (s, 3H), 2.21 (tdd, *J* = 10.6, 5.1, 2.4 Hz, 1H), 2.05 (dd, *J* = 13.7, 11.2 Hz, 1H), 1.50 (s, 3H), 0.52 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.8, 139.5, 138.6, 136.7, 132.3, 131.3, 128.8, 128.8, 126.6, 124.5, 122.9, 65.6, 47.1, 37.7, 31.7, 24.8, 21.5, 13.5. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1806. IR (neat): ν_{max} 3024, 2965, 2924, 2876, 1698, 1490, 1469, 1429, 1391, 1370, 1287, 1197, 1108, 1033, 1011, 998, 97, 911, 842, 780, 764, 744, 729, 701, 615, 549, 527, 511 cm^{-1}

2b (minor): R_f = 0.59 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.38 – 7.29 (m, 4H), 7.24 (dd, *J* = 9.0, 4.1 Hz, 4H), 4.65 (s, 1H), 4.15 (dt, *J* = 11.8, 1.7 Hz, 1H), 3.81 (dd, *J* = 11.7, 1.5 Hz, 1H), 3.17 – 2.97 (m, 2H), 2.43 (s, 3H), 1.60 (dd, *J* = 10.8, 4.9 Hz, 1H), 1.51 (s, 3H), 0.65 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.5, 140.1, 138.7, 137.4, 132.3, 129.6, 128.8, 126.6, 124.7, 122.7, 70.3, 61.8, 47.2, 36.8, 32.1, 25.6, 21.9, 21.6. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1803. IR (neat): ν_{max} 3026, 2970, 2925, 1709, 1625, 1601, 1488, 1455, 1371, 1285, 1205, 1140, 1105, 1049, 1008, 968, 927, 844, 813, 772, 750, 728, 702, 554, 532, 515 cm^{-1}

3-benzyl-4,4,6-trimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



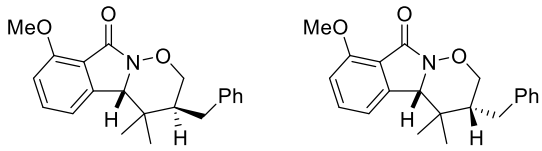
2c (major) **2c (minor)**

White solid; 53.0 mg, 83% yield, dr = 4.7:1;

2c (major): R_f = 0.55 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 7.9 Hz, 3H), 7.25 (d, *J* = 7.2 Hz, 2H), 7.15 (d, *J* = 7.3 Hz, 2H), 4.30 (s, 1H), 4.00 – 3.82 (m, 2H), 2.97 (dd, *J* = 13.6, 2.4 Hz, 1H), 2.46 (s, 3H), 2.21 (tdd, *J* = 10.6, 5.1, 2.2 Hz, 1H), 2.06 (dd, *J* = 13.6, 11.1 Hz, 1H), 1.52 (s, 3H), 0.54 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.9, 142.0, 140.0, 139.5, 129.5, 128.9, 128.9, 128.7, 126.7, 124.1, 123.8, 72.7, 65.7, 47.2, 37.8, 31.7, 24.9, 22.3, 13.6. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1804. IR (neat): ν_{max} 3019, 2969, 2920, 2866, 1695, 1619, 1492, 1450, 1392, 1370, 1217, 1193, 1103, 1035, 1006, 970, 918, 833, 782, 764, 740, 700, 682, 584, 552, 535 cm^{-1}

2c (minor): R_f = 0.56 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.7 Hz, 1H), 7.31 (d, *J* = 7.0 Hz, 2H), 7.27 (s, 1H), 7.26 – 7.21 (m, 4H), 4.65 (s, 1H), 4.16 (d, *J* = 12.0 Hz, 1H), 3.81 (dd, *J* = 11.7, 1.5 Hz, 1H), 3.19 – 2.97 (m, 2H), 2.47 (s, 3H), 1.60 (dd, *J* = 11.1, 4.7 Hz, 1H), 1.53 (s, 3H), 0.67 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.6, 142.0, 140.6, 140.1, 129.5, 129.5, 128.8, 128.6, 126.6, 124.2, 123.5, 70.2, 61.9, 47.2, 36.8, 32.1, 25.7, 22.3, 21.9. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1805. IR (neat): ν_{max} 3025, 2970, 2927, 1709, 1620, 1493, 1455, 1371, 1289, 1239, 1207, 1105, 1049, 994, 951, 914, 895, 830, 782, 728, 701, 688, 644, 554, 514 cm^{-1}

3-benzyl-8-methoxy-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2d (major) **2d (minor)**

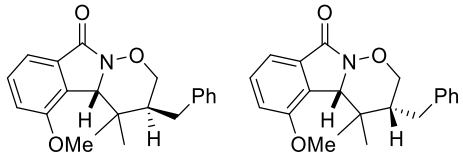
White solid; 49.0 mg, 73% yield, dr = 5.8:1;

2d (major): R_f = 0.58 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 8.4, 7.5 Hz, 1H), 7.34 – 7.25 (m, 2H), 7.24 – 7.17 (m, 1H), 7.16 – 7.08 (m, 2H), 7.04 (dt, *J* = 7.6, 0.7 Hz, 1H), 6.91 (d, *J* = 8.4 Hz, 1H), 4.24 (s, 1H), 3.93 (s, 3H), 3.90 – 3.78 (m, 2H), 2.92 (dd, *J* = 13.6, 2.3 Hz, 1H), 2.16 (dddd, *J* = 11.7, 9.3, 5.7, 2.3 Hz, 1H), 2.03 (dd, *J* = 13.6, 11.1 Hz, 1H), 1.47 (s, 3H), 0.51 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.1, 157.8, 142.3, 139.5, 133.0, 128.8, 128.7, 126.6, 115.3, 111.0, 72.3, 65.1, 55.9, 47.0, 37.8, 31.7, 24.6, 13.5. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_3$ $[M+H]^+$: 338.1751, found: 338.1753. IR (neat): ν_{max} 2969, 2936, 2874, 1702, 1607, 1593, 1485, 1456, 1440, 1392, 1371, 1332, 1310, 1284, 1268, 1195, 1167, 1084, 1067, 1030, 997, 953, 913, 864, 845, 809, 756, 729, 702, 687, 645, 618, 588, 556, 520 cm^{-1}

2d (minor): R_f = 0.58 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 8.4, 7.5 Hz, 1H), 7.34 – 7.27 (m, 2H), 7.22 (dt, *J* = 6.0, 1.6 Hz, 3H), 6.99 (d, *J* = 7.5 Hz, 1H), 6.93 (d, *J* = 8.4 Hz, 1H), 4.62 (s, 1H), 4.11 (dt, *J* = 11.6, 1.7 Hz, 1H), 3.96 (s, 3H), 3.78 (dd, *J* = 11.7, 1.5 Hz, 1H),

3.13 – 2.98 (m, 2H), 1.60 – 1.54 (m, 1H), 1.49 (s, 3H), 0.66 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.9, 158.0, 143.1, 140.1, 133.0, 129.5, 128.7, 126.5, 118.2, 115.2, 110.9, 69.9, 61.4, 56.0, 47.2, 36.9, 32.0, 25.6, 22.0. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_3$ $[M+H]^+$: 338.1751, found: 338.1754. IR (neat): ν_{max} 3025, 2968, 2928, 1702, 1607, 1593, 1485, 1455, 1440, 1390, 1370, 1355, 1325, 1284, 1267, 1197, 1179, 1081, 1067, 1050, 992, 970, 946, 914, 809, 769, 731, 701, 685, 644, 619, 592, 580, 517 cm^{-1}

3-benzyl-5-methoxy-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



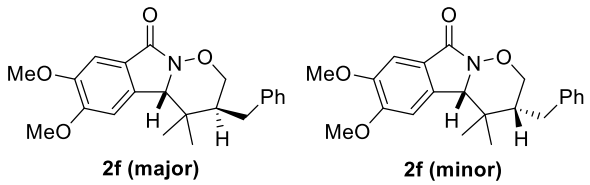
2e (major) **2e (minor)**

White solid; 50.0 mg, 74% yield, dr = 6.7:1;

2e (major): R_f = 0.49 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.31 (dd, *J* = 8.0, 6.4 Hz, 2H), 7.27 – 7.18 (m, 1H), 7.15 (dd, *J* = 6.9, 1.8 Hz, 2H), 7.05 (dd, *J* = 8.1, 1.1 Hz, 1H), 4.47 (s, 1H), 3.87 (d, *J* = 12.5 Hz, 5H), 2.98 (dd, *J* = 13.7, 2.4 Hz, 1H), 2.27 – 2.15 (m, 1H), 2.02 (dd, *J* = 13.7, 11.2 Hz, 1H), 1.58 (s, 3H), 0.49 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.2, 154.5, 139.8, 133.4, 130.1, 128.9, 128.8, 127.9, 126.6, 116.4, 113.9, 72.4, 65.3, 55.5, 47.1, 39.0, 31.9, 25.7, 14.6. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_3$ $[M+H]^+$: 338.1751, found: 338.1753. IR (neat): ν_{max} 3022, 2969, 2940, 1700, 1594, 1489, 1460, 1431, 1385, 1373, 1338, 1265, 1186, 1160, 1073, 1062, 1035, 1001, 966, 948, 910, 852, 829, 795, 745, 732, 702, 670, 622, 566, 548, 529, 517 cm^{-1}

2e (minor): R_f = 0.50 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 1H), 7.35 – 7.29 (m, 2H), 7.24 (d, *J* = 7.1 Hz, 3H), 7.05 (dd, *J* = 8.1, 1.0 Hz, 1H), 4.81 (s, 1H), 4.13 (dt, *J* = 11.6, 1.8 Hz, 1H), 3.90 (s, 3H), 3.78 (dd, *J* = 11.6, 1.6 Hz, 1H), 3.19 – 3.01 (m, 2H), 1.61 – 1.55 (m, 1H), 1.53 (s, 3H), 0.65 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.0, 154.5, 140.3, 133.2, 130.0, 129.5, 128.8, 128.5, 126.5, 116.5, 113.6, 69.9, 61.6, 55.4, 47.7, 38.1, 31.9, 27.5, 22.8. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_3$ $[M+H]^+$: 338.1751, found: 338.1750. IR (neat): ν_{max} 3025, 2968, 2931, 2841, 1707, 1596, 1490, 1455, 1392, 1372, 1356, 1272, 1180, 1074, 1062, 1031, 1009, 994, 968, 909, 846, 825, 802, 786, 769, 730, 700, 644, 614, 576, 548, 516 cm^{-1}

3-benzyl-6,7-dimethoxy-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2f (major) **2f (minor)**

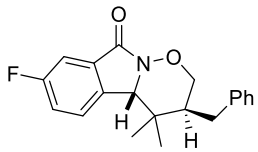
White solid; 51.0 mg, 69% yield, dr = 5.4:1;

2f (major): R_f = 0.2 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 – 7.28 (m, 3H), 7.27 – 7.21 (m, 1H), 7.16 (dd, *J* = 6.9, 1.8 Hz, 2H), 6.94 (s, 1H), 4.26 (s, 1H), 4.01 – 3.83 (m, 8H), 2.96 (dd, *J* = 13.5, 2.3 Hz, 1H), 2.21 (tdd, *J* = 10.3, 4.9, 2.3 Hz, 1H), 2.07 (dd, *J* = 13.6, 11.2 Hz, 1H), 1.51 (s, 3H), 0.55 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.3, 152.2, 149.9, 139.5, 133.0, 128.9, 128.8, 126.7, 123.7, 106.2, 105.9, 72.7, 65.5, 56.5, 56.3, 47.0, 37.8, 31.7, 24.9, 13.6. HRMS (ESI) m/z calcd

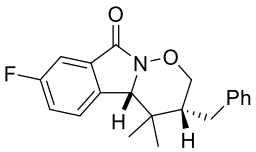
for $C_{22}H_{25}NO_4$ $[M+H]^+$: 368.1856, found: 368.1859. IR (neat): ν_{max} 2968, 2935, 2875, 1699, 1614, 1495, 1466, 1422, 1373, 1293, 1256, 1193, 1101, 1011, 984, 912, 864, 822, 769, 727, 701, 683, 648, 601, 528 cm^{-1}

2f (minor): R_f = 0.21 (2:1 petroleum ether/ethyl acetate); ^1H NMR (600 MHz, $CDCl_3$) δ 7.40 (s, 1H), 7.33 (dd, *J* = 8.2, 7.0 Hz, 2H), 7.26 – 7.21 (m, 3H), 6.87 (s, 1H), 4.62 (s, 1H), 4.14 (dt, *J* = 11.6, 1.8 Hz, 1H), 3.97 (s, 3H), 3.94 (s, 3H), 3.81 (dd, *J* = 11.7, 1.5 Hz, 1H), 3.12 – 3.03 (m, 2H), 1.62 – 1.59 (m, 1H), 1.52 (s, 3H), 0.68 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.0, 152.3, 140.0, 133.7, 129.6, 128.8, 126.6, 106.3, 105.6, 70.2, 61.7, 56.5, 56.4, 47.2, 36.9, 32.0, 25.7, 22.0. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_4$ $[M+H]^+$: 368.1856, found: 368.1864. IR (neat): ν_{max} 2967, 2931, 1705, 1615, 1499, 1460, 1371, 1294, 1254, 1226, 1207, 1103, 1049, 1009, 864, 769, 728, 702, 685 cm^{-1}

3-benzyl-7-fluoro-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2g (major)



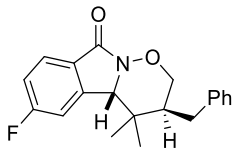
2g (minor)

White solid; 50.0 mg, 76% yield, dr = 5.0:1;

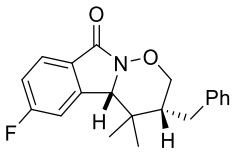
2g (major): R_f = 0.69 (2:1 petroleum ether/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 7.6, 2.5 Hz, 1H), 7.47 (dd, *J* = 8.4, 4.4 Hz, 1H), 7.32 (t, *J* = 7.1 Hz, 2H), 7.27 – 7.20 (m, 2H), 7.19 – 7.09 (m, 2H), 4.32 (s, 1H), 4.00 – 3.84 (m, 2H), 2.96 (dd, *J* = 13.7, 2.5 Hz, 1H), 2.22 (tdd, *J* = 10.5, 5.4, 2.6 Hz, 1H), 2.06 (dd, *J* = 13.6, 11.2 Hz, 1H), 1.51 (s, 3H), 0.53 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ163.0 (d, *J* = 248.8 Hz), 159.6 (d, *J* = 3.3 Hz), 139.3, 135.1 (d, *J* = 2.9 Hz), 133.6 (d, *J* = 8.5 Hz), 128.9 (d, *J* = 2.4 Hz), 126.8, 124.8 (d, *J* = 8.1 Hz), 118.8 (d, *J* = 23.2 Hz), 111.4 (d, *J* = 23.7 Hz), 72.9, 65.6, 47.0, 37.9, 31.6, 24.8, 13.5. ^{19}F NMR (282 MHz, $CDCl_3$) δ -111.5 (td, *J* = 8.2, 4.3 Hz). HRMS (ESI) m/z calcd for $C_{20}H_{20}FNO_2$ $[M+H]^+$: 326.1551, found: 326.1553. IR (neat): ν_{max} 3054, 2968, 2939, 2874, 1704, 1621, 1600, 1482, 1389, 1371, 1269, 1241, 1196, 1170, 1138, 1094, 1070, 1032, 1003, 968, 873, 853, 816, 781, 767, 746, 701, 615, 572, 554, 537, 515 cm^{-1}

2g (minor): R_f = 0.70 (2:1 petroleum ether/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 7.6, 2.5 Hz, 1H), 7.41 (dd, *J* = 8.4, 4.5 Hz, 1H), 7.36 – 7.30 (m, 2H), 7.28 (d, *J* = 2.5 Hz, 1H), 7.25 – 7.20 (m, 3H), 4.68 (s, 1H), 4.17 (dt, *J* = 11.8, 1.7 Hz, 1H), 3.84 (dd, *J* = 11.8, 1.5 Hz, 1H), 3.15 – 2.99 (m, 2H), 1.64 (s, 1H), 1.53 (s, 3H), 0.67 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.0 (d, *J* = 248.8 Hz), 160.3 (d, *J* = 3.2 Hz), 139.8, 135.7 (d, *J* = 2.8 Hz), 133.5 (d, *J* = 8.8 Hz), 129.5, 128.9, 126.7, 124.6 (d, *J* = 8.1 Hz), 118.9 (d, *J* = 23.3 Hz), 111.5 (d, *J* = 23.8 Hz), 70.5, 61.8, 47.1, 36.9, 32.0, 25.6, 21.8. ^{19}F NMR (282 MHz, $CDCl_3$) δ -111.5 (td, *J* = 8.2, 4.3 Hz). HRMS (ESI) m/z calcd for $C_{20}H_{20}FNO_2$ $[M+H]^+$: 326.1551, found: 326.1550. IR (neat): ν_{max} 3027, 2970, 2930, 1715, 1621, 1601, 1483, 1456, 1373, 1270, 1243, 1204, 1135, 1091, 1049, 1003, 927, 877, 853, 813, 778, 750, 730, 702, 672, 559, 515 cm^{-1}

3-benzyl-6-fluoro-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2h (major)



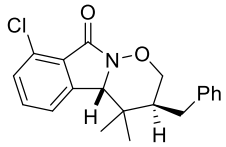
2h (minor)

White solid; 52.0 mg, 79% yield, dr = 5.0:1;

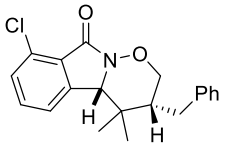
2h (major): R_f = 0.68 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 8.3, 5.1 Hz, 1H), 7.34 (dd, *J* = 8.0, 6.4 Hz, 2H), 7.30 – 7.14 (m, 5H), 4.35 (s, 1H), 4.03 – 3.85 (m, 2H), 2.99 (dd, *J* = 13.7, 2.4 Hz, 1H), 2.24 (tdd, *J* = 10.4, 5.2, 2.4 Hz, 1H), 2.09 (dd, *J* = 13.6, 11.2 Hz, 1H), 1.53 (s, 3H), 0.58 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.8 (d, *J* = 251.6 Hz), 159.8, 141.8 (d, *J* = 9.4 Hz), 139.3, 128.8 (d, *J* = 1.9 Hz), 127.4 (d, *J* = 2.4 Hz), 126.7, 126.3 (d, *J* = 9.7 Hz), 116.2 (d, *J* = 23.0 Hz), 110.9 (d, *J* = 24.6 Hz), 72.7, 65.6, 65.5, 47.0, 37.8, 31.6, 24.6, 13.5. ^{19}F NMR (282 MHz, $CDCl_3$) δ -106.5 (td, *J* = 8.7, 5.1 Hz). HRMS (ESI) m/z calcd for $C_{20}H_{20}FNO_2$ $[M+H]^+$: 326.1551, found: 326.1552. IR (neat): ν_{max} 3022, 2976, 2922, 2869, 1698, 1624, 1594, 1492, 1475, 1396, 1371, 1330, 1270, 1244, 1226, 1180, 1126, 1087, 1034, 1006, 971, 954, 921, 866, 841, 783, 765, 745, 731, 701, 680, 640, 585, 561, 540 cm^{-1}

2h (minor): R_f = 0.69 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 8.3, 5.1 Hz, 1H), 7.36 – 7.29 (m, 2H), 7.26 – 7.11 (m, 5H), 4.68 (s, 1H), 4.15 (dt, *J* = 11.7, 1.8 Hz, 1H), 3.82 (dd, *J* = 11.8, 1.5 Hz, 1H), 3.15 – 2.97 (m, 2H), 1.66 – 1.58 (m, 1H), 1.52 (s, 3H), 0.69 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.9 (d, *J* = 251.7 Hz), 160.4, 142.5 (d, *J* = 9.5 Hz), 139.8, 129.5, 128.8, 127.3 (d, *J* = 2.5 Hz), 126.6, 126.4 (d, *J* = 9.7 Hz), 116.3 (d, *J* = 23.1 Hz), 110.7 (d, *J* = 24.5 Hz), 70.3, 61.8, 61.8, 47.1, 36.9, 32.0, 25.46, 21.8. ^{19}F NMR (282 MHz, $CDCl_3$) δ -106.6 (td, *J* = 8.7, 5.1 Hz). HRMS (ESI) m/z calcd for $C_{20}H_{20}FNO_2$ $[M+H]^+$: 326.1551, found: 326.1553. IR (neat): ν_{max} 3027, 2971, 2932, 2886, 1707, 1624, 1597, 1493, 1476, 1455, 1373, 1357, 1326, 1272, 1242, 1206, 1180, 1125, 1086, 1068, 1048, 994, 961, 949, 912, 896, 870, 835, 772, 749, 729, 701, 688, 676, 666, 646, 622, 589, 558, 516 cm^{-1}

3-benzyl-8-chloro-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2i (major)



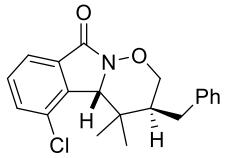
2i (minor)

White solid; 52.0 mg, 76% yield, dr = 5.3:1;

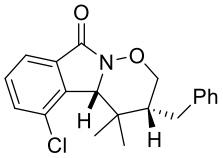
2i (major): R_f = 0.57 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 (q, *J* = 5.4 Hz, 3H), 7.32 (dd, *J* = 8.0, 6.4 Hz, 2H), 7.22 (d, *J* = 7.3 Hz, 1H), 7.19 – 7.10 (m, 2H), 4.29 (s, 1H), 3.90 (q, *J* = 5.5, 4.7 Hz, 2H), 2.96 (dd, *J* = 13.7, 2.4 Hz, 1H), 2.27 – 2.14 (m, 1H), 2.06 (dd, *J* = 13.6, 11.2 Hz, 1H), 1.51 (s, 3H), 0.54 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.8, 142.2, 139.3, 132.3, 132.1, 130.5, 128.9, 126.7, 121.7, 72.6, 64.8, 47.0, 37.9, 31.7, 24.8, 13.6. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1255. IR (neat): ν_{max} 2970, 2932, 2874, 1711, 1604, 1578, 1494, 1461, 1373, 1327, 1267, 1197, 1166, 1136, 1062, 1031, 997, 938, 921, 840, 796, 776, 758, 727, 701, 682, 645, 587, 567, 524 cm^{-1}

2i (minor): R_f = 0.58 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 – 7.40 (m, 2H), 7.32 (ddd, *J* = 7.5, 5.8, 1.1 Hz, 3H), 7.24 – 7.20 (m, 2H), 4.65 (s, 1H), 4.14 (dt, *J* = 11.8, 1.8 Hz, 1H), 3.82 (dd, *J* = 11.8, 1.6 Hz, 1H), 3.16 – 2.96 (m, 2H), 1.64 – 1.60 (m, 1H), 1.52 (s, 3H), 0.67 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.4, 142.9, 139.9, 132.5, 132.1, 130.4, 129.5, 128.8, 126.6, 121.5, 70.1, 61.05, 47.2, 36.9, 32.0, 25.7, 21.9. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1255. IR (neat): ν_{max} 2971, 2933, 2884, 1714, 1605, 1578, 1493, 1461, 1390, 1373, 1265, 1201, 1049, 997, 947, 916, 900, 801, 777, 758, 733, 702, 677, 646, 569, 527, 508 cm^{-1}

3-benzyl-5-chloro-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2j (major)



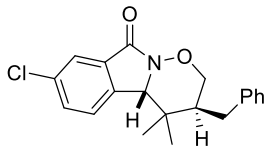
2j (minor)

White solid; 49.0 mg, 71% yield, dr = 10.5:1;

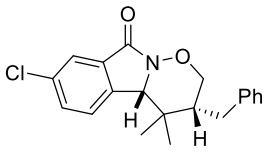
2j (major): R_f = 0.38 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 7.3, 1.1 Hz, 1H), 7.51 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.34 – 7.25 (m, 2H), 7.25 – 7.18 (m, 1H), 7.17 – 7.07 (m, 2H), 4.54 (s, 1H), 4.00 – 3.73 (m, 2H), 2.97 (dd, *J* = 13.9, 2.5 Hz, 1H), 2.30 – 2.18 (m, 1H), 1.99 (dd, *J* = 13.8, 11.1 Hz, 1H), 1.63 (s, 3H), 0.47 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.8, 139.4, 138.5, 134.3, 133.0, 130.0, 129.3, 128.8, 128.8, 126.6, 122.6, 72.1, 66.0, 46.3, 40.5, 31.7, 26.9, 14.6. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1257. IR (neat): ν_{max} 3025, 2970, 2930, 2875, 1714, 1604, 1574, 1494, 1461, 1395, 1374, 1328, 1258, 1185, 1156, 1129, 1030, 1002, 959, 939, 910, 831, 813, 748, 729, 701, 661, 646, 621, 595, 558, 539, 519 cm^{-1}

2j (minor): R_f = 0.39 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 7.4, 1.1 Hz, 1H), 7.54 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 7.36 – 7.30 (m, 2H), 7.26 – 7.20 (m, 3H), 4.90 (s, 1H), 4.17 (dt, *J* = 11.7, 1.9 Hz, 1H), 3.78 (dd, *J* = 11.7, 1.5 Hz, 1H), 3.21 – 3.04 (m, 2H), 1.63 (s, 3H), 1.60 – 1.54 (m, 1H), 0.65 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.8, 140.0, 139.1, 134.1, 133.0, 130.1, 129.5, 129.4, 128.8, 126.6, 122.8, 69.6, 62.6, 47.8, 39.4, 31.9, 29.2, 22.8. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1251. IR (neat): ν_{max} 3025, 2972, 2931, 1719, 1606, 1575, 1494, 1461, 1394, 1373, 1324, 1260, 1178, 1128, 1092, 1053, 1009, 994, 962, 907, 827, 811, 777, 762, 730, 701, 626 cm^{-1}

3-benzyl-7-chloro-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2k (major)



2k (minor)

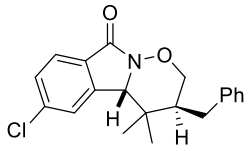
White solid; 53.0 mg, 79% yield, dr = 4.9:1;

2k (major): R_f = 0.73 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 – 7.70 (m, 1H), 7.57 – 7.40 (m, 2H), 7.28 (dq, *J* = 14.2, 7.3 Hz, 3H), 7.14 (d, *J* = 7.3 Hz, 2H), 4.32 (s, 1H), 4.02 – 3.81 (m, 2H), 3.06 – 2.86 (m, 1H), 2.29 – 2.14 (m, 1H), 2.13 – 2.00 (m, 1H), 1.51 (s, 3H), 0.53 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3, 139.3, 137.7, 135.0, 133.2, 131.5, 128.9, 128.8, 126.8, 124.5, 124.4,

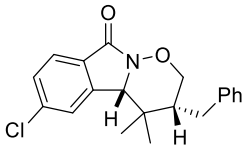
72.8, 65.6, 47.0, 37.9, 31.6, 24.8, 13.6. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1259. IR (neat): ν_{max} 3069, 2964, 2937, 1706, 1600, 1494, 1465, 1429, 1390, 1372, 1261, 1196, 1175, 1116, 1074, 1033, 1015, 975, 942, 914, 885, 867, 852, 832, 809, 774, 755, 715, 702, 610, 563, 542, 518 cm^{-1}

2k (minor): R_f = 0.74 (2:1 petroleum ether/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 7.89 (d, *J* = 2.0 Hz, 1H), 7.52 (dd, *J* = 8.1, 2.0 Hz, 1H), 7.41 – 7.29 (m, 3H), 7.23 (dd, *J* = 7.7, 1.6 Hz, 3H), 4.68 (s, 1H), 4.16 (dt, *J* = 11.7, 1.9 Hz, 1H), 3.83 (dd, *J* = 11.8, 1.5 Hz, 1H), 3.16 – 2.98 (m, 2H), 1.65 – 1.59 (m, 1H), 1.53 (s, 3H), 0.68 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.0, 139.8, 138.4, 135.0, 133.1, 131.6, 129.5, 128.9, 126.7, 124.7, 124.2, 70.4, 61.8, 47.1, 36.9, 32.0, 25.6, 21.8. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1257. IR (neat): ν_{max} 2967, 2926, 1712, 1465, 1426, 1391, 1372, 1263, 1199, 1181, 1116, 1049, 1005, 924, 897, 825, 812, 741, 719, 701, 654, 544, 511 cm^{-1}

3-benzyl-6-chloro-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2l (major)



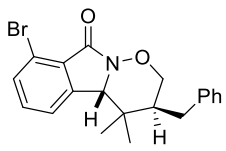
2l (minor)

White solid; 51.0 mg, 74% yield, dr = 5.9:1;

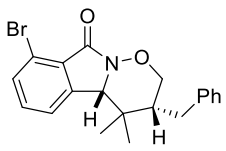
2l (major): R_f = 0.71 (2:1 petroleum ether/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.1 Hz, 1H), 7.53 – 7.41 (m, 2H), 7.32 (dd, *J* = 8.0, 6.3 Hz, 2H), 7.23 (td, *J* = 5.1, 4.5, 2.4 Hz, 1H), 7.19 – 7.09 (m, 2H), 4.32 (s, 1H), 3.99 – 3.83 (m, 2H), 2.96 (dd, *J* = 13.6, 2.4 Hz, 1H), 2.21 (tdd, *J* = 10.3, 5.2, 2.4 Hz, 1H), 2.06 (dd, *J* = 13.7, 11.2 Hz, 1H), 1.51 (s, 3H), 0.56 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.7, 141.2, 139.3, 137.8, 129.9, 129.2, 128.9, 128.8, 126.8, 125.5, 123.6, 72.8, 65.5, 47.0, 37.9, 31.6, 24.8, 13.6. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1259. IR (neat): ν_{max} 3019, 2971, 2921, 2868, 1698, 1611, 1579, 1492, 1455, 1422, 1392, 1370, 1258, 1201, 1107, 1072, 1035, 1004, 971, 930, 909, 838, 779, 758, 733, 714, 700, 676, 576, 532, 508 cm^{-1}

2l (minor): R_f = 0.72 (2:1 petroleum ether/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.1 Hz, 1H), 7.51 – 7.42 (m, 2H), 7.33 (dd, *J* = 8.2, 6.1 Hz, 2H), 7.26 – 7.18 (m, 3H), 4.68 (s, 1H), 4.16 (dt, *J* = 11.7, 1.8 Hz, 1H), 3.83 (dd, *J* = 11.7, 1.5 Hz, 1H), 3.15 – 2.98 (m, 2H), 1.65 – 1.60 (m, 1H), 1.54 (s, 3H), 0.70 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.3, 141.8, 139.8, 137.9, 129.8, 129.5, 129.2, 128.9, 126.7, 125.6, 123.4, 70.4, 61.8, 47.2, 36.9, 32.0, 25.6, 21.9. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClNO_2$ $[M+H]^+$: 342.1255, found: 342.1262. IR (neat): ν_{max} 2969, 2925, 1712, 1612, 1581, 1493, 1459, 1423, 1374, 1268, 1204, 1095, 1069, 1049, 994, 950, 834, 781, 739, 701, 676, 642, 581, 540, 513 cm^{-1}

3-benzyl-8-bromo-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2m (major)



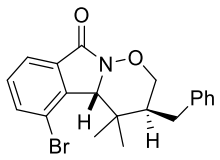
2m (minor)

White solid; 59.0 mg, 77% yield, dr = 6.2:1;

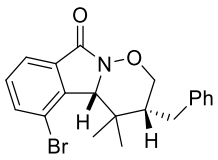
2m (major): R_f = 0.70 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.8 Hz, 1H), 7.45 (d, *J* = 7.5 Hz, 1H), 7.40 – 7.28 (m, 3H), 7.26 – 7.19 (m, 1H), 7.18 – 7.08 (m, 2H), 4.27 (s, 1H), 3.96 – 3.82 (m, 2H), 2.95 (dd, *J* = 13.6, 2.4 Hz, 1H), 2.21 (dddd, *J* = 11.6, 8.8, 6.0, 2.4 Hz, 1H), 2.05 (dd, *J* = 13.6, 11.2 Hz, 1H), 1.50 (s, 3H), 0.52 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.0, 142.4, 139.3, 133.7, 132.2, 129.0, 128.8, 126.7, 122.3, 119.7, 72.5, 64.5, 47.0, 37.9, 31.6, 24.8, 13.6. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0751. IR (neat): ν_{max} 3026, 2972, 2876, 1706, 1599, 1569, 1493, 1452, 1392, 1373, 1312, 1267, 1200, 1165, 1121, 1062, 1042, 990, 918, 863, 843, 796, 779, 757, 733, 712, 700, 681, 586, 561, 538, 523, 507 cm^{-1}

2m (minor): R_f = 0.71 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.66 – 7.57 (m, 1H), 7.42 – 7.28 (m, 4H), 7.26 – 7.19 (m, 3H), 4.63 (s, 1H), 4.14 (dt, *J* = 11.7, 1.9 Hz, 1H), 3.82 (dd, *J* = 11.8, 1.5 Hz, 1H), 3.15 – 2.98 (m, 2H), 1.59 (d, *J* = 4.5 Hz, 1H), 1.52 (s, 3H), 0.66 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.7, 143.1, 139.9, 133.7, 132.2, 129.5, 129.0, 128.8, 126.6, 122.1, 119.9, 70.1, 60.9, 47.2, 36.9, 32.0, 25.7, 21.9. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0746. IR (neat): ν_{max} 2970, 2931, 1714, 1601, 1571, 1493, 1458, 1372, 1266, 1200, 1050, 996, 949, 914, 796, 777, 756, 733, 716, 701, 676, 644, 563, 518 cm^{-1}

3-benzyl-5-bromo-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2n (major)



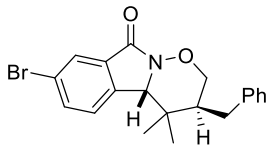
2n (minor)

White solid; 61.0 mg, 79% yield, dr = 9.3:1;

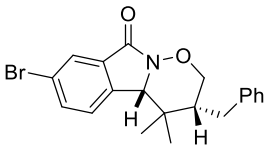
2n (major): R_f = 0.71 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.4 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.33 (q, *J* = 7.6 Hz, 3H), 7.22 (d, *J* = 7.4 Hz, 1H), 7.14 (d, *J* = 7.3 Hz, 2H), 4.52 (s, 1H), 4.03 – 3.78 (m, 2H), 2.98 (dd, *J* = 13.8, 2.6 Hz, 1H), 2.26 (tt, *J* = 11.3, 3.5 Hz, 1H), 2.01 (dd, *J* = 13.8, 11.1 Hz, 1H), 1.69 (s, 3H), 0.47 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.3, 141.2, 139.5, 136.3, 134.7, 130.3, 128.9, 128.9, 126.8, 123.3, 117.93, 72.09, 67.02, 46.39, 41.15, 31.75, 27.88, 14.76. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0750. IR (neat): ν_{max} 2970, 2934, 1714, 1604, 1568, 1494, 1456, 1395, 1374, 1257, 1184, 1155, 1115, 1030, 998, 957, 934, 910, 828, 805, 748, 727, 700, 659, 593, 554, 518 cm^{-1}

2n (minor): R_f = 0.72 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.72 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.40 – 7.30 (m, 3H), 7.26 – 7.21 (m, 3H), 4.86 (s, 1H), 4.18 (dt, *J* = 11.7, 1.8 Hz, 1H), 3.78 (dd, *J* = 11.8, 1.5 Hz, 1H), 3.21 – 3.05 (m, 2H), 1.68 (s, 3H), 1.59 – 1.52 (m, 1H), 0.63 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.2, 141.6, 140.0, 136.3, 134.4, 130.3, 129.5, 128.8, 126.6, 123.3, 117.8, 69.5, 63.5, 47.8, 39.8, 31.9, 30.1, 22.8. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0746. IR (neat): ν_{max} 2972, 2930, 1715, 1604, 1569, 1493, 1455, 1422, 1393, 1372, 1321, 1259, 1175, 1115, 1093, 1052, 1007, 992, 957, 907, 825, 802, 774, 747, 727, 700, 646, 625, 519, 506 cm^{-1}

3-benzyl-7-bromo-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2o (major)



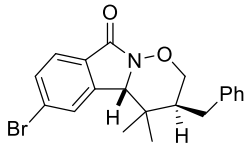
2o (minor)

White solid; 61.0 mg, 78% yield, dr = 5.0:1;

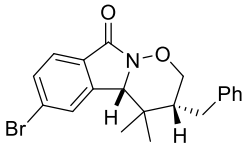
2o (major): R_f = 0.43 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 (d, *J* = 1.9 Hz, 1H), 7.66 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.41 – 7.28 (m, 3H), 7.27 – 7.20 (m, 1H), 7.14 (dd, *J* = 6.9, 1.8 Hz, 2H), 4.30 (s, 1H), 3.99 – 3.84 (m, 2H), 2.96 (dd, *J* = 13.7, 2.4 Hz, 1H), 2.21 (tdd, *J* = 10.2, 5.2, 2.5 Hz, 1H), 2.06 (dd, *J* = 13.7, 11.2 Hz, 1H), 1.51 (s, 3H), 0.53 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 139.2, 138.2, 134.4, 133.4, 128.9, 128.8, 127.4, 126.7, 124.7, 122.8, 72.8, 65.6, 47.0, 37.8, 31.6, 24.8, 13.5. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0747. IR (neat): ν_{max} 2966, 2929, 2874, 1706, 1601, 1494, 1459, 1421, 1392, 1371, 1262, 1195, 1171, 1114, 1031, 1002, 972, 935, 908, 865, 850, 809, 774, 753, 729, 703, 687, 667, 646, 604, 558, 538, 517 cm^{-1}

2o (minor): R_f = 0.44 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (d, *J* = 1.9 Hz, 1H), 7.67 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.37 – 7.29 (m, 3H), 7.22 (dd, *J* = 7.7, 1.6 Hz, 3H), 4.66 (s, 1H), 4.16 (dt, *J* = 11.8, 1.8 Hz, 1H), 3.83 (dd, *J* = 11.8, 1.5 Hz, 1H), 3.14 – 2.98 (m, 2H), 1.63 – 1.58 (m, 1H), 1.52 (s, 3H), 0.67 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.8, 139.8, 138.9, 134.4, 133.3, 129.5, 128.9, 127.6, 126.7, 124.5, 122.8, 70.4, 61.9, 47.1, 36.9, 32.0, 25.6, 21.8. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0745. IR (neat): ν_{max} 2967, 2925, 1708, 1606, 1494, 1459, 1420, 1391, 1372, 1263, 1197, 1181, 1167, 1113, 1093, 1048, 1005, 995, 960, 941, 922, 909, 895, 872, 810, 783, 734, 712, 701, 683, 643, 598, 568, 538, 511 cm^{-1}

3-benzyl-6-bromo-4,4-dimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2p (major)



2p (minor)

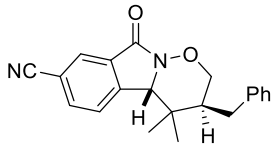
White solid; 58.0 mg, 75% yield, dr = 5.2:1;

2p (major): R_f = 0.33 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.0 Hz, 1H), 7.68 – 7.57 (m, 2H), 7.32 (dd, *J* = 8.0, 6.4 Hz, 2H), 7.25 (d, *J* = 6.7 Hz, 1H), 7.19 – 7.08 (m, 2H), 4.32 (s, 1H), 3.98 – 3.83 (m, 2H), 2.97 (dd, *J* = 13.7, 2.4 Hz, 1H), 2.21 (tdd, *J* = 10.2, 5.2, 2.4 Hz, 1H), 2.06 (dd, *J* = 13.7, 11.2 Hz, 1H), 1.52 (s, 3H), 0.56 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.8, 141.4, 139.3, 132.1, 130.4, 128.9, 128.9, 126.8, 126.5, 126.2, 125.7, 72.8, 65.5, 47.0, 37.9, 31.6, 24.8, 13.6. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0747. IR (neat): ν_{max} 2969, 2921, 1699, 1606, 1574, 1493, 1453, 1418, 1391, 1370, 1200, 1109, 1060, 1032, 1003, 969, 926, 908, 835, 778, 757, 731, 704, 675, 662, 567, 527 cm^{-1}

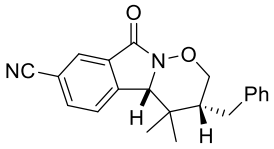
2p (minor): R_f = 0.34 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.67 – 7.59 (m, 2H), 7.36 – 7.30 (m, 2H), 7.26 – 7.20 (m, 4H), 4.68 (s, 1H), 4.16 (dt, *J* = 11.7, 1.8 Hz, 1H), 3.83 (dd, *J* = 11.8, 1.5 Hz, 1H), 3.14 – 2.98 (m, 2H), 1.67 – 1.61 (m, 1H), 1.54 (s, 3H), 0.70 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.4, 142.0, 139.8, 132.1, 130.3, 129.5, 128.9, 126.7, 126.3,

126.2, 125.8, 70.4, 61.7, 47.1, 36.9, 32.0, 25.6, 21.9. HRMS (ESI) m/z calcd for $C_{20}H_{20}BrNO_2$ $[M+H]^+$: 386.0750, found: 386.0746. IR (neat): ν_{max} 2970, 2931, 1712, 1608, 1493, 1457, 1418, 1372, 1203, 1108, 1093, 1056, 994, 950, 923, 894, 833, 781, 736, 701, 674, 513 cm^{-1}

3-benzyl-4,4-dimethyl-9-oxo-3,4,4a,9-tetrahydro-2H-[1,2]oxazino[3,2-a]isoindole-7-carbonitrile



2q (major)



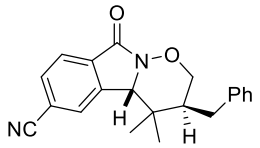
2q (minor)

White solid; 28.0 mg, 42% yield, dr = 3.7:1;

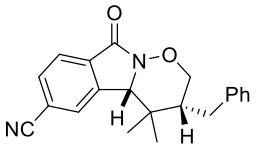
2q (major): R_f = 0.61 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.0 Hz, 1H), 7.70 – 7.57 (m, 2H), 7.32 (dd, *J* = 8.0, 6.4 Hz, 2H), 7.25 (d, *J* = 6.7 Hz, 1H), 7.19 – 7.06 (m, 2H), 4.32 (s, 1H), 3.99 – 3.84 (m, 2H), 2.97 (dd, *J* = 13.7, 2.4 Hz, 1H), 2.21 (tdd, *J* = 10.2, 5.2, 2.4 Hz, 1H), 2.06 (dd, *J* = 13.6, 11.2 Hz, 1H), 1.52 (s, 3H), 0.56 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.4, 143.9, 139.0, 134.9, 132.9, 129.0, 128.8, 128.0, 126.9, 124.3, 117.9, 113.1, 72.9, 66.0, 47.0, 38.1, 31.6, 24.9, 13.7. HRMS (ESI) m/z calcd for $C_{21}H_{20}N_2O_2$ $[M+H]^+$: 333.1598, found: 333.1596. IR (neat): ν_{max} 2971, 2927, 2231, 1712, 1624, 1495, 1478, 1454, 1393, 1373, 1200, 1099, 1030, 1006, 966, 909, 868, 844, 816, 781, 762, 730, 701, 647, 616, 586, 570, 543, 527 cm^{-1}

2q (minor): R_f = 0.62 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.19 (d, *J* = 1.5 Hz, 1H), 7.84 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.33 (td, *J* = 6.8, 1.2 Hz, 2H), 7.23 (dd, *J* = 8.2, 1.5 Hz, 3H), 4.77 (s, 1H), 4.17 (dd, *J* = 11.7, 2.0 Hz, 1H), 3.86 (dd, *J* = 11.8, 1.5 Hz, 1H), 3.16 – 2.98 (m, 2H), 1.68 – 1.62 (m, 1H), 1.56 (s, 3H), 0.68 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.0, 144.6, 139.5, 134.9, 132.8, 129.5, 128.9, 128.2, 126.8, 124.1, 113.1, 70.5, 62.2, 47.1, 37.1, 32.0, 25.7, 21.8. HRMS (ESI) m/z calcd for $C_{21}H_{20}N_2O_2$ $[M+H]^+$: 333.1598, found: 333.1604. IR (neat): ν_{max} 2970, 2932, 2231, 1716, 1624, 1478, 1456, 1391, 1374, 1207, 1098, 1048, 1004, 973, 908, 843, 817, 727, 702, 664, 646, 605, 573 cm^{-1}

3-benzyl-4,4-dimethyl-9-oxo-3,4,4a,9-tetrahydro-2H-[1,2]oxazino[3,2-a]isoindole-6-carbonitrile



2r (major)



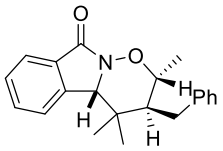
2r (minor)

White solid; 28.0 mg, 40% yield, dr = 4.6:1;

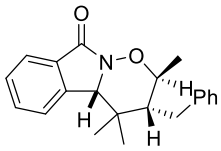
2r (major): R_f = 0.51 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 – 7.95 (m, 1H), 7.80 (d, *J* = 7.2 Hz, 2H), 7.34 (dd, *J* = 8.1, 6.4 Hz, 2H), 7.26 (s, 2H), 7.16 (dd, *J* = 6.8, 1.9 Hz, 2H), 4.41 (s, 1H), 3.94 (q, *J* = 5.4, 4.5 Hz, 2H), 2.99 (dd, *J* = 13.7, 2.5 Hz, 1H), 2.26 (tdd, *J* = 9.0, 7.5, 2.5 Hz, 1H), 2.08 (dd, *J* = 13.7, 11.2 Hz, 1H), 1.62 (s, 1H), 1.56 (s, 3H), 0.56 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.6, 140.2, 139.0, 135.7, 132.8, 129.0, 128.9, 126.9, 126.9, 125.2, 115.1, 73.0, 65.7, 47.0, 38.1, 31.6, 24.9, 13.6. HRMS (ESI) m/z calcd for $C_{21}H_{20}N_2O_2$ $[M+H]^+$: 333.1598, found: 333.1596. IR (neat): ν_{max} 2970, 2926, 2233, 1704, 1494, 1459, 1393, 1214, 1183, 1105, 1002, 916, 851, 760, 728, 700, 675, 587, 563, 526 cm^{-1}

2r (minor): R_f = 0.52 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 7.8, 0.8 Hz, 1H), 7.81 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.74 (dt, *J* = 1.5, 0.8 Hz, 1H), 7.38 – 7.31 (m, 2H), 7.29 – 7.26 (m, 1H), 7.23 (dd, *J* = 8.0, 1.4 Hz, 2H), 4.76 (s, 1H), 4.18 (dt, *J* = 11.7, 1.9 Hz, 1H), 3.87 (dd, *J* = 11.8, 1.5 Hz, 1H), 3.17 – 2.99 (m, 2H), 1.66 (dt, *J* = 12.1, 2.1 Hz, 1H), 1.59 (s, 3H), 0.69 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1, 140.8, 139.5, 135.5, 132.7, 129.5, 128.9, 126.8, 126.7, 125.2, 115.1, 70.6, 61.9, 47.1, 37.1, 32.0, 25.7, 21.8. HRMS (ESI) m/z calcd for $C_{21}H_{20}N_2O_2$ $[M+H]^+$: 333.1598, found: 333.1598. IR (neat): ν_{max} 2922, 2851, 2229, 1712, 1494, 1455, 1426, 1373, 1280, 1209, 1185, 1105, 1048, 994, 954, 912, 846, 784, 728, 702, 677, 647, 618, 564, 518 cm^{-1}

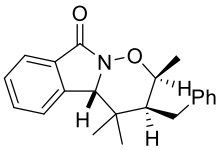
3-benzyl-2,4,4-trimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2s (major)



2s (minor 1)



2s (minor 2)

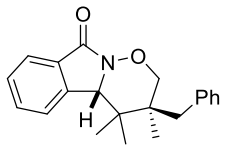
White solid; 60.0 mg, 92% yield, dr = 3.6:1.2:1;

2s (major): R_f = 0.23 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.56 – 7.46 (m, 3H), 7.35 – 7.29 (m, 2H), 7.26 – 7.19 (m, 3H), 4.39 (s, 1H), 4.14 (dq, *J* = 10.0, 6.2 Hz, 1H), 2.94 (dt, *J* = 15.6, 1.5 Hz, 1H), 2.19 (dd, *J* = 15.6, 7.8 Hz, 1H), 2.09 (ddd, *J* = 10.1, 7.8, 2.3 Hz, 1H), 1.49 (s, 3H), 1.16 (d, *J* = 6.2 Hz, 3H), 0.53 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.4, 141.6, 139.8, 131.3, 128.8, 128.7, 128.6, 126.3, 124.3, 123.2, 80.8, 65.8, 52.4, 38.6, 32.5, 25.3, 18.7, 14.4. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1801. IR (neat): ν_{max} 2971, 2934, 1709, 1616, 1603, 1496, 1468, 1393, 1372, 1326, 1300, 1202, 1135, 1087, 1063, 991, 966, 946, 913, 781, 736, 700, 685, 564, 525 cm^{-1}

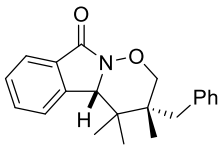
2s (minor 1): R_f = 0.30 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (dt, *J* = 7.4, 1.0 Hz, 1H), 7.54 (td, *J* = 7.5, 1.3 Hz, 1H), 7.49 (td, *J* = 7.6, 1.1 Hz, 1H), 7.45 (dq, *J* = 7.5, 0.9 Hz, 1H), 7.33 (dd, *J* = 8.2, 6.9 Hz, 2H), 7.25 – 7.23 (m, 1H), 7.22 – 7.20 (m, 2H), 4.61 (s, 1H), 4.31 (qd, *J* = 7.0, 1.5 Hz, 1H), 3.14 (dd, *J* = 13.5, 3.7 Hz, 1H), 2.90 (dd, *J* = 13.5, 11.9 Hz, 1H), 1.63 (ddd, *J* = 11.9, 3.7, 1.5 Hz, 1H), 1.53 (s, 3H), 1.36 (d, *J* = 7.0 Hz, 3H), 0.79 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.1, 140.5, 140.2, 131.3, 129.5, 128.9, 128.5, 126.6, 124.2, 123.1, 78.7, 62.0, 51.0, 37.1, 35.0, 27.7, 25.1, 20.7. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1799. IR (neat): ν_{max} 2975, 2935, 1704, 1618, 1494, 1467, 1453, 1394, 1382, 1203, 1152, 1117, 1089, 1029, 960, 937, 862, 791, 762, 736, 699, 678, 516 cm^{-1}

2s (minor 2): R_f = 0.28 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.55 – 7.52 (m, 2H), 7.50 – 7.47 (m, 1H), 7.35 – 7.31 (m, 2H), 7.26 – 7.23 (m, 1H), 7.21 (dd, *J* = 7.8, 1.3 Hz, 2H), 4.36 (s, 1H), 4.08 (qd, *J* = 6.9, 5.1 Hz, 1H), 3.04 (dd, *J* = 14.0, 3.4 Hz, 1H), 2.46 (ddd, *J* = 11.9, 5.1, 3.4 Hz, 1H), 2.33 (dd, *J* = 14.0, 11.9 Hz, 1H), 1.52 (s, 3H), 1.45 (d, *J* = 6.9 Hz, 3H), 0.64 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.6, 139.3, 131.6, 131.3, 128.9, 128.8, 128.6, 126.7, 124.2, 123.1, 79.3, 65.8, 50.0, 38.0, 31.8, 27.5, 17.6, 14.3. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1806. IR (neat): ν_{max} 2972, 2939, 1712, 1616, 1494, 1469, 1386, 1198, 1086, 1048, 982, 950, 746, 698, 681 cm^{-1}

3-benzyl-3,4,4-trimethyl-2,3,4,4a-tetrahydro-9H-[1,2]oxazino[3,2-a]isoindol-9-one



2t (major)



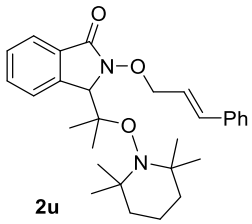
2t (minor)

White solid; 55.0 mg, 84% yield, dr = 3.8:1;

2t (major): R_f = 0.33 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (dt, *J* = 7.5, 0.9 Hz, 1H), 7.55 (td, *J* = 7.5, 1.3 Hz, 1H), 7.49 (td, *J* = 7.5, 1.0 Hz, 1H), 7.46 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.31 (dd, *J* = 8.1, 6.5 Hz, 2H), 7.28 – 7.25 (m, 1H), 7.09 – 7.06 (m, 2H), 4.74 (s, 1H), 4.33 – 4.30 (m, 1H), 3.65 (d, *J* = 11.2 Hz, 1H), 2.70 (d, *J* = 13.4 Hz, 1H), 2.54 (d, *J* = 13.4 Hz, 1H), 1.42 (s, 3H), 1.21 (s, 3H), 0.67 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.9, 140.6, 136.8, 131.4, 130.8, 128.5, 128.3, 126.7, 124.3, 123.1, 78.1, 62.4, 40.4, 39.3, 38.5, 20.7, 17.6, 16.2. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1801. IR (neat): ν_{max} 2975, 1710, 1617, 1495, 1468, 1383, 1299, 1205, 1120, 1088, 1001, 924, 787, 747, 697, 683, 652, 618, 599, 549 cm^{-1}

2t (minor): R_f = 0.38 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (dt, *J* = 7.4, 1.0 Hz, 1H), 7.55 (td, *J* = 7.5, 1.3 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.33 – 7.28 (m, 4H), 7.26 – 7.23 (m, 1H), 4.95 (s, 1H), 3.81 (dd, *J* = 11.9, 1.5 Hz, 1H), 3.64 (d, *J* = 11.9 Hz, 1H), 3.48 (d, *J* = 12.9 Hz, 1H), 2.66 (dd, *J* = 12.9, 1.5 Hz, 1H), 1.43 (s, 3H), 0.72 (d, *J* = 0.8 Hz, 3H), 0.59 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.1, 140.8, 137.4, 131.6, 131.4, 128.5, 128.3, 126.7, 124.4, 123.1, 73.8, 62.0, 40.2, 39.9, 37.6, 20.5, 17.3, 14.7. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1801. IR (neat): ν_{max} 2973, 2926, 1707, 1617, 1493, 1468, 1396, 1374, 1299, 1197, 1144, 1095, 996, 938, 911, 805, 762, 729, 708, 685, 645, 531, 511 cm^{-1}

2-(cinnamyloxy)-3-(2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)propan-2-yl)isoindolin-1-one

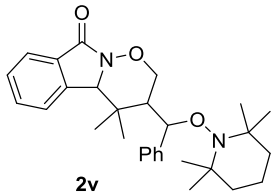


2u

White solid; R_f = 0.79 (2:1 petroleum ether/ethyl acetate); 17.2 mg, 19% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 15.8, 7.6 Hz, 2H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.38 – 7.25 (m, 5H), 6.67 (d, *J* = 15.8 Hz, 1H), 6.43 (dt, *J* = 16.2, 7.0 Hz, 1H), 5.01 (s, 1H), 4.86 (dd, *J* = 11.2, 7.2 Hz, 1H), 4.76 (dd, *J* = 11.0, 6.8 Hz, 1H), 1.59 (d, *J* = 25.0 Hz, 8H), 1.35 (d, *J* = 9.2 Hz, 1H), 1.24 (d, *J* = 4.3 Hz, 6H), 1.19 (s, 3H), 1.15 (s, 3H), 0.93 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.7, 141.9, 136.3, 136.2, 132.0, 128.7, 128.4, 128.3, 126.9, 125.5, 123.5, 122.9, 82.2, 75.8, 67.6, 59.9, 59.6, 41.2, 41.1, 35.5, 34.9, 24.2, 23.9, 22.3, 21.5, 17.3. HRMS (ESI) m/z calcd for $C_{29}H_{38}N_2O_3$ $[M+H]^+$: 463.2955, found: 463.2960. IR (neat): ν_{max} 2999, 2974, 2931, 2870, 1713, 1616, 1468, 1450, 1375, 1363, 1257, 1228, 1205, 1181, 1131, 1087, 962, 911, 877, 813, 785, 732, 687, 646, 570 cm^{-1}

4,4-dimethyl-3-(phenyl((2,2,6,6-tetramethylpiperidin-1-yl)oxy)methyl)-2,3,4,4a-tetrahydro-9H-

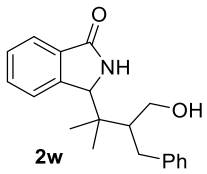
[1,2]oxazino[3,2-a]isoindol-9-one



2v

White solid; R_f = 0.71 (2:1 petroleum ether/ethyl acetate); 30.0 mg, 33% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93 – 7.86 (m, 1H), 7.46 (tt, *J* = 4.3, 2.0 Hz, 4H), 7.33 (td, *J* = 6.4, 5.0, 2.9 Hz, 4H), 4.97 – 4.75 (m, 2H), 4.46 (t, *J* = 11.7 Hz, 1H), 4.28 (s, 1H), 3.03 (ddd, *J* = 11.9, 8.1, 4.0 Hz, 1H), 1.53 – 1.09 (m, 12H), 0.91 (s, 3H), 0.84 (s, 3H), 0.63 (s, 3H), -0.01 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.6, 142.1, 139.4, 131.4, 131.2, 130.7, 128.5, 128.3, 127.7, 124.1, 123.2, 81.8, 71.9, 65.8, 61.0, 58.9, 49.3, 40.8, 40.1, 38.2, 35.3, 32.9, 26.2, 21.0, 20.8, 17.0, 14.9. HRMS (ESI) m/z calcd for $C_{29}H_{38}N_2O_3$ $[M+H]^+$: 463.2955, found: 463.2953. IR (neat): ν_{max} 2972, 2935, 2876, 1714, 1617, 1466, 1375, 1300, 1240, 1201, 1173, 1131, 1089, 1057, 1000, 954, 927, 878, 854, 789, 757, 730, 702, 686, 644, 603, 560, 527 cm^{-1}

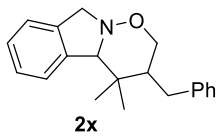
3-(3-benzyl-4-hydroxy-2-methylbutan-2-yl)isoindolin-1-one



2w

White solid; R_f = 0.16 (1:2 petroleum ether/ethyl acetate); 61.3 mg, 99% yield; ^{1}H NMR (300 MHz, CD_3OD) δ 7.82 – 7.75 (m, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.58 (td, *J* = 7.6, 1.4 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.30 – 7.11 (m, 5H), 4.98 (s, 1H), 3.78 – 3.65 (m, 2H), 2.87 (dd, *J* = 13.7, 3.4 Hz, 1H), 2.61 (dd, *J* = 13.7, 10.2 Hz, 1H), 2.02 (dq, *J* = 8.0, 3.8 Hz, 1H), 1.02 (s, 3H), 0.96 (s, 3H). ^{13}C NMR (75 MHz, CD_3OD) δ 173.3, 147.6, 143.1, 134.2, 132.6, 130.3, 129.4, 129.2, 126.9, 126.3, 124.3, 65.4, 61.4, 50.2, 41.7, 34.3, 22.4, 21.6. HRMS (ESI) m/z calcd for $C_{20}H_{23}NO_2$ $[M+H]^+$: 310.1802, found: 310.1802. IR (neat): ν_{max} 3456, 3179, 3060, 2973, 2926, 2894, 1669, 1615, 1471, 1370, 1322, 1252, 1207, 1143, 1098, 1056, 1030, 991, 947, 915, 812, 759, 718, 698, 623, 601, 578, 536 cm^{-1}

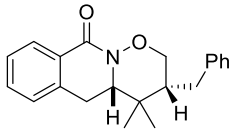
3-benzyl-4,4-dimethyl-3,4,4a,9-tetrahydro-2H-[1,2]oxazino[3,2-a]isoindole



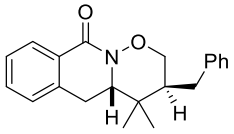
2x

White solid; R_f = 0.39 (10:1 petroleum ether/ethyl acetate); 53.1 mg, 91% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (q, *J* = 2.9, 2.2 Hz, 1H), 7.31 – 7.14 (m, 8H), 4.27 (d, *J* = 11.2 Hz, 1H), 3.87 (t, *J* = 11.4 Hz, 1H), 3.76 (dd, *J* = 11.2, 1.8 Hz, 1H), 3.67 (dd, *J* = 11.5, 4.9 Hz, 1H), 3.62 (d, *J* = 1.7 Hz, 1H), 2.97 (dd, *J* = 13.8, 2.6 Hz, 1H), 2.11 (dd, *J* = 13.7, 11.3 Hz, 1H), 1.84 (tdd, *J* = 11.3, 4.9, 2.6 Hz, 1H), 1.48 (s, 3H), 1.06 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.7, 138.7, 137.7, 128.9, 128.6, 127.3, 127.2, 126.2, 123.3, 123.3, 77.8, 71.1, 57.7, 48.5, 36.6, 32.0, 25.3, 15.0. HRMS (ESI) m/z calcd for $C_{20}H_{23}NO$ $[M+H]^+$: 294.1852, found: 294.1852. IR (neat): ν_{max} 3025, 2961, 2901, 2804, 1602, 1493, 1460, 1390, 1368, 1177, 1051, 1035, 1000, 882, 769, 741, 700, 658, 608, 519 cm^{-1}

3-benzyl-4,4-dimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4a (major)



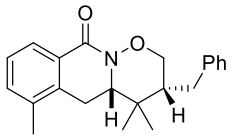
4a (minor)

White solid; 53.0 mg, 83% yield, dr = 4.3:1;

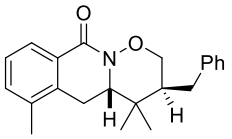
4a (major): R_f = 0.58 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.43 (td, *J* = 7.4, 1.5 Hz, 1H), 7.35 – 7.26 (m, 3H), 7.24 – 7.08 (m, 4H), 4.06 – 3.94 (m, 2H), 3.84 – 3.76 (m, 1H), 3.55 (dd, *J* = 17.3, 8.6 Hz, 1H), 3.18 (dd, *J* = 17.3, 2.1 Hz, 1H), 2.87 – 2.76 (m, 1H), 2.10 – 1.98 (m, 2H), 1.18 (s, 3H), 0.68 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.4, 139.6, 136.2, 132.6, 128.8, 128.7, 128.1, 126.9, 126.8, 126.5, 71.3, 66.0, 48.0, 38.3, 32.5, 27.4, 23.6, 15.2. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1800. IR (neat): ν_{max} 2966, 2953, 2934, 1664, 1601, 1581, 1493, 1459, 1413, 1399, 1365, 1342, 1295, 1272, 1243, 1213, 1199, 1181, 1154, 1092, 1053, 1037, 1018, 994, 925, 910, 796, 757, 737, 701, 672, 652, 584, 526 cm^{-1}

4a (minor): R_f = 0.59 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.19 – 8.12 (m, 1H), 7.47 – 7.41 (m, 1H), 7.37 – 7.27 (m, 3H), 7.24 – 7.14 (m, 4H), 4.33 – 4.21 (m, 2H), 3.79 (dd, *J* = 12.2, 1.4 Hz, 1H), 3.35 (dd, *J* = 16.9, 7.4 Hz, 1H), 3.12 (dd, *J* = 16.9, 5.8 Hz, 1H), 3.03 – 2.90 (m, 2H), 1.57 – 1.50 (m, 1H), 1.21 (s, 3H), 1.02 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.8, 140.3, 136.1, 132.6, 129.6, 128.7, 128.5, 127.9, 127.1, 126.9, 126.4, 68.5, 62.0, 47.9, 36.5, 32.1, 27.7, 24.8, 23.4. HRMS (ESI) m/z calcd for $C_{21}H_{23}NO_2$ $[M+H]^+$: 322.1802, found: 322.1799. IR (neat): ν_{max} 3026, 2965, 2886, 1669, 1604, 1492, 1460, 1394, 1371, 1351, 1295, 1267, 1238, 1096, 1065, 1043, 999, 945, 792, 740, 705, 502 cm^{-1}

3-benzyl-4,4,6-trimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4b (major)



4b (minor)

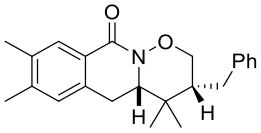
White solid; 49.0 mg, 73% yield, dr = 4.0:1;

4b (major): R_f = 0.65 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.31 – 7.17 (m, 5H), 7.14 – 7.04 (m, 2H), 4.10 – 3.94 (m, 2H), 3.79 (dd, *J* = 12.1, 3.8 Hz, 1H), 3.22 (qd, *J* = 17.7, 5.4 Hz, 2H), 2.89 – 2.73 (m, 1H), 2.30 (s, 3H), 2.11 – 1.98 (m, 2H), 1.18 (s, 3H), 0.65 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.6, 139.6, 134.4, 134.0, 128.9, 128.7, 126.6, 126.5, 126.1, 71.1, 65.4, 48.0, 38.4, 32.6, 24.6, 23.8, 19.3, 15.2. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_2$ $[M+H]^+$: 336.1958, found: 336.1952. IR (neat): ν_{max} 3026, 2966, 2879, 1666, 1596, 1492, 1467, 1451, 1415, 1399, 1372, 1344, 1303, 1272, 1246, 1215, 1084, 1054, 1041, 1019, 993, 940, 910, 887, 818, 805, 744, 701, 664, 645, 626, 608, 575, 538, 523 cm^{-1}

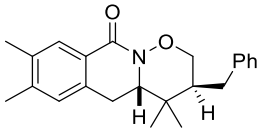
4b (minor): R_f = 0.66 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.34 – 7.27 (m, 3H), 7.21 (dd, *J* = 8.0, 6.3 Hz, 4H), 4.35 – 4.21 (m, 2H), 3.78 (dd, *J* = 12.3, 1.5 Hz, 1H), 3.20 (dd, *J* = 17.3, 7.7 Hz, 1H), 3.08 – 2.90 (m, 3H), 2.30 (s, 3H), 1.54 (ddt, *J* = 11.1,

4.1, 1.8 Hz, 1H), 1.22 (s, 3H), 1.01 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.0, 140.4, 134.5, 134.4, 134.1, 129.6, 128.7, 127.9, 126.8, 126.4, 126.4, 68.4, 61.4, 47.9, 36.6, 32.2, 24.9, 24.7, 23.4, 19.3. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_2$ $[M+H]^+$: 336.1958, found: 336.1957. IR (neat): ν_{max} 3024, 2966, 2879, 1669, 1596, 1493, 1469, 1395, 1351, 1302, 1270, 1241, 1212, 1156, 1069, 1045, 1012, 965, 946, 917, 806, 744, 701, 642, 602, 559, 519 cm^{-1}

3-benzyl-4,4,7,8-tetramethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4c (major)



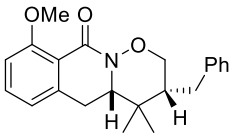
4c (minor)

White solid; 47.0 mg, 67% yield, dr = 4.2:1;

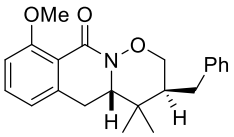
4c (major): R_f = 0.61 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.31 – 7.25 (m, 2H), 7.23 – 7.16 (m, 1H), 7.13 – 7.05 (m, 2H), 6.90 (s, 1H), 4.04 – 3.88 (m, 2H), 3.78 (dd, *J* = 12.1, 4.0 Hz, 1H), 3.45 (dd, *J* = 17.2, 8.6 Hz, 1H), 3.09 (dd, *J* = 17.2, 2.0 Hz, 1H), 2.86 – 2.73 (m, 1H), 2.26 (s, 6H), 2.07 – 1.95 (m, 2H), 1.15 (s, 3H), 0.67 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.9, 141.9, 139.6, 135.3, 133.5, 128.9, 128.8, 128.6, 128.0, 126.4, 71.2, 66.1, 48.0, 38.2, 32.5, 26.9, 23.6, 12.0, 19.3, 15.2. HRMS (ESI) m/z calcd for $C_{23}H_{27}NO_2$ $[M+H]^+$: 350.2115, found: 350.2114. IR (neat): ν_{max} 3024, 2967, 2938, 1664, 1615, 1495, 1453, 1420, 1392, 1371, 1324, 1273, 1227, 1178, 1080, 1050, 1022, 984, 910, 873, 824, 809, 753, 729, 700, 661, 644, 617, 585, 561, 544, 515 cm^{-1}

4c (minor): R_f = 0.64 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.32 – 7.26 (m, 2H), 7.20 (td, *J* = 7.0, 1.3 Hz, 3H), 6.91 (s, 1H), 4.29 – 4.19 (m, 2H), 3.77 (dd, *J* = 12.3, 1.5 Hz, 1H), 3.28 (dd, *J* = 16.8, 7.5 Hz, 1H), 3.07 – 2.88 (m, 3H), 2.30 – 2.23 (m, 6H), 1.56 – 1.47 (m, 1H), 1.19 (s, 3H), 1.01 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.2, 141.9, 140.4, 135.5, 133.5, 129.6, 129.2, 128.6, 128.1, 126.3, 68.4, 62.2, 47.9, 36.5, 32.1, 27.1, 24.8, 23.4, 20.0, 19.4. HRMS (ESI) m/z calcd for $C_{23}H_{27}NO_2$ $[M+H]^+$: 350.2115, found: 350.2114. IR (neat): ν_{max} 3025, 2967, 2884, 1667, 1615, 1495, 1454, 1419, 1390, 1351, 1275, 1251, 1223, 1066, 1022, 993, 955, 937, 911, 808, 730, 701, 644, 615, 562, 519 cm^{-1}

3-benzyl-9-methoxy-4,4-dimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4d (major)



4d (minor)

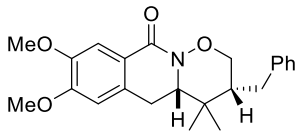
White solid; 49.0 mg, 64% yield, dr = 4.9:1;

4d (major): R_f = 0.13 (1:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (t, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 6.8 Hz, 2H), 7.19 (t, *J* = 7.1 Hz, 1H), 7.12 – 7.02 (m, 2H), 6.85 (d, *J* = 8.4 Hz, 1H), 6.73 (d, *J* = 7.5 Hz, 1H), 4.02 (td, *J* = 10.1, 8.8, 3.3 Hz, 1H), 3.96 – 3.86 (m, 4H), 3.80 – 3.72 (m, 1H), 3.53 (dd, *J* = 17.1, 8.6 Hz, 1H), 3.12 (dd, *J* = 17.2, 1.8 Hz, 1H), 2.85 – 2.73 (m, 1H), 2.07 – 1.95 (m, 2H), 1.15 (s, 3H), 0.70 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.0, 139.7, 139.5, 133.6, 128.9, 128.7, 126.5, 119.4, 110.9, 71.1, 65.4, 56.4, 48.0, 38.1, 32.6, 28.3, 23.6, 15.5. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_3$

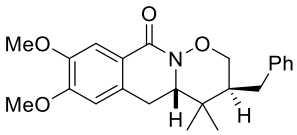
$[M+H]^+$: 352.1907, found: 352.1906. IR (neat): ν_{max} 3024, 2965, 2932, 1667, 1595, 1493, 1471, 1455, 1437, 1394, 1370, 1273, 1225, 1100, 1078, 1051, 988, 954, 914, 891, 860, 828, 785, 755, 731, 700, 667, 644, 628, 547, 514 cm^{-1}

4d (minor): R_f = 0.14 (1:1 petroleum ether/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 7.36 (t, *J* = 8.0 Hz, 1H), 7.33 – 7.27 (m, 2H), 7.24 – 7.14 (m, 3H), 6.86 (d, *J* = 8.5 Hz, 1H), 6.73 (d, *J* = 7.5 Hz, 1H), 4.28 – 4.15 (m, 2H), 3.92 (s, 3H), 3.74 (dd, *J* = 12.3, 1.5 Hz, 1H), 3.36 (dd, *J* = 16.8, 7.5 Hz, 1H), 3.12 – 2.88 (m, 3H), 1.55 – 1.45 (m, 1H), 1.18 (s, 3H), 0.99 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.9, 161.0, 140.5, 139.4, 133.5, 129.6, 128.6, 126.3, 119.4, 116.0, 110.9, 68.4, 61.4, 56.4, 47.8, 36.4, 32.3, 28.5, 24.6, 23.5. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_3$ $[M+H]^+$: 352.1907, found: 352.1914. IR (neat): ν_{max} 3024, 2962, 2885, 1674, 1595, 1472, 1390, 1275, 1223, 1094, 1001, 956, 929, 783, 753, 732, 701 cm^{-1}

3-benzyl-7,8-dimethoxy-4,4-dimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4e (major)



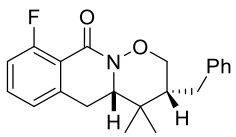
4e (minor)

White solid; 69.0 mg, 69% yield, dr = 3.4:1;

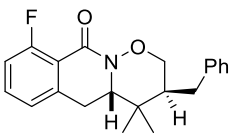
4e (major): R_f = 0.40 (1:1 petroleum ether/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.31 – 7.25 (m, 2H), 7.22 – 7.17 (m, 1H), 7.12 – 7.06 (m, 2H), 6.58 (s, 1H), 4.06 – 3.88 (m, 9H), 3.78 (dd, *J* = 12.1, 3.8 Hz, 1H), 3.47 (dd, *J* = 17.1, 8.6 Hz, 1H), 3.08 (dd, *J* = 17.2, 2.3 Hz, 1H), 2.86 – 2.76 (m, 1H), 2.08 – 1.98 (m, 2H), 1.17 (s, 3H), 0.71 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.9, 152.5, 147.9, 139.6, 129.8, 128.9, 128.7, 126.5, 110.1, 109.0, 71.1, 66.2, 56.2, 56.2, 48.0, 38.1, 32.6, 27.2, 23.7, 15.3. HRMS (ESI) m/z calcd for $C_{23}H_{27}NO_4$ $[M+H]^+$: 382.2013, found: 382.2001. IR (neat): ν_{max} 2965, 2937, 1659, 1602, 1511, 1454, 1423, 1391, 1364, 1274, 1237, 1209, 1166, 1092, 1053, 1037, 1010, 985, 913, 882, 783, 755, 728, 700, 671, 645, 623 cm^{-1}

4e (minor): R_f = 0.41 (1:1 petroleum ether/ethyl acetate); ^1H NMR (600 MHz, $CDCl_3$) δ 7.62 (s, 1H), 7.30 (d, *J* = 7.4 Hz, 2H), 7.19 (d, *J* = 7.6 Hz, 3H), 6.59 (s, 1H), 4.23 (d, *J* = 9.9 Hz, 2H), 3.93 (d, *J* = 2.4 Hz, 6H), 3.78 (d, *J* = 12.2 Hz, 1H), 3.27 (dd, *J* = 16.8, 7.3 Hz, 1H), 3.08 – 2.90 (m, 3H), 1.53 (d, *J* = 11.9 Hz, 1H), 1.20 (s, 3H), 1.05 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.3, 152.6, 148.1, 140.4, 129.9, 129.6, 128.7, 126.4, 120.5, 110.5, 109.1, 68.3, 62.4, 56.3, 56.2, 47.9, 36.3, 32.1, 27.4, 24.8, 23.5. HRMS (ESI) m/z calcd for $C_{23}H_{27}NO_4$ $[M+H]^+$: 382.2013, found: 382.2009. IR (neat): ν_{max} 3024, 2967, 2937, 2875, 1659, 1601, 1513, 1464, 1428, 1396, 1365, 1280, 1243, 1222, 1209, 1169, 1097, 1010, 976, 912, 883, 852, 817, 787, 763, 731, 701, 669, 647, 621, 593, 528 cm^{-1}

3-benzyl-9-fluoro-4,4-dimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4f (major)



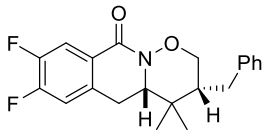
4f (minor)

White solid; 49.0 mg, 72% yield, dr = 4.5:1;

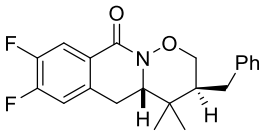
4f (major): R_f = 0.33 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 (td, *J* = 8.0, 4.9 Hz, 1H), 7.31 – 7.25 (m, 2H), 7.23 – 7.17 (m, 1H), 7.11 – 7.06 (m, 2H), 7.03 – 6.93 (m, 2H), 4.04 – 3.90 (m, 2H), 3.81 – 3.74 (m, 1H), 3.58 – 3.48 (m, 1H), 3.18 (dd, *J* = 17.4, 2.0 Hz, 1H), 2.79 (t, *J* = 10.0 Hz, 1H), 2.08 – 1.98 (m, 2H), 1.16 (s, 3H), 0.71 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.6 (d, *J* = 264.6 Hz), 158.8 (d, *J* = 4.4 Hz), 139.4 (d, *J* = 17.9 Hz), 133.9 (d, *J* = 10.2 Hz), 128.8, 128.7, 126.5, 122.8 (d, *J* = 4.1 Hz), 116.0 (d, *J* = 6.8 Hz), 115.8 (d, *J* = 11.8 Hz), 71.3, 65.6, 48.0, 38.2, 32.5, 27.8, 23.6, 15.3. ^{19}F NMR (282 MHz, $CDCl_3$) δ -110.1 (dd, *J* = 11.4, 4.8 Hz). HRMS (ESI) m/z calcd for $C_{21}H_{22}FNO_2$ $[M+H]^+$: 340.1707, found: 340.1706. IR (neat): ν_{max} 2979, 2963, 2952, 2934, 1671, 1610, 1492, 1465, 1411, 1398, 1370, 1342, 1307, 1256, 1201, 1180, 1162, 1037, 1008, 984, 901, 831, 796, 774, 752, 733, 699, 689, 660, 619, 575, 549, 513 cm^{-1}

4f (minor): R_f = 0.34 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 (td, *J* = 8.0, 4.8 Hz, 1H), 7.29 (dd, *J* = 7.8, 6.3 Hz, 2H), 7.24 – 7.16 (m, 3H), 7.05 – 6.93 (m, 2H), 4.28 – 4.20 (m, 2H), 3.77 (dd, *J* = 12.3, 1.5 Hz, 1H), 3.36 (dd, *J* = 17.0, 7.4 Hz, 1H), 3.11 (dd, *J* = 17.0, 5.3 Hz, 1H), 2.94 (d, *J* = 9.8 Hz, 2H), 1.58 – 1.50 (m, 1H), 1.20 (s, 3H), 1.02 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.7 (d, *J* = 264.9 Hz), 160.1 (d, *J* = 4.5 Hz), 140.2, 139.1, 133.9 (d, *J* = 10.2 Hz), 129.6, 128.7, 126.4, 122.9 (d, *J* = 4.0 Hz), 116.1 (d, *J* = 4.6 Hz), 116.0 (d, *J* = 14.1 Hz), 77.4, 68.6, 61.6, 47.7, 36.4, 32.2, 28.0, 24.6, 23.4. ^{19}F NMR (282 MHz, $CDCl_3$) δ -109.9 (dd, *J* = 11.4, 4.8 Hz). HRMS (ESI) m/z calcd for $C_{21}H_{22}FNO_2$ $[M+H]^+$: 340.1707, found: 340.1706. IR (neat): ν_{max} 3025, 2966, 2881, 1672, 1612, 1582, 1493, 1468, 1426, 1392, 1371, 1351, 1305, 1284, 1259, 1231, 1165, 1129, 1095, 1075, 1059, 1033, 1020, 986, 953, 932, 889, 846, 829, 805, 785, 753, 731, 701, 679, 645, 624, 595, 576, 557, 540, 521 cm^{-1}

3-benzyl-7,8-difluoro-4,4-dimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4g (major)



4g (minor)

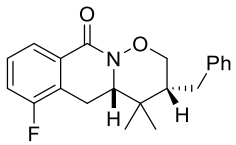
White solid; 50.0 mg, 69% yield, dr = 3.4:1;

4g (major): R_f = 0.51 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 10.6, 8.1 Hz, 1H), 7.27 (d, *J* = 7.2 Hz, 2H), 7.24 – 7.17 (m, 1H), 7.09 (d, *J* = 7.3 Hz, 2H), 6.96 (dd, *J* = 10.1, 7.1 Hz, 1H), 4.03 – 3.90 (m, 2H), 3.79 (dd, *J* = 12.2, 3.5 Hz, 1H), 3.48 (dd, *J* = 17.5, 8.6 Hz, 1H), 3.12 (d, *J* = 17.4 Hz, 1H), 2.80 (t, *J* = 9.9 Hz, 1H), 2.10 – 1.98 (m, 2H), 1.17 (s, 3H), 0.69 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 154.6 (d, *J* = 13.4 Hz), 151.2 (dd, *J* = 13.0, 5.8 Hz), 147.9 (d, *J* = 12.7 Hz), 139.4, 133.4 (dd, *J* = 7.0, 4.0 Hz), 128.8 (d, *J* = 6.4 Hz), 126.6, 125.0 (dd, *J* = 5.6, 3.4 Hz), 117.5 (dd, *J* = 19.1, 1.8 Hz), 115.8 (d, *J* = 18.2 Hz), 71.4, 65.9, 47.9, 38.3, 32.5, 26.7, 23.6, 15.2. ^{19}F NMR (282 MHz, $CDCl_3$) δ -131.1 (dt, *J* = 21.3, 9.1 Hz), -138.6 – -139.8 (m). HRMS (ESI) m/z calcd for $C_{21}H_{21}F_2NO_2$ $[M+H]^+$: 358.1613, found: 358.1613. IR (neat): ν_{max} 2964, 2937, 1659, 1620, 1602, 1511, 1492, 1465, 1444, 1406, 1369, 1317, 1297, 1268, 1218, 1175, 1153, 1081, 1051, 1037, 982, 921, 893, 786, 754, 731, 698, 670, 628, 604, 525 cm^{-1}

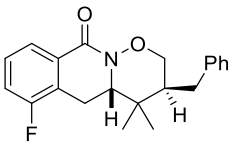
4g (minor): R_f = 0.52 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 10.7, 8.1 Hz, 1H), 7.30 (ddd, *J* = 7.6, 6.2, 1.5 Hz, 2H), 7.24 – 7.16 (m, 3H), 6.97 (dd, *J* = 10.1, 7.1 Hz,

1H), 4.31 – 4.18 (m, 2H), 3.78 (dd, *J* = 12.2, 1.5 Hz, 1H), 3.29 (dd, *J* = 17.1, 7.4 Hz, 1H), 3.06 (dd, *J* = 17.0, 5.8 Hz, 1H), 2.95 (d, *J* = 9.2 Hz, 2H), 1.55 (t, *J* = 8.0 Hz, 1H), 1.21 (s, 3H), 1.03 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.0, 153.8 (d, *J* = 13.4 Hz), 152.1 (d, *J* = 13.5 Hz), 150.5 (d, *J* = 12.8 Hz), 148.8 (d, *J* = 12.7 Hz), 140.1, 133.3 (dd, *J* = 7.1, 3.9 Hz), 129.6, 128.7, 126.5, 125.0 (dd, *J* = 5.5, 3.4 Hz), 117.8 (d, *J* = 18.5 Hz), 115.9 (d, *J* = 18.0 Hz), 68.6, 62.0, 47.7, 36.5, 32.1, 27.0, 24.7, 23.4. ^{19}F NMR (282 MHz, $CDCl_3$) δ -131.0 (dt, *J* = 21.4, 9.0 Hz), -139.0 (ddd, *J* = 21.4, 10.6, 7.3 Hz). HRMS (ESI) m/z calcd for $C_{21}H_{21}F_2NO_2$ $[M+H]^+$: 358.1613, found: 358.1616. IR (neat): ν_{max} 3025, 2966, 2881, 1672, 1612, 1582, 1493, 1468, 1426, 1392, 1371, 1351, 1305, 1284, 1259, 1231, 1165, 1129, 1095, 1075, 1059, 1033, 1020, 986, 953, 932, 889, 846, 829, 805, 785, 753, 731, 701, 679, 645, 624, 595, 576, 557, 540, 521 cm^{-1}

3-benzyl-6-fluoro-4,4-dimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4h (major)



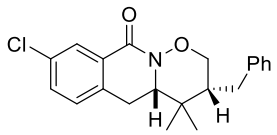
4h (minor)

White solid; 47.0 mg, 69% yield, dr = 3.9:1;

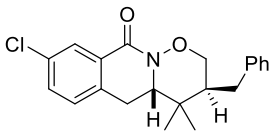
4h (major): R_f = 0.70 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.33 – 7.24 (m, 3H), 7.18 (q, *J* = 9.3, 8.3 Hz, 2H), 7.12 – 7.05 (m, 2H), 4.00 (td, *J* = 10.4, 9.0, 4.5 Hz, 2H), 3.80 (dd, *J* = 12.1, 3.7 Hz, 1H), 3.39 – 3.25 (m, 2H), 2.87 – 2.76 (m, 1H), 2.11 – 1.98 (m, 2H), 1.19 (s, 3H), 0.68 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.4, 158.7 (d, *J* = 231.6 Hz), 157.2, 139.4, 129.9, 128.8 (d, *J* = 9.0 Hz), 128.0 (d, *J* = 8.0 Hz), 126.5, 123.7, 123.2 (d, *J* = 17.9 Hz), 119.0 (d, *J* = 21.5 Hz), 71.3, 65.4, 48.0, 38.4, 32.6, 23.5, 20.2, 14.9. ^{19}F NMR (282 MHz, $CDCl_3$) δ -119.6 (dd, *J* = 9.2, 5.2 Hz). HRMS (ESI) m/z calcd for $C_{21}H_{22}FNO_2$ $[M+H]^+$: 340.1707, found: 340.1702. IR (neat): ν_{max} 3026, 2967, 2929, 2876, 1671, 1616, 1585, 1494, 1472, 1453, 1429, 1400, 1372, 1339, 1306, 1269, 1248, 1217, 1153, 1054, 1037, 1006, 956, 911, 890, 819, 804, 744, 700, 662, 645, 627, 606, 579, 552, 523, 505 cm^{-1}

4h (minor): R_f = 0.71 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.30 (td, *J* = 7.8, 3.2 Hz, 3H), 7.22 – 7.17 (m, 4H), 4.33 (dd, *J* = 7.8, 5.4 Hz, 1H), 4.24 (ddd, *J* = 12.2, 2.5, 1.3 Hz, 1H), 3.79 (dd, *J* = 12.3, 1.5 Hz, 1H), 3.29 (dd, *J* = 17.5, 7.8 Hz, 1H), 3.17 (dd, *J* = 17.5, 5.4 Hz, 1H), 2.98 – 2.93 (m, 2H), 1.58 – 1.54 (m, 1H), 1.23 (s, 3H), 1.03 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.6 (d, *J* = 3.4 Hz), 158.9 (d, *J* = 245.6 Hz), 140.2, 129.9 (d, *J* = 3.8 Hz), 129.6, 128.7, 128.1 (d, *J* = 8.2 Hz), 126.4, 124.1 (d, *J* = 3.4 Hz), 123.1 (d, *J* = 17.9 Hz), 119.0 (d, *J* = 21.4 Hz), 68.6, 61.4, 47.8, 36.6, 32.1, 24.6, 23.1, 20.4. ^{19}F NMR (282 MHz, $CDCl_3$) δ -120.0 (dd, *J* = 9.1, 5.3 Hz). HRMS (ESI) m/z calcd for $C_{21}H_{22}FNO_2$ $[M+H]^+$: 340.1707, found: 340.1703. IR (neat): ν_{max} 3026, 2967, 2884, 1675, 1615, 1586, 1493, 1473, 1455, 1431, 1395, 1372, 1352, 1304, 1270, 1247, 1215, 1152, 1095, 1066, 1044, 1006, 985, 949, 926, 878, 834, 805, 746, 721, 701, 665, 643, 603, 583, 528, 506 cm^{-1}

3-benzyl-8-chloro-4,4-dimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4i (major)



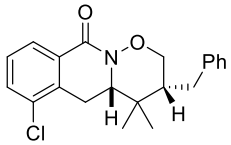
4i (minor)

White solid; 49.0 mg, 68% yield, dr = 3.8:1;

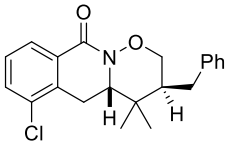
4i (major): R_f = 0.57 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12 (d, *J* = 2.4 Hz, 1H), 7.43 – 7.34 (m, 1H), 7.29 (t, *J* = 7.5 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.15 – 7.03 (m, 3H), 3.98 (dd, *J* = 13.8, 9.3 Hz, 2H), 3.79 (dd, *J* = 12.1, 3.4 Hz, 1H), 3.49 (dd, *J* = 17.4, 8.7 Hz, 1H), 3.15 (d, *J* = 17.4 Hz, 1H), 2.81 (d, *J* = 10.1 Hz, 1H), 2.11 – 1.95 (m, 2H), 1.17 (s, 3H), 0.66 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.1, 139.4, 134.4, 133.1, 132.5, 128.8, 128.7, 128.4, 128.0, 126.6, 71.5, 65.8, 47.9, 38.4, 32.5, 26.8, 23.6, 15.2. HRMS (ESI) m/z calcd for $C_{21}H_{22}ClNO_2$ $[M+H]^+$: 356.1412, found: 356.1413. IR (neat): ν_{max} 3026, 2968, 2934, 1671, 1600, 1576, 1480, 1452, 1428, 1394, 1371, 1336, 1296, 1271, 1237, 1181, 1154, 1112, 1079, 1052, 1037, 1000, 984, 940, 909, 872, 812, 768, 752, 730, 700, 676, 652, 640, 575, 536, 520 cm^{-1}

4i (minor): R_f = 0.59 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 2.3 Hz, 1H), 7.38 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.33 – 7.24 (m, 2H), 7.23 – 7.14 (m, 3H), 7.10 (d, *J* = 8.1 Hz, 1H), 4.32 – 4.18 (m, 2H), 3.78 (d, *J* = 12.2 Hz, 1H), 3.31 (dd, *J* = 17.1, 7.5 Hz, 1H), 3.08 (dd, *J* = 17.1, 5.5 Hz, 1H), 3.01 – 2.90 (m, 2H), 1.54 (t, *J* = 7.8 Hz, 1H), 1.20 (s, 3H), 1.00 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.4, 140.1, 134.3, 133.2, 132.5, 129.6, 129.4, 128.7, 128.5, 128.3, 126.4, 68.6, 61.8, 47.7, 36.5, 32.1, 27.0, 24.7, 23.4. HRMS (ESI) m/z calcd for $C_{21}H_{22}ClNO_2$ $[M+H]^+$: 356.1412, found: 356.1410. IR (neat): ν_{max} 3026, 2967, 2881, 1667, 1599, 1577, 1479, 1454, 1426, 1391, 1371, 1352, 1296, 1267, 1230, 1172, 1113, 1096, 1063, 1040, 1012, 1002, 963, 948, 906, 869, 817, 765, 725, 701, 684, 643, 612, 580, 553, 519 cm^{-1}

3-benzyl-6-chloro-4,4-dimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4j (major)



4j (minor)

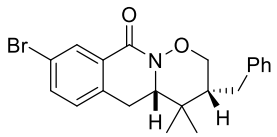
White solid; 50.0 mg, 69% yield, dr = 3.7:1;

4j (major): R_f = 0.48 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.8 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.33 – 7.16 (m, 4H), 7.09 (d, *J* = 7.4 Hz, 2H), 4.00 (t, *J* = 10.1 Hz, 2H), 3.80 (dd, *J* = 11.9, 3.5 Hz, 1H), 3.50 – 3.27 (m, 2H), 2.82 (d, *J* = 10.8 Hz, 1H), 2.12 – 1.97 (m, 2H), 1.20 (s, 3H), 0.65 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.1, 139.4, 133.8, 133.0, 132.2, 129.6, 128.8, 128.7, 127.9, 126.8, 126.5, 71.3, 65.1, 47.9, 38.5, 32.6, 24.9, 23.6, 15.0. HRMS (ESI) m/z calcd for $C_{21}H_{22}ClNO_2$ $[M+H]^+$: 356.1412, found: 356.1403. IR (neat): ν_{max} 3026, 2967, 2937, 2875, 1671, 1593, 1572, 1494, 1453, 1402, 1372, 1338, 1299, 1266, 1245, 1222, 1177, 1146, 1121, 1053, 1038, 995, 929, 912, 870, 804, 784, 743, 731, 700, 661, 646, 619, 596, 565, 539, 507 cm^{-1}

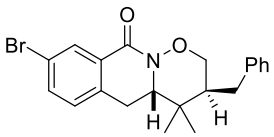
4j (minor): R_f = 0.49 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.8 Hz, 1H), 7.50 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.34 – 7.25 (m, 3H), 7.24 – 7.16 (m, 3H), 4.34 (dd, *J* = 7.6, 5.6

Hz, 1H), 4.23 (d, J = 12.3 Hz, 1H), 3.83 – 3.75 (m, 1H), 3.39 – 3.20 (m, 2H), 2.97 (d, J = 7.2 Hz, 2H), 1.56 (t, J = 7.9 Hz, 1H), 1.24 (s, 3H), 1.00 (d, J = 2.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.4, 140.2, 133.8, 133.1, 132.3, 129.6, 129.6, 128.7, 128.0, 127.1, 126.4, 68.6, 61.1, 47.7, 36.7, 32.1, 25.0, 24.7, 23.2. HRMS (ESI) m/z calcd for $C_{21}H_{22}ClNO_2$ $[M+H]^+$: 356.1412, found: 356.1403. IR (neat): ν_{max} 3026, 2966, 2882, 1674, 1594, 1572, 1493, 1453, 1395, 1371, 1352, 1299, 1266, 1238, 1167, 1119, 1066, 1045, 999, 960, 946, 914, 806, 789, 744, 728, 701 cm^{-1}

3-benzyl-8-bromo-4,4-dimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4k (major)



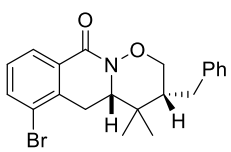
4k (minor)

White solid; 53.0 mg, 67% yield, dr = 4.2:1;

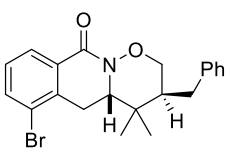
4k (major): R_f = 0.68 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.28 (d, J = 2.2 Hz, 1H), 7.54 (dd, J = 8.1, 2.2 Hz, 1H), 7.33 – 7.26 (m, 2H), 7.24 – 7.18 (m, 1H), 7.12 – 7.01 (m, 3H), 3.99 (ddd, J = 13.2, 8.8, 2.2 Hz, 2H), 3.80 (dd, J = 12.1, 3.9 Hz, 1H), 3.52 – 3.41 (m, 1H), 3.14 (dd, J = 17.5, 2.0 Hz, 1H), 2.80 (dd, J = 10.9, 8.6 Hz, 1H), 2.10 – 1.98 (m, 2H), 1.17 (s, 3H), 0.67 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.0, 139.4, 135.5, 135.0, 131.0, 129.6, 128.9, 128.8, 128.7, 126.6, 120.9, 71.5, 65.8, 48.0, 38.4, 32.6, 27.0, 23.6, 15.3. HRMS (ESI) m/z calcd for $C_{21}H_{22}BrNO_2$ $[M+H]^+$: 400.0907, found: 400.0900. IR (neat): ν_{max} 3026, 2968, 2935, 1669, 1594, 1574, 1495, 1475, 1453, 1427, 1395, 1372, 1336, 1295, 1270, 1236, 1181, 1106, 1052, 1037, 999, 984, 937, 909, 868, 811, 751, 731, 702, 674, 651, 615, 573, 533, 513 cm^{-1}

4k (minor): R_f = 0.69 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.29 (d, J = 2.1 Hz, 1H), 7.54 (dd, J = 8.1, 2.2 Hz, 1H), 7.33 – 7.26 (m, 2H), 7.24 – 7.15 (m, 3H), 7.04 (d, J = 8.1 Hz, 1H), 4.29 (dd, J = 7.6, 5.5 Hz, 1H), 4.26 – 4.18 (m, 1H), 3.78 (dd, J = 12.3, 1.5 Hz, 1H), 3.30 (dd, J = 17.1, 7.6 Hz, 1H), 3.06 (dd, J = 17.1, 5.5 Hz, 1H), 3.00 – 2.88 (m, 2H), 1.55 (t, J = 8.0 Hz, 1H), 1.20 (s, 3H), 1.01 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.3, 140.2, 135.5, 134.9, 131.3, 129.6, 129.6, 128.7, 128.7, 126.5, 68.7, 61.8, 47.7, 36.6, 32.1, 27.1, 24.7, 23.4. HRMS (ESI) m/z calcd for $C_{21}H_{22}BrNO_2$ $[M+H]^+$: 400.0907, found: 400.0892. IR (neat): ν_{max} 3025, 2966, 2880, 2239, 1666, 1594, 1574, 1493, 1477, 1454, 1424, 1391, 1371, 1352, 1295, 1268, 1230, 1172, 1107, 1065, 1040, 1012, 1001, 958, 908, 865, 814, 763, 727, 701, 681, 645, 612, 576, 550, 512 cm^{-1}

3-benzyl-6-bromo-4,4-dimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4l (major)



4l (minor)

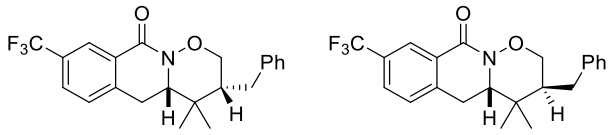
White solid; 55.0 mg, 69% yield, dr = 4.1:1;

4l (major): R_f = 0.58 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (d, J = 7.8 Hz, 1H), 7.67 (d, J = 7.9 Hz, 1H), 7.28 (t, J = 7.4 Hz, 2H), 7.20 (t, J = 7.8 Hz, 2H), 7.09 (d, J = 7.3 Hz, 2H), 4.00 (dt, J = 9.6, 6.4 Hz, 2H), 3.79 (dd, J = 11.9, 3.6 Hz, 1H), 3.50 – 3.38 (m, 1H), 3.32 (dd, J =

18.1, 8.5 Hz, 1H), 2.82 (d, J = 10.9 Hz, 1H), 2.11 – 1.97 (m, 2H), 1.20 (s, 3H), 0.65 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.0, 139.4, 136.3, 135.5, 129.7, 128.8, 128.7, 128.2, 127.5, 126.5, 122.6, 71.3, 65.1, 47.8, 38.5, 32.6, 27.8, 23.7, 15.1. HRMS (ESI) m/z calcd for $C_{21}H_{22}BrNO_2$ $[M+H]^+$: 400.0907, found: 400.0900. IR (neat): ν_{max} 2967, 2937, 2875, 1667, 1592, 1566, 1494, 1450, 1399, 1372, 1337, 1298, 1264, 1244, 1222, 1175, 1109, 1053, 1038, 992, 909, 860, 802, 772, 727, 699, 659, 645, 616, 592, 562, 536, 513 cm^{-1}

4l (minor): R_f = 0.59 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.15 (dd, J = 7.8, 1.3 Hz, 1H), 7.68 (dd, J = 8.0, 1.3 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.25 – 7.16 (m, 4H), 4.33 (dd, J = 7.9, 5.2 Hz, 1H), 4.24 (ddd, J = 12.2, 2.5, 1.3 Hz, 1H), 3.79 (dd, J = 12.2, 1.5 Hz, 1H), 3.33 (dd, J = 17.6, 7.8 Hz, 1H), 3.25 (dd, J = 17.6, 5.2 Hz, 1H), 3.01 – 2.94 (m, 2H), 1.57 – 1.54 (m, 1H), 1.24 (s, 3H), 1.01 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.3, 140.2, 136.4, 135.5, 129.6, 128.7, 128.3, 127.9, 126.5, 68.6, 61.2, 47.8, 36.7, 32.2, 28.0, 24.7, 23.2. HRMS (ESI) m/z calcd for $C_{21}H_{22}BrNO_2$ $[M+H]^+$: 400.0907, found: 400.0892. IR (neat): ν_{max} 3026, 2965, 2929, 1673, 1592, 1566, 1493, 1449, 1394, 1371, 1299, 1264, 1239, 1167, 1107, 1065, 998, 946, 861, 804, 776, 744, 716, 701, 585, 531, 516 cm^{-1}

3-benzyl-4,4-dimethyl-8-(trifluoromethyl)-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



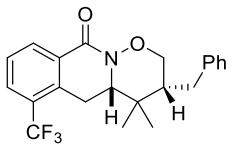
4m (major) **4m (minor)**

White solid; 53.0 mg, 68% yield, dr = 4.0:1;

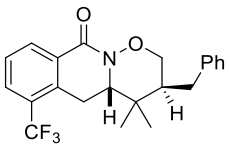
4m (major): R_f = 0.68 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.42 (d, J = 2.0 Hz, 1H), 7.66 (dd, J = 8.1, 1.9 Hz, 1H), 7.33 – 7.24 (m, 3H), 7.24 – 7.17 (m, 1H), 7.13 – 7.05 (m, 2H), 4.07 – 3.94 (m, 2H), 3.81 (dd, J = 11.9, 3.7 Hz, 1H), 3.57 (dd, J = 17.7, 8.7 Hz, 1H), 3.25 (dd, J = 17.7, 1.9 Hz, 1H), 2.87 – 2.75 (m, 1H), 2.11 – 1.97 (m, 2H), 1.19 (s, 3H), 0.65 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.9, 140.0, 139.3, 129.0, 129.0, 128.8, 128.7, 128.5, 127.6, 126.6, 125.3, 125.2, 71.5, 65.6, 47.9, 38.4, 32.5, 27.3, 23.5, 15.2. ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.5. HRMS (ESI) m/z calcd for $C_{22}H_{22}F_3NO_2$ $[M+H]^+$: 390.1675, found: 390.1680. IR (neat): ν_{max} 3028, 2969, 2938, 1669, 1621, 1496, 1469, 1453, 1397, 1373, 1328, 1294, 1272, 1251, 1235, 1167, 1122, 1104, 1068, 1037, 1001, 983, 941, 911, 878, 835, 818, 784, 753, 731, 700, 688, 656, 618, 599, 573, 532, 50 cm^{-1}

4m (minor): R_f = 0.69 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.47 – 8.42 (m, 1H), 7.70 – 7.66 (m, 1H), 7.32 – 7.28 (m, 3H), 7.23 – 7.17 (m, 3H), 4.34 (dd, J = 7.7, 5.3 Hz, 1H), 4.24 (ddd, J = 12.2, 2.5, 1.2 Hz, 1H), 3.81 (dd, J = 12.3, 1.5 Hz, 1H), 3.44 – 3.39 (m, 1H), 3.18 (dd, J = 17.3, 5.3 Hz, 1H), 2.99 – 2.94 (m, 2H), 1.59 – 1.55 (m, 1H), 1.22 (s, 3H), 1.01 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.2, 140.1, 139.8, 129.6, 129.0, 129.0, 128.7, 128.6, 127.7, 126.5, 125.7, 125.7, 68.7, 61.7, 47.7, 36.6, 32.1, 27.5, 24.7, 23.3. ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.6. HRMS (ESI) m/z calcd for $C_{22}H_{22}F_3NO_2$ $[M+H]^+$: 390.1675, found: 390.1679. IR (neat): ν_{max} 3027, 2969, 2882, 1672, 1621, 1494, 1455, 1394, 1354, 1329, 1293, 1270, 1254, 1230, 1167, 1124, 1105, 1069, 1041, 1013, 965, 950, 924, 875, 832, 783, 765, 715, 701, 680, 646, 626, 599, 547, 515 cm^{-1}

3-benzyl-4,4-dimethyl-6-(trifluoromethyl)-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4n (major)



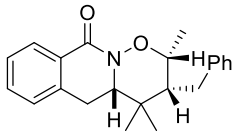
4n (minor)

White solid; 54.0 mg, 68% yield, dr = 5.0:1;

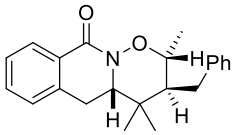
4n (major): R_f = 0.44 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.77 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.33 – 7.26 (m, 2H), 7.23 – 7.18 (m, 1H), 7.11 – 7.07 (m, 2H), 4.04 – 3.96 (m, 2H), 3.84 – 3.77 (m, 1H), 3.51 (d, *J* = 6.9 Hz, 2H), 2.82 (d, *J* = 11.3 Hz, 1H), 2.12 – 1.97 (m, 2H), 1.19 (s, 3H), 0.62 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.8, 139.4, 134.9, 134.9, 131.9, 130.0, 129.7, 129.6, 128.8, 128.7, 127.0, 126.6, 71.6, 65.3, 47.9, 38.5, 32.5, 24.4, 24.4, 23.5, 15.2. ^{19}F NMR (282 MHz, $CDCl_3$) δ -61.1. HRMS (ESI) m/z calcd for $C_{22}H_{22}F_3NO_2$ $[M+H]^+$: 390.1675, found: 390.1680. IR (neat): ν_{max} 3027, 2969, 2940, 1673, 1603, 1495, 1473, 1454, 1411, 1357, 1322, 1265, 1250, 1233, 1155, 1117, 1098, 1055, 1039, 995, 930, 874, 823, 744, 701, 689, 667, 646, 620, 600, 556, 526 cm^{-1}

4n (minor): R_f = 0.45 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 – 8.38 (m, 1H), 7.78 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.23 – 7.18 (m, 3H), 4.35 (dd, *J* = 7.6, 4.6 Hz, 1H), 4.26 – 4.22 (m, 1H), 3.79 (dd, *J* = 12.3, 1.4 Hz, 1H), 3.46 (dd, *J* = 17.6, 7.5 Hz, 1H), 3.37 (dd, *J* = 17.6, 4.6 Hz, 1H), 3.01 – 2.95 (m, 2H), 1.57 – 1.53 (m, 1H), 1.23 (s, 3H), 0.95 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.0, 140.1, 134.9, 132.2, 130.0, 129.7, 129.7, 129.6, 128.7, 127.1, 126.5, 68.8, 61.2, 47.7, 36.8, 32.2, 24.6, 24.5, 24.5, 23.3. ^{19}F NMR (564 MHz, $CDCl_3$) δ -60.9. HRMS (ESI) m/z calcd for $C_{22}H_{22}F_3NO_2$ $[M+H]^+$: 390.1675, found: 390.1677. IR (neat): ν_{max} 3027, 2968, 2884, 1672, 1601, 1494, 1475, 1455, 1407, 1395, 1373, 1353, 1321, 1269, 1246, 1234, 1156, 1117, 1097, 1080, 1067, 1045, 999, 960, 947, 912, 869, 821, 745, 728, 702, 687, 646, 629, 608, 593, 538, 513 cm^{-1}

3-benzyl-2,4,4-trimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4o (major)



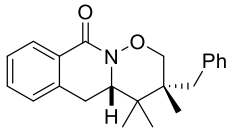
4o (minor)

White solid; 63.0 mg, 90% yield, dr = 1.2:1;

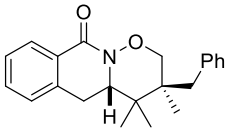
4o (major): R_f = 0.32 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.42 (td, *J* = 7.4, 1.6 Hz, 1H), 7.37 – 7.27 (m, 3H), 7.19 (ddd, *J* = 11.3, 7.1, 2.0 Hz, 4H), 4.06 – 3.96 (m, 2H), 3.13 (t, *J* = 14.5 Hz, 1H), 2.97 (dd, *J* = 13.8, 5.0 Hz, 1H), 2.84 (dd, *J* = 15.4, 3.6 Hz, 1H), 2.48 (dd, *J* = 13.8, 8.7 Hz, 1H), 1.87 (td, *J* = 8.4, 4.9 Hz, 1H), 1.34 (s, 3H), 1.09 (s, 3H), 0.96 (d, *J* = 6.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.9, 140.6, 136.7, 132.1, 129.0, 128.8, 128.3, 127.6, 127.3, 126.5, 80.6, 65.6, 47.8, 36.2, 35.0, 30.9, 26.0, 25.3, 19.8. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_2$ $[M+H]^+$: 336.1958, found: 336.1960. IR (neat): ν_{max} 3026, 2969, 2928, 2879, 1672, 1604, 1494, 1458, 1376, 1348, 1315, 1048, 987, 953, 738, 700, 503 cm^{-1}

4o (minor): R_f = 0.42 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.43 (td, *J* = 7.5, 1.5 Hz, 1H), 7.36 – 7.26 (m, 3H), 7.21 – 7.13 (m, 4H), 4.17 (dq, *J* = 10.1, 6.2 Hz, 1H), 4.04 (dd, *J* = 8.8, 1.9 Hz, 1H), 3.57 (dd, *J* = 17.3, 8.8 Hz, 1H), 3.18 (dd, *J* = 17.5, 2.0 Hz, 1H), 2.84 – 2.76 (m, 1H), 2.13 (dd, *J* = 15.4, 8.2 Hz, 1H), 1.91 (ddd, *J* = 10.3, 8.1, 2.2 Hz, 1H), 1.13 (s, 3H), 1.06 (d, *J* = 6.2 Hz, 3H), 0.68 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.1, 141.9, 136.2, 132.5, 128.7, 128.2, 126.9, 126.9, 126.2, 78.9, 66.0, 53.9, 39.2, 33.3, 27.6, 24.2, 19.1, 15.9. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_2$ $[M+H]^+$: 336.1958, found: 336.1951. IR (neat): ν_{max} 3027, 2969, 2934, 1669, 1604, 1494, 1461, 1403, 1375, 1341, 1265, 1185, 1137, 1090, 1066, 999, 949, 791, 737, 700, 649, 575, 520, 504 cm^{-1}

3-benzyl-3,4,4-trimethyl-3,4,4a,5-tetrahydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one



4p (major)



4p (minor)

White solid; 49.0 mg, 72% yield, dr = 3.7:1;

4p (major): R_f = 0.56 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.43 (td, *J* = 7.5, 1.5 Hz, 1H), 7.29 (d, *J* = 18.7 Hz, 2H), 7.25 – 7.17 (m, 2H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.08 – 6.96 (m, 2H), 4.47 – 4.25 (m, 2H), 3.62 – 3.44 (m, 2H), 3.11 (dd, *J* = 17.5, 2.3 Hz, 1H), 2.52 (s, 2H), 1.05 (d, *J* = 7.2 Hz, 6H), 0.85 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.6, 137.0, 132.6, 130.8, 128.3, 128.2, 127.9, 126.9, 126.8, 126.5, 61.5, 40.5, 39.7, 39.1, 27.5, 19.8, 18.1, 18.0. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_2$ $[M+H]^+$: 336.1958, found: 336.1954. IR (neat): ν_{max} 3027, 2972, 2879, 1668, 1604, 1584, 1493, 1459, 1399, 1384, 1337, 1276, 1252, 1091, 1032, 994, 924, 788, 759, 732, 705, 686, 663, 590, 554, 535, 507 cm^{-1}

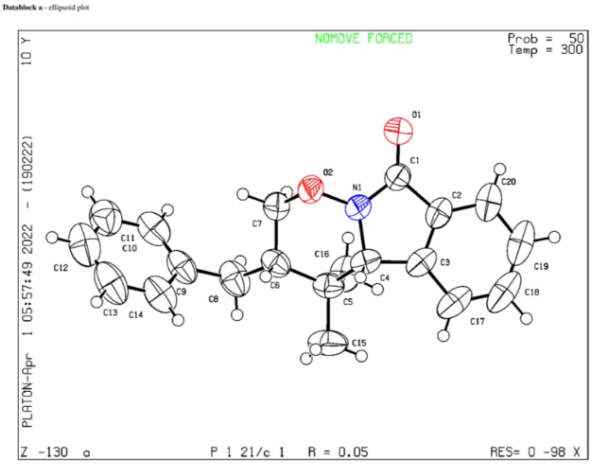
4p (minor): R_f = 0.60 (2:1 petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.44 (td, *J* = 7.5, 1.5 Hz, 1H), 7.31 (dd, *J* = 17.7, 6.8 Hz, 3H), 7.23 (d, *J* = 7.2 Hz, 3H), 7.16 (d, *J* = 7.5 Hz, 1H), 4.64 (dd, *J* = 8.6, 2.7 Hz, 1H), 3.82 (dd, *J* = 12.4, 1.5 Hz, 1H), 3.62 – 3.51 (m, 2H), 3.39 (d, *J* = 12.8 Hz, 1H), 3.14 (dd, *J* = 17.3, 2.8 Hz, 1H), 2.47 (dd, *J* = 12.8, 1.6 Hz, 1H), 1.07 (s, 3H), 0.79 (s, 3H), 0.62 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.9, 136.3, 132.6, 131.7, 128.4, 128.2, 127.9, 126.9, 126.8, 126.5, 72.3, 61.2, 40.3, 40.2, 37.7, 27.6, 19.5, 19.0, 15.2. HRMS (ESI) m/z calcd for $C_{22}H_{25}NO_2$ $[M+H]^+$: 336.1958, found: 336.1957. IR (neat): ν_{max} 3027, 2972, 2881, 1668, 1604, 1583, 1491, 1460, 1397, 1374, 1342, 1275, 1251, 1216, 1153, 1125, 1091, 1032, 994, 975, 912, 878, 854, 792, 732, 706, 687, 670, 643, 516 cm^{-1}

11. X-ray structure of products 2a (major), 2a (minor), 2s (major), 4a (major), 4a (minor) and 4p (major)

The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The refinements were carried out using full-matrix least-squares techniques on F^2 using the program SHELXL. In each case, the locations of the largest peaks in the final difference Fourier map calculations and the magnitude of the residual electron densities were of no chemical

significance. Positional parameters, hydrogen atom parameters, thermal parameters, bond distances, and angles have been deposited as supporting information.

