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Supporting Information

Catalytic asymmetric Michael and Nef-type sequential reaction of nitroolefin with azlactone to construct oxazole-fused succinimide

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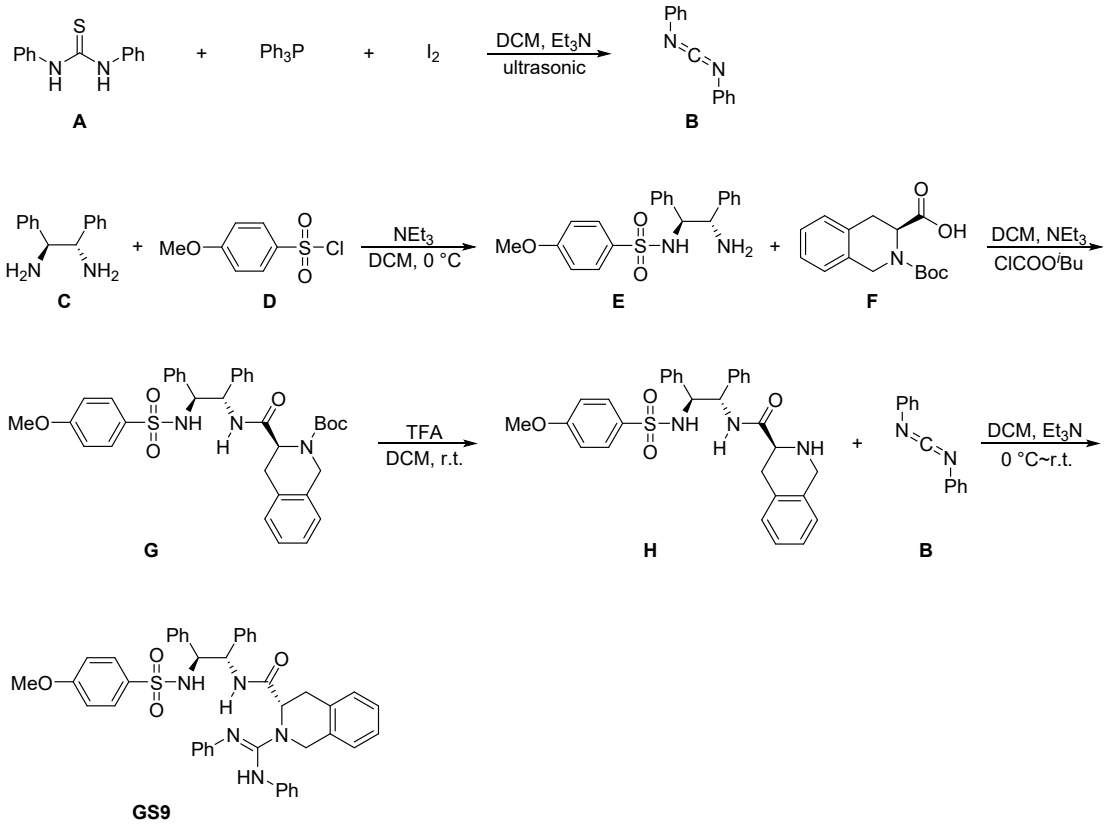
contents

1. General information

^{1}H NMR spectra were recorded on Bruker ASCEND™ (400 MHz). Chemical shifts are reported in ppm from the tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$, δ = 7.26). Data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz), integration. $^{13}C\{^{1}H\}$ NMR data were collected on Bruker ASCEND™ (100 MHz) with complete proton decoupling. $^{19}F\{^{1}H\}$ NMR spectra were collected on Bruker ASCEND™ (376 MHz) with complete proton decoupling. Melting points (M.p.) were determined using OptiMelt automated melting point system. High resolution mass spectra (HRMS) analyses were recorded on Thermo Scientific Q Exactive hybrid quadrupole-Orbitrap mass spectrometer (ESI Source) and methanol were used to dissolve the sample. Enantiomeric excesses (ee) were determined by UPC^2 analysis by using the corresponding commercial chiralpak column as stated in the experimental procedures at 35 °C with PDA detector. Optical rotations were measured on a Rudolph Autopol V automatic polarimeter and are reported as follows: $[\alpha]^{T}_{\lambda}$ = (c = g/100 mL, in solvent). IR spectra were recorded on Bruker TENSOR II IR spectrophotometer. Unless otherwise indicated, reagents obtained from commercial sources were used without further purification. Chemical reagents were purchased from Alfa, Adamas, Ark, Aladdin, Innochem, TCI, etc. Solvents were dried and distilled prior to use according to the standard methods. The azlactones were prepared according to literature procedure.[1] The nitroolefins were synthesized by following the literature procedure.[2] Unless otherwise indicated, all reactions below were carried out without the protection of inert gas.

2. Typical procedure for the preparation of guanidines



GS9

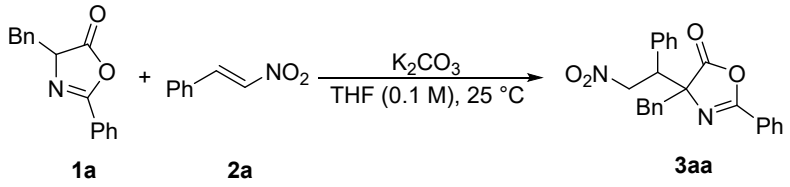
To a solution of iodine (12.0 mmol) and triphenylphosphine (12.0 mmol) in DCM (70 mL) was added a solution of thiourea or urea (10.0 mmol) and NEt_3 (25.0 mmol) in DCM (70 mL) under sonication. The reaction mixture was further sonicated until completion of the reaction as indicated by TLC. The crude mixture was concentrated under reduced pressure then purified by flash chromatograph using hexane to give the carbodiimide (75% yield).

A solution of sulfonyl chloride **D** (10.0 mmol) was slowly added to a stirred solution of diamine **C** (10.0 mmol), NEt_3 (11.0 mmol) in DCM (25 mL). The resulting mixture was stirred for another 2 hours, washed twice with water (25 mL) and dried over Na_2SO_4. The solvent was removed *in vacuo* to give a white solid **E**. To a solution of **F** in DCM (40 mL) was added NEt_3 (11.0 mmol), isobutyl carbonochloridate (11.0 mmol) at 0 °C under stirring. After 10 min, **E** was added. The reaction was allowed to warm to room temperature for another 2 hours. The mixture was washed with 1 N $KHSO_4$ solution, saturated $NaHCO_3$ solution, and brine, dried over anhydrous Na_2SO_4 and concentrated to get a white solid **G**. Then, TFA (10 mL) was added to the DCM (10 mL) solution of **G**, and stirred until the reaction finished (1 h). The *p*H value of the mixture was brought into the range of 10–12 by the addition of 2 N NaOH solution. The aqueous phase was extracted with DCM (3 × 30 mL). The combined organic phase was washed with brine, dried over anhydrous Na_2SO_4 and concentrated and then purified through flash chromatograph to give a white solid **H** (70% yield). To a solution of **H** (3.0 mmol) and **B** (3.6 mmol) in DCM (15 mL) was added NEt_3 (3.0 mmol). The resulting mixture was stirred for another 4 hours at room temperature. The crude mixture was concentrated under reduced pressure then purified by flash chromatograph to give the guanidine (50% yield)

For other catalysts, the synthesis method could be found in the literature.[3]

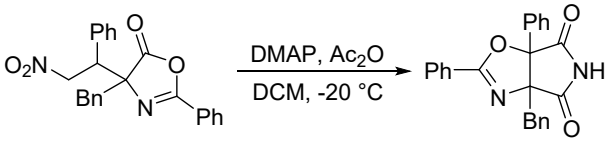
3. General procedure for the catalytic asymmetric reaction

3.1 General procedure for the preparation of the racemic products



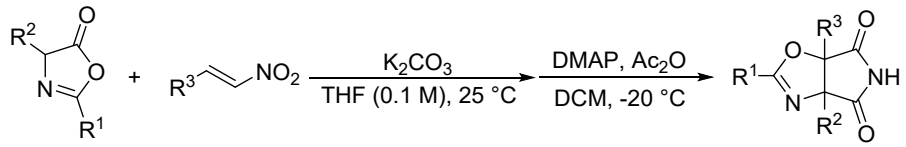
1a **2a** **3aa**

The reaction was conducted with azlactone **1a** (0.10 mmol), nitroolefin **2a** (1.0 equiv, 0.10 mmol), and potassium carbonate (K_2CO_3, 20 mol %, 2.8 mg) in THF (1.0 mL) at 25 °C. Upon the completion of this reaction, the mixture was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:15) to afford the corresponding product **3aa**.



3aa **4aa**

The reaction was conducted with **3aa** (0.10 mmol), 4-dimethylaminopyridine (DMAP, 4.0 equiv, 48.8 mg), and acetic anhydride (Ac_2O, 4.0 equiv, 37.6 μL) in DCM (1.0 mL) at –20 °C. Upon the completion of this reaction, the solution was dilute with water (1 mL) and then was extracted with DCM (3 x 5 mL) and the organic phase was washed with brine (10 mL), dried (Na_2SO_4) and concentrated. The resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:4, v/v) to afford the corresponding racemic product **4aa** (>95:5 dr).

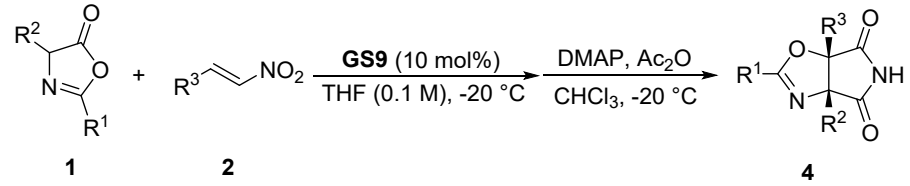


1 **2** **4**

The reaction was conducted with azlactone **1** (0.10 mmol), nitroolefin **2** (1.0 equiv, 0.10 mmol), and potassium carbonate (K_2CO_3, 20 mol %, 2.8 mg) in THF (1.0 mL) at 25 °C. Upon the completion of this reaction, the mixture was filtered on Celite and concentrated *in vacuo*. then the residue was dissolved in DCM (1.0 mL), 4-dimethylaminopyridine (DMAP, 4.0 equiv, 48.8 mg), and acetic anhydride (Ac_2O, 4.0 equiv, 37.6 μL) was added to this solution at –20 °C, Then the mixture was stirred at the same temperature. Upon the completion of this reaction, the solution was dilute with water (1 mL) and then was extracted with DCM (3 x 5 mL) and the organic phase was washed with brine (10 mL), dried (Na_2SO_4) and concentrated. The resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:5–1:2, v/v) to afford

the corresponding racemic product **4**.

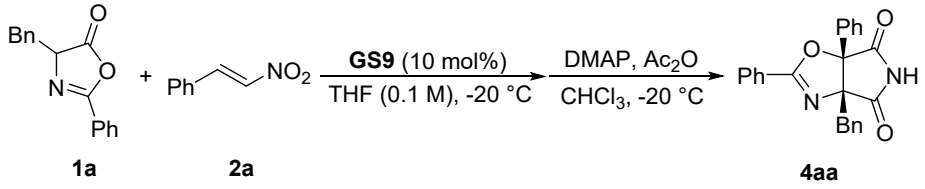
3.2 General procedure for the catalytic asymmetric reactions



1 **2** **4**

Nitroolefin **2** (1.0 equiv, 0.10 mmol), **GS9** (10 mol%, 7.4 mg) and THF (1.0 mL) were added to an oven-dried reaction tube. After the mixture has been stirred at –20 °C for 10 min, azlactone **1** (0.10 mmol) was added. Then the mixture was stirred at –20 °C for indicated time. Upon the completion of this reaction, the volatile was removed under reduced pressure, then the residue was dissolved in $CHCl_3$ (1.0 mL), 4-dimethylaminopyridine (DMAP, 3.2 equiv, 39.0 mg), and acetic anhydride (Ac_2O, 3.2 equiv, 30.1 μL) were added to this solution at –20 °C. Then the mixture was stirred at the same temperature for 72 h. Upon the completion of this reaction, the solution was dilute with water (1 mL) and then was extracted with DCM (3 x 5 mL). The organic phase was washed with brine (10 mL), dried (Na_2SO_4) and concentrated. The resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:5–1:2, v/v) to afford the corresponding chiral product **4**.

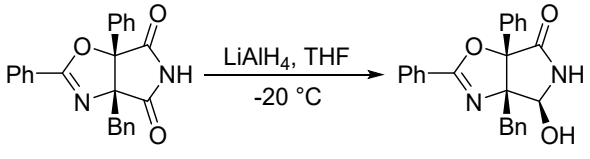
3.3 Experimental procedure for the scale-up reaction



1a **2a** **4aa**

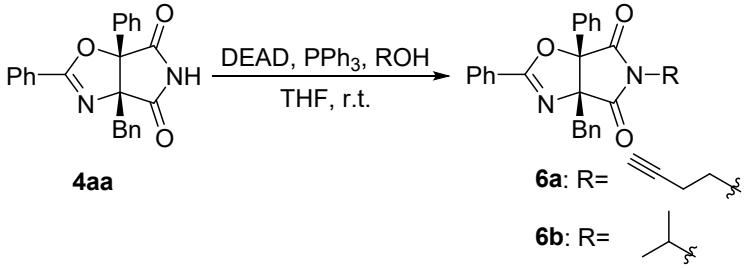
Nitroolefin **2** (4.0 mmol, 0.596 g), **GS9** (10 mol%, 0.294 g) and THF (40 mL) were added to an oven-dried flask. After the mixture has been stirred at -20 °C for 10 min, azlactone **1** (4.0 mmol, 1.00 g) was added in portions. Then the mixture was stirred at -20 °C for 48 h. Upon the completion of this reaction, the volatile was removed under reduced pressure, then the residue was dissolved in $CHCl_3$ (40 mL), 4-dimethylaminopyridine (DMAP, 12.8 mmol, 1.5616 g), and acetic anhydride (Ac_2O, 12.8 mmol, 1.2 mL) were added to this solution at -20 °C. Then the mixture was stirred at the same temperature for 72 h. Upon the completion of this reaction, the solution was dilute with water (40 mL) and then was extracted with DCM (3 x 20 mL) and the organic phase was washed with brine, dried (Na_2SO_4) and concentrated. The resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:4) to afford the corresponding product **4aa** (1.419 g, 93% yield, >95:5 dr, 92% ee).

3.4 Experimental procedure for further transformation



4aa **5**

To a suspension of $LiAlH_4$ (0.25 mmol) in dry THF (1.25 mL), was added a solution of **4aa** (76.4 mg, 0.2 mmol) in dry THF (40 mL) at −20 °C under a nitrogen atmosphere. Then the mixture was stirred at −20 °C for 3 h. Saturated Na_2SO_4 (aq, 0.2 mL) was added to the mixture. After being stirred for 10 min, Na_2SO_4 (56.8 mg, 0.4 mmol) was added to the mixture. The resulting mixture was filtered on Celite and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:1.5, v/v, then ethyl acetate/dichloromethane = 1:15, v/v) to afford product **5**.



4aa

6a: R=

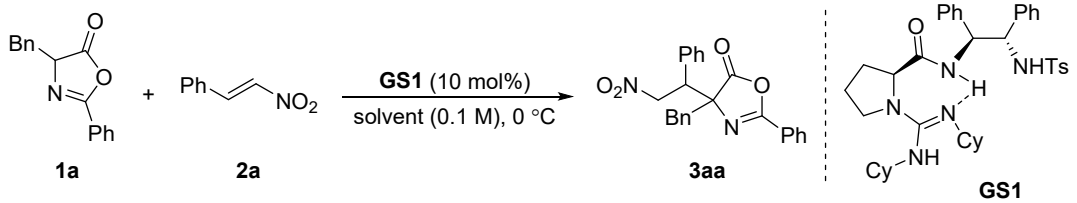
6b: R=

Diethyl azodicarboxylate (DEAD, 1.3 equiv, 0.13 mmol, 20.5 μL) was added to a stirred solution of **4aa** (0.1 mmol, 38.2 mg), triphenylphosphine (PPh_3, 1.3 equiv, 0.13 mmol, 34.1 mg) and alcohol (1.2 equiv, 0.12 mmol) in THF (0.5 mL). After 24 h at room temperature, the reaction mixture was concentrated under reduced pressure, the residue was purified by column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:15, v/v) to afford the product **6**.

4. Optimization of the reaction conditions

4.1 Optimization of the Michael reaction conditions

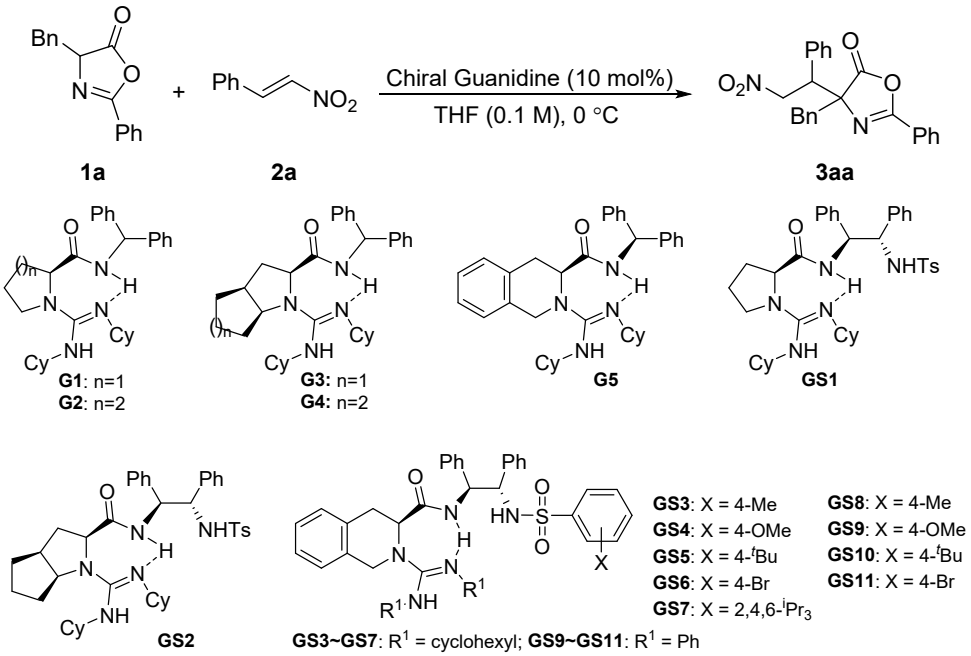
4.1.1 Screening of solvents



Entry[a]	Solvent	Yield (%)[b]	dr[c]	ee (%)[c]
1	DCM	34	88:12	58
2	toluene	51	91:9	62
3	THF	60	92:8	65
4	EtOAc	60	94:6	58
5	Et_2O	58	93:7	55
6	MeOH	20	48:52	18/9
7	MeCN	39	64:36	31/0

[a]Unless otherwise noted, all reactions were carried out with **1a** (0.12 mmol), **2a** (0.10 mmol), and the catalyst (10 mol%) in solvent (0.1 M) at 0 °C for 18 h. [b]Isolated yield. [c]Determined by UPC[2] analysis on a chiral stationary phase.

4.1.2 Screening of guanidines

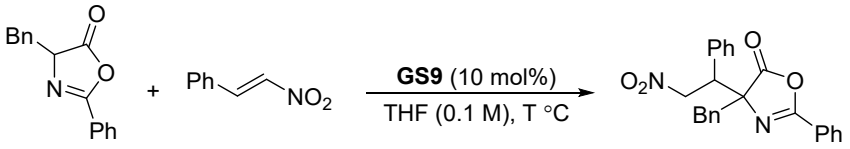


Entry[a]	**Guanidine**	Yield (%)[b]	dr[c]	ee (%)[c]
1	**G1**	51	78:22	32/0
2	**G2**	61	85:15	24/0
3	**G3**	53	79:21	30/25
4	**G4**	48	76:24	31/34
5	**G5**	75	93:7	46
6	**GS1**	60	92:8	65
7	**GS2**	85	91:9	54

8	**GS3**	82	>95:5	72
9	**GS4**	88	95:5	70
10	**GS5**	79	>95:5	77
11	**GS6**	90	94:6	71
12	**GS7**	82	92:8	31
13	**GS8**	87	>95:5	86
14	**GS9**	99	>95:5	90
15	**GS10**	97	>95:5	90
16	**GS11**	93	>95:5	87

[a]Unless otherwise noted, all reactions were carried out with **1a** (0.12 mmol), **2a** (0.10 mmol), and the catalyst (10 mol%) in THF (0.1 M) at 0 °C for 18 h. [b]Isolated yield. [c]Determined by UPC[2] analysis on a chiral stationary phase.

4.1.3. Screening of temperature



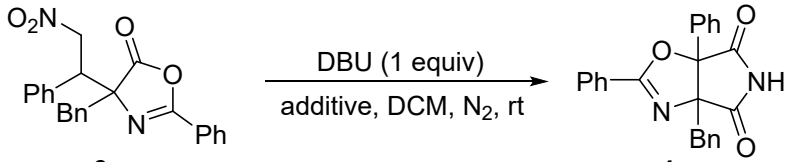
1a **2a** **3aa**

Entry[a]	T (°C)	Yield (%)[b]	dr[c]	ee (%)[c]
1	0	>99	99:1	90
2	−10	>99	>99:1	90
3	−20	>99	>99:1	92
4	−30	98	>99:1	91
5	−40	90	98:2	84

[a]Unless otherwise noted, all reactions were carried out with **1a** (0.12 mmol), **2a** (0.10 mmol), and the catalyst (10 mol%) in THF (0.1 M) at 0 °C for 48 h. [b]Isolated yield. [c]Determined by UPC[2] analysis on a chiral stationary phase.

4.2 Optimization of the Nef-type reaction conditions

4.2.1 Screening of dehydrating agent

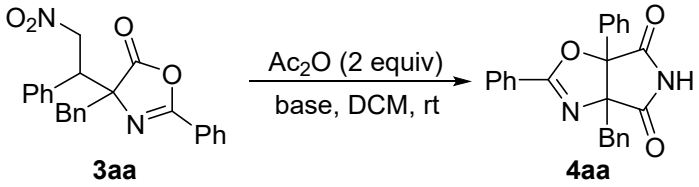


3aa **4aa**

Entry[a]	dehydrating agent	Yield (%)[b]	dr[c]
1	-	18	>95:5
2	DCC (1 equiv)	42	>95:5
3	HBTU (1.2 equiv)	complex	n.d.
4	MsCl (1 equiv)	trace	n.d.
5	$SOCl_2$ (1 equiv)	complex	n.d.
6	Tf_2O (1 equiv)	complex	n.d.
7	Ac_2O (1 equiv)	59	>95:5
8	3Å MS (20 mg)	17	>95:5
9	4Å MS (20 mg)	15	>95:5
10	5Å MS (20 mg)	17	>95:5

[a]Unless otherwise noted, all reactions were carried out with **3aa** (0.10 mmol), DBU (0.1 mmol) and the dehydrating agent in DCM (1.0 mL) at room temperature for 24 h. [b]Isolated yield. [c]Determined by ^1H NMR.

4.2.2 Screening of base

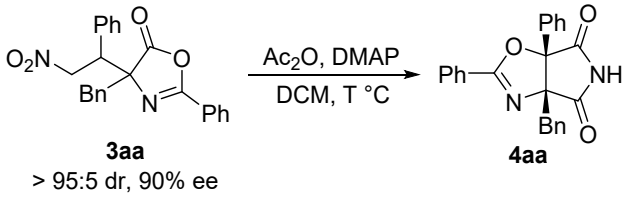


3aa **4aa**

Entry[a]	base	Yield (%)[b]	dr[c]
1	-	n.r.	n.d.
2	DABCO (2.0 equiv)	35	>95:5
3	DBU (3.0 equiv)	63	>95:5
4	KO^{t}Bu (3.0 equiv)	23	>95:5
5	Cs_2CO_3 (3.0 equiv)	10	>95:5
6	DMAP (3.0 equiv)	79	>95:5
7[d]	DMAP (4.0 equiv)	91	>95:5

[a]Unless otherwise noted, all reactions were carried out with **3aa** (0.10 mmol), Ac_2O (0.2 mmol) and base (2–4 equiv) in DCM (1.0 mL) at room temperature for 24 h. [b]Isolated yield. [c]Determined by ^{1}H NMR. [d]Ac_2O (0.4 mmol) was used.

4.2.3. Screening of temperature



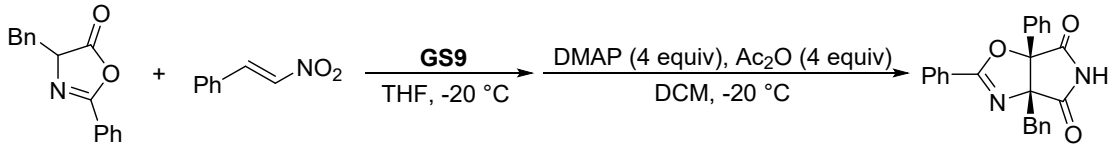
3aa
> 95:5 dr, 90% ee

4aa

Entry[a]	T (°C)	Yield (%)[b]	dr[c]	ee (%)[d]
1	0	80	>95:5	88
2	–10	78	>95:5	88
3	–20	83	>95:5	89
4	–30	79	>95:5	89
5	–40	73	>95:5	89

[a]Unless otherwise noted, all reactions were carried out with **3aa** (0.1 mmol), DMAP (0.40 mmol) and Ac_2O (0.4 mmol) in DCM (0.1 M) at T °C for 72 h. [b]Isolated yield. [c]Determined by ^{1}H NMR. [d]Determined by UPC^2 analysis on a chiral stationary phase.

4.3. Optimization of the sequential reaction conditions



1a **2a** **4aa**

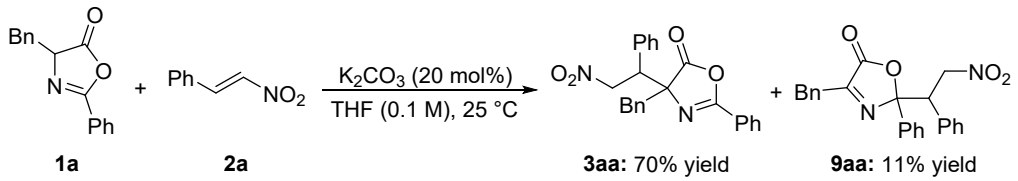
Entry[a]	Solvent	Yield (%)[b]	dr[c]	ee (%)[d]
1	DCM	61	>95:5	82
2	Toluene	53	>95:5	88
3	EtOAc	64	>95:5	84
4	THF	59	>95:5	80
5	$CHCl_3$	70	>95:5	89

6[e]	$CHCl_3$	78	>95:5	90
7[f]	$CHCl_3$	66	>95:5	88
8[e,g]	$CHCl_3$	86	>95:5	90

[a]Unless otherwise noted, all reactions were carried out with **1a** (0.12 mmol), **2a** (0.10 mmol) and **GS9** (10 mol%) in THF (0.1 M) at −20 °C for 48 h. After removal of solvent, DMAP (0.4 mmol), Ac_2O (0.4 mmol) in solvent (1.0 mL) were added, and the mixture continued stirring at −20 °C for 72 h. [b]Isolated yield. [c]Determined by ^1H NMR. [d]Determined by UPC2 analysis on a chiral stationary phase. [e]**1a** (0.1 mmol), **2a** (0.10 mmol) were used. [f]**1a** (0.1 mmol), **2a** (0.12 mmol) were used. [g]DMAP (0.32 mmol), Ac_2O (0.32 mmol) were used.

5. Determination of the structure of the Michael addition product

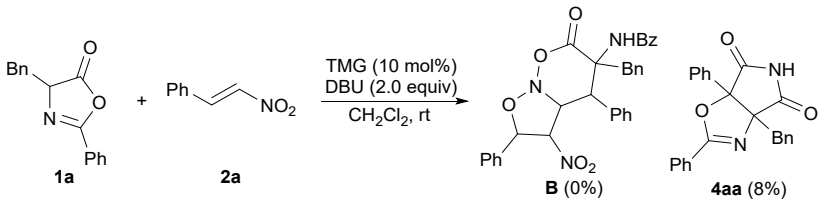
5.1 Preparation of Michael addition products



1a **2a** **3aa:** 70% yield **9aa:** 11% yield

The reaction was conducted with azlactone **1a** (0.10 mmol), nitroolefin **2a** (1.0 equiv, 0.10 mmol), and potassium carbonate (K_2CO_3, 20 mol %, 2.8 mg) in THF (1.0 mL) at 25 °C. Upon the completion of this reaction, the mixture was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:25) to afford the corresponding product **3aa** and **9aa**.

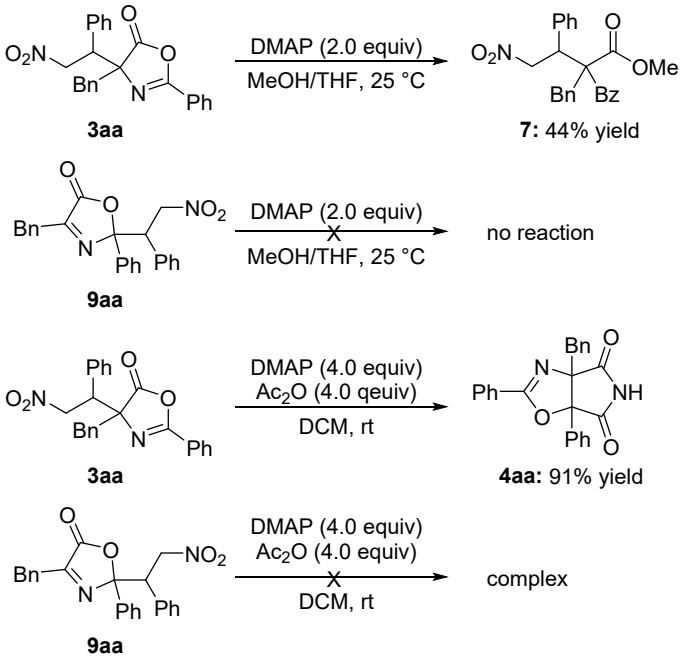
When the Michael addition reaction was catalyzed by potassium carbonate, C4 adduct (**3aa**) and C2 adduct (**9aa**) could be obtained at the same time. Additionally, the pair of diastereoisomers of **3aa** could be isolated by silica gel column chromatography. When the Michael addition reaction was catalyzed by chiral guanidine-sulfonamide, the formation of C2 adduct would be repressed obviously and no **9aa** was observed.



1a **2a** **B** (0%) **4aa** (8%)

To our surprise when azlactone 1a and nitroolefin 2a were treated with TMG and excessive DBU, a fused succinimide oxazoline **4aa** was isolated in trace amount, which intrigued us for sequential transformation.

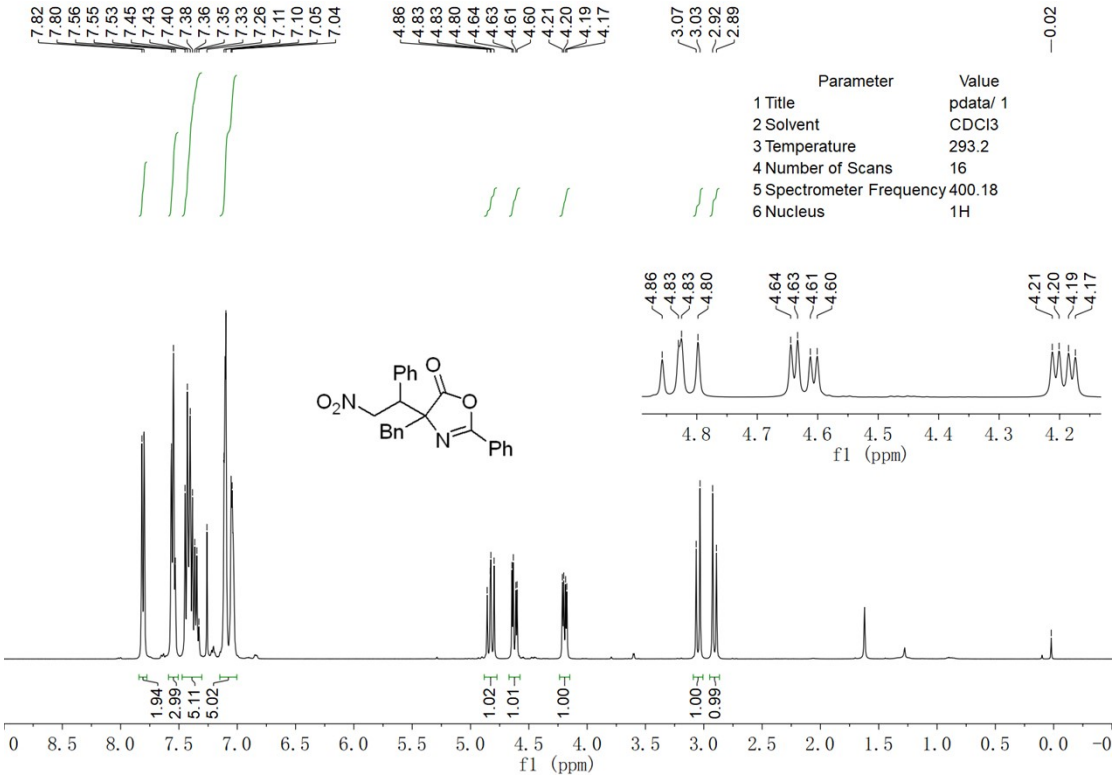
5.2 Transformation of Michael addition products

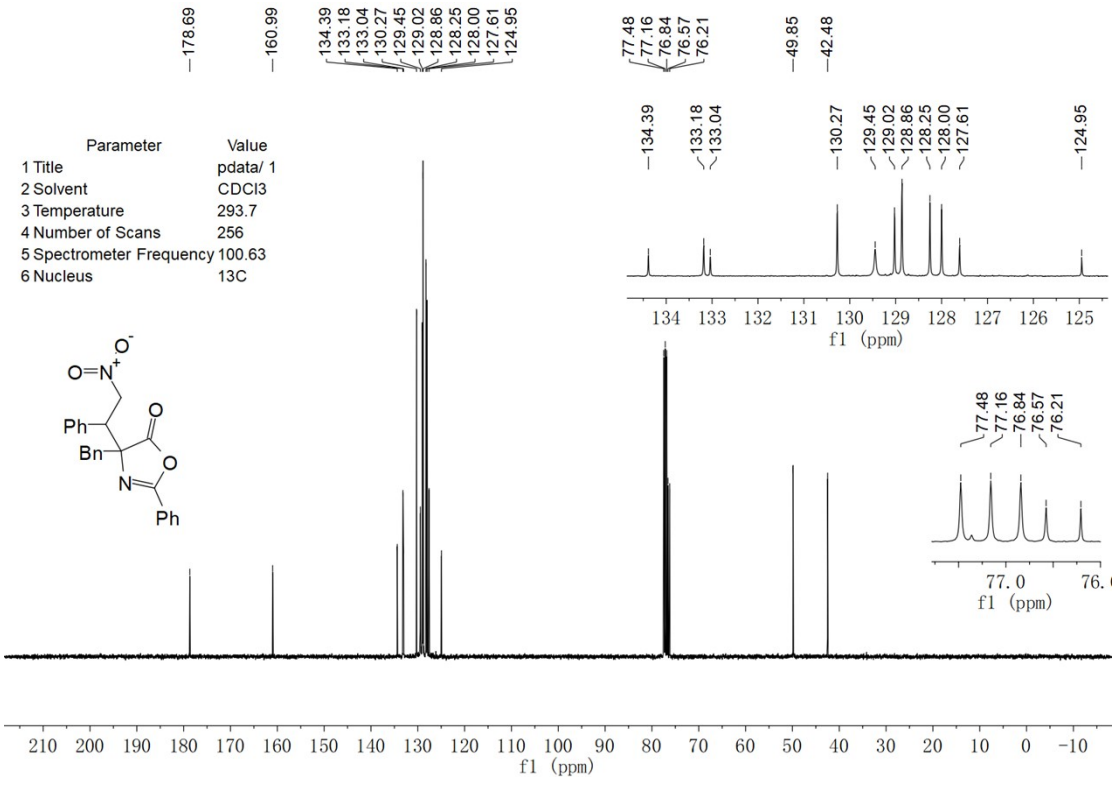


In order to confirm the structure of the Michael addition products, the following transformation experiments were designed. The ring-opening reaction of **3aa** in methanol could be readily carried out to yield the lactonization product **7**, whereas **9aa** fails to react under the same conditions. The Nef-type reaction of **3aa** could also be readily carried out under standard conditions to yield **4aa**, whereas **9aa** will decompose under the same conditions. These results indicate that **3aa** is the C4 adduct and **9aa** might be the C2 adduct.

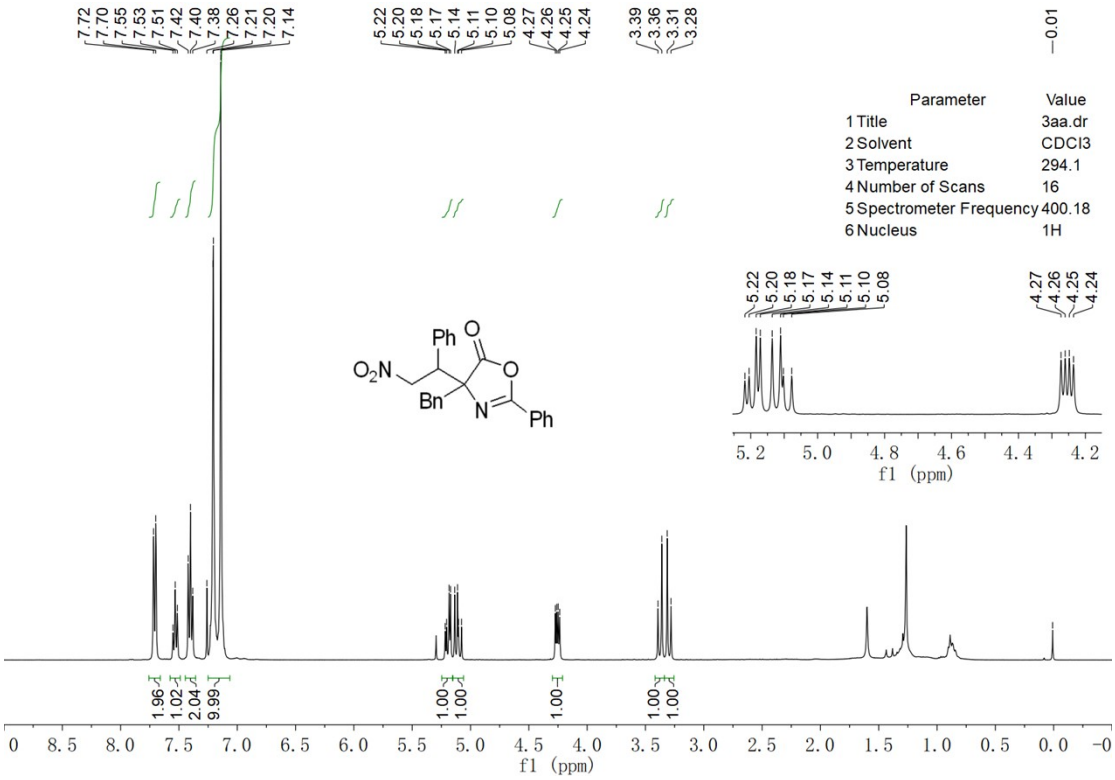
5.3 Copies of NMR spectra

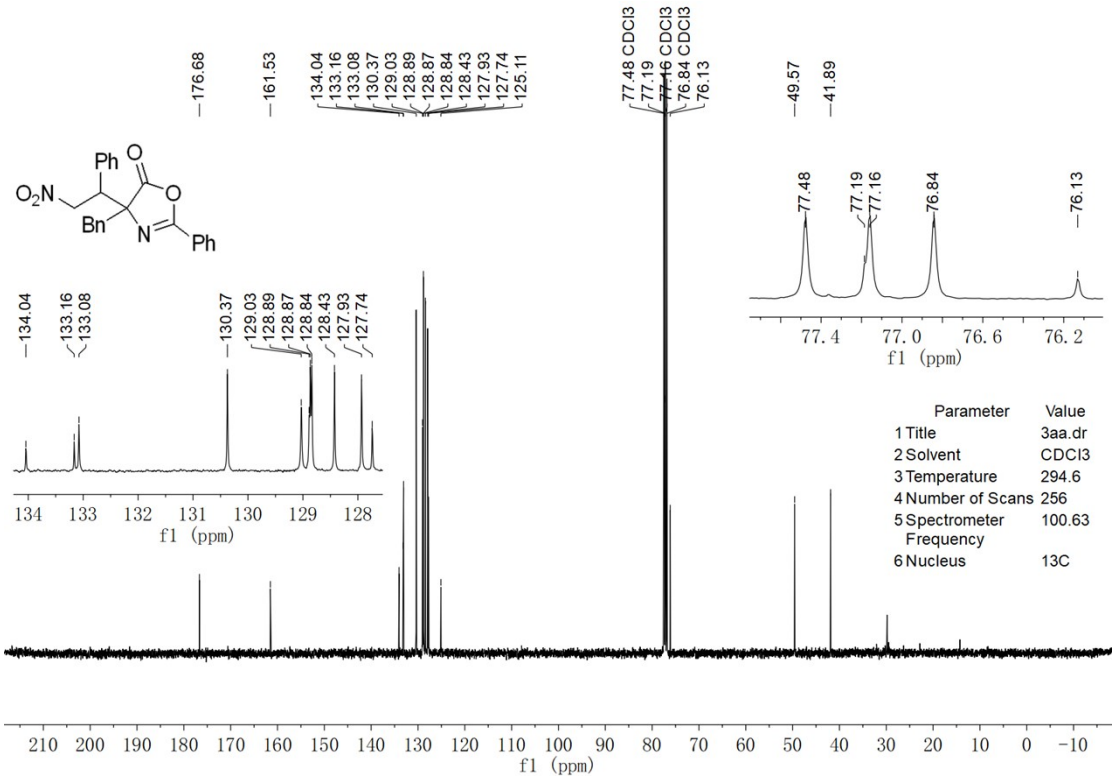
3aa



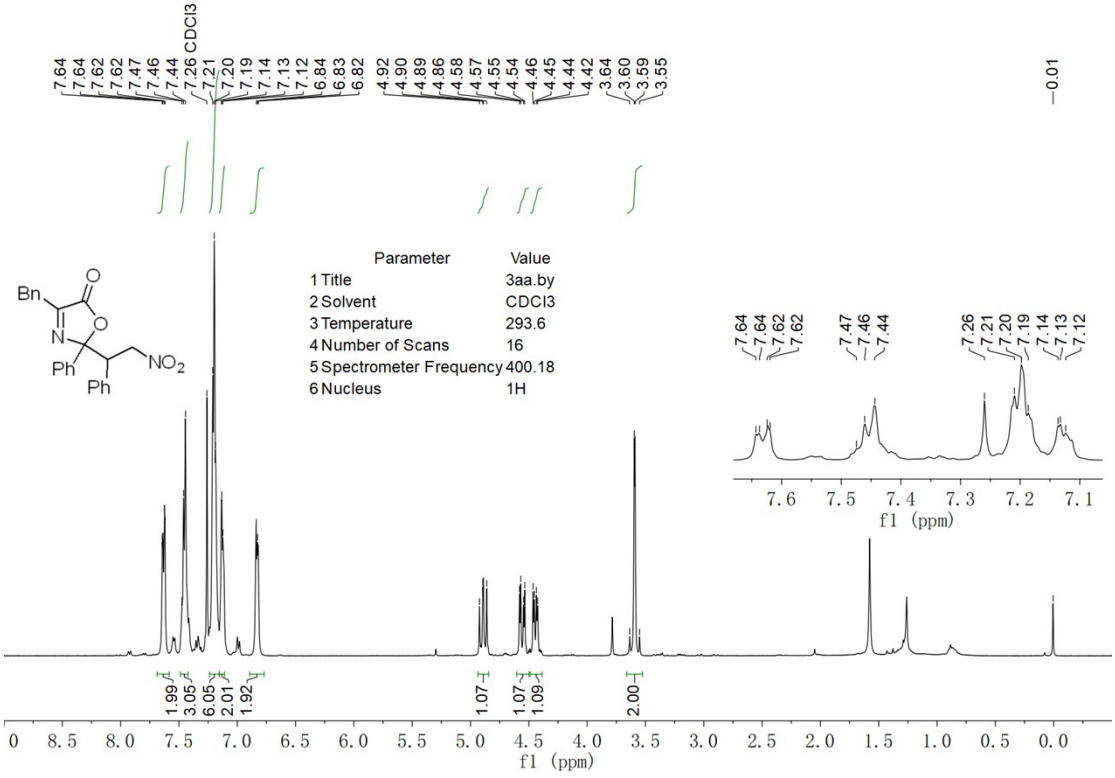


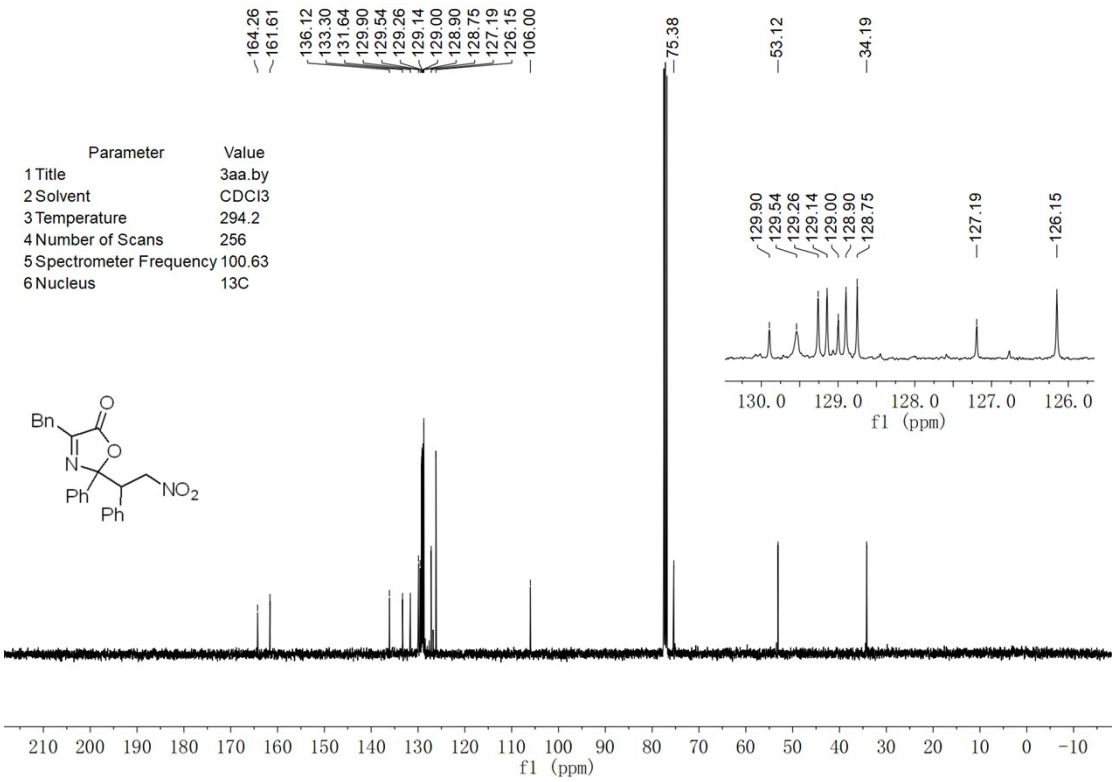
The diastereoisomer of **3aa**



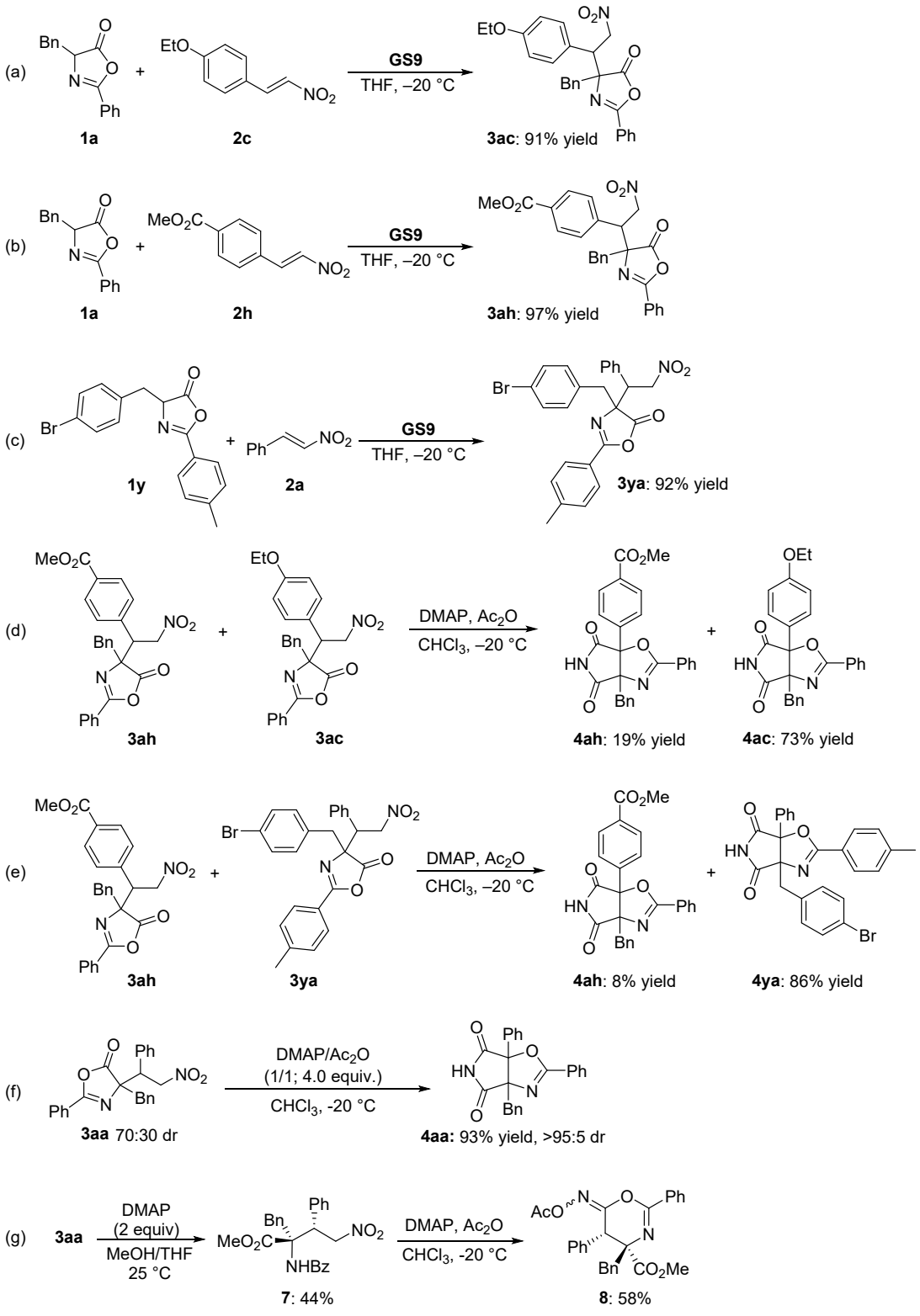


9aa (C2 adduct)





6. Control experiments



Procedure:

(a) Nitroolefin **2c** (0.10 mmol, 19.3 mg), **GS9** (10 mol %, 7.4 mg) and THF (1.0 mL) were added to an oven-dried reaction tube. After the mixture has been stirred at –20 °C for 10 min, azlactone **1a** (0.10 mmol, 25.1 mg) was added. Then the mixture was stirred at –20 °C for 48 h. Upon the

completion of this reaction, the resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:10, v/v) to afford the corresponding product **3ac**.

(b) Nitroolefin **2h** (0.10 mmol, 20.7 mg), **GS9** (10 mol %, 7.4 mg) and THF (1.0 mL) were added to an oven-dried reaction tube. After the mixture has been stirred at –20 °C for 10 min, azlactone **1a** (0.10 mmol, 25.1 mg) was added. Then the mixture was stirred at –20 °C for 48 h. Upon the completion of this reaction, the resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:10, v/v) to afford the corresponding product **3ah**.

(c) Nitroolefin **2a** (0.10 mmol, 14.9 mg), **GS9** (10 mol %, 7.4 mg) and THF (1.0 mL) were added to an oven-dried reaction tube. After the mixture has been stirred at –20 °C for 10 min, azlactone **1y** (0.10 mmol, 34.4 mg) was added. Then the mixture was stirred at –20 °C for 48 h. Upon the completion of this reaction, the resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:15, v/v) to afford the corresponding product **3ya**.

(d) **3ah** (0.09 mmol, 41.2 mg), **3ac** (0.09 mmol, 40.0 mg) and $CHCl_3$ (2.0 mL) were added to an oven-dried reaction tube, 4-dimethylaminopyridine (DMAP, 0.72 mmol, 87.8 g), and acetic anhydride (Ac_2O, 0.72 mmol, 67.7 μL) was added to this solution at –20 °C, then the mixture was stirred at the same temperature for 72 h. Upon the completion of this reaction, the solution was dilute with water (1 mL) and then was extracted with DCM (3 x 5 mL) and the organic phase was washed with brine (10 mL), dried (Na_2SO_4) and concentrated. The resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:5–1:2, v/v) to afford the corresponding product **4ah** and **4ac**.

(e) **3ah** (0.09 mmol, 41.2 mg), **3ya** (0.09 mmol, 44.4 mg) and $CHCl_3$ (2.0 mL) were added to an oven-dried reaction tube, 4-dimethylaminopyridine (DMAP, 0.72 mmol, 87.8 g), and acetic anhydride (Ac_2O, 0.72 mmol, 67.7 μL) was added to this solution at –20 °C, then the mixture was stirred at the same temperature for 72 h. Upon the completion of this reaction, the solution was dilute with water (1 mL) and then was extracted with DCM (3 x 5 mL) and the organic phase was washed with brine (10 mL), dried (Na_2SO_4) and concentrated. The resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:5–1:2, v/v) to afford the corresponding product **4ah** and **4ya**.

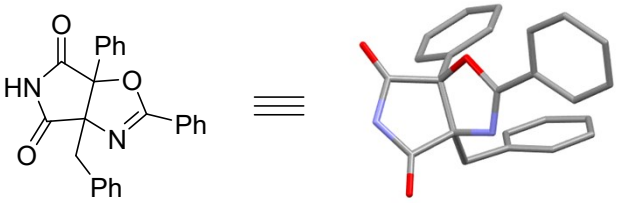
(f) **3aa** (0.10 mmol, 40.0 mg) and $CHCl_3$ (1.0 mL) were added to an oven-dried reaction tube, 4-dimethylaminopyridine (DMAP, 0.40 mmol, 48.8 g), and acetic anhydride (Ac_2O, 0.40 mmol, 37.6 μL) were added to this solution at –20 °C, then the mixture was stirred at the same temperature for 72 h. Upon the completion of this reaction, the solution was dilute with water (1 mL) and then was extracted with DCM (3 x 5 mL) and the organic phase was washed with brine (10 mL), dried (Na_2SO_4) and concentrated. The resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:4, v/v) to afford the corresponding product **4aa**.