Crystal Structure Report for 2a (major).



A single crystal with approximate dimensions of 0.25 mm x 0.20 mm x 0.18 mm was formed by recrystallization of **2a (major)** from a 2:1 petroleum ether/ethyl acetate mixture at room temperature and was used for the single-crystal X-ray crystallographic analysis. The X-ray intensity data were measured. All structures were solved by using the program SHELXS/T and Olex2. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication **no. CCDC 2243178**. Copies of the data can be obtained free of charge by application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk)

Crystal data and structure refinement for a.

Identification code	A
Empirical formula	$C_{20}H_{21}NO_2$
Formula weight	307.38
Temperature/K	300
Crystal system	Monoclinic
Space group	$P2_1/c$
a /Å	8.3899(2)
b/Å	17.2182(5)
c/Å	11.7013(3)
α/°	90
β/°	96.7210(10)
γ/°	90
Volume/Å^3	1678.74(8)
Z	4
ρ_{calc}g/cm^3	1.216
μ/mm^{-1}	0.618
F(000)	656.0

Crystal size/mm^3	0.25 × 0.2 × 0.18
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	9.18 to 148.906
Index ranges	-10 ≤ h ≤ 10, -21 ≤ k ≤ 21, -14 ≤ l ≤ 14
Reflections collected	32515
Independent reflections	3418 [R_{int} = 0.0340, R_{sigma} = 0.0180]
Data/restraints/parameters	3418/1/211
Goodness-of-fit on F^2	1.080
Final R indexes [I>=2σ (I)]	R_1 = 0.0477, wR_2 = 0.1381
Final R indexes [all data]	R_1 = 0.0497, wR_2 = 0.1400
Largest diff. peak/hole / e Å^{-3}	0.25/-0.20

Bond Lengths for a.

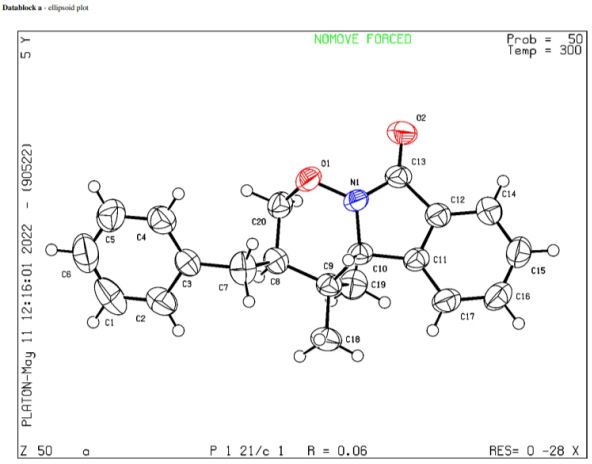
Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.2144(17)	C5	C16	1.5284(19)
O2	N1	1.3874(13)	C6	C7	1.5130(19)
O2	C7	1.4441(16)	C6	C8	1.5447(19)
N1	C1	1.3465(18)	C8	C9	1.509(2)
N1	C4	1.4522(16)	C9	C10	1.384(3)
C1	C2	1.4848(18)	C9	C14	1.387(2)
C2	C3	1.385(2)	C10	C11	1.377(2)
C2	C20	1.381(2)	C11	C12	1.361(3)
C3	C4	1.508(2)	C12	C13	1.371(3)
C3	C17	1.3919(19)	C13	C14	1.396(3)
C4	C5	1.5567(19)	C17	C18	1.379(3)
C5	C6	1.553(2)	C18	C19	1.379(3)
C5	C15	1.533(2)	C19	C20	1.388(3)

Bond Angles for a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	O2	C7	107.46(9)	C16	C5	C6	112.06(12)
O2	N1	C4	118.90(11)	C16	C5	C15	110.45(13)
C1	N1	O2	123.19(10)	C7	C6	C5	112.30(10)
C1	N1	C4	117.88(11)	C7	C6	C8	108.47(12)
O1	C1	N1	127.12(12)	C8	C6	C5	114.18(11)
O1	C1	C2	129.60(13)	O2	C7	C6	111.37(11)
N1	C1	C2	103.26(11)	C9	C8	C6	113.24(12)
C3	C2	C1	109.45(12)	C10	C9	C8	121.21(14)
C20	C2	C1	127.81(15)	C10	C9	C14	117.63(16)
C20	C2	C3	122.71(14)	C14	C9	C8	121.16(17)
C2	C3	C4	110.10(11)	C11	C10	C9	121.59(16)
C2	C3	C17	119.32(16)	C12	C11	C10	120.4(2)
C17	C3	C4	130.58(16)	C11	C12	C13	119.52(19)

N1	C4	C3	99.22(11)	C12	C13	C14	120.50(17)
N1	C4	C5	111.02(11)	C9	C14	C13	120.30(19)
C3	C4	C5	118.22(11)	C18	C17	C3	118.37(19)
C6	C5	C4	106.60(10)	C19	C18	C17	121.58(16)
C15	C5	C4	107.71(13)	C18	C19	C20	120.87(18)
C15	C5	C6	109.32(13)	C2	C20	C19	117.1(2)
C16	C5	C4	110.54(12)	-	-	-	-

Crystal Structure Report for 2a (minor).



A single crystal with approximate dimensions of 0.20 mm x 0.15 mm x 0.13 mm was formed by recrystallization of **2a (minor)** from a 2:1 petroleum ether/ethyl acetate mixture at room temperature and was used for the single-crystal X-ray crystallographic analysis. The X-ray intensity data were measured. All structures were solved by using the program SHELXS/T and Olex2. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication **no. CCDC 2244760**. Copies of the data can be obtained free of charge by application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk)

Crystal data and structure refinement for a.

Identification code	A
Empirical formula	$C_{20}H_{21}NO_2$
Formula weight	307.38
Temperature/K	300
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.5000(10)
b/Å	14.8211(17)
c/Å	13.0677(16)
α/°	90
β/°	91.708(5)
γ/°	90
Volume/Å^3	1645.5(3)

Z	4
ρ_{calc}g/cm^3	1.241
μ/mm^{-1}	0.630
F(000)	656.0
Crystal size/mm^3	0.20 × 0.15 × 0.13
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	9.024 to 140.376
Index ranges	-10 ≤ h ≤ 10, -18 ≤ k ≤ 18, -14 ≤ l ≤ 13
Reflections collected	14313
Independent reflections	3002 [R_{int} = 0.0812, R_{sigma} = 0.0515]
Data/restraints/parameters	3002/0/211
Goodness-of-fit on F^2	1.096
Final R indexes [I>=2σ (I)]	R_1 = 0.0626, wR_2 = 0.1966
Final R indexes [all data]	R_1 = 0.0705, wR_2 = 0.2064
Largest diff. peak/hole / e Å^{-3}	0.23/-0.25

Bond Lengths for a.

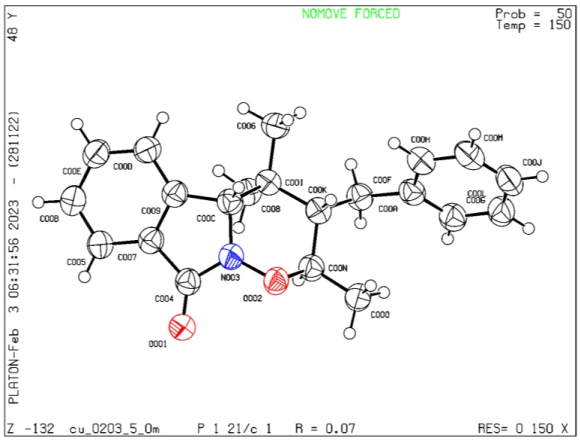
Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	N1	1.391(2)	C8	C9	1.557(3)
O1	C20	1.457(2)	C8	C20	1.522(3)
O2	C13	1.220(2)	C9	C10	1.552(2)
N1	C10	1.458(2)	C9	C18	1.527(3)
N1	C13	1.350(3)	C9	C19	1.527(3)
C1	C2	1.392(4)	C10	C11	1.507(2)
C1	C6	1.374(5)	C11	C12	1.383(3)
C2	C3	1.387(3)	C11	C17	1.391(3)
C3	C4	1.380(3)	C12	C13	1.486(3)
C3	C7	1.505(3)	C12	C14	1.383(3)
C4	C5	1.377(4)	C14	C15	1.381(3)
C5	C6	1.355(5)	C15	C16	1.378(4)
C7	C8	1.538(3)	C16	C17	1.388(3)

Bond Angles for a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	O1	C20	108.54(13)	C19	C9	C10	111.48(16)
O1	N1	C10	118.64(15)	C19	C9	C18	108.42(16)
C13	N1	O1	123.57(15)	N1	C10	C9	109.55(14)
C13	N1	C10	117.16(15)	N1	C10	C11	99.42(14)
C6	C1	C2	120.5(3)	C11	C10	C9	116.21(14)
C3	C2	C1	119.9(2)	C12	C11	C10	119.89(18)
C2	C3	C7	120.1(2)	C12	C11	C17	110.02(15)
C4	C3	C2	118.3(2)	C17	C11	C10	130.10(18)
C4	C3	C7	121.60(19)	C11	C12	C13	109.56(16)

C5	C4	C3	121.1(2)	C14	C12	C11	121.80(18)
C6	C5	C4	120.7(3)	C14	C12	C13	128.64(19)
C5	C6	C1	119.5(2)	O2	C13	N1	126.99(18)
C3	C7	C8	113.12(17)	O2	C13	C12	129.56(19)
C7	C8	C9	114.98(16)	N1	C13	C12	103.41(15)
C20	C8	C7	110.08(17)	C15	C14	C12	117.9(2)
C20	C8	C9	110.40(15)	C16	C15	C14	120.9(2)
C10	C9	C8	107.56(13)	C15	C16	C17	121.19(19)
C18	C9	C8	111.24(16)	C16	C17	C11	118.2(2)
C18	C9	C10	108.91(15)	O1	C20	C8	110.21(15)
C19	C9	C8	109.26(16)	-	-	-	-

Crystal Structure Report for 2s (major).



A single crystal with approximate dimensions of 0.20 mm x 0.15 mm x 0.10 mm was formed by recrystallization of **2s (major)** from a 2:1 petroleum ether/ethyl acetate mixture at room temperature and was used for the single-crystal X-ray crystallographic analysis. The X-ray intensity data were measured. All structures were solved by using the program SHELXS/T and Olex2. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication **no. CCDC 2244761**. Copies of the data can be obtained free of charge by application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk)

Crystal data and structure refinement for cu_0203_5_0m.

Identification code	cu_0203_5_0m
Empirical formula	$C_{21}H_{23}NO_2$
Formula weight	321.40
Temperature/K	150
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	10.8205(2)
b/Å	15.6904(4)

c/Å	11.3118(3)
α/°	90
β/°	117.9190(10)
γ/°	90
Volume/Å^3	1696.97(7)
Z	4
ρ_{calc}g/cm^3	1.258
μ/mm^{-1}	0.633
F(000)	688.0
Crystal size/mm^3	0.20 × 0.15 × 0.10
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	9.25 to 149.498
Index ranges	-13 ≤ h ≤ 13, -19 ≤ k ≤ 19, -14 ≤ l ≤ 14
Reflections collected	17442
Independent reflections	3457 [R_{int} = 0.0276, R_{sigma} = 0.0245]
Data/restraints/parameters	3457/0/220
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0730, wR_2 = 0.1799
Final R indexes [all data]	R_1 = 0.0742, wR_2 = 0.1827
Largest diff. peak/hole / e Å^{-3}	0.34/-0.25

Bond Lengths for cu_0203_5_0m.

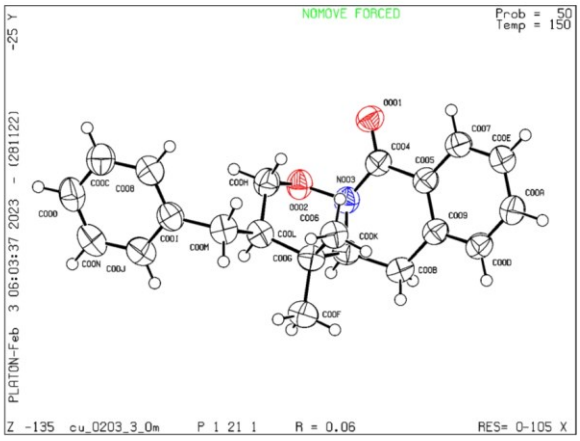
Atom	Atom	Length/Å	Atom	Atom	Length/Å
O001	C004	1.2184(18)	C00A	C00G	1.394(2)
O002	N003	1.3805(15)	C00A	C00H	1.398(2)
O002	C00N	1.4540(17)	C00B	C00E	1.395(2)
N003	C004	1.3573(18)	C00C	C00I	1.5598(18)
N003	C00C	1.4563(18)	C00D	C00E	1.392(2)
C004	C007	1.4870(19)	C00F	C00K	1.5512(18)
C005	C007	1.3883(19)	C00G	C00L	1.394(2)
C005	C00B	1.387(2)	C00H	C00M	1.390(2)
C006	C00I	1.5322(18)	C00I	C00K	1.5538(18)
C007	C009	1.396(2)	C00J	C00L	1.388(3)
C008	C00I	1.5369(18)	C00J	C00M	1.382(3)
C009	C00C	1.5106(19)	C00K	C00N	1.5311(19)
C009	C00D	1.391(2)	C00N	C00O	1.5093(19)
C00A	C00F	1.5143(19)	-	-	-

Bond Angles for cu_0203_5_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°

N003	O002	C00N	109.29(10)	C009	C00D	C00E	118.34(14)
O002	N003	C00C	119.70(11)	C00D	C00E	C00B	121.42(14)
C004	N003	O002	122.52(11)	C00A	C00F	C00K	115.03(11)
C004	N003	C00C	117.64(12)	C00A	C00G	C00L	120.93(15)
O001	C004	N003	127.07(13)	C00M	C00H	C00A	120.90(16)
O001	C004	C007	129.85(13)	C006	C00I	C008	110.14(11)
N003	C004	C007	103.08(12)	C006	C00I	C00C	107.79(11)
C00B	C005	C007	117.71(14)	C006	C00I	C00K	109.85(11)
C005	C007	C004	127.84(13)	C008	C00I	C00C	110.24(11)
C005	C007	C009	122.30(13)	C008	C00I	C00K	111.65(11)
C009	C007	C004	109.86(12)	C00K	C00I	C00C	107.04(10)
C007	C009	C00C	109.57(12)	C00M	C00J	C00L	119.41(15)
C00D	C009	C007	119.65(13)	C00F	C00K	C00I	113.27(11)
C00D	C009	C00C	130.77(13)	C00N	C00K	C00F	110.04(11)
C00G	C00A	C00F	121.28(13)	C00N	C00K	C00I	112.42(11)
C00G	C00A	C00H	118.06(14)	C00J	C00L	C00G	120.21(16)
C00H	C00A	C00F	120.61(13)	C00J	C00M	C00H	120.48(16)
C005	C00B	C00E	120.58(14)	O002	C00N	C00K	109.89(11)
N003	C00C	C009	99.74(10)	O002	C00N	C00O	103.36(10)
N003	C00C	C00I	110.09(11)	C00O	C00N	C00K	115.16(12)
C009	C00C	C00I	117.61(11)	-	-	-	-

Crystal Structure Report for 4a (major).



A single crystal with approximate dimensions of 0.20 mm x 0.15 mm x 0.10 mm was formed by recrystallization of **4a (major)** from a 2:1 petroleum ether/ethyl acetate mixture at room temperature and was used for the single-crystal X-ray crystallographic analysis. The X-ray intensity data were measured. All structures were solved by using the program SHELXS/T and Olex2. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication **no. CCDC 2244762**. Copies of the data can be obtained free of charge by application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk)

Crystal data and structure refinement for cu_0203_3_0m.

Identification code	cu_0203_3_0m
Empirical formula	$C_{21}H_{23}NO_2$
Formula weight	321.40
Temperature/K	150
Crystal system	Monoclinic
Space group	$P2_1$
a/Å	7.9121(3)
b/Å	9.1248(3)
c/Å	11.9813(4)
α/°	90
β/°	101.4770(10)
γ/°	90
Volume/Å^3	847.71(5)
Z	2
ρ_{calc}g/cm^3	1.259
μ/mm^{-1}	0.633
F(000)	344.0
Crystal size/mm^3	0.20 × 0.15 × 0.10
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	12.284 to 149.31
Index ranges	$-9 \le h \le 9$, $-11 \le k \le 11$, $-14 \le l \le 14$
Reflections collected	14417
Independent reflections	3392 [R_{int} = 0.0288, R_{sigma} = 0.0309]
Data/restraints/parameters	3392/1/219
Goodness-of-fit on F^2	1.091
Final R indexes [I>=2σ (I)]	R_1 = 0.0599, wR_2 = 0.1450
Final R indexes [all data]	R_1 = 0.0601, wR_2 = 0.1453
Largest diff. peak/hole / e Å^{-3}	0.31/-0.22
Flack parameter	0.01(7)

Bond Lengths for cu_0203_3_0m.

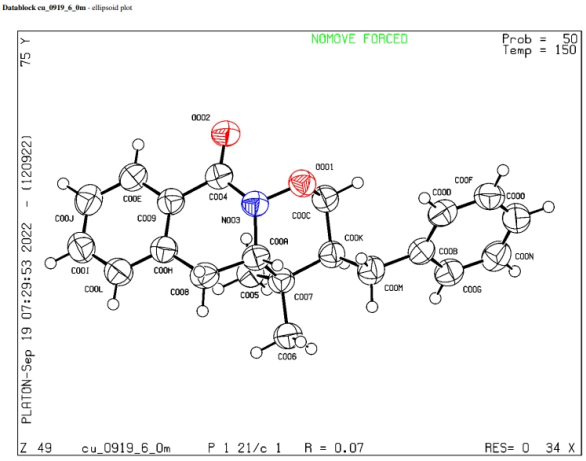
Atom	Atom	Length/Å	Atom	Atom	Length/Å
O001	C004	1.215(3)	C00A	C00D	1.387(4)
O002	N003	1.402(2)	C00A	C00E	1.392(4)
O002	C00H	1.441(3)	C00B	C00K	1.532(3)
N003	C004	1.364(3)	C00C	C00O	1.379(5)
N003	C00K	1.468(3)	C00F	C00G	1.533(3)
C004	C005	1.498(3)	C00G	C00K	1.557(3)

C005	C007	1.387(3)	C00G	C00L	1.560(3)
C005	C009	1.407(3)	C00H	C00L	1.527(3)
C006	C00G	1.535(3)	C00I	C00J	1.393(4)
C007	C00E	1.389(3)	C00I	C00M	1.520(3)
C008	C00C	1.385(4)	C00J	C00N	1.388(4)
C008	C00I	1.380(4)	C00L	C00M	1.535(4)
C009	C00B	1.502(3)	C00N	C00O	1.379(5)
C009	C00D	1.385(3)	-	-	-

Bond Angles for cu_0203_3_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N003	O002	C00H	107.89(16)	C006	C00G	C00K	112.06(19)
O002	N003	C00K	111.99(17)	C006	C00G	C00L	112.11(19)
C004	N003	O002	115.34(18)	C00F	C00G	C006	109.6(2)
C004	N003	C00K	127.66(18)	C00F	C00G	C00K	107.4(2)
O001	C004	N003	123.0(2)	C00F	C00G	C00L	108.62(19)
O001	C004	C005	122.4(2)	C00K	C00G	C00L	106.85(18)
N003	C004	C005	114.62(19)	O002	C00H	C00L	111.5(2)
C007	C005	C004	118.16(19)	C008	C00I	C00J	118.4(2)
C007	C005	C009	120.9(2)	C008	C00I	C00M	121.1(2)
C009	C005	C004	121.0(2)	C00J	C00I	C00M	120.5(2)
C005	C007	C00E	120.0(2)	C00N	C00J	C00I	120.7(3)
C00I	C008	C00C	121.2(3)	N003	C00K	C00B	108.36(18)
C005	C009	C00B	120.16(19)	N003	C00K	C00G	111.12(18)
C00D	C009	C005	118.6(2)	C00B	C00K	C00G	116.77(19)
C00D	C009	C00B	121.2(2)	C00H	C00L	C00G	111.89(18)
C00D	C00A	C00E	120.8(2)	C00H	C00L	C00M	109.1(2)
C009	C00B	C00K	115.04(19)	C00M	C00L	C00G	113.73(19)
C00O	C00C	C008	119.9(3)	C00I	C00M	C00L	114.1(2)
C009	C00D	C00A	120.5(2)	C00O	C00N	C00J	119.9(3)
C007	C00E	C00A	119.3(2)	C00C	C00O	C00N	120.0(2)

Crystal Structure Report for 4a (minor).



A single crystal with approximate dimensions of 0.20 mm x 0.15 mm x 0.10 mm was formed by recrystallization of **4a (minor)** from a 2:1 petroleum ether/ethyl acetate mixture at room temperature and was used for the single-crystal X-ray crystallographic analysis. The X-ray intensity data were measured. All structures were solved by using the program SHELXS/T and Olex2. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication **no. CCDC 2244763**. Copies of the data can be obtained free of charge by application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk)

Crystal data and structure refinement for cu_0919_6_0m.

Identification code	cu_0919_6_0m
Empirical formula	$C_{21}H_{23}NO_2$
Formula weight	321.40
Temperature/K	150
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.1681(4)
b/Å	16.0212(8)
c/Å	11.4696(5)
α/°	90
β/°	93.233(2)
γ/°	90
Volume/Å^3	1682.02(13)
Z	4
ρ_{calc}g/cm^3	1.269
μ/mm^{-1}	0.638
F(000)	688.0
Crystal size/mm^3	0.20 × 0.15 × 0.10
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	9.662 to 155.602
Index ranges	$-11 \le h \le 11$, $-20 \le k \le 20$, $-14 \le l \le 12$
Reflections collected	34118
Independent reflections	3563 [R_{int} = 0.0368, R_{sigma} = 0.0239]
Data/restraints/parameters	3563/0/219
Goodness-of-fit on F^2	1.073
Final R indexes [I>=2σ (I)]	R_1 = 0.0656, wR_2 = 0.1668
Final R indexes [all data]	R_1 = 0.0676, wR_2 = 0.1709
Largest diff. peak/hole / e Å^{-3}	0.34/-0.17

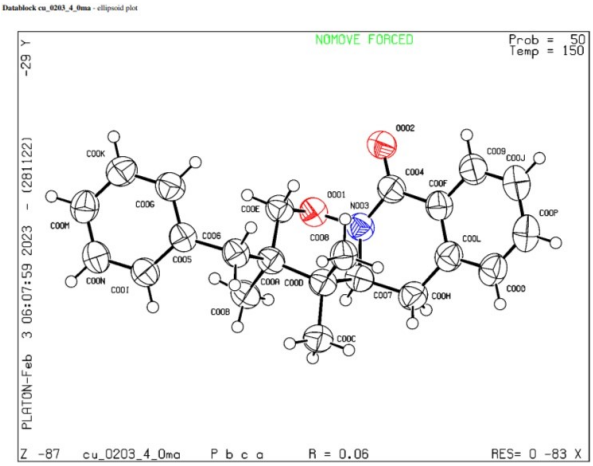
Bond Lengths for cu_0919_6_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O001	N003	1.4048(14)	C00B	C00D	1.3922(19)
O001	C00C	1.4471(16)	C00B	C00G	1.3972(19)
O002	C004	1.2232(15)	C00B	C00M	1.5091(19)
N003	C004	1.3660(16)	C00C	C00K	1.5242(17)
N003	C00A	1.4675(16)	C00D	C00F	1.384(2)
C004	C009	1.4938(18)	C00E	C00J	1.382(2)
C005	C007	1.5368(17)	C00F	C00O	1.383(2)
C006	C007	1.5327(17)	C00G	C00N	1.389(2)
C007	C00A	1.5490(17)	C00H	C00L	1.394(2)
C007	C00K	1.5635(17)	C00I	C00J	1.395(2)
C008	C00A	1.5285(18)	C00I	C00L	1.383(2)
C008	C00H	1.5045(19)	C00K	C00M	1.5475(18)
C009	C00E	1.3949(19)	C00N	C00O	1.380(2)
C009	C00H	1.4002(18)	-	-	-

Bond Angles for cu_0919_6_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N003	O001	C00C	107.93(9)	C00D	C00B	C00G	117.93(13)
O001	N003	C00A	112.20(9)	C00D	C00B	C00M	121.41(12)
C004	N003	O001	115.46(9)	C00G	C00B	C00M	120.63(12)
C004	N003	C00A	126.77(11)	O001	C00C	C00K	110.84(10)
O002	C004	N003	122.57(12)	C00F	C00D	C00B	121.24(14)
O002	C004	C009	122.54(12)	C00J	C00E	C009	120.26(13)
N003	C004	C009	114.89(10)	C00O	C00F	C00D	120.11(14)
C005	C007	C00A	111.83(10)	C00N	C00G	C00B	120.73(13)
C005	C007	C00K	109.13(10)	C009	C00H	C008	120.17(12)
C006	C007	C005	107.53(10)	C00L	C00H	C008	121.06(12)
C006	C007	C00A	109.67(10)	C00L	C00H	C009	118.74(13)
C006	C007	C00K	111.02(10)	C00L	C00I	C00J	120.52(14)
C00A	C007	C00K	107.68(10)	C00E	C00J	C00I	119.44(14)
C00H	C008	C00A	114.68(10)	C00C	C00K	C007	110.35(10)
C00E	C009	C004	118.48(11)	C00C	C00K	C00M	110.24(11)
C00E	C009	C00H	120.44(12)	C00M	C00K	C007	113.71(10)
C00H	C009	C004	121.05(11)	C00I	C00L	C00H	120.59(14)
N003	C00A	C007	110.14(9)	C00B	C00M	C00K	112.98(11)
N003	C00A	C008	108.64(10)	C00O	C00N	C00G	120.36(14)
C008	C00A	C007	117.31(11)	C00N	C00O	C00F	119.62(14)

Crystal Structure Report for 4p (major).



A single crystal with approximate dimensions of 0.20 mm x 0.15 mm x 0.10 mm was formed by recrystallization of **4p (major)** from a 2:1 petroleum ether/ethyl acetate mixture at room temperature and was used for the single-crystal X-ray crystallographic analysis. The X-ray intensity data were measured. All structures were solved by using the program SHELXS/T and Olex2. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication **no. CCDC 2244764**. Copies of the data can be obtained free of charge by application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk)

Crystal data and structure refinement for cu_0203_4_0ma.

Identification code	cu_0203_4_0ma
Empirical formula	$C_{22}H_{25}NO_2$
Formula weight	335.43
Temperature/K	150
Crystal system	orthorhombic
Space group	Pbca
a/Å	12.8140(4)
b/Å	9.0568(3)
c/Å	30.5543(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3545.9(2)
Z	8
ρ_{calc}g/cm^3	1.257
μ/mm^{-1}	0.626
F(000)	1440.0
Crystal size/mm^3	0.20 × 0.15 × 0.10
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5.784 to 149.066

Index ranges	$-15 \leq h \leq 16, -11 \leq k \leq 8, -38 \leq l \leq 37$
Reflections collected	41144
Independent reflections	3621 [$R_{int} = 0.0423$, $R_{sigma} = 0.0263$]
Data/restraints/parameters	3621/0/229
Goodness-of-fit on F^2	1.084
Final R indexes [I>=2σ (I)]	$R_1 = 0.0644$, $wR_2 = 0.1671$
Final R indexes [all data]	$R_1 = 0.0678$, $wR_2 = 0.1736$
Largest diff. peak/hole / e $Å^{-3}$	0.31/-0.17

Bond Lengths for cu_0203_4_0ma.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O001	N003	1.4019(15)	C009	C00J	1.385(2)
O001	C00E	1.4428(16)	C00A	C00B	1.5389(18)
O002	C004	1.2249(18)	C00A	C00D	1.5794(19)
N003	C004	1.3625(18)	C00A	C00E	1.5353(18)
N003	C007	1.4709(17)	C00C	C00D	1.5397(18)
C004	C00F	1.495(2)	C00F	C00L	1.400(2)
C005	C006	1.5131(19)	C00G	C00K	1.386(2)
C005	C00G	1.393(2)	C00H	C00L	1.502(2)
C005	C00I	1.3936(19)	C00I	C00N	1.389(2)
C006	C00A	1.5528(18)	C00J	C00P	1.385(3)
C007	C00D	1.5554(18)	C00K	C00M	1.388(2)
C007	C00H	1.5271(19)	C00L	C00O	1.394(2)
C008	C00D	1.5419(18)	C00M	C00N	1.383(2)
C009	C00F	1.393(2)	C00O	C00P	1.384(3)

Bond Angles for cu_0203_4_0ma.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N003	O001	C00E	108.30(9)	C008	C00D	C007	110.74(11)
O001	N003	C007	111.90(10)	C008	C00D	C00A	111.90(11)
C004	N003	O001	115.58(11)	C00C	C00D	C007	107.44(11)
C004	N003	C007	127.22(12)	C00C	C00D	C008	108.12(11)
O002	C004	N003	122.38(13)	C00C	C00D	C00A	110.83(11)
O002	C004	C00F	122.70(13)	O001	C00E	C00A	111.45(11)
N003	C004	C00F	114.90(12)	C009	C00F	C004	118.72(13)
C00G	C005	C006	120.29(12)	C009	C00F	C00L	120.21(14)
C00G	C005	C00I	117.88(13)	C00L	C00F	C004	121.02(13)
C00I	C005	C006	121.78(13)	C00K	C00G	C005	121.40(14)
C005	C006	C00A	115.80(11)	C00L	C00H	C007	115.81(12)
N003	C007	C00D	110.94(11)	C00N	C00I	C005	121.03(14)
N003	C007	C00H	108.96(11)	C009	C00J	C00P	119.58(16)
C00H	C007	C00D	116.61(11)	C00G	C00K	C00M	119.91(15)

C00J	C009	C00F	120.35(16)	C00F	C00L	C00H	120.43(13)
C006	C00A	C00D	110.59(10)	C00O	C00L	C00F	118.74(15)
C00B	C00A	C006	109.86(11)	C00O	C00L	C00H	120.81(14)
C00B	C00A	C00D	111.32(11)	C00N	C00M	C00K	119.53(14)
C00E	C00A	C006	107.86(11)	C00M	C00N	C00I	120.24(14)
C00E	C00A	C00B	108.29(11)	C00P	C00O	C00L	120.65(16)
C00E	C00A	C00D	108.84(11)	C00O	C00P	C00J	120.46(15)
C007	C00D	C00A	107.73(10)	-	-	-	-

12. Copies of ^{1}H, ^{13}C and ^{19}F NMR spectra

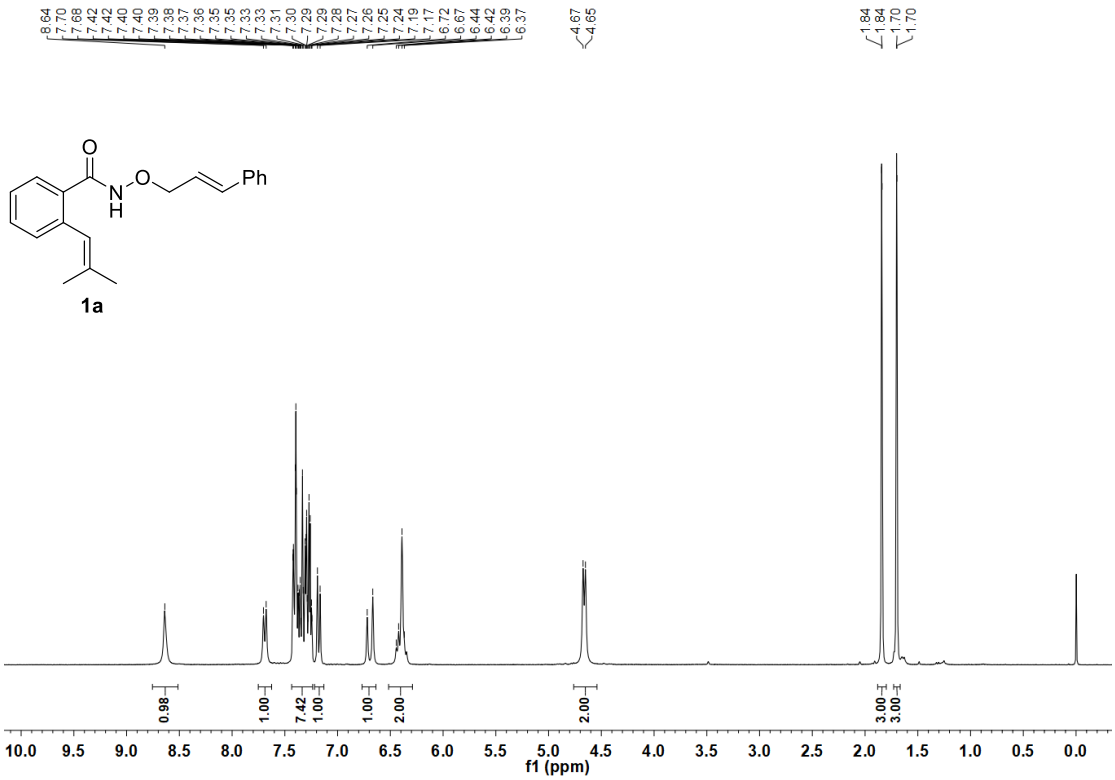


Figure S9. ^{1}H NMR spectra of **1a** (300 MHz, $CDCl_3$)

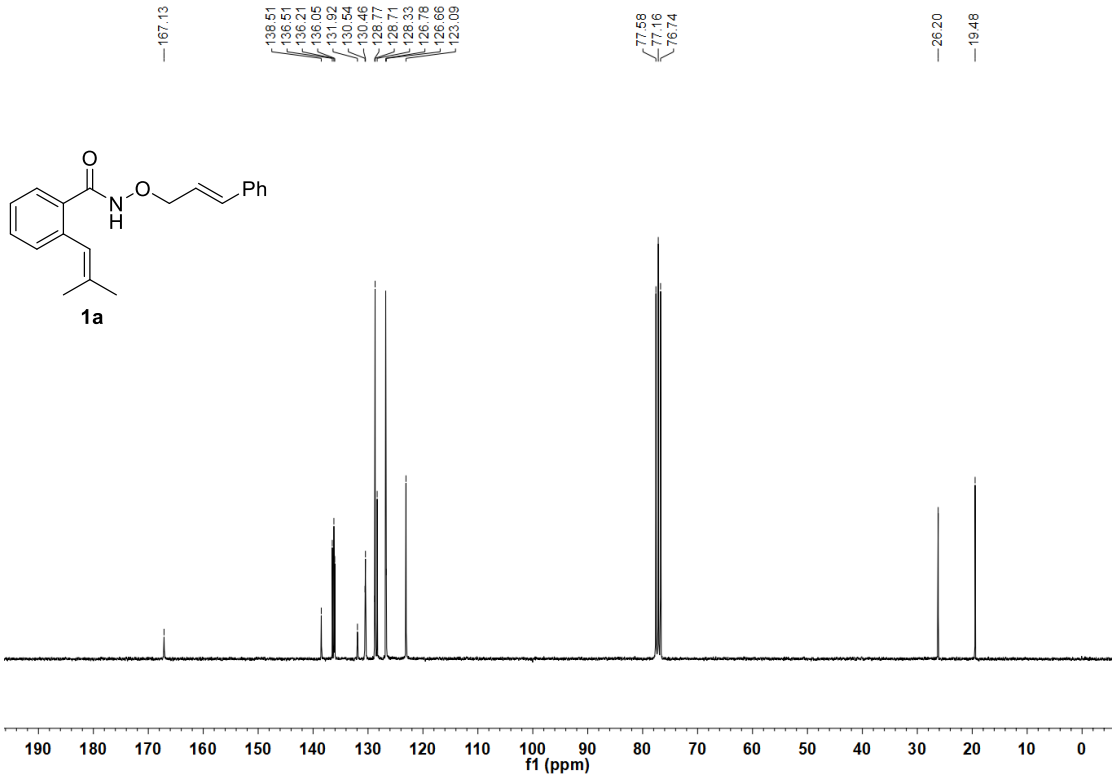


Figure S10. ^{13}C NMR spectra of **1a** (75 MHz, $CDCl_3$)

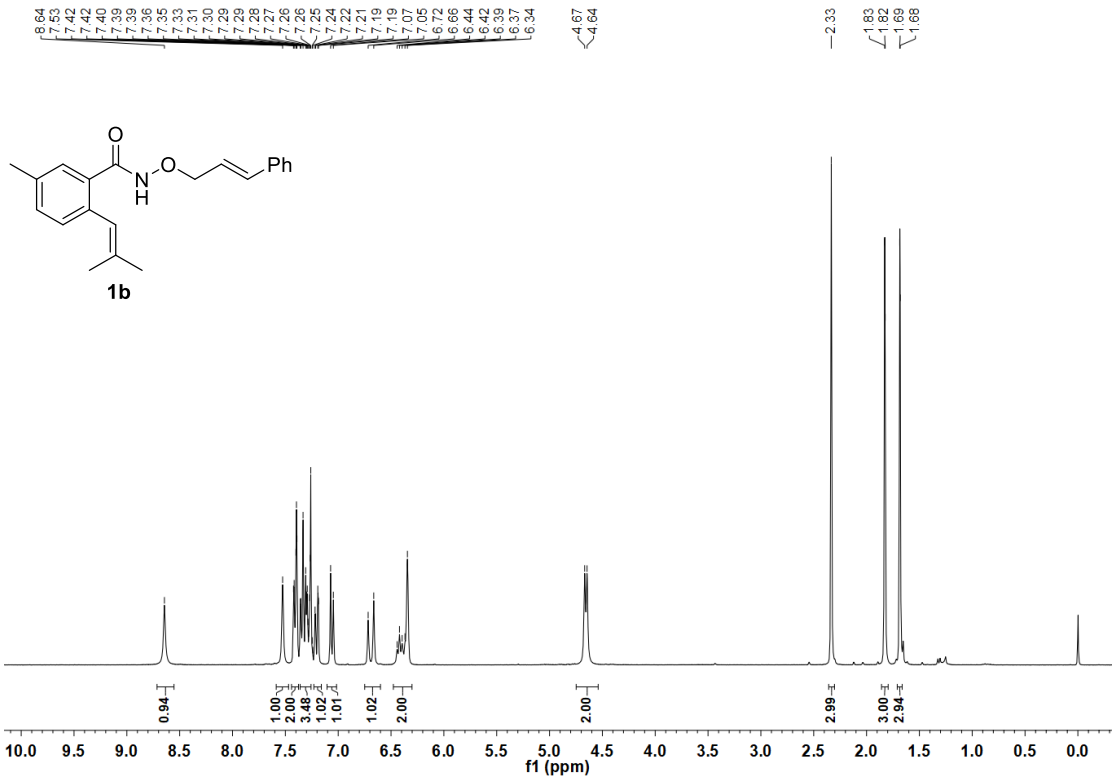


Figure S11. ^{1}H NMR spectra of **1b** (300 MHz, $CDCl_3$)

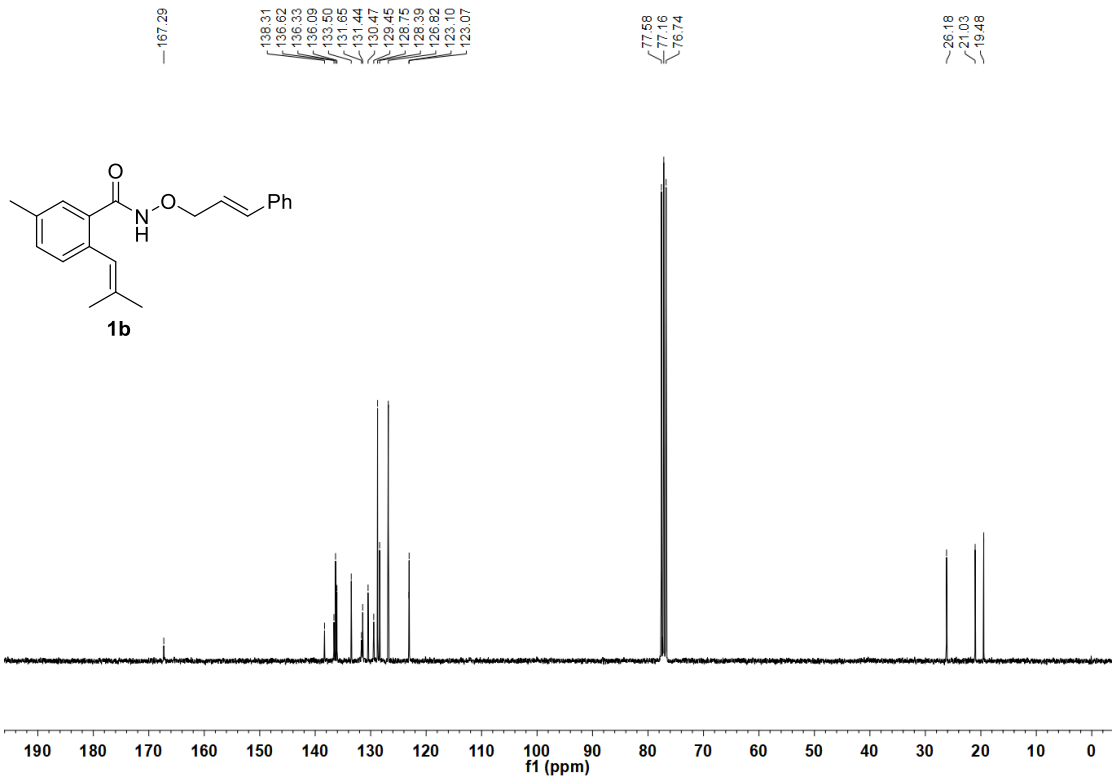


Figure S12. ^{13}C NMR spectra of **1b** (75 MHz, $CDCl_3$)

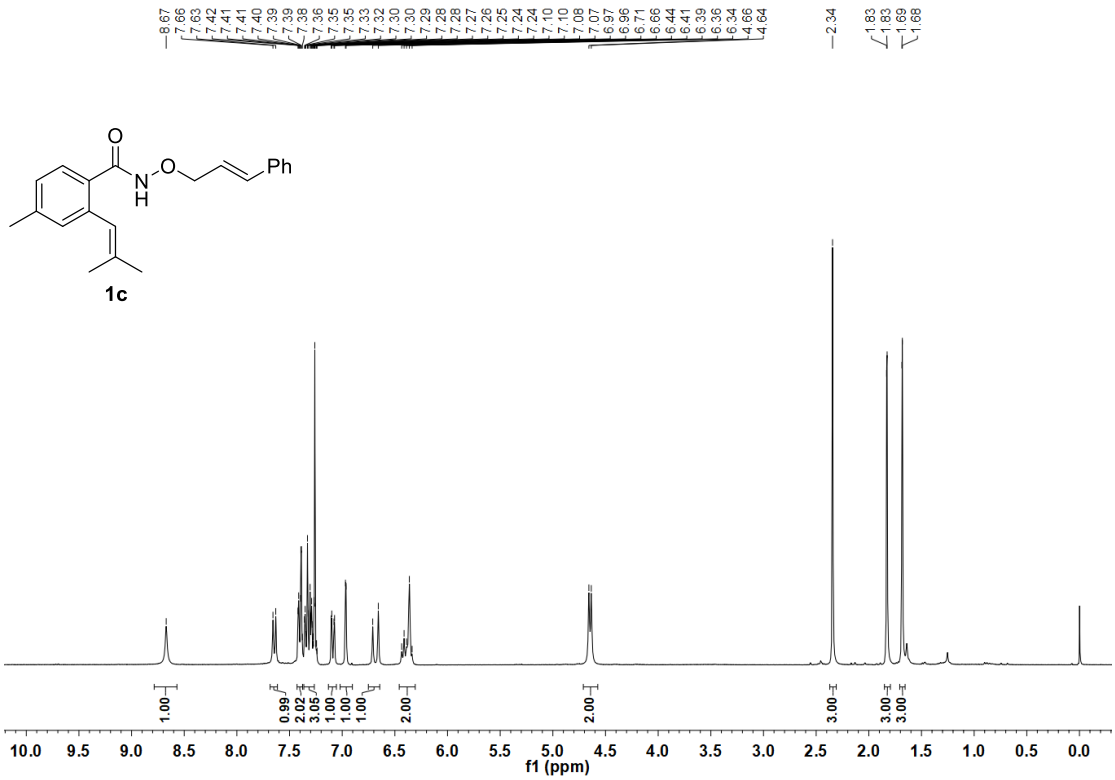


Figure S13. ^{1}H NMR spectra of **1c** (300 MHz, $CDCl_3$)

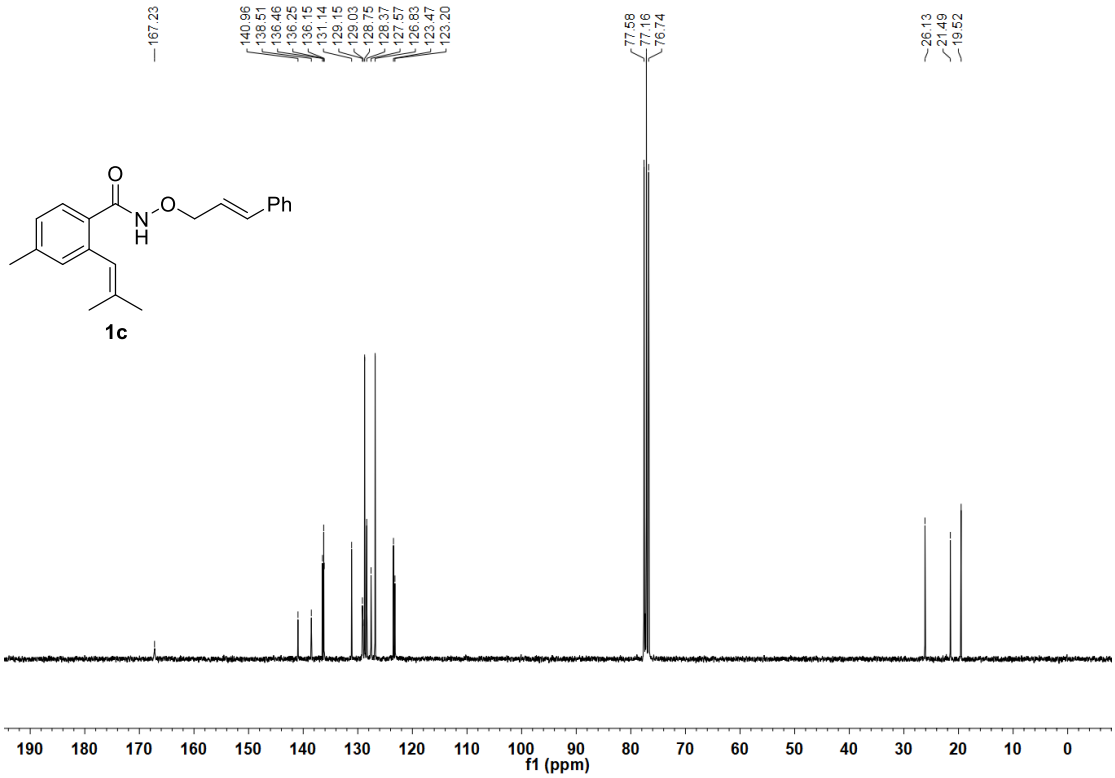


Figure S14. ^{13}C NMR spectra of **1c** (75 MHz, $CDCl_3$)

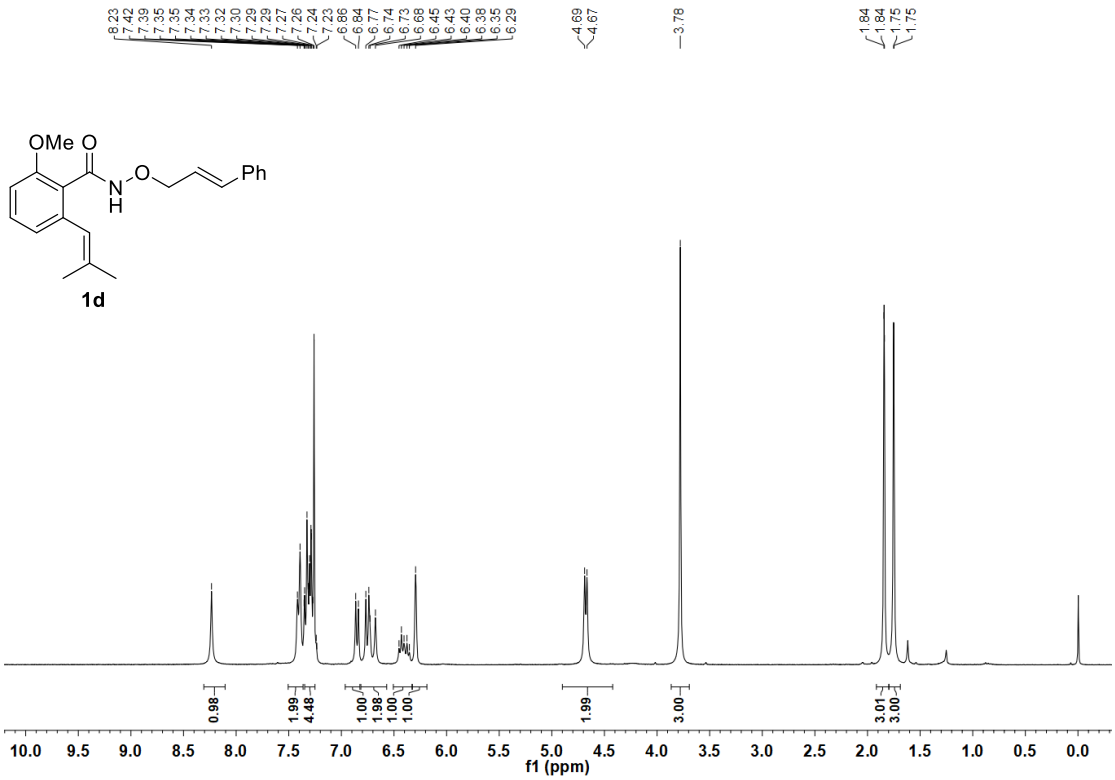


Figure S15. ^{1}H NMR spectra of **1d** (300 MHz, $CDCl_3$)

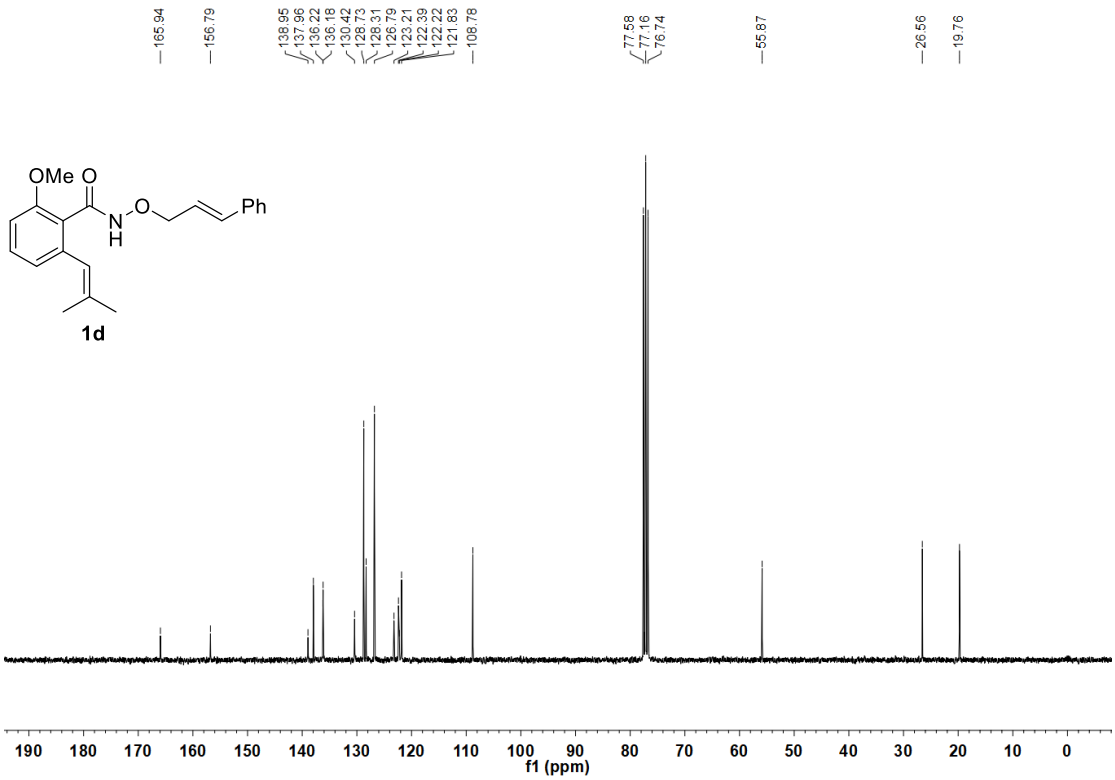


Figure S16. ^{13}C NMR spectra of **1d** (75 MHz, $CDCl_3$)

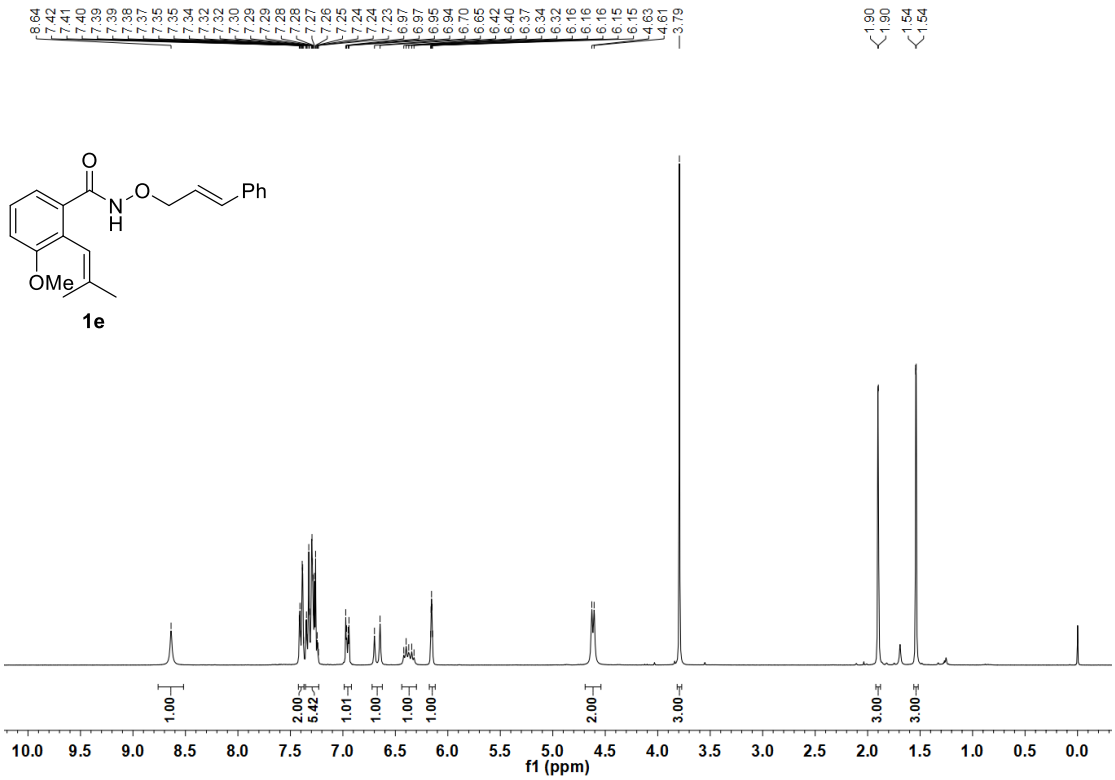


Figure S17. ^{1}H NMR spectra of **1e** (300 MHz, $CDCl_3$)

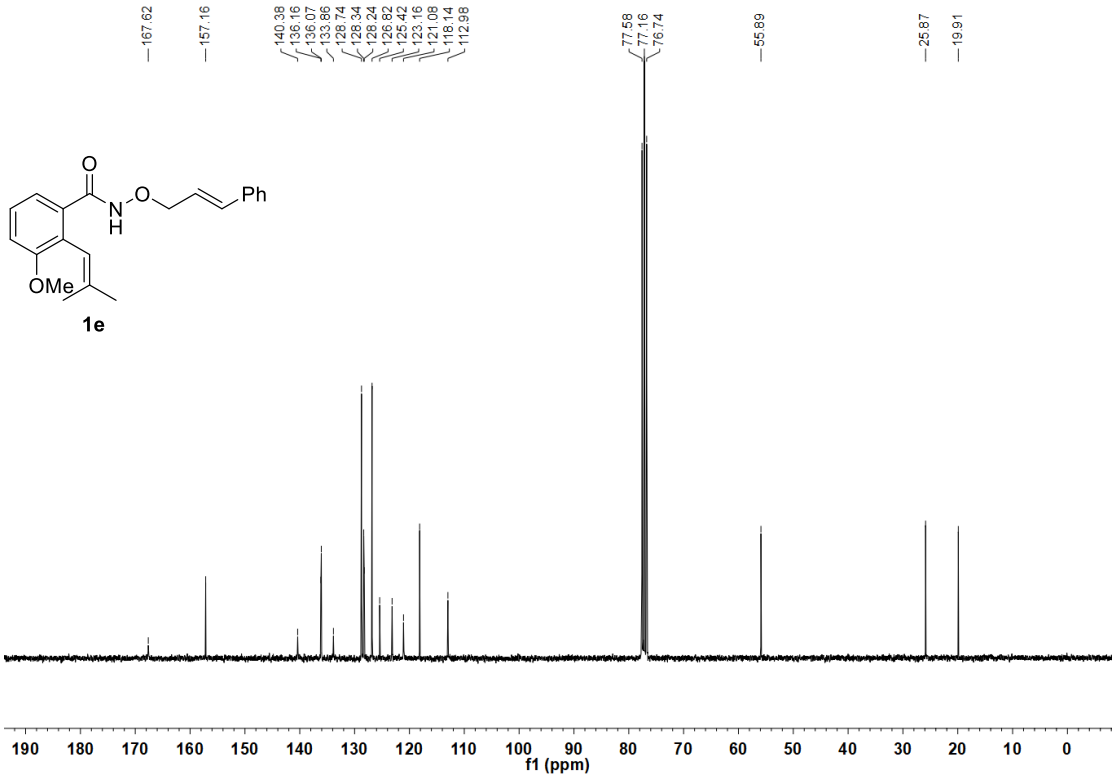


Figure S18. ^{13}C NMR spectra of **1e** (75 MHz, $CDCl_3$)

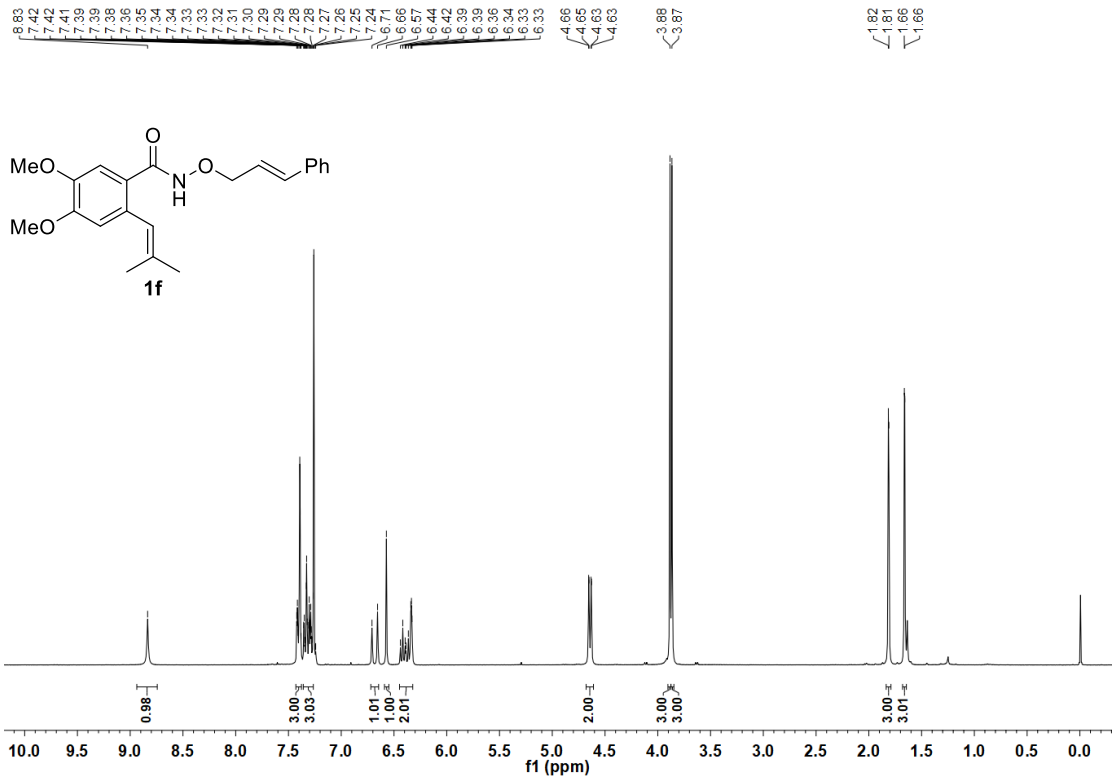


Figure S19. ^{1}H NMR spectra of **1f** (300 MHz, $CDCl_3$)

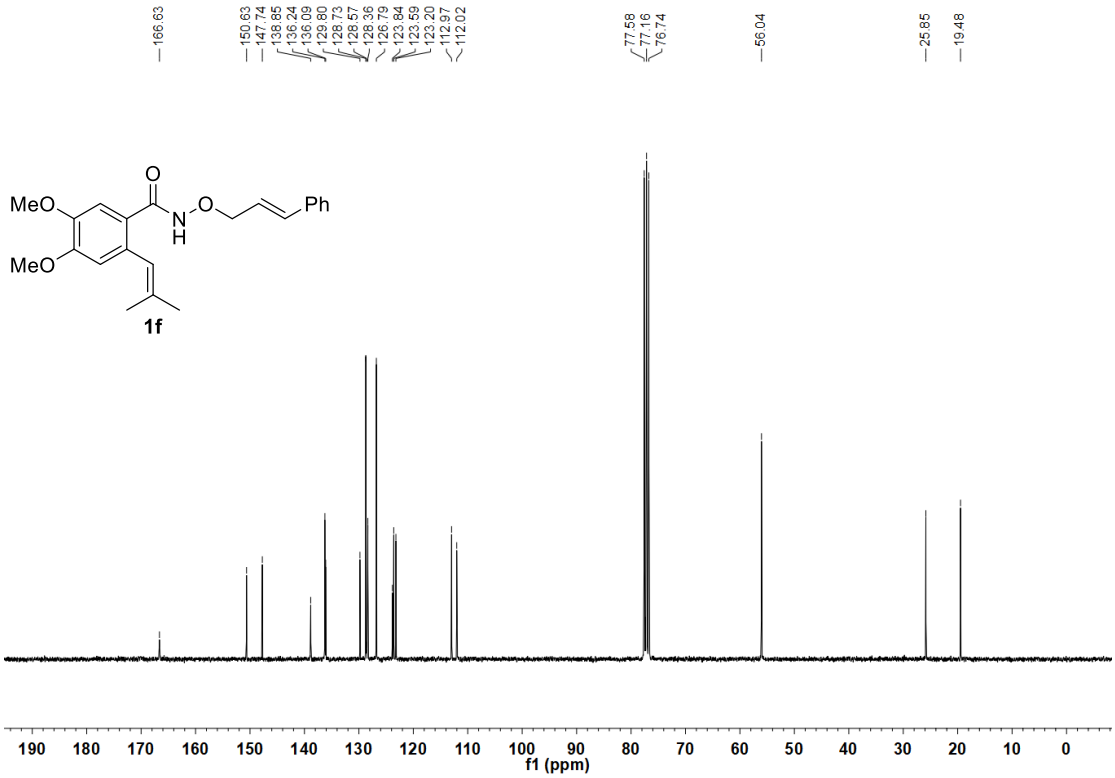


Figure S20. ^{13}C NMR spectra of **1f** (75 MHz, $CDCl_3$)

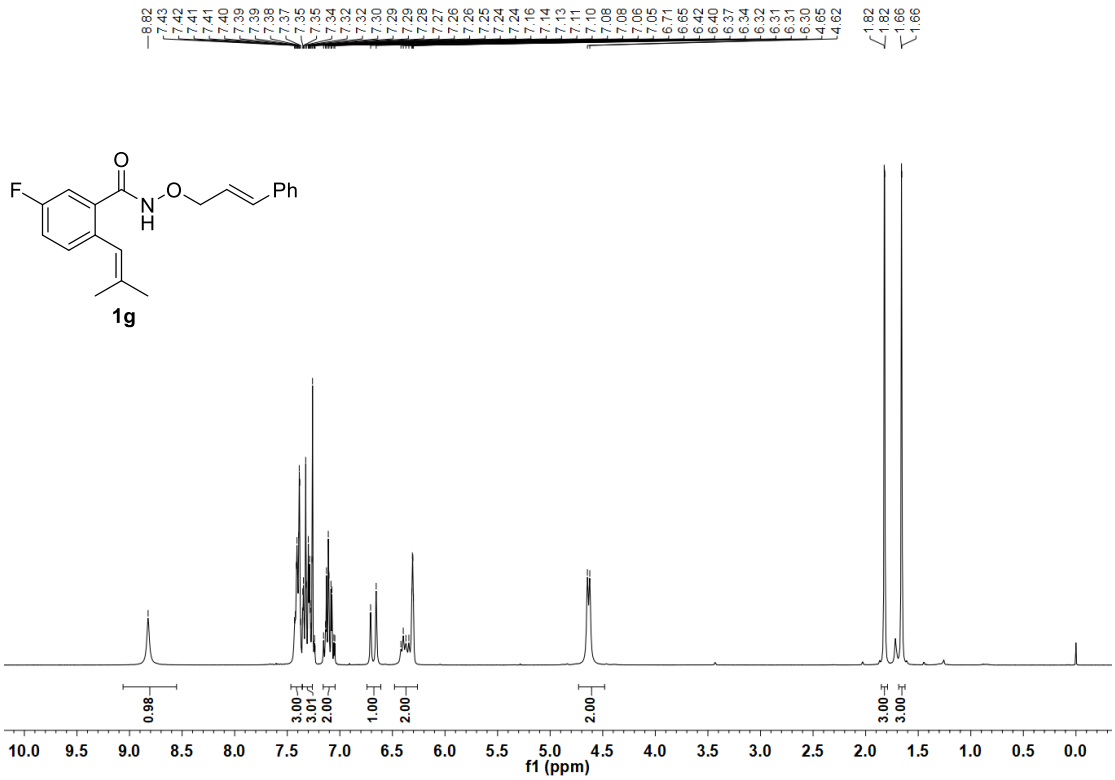


Figure S21. ^{1}H NMR spectra of **1g** (300 MHz, $CDCl_3$)

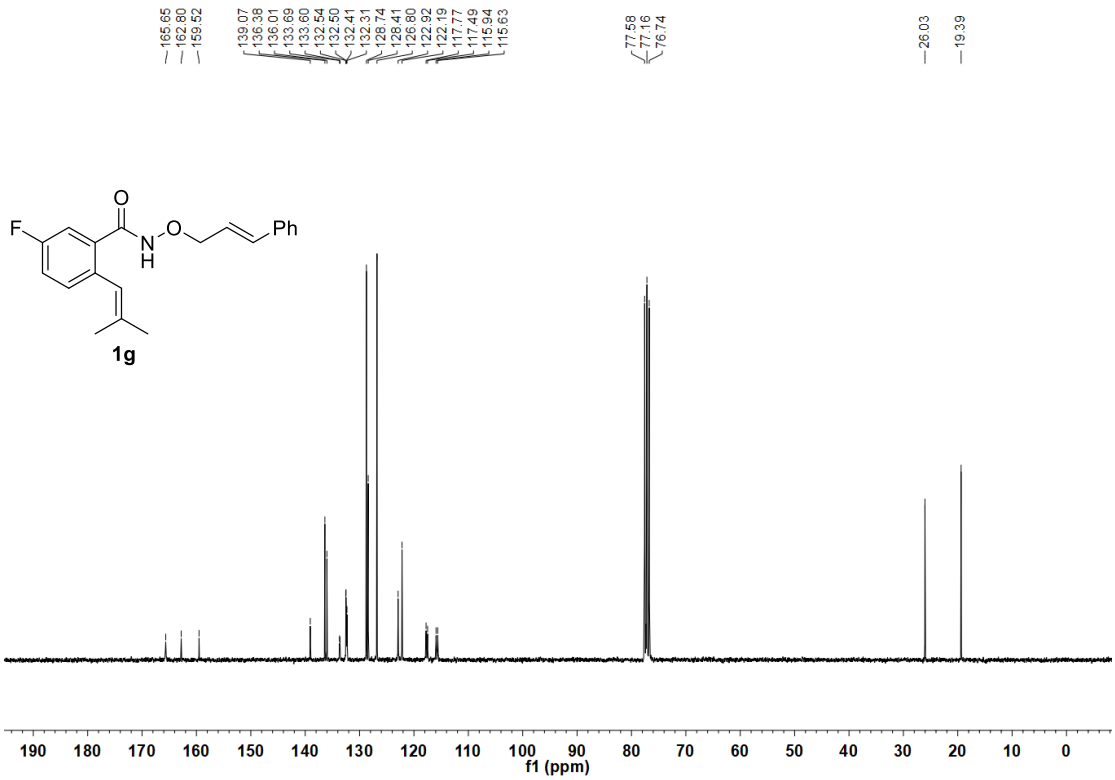


Figure S22. ^{13}C NMR spectra of **1g** (75 MHz, $CDCl_3$)

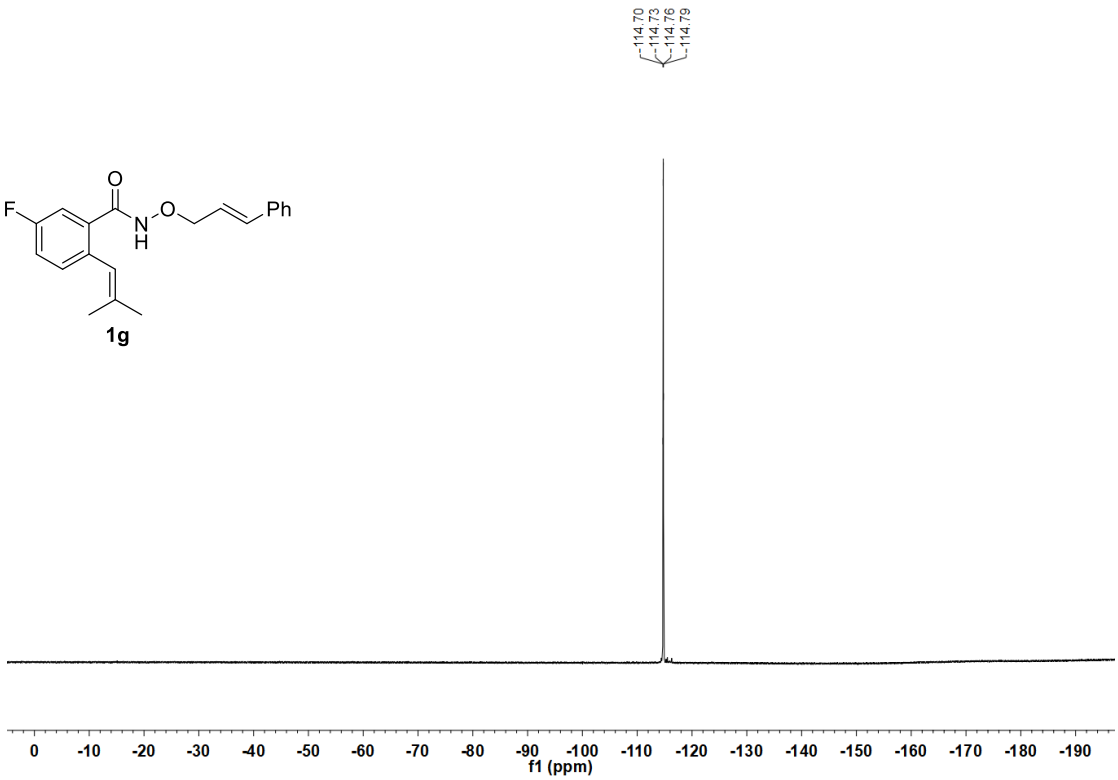


Figure S23. ^{19}F NMR spectra of **1g** (282 MHz, $CDCl_3$)

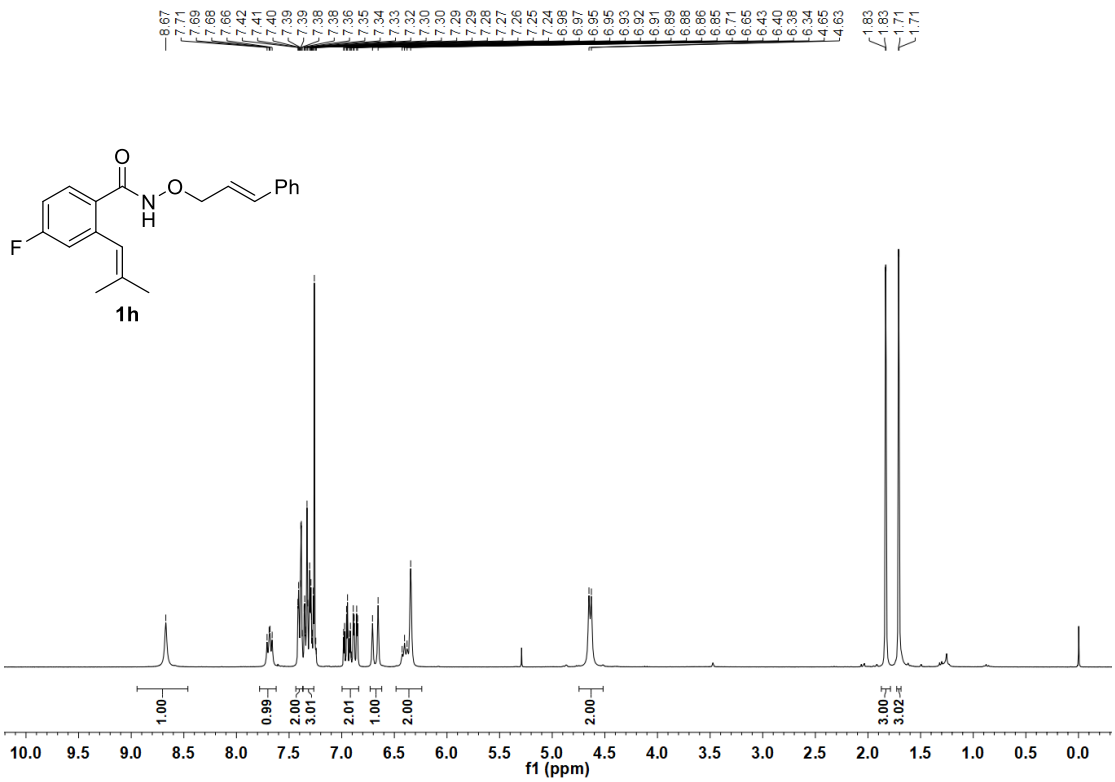


Figure S24. ^{1}H NMR spectra of **1h** (300 MHz, $CDCl_3$)

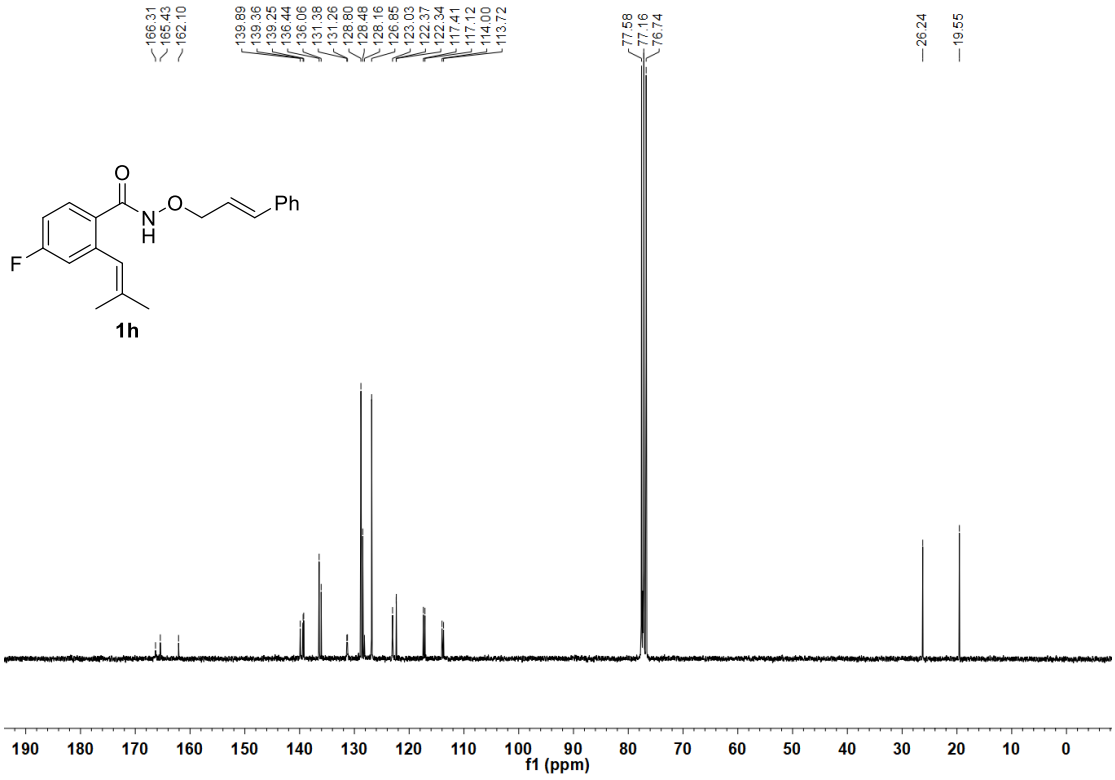


Figure S25. ^{13}C NMR spectra of **1h** (75 MHz, $CDCl_3$)

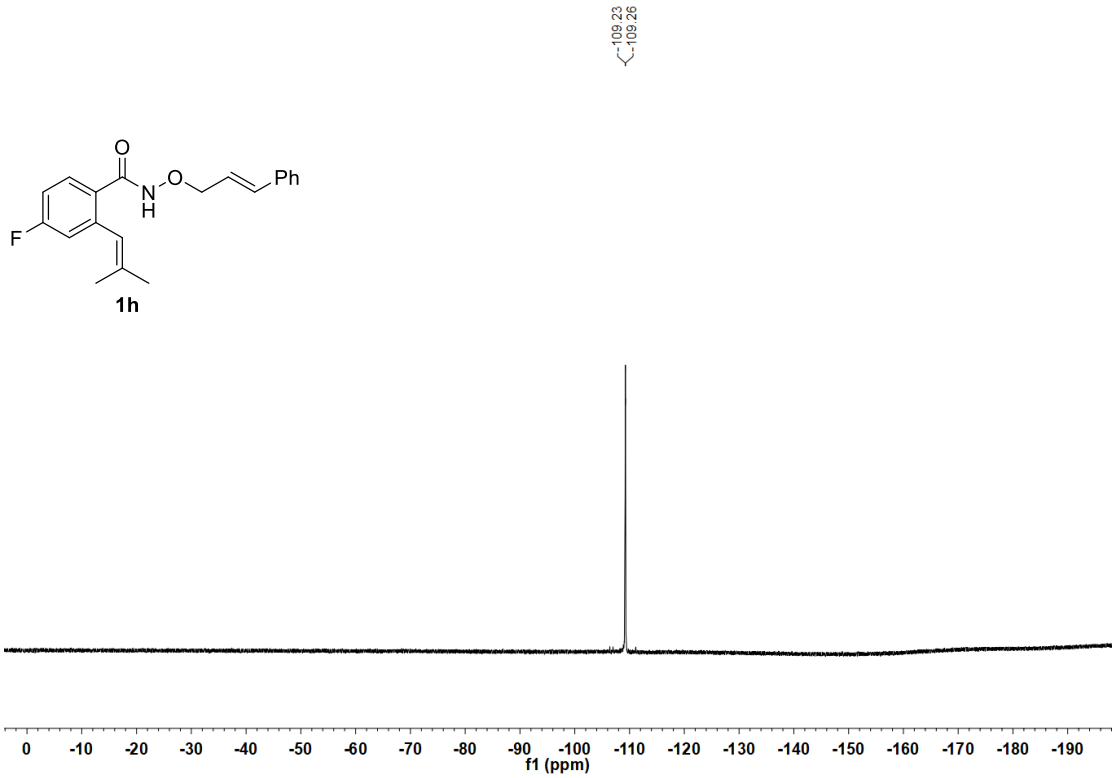


Figure S26. ^{19}F NMR spectra of **1h** (282 MHz, $CDCl_3$)

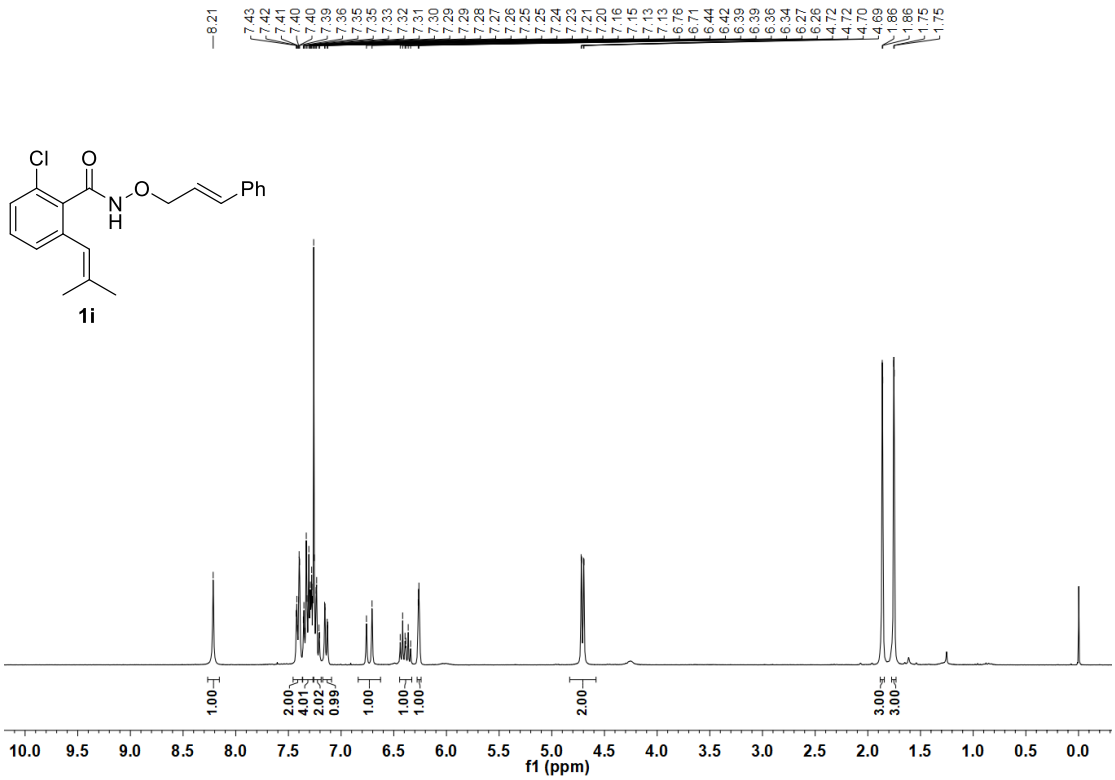


Figure S27. ^{1}H NMR spectra of **1i** (300 MHz, $CDCl_3$)

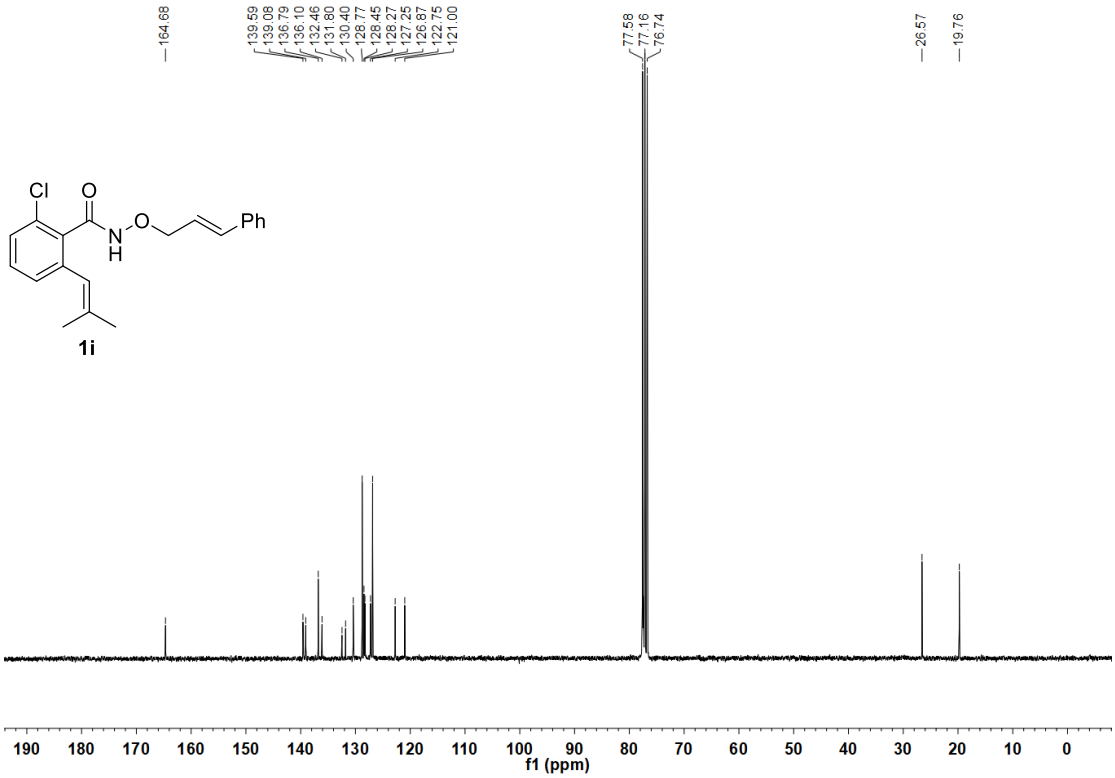


Figure S28. ^{13}C NMR spectra of **1i** (75 MHz, $CDCl_3$)

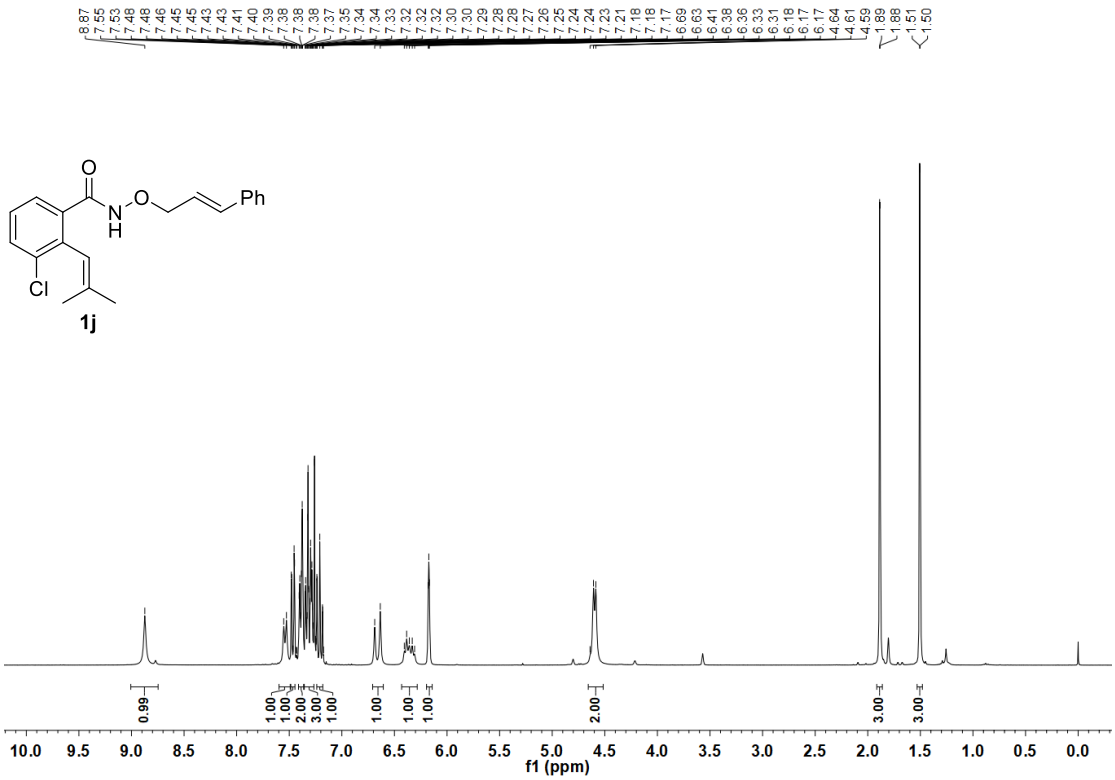


Figure S29. ^{1}H NMR spectra of **1j** (300 MHz, $CDCl_3$)

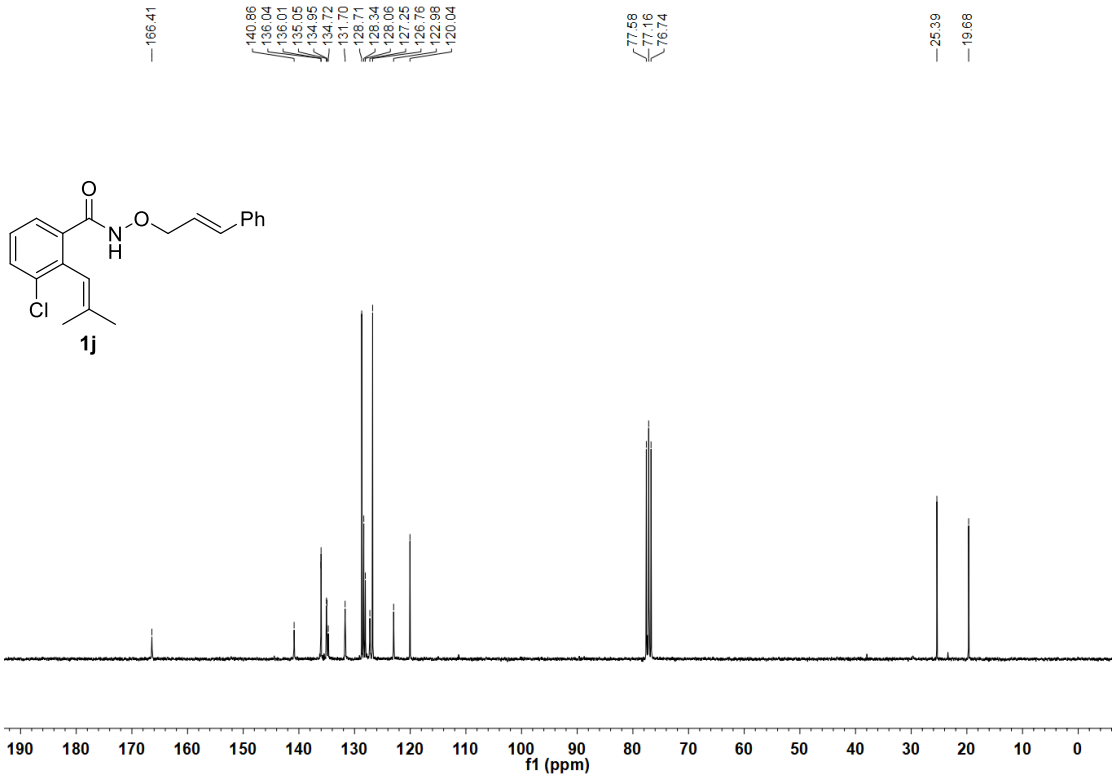


Figure S30. ^{13}C NMR spectra of **1j** (75 MHz, $CDCl_3$)

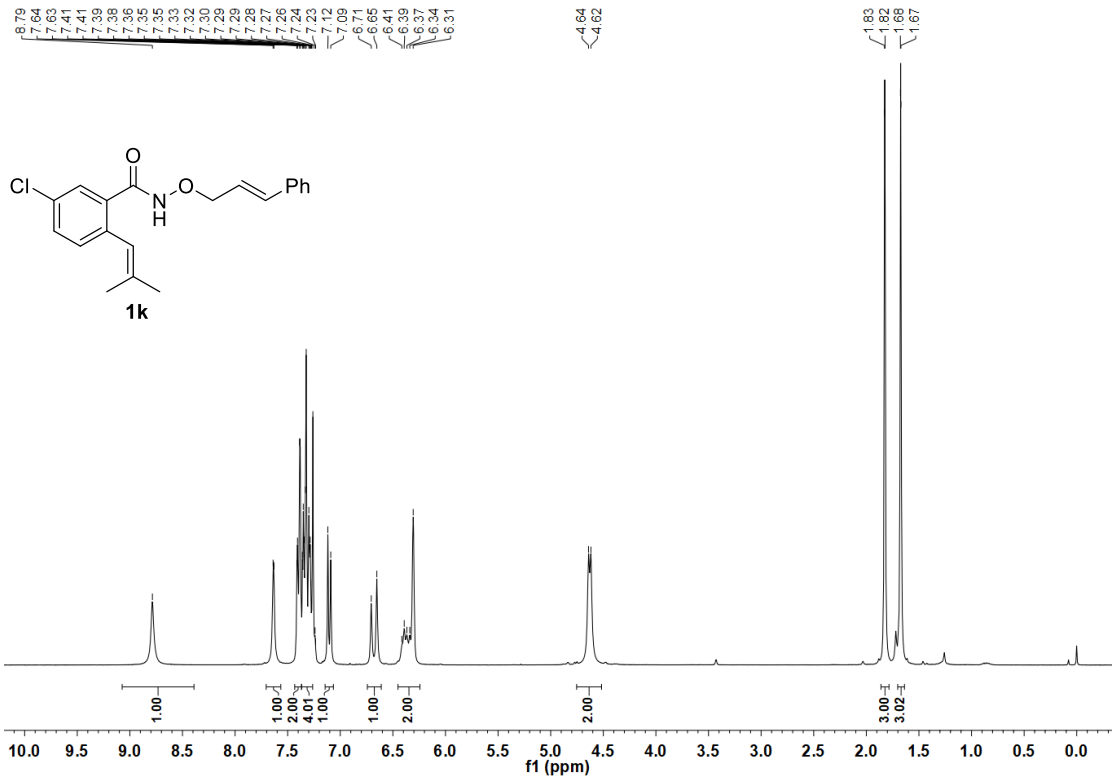


Figure S31. ^{1}H NMR spectra of **1k** (300 MHz, $CDCl_3$)

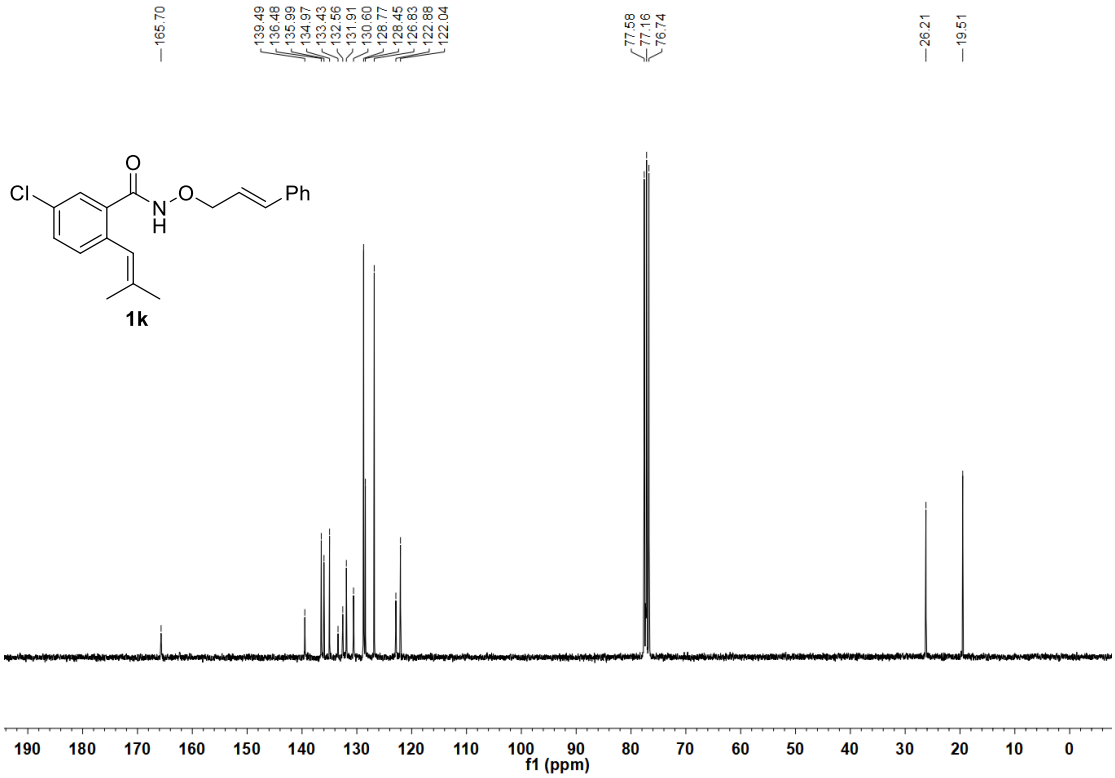


Figure S32. ^{13}C NMR spectra of **1k** (75 MHz, $CDCl_3$)

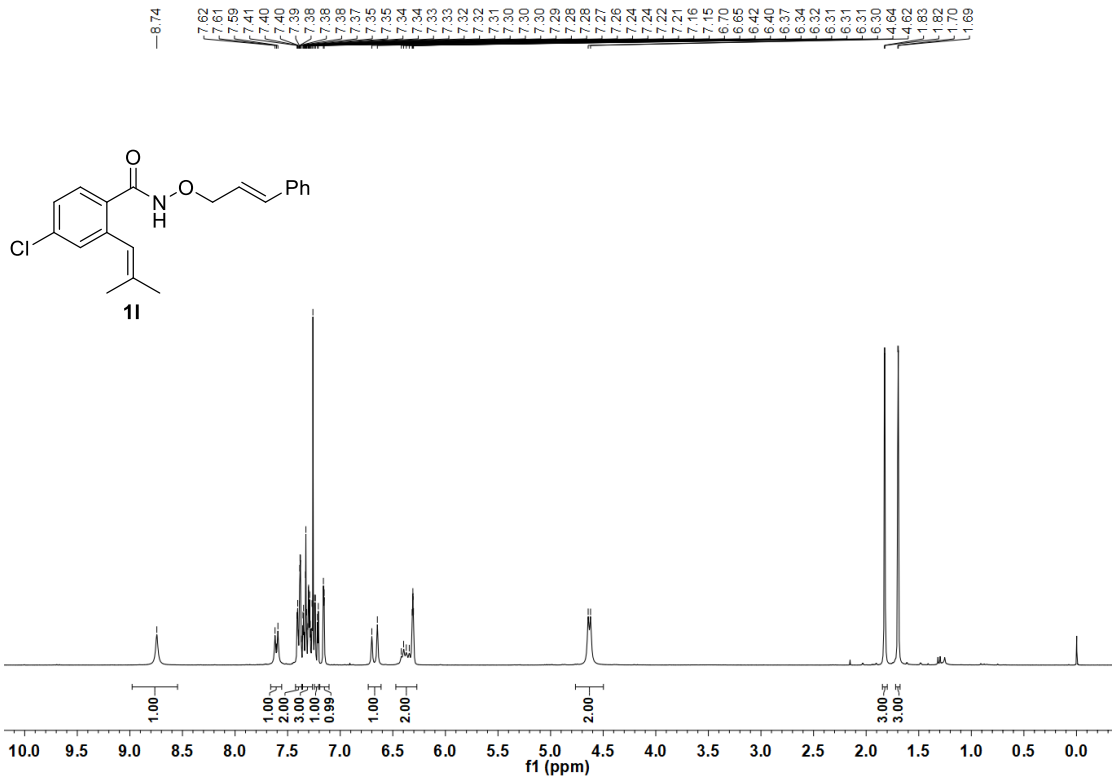


Figure S33. ^{1}H NMR spectra of **1l** (300 MHz, $CDCl_3$)

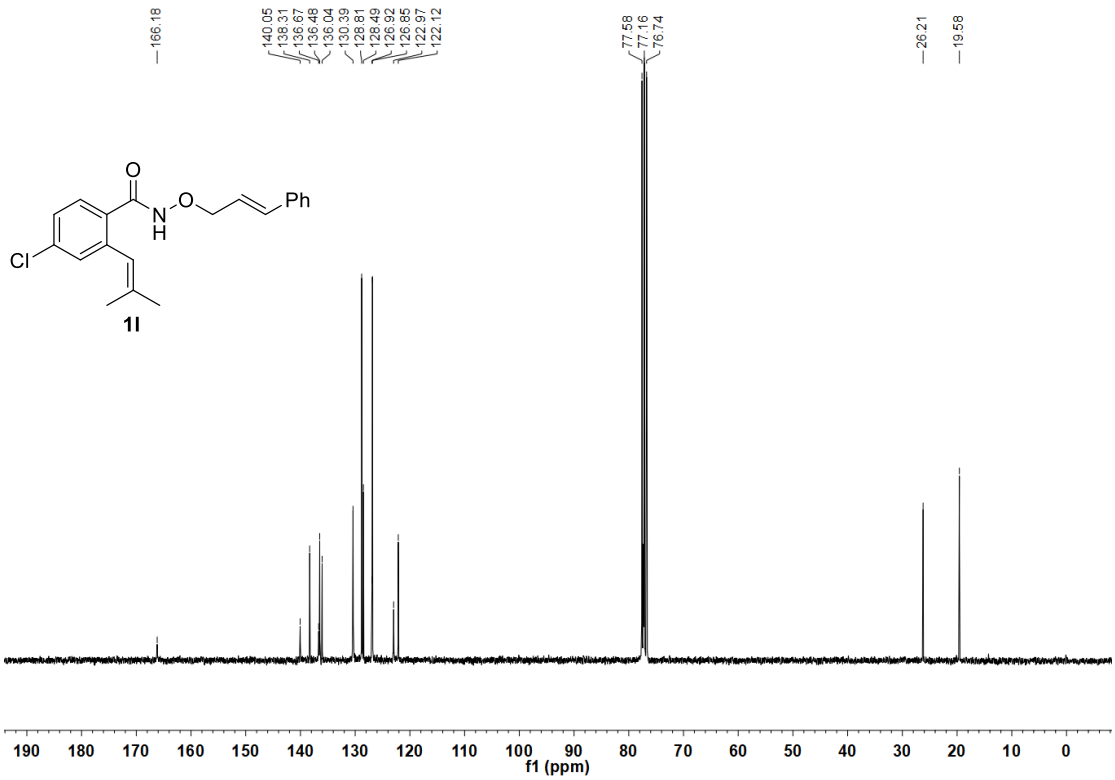


Figure S34. ^{13}C NMR spectra of **1l** (75 MHz, $CDCl_3$)

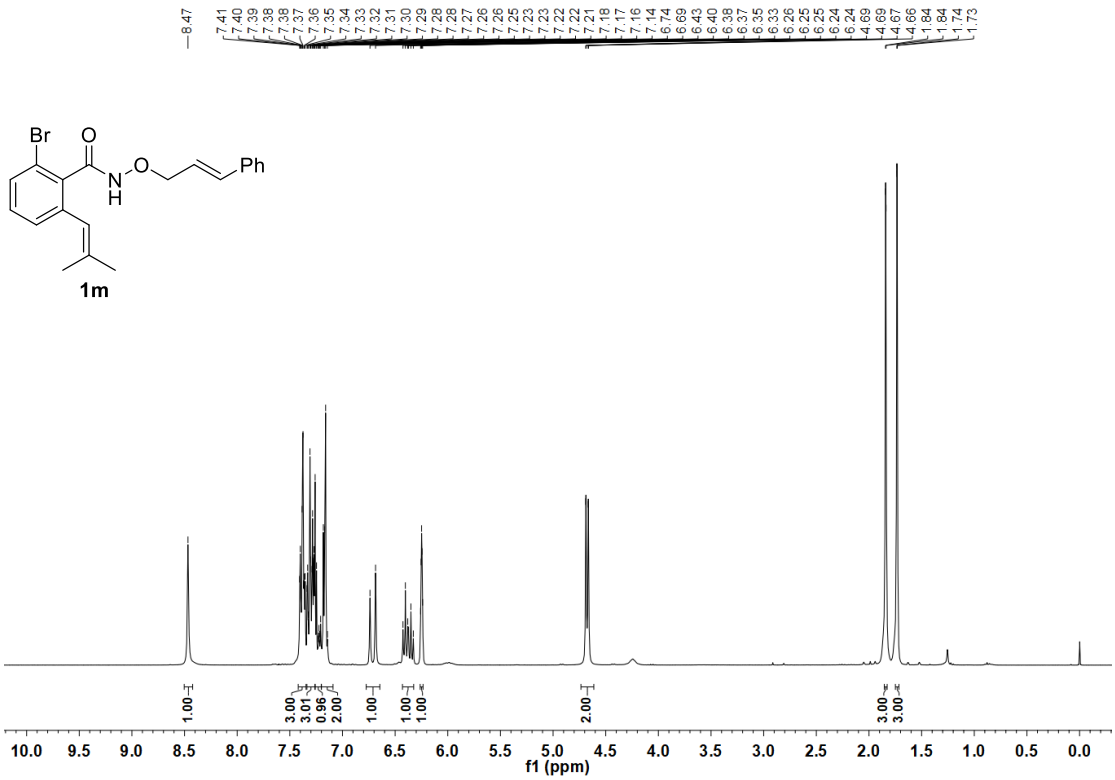


Figure S35. ^{1}H NMR spectra of **1m** (300 MHz, $CDCl_3$)

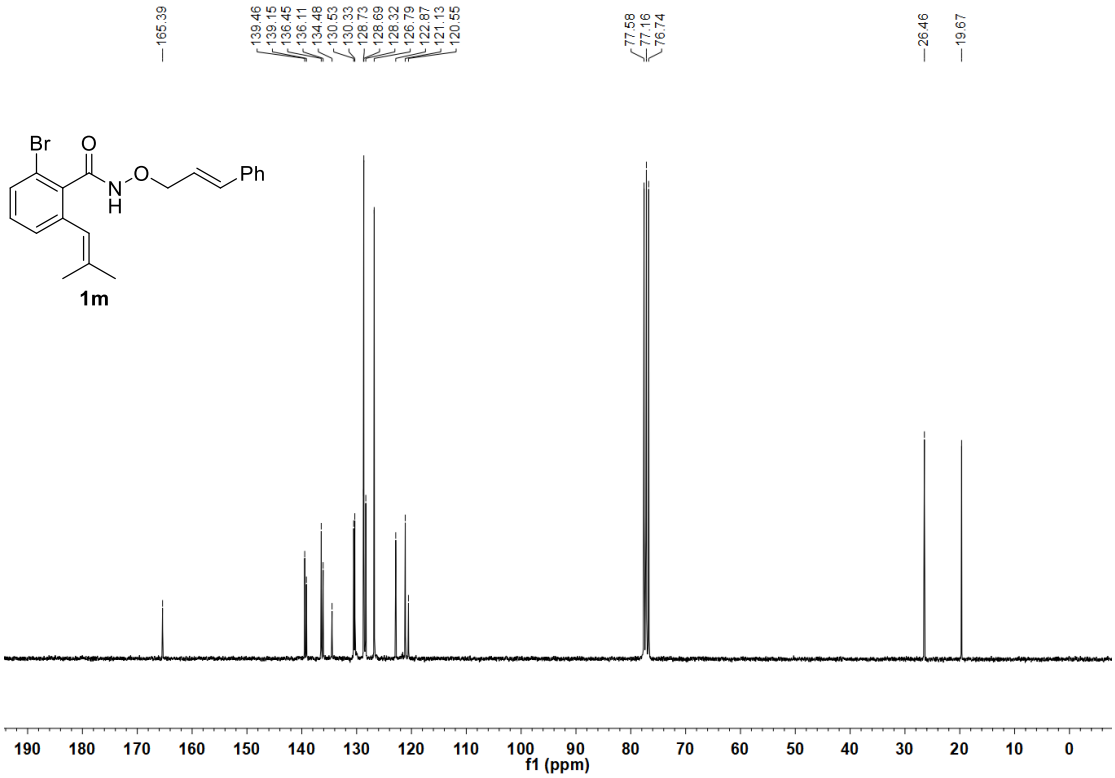


Figure S36. ^{13}C NMR spectra of **1m** (75 MHz, $CDCl_3$)

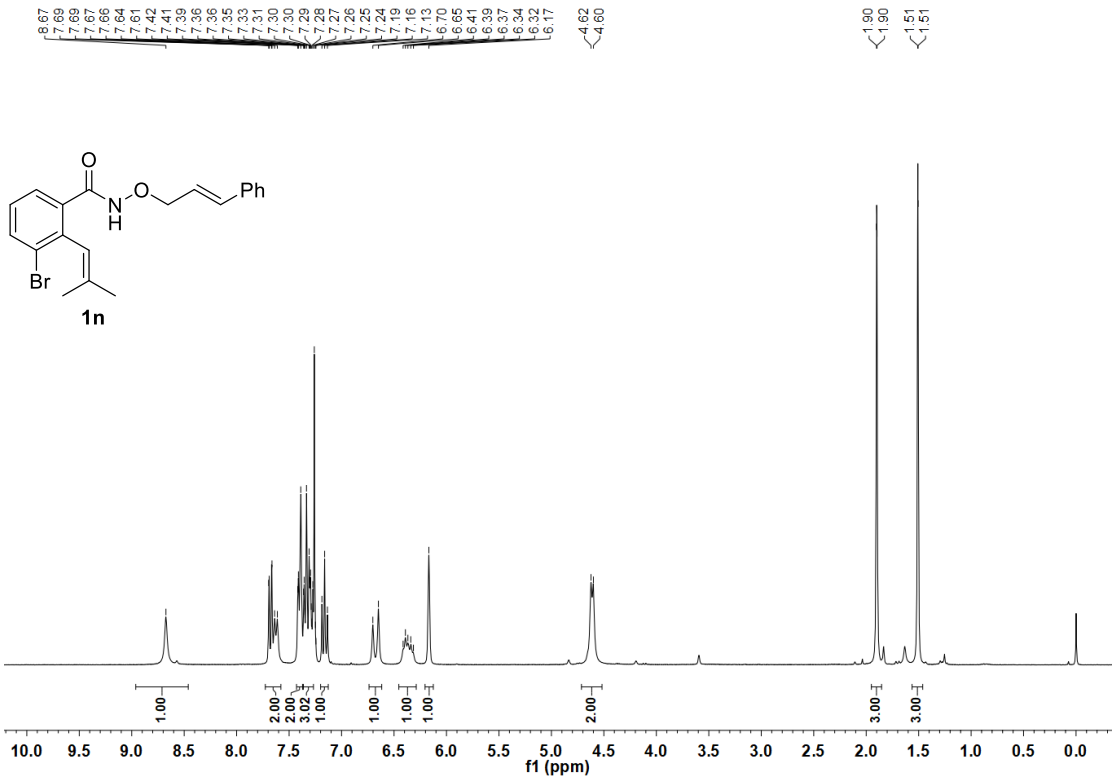


Figure S37. ^{1}H NMR spectra of **1n** (300 MHz, $CDCl_3$)

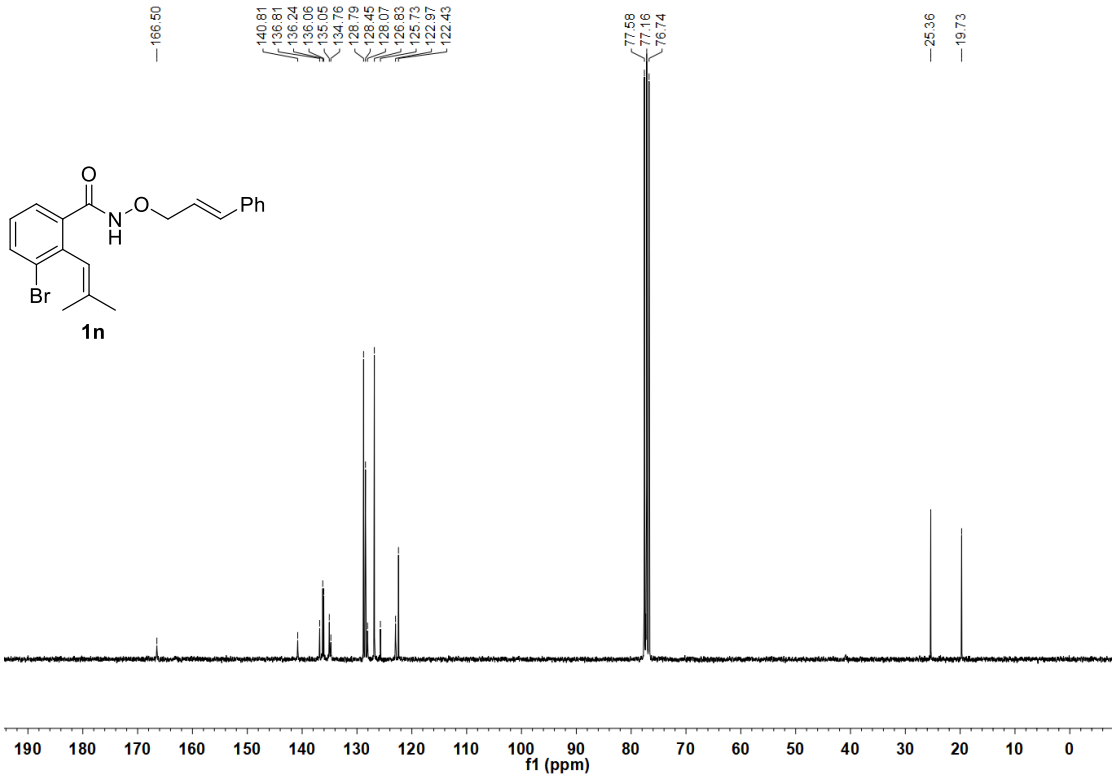


Figure S38. ^{13}C NMR spectra of **1n** (75 MHz, $CDCl_3$)

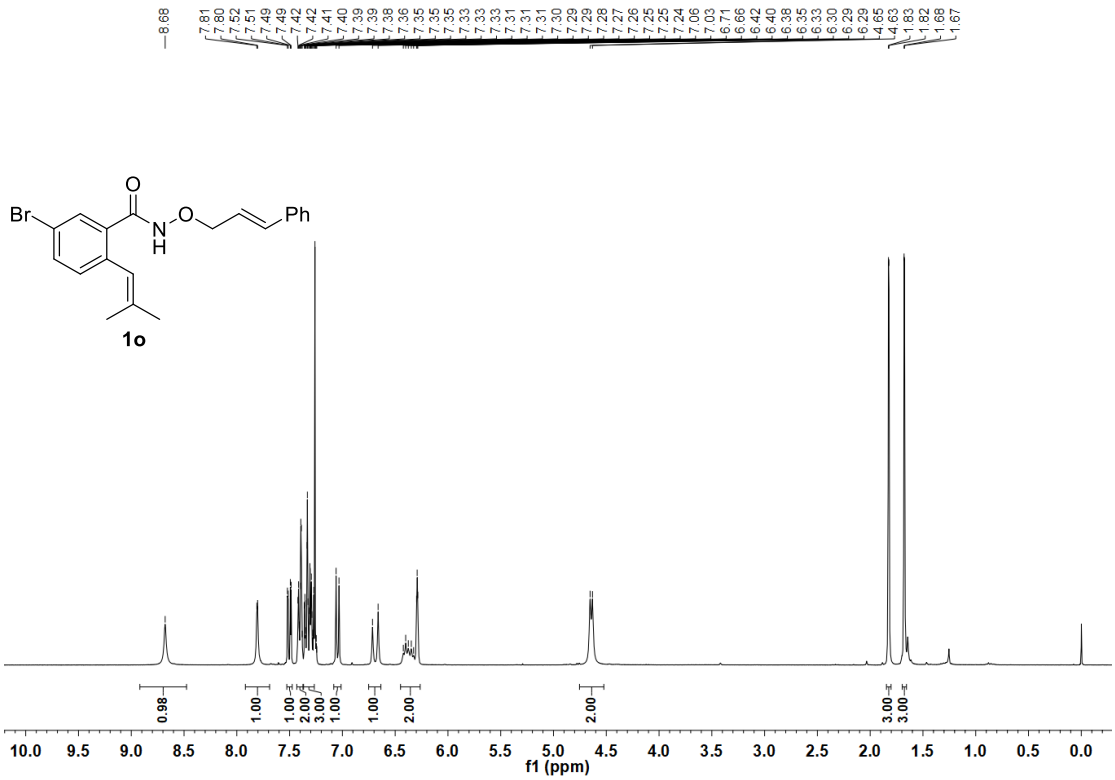


Figure S39. ^{1}H NMR spectra of **1o** (300 MHz, $CDCl_3$)

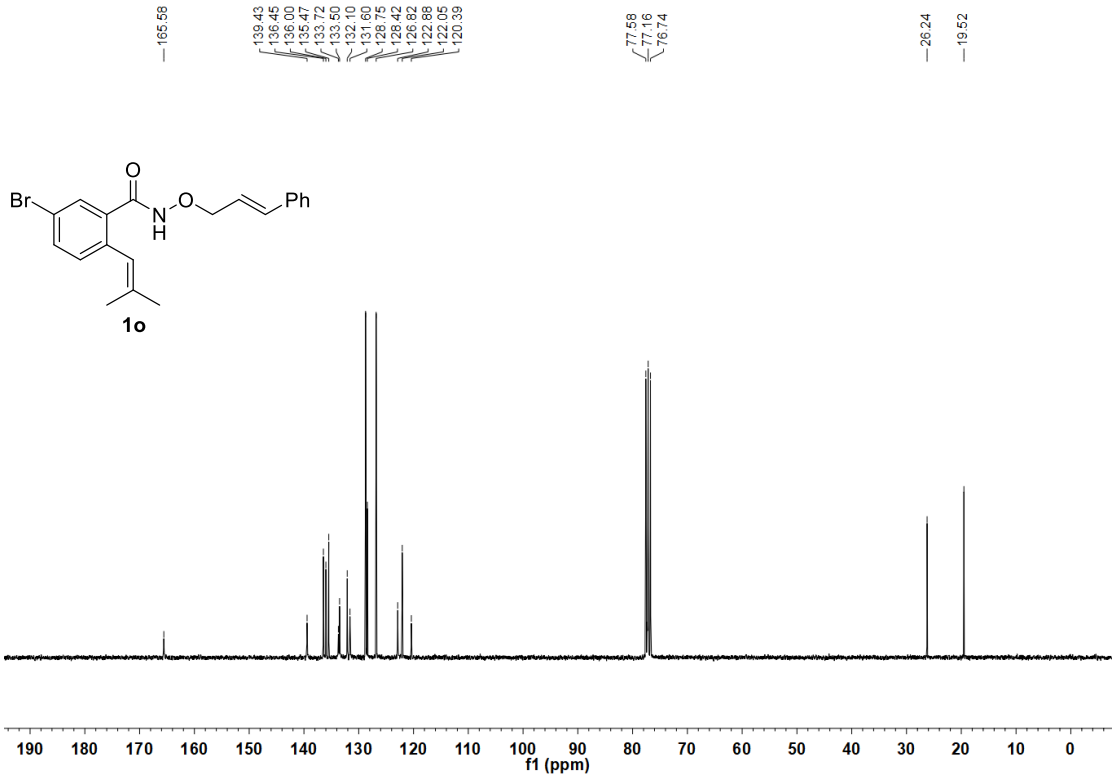


Figure S40. ^{13}C NMR spectra of **1o** (75 MHz, $CDCl_3$)

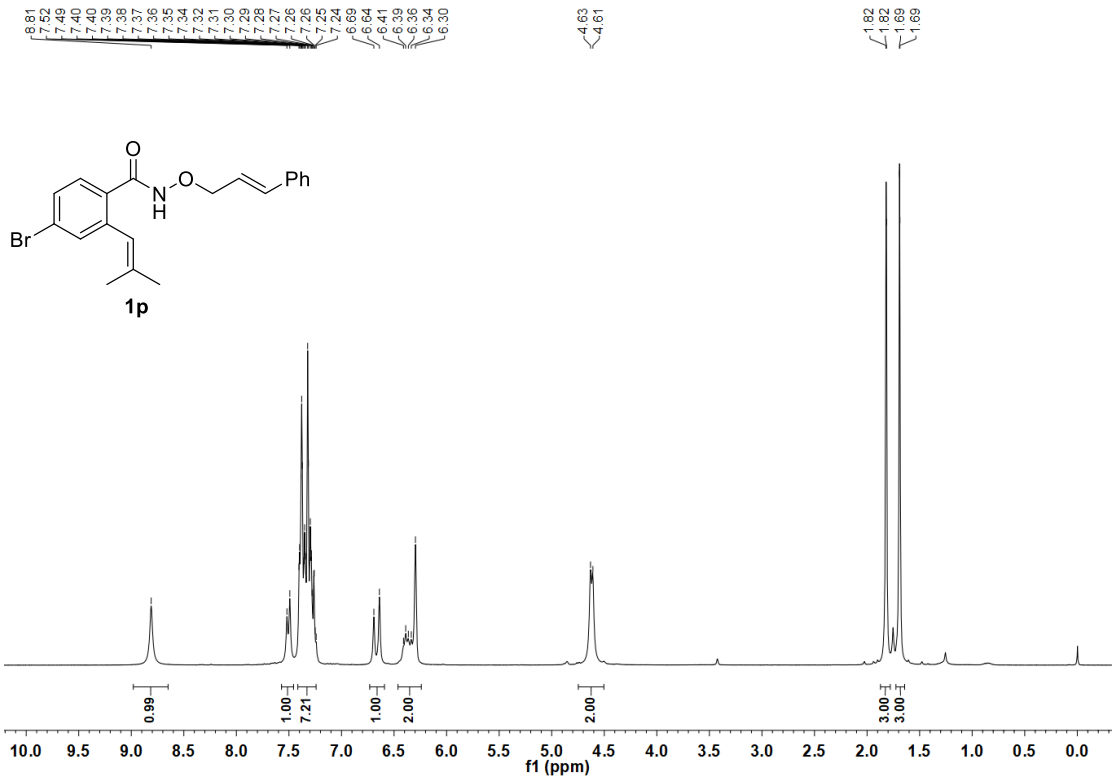


Figure S41. ^{1}H NMR spectra of **1p** (300 MHz, $CDCl_3$)

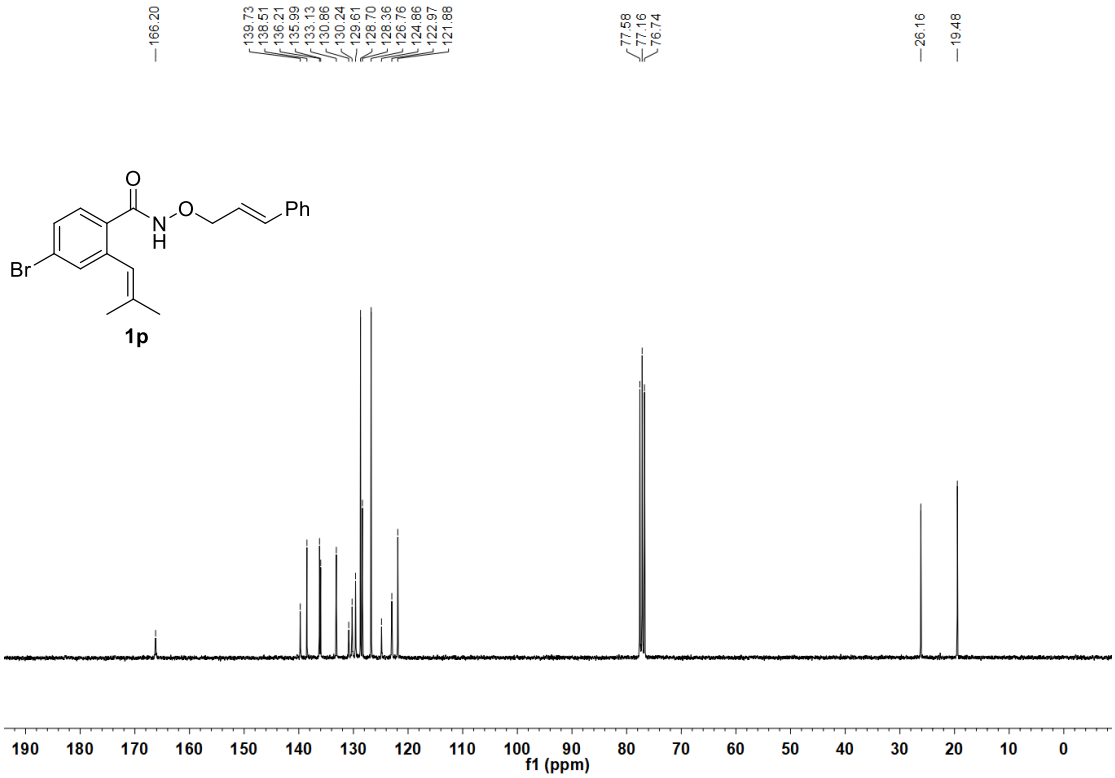


Figure S42. ^{13}C NMR spectra of **1p** (75 MHz, $CDCl_3$)

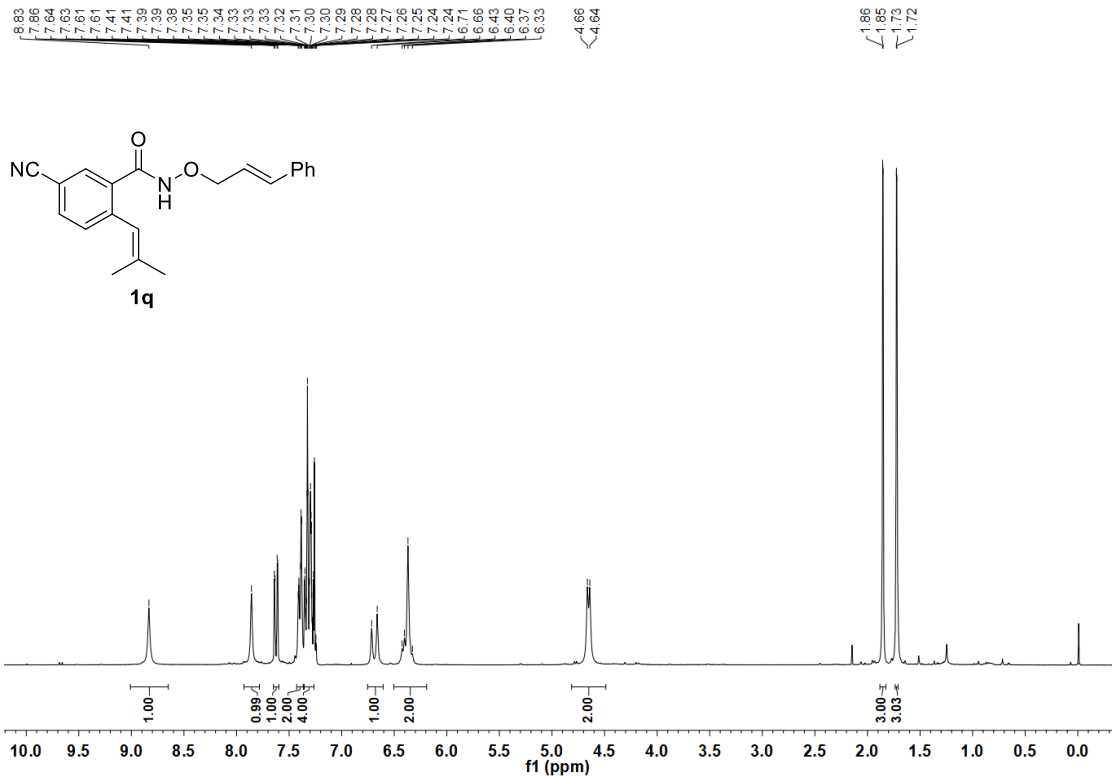


Figure S43. ^{1}H NMR spectra of **1q** (300 MHz, $CDCl_3$)

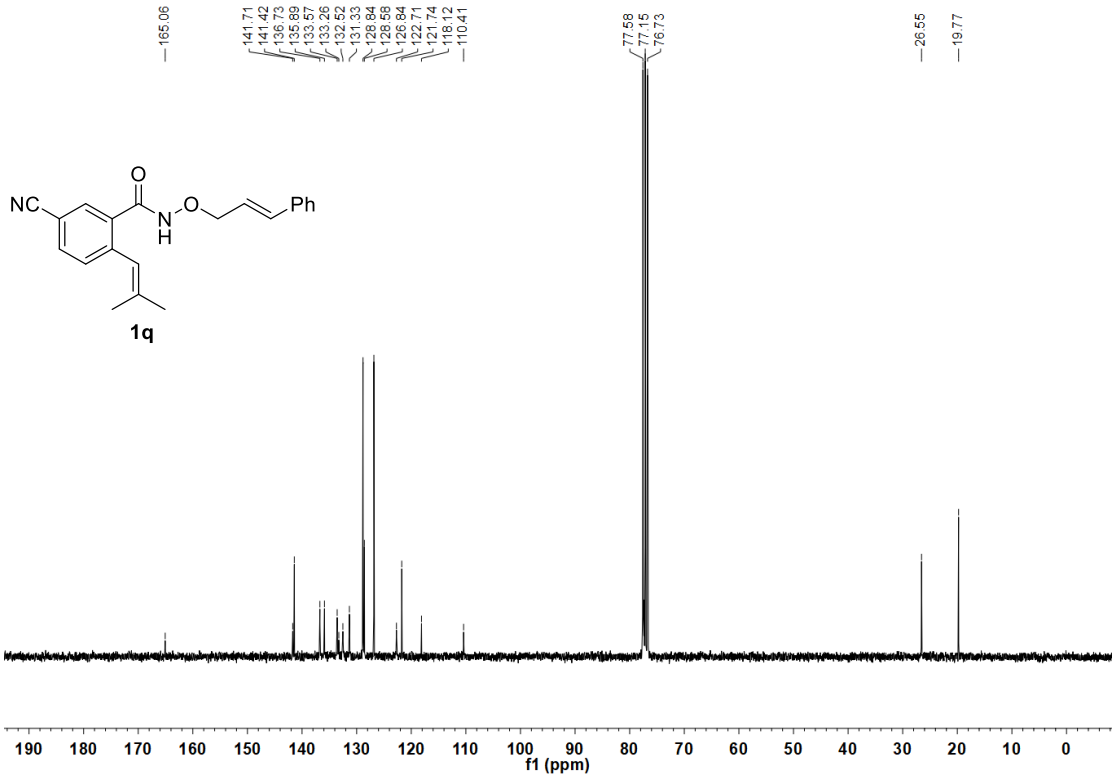


Figure S44. ^{13}C NMR spectra of **1q** (75 MHz, $CDCl_3$)

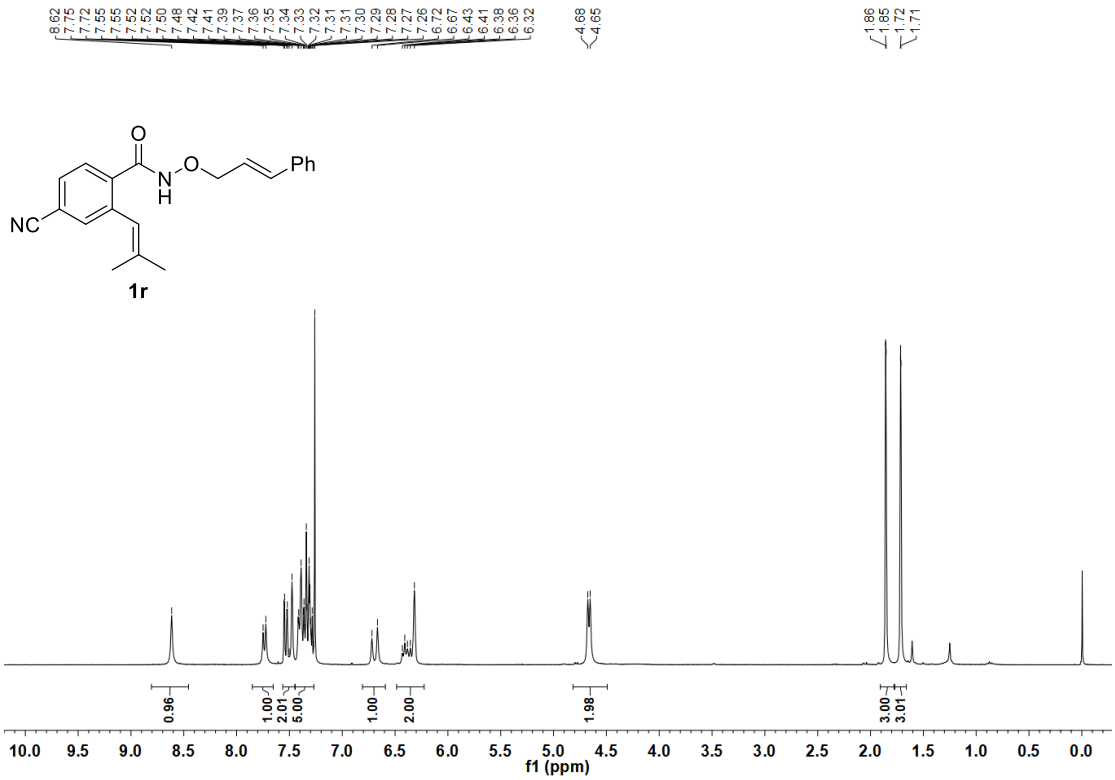


Figure S45. ^{1}H NMR spectra of **1r** (300 MHz, $CDCl_3$)

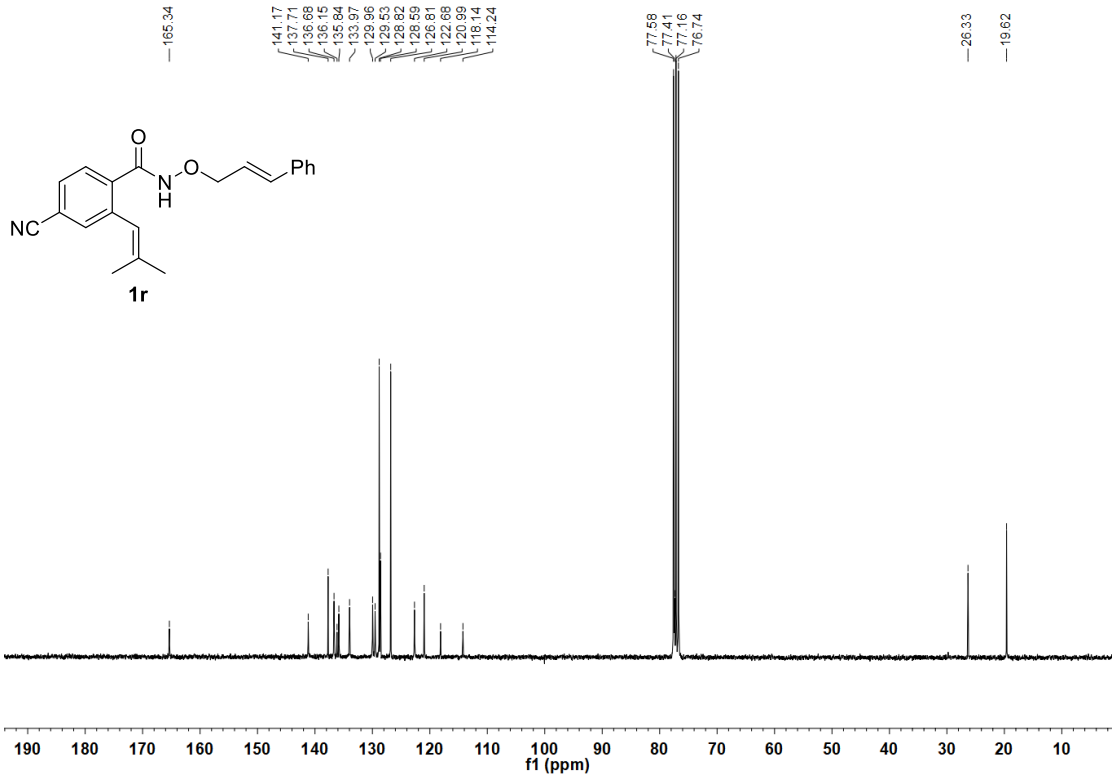


Figure S46. ^{13}C NMR spectra of **1r** (75 MHz, $CDCl_3$)

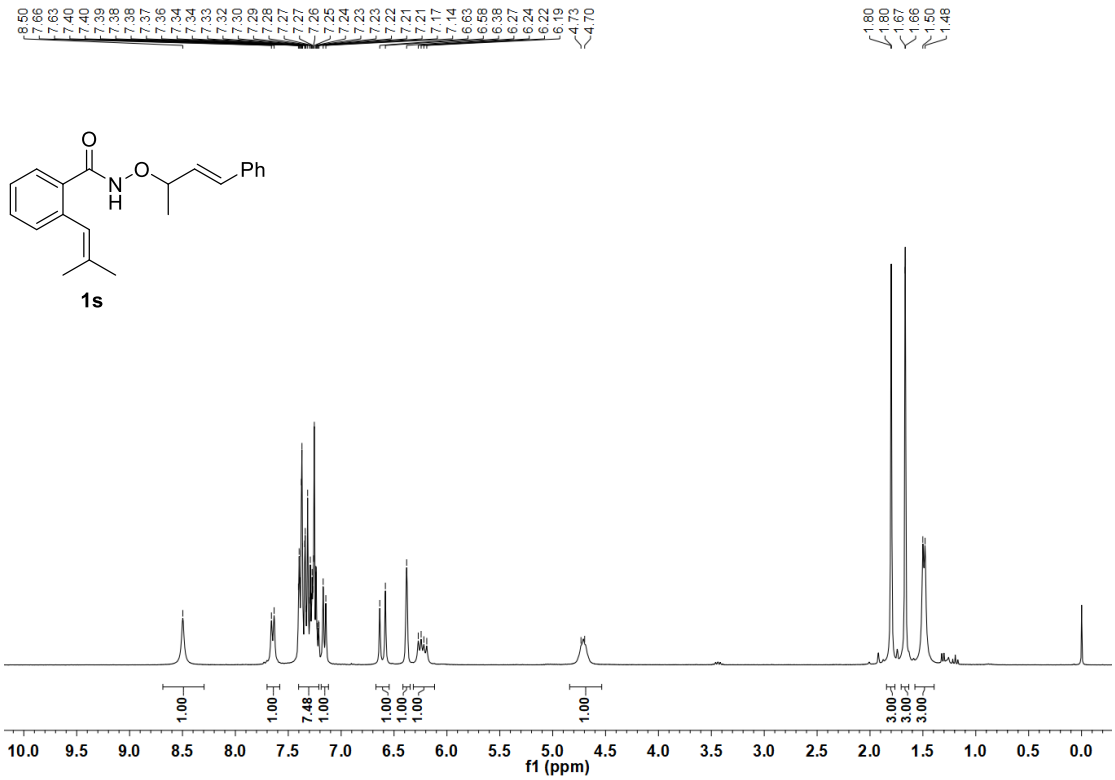


Figure S47. ^{1}H NMR spectra of **1s** (300 MHz, $CDCl_3$)

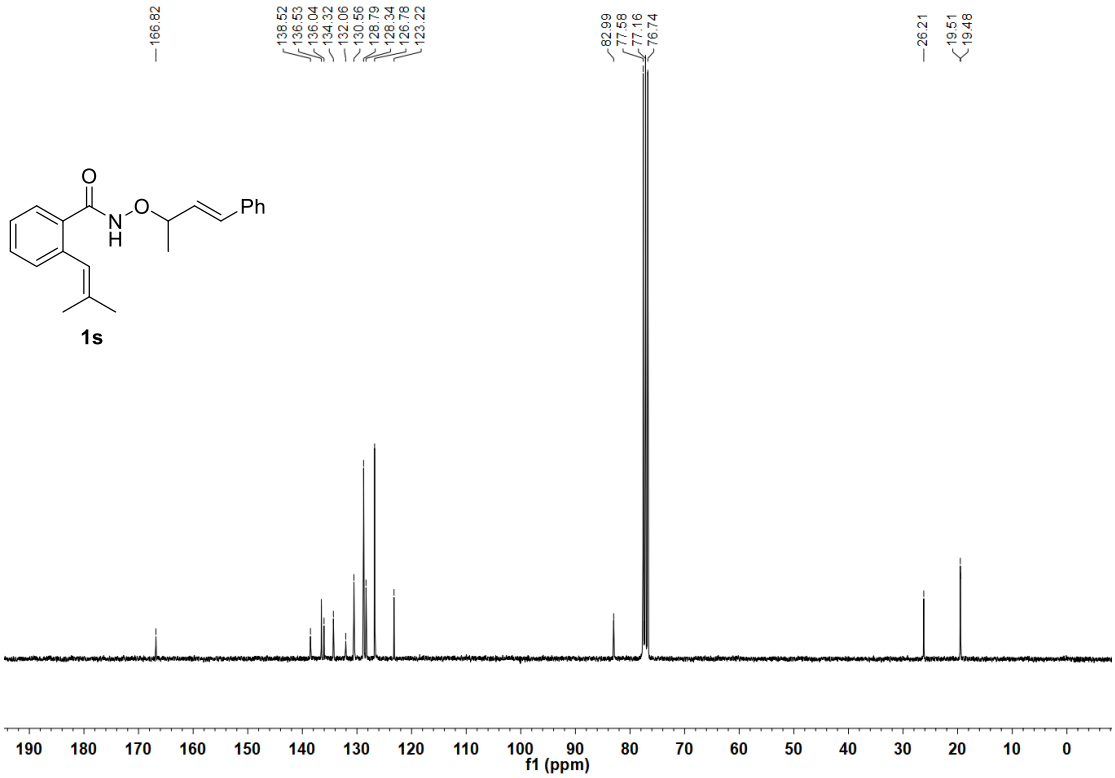


Figure S48. ^{13}C NMR spectra of **1s** (75 MHz, $CDCl_3$)

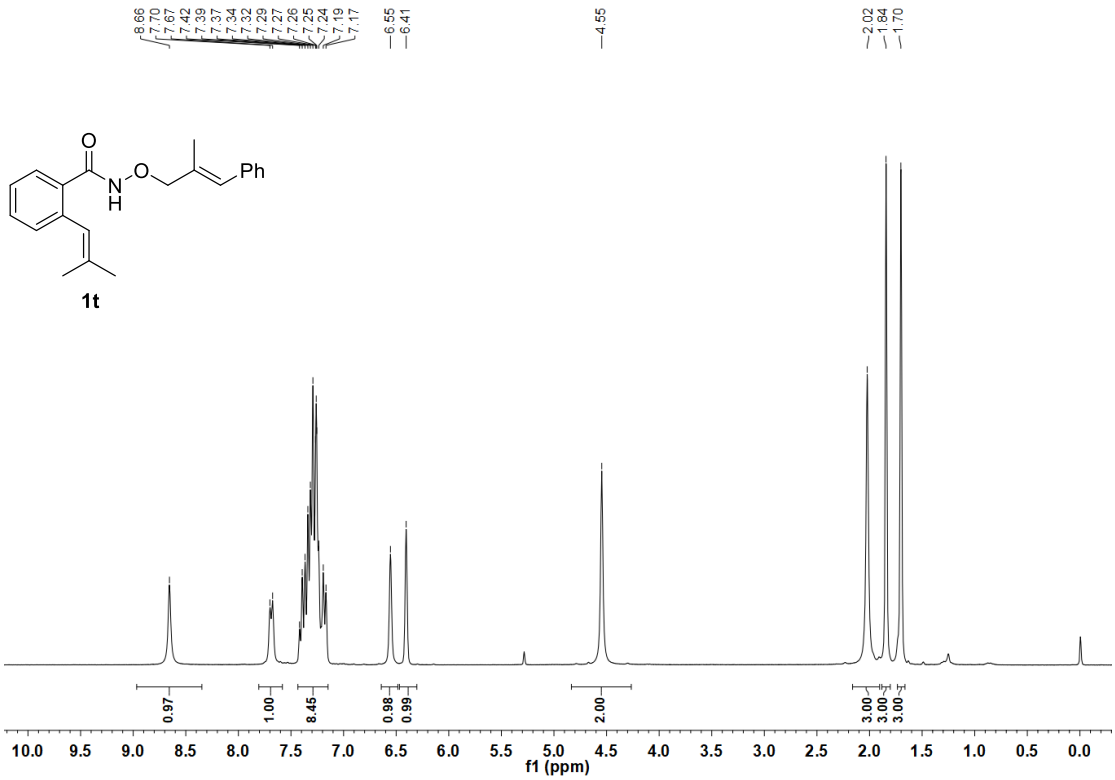


Figure S49. ^{1}H NMR spectra of **1t** (300 MHz, $CDCl_3$)

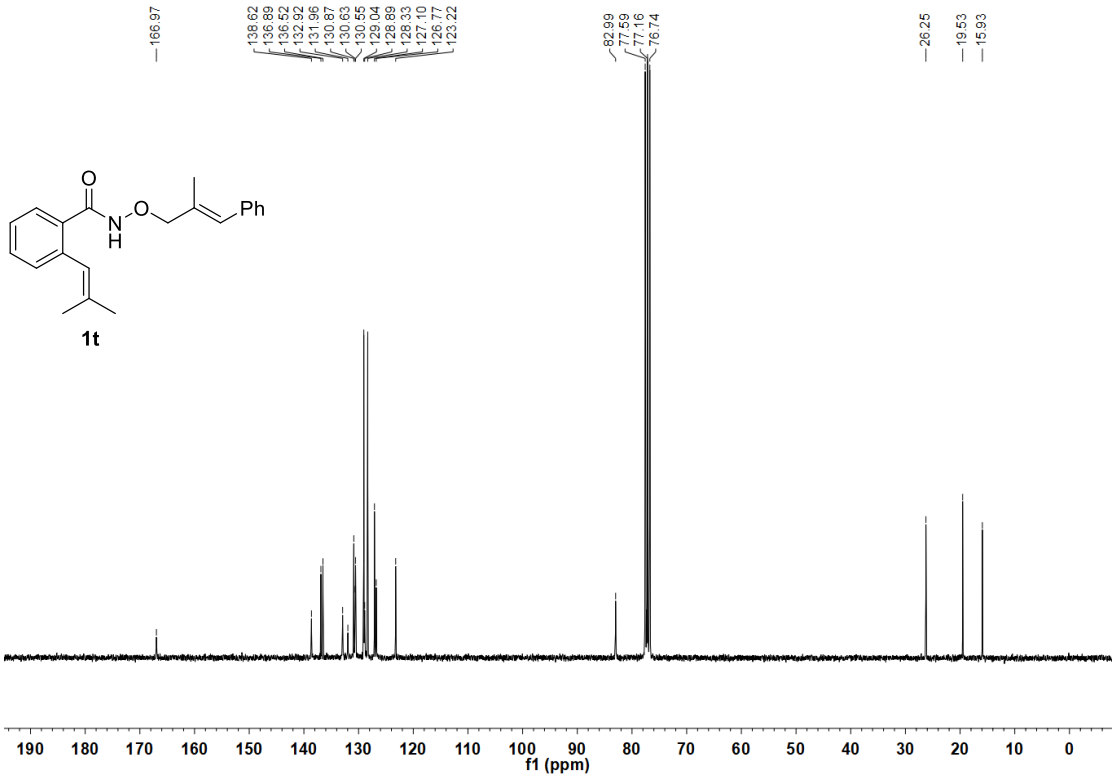


Figure S50. ^{13}C NMR spectra of **1t** (75 MHz, $CDCl_3$)

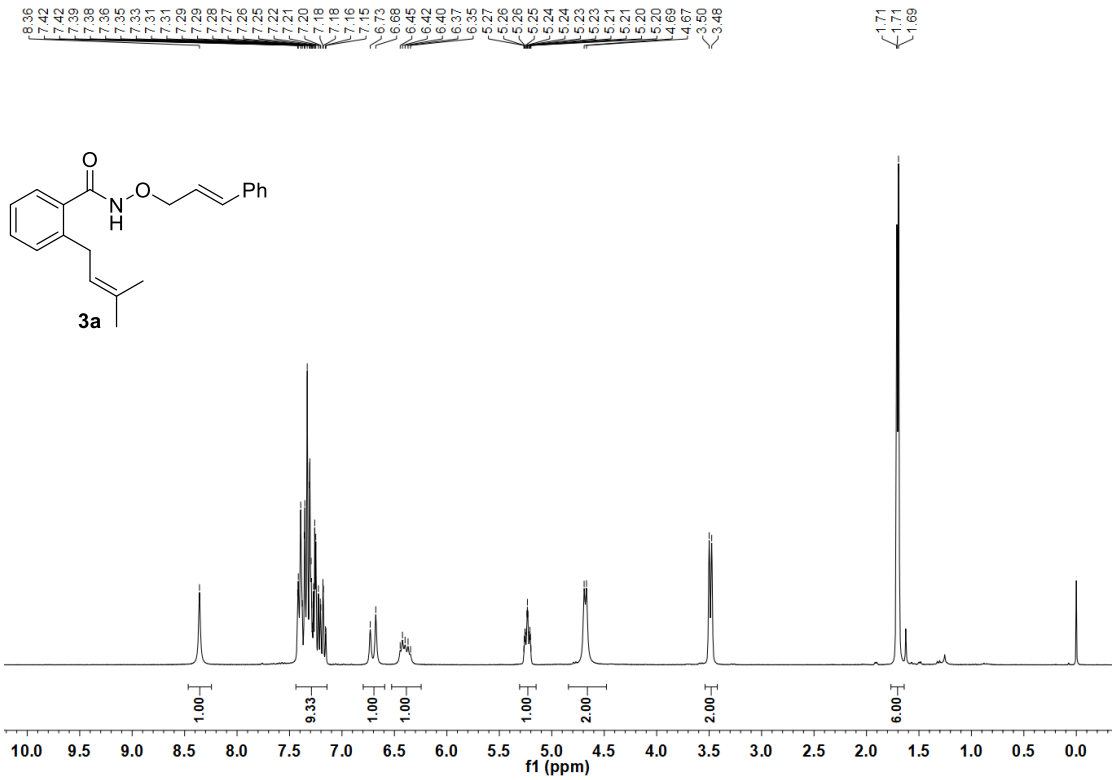


Figure S51. ^{1}H NMR spectra of **3a** (300 MHz, $CDCl_3$)

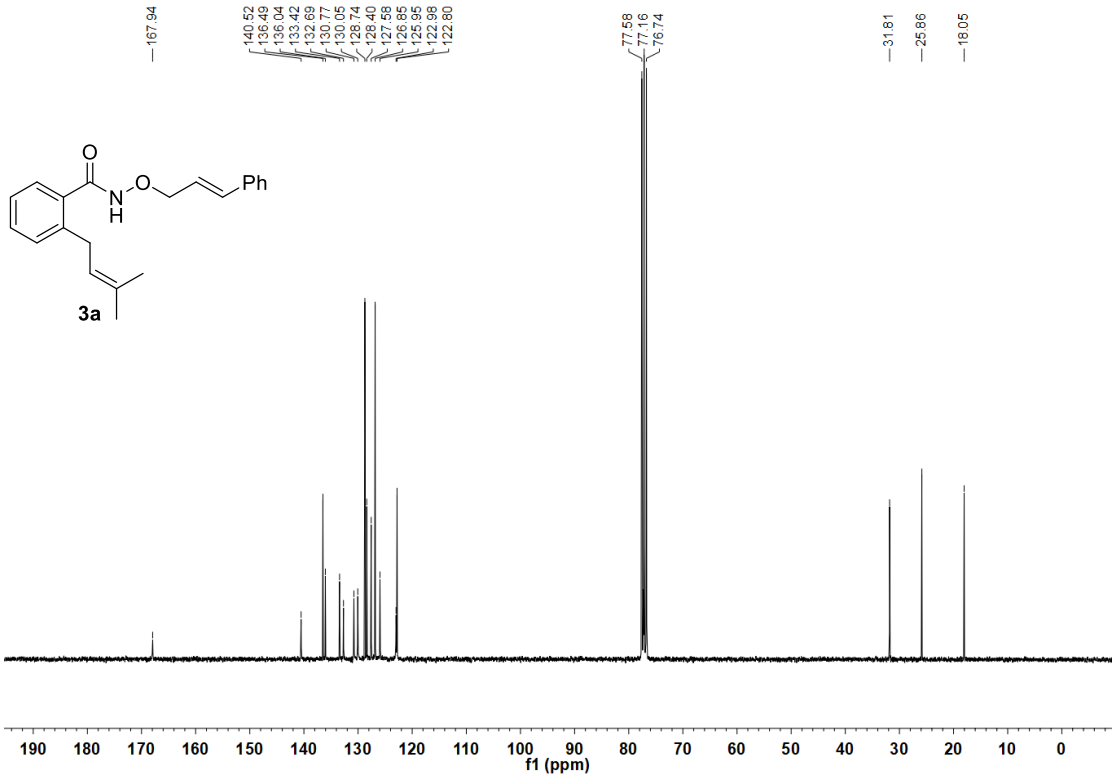


Figure S52. ^{13}C NMR spectra of **3a** (75 MHz, $CDCl_3$)

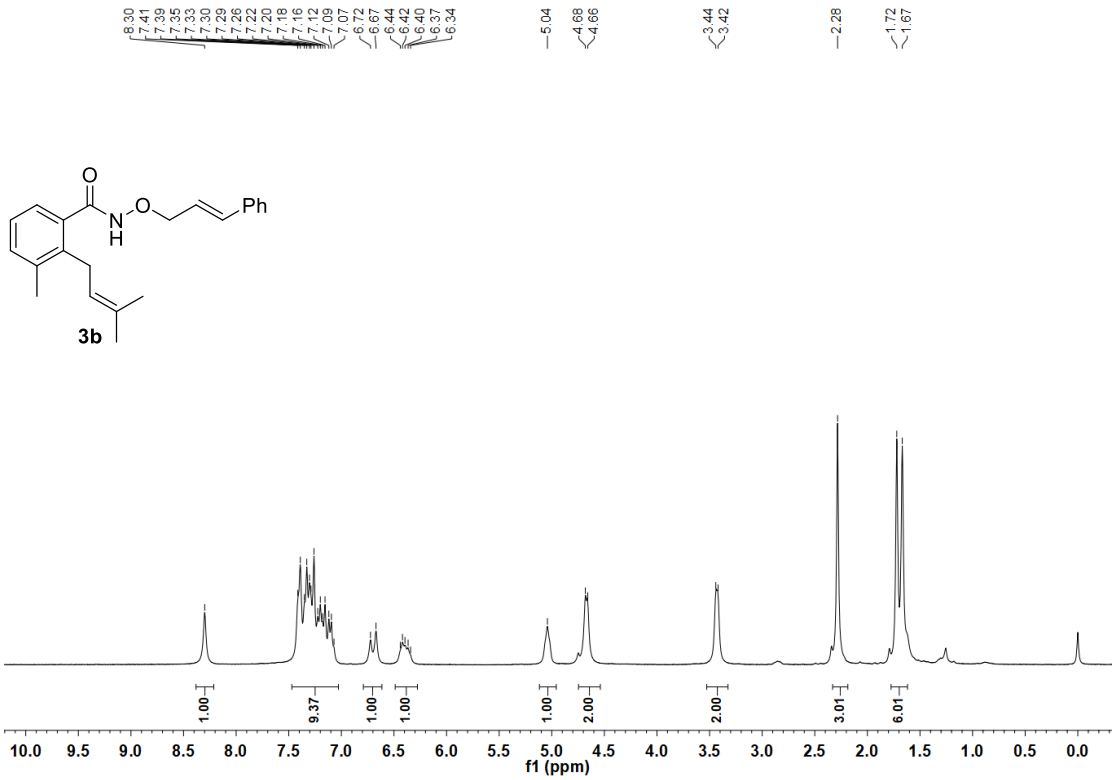


Figure S53. ^{1}H NMR spectra of **3b** (300 MHz, $CDCl_3$)

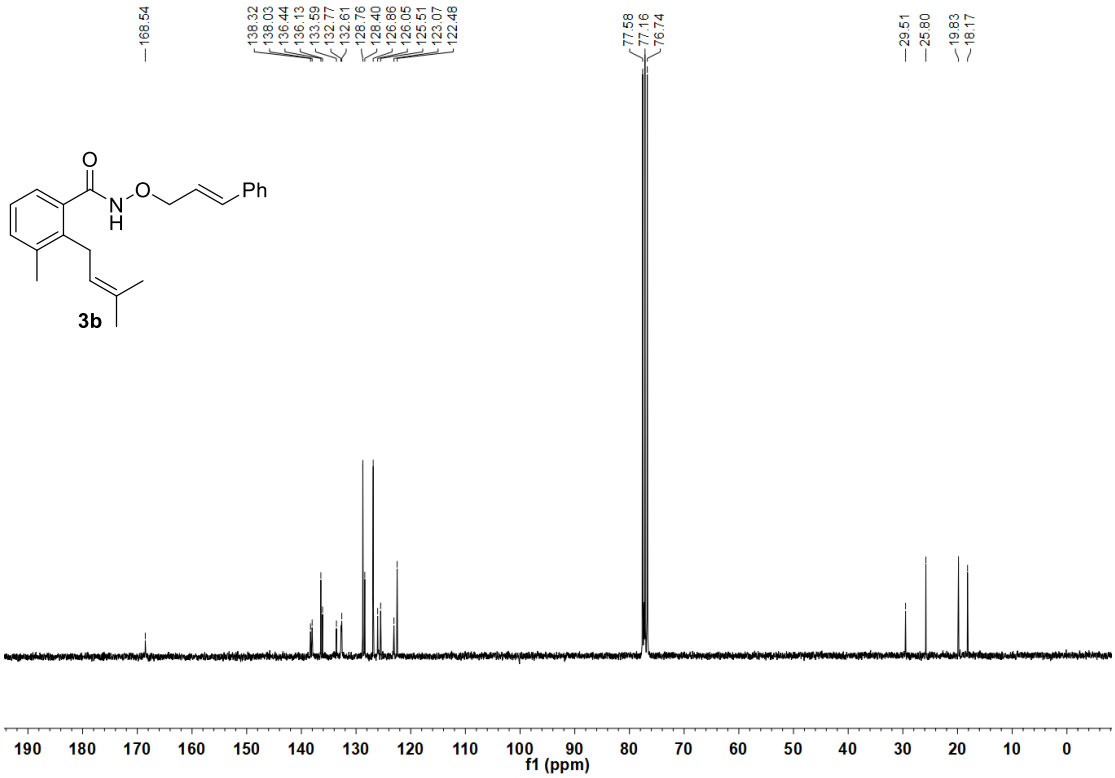


Figure S54. ^{13}C NMR spectra of **3b** (75 MHz, $CDCl_3$)

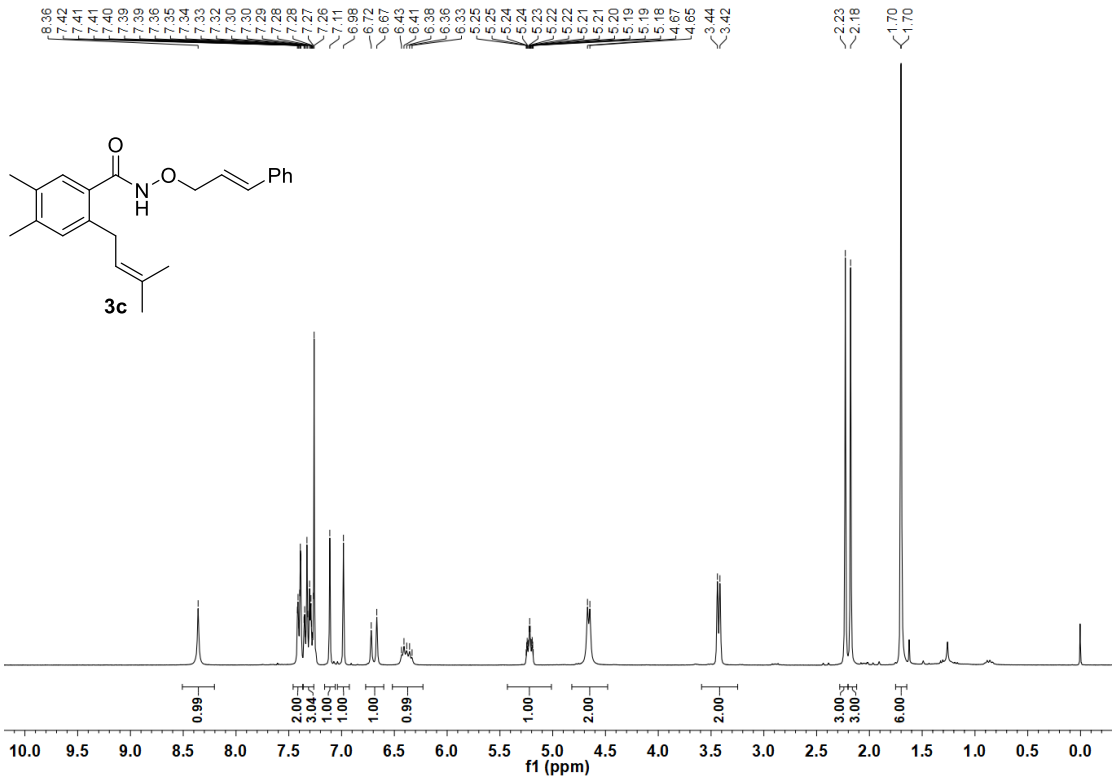


Figure S55. ^{1}H NMR spectra of **3c** (300 MHz, $CDCl_3$)

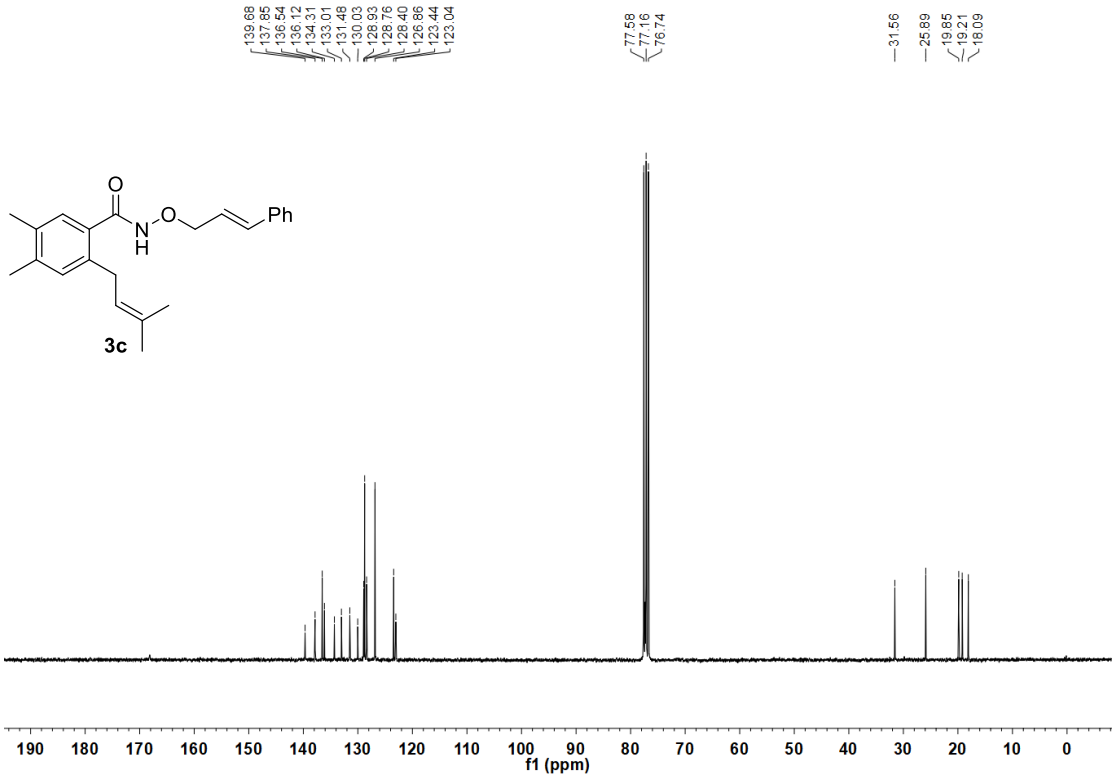


Figure S56. ^{13}C NMR spectra of **3c** (75 MHz, $CDCl_3$)

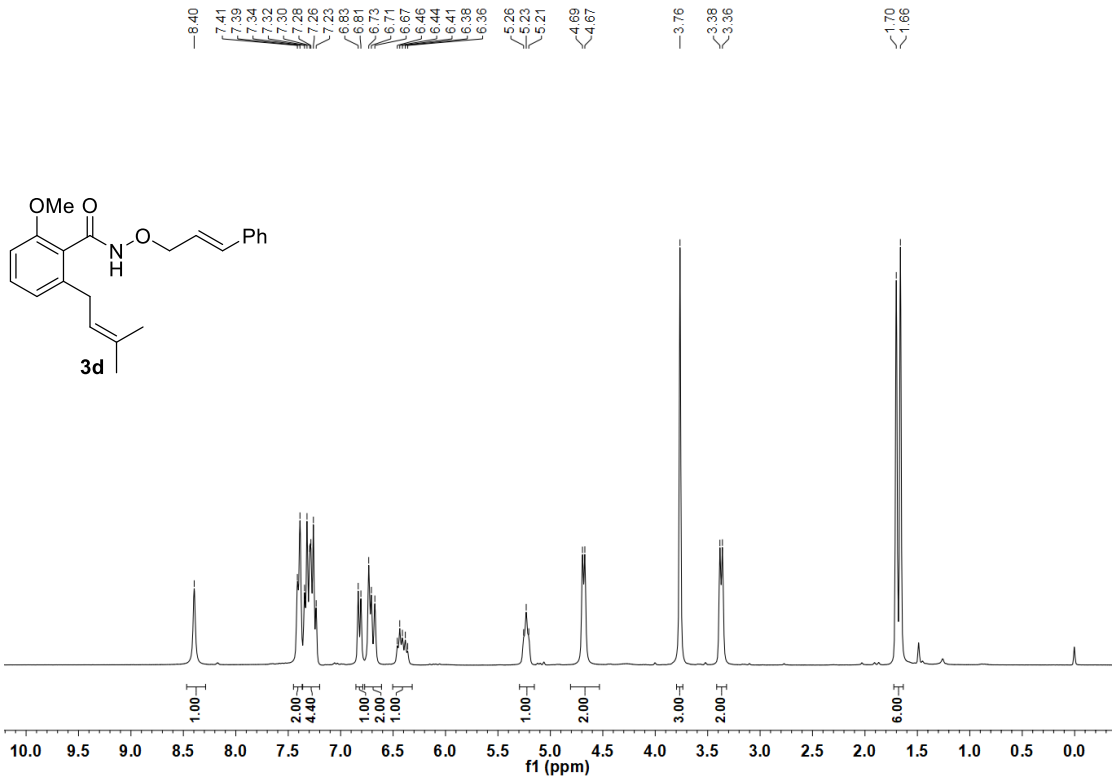


Figure S57. ^{1}H NMR spectra of **3d** (300 MHz, $CDCl_3$)

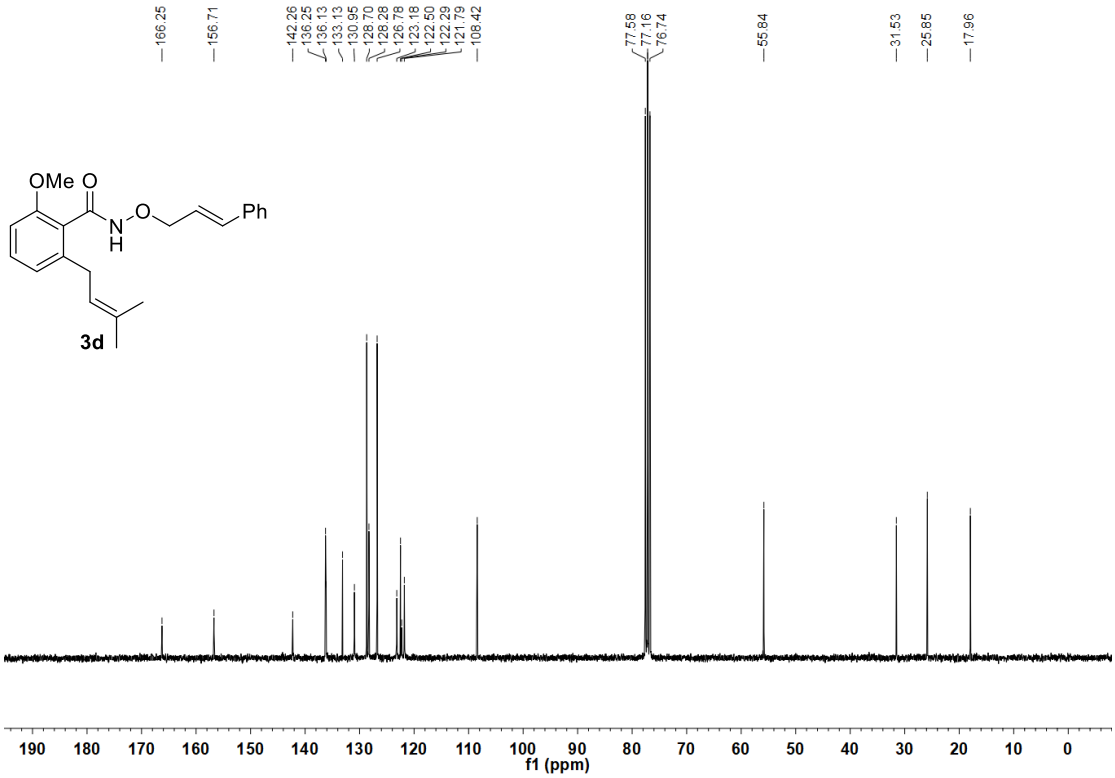


Figure S58. ^{13}C NMR spectra of **3d** (75 MHz, $CDCl_3$)

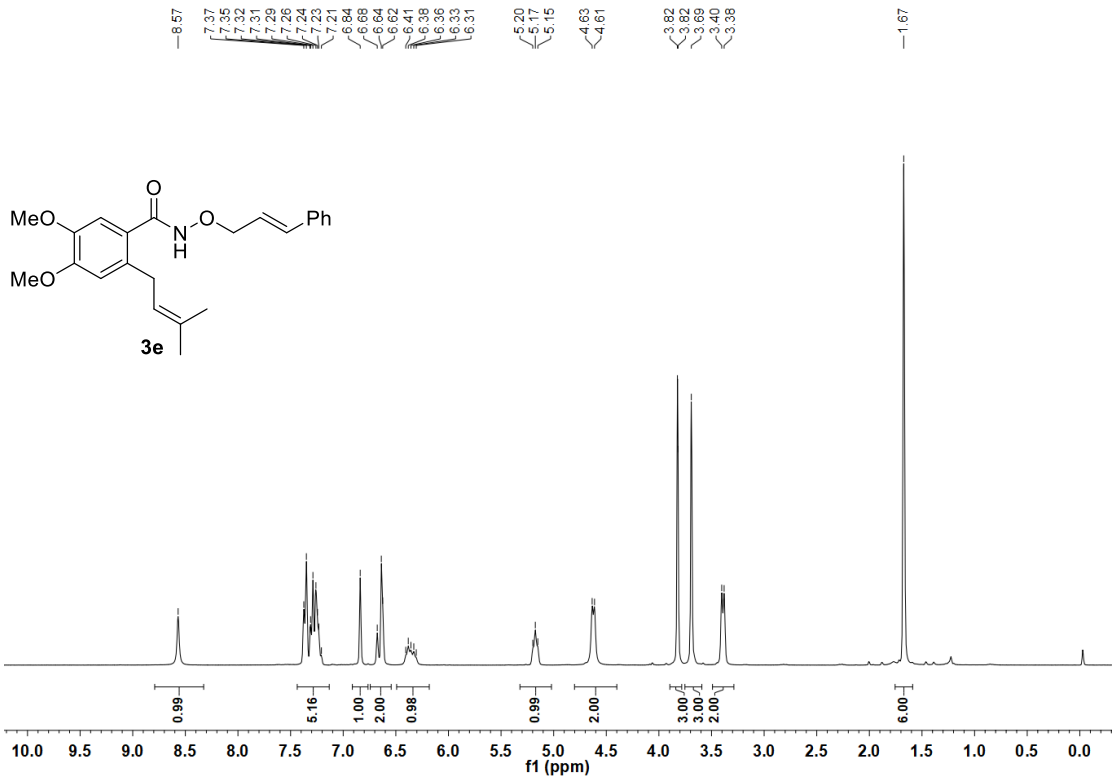


Figure S59. ^{1}H NMR spectra of **3e** (300 MHz, $CDCl_3$)

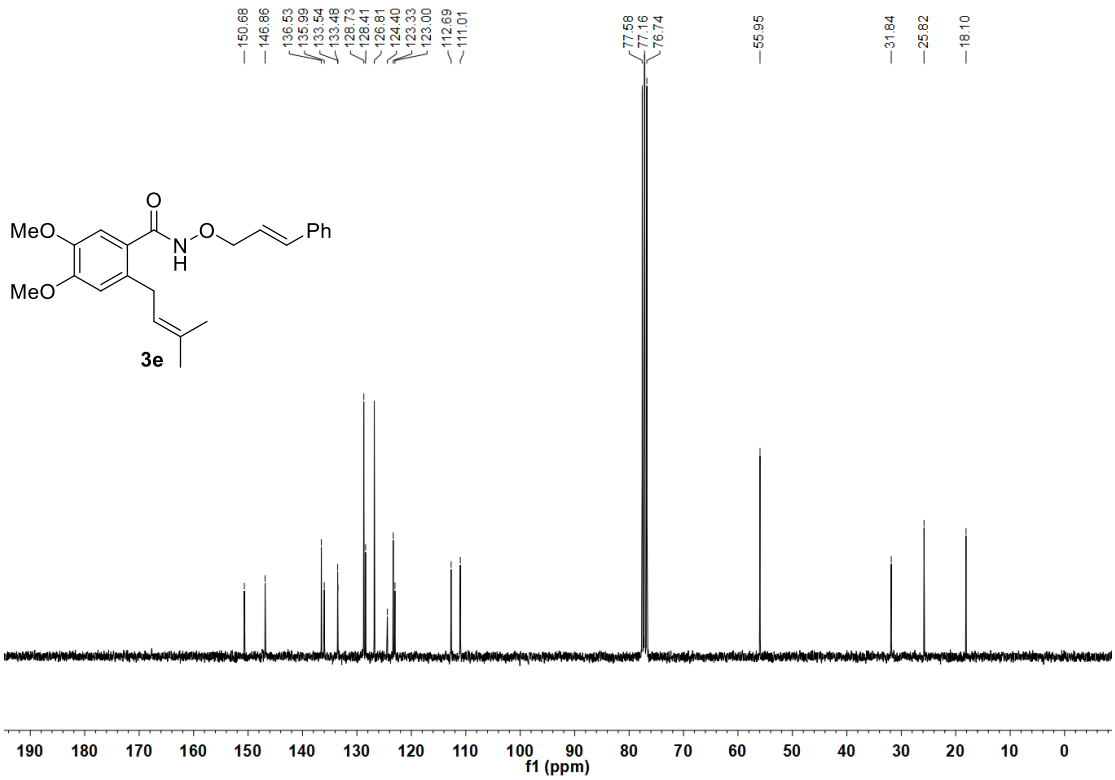


Figure S60. ^{13}C NMR spectra of **3e** (75 MHz, $CDCl_3$)

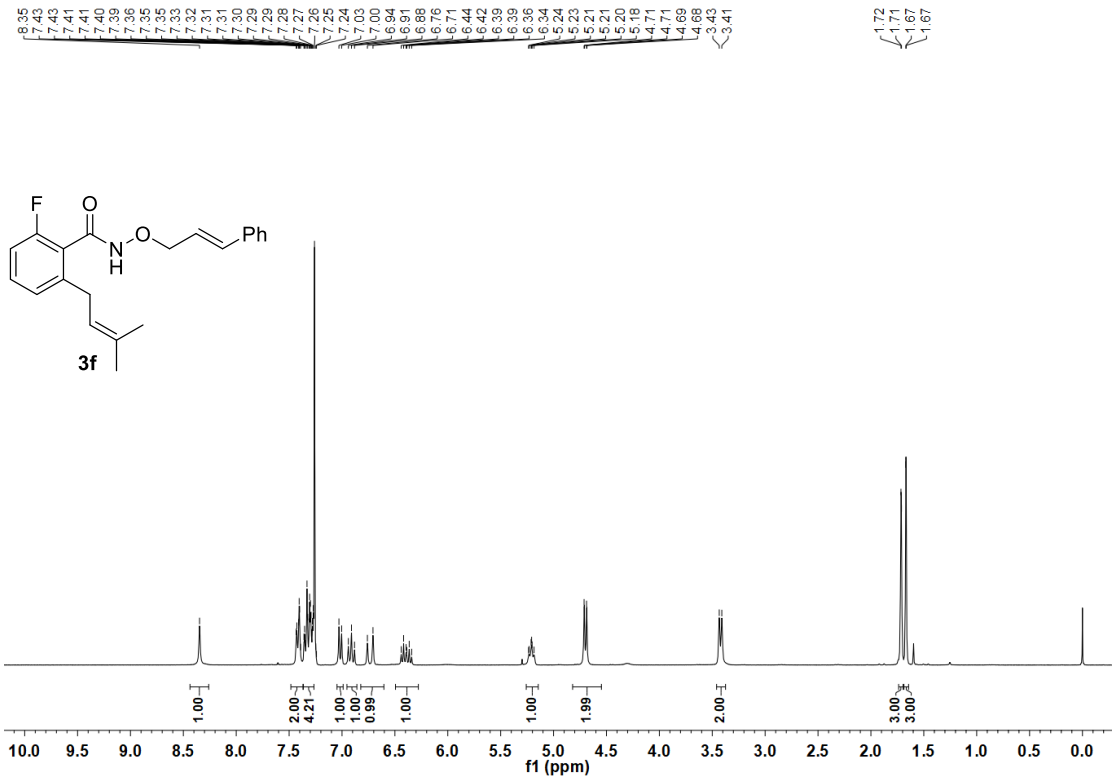


Figure S61. ^{1}H NMR spectra of **3f** (300 MHz, $CDCl_3$)

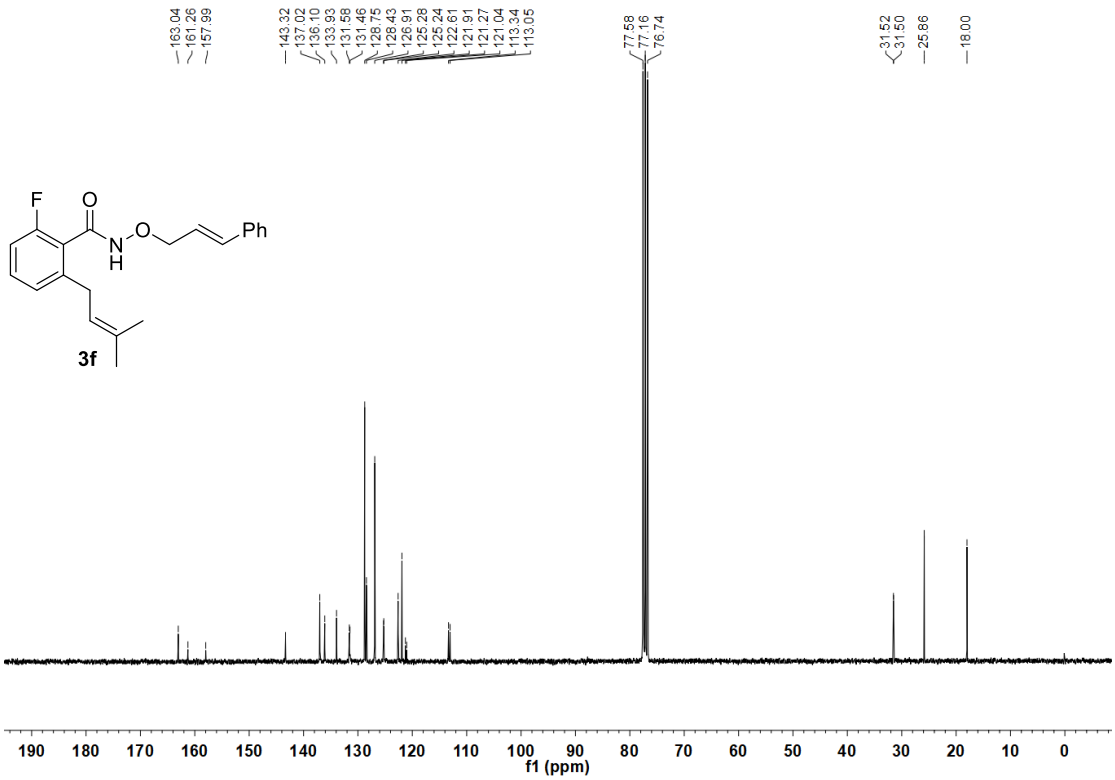


Figure S62. ^{13}C NMR spectra of **3f** (75 MHz, $CDCl_3$)

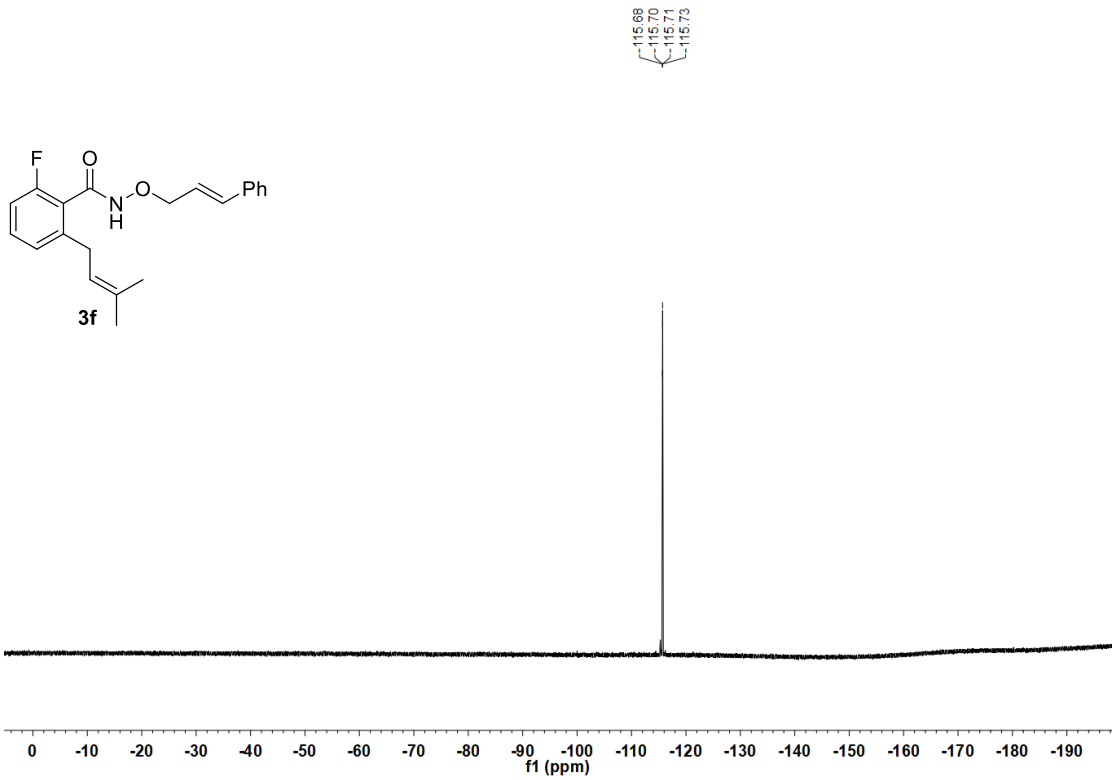


Figure S63. ^{19}F NMR spectra of **3f** (282 MHz, $CDCl_3$)

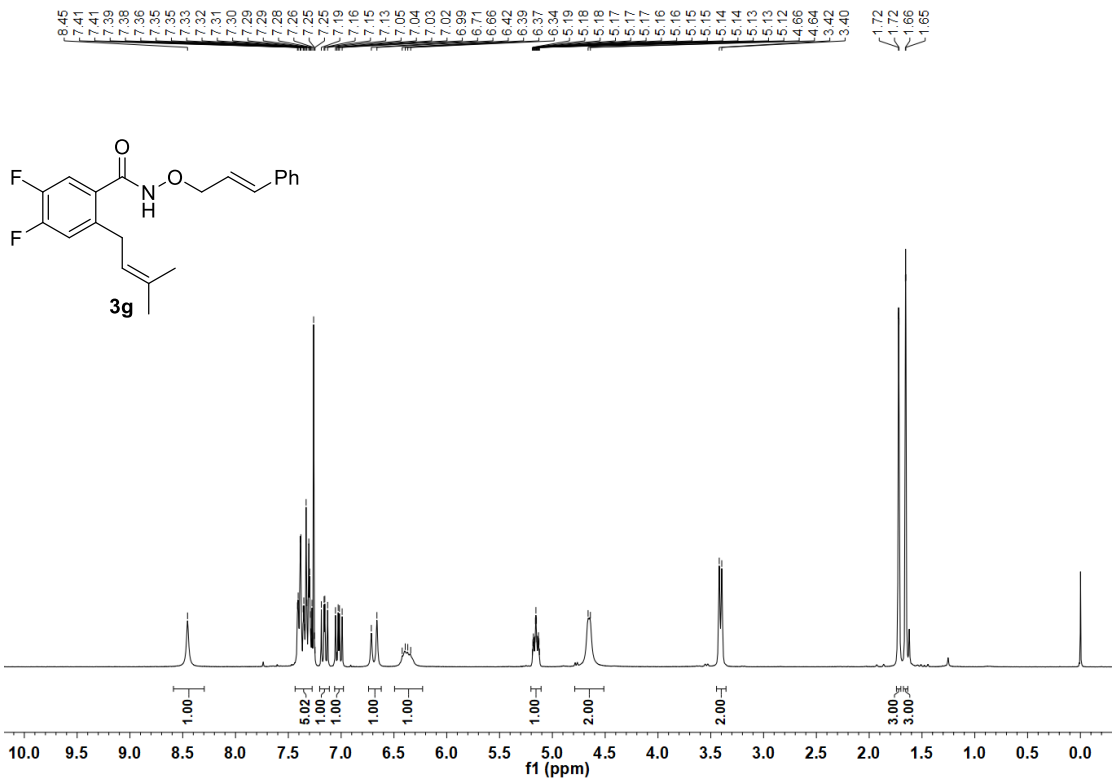


Figure S64. ^{1}H NMR spectra of **3g** (300 MHz, $CDCl_3$)

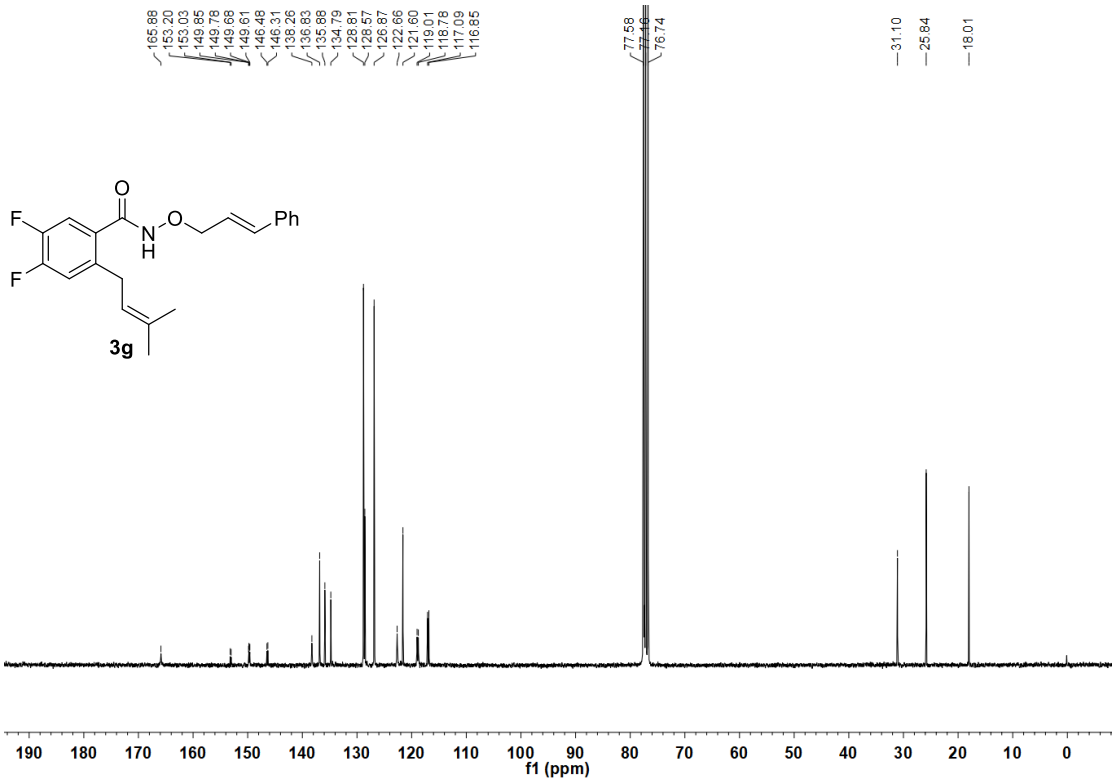


Figure S65. ^{13}C NMR spectra of **3g** (75 MHz, $CDCl_3$)

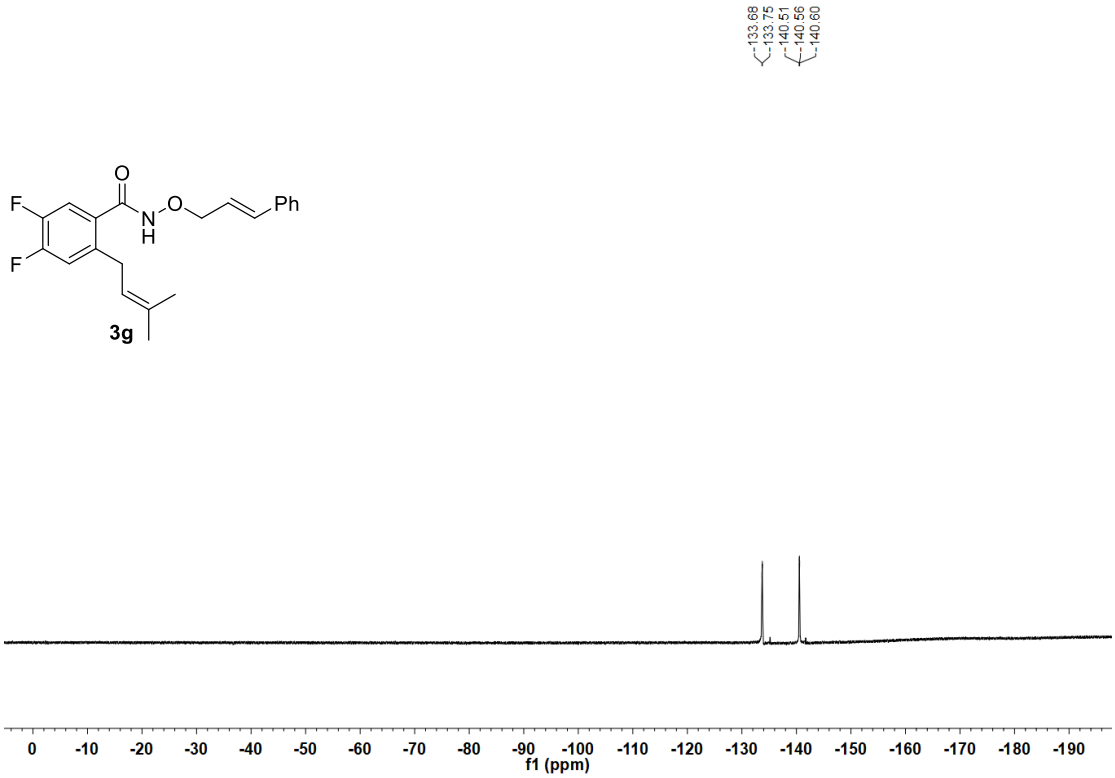


Figure S66. ^{19}F NMR spectra of **3g** (282 MHz, $CDCl_3$)

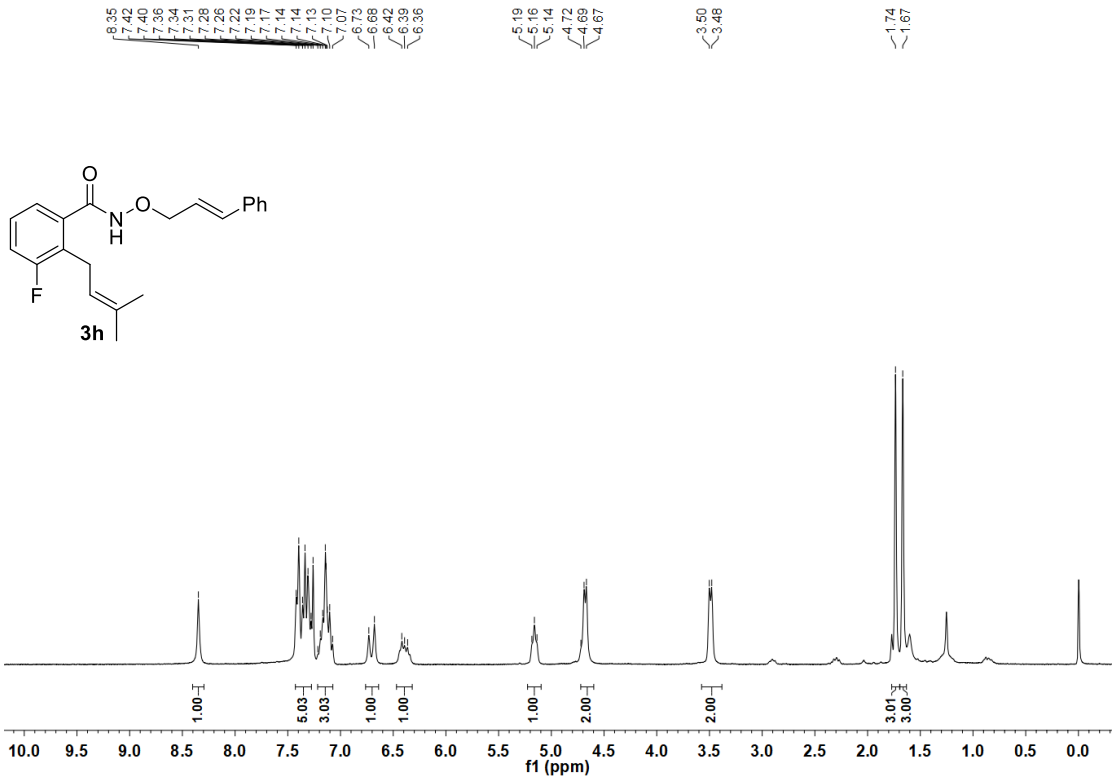


Figure S67. ^{1}H NMR spectra of **3h** (300 MHz, $CDCl_3$)

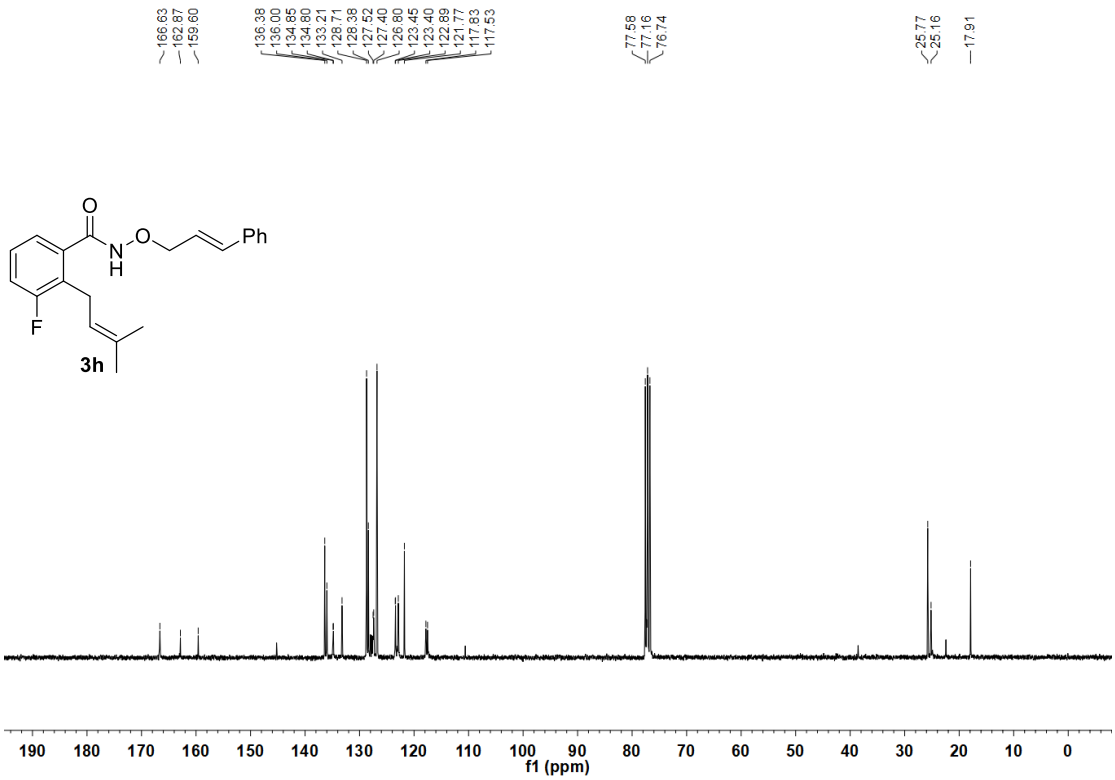


Figure S68. ^{13}C NMR spectra of **3h** (75 MHz, $CDCl_3$)

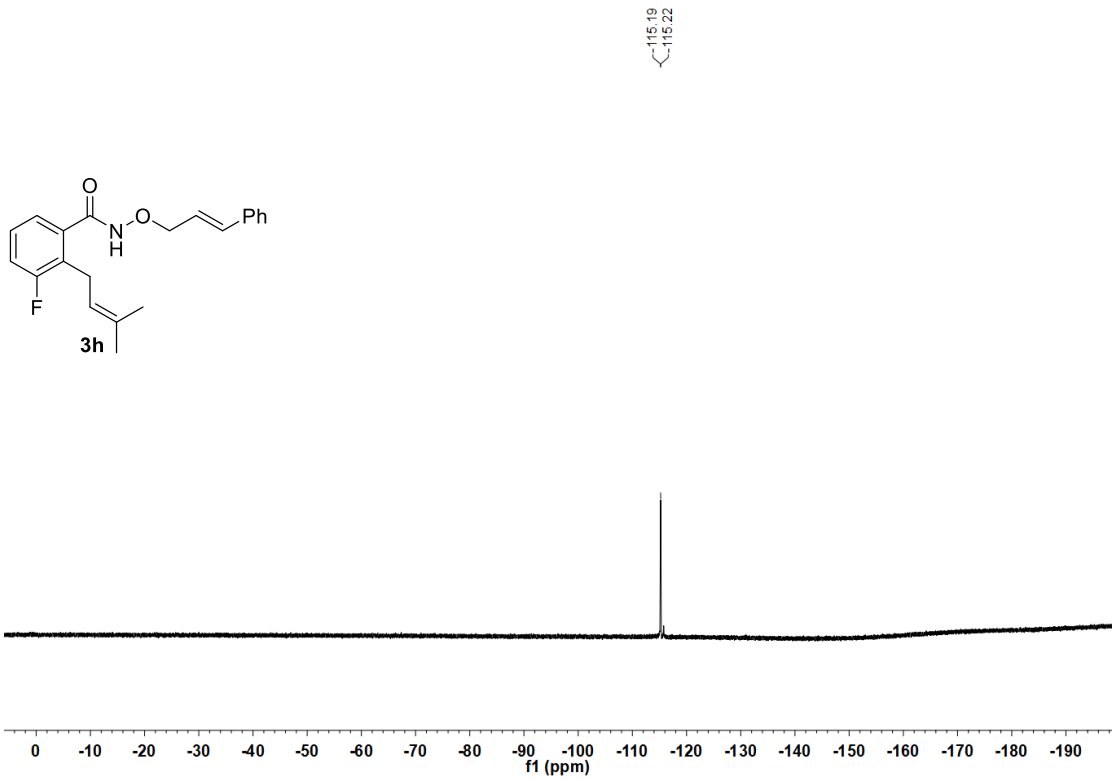


Figure S69. ^{19}F NMR spectra of **3h** (282 MHz, $CDCl_3$)

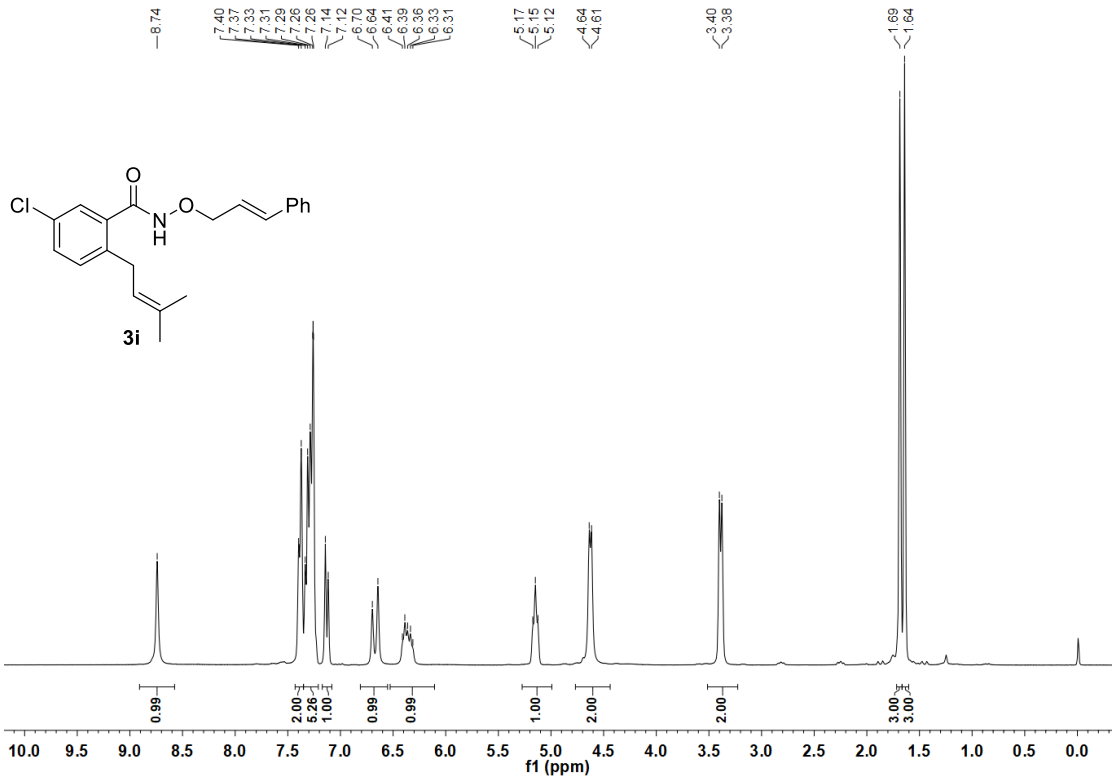


Figure S70. ^{1}H NMR spectra of **3i** (300 MHz, $CDCl_3$)