(g) **3aa** (0.30 mmol, 12.0 mg), 4-dimethylaminopyridine (DMAP, 0.60 mmol, 73.2 g), MeOH (0.6 mL) and THF (2.4 mL) were added to an oven-dried reaction tube, then the mixture was stirred at the room temperature for 72 h. The mixture was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:6) to afford the corresponding product **7**. Then, **7** (0.10 mmol, 43.2 mg) and $CHCl_3$ (1.0 mL) were added to an oven-dried reaction tube,

4-dimethylaminopyridine (DMAP, 0.40 mmol, 48.8 g), and acetic anhydride (Ac_2O, 0.40 mmol, 37.6 μL) were added to this solution at −20 °C, then the mixture was stirred at the same temperature for 72 h. Upon the completion of this reaction, the solution was dilute with water (1 mL) and then was extracted with DCM (3 x 5 mL) and the organic phase was washed with brine (10 mL), dried (Na_2SO_4) and concentrated. The resulting crude product was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether = 1:5, v/v) to afford the corresponding product **8**.

7. X-ray crystallography of (±)-4aa

The colourless crystal in block-shape, with approximate dimensions of 0.138 × 0.300 × 0.500 mm^3, was selected and mounted for the single-crystal X-ray diffraction. The data set was collected by Bruker D8 Venture Photon II diffractometer at 173(2)K equipped with micro-focus Cu radiation source (K_α = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package[a, b, c, d]. The relatively large standard uncertainty indicates that the structural data alone should not be used to confirm absolute stereochemistry, but should be used in conjunction with the established stereochemistry of the precursor compound. The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested[e]. CCDC 2336953 contains the supplementary crystallographic data which can be obtained free of charge from The Cambrige Crystallographic Data Centere via https://www.ccdc.cam.ac.uk/structures/.



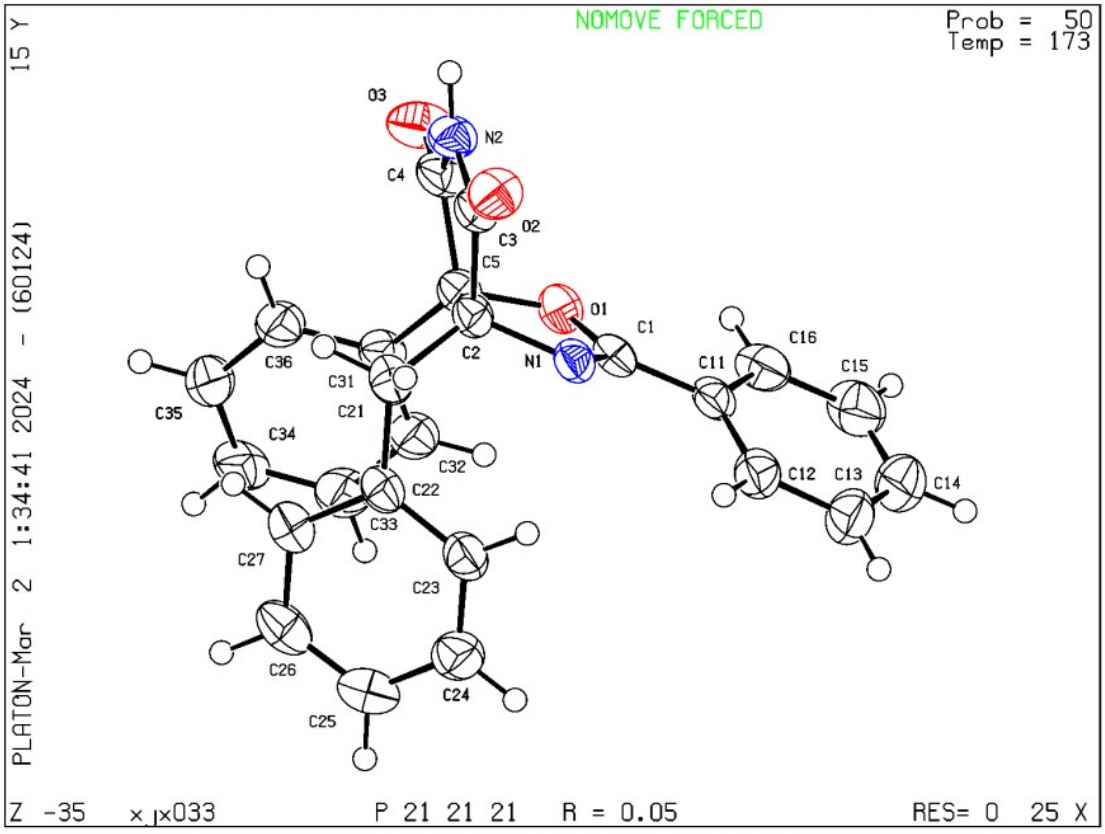


Figure 1. The thermal ellipsoid figure of **4aa** with 50% probabilities.

The crystal of product **4aa** was obtained in the solvents of toluene and hexane by diffusion. CCDC: 2336953.

Crystallographic Data for C24 H18 N2 O3.

Formula	C24 H18 N2 O3
Formula mass (amu)	382.40
Space group	$P2_12_12_1$
a (Å)	8.6718(3)
b (Å)	9.0165(3)
c (Å)	24.3506(9)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å^3)	1903.96(12)
Z	4
λ (Å)	1.54178
T (K)	173(2) K
ρ_{calcd} (g cm^{-3})	1.334
μ (mm^{-1})	0.720
Transmission factors	0.587–1.000
θ_{max} (deg)	79.911
No. of unique data, including $F_o^2 < 0$	4015
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	3719
No. of variables	266
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0533
$R_w(F_o^2)$ [b]	0.1429
Goodness of fit	1.068

[a] $R(F) = \sum||F_o| - |F_c|| / \sum|F_o|$.

[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] / \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)^2 + Bp]$, where $p = [\max(F_o^2,0) + 2F_c^2] / 3$.

References:

[a] Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112–122.

[b] Sheldrick, G. M. *Acta Cryst.* **2015**, *A71*, 3–8.

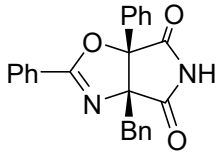
[c] Sheldrick, G. M. *Acta Cryst*. **2015**, *C71*, 3–8.

[d] Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst*. **2009**, *42*, 339-341.

[e] Spek, A. L. *J. Appl. Cryst.* **2003**, *36*, 7–13.

8. Characterization of the products

3a-Benzyl-2,6a-diphenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4aa)



White solid, **M.p.** 88 – 89 °C; 32.9 mg, 86% yield, >95:5 dr, 92% ee. $[\alpha]^{25}_{D}$ = +24.3 (*c* = 0.61, in CH_2Cl_2).

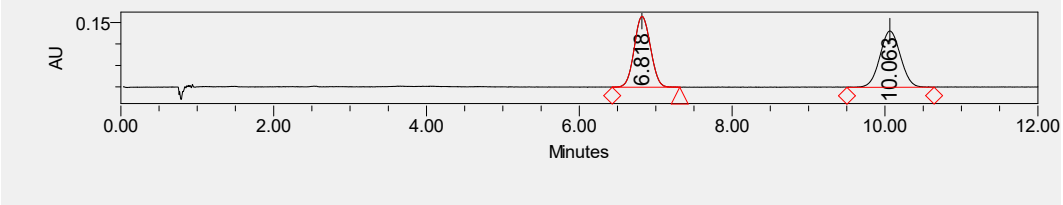
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 6.8 min, 10.0 min. dr >95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.31 (s, 1H), 8.10 – 8.08 (m, 2H), 7.58 – 7.55 (m, 1H), 7.48 – 7.44 (m, 2H), 7.41 – 7.38 (m, 1H), 7.34 – 7.30 (m, 2H), 7.11 – 7.10 (m, 2H), 7.02 – 6.98 (m, 1H), 6.91 – 6.87 (m, 2H), 6.50 – 6.48 (m, 2H), 3.45 (d, *J* = 14.6 Hz, 1H), 2.98 (d, *J* = 14.6 Hz, 1H) ppm.

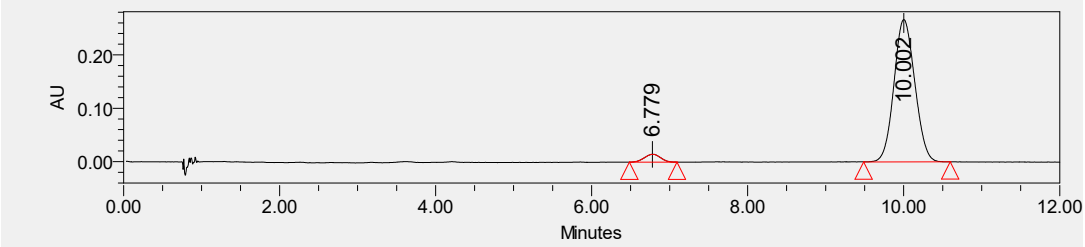
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ= 175.4, 174.1, 164.1, 133.6, 132.9, 131.9, 130.5, 129.4, 129.1 128.8, 127.6, 126.5, 126.2, 125.7, 91.4, 83.2, 36.6 ppm.

IR (neat): ν (cm^{-1}) 3213, 3064, 3033, 2761, 2351, 1792, 1733, 1642, 1603, 1580, 1496, 1451, 1330, 1215, 1093, 1066, 1027, 975, 761, 696, 641, 501.

HRMS (ESI-FT) calcd for $C_{24}H_{19}N_2O_3^+$ ([M]+H$^+$) = 383.1390, found 383.1394.

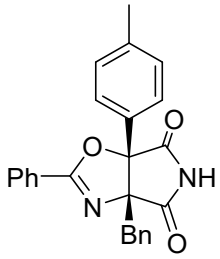


	Retention Time	% Area
1	6.818	49.81
2	10.063	50.19



	Retention Time	% Area
1	6.779	4.06
2	10.002	95.94

3a-Benzyl-2-phenyl-6a-(*p*-tolyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ab)



White solid, **M.p.** 98 – 99 °C; 29.6 mg, 75% yield, >95:5 dr, 83% ee. $[\alpha]^{25}_{D}$ = +39.1 (*c* = 0.58, in CH_2Cl_2).

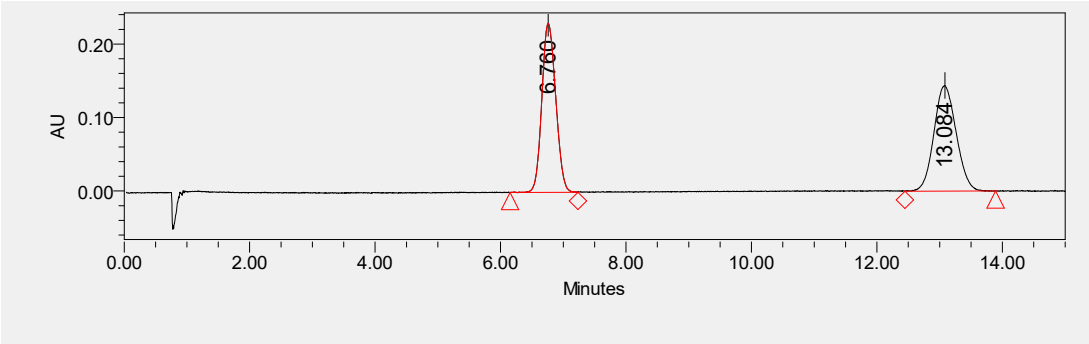
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 6.9 min, 12.8 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.30 (s, 1H), 8.12 – 8.03 (m, 2H), 7.58 – 7.54 (m, 1H), 7.47 – 7.44 (m, 2H), 7.13 – 7.11 (m, 2H), 7.03 – 6.96 (m, 3H), 6.92 – 6.88 (m, 2H), 6.53 – 6.52 (m, 2H), 3.40 (d, *J* = 14.6 Hz, 1H), 2.97 (d, *J* = 14.6 Hz, 1H), 2.39 (s, 3H) ppm.

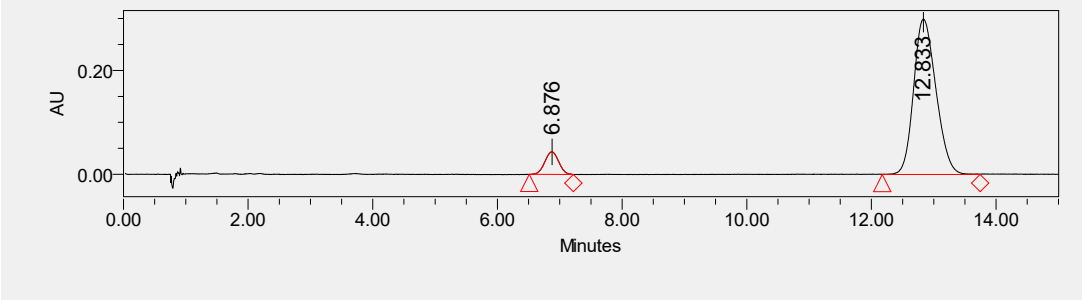
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ= 175.5, 174.2, 164.1, 139.4, 133.7, 132.8, 130.5, 129.4, 129.1, 128. 9, 128.8, 127.5, 126.5, 126.1, 125.8, 91.4, 83.1, 36.7, 21.4 ppm.

IR (neat): ν (cm^{-1}) 3212, 3063, 3031, 2924, 2761, 1793, 1732, 1642, 1580, 1517, 1496, 1452, 1331, 1215, 1187, 1092, 1066, 1030, 976, 812, 782, 734, 697, 649, 608, 584, 504.

HRMS (ESI-FT) calcd for $C_{25}H_{21}N_2O_3^+$ ([M]+H$^+$) = 397.1547, found 397.1553.

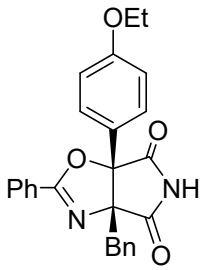


	Retention Time	% Area
1	6.760	49.97
2	13.084	50.03



	Retention Time	% Area
1	6.876	8.26
2	12.833	91.74

3a-Benzyl-6a-(4-ethoxyphenyl)-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ac)



Yellow solid, **M.p.** 96 – 97 °C; 33.2 mg, 78% yield, >95:5 dr, 88% ee. $[\alpha]^{25}_{D}$ = +49.0 (*c* = 0.73, in CH_2Cl_2).

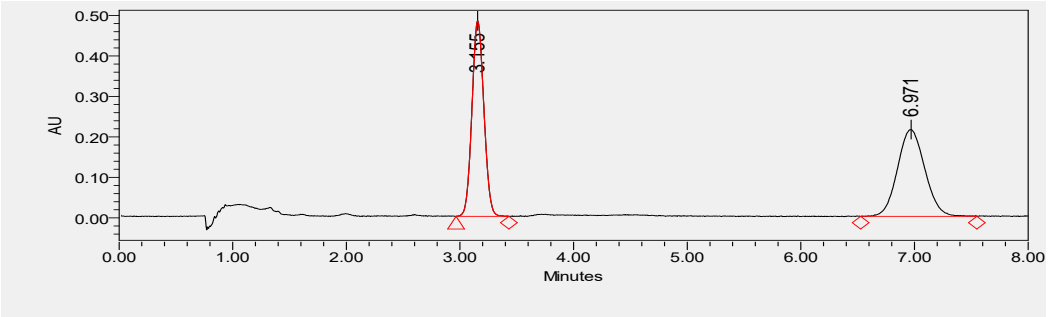
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 3.1 min, 6.9 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.33 (s, 1H), 8.08 – 8.07 (m, 2H), 7.57 – 7.53 (m, 1H), 7.47 – 7.43 (m, 2H), 7.03 – 6.98 (m, 3H), 6.95 – 6.91 (m, 2H), 6.83 – 6.81 (m, 2H), 6.57 – 6.55 (m, 2H), 4.06 (q, *J* = 7.0 Hz, 2H), 3.39 (d, *J* = 14.6 Hz, 1H), 3.01 (d, *J* = 14.6 Hz, 1H), 1.45 (t, *J* = 7.0 Hz, 3H) ppm.

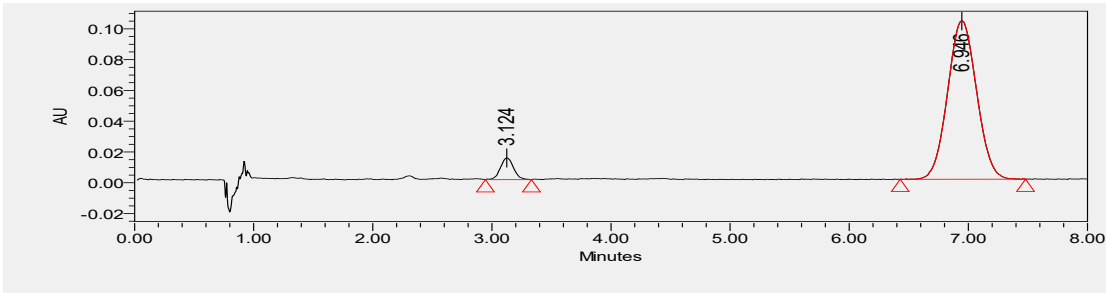
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.5, 174.3, 164.1, 159.8, 133.8, 132.8, 130.5, 129.1, 128.8, 127.6, 127.5, 126.5, 125.8, 123.6, 114.7, 91.3, 83.1, 63.8, 36.8, 14.9 ppm.

IR (neat): ν (cm^{-1}) 3199, 3063, 2981, 2930, 2762, 1792, 1729, 1641, 1614, 1580, 1515, 1496, 1478, 1452, 1392, 1306, 1249, 1217, 1181, 1091, 1066, 1047, 1029, 975, 923, 827, 782, 735, 697, 624, 571, 523, 500, 432.

HRMS (ESI-FT) calcd for $C_{26}H_{23}N_2O_4^+$ ([M]+H$^+$) = 427.1652, found 427.1657.

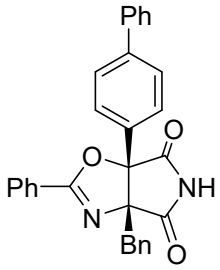


	Retention Time	% Area
1	3.155	49.54
2	6.971	50.46



	Retention Time	% Area
2	6.946	94.11
1	3.124	5.89

6a-([1,1'-biphenyl]-4-yl)-3a-Benzyl-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ad)



White solid, **M.p.** 116 – 117 °C; 38.5 mg, 84% yield, >95:5 dr, 90% ee. $[\alpha]^{25}_{D}$ = +94.3 (*c* = 0.57, in CH_2Cl_2).

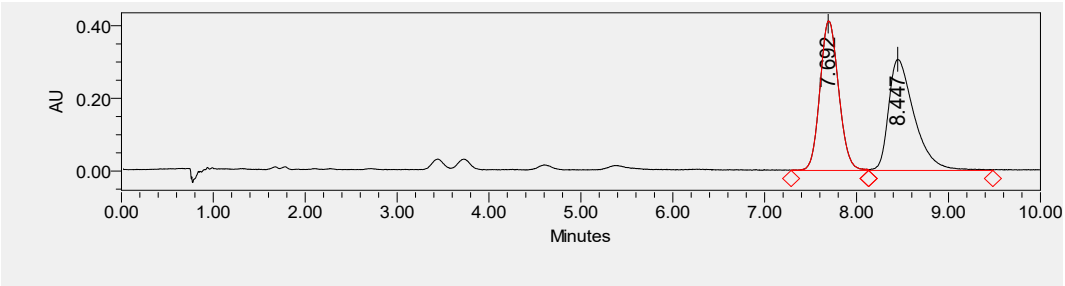
Dissolved in MeOH for UPC^2; **UPC^2** (Daicel CHIRALPAK **OD-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 7.6 min, 8.5, min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.25 (s, 1H), 8.13 – 8.11 (m, 2H), 7.61 – 7.56 (m, 3H), 7.52 – 7.46 (m, 6H), 7.43 – 7.39 (m, 1H), 7.16 – 7.14 (m, 2H), 7.03 – 7.00 (m, 1H), 6.91 – 6.87 (m, 2H), 6.57 – 6.55 (m, 2H), 3.47 (d, *J* = 14.8 Hz, 1H), 3.06 (d, *J* = 14.8 Hz, 1H) ppm.

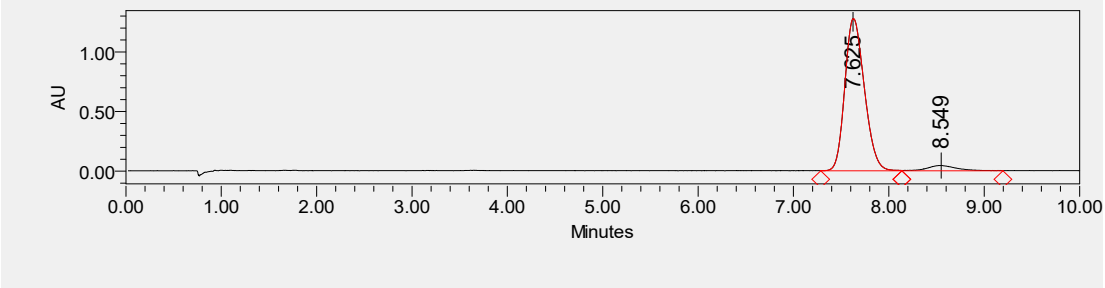
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.4, 174.0, 164.2, 142.4, 140.4, 133.7, 132.9, 130.8, 130.3, 129.1, 129.0, 128.8, 128.0, 127.6, 127.4, 127.3, 126.6, 126.5, 125.7, 91.3, 83.5, 36.8 ppm.

IR (neat): ν (cm^{-1}) 3193, 3061, 3031, 2760, 1792, 1729, 1641, 1602, 1580, 1521, 1491, 1451, 1430, 1405, 1329, 1264, 1215, 1160, 1091, 1066, 1029, 1007, 977, 954, 901, 834, 762, 733, 695, 652, 634, 591, 575, 546, 502, 475, 440.

HRMS (ESI-FT) calcd for $C_{30}H_{22}N_2O_3K^+$ ([M]+K$^+$) = 497.1262, found 497.1265.

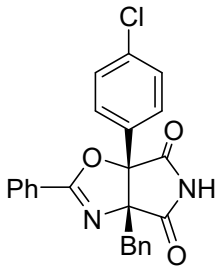


	Retention Time	% Area
1	7.692	49.48
2	8.447	50.52



	Retention Time	% Area
1	7.625	95.09
2	8.549	4.91

3a-Benzyl-6a-(4-chlorophenyl)-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ae)



White solid, **M.p.** 90 – 91 °C; 28.1 mg, 67% yield, >95:5 dr, 85% ee. $[\alpha]^{25}_{D}$ = +44.5 (*c* = 0.53, in CH_2Cl_2).

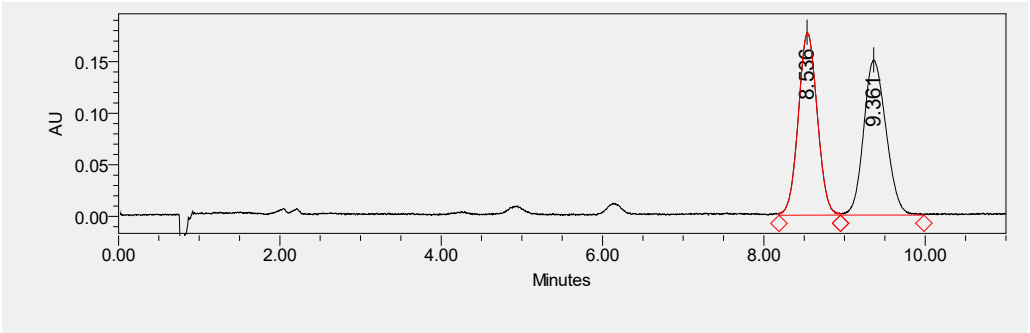
Dissolved in MeOH for UPC^2; **UPC^2** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 8.4 min, 9.2 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.34 (s, 1H), 8.08 – 8.07 (m, 2H), 7.59 – 7.56 (m, 1H), 7.49 – 7.45 (m, 2H), 7.26 – 7.24 (m, 2H), 7.04 – 6.98 (m, 3H), 6.95 – 6.91 (m, 2H), 6.55 – 6.53 (m, 2H), 3.43 (d, *J* = 14.8 Hz, 1H), 2.98 (d, *J* = 14.8 Hz, 1H) ppm.

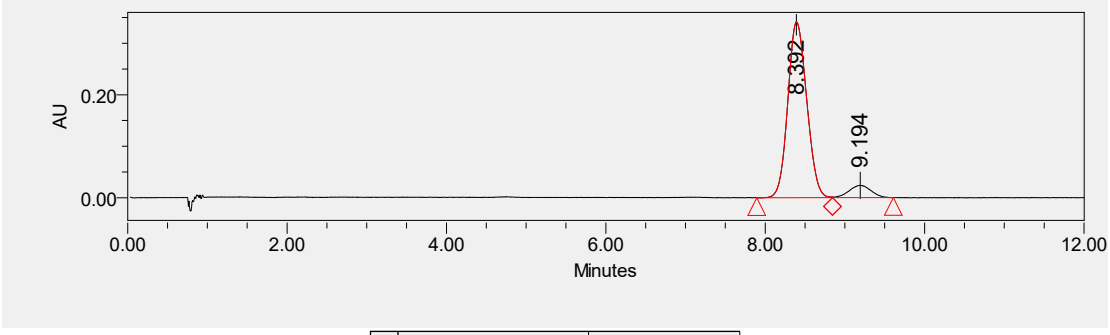
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.2, 173.6, 164.1, 135.5, 133.5, 133.0, 130.6, 130.1, 129.1, 128.9, 128.9, 127.8, 127.6, 126.7, 125.5, 90.9, 83.4, 36.77 ppm.

IR (neat): ν (cm^{-1}) 3212, 3063, 2926, 2762, 1793, 1729, 1642, 1601, 1580, 1494, 1452, 1430, 1403, 1330, 1214, 1091, 1066, 1029, 1012, 978, 954, 901, 821, 782, 757, 738, 696, 647, 622, 590, 504, 484, 448.

HRMS (ESI-FT) calcd for $C_{24}H_{18}{}^{34.9659}ClN_2O_3^+$ ([M]+H$^+$) = 417.1000, found 417.1001.

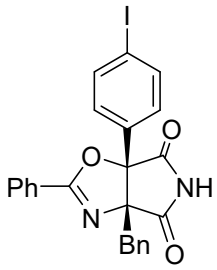


	Retention Time	% Area
1	8.536	49.84
2	9.361	50.16



	Retention Time	% Area
1	8.392	92.43
2	9.194	7.57

3a-Benzyl-6a-(4-iodophenyl)-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4af)



White solid, **M.p.** 113 – 114 °C; 40.2 mg, 79% yield, >95:5 dr, 88% ee. $[\alpha]^{25}_{D}$ = +58.4 (*c* = 0.78, in CH_2Cl_2).

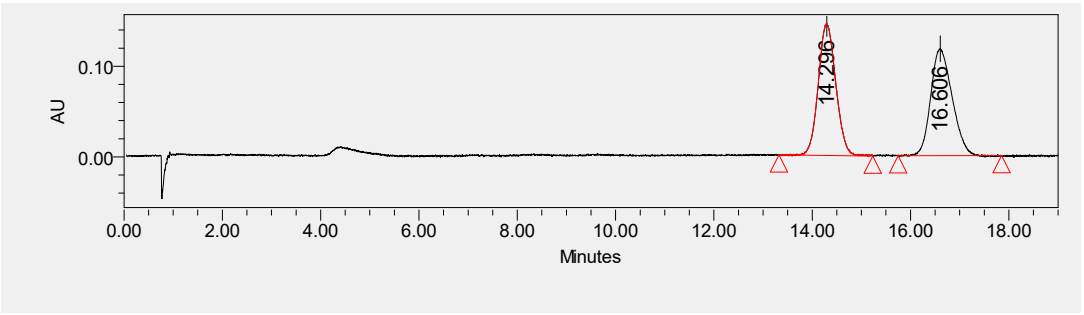
Dissolved in MeOH for UPC^2; **UPC^2** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 14.2 min, 16.5 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.38 (s, 1H), 8.08 – 8.06 (m, 2H), 7.61 – 7.57 (m, 3H), 7.49 – 7.45 (m, 2H), 7.05 – 7.01 (m, 1H), 6.95 – 6.91 (m, 2H), 6.79 – 6.77 (m, 2H), 6.54 – 6.52 (m, 2H), 3.42 (d, *J* = 14.8 Hz, 1H), 2.98 (d, *J* = 14.8 Hz, 1H) ppm.

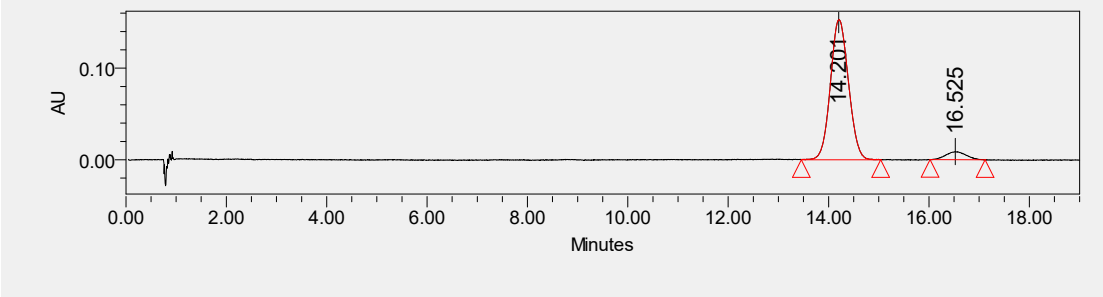
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.2, 173.5, 164.1, 137.8, 133.5, 133.0, 131.8, 130.1, 129.1, 128.9, 127.9, 127.8, 126.7, 125.5, 95.2, 90.1, 83.4, 36.76 ppm.

IR (neat): ν (cm^{-1}) 3194, 3062, 2920, 2851, 2761, 1793, 1725, 1641, 1602, 1580, 1489, 1451, 1430, 1394, 1264, 1214, 1161, 1090, 1065, 1028, 1004, 978, 951, 900, 814, 781, 734, 694, 646, 622, 589, 571, 502, 474, 436.

HRMS (ESI-FT) calcd for $C_{24}H_{18}IN_2O_3^+$ ([M]+H$^+$) = 509.0357, found 509.0363.

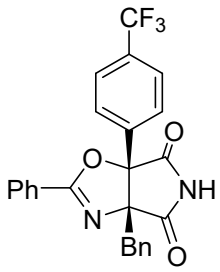


	Retention Time	% Area
1	14.296	50.20
2	16.606	49.80



	Retention Time	% Area
1	14.201	94.03
2	16.525	5.97

3a-Benzyl-2-phenyl-6a-(4-(trifluoromethyl)phenyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ag)



White solid, **M.p.** 93 – 94 °C; 20.3 mg, 45% yield, >95:5 dr, 88% ee. $[\alpha]^{25}_{D}$ = +19.7 (*c* = 0.30, in CH_2Cl_2).

Dissolved in MeOH for UPC^2; **UPC^2** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 95/5, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 6.9 min, 10.0 min. dr > 95:5 determined by ^{1}H NMR.

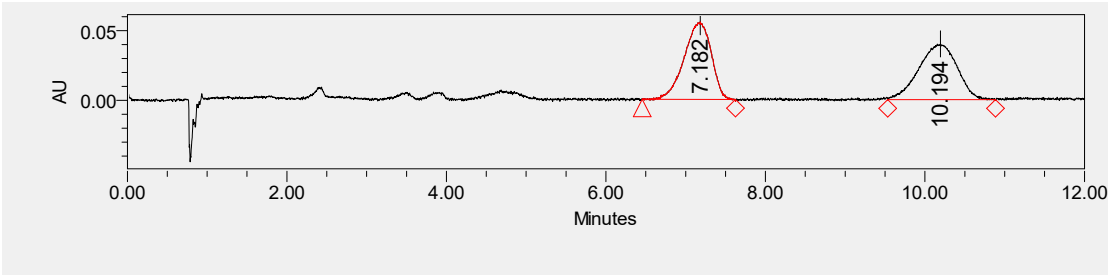
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.03 (s, 1H), 8.11 – 8.09 (m, 2H), 7.62 – 7.58 (m, 1H), 7.52 – 7.47 (m, 4H), 7.17 – 7.15 (m, 2H), 7.02 – 6.99 (m, 1H), 6.89 – 6.85 (m, 2H), 6.48 – 6.46 (m, 2H), 3.46 (d, *J* = 15.0 Hz, 1H), 3.00 (d, *J* = 15.0 Hz, 1H) ppm.

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 174.8, 173.1, 164.1, 136.0, 133.4, 133.2, 129.9, 129.2, 129.0, 127.9, 126.7, 126.6, 125.6 (q, *J* = 3.7 Hz), 125.4, 125.1, 122.4, 90.8, 83.8, 36.8 ppm.

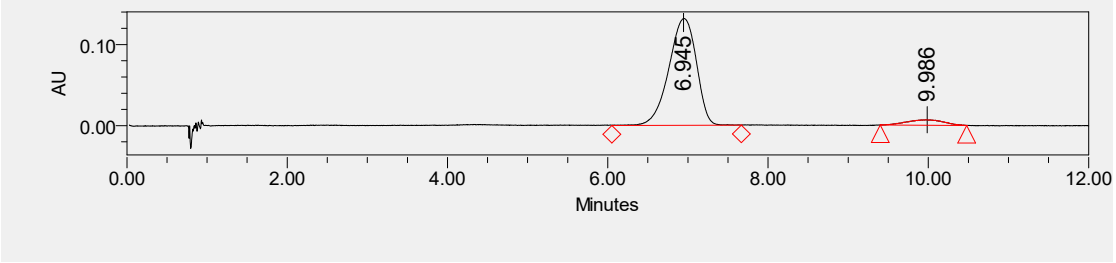
^{19}F{^{1}H} NMR (376 MHz, Chloroform-*d*) δ = −62.82 ppm.

IR (neat): ν (cm^{-1}) 3221, 3066, 2927, 2764, 1795, 1734, 1644, 1581, 1496, 1452, 1414, 1326, 1215, 1170, 1125, 1092, 1070, 1029, 1015, 980, 835, 781, 753, 695, 647, 607, 503, 441.

HRMS (ESI-FT) calcd for $C_{25}H_{18}F_3N_2O_3^+$ ([M]+H$^+$) = 451.1264, found 451.1260.

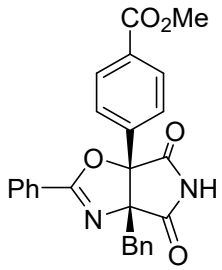


	Retention Time	% Area
1	7.182	49.60
2	10.194	50.40



	Retention Time	% Area
2	9.986	6.25
1	6.945	93.75

Methyl 4-(3a-benzyl-4,6-dioxo-2-phenyl-3a,4,5,6-tetrahydro-6a*H*-pyrrolo[3,4-*d*]oxazol-6a-yl)benzoate (4ah)



White solid, **M.p.** 102 – 103 °C; 24.9 mg, 57% yield, >95:5 dr, 87% ee. $[\alpha]^{25}_{D}$ = +64.6 (*c* = 0.40, in CH_2Cl_2).

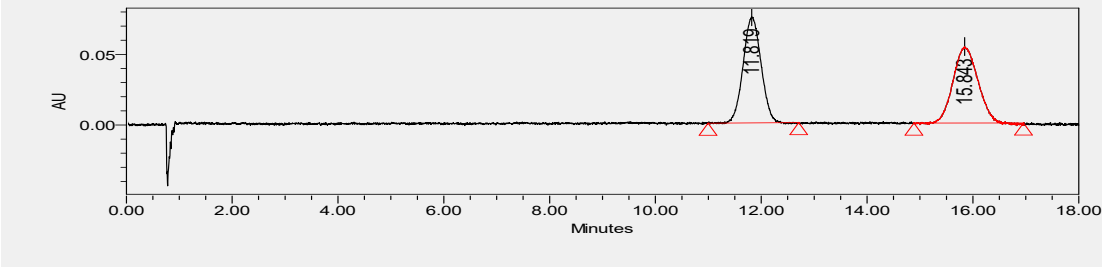
Dissolved in MeOH for UPC^2; **UPC^2** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 11.6 min, 15.5 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.27 (s, 1H), 8.09 – 8.08 (m, 2H), 7.97 – 7.95 (m, 2H), 7.60 – 7.56 (m, 1H), 7.49 – 7.46 (m, 2H), 7.17 – 7.15 (m, 2H), 7.02 – 6.98 (m, 1H), 6.88 – 6.84 (m, 2H), 6.48 – 6.46 (m, 2H), 3.97 (s, 3H), 3.47 (d, *J* = 14.8 Hz, 1H), 2.96 (d, *J* = 14.8 Hz, 1H) ppm.

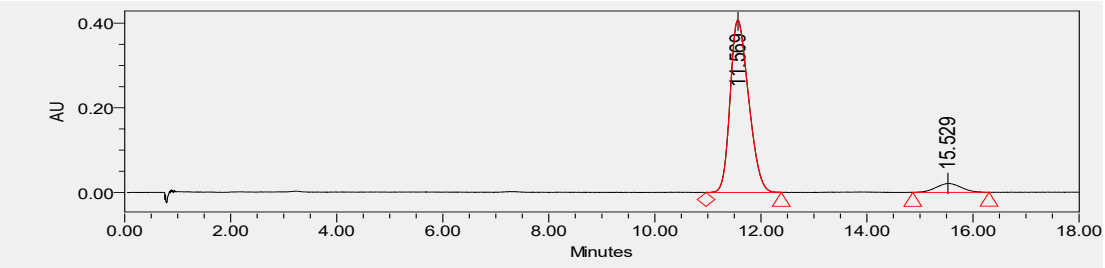
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.0, 173.4, 164.1, 136.9, 133.3, 133.1, 131.0, 130.2, 129.9, 129.1, 128.9, 127.7, 126.7, 126.4, 125.5, 91.1, 83.6, 52.6, 36.6 ppm.

IR (neat): ν (cm^{-1}) 3199, 3064, 2953, 2762, 1794, 1726, 1643, 1580, 1495, 1452, 1436, 1410, 1329, 1282, 1215, 1195, 1112, 1091, 1066, 1030, 1015, 957, 902, 852, 827, 772, 733, 697, 647, 591, 504, 439.

HRMS (ESI-FT) calcd for $C_{26}H_{21}N_2O_5^+$ ([M]+H$^+$) = 441.1445, found 441.1447.

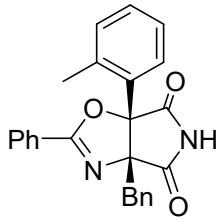


	Retention Time	% Area
1	11.819	50.18
2	15.843	49.82



	Retention Time	% Area
1	11.569	93.42
2	15.529	6.58

3a-Benzyl-2-phenyl-6a-(*o*-tolyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-d]oxazole-4,6(5*H*)-dione (4ai)



White solid, **M.p.** 88 – 89 °C; 34.6 mg, 87% yield, >95:5 dr, 88% ee. $[\alpha]^{25}_{D}$ = +22.8 (*c* = 0.69, in CH_2Cl_2).

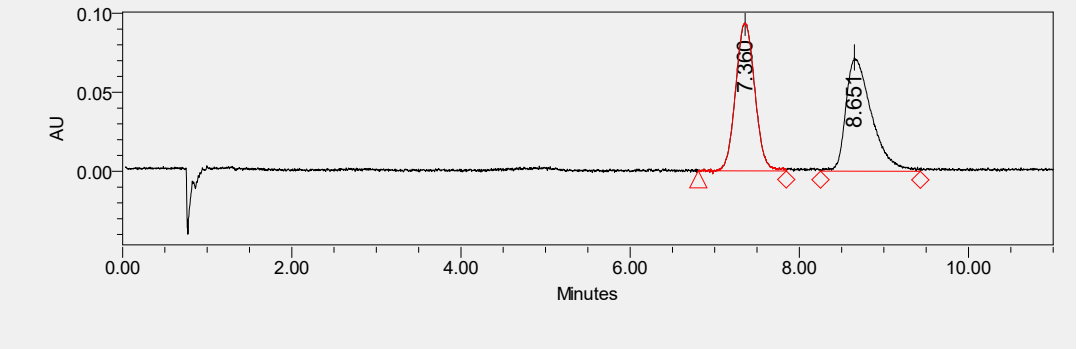
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OD-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 7.2 min, 8.8 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ=9.33 (s, 1H), 8.10 – 8.08 (m, 2H), 7.58 – 7.55 (m, 1H), 7.49 – 7.45 (m, 2H), 7.24 – 7.18 (m, 2H), 7.02 – 6.98 (m, 1H), 6.95 – 6.88 (m, 3H), 6.81 (s, 1H), 6.49 – 6.48 (m, 2H), 3.45 (d, *J* = 14.6 Hz, 1H), 2.97 (d, *J* = 14.6 Hz, 1H), 2.26 (s, 3H) ppm.

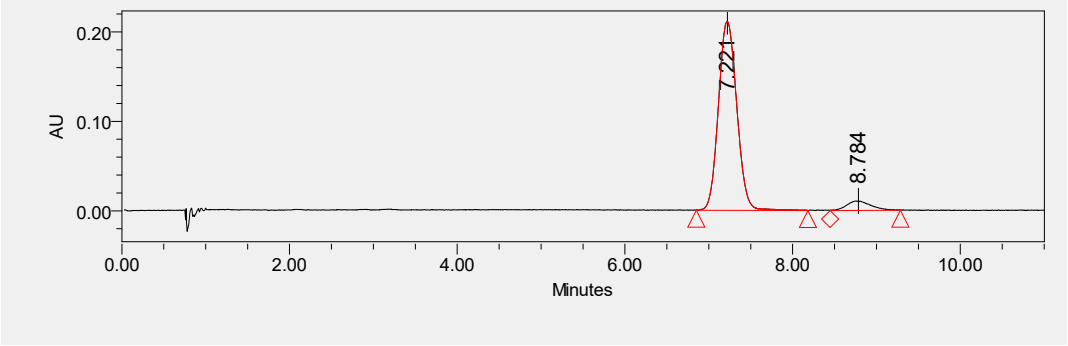
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ= 175.5, 174.3, 164.1, 138.6, 133.6, 132.8, 131.7, 130.5, 130.1, 129.1, 128. 8, 128.7, 127.4, 127.1, 126.5, 125.8, 123.1, 91.4, 83.1, 36.6, 21.5 ppm.

IR (neat): ν (cm^{-1}) 3195, 3062, 2921, 2759, 1792, 1729, 1641, 1607, 1580, 1494, 1451, 1330, 1269, 1222, 1179, 1091, 1067, 1029, 1000, 976, 836, 782, 735, 696, 642, 623, 577, 526, 497, 472, 437.

HRMS (ESI-FT) calcd for $C_{25}H_{21}N_2O_3^+$ ([M]+H$^+$) = 397.1547, found 397.1549.

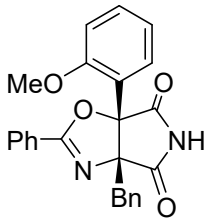


	Retention Time	% Area
1	7.360	49.42
2	8.651	50.58



	Retention Time	% Area
1	7.221	93.78
2	8.784	6.22

3a-Benzyl-6a-(2-methoxyphenyl)-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4aj)



White solid, **M.p.** 108 – 109 °C; 36.3 mg, 88% yield, >95:5 dr, 92% ee. $[\alpha]^{25}_{D}$ = +98.1 (*c* = 0.75, in CH_2Cl_2).

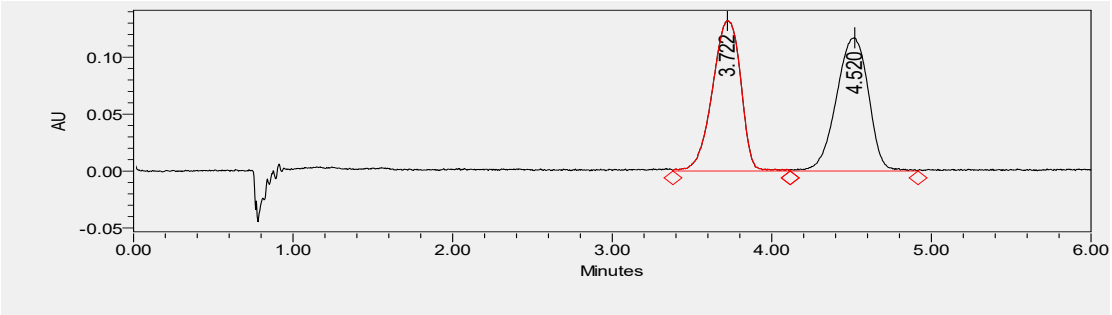
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 3.9 min, 4.7 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.85 (s, 1H), 8.06 – 8.05 (m, 2H), 7.56 – 7.52 (m, 1H), 7.46 – 7.38 (m, 3H), 7.12 – 7.09 (m, 1H), 7.00 – 6.93 (m, 2H), 6.87 – 6.83 (m, 3H), 6.49 – 6.47 (m, 2H), 3.85 (s, 3H), 3.70 (d, *J* = 14.6 Hz, 1H), 2.75 (d, *J* = 14.6 Hz, 1H) ppm.

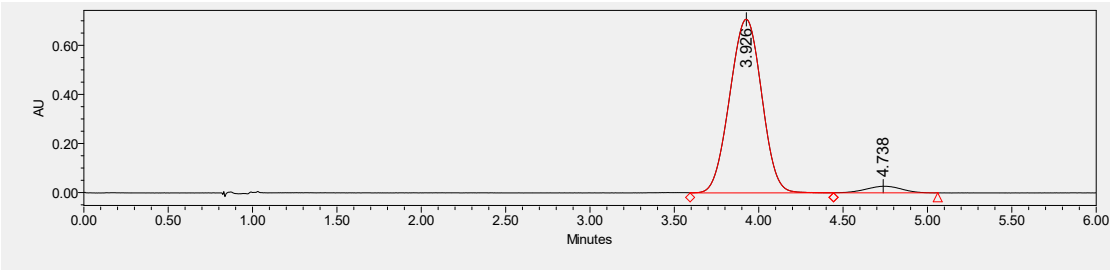
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.6, 174.5, 163.2, 155.0, 134.2, 132.6, 130.7, 129.0, 128.7, 128.2, 127.2, 126.2, 126.0, 121.7, 121.6, 111.1, 90.2, 82.5, 55.6, 35.9 ppm.

IR (neat): ν (cm^{-1}) 3213, 3062, 2940, 2841, 2765, 1793, 1724, 1645, 1603, 1582, 1493, 1452, 1331, 1293, 1256, 1215, 1182, 1163, 1124, 1091, 1067, 1023, 976, 954, 753, 737, 696, 638, 596, 572, 509, 477, 456, 430.

HRMS (ESI-FT) calcd for $C_{25}H_{21}N_2O_4^+$ ([M]+H$^+$) = 413.1496, found 413.1501.

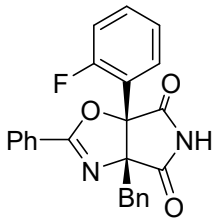


	Retention Time	% Area
1	3.722	49.91
2	4.520	50.09



	Retention Time	% Area
1	3.926	95.91
2	4.738	4.09

3a-Benzyl-6a-(2-fluorophenyl)-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ak)



White solid, **M.p.** 88 – 89 °C; 26.9 mg, 67% yield, >95:5 dr, 79% ee. $[\alpha]^{25}_{D}$ = +40.1 (*c* = 0.30, in CH_2Cl_2).

Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 4.7 min, 5.8 min. dr > 95:5 determined by ^{1}H NMR.

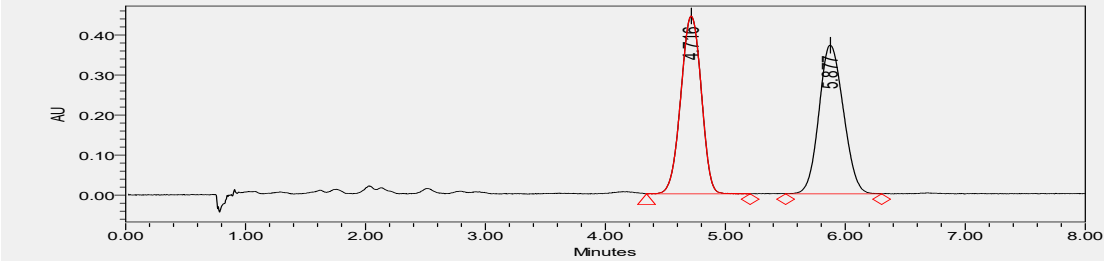
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.75 (s, 1H), 8.08 – 8.02 (m, 2H), 7.59 – 7.55 (m, 1H), 7.49 – 7.45 (m, 2H), 7.43 – 7.39 (m, 1H), 7.21 – 7.17 (m, 1H), 7.13 – 7.09 (m, 1H), 7.03 - 6.95 (m, 2H), 6.88 – 6.84 (m, 2H), 6.54 – 6.52 (m, 2H), 3.76 (d, *J* = 15.0 Hz, 1H), 2.82 (d, *J* = 15.0 Hz, 1H) ppm.

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 174.6, 172.9, 163.3, 133.7, 132.9, 131.4, 131.3, 129.1, 128.9 (d, *J* = 286.0 Hz), 128.8, 126.5, 125.6, 124.9, 124.8, 120.8, 120.6, 115.7 (d, *J* = 20.1 Hz), 88.9, 83.0, 36.1 ppm.

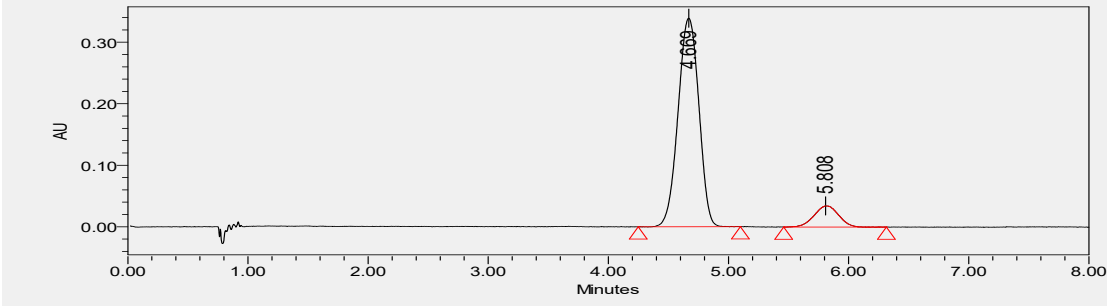
^{19}F{^{1}H} NMR (376 MHz, Chloroform-*d*) δ = −111.18 ppm.

IR (neat): ν (cm^{-1}) 3213, 3064, 2763, 1796, 1730, 1645, 1603, 1582, 1491, 1454, 1329, 1288, 1221, 1198, 1160, 1089, 1066, 1027, 977, 953, 815, 759, 735, 695, 655, 635, 575, 541, 497, 456.

HRMS (ESI-FT) calcd for $C_{24}H_{18}FN_2O_3^+$ ([M]+H$^+$) = 439.1264, found 439.1263.

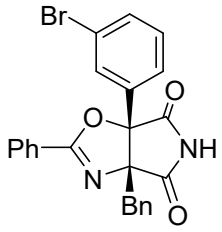


	Retention Time	% Area
1	4.716	50.02
2	5.877	49.98



	Retention Time	% Area
1	4.669	89.28
2	5.808	10.72

3a-Benzyl-6a-(3-bromophenyl)-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4al)



White solid, **M.p.** 109 – 110 °C; 23.4 mg, 51% yield, >95:5 dr, 86% ee. $[\alpha]^{25}_{D}$ = +20.9 (*c* = 1.21, in CH_2Cl_2).

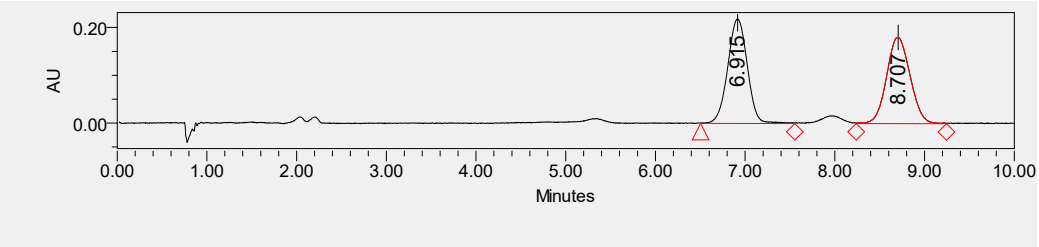
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 6.8 min, 8.6 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.58 (s, 1H), 8.09 – 8.07 (m, 2H), 7.59 – 7.56 (m, 1H), 7.53– 7.45 (m, 3H), 7.22 – 7.18 (m, 1H), 7.14 (s, 1H), 7.05 – 7.03 (m, 2H), 6.96 – 6.92 (m, 2H), 6.52 – 6.50 (m, 2H), 3.50 (d, *J* = 14.8 Hz, 1H), 2.96 (d, *J* = 14.8 Hz, 1H) ppm.

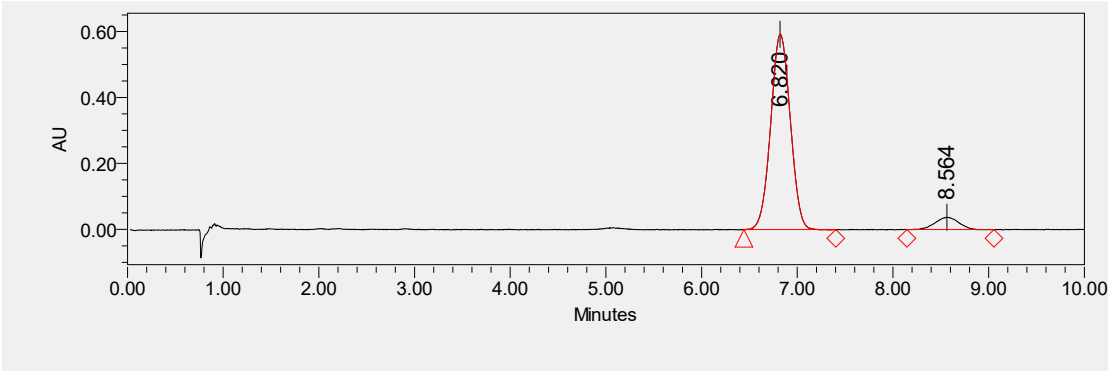
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ= 175.3, 173.6, 164.1, 134.1, 133.2, 133.0, 132.5, 130.2, 130.1, 129.7, 129.1, 128.9, 127.7, 126.8, 125.4, 124.6, 123.2, 90.6, 83.3, 36.6 ppm.

IR (neat): ν (cm^{-1}) 3120, 3063, 2760, 1793, 1725, 1641, 1600, 1578, 1495, 1476, 1452, 1428, 1329, 1264, 1214, 1090, 1067, 1028, 999, 977, 879, 783, 759, 737, 695, 639, 622, 576, 498, 472, 434.

HRMS (ESI-FT) calcd for $C_{24}H_{18}{}^{78.9183}BrN_2O_3^+$ ([M]+H$^+$) = 461.0495, found 461.0497, $C_{24}H_{18}{}^{80.9163}BrN_2O_3^+$ ([M]+H$^+$) = 463.0475, found 463.0474.

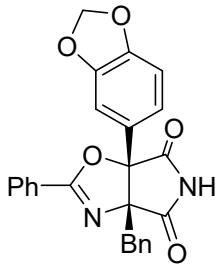


	Retention Time	% Area
1	6.915	50.24
2	8.707	49.76



	Retention Time	% Area
1	6.820	92.86
2	8.564	7.14

6a-(Benzo[*d*][1,3]dioxol-5-yl)-3a-benzyl-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4am)



White solid, **M.p.** 105 – 106 °C; 33.9 mg, 80% yield, >95:5 dr, 88% ee. $[\alpha]^{25}_{D}$ = +41.2 (*c* = 0.79, in CH_2Cl_2).