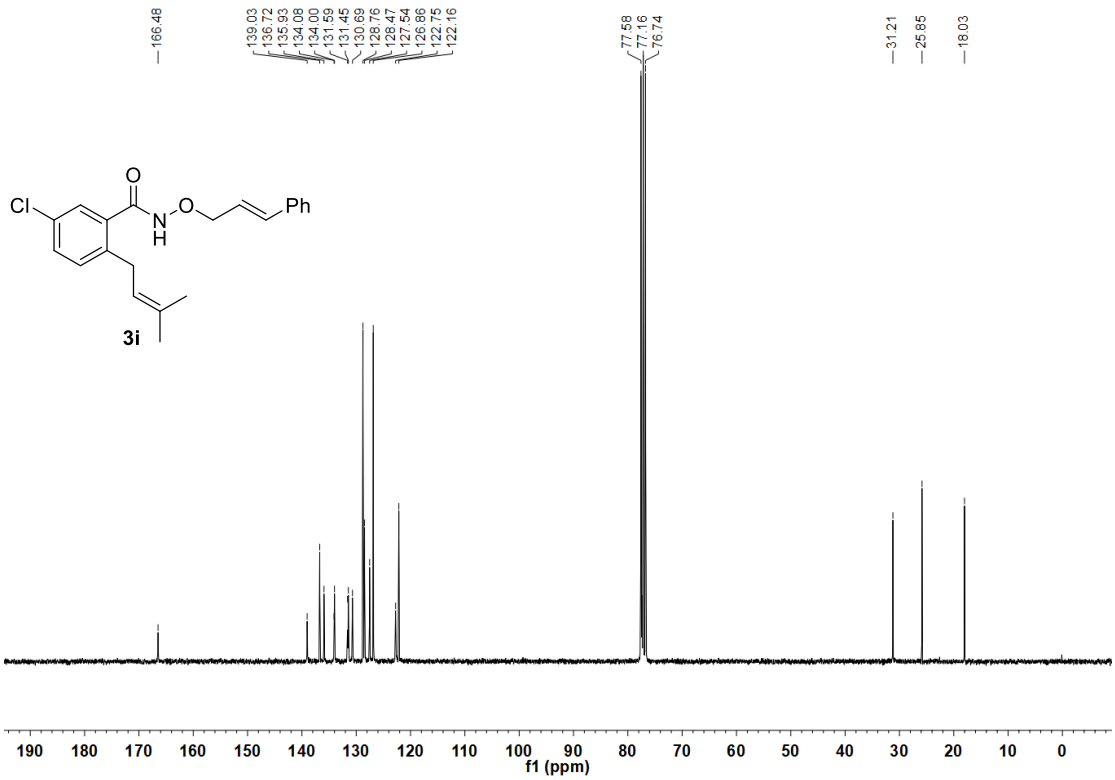


Figure S71. ^{13}C NMR spectra of **3i** (75 MHz, $CDCl_3$)

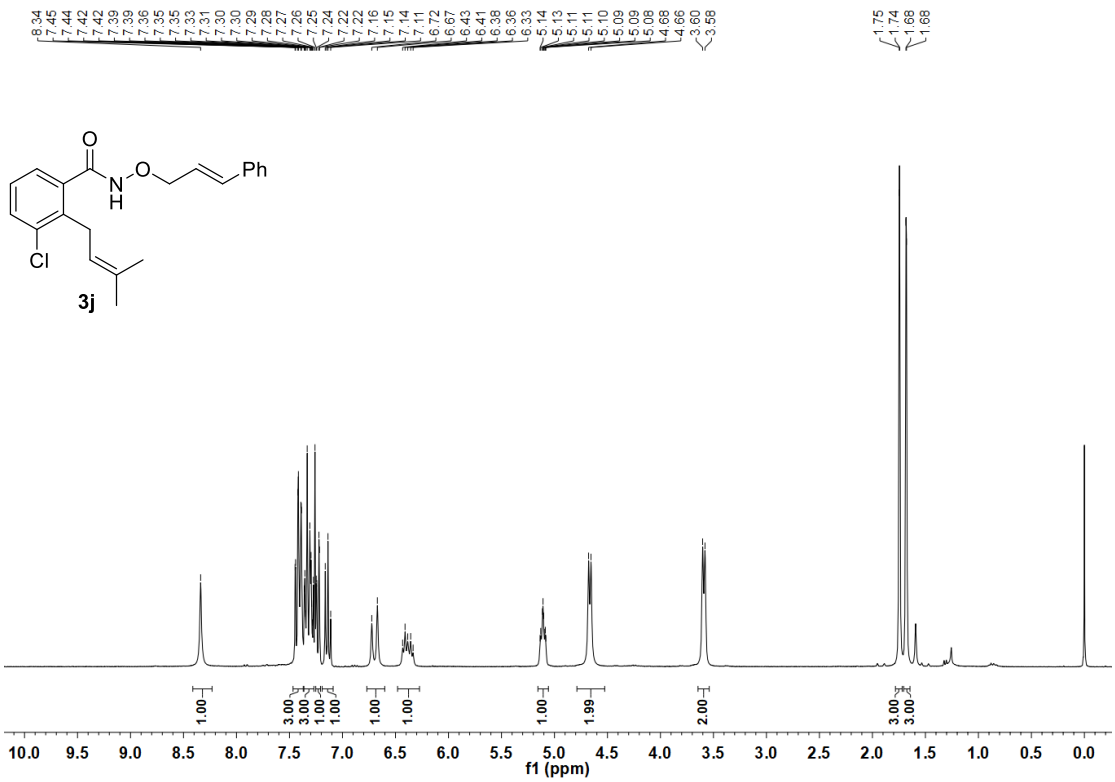


Figure S72. ^{1}H NMR spectra of **3j** (300 MHz, $CDCl_3$)

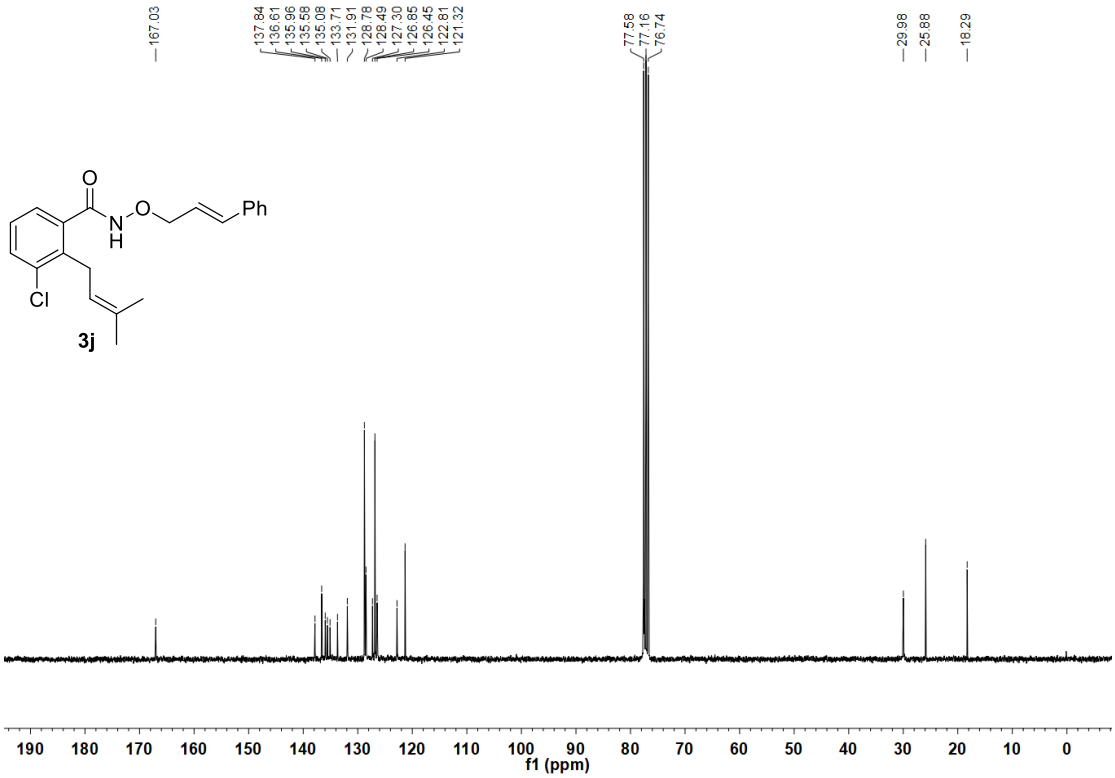


Figure S73. ^{13}C NMR spectra of **3j** (75 MHz, $CDCl_3$)

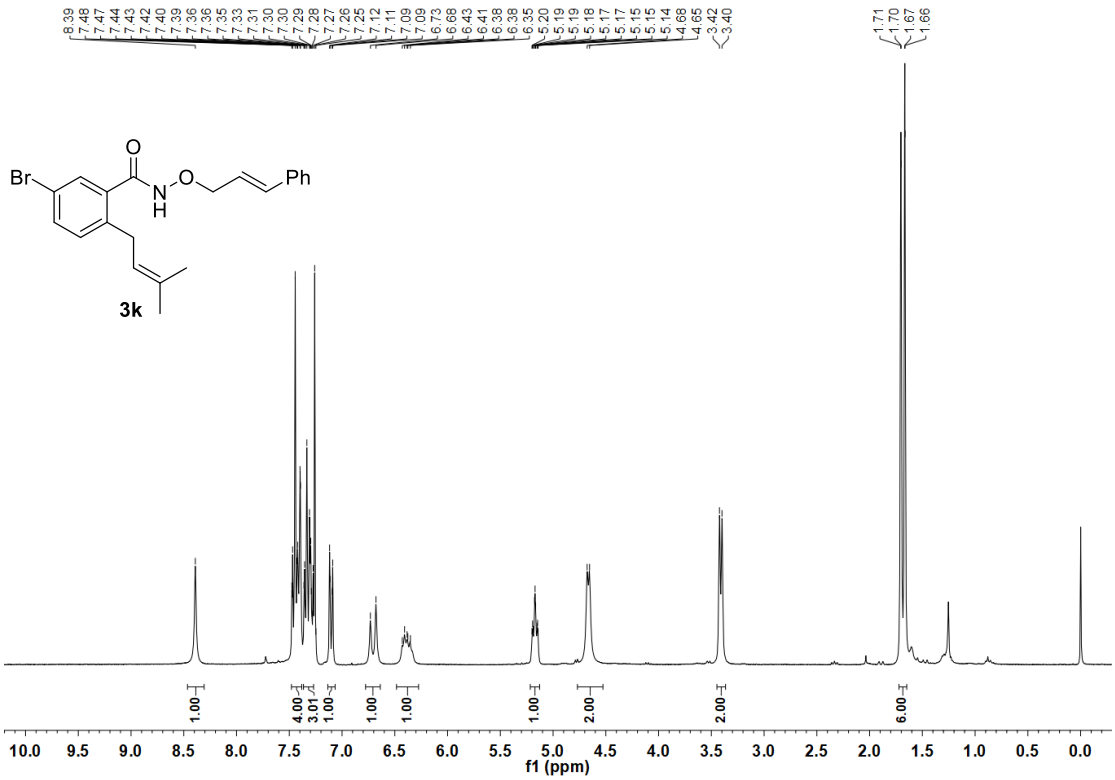


Figure S74. ^{1}H NMR spectra of **3k** (300 MHz, $CDCl_3$)

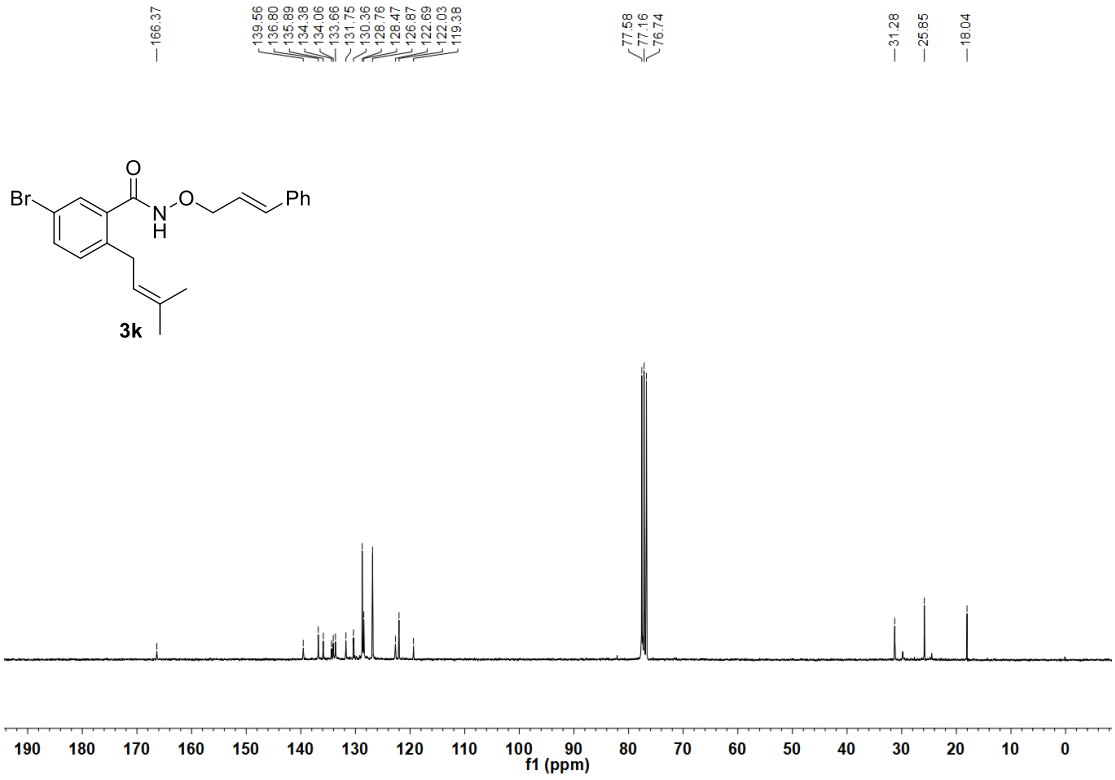


Figure S75. ^{13}C NMR spectra of **3k** (75 MHz, $CDCl_3$)

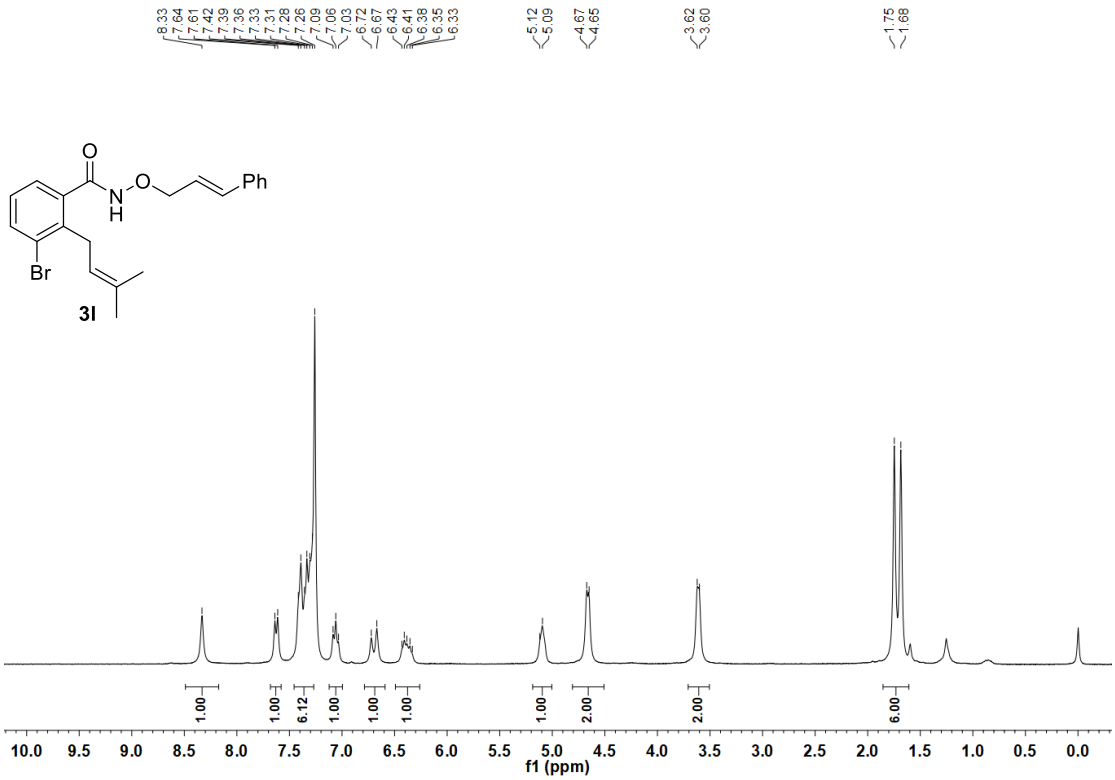


Figure S76. ^{1}H NMR spectra of **3l** (300 MHz, $CDCl_3$)

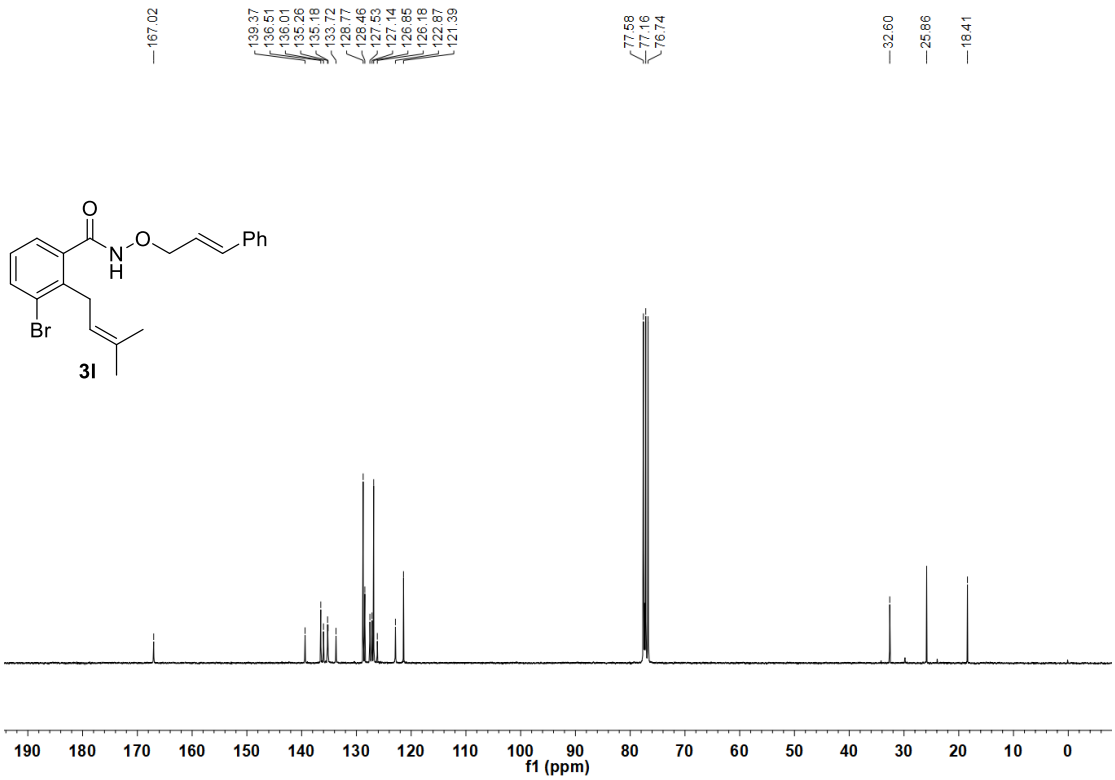


Figure S77. ^{13}C NMR spectra of **3l** (75 MHz, $CDCl_3$)

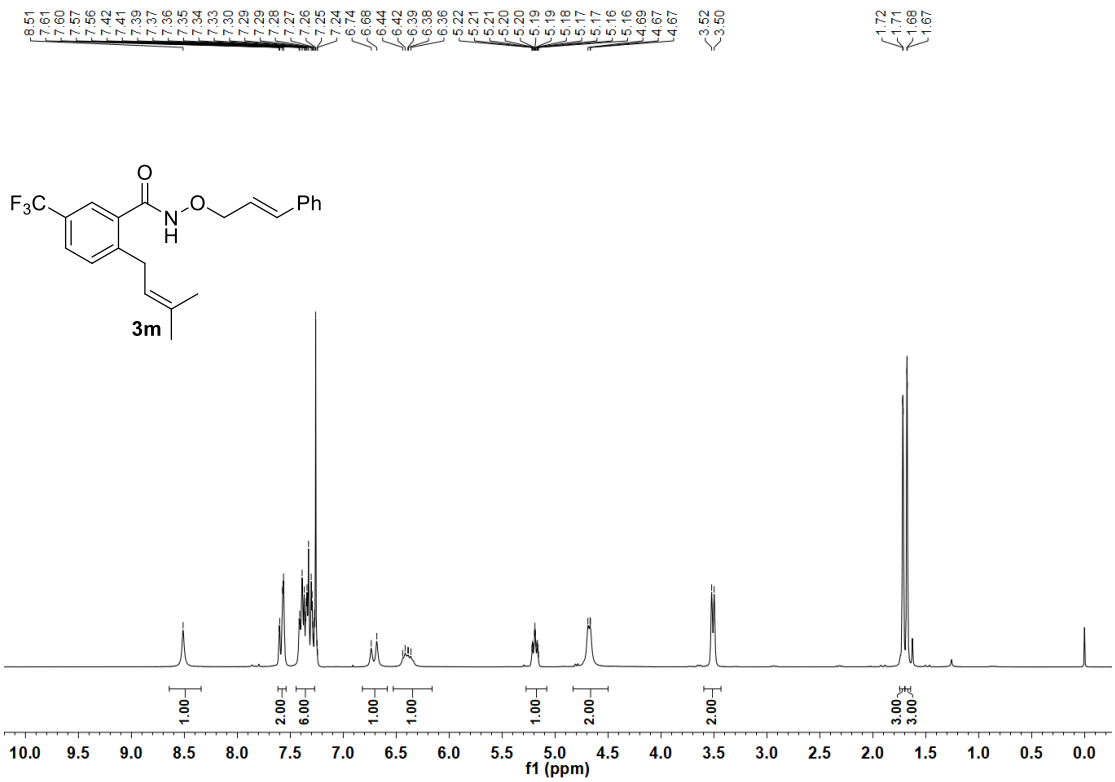


Figure S78. ^{1}H NMR spectra of **3m** (300 MHz, $CDCl_3$)

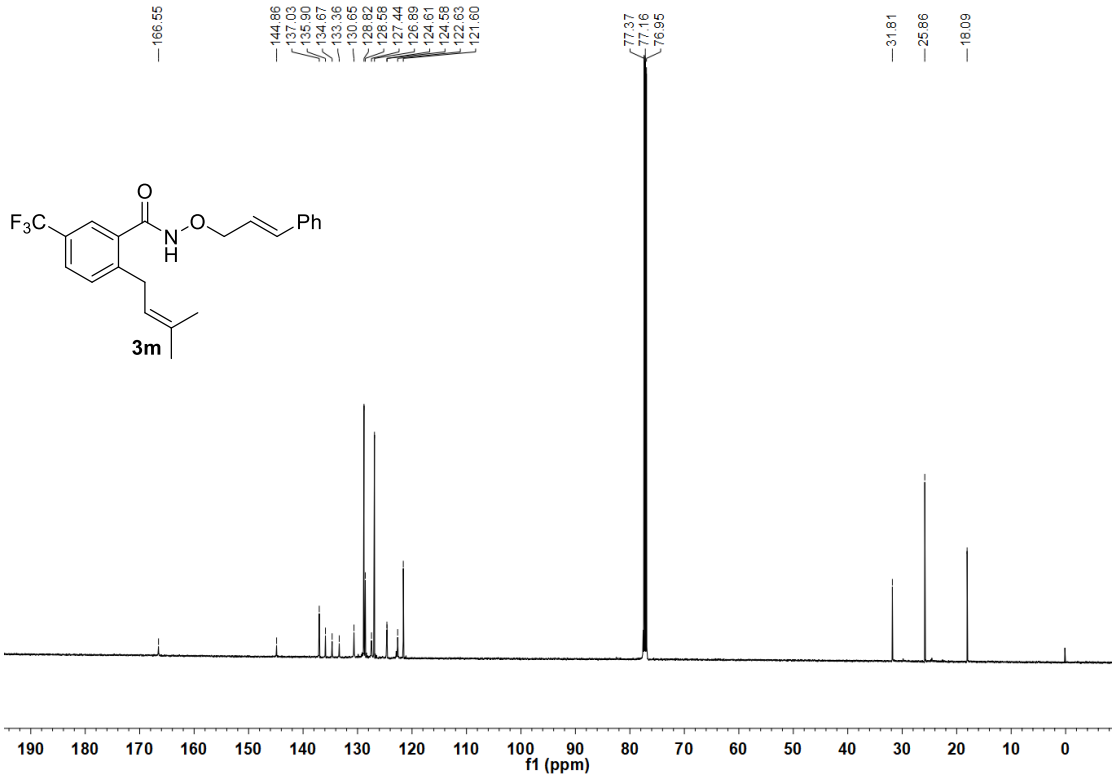


Figure S79. ^{13}C NMR spectra of **3m** (75 MHz, $CDCl_3$)

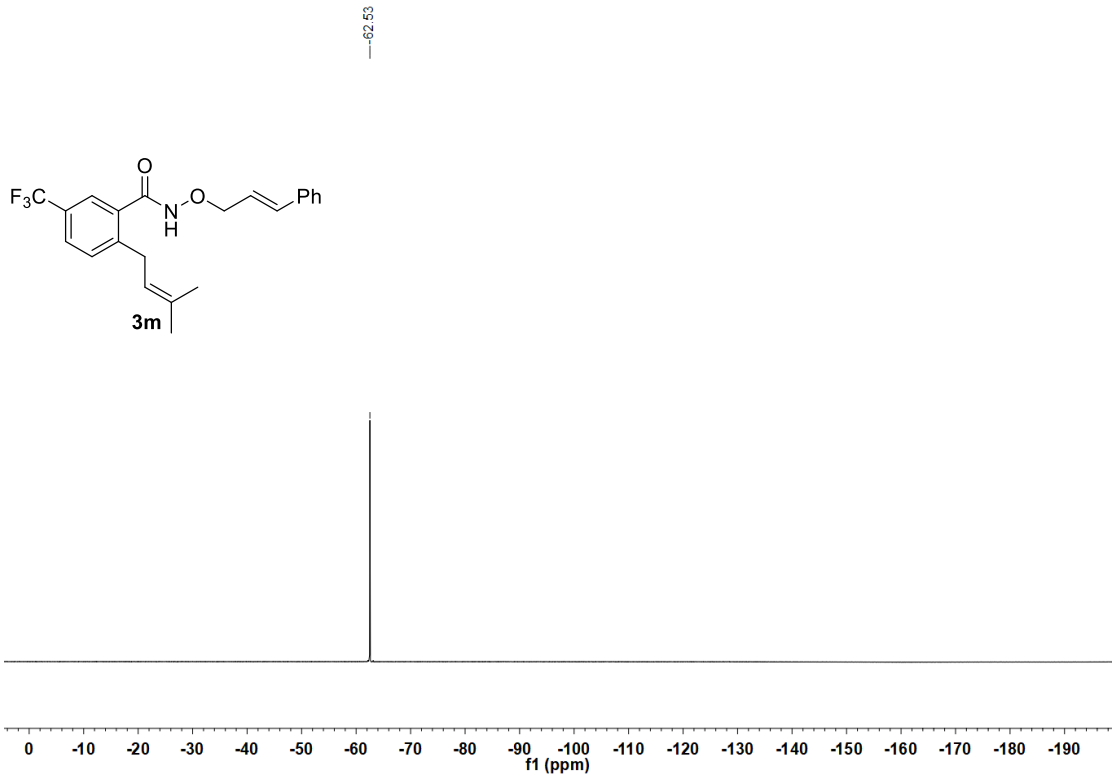


Figure S80. ^{19}F NMR spectra of **3m** (282 MHz, $CDCl_3$)

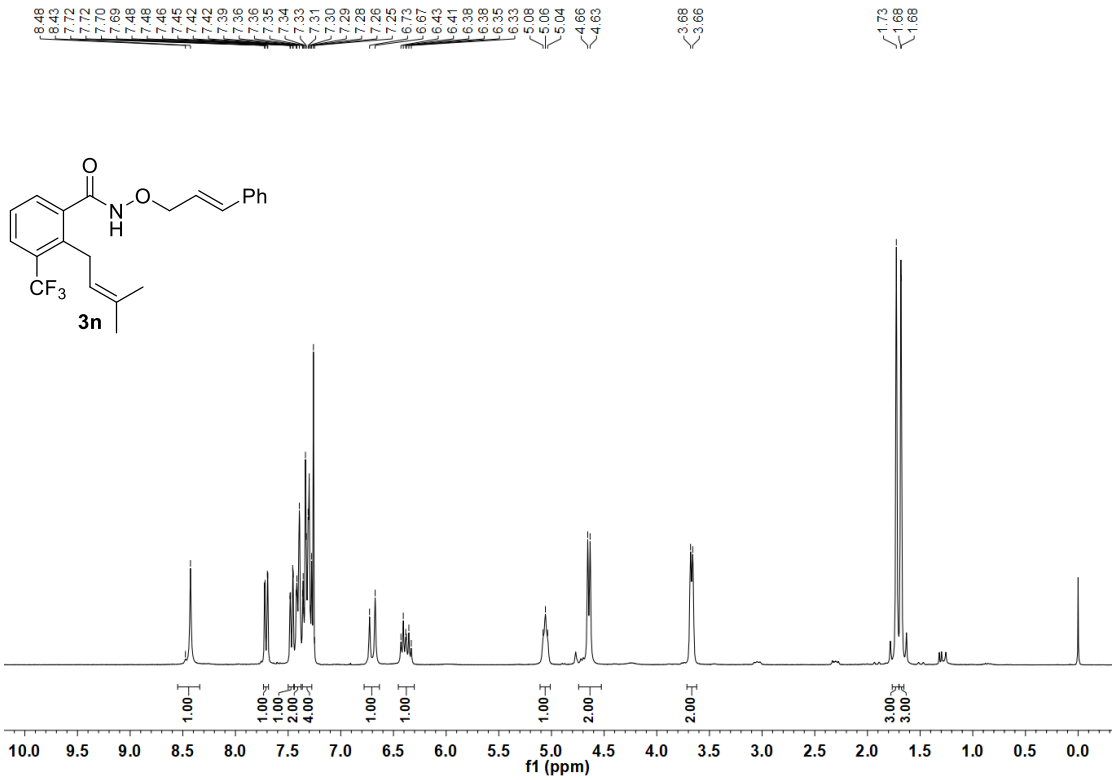


Figure S81. ^{1}H NMR spectra of **3n** (300 MHz, $CDCl_3$)

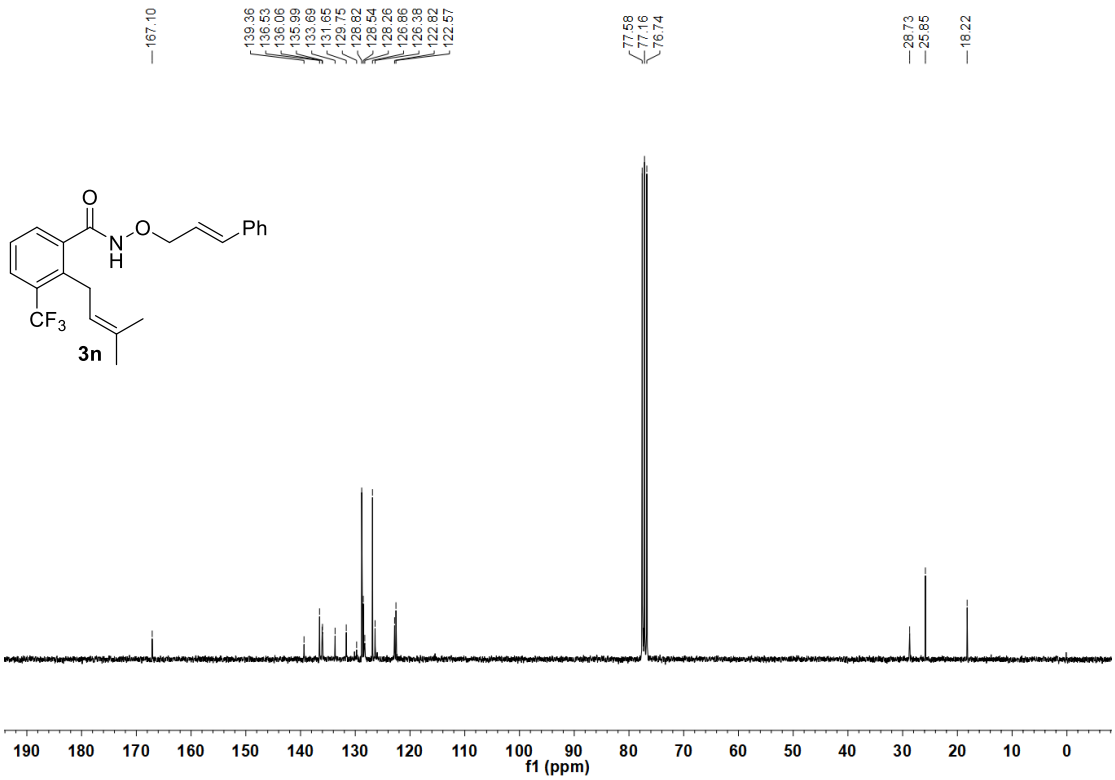


Figure S82. ^{13}C NMR spectra of **3n** (75 MHz, $CDCl_3$)

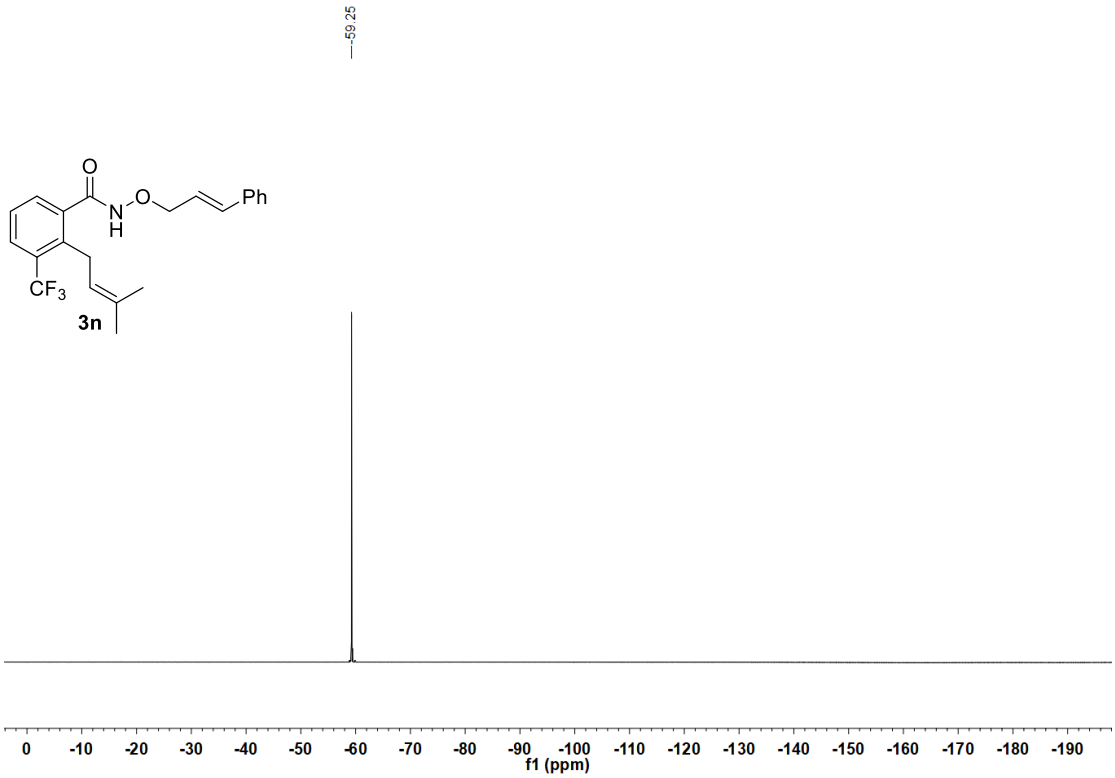


Figure S83. ^{19}F NMR spectra of **3n** (282 MHz, $CDCl_3$)

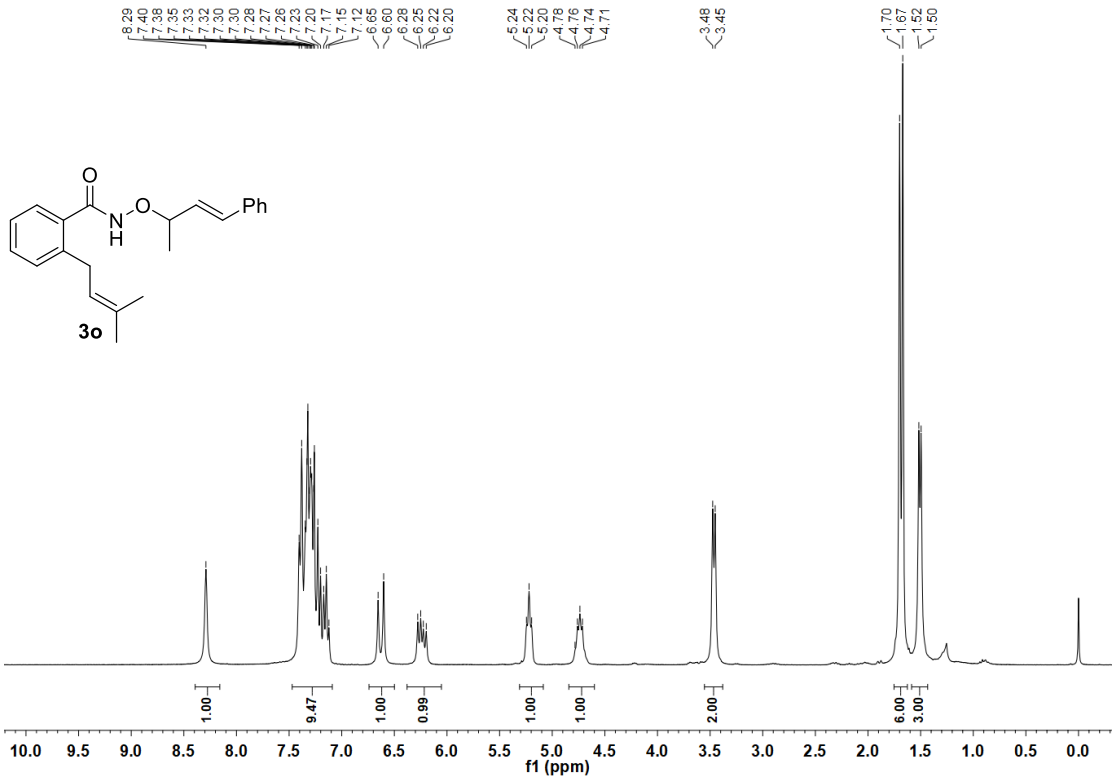


Figure S84. ^{1}H NMR spectra of **3o** (300 MHz, $CDCl_3$)

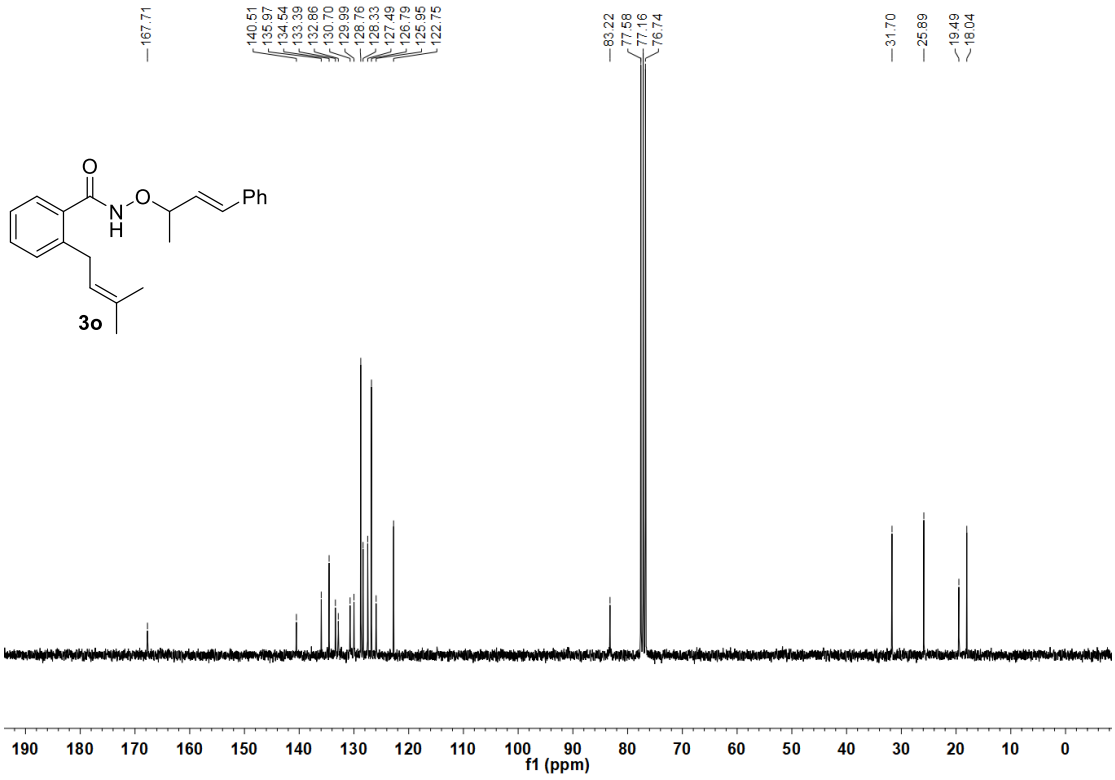


Figure S85. ^{13}C NMR spectra of **3o** (75 MHz, $CDCl_3$)

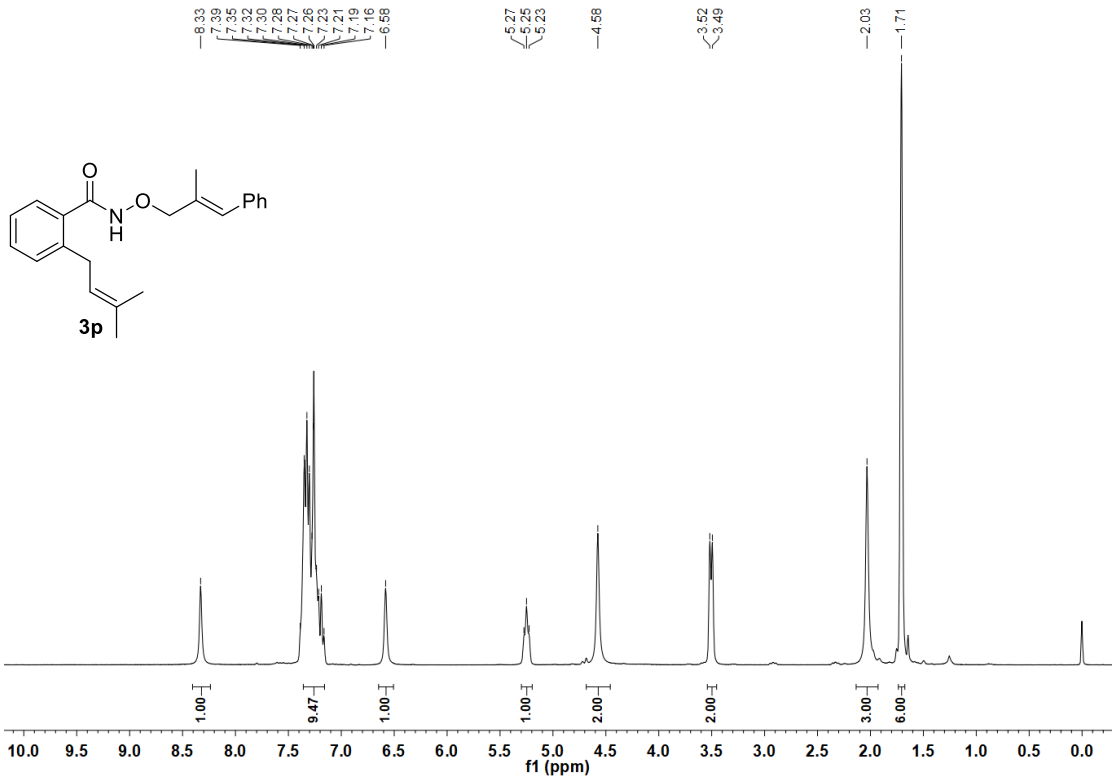


Figure S86. ^{1}H NMR spectra of **3p** (300 MHz, $CDCl_3$)

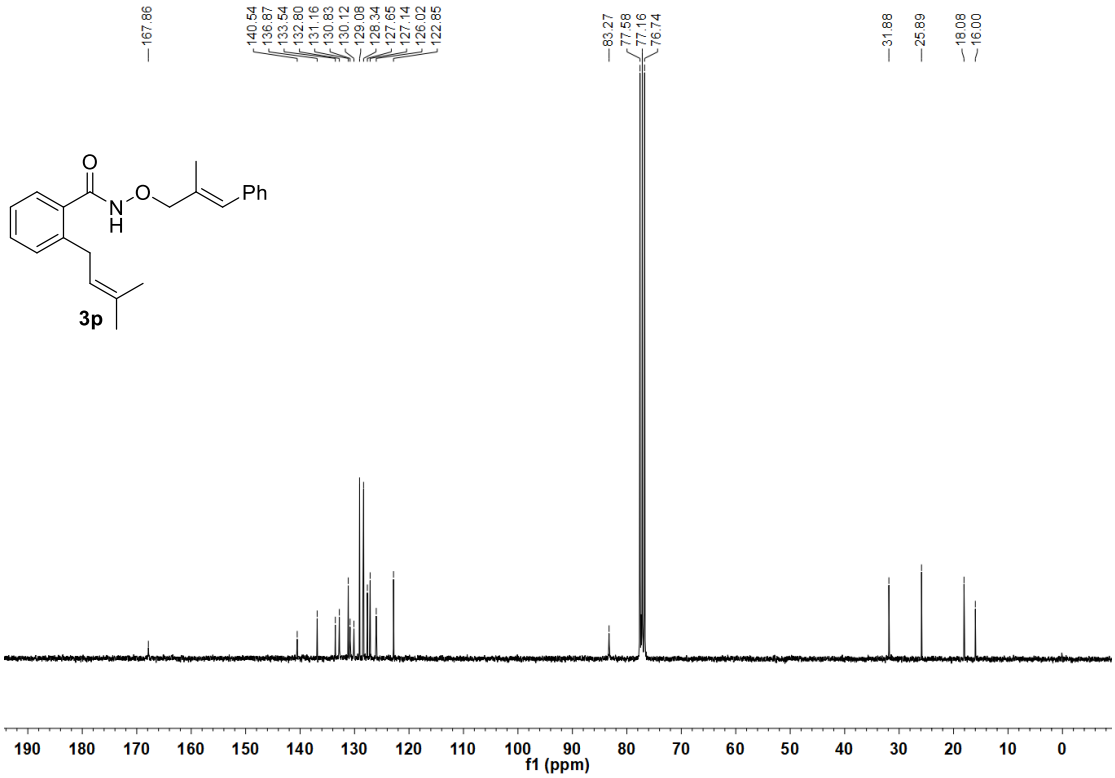


Figure S87. ^{13}C NMR spectra of **3p** (75 MHz, $CDCl_3$)

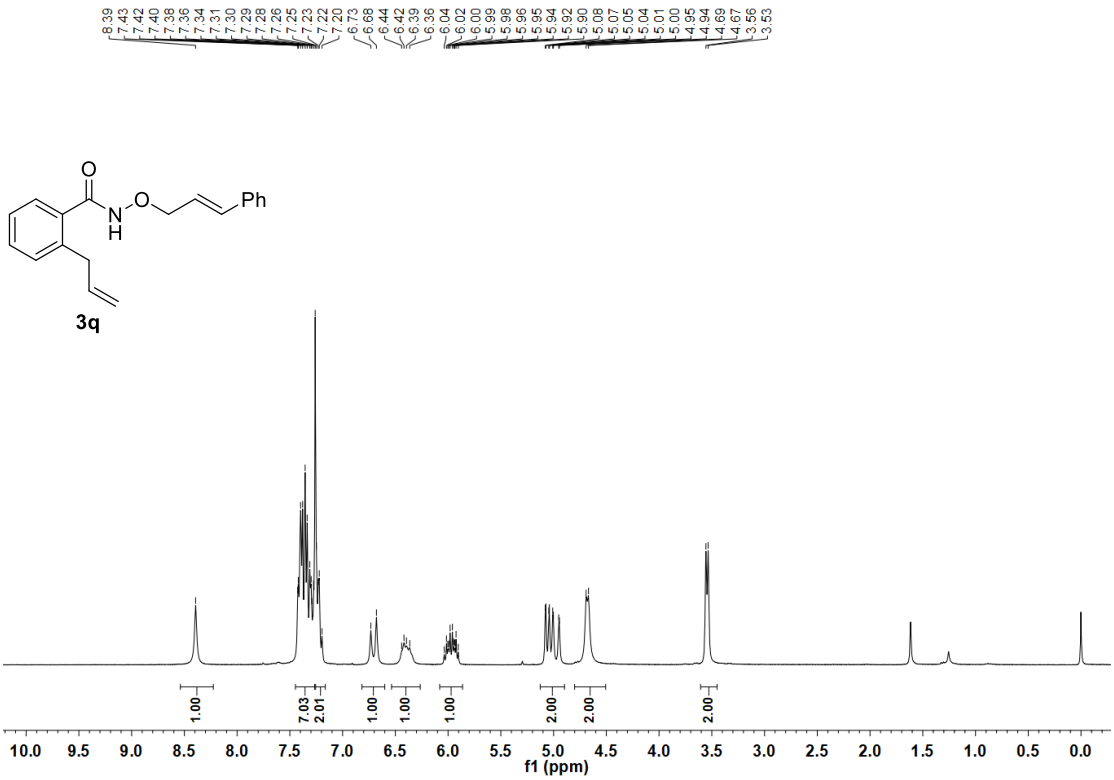


Figure S88. ^{1}H NMR spectra of **3q** (300 MHz, $CDCl_3$)

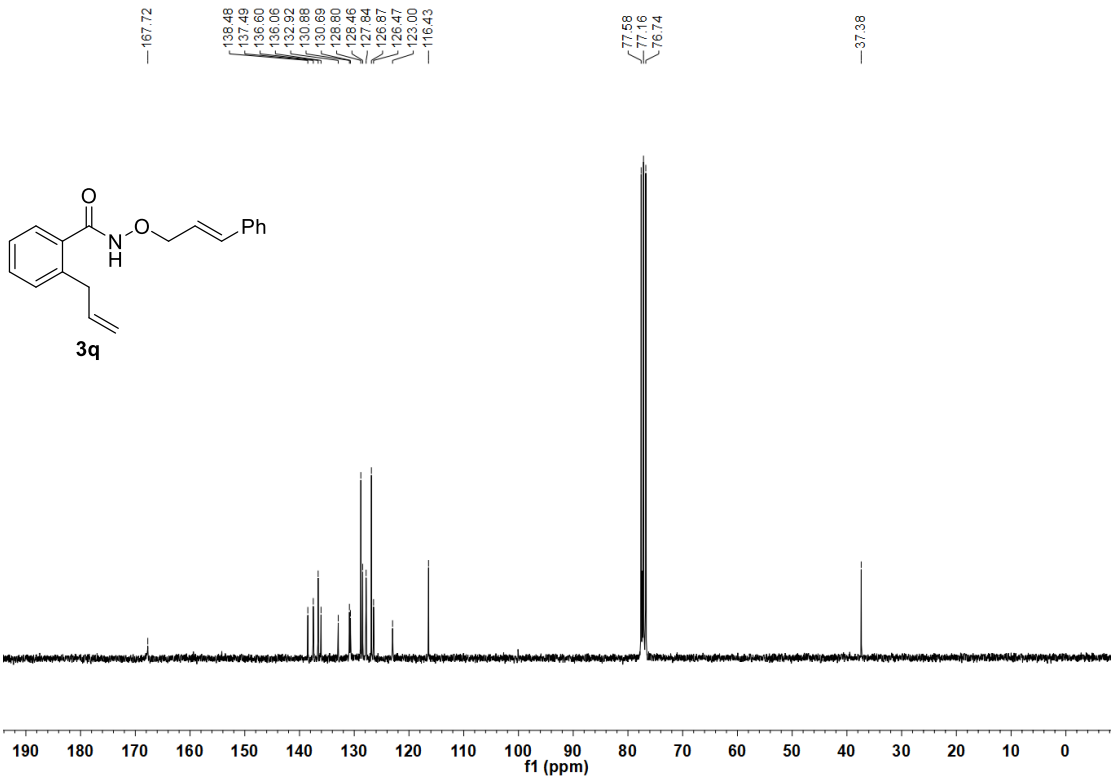


Figure S89. ^{13}C NMR spectra of **3q** (75 MHz, $CDCl_3$)

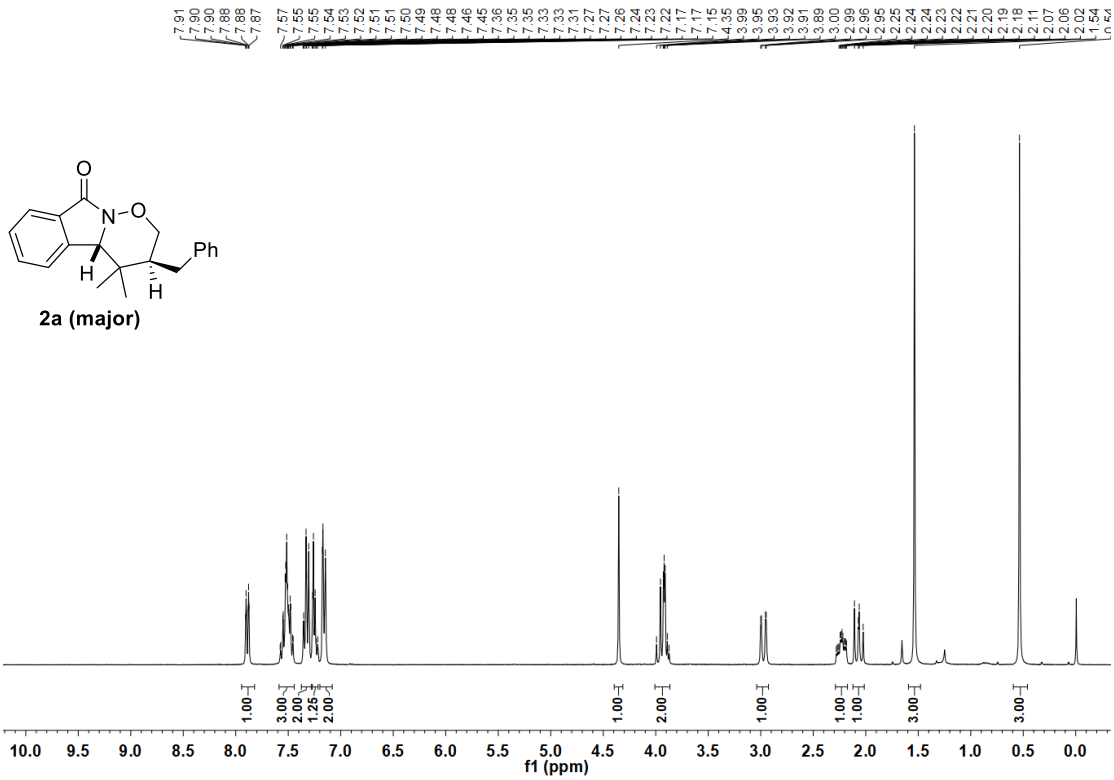


Figure S90. ^{1}H NMR spectra of **2a (major)** (300 MHz, $CDCl_3$)

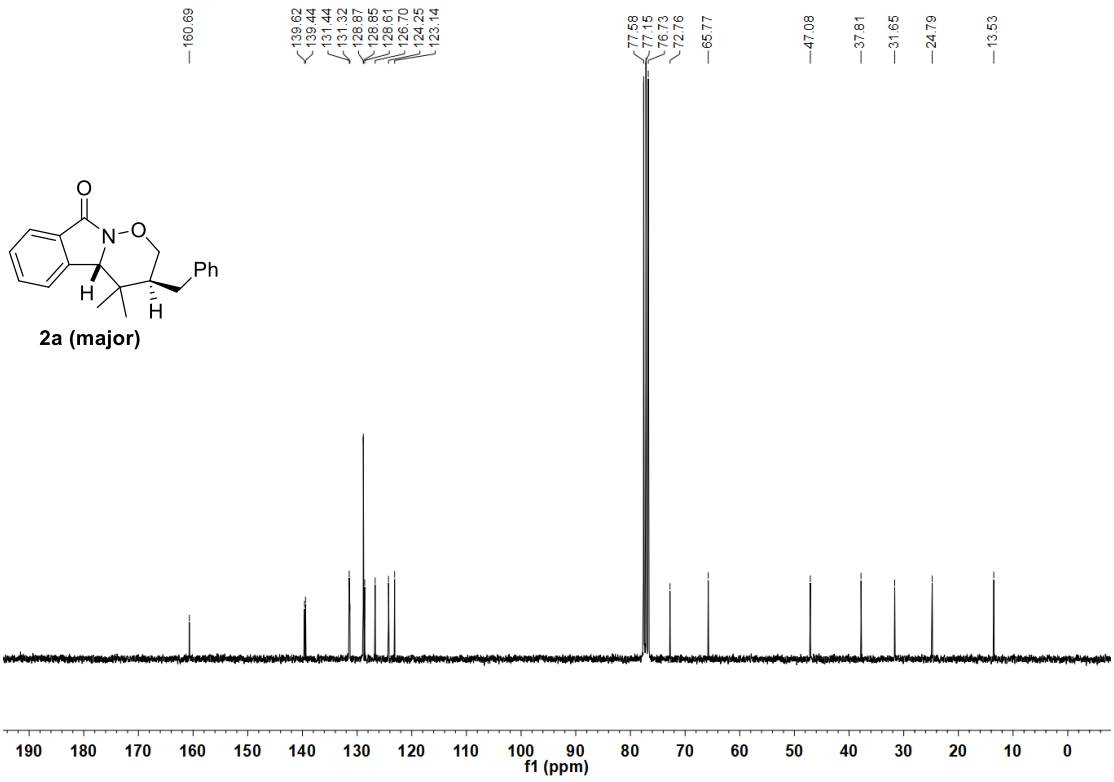


Figure S91. ^{13}C NMR spectra of **2a (major)** (75 MHz, $CDCl_3$)

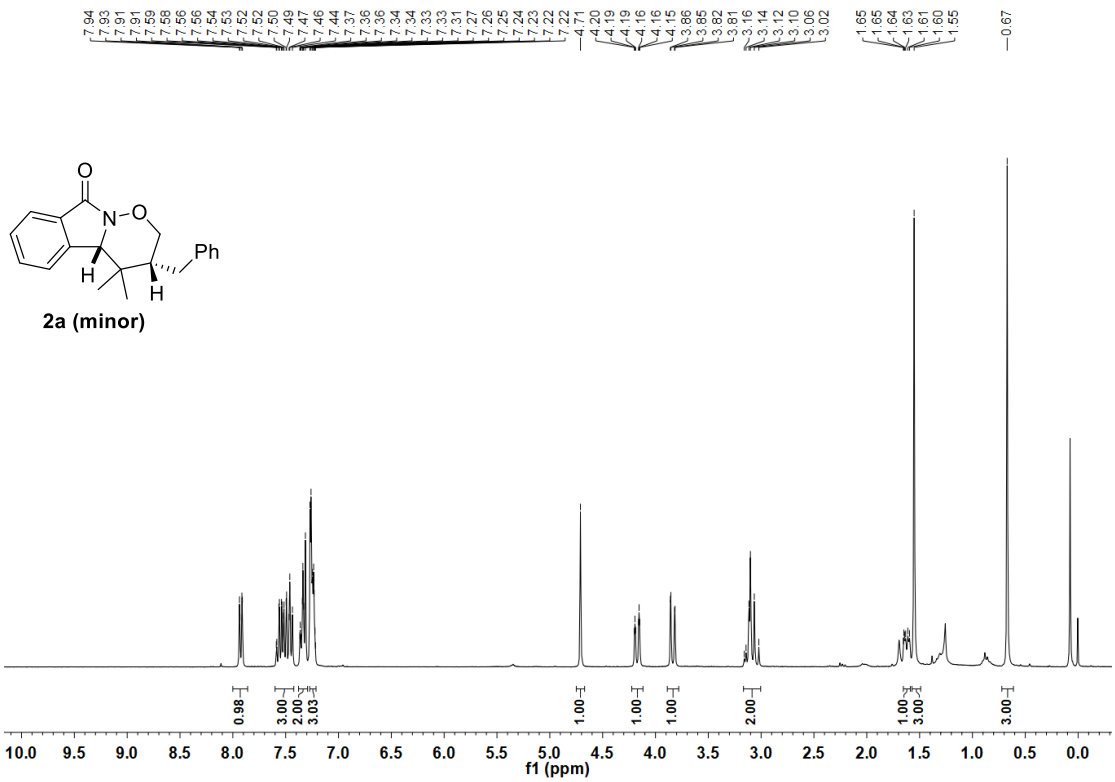


Figure S92. ^{1}H NMR spectra of **2a (minor)** (300 MHz, $CDCl_3$)

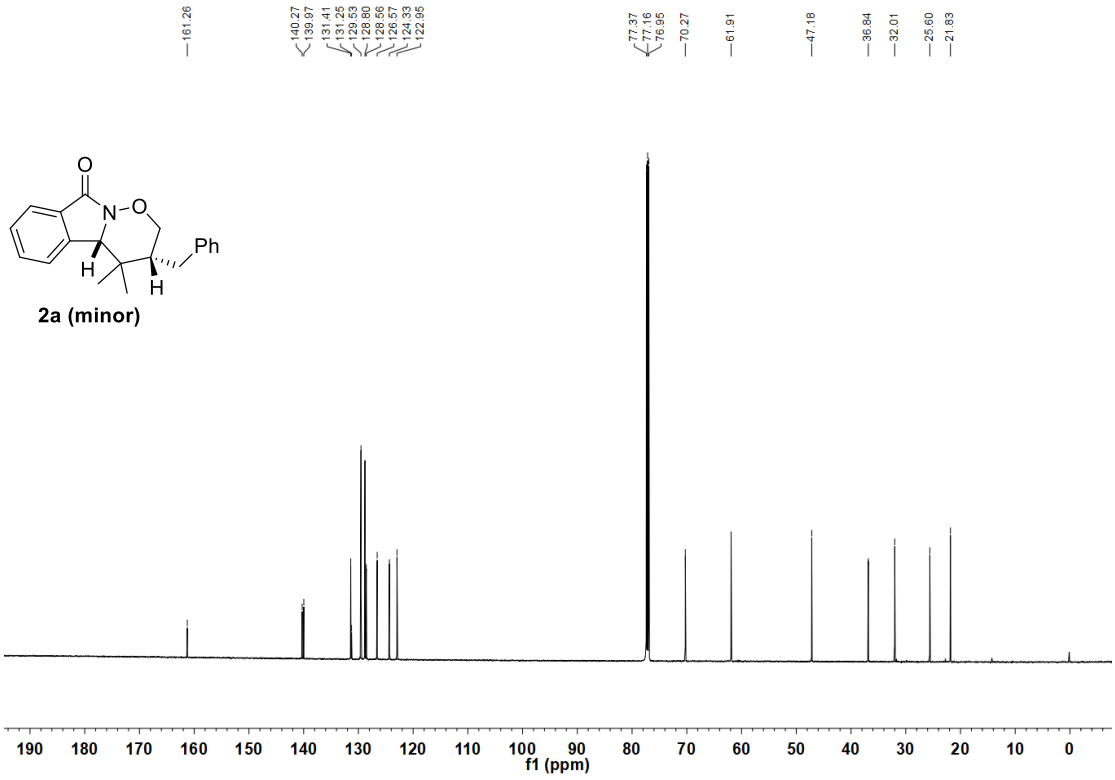


Figure S93. ^{13}C NMR spectra of **2a (minor)** (75 MHz, $CDCl_3$)

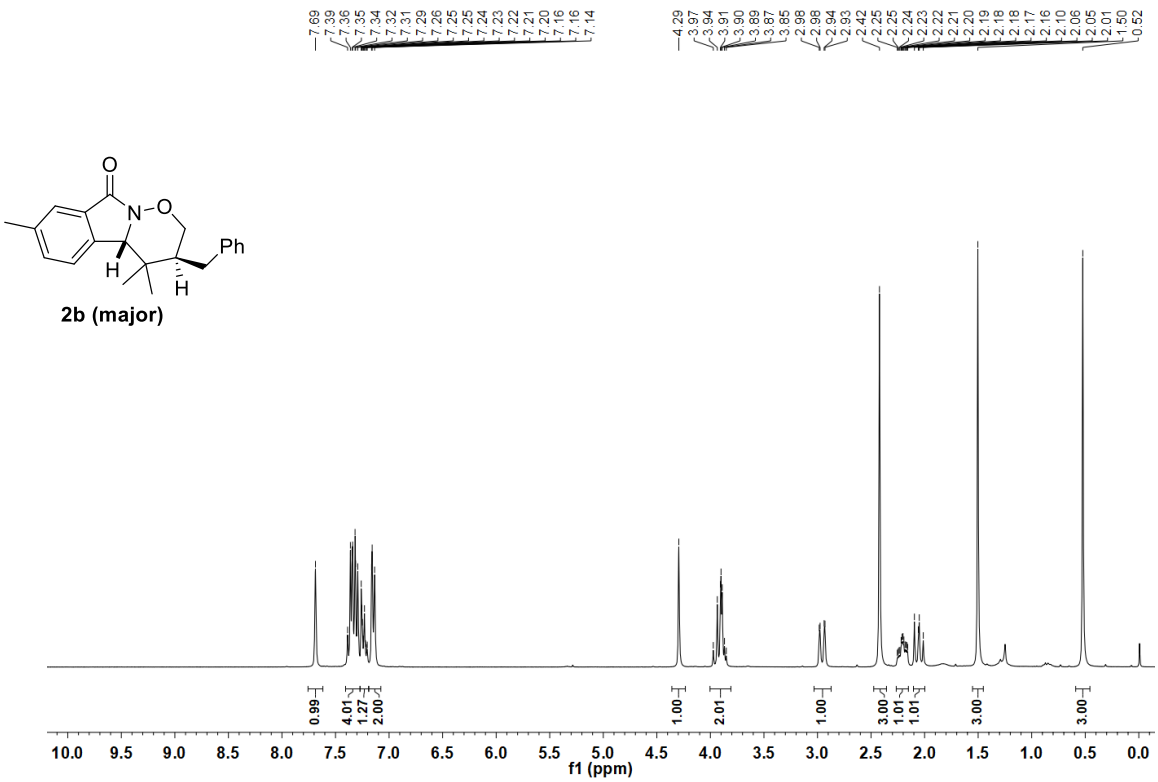


Figure S94. ^{1}H NMR spectra of **2b (major)** (300 MHz, $CDCl_3$)

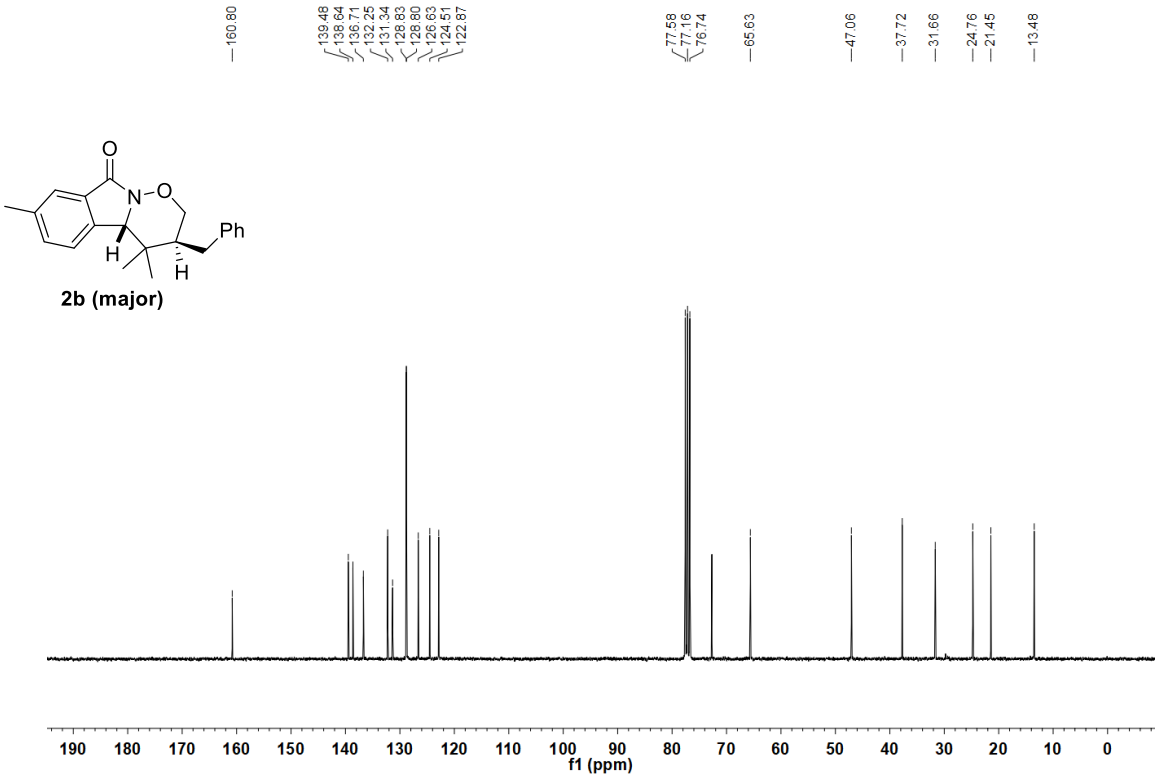


Figure S95. ^{13}C NMR spectra of **2b (major)** (75 MHz, $CDCl_3$)

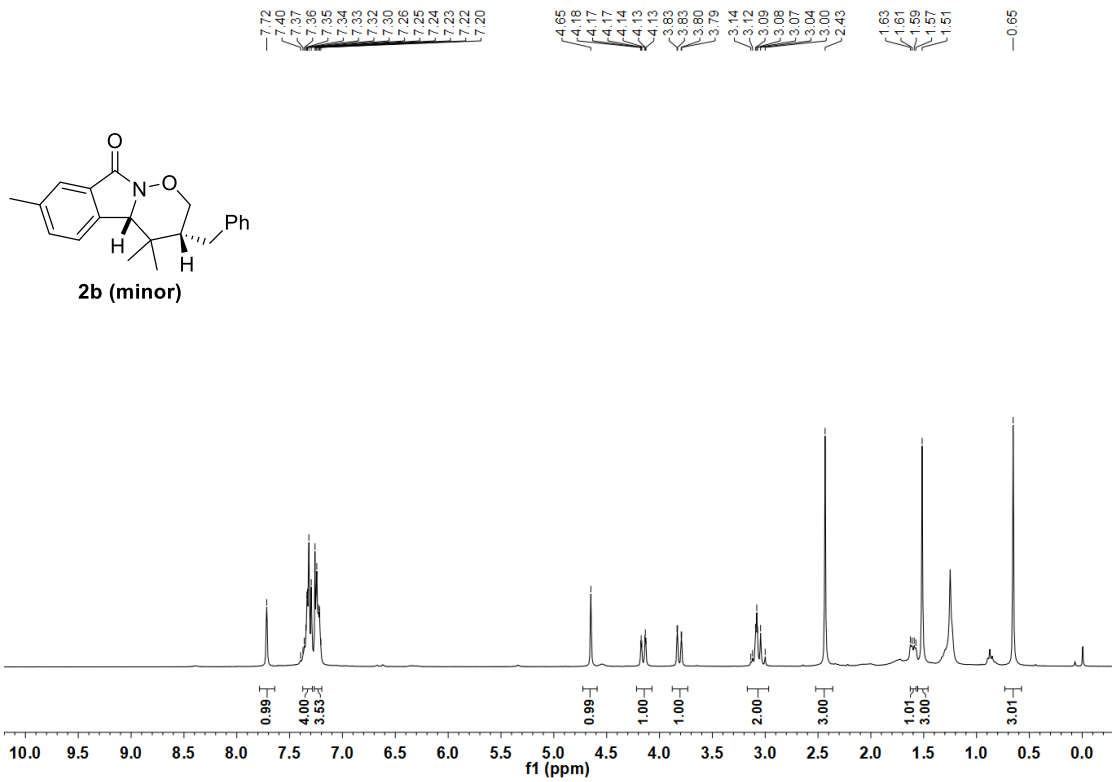


Figure S96. ^{1}H NMR spectra of **2b (minor)** (300 MHz, $CDCl_3$)

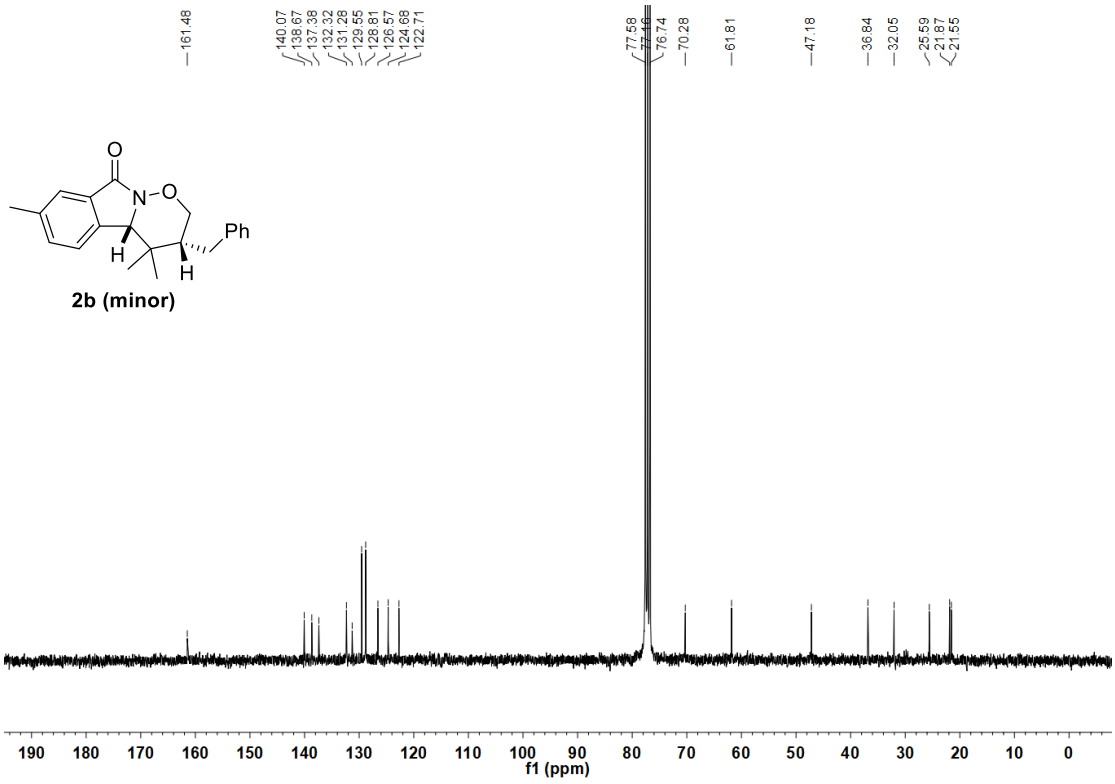


Figure S97. ^{13}C NMR spectra of **2b (minor)** (75 MHz, $CDCl_3$)

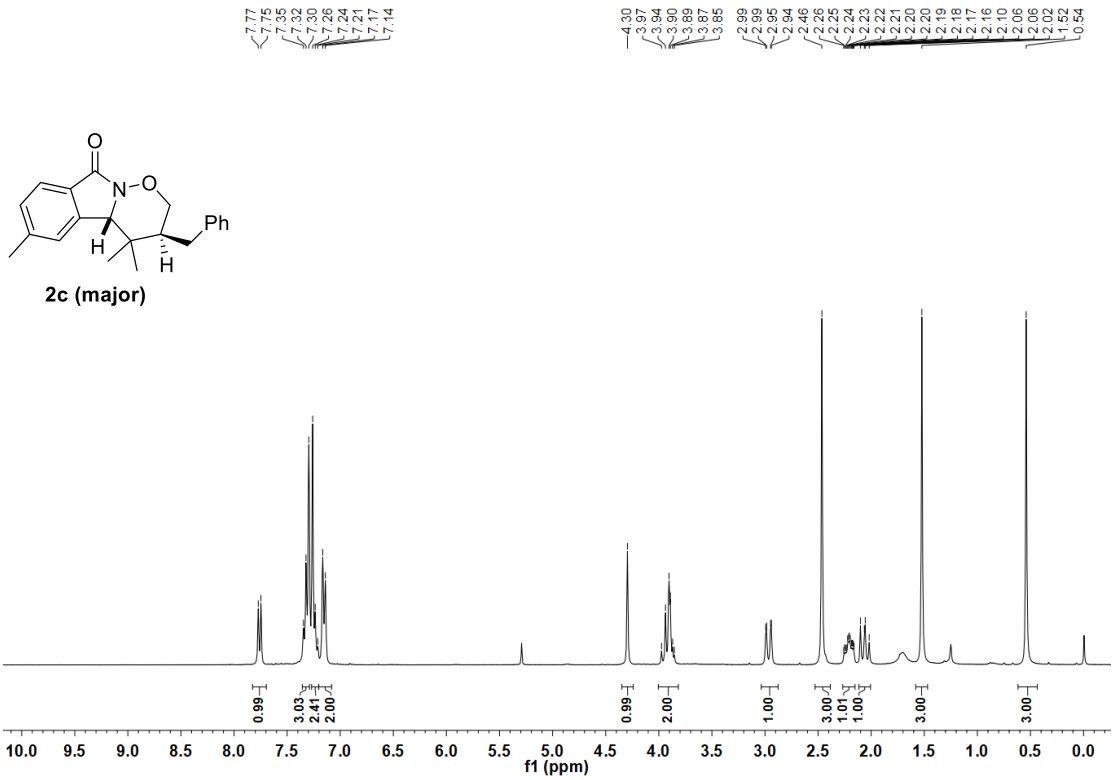


Figure S98. ^{1}H NMR spectra of **2c (major)** (300 MHz, $CDCl_3$)

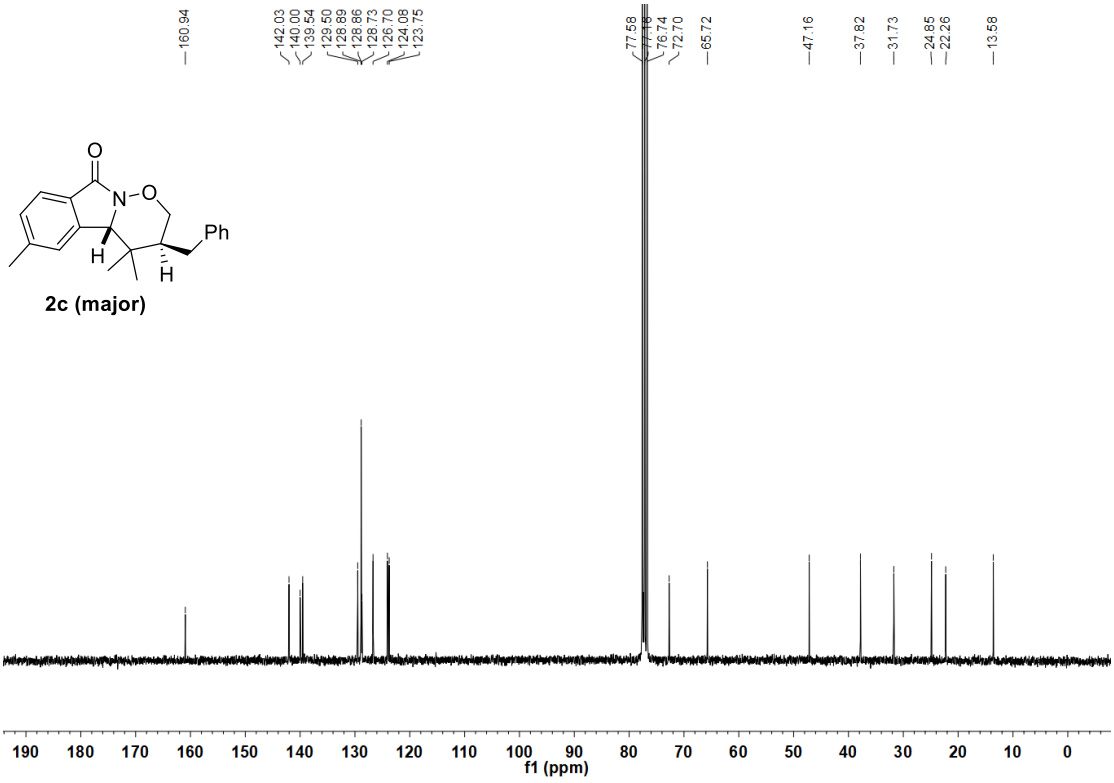


Figure S99. ^{13}C NMR spectra of **2c (major)** (75 MHz, $CDCl_3$)

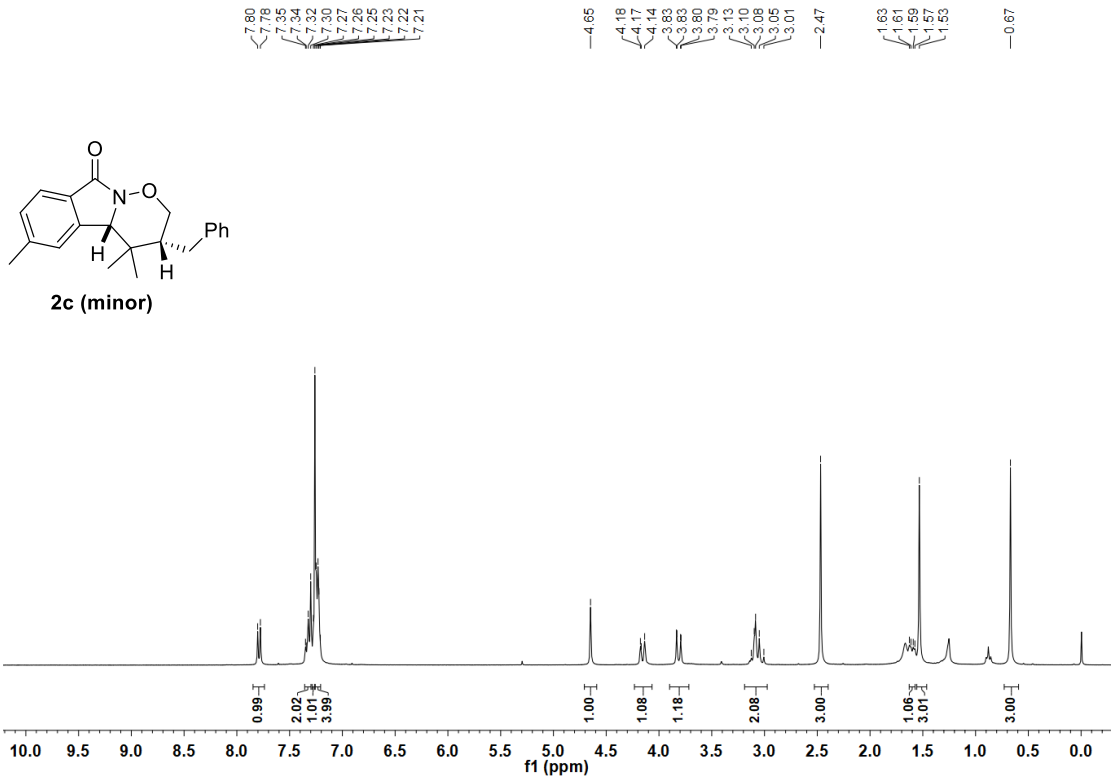


Figure S100. ^{1}H NMR spectra of **2c (minor)** (300 MHz, $CDCl_3$)

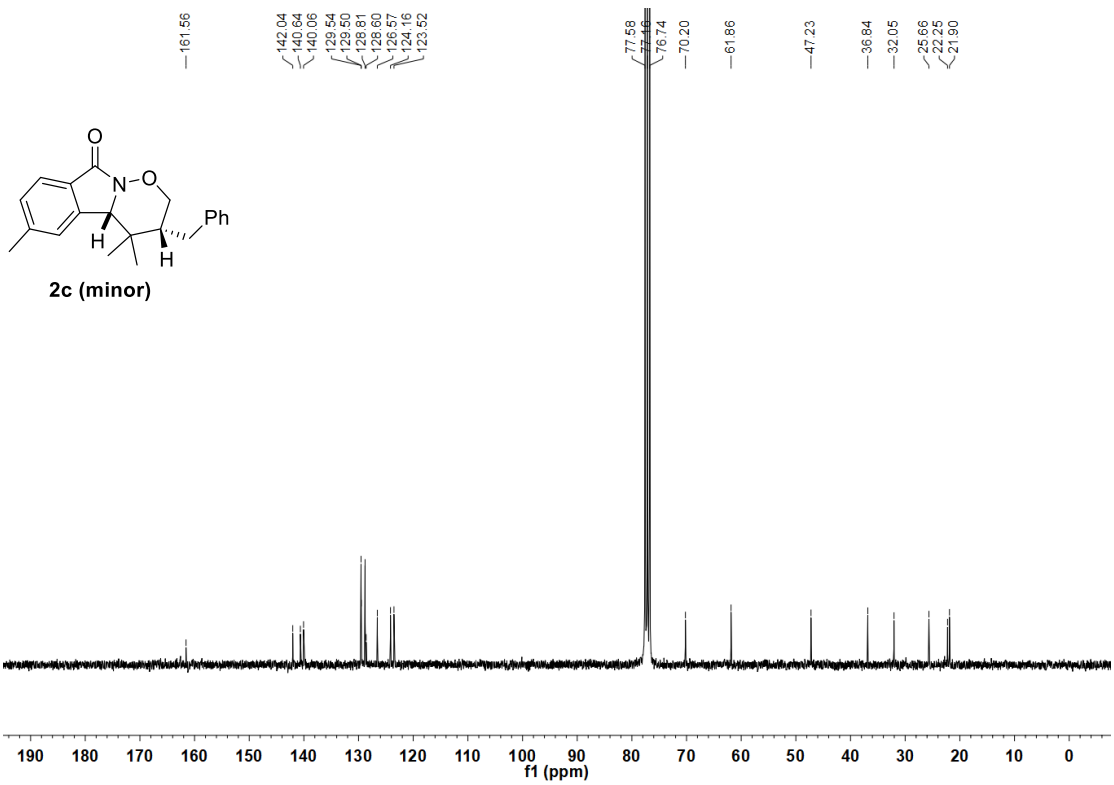


Figure S101. ^{13}C NMR spectra of **2c (minor)** (75 MHz, $CDCl_3$)

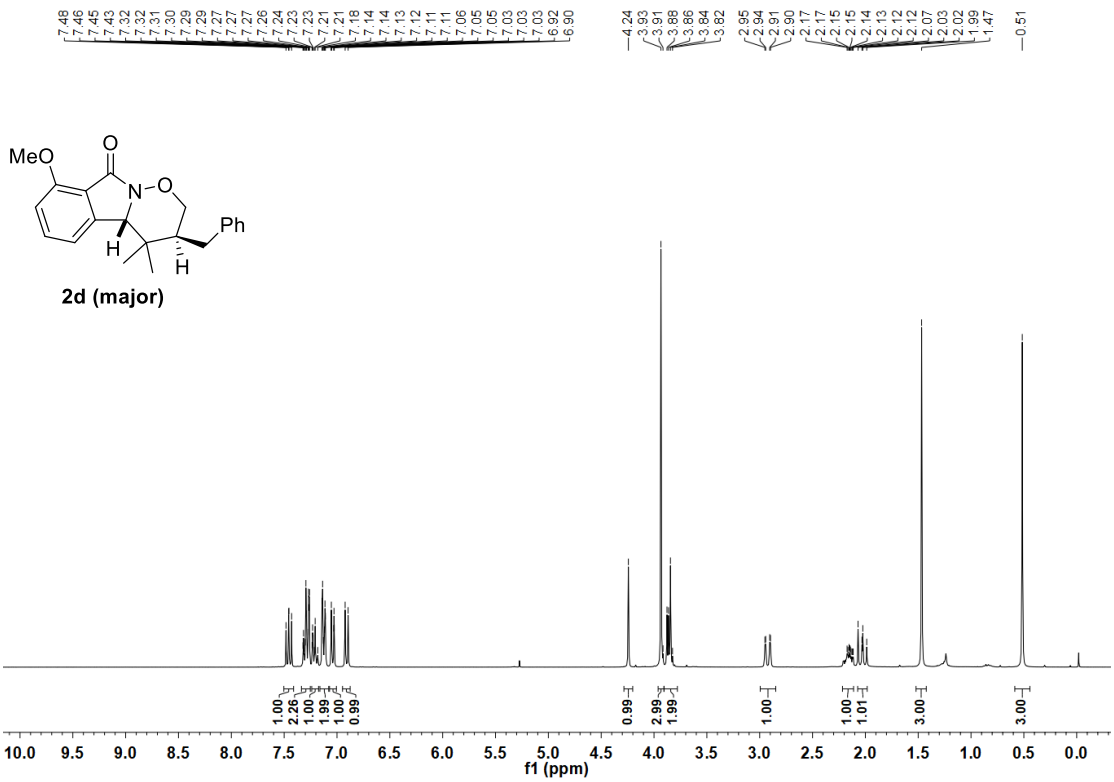


Figure S102. ^{1}H NMR spectra of **2d (major)** (300 MHz, $CDCl_3$)

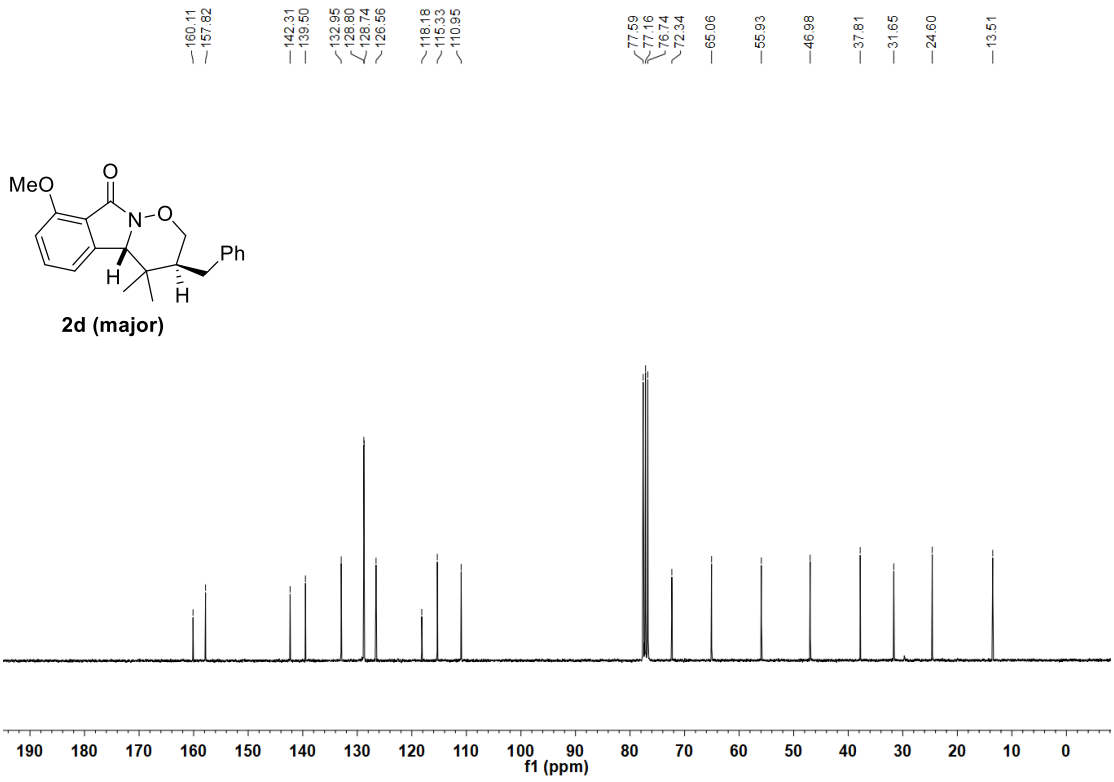


Figure S103. ^{13}C NMR spectra of **2d (major)** (75 MHz, $CDCl_3$)

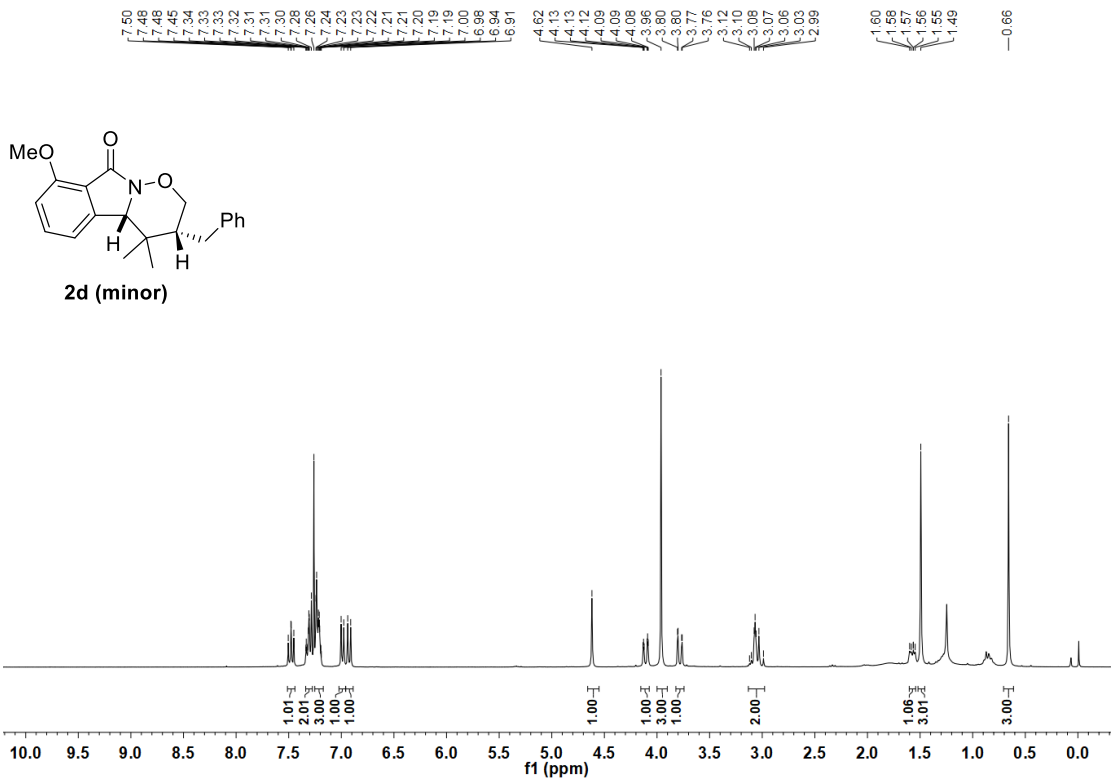


Figure S104. ^{1}H NMR spectra of **2d (minor)** (300 MHz, $CDCl_3$)

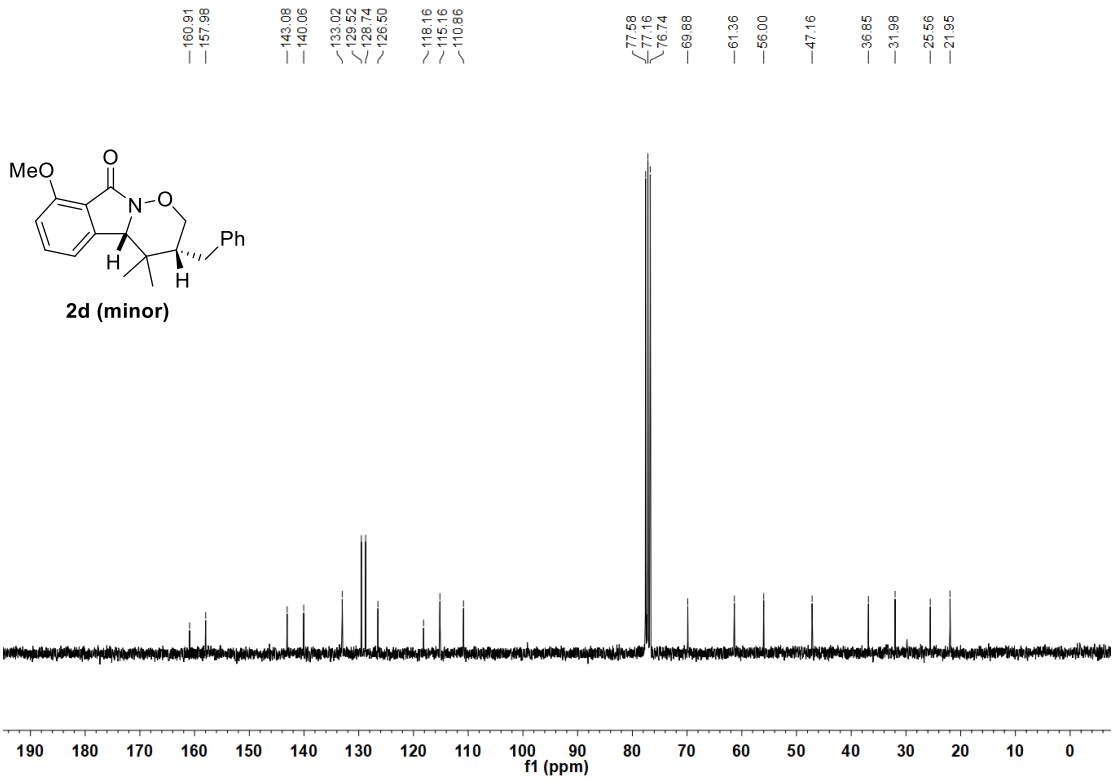


Figure S105. ^{13}C NMR spectra of **2d (minor)** (75 MHz, $CDCl_3$)

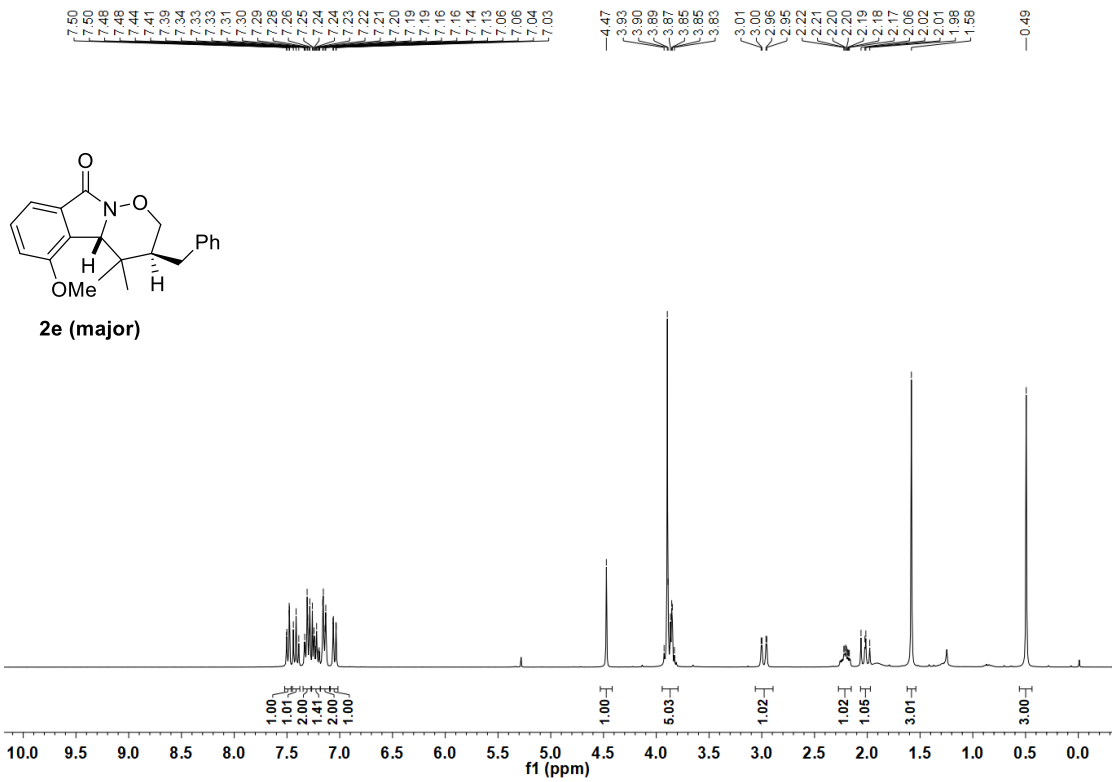


Figure S106. ^{1}H NMR spectra of **2e (major)** (300 MHz, $CDCl_3$)

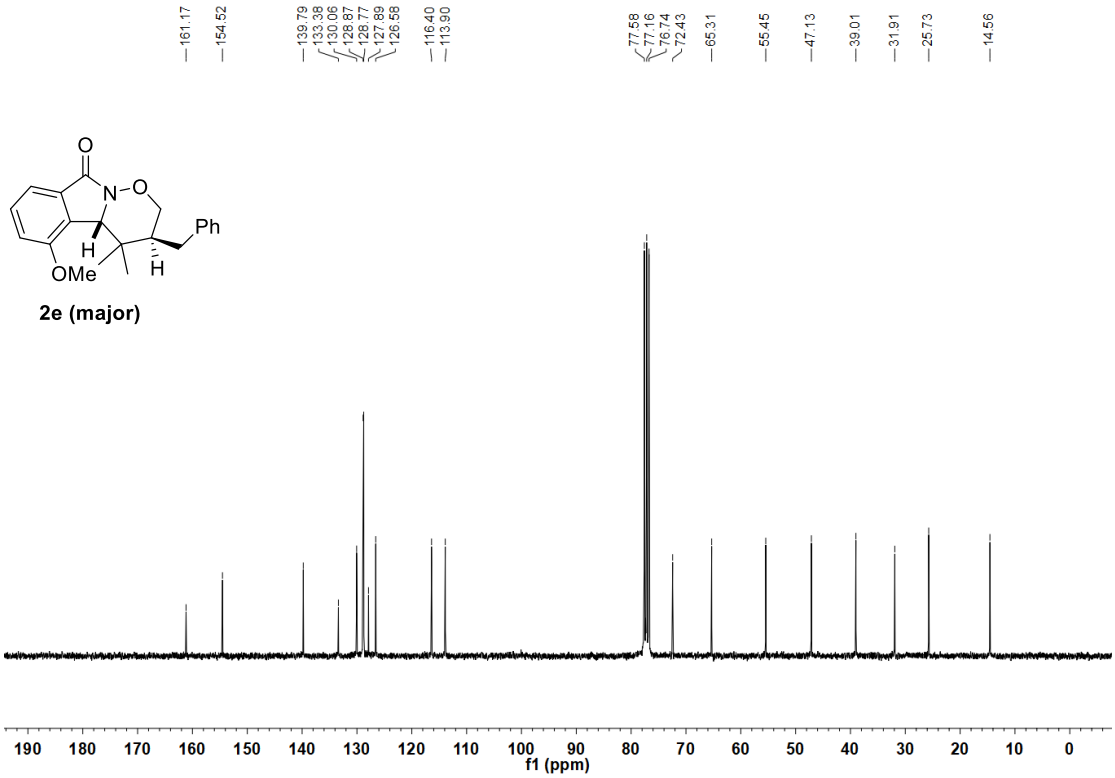


Figure S107. ^{13}C NMR spectra of **2e (major)** (75 MHz, $CDCl_3$)

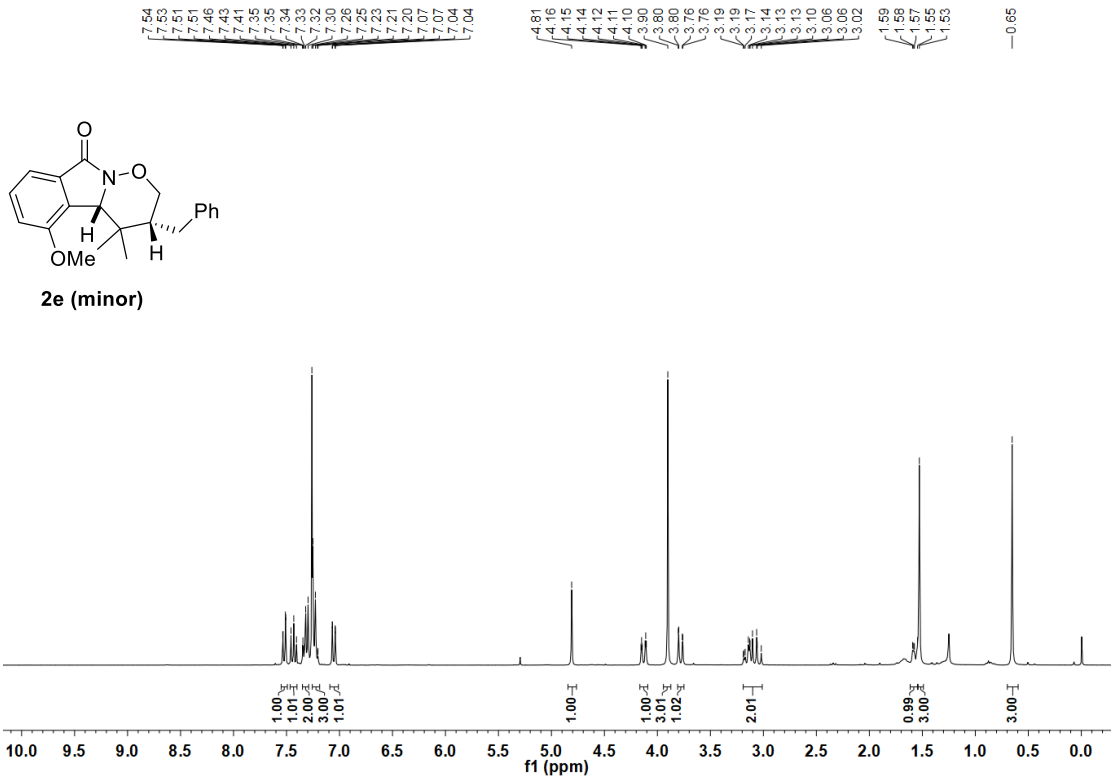


Figure S108. ^{1}H NMR spectra of **2e (minor)** (300 MHz, $CDCl_3$)

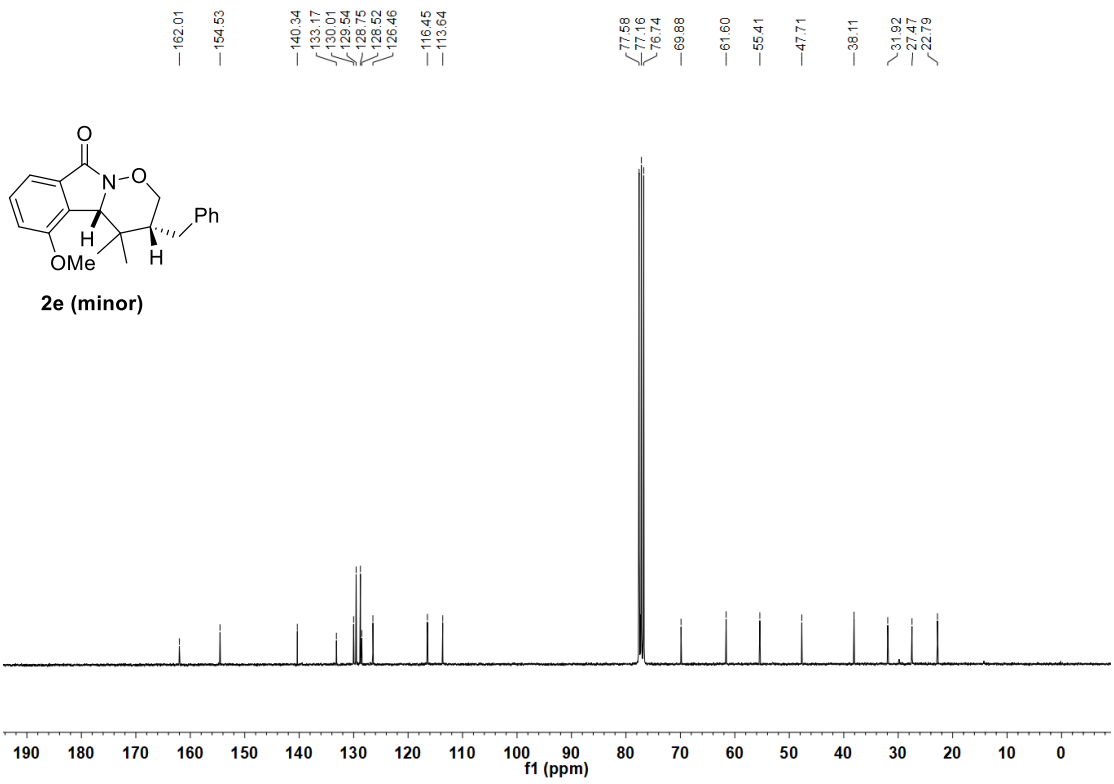


Figure S109. ^{13}C NMR spectra of **2e (minor)** (75 MHz, $CDCl_3$)

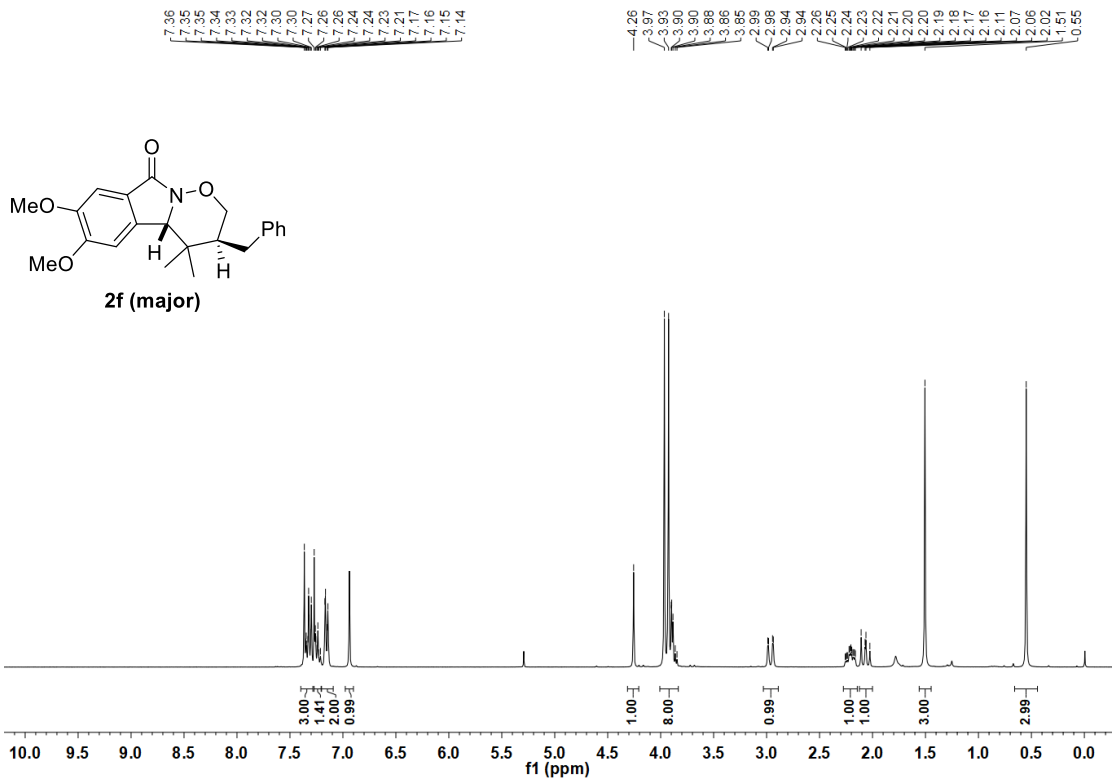


Figure S110. ^{1}H NMR spectra of **2f (major)** (300 MHz, $CDCl_3$)

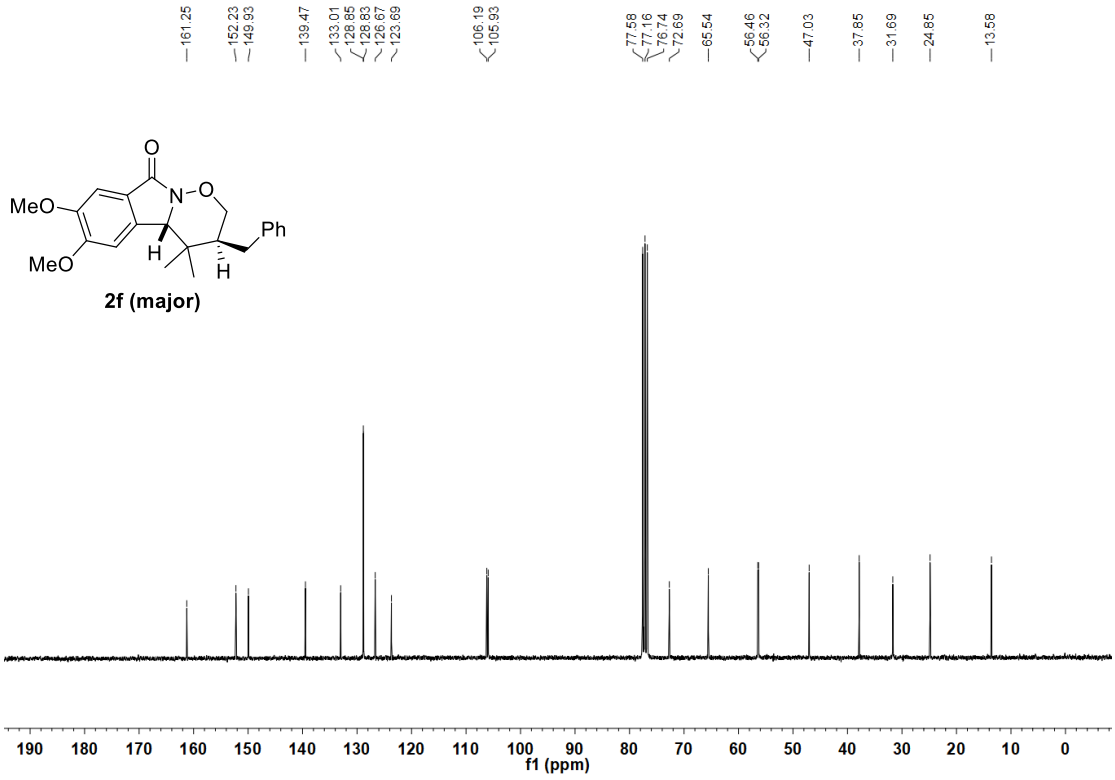


Figure S111. ^{13}C NMR spectra of **2f (major)** (75 MHz, $CDCl_3$)

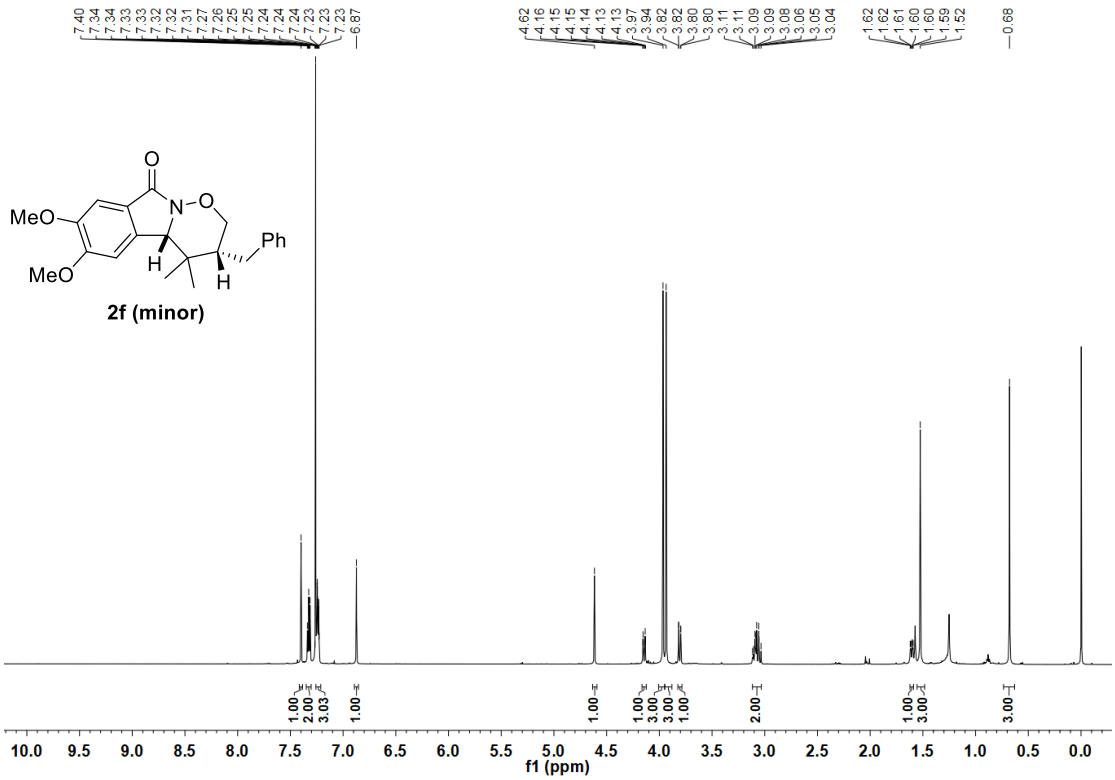


Figure S112. ^{1}H NMR spectra of **2f (minor)** (600 MHz, $CDCl_3$)

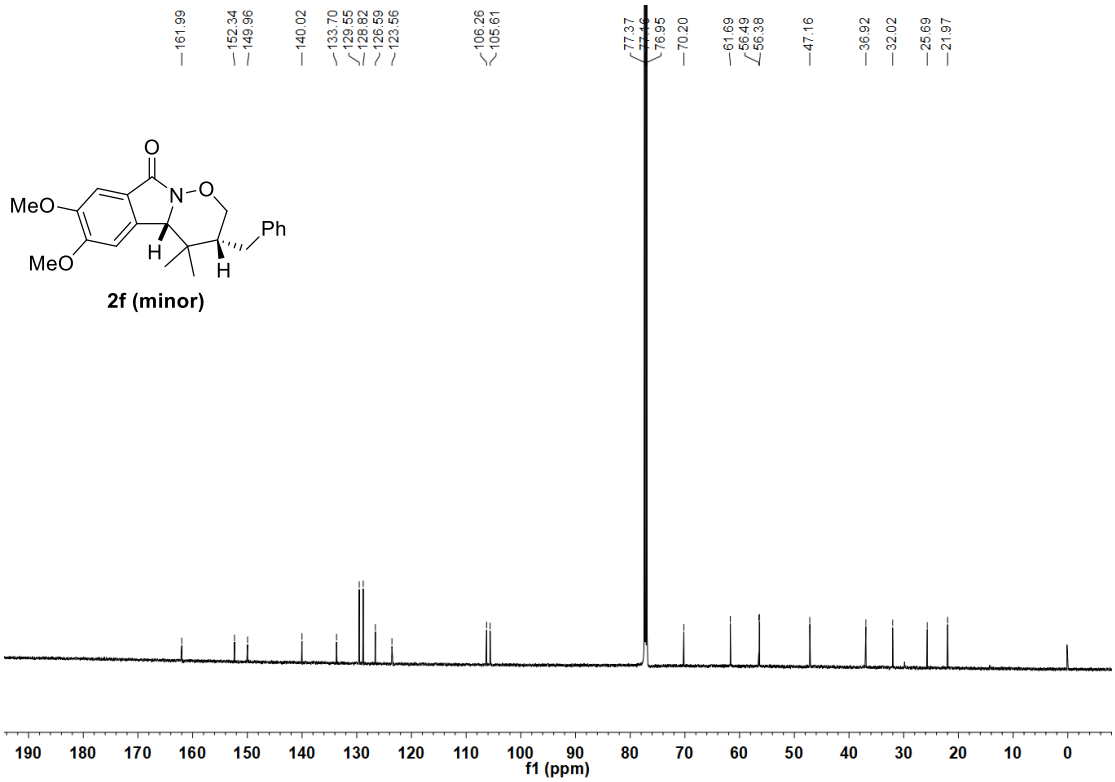


Figure S113. ^{13}C NMR spectra of **2f (minor)** (151 MHz, $CDCl_3$)

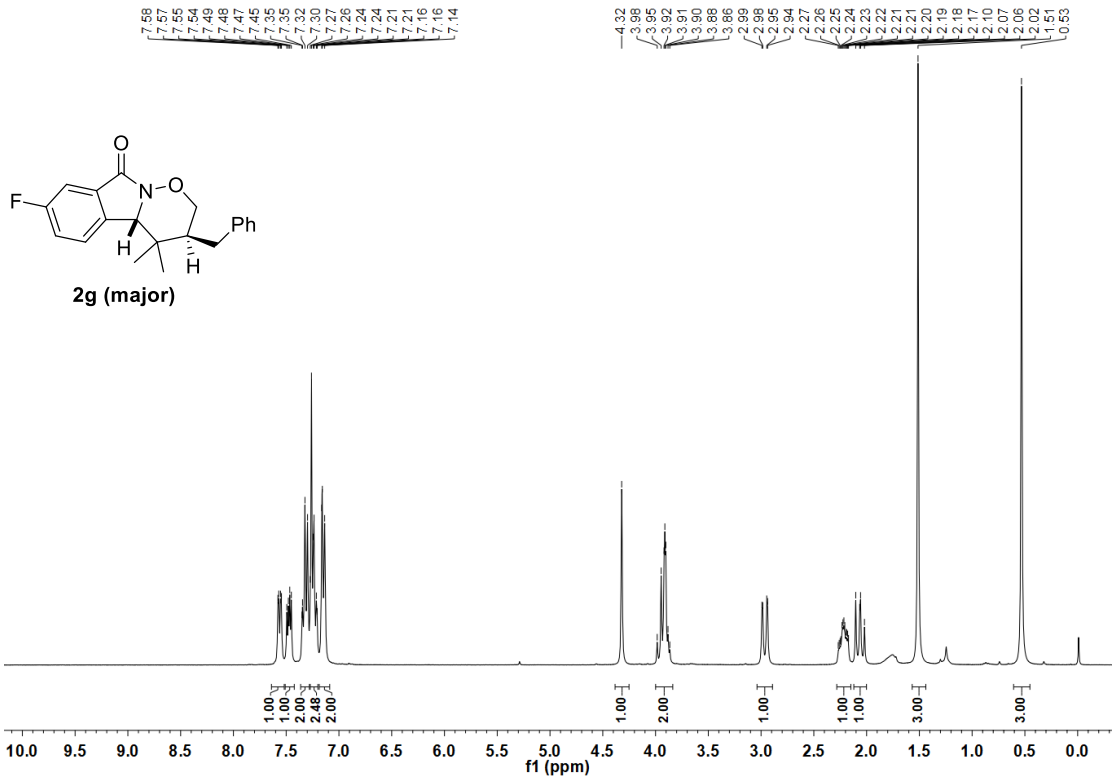


Figure S114. ^{1}H NMR spectra of **2g (major)** (300 MHz, $CDCl_3$)

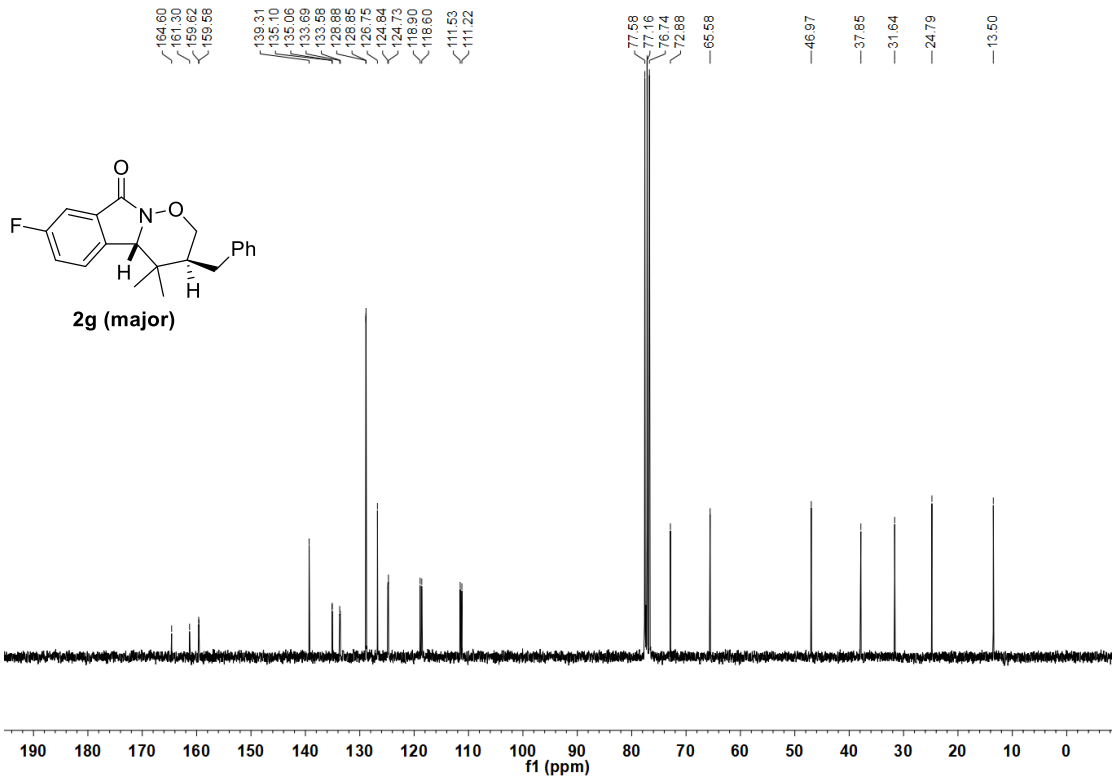


Figure S115. ^{13}C NMR spectra of **2g (major)** (75 MHz, $CDCl_3$)

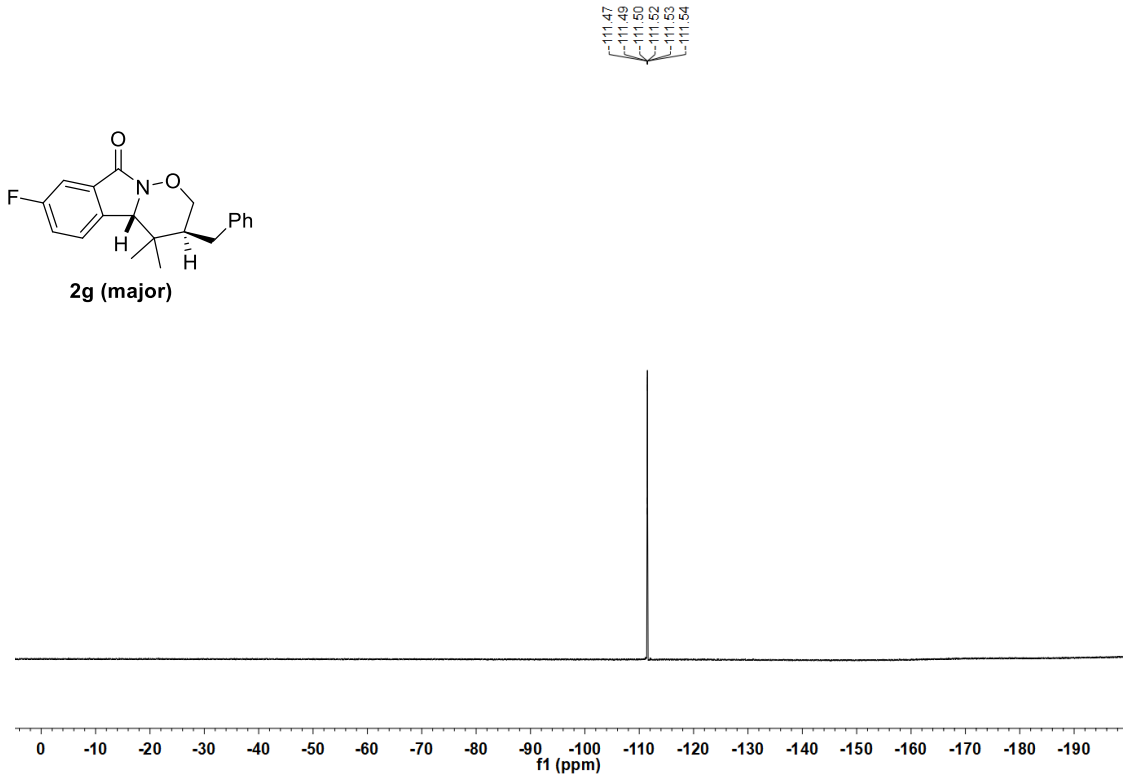


Figure S116. ^{19}F NMR spectra of **2g (major)** (282 MHz, $CDCl_3$)

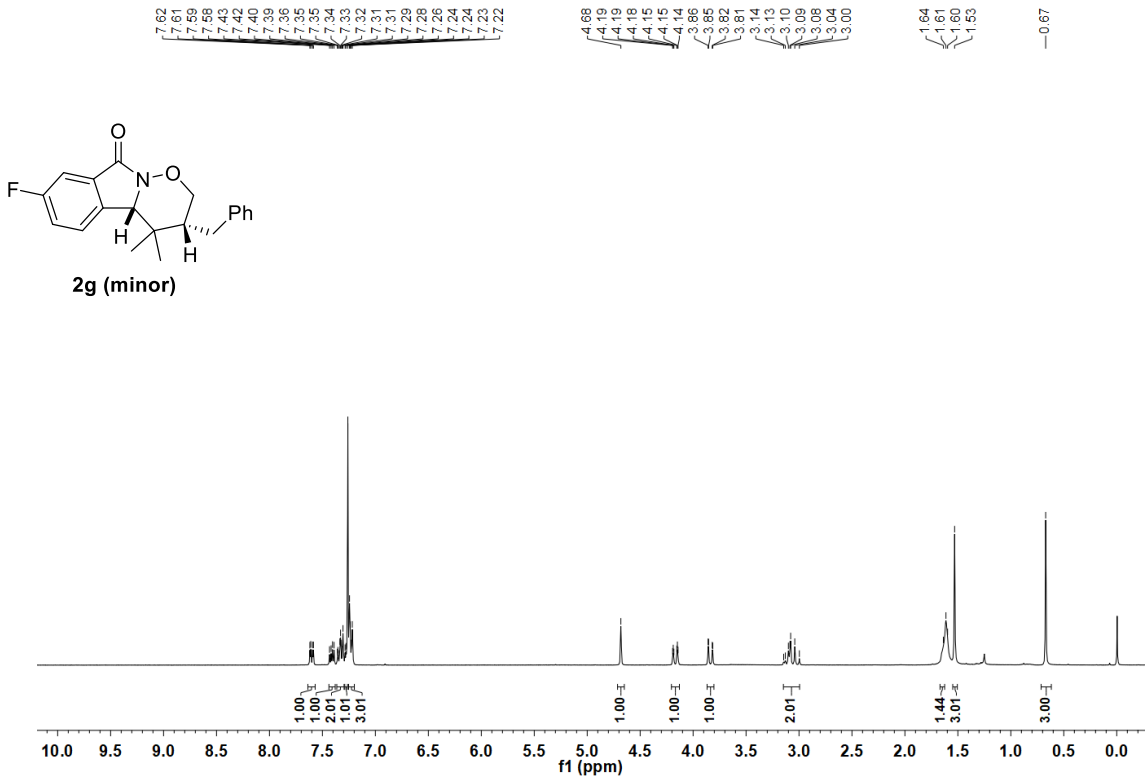


Figure S117. ^{1}H NMR spectra of **2g (minor)** (300 MHz, $CDCl_3$)

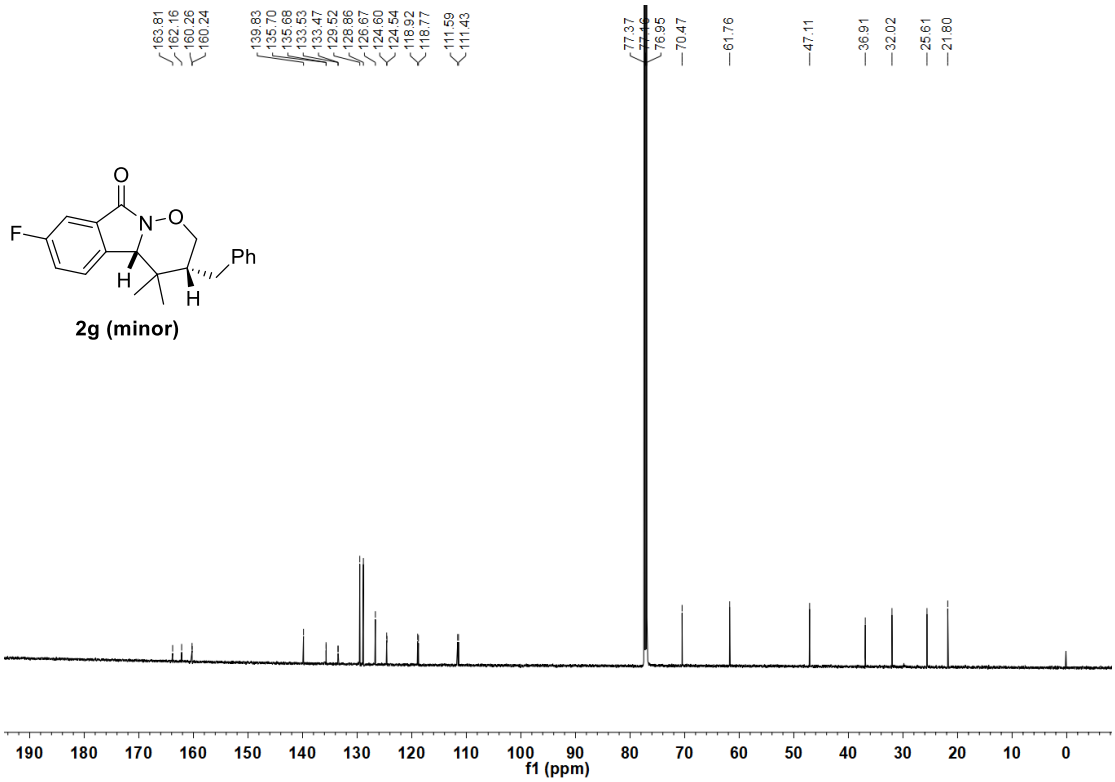


Figure S118. ^{13}C NMR spectra of **2g (minor)** (75 MHz, $CDCl_3$)

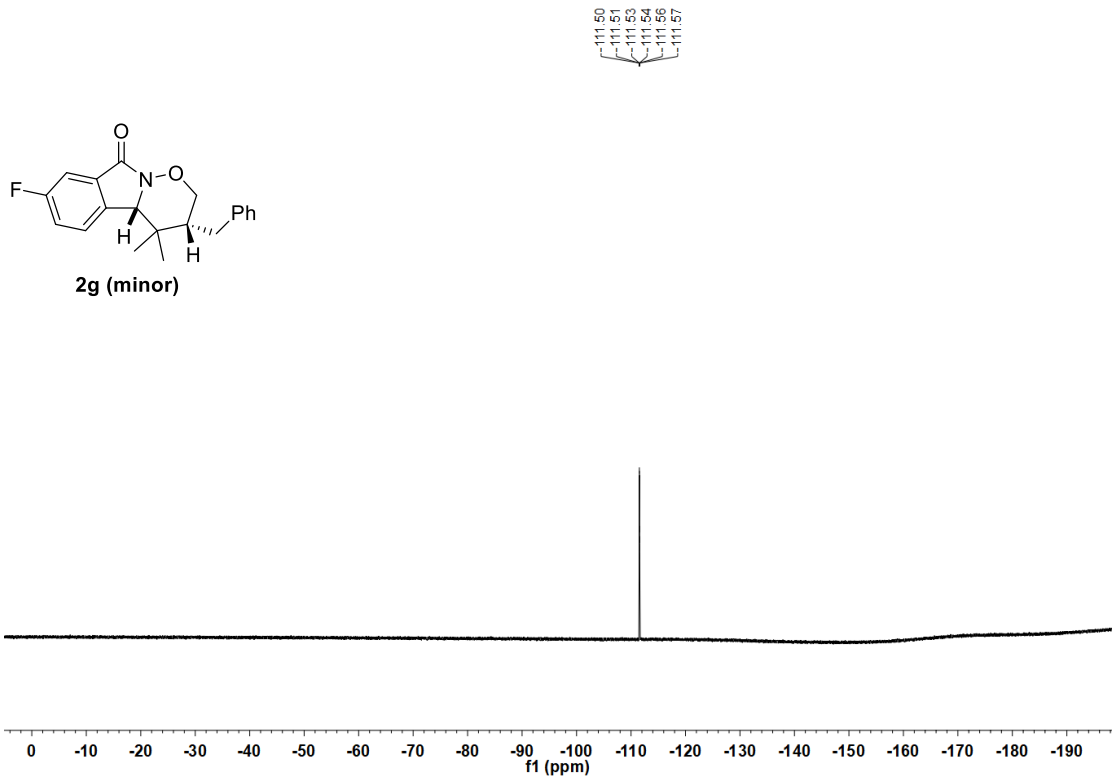


Figure S119. ^{19}F NMR spectra of **2g (minor)** (282 MHz, $CDCl_3$)

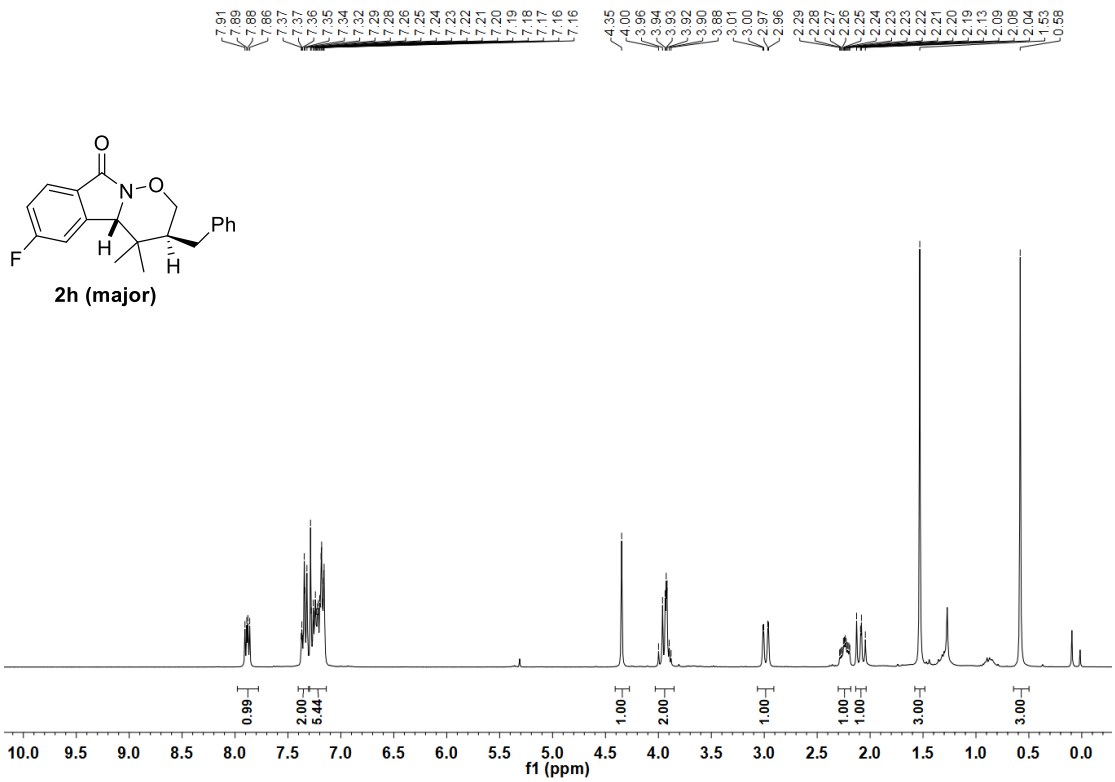


Figure S120. ^{1}H NMR spectra of **2h (major)** (300 MHz, $CDCl_3$)

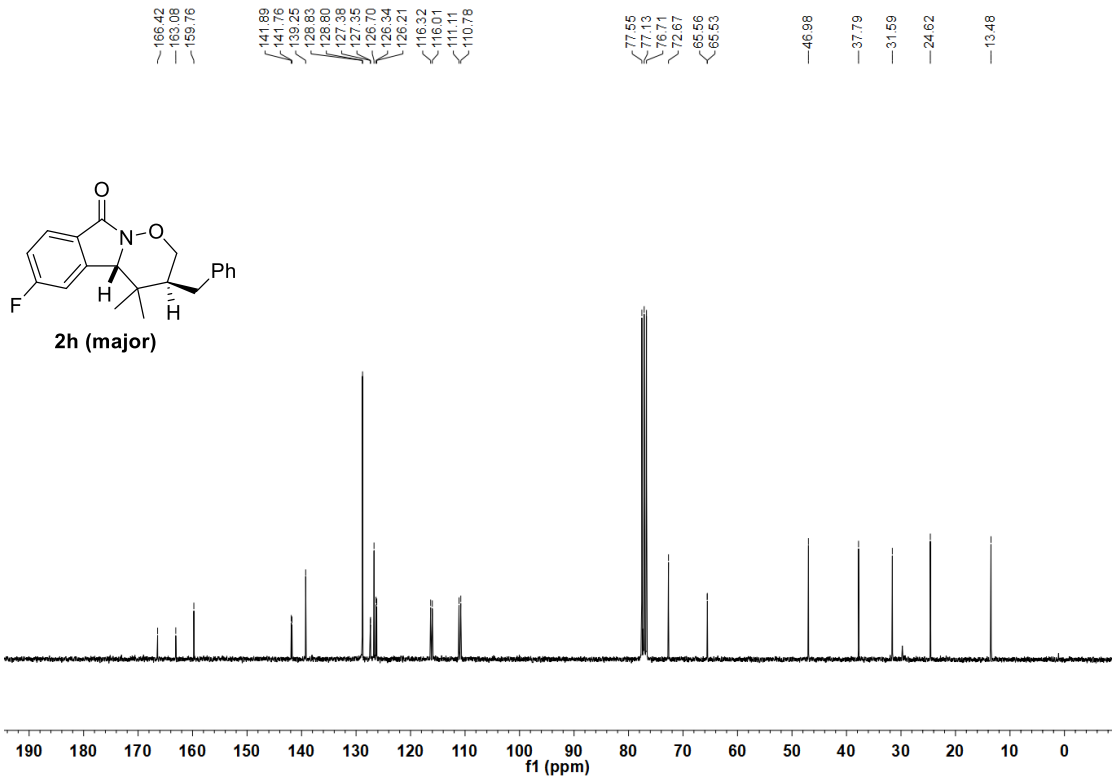


Figure S121. ^{13}C NMR spectra of **2h (major)** (75 MHz, $CDCl_3$)

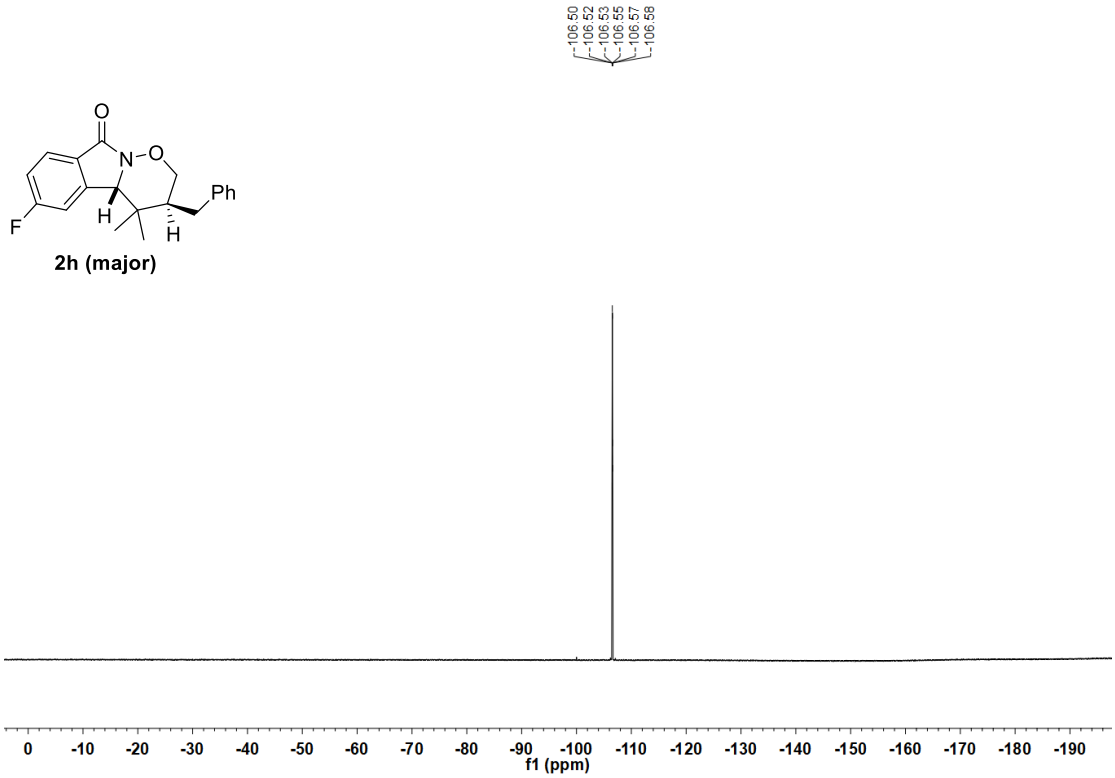


Figure S122. ^{19}F NMR spectra of **2h (major)** (282 MHz, $CDCl_3$)

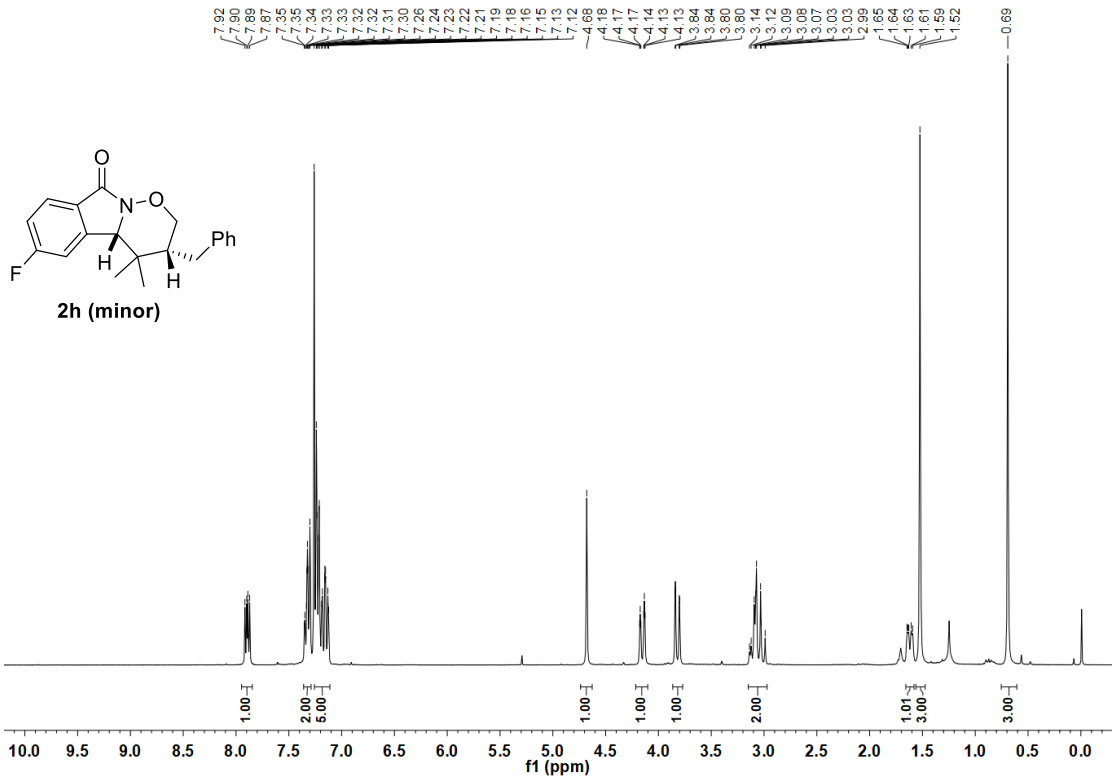


Figure S123. ^{1}H NMR spectra of **2h (minor)** (300 MHz, $CDCl_3$)

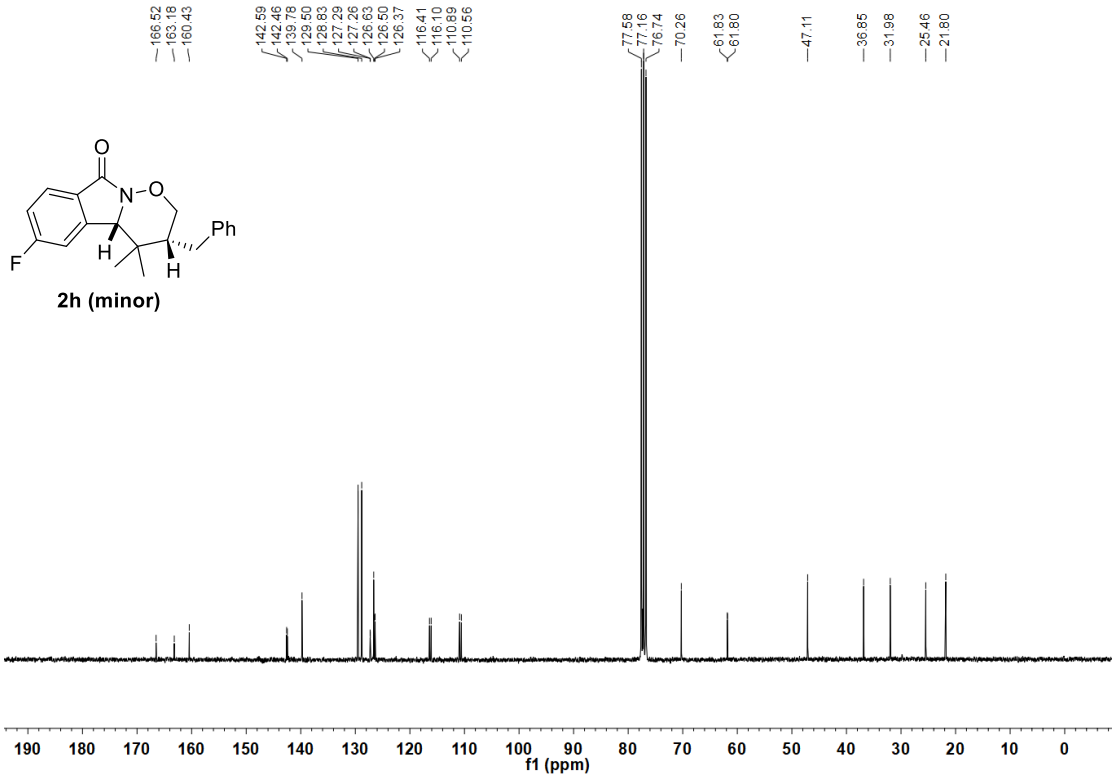


Figure S124. ^{13}C NMR spectra of **2h (minor)** (75 MHz, $CDCl_3$)

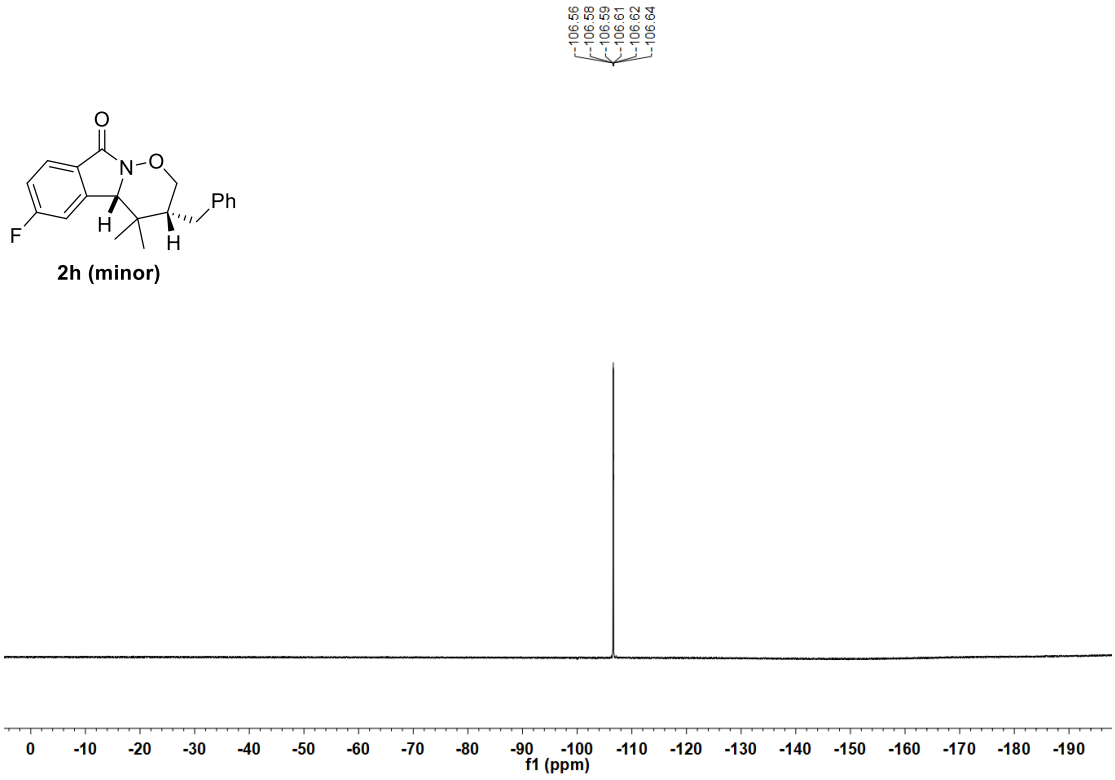


Figure S125. ^{19}F NMR spectra of **2h (minor)** (282 MHz, $CDCl_3$)

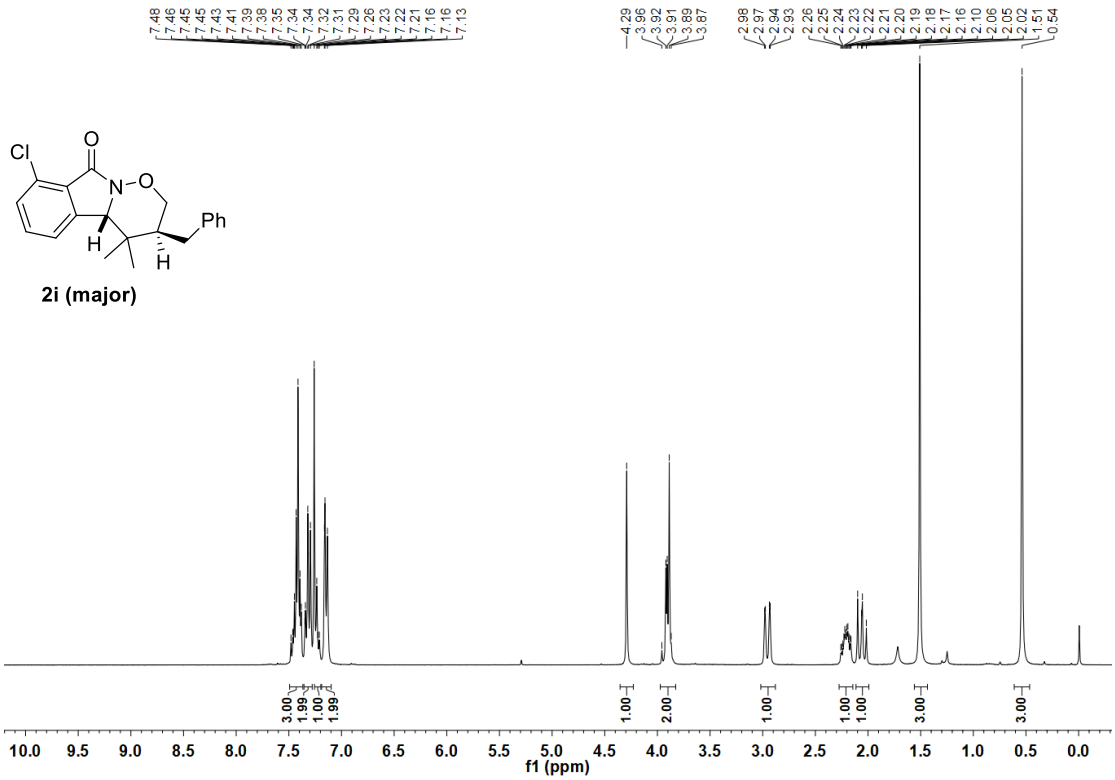


Figure S126. ^{1}H NMR spectra of **2i (major)** (300 MHz, $CDCl_3$)

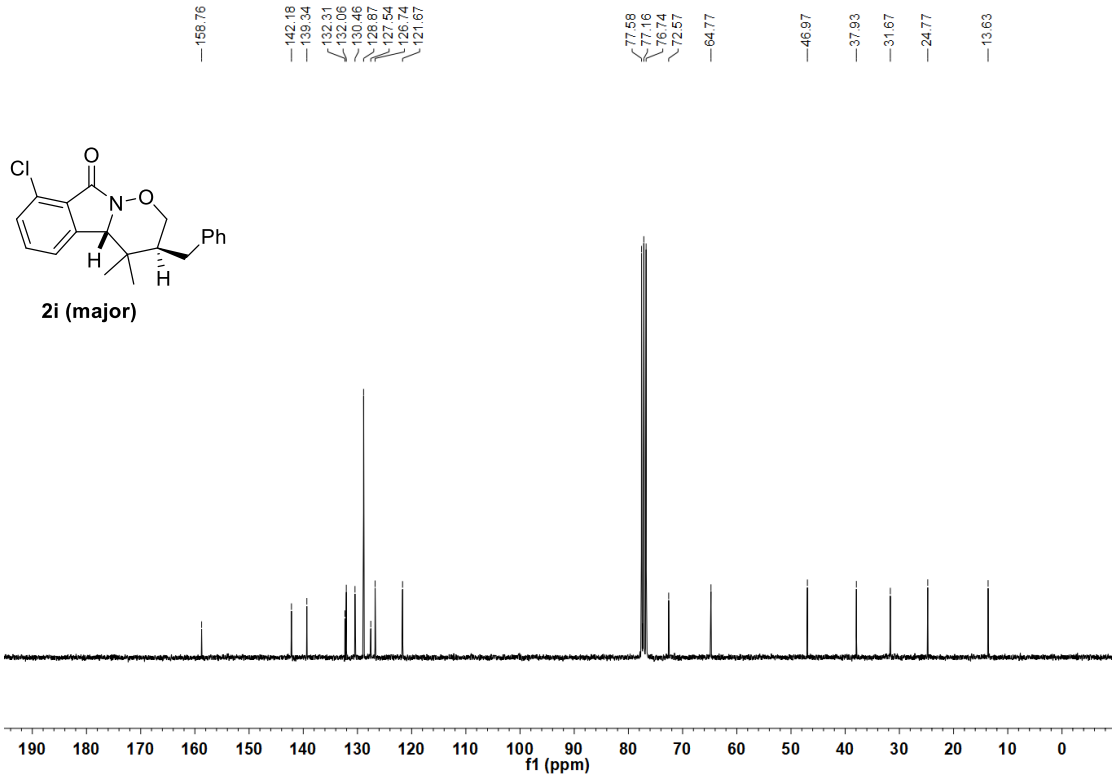


Figure S127. ^{13}C NMR spectra of **2i (major)** (75 MHz, $CDCl_3$)

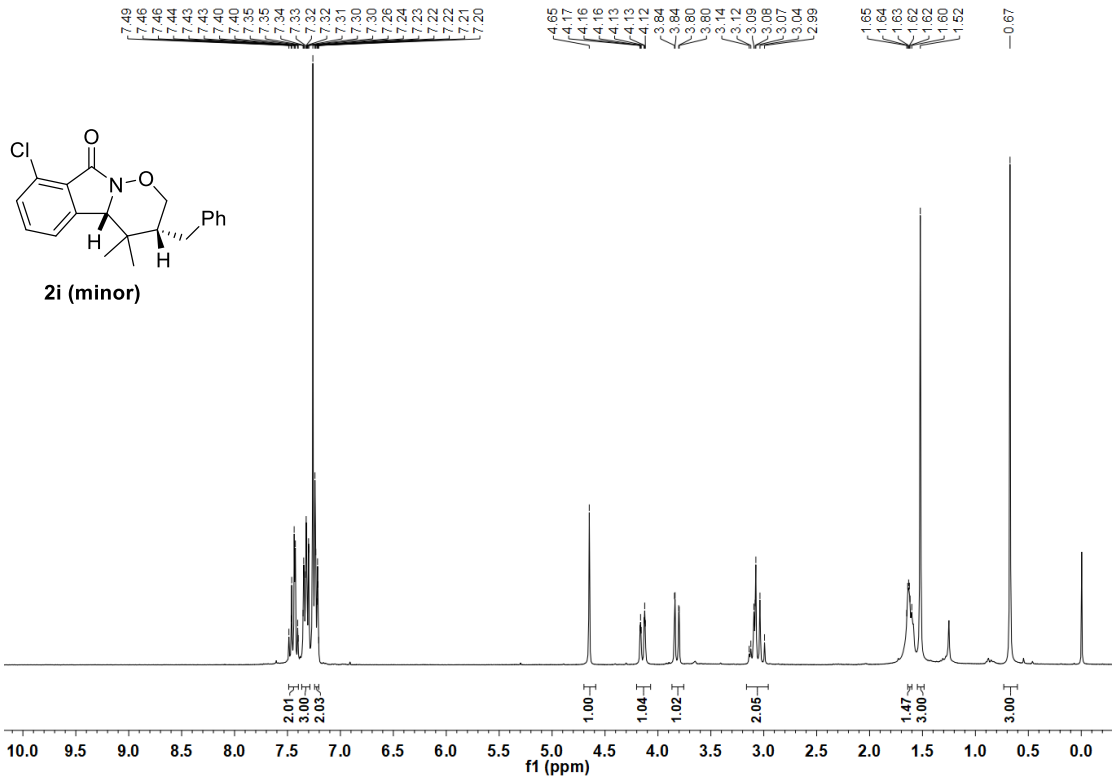


Figure S128. ^{1}H NMR spectra of **2i (minor)** (300 MHz, $CDCl_3$)

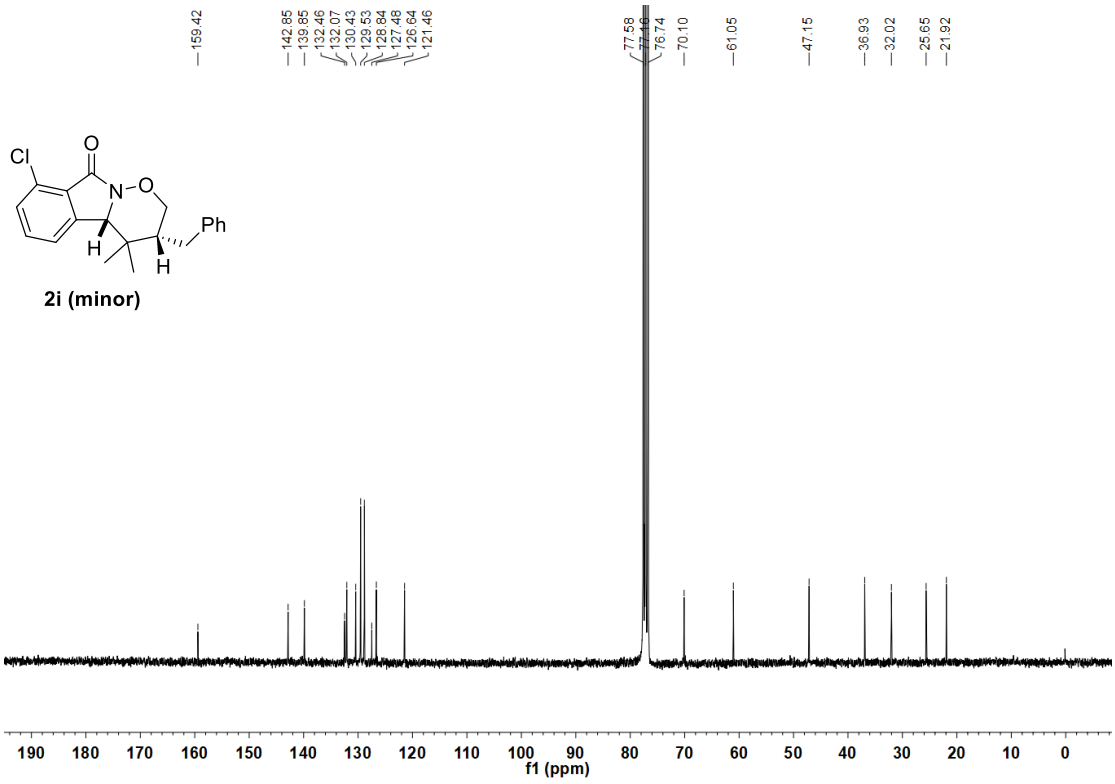


Figure S129. ^{13}C NMR spectra of **2i (minor)** (75 MHz, $CDCl_3$)

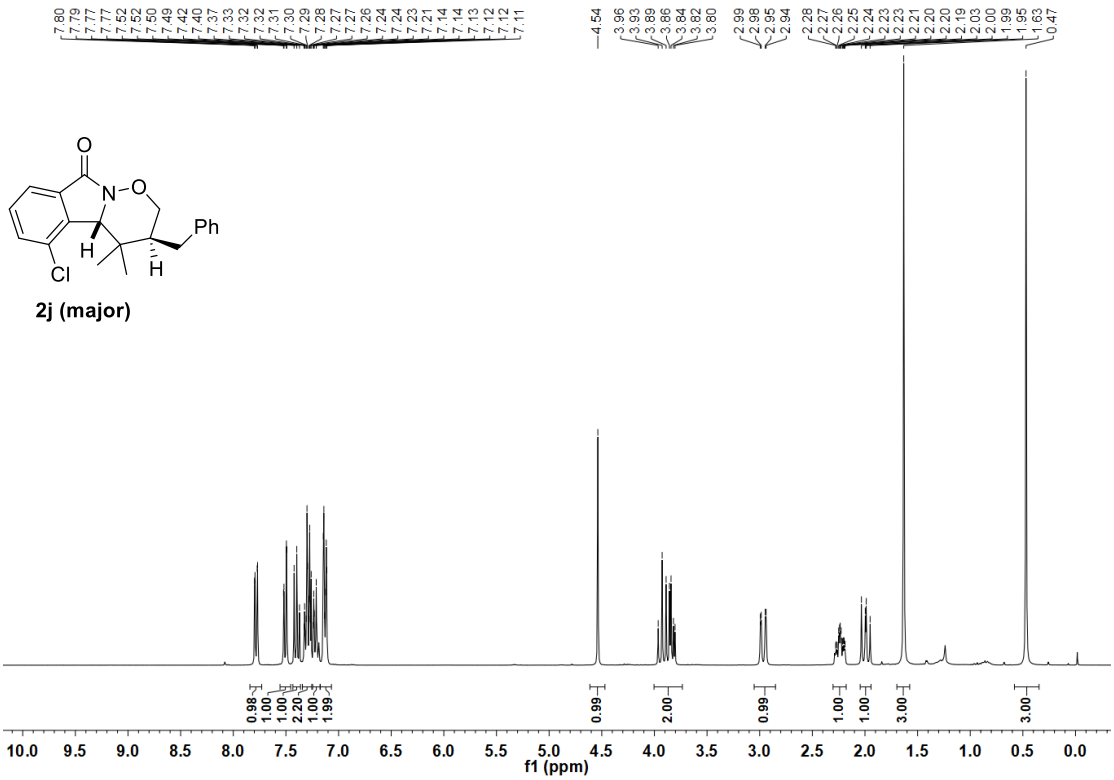


Figure S130. ^{1}H NMR spectra of **2j (major)** (300 MHz, $CDCl_3$)

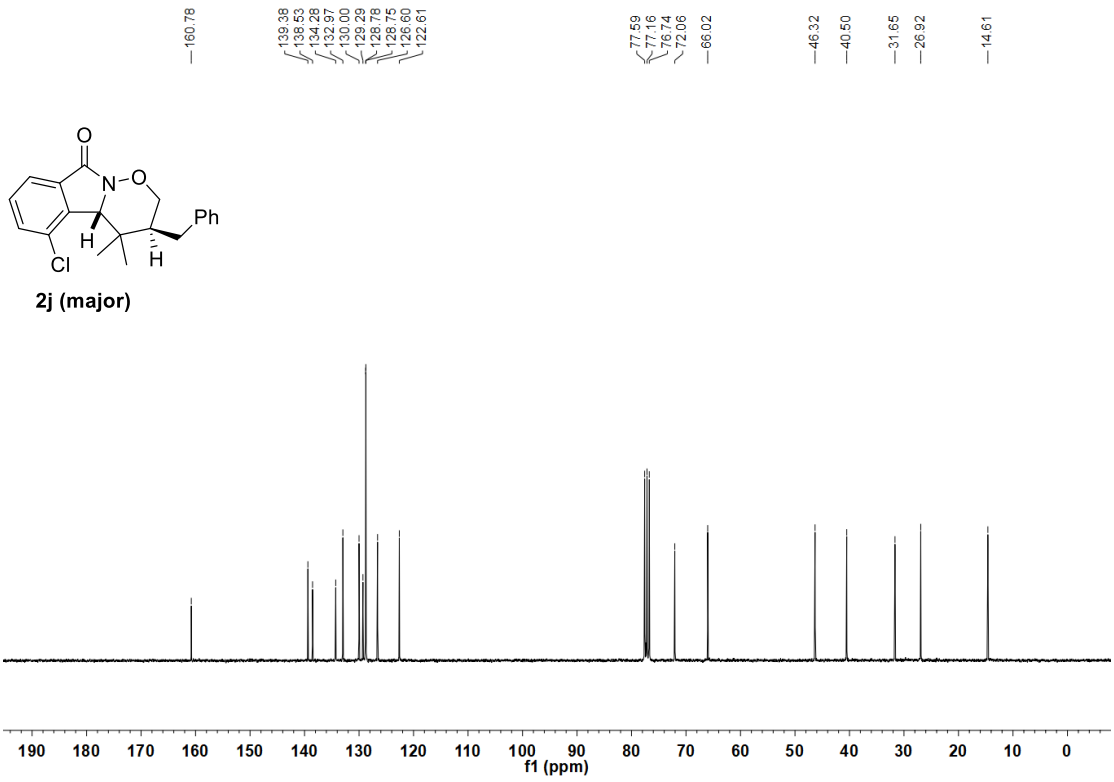


Figure S131. ^{13}C NMR spectra of **2j (major)** (75 MHz, $CDCl_3$)

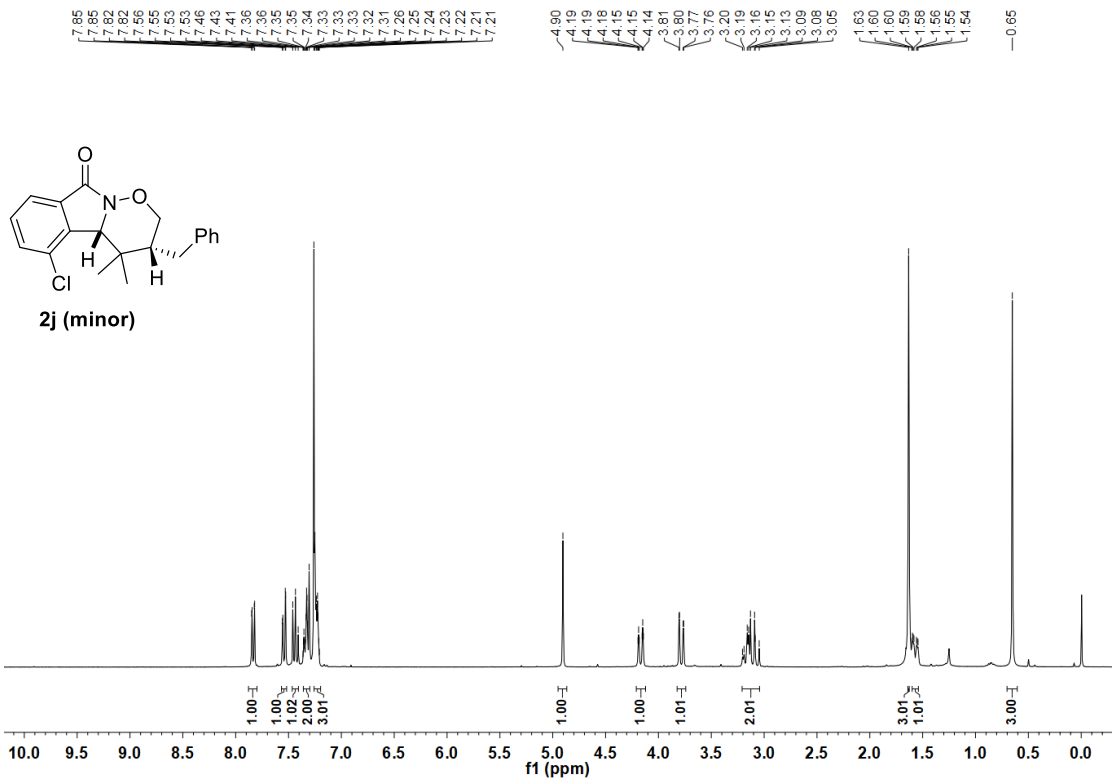


Figure S132. ^{1}H NMR spectra of **2j (minor)** (300 MHz, $CDCl_3$)

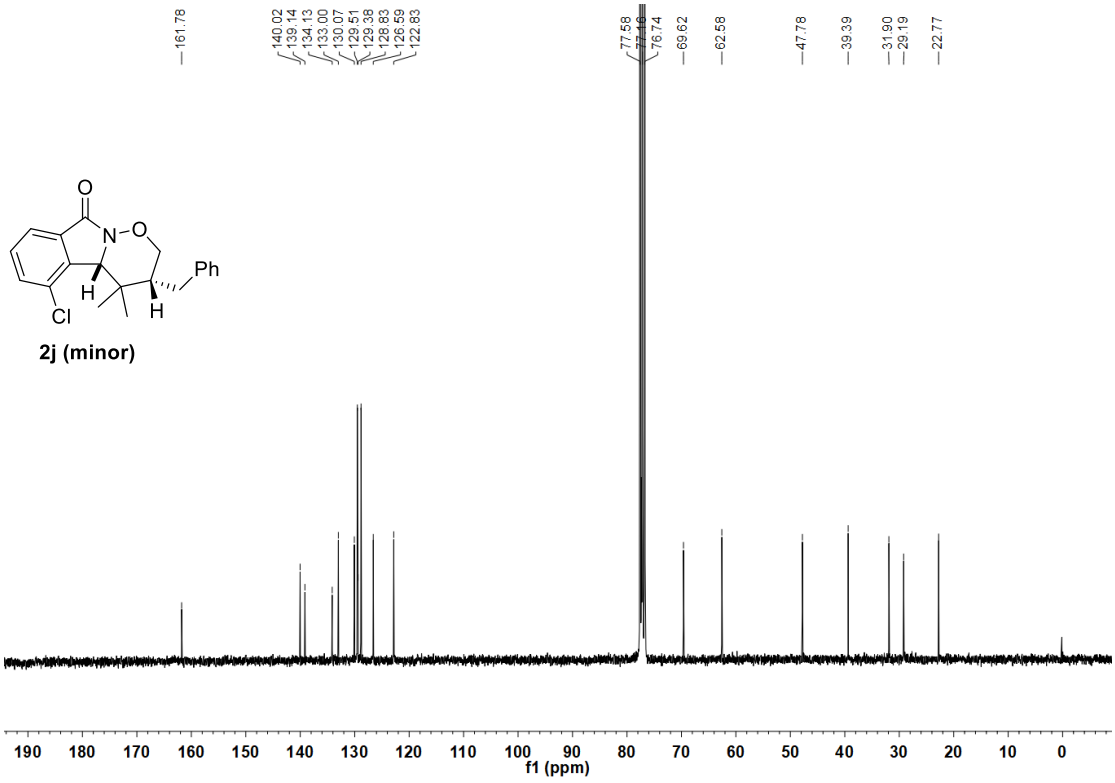


Figure S133. ^{13}C NMR spectra of **2j (minor)** (75 MHz, $CDCl_3$)

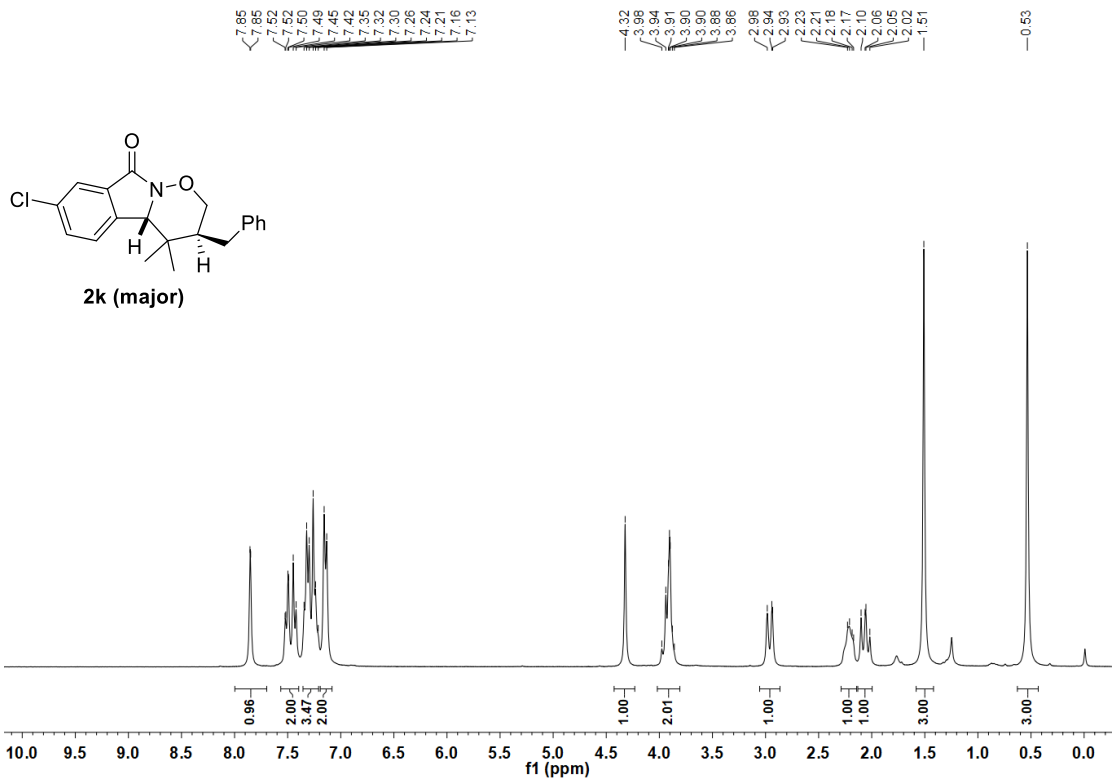


Figure S134. ^{1}H NMR spectra of **2k (major)** (300 MHz, $CDCl_3$)

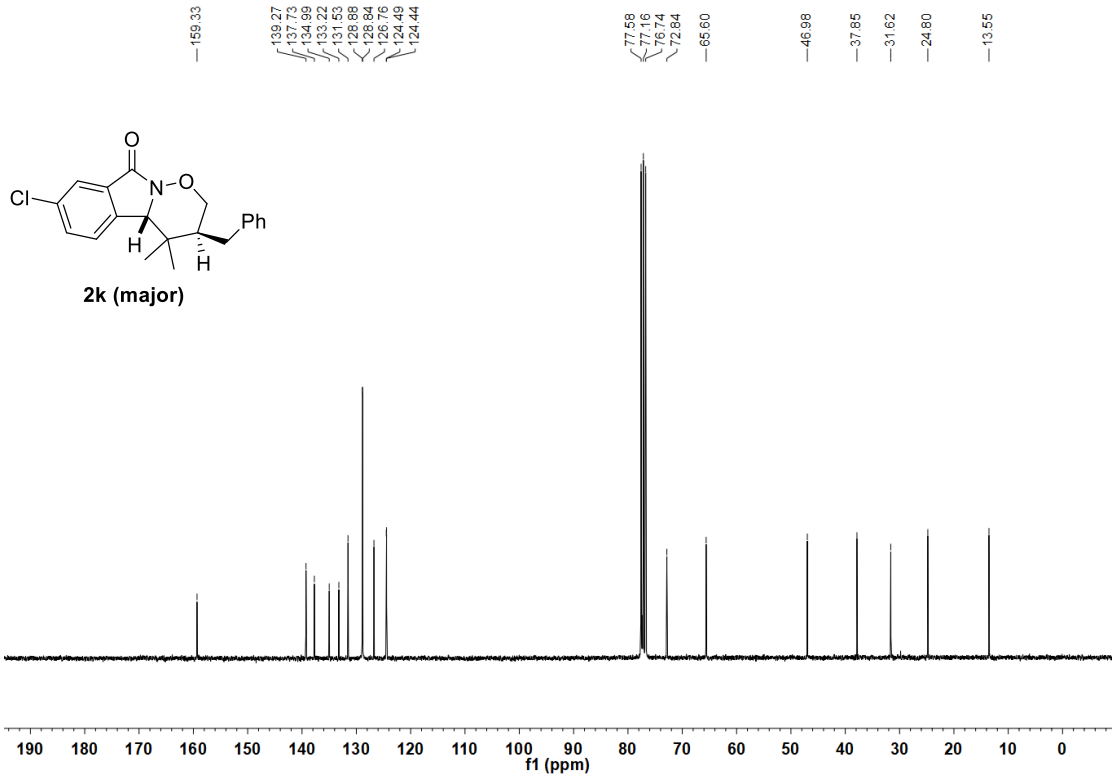


Figure S135. ^{13}C NMR spectra of **2k (major)** (75 MHz, $CDCl_3$)

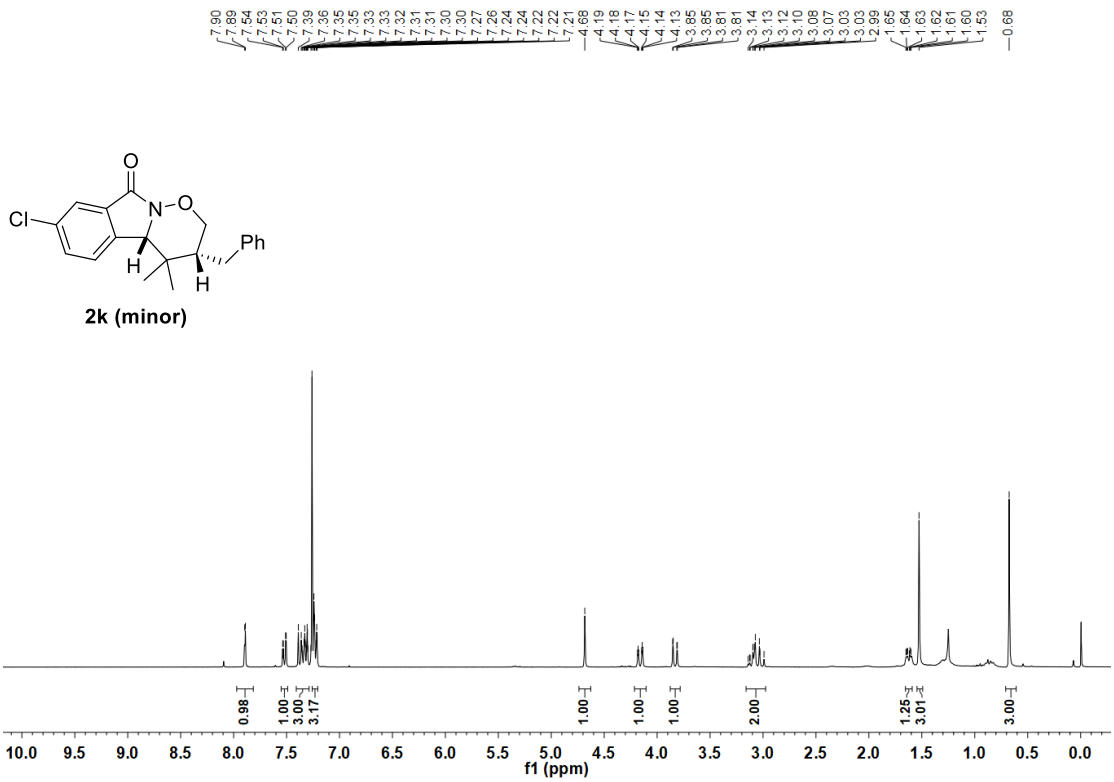


Figure S136. ^{1}H NMR spectra of **2k (minor)** (300 MHz, $CDCl_3$)

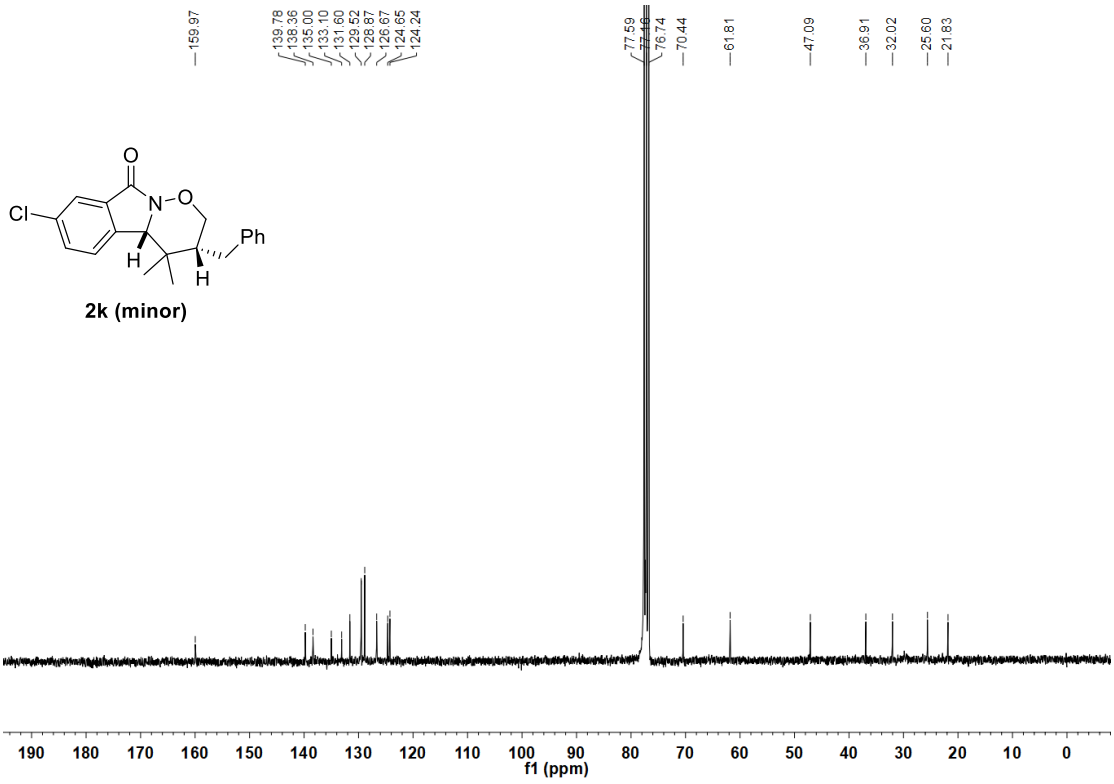


Figure S137. ^{13}C NMR spectra of **2k (minor)** (75 MHz, $CDCl_3$)

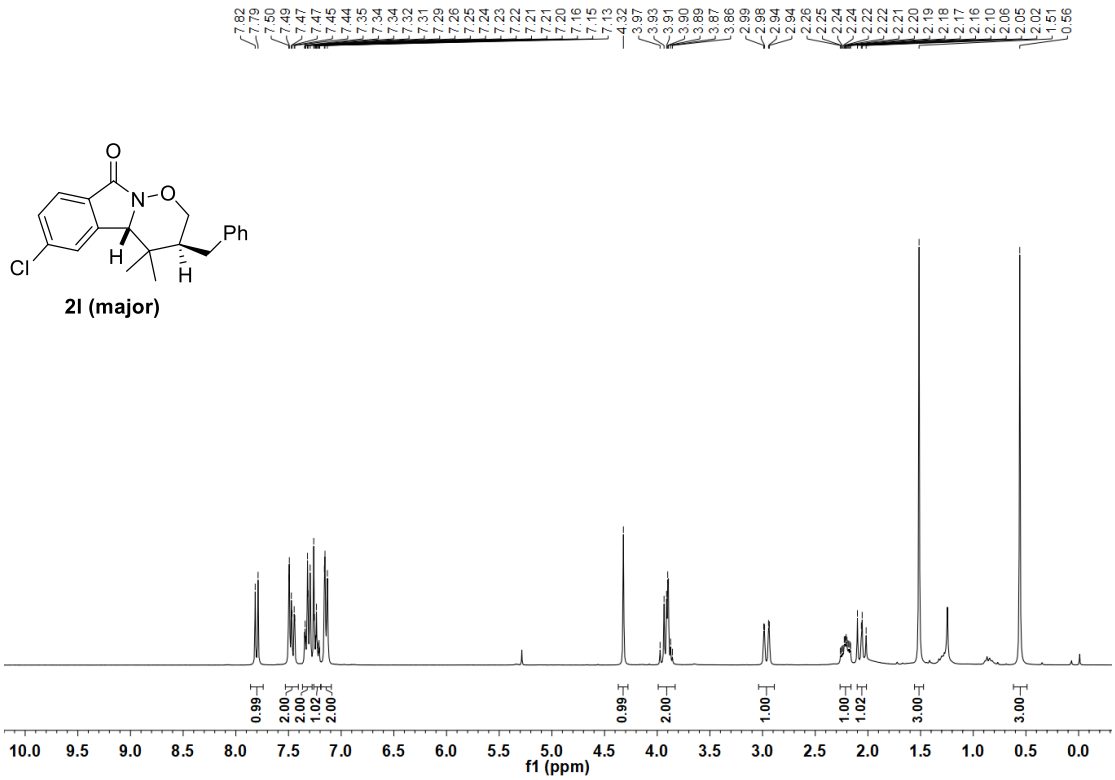


Figure S138. ^{1}H NMR spectra of **2l (major)** (300 MHz, $CDCl_3$)

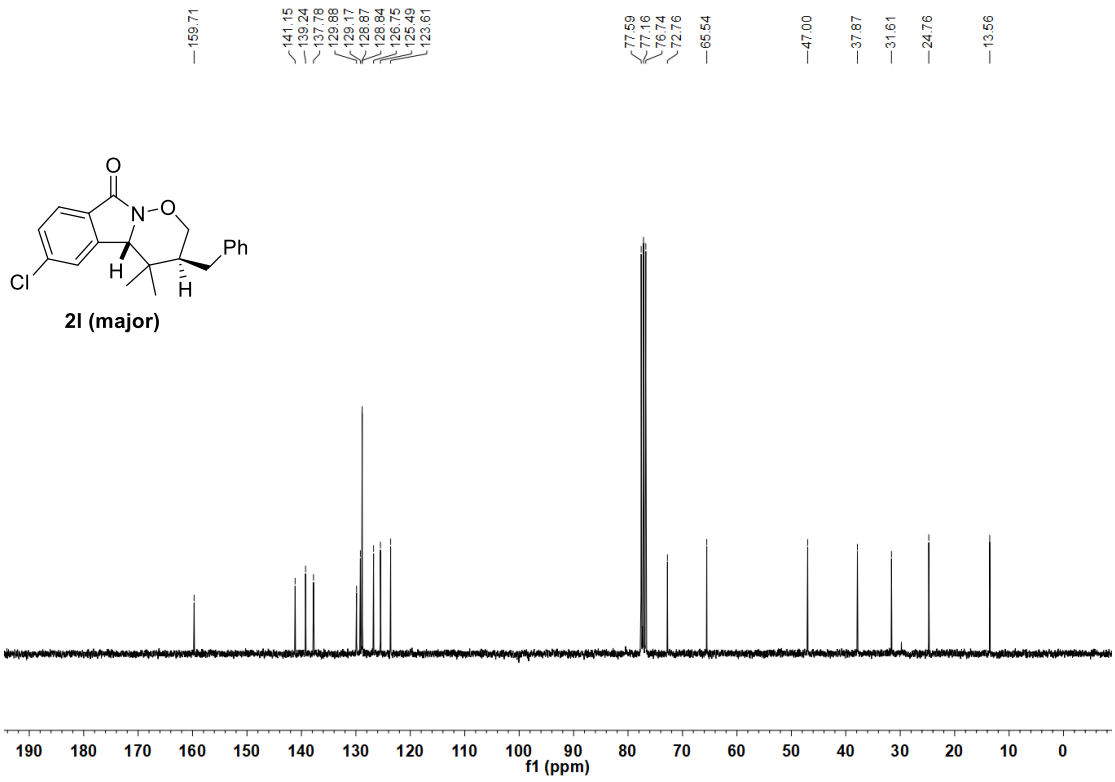


Figure S139. ^{13}C NMR spectra of **2l (major)** (75 MHz, $CDCl_3$)

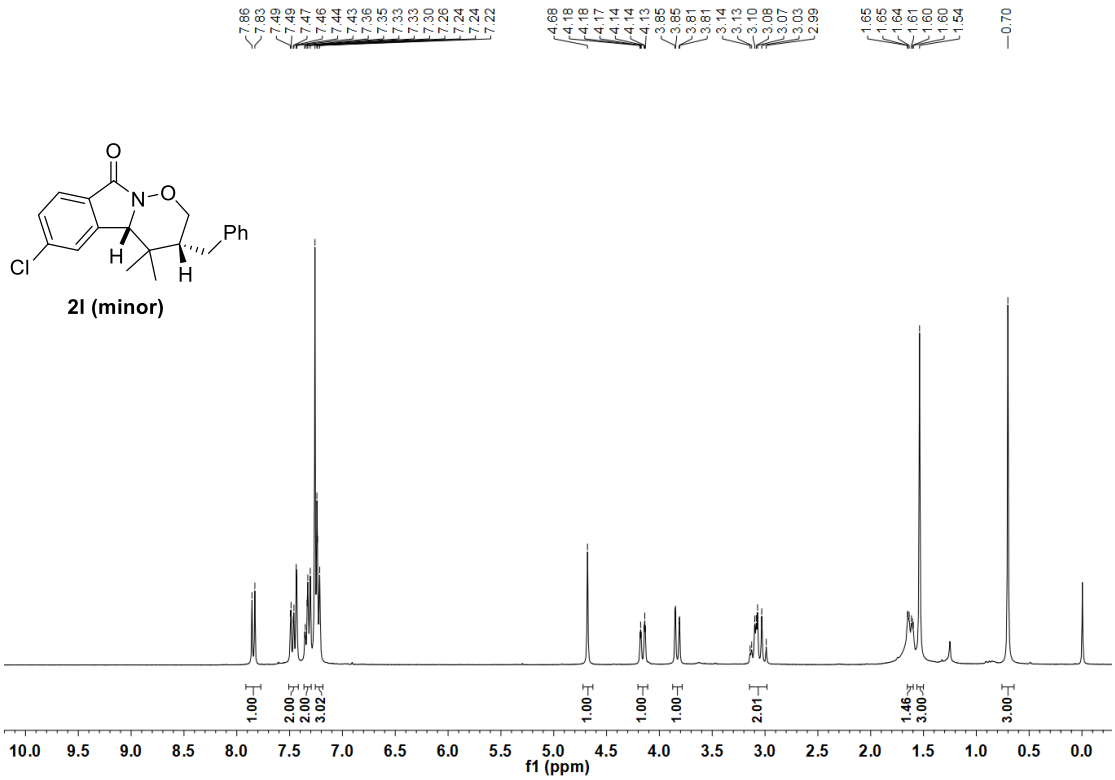


Figure S140. ^{1}H NMR spectra of **2l (minor)** (300 MHz, $CDCl_3$)

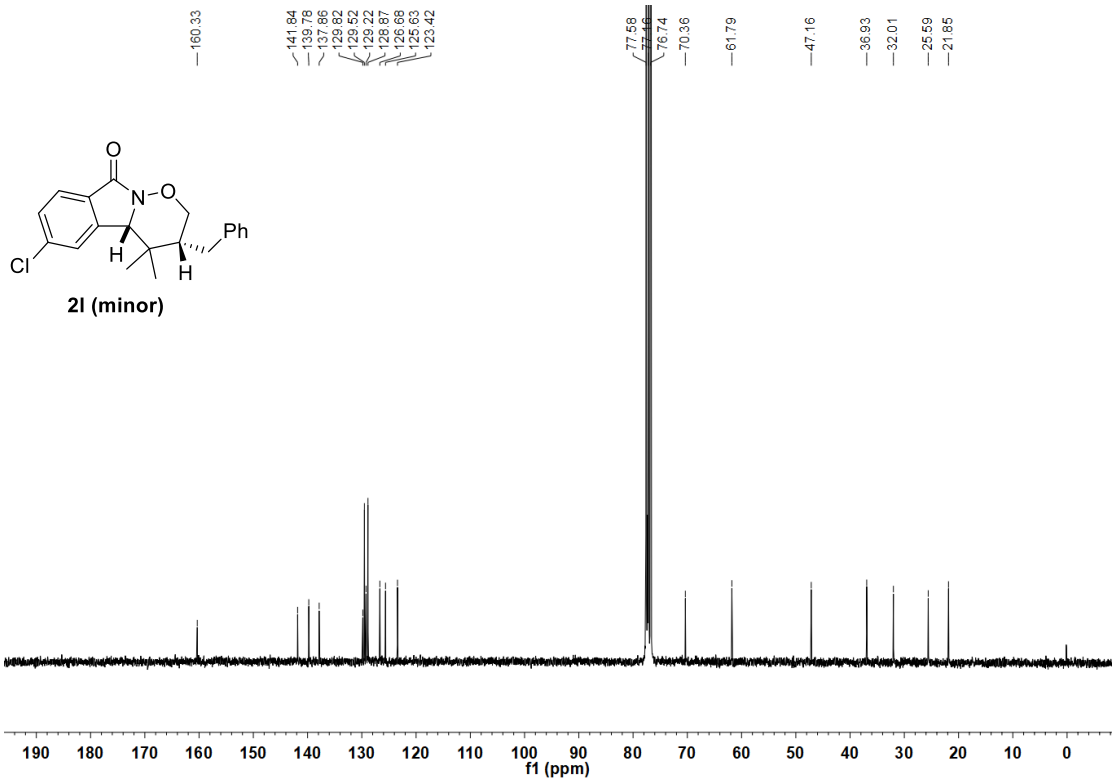


Figure S141. ^{13}C NMR spectra of **2l (minor)** (75 MHz, $CDCl_3$)

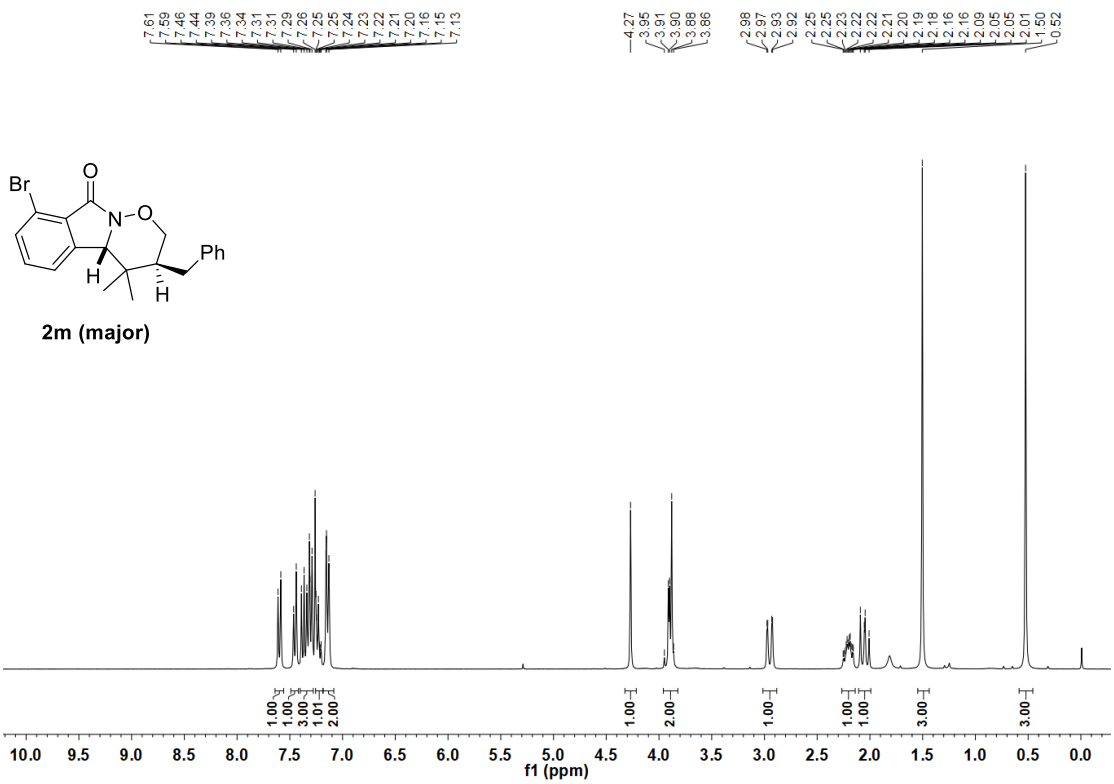


Figure S142. ^{1}H NMR spectra of **2m (major)** (300 MHz, $CDCl_3$)

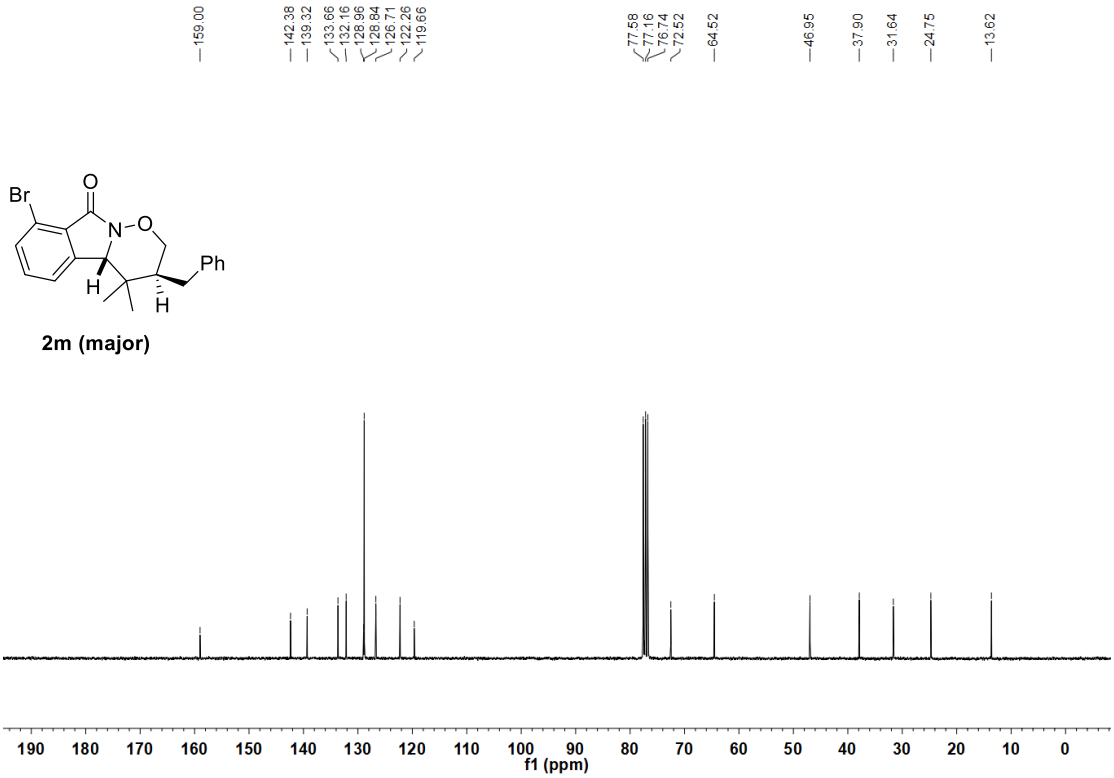


Figure S143. ^{13}C NMR spectra of **2m (major)** (75 MHz, $CDCl_3$)

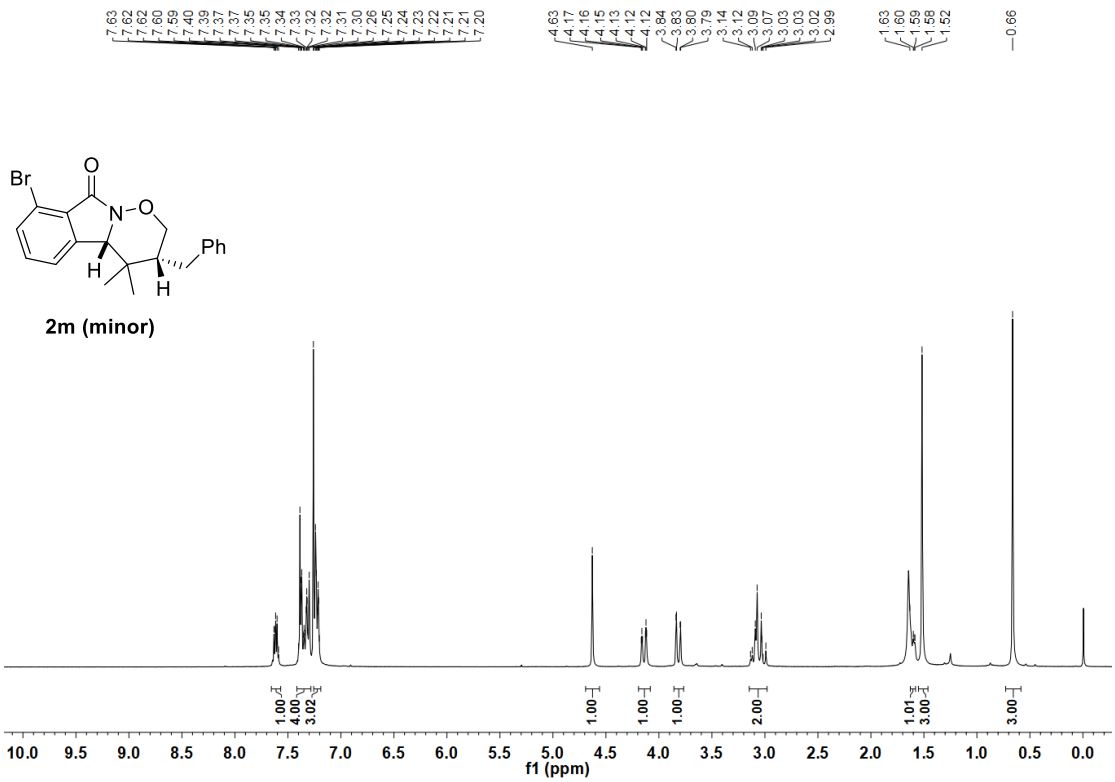


Figure S144. ^{1}H NMR spectra of **2m (minor)** (300 MHz, $CDCl_3$)

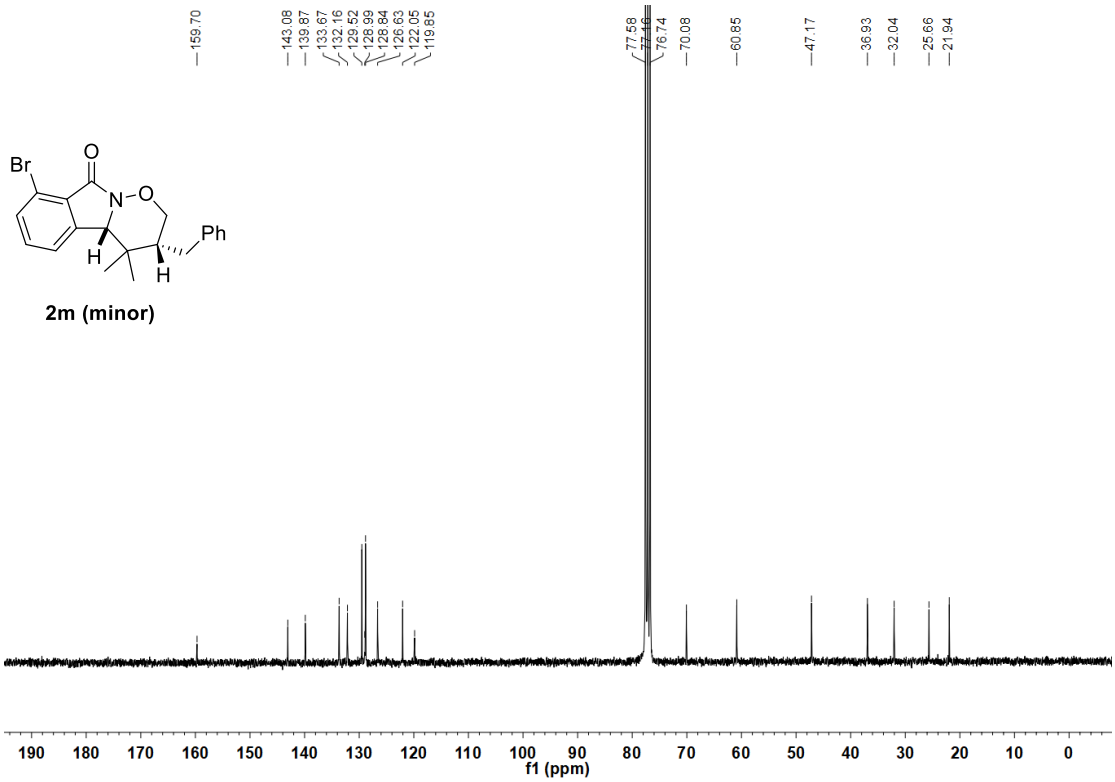


Figure S145. ^{13}C NMR spectra of **2m (minor)** (75 MHz, $CDCl_3$)