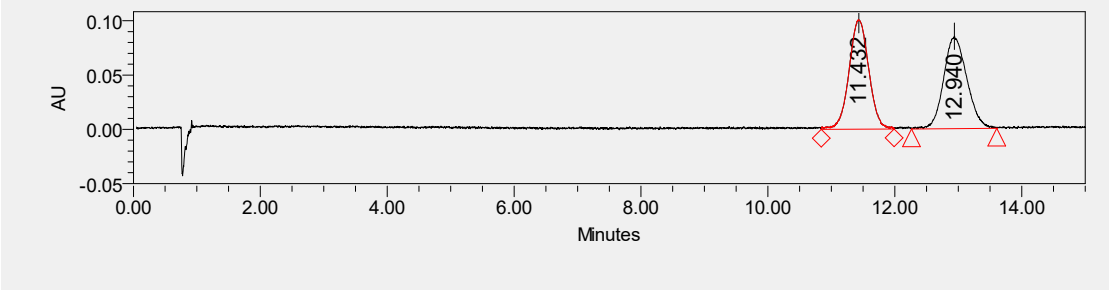
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 11.2 min, 12.8 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.36 (s, 1H), 8.08 – 8.06 (m, 2H), 7.58 – 7.54 (m, 1H), 7.48 – 7.44 (m, 2H), 7.05 – 7.02 (m, 1H), 6.98 – 6.95 (m, 2H), 6.76 – 6.74 (m, 1H), 6.65 – 6.63 (m, 2H), 6.60 – 6.57 (m, 1H), 6.49 – 6.48 (m, 1H), 5.99 – 5.98 (m, 2H), 3.43 (d, *J* = 14.8 Hz, 1H), 3.02 (d, *J* = 14.8 Hz, 1H) ppm.

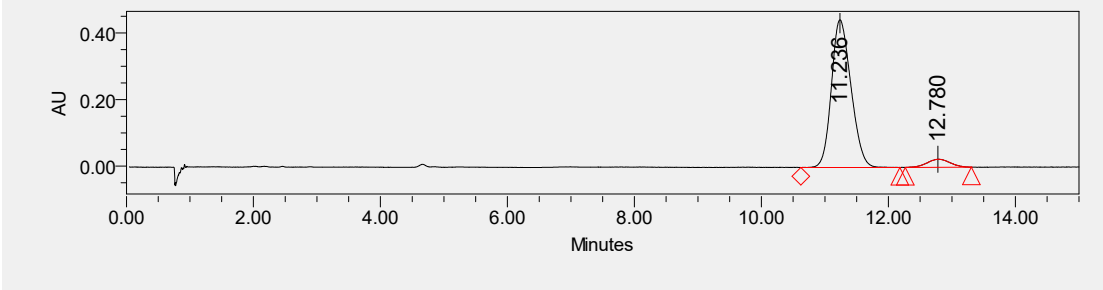
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.4, 174.1, 164.0, 148.5, 148.2, 133.9, 132.9, 130.3, 129.1, 128.8, 127.6, 126.6, 125.6, 125.6, 120.0, 108.5, 107.2, 101.6, 91.2, 83.3, 36.8 ppm.

IR (neat): ν (cm^{-1}) 3196, 3063, 2771, 1792, 1731, 1642, 1580, 1493, 1449, 1330, 1284, 1250, 1146, 1108, 1091, 977, 933, 871, 812, 782, 734, 696, 644, 621, 573, 499, 472, 422.

HRMS (ESI-FT) calcd for $C_{25}H_{19}N_2O_5^+$ ([M]+H$^+$) = 427.1288, found 427.1287.

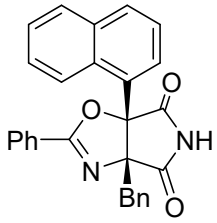


	Retention Time	% Area
1	11.432	50.26
2	12.940	49.74



	Retention Time	% Area
1	11.236	93.92
2	12.780	6.08

3a-Benzyl-6a-(naphthalen-1-yl)-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4an)



White solid, **M.p.** 114 – 115 °C; 16.7 mg, 39% yield, >95:5 dr, 88% ee. $[\alpha]^{25}_{D}$ = +172.7 (*c* = 0.26, in CH_2Cl_2).

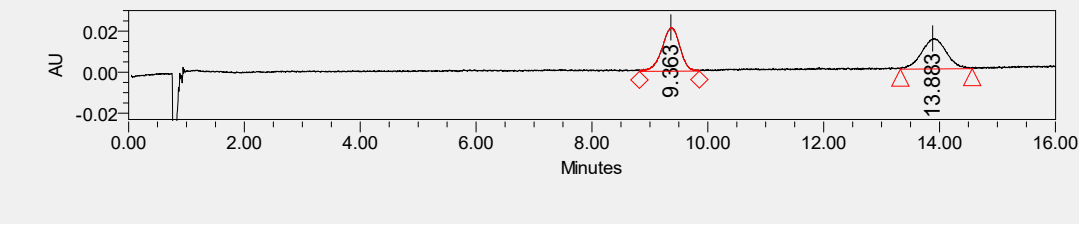
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 9.3 min, 14.1 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ= 8.99 (s, 1H), 8.16 – 8.15 (m, 2H), 8.00 – 7.98 (m, 1H), 7.90 – 7.88 (m, 1H), 7.62 – 7.58 (m, 4H), 7.52 – 7.48 (m, 2H), 7.39 – 7.37 (m, 1H), 7.25 – 7.21 (m, 1H), 6.89 – 6.85 (m, 1H), 6.74 – 6.70 (m, 2H), 6.13 – 6.11 (m, 2H), 3.73 (d, *J* = 14.8 Hz, 1H), 2.78 (d, *J* = 14.8 Hz, 1H) ppm.

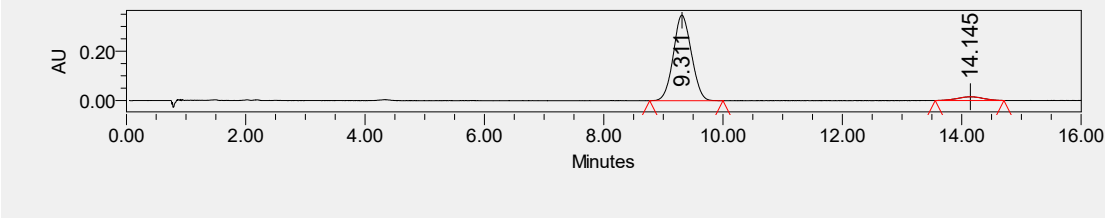
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ= 175.0, 173.3, 163.1, 134.3, 133.9, 132.9, 130.5, 130.1, 130.0, 129.5, 129.1, 128.9, 128.0, 127.4, 127.2, 127.0, 126.2, 126.0, 125.8, 125.4, 122.8, 91.4, 83.5, 35.9 ppm.

IR (neat): ν (cm^{-1}) 3193, 3061, 2758, 1792, 1733, 1646, 1601, 1580, 1513, 1496, 1452, 1329, 1216, 1178, 1109, 1093, 1073, 1028, 984, 931, 857, 798, 775, 754, 734, 696, 641, 622, 528, 489, 417.

HRMS (ESI-FT) calcd for $C_{28}H_{21}N_2O_3^+$ ([M]+H$^+$) = 433.1547, found 433.1547.

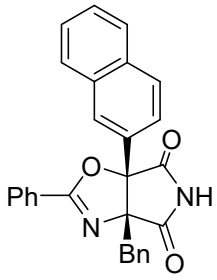


	Retention Time	% Area
1	9.363	50.81
2	13.883	49.19



	Retention Time	% Area
1	9.311	94.07
2	14.145	5.93

3a-Benzyl-6a-(naphthalen-2-yl)-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ao)



White solid, **M.p.** 128 – 129 °C; 32.2 mg, 75% yield, >95:5 dr, 85% ee. $[\alpha]^{25}_{D}$ = +93.4 (*c* = 0.47, in CH_2Cl_2).

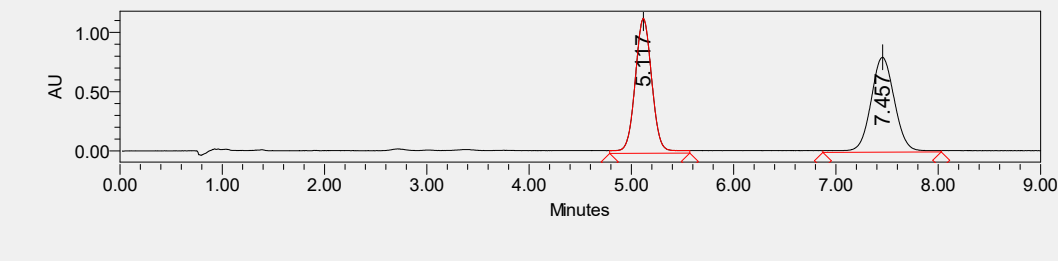
Dissolved in MeOH for UPC^2; **UPC^2** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 5.2 min, 7.4 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.28 (s, 1H), 8.16 – 8.13 (m, 2H), 7.88 – 7.82 (m, 2H), 7.69 – 7.67 (m, 1H), 7.61 – 7.48 (m, 6H), 7.20 – 7.18 (m, 1H), 6.90 – 6.86 (m, 1H), 6.68 – 6.64 (m, 2H), 6.36 – 6.34 (m, 2H), 3.46 (d, *J* = 14.6 Hz, 1H), 3.02 (d, *J* = 14.6 Hz, 1H) ppm.

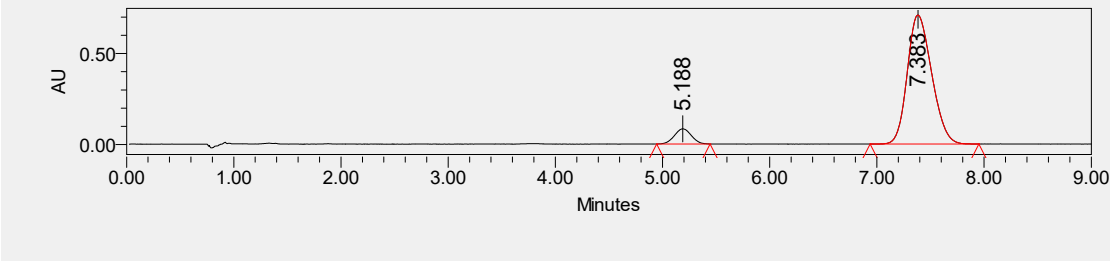
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.4, 174.0, 164.2, 133.4, 133.3, 133.0, 132.9, 130.3, 129.2, 128.9, 128.8, 128.7, 128.5, 127.8, 127.4, 127.2, 127.0 126.6, 126.5, 125.8, 122.8, 91.6, 83.1, 36.8 ppm.

IR (neat): ν (cm^{-1}) 3217, 3061, 2760, 1793, 1731, 1642, 1602, 1580, 1495, 1452, 1431, 1330, 1273, 1215, 1186, 1131, 1092, 1067, 1029, 978, 935, 905, 858, 816, 781, 743, 696, 647, 624, 495, 476.

HRMS (ESI-FT) calcd for $C_{28}H_{21}N_2O_3^+$ ([M]+H$^+$) = 433.1547, found 433.1549.

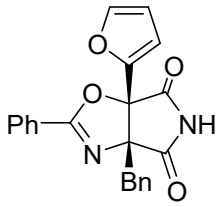


	Retention Time	% Area
1	5.117	50.16
2	7.457	49.84



	Retention Time	% Area
1	5.188	7.59
2	7.383	92.41

3a-Benzyl-6a-(furan-2-yl)-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ap)



White solid, **M.p.** 82 – 83 °C; 18.6 mg, 50% yield, >95:5 dr, 86% ee. $[\alpha]^{25}_{436}$ = –37.1 (*c* = 0.55, in CH_2Cl_2).

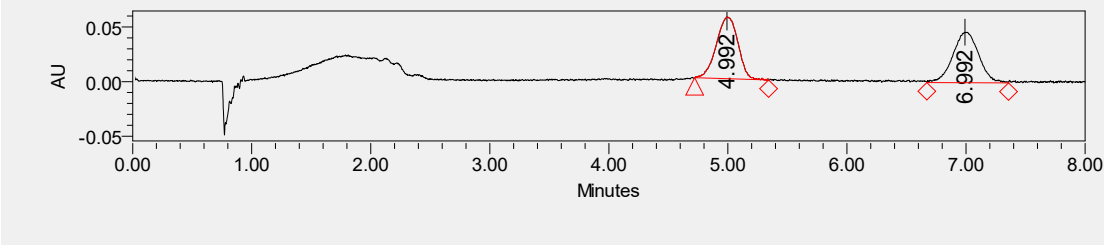
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 4.9 min, 6.9 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.05 (s, 1H), 8.04 – 8.02 (m, 2H), 7.57 – 7.51 (m, 2H), 7.46 – 7.42 (m, 2H), 7.10 – 7.00 (m, 3H), 6.76 – 6.74 (m, 2H), 6.39 – 6.38 (m, 1H), 6.35 – 6.34 (m, 1H), 3.43 (m, 2H) ppm.

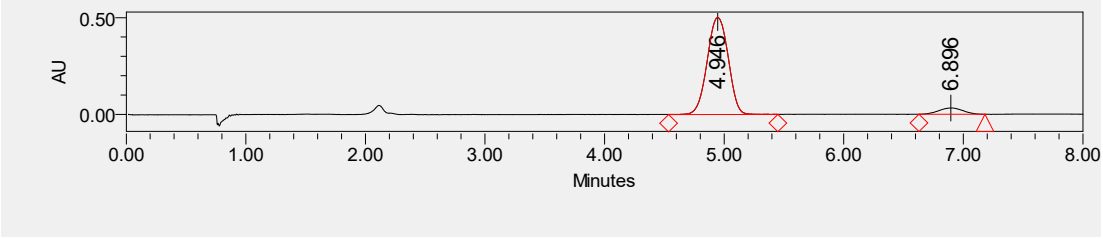
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 174.7, 171.1, 163.7, 144.3, 144.0, 133.8, 132.9, 129.8, 129.1, 128.7, 127.9, 127.0, 125.6, 112.5, 111.3, 86.4, 83.6, 37.2 ppm.

IR (neat): ν (cm^{-1}) 3200, 3064, 2763, 1794, 1732, 1643, 1603, 1580, 1496, 1452, 1329, 1294, 1267, 1235, 1216, 1154, 1094, 1066, 1030, 1005, 961, 886, 819, 782, 741, 696, 640, 594, 501, 431.

HRMS (ESI-FT) calcd for $C_{22}H_{17}N_2O_4^+$ ([M]+H$^+$) = 373.1183, found 373.1183.

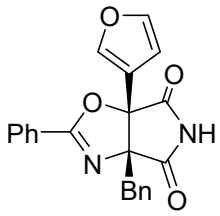


	Retention Time	% Area
1	4.992	50.33
2	6.992	49.67



	Retention Time	% Area
1	4.946	92.99
2	6.896	7.01

3a-Benzyl-6a-(furan-3-yl)-2-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4aq)



White solid, **M.p.** 76 – 77 °C; 16.9 mg, 45% yield, >95:5 dr, 87% ee. $[\alpha]^{25}_{436}$ = –25.4 (*c* = 0.98, in CH_2Cl_2).

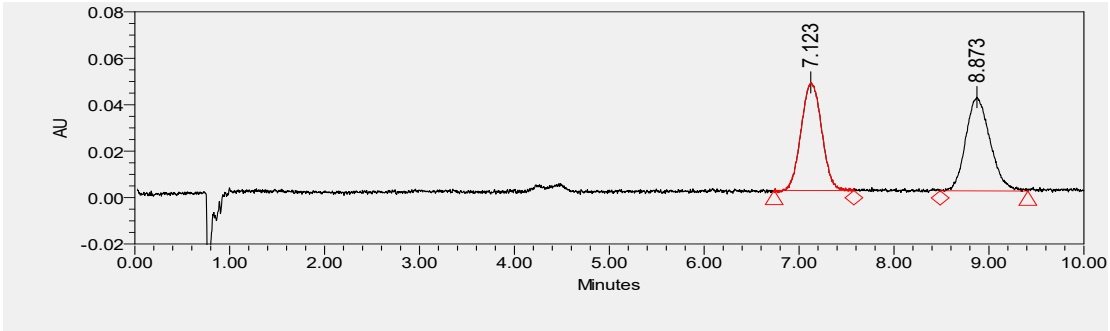
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OD-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 6.7 min, 8.3 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.20 (s, 1H), 8.04 – 8.02 (m, 2H), 7.56 – 7.52 (m, 1H), 7.50 – 7.49 (m, 1H) 7.46 – 7.42 (m, 2H), 7.18 (m, 1H), 7.11 – 7.03 (m, 3H), 6.81 – 6.80 (m, 2H), 6.30 – 6.29 (m, 1H), 3.34 (d, *J* = 14.6 Hz, 1H), 3.28 (d, *J* = 14.6 Hz, 1H) ppm.

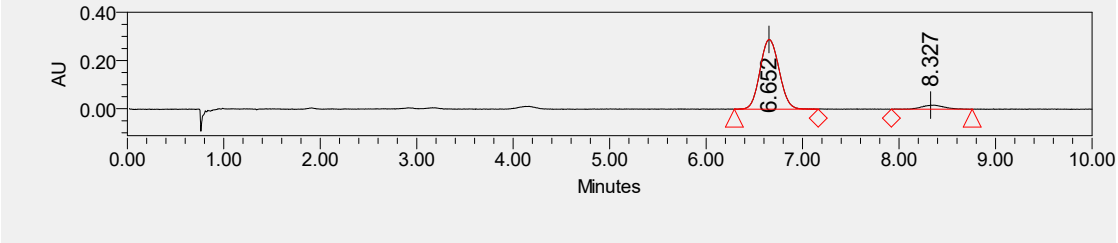
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.0, 172.7, 164.0, 144.0, 142.0, 133.7, 132.8, 130.1, 129.0, 128.7, 127.8, 126.9, 125.5, 117.0, 108.7, 87.1, 82.4, 37.2 ppm.

IR (neat): ν (cm^{-1}) 3152, 3064, 2761, 1793, 1729, 1641, 1602, 1580, 1497, 1452, 1432, 1330, 1295, 1265, 1219, 1163, 1092, 1065, 1029, 968, 893, 875, 799, 784, 735, 696, 640, 600, 502, 474, 434.

HRMS (ESI-FT) calcd for $C_{22}H_{17}N_2O_4^+$ ([M]+H$^+$) = 373.1183, found 373.1189.

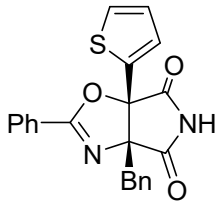


	Retention Time	% Area
1	7.123	49.41
2	8.873	50.59



	Retention Time	% Area
1	6.652	93.72
2	8.327	6.28

3a-Benzyl-2-phenyl-6a-(thiophen-2-yl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ar)



Yellow solid, **M.p.** 189 – 190 °C; 23.7 mg, 61% yield, >95:5 dr, 88% ee. $[\alpha]^{25}_{436} = -25.7$ ($c = 0.41$, in CH_2Cl_2).

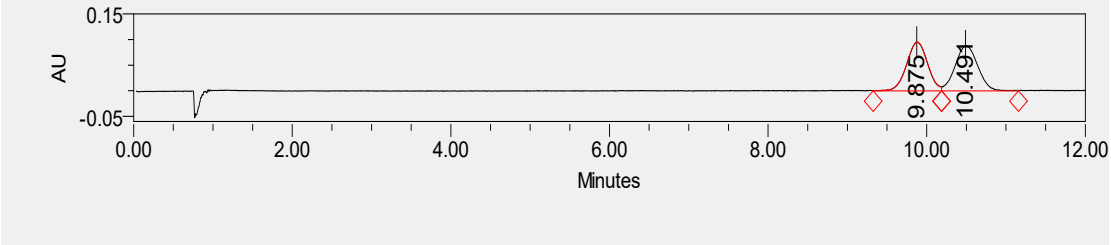
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 9.8 min, 10.6 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.11 (s, 1H), 8.06 – 8.04 (m, 2H), 7.58 – 7.54 (m, 1H), 7.47 – 7.43 (m, 2H), 7.39 – 7.37 (m, 1H), 7.08 – 6.97 (m, 4H), 6.84 – 6.83 (m, 1H), 6.67 – 6.66 (m, 2H), 3.39 (d, J = 14.6 Hz, 1H), 3.29 (d, J = 14.6 Hz, 1H) ppm.

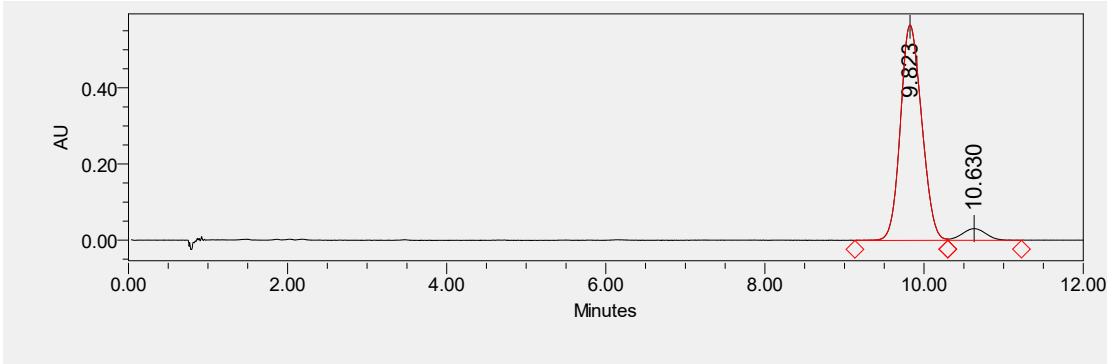
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 174.6 172.4, 163.7, 134.3, 133.8, 132.9, 130.1, 129.2, 128.8, 127.9, 127.5, 127.3, 127.2, 126.7, 125.5, 89.4, 83.7, 37.2 ppm.

IR (neat): ν (cm^{-1}) 3211, 3065, 2762, 1794, 1733, 1643, 1603, 1580, 1495, 1452, 1432, 1328, 1245, 1197, 1091, 1066, 1028, 968, 913, 850, 782, 736, 696, 640, 499, 428.

HRMS (ESI-FT) calcd for $C_{22}H_{16}N_2O_3SNa^+$ ([M]+Na$^+$) = 411.0774, found 411.0762.

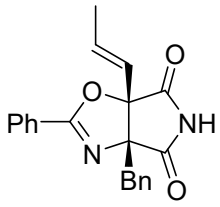


	Retention Time	% Area
1	9.875	50.04
2	10.491	49.96



	Retention Time	% Area
1	9.823	94.20
2	10.630	5.80

3a-Benzyl-2-phenyl-6a-((*E*)-prop-1-en-1-yl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4as)



White solid, **M.p.** 100 – 101 °C; 12.2 mg, 35% yield, >95:5 dr, 81% ee. $[\alpha]^{25}_{D}$ = –36.9 (*c* = 0.16, in CH_2Cl_2).

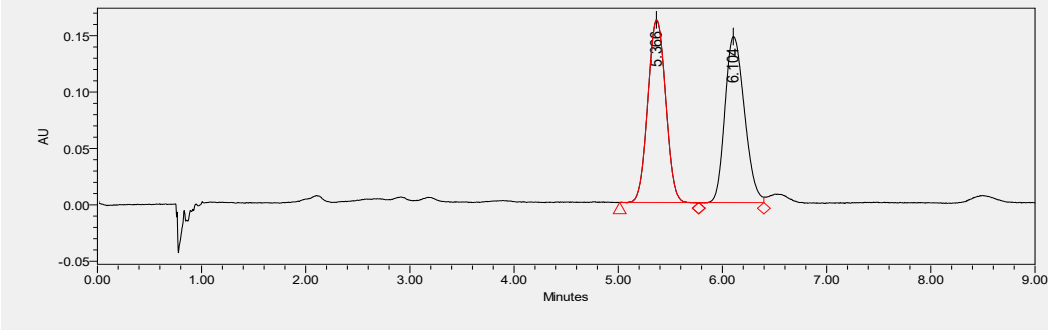
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OD-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 5.3 min, 6.1 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.83 (s, 1H), 8.00 – 7.99 (m, 2H), 7.54 – 7.51 (m, 1H), 7.44 – 7.40 (m, 2H), 7.26 – 7.17 (m, 5H), 5.97 –5.88 (m, 1H), 5.36 (dd, *J* = 16.0, 1.2 Hz, 1H), 3.43 (d, *J* = 14.8 Hz, 1H), 3.31 (d, *J* = 14.8 Hz, 1H), 1.78 – 1.76 (m, 3H) ppm.

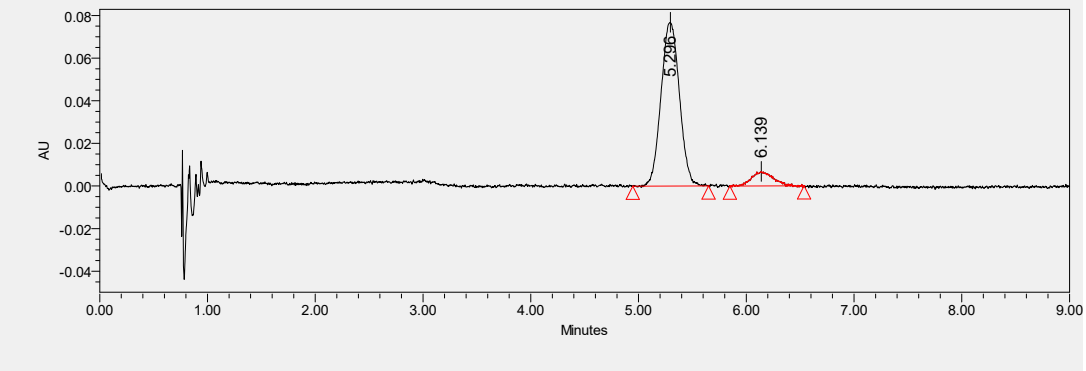
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.1, 173.3, 164.0, 134.6, 132.7, 132.4, 131.1, 129.0, 128.7, 128.1, 127.1, 125.9, 121.6, 89.8, 83.0, 37.4, 18.3 ppm.

IR (neat): ν (cm^{-1}) 3212, 3063, 2922, 2854, 2761, 1792, 1730, 1672, 1640, 1602, 1580, 1496, 1451, 1332, 1296, 1224, 1159, 1090, 1068, 1028, 965, 934, 781, 735, 696, 625, 501, 432.

HRMS (ESI-FT) calcd for $C_{21}H_{18}N_2O_3Na^+$ ([M]+Na$^+$) = 369.1210, found 369.1212.

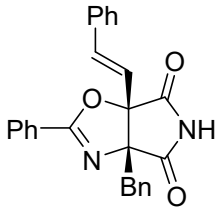


	Retention Time	% Area
1	5.366	50.17
2	6.104	49.83



	Retention Time	% Area
1	5.296	90.58
2	6.139	9.42

3a-Benzyl-2-phenyl-6a-((*E*)-styryl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4at)



White solid, **M.p.** 83 – 84 °C; 17.3 mg, 42% yield, >95:5 dr, 67% ee. $[\alpha]^{25}_{D}$ = +45.0 (*c* = 0.26, in CH_2Cl_2).

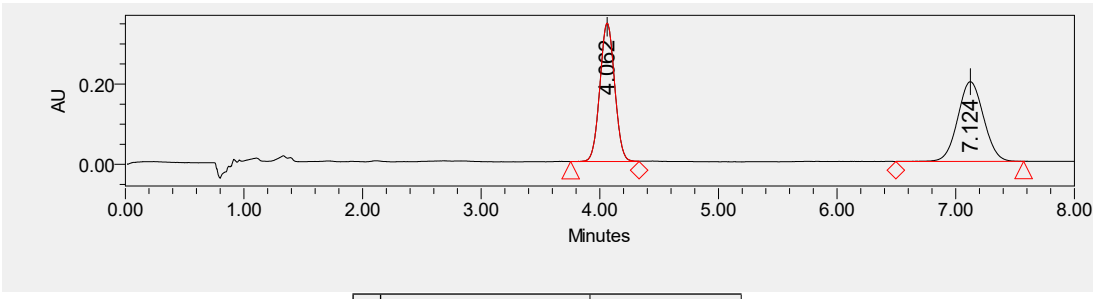
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 4.1 min, 7.1 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.70 (s, 1H), 8.07 – 8.06 (m, 2H), 7.58 – 7.55 (m, 1H), 7.48 – 7.44 (m, 2H), 7.39 – 7.30 (m, 5H), 7.21 – 7.12 (m, 5H), 6.77 (d, *J* = 16.2 Hz, 1H), 5.93 (d, *J* = 16.2 Hz, 1H), 3.44 (d, *J* = 14.8 Hz, 1H), 3.40 (d, *J* = 14.8 Hz, 1H) ppm.

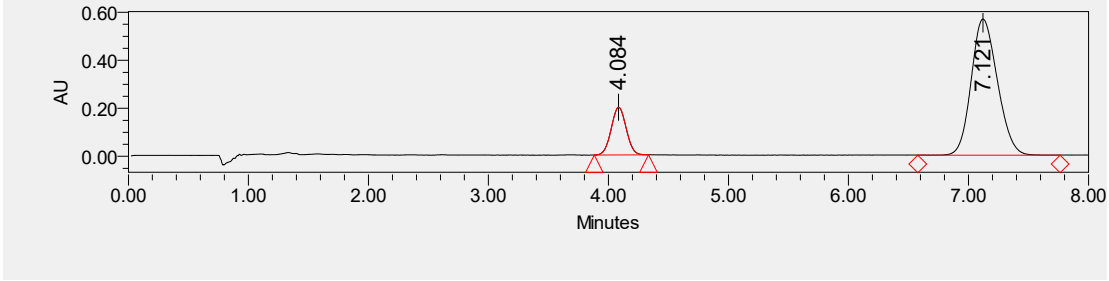
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 174.8, 172.8, 164.1, 134.9, 134.5, 134.4, 132.9, 131.1, 129.1, 129.0, 128.9, 128.8, 128.3, 127.3, 127.2, 125.8, 119.2, 90.2, 84.1, 37.5 ppm.

IR (neat): ν (cm^{-1}) 3216, 3062, 3030, 2925, 2761, 1792, 1733, 1640, 1602, 1580, 1496, 1451, 1330, 1216, 1155, 1091, 1067, 1029, 965, 782, 738, 695, 645, 567, 546, 492.

HRMS (ESI-FT) calcd for $C_{26}H_{20}N_2O_3K^+$ ([M]+K$^+$) = 447.1106, found 447.1106.

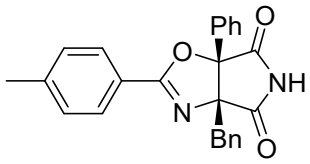


	Retention Time	% Area
1	4.062	49.77
2	7.124	50.23



	Retention Time	% Area
1	4.084	16.64
2	7.121	83.36

3a-Benzyl-6a-phenyl-2-(*p*-tolyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ba)



White solid, **M.p.** 86 – 87 °C; 35.9 mg, 91% yield, >95:5 dr, 89% ee. $[\alpha]^{25}_{D}$ = +12.4 (*c* = 0.71, in CH_2Cl_2).

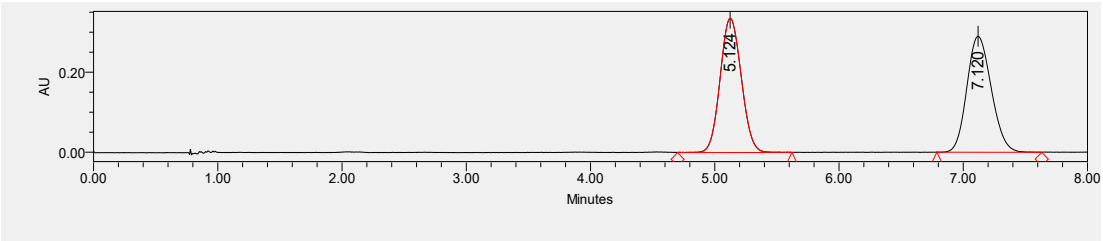
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 5.5 min, 7.3 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.40 (s, 1H), 7.98 – 7.96 (m, 2H), 7.40 – 7.37 (m, 1H), 7.33 – 7.25 (m, 4H), 7.10 – 7.09 (m, 2H), 7.01 – 6.97 (m, 1H), 6.90 – 6.86 (m, 2H), 6.49 – 6.47 (m, 2H), 3.44 (d, *J* = 14.6 Hz, 1H), 2.96 (d, *J* = 14.6 Hz, 1H), 2.42 (s, 3H) ppm.

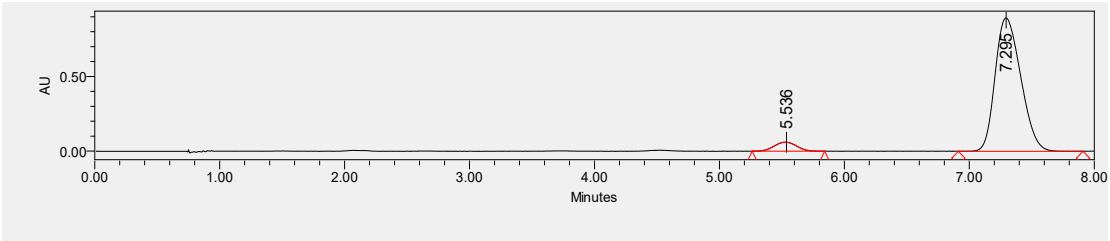
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.6, 174.3, 164.2, 143.6, 133.6, 132.0, 130.5, 129.5, 129.3, 129.1, 128.7, 127.5, 126.4, 126.2, 122.9, 91.3, 83.1, 36.6, 21.8 ppm.

IR (neat): ν (cm^{-1}) 3195, 3063, 3033, 2924, 2760, 1792, 1730, 1640, 1573, 1498, 1452, 1430, 1411, 1328, 1264, 1215, 1182, 1160, 1092, 1049, 1019, 975, 917, 829, 762, 729, 699, 644, 476.

HRMS (ESI-FT) calcd for $C_{25}H_{21}N_2O_3^+$ ([M]+H$^+$) = 397.1547, found 397.1550.

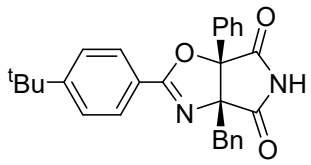


	Retention Time	% Area
1	5.124	50.07
2	7.120	49.93



	Retention Time	% Area
1	5.536	5.60
2	7.295	94.40

3a-Benzyl-2-(4-(*tert*-butyl)phenyl)-6a-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ca)



White solid, **M.p.** 113 – 114 °C; 41.8 mg, 95% yield, >95:5 dr, 91% ee. $[\alpha]^{25}_{D}$ = +10.3 (*c* = 0.80, in CH_2Cl_2).

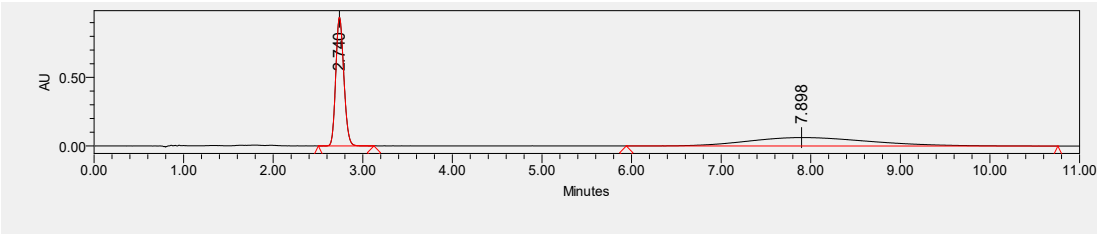
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 2.6 min, 7.2 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.42 (s, 1H), 8.04 – 8.02 (m, 2H), 7.50 – 7.47 (m, 2H), 7.40 – 7.37 (m, 1H), 7.32 – 7.29 (m, 2H), 7.11 – 7.09 (m, 2H), 7.01 – 6.98 (m, 1H), 6.91 – 6.87 (m, 2H), 6.50 – 6.49 (m, 2H), 3.45 (d, *J* = 14.8 Hz, 1H), 2.96 (d, *J* = 14.8 Hz, 1H), 1.35 (s, 9H) ppm.

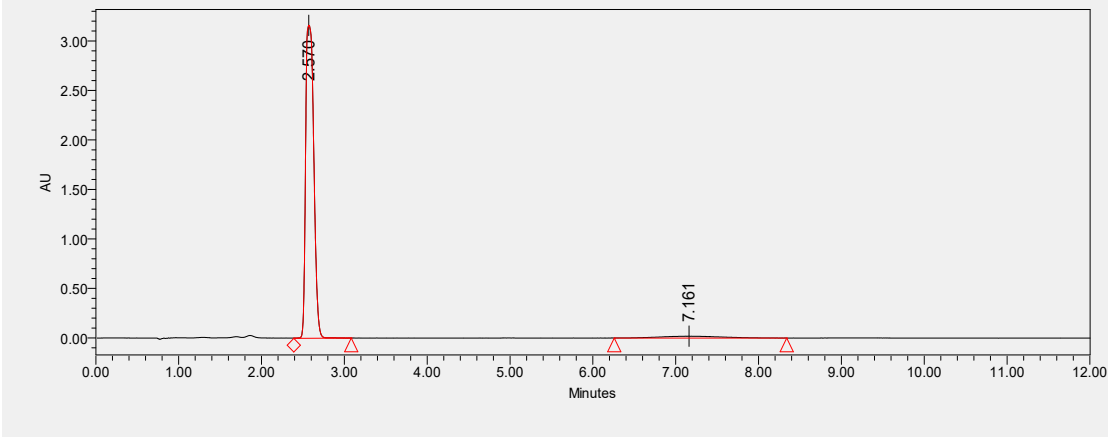
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.6, 174.3, 164.2, 156.6, 133.7, 132.0, 130.5, 129.3, 129.0, 128.7, 127.6, 126.4, 126.3, 125.8, 122.9, 91.2, 83.1, 36.7, 35.3, 31.2 ppm.

IR (neat): ν (cm^{-1}) 3201, 3063, 3033, 2963, 2870, 2760, 1793, 1732, 1641, 1568, 1499, 1453, 1411, 1364, 1329, 1267, 1215, 1160, 1114, 1089, 1050, 1018, 975, 918, 847, 755, 735, 698, 646, 552, 494.

HRMS (ESI-FT) calcd for $C_{28}H_{27}N_2O_3^+$ ([M]+H$^+$) = 439.2016, found 439.2015.

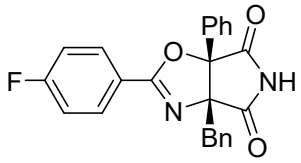


	Retention Time	% Area
1	2.740	50.10
2	7.898	49.90



	Retention Time	% Area
1	2.570	95.67
2	7.161	4.33

3a-Benzyl-2-(4-fluorophenyl)-6a-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4da)



White solid, **M.p.** 93 – 94 °C; 32.4 mg, 81% yield, >95:5 dr, 92% ee. $[\alpha]^{25}_{D}$ = +19.3 (*c* = 0.70, in CH_2Cl_2).

Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 5.7 min, 6.3 min. dr > 95:5 determined by ^{1}H NMR.

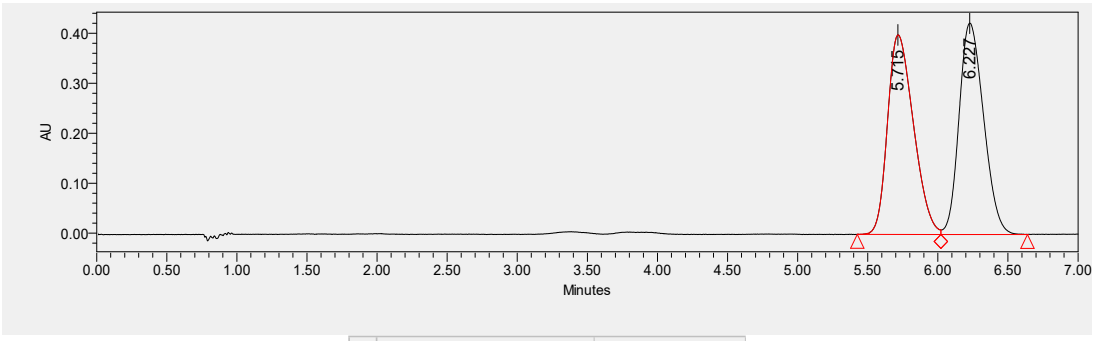
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.36 (s, 1H), 8.10 – 8.07 (m, 2H), 7.42 – 7.38 (m, 1H), 7.34 – 7.30 (m, 2H), 7.16 – 7.08 (m, 4H), 7.02 – 6.98 (m, 1H), 6.91 – 6.87 (m, 2H), 6.47 – 6.46 (m, 2H), 3.43 (d, *J* = 14.6 Hz, 1H), 2.96 (d, *J* = 14.6 Hz, 1H) ppm.

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.4, 174.1, 165.6 (d, *J* = 253.6 Hz), 163.2, 133.4, 131.7, 131.5 (d, *J* = 9.1 Hz), 130.4, 129.4, 128.8, 127.6, 126.6, 126.2, 121.9 (d, *J* = 3.1 Hz), 116.1 (d, *J* = 22.0 Hz), 91.5, 83.1, 36.6 ppm.

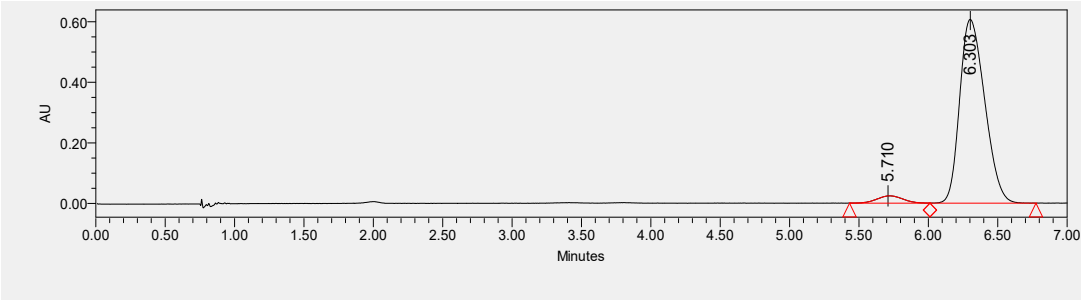
^{19}F{^{1}H} NMR (376 MHz, Chloroform-*d*) δ = −105.27 ppm.

IR (neat): ν (cm^{-1}) 3195, 3065, 2762, 1793, 1733, 1644, 1604, 1509, 1452, 1414, 1328, 1297, 1234, 1157, 1090, 1049, 1016, 974, 848, 814, 762, 699, 643, 597, 487.

HRMS (ESI-FT) calcd for $C_{24}H_{18}FN_2O_3^+$ ([M]+H$^+$) = 401.1296, found 401.1299.

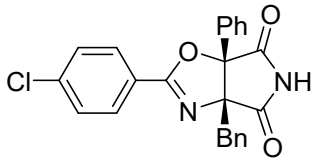


	Retention Time	% Area
1	5.715	49.94
2	6.227	50.06



	Retention Time	% Area
1	5.710	3.95
2	6.303	96.05

3a-Benzyl-2-(4-chlorophenyl)-6a-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ea)



White solid, **M.p.** 98 – 99 °C; 41.3 mg, 98% yield, >95:5 dr, 91% ee. $[\alpha]^{25}_{D}$ = +6.7 (*c* = 0.68, in CH_2Cl_2).

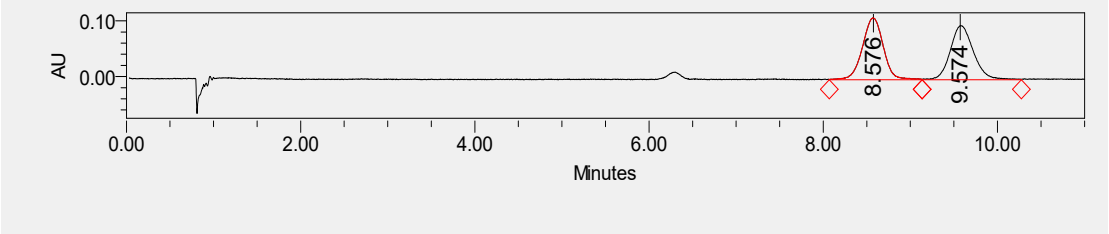
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **IB-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 8.5 min, 9.6 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.37 (s, 1H), 8.03 – 7.99 (m, 2H), 7.45 – 7.43 (m, 2H), 7.42 – 7.40 (m, 1H), 7.34 – 7.31 (m, 2H), 7.09 – 7.07 (m, 2H), 7.02 – 6.98 (m, 1H), 6.91 – 6.87 (m, 2H), 6.46 – 6.45 (m, 2H), 3.44 (d, *J* = 14.8 Hz, 1H), 2.96 (d, *J* = 14.8 Hz, 1H) ppm.

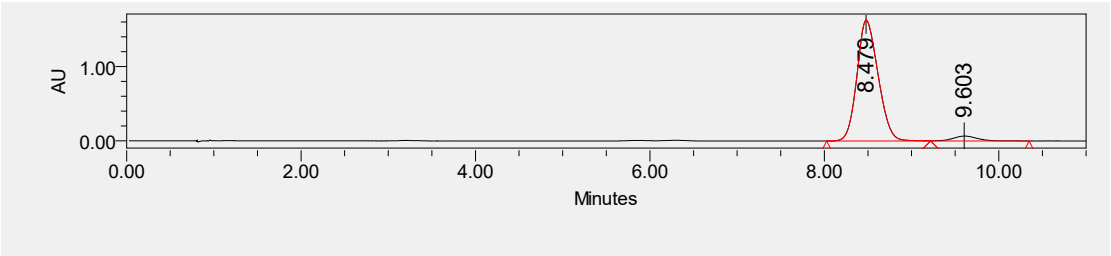
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.3, 174.0, 163.2, 139.3, 133.4, 131.7, 130.4, 130.3, 129.5, 129.2, 128.8, 127.6, 126.6, 126.2, 124.2, 91.6, 83.2, 36.6 ppm.

IR (neat): ν (cm^{-1}) 3207, 3064, 3033, 2765, 1793, 1734, 1644, 1597, 1492, 1452, 1430, 1404, 1327, 1264, 1216, 1093, 1049, 1015, 974, 917, 841, 756, 731, 699, 678, 642, 589, 510, 475, 451.

HRMS (ESI-FT) calcd for $C_{24}H_{18}{}^{34.9659}ClN_2O_3^+$ ([M]+H$^+$) = 417.1000, found 417.1004, $C_{24}H_{18}{}^{36.9659}ClN_2O_3^+$ ([M]+H$^+$) = 419.0971, found 419.0970.

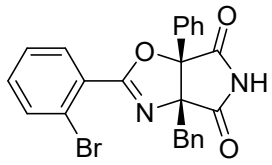


	Retention Time	% Area
1	8.576	50.82
2	9.574	49.18



	Retention Time	% Area
1	8.479	95.56
2	9.603	4.44

3a-Benzyl-2-(2-bromophenyl)-6a-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4fa)



White solid, **M.p.** 104 – 106 °C; 45.1 mg, 98% yield, >95:5 dr, 90% ee. $[\alpha]^{25}_{D}$ = +74.3 (*c* = 0.60, in CH_2Cl_2).

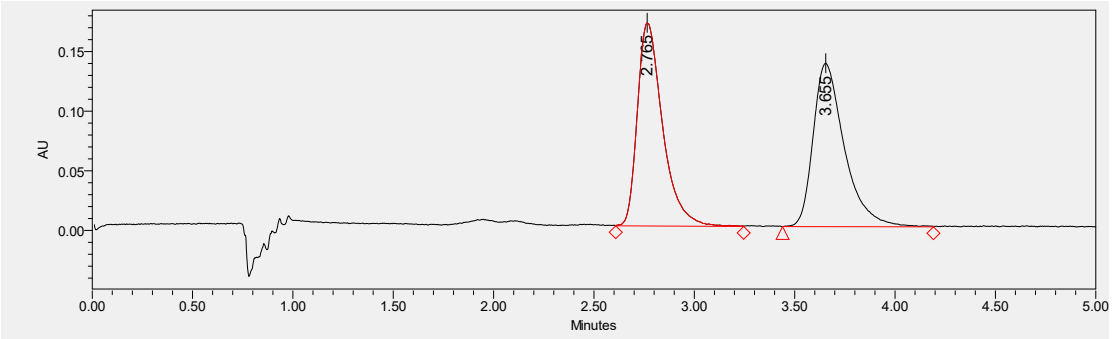
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 2.8 min, 3.7 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.30 (s, 1H), 7.71 – 7.65 (m, 2H), 7.44 – 7.34 (m, 5H), 7.19 – 7.17 (m, 2H), 7.08 – 7.04 (m, 1H), 6.98 – 6.94 (m, 2H), 6.52 – 6.50 (m, 2H), 3.52 (d, *J* = 14.4 Hz, 1H), 2.99 (d, *J* = 14.4 Hz, 1H) ppm.

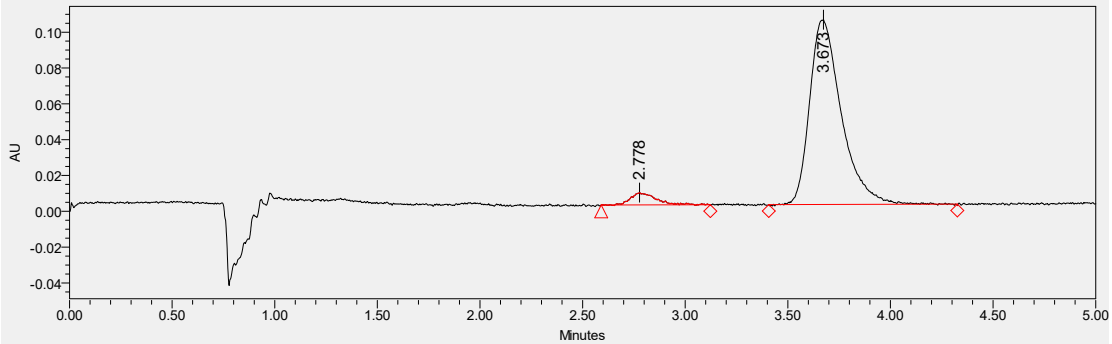
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.0, 173.6, 163.9, 134.2, 133.3, 132.9, 132.0, 131.7, 130.8, 129.5, 128.9, 127.6, 127.4, 126.7, 126.3, 122.3, 91.7, 83.0, 36.1 ppm.

IR (neat): ν (cm^{-1}) 3201, 3063, 2760, 1794, 1729, 1642, 1588, 1497, 1473, 1451, 1432, 1326, 1262, 1214, 1160, 1106, 1031, 972, 918, 732, 700, 676, 639, 491.

HRMS (ESI-FT) calcd for $C_{24}H_{18}{}^{78.9183}BrN_2O_3^+$ ([M]+H$^+$) = 461.0495, found 461.0490, $C_{24}H_{18}{}^{80.9163}BrN_2O_3^+$ ([M]+H$^+$) = 463.0475, found 463.0472.

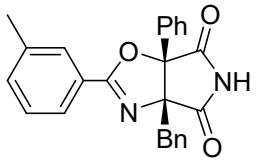


	Retention Time	% Area
1	2.765	50.13
2	3.655	49.87



	Retention Time	% Area
1	2.778	5.10
2	3.673	94.90

3a-Benzyl-6a-phenyl-2-(*m*-tolyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ga)



White solid, **M.p.** 86 – 87 °C; 33.1 mg, 84% yield, >95:5 dr, 88% ee. $[\alpha]^{25}_{D}$ = +21.6 (*c* = 0.56, in CH_2Cl_2).

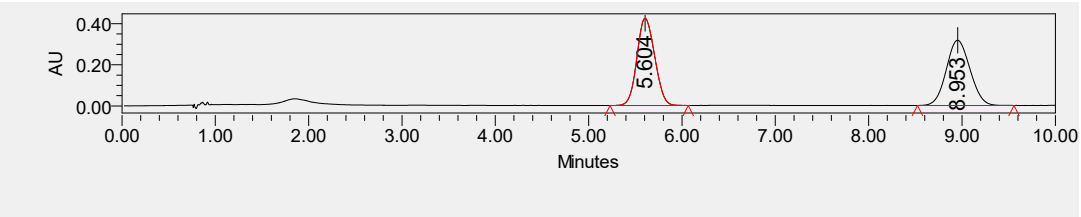
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 5.7 min, 8.9 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.34 (s, 1H), 7.91 – 7.88 (m, 2H), 7.41 – 7.35 (m, 3H), 7.33 – 7.29 (m, 2H), 7.11 – 7.09 (m, 2H), 7.02 – 6.98 (m, 1H), 6.91 – 6.87 (m, 2H), 6.50 – 6.48 (m, 2H), 3.43 (d, *J* = 14.6 Hz, 1H), 2.98 (d, *J* = 14.6 Hz, 1H), 2.41 (s, 3H) ppm.

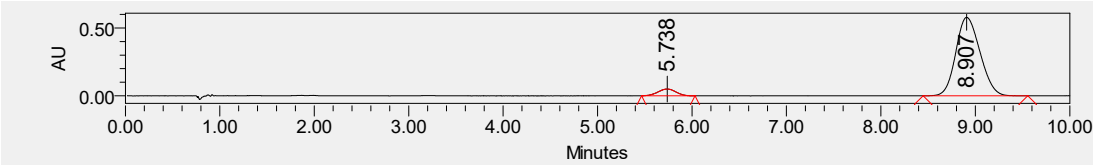
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.5, 174.2, 164.3, 138.7, 133.7, 133.6, 131.9, 130.4, 129.6, 129.3, 128.8, 128.7, 127.6, 126.5, 126.3, 125.6, 91.3, 83.2, 36.7, 21.4 ppm.

IR (neat): ν (cm^{-1}) 3206, 3063, 3032, 2924, 2760, 1793, 1733, 1642, 1603, 1586, 1496, 1452, 1431, 1328, 1265, 1202, 1098, 1049, 1019, 1049, 1019, 976, 925, 830, 800, 762, 738, 700, 641, 623, 573, 481, 425.

HRMS (ESI-FT) calcd for $C_{25}H_{21}N_2O_3^+$ ([M]+H$^+$) = 397.1547, found 397.1550.

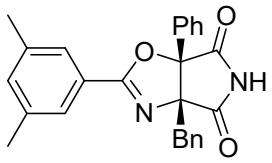


	Retention Time	% Area
1	5.604	50.09
2	8.953	49.91



	Retention Time	% Area
1	5.738	6.00
2	8.907	94.00

3a-Benzyl-2-(3,5-dimethylphenyl)-6a-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ha)



White solid, **M.p.** 95 – 96 °C; 36.6 mg, 89% yield, >95:5 dr, 77% ee. $[\alpha]^{25}_{D}$ = +17.2 (*c* = 0.65, in CH_2Cl_2).