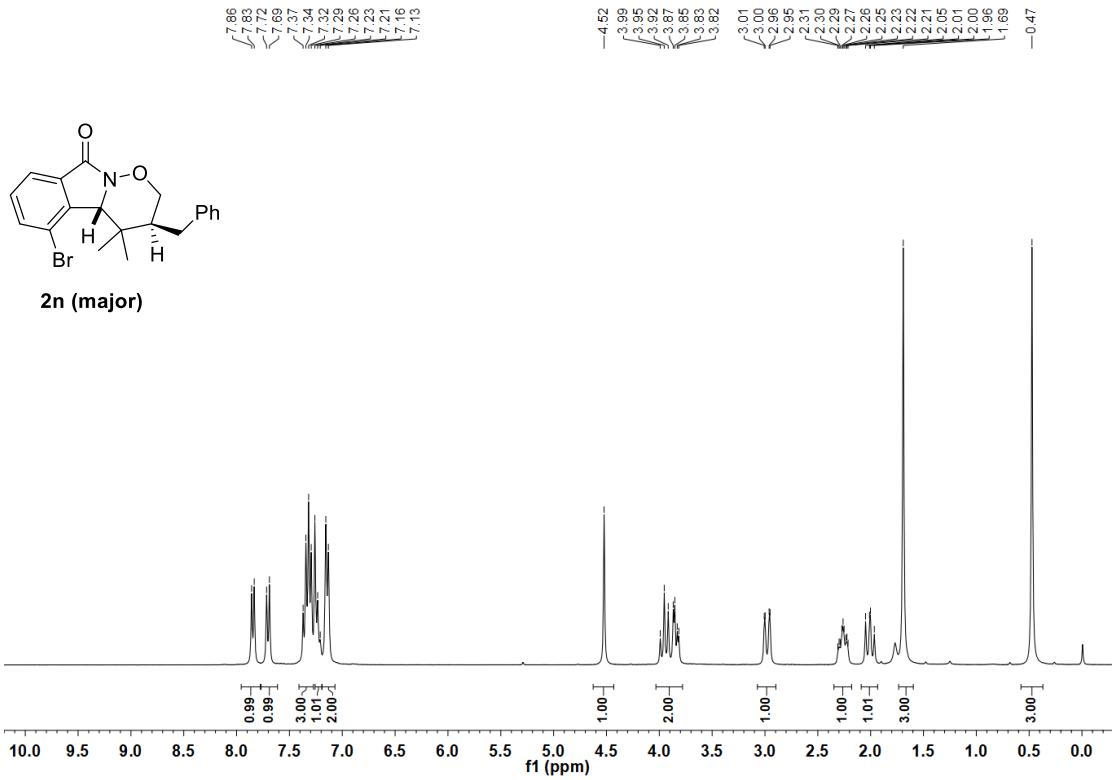


Figure S146. ^{1}H NMR spectra of **2n (major)** (300 MHz, $CDCl_3$)

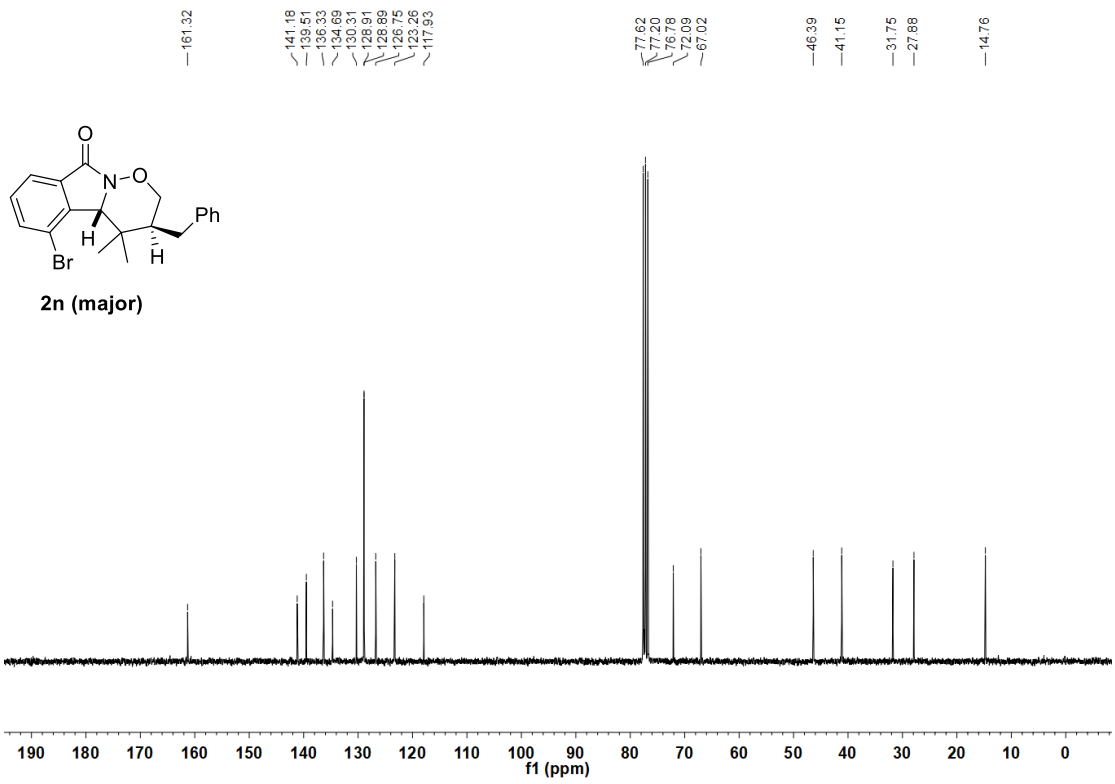


Figure S147. ^{13}C NMR spectra of **2n (major)** (75 MHz, $CDCl_3$)

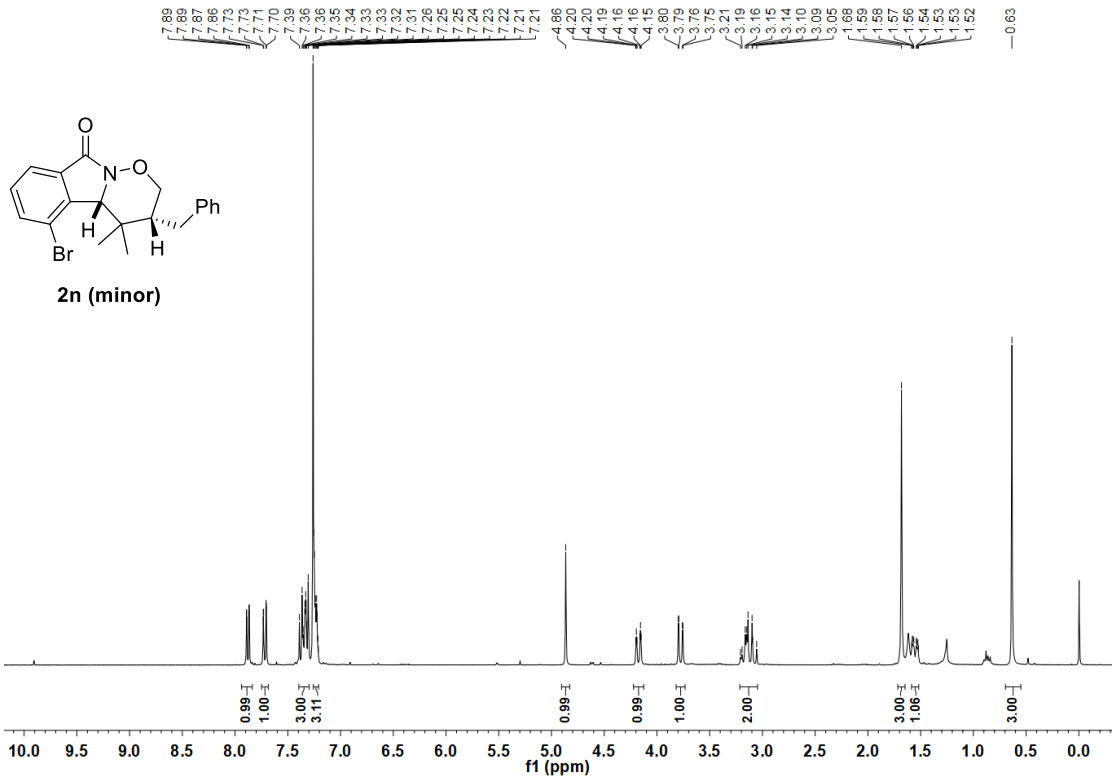


Figure S148. ^{1}H NMR spectra of **2n (minor)** (300 MHz, $CDCl_3$)

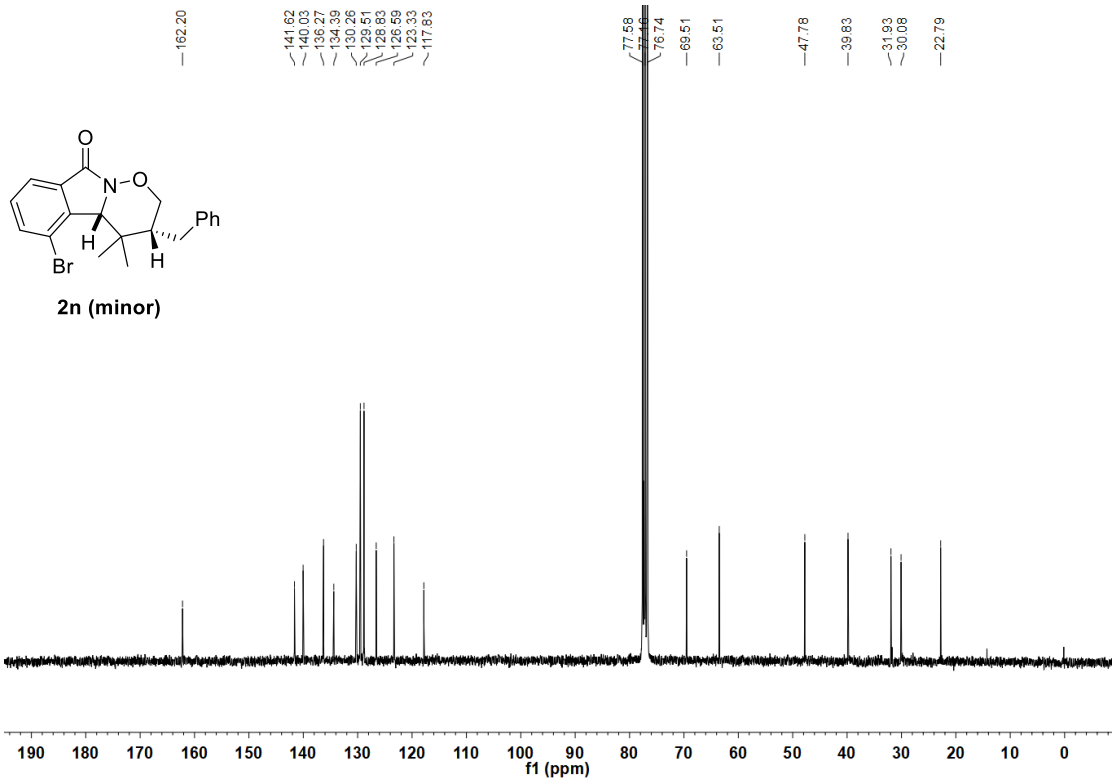


Figure S149. ^{13}C NMR spectra of **2n (minor)** (75 MHz, $CDCl_3$)

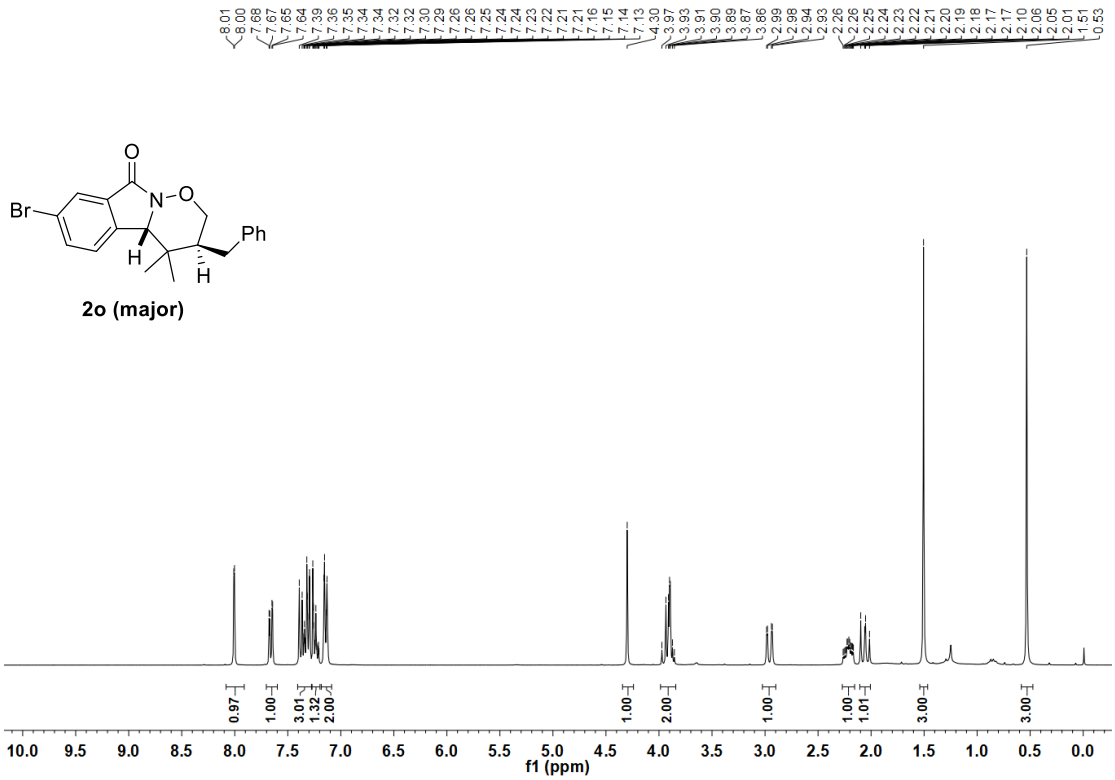


Figure S150. ^{1}H NMR spectra of **2o (major)** (300 MHz, $CDCl_3$)

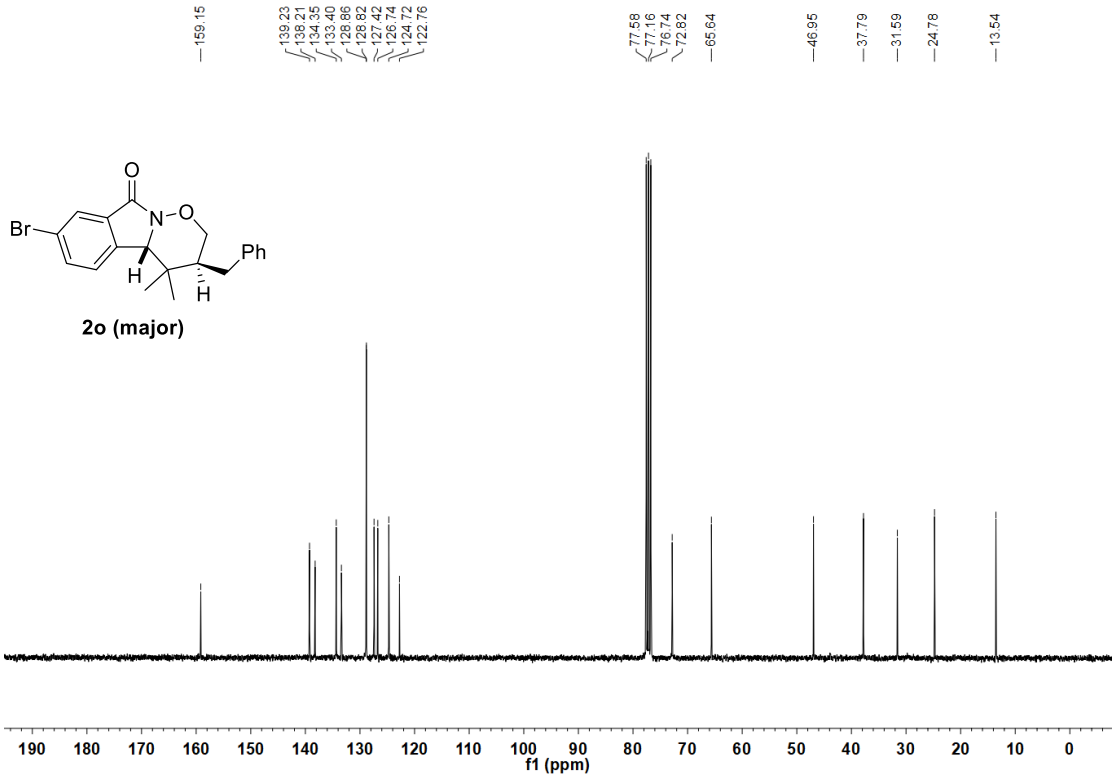


Figure S151. ^{13}C NMR spectra of **2o (major)** (75 MHz, $CDCl_3$)

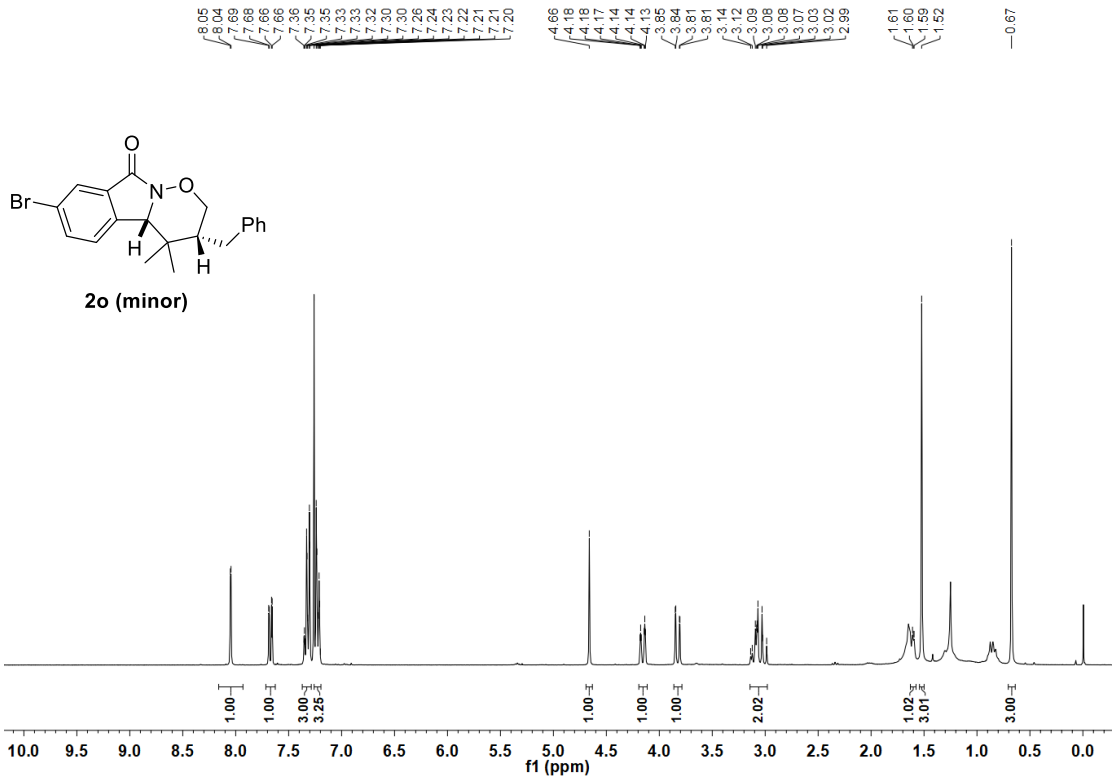


Figure S152. ^{1}H NMR spectra of **2o (minor)** (300 MHz, $CDCl_3$)

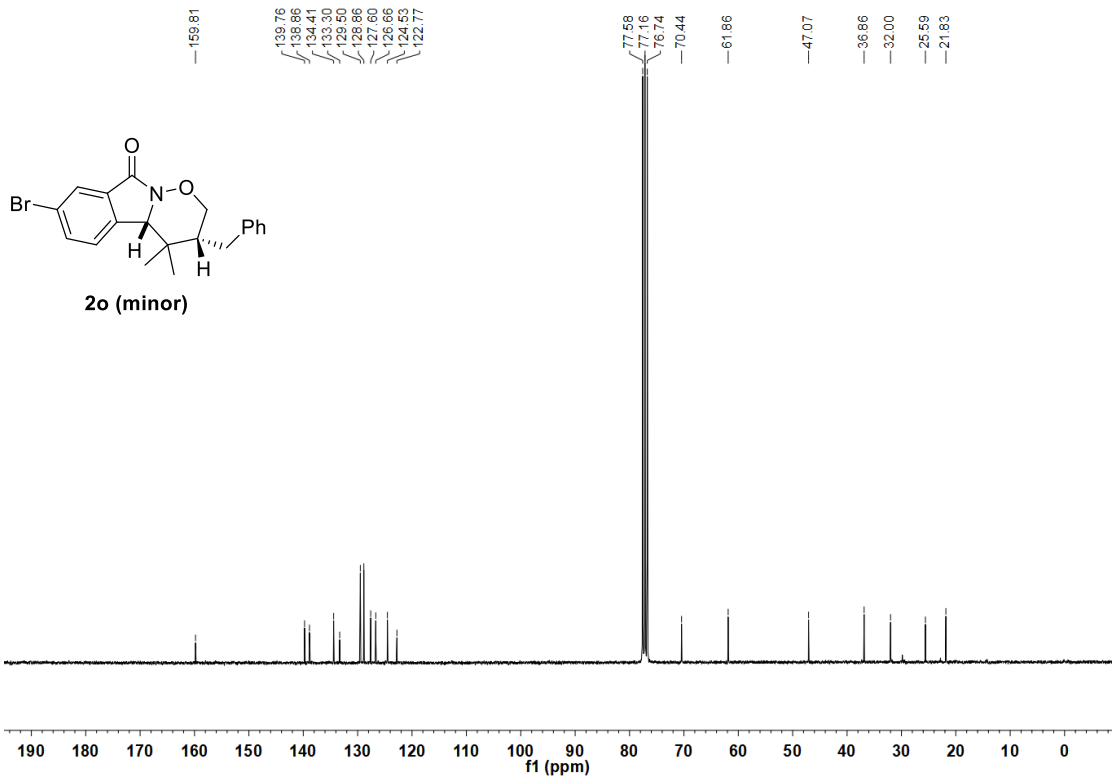


Figure S153. ^{13}C NMR spectra of **2o (minor)** (75 MHz, $CDCl_3$)

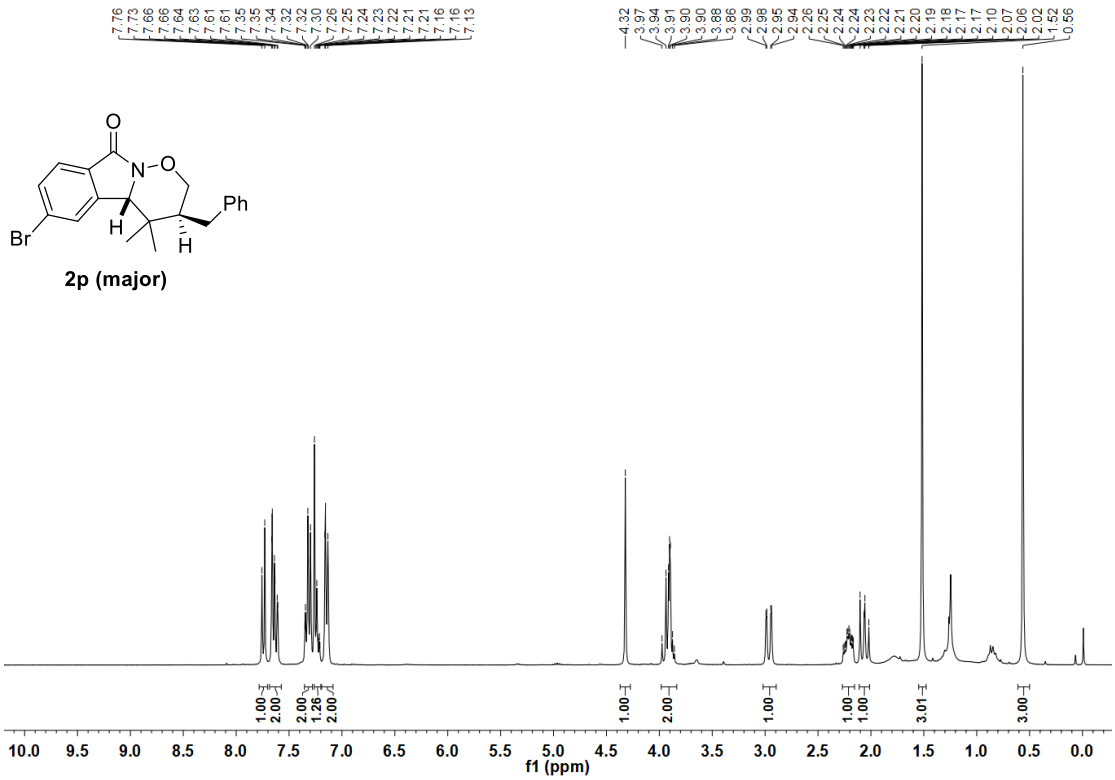


Figure S154. ^{1}H NMR spectra of **2p (major)** (300 MHz, $CDCl_3$)

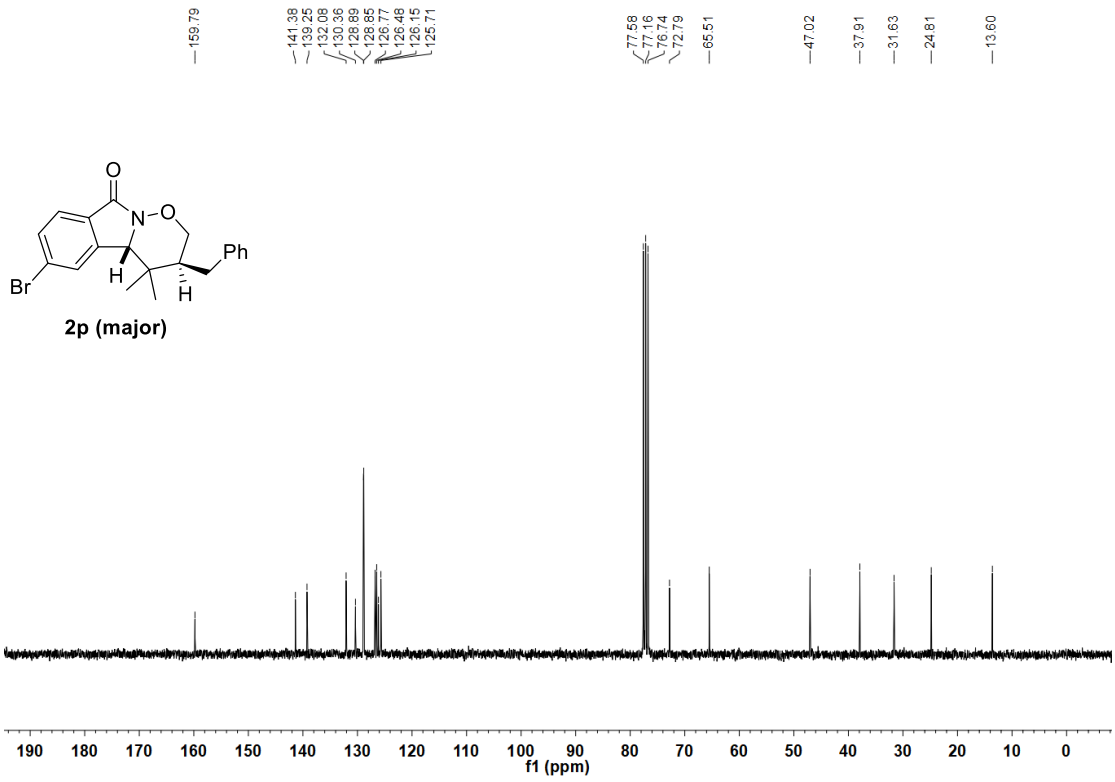


Figure S155. ^{13}C NMR spectra of **2p (major)** (75 MHz, $CDCl_3$)

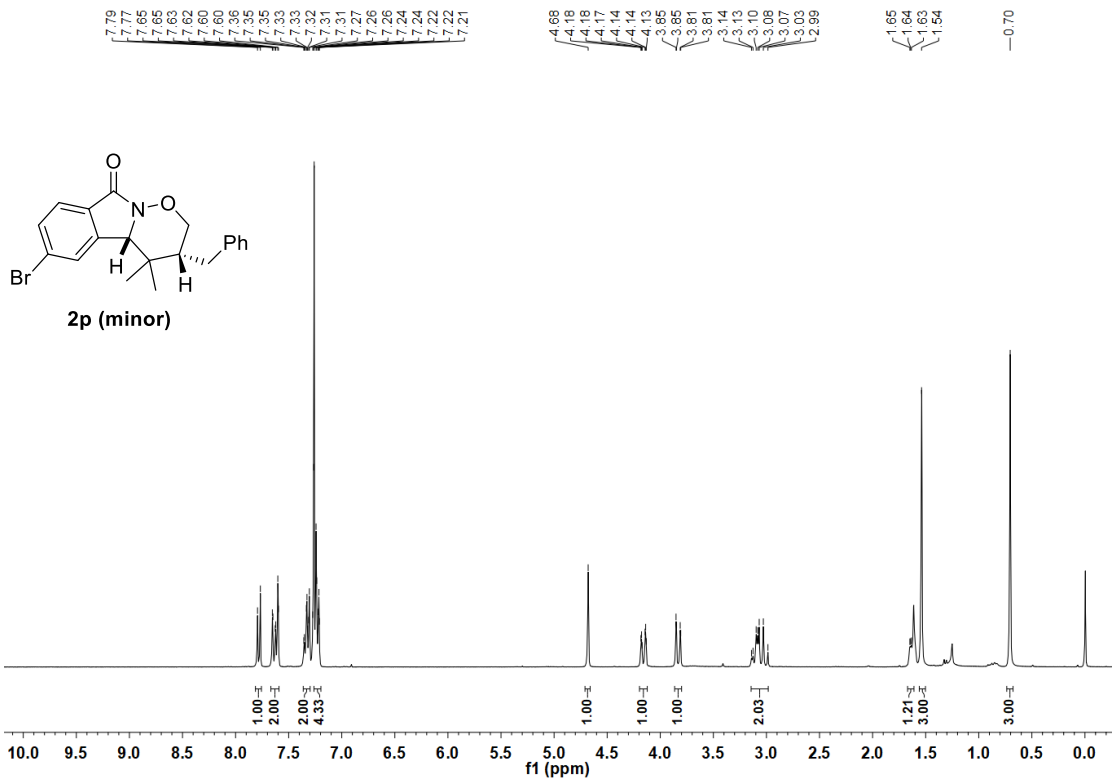


Figure S156. ^{1}H NMR spectra of **2p (minor)** (300 MHz, $CDCl_3$)

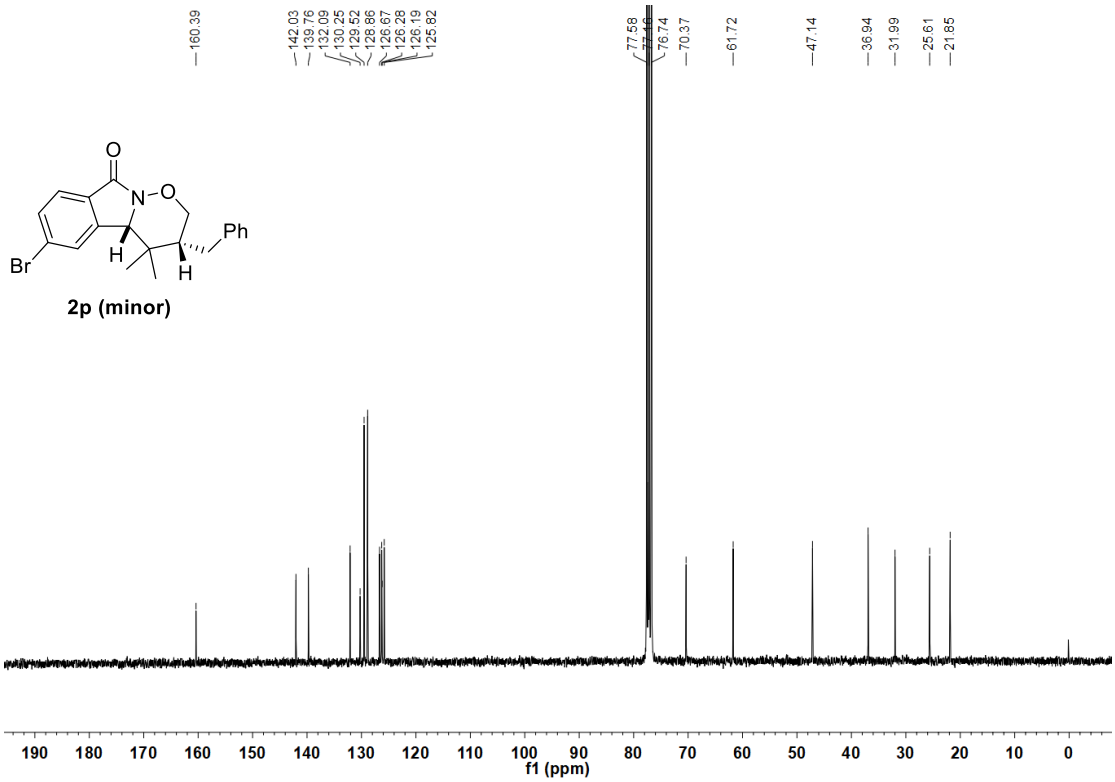


Figure S157. ^{13}C NMR spectra of **2p (minor)** (75 MHz, $CDCl_3$)

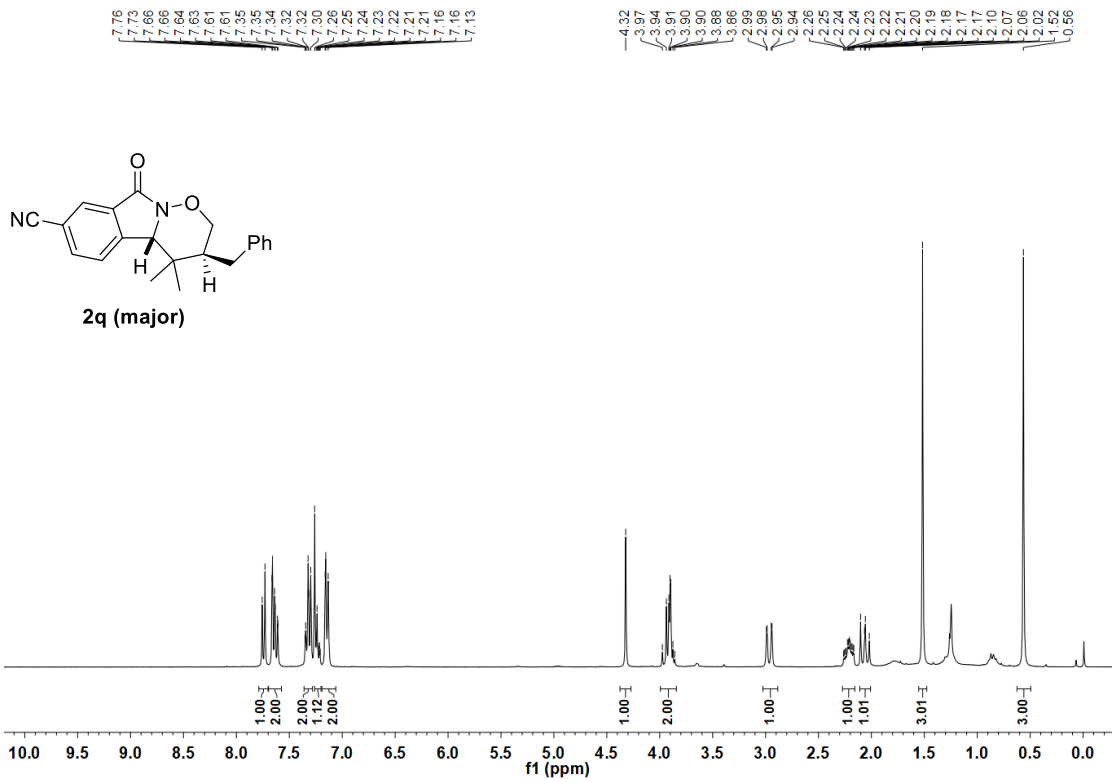


Figure S158. ^{1}H NMR spectra of **2q (major)** (300 MHz, $CDCl_3$)

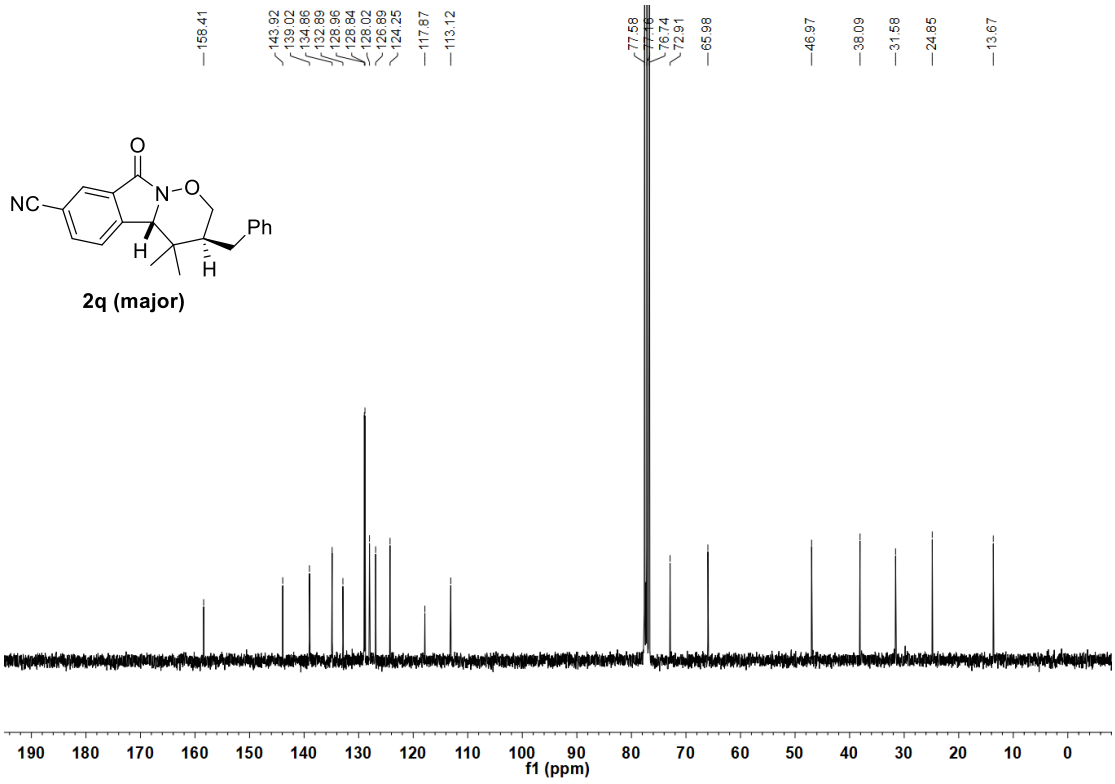


Figure S159. ^{13}C NMR spectra of **2q (major)** (75 MHz, $CDCl_3$)

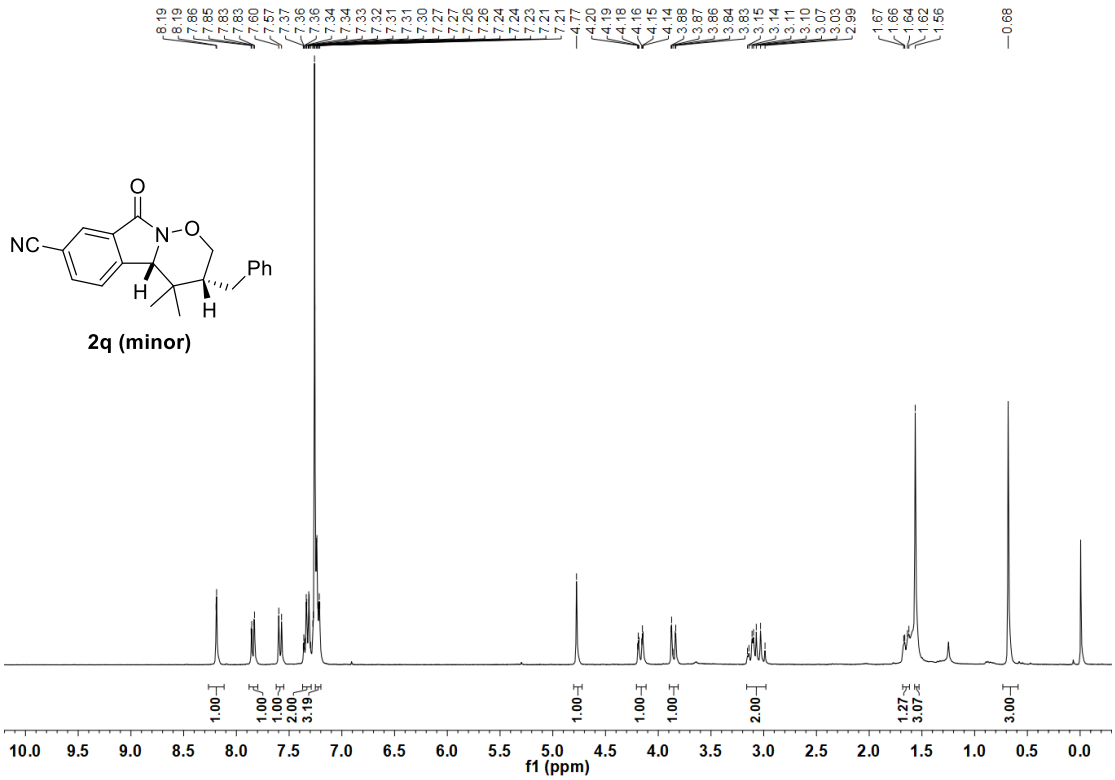


Figure S160. ^{1}H NMR spectra of **2q (minor)** (300 MHz, $CDCl_3$)

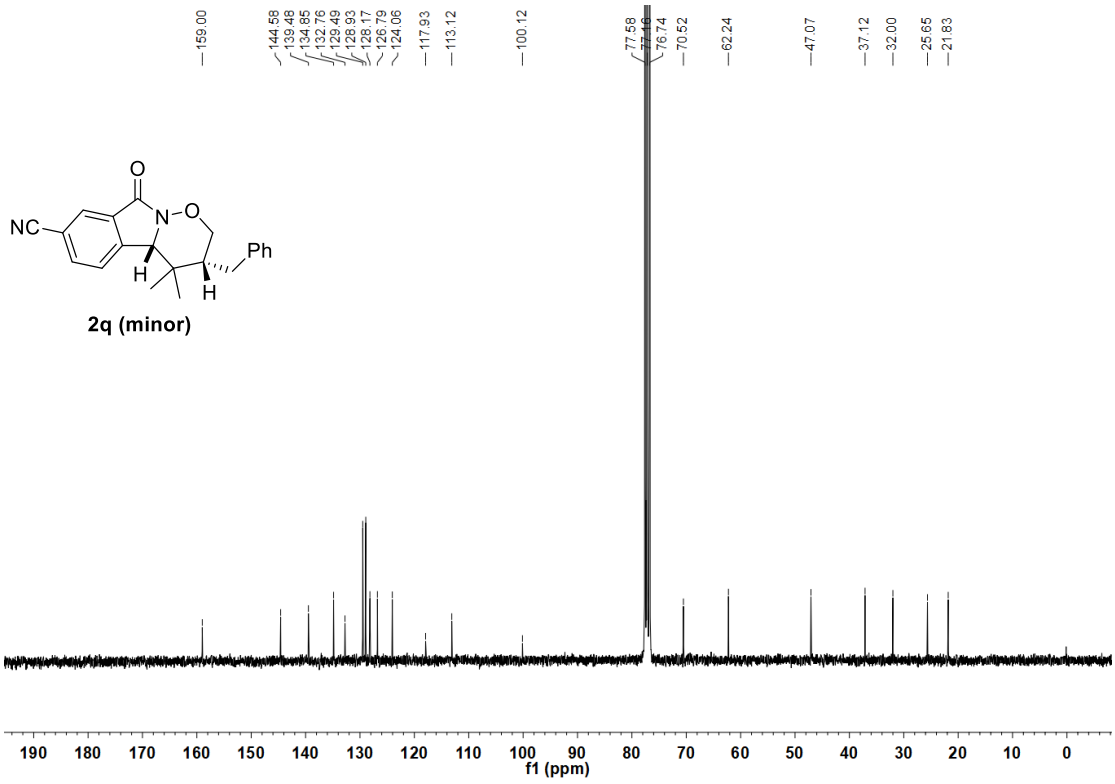


Figure S161. ^{13}C NMR spectra of **2q (minor)** (75 MHz, $CDCl_3$)

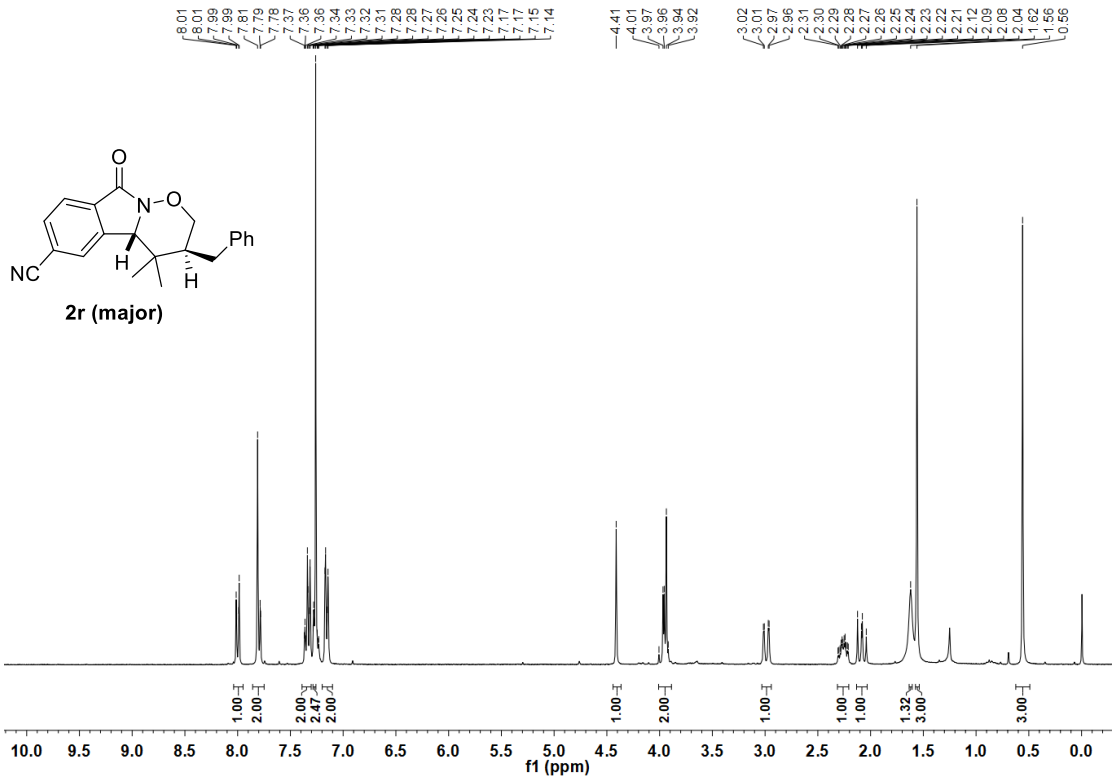


Figure S162. ^{1}H NMR spectra of **2r (major)** (300 MHz, $CDCl_3$)

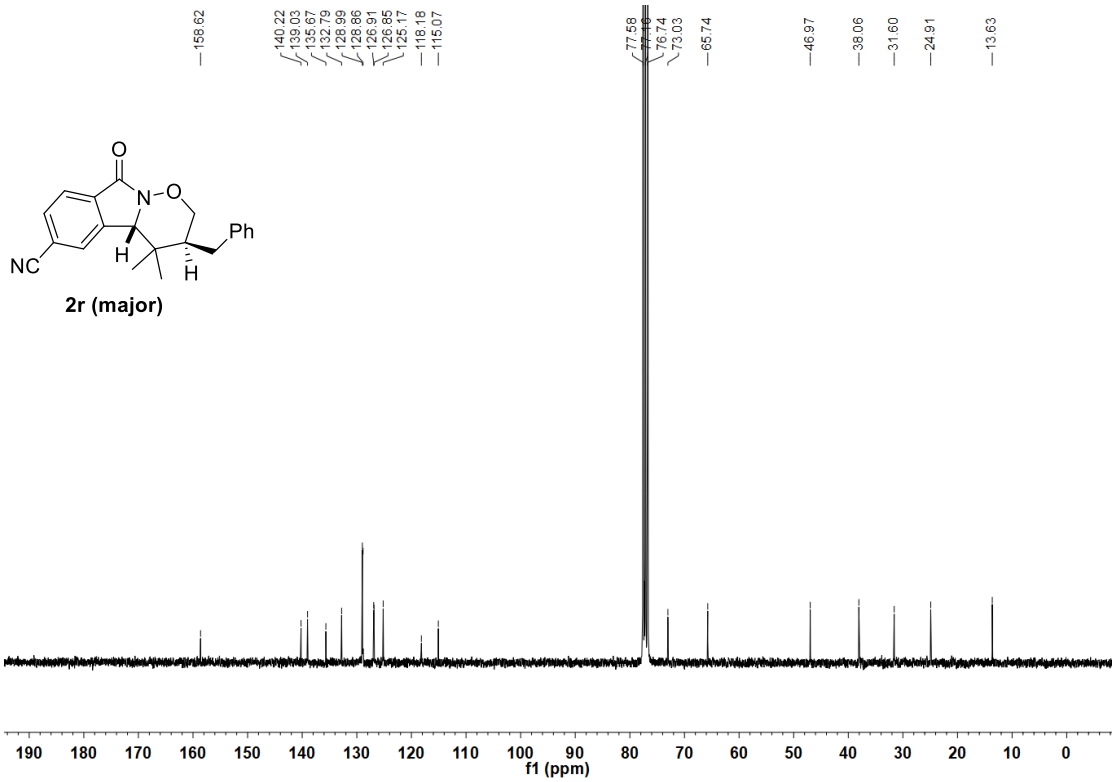


Figure S163. ^{13}C NMR spectra of **2r (major)** (75 MHz, $CDCl_3$)

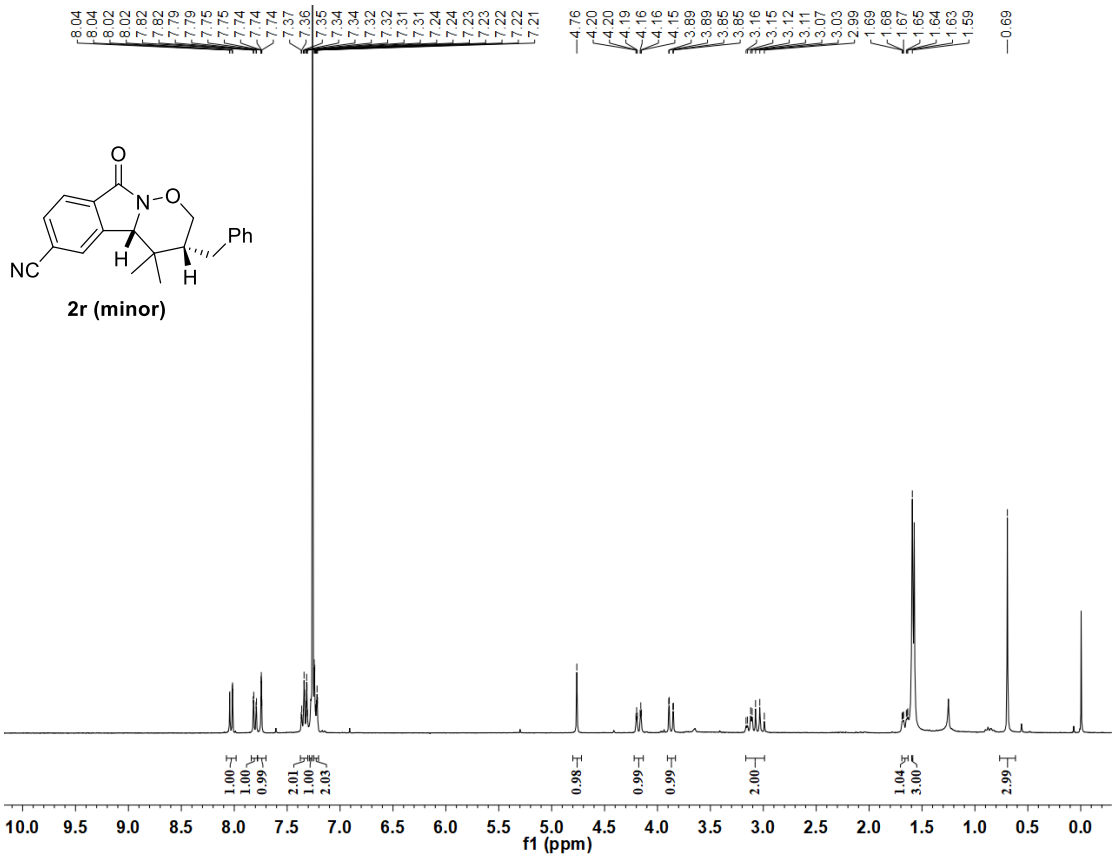


Figure S164. ^{1}H NMR spectra of **2r (minor)** (300 MHz, $CDCl_3$)

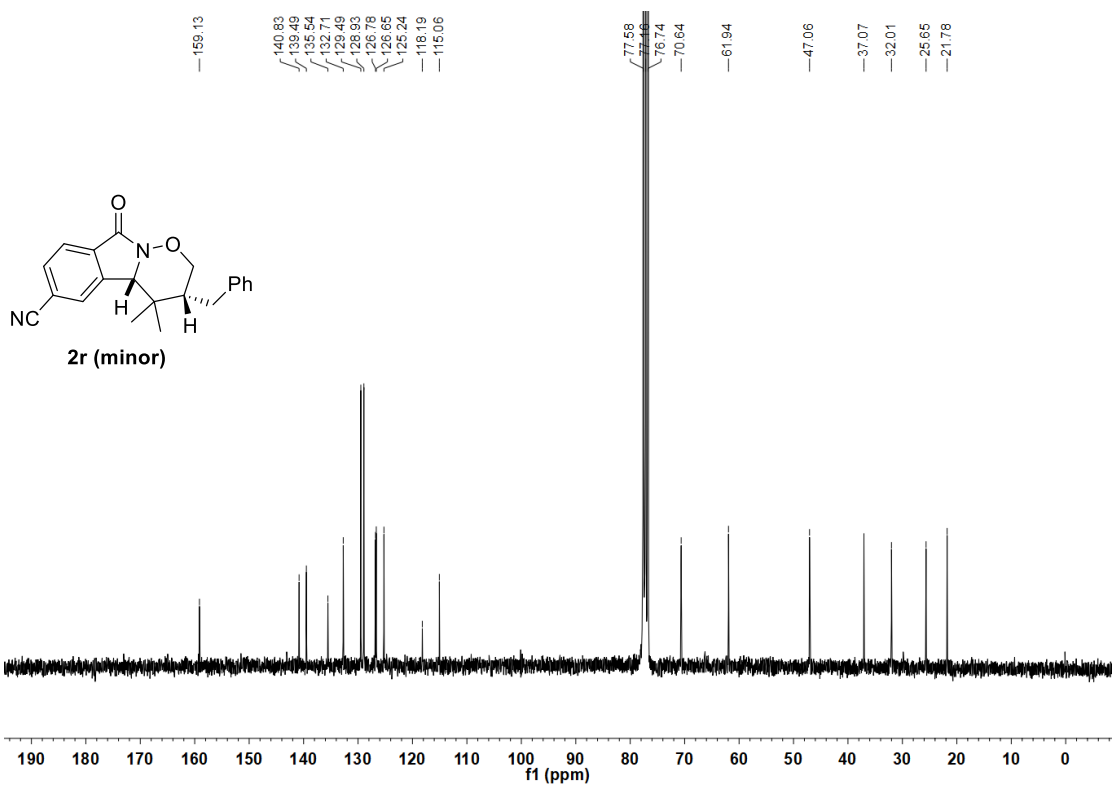


Figure S165. ^{13}C NMR spectra of **2r (minor)** (75 MHz, $CDCl_3$)

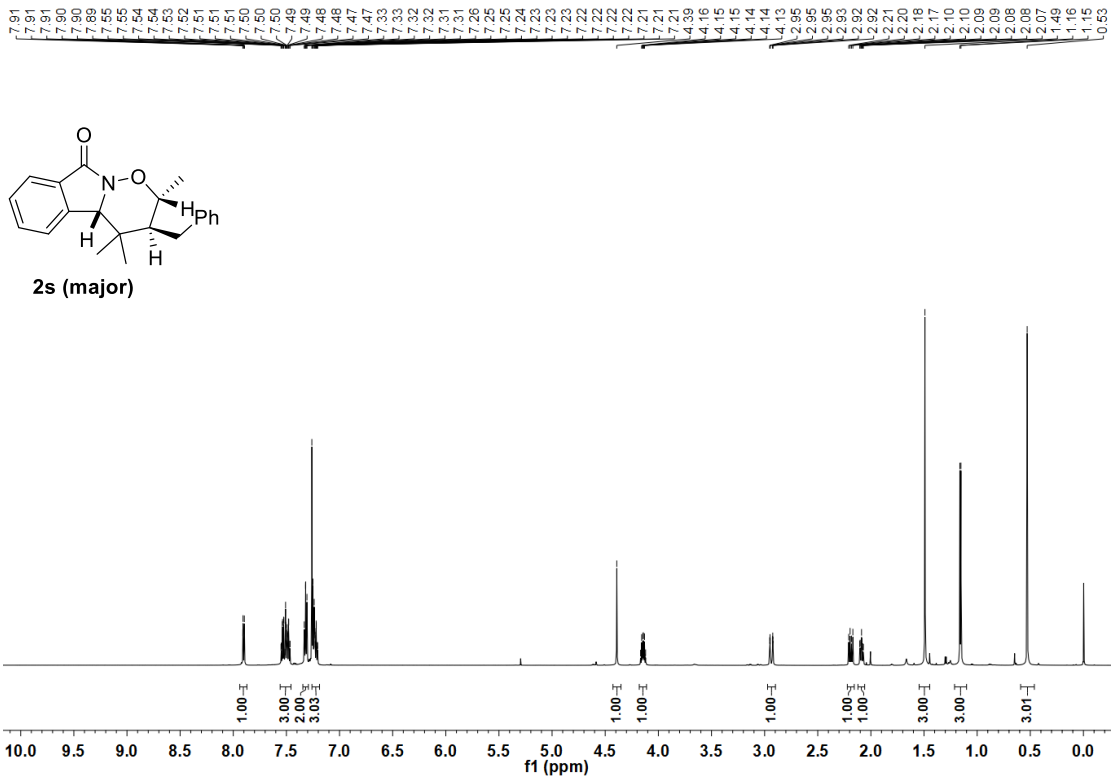


Figure S166. ^{1}H NMR spectra of **2s (major)** (600 MHz, $CDCl_3$)

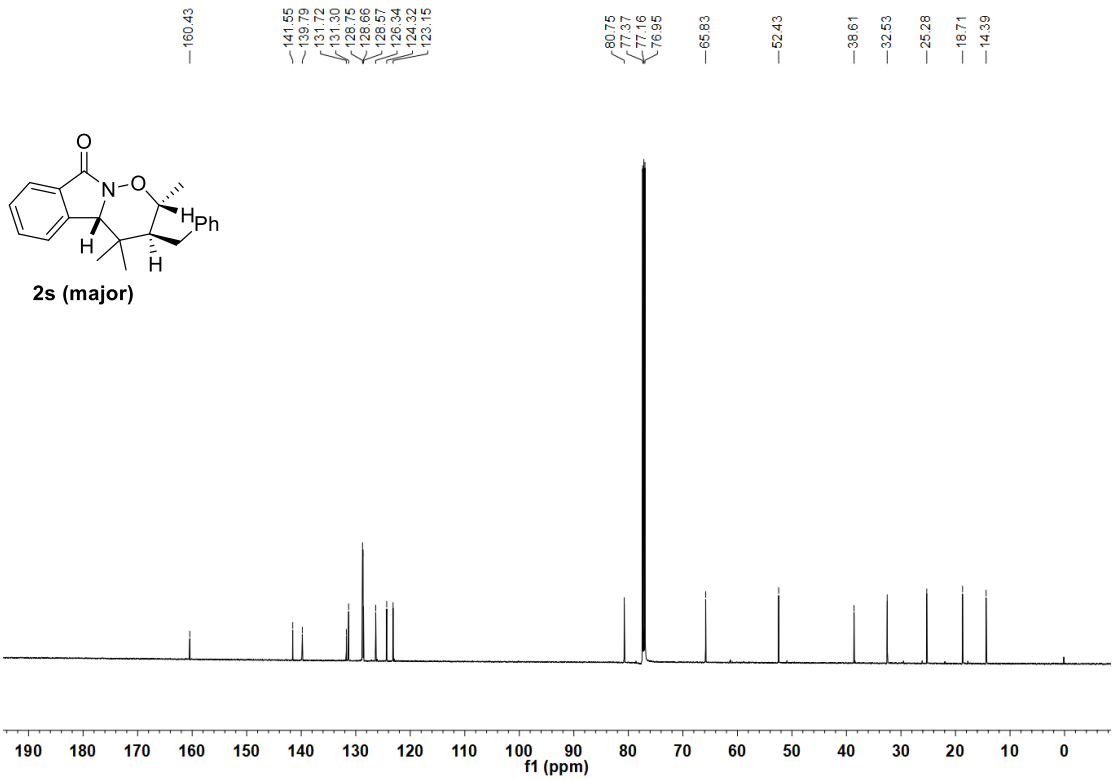


Figure S167. ^{13}C NMR spectra of **2s (major)** (151 MHz, $CDCl_3$)

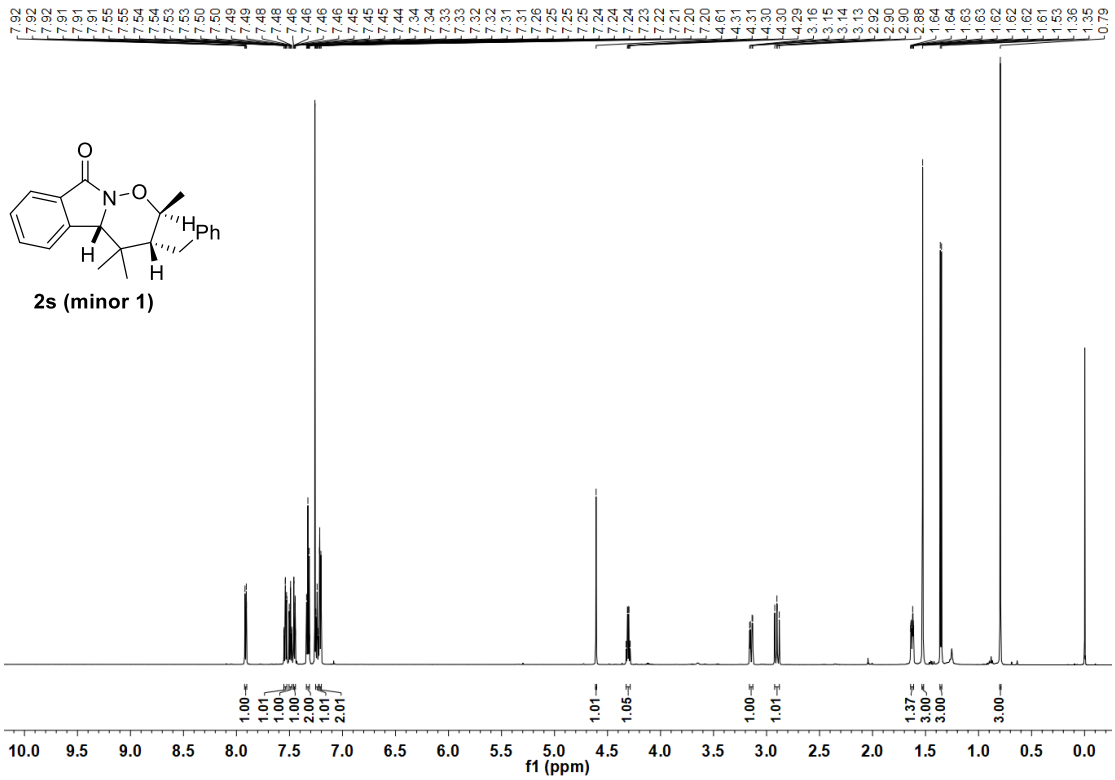


Figure S168. ^{1}H NMR spectra of **2s (minor 1)** (600 MHz, $CDCl_3$)

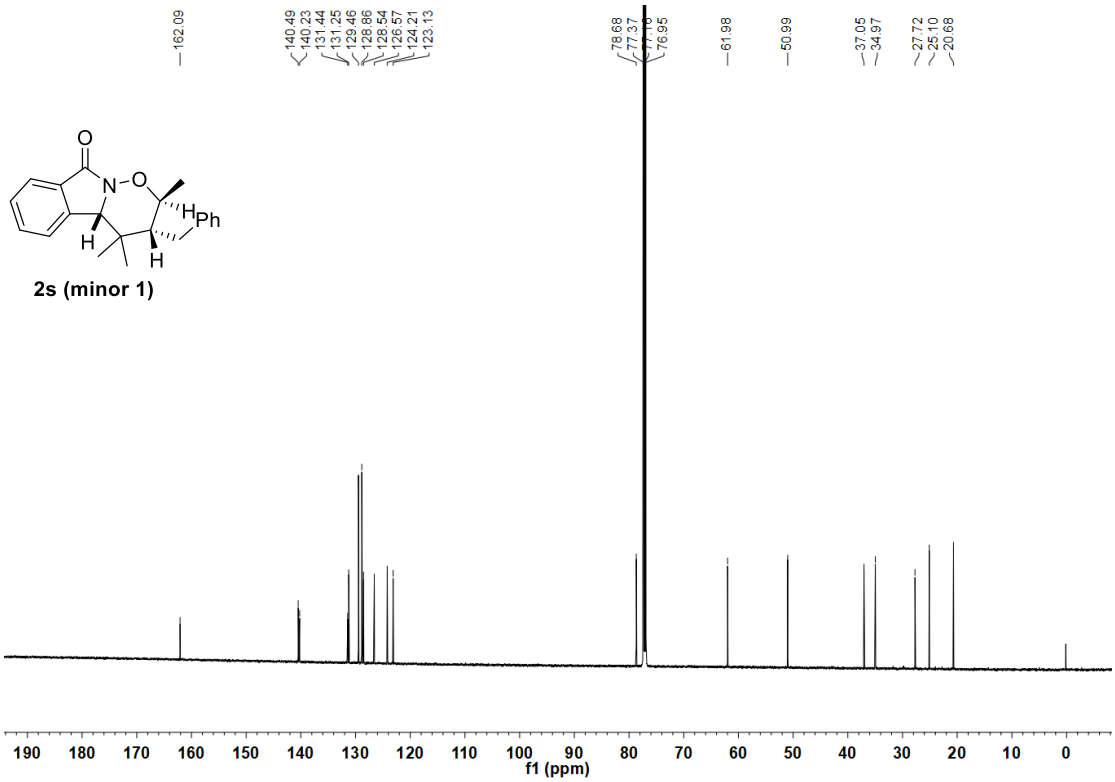


Figure S169. ^{13}C NMR spectra of **2s (minor 1)** (151 MHz, $CDCl_3$)

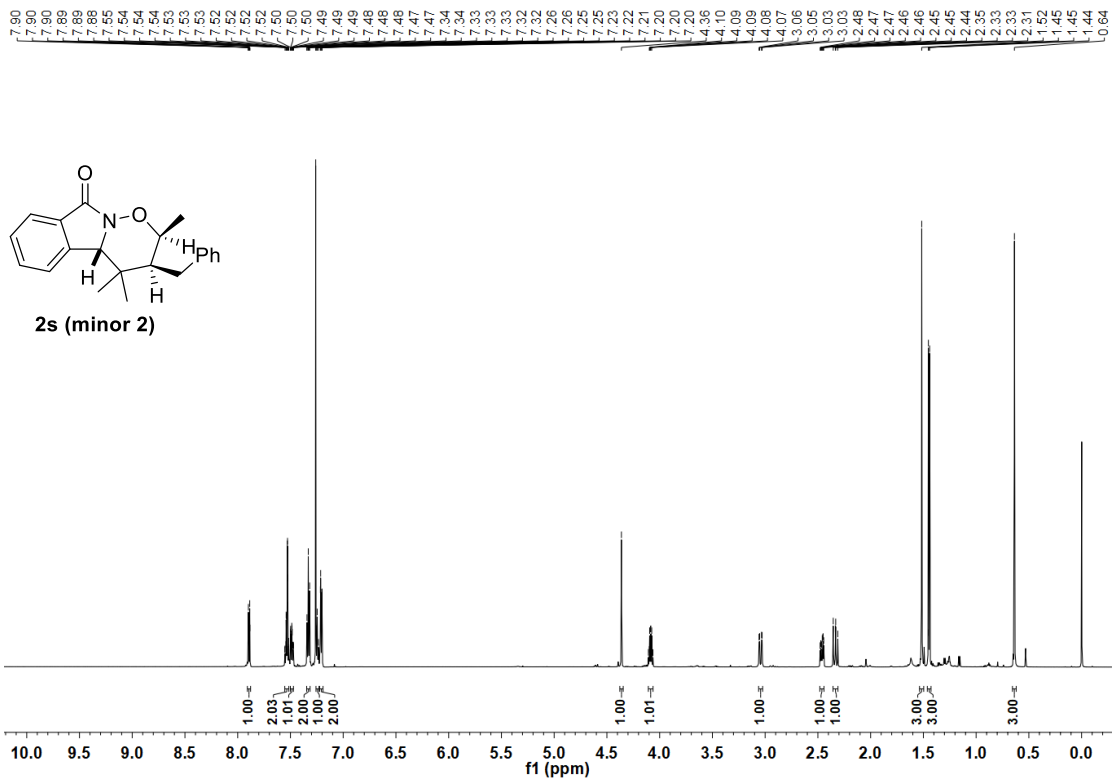


Figure S170. ^{1}H NMR spectra of **2s (minor 2)** (600 MHz, $CDCl_3$)

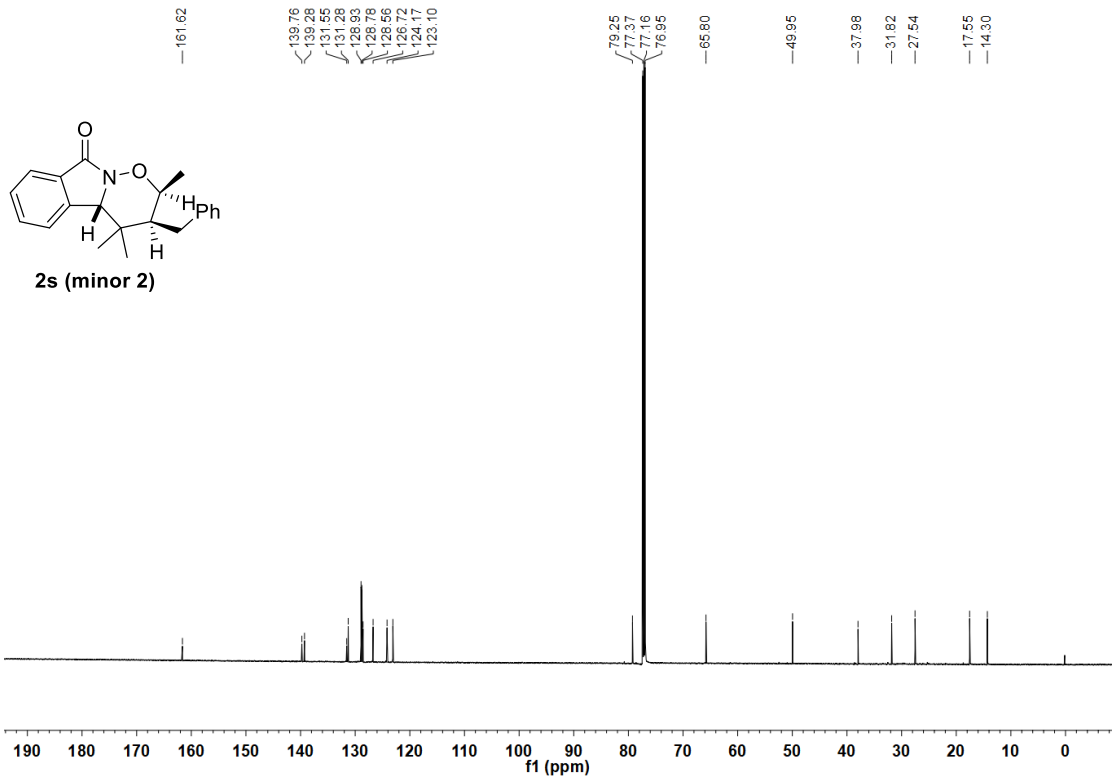


Figure S171. ^{13}C NMR spectra of **2s (minor 2)** (151 MHz, $CDCl_3$)

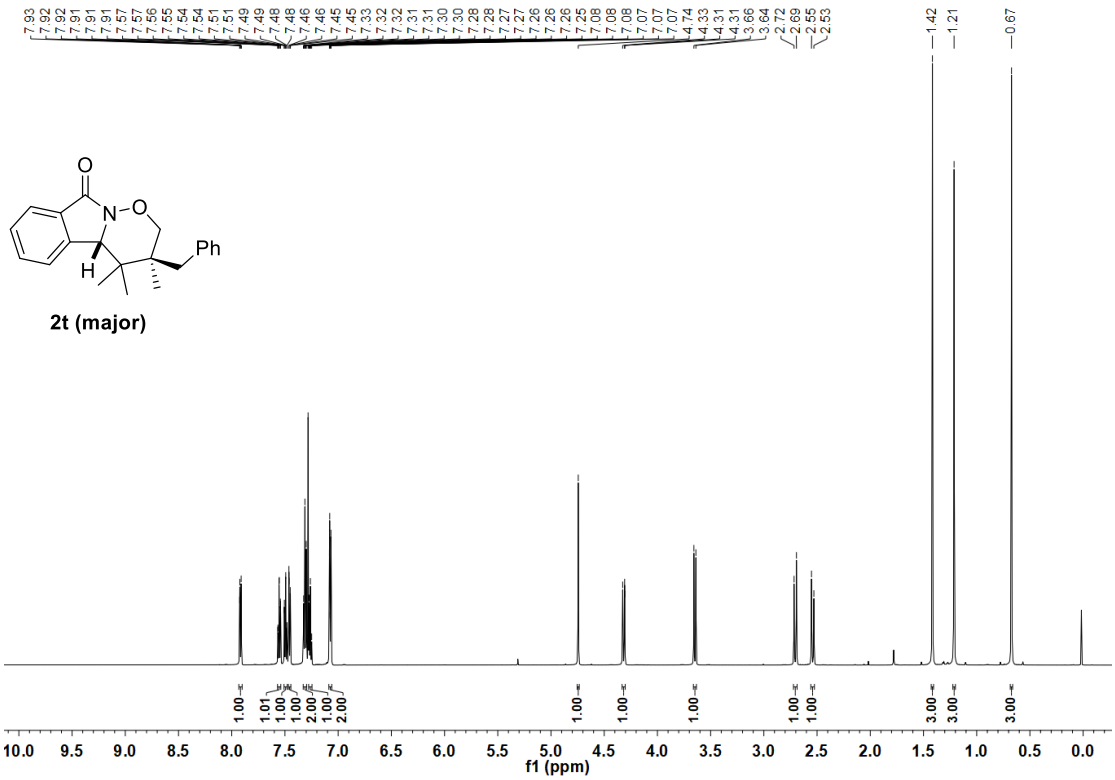


Figure S172. ^{1}H NMR spectra of **2t (major)** (600 MHz, $CDCl_3$)

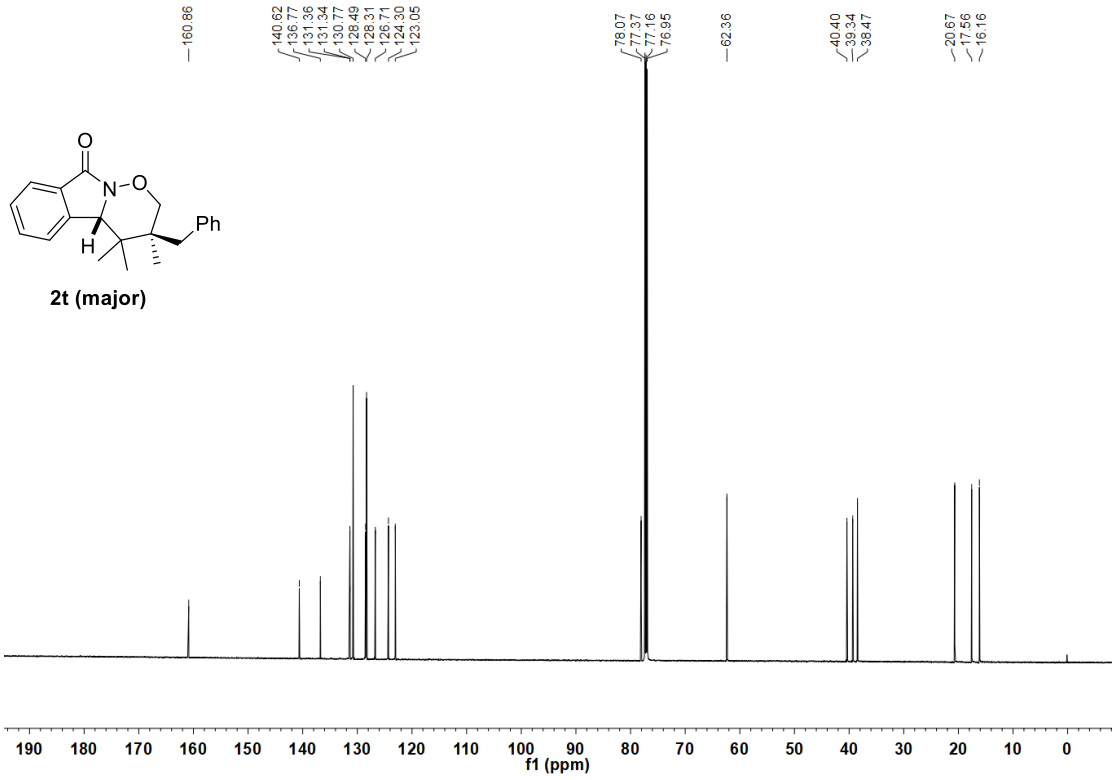


Figure S173. ^{13}C NMR spectra of **2t (major)** (151 MHz, $CDCl_3$)

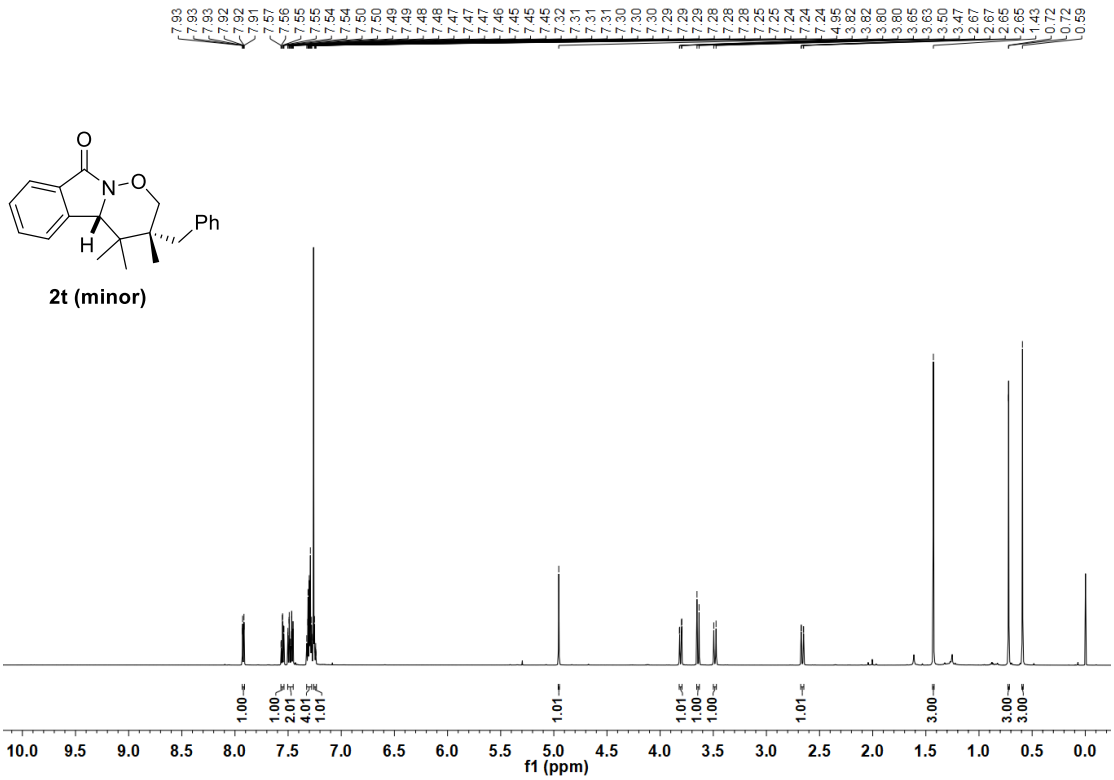


Figure S174. ^{1}H NMR spectra of **2t (minor)** (600 MHz, $CDCl_3$)

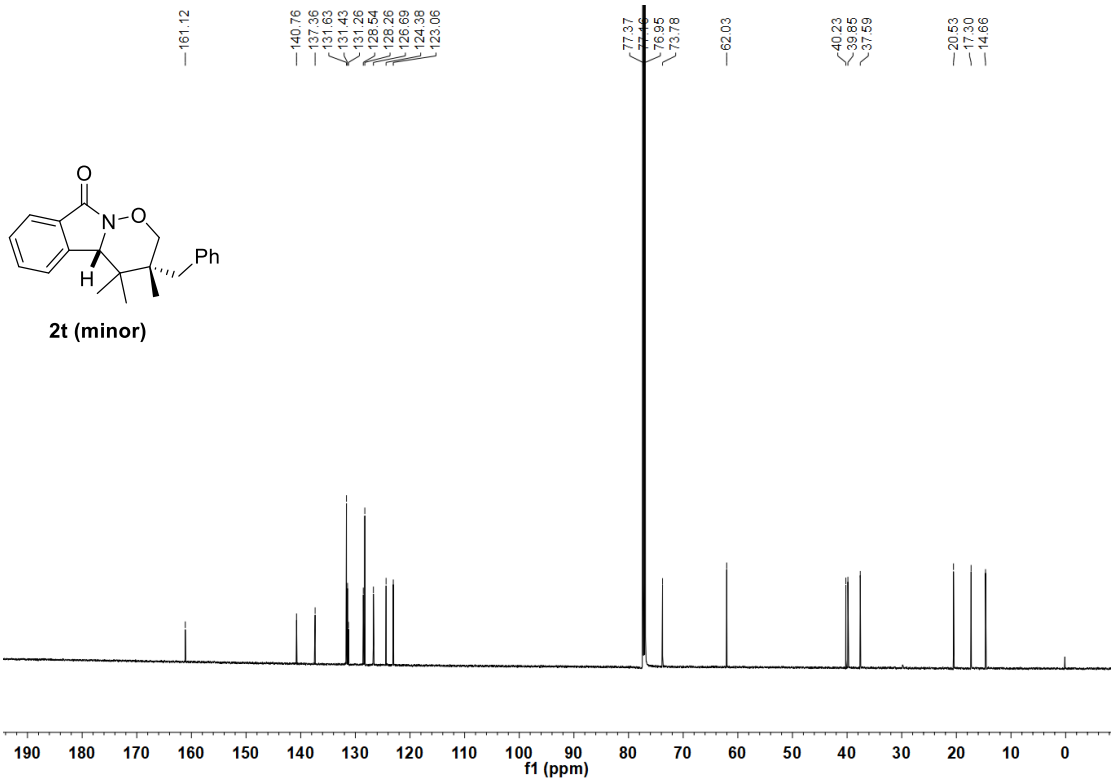


Figure S175. ^{13}C NMR spectra of **2t (minor)** (151 MHz, $CDCl_3$)

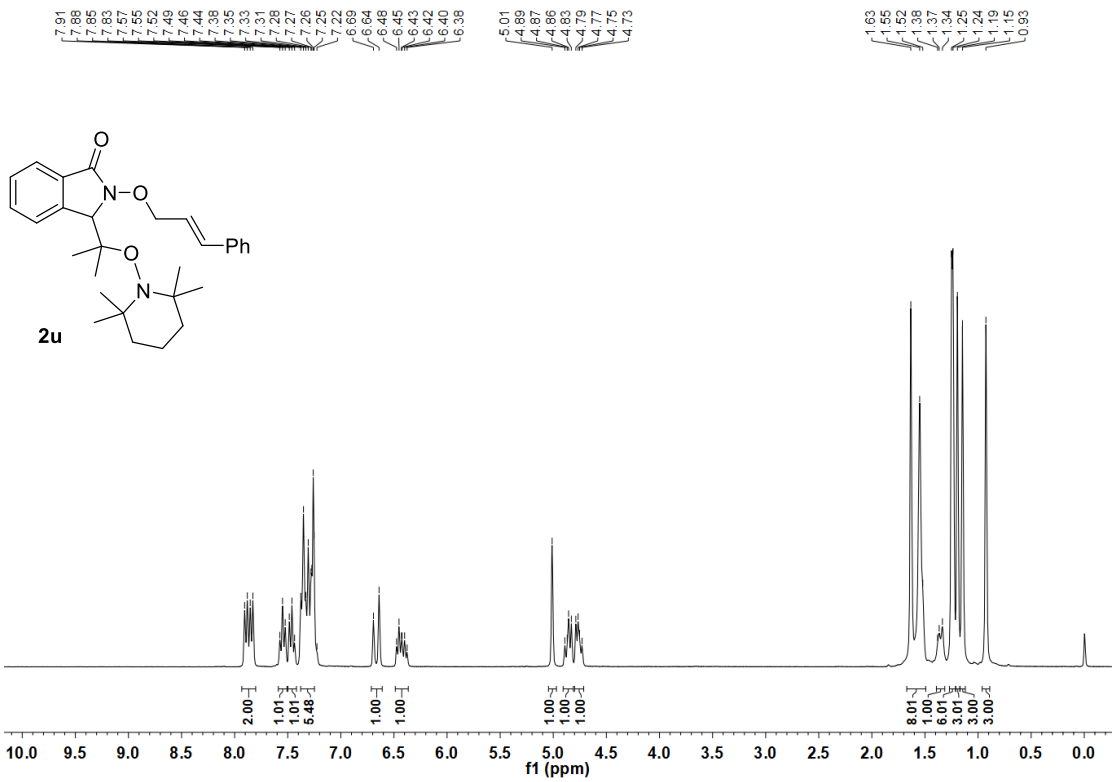


Figure S176. ^{1}H NMR spectra of **2u** (300 MHz, $CDCl_3$)

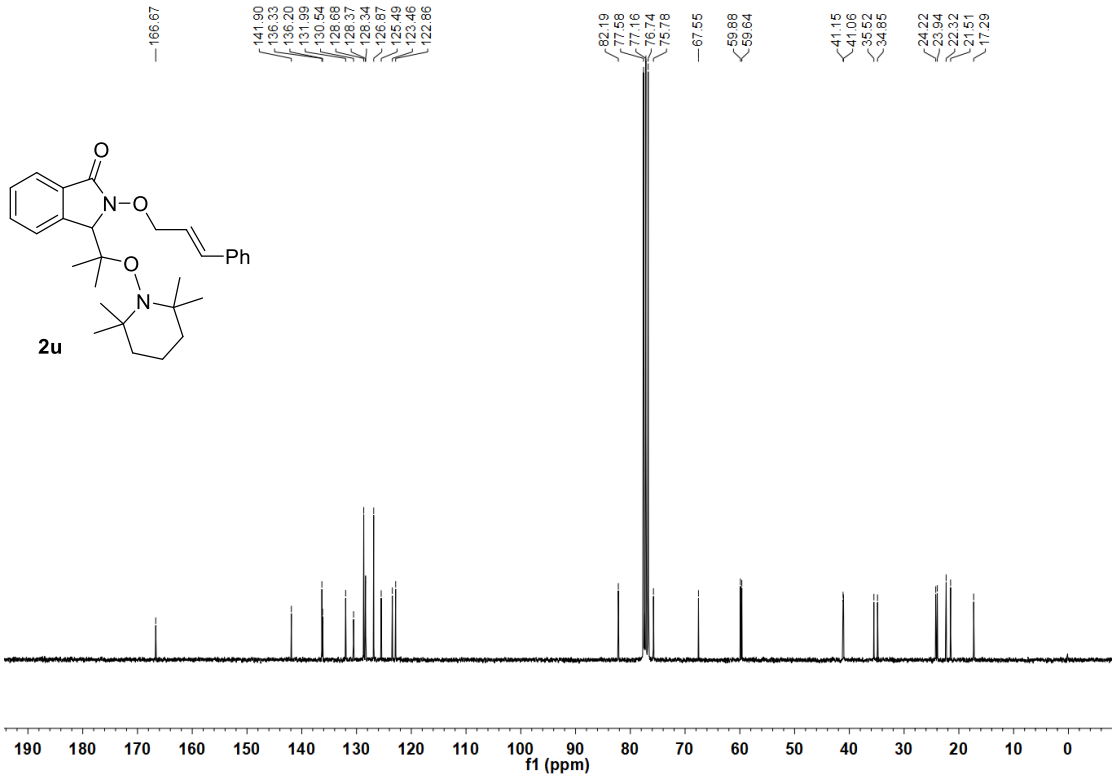


Figure S177. ^{13}C NMR spectra of **2u** (75 MHz, $CDCl_3$)

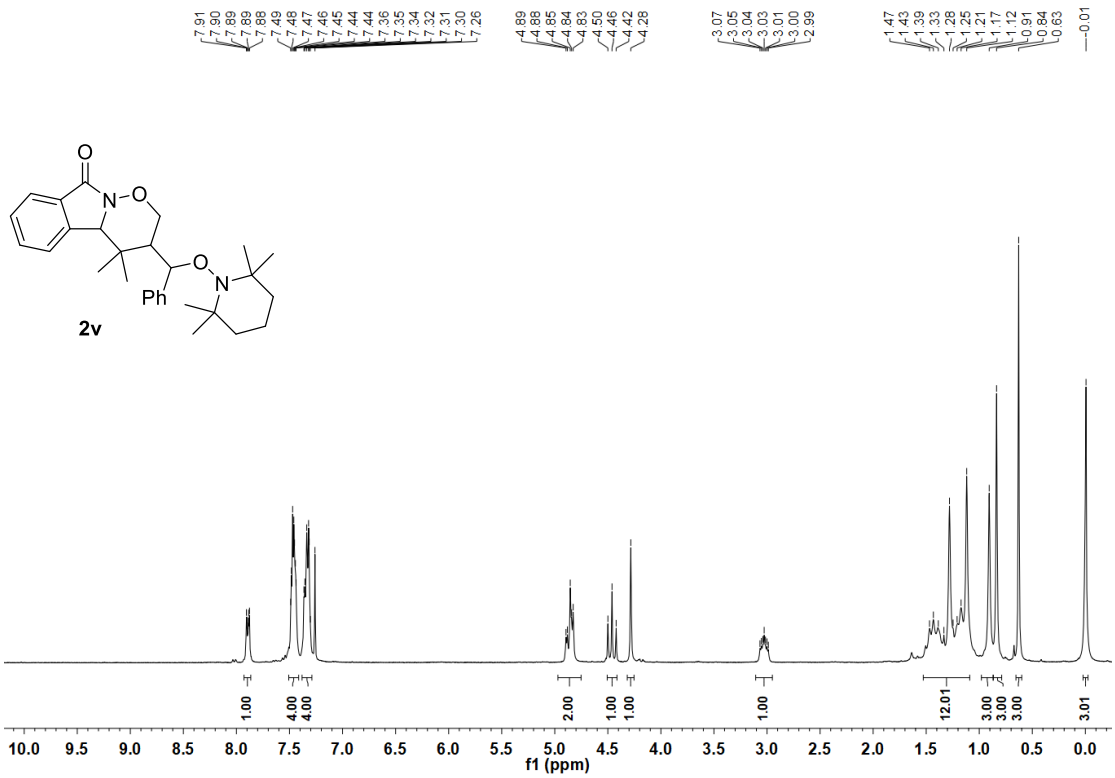


Figure S178. ^{1}H NMR spectra of **2v** (300 MHz, $CDCl_3$)

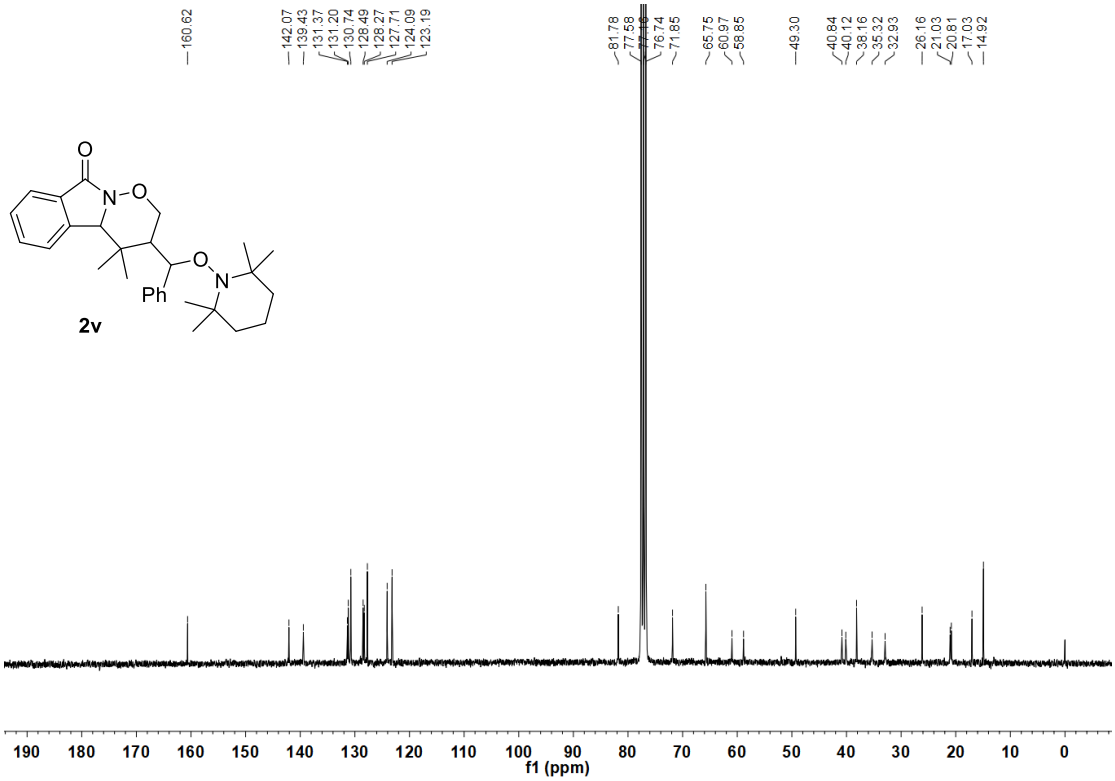


Figure S179. ^{13}C NMR spectra of **2v** (75 MHz, $CDCl_3$)

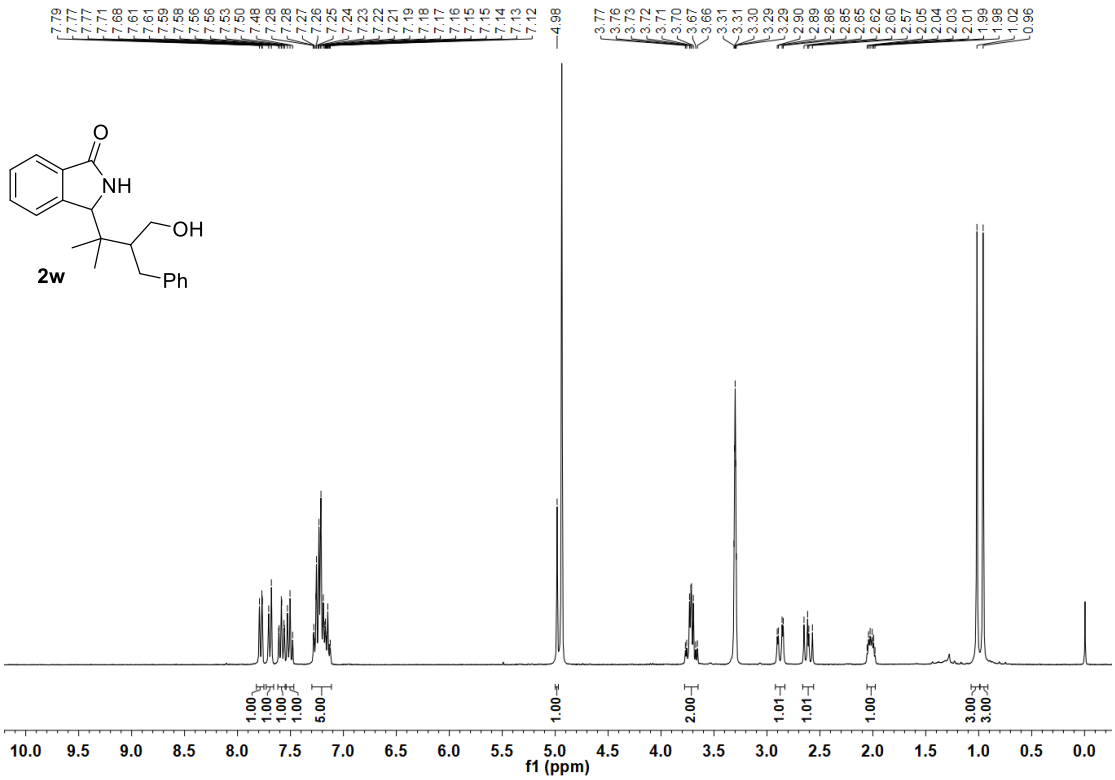


Figure S180. ^{1}H NMR spectra of **2w** (300 MHz, CD_3OD)

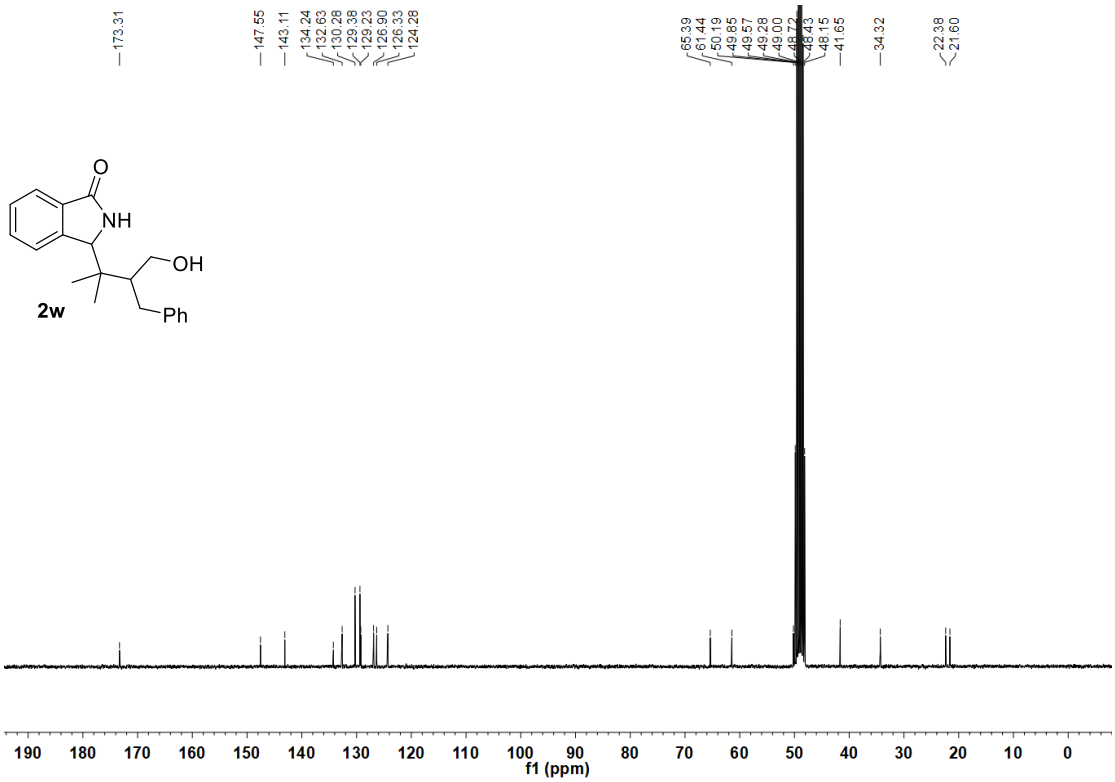


Figure S181. ^{13}C NMR spectra of **2w** (75 MHz, CD_3OD)

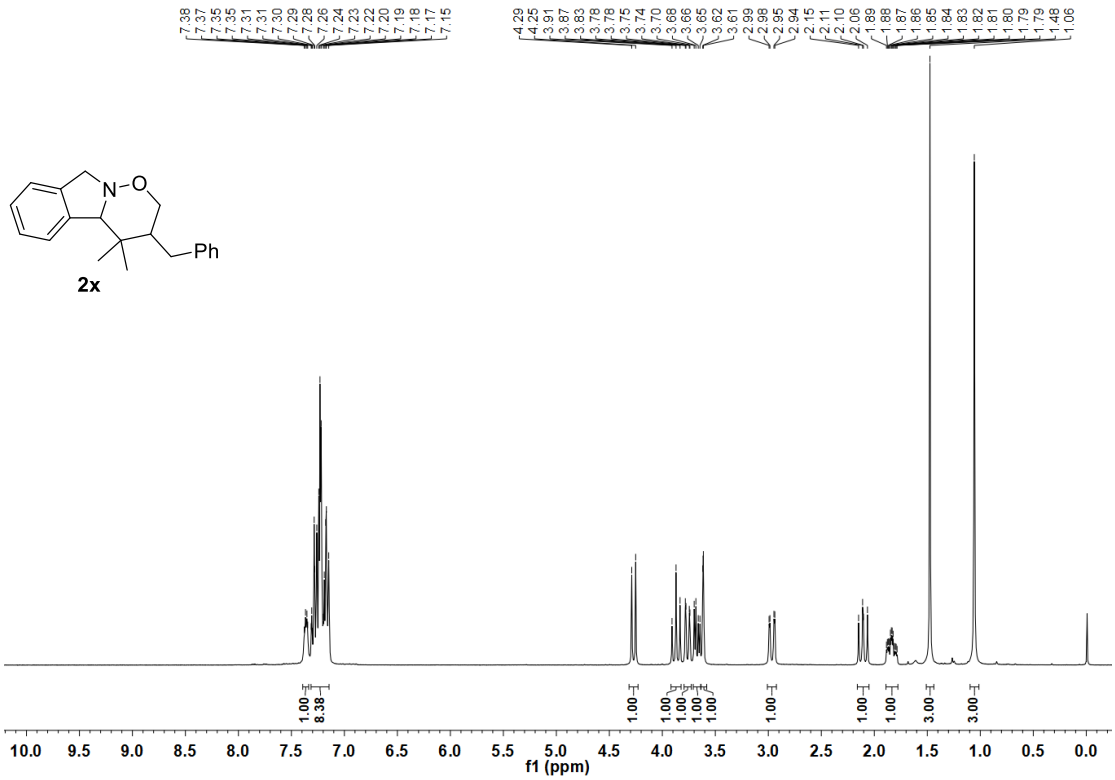


Figure S182. ^{1}H NMR spectra of **2x** (300 MHz, $CDCl_3$)

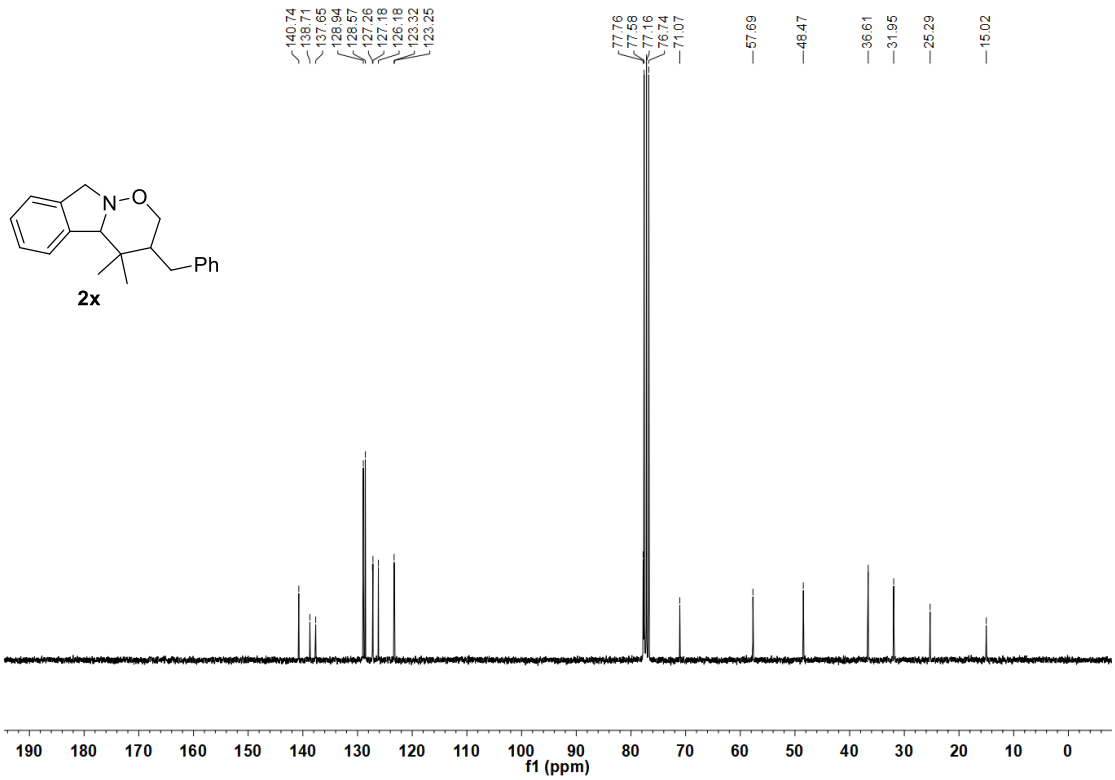


Figure S183. ^{13}C NMR spectra of **2x** (75 MHz, $CDCl_3$)

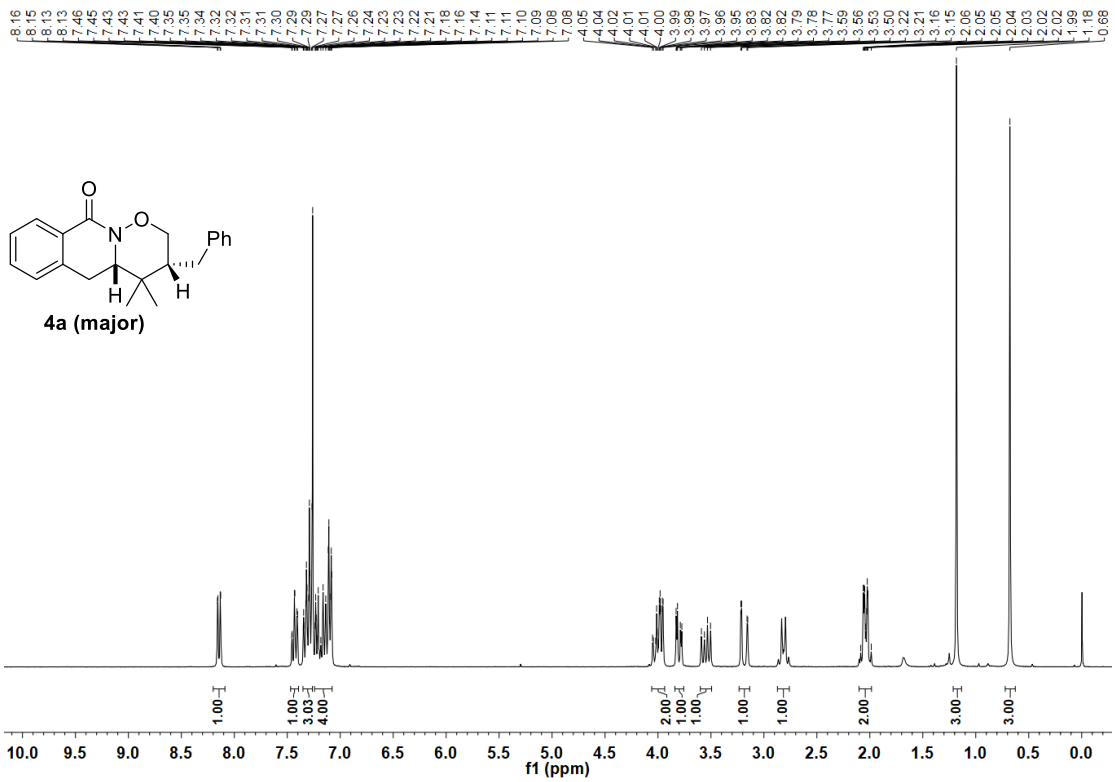


Figure S184. ^{1}H NMR spectra of **4a (major)** (300 MHz, $CDCl_3$)

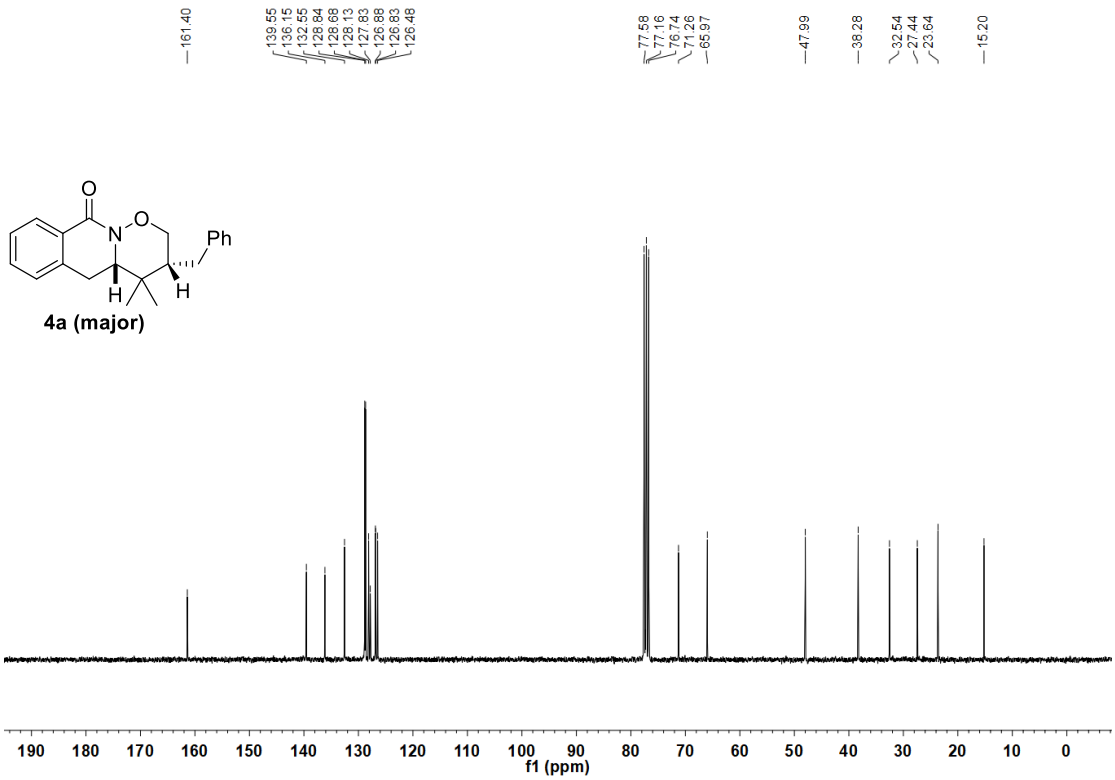


Figure S185. ^{13}C NMR spectra of **4a (major)** (75 MHz, $CDCl_3$)

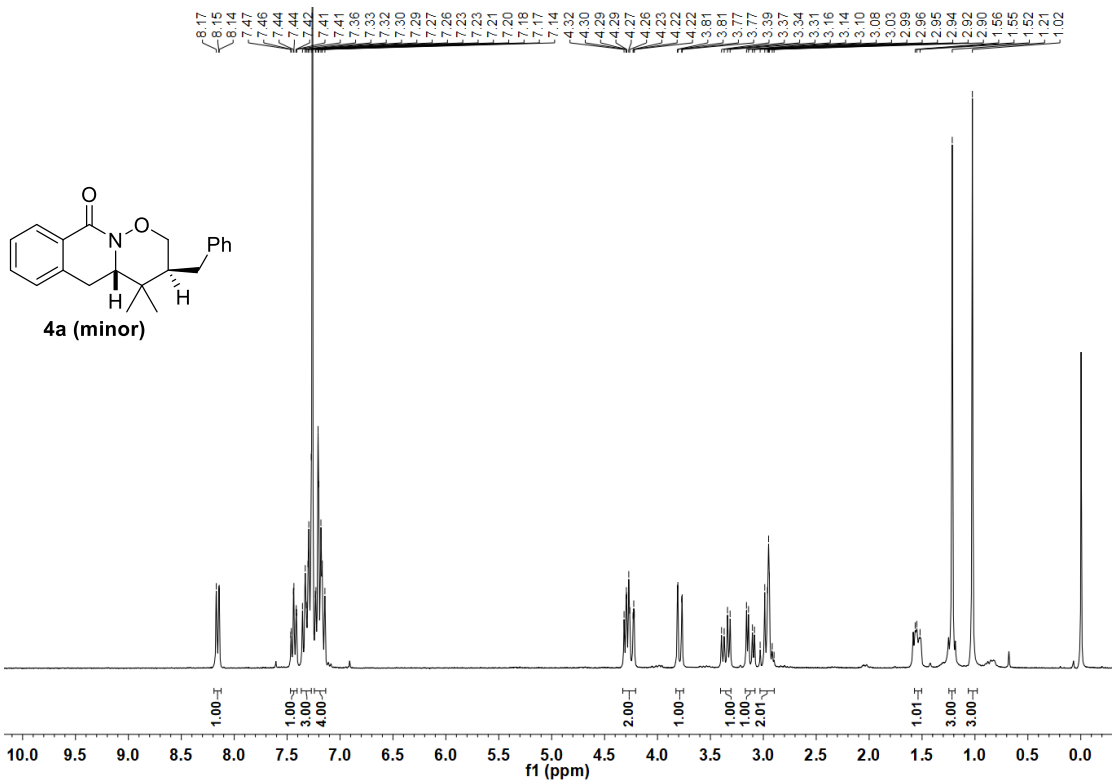


Figure S186. ^{1}H NMR spectra of **4a (minor)** (300 MHz, $CDCl_3$)

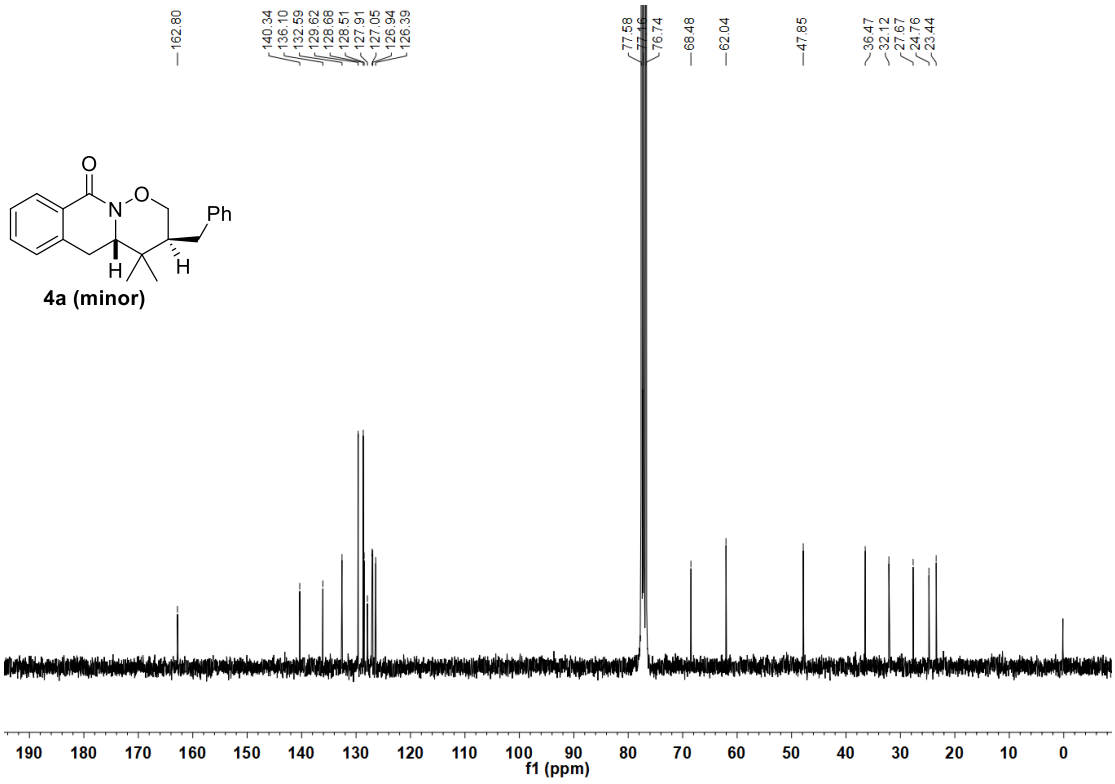


Figure S187. ^{13}C NMR spectra of **4a (minor)** (75 MHz, $CDCl_3$)

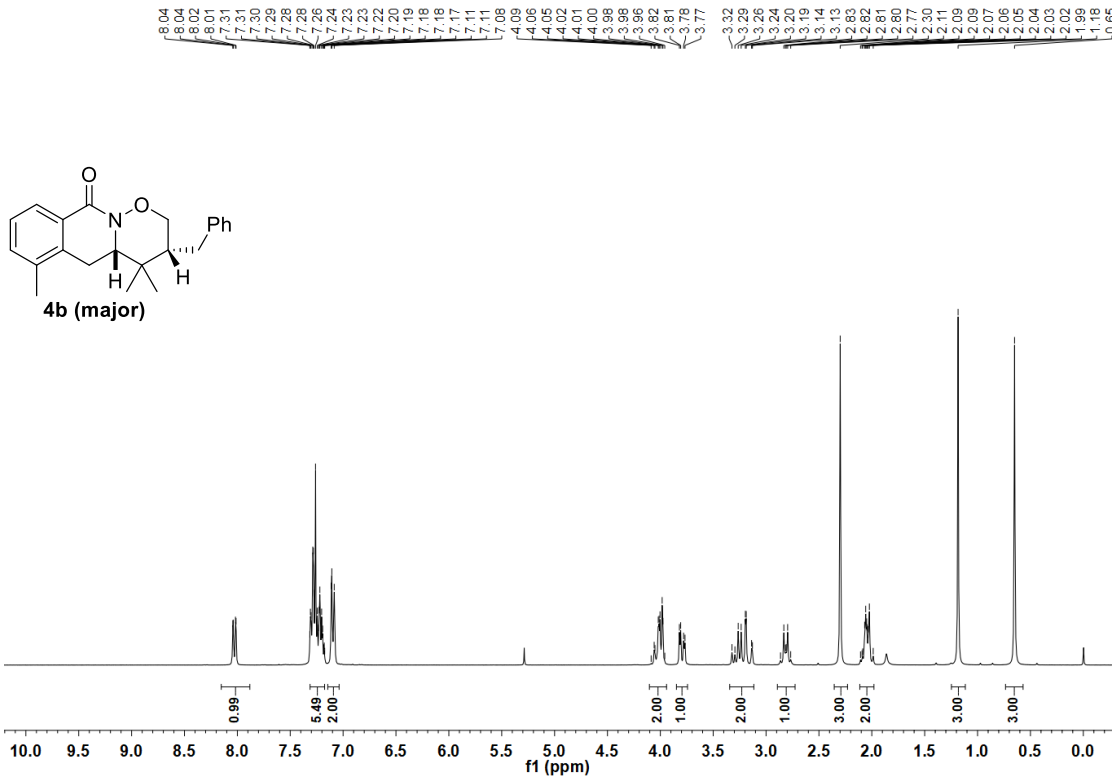


Figure S188. ^{1}H NMR spectra of **4b (major)** (300 MHz, $CDCl_3$)

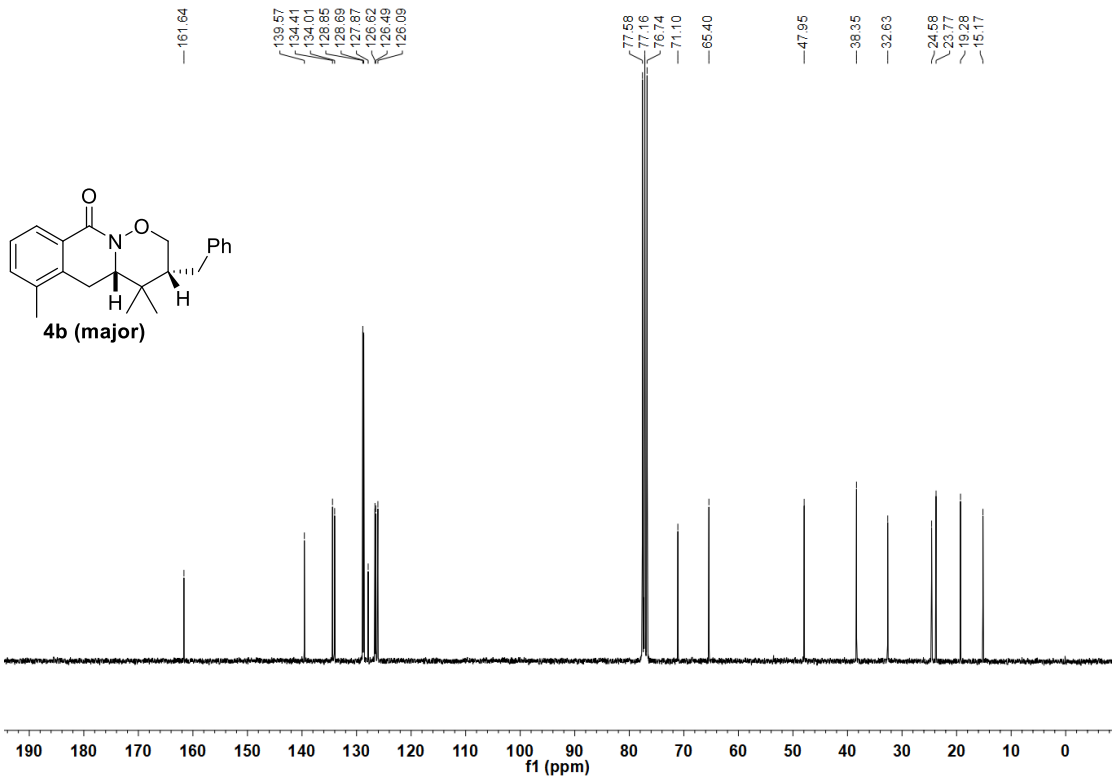


Figure S189. ^{13}C NMR spectra of **4b (major)** (75 MHz, $CDCl_3$)

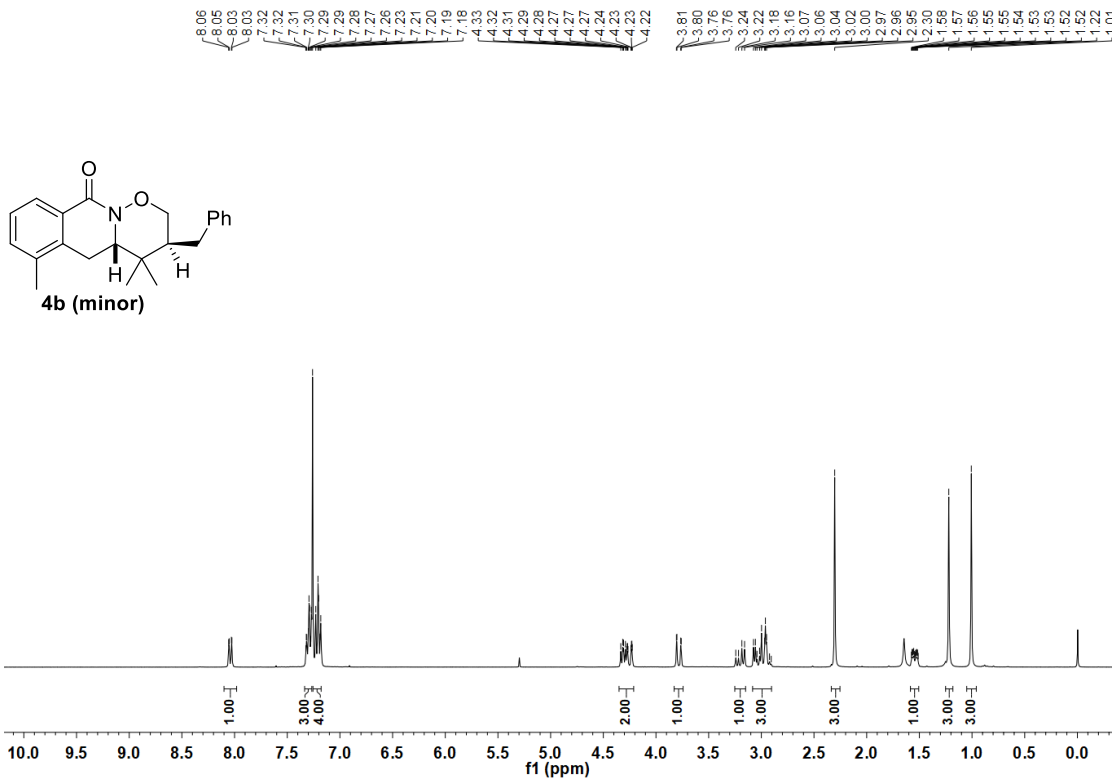


Figure S 190. ^{1}H NMR spectra of **4b (minor)** (300 MHz, $CDCl_3$)

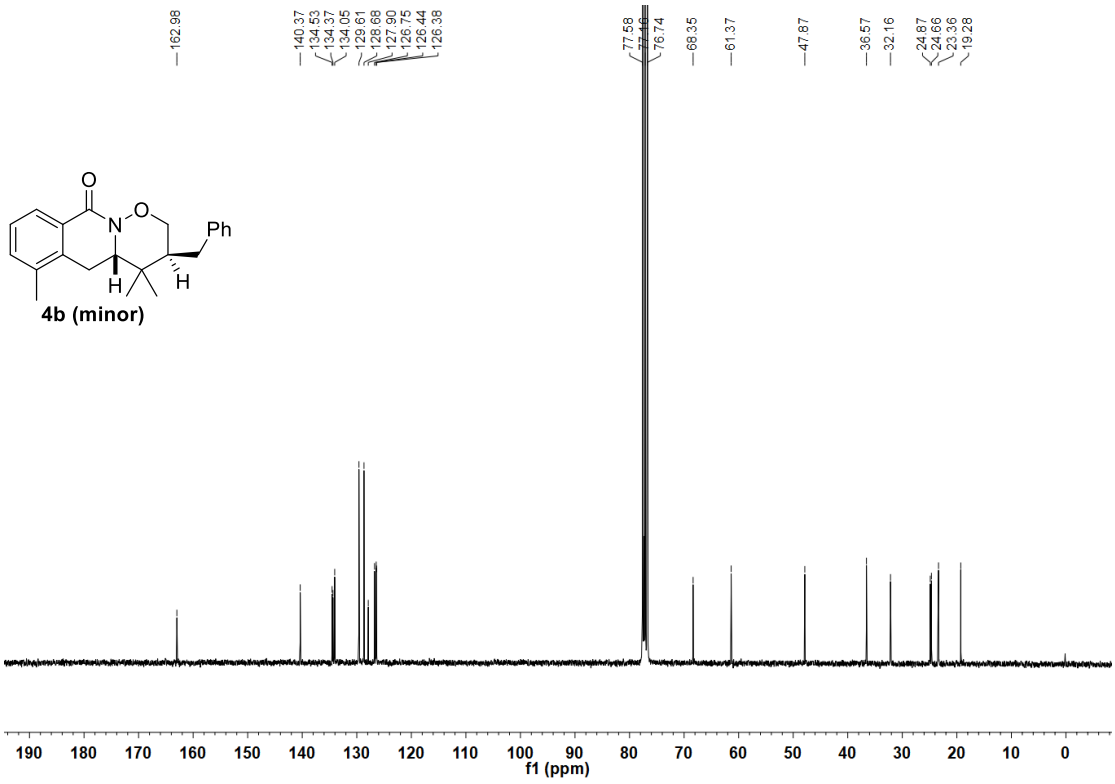


Figure S191. ^{13}C NMR spectra of **4b (minor)** (75 MHz, $CDCl_3$)

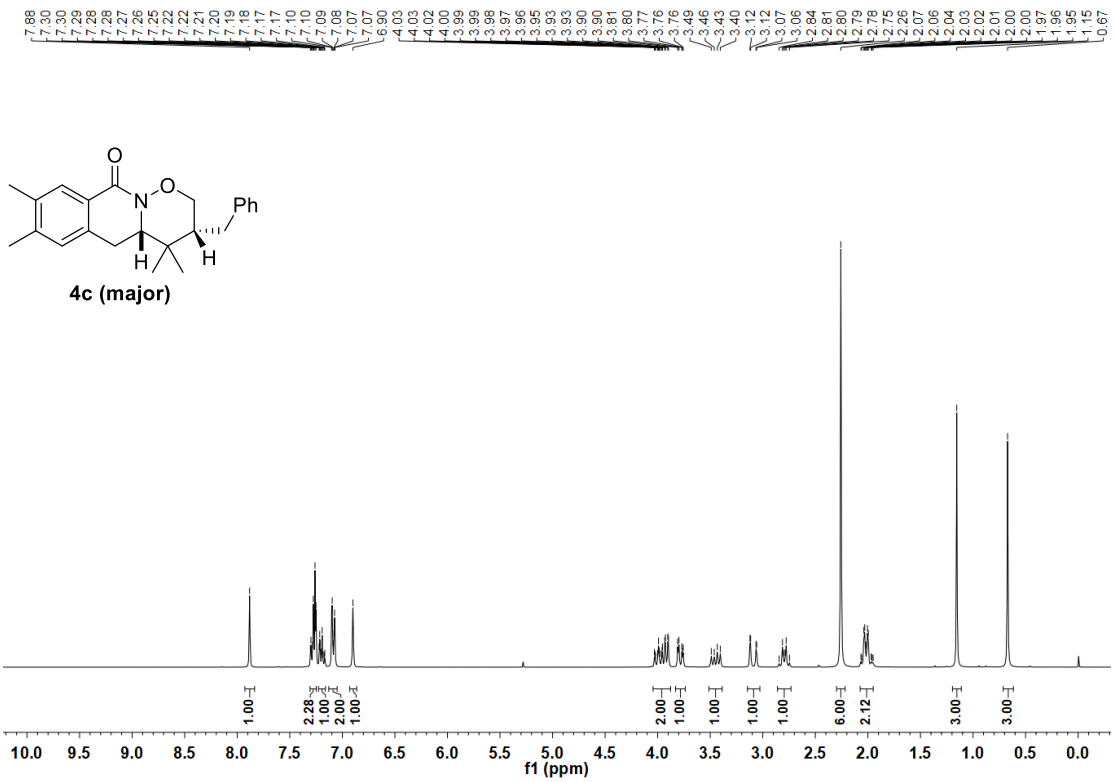


Figure S192. ^{1}H NMR spectra of **4c (major)** (300 MHz, $CDCl_3$)

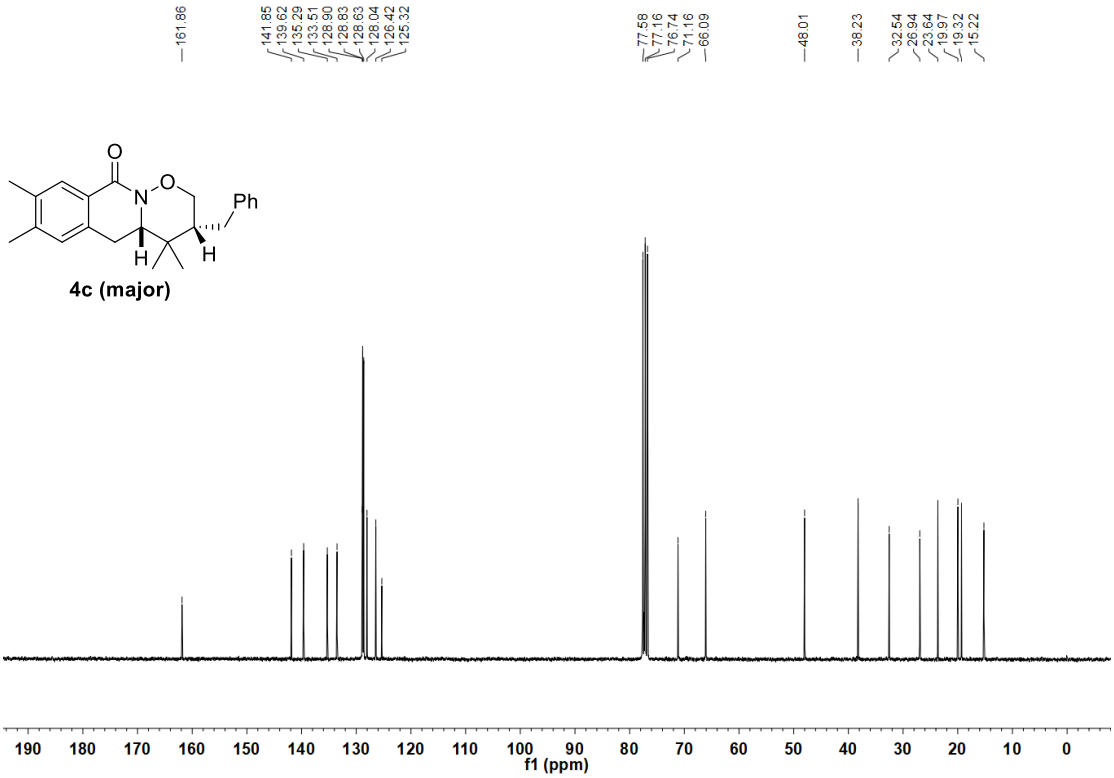


Figure S193. ^{13}C NMR spectra of **4c (major)** (75 MHz, $CDCl_3$)

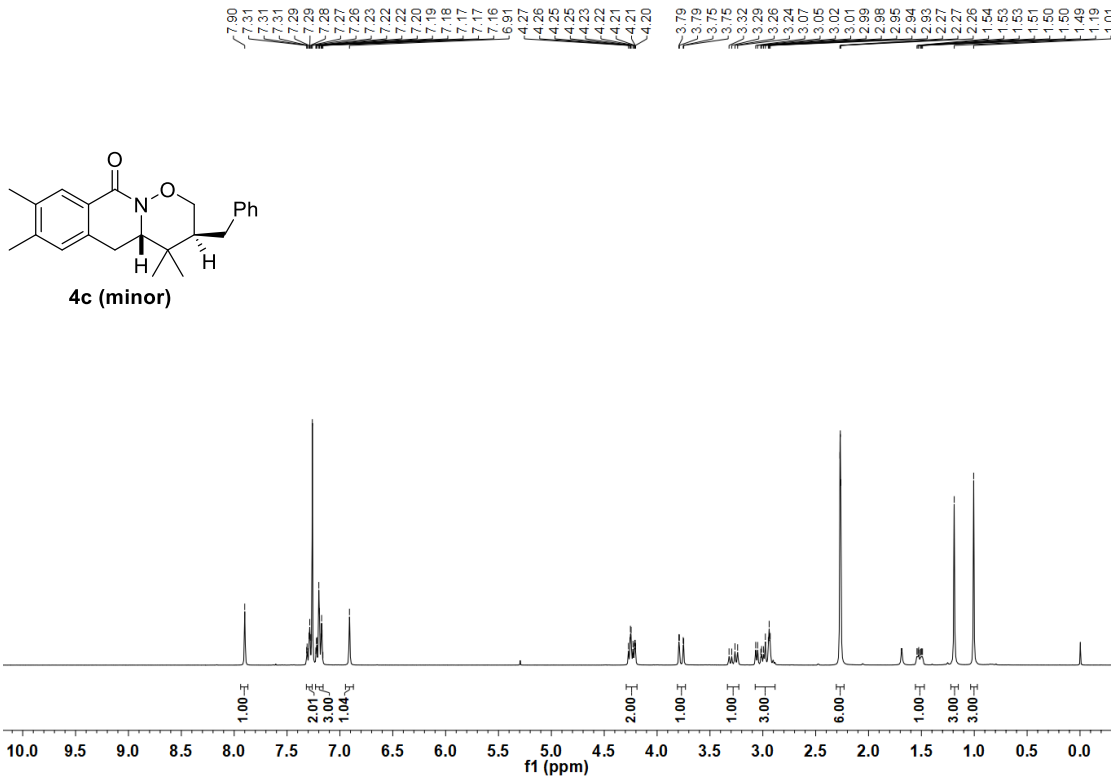


Figure S194. ^{1}H NMR spectra of **4c (minor)** (300 MHz, $CDCl_3$)

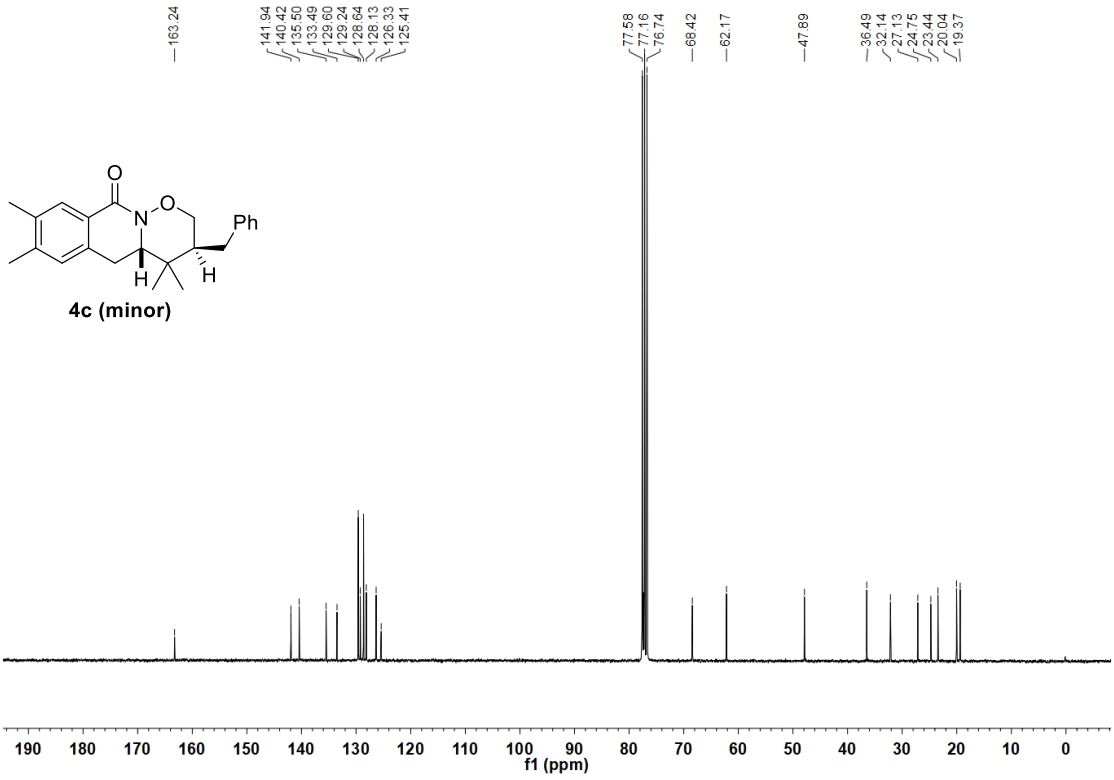


Figure S195. ^{13}C NMR spectra of **4c (minor)** (75 MHz, $CDCl_3$)

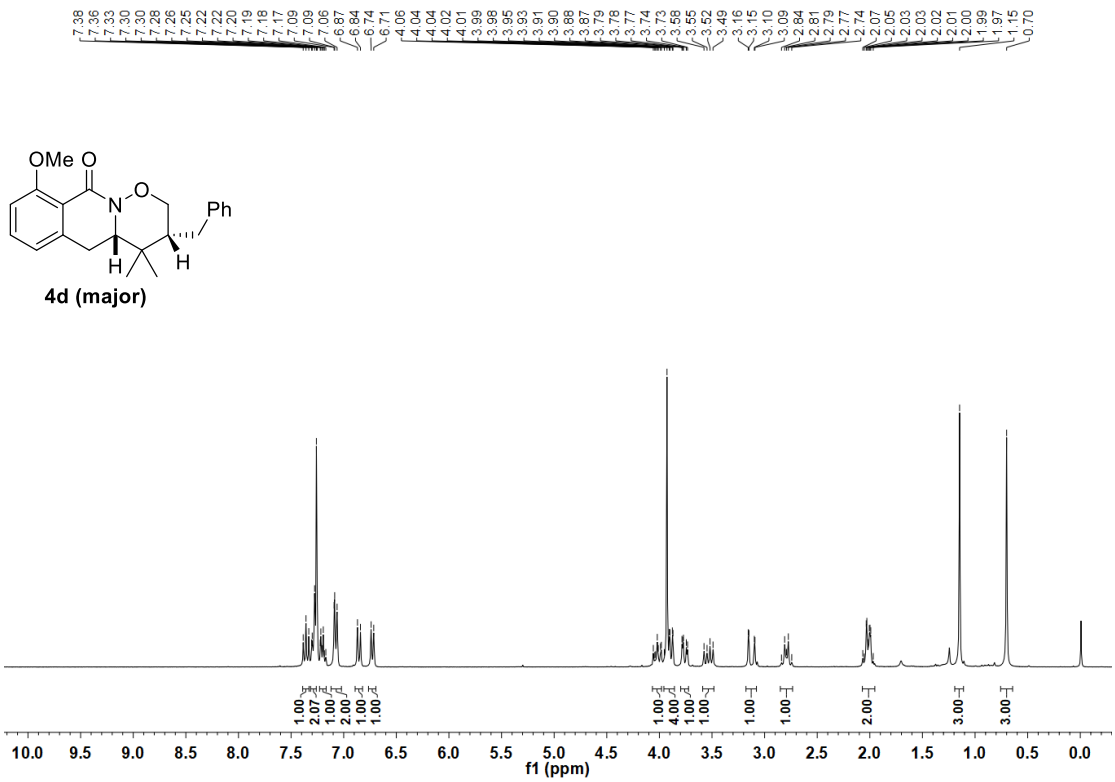


Figure S196. ^{1}H NMR spectra of **4d (major)** (300 MHz, $CDCl_3$)

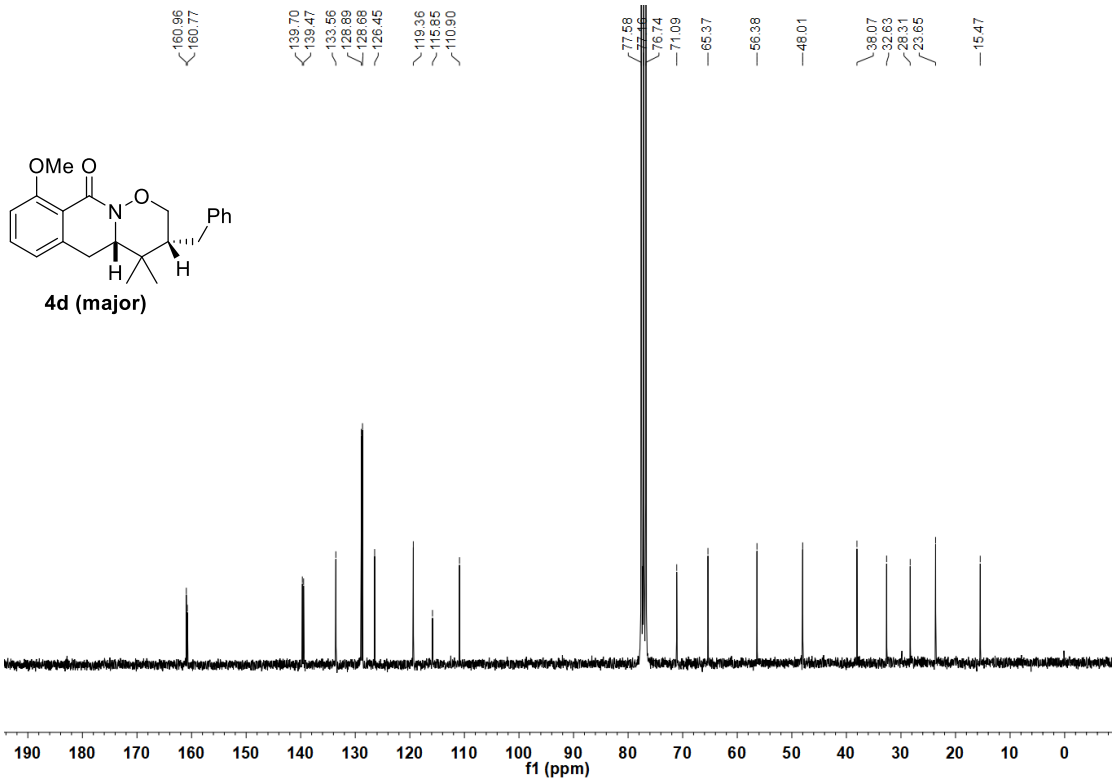


Figure S197. ^{13}C NMR spectra of **4d (major)** (75 MHz, $CDCl_3$)

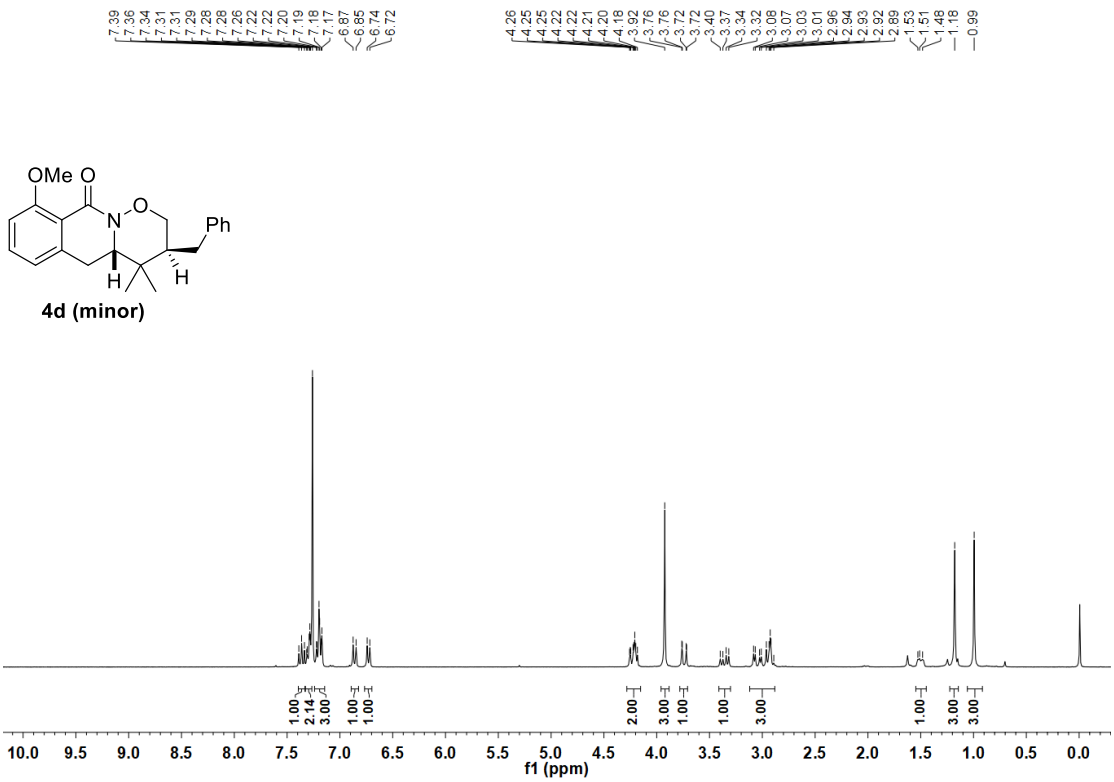


Figure S198. ^{1}H NMR spectra of **4d (minor)** (300 MHz, $CDCl_3$)

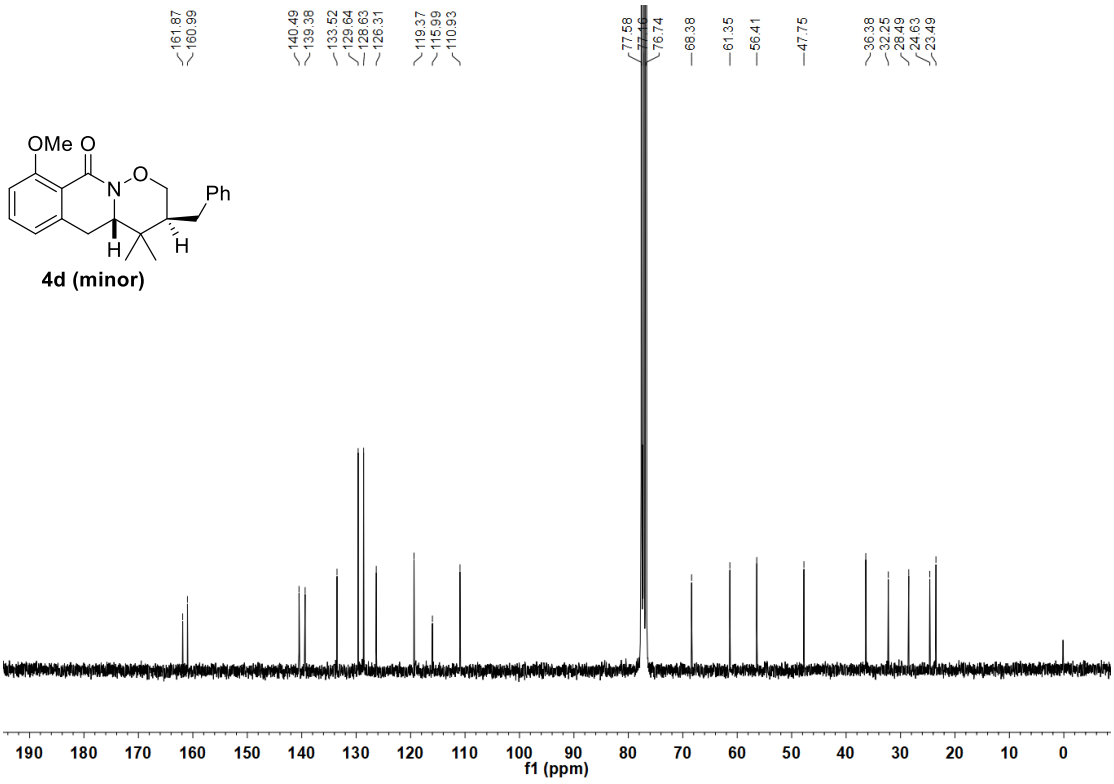


Figure S199. ^{13}C NMR spectra of **4d (minor)** (75 MHz, $CDCl_3$)

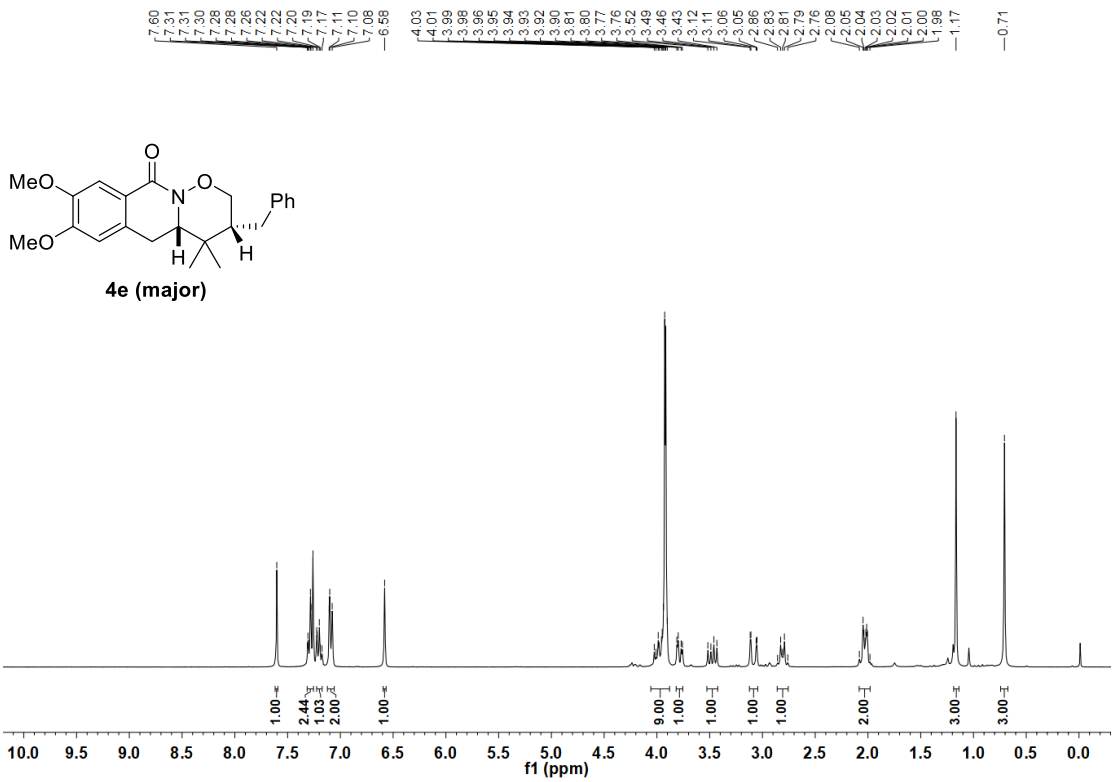


Figure S200. ^{1}H NMR spectra of **4e (major)** (300 MHz, $CDCl_3$)

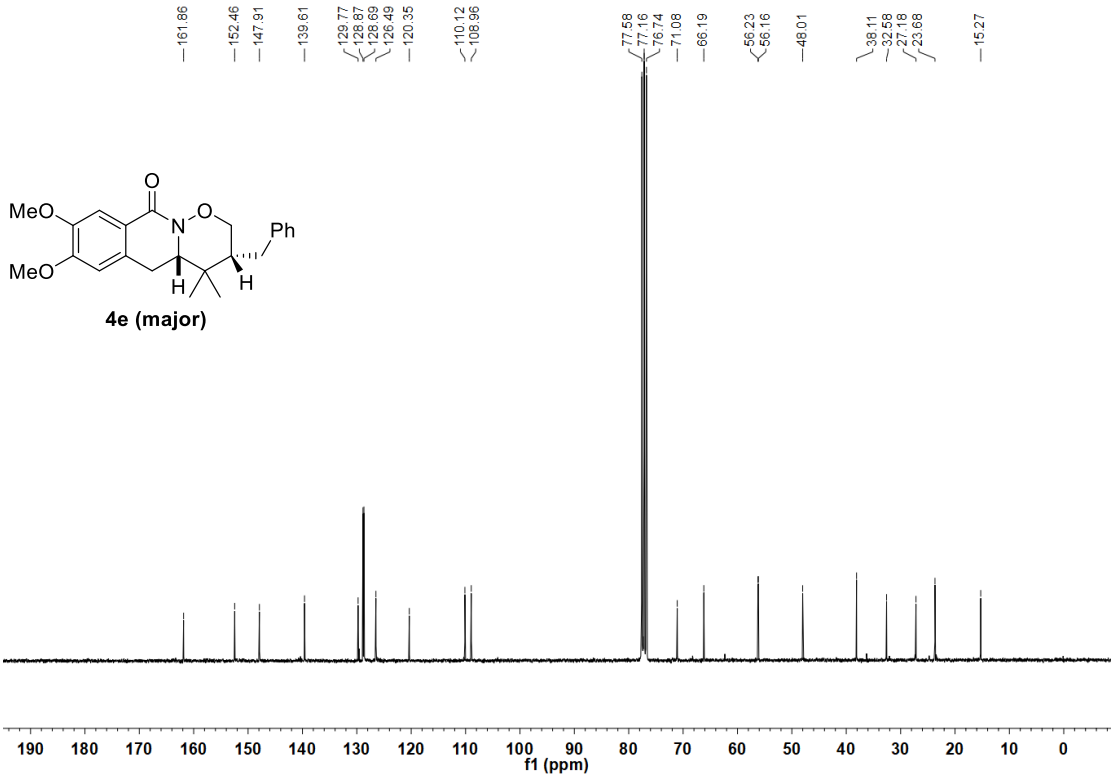


Figure S201. ^{13}C NMR spectra of **4e (major)** (75 MHz, $CDCl_3$)

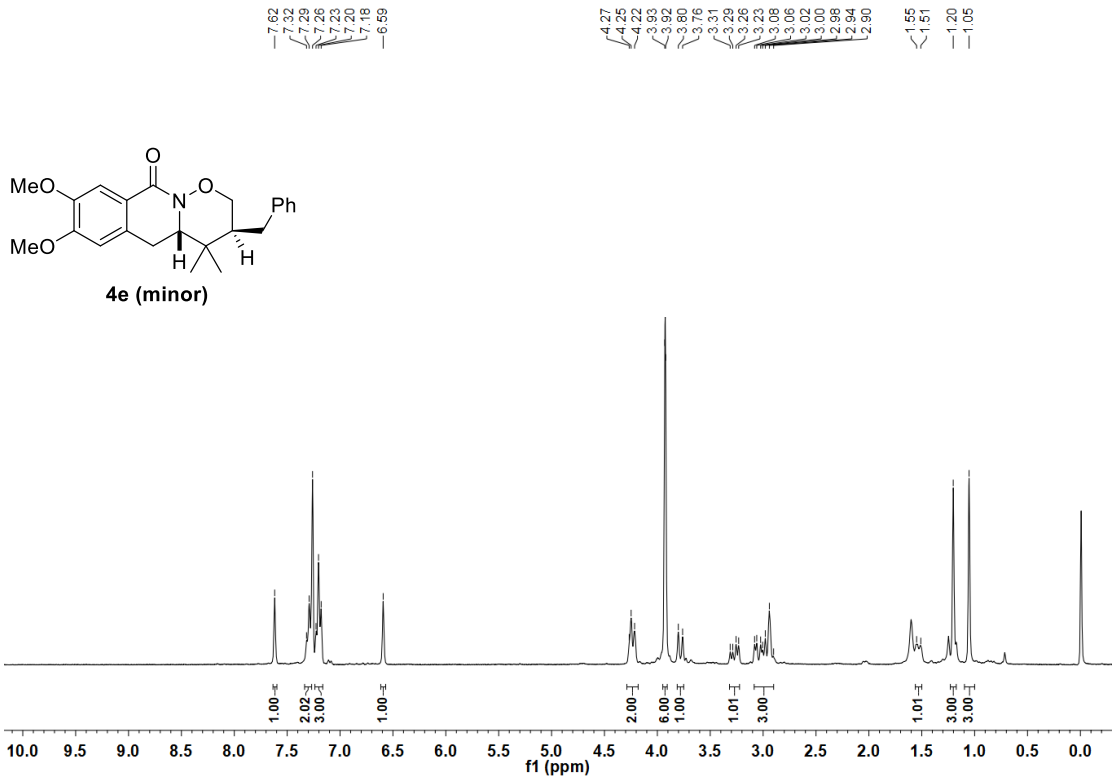


Figure S202. ^{1}H NMR spectra of **4e (minor)** (600 MHz, $CDCl_3$)

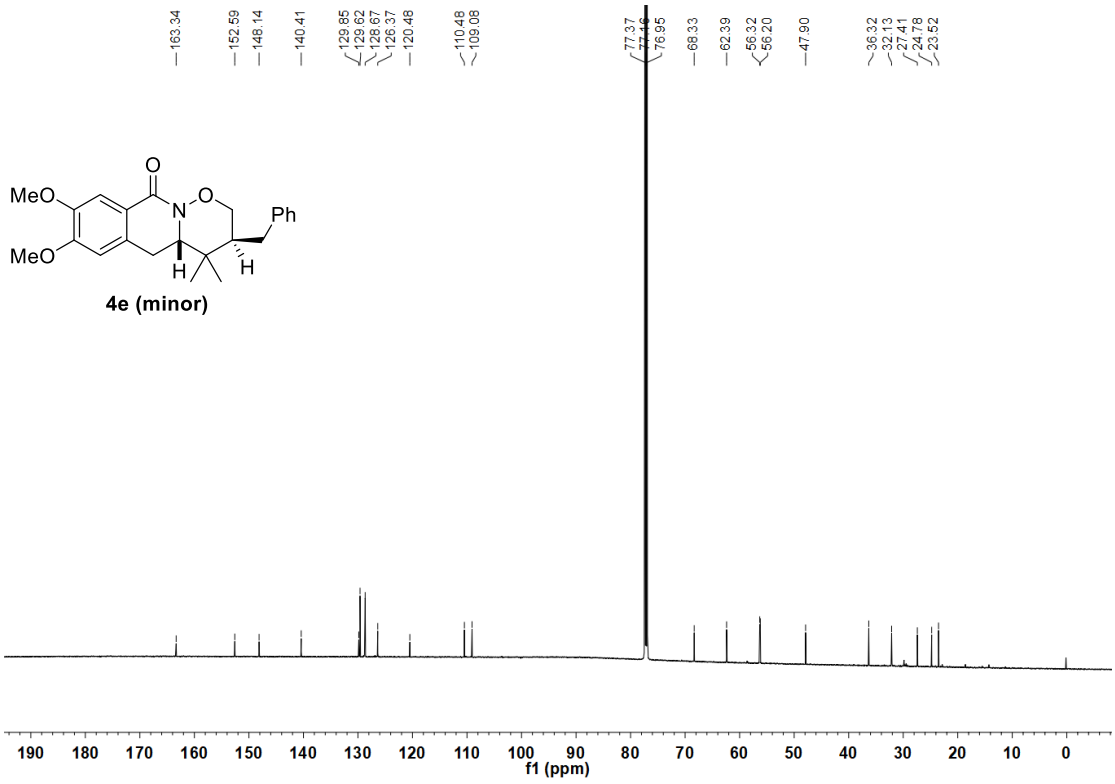


Figure S203. ^{13}C NMR spectra of **4e (minor)** (151 MHz, $CDCl_3$)

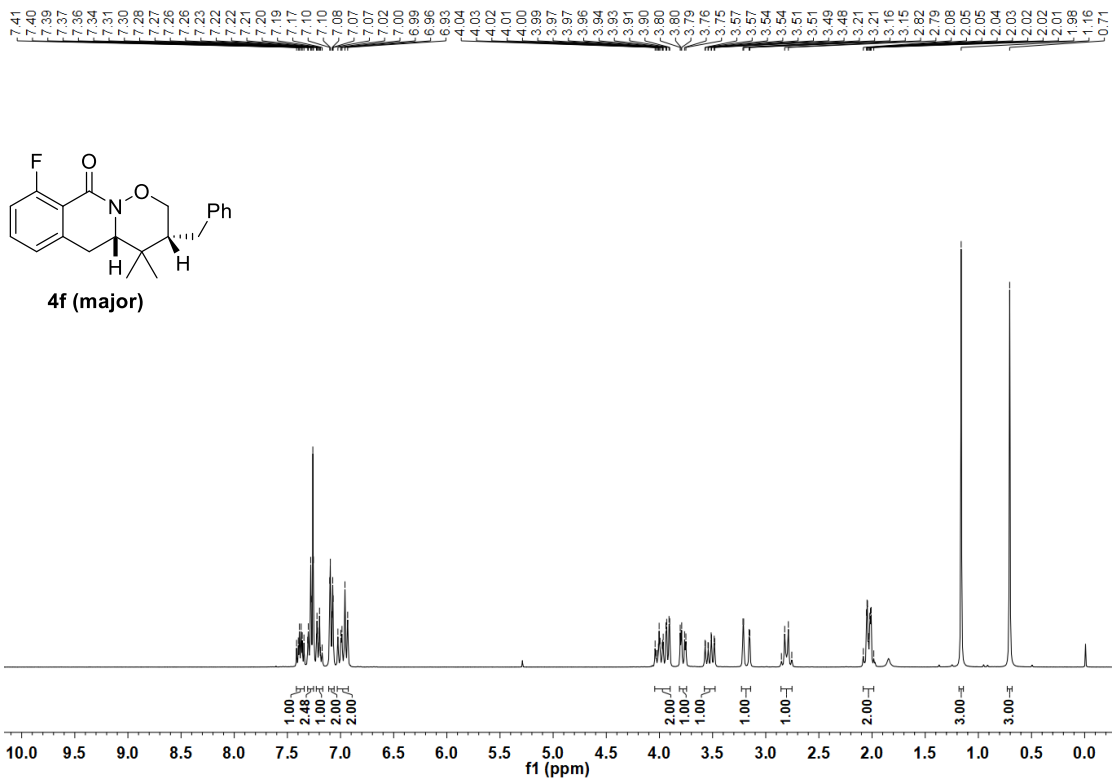


Figure S204. ^{1}H NMR spectra of **4f (major)** (300 MHz, $CDCl_3$)

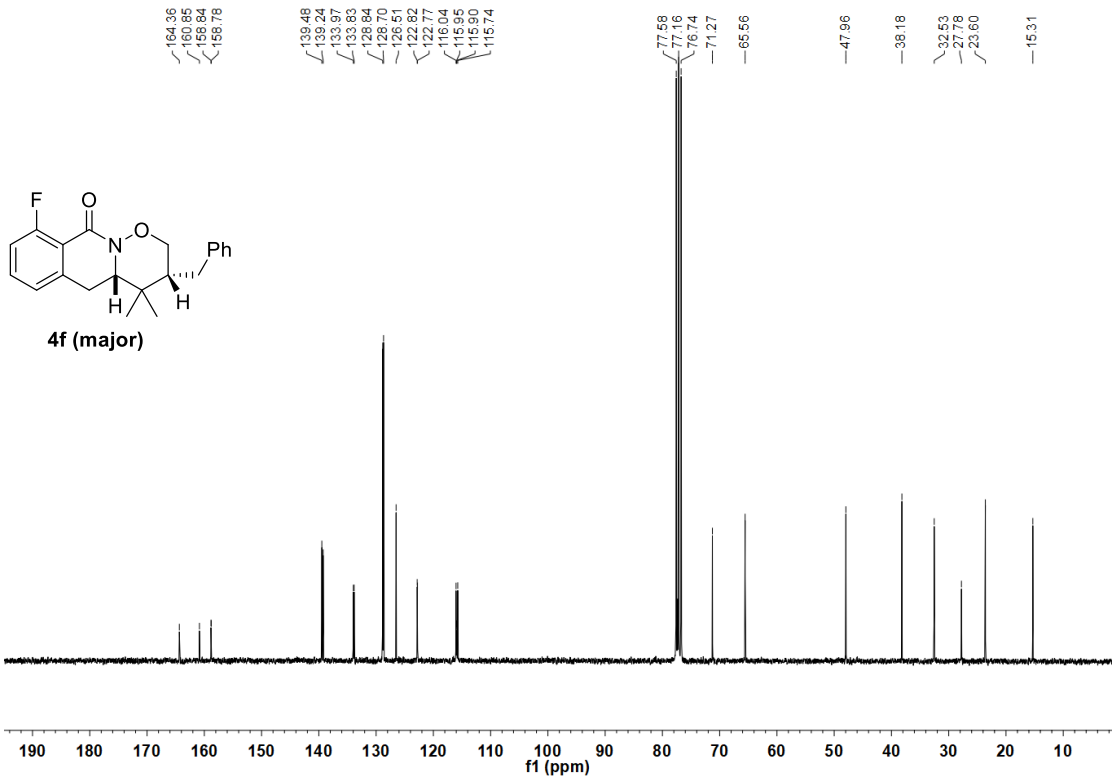


Figure S205. ^{13}C NMR spectra of **4f (major)** (75 MHz, $CDCl_3$)

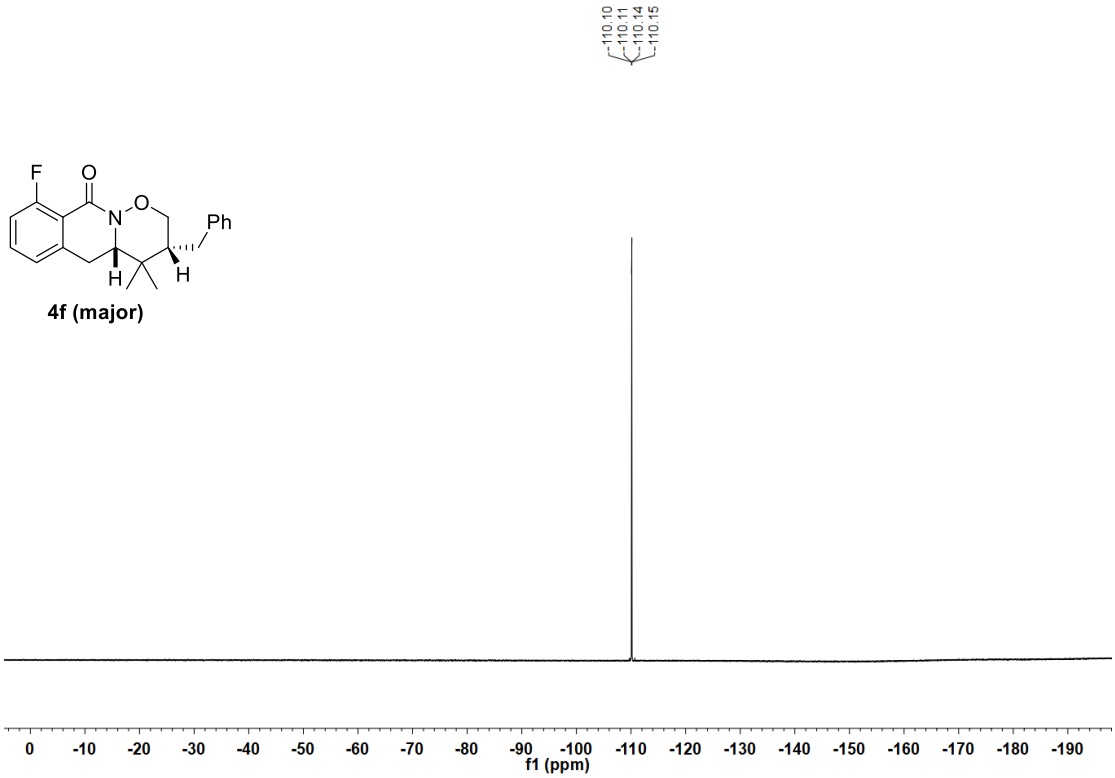


Figure S206. ^{19}F NMR spectra of **4f (major)** (282 MHz, $CDCl_3$)

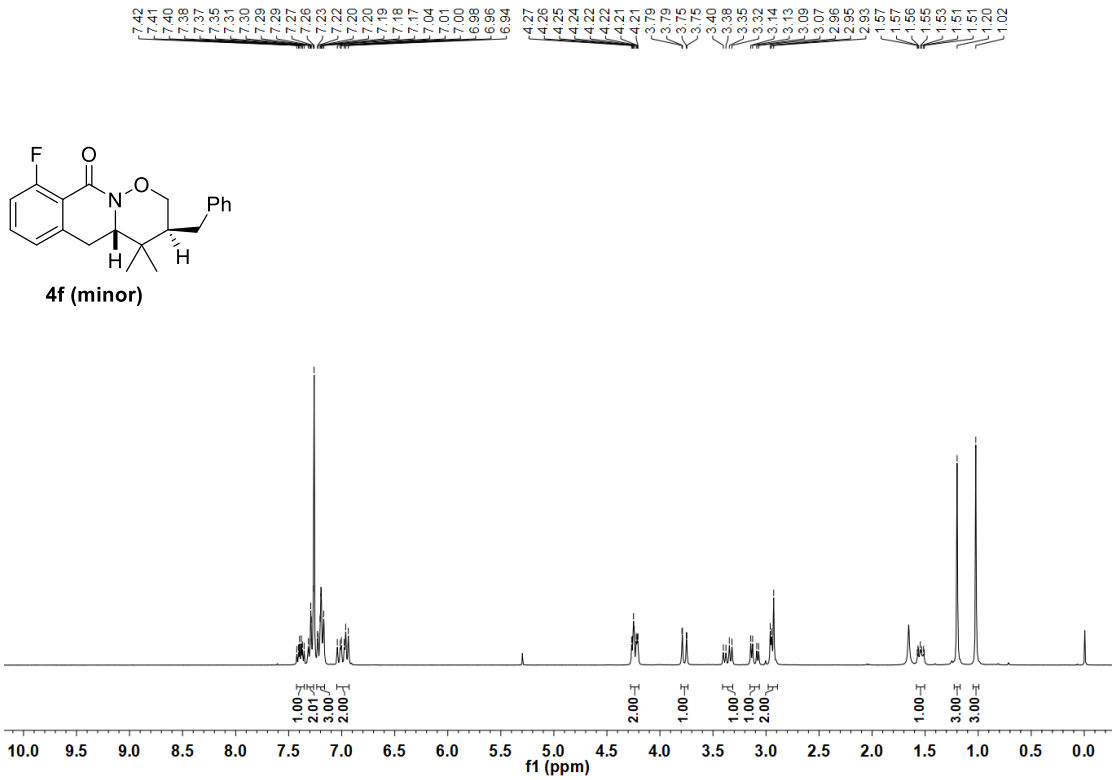


Figure S207. ^{1}H NMR spectra of **4f (minor)** (300 MHz, $CDCl_3$)

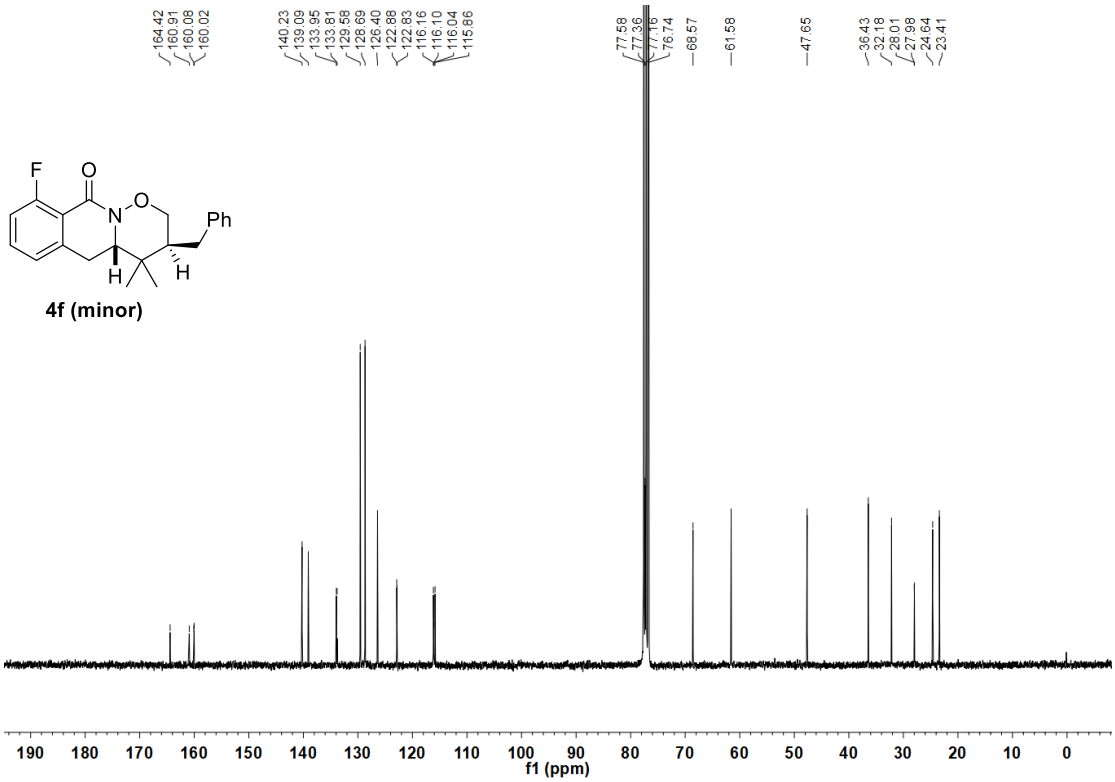


Figure S208. ^{13}C NMR spectra of **4f (minor)** (75 MHz, $CDCl_3$)

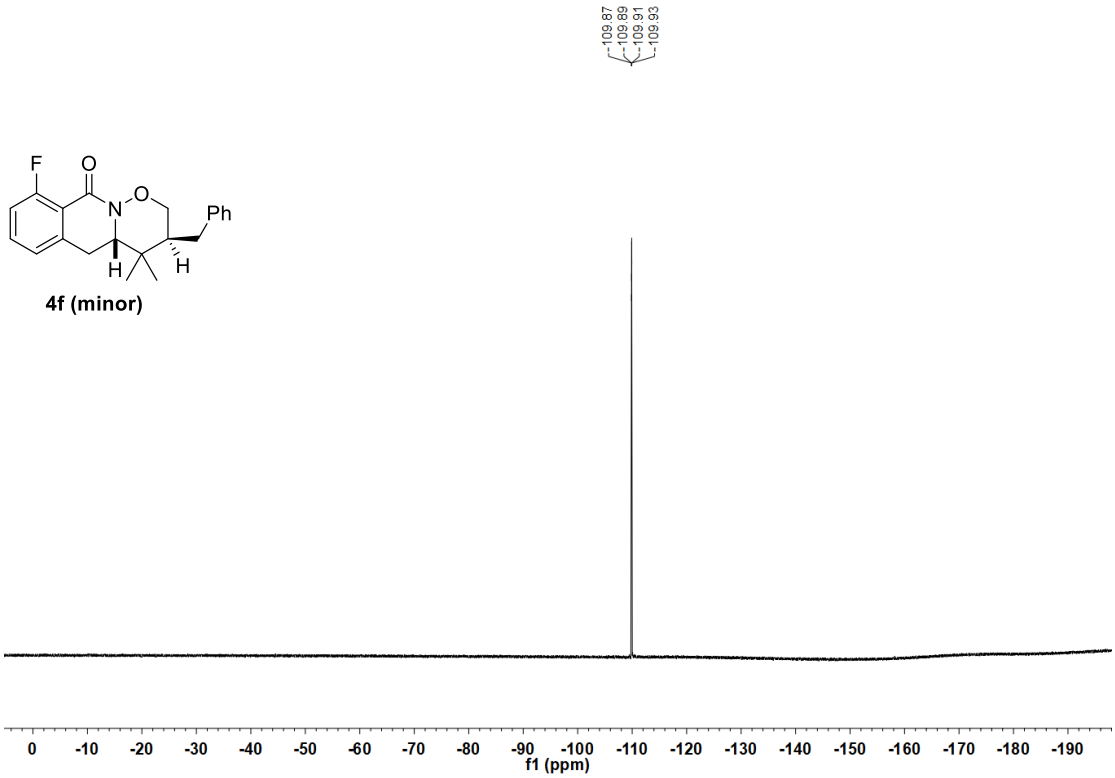


Figure S209. ^{19}F NMR spectra of **4f (minor)** (282 MHz, $CDCl_3$)

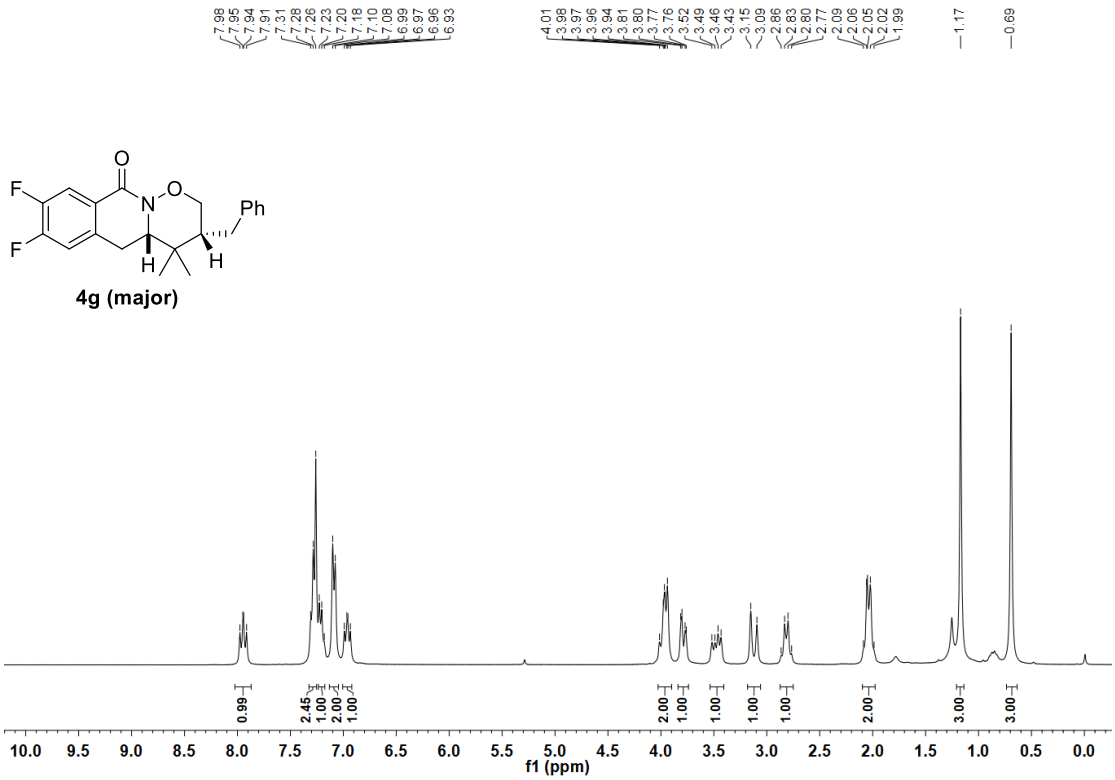


Figure S210. ^{1}H NMR spectra of **4g (major)** (300 MHz, $CDCl_3$)

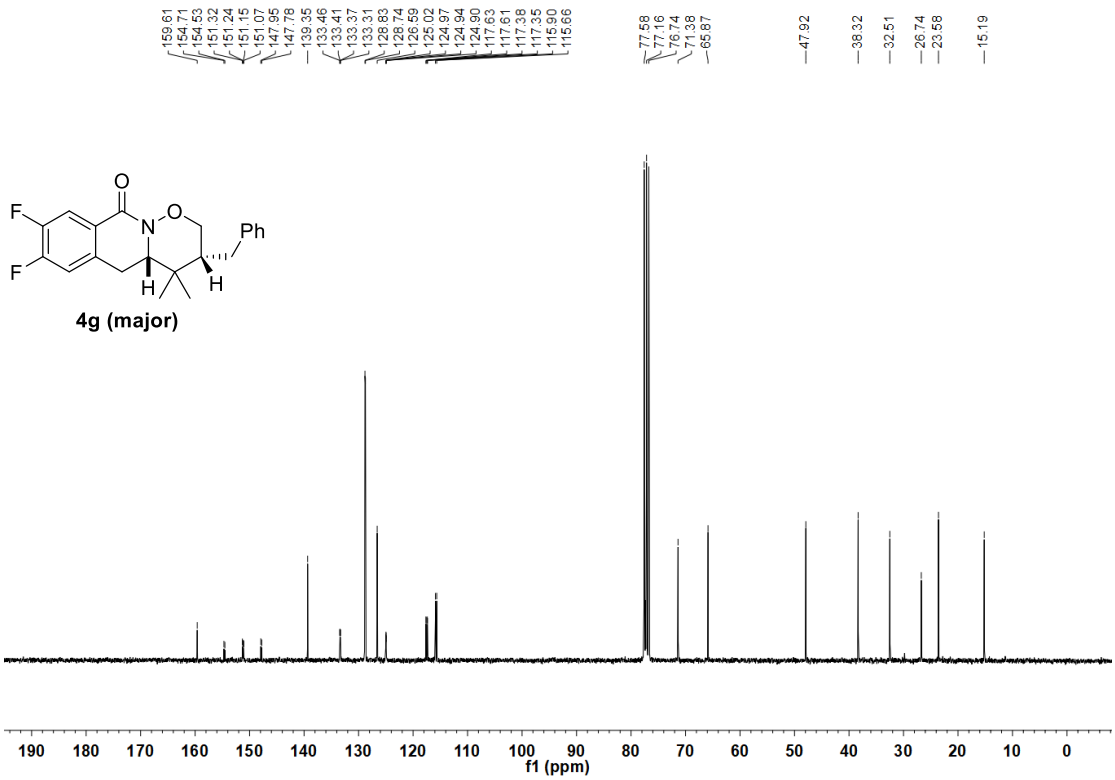


Figure S211. ^{13}C NMR spectra of **4g (major)** (75 MHz, $CDCl_3$)

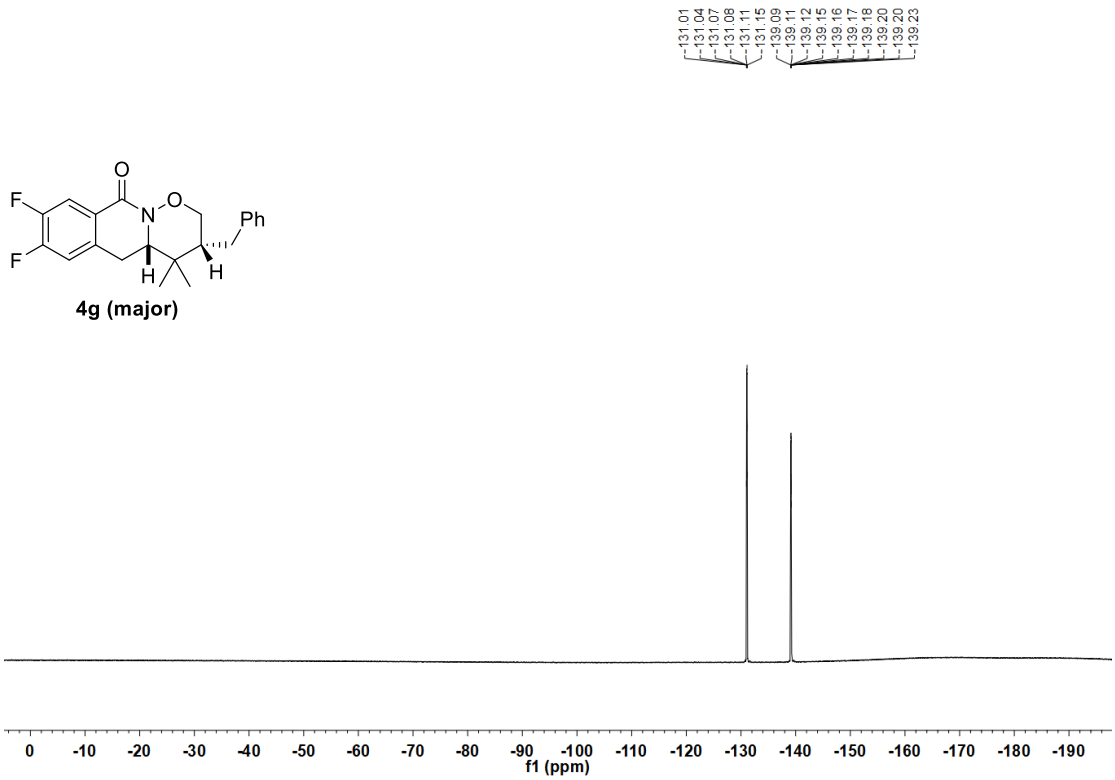


Figure S212. ^{19}F NMR spectra of **4g (major)** (282 MHz, $CDCl_3$)

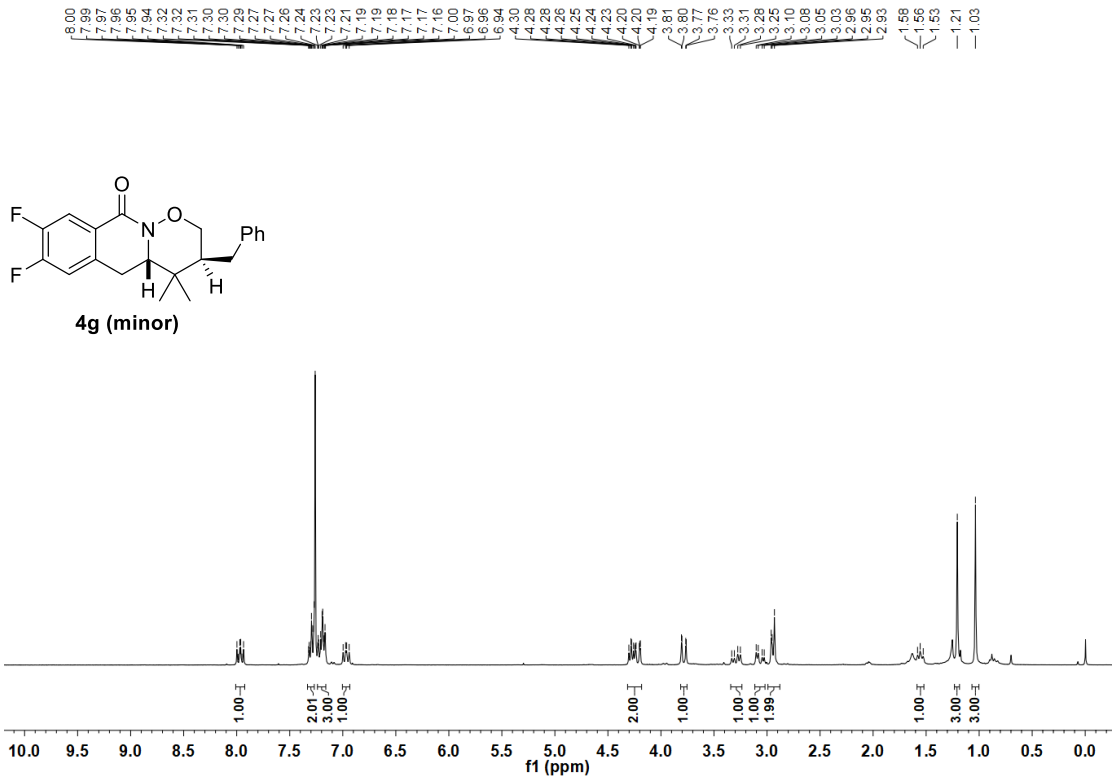


Figure S213. ^{1}H NMR spectra of **4g (minor)** (300 MHz, $CDCl_3$)

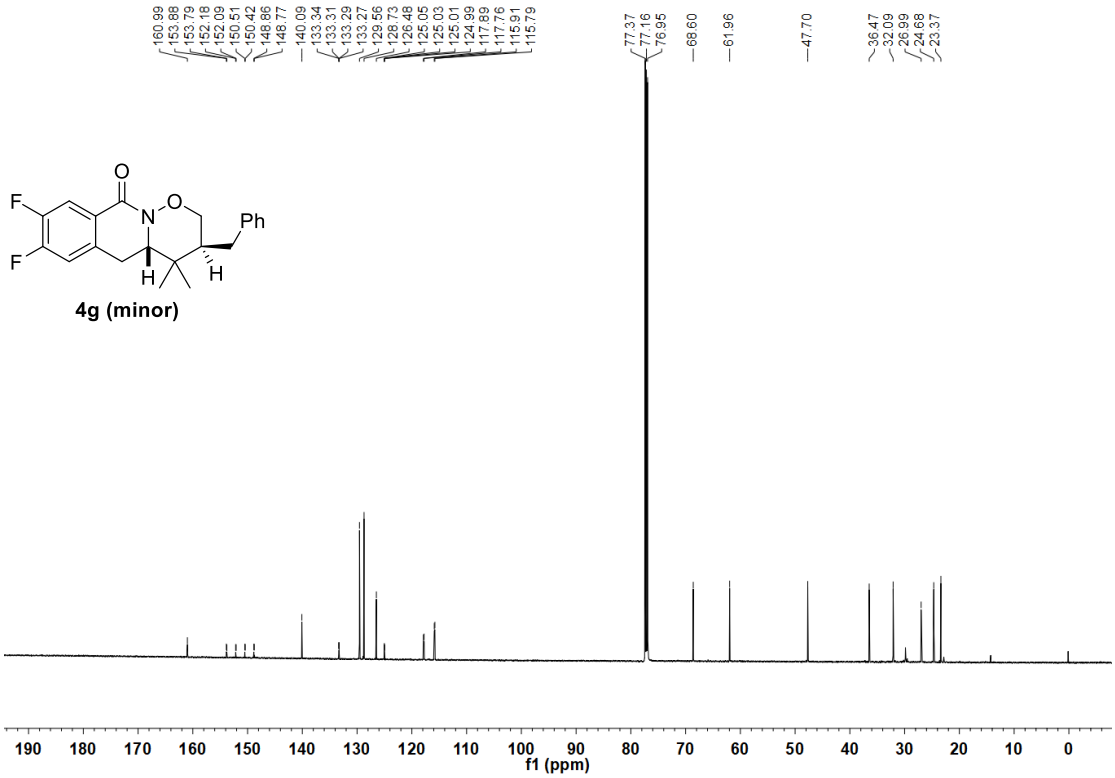


Figure S214. ^{13}C NMR spectra of **4g (minor)** (75 MHz, $CDCl_3$)

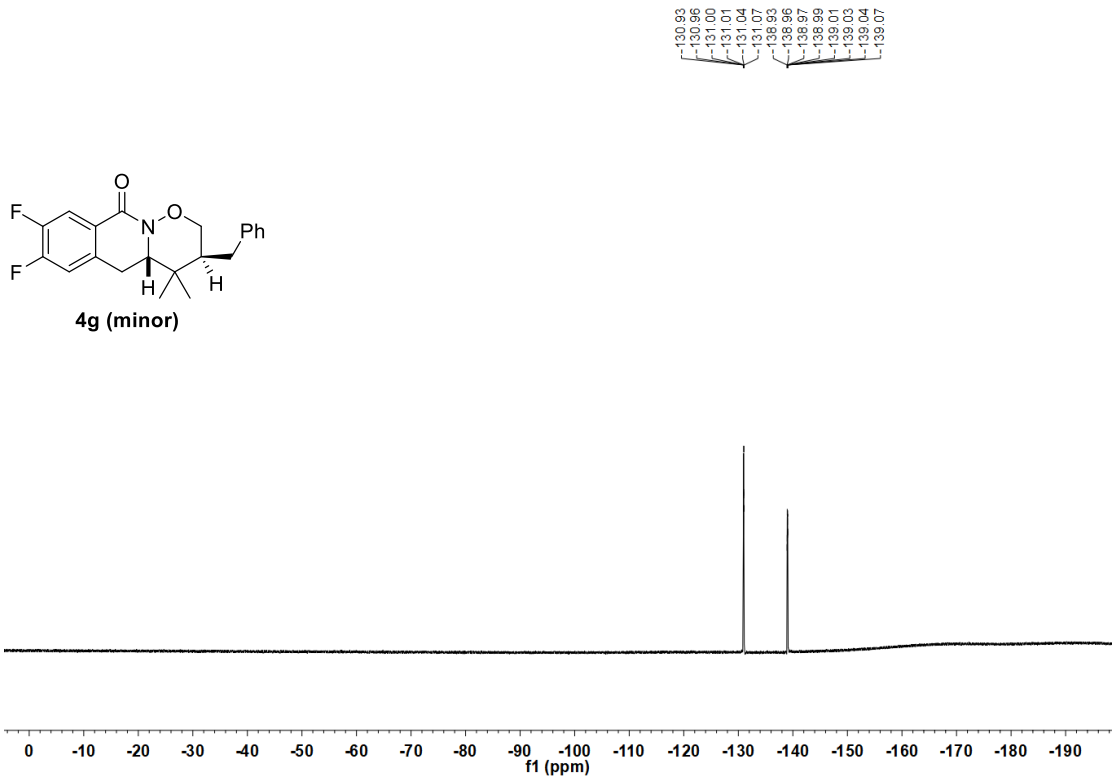


Figure S215. ^{19}F NMR spectra of **4g (minor)** (282 MHz, $CDCl_3$)

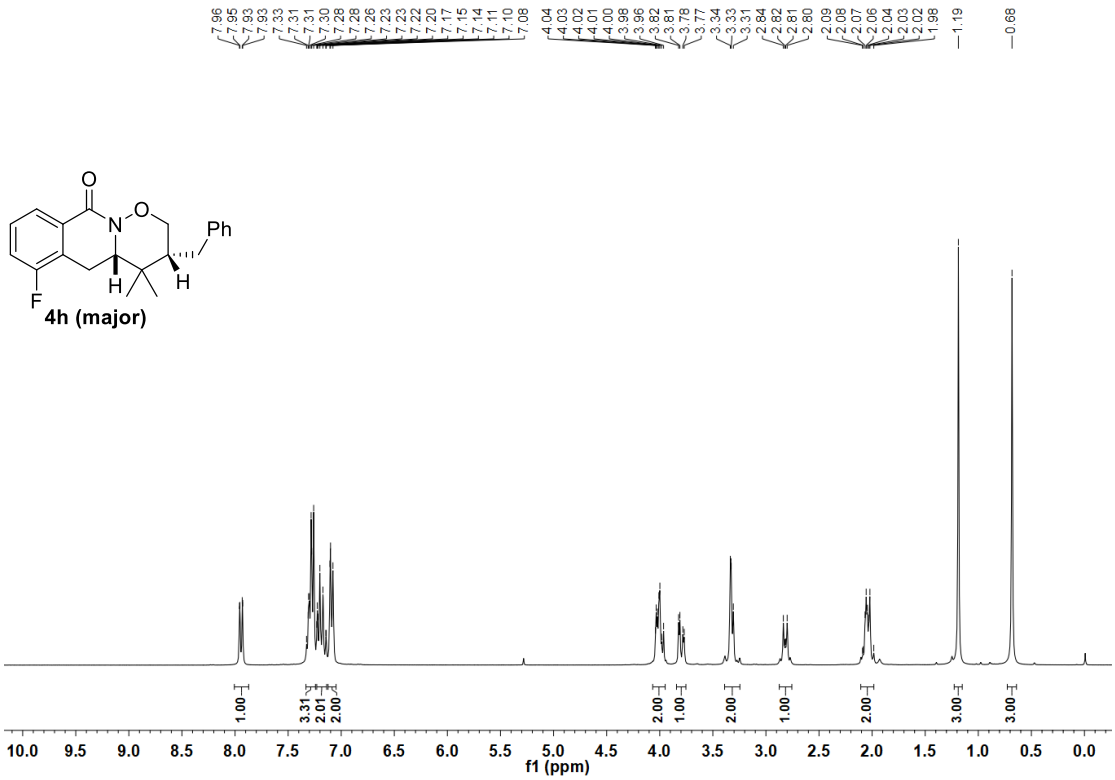


Figure S216. ^{1}H NMR spectra of **4h (major)** (300 MHz, $CDCl_3$)

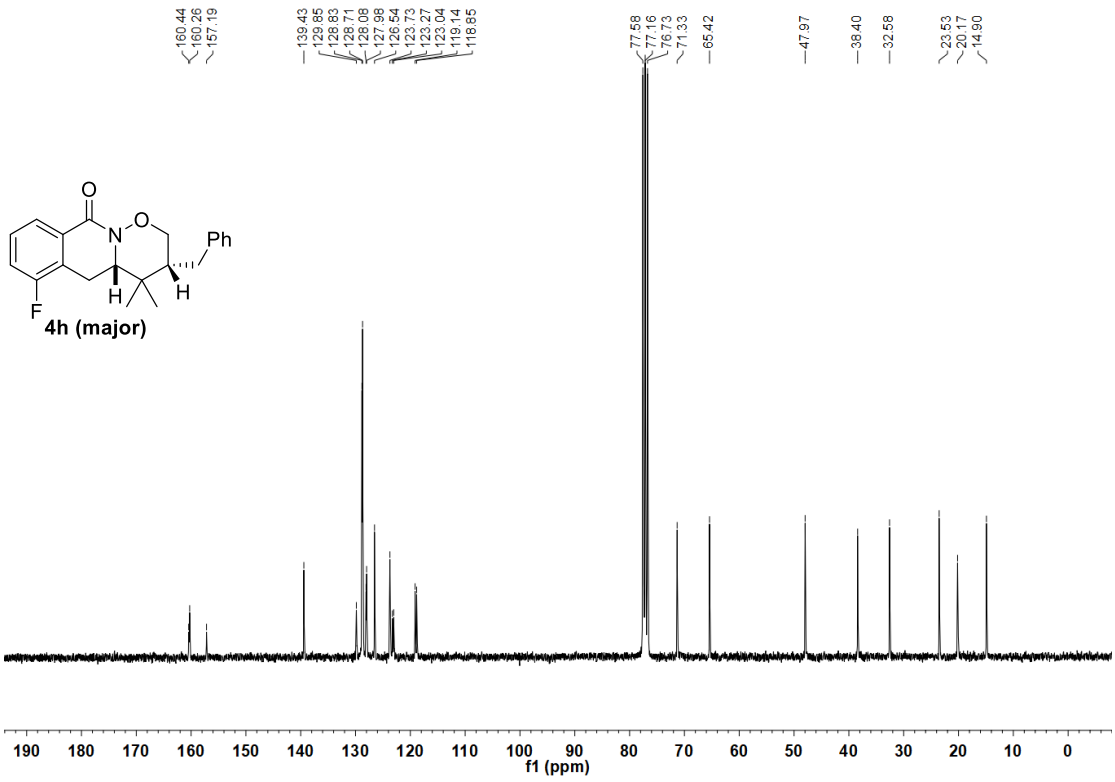


Figure S217. ^{13}C NMR spectra of **4h (major)** (75 MHz, $CDCl_3$)

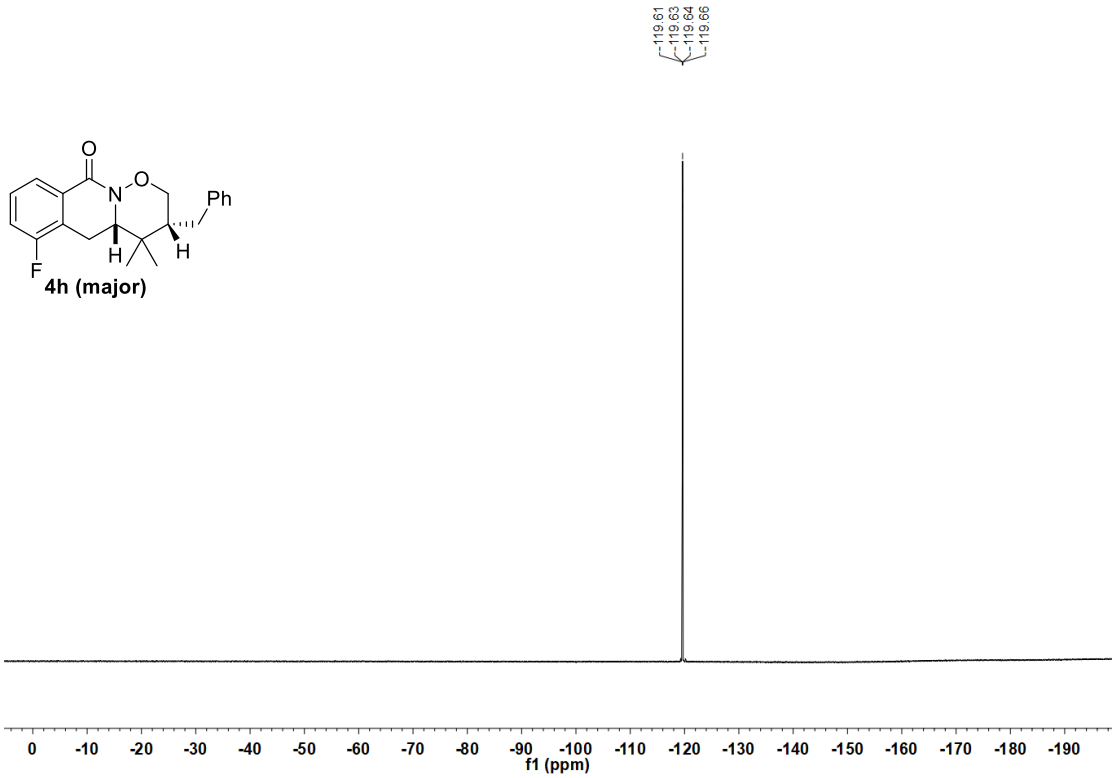


Figure S218. ^{19}F NMR spectra of **4h (major)** (282 MHz, $CDCl_3$)

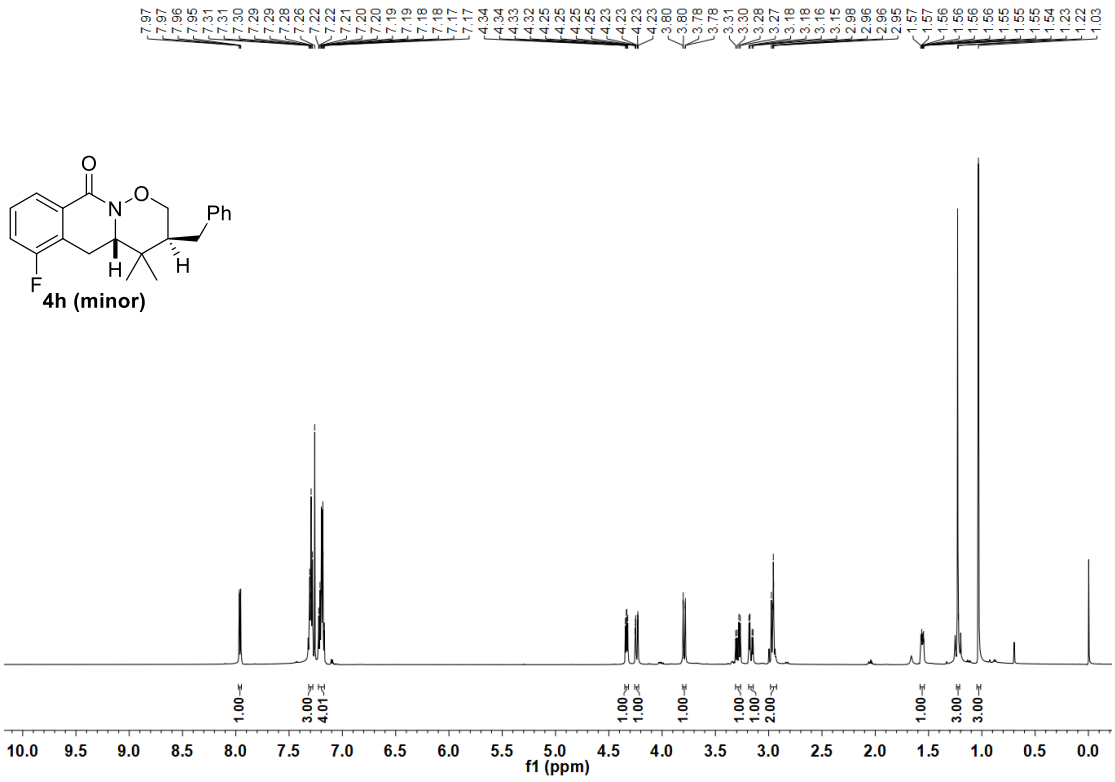


Figure S219. ^{1}H NMR spectra of **4h (minor)** (600 MHz, $CDCl_3$)