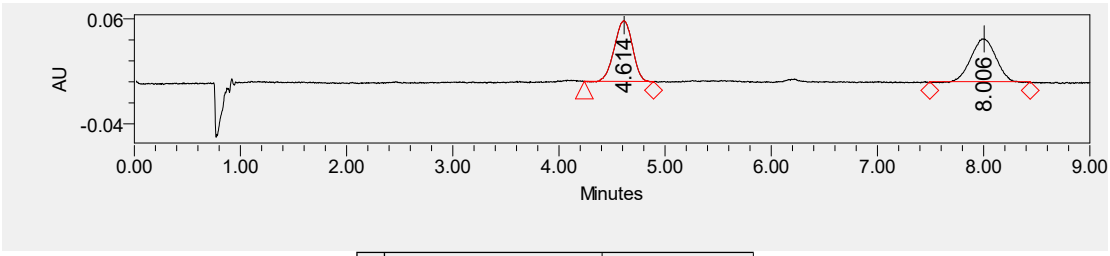
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 4.6 min, 8.0 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.32 (s, 1H), 7.72 – 7.71 (m, 2H), 7.41 – 7.37 (m, 1H), 7.33 – 7.29 (m, 2H), 7.19 (s, 1H), 7.10 – 7.09 (m, 2H), 7.02 – 6.98 (m, 1H), 6.91 – 6.87 (m, 2H), 6.50 – 6.48 (m, 2H), 3.42 (d, *J* = 14.8 Hz, 1H), 2.99 (d, *J* = 14.8 Hz, 1H), 2.36 (s, 6H) ppm.

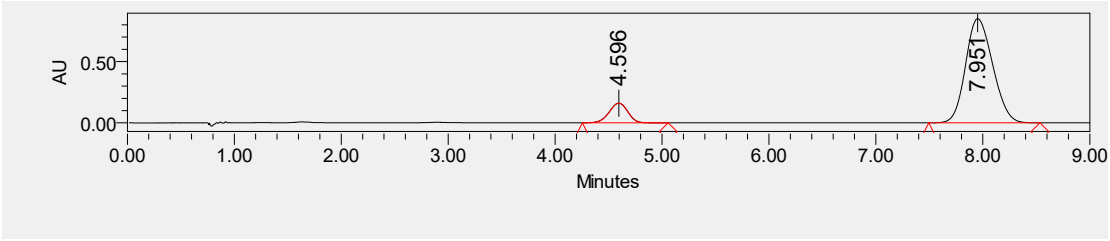
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.5, 174.2, 164.5, 138.5, 134.6, 133.6, 132.0, 130.4, 129.3, 128.7, 127.6, 126.8, 126.5, 126.3, 125.5, 91.2, 83.1, 36.7, 21.2 ppm.

IR (neat): ν (cm^{-1}) 3213, 3063, 3032, 2921, 2759, 1793, 1734, 1641, 1599, 1497, 1452, 1381, 1338, 1222, 1159, 1111, 1085, 1021, 975, 929, 863, 815, 761, 726, 700, 678, 642, 623, 574, 523, 478, 450.

HRMS (ESI-FT) calcd for $C_{26}H_{23}N_2O_3^+$ ([M]+H$^+$) = 411.1703, found 411.1702.

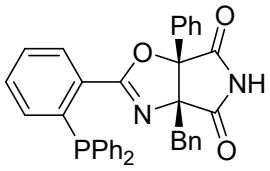


	Retention Time	% Area
1	4.614	50.53
2	8.006	49.47



	Retention Time	% Area
1	4.596	11.42
2	7.951	88.58

3a-Benzyl-2-(2-(diphenylphosphaneyl)phenyl)-6a-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ia)



White solid, **M.p.** 112 – 113 °C; 39.2 mg, 69% yield, >95:5 dr, 94% ee. $[\alpha]^{25}_{D}$ = +96.5 (*c* = 0.45, in CH_2Cl_2).

Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **IA-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 8.3 min, 9.6 min. dr > 95:5 determined by ^{1}H NMR.

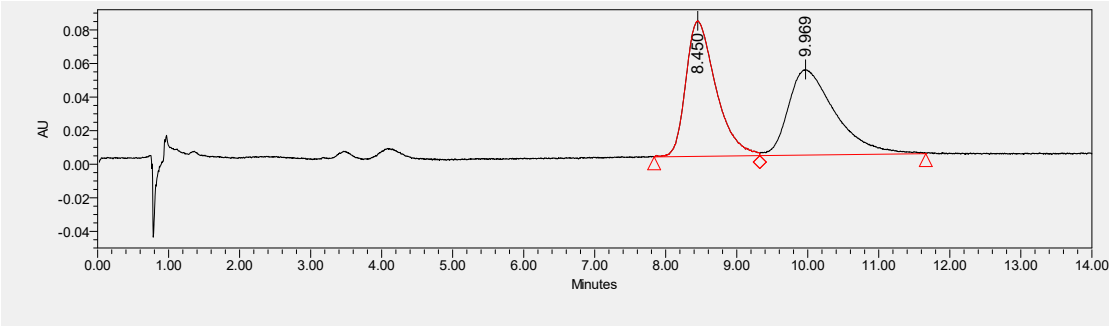
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 11.13 (s, 1H), 7.74 – 7.58 (m, 6H), 7.52 – 7.39 (m, 7H), 7.30 –7.25 (m, 2H), 7.19 – 7.15 (m, 2H), 6.99 – 6.97 (m, 1H), 6.88 – 6.81 (m, 4H), 6.32 – 6.30 (m, 2H), 3.32 (d, *J* = 14.8 Hz, 1H), 2.81 (d, *J* = 14.8 Hz, 1H) ppm.

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.1, 173.5, 163.5 (d, *J* = 3.2 Hz), 134.3, 134.0 (d, J = 11.2 Hz), 133.4, 133.0, 132.4 (d, J = 17.1 Hz), 132.3 (d, J = 2.9 Hz), 131.9 (d, J = 5.1 Hz), 131.8, 131.2 (d, J = 8.7 Hz), 130.7, 130.3 (d, J = 12.1 Hz), 128.6 (d, J = 19.3 Hz), 128.5 (d, J = 12.6 Hz), 128.3, 128.3, 127.2, 126.4, 126.1, 91.6, 83.0, 36.3 ppm.

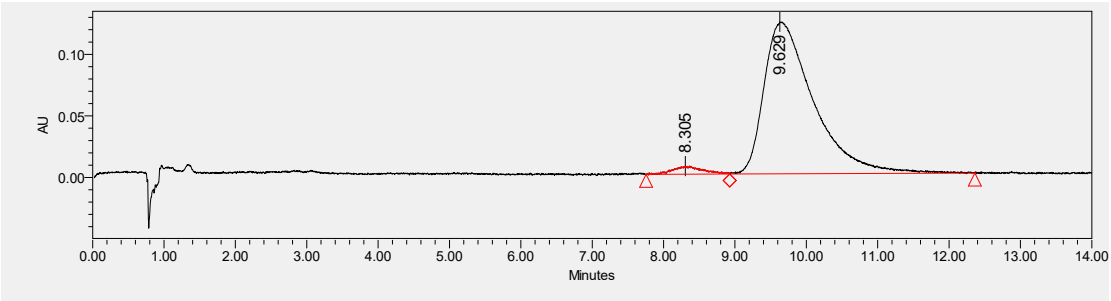
^{31}P{^{1}H} NMR (162 MHz, Chloroform-*d*) δ = 32.26 ppm.

IR (neat): ν (cm^{-1}) 3059, 2924, 2751, 1791, 1736, 1664, 1588, 1496, 1437, 1376, 1323, 1260, 1218, 1174, 1116, 1064, 971, 803, 755, 723, 697, 624, 573, 545, 517, 493.

HRMS (ESI-FT) calcd for $C_{36}H_{27}N_2O_3PNa^+$ ([M]+Na^+) = 589.1652, found 589.1633.

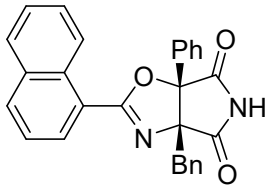


	Retention Time	% Area
1	8.450	50.37
2	9.969	49.63



	Retention Time	% Area
1	8.305	3.09
2	9.629	96.91

3a-Benzyl-2-(naphthalen-1-yl)-6a-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ja)



White solid, **M.p.** 96 – 98 °C; 36.7 mg, 85% yield, >95:5 dr, 91% ee. $[\alpha]^{25}_{D}$ = +26.8 (*c* = 0.75, in CH_2Cl_2).

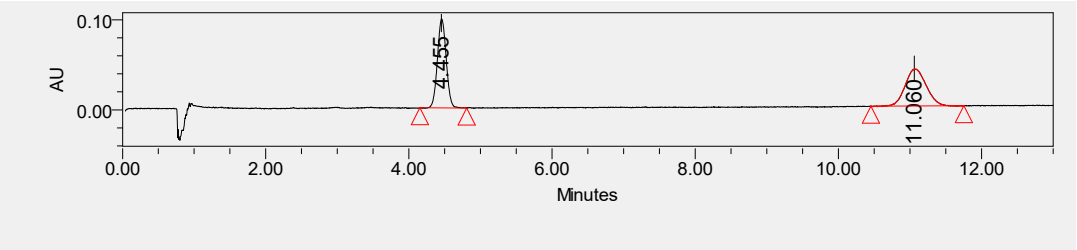
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 4.5 min, 11.0 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.22 (d, *J* = 8.6 Hz, 1H), 8.26 – 8.24 (m, 1H), 8.04 – 8.02 (m, 1H), 7.91 – 7.89 (m, 1H), 7.67 – 7.63 (m, 1H), 7.58 – 7.55 (m, 1H), 7.52 – 7.48 (m, 1H), 7.44 – 7.40 (m, 1H), 7.37 – 7.33 (m, 2H), 7.19 – 7.18 (m, 2H), 7.03 – 6.99 (m, 1H), 6.92 – 6.89 (m, 2H), 6.57 – 6.55 (m, 2H), 3.52 (d, *J* = 14.6 Hz, 1H), 3.08 (d, *J* = 14.6 Hz, 1H) ppm.

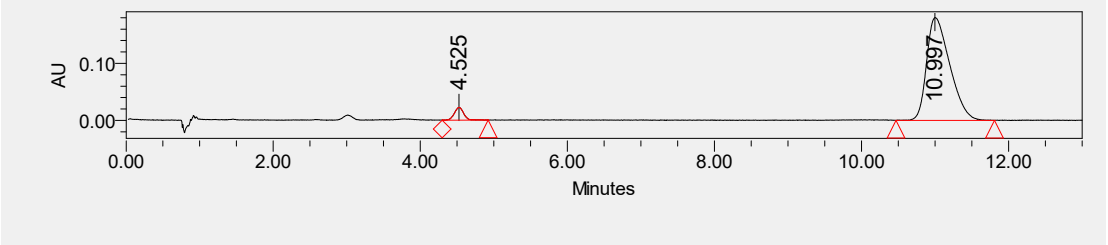
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.3, 174.1, 164.0, 133.9, 133.8, 133.7, 132.0, 131.2, 130.7, 130.6, 129.4, 128.9, 128.8, 128.3, 127.7, 126.6, 126.5, 126.3, 124.7, 122.0, 90.2, 84.0, 36.8 ppm.

IR (neat): ν (cm^{-1}) 3203, 3062, 2760, 1793, 1729, 1636, 1616, 1589, 1512, 1497, 1452, 1327, 1300, 1251, 1214, 1130, 1085, 1051, 1019, 968, 916, 809, 777, 642, 574, 528, 485.

HRMS (ESI-FT) calcd for $C_{28}H_{21}N_2O_3^+$ ([M]+H$^+$) = 433.1547, found 433.1548.

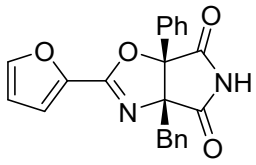


	Retention Time	% Area
1	4.455	50.13
2	11.060	49.87



	Retention Time	% Area
1	4.525	4.75
2	10.997	95.25

3a-Benzyl-2-(furan-2-yl)-6a-phenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ka)



White solid, **M.p.** 112 – 113 °C; 27.7 mg, 74% yield, >95:5 dr, 92% ee. $[\alpha]^{25}_{D}$ = +7.5 (*c* = 0.21, in CH_2Cl_2).

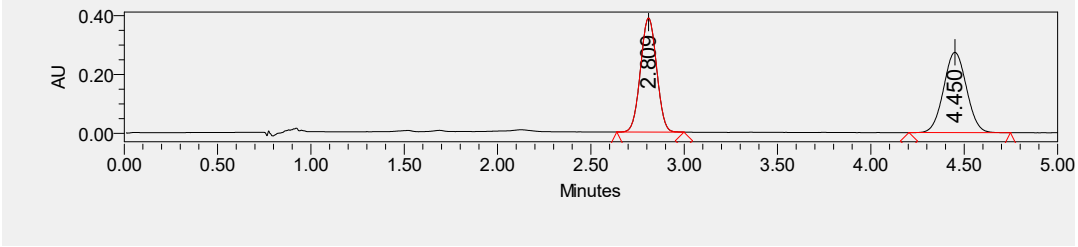
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 2.9 min, 4.4 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.94 (s, 1H), 7.78 – 7.77 (m, 1H), 7.59 – 7.58 (m, 1H), 7.42 – 7.39 (m, 1H), 7.34 – 7.30 (m, 2H), 7.14 – 7.08 (m, 3H), 7.03 – 6.99 (m, 1H), 6.92 – 6.88 (m, 2H), 6.48 – 6.46 (m, 2H), 3.42 (d, *J* = 14.6 Hz, 1H), 2.97 (d, *J* = 14.6 Hz, 1H) ppm.

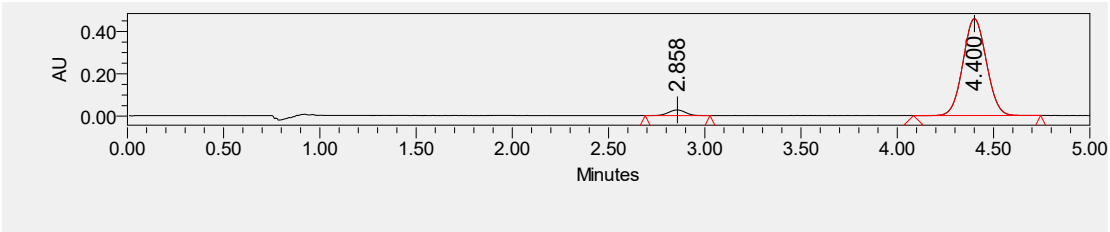
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 174.9, 173.6, 159.9, 133.4, 132.7, 132.3, 131.7, 130.5, 129.5, 128.8, 128.1, 127.9, 127.6, 126.5, 126.2, 91.6, 83.2, 36.6 ppm.

IR (neat): ν (cm^{-1}) 3206, 3091, 2758, 1793, 1734, 1639, 1518, 1498, 1451, 1427, 1370, 1326, 1216, 1159, 1088, 1066, 1032, 1006, 971, 855, 762, 723, 701, 650, 629, 578, 498, 452.

HRMS (ESI-FT) calcd for $C_{22}H_{16}N_2O_4K^+$ ([M]+K$^+$) = 411.0742, found 411.0746.

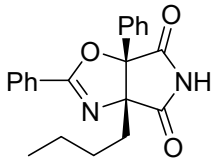


	Retention Time	% Area
1	2.809	50.04
2	4.450	49.96



	Retention Time	% Area
1	2.858	4.08
2	4.400	95.92

(3a*R*,6a*S*)-3a-Butyl-2,6a-diphenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4la)



White solid, **M.p.** 174 – 176 °C; 25.0 mg, 72% yield, >95:5 dr, 88% ee. $[\alpha]^{25}_{D}$ = +66.6 (*c* = 0.50, in CH_2Cl_2). Reference report: $[\alpha]^{23}_{D}$ = +86.8 (*c* = 0.191, CH_2Cl_2, sample with ee = 94%), see *Angew. Chem., Int. Ed.*, **2013**, *52*, 13223.

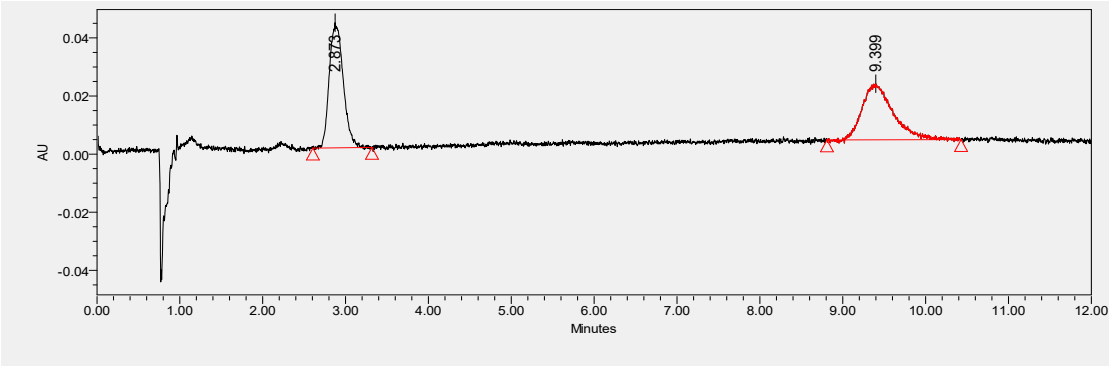
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 2.9 min, 9.3 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.23 (s, 1H), 8.18 – 8.05 (m, 2H), 7.59 – 7.55 (m, 1H), 7.49 – 7.36 (m, 7H), 1.95 – 1.88 (m, 1H), 1.61 – 1.53 (m, 1H), 1.11 – 1.03 (m, 1H), 1.01 – 0.78 (m, 3H), 0.55 (t, *J* = 7.2 Hz, 3H) ppm.

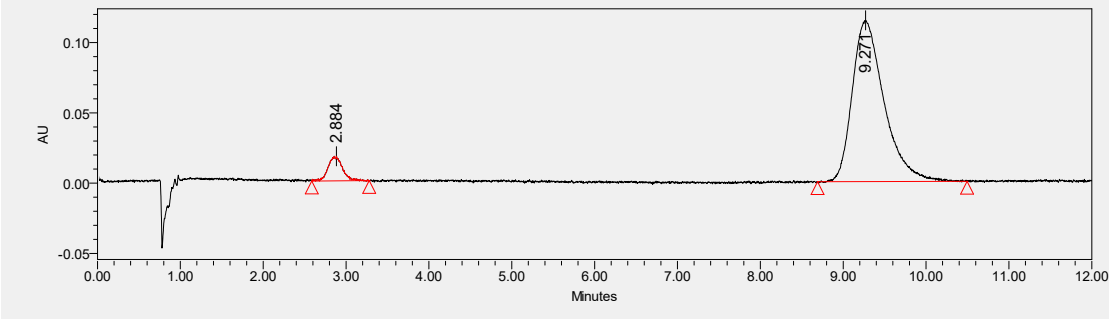
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.7, 174.1, 163.9, 132.8, 132.2, 129.5, 129.1, 128.8, 128.8, 126.0, 125.8, 91.5, 83.3, 31.2, 24.6, 22.7, 13.5 ppm.

IR (neat): ν (cm^{-1}) 3201, 3066, 2958, 2870, 2759, 1792, 1732, 1643, 1580, 1496, 1451, 1329, 1214, 1179, 1115, 1090, 1067, 1025, 771, 696, 639, 515.

HRMS (ESI-FT) calcd for $C_{21}H_{21}N_2O_3^+$ ([M]+H$^+$) = 349.1547, found 349.1547.

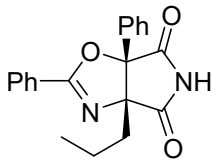


	Retention Time	% Area
1	2.873	50.10
2	9.399	49.90



	Retention Time	% Area
1	2.884	6.05
2	9.271	93.95

2,6a-Diphenyl-3a-propyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ma)



White solid, **M.p.** 180 – 182 °C; 19.6 mg, 59% yield, >95:5 dr, 84% ee. $[\alpha]^{25}_{D}$ = +66.6 (*c* = 0.36, in CH_2Cl_2).

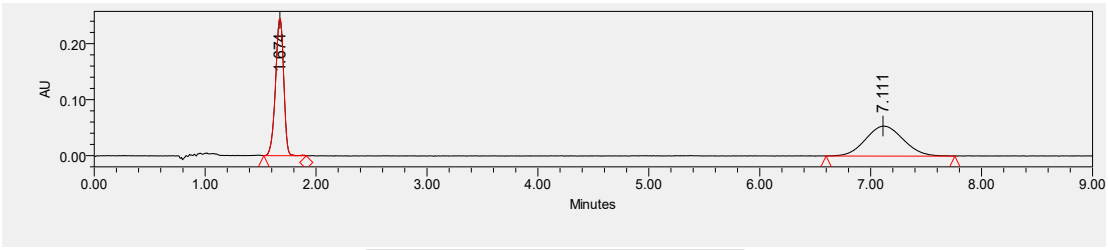
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 1.7 min, 6.8 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.04 (s, 1H), 8.12 – 8.10 (m, 2H), 7.59 – 7.55 (m, 1H), 7.49 – 7.41 (m, 5H), 7.38 – 7.35 (m, 2H), 1.92 – 1.84 (m, 1H), 1.55 – 1.48 (m, 1H), 1.21 – 1.11 (m, 1H), 0.95 – 0.85 (m, 1H), 0.57 (t, *J* = 7.2 Hz, 3H) ppm.

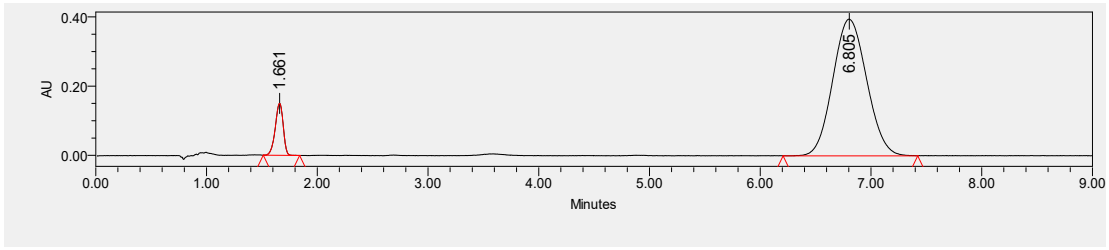
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.5, 174.0, 164.0, 132.8, 132.2, 129.5, 129.1, 128.8, 128.8, 126.0, 125.8, 91.5, 83.4, 33.7, 16.2, 14.3 ppm.

IR (neat): ν (cm^{-1}) 3211, 3066, 2964, 2874, 2761, 1792, 1732, 1643, 1580, 1496, 1451, 1330, 1217, 1179, 1118, 1090, 1067, 1048, 1026, 1002, 773, 696, 641, 515.

HRMS (ESI-FT) calcd for $C_{20}H_{19}N_2O_3^+$ ([M]+H$^+$) = 335.1390, found 335.1393.

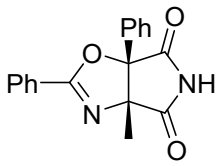


	Retention Time	% Area
1	1.674	49.69
2	7.111	50.31



	Retention Time	% Area
1	1.661	8.18
2	6.805	91.82

3a-Methyl-2,6a-diphenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4na)



White solid, **M.p.** 93 – 95 °C; 18.0 mg, 59% yield, >95:5 dr, 84% ee. $[\alpha]^{25}_{D}$ = +66.3 (*c* = 0.32, in CH_2Cl_2).

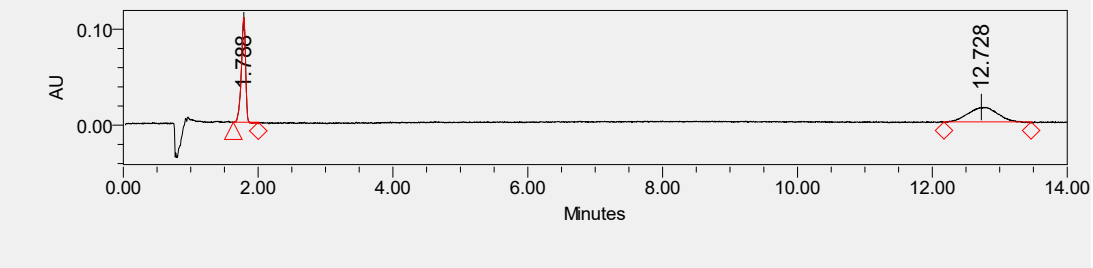
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 1.8 min, 12.7 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.11 – 8.09 (m, 2H), 7.58 – 7.55 (m, 1H), 7.48 – 7.41 (m, 5H), 7.32 – 7.30 (m, 2H), 5.43 (s, 1H), 1.17 (s, 3H) ppm.

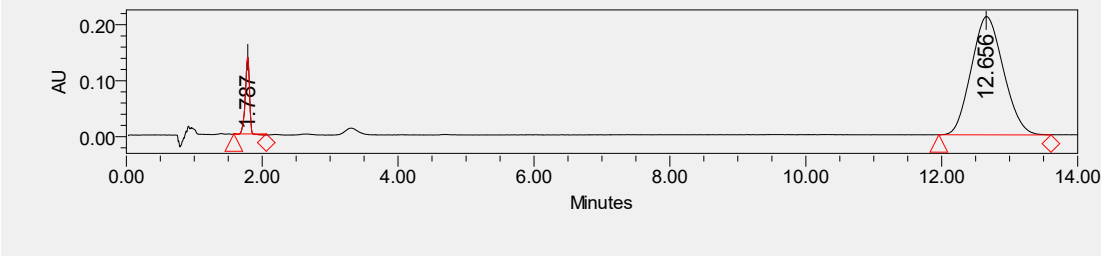
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 176.6, 174.6, 164.0, 132.9, 132.5, 129.5, 129.1, 129.0, 128.8, 125.8, 91.8, 80.9, 18.8 ppm.

IR (neat): ν (cm^{-1}) 3191, 3065, 2931, 2760, 1793, 1733, 1642, 1602, 1580, 1496, 1451, 1377, 1328, 1229, 1179, 1146, 1120, 1087, 1068, 1031, 1003, 970, 771, 696, 627, 604, 500, 432.

HRMS (ESI-FT) calcd for $C_{18}H_{14}N_2O_3Na^+$ ([M]+Na$^+$) = 329.0897, found 329.0894.

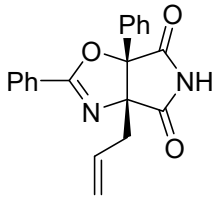


	Retention Time	% Area
1	1.788	50.84
2	12.728	49.16



	Retention Time	% Area
1	1.787	7.95
2	12.656	92.05

3a-Allyl-2,6a-diphenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4oa)



White solid, **M.p.** 183 – 185 °C; 27.9 mg, 84% yield, >95:5 dr, 92% ee. $[\alpha]^{25}_{D}$ = +55.3 (*c* = 0.55, in CH_2Cl_2).

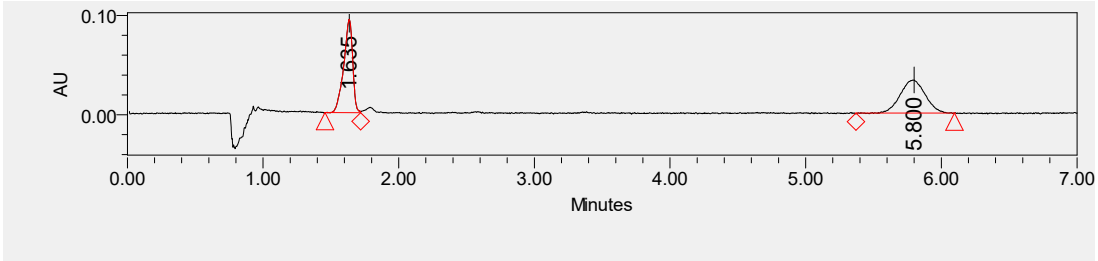
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 1.6 min, 5.7 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.38 (s, 1H), 8.12 – 8.10 (m, 2H), 7.59 – 7.55 (m, 1H), 7.49 – 7.45 (m, 2H), 7.41 – 7.40 (m, 3H), 7.35 – 7.32 (m, 2H), 5.32 – 5.21 (m, 1H), 4.76 (dd, *J* = 10.2, 1.8 Hz, 1H), 4.56 (dd, *J* = 17.2, 1.8 Hz, 1H), 2.67 (dd, *J* = 14.8, 6.8 Hz, 1H), 2.44 (dd, *J* = 14.8, 7.2 Hz, 1H) ppm.

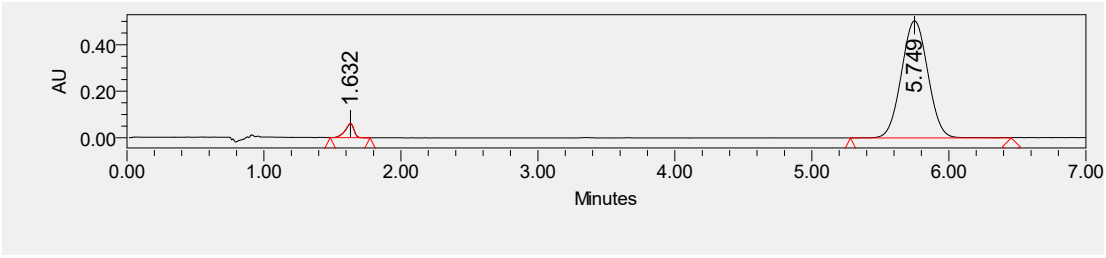
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.1, 174.0, 164.3, 132.9, 131.9, 129.7, 129.6, 129.2, 128.8, 128.7, 126.4, 125.7, 120.0, 91.3, 82.7, 35.9 ppm.

IR (neat): ν (cm^{-1}) 3214, 3073, 2760, 1793, 1735, 1642, 1580, 1495, 1451, 1431, 1330, 1215, 1160, 1093, 1067, 1027, 999, 925, 770, 696, 652, 625, 564, 505.

HRMS (ESI-FT) calcd for $C_{20}H_{17}N_2O_3^+$ ([M]+H$^+$) = 333.1234, found 333.1234.

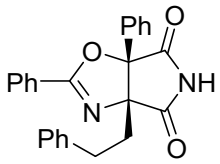


	Retention Time	% Area
1	1.635	50.28
2	5.800	49.72



	Retention Time	% Area
1	1.632	3.87
2	5.749	96.13

3a-Phenethyl-2,6a-diphenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4pa)



White solid, **M.p.** 94 – 96 °C; 21.9 mg, 55% yield, >95:5 dr, 60% ee. $[\alpha]^{25}_{D}$ = +28.3 (*c* = 0.27, in CH_2Cl_2).

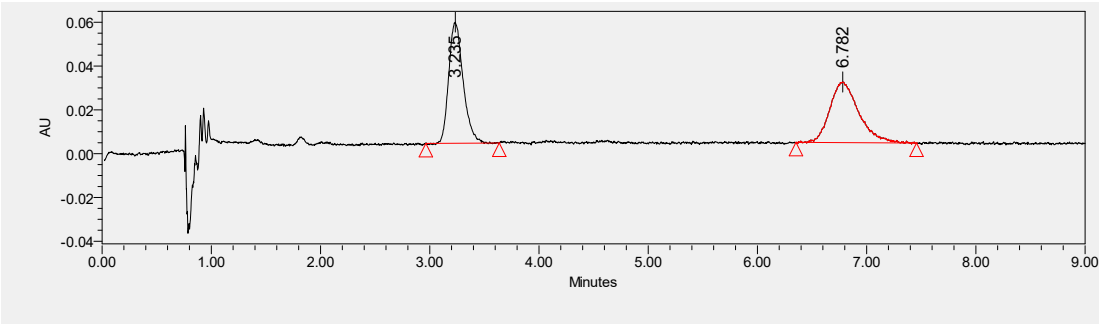
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 3.2 min, 6.8 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.96 (s, 1H), 8.17 – 8.15 (m, 2H), 7.61 – 7.57 (m, 1H), 7.51 – 7.44 (m, 7H), 7.14 – 7.05 (m, 3H), 6.65 – 6.64 (m, 2H), 2.47 (td, *J* = 12.8, 4.8 Hz, 1H), 2.31 (td, *J* = 13.2, 4.8 Hz, 1H), 2.12 (m, 1H), 1.80 (m, 1H) ppm.

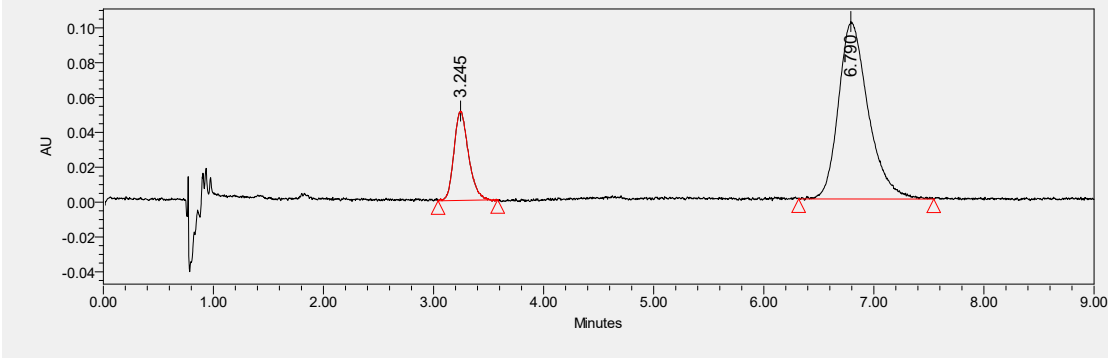
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.1, 173.7, 164.3, 141.0, 133.0, 132.2, 129.8, 129.2, 129.1, 128.9, 128.4, 128.3, 126.1, 125.7, 91.5, 83.0, 33.8, 29.2 ppm.

IR (neat): ν (cm^{-1}) 3196, 3064, 3028, 2920, 2850, 2763, 1792, 1737, 1642, 1603, 1581, 1496, 1451, 1330, 1218, 1095, 1068, 1029, 997, 751, 696, 627, 560, 498.

HRMS (ESI-FT) calcd for $C_{25}H_{21}N_2O_3^+$ ([M]+H$^+$) = 397.1547, found 397.1549.

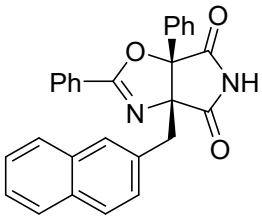


	Retention Time	% Area
1	3.235	49.90
2	6.782	50.10



	Retention Time	% Area
1	3.245	19.83
2	6.790	80.17

3a-(Naphthalen-2-ylmethyl)-2,6a-diphenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4qa)



White solid, **M.p.** 98 – 100 °C; 43.0 mg, 99% yield, >95:5 dr, 94% ee. $[\alpha]^{25}_{436}$ = –42.8 (*c* = 0.59, in CH_2Cl_2).

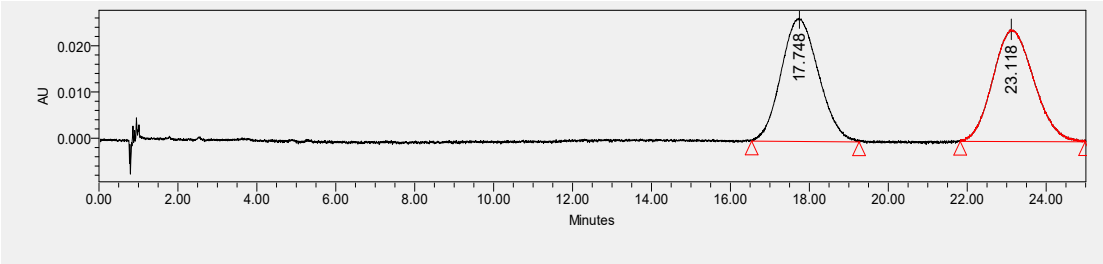
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 17.3 min, 22.6 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.34 (s, 1H), 8.09 – 8.07 (m, 2H), 7.66 – 7.64 (m, 1H), 7.56 – 7.53 (m, 1H), 7.47 – 7.42 (m, 4H), 7.37 – 7.29 (m, 5H), 7.11 – 7.09 (m, 2H), 6.95 – 6.93 (m, 1H), 6.52 – 6.51 (m, 1H), 3.68 (d, *J* = 14.6 Hz, 1H), 3.14 (d, *J* = 14.6 Hz, 1H) ppm.

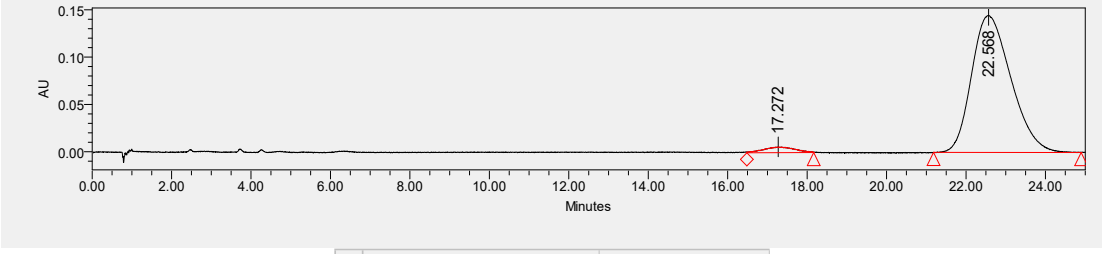
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.4, 174.1, 164.2, 132.9, 132.7, 132.1, 131.9, 130.9, 129.7, 129.5, 129.1, 128.9, 128.8, 127.9, 127.4, 126.8, 126.4, 125.6, 125.6, 91.4, 83.0, 36.6 ppm.

IR (neat): ν (cm^{-1}) 3211, 3060, 2760, 1793, 1731, 1641, 1602, 1580, 1497, 1450, 1429, 1329, 1265, 1215, 1160, 1092, 1067, 1024, 977, 899, 859, 821, 763, 736, 696, 653, 627, 587, 539, 479, 455, 436.

HRMS (ESI-FT) calcd for $C_{28}H_{21}N_2O_3^+$ ([M]+H$^+$) = 433.1547, found 433.1554.

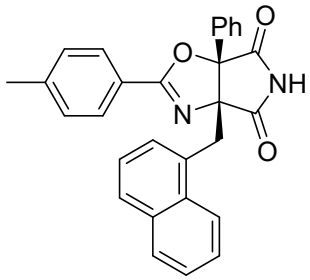


	Retention Time	% Area
1	17.748	50.17
2	23.118	49.83



	Retention Time	% Area
1	17.272	3.16
2	22.568	96.84

3a-(Naphthalen-1-ylmethyl)-6a-phenyl-2-(*p*-tolyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ra)



White solid, **M.p.** 99 – 101 °C; 44.6 mg, 99% yield, >95:5 dr, 91% ee. $[\alpha]^{25}_{D}$ = +57.6 (*c* = 0.82, in CH_2Cl_2).

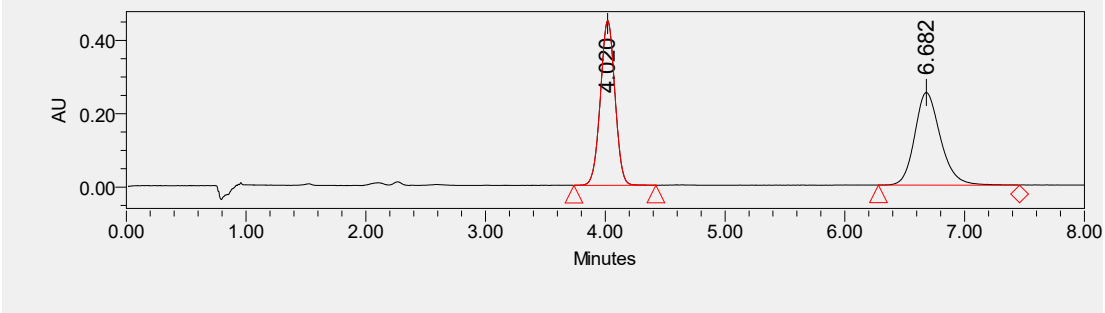
Dissolved in MeOH for UPC^2; **UPC^2** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 4.1 min, 6.7 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.39 (s, 1H), 7.99 – 7.97 (m, 1H), 7.67 – 7.64 (m, 3H), 7.58 – 7.56 (m, 1H), 7.39 – 7.34 (m, 2H), 7.30 – 7.28 (m, 3H), 7.24 – 7.22 (m, 2H), 7.12 – 7.10 (m, 2H), 7.07 – 7.04 (m, 1H), 6.54 – 6.52 (m, 1H), 3.94 (d, *J* = 15.2 Hz, 1H), 3.22 (d, *J* = 15.2 Hz, 1H) ppm.

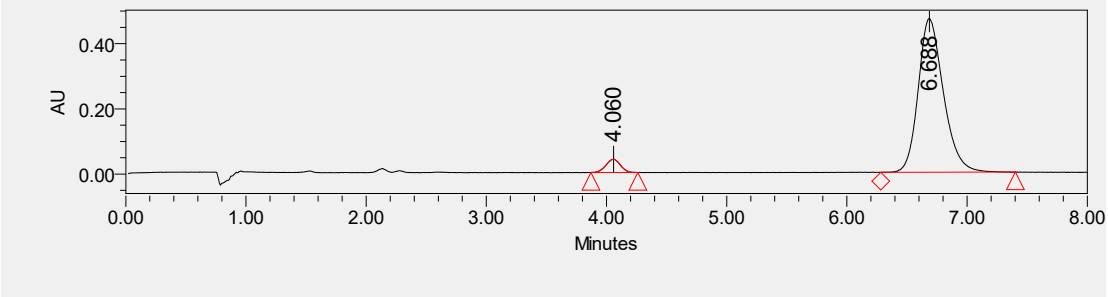
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.6, 174.3, 164.0, 143.3, 133.6, 133.2, 132.0, 130.5, 129.4, 129.3, 129.0, 128.9, 128.7, 128.2, 127.8, 126.1, 125.4, 125.3, 125.1, 124.7, 122.8, 92.1, 83.1, 32.9, 21.8 ppm.

IR (neat): ν (cm^{-1}) 3207, 3063, 2926, 2759, 1792, 1729, 1640, 1573, 1512, 1450, 1398, 1328, 1265, 1214, 1182, 1092, 972, 915, 829, 780, 729, 698, 661, 630, 588, 536, 512, 462, 417.

HRMS (ESI-FT) calcd for $C_{29}H_{23}N_2O_3^+$ ([M]+H$^+$) = 447.1703, found 447.1708.

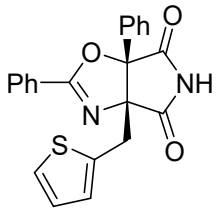


	Retention Time	% Area
1	4.020	50.08
2	6.682	49.92



	Retention Time	% Area
1	4.060	4.73
2	6.688	95.27

2,6a-Diphenyl-3a-(thiophen-2-ylmethyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4sa)



White solid, **M.p.** 116 – 118 °C; 37.4 mg, 96% yield, >95:5 dr, 93% ee. $[\alpha]^{25}_{D}$ = +21.2 (*c* = 0.59, in CH_2Cl_2).

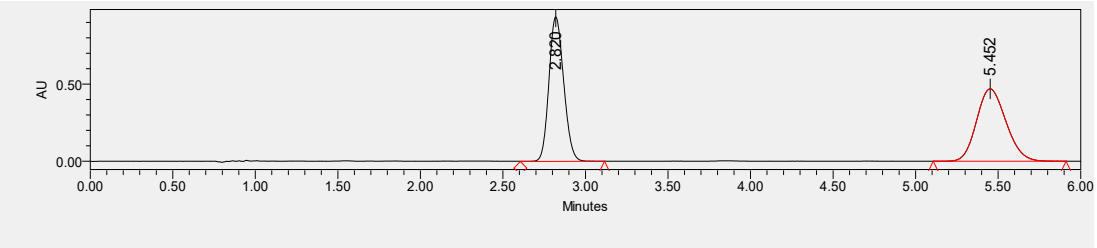
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 2.8 min, 5.2 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.43 (s, 1H), 8.14 – 8.13 (m, 2H), 7.60 – 7.56 (m, 1H), 7.50 – 7.46 (m, 2H), 7.34 – 7.31 (m, 1H), 7.28 – 7.24 (m, 2H), 7.09 – 7.07 (m, 2H), 6.91 – 6.90 (m, 1H), 6.51 – 6.48 (m, 1H), 5.72 – 5.71 (m, 1H), 3.65 (d, *J* = 15.6 Hz, 1H), 3.25 (d, *J* = 15.6 Hz, 1H) ppm.

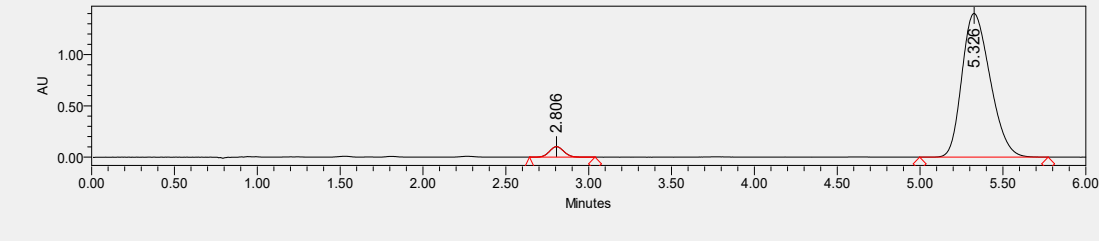
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.2, 174.1, 165.2 134.9, 133.0, 131.7, 129.3, 129.2, 128.8, 128.6, 127.5, 125.8, 125.7, 125.3, 91.2, 82.7, 31.7 ppm.

IR (neat): ν (cm^{-1}) 3193, 3067, 2759, 1792, 1732, 1640, 1603, 1580, 1496, 1450, 1423, 1330, 1269, 1227, 1207, 1178, 1156, 1093, 1067, 1046, 1026, 976, 851, 765, 736, 695, 651, 625, 587, 504.

HRMS (ESI-FT) calcd for $C_{22}H_{17}N_2O_3S^+$ ([M]+H$^+$) = 389.0954, found 389.0944.

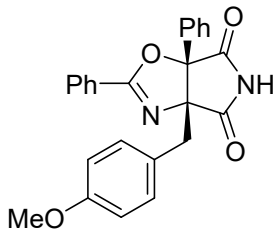


	Retention Time	% Area
1	2.820	50.13
2	5.452	49.87



	Retention Time	% Area
1	2.806	3.54
2	5.326	96.46

3a-(4-Methoxybenzyl)-2,6a-diphenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ta)



White solid, **M.p.** 95 – 97 °C; 36.3 mg, 88% yield, >95:5 dr, 87% ee. $[\alpha]^{25}_{D}$ = +35.0 (*c* = 0.60, in CH_2Cl_2).

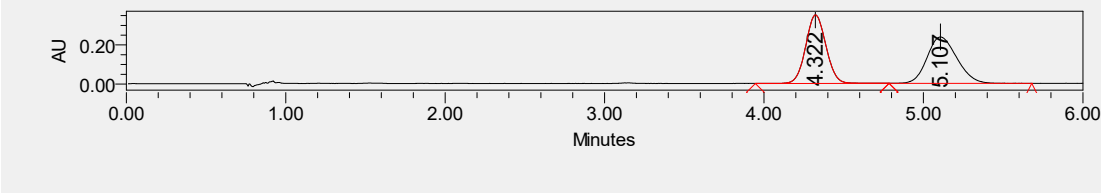
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 4.3 min, 5.2 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.32 (s, 1H), 8.09 – 8.07 (m, 2H), 7.58 – 7.54 (m, 1H), 7.48 – 7.44 (m, 2H), 7.42 – 7.38 (m, 1H), 7.36 – 7.32 (m, 2H), 7.13 – 7.11 (m, 2H), 6.44 – 6.42 (m, 2H), 6.38 – 6.36 (m, 2H), 3.66 (s, 3H), 3.39 (d, *J* = 14.8 Hz, 1H), 2.92 (d, *J* = 14.8 Hz, 1H) ppm.

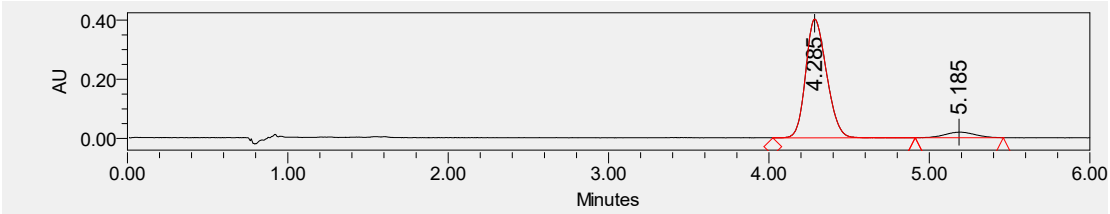
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.5, 174.2, 164.0, 158.2, 132.8, 132.0, 131.6, 129.4, 129.1, 128.8, 126.3, 125.8, 125.4, 112.9, 91.3, 83.2, 55.2, 35.7 ppm.

IR (neat): ν (cm^{-1}) 3193, 3064, 2934, 2836, 2761, 1792, 1733, 1642, 1612, 1581, 1513, 1496, 1450, 1331, 1303, 1251, 1216, 1180, 1112, 1093, 1067, 1030, 975, 827, 766, 737, 696, 643, 589, 551, 507, 430.

HRMS (ESI-FT) calcd for $C_{25}H_{21}N_2O_4^+$ ([M]+H$^+$) = 413.1496, found 413.1493.

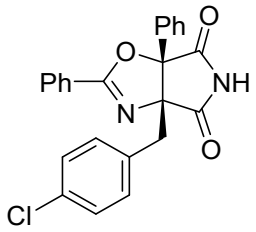


	Retention Time	% Area
1	4.322	50.18
2	5.107	49.82



	Retention Time	% Area
1	4.285	93.59
2	5.185	6.41

3a-(4-Chlorobenzyl)-2,6a-diphenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ua)



White solid, **M.p.** 94 – 96 °C; 41.5 mg, 99% yield, >95:5 dr, 90% ee. $[\alpha]^{25}_{D}$ = +40.8 (*c* = 1.15, in CH_2Cl_2).

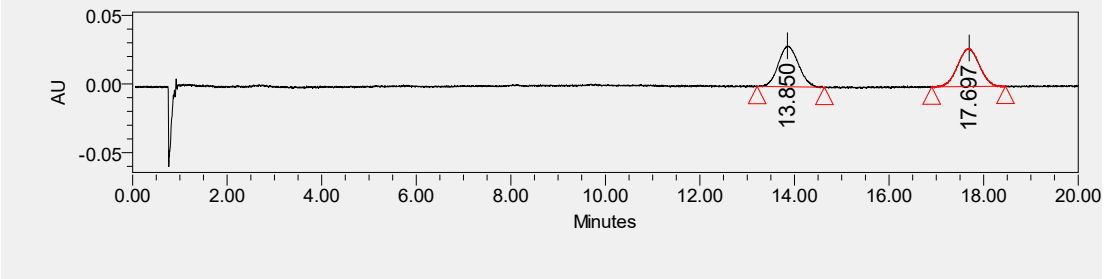
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 13.8 min, 17.4 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.70 (s, 1H), 8.08 – 8.06 (m, 2H), 7.58 – 7.55 (m, 1H), 7.48 – 7.44 (m, 2H), 7.42 – 7.39 (m, 1H), 7.36 – 7.32 (m, 2H), 7.13 – 7.11 (m, 2H), 6.87 – 6.85 (m, 2H), 6.41 – 6.39 (m, 2H), 3.44 (d, *J* = 14.8 Hz, 1H), 2.87 (d, *J* = 14.8 Hz, 1H) ppm.

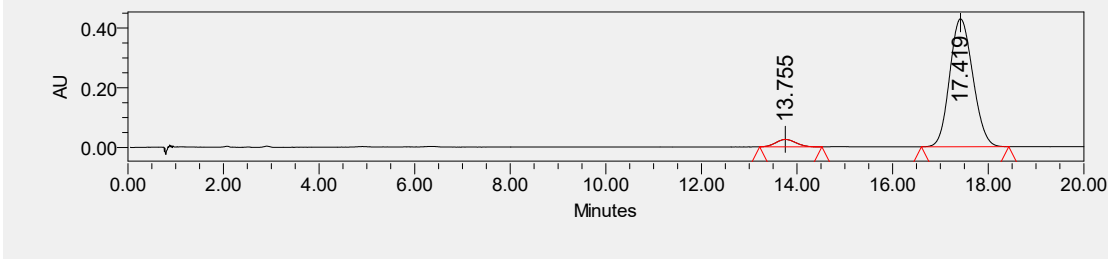
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.5, 174.2, 164.3, 133.0, 132.5, 132.0, 131.9, 131.8, 129.5, 129.1, 128.9, 127.6, 126.2, 125.5, 91.3, 82.9, 35.8 ppm.

IR (neat): ν (cm^{-1}) 3198, 3065, 2926, 2762, 1793, 1726, 1641, 1601, 1580, 1493, 1450, 1431, 1409, 1330, 1264, 1214, 1091, 1067, 1050, 1016, 976, 916, 837, 815, 766, 737, 695, 641, 585, 519, 491.

HRMS (ESI-FT) calcd for $C_{24}H_{17}{}^{34.9659}ClN_2O_3K^+$ ([M]+K$^+$) = 455.0559, found 455.0548, $C_{24}H_{17}{}^{36.9659}ClN_2O_3K^+$ ([M]+K$^+$) = 457.0530, found 457.0532.

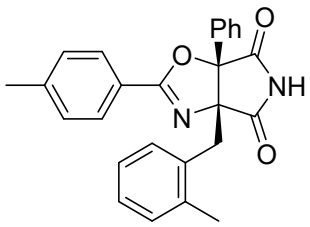


	Retention Time	% Area
1	13.850	49.84
2	17.697	50.16



	Retention Time	% Area
1	13.755	4.82
2	17.419	95.18

3a-(2-Methylbenzyl)-6a-phenyl-2-(*p*-tolyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4va)



White solid, **M.p.** 102 – 104 °C; 35.7 mg, 87% yield, >95:5 dr, 91% ee. $[\alpha]^{25}_{D}$ = +68.8 (*c* = 0.65, in CH_2Cl_2).

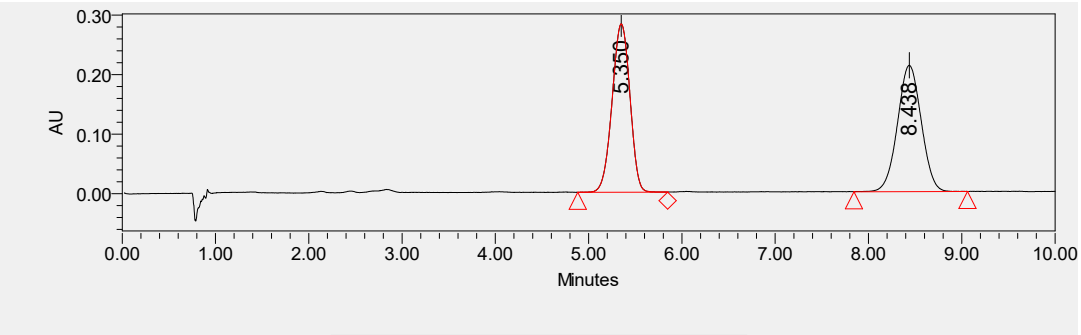
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 5.4 min, 8.5 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.25 (s, 1H), 7.93 – 7.91 (m, 2H), 7.38 – 7.33 (m, 3H), 7.25 – 7.20 (m, 4H), 6.99 – 6.96 (m, 1H), 6.92 – 6.86 (m, 2H), 6.72 – 6.70 (m, 1H), 3.27 (d, *J* = 15.0 Hz, 1H), 2.80 (d, *J* = 15.0 Hz, 1H), 2.40 (s, 3H), 2.00 (s, 3H) ppm.

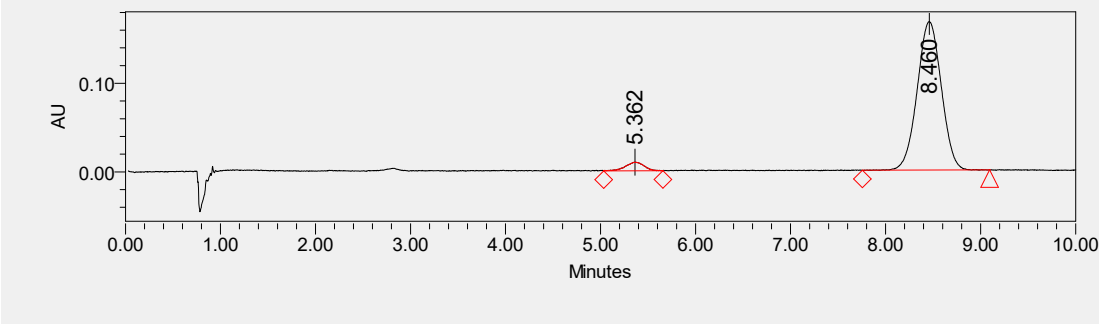
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.4, 174.2, 164.1, 143.5, 138.2, 132.9, 132.0, 130.5, 130.1, 129.5, 129.4, 129.1, 128.8, 126.9, 126.3, 125.3, 123.0, 92.1, 83.3, 33.7, 21.8, 20.2 ppm.

IR (neat): ν (cm^{-1}) 3212, 3064, 2925, 2760, 1792, 1732, 1640, 1573, 1512, 1496, 1450, 1411, 1329, 1265, 1214, 1181, 1116, 1080, 1045, 1019, 973, 829, 729, 696, 644, 537, 467.

HRMS (ESI-FT) calcd for $C_{26}H_{23}N_2O_3^+$ ([M]+H$^+$) = 411.1703, found 411.1710.

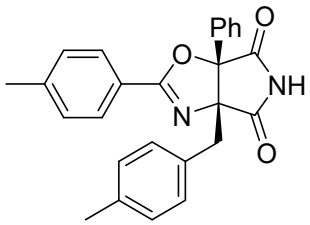


	Retention Time	% Area
1	5.350	49.98
2	8.438	50.02



	Retention Time	% Area
1	5.362	4.26
2	8.460	95.74

3a-(4-Methylbenzyl)-6a-phenyl-2-(*p*-tolyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4wa)



Pale yellow solid, **M.p.** 106 – 108 °C; 40.0 mg, 98% yield, > 95:5 dr, 90% ee. $[\alpha]^{25}_{D}$ = +25.1 (*c* = 0.54, in CH_2Cl_2).

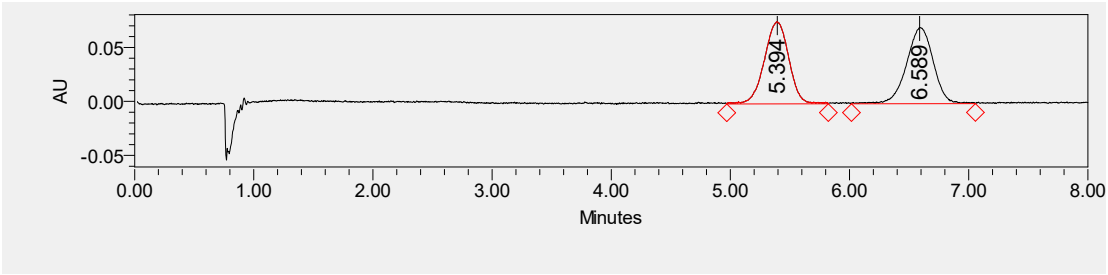
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 5.4 min, 6.5 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.23 (s, 1H), 7.98 – 7.96 (m, 2H), 7.41 – 7.38 (m, 1H), 7.34 – 7.30 (m, 2H), 7.25 (s, 2H), 7.12 – 7.10 (m, 2H), 6.71 – 6.69 (m, 2H), 6.37 – 6.35 (m, 2H), 3.38 (d, *J* = 14.6 Hz, 1H), 2.93 (d, *J* = 14.6 Hz, 1H), 2.42 (s, 3H), 2.16 (s, 3H) ppm.

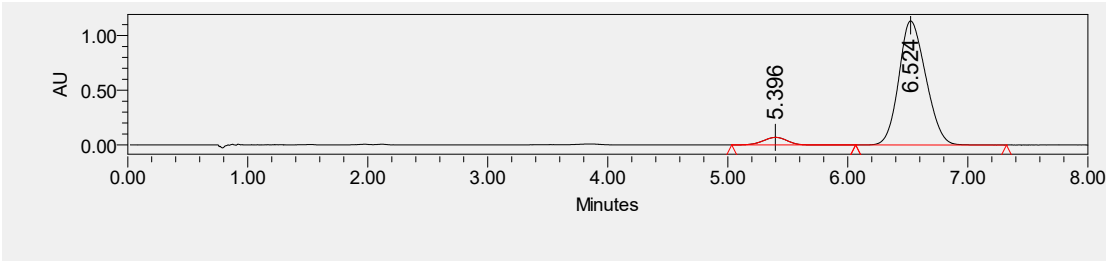
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.6, 174.2, 164.2, 143.5, 136.0, 132.0, 130.4, 130.3, 129.5, 129.3, 129.1, 128.7, 128.3, 126.3, 123.0, 91.3, 83.2, 36.3, 21.8, 21.1 ppm.

IR (neat): ν (cm^{-1}) 3204, 3032, 2922, 2760, 1794, 1734, 1640, 1573, 1514, 1450, 1411, 1329, 1213, 1182, 1092, 1050, 1019, 973, 828, 766, 727, 695, 645, 539, 456,

HRMS (ESI-FT) calcd for $C_{26}H_{23}N_2O_3^+$ ([M]+H$^+$) = 411.1703, found 411.1701.

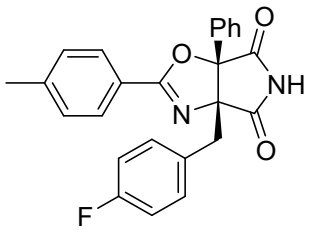


	Retention Time	% Area
1	5.394	49.57
2	6.589	50.43



	Retention Time	% Area
1	5.396	5.18
2	6.524	94.82

3a-(4-Fluorobenzyl)-6a-phenyl-2-(*p*-tolyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4xa)



White solid, **M.p.** 93 – 95 °C; 41.0 mg, 98% yield, >95:5 dr, 90% ee. $[\alpha]^{25}_{D}$ = +5.1 (*c* = 0.73, in CH_2Cl_2).

Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 5.4 min, 6.2 min. dr > 95:5 determined by ^{1}H NMR.

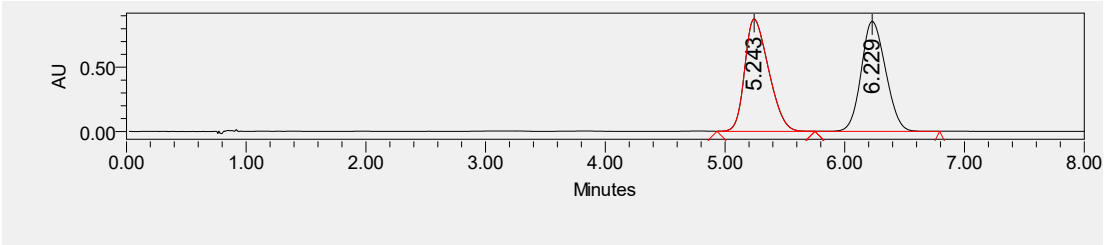
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.41 (s, 1H), 7.97 – 7.95 (m, 2H), 7.42 – 7.38 (m, 1H), 7.35 – 7.32 (m, 2H), 7.27 – 7.25 (m, 2H), 7.12 – 7.10 (m, 2H), 6.59 – 6.55 (m, 2H), 6.43 – 6.40 (m, 2H), 3.43 (d, *J* = 14.8 Hz, 1H), 2.89 (d, *J* = 14.8 Hz, 1H), 2.42 (s, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.5, 174.2, 164.4, 161.7 (d, *J* = 245.0 Hz),143.7, 132.0, 131.9, 129.6, 129.4, 129.2 (d, *J* = 3.2 Hz), 129.0, 128.8, 126.2, 122.8, 114.3 (d, *J* = 21.1 Hz), 91.2, 82.9, 35.7, 21.8 ppm.

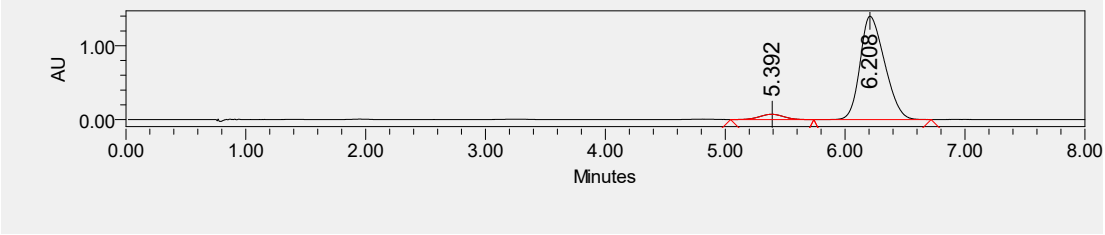
^{19}F{^{1}H} NMR (376 MHz, Chloroform-*d*) δ = −116.39 ppm.

IR (neat): ν (cm^{-1}) 3193, 3066, 2925, 2760, 1793, 1729, 1639, 1606, 1573, 1510, 1450, 1432, 1412, 1328, 1265, 1220, 1182, 1159, 1093, 1049, 1019, 976, 830, 766, 728, 696, 682, 644, 586, 538, 506, 455.

HRMS (ESI-FT) calcd for $C_{25}H_{20}FN_2O_3^+$ ([M]+H$^+$) = 415.1452, found 415.1451.

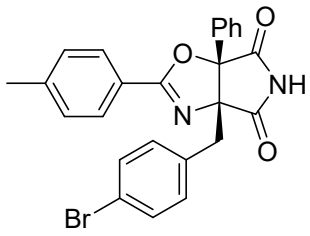


	Retention Time	% Area
1	5.243	50.02
2	6.229	49.98



	Retention Time	% Area
1	5.392	4.80
2	6.208	95.20

3a-(4-Bromobenzyl)-6a-phenyl-2-(*p*-tolyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4ya)



White solid, **M.p.** 136 – 138 °C; 47.1 mg, 99% yield, >95:5 dr, 92% ee. $[\alpha]^{25}_{D}$ = +34.8 (*c* = 0.82, in CH_2Cl_2).

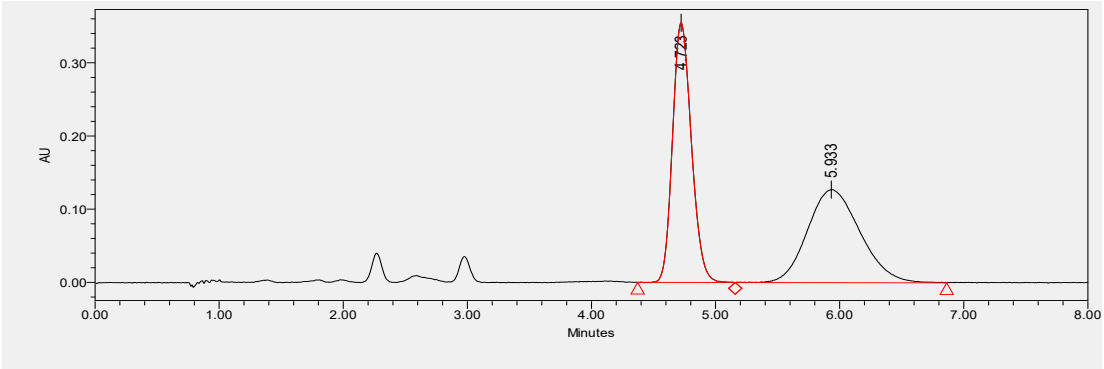
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 4.5 min, 5.7 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.44 (s, 1H), 7.97 – 7.95 (m, 2H), 7.42 – 7.39 (m, 1H), 7.35 – 7.32 (m, 2H), 7.27 – 7.25 (m, 2H), 7.12 – 7.10 (m, 2H), 7.01 – 6.99 (m, 2H), 6.35 – 6.32 (m, 2H), 3.41 (d, *J* = 14.8 Hz, 1H), 2.84 (d, *J* = 14.8 Hz, 1H), 2.42 (s, 3H) ppm.

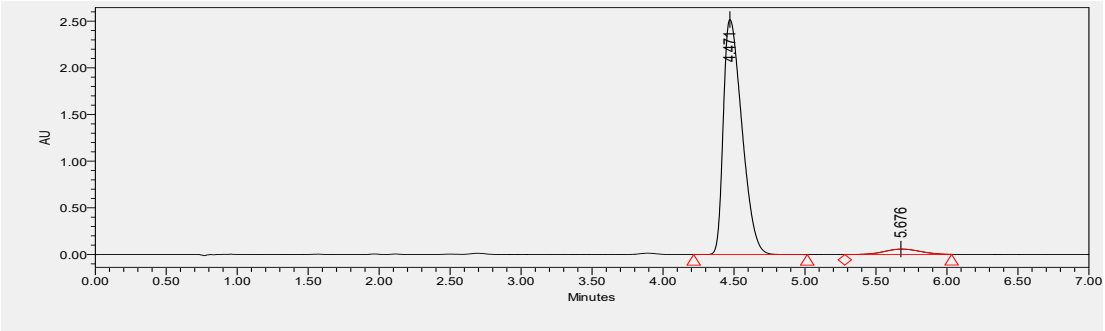
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.4, 174.1, 164.4, 143.8, 132.6, 132.2, 132.0, 130.5, 129.6, 129.5, 129.1, 128.9, 126.2, 122.7, 120.7, 91.2, 82.8, 35.9, 21.9 ppm.

IR (neat): ν (cm^{-1}) 3204, 3065, 2924, 2762, 1793, 1733, 1639, 1573, 1512, 1488, 1450, 1432, 1409, 1328, 1214, 1182, 1076, 1050, 1015, 976, 829, 767, 728, 695, 644, 582, 514, 491, 466.

HRMS (ESI-FT) calcd for $C_{25}H_{20}{}^{78.9183}BrN_2O_3^+$ ([M]+H$^+$) = 475.0652, found 475.0061, $C_{25}H_{20}{}^{80.9163}BrN_2O_3^+$ ([M]+H$^+$) = 477.0631, found 477.0636.

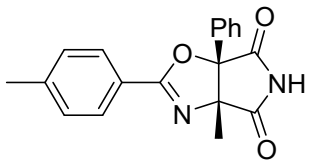


	Retention Time	% Area
1	4.723	49.99
2	5.933	50.01



	Retention Time	% Area
1	4.471	95.75
2	5.676	4.25

3a-Methyl-6a-phenyl-2-(*p*-tolyl)-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (4za)



White solid, **M.p.** 172 – 174 °C; 23.2 mg, 73% yield, >95:5 dr, 89% ee. $[\alpha]^{25}_{D}$ = +87.3 (*c* = 0.40, in CH_2Cl_2).

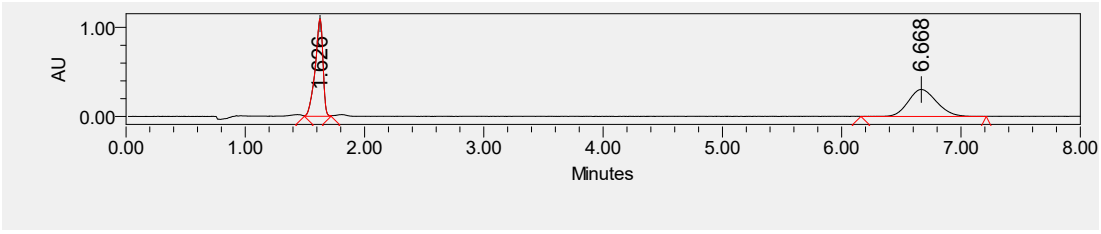
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 1.6 min, 6.6 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ= 9.27 (s, 1H), 7.99 – 7.97 (m, 2H), 7.46 – 7.39 (m, 3H), 7.31 – 7.26 (m, 4H), 2.42 (s, 3H), 1.17 (s, 3H) ppm.

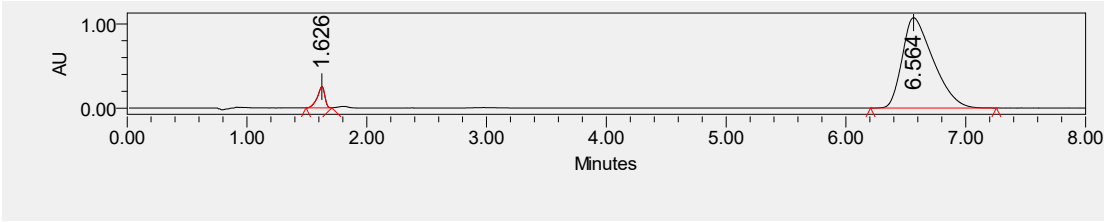
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ= 175.9, 174.0, 164.3, 143.6, 132.4, 129.5, 129.1, 129.0, 125.8, 122.9, 91.5, 80.7, 21.8, 18.8 ppm.

IR (neat): ν (cm^{-1}) 3202, 3066, 2762, 1793, 1734, 1639, 1574, 1511, 1451, 1411, 1377, 1325, 1229, 1182, 1146, 1118, 1079, 1037, 1003, 967, 830, 770, 728, 697, 631, 451.

HRMS (ESI-FT) calcd for $C_{19}H_{17}N_2O_3^+$ ([M]+H$^+$) = 321.1234, found 321.1234.

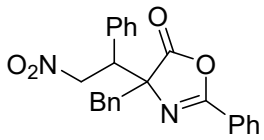


	Retention Time	% Area
1	1.626	49.73
2	6.668	50.27



	Retention Time	% Area
1	1.626	5.45
2	6.564	94.55

4-Benzyl-4-(2-nitro-1-phenylethyl)-2-phenyloxazol-5(4H)-one (3aa)



White solid, **M.p.** 117 – 119 °C; 39.8 mg, 99% yield, >95:5 dr, 92% ee. $[\alpha]^{25}_{D}$ = +172.0 (*c* = 1.38, in CH_2Cl_2).

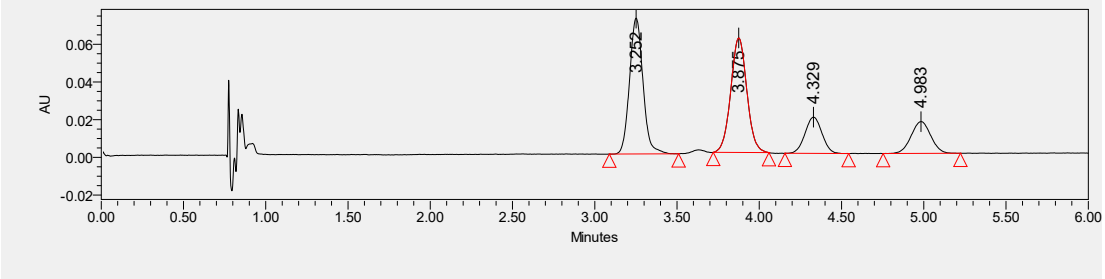
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OZ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 1.6 min, 6.6 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.82 – 7.80 (m, 2H), 7.56 – 7.53 (m, 3H), 7.45 – 7.33 (m, 5H), 7.11 – 7.10 (m, 3H), 7.05 – 7.04 (M, 2H), 4.83 (dd, *J* = 12.8, 10.8 Hz, 1H), 4.62 (dd, *J* = 12.8, 4.8 Hz, 1H), 4.19 (dd, *J* = 10.8, 4.8 Hz, 1H), 3.05 (d, *J* = 13.2 Hz, 1H), 2.91 (d, *J* = 13.2 Hz, 1H) ppm.

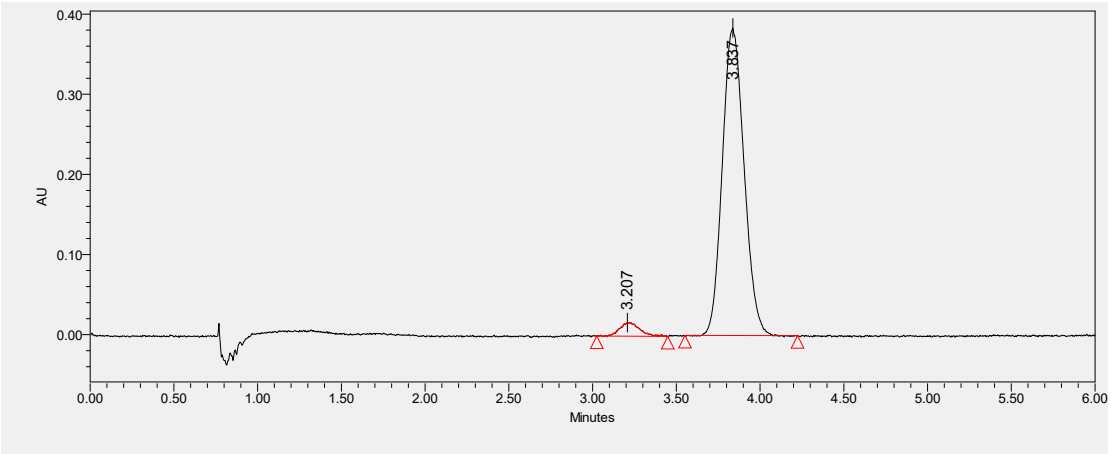
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 178.7, 161.0, 134.4, 133.2, 133.0, 130.3, 129.5, 129.0, 128.9, 128.3, 128.0, 127.6, 125.0, 76.6, 76.2, 50.0, 42.5 ppm.

IR (neat): ν (cm^{-1}) 3034, 2925, 1812, 1652, 1555, 1494, 1451, 1377, 1293, 1170, 1104, 1060, 963, 894, 778, 742, 697, 664, 593, 539, 480.

HRMS (ESI-FT) calcd for $C_{24}H_{21}N_2O_4^+$ ([M]+H$^+$) = 401.1496, found 401.1493.

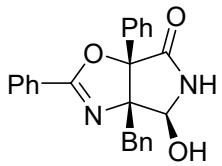


	Retention Time	% Area
1	3.252	37.28
2	3.875	37.47
3	4.329	12.55
4	4.983	12.70



	Retention Time	% Area
1	3.207	3.95
2	3.837	96.05

3a-Benzyl-4-hydroxy-2,6a-diphenyl-3a,4,5,6a-tetrahydro-6*H*-pyrrolo[3,4-*d*]oxazol-6-one (5)



White solid, **M.p.** 93 – 95 °C; 30.7 mg, 80% yield, >95:5 dr, 92% ee. $[\alpha]^{25}_{D}$ = +233.8 (*c* = 0.23, in CH_2Cl_2).

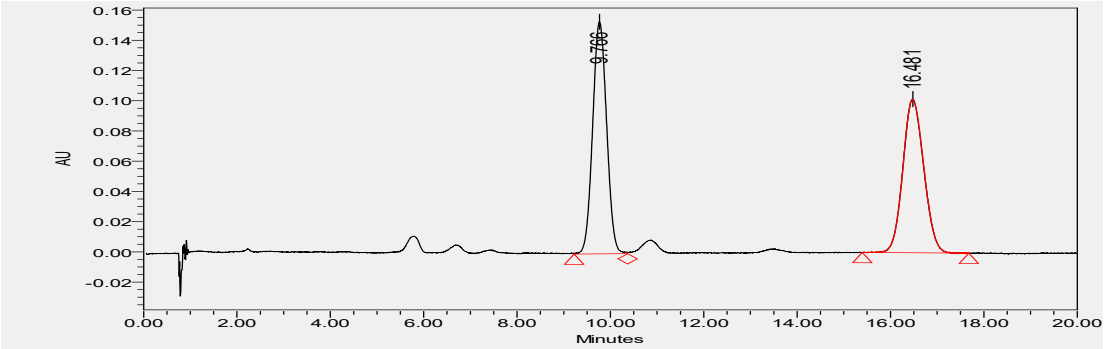
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 9.8 min, 16.4 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.12 – 8.11 (m, 2H), 7.59 – 7.56 (m, 1H), 7.49 – 7.42 (m, 5H), 7.33 – 7.30 (m, 2H), 7.11 – 7.05 (m, 3H), 6.98 (s, 1H), 6.83 – 6.81 (m, 2H), 5.47 (d, *J* = 10.4 Hz, 1H), 4.10 (d, *J* = 10.4 Hz, 1H), 2.75 (d, *J* = 14.0 Hz, 1H), 2.64 (d, *J* = 14.0 Hz, 1H) ppm.

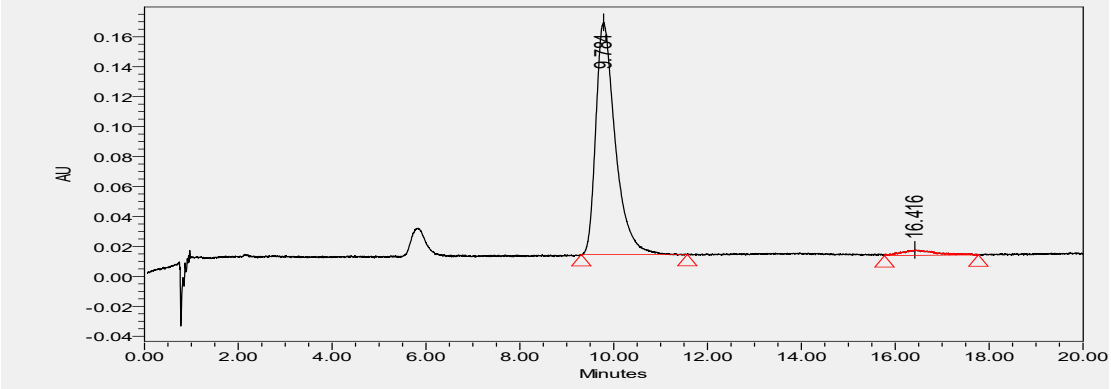
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 171.7, 164.5, 134.5, 133.0, 132.9, 130.7, 129.2, 129.1, 128.9, 128.7, 127.7, 126.8, 126.1, 126.0, 93.5, 83.0, 81.6, 40.6 ppm.

IR (neat): ν (cm^{-1}) 3240, 3062, 3031, 2924, 1719, 1644, 1604, 1581, 1496, 1450, 1333, 1296, 1257, 1162, 1090, 1069, 1030, 971, 955, 918, 798, 764, 739, 698, 635, 559, 475, 427.

HRMS (ESI-FT) calcd for $C_{24}H_{21}N_2O_3^+$ ([M]+H$^+$) = 385.1547, found 385.1547.

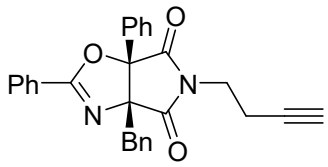


	Retention Time	% Area
1	9.766	50.30
2	16.481	49.70



	Retention Time	% Area
1	9.784	96.23
2	16.416	3.77

3a-Benzyl-5-(but-3-yn-1-yl)-2,6a-diphenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (6a)



White solid, **M.p.** 133 – 135 °C; 38.3 mg, 88% yield, >95:5 dr, 91% ee. $[\alpha]^{25}_{D}$ = +26.0 (*c* = 0.87, in CH_2Cl_2).

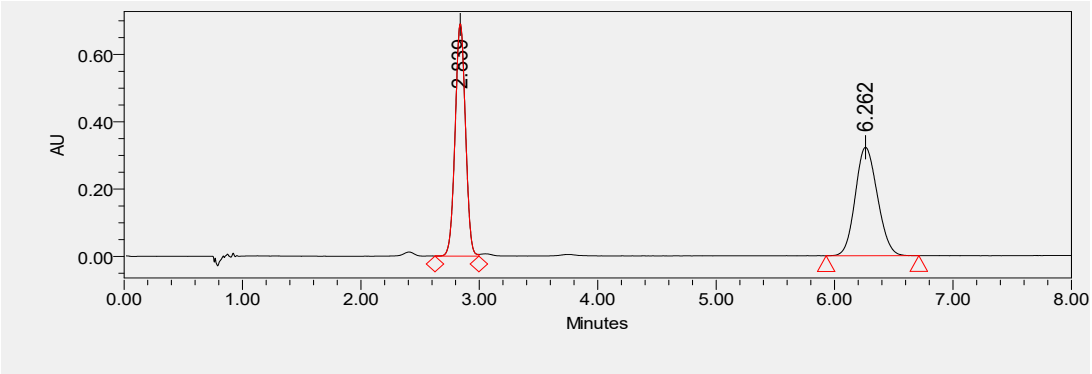
Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 2.8 min, 6.3 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.10 – 8.08 (m, 2H), 7.58 – 7.55 (m, 1H), 7.48 – 7.44 (m, 2H), 7.42 – 7.38 (m, 1H), 7.33 – 7.30 (m, 2H), 7.16 – 7.14 (m, 2H), 7.02 – 6.99 (m, 1H), 6.92 – 6.88 (m, 2H), 6.51 – 6.49 (m, 2H), 3.91 – 3.88 (m, 2H), 3.47 (d, *J* = 14.8 Hz, 1H), 2.98 (d, *J* = 14.8 Hz, 1H), 2.69 (td, *J* = 6.8, 2.4 Hz, 2H), 1.93 (t, *J* = 2.4 Hz, 1H) ppm.

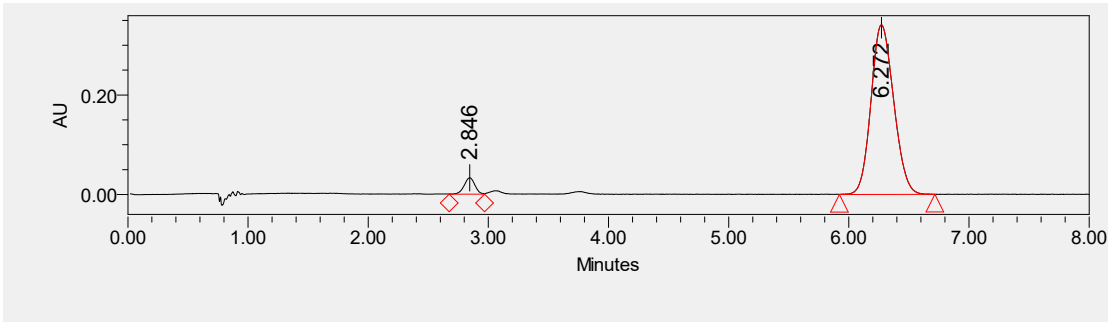
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.2, 173.8, 163.9, 133.8, 132.8, 132.3, 130.5, 129.3, 129.1, 128.7, 128.7, 127.5, 126.4, 125.9, 90.5, 82.2, 79.8, 71.0, 37.9, 37.1, 17.3 ppm.

IR (neat): ν (cm^{-1}) 3296, 3063, 3032, 2921, 1790, 1719, 1645, 1603, 1581, 1496, 1450, 1392, 1358, 1331, 1307, 1263, 1192, 1091, 1067, 996, 838, 781, 738, 697, 640, 472.

HRMS (ESI-FT) calcd for $C_{28}H_{23}N_2O_3^+$ ([M]+H$^+$) = 435.1703, found 435.1712.

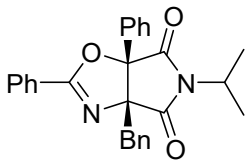


	Retention Time	% Area
1	2.839	49.99
2	6.262	50.01



	Retention Time	% Area
1	2.846	4.40
2	6.272	95.60

3a-Benzyl-5-isopropyl-2,6a-diphenyl-3a,6a-dihydro-4*H*-pyrrolo[3,4-*d*]oxazole-4,6(5*H*)-dione (6b)



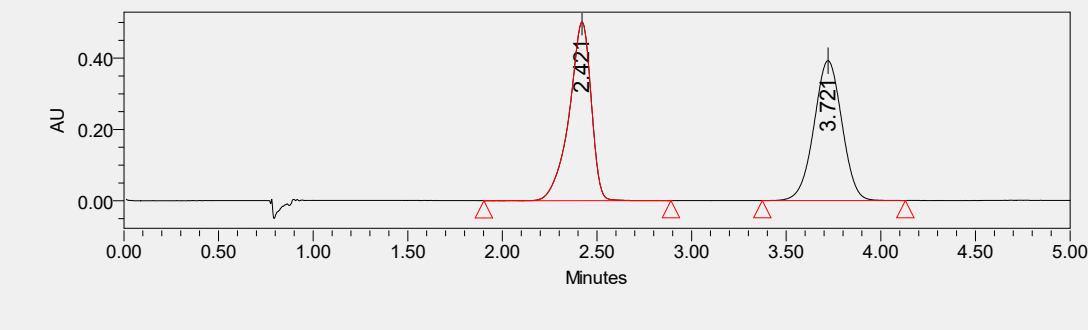
Colorless oil; 35.1 mg, 83% yield, >95:5 dr, 92% ee. $[\alpha]^{25}_{436}$ = –6.8 (*c* = 0.59, in CH_2Cl_2). Dissolved in MeOH for UPC²; **UPC²** (Daicel CHIRALPAK **OJ-3**, CO_2/MeOH = 95/5, flow rate = 1.5 mL/min, λ = 254 nm) retention time: 2.4 min, 3.7 min. dr > 95:5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.10 – 8.08 (m, 2H), 7.59 – 7.55 (m, 1H), 7.48 – 7.45 (m, 2H), 7.41 – 7.38 (m, 1H), 7.34 – 7.30 (m, 2H), 7.05 – 6.98 (m, 3H), 6.91 – 6.87 (m, 2H), 6.49 – 6.47 (m, 2H), 4.57 (m, 1H), 3.40 (d, *J* = 14.4 Hz, 1H), 2.99 (d, *J* = 14.4 Hz, 1H), 1.49 (dd, *J* = 6.8, 1.6 Hz, 6H) ppm.

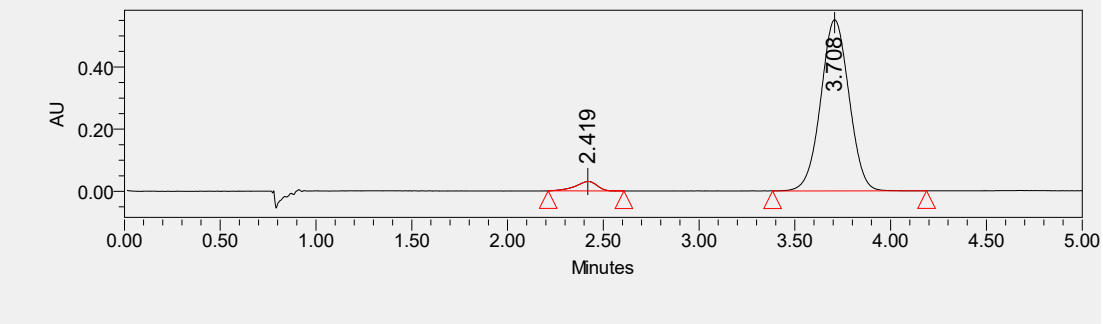
^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 175.4, 174.0, 163.8, 133.9, 132.7, 132.6, 130.4, 129.2, 129.1, 128.7, 127.5, 126.4, 126.2, 125.9, 90.1, 81.6, 45.2, 37.0, 19.6, 19.1 ppm.

IR (neat): ν (cm^{-1}) 3063, 3032, 2977, 1785, 1715, 1643, 1603, 1581, 1496, 1452, 1397, 1356, 1331, 1228, 1178, 1092, 1066, 1028, 985, 916, 873, 824, 780, 739, 697, 638, 505, 422.

HRMS (ESI-FT) calcd for $C_{27}H_{25}N_2O_3^+$ ([M]+H$^+$) = 425.1860, found 425.1861.

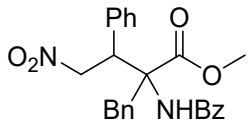


	Retention Time	% Area
1	2.421	50.06
2	3.721	49.94



	Retention Time	% Area
1	2.419	4.05
2	3.708	95.95

Methyl 2-benzamido-2-benzyl-4-nitro-3-phenylbutanoate (7)



White solid, **M.p.** 74 – 76 °C.

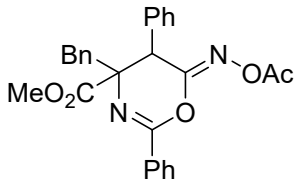
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.47 – 7.41 (m, 3H), 7.36 – 7.32 (m, 2H), 7.23 – 7.19 (m, 6H), 7.12 – 7.05 (m, 4H), 6.59 (s, 1H), 5.31 – 5.24 (m, 3H), 4.20 (d, *J* = 13.0 Hz, 1H), 3.89 (s, 3H), 3.37 (d, *J* = 13.0 Hz, 1H) ppm.

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 171.4, 167.8, 135.7, 135.3, 135.1, 131.7, 129.7, 128.9, 128.8, 128.6, 128.6, 128.3, 127.5, 126.8, 68.8, 53.3, 46.8, 38.8 ppm.

IR (neat): ν (cm^{-1}) 3408, 3033, 2954, 1738, 1662, 1554, 1511, 1487, 1443, 1359, 1288, 1233, 1089, 958, 883, 838, 704, 614, 556.

HRMS (ESI-FT) calcd for $C_{25}H_{25}N_2O_5^+$ ([M]+H$^+$) = 433.1758, found 433.1760.

Methyl (Z)-6-(acetoxyimino)-4-benzyl-2,5-diphenyl-5,6-dihydro-4H-1,3-oxazine-4-carboxylate (8)



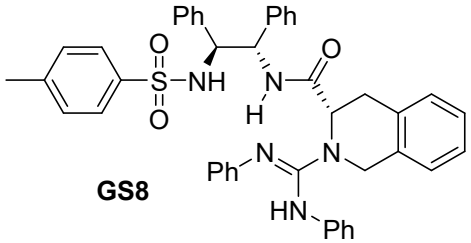
White solid, **M.p.** 97 – 99 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.20 – 8.18 (m, 2H), 7.63 – 7.59 (m, 1H), 7.55 – 7.51 (m, 2H), 7.32 – 7.23 (m, 10H), 4.51 (s, 1H), 3.62 (s, 3H), 3.13 (d, J = 13.6 Hz, 1H), 2.67 (d, J = 13.6 Hz, 1H), 2.21 (s, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 171.0, 167.7, 154.2, 150.9, 135.6, 134.1, 132.6, 130.9, 129.3, 128.8, 128.7, 128.6, 128.4, 128.0, 127.0, 67.6, 53.2, 45.7, 42.2, 19.5 ppm.

IR (neat): ν (cm^{-1}) 3032, 2952, 1777, 1739, 1669, 1494, 1448, 1367, 1244, 1187, 1126, 1094, 1046, 1000, 963, 919, 830, 750, 699, 540.

HRMS (ESI-FT) calcd for $C_{27}H_{25}N_2O_5^+$ ([M]+H$^+$) = 457.1758, found 457.1763.



GS8

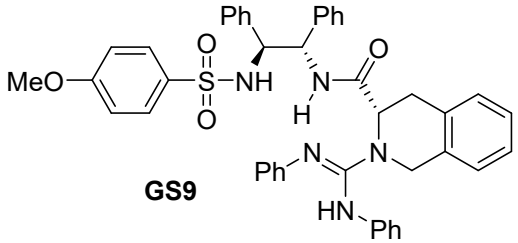
White solid, **M.p.** 107 – 109 °C; $[\alpha]^{25}_{D} = -146.6$ (c = 0.69, in CH_2Cl_2).

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.82 (d, J = 7.6 Hz, 1H), 7.47 – 7.45 (m, 2H), 7.24 – 7.22 (m, 3H), 7.19 – 7.12 (m, 6H), 7.07 – 7.00 (m, 5H), 6.97 – 6.94 (m, 5H), 6.84 – 6.83 (m, 6H), 6.79 – 6.77 (m, 1H), 6.43 (s, 1H), 5.76 (s, 1H), 5.14 – 5.10 (m, 1H), 4.92 – 4.91 (m, 1H), 4.65 (d, J = 9.6 Hz, 1H), 4.40 (d, J = 16.4 Hz, 1H), 4.14 (d, J = 16.4 Hz, 1H), 3.40 – 3.36 (m, 1H), 3.09 – 3.03 (m, 1H), 2.25 (s, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 173.6, 151.8, 142.7, 138.5, 138.3, 137.8, 133.3, 131.7, 129.5, 129.3, 128.7, 128.1, 128.0, 127.8, 127.6, 127.4, 127.0, 126.8, 126.1, 126.0, 123.0, 64.9, 59.0, 55.4, 46.3, 29.4, 21.5 ppm.

IR (neat): ν (cm^{-1}) 3030, 1664, 1619, 1580, 1496, 1453, 1403, 1313, 1232, 1157, 1090, 1027, 938, 814, 751, 698, 669, 563.

HRMS (ESI-FT) calcd for $C_{44}H_{42}N_5O_3S^+$ ([M]+H$^+$) = 720.3003, found 720.3004.



GS9

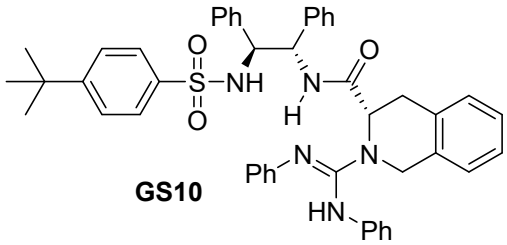
White solid, **M.p.** 116 – 118 °C; $[\alpha]^{25}_{D} = -126.1$ (c = 0.69, in CH_2Cl_2).

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.79 (d, J = 7.2 Hz, 1H), 7.49 – 7.47 (m, 2H), 7.13 – 7.11 (m, 9H), 7.07 – 6.94 (m, 8H), 6.85 – 6.78 (m, 7H), 6.69 – 6.66 (m, 2H), 6.41 (s, 1H), 5.79 (s, 1H), 5.14 – 5.10 (m, 1H), 4.98 – 4.97 (m, 1H), 4.64 (d, J = 9.6 Hz, 1H), 4.40 (d, J = 16.4 Hz, 1H), 4.16 (d, J = 16.4 Hz, 1H), 3.69 (s, 3H), 3.40 – 3.36 (m, 1H), 3.09 – 3.04 (m, 1H) ppm.

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 173.5, 162.4, 151.8, 138.4, 137.9, 133.3, 133.0, 131.8, 129.5, 128.9, 128.7, 128.1, 127.9, 127.8, 127.6, 127.5, 127.0, 126.1, 126.0, 123.0, 113.8, 64.8, 59.0, 55.6, 55.5, 46.4, 29.4 ppm.

IR (neat): ν (cm^{-1}) 3030, 1664, 1618, 1580, 1497, 1455, 1408, 1308, 1258, 1153, 1092, 1027, 937, 833, 751, 698, 565.

HRMS (ESI-FT) calcd for $C_{44}H_{42}N_5O_4S^+$ ([M]+H$^+$) = 736.2952, found 736.2951.



GS10

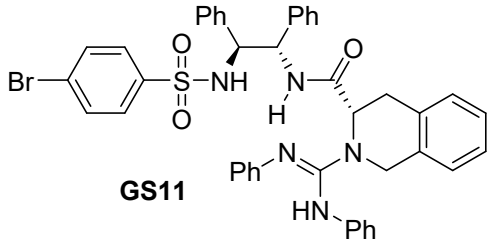
White solid, **M.p.** 127 – 129 °C; $[\alpha]^{25}_{D} = -150.3$ (c = 0.71, in CH_2Cl_2).

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.82 (d, J = 7.6 Hz, 1H), 7.48 – 7.45 (m, 2H), 7.23 – 7.11 (m, 11H), 7.07 – 7.03 (m, 2H), 6.99 – 6.89 (m, 6H), 6.85 – 6.79 (m, 7H), 6.42 (s, 1H), 5.79 (s, 1H), 5.16 – 5.11 (m, 1H), 4.89 – 4.88 (m, 1H), 4.68 (d, J = 9.6 Hz, 1H), 4.41 (d, J = 16.4 Hz, 1H), 4.16 (d, J = 16.4 Hz, 1H), 3.38 – 3.34 (m, 1H), 3.07 – 3.01 (m, 1H), 1.23 (s, 9H).

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 173.5, 155.6, 151.8, 138.3, 138.2, 137.9, 133.3, 131.8, 129.5, 128.7, 128.1, 128.0, 127.8, 127.5, 127.4, 127.0, 126.7, 126.1, 126.0, 125.6, 123.0, 65.0, 58.9, 55.3, 46.4, 35.0, 31.1, 29.5 ppm.

IR (neat): ν (cm^{-1}) 3031, 2963, 1664, 1619, 1580, 1496, 1454, 1399, 1321, 1233, 1161, 1113, 1086, 1027, 932, 836, 750, 697, 632, 574.

HRMS (ESI-FT) calcd for $C_{47}H_{48}N_5O_3S^+$ ([M]+H$^+$) = 762.3472, found 762.3467.



GS11

White solid, **M.p.** 129 – 131 °C; $[\alpha]^{25}_{D} = -157.7$ (c = 0.72, in CH_2Cl_2).

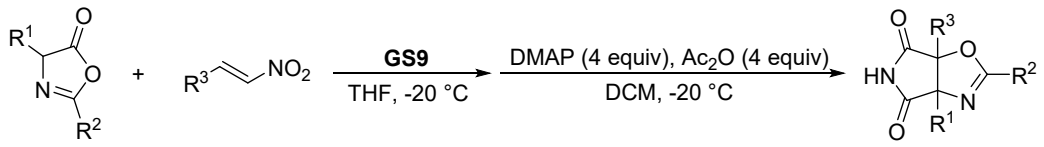
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.05 (d, J = 7.6 Hz, 1H), 7.35 – 7.27 (m, 5H), 7.24 – 7.13 (m, 8H), 7.05 – 6.91 (m, 8H), 6.86 – 6.78 (m, 7H), 5.75 (s, 1H), 5.16 – 5.11 (m, 1H), 4.93 – 4.92 (m, 1H), 4.71 (d, J = 10.0 Hz, 1H), 4.38 (d, J = 16.4 Hz, 1H), 4.12 (d, J = 16.4 Hz, 1H), 3.40 – 3.36 (m, 1H), 3.10 – 3.05 (m, 1H) ppm.

^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 173.9, 152.0, 140.5, 138.0, 137.6, 133.2, 131.8, 131.6, 129.6, 128.8, 128.7, 128.3, 128.2, 128.1, 127.8, 127.6, 127.0, 126.7, 126.1, 126.0, 123.2, 65.3, 59.1, 55.3, 46.4, 29.3 ppm.

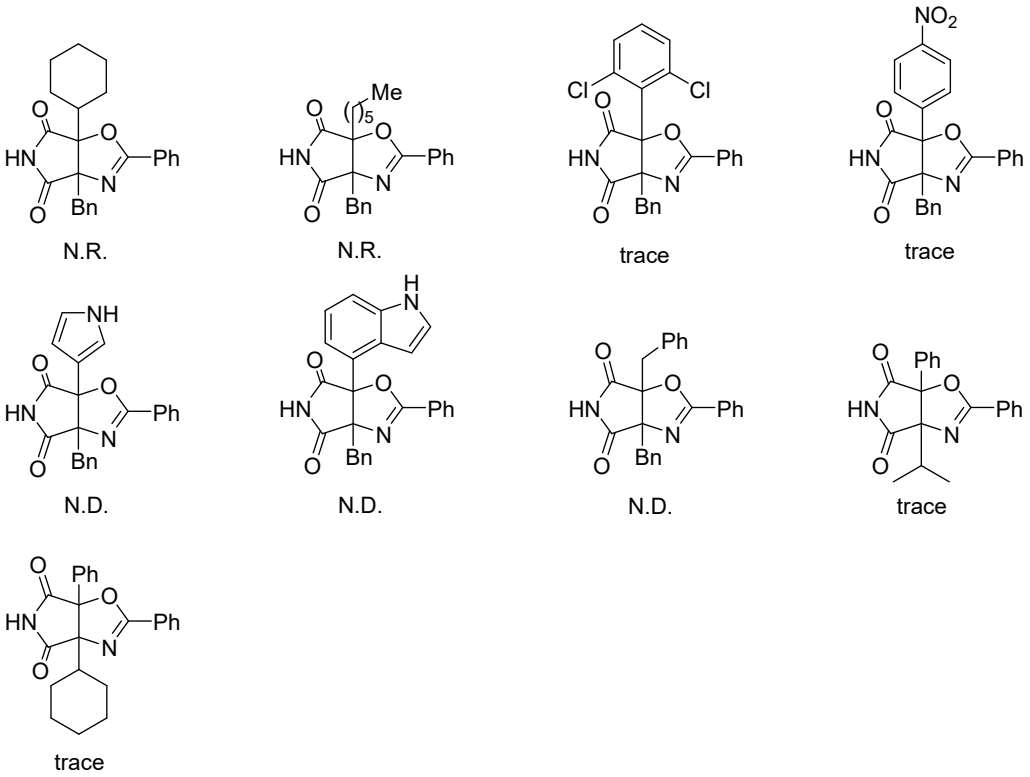
IR (neat): ν (cm^{-1}) 3030, 1662, 1618, 1578, 1496, 1453, 1392, 1330, 1234, 1159, 1089, 1068, 1010, 935, 822, 742, 698, 605, 541, 421.

HRMS (ESI-FT) calcd for $C_{43}H_{39}{}^{78.9183}BrN_5O_3S^+$ ([M]+H^+) = 784.1951, found 784.1943, $C_{43}H_{39}{}^{80.9163}BrN_5O_3S^+$ ([M]+H^+) = 786.1931, found 786.1933.

9. Substrate scope limitation



1 **2** **4**



[a]Unless otherwise noted, all reactions were carried out with **1** (0.10 mmol), **2** (0.10 mmol), and **GS9** (10 mol%) in THF (1.0 mL) at –20 °C. [b] N.R. = no reaction, N.D. = no detection.

Nitroolefins derived from heptaldehyde and cyclohexanecarboxaldehyde could not react with azlactones under the standard conditions. Dichloro-substituted or nitro-substituted nitroolefins were difficult to undergo Nef-type reactions due to the strong electron-withdrawing nature of the substituent group. Nitroolefins derived from pyrrole-3-carboxaldehyde and indole-4-carboxaldehyde could not give the desired C4 adduct under the standard conditions. Azlactones derived from valine and Cyclohexylglycine failed to give the Michael addition product.

10.References

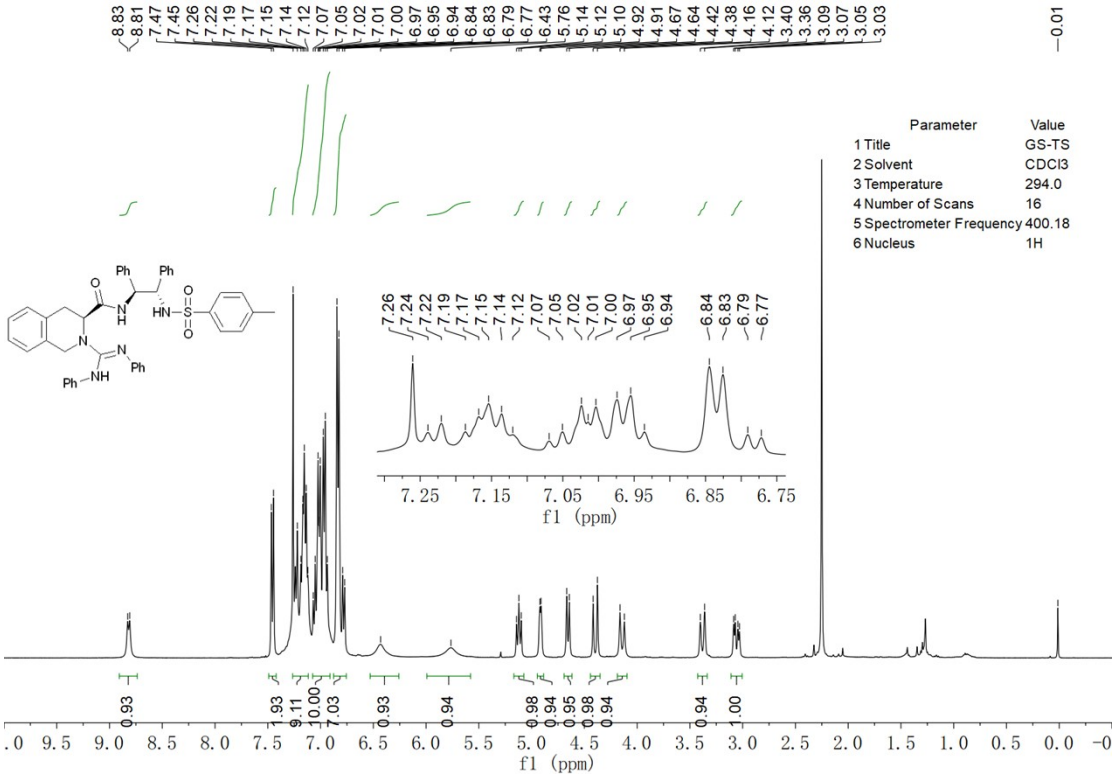
(1) (a) Dong, S. X.; Liu, X. H.; Chen, X. H.; Mei, F.; Zhang, Y. L.; Gao, B.; Lin, L. L.; Feng, X. M. *J. Am. Chem. Soc.* **2010**, *132*, 10650–10651. (b) Teegardina, K. A.; Weaver, J. D. *Chem. Commun.* **2017**, *53*, 4771−4774.

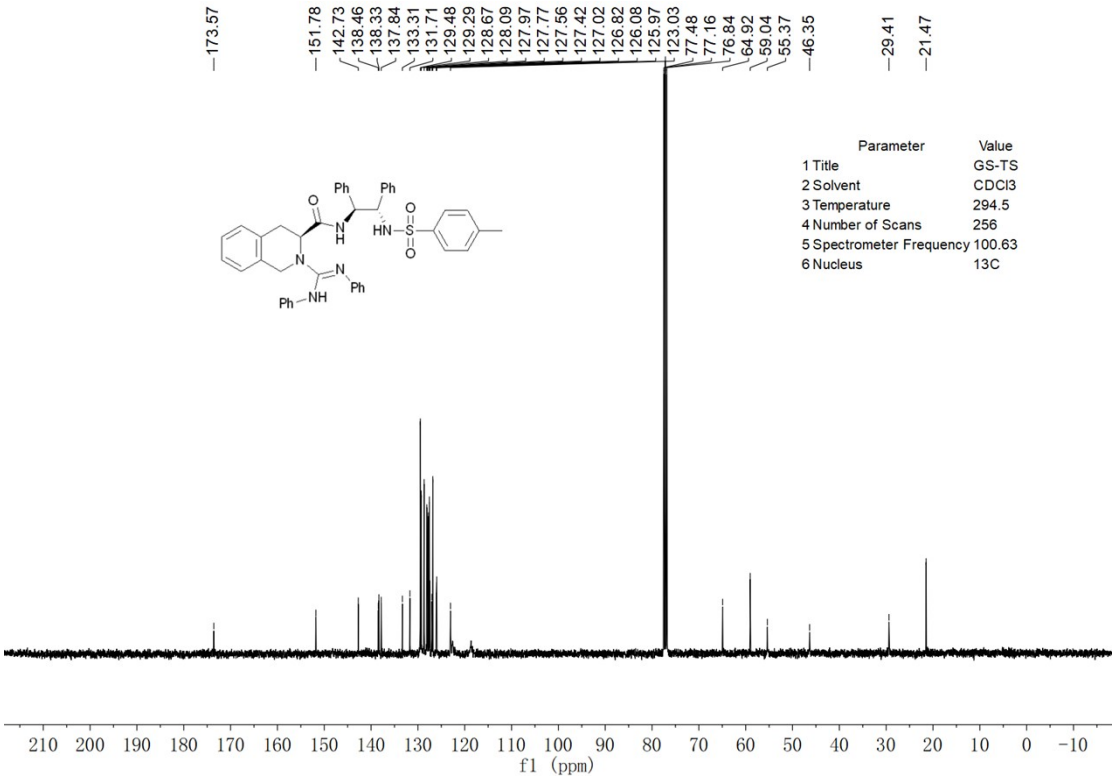
(2) (a) Zheng, C. G.; Huang, S.; Liu, Y.; Jiang, C.; Zhang, W.; Fang, G.; Hong, J. Q. *Org. Lett.* **2020**, *22*, 4868−4872. (b) Kyle, A. F.; Jakubec, P.; Cockfield, D. M.; Cleator, E.; Skidmore. J.; Dixon, D. J. *Chem. Commun.* **2011**, *47*, 10037−10039. (c) Gao, S. H.; Tu, Y. Q.; Hu, X. D.; Wang, S. H.; Hua, R. B.; Jiang, Y. J.; Zhao, Y. M.; Fan, X. H.; Zhang, S. Y. *Org. Lett.* **2006**, *8*, 2373−2376. (d) Betke, T.; Rommelmann, P.; Oike, K.; Asano, Y.; Gröger, H. *Angew. Chem. Int. Ed.* **2017**, *56*, 12361−12366. (e) Dhakal, R. C.; Dieter, R. K. *Org. Lett.* **2014**, *16*, 1362−1365.

(3) (a) Yu, Z. P.; Liu, X. H.; Zhou, L.; Lin, L. L.; Feng, X. M. *Angew. Chem. Int. Ed.* **2009**, *48*, 5195–5198. (b) Dong, S. X.; Liu, X. H.; Zhang, Y. L.; Lin, L. L.; Feng, X. M. *Org. Lett.* **2011**, *13*, 5060–5063.

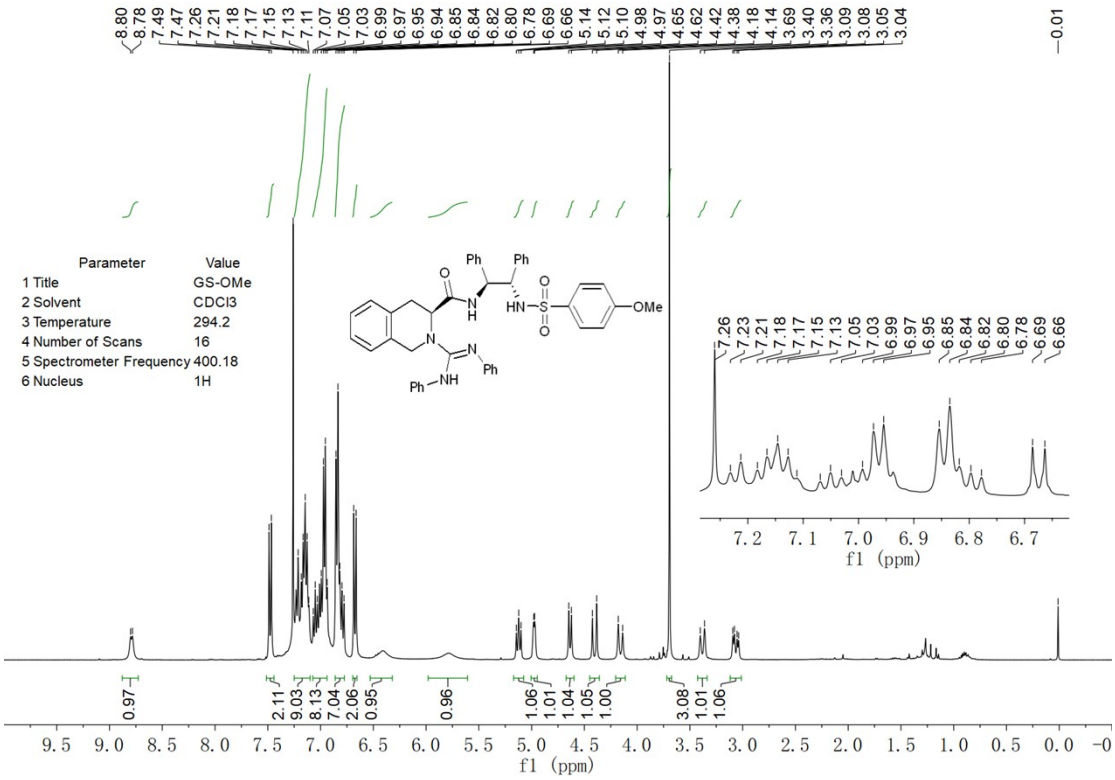
11. Copies of NMR spectra

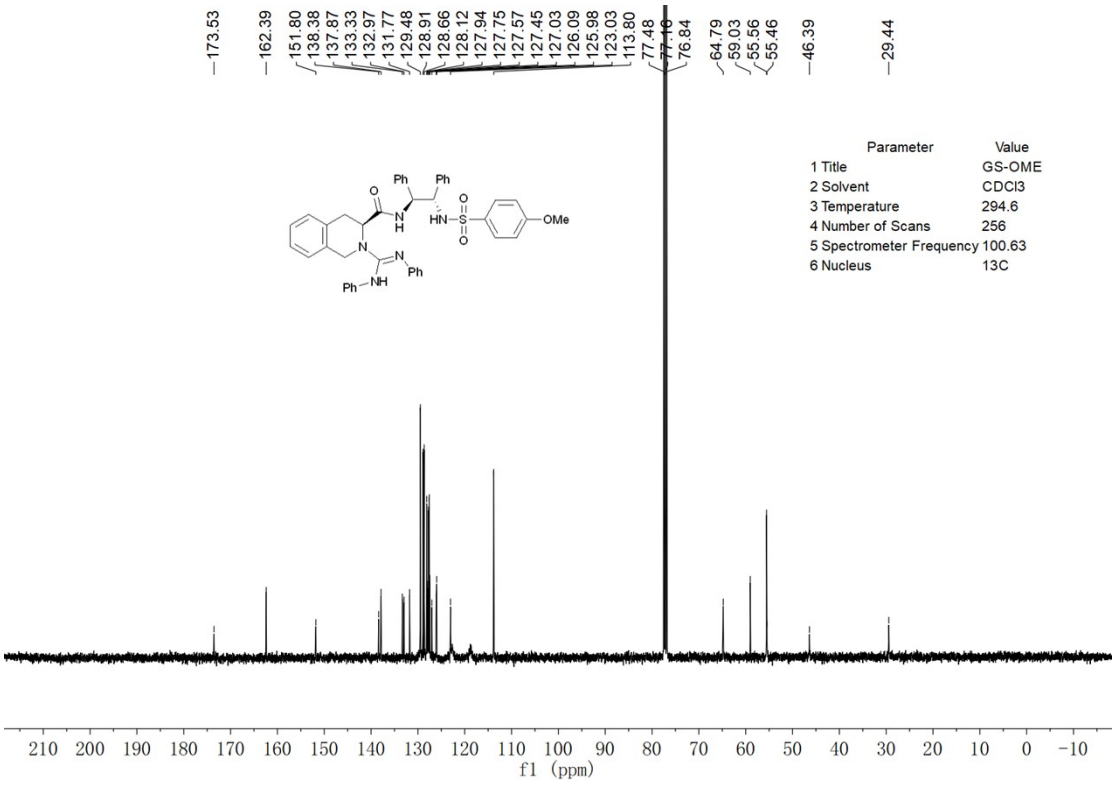
GS8





GS9


Parameter Value
1 Title GS-OMe
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)


Parameter Value
1 Title GS-OME
2 Solvent CDCl3
3 Temperature 294.6
4 Number of Scans 256
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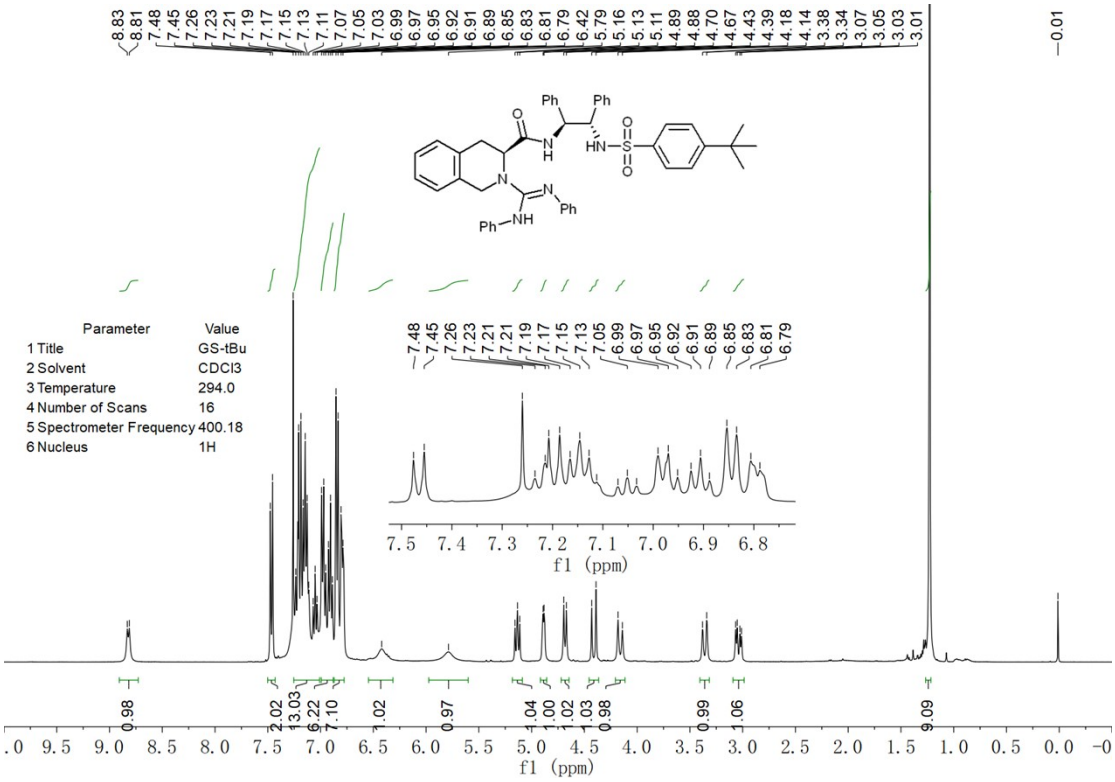
6 Nucleus 13C
f1 (ppm)

GS10


Parameter Value
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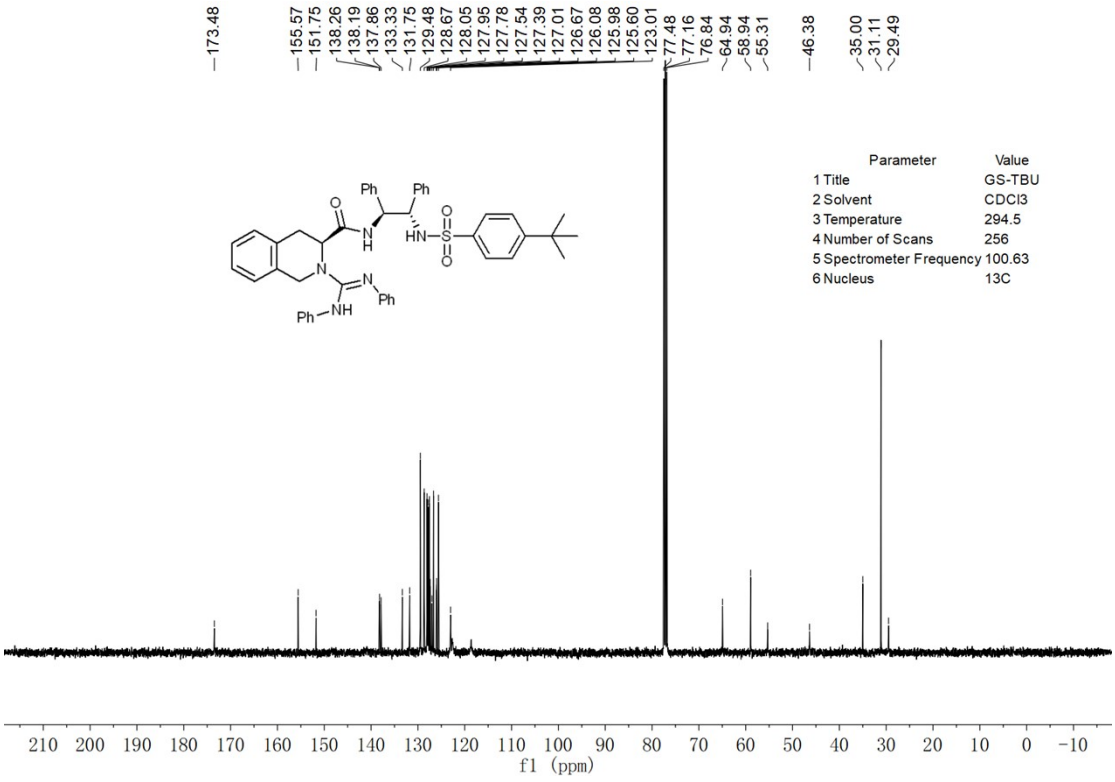
f1 (ppm)


Parameter Value
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3 Temperature 294.5
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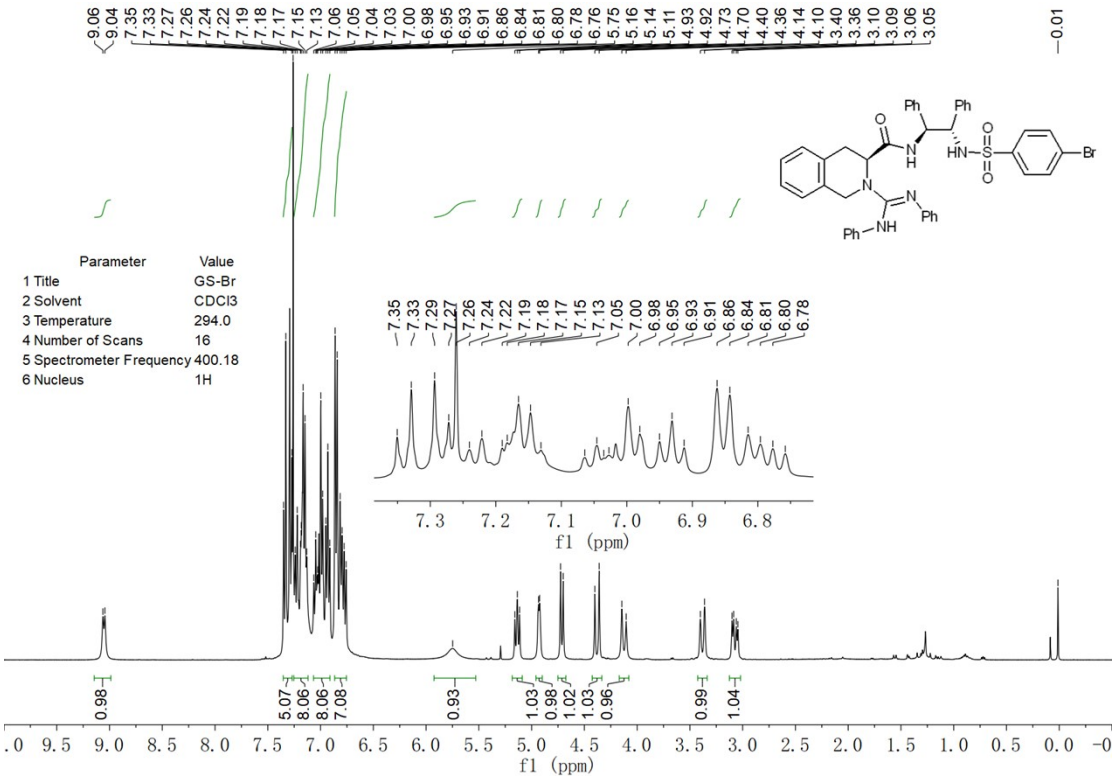
6 Nucleus 13C
f1 (ppm)

GS11


Parameter Value
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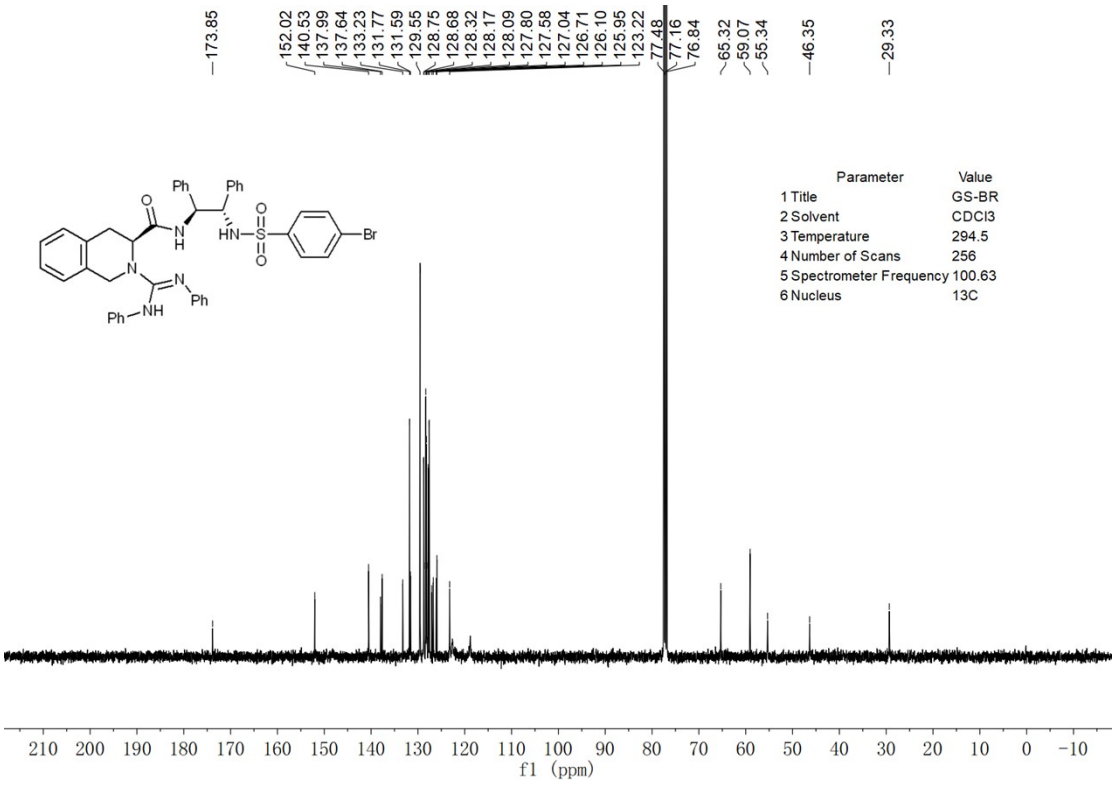
3 Temperature 294.0
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)


Parameter Value
1 Title GS-BR
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3 Temperature 294.5
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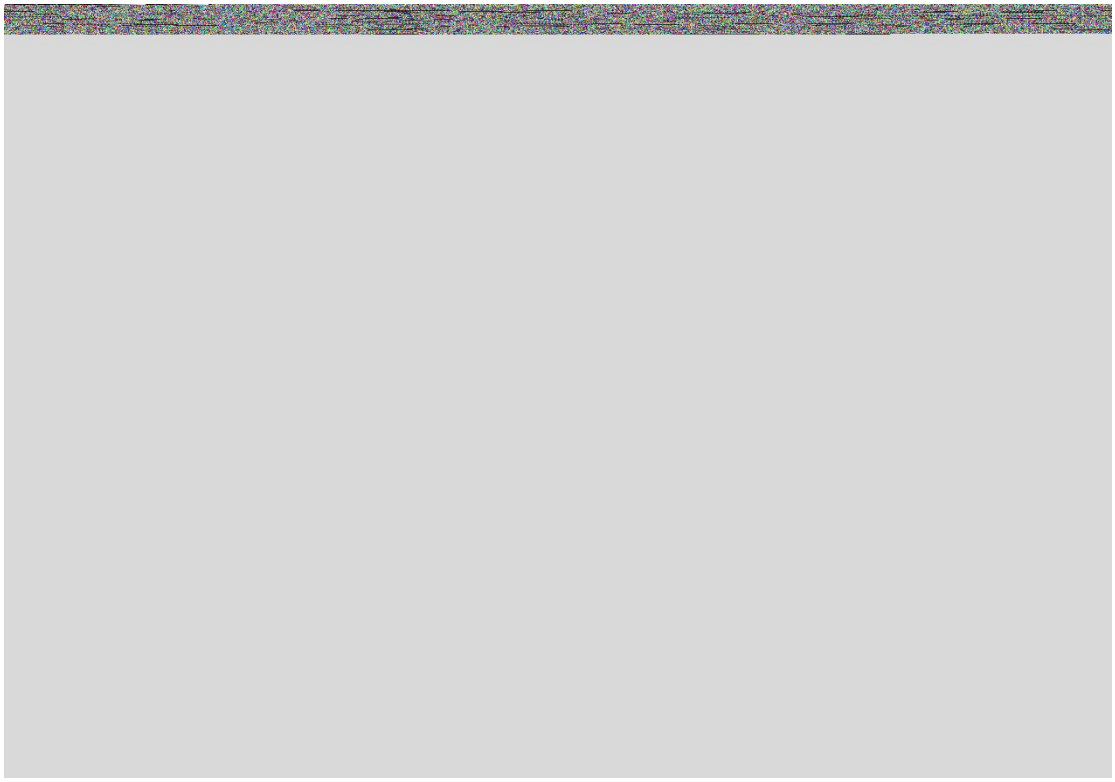
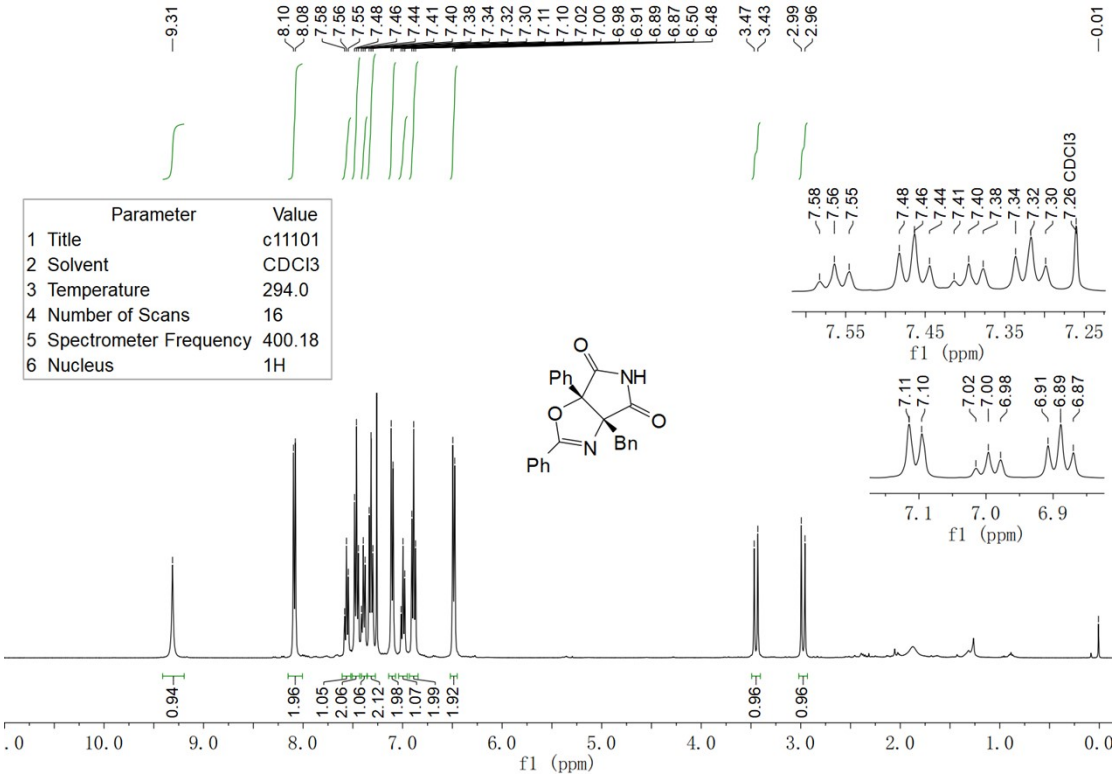
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

3aa



4aa


Parameter Value
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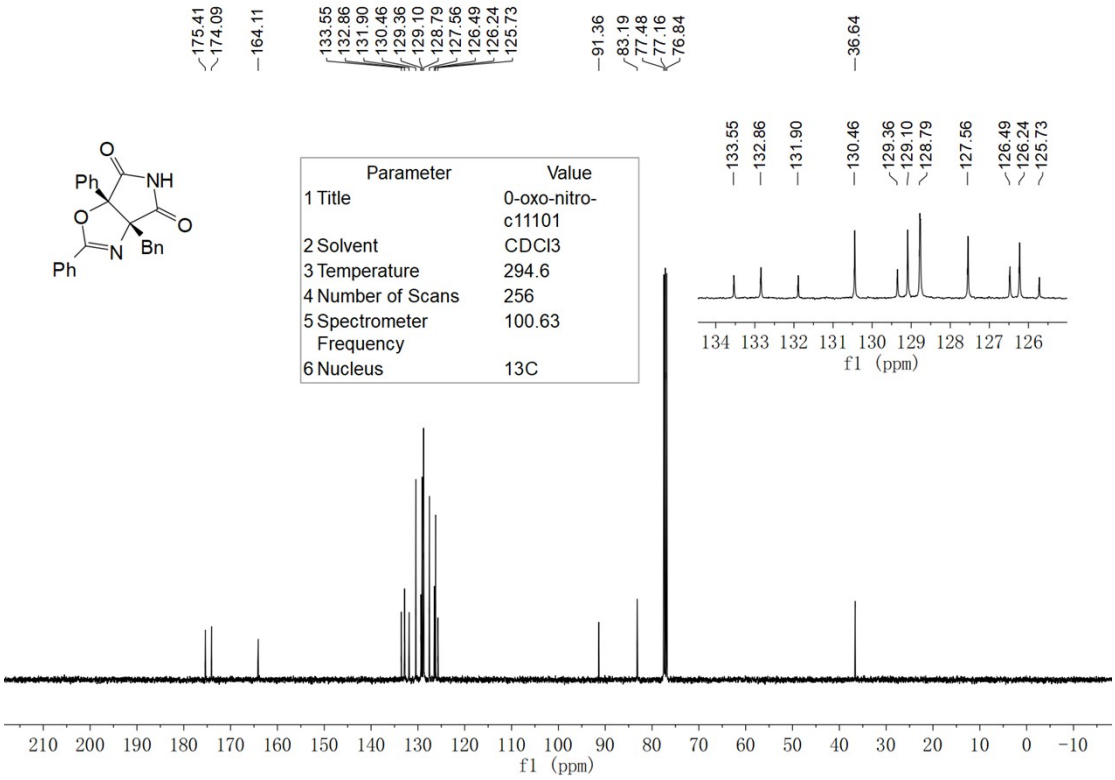
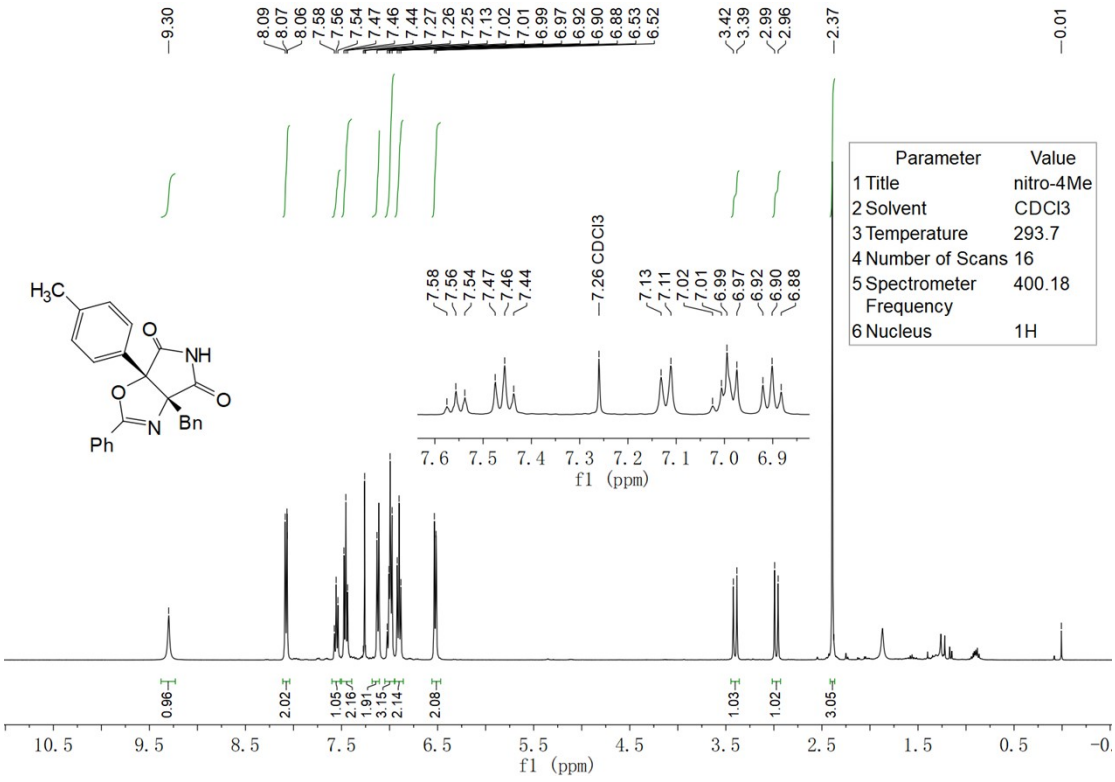
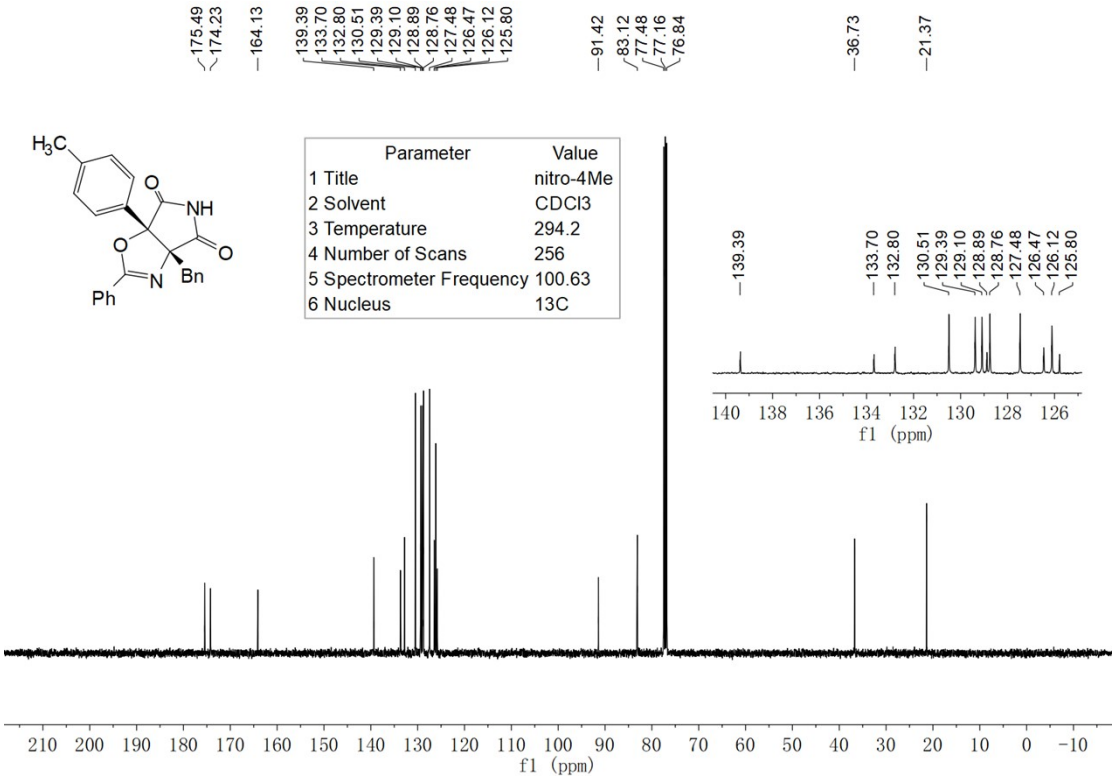
6 Nucleus 1H
f1 (ppm)

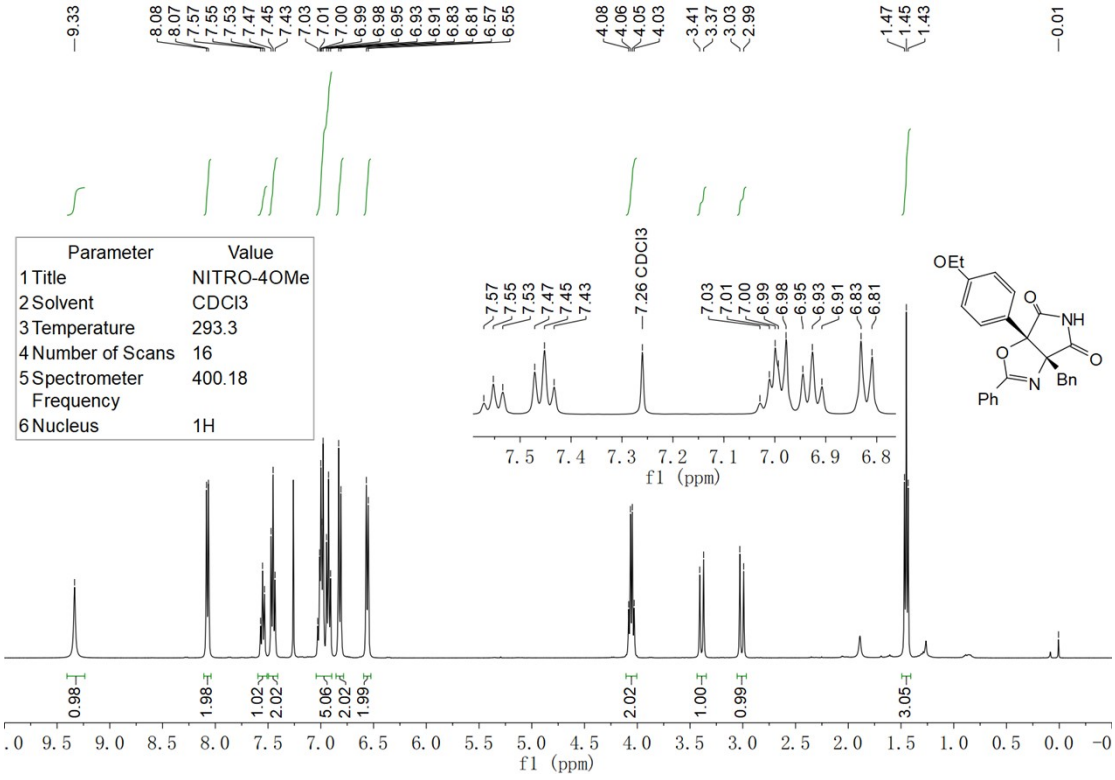

Parameter Value
1 Title 0-oxo-nitro-c11101
2 Solvent CDCl3
3 Temperature 294.6
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

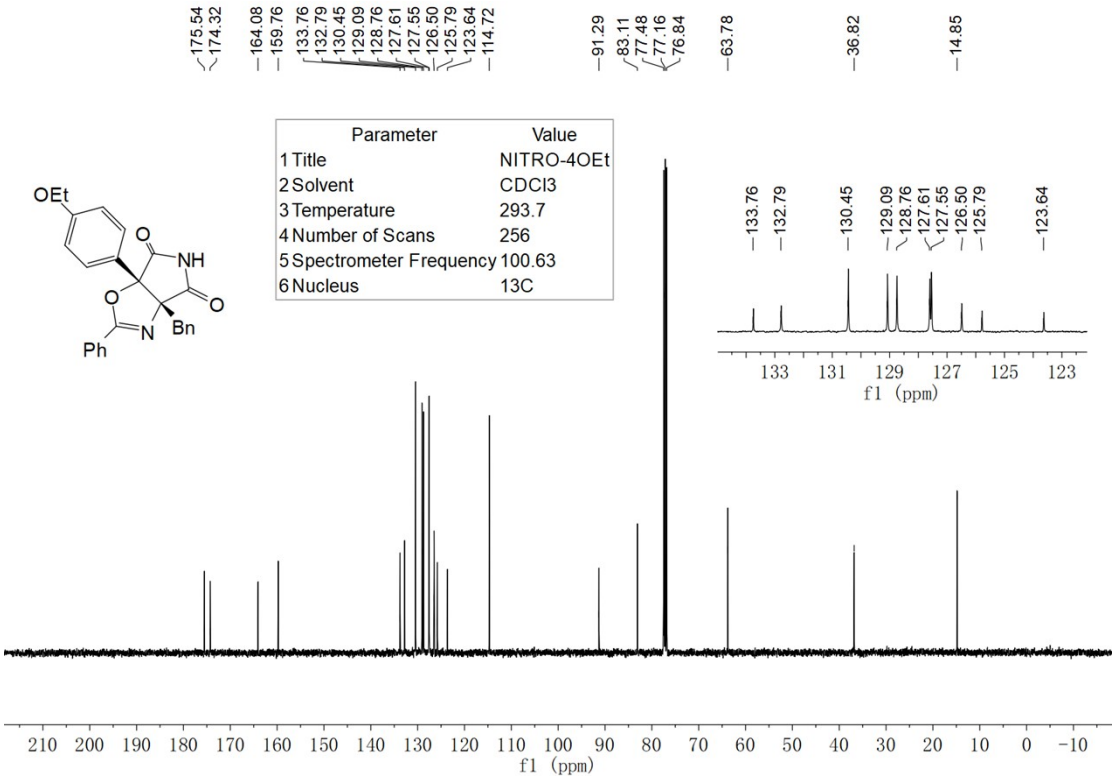
4ab


9.30
8.09
8.07
8.06
7.58
7.56
7.54
7.47
7.46
7.44
7.27
7.26
7.25
7.13
7.02
7.01
6.99
6.97
6.92
6.90
6.88
6.53
6.52
3.42
3.39
2.99
2.96
2.37
0.01
7.26 CDCl3
Parameter Value
1 Title nitro-4Me
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
H3C
O
NH
O
O
N
Bn
Ph
0.96
2.02
1.05
2.16
1.91
3.15
2.14
2.08
1.03
1.02
3.05
f1 (ppm)

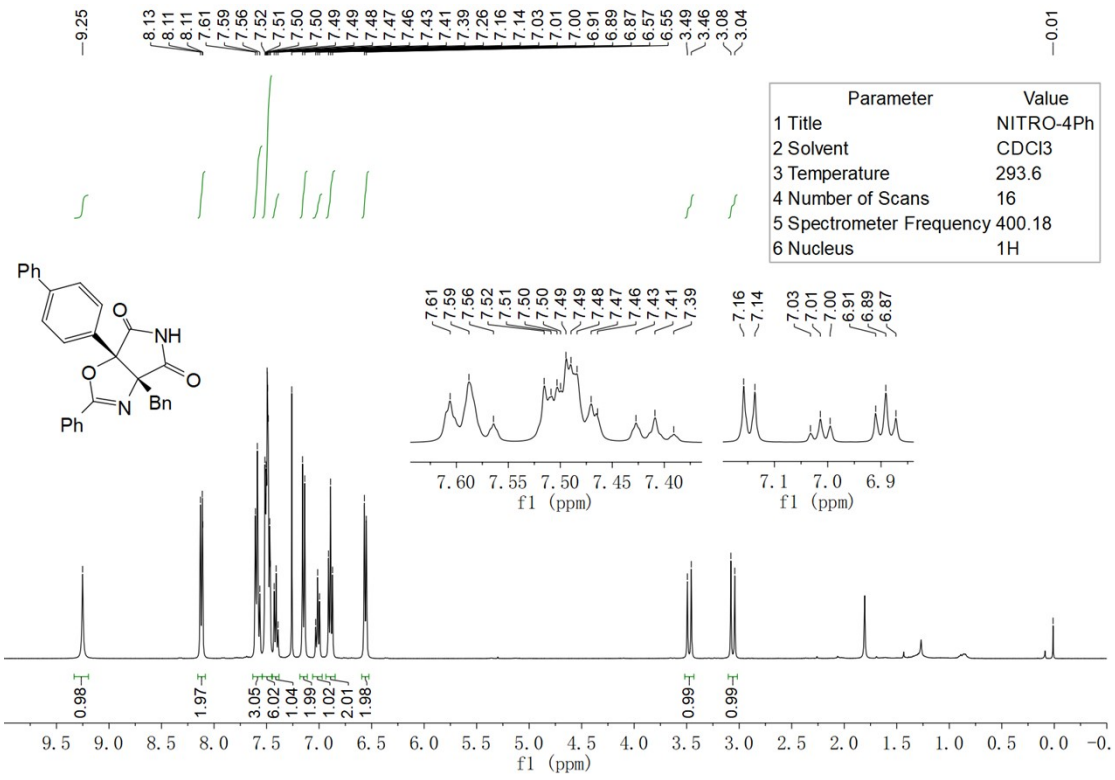

175.49
174.23
164.13
139.39
133.70
132.80
130.51
129.39
129.10
128.89
128.76
127.48
126.47
126.12
125.80
91.42
83.12
77.48
77.16
76.84
36.73
21.37
Parameter Value
1 Title nitro-4Me
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
H3C
O
NH
O
O
N
Bn
Ph
f1 (ppm)

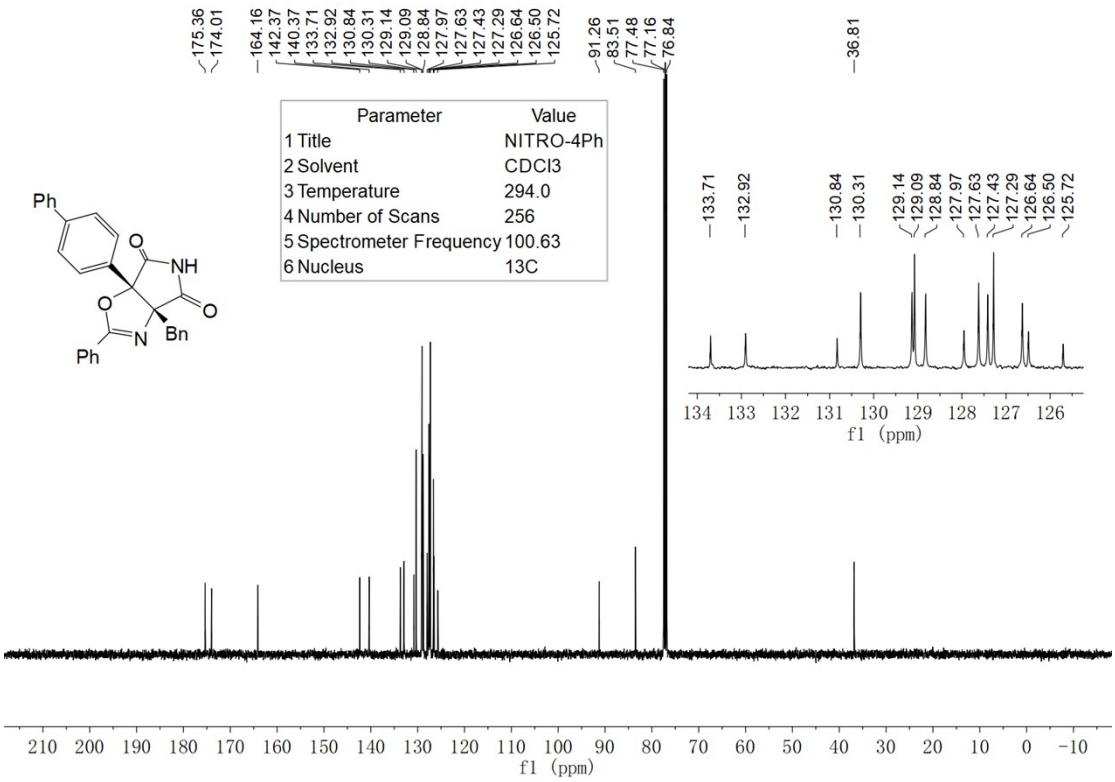
4ac


Parameter Value
1 Title NITRO-4OMe
2 Solvent CDCl3
3 Temperature 293.3
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

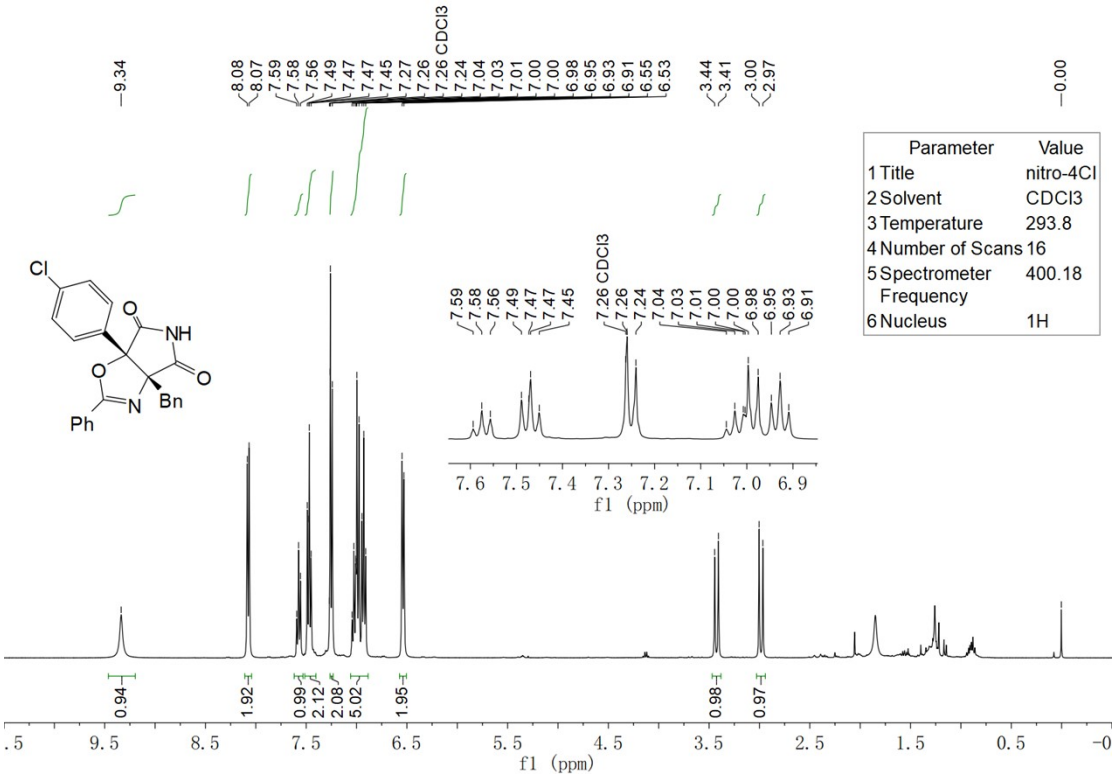

Parameter Value
1 Title NITRO-4OEt
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

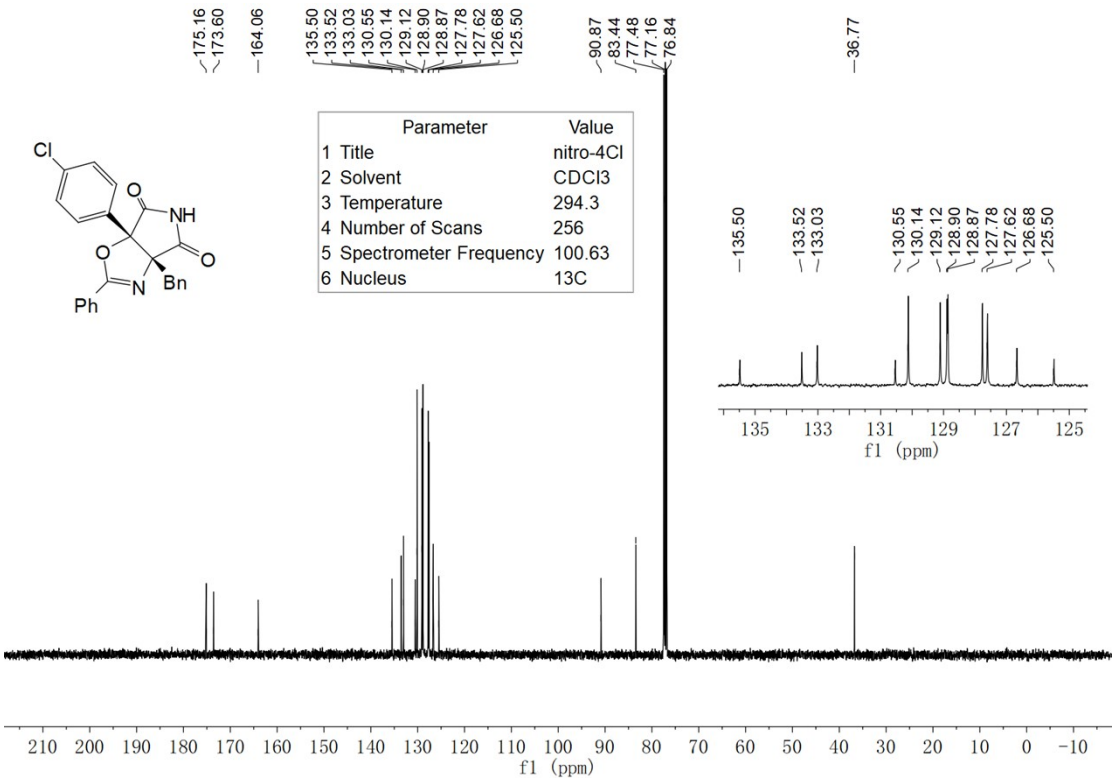
4ad


Parameter Value
1 Title NITRO-4Ph
2 Solvent CDCl3
3 Temperature 293.6
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

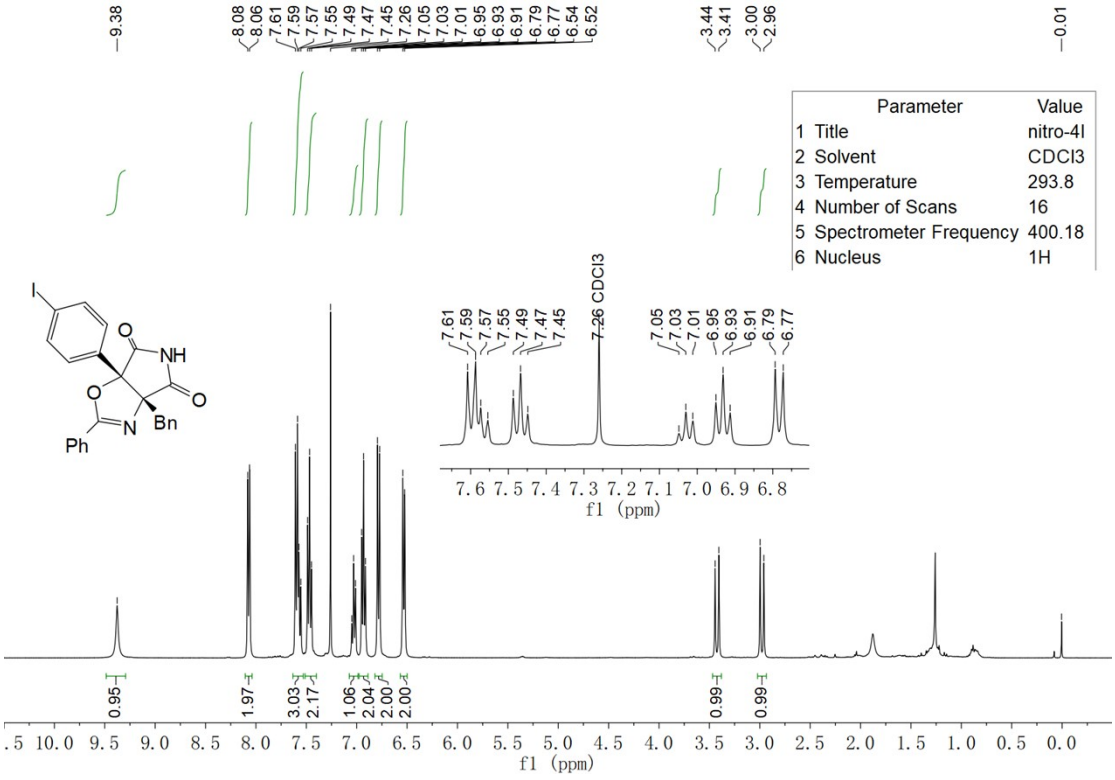

Parameter Value
1 Title NITRO-4Ph
2 Solvent CDCl3
3 Temperature 294.0
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

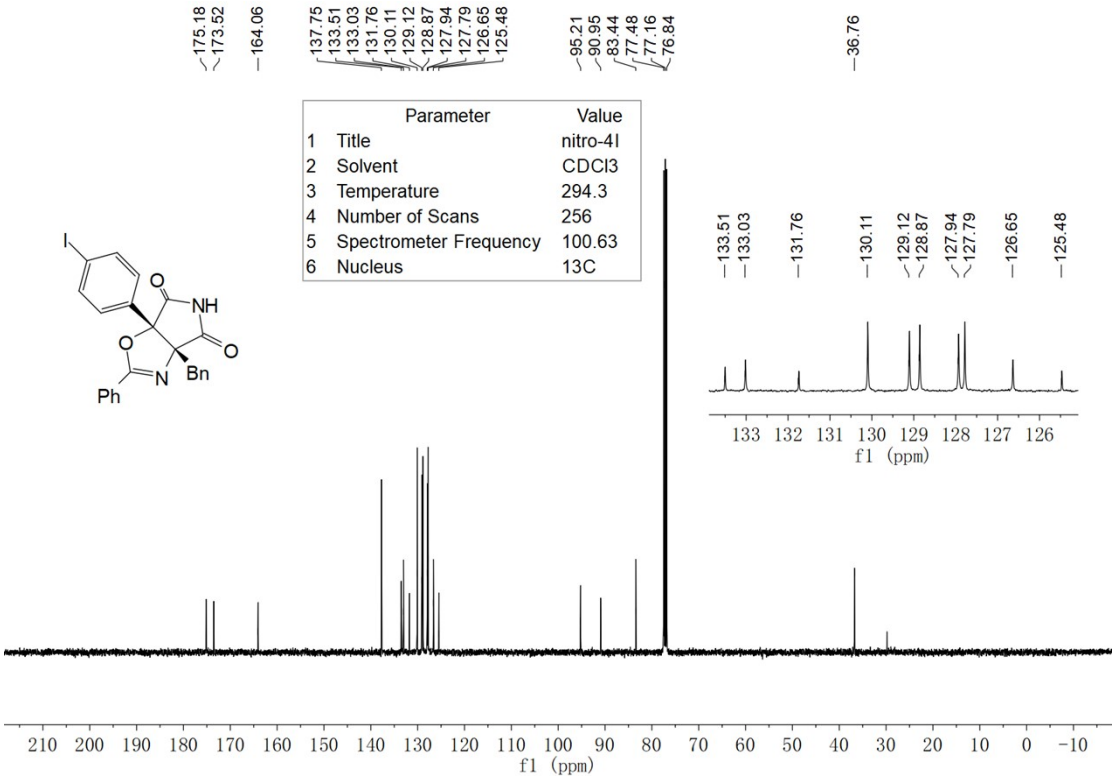
4ae


9.34
8.08
8.07
7.59
7.58
7.56
7.49
7.47
7.47
7.45
7.27
7.26 CDCl3
7.24
7.04
7.03
7.01
7.00
7.00
6.98
6.95
6.93
6.91
6.55
6.53
3.44
3.41
3.00
2.97
0.00
Parameter Value
1 Title nitro-4Cl
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Cl
O
NH
O
O
N
Bn
Ph
0.94
1.92
0.99
2.12
2.08
5.02
1.95
0.98
0.97
f1 (ppm)

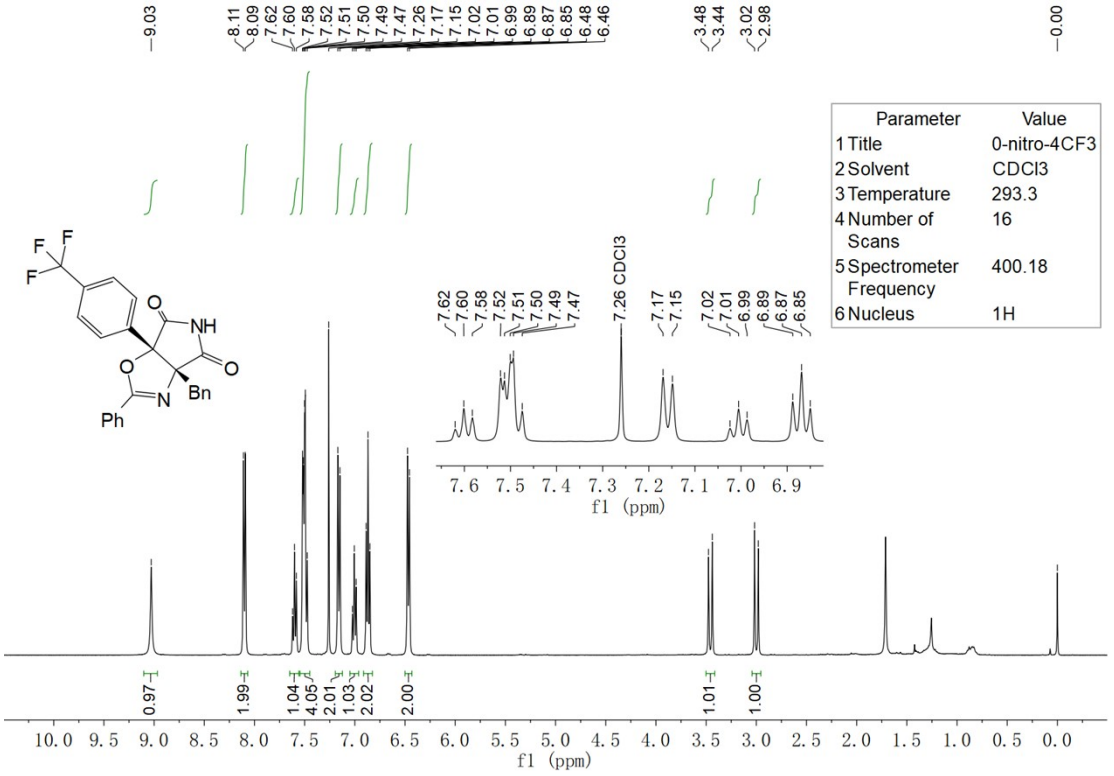

175.16
173.60
164.06
135.50
133.52
133.03
130.55
130.14
129.12
128.90
128.87
127.78
127.62
126.68
125.50
90.87
83.44
77.48
77.16
76.84
36.77
Parameter Value
1 Title nitro-4Cl
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Cl
O
NH
O
O
N
Bn
Ph
f1 (ppm)

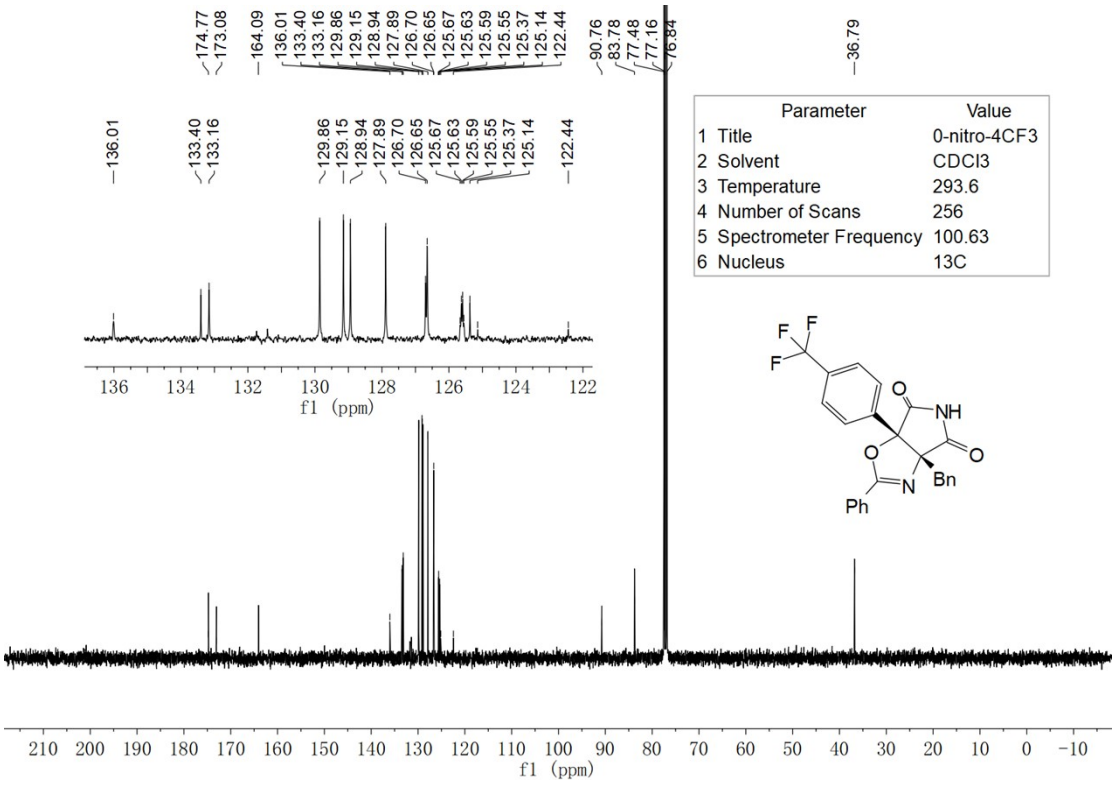
4af

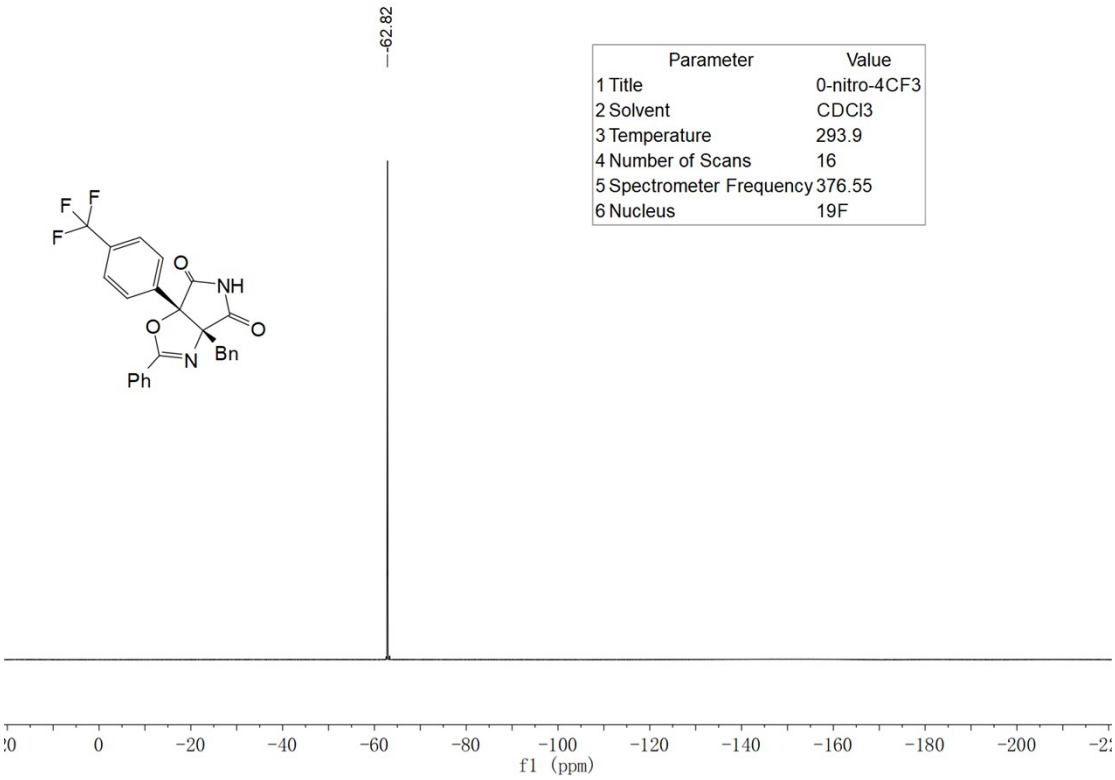

9.38
8.08
8.06
7.61
7.59
7.57
7.55
7.49
7.47
7.45
7.26
7.05
7.03
7.01
6.95
6.93
6.91
6.79
6.77
6.54
6.52
3.44
3.41
3.00
2.96
0.01
Parameter Value
1 Title nitro-4l
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
7.26 CDCl3
f1 (ppm)
0.95
1.97
3.03
2.17
1.06
2.04
2.00
2.00
0.99
0.99
f1 (ppm)


175.18
173.52
164.06
137.75
133.51
133.03
131.76
130.11
129.12
128.87
127.94
127.79
126.65
125.48
95.21
90.95
83.44
77.48
77.16
76.84
36.76
Parameter Value
1 Title nitro-4l
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)
f1 (ppm)

4ag

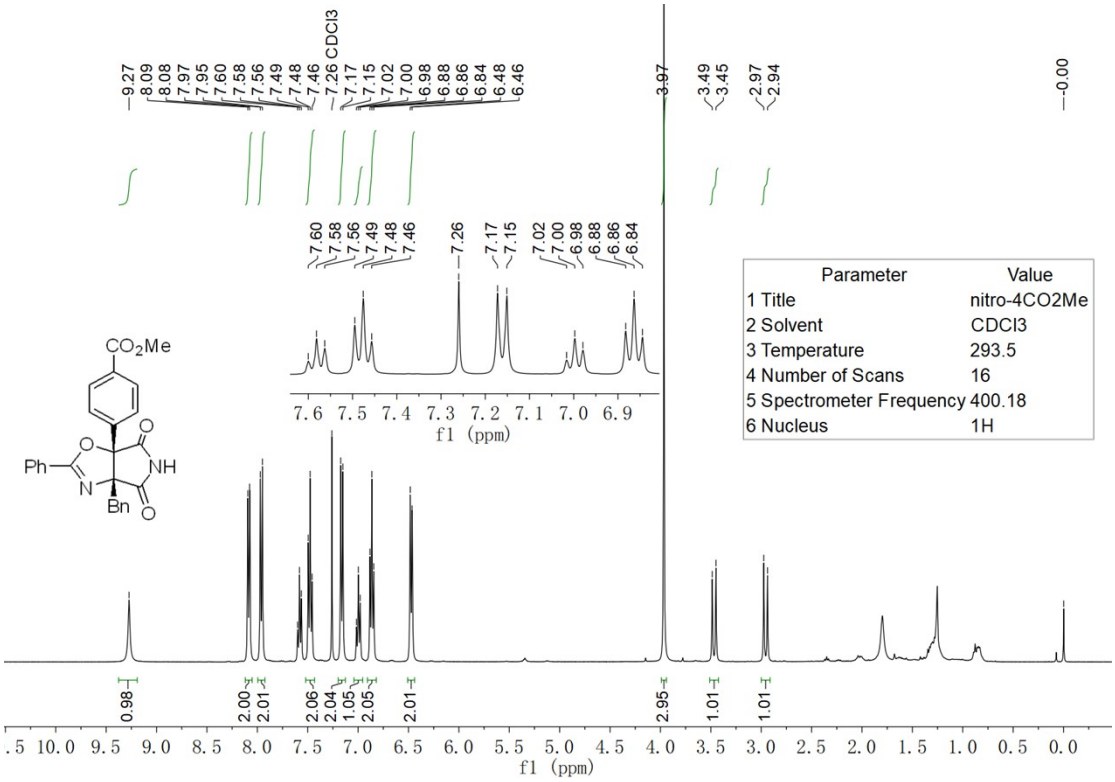

9.03
8.11
8.09
7.62
7.60
7.58
7.52
7.51
7.50
7.49
7.47
7.26
7.17
7.15
7.02
7.01
6.99
6.89
6.87
6.85
6.48
6.46
3.48
3.44
3.02
2.98
0.00
Parameter Value
1 Title 0-nitro-4CF3
2 Solvent CDCl3
3 Temperature 293.3
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
7.26 CDCl3
f1 (ppm)
0.97
1.99
1.04
4.05
2.01
1.03
2.02
2.00
1.01
1.00
f1 (ppm)

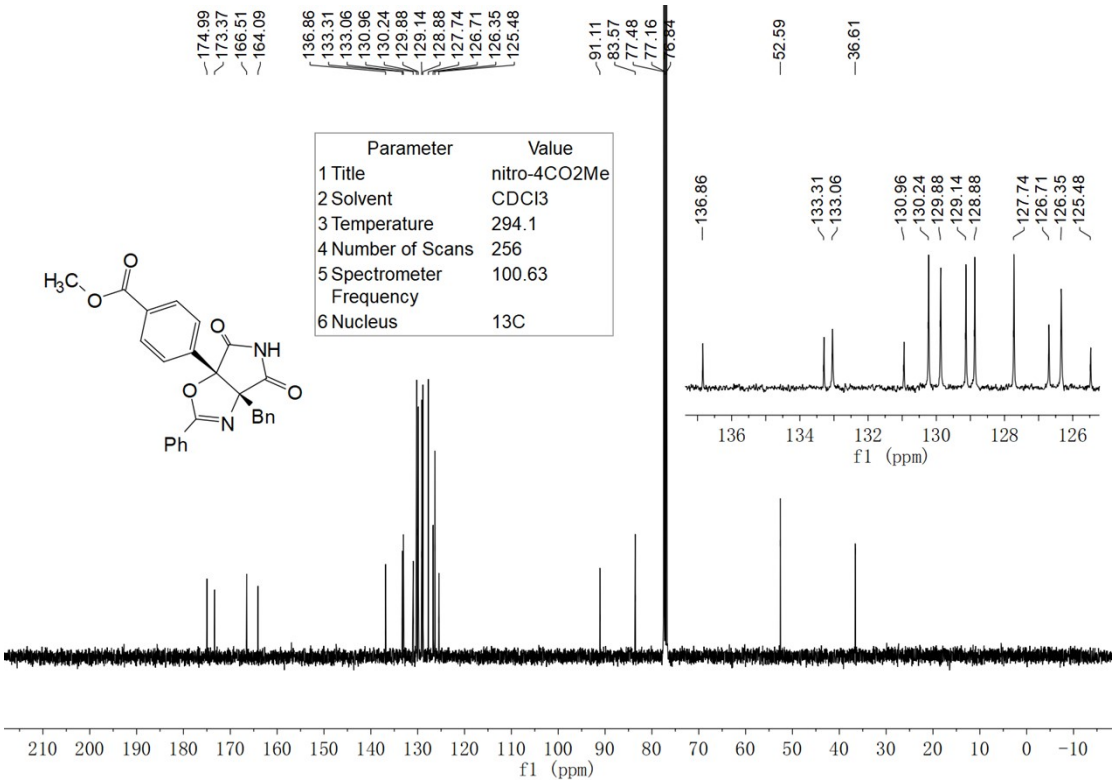

174.77
173.08
164.09
136.01
133.40
133.16
129.86
129.15
128.94
127.89
126.70
126.65
125.67
125.63
125.59
125.55
125.37
125.14
122.44
90.76
83.78
77.48
77.16
76.84
36.79
Parameter Value
1 Title 0-nitro-4CF3
2 Solvent CDCl3
3 Temperature 293.6
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)
f1 (ppm)



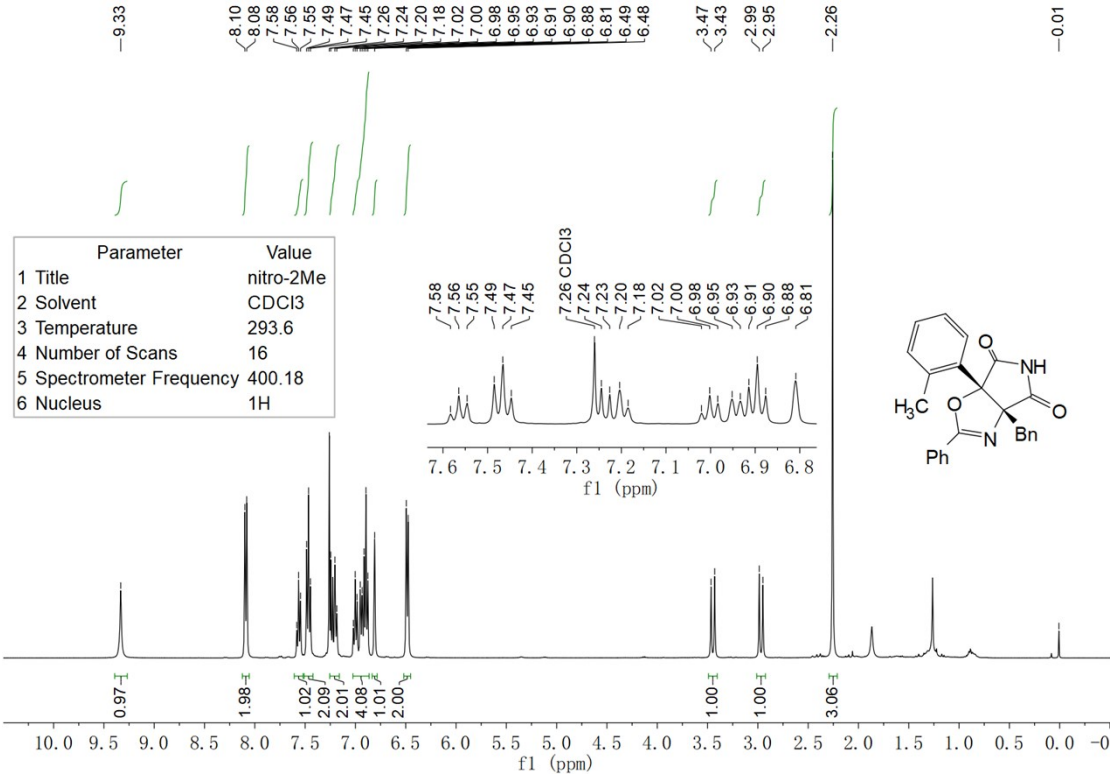
Parameter	Value
1 Title	0-nitro-4CF3
2 Solvent	CDCl3
3 Temperature	293.9
4 Number of Scans	16
5 Spectrometer Frequency	376.55
6 Nucleus	19F

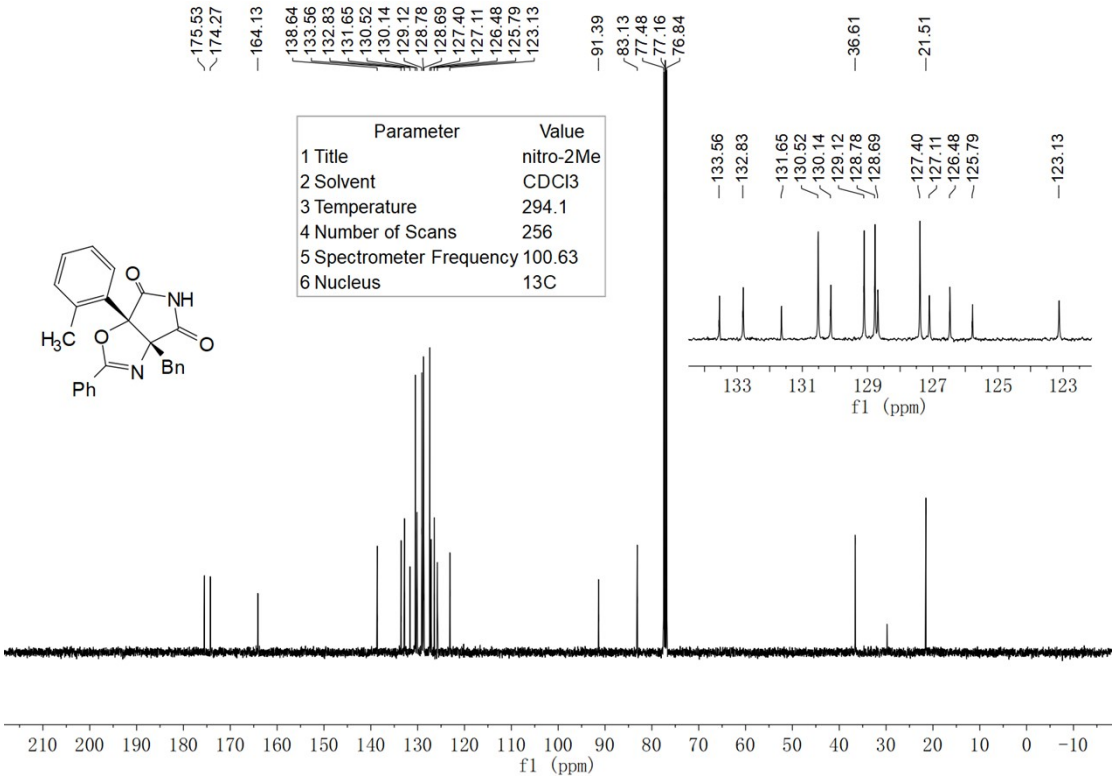
4ah


9.27
8.09
8.08
7.97
7.95
7.60
7.58
7.56
7.49
7.48
7.46
7.26 CDCl3
7.17
7.15
7.02
7.00
6.98
6.88
6.86
6.84
6.48
6.46
3.97
3.49
3.45
2.97
2.94
0.00
CO2Me
Ph
N
O
NH
Bn
Parameter Value
1 Title nitro-4CO2Me
2 Solvent CDCl3
3 Temperature 293.5
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

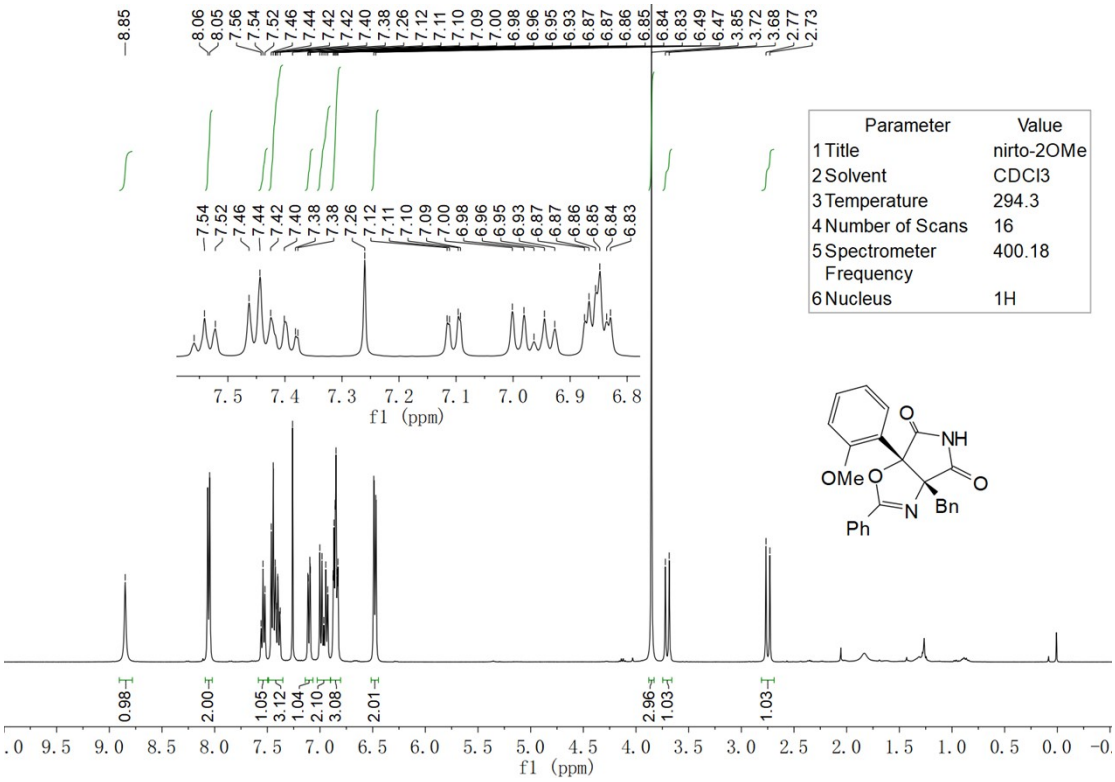

174.99
173.37
166.51
164.09
136.86
133.31
133.06
130.96
130.24
129.88
129.14
128.88
127.74
126.71
126.35
125.48
91.11
83.57
77.48
77.16
76.84
52.59
36.61
H3C
O
NH
N
Bn
Ph
Parameter Value
1 Title nitro-4CO2Me
2 Solvent CDCl3
3 Temperature 294.1
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

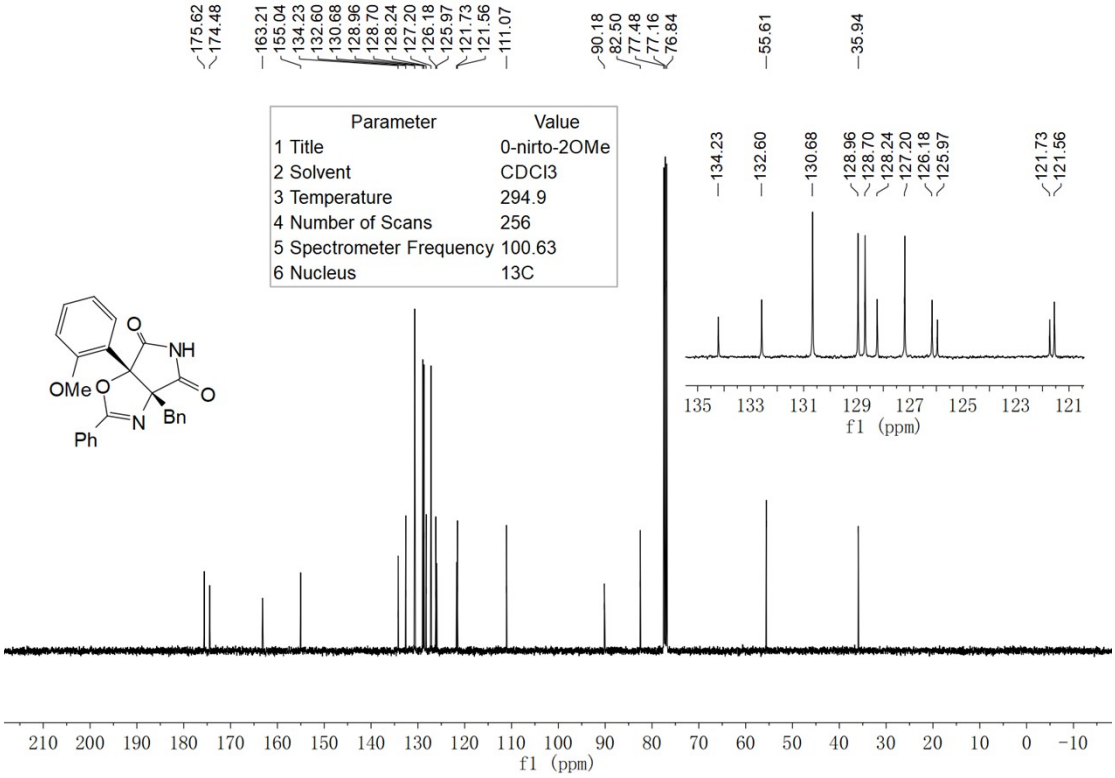
4ai


Parameter Value
1 Title nitro-2Me
2 Solvent CDCl3
3 Temperature 293.6
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

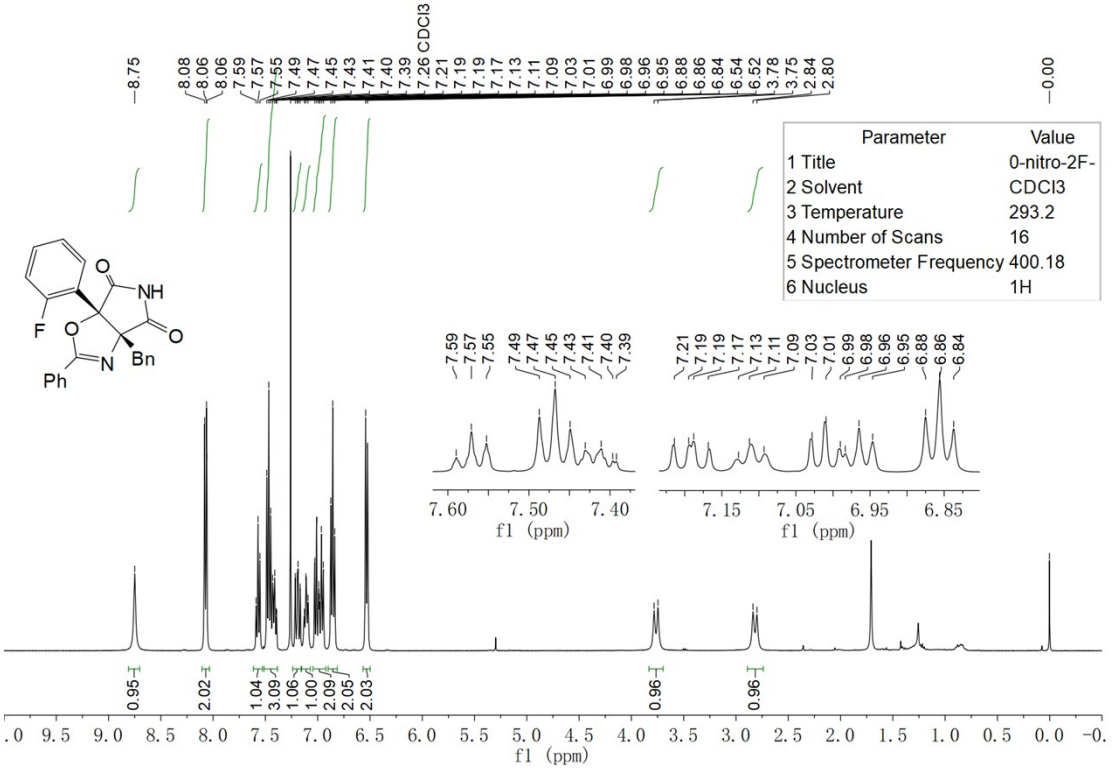

Parameter Value
1 Title nitro-2Me
2 Solvent CDCl3
3 Temperature 294.1
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

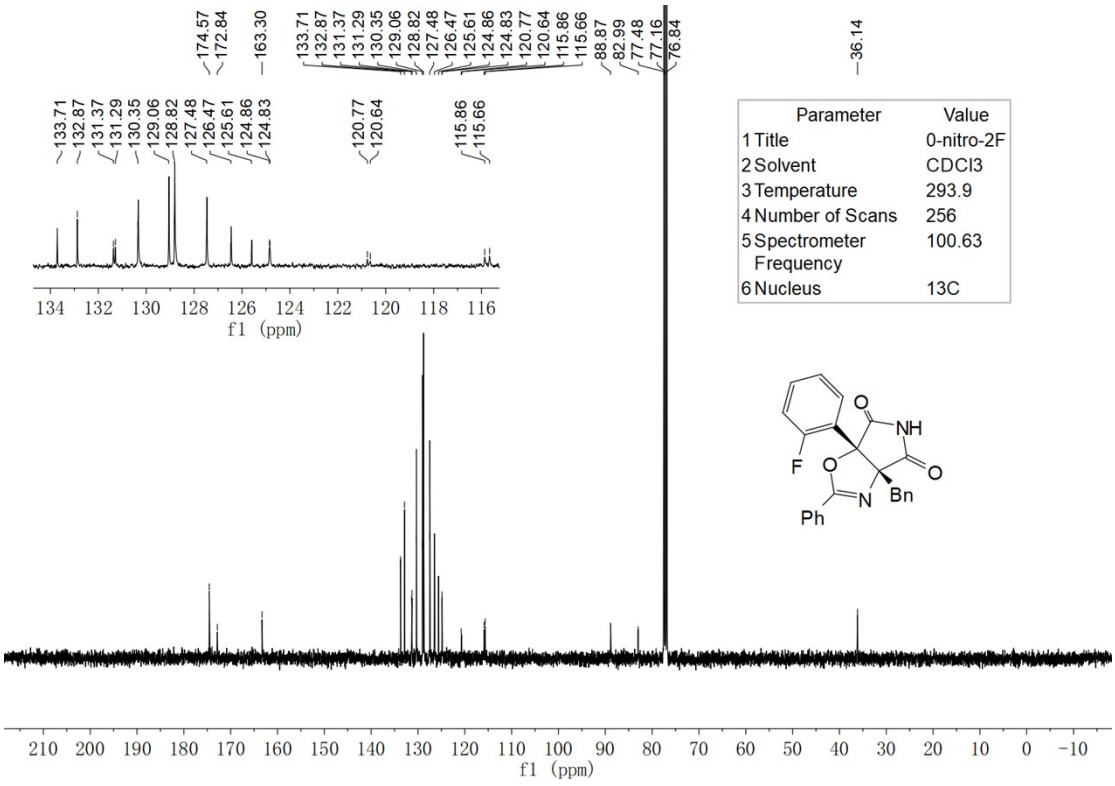
4aj

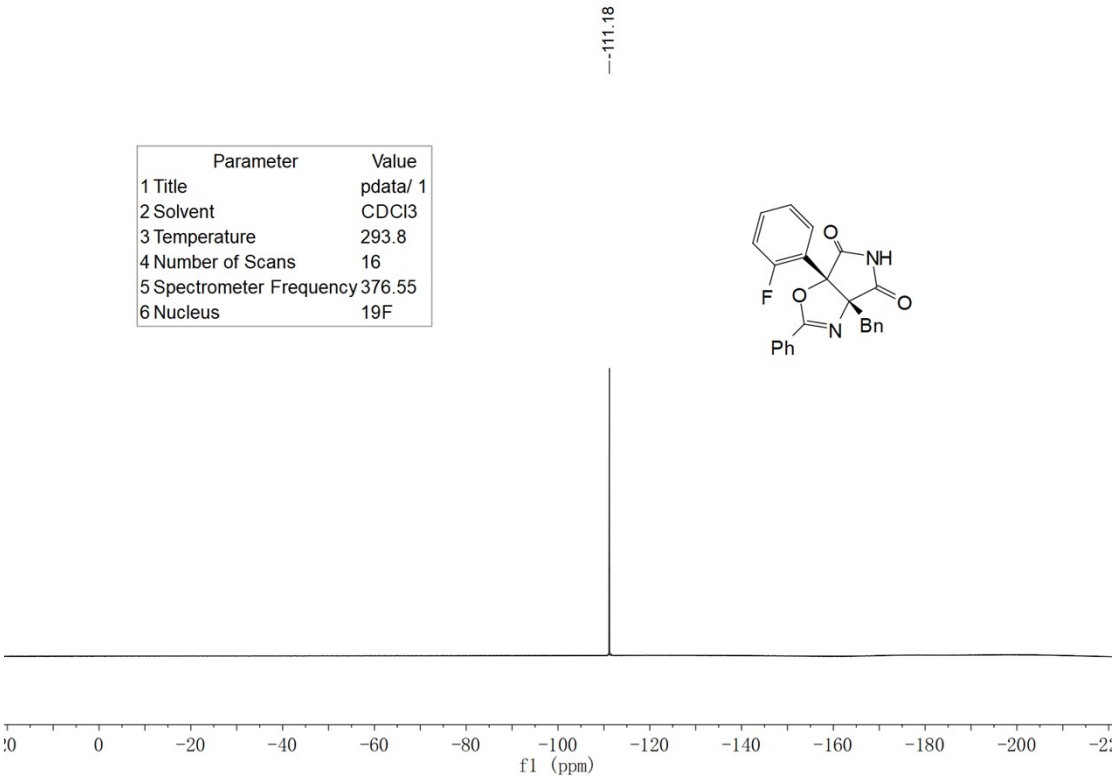

Parameter Value
1 Title nirto-2OMe
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)


Parameter Value
1 Title 0-nirto-2OMe
2 Solvent CDCl3
3 Temperature 294.9
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

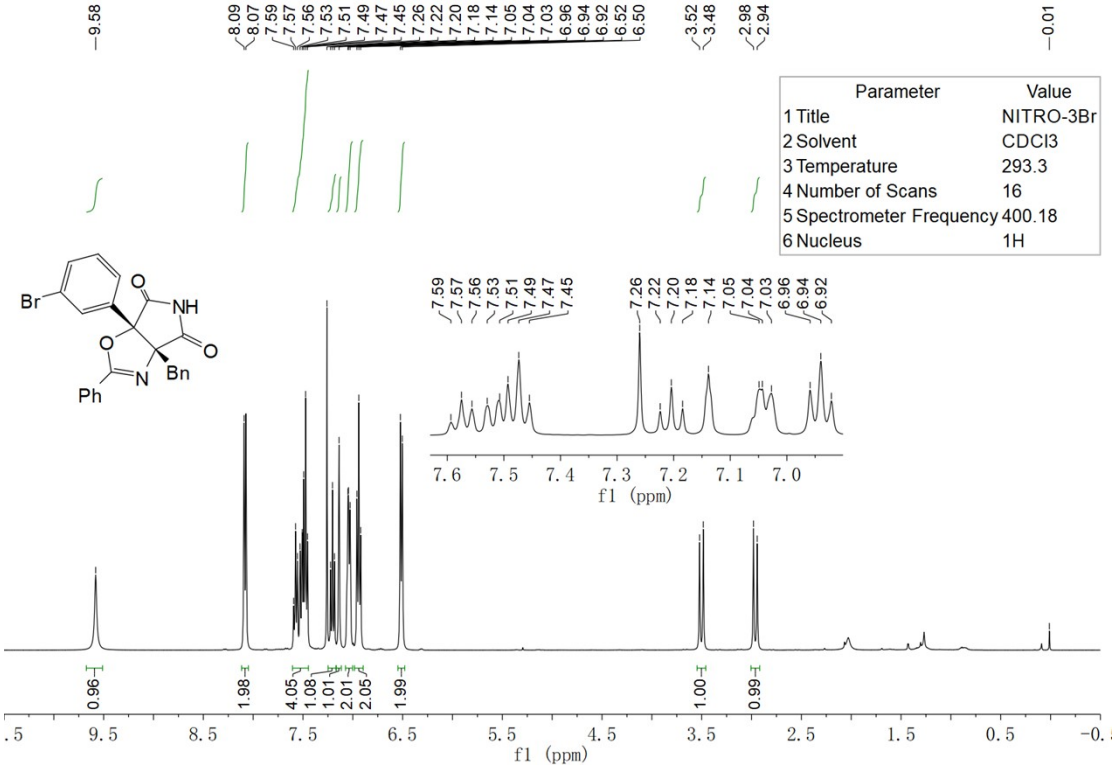
4ak

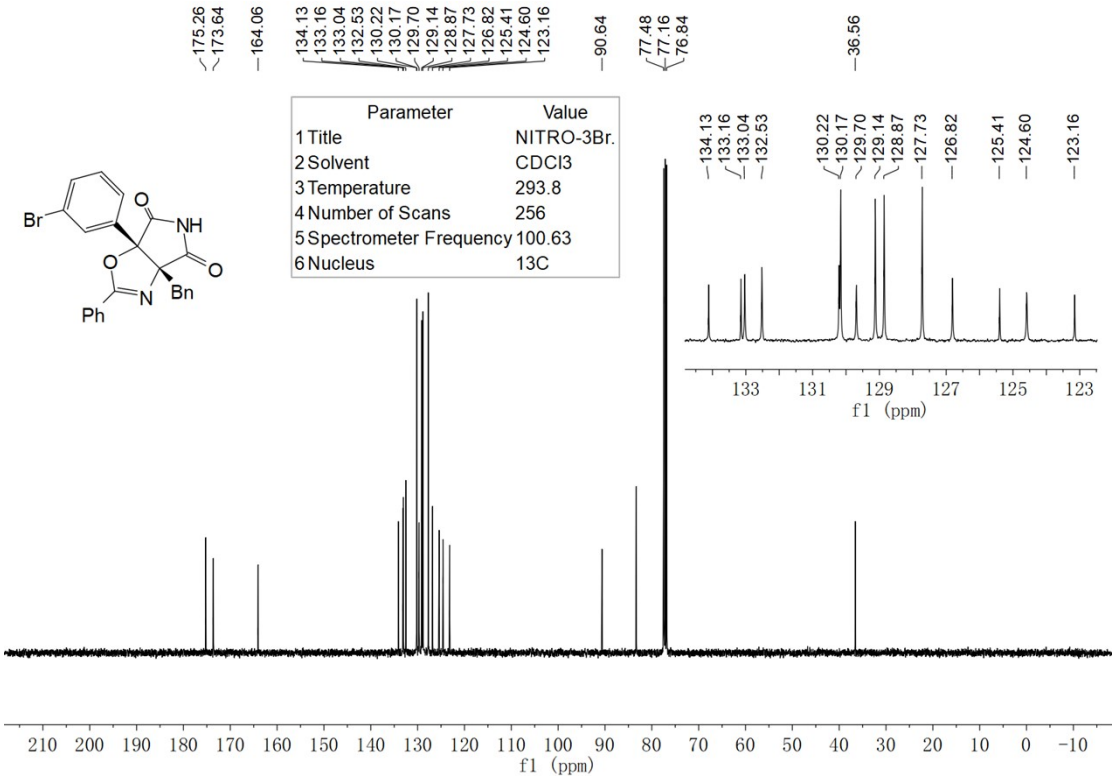

Parameter Value
1 Title 0-nitro-2F-
2 Solvent CDCl3
3 Temperature 293.2
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)


Parameter Value
1 Title 0-nitro-2F
2 Solvent CDCl3
3 Temperature 293.9
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

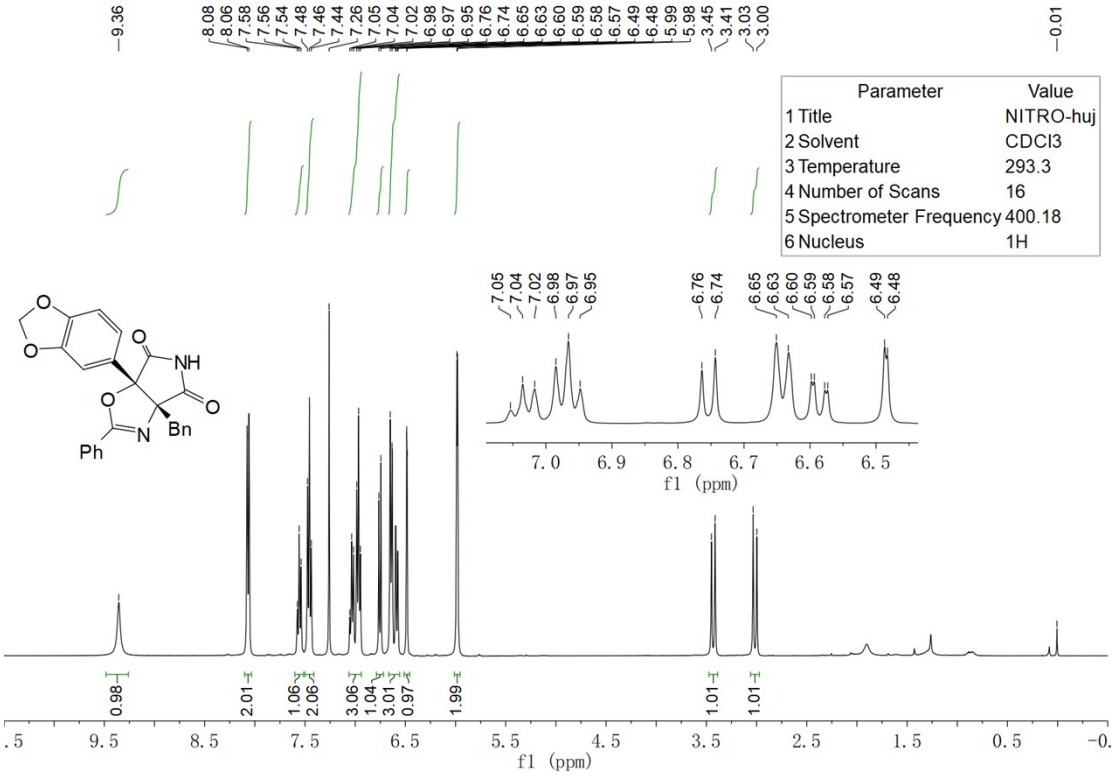

-111.18
Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 16
5 Spectrometer Frequency 376.55
6 Nucleus 19F
O
NH
F
O
O
N
Bn
Ph
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
f1 (ppm)

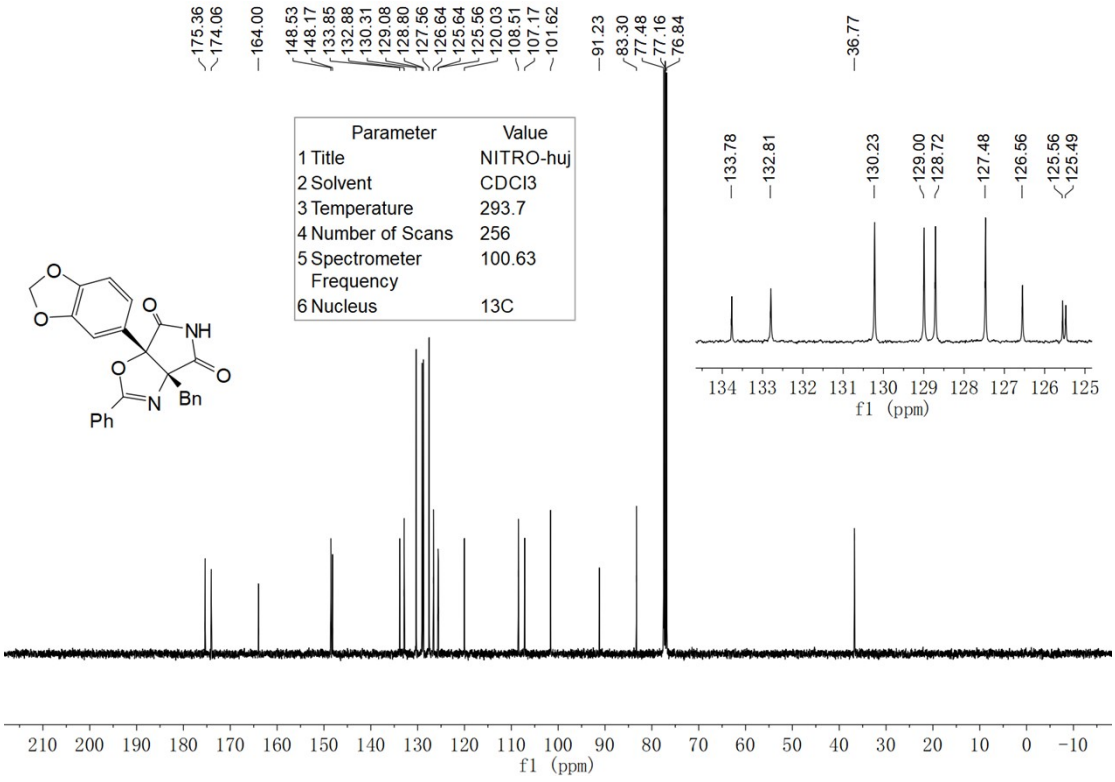
4al


9.58
8.09
8.07
7.59
7.57
7.56
7.53
7.51
7.49
7.47
7.45
7.26
7.22
7.20
7.18
7.14
7.05
7.04
7.03
6.96
6.94
6.92
6.52
6.50
3.52
3.48
2.98
2.94
0.01
Parameter Value
1 Title NITRO-3Br
2 Solvent CDCl3
3 Temperature 293.3
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Br
O
NH
O
O
N
Bn
Ph
0.96
1.98
4.05
1.08
1.01
2.01
2.05
1.99
1.00
0.99
f1 (ppm)

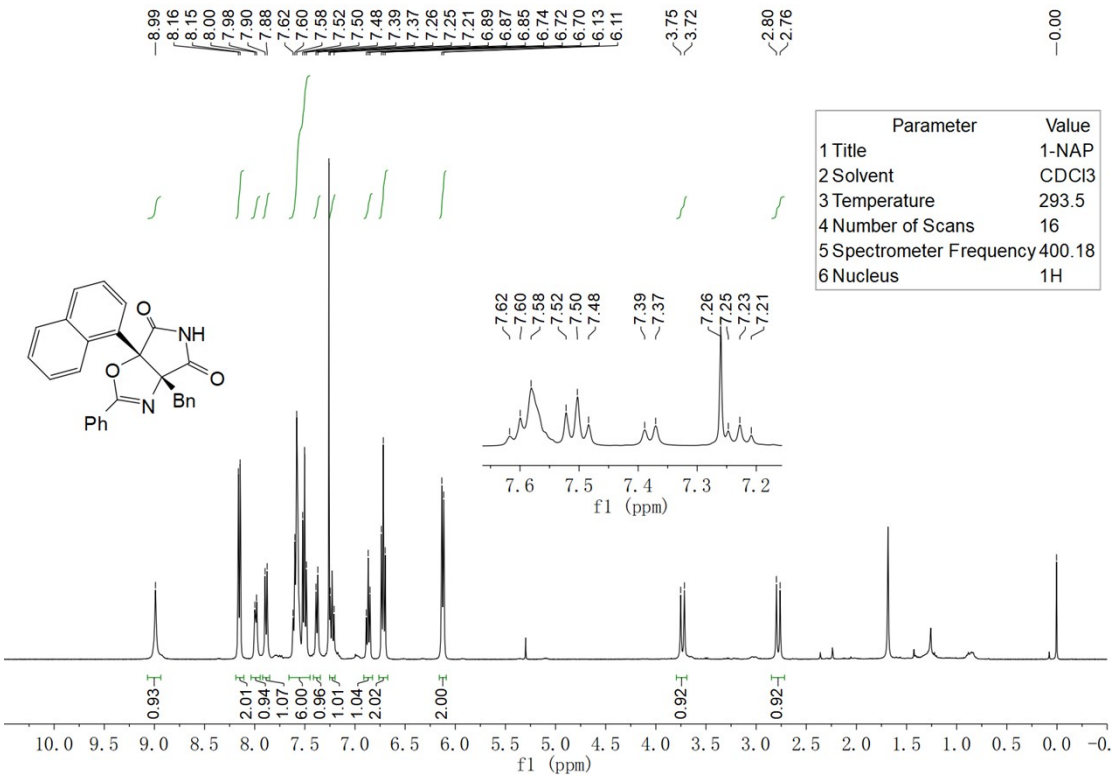

175.26
173.64
164.06
134.13
133.16
133.04
132.53
130.22
130.17
129.70
129.14
128.87
127.73
126.82
125.41
124.60
123.16
90.64
77.48
77.16
76.84
36.56
Parameter Value
1 Title NITRO-3Br.
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Br
O
NH
O
O
N
Bn
Ph
f1 (ppm)

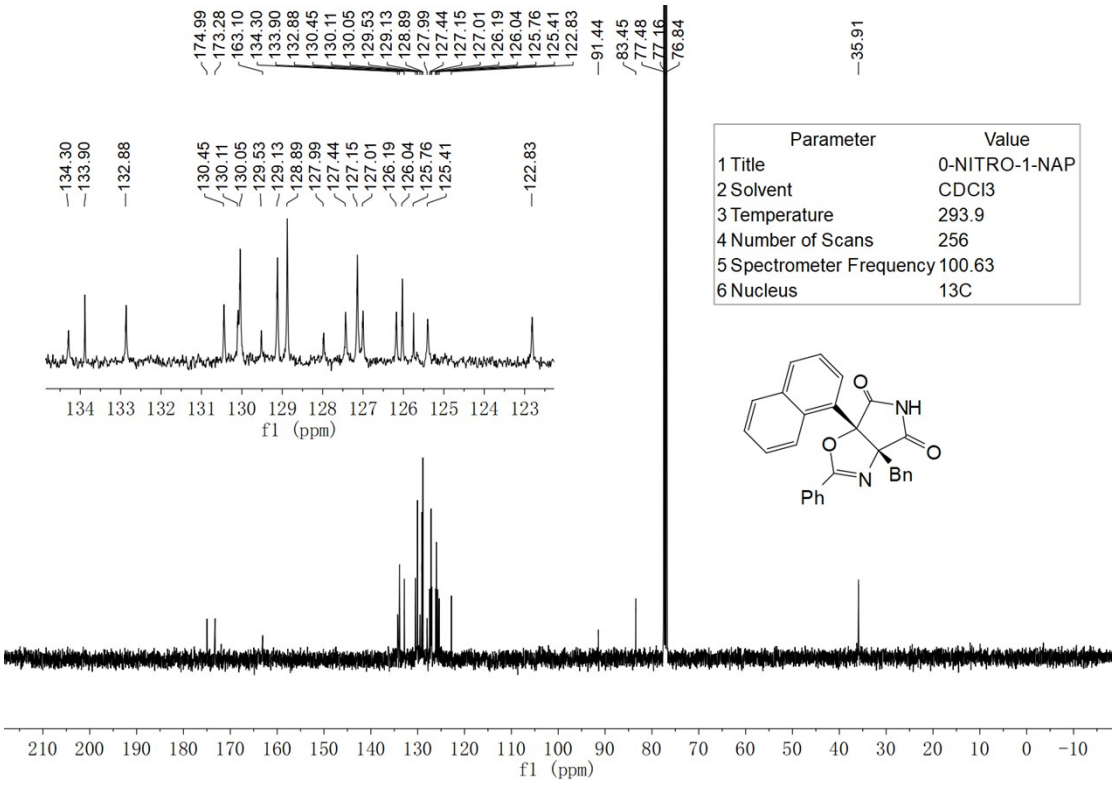
4am


Parameter Value
1 Title NITRO-huj
2 Solvent CDCl3
3 Temperature 293.3
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

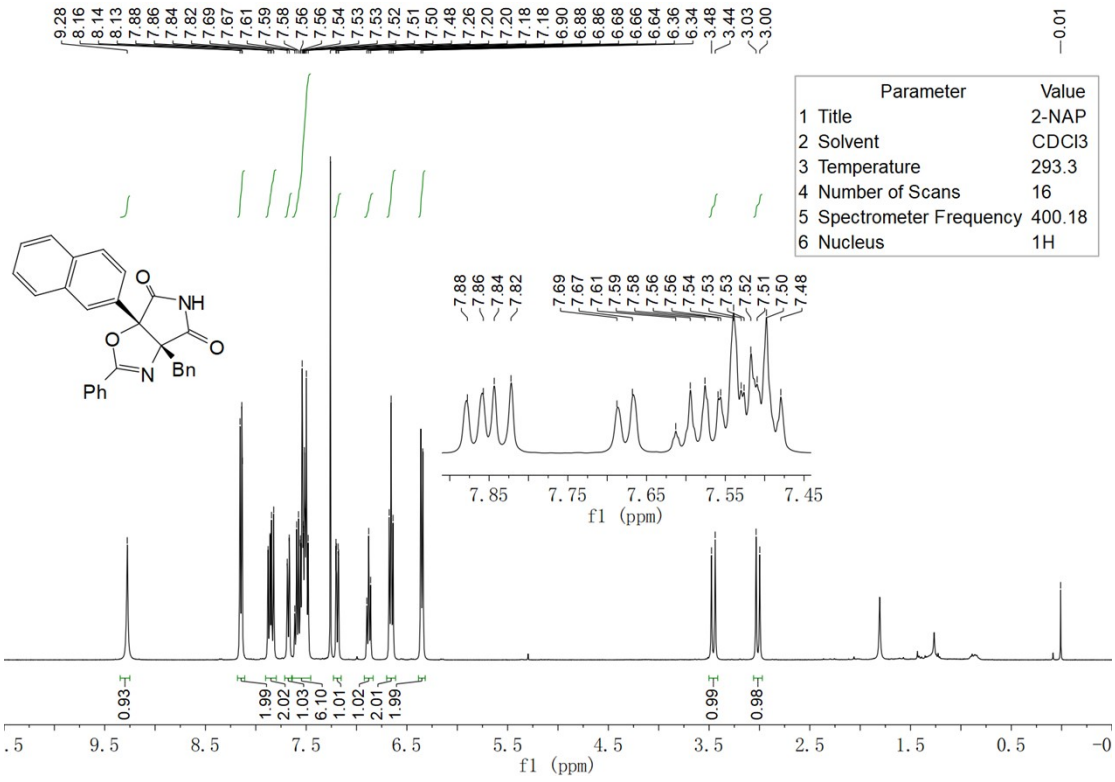

Parameter Value
1 Title NITRO-huj
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

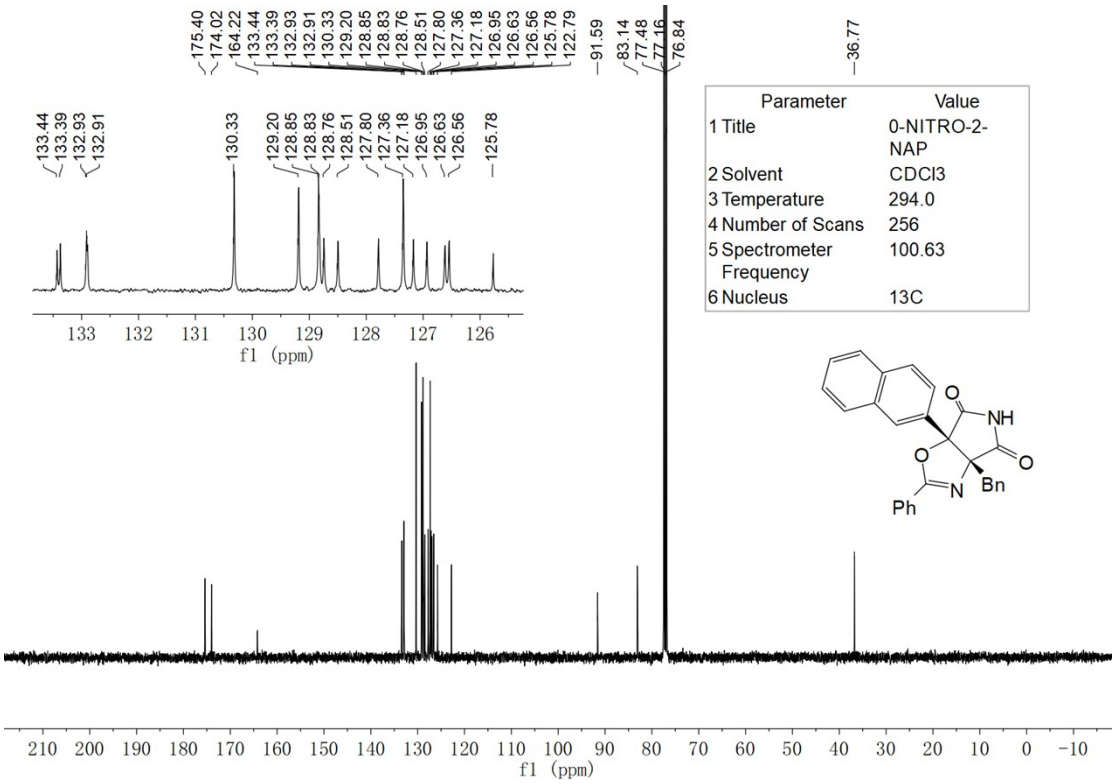
4an


8.99 8.16 8.15 8.00 7.98 7.90 7.88 7.62 7.60 7.58 7.52 7.50 7.48 7.39 7.37 7.26 7.25 7.21 6.89 6.87 6.85 6.74 6.72 6.70 6.13 6.11 3.75 3.72 2.80 2.76 0.00
Parameter Value
1 Title 1-NAP
2 Solvent CDCl3
3 Temperature 293.5
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
O NH O O N Bn Ph
7.62 7.60 7.58 7.52 7.50 7.48 7.39 7.37 7.26 7.25 7.23 7.21
7.6 7.5 7.4 7.3 7.2
f1 (ppm)
0.93 2.01 0.94 1.07 6.00 0.96 1.01 1.04 2.02 2.00 0.92 0.92
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

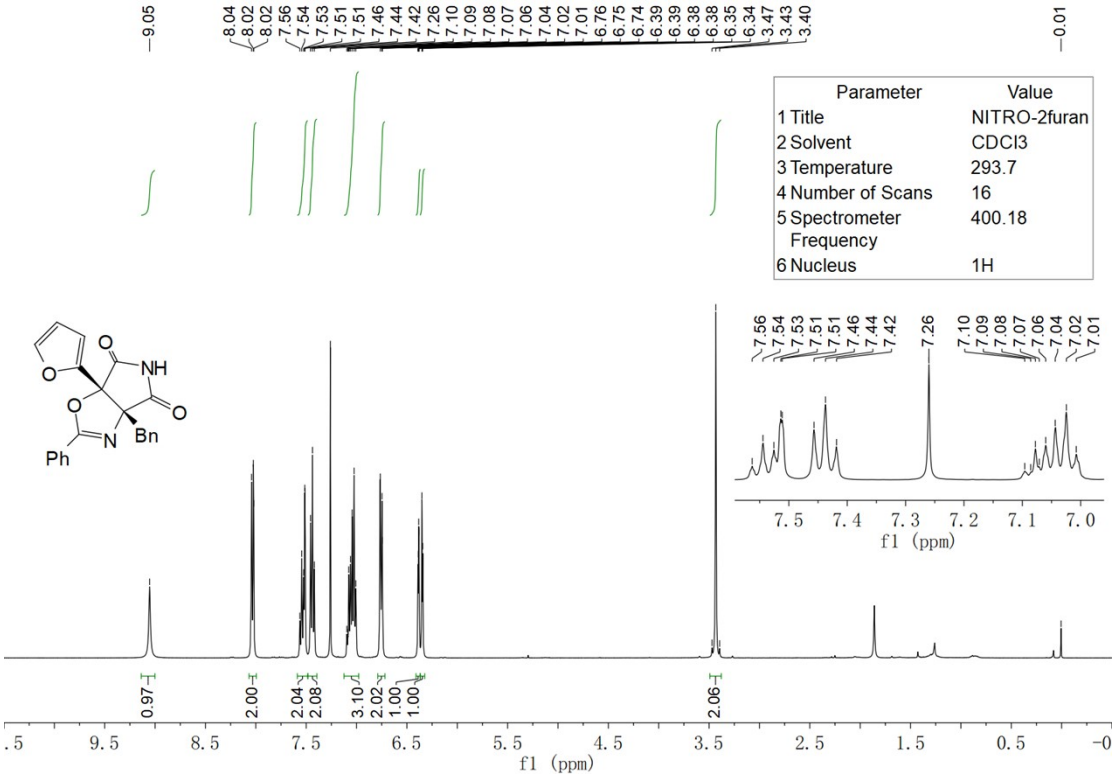

174.99 173.28 163.10 134.30 133.90 132.88 130.45 130.11 130.05 129.53 129.13 128.89 127.99 127.44 127.15 127.01 126.19 126.04 125.76 125.41 122.83 91.44 83.45 77.48 77.16 76.84 35.91
Parameter Value
1 Title 0-NITRO-1-NAP
2 Solvent CDCl3
3 Temperature 293.9
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
134.30 133.90 132.88 130.45 130.11 130.05 129.53 129.13 128.89 127.99 127.44 127.15 127.01 126.19 126.04 125.76 125.41 122.83
134 133 132 131 130 129 128 127 126 125 124 123
f1 (ppm)
O NH O O N Bn Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

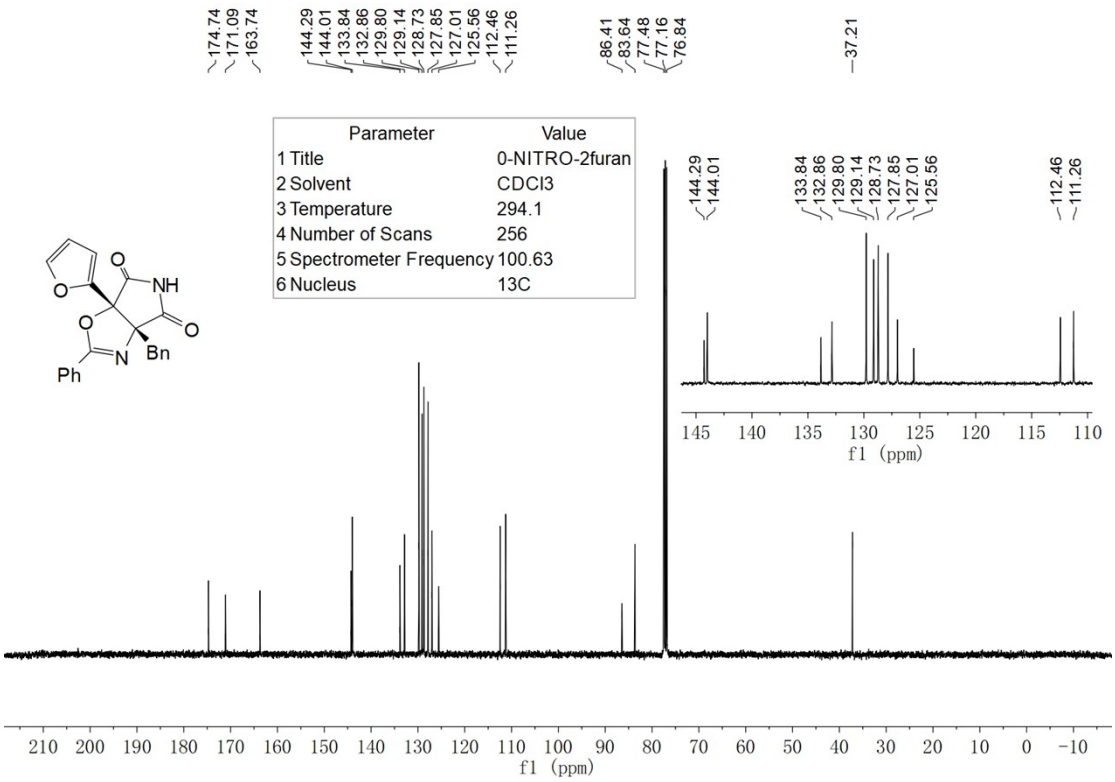
4ao


Parameter Value
1 Title 2-NAP
2 Solvent CDCl3
3 Temperature 293.3
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

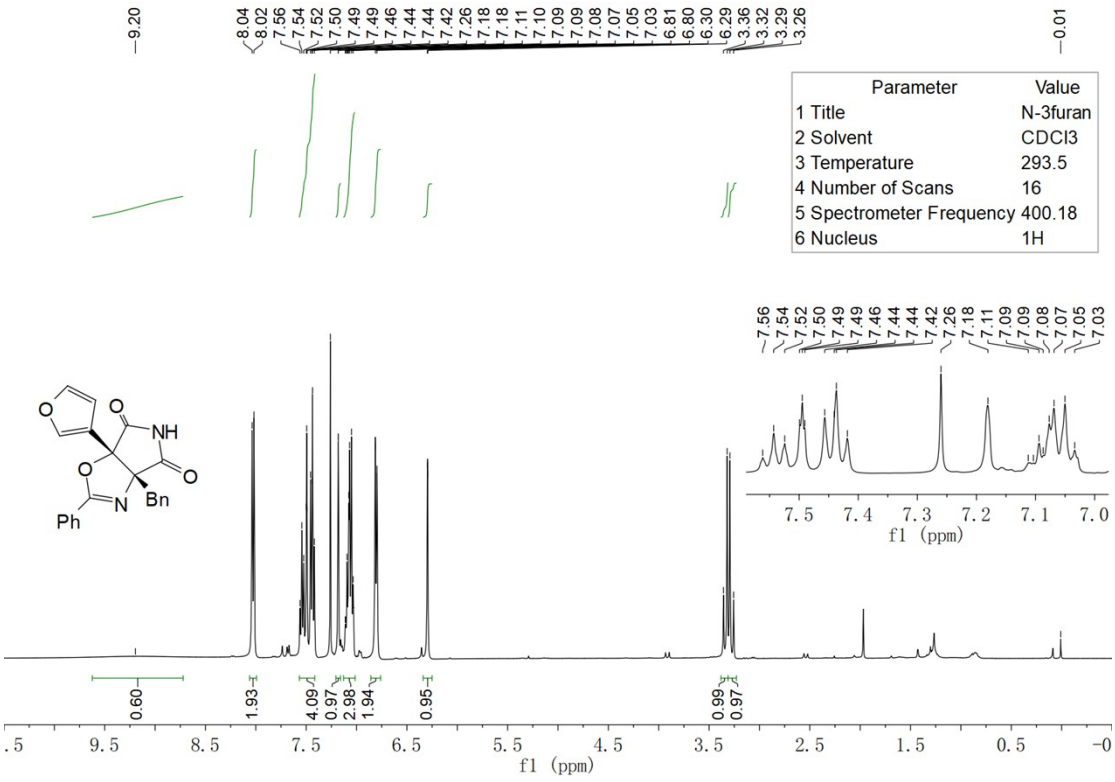

Parameter Value
1 Title 0-NITRO-2-NAP
2 Solvent CDCl3
3 Temperature 294.0
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

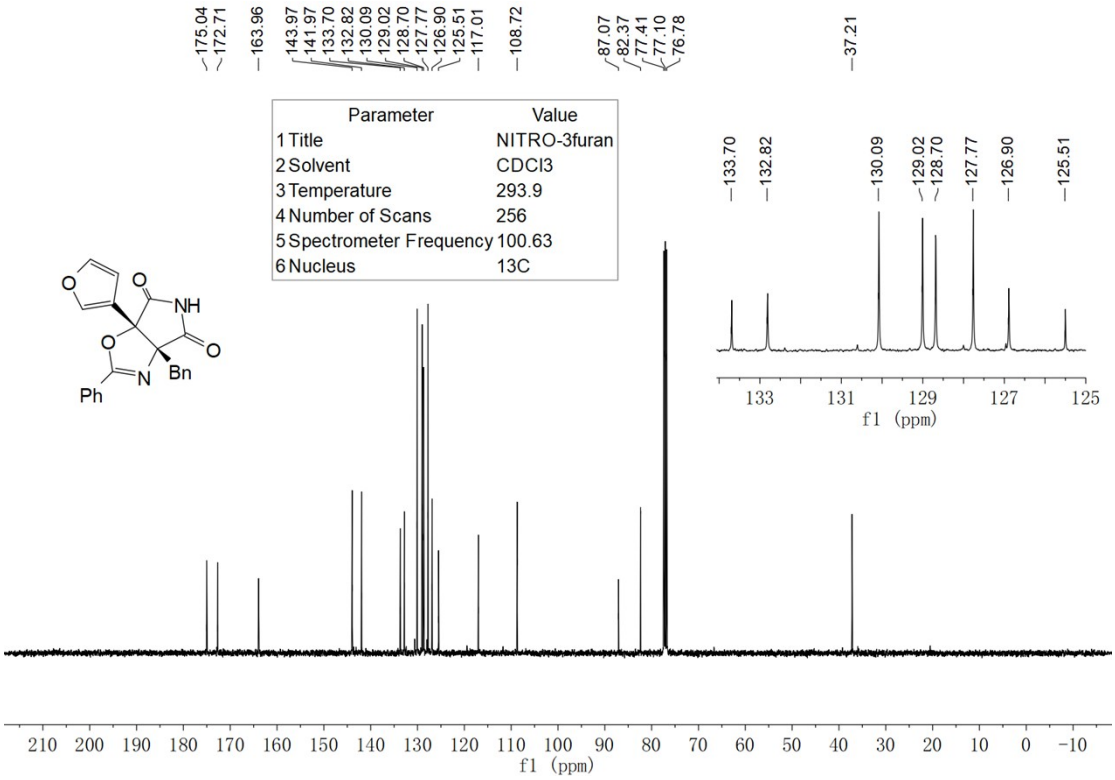
4ap


9.05
8.04
8.02
8.02
7.56
7.54
7.53
7.51
7.51
7.46
7.44
7.42
7.26
7.10
7.09
7.08
7.07
7.06
7.04
7.02
7.01
6.76
6.75
6.74
6.39
6.39
6.38
6.38
6.35
6.34
3.47
3.43
3.40
0.01
Parameter Value
1 Title NITRO-2furan
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
O
NH
O
O
N
Bn
Ph
0.97
2.00
2.04
2.08
3.10
2.02
1.00
1.00
2.06
f1 (ppm)

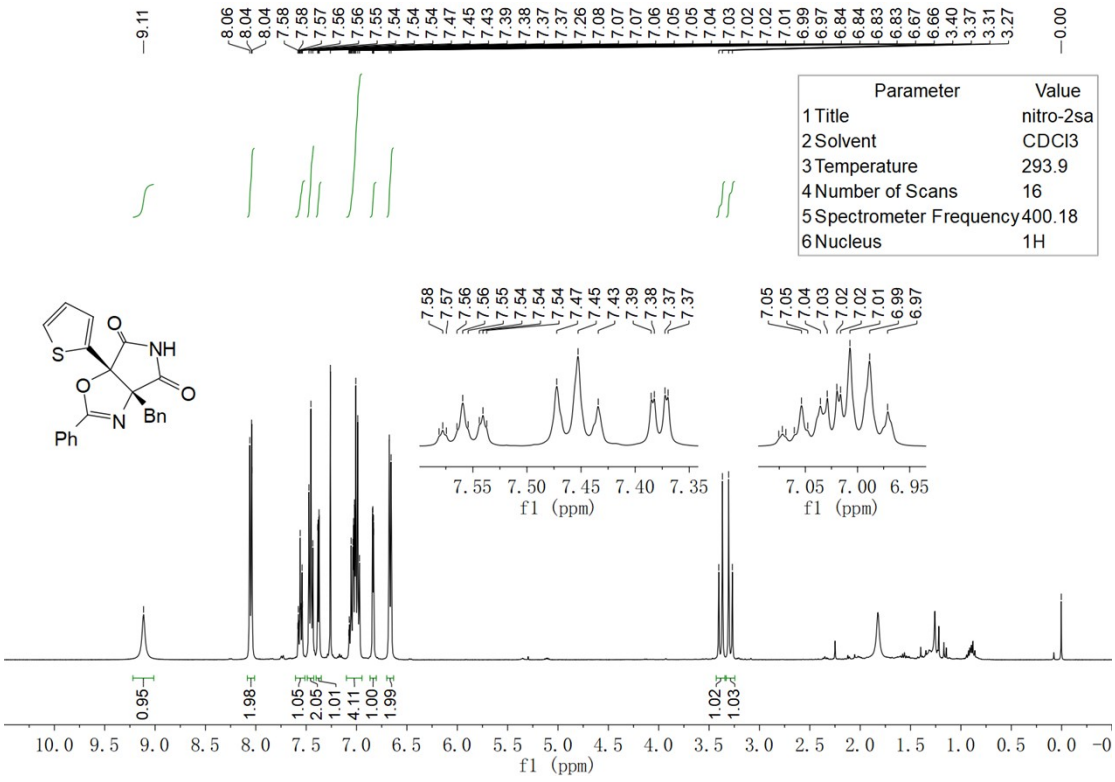

174.74
171.09
163.74
144.29
144.01
133.84
132.86
129.80
129.14
128.73
127.85
127.01
125.56
112.46
111.26
86.41
83.64
77.48
77.16
76.84
37.21
Parameter Value
1 Title 0-NITRO-2furan
2 Solvent CDCl3
3 Temperature 294.1
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
O
NH
O
O
N
Bn
Ph
f1 (ppm)

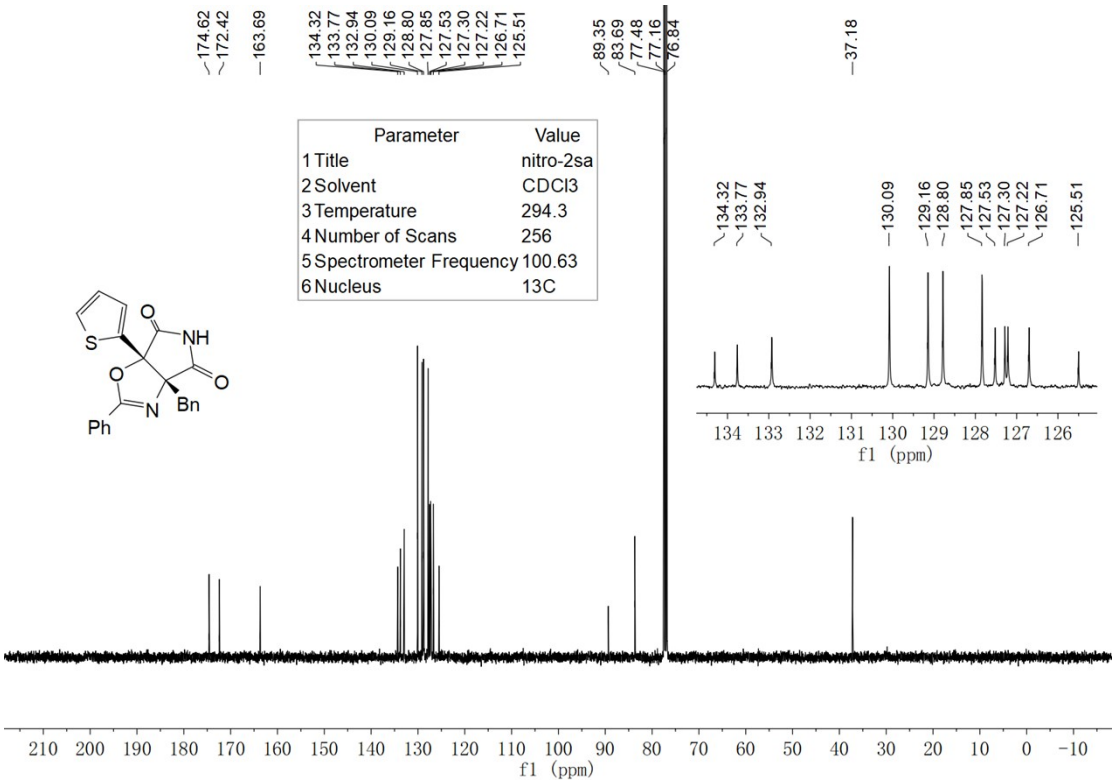
4aq


9.20
8.04
8.02
7.56
7.54
7.52
7.50
7.49
7.49
7.46
7.44
7.44
7.42
7.26
7.18
7.18
7.11
7.10
7.09
7.09
7.08
7.07
7.05
7.03
6.81
6.80
6.30
6.29
3.36
3.32
3.29
3.26
0.01
Parameter Value
1 Title N-3furan
2 Solvent CDCl3
3 Temperature 293.5
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
O
NH
O
O
N
Bn
Ph
0.60
1.93
4.09
0.97
2.98
1.94
0.95
0.99
0.97
f1 (ppm)

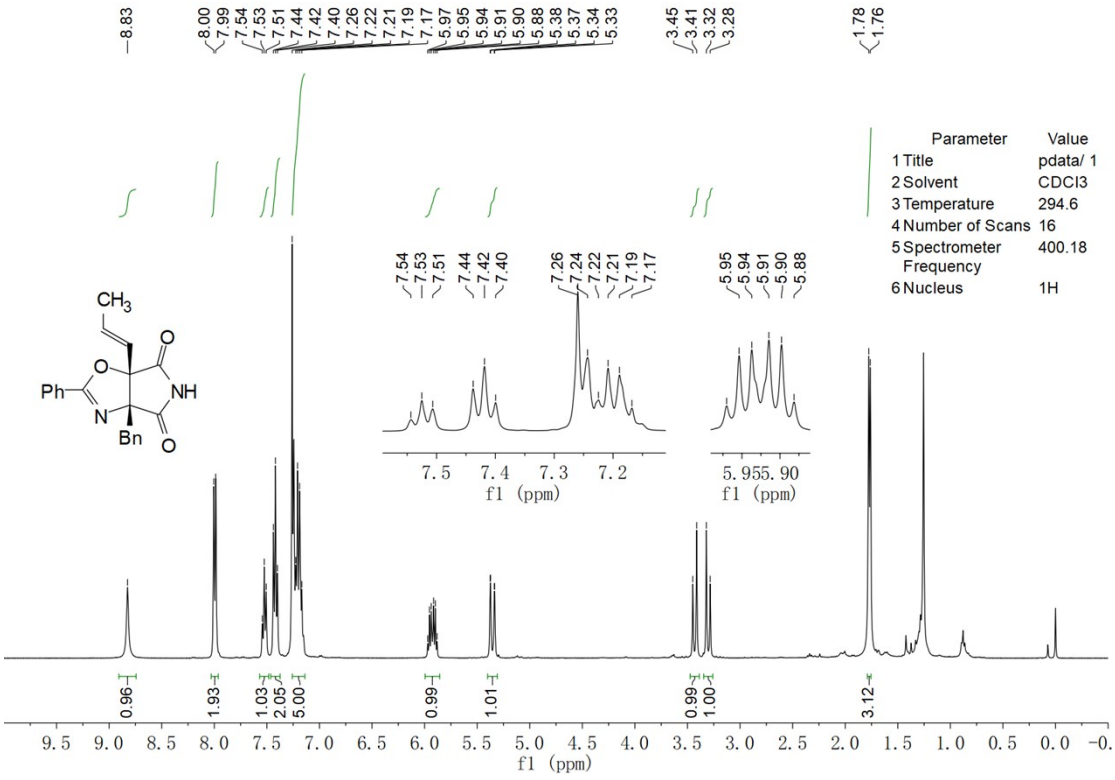

175.04
172.71
163.96
143.97
141.97
133.70
132.82
130.09
129.02
128.70
127.77
126.90
125.51
117.01
108.72
87.07
82.37
77.41
77.10
76.78
37.21
Parameter Value
1 Title NITRO-3furan
2 Solvent CDCl3
3 Temperature 293.9
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
O
NH
O
O
N
Bn
Ph
f1 (ppm)

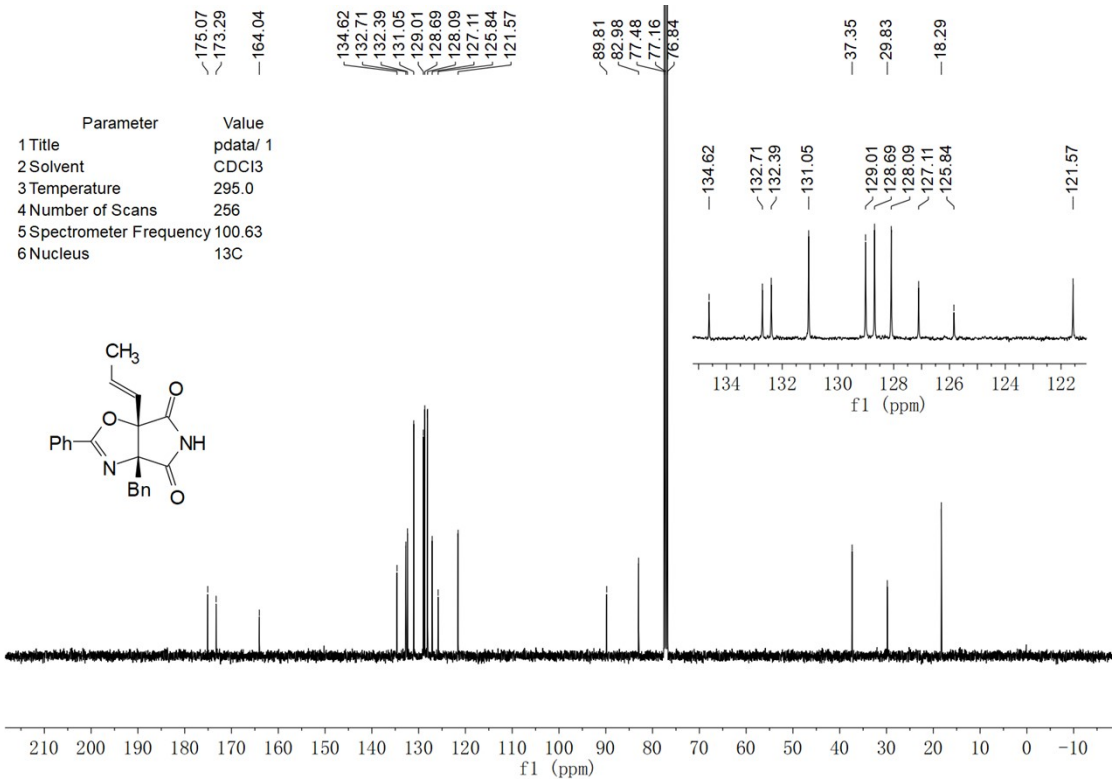
4ar


Parameter Value
1 Title nitro-2sa
2 Solvent CDCl3
3 Temperature 293.9
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

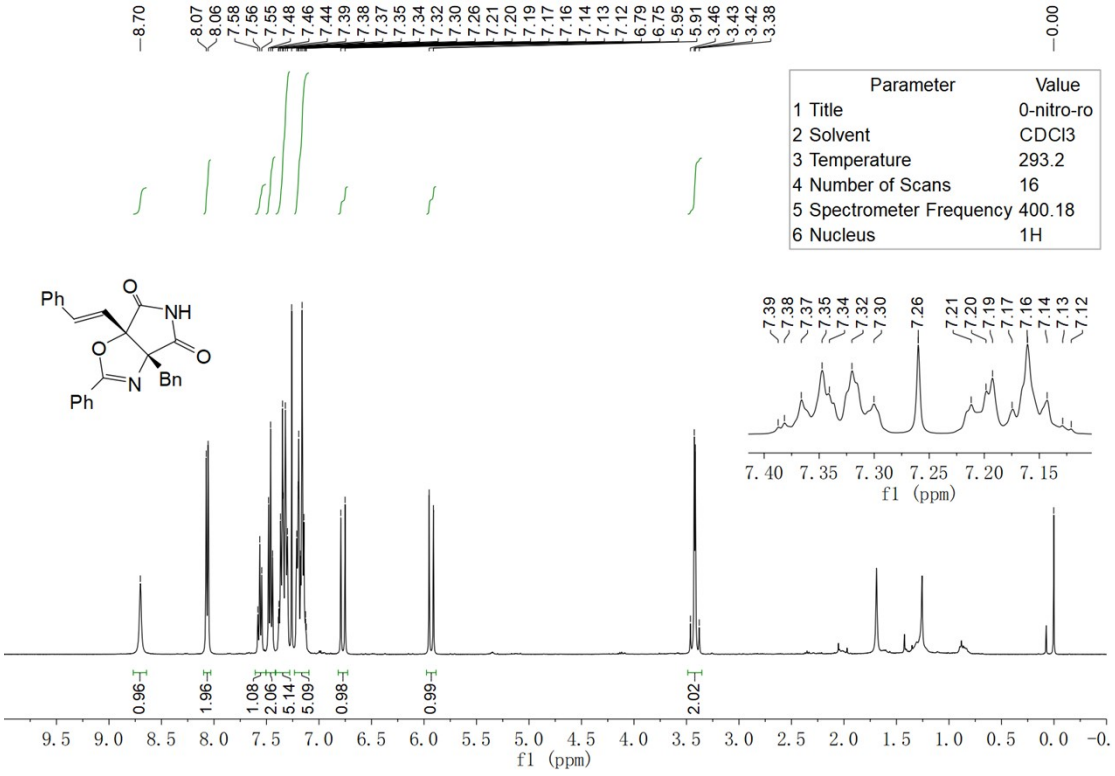

Parameter Value
1 Title nitro-2sa
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

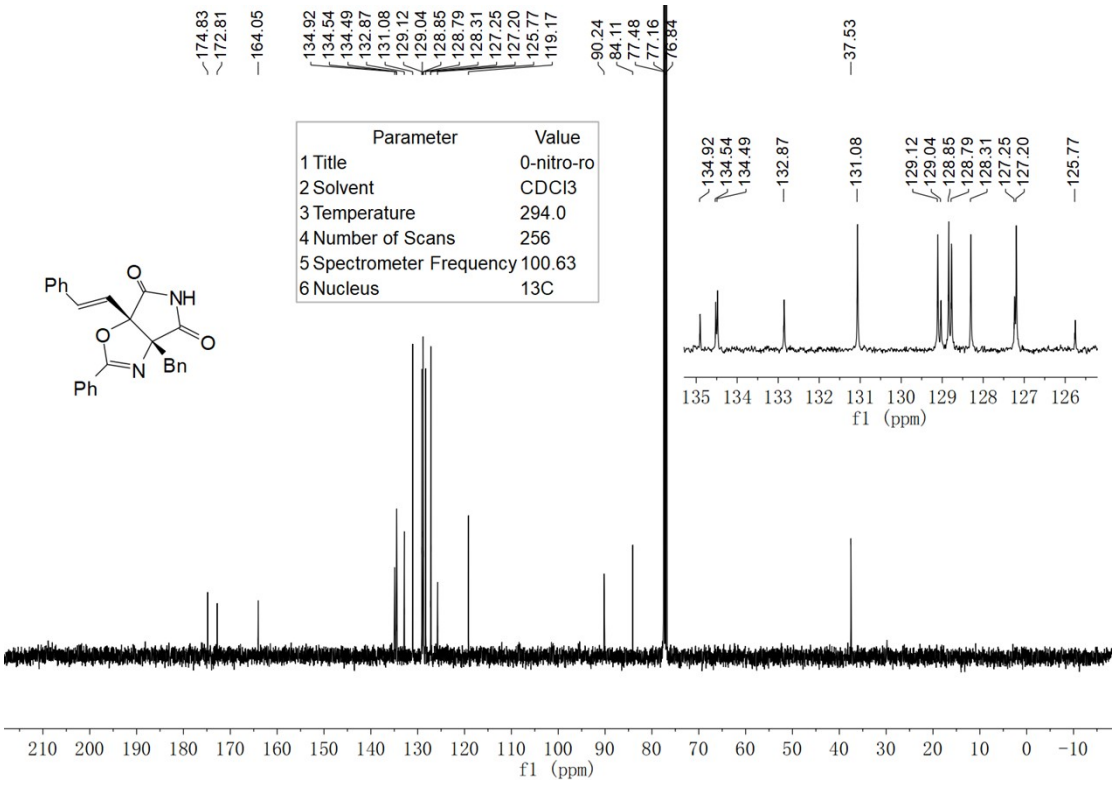
4as


8.83
8.00
7.99
7.54
7.53
7.51
7.44
7.42
7.40
7.26
7.22
7.21
7.19
7.17
5.97
5.95
5.94
5.91
5.90
5.88
5.38
5.37
5.34
5.33
3.45
3.41
3.32
3.28
1.78
1.76
Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 294.6
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
CH3
O
O
Ph
NH
N
Bn
O
0.96
1.93
1.03
2.05
5.00
0.99
1.01
0.99
1.00
3.12
f1 (ppm)

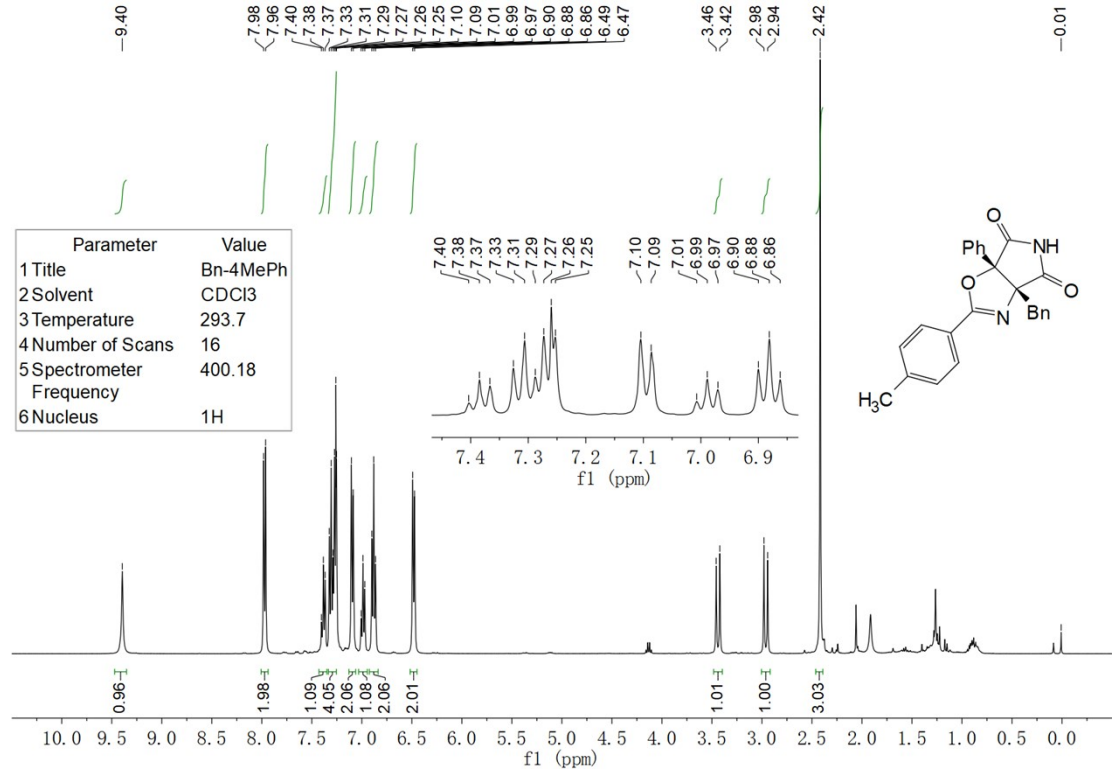

175.07
173.29
164.04
134.62
132.71
132.39
131.05
129.01
128.69
128.09
127.11
125.84
121.57
89.81
82.98
77.48
77.16
76.84
37.35
29.83
18.29
Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 295.0
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
CH3
O
O
Ph
NH
N
Bn
O
f1 (ppm)

4at


8.70
8.07
8.06
7.58
7.56
7.55
7.48
7.46
7.44
7.39
7.38
7.37
7.35
7.34
7.32
7.30
7.26
7.21
7.20
7.19
7.17
7.16
7.14
7.13
7.12
6.79
6.75
5.95
5.91
3.46
3.43
3.42
3.38
0.00
Parameter Value
1 Title 0-nitro-ro
2 Solvent CDCl3
3 Temperature 293.2
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph
O
NH
O
O
N
Bn
Ph
0.96
1.96
1.08
2.06
5.14
5.09
0.98
0.99
2.02
f1 (ppm)


174.83
172.81
164.05
134.92
134.54
134.49
132.87
131.08
129.12
129.04
128.85
128.79
128.31
127.25
127.20
125.77
119.17
90.24
84.11
77.48
77.16
76.84
37.53
Parameter Value
1 Title 0-nitro-ro
2 Solvent CDCl3
3 Temperature 294.0
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Ph
O
NH
O
O
N
Bn
Ph
f1 (ppm)

4ba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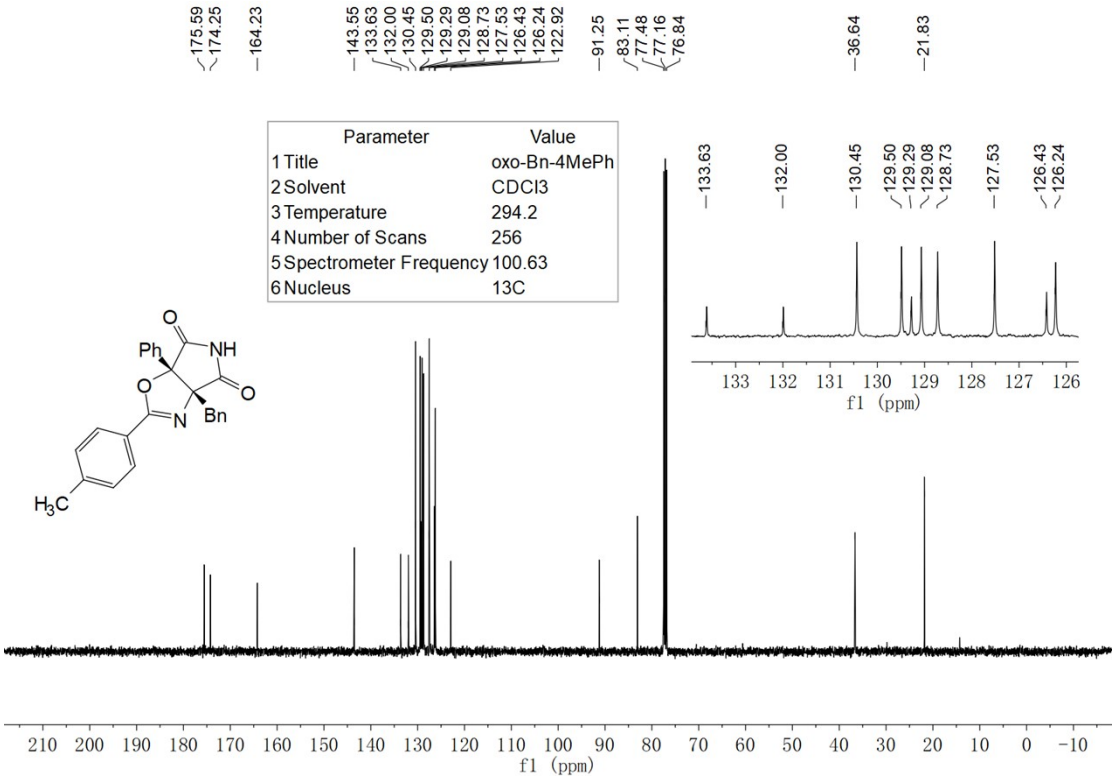
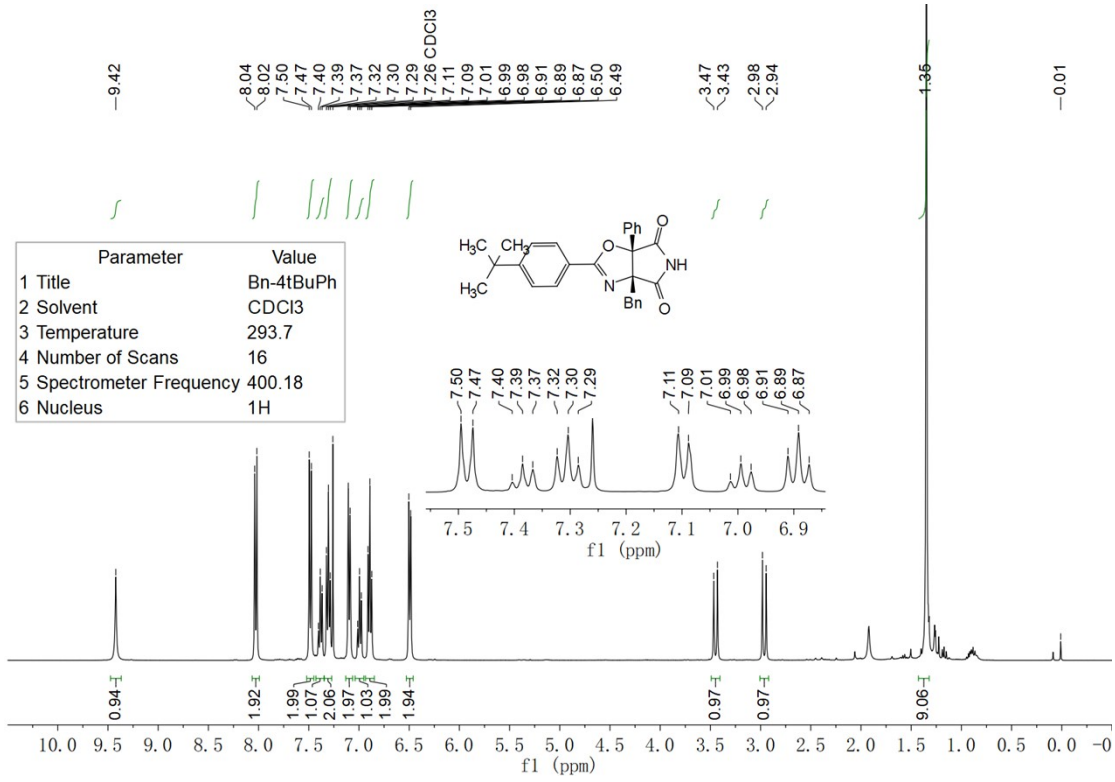
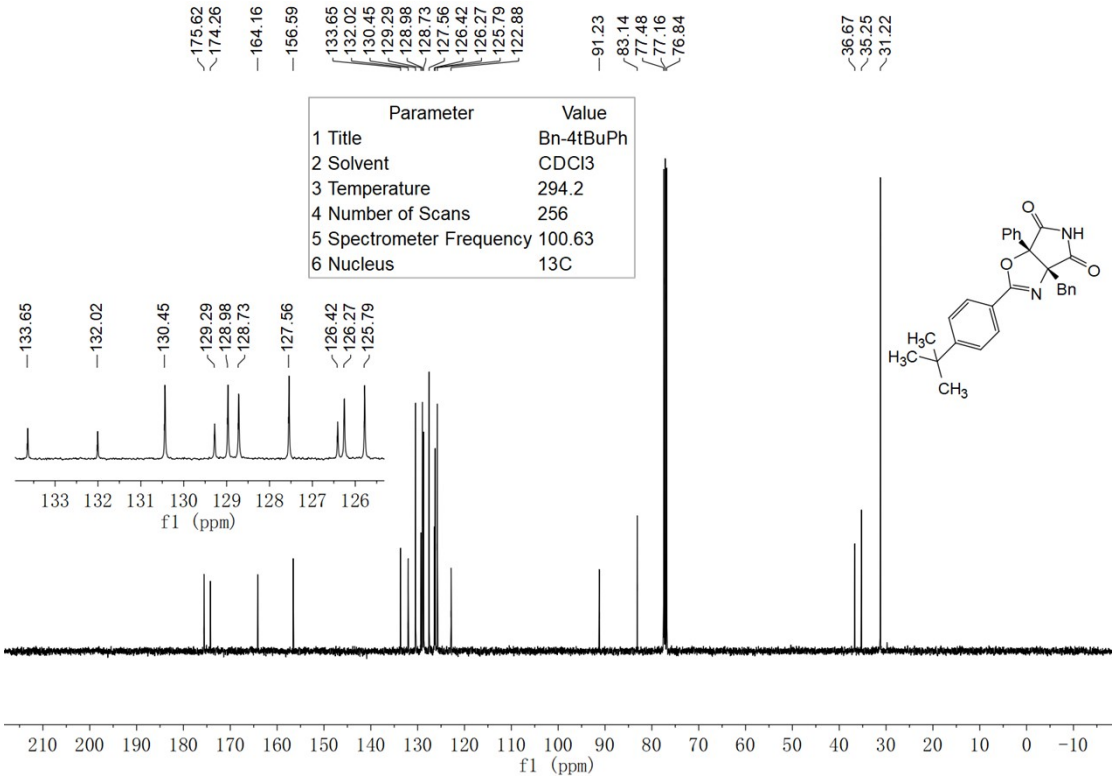
7.98
7.96
7.40
7.38
7.37
7.33
7.31
7.29
7.27
7.26
7.25
7.10
7.09
7.01
6.99
6.97
6.90
6.88
6.86
6.49
6.47
3.46
3.42
2.98
2.94
2.42
0.01
Parameter Value
1 Title Bn-4MePh
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
0.96
1.98
1.09
4.05
2.06
1.08
2.06
2.01
1.01
1.00
3.03
f1 (ppm)
Ph
NH
O
N
Bn
H3C


175.59
174.25
164.23
143.55
133.63
132.00
130.45
129.50
129.29
129.08
128.73
127.53
126.43
126.24
122.92
91.25
83.11
77.48
77.16
76.84
36.64
21.83
Parameter Value
1 Title oxo-Bn-4MePh
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)
Ph
NH
O
N
Bn
H3C

4ca


9.42
8.04
8.02
7.50
7.47
7.40
7.39
7.37
7.32
7.30
7.29
7.26 CDCl3
7.11
7.09
7.01
6.99
6.98
6.91
6.89
6.87
6.50
6.49
3.47
3.43
2.98
2.94
1.36
0.01
Parameter Value
1 Title Bn-4tBuPh
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph
O
NH
O
N
Bn
O
H3C
CH3
H3C
f1 (ppm)
0.94
1.92
1.99
1.07
2.06
1.97
1.03
1.99
1.94
0.97
0.97
9.06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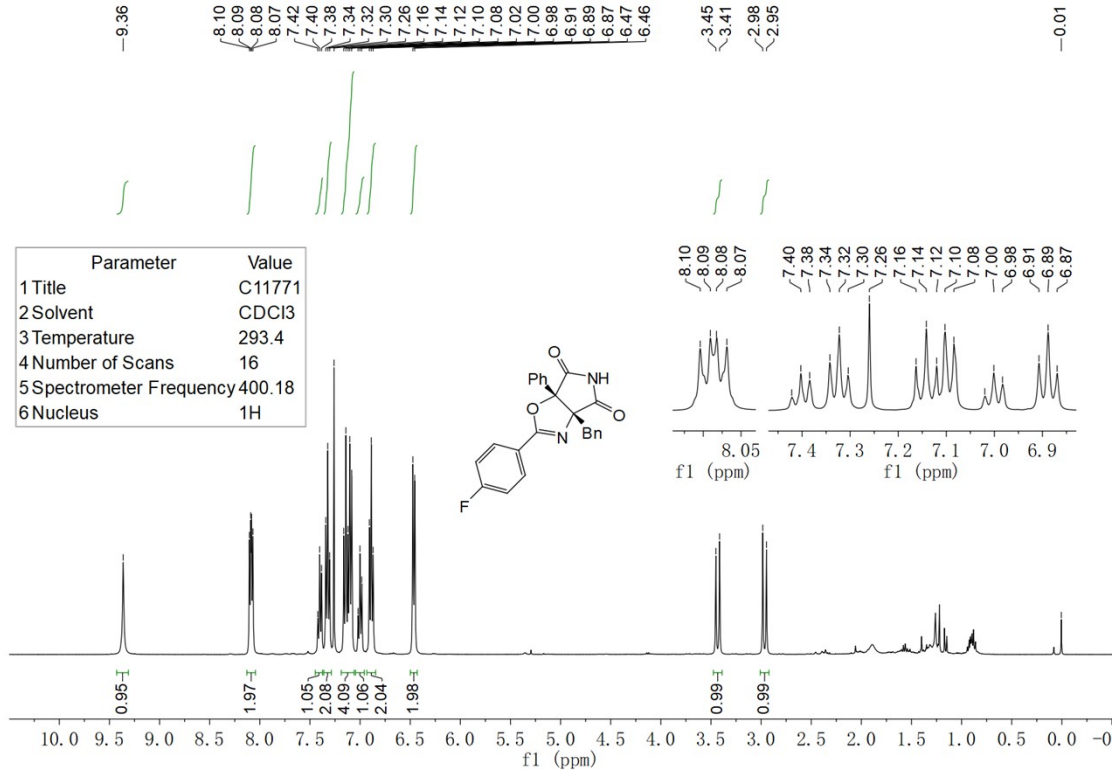
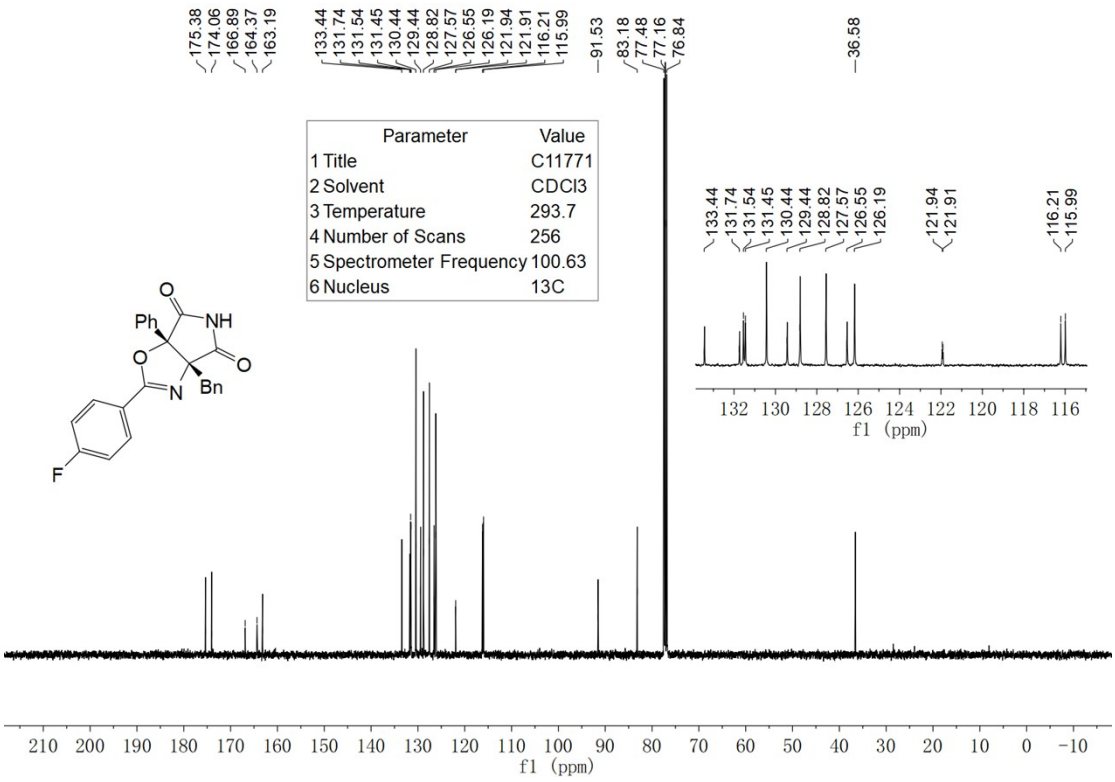