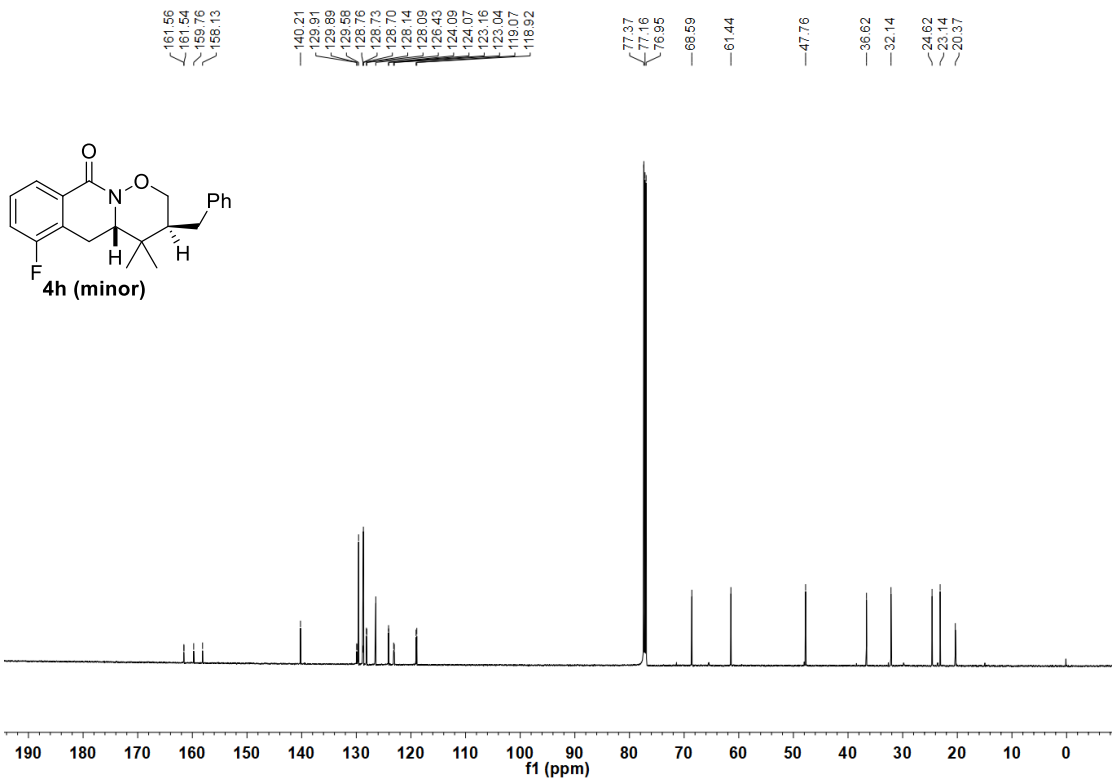


Figure S220. ^{13}C NMR spectra of **4h (minor)** (151 MHz, $CDCl_3$)

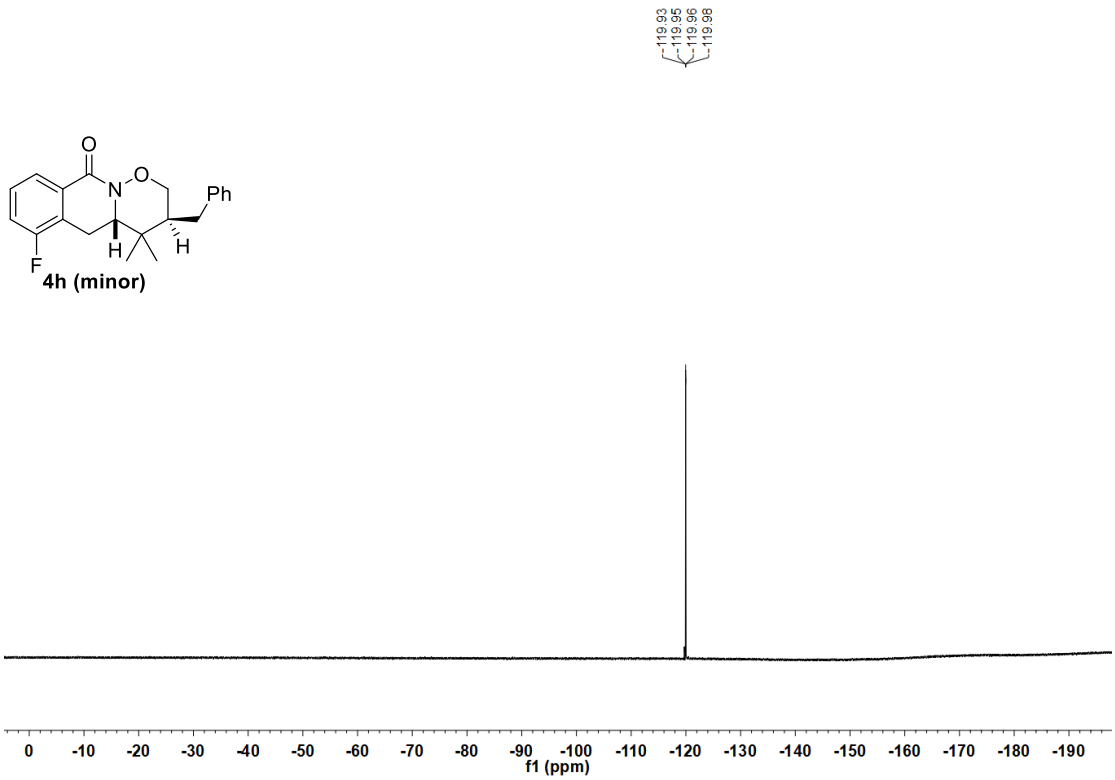


Figure S221. ^{19}F NMR spectra of **4h (minor)** (282 MHz, $CDCl_3$)

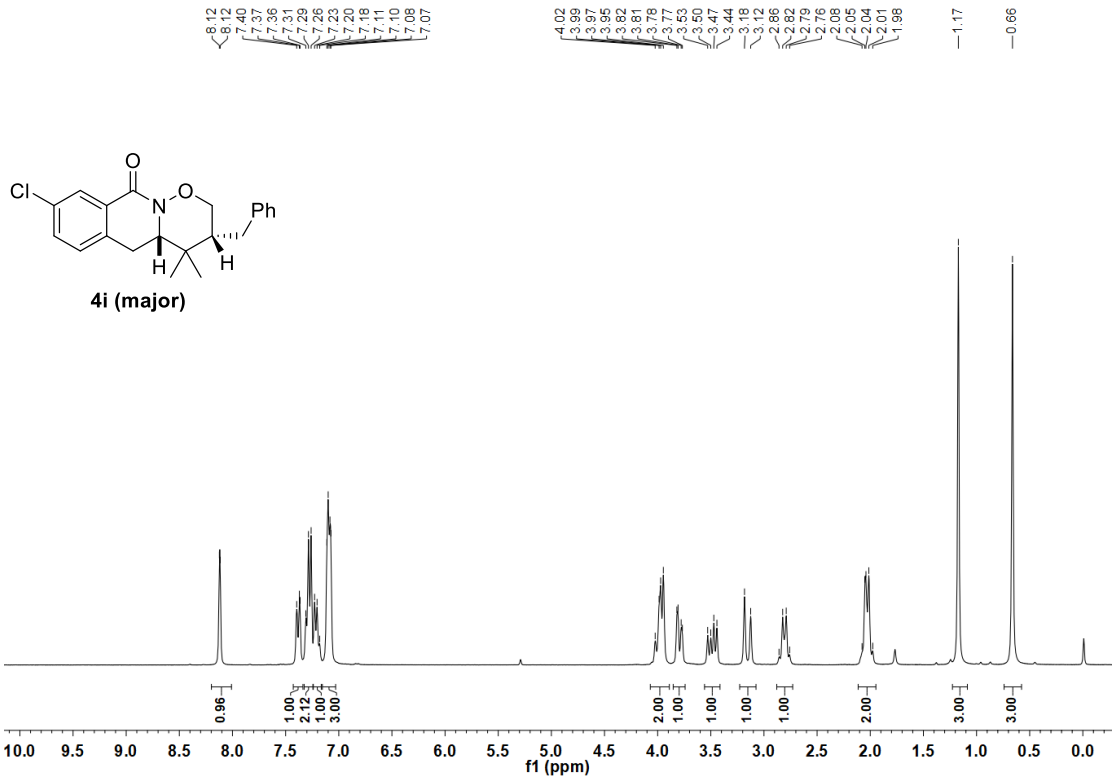


Figure S222. ^{1}H NMR spectra of **4i (major)** (300 MHz, $CDCl_3$)

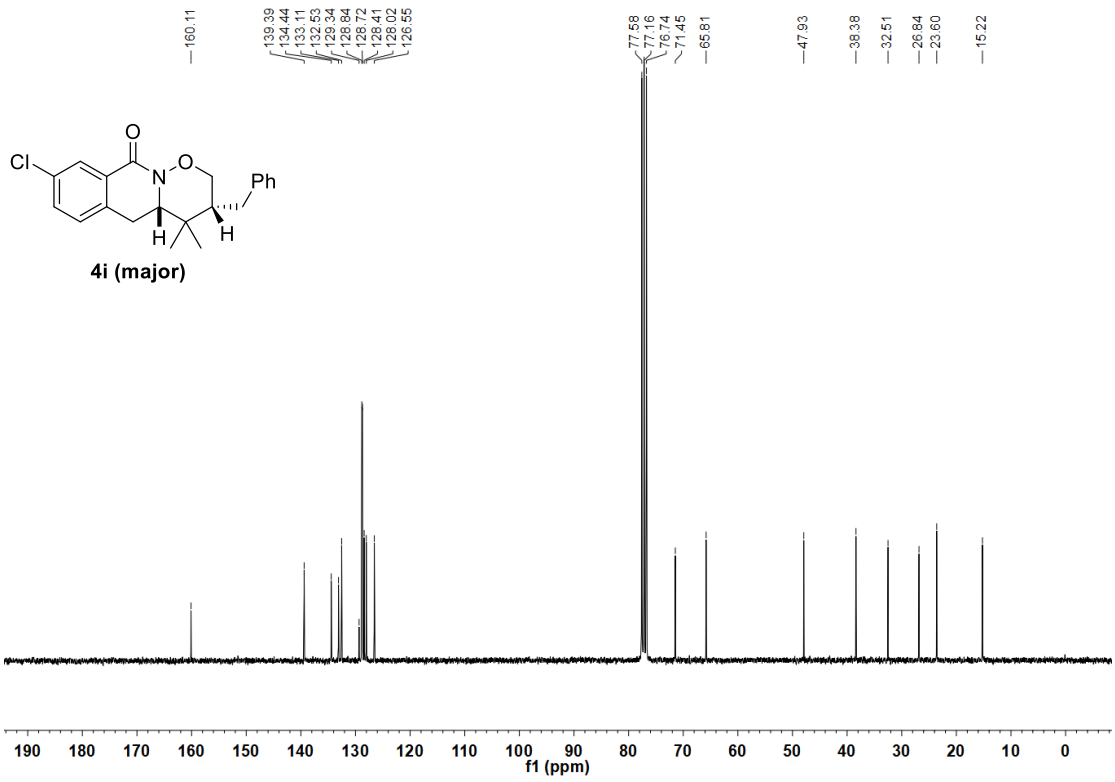


Figure S223. ^{13}C NMR spectra of **4i (major)** (75 MHz, $CDCl_3$)

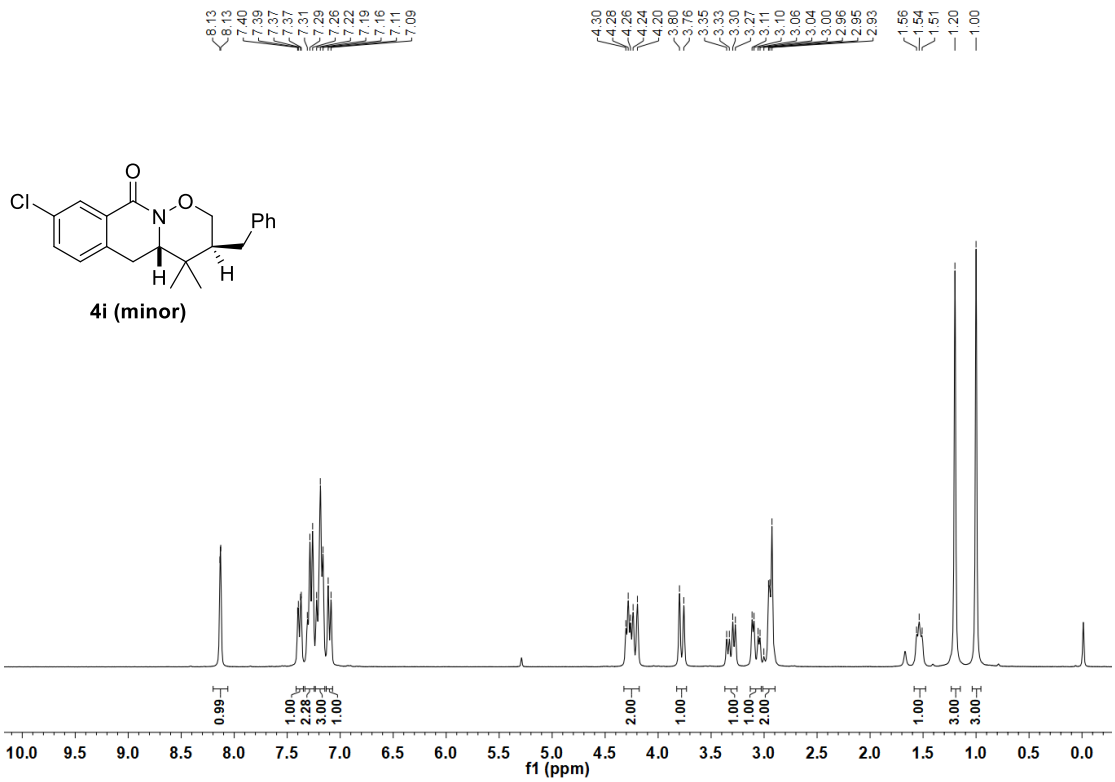


Figure S224. ^{1}H NMR spectra of **4i (minor)** (300 MHz, $CDCl_3$)

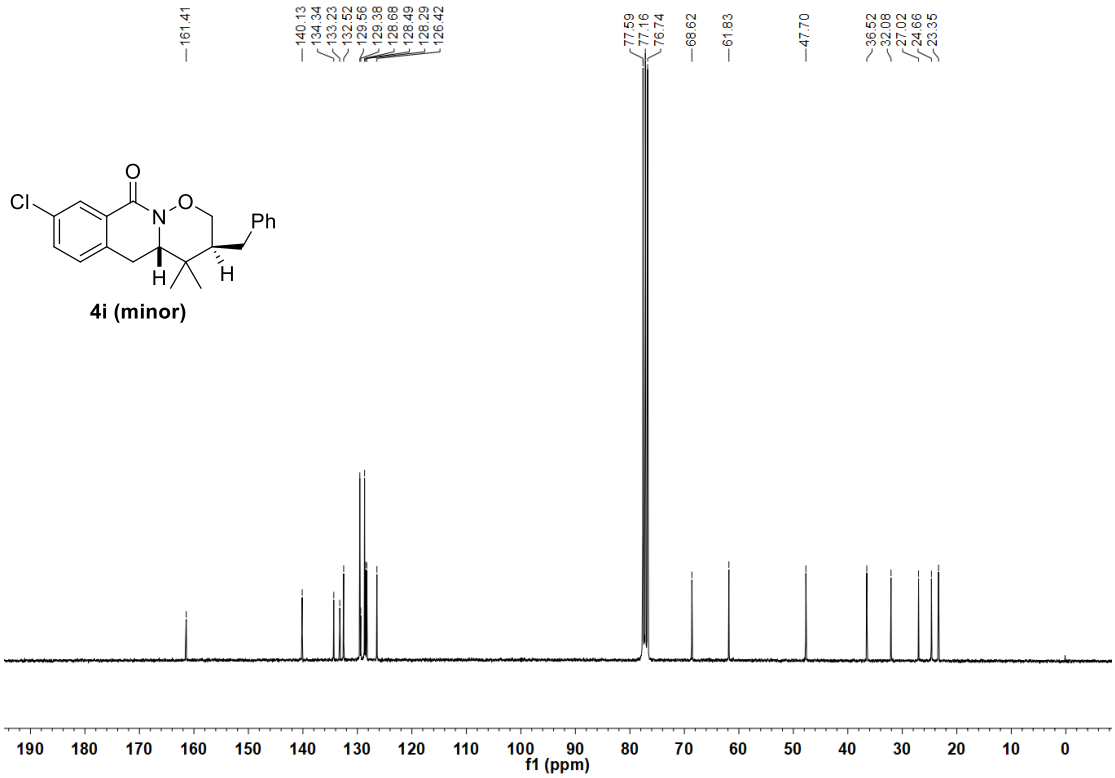


Figure S225. ^{13}C NMR spectra of **4i (minor)** (75 MHz, $CDCl_3$)

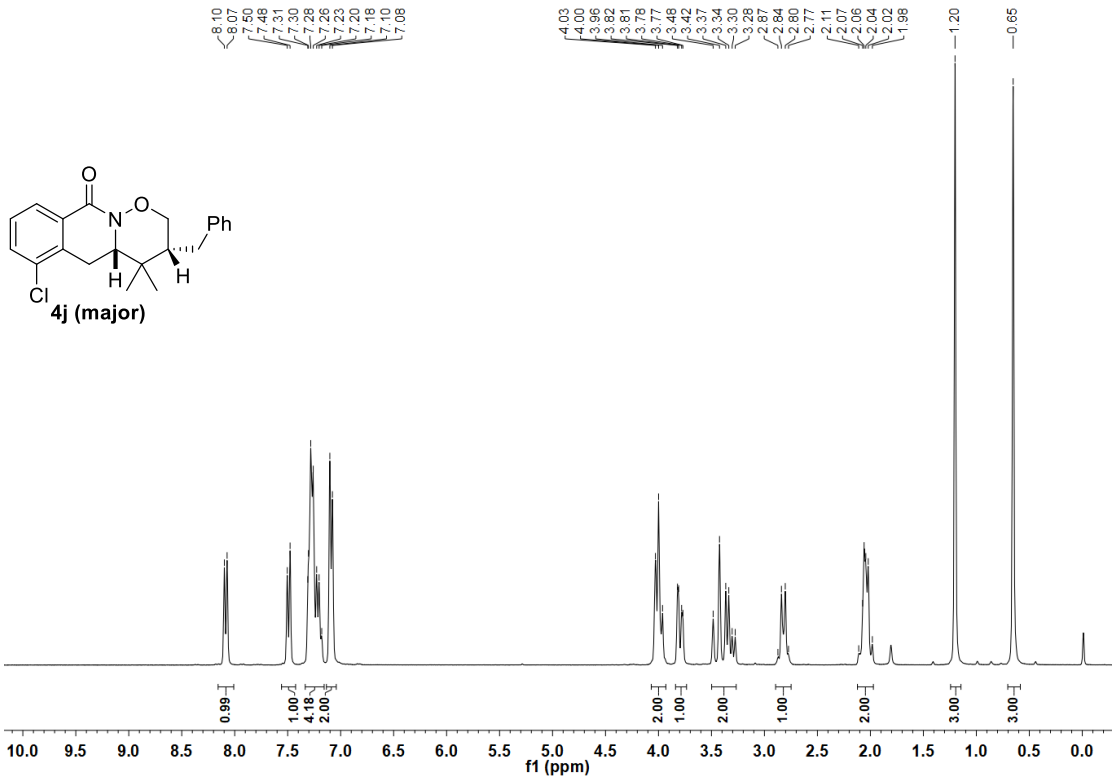


Figure S226. ^{1}H NMR spectra of **4j (major)** (300 MHz, $CDCl_3$)

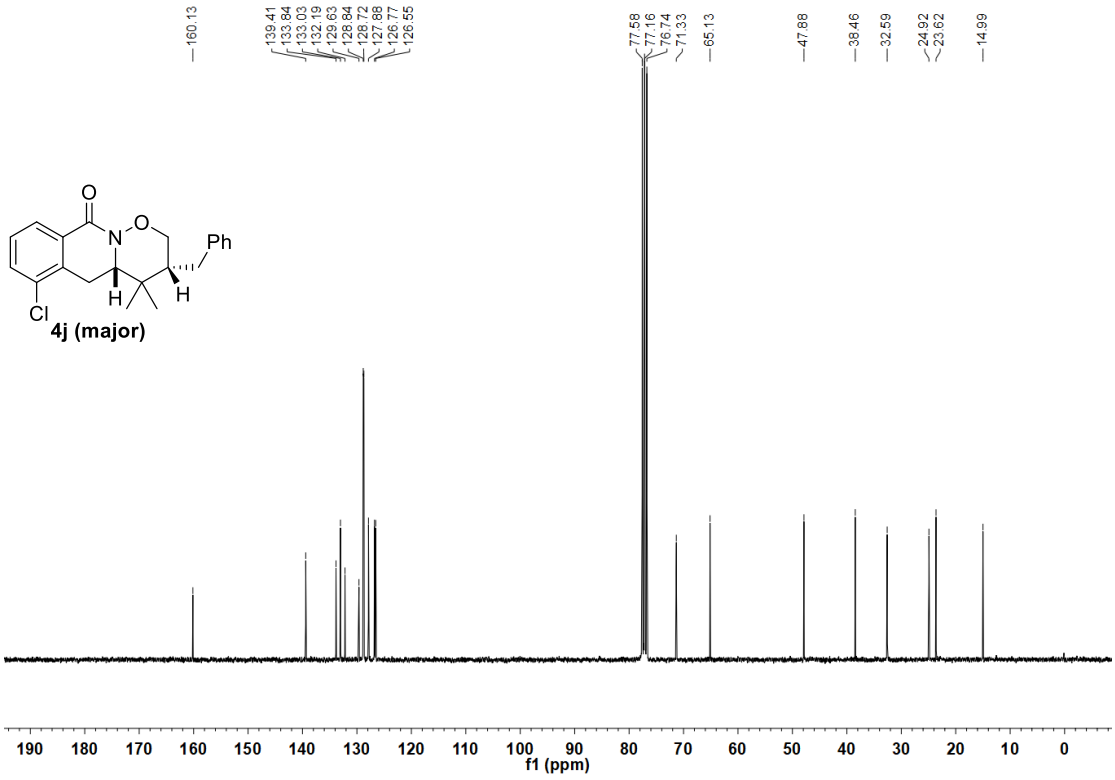


Figure S227. ^{13}C NMR spectra of **4j (major)** (75 MHz, $CDCl_3$)

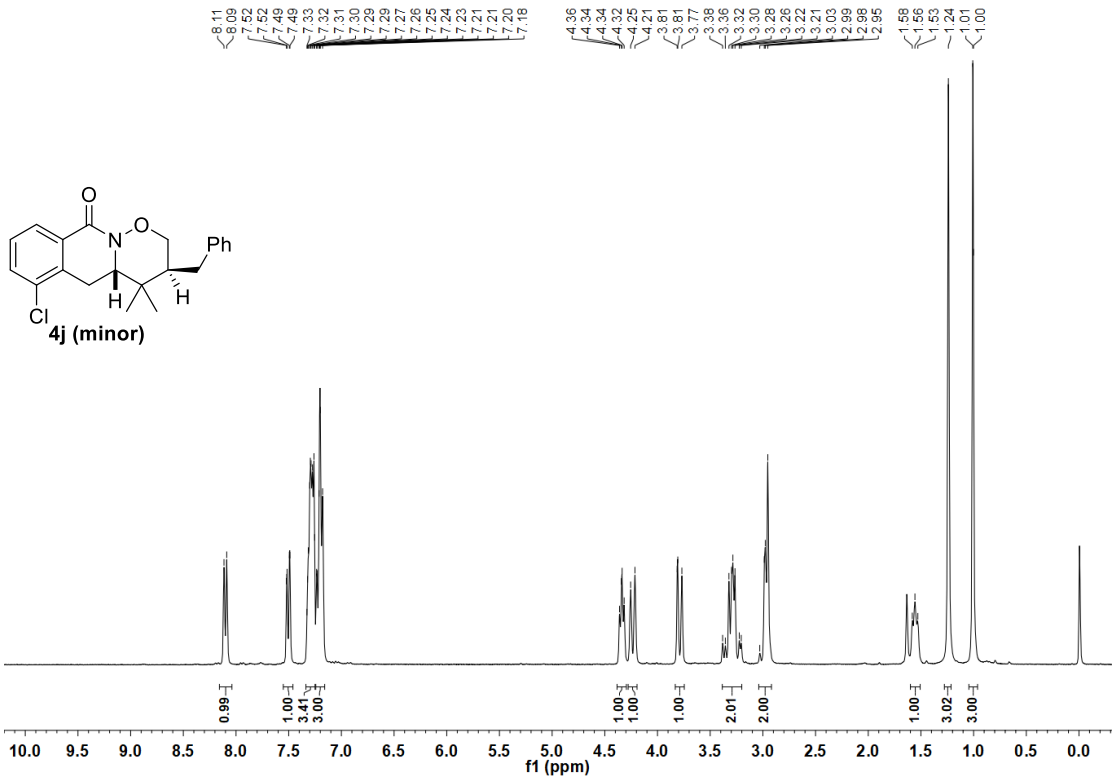


Figure S228. ^{1}H NMR spectra of **4j (minor)** (300 MHz, $CDCl_3$)

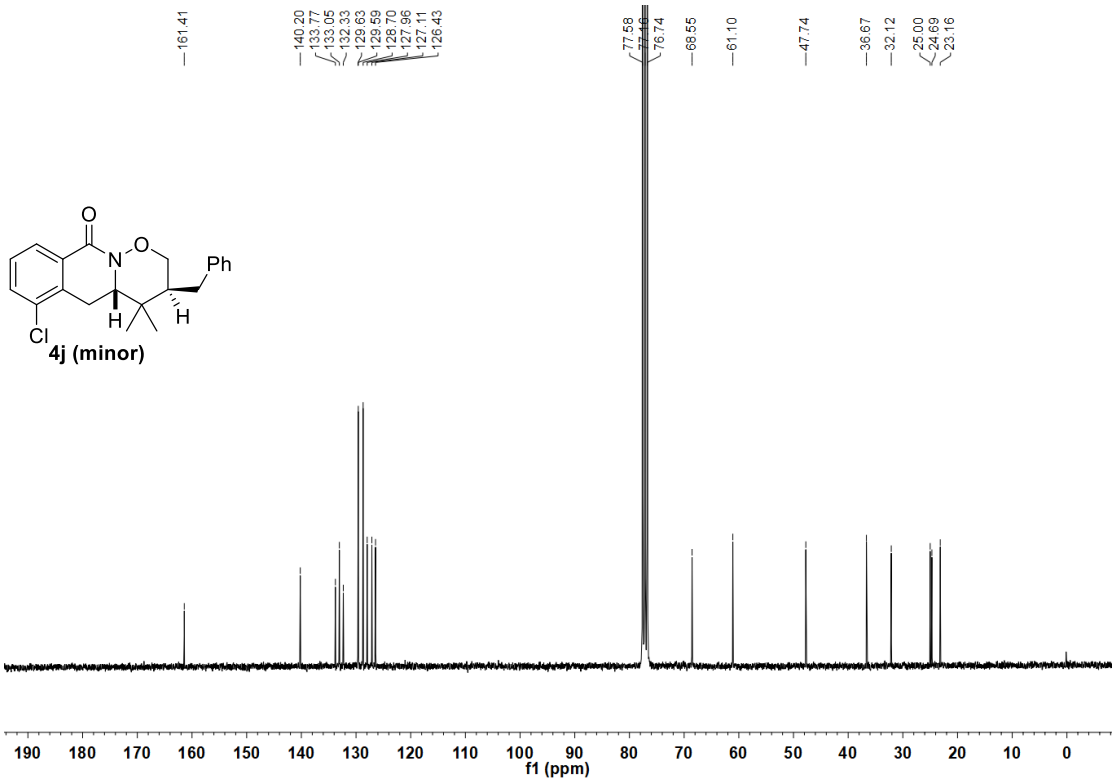


Figure S229. ^{13}C NMR spectra of **4j (minor)** (75 MHz, $CDCl_3$)

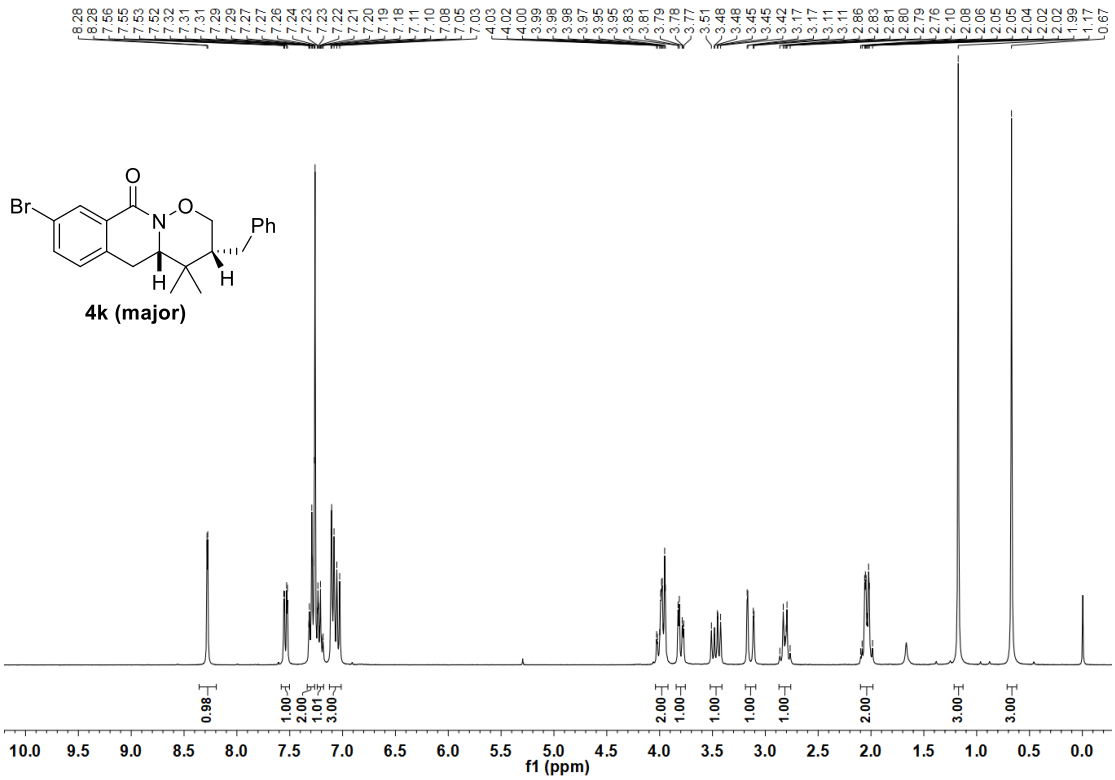


Figure S230. ^{1}H NMR spectra of **4k (major)** (300 MHz, $CDCl_3$)

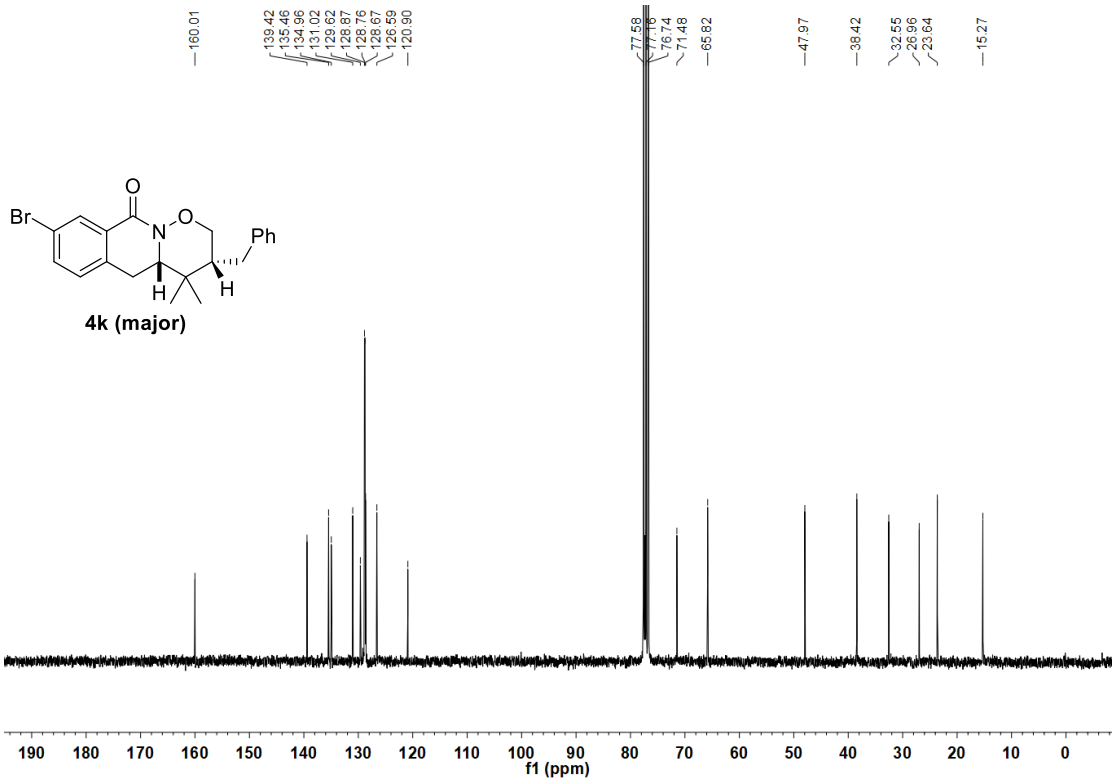


Figure S231. ^{13}C NMR spectra of **4k (major)** (75 MHz, $CDCl_3$)

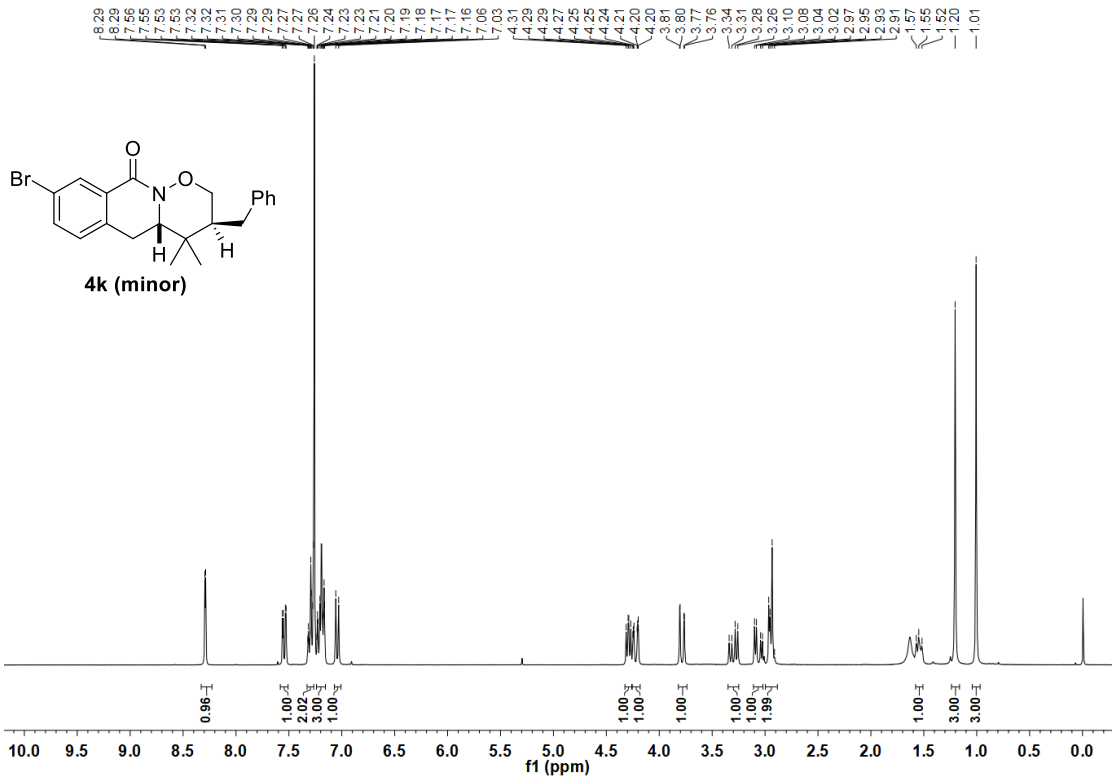


Figure S232. ^{1}H NMR spectra of **4k (minor)** (300 MHz, $CDCl_3$)

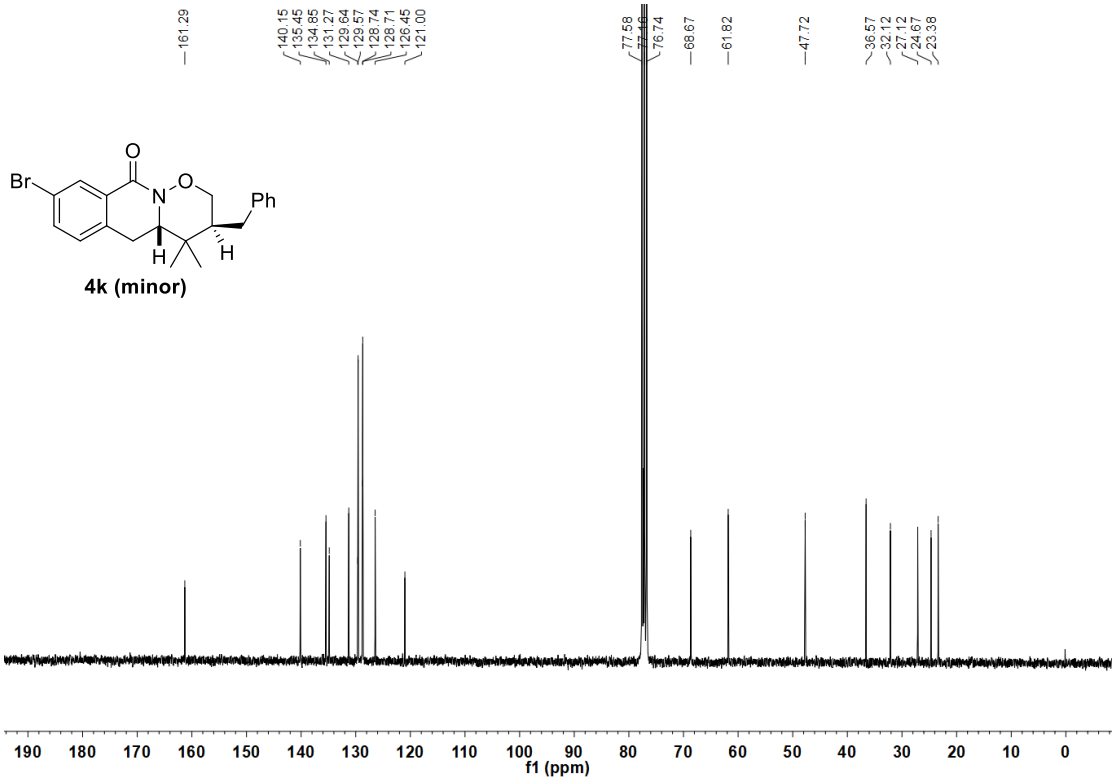


Figure S233. ^{13}C NMR spectra of **4k (minor)** (75 MHz, $CDCl_3$)

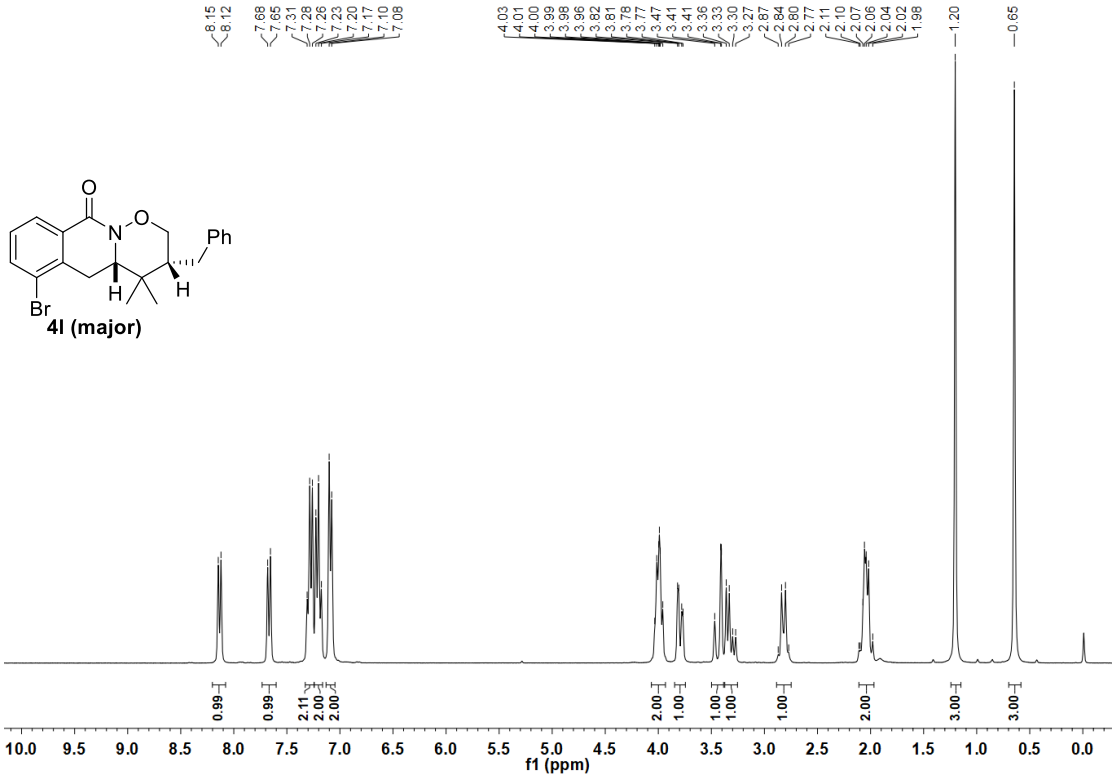


Figure S234. ^{1}H NMR spectra of **4l (major)** (300 MHz, $CDCl_3$)

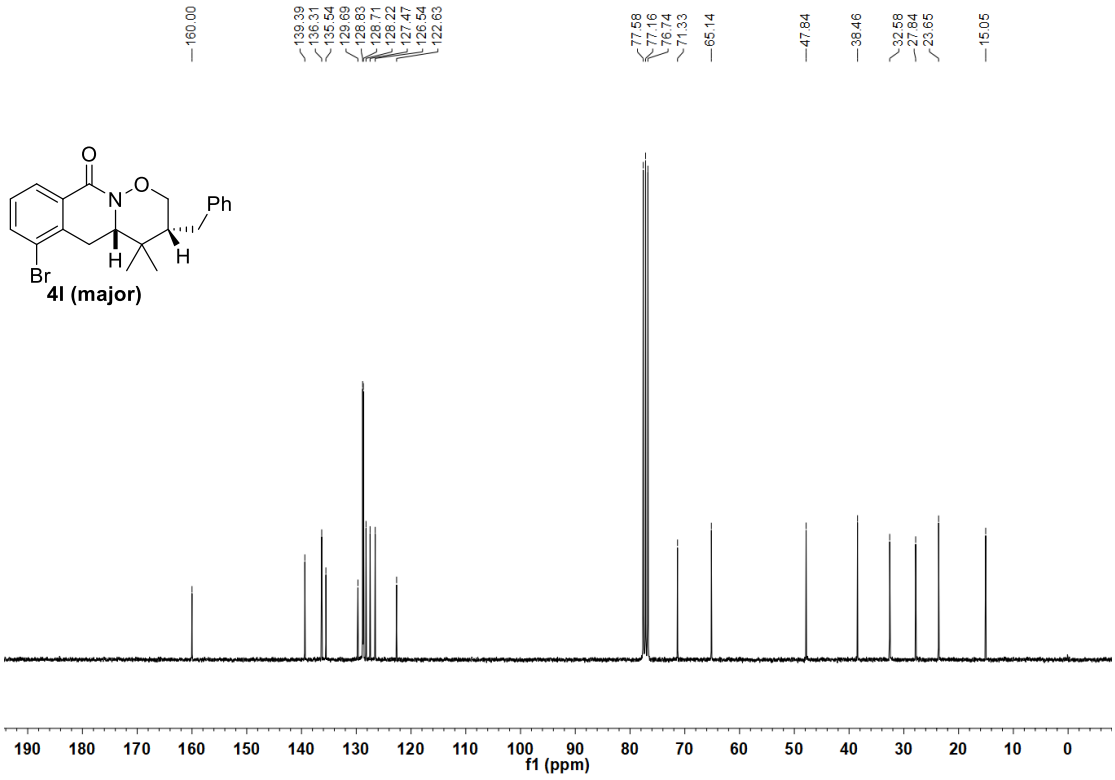


Figure S235. ^{13}C NMR spectra of **4l (major)** (75 MHz, $CDCl_3$)

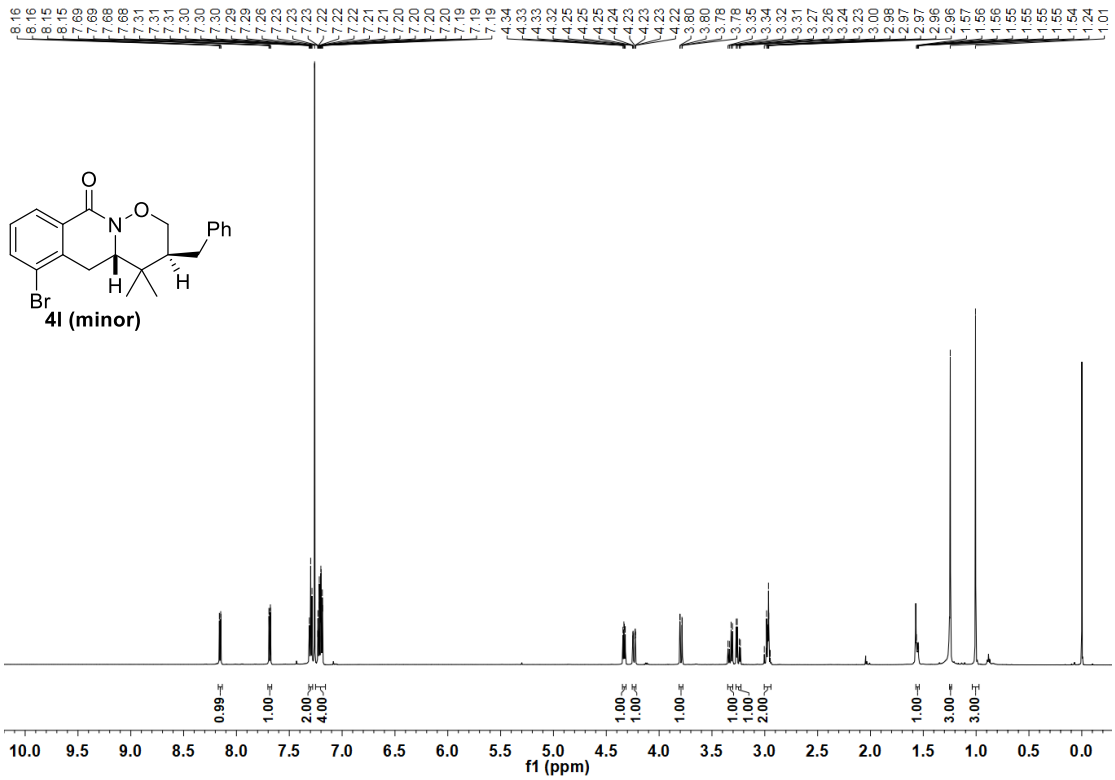


Figure S236. ^{1}H NMR spectra of **4l (minor)** (600 MHz, $CDCl_3$)

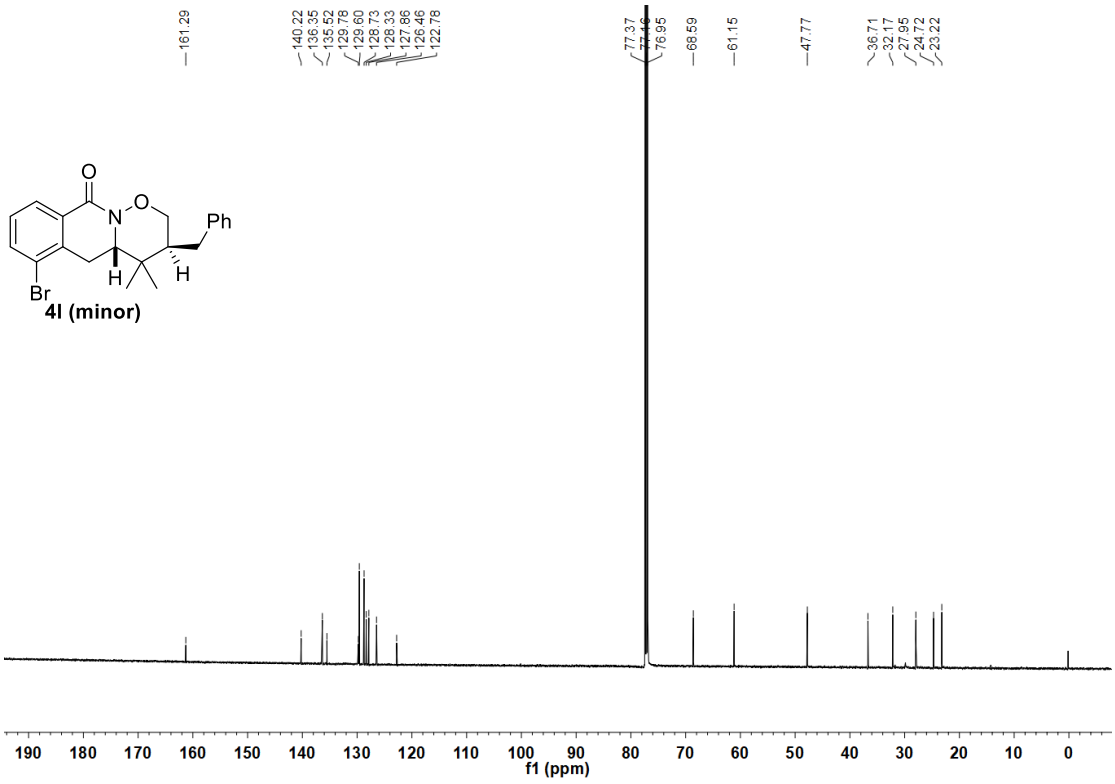


Figure S237. ^{13}C NMR spectra of **4l (minor)** (151 MHz, $CDCl_3$)

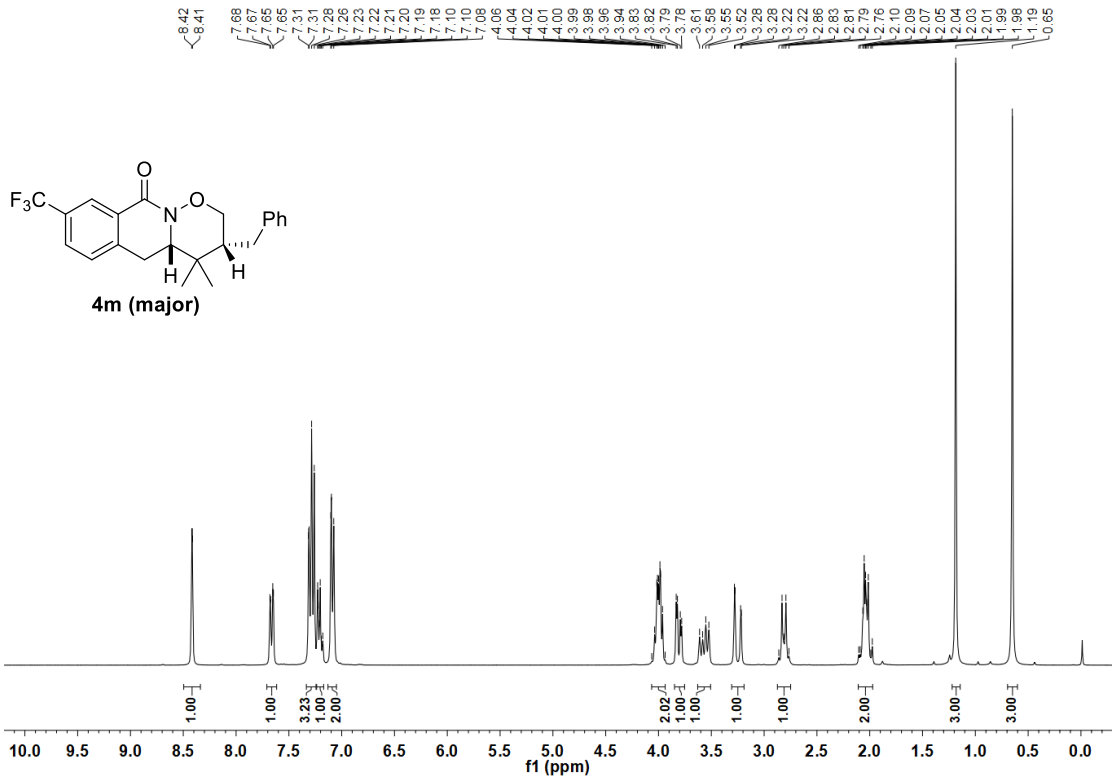


Figure S238. ^{1}H NMR spectra of **4m (major)** (300 MHz, $CDCl_3$)

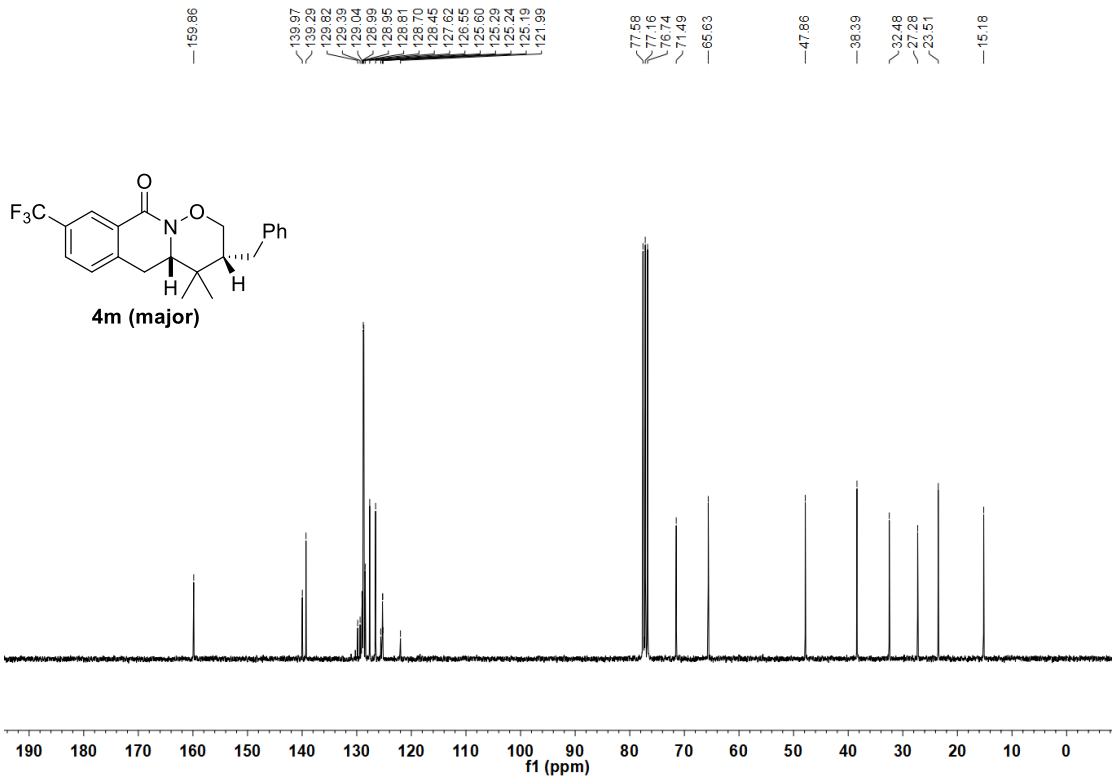


Figure S239. ^{13}C NMR spectra of **4m (major)** (75 MHz, $CDCl_3$)

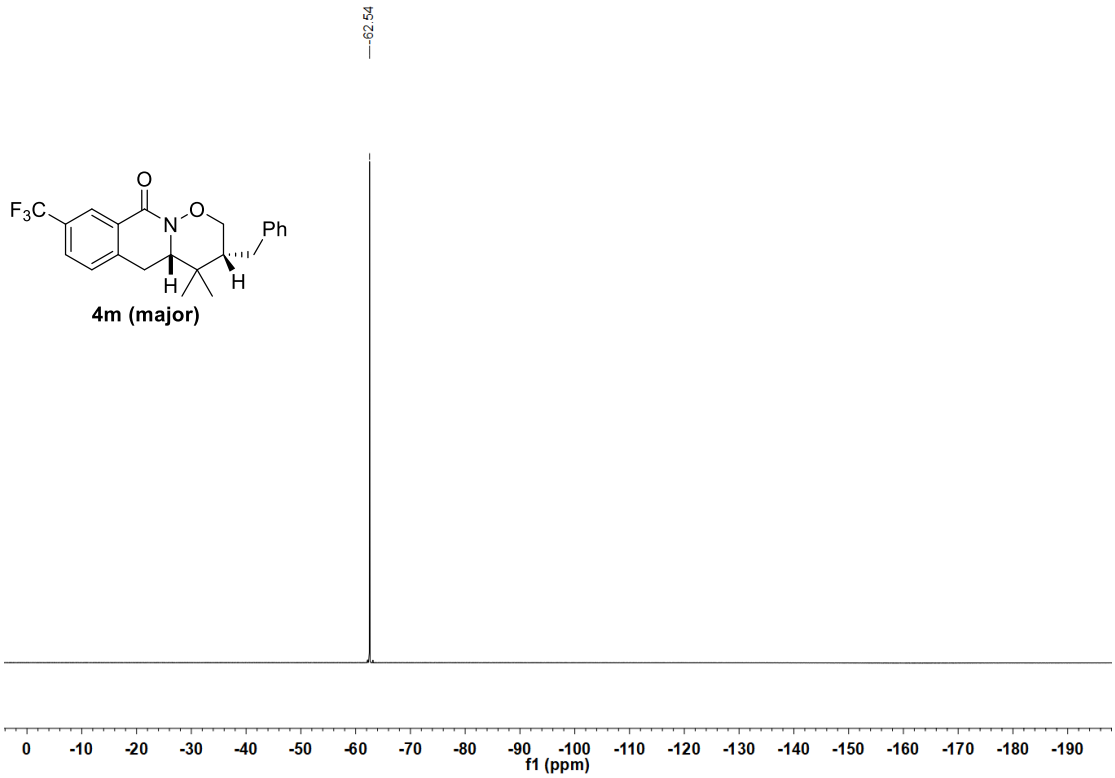


Figure S240. ^{19}F NMR spectra of **4m (major)** (282 MHz, $CDCl_3$)

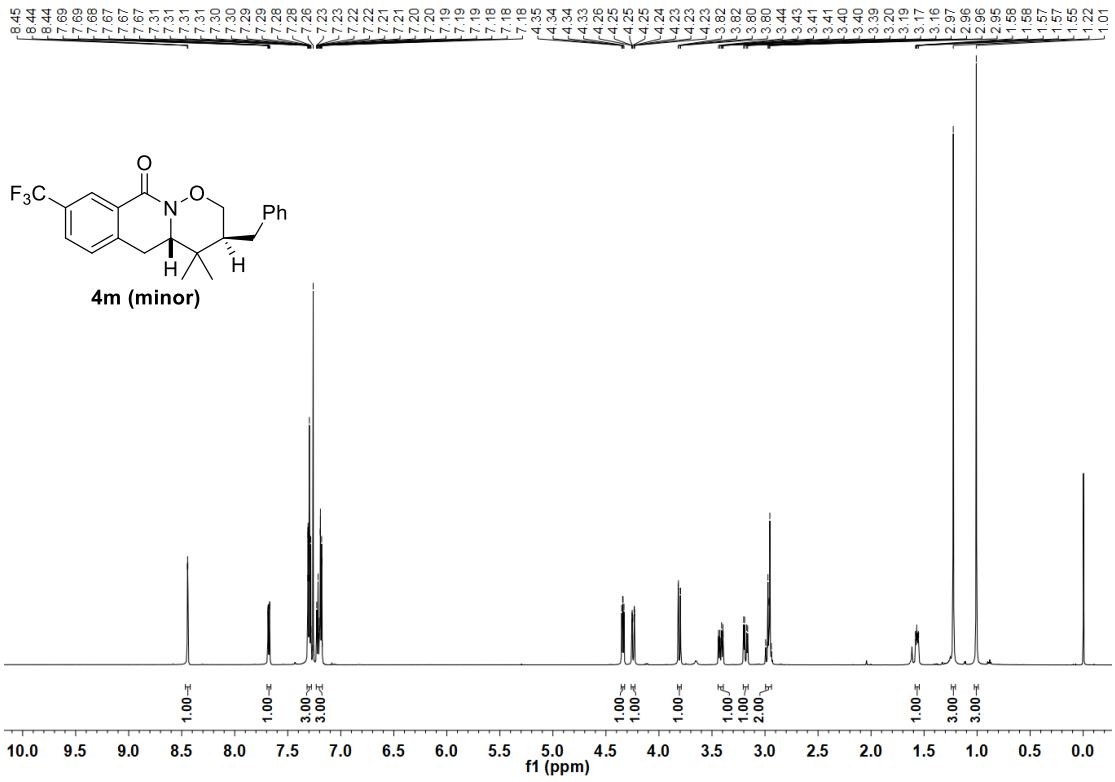


Figure S241. ^{1}H NMR spectra of **4m (minor)** (600 MHz, $CDCl_3$)

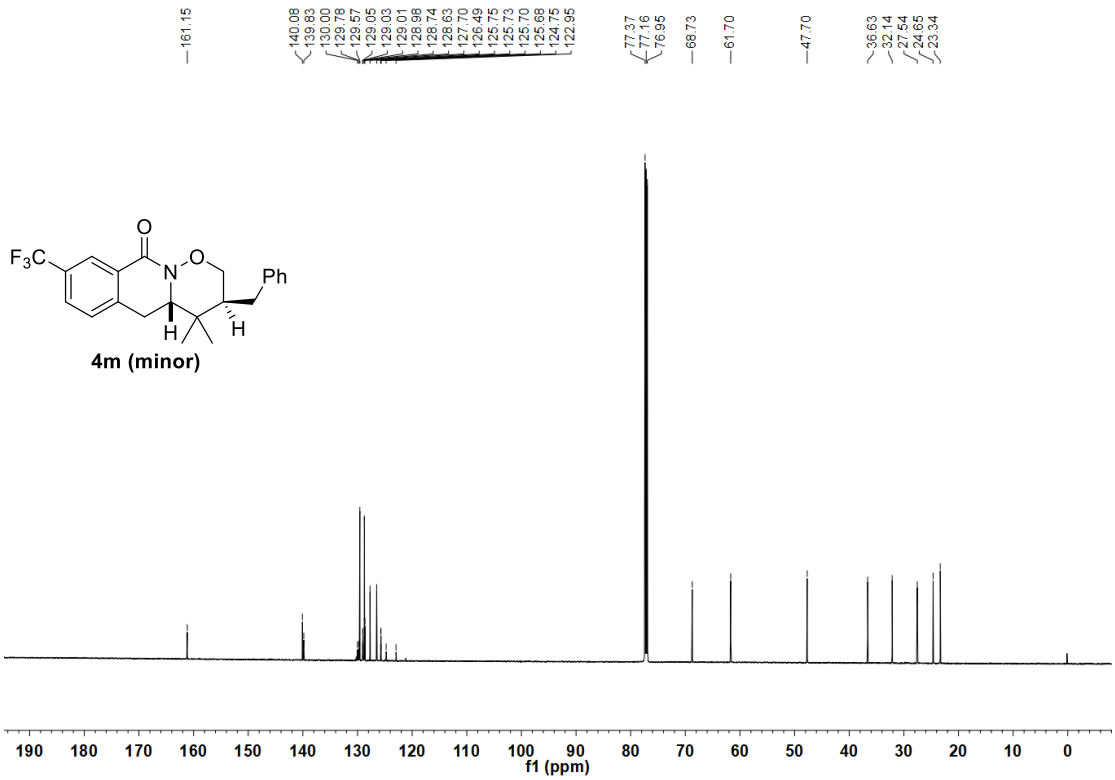


Figure S242. ^{13}C NMR spectra of **4m (minor)** (151 MHz, $CDCl_3$)

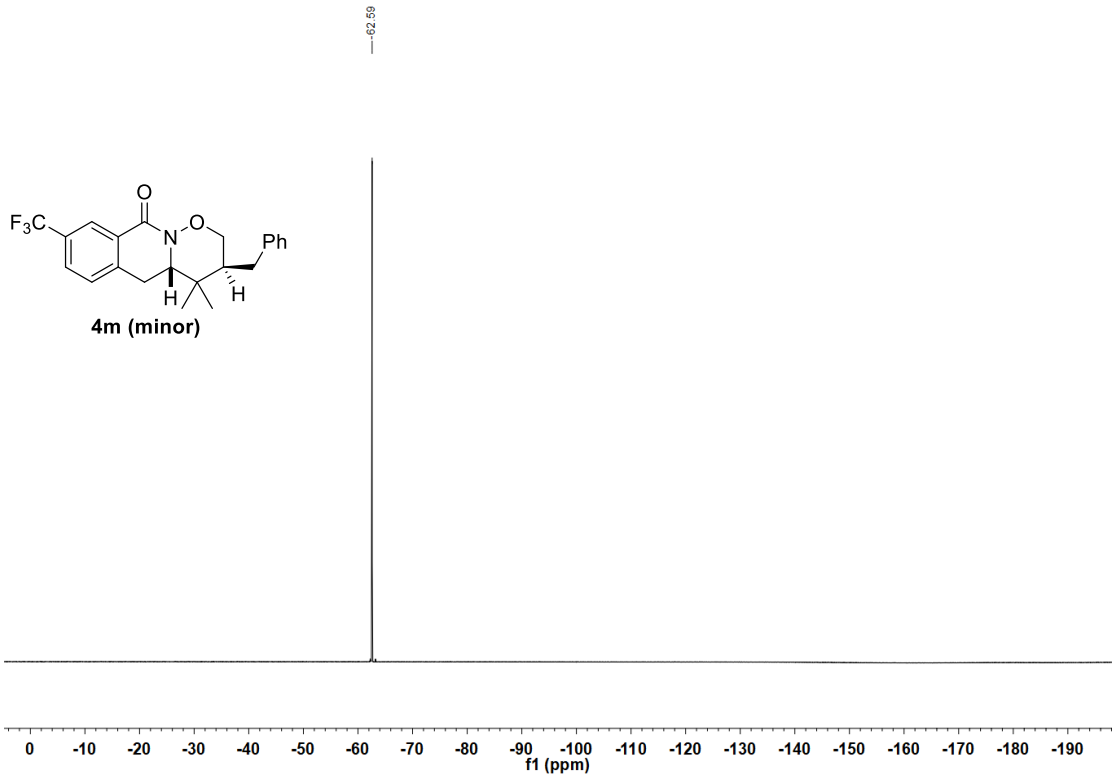


Figure S243. ^{19}F NMR spectra of **4m (minor)** (282 MHz, $CDCl_3$)

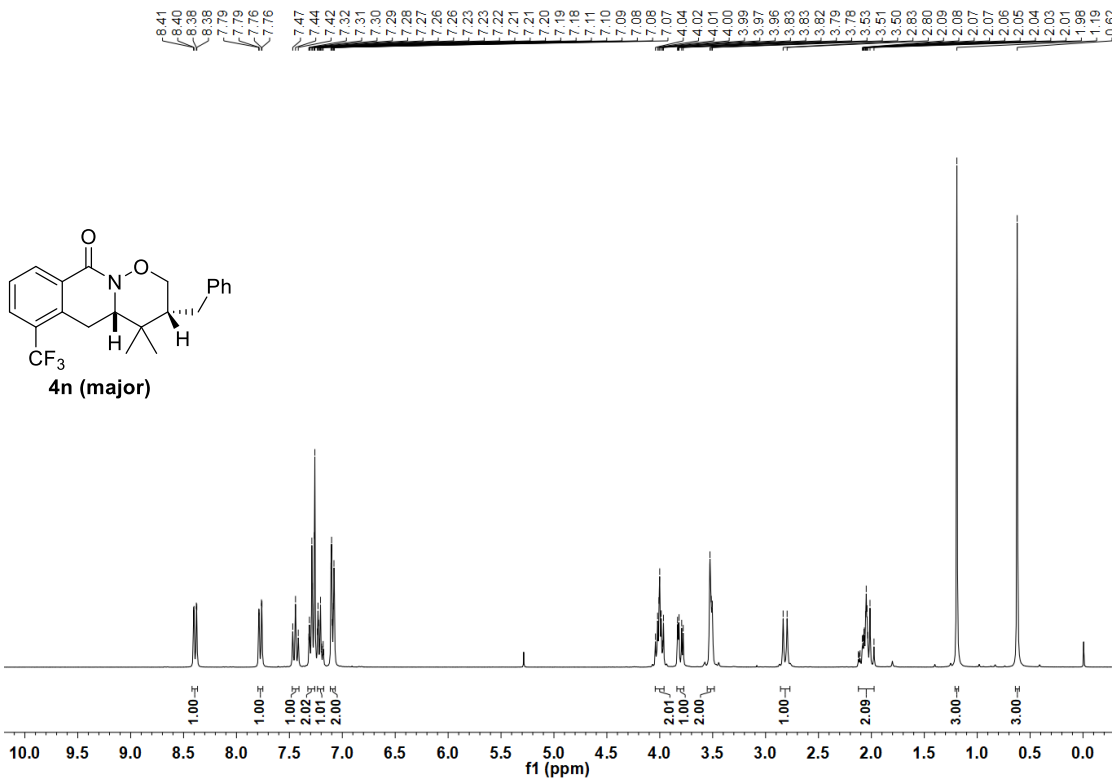


Figure S244. ^{1}H NMR spectra of **4n (major)** (300 MHz, $CDCl_3$)

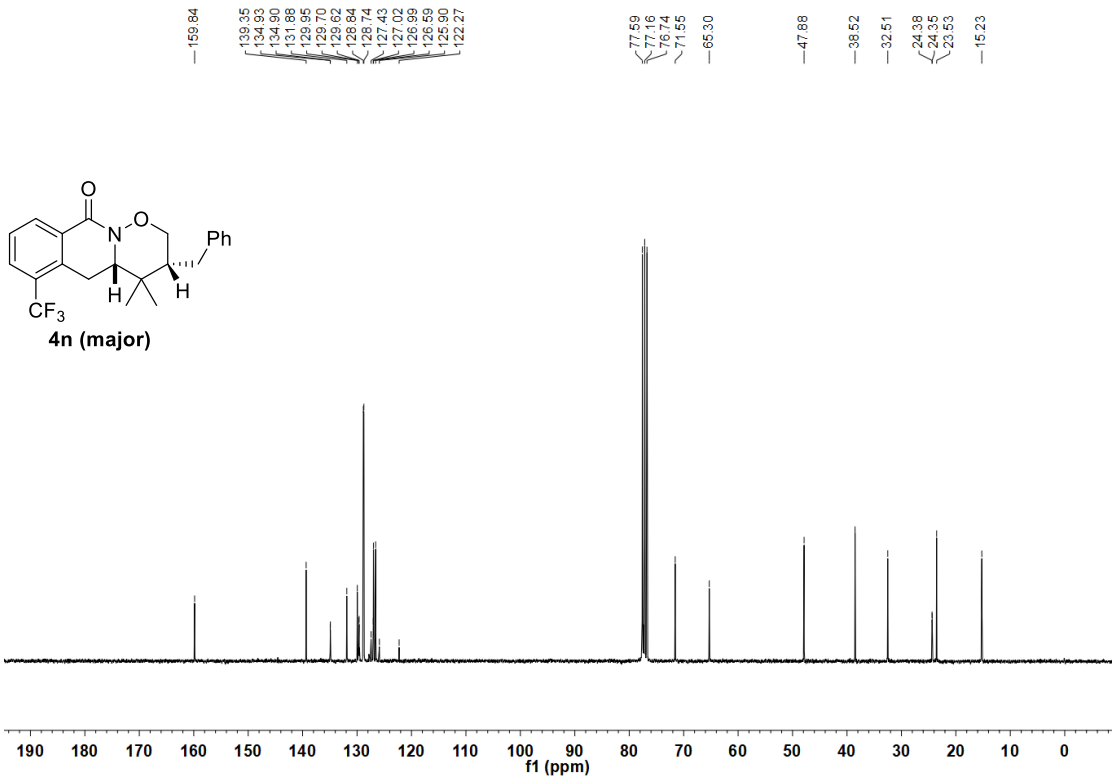


Figure S245. ^{13}C NMR spectra of **4n (major)** (75 MHz, $CDCl_3$)

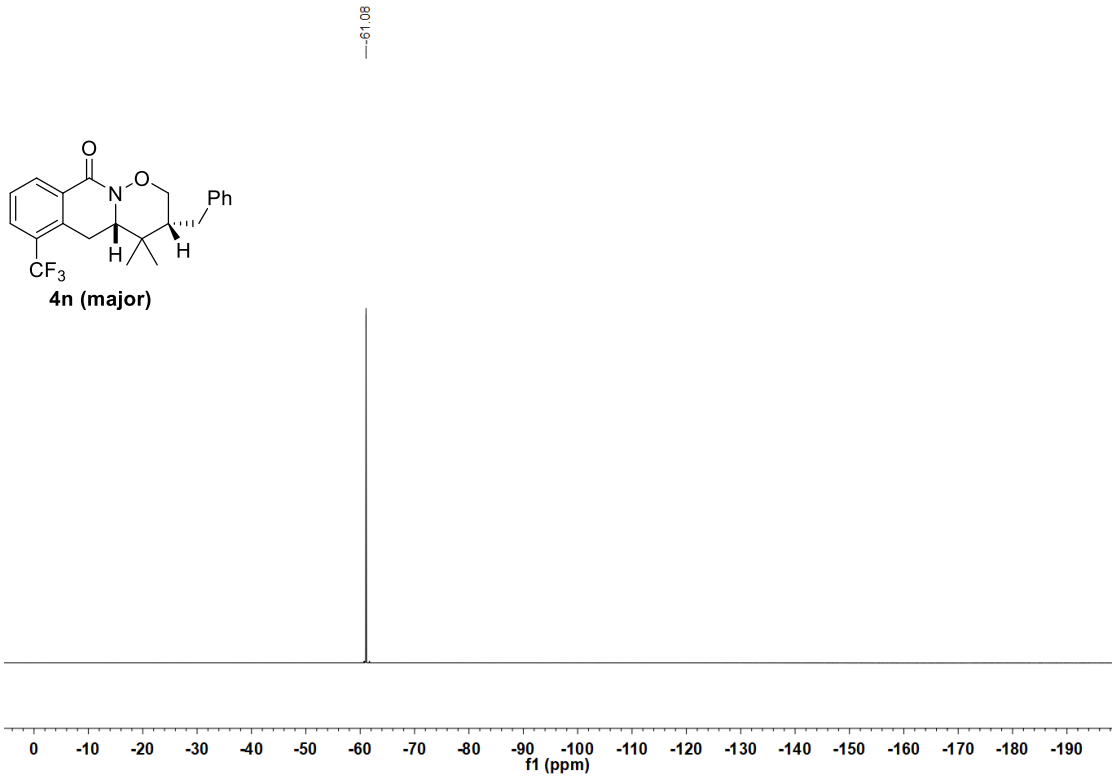


Figure S246. ^{19}F NMR spectra of **4n (major)** (282 MHz, $CDCl_3$)

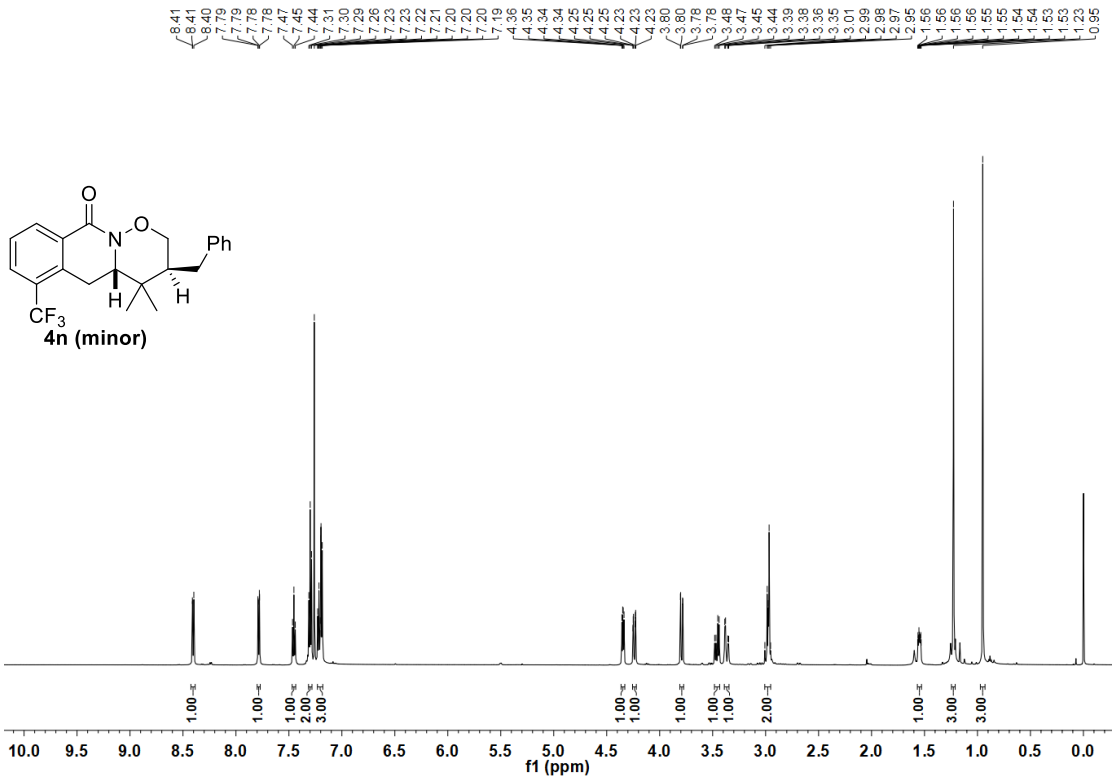


Figure S247. ^{1}H NMR spectra of **4n (minor)** (600 MHz, $CDCl_3$)

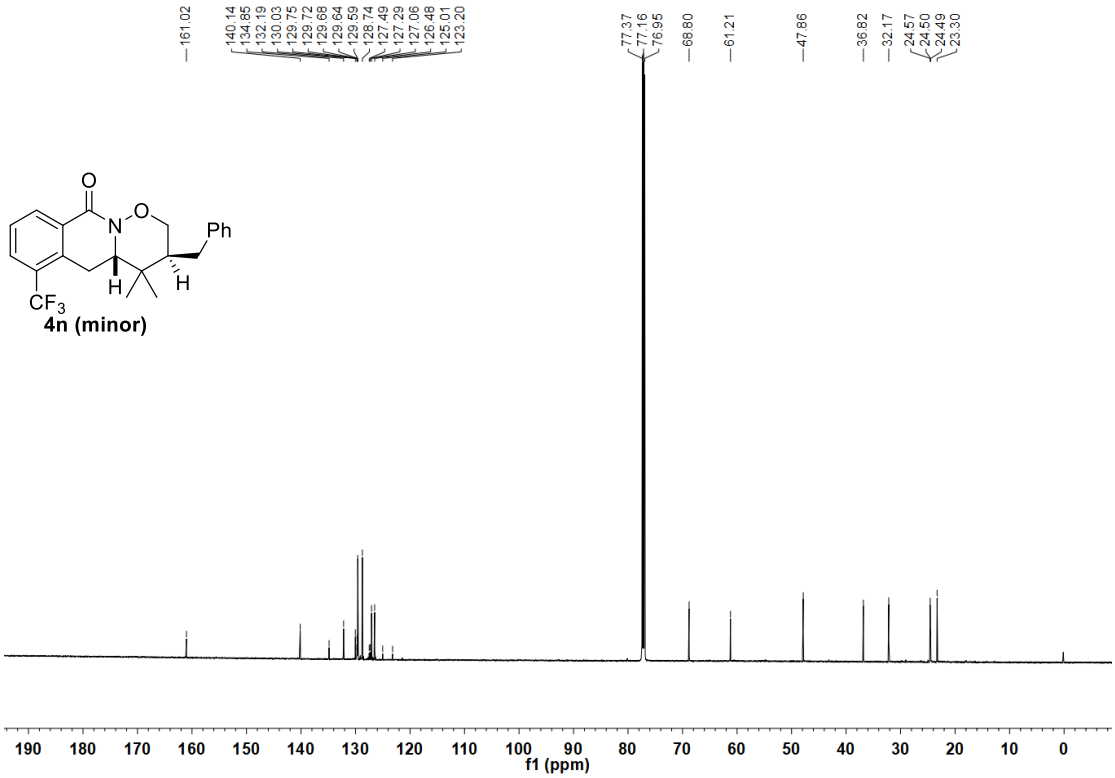


Figure S248. ^{13}C NMR spectra of **4n (minor)** (151 MHz, $CDCl_3$)

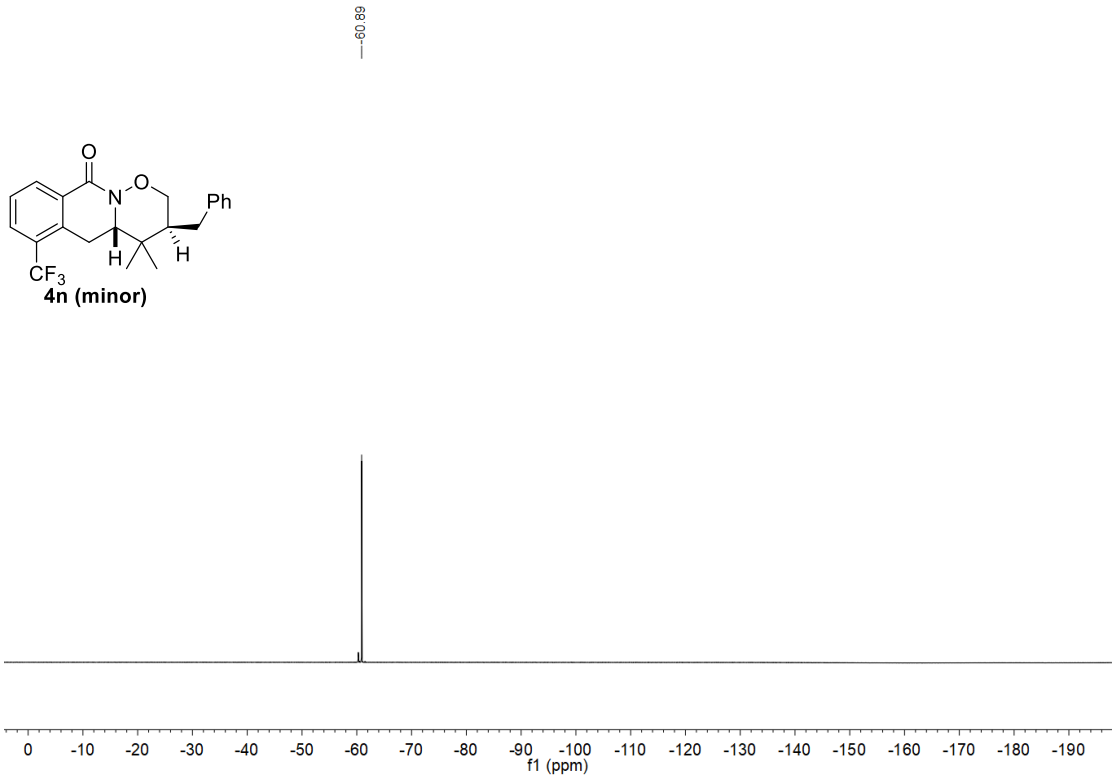


Figure S249. ^{19}F NMR spectra of **4n (minor)** (282 MHz, $CDCl_3$)

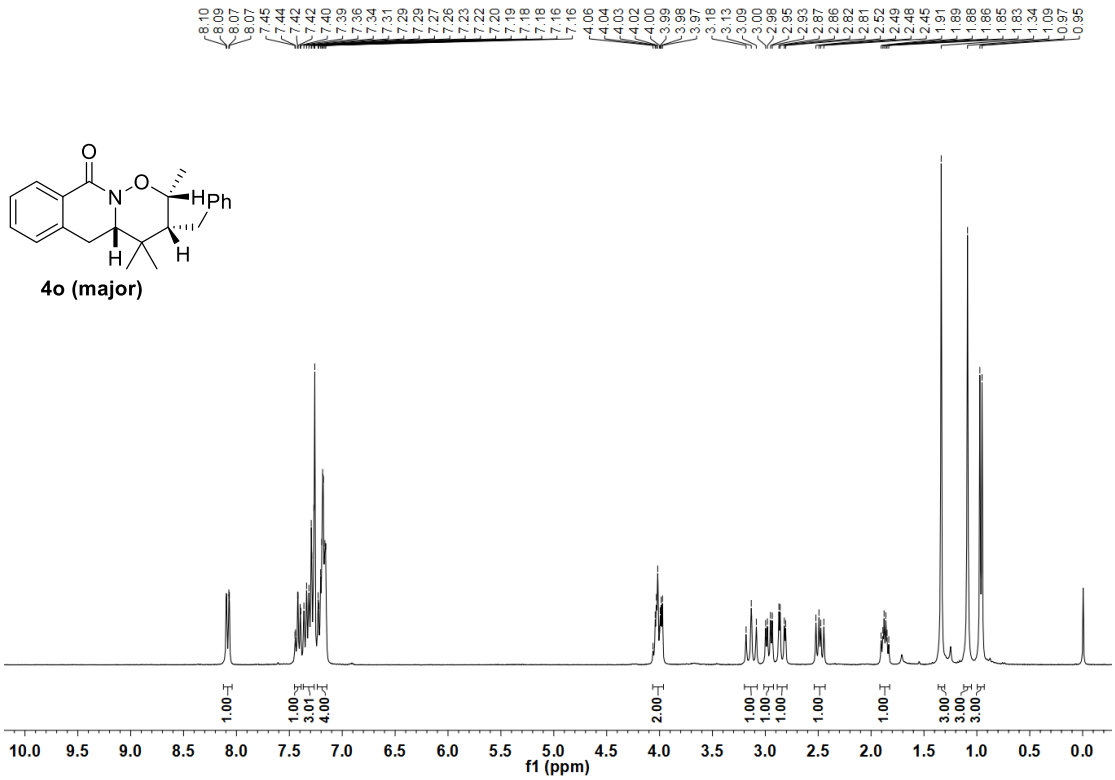


Figure S250. ^{1}H NMR spectra of **4o (major)** (600 MHz, $CDCl_3$)

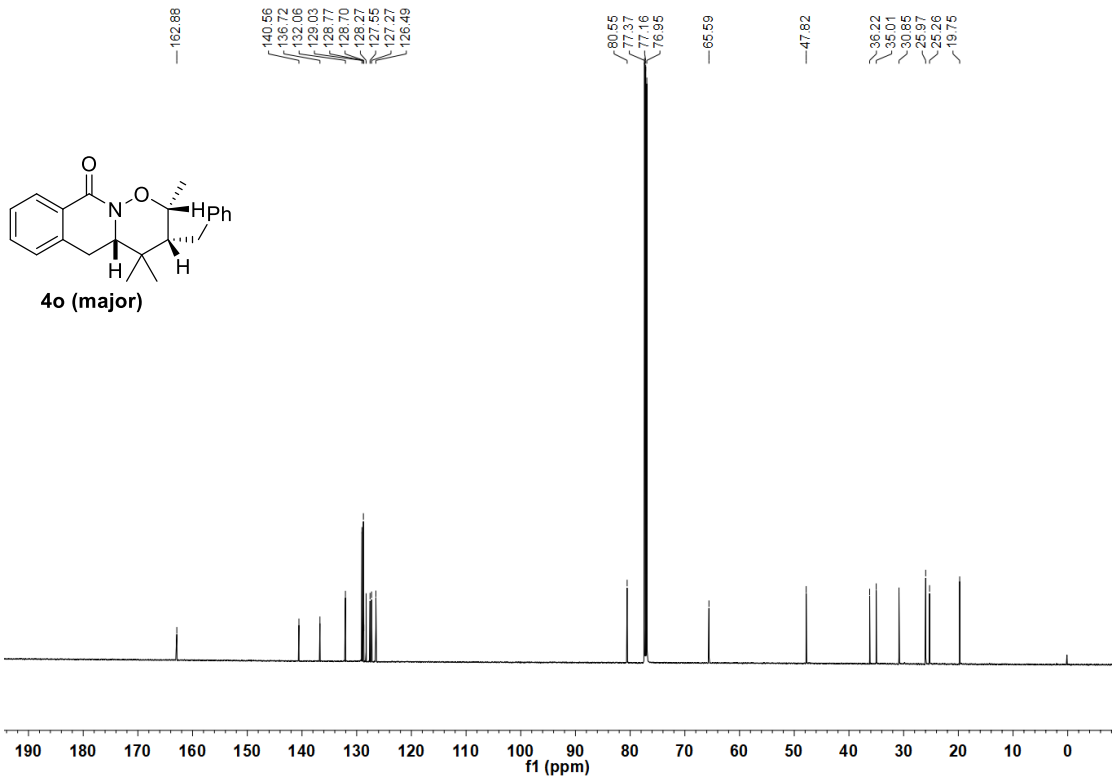


Figure S251. ^{13}C NMR spectra of **4o (major)** (151 MHz, $CDCl_3$)

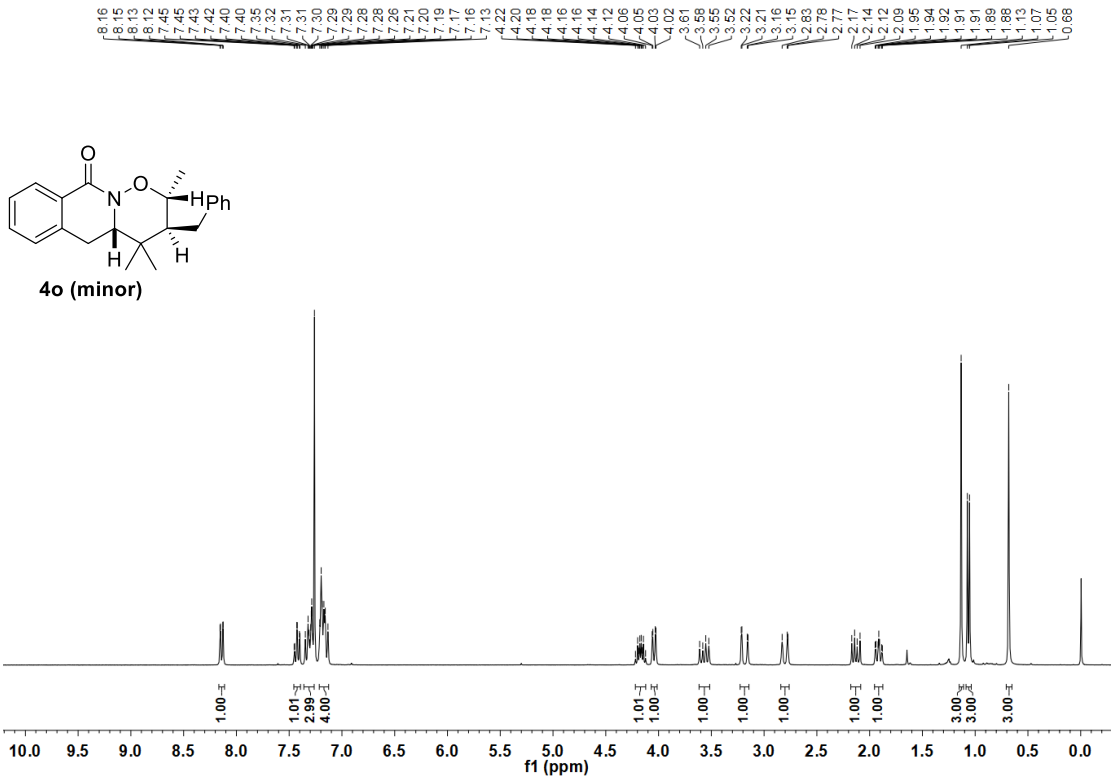


Figure S252. ^{1}H NMR spectra of **4o (minor)** (600 MHz, $CDCl_3$)

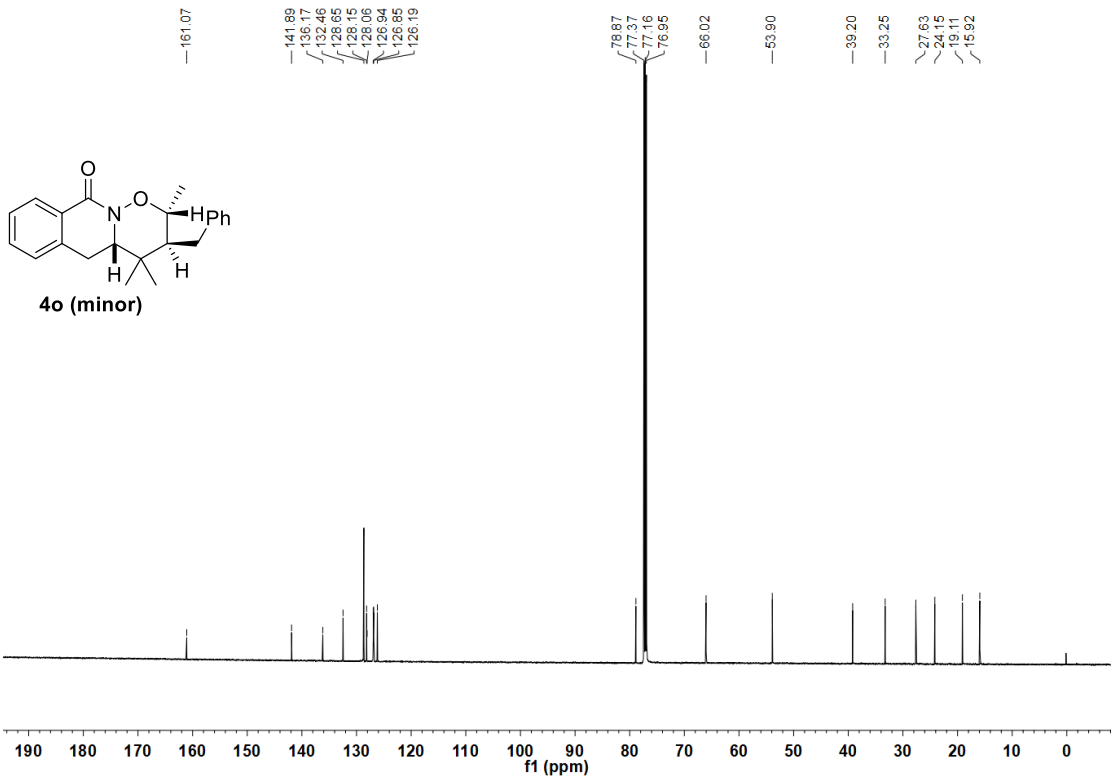


Figure S253. ^{13}C NMR spectra of **4o (minor)** (151 MHz, $CDCl_3$)

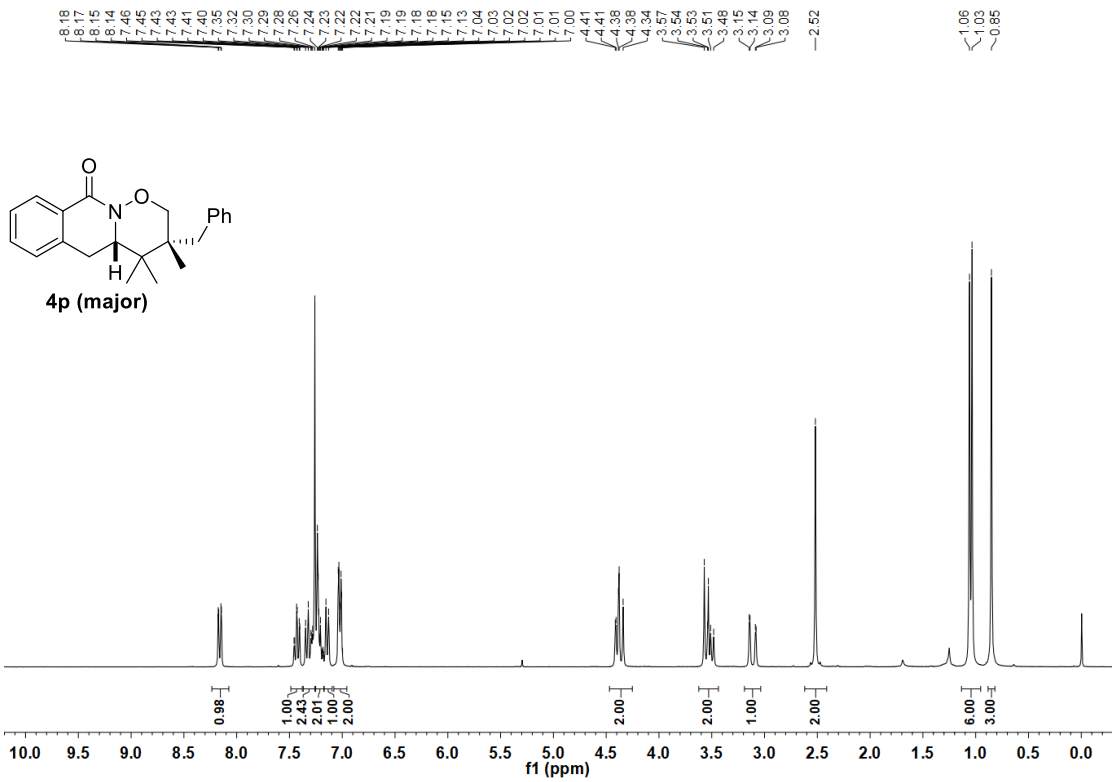


Figure S254. ^{1}H NMR spectra of **4p (major)** (600 MHz, $CDCl_3$)

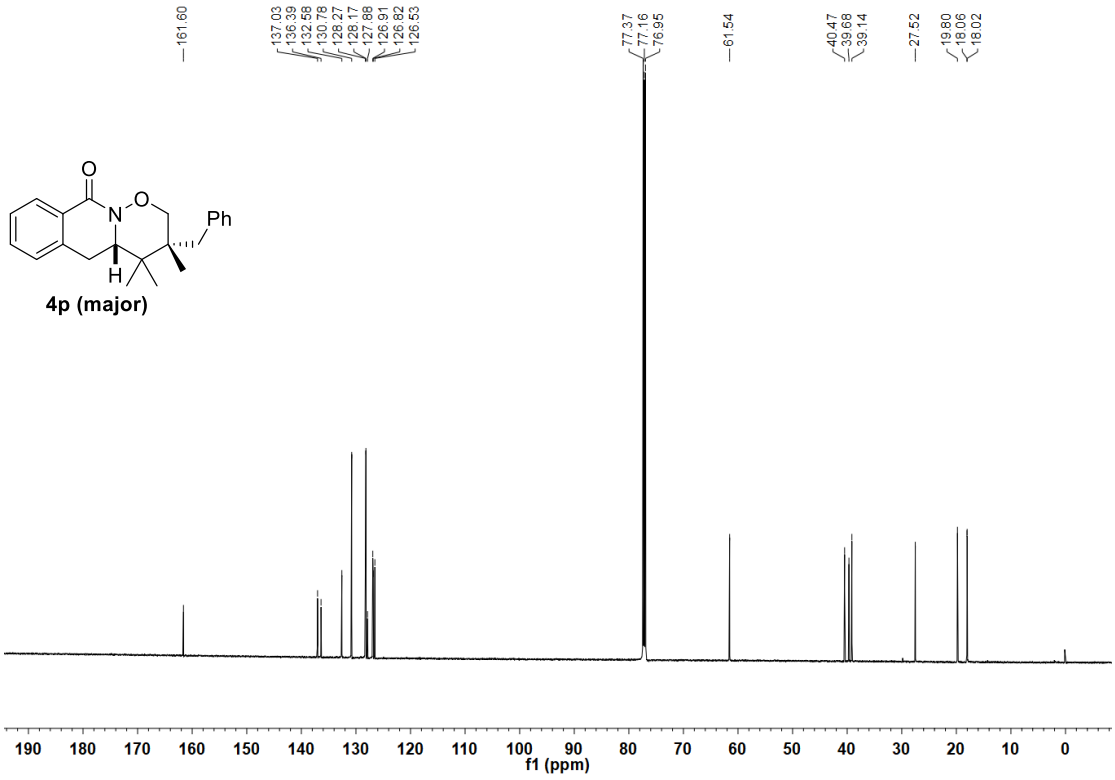


Figure S255. ^{13}C NMR spectra of **4p (major)** (151 MHz, $CDCl_3$)

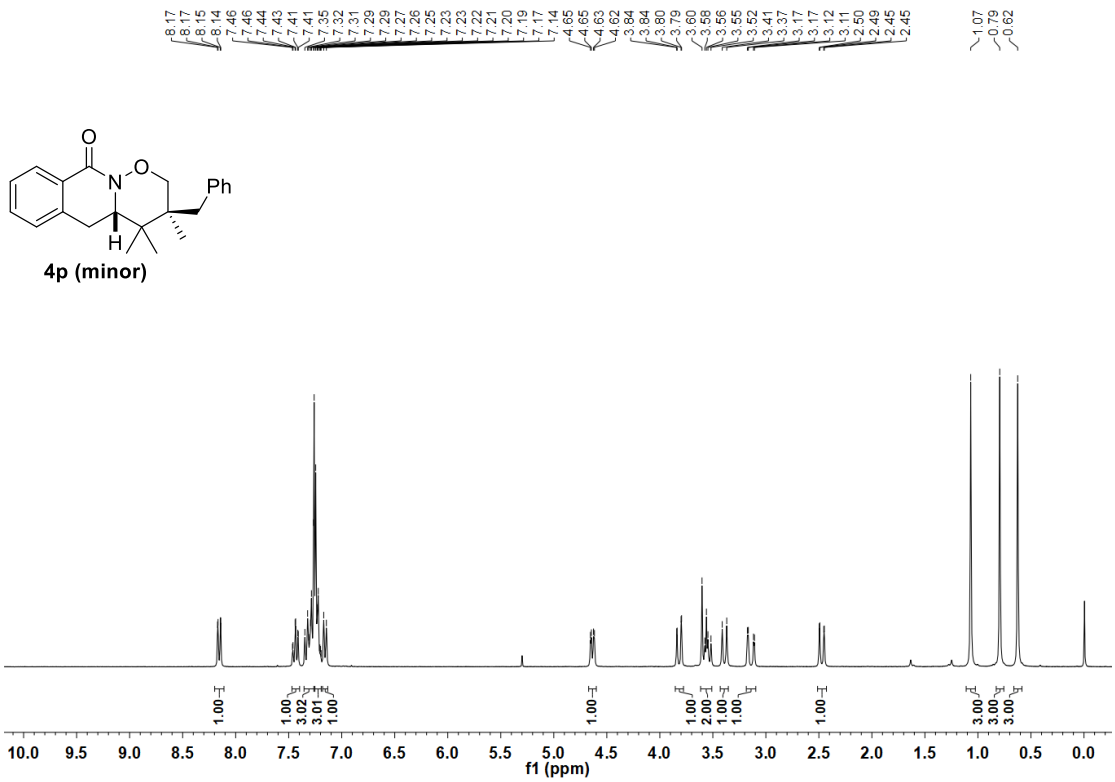


Figure S256. ^{1}H NMR spectra of **4p (minor)** (600 MHz, $CDCl_3$)

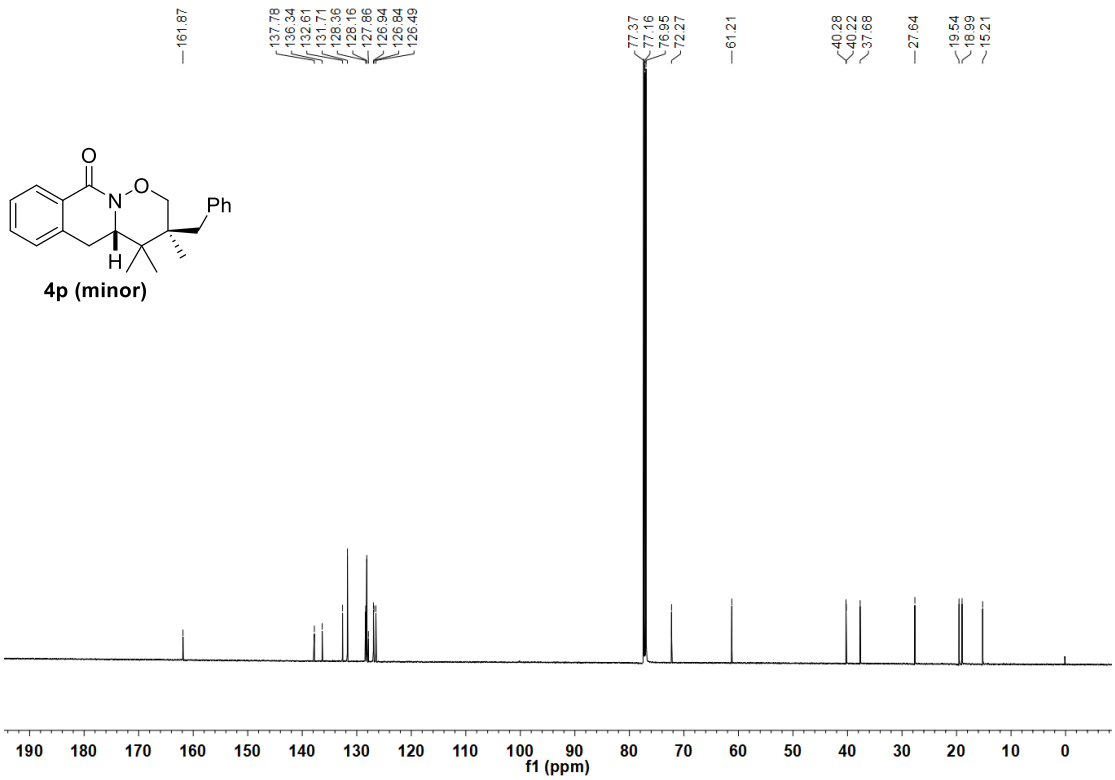


Figure S257. ^{13}C NMR spectra of **4p (minor)** (151 MHz, $CDCl_3$)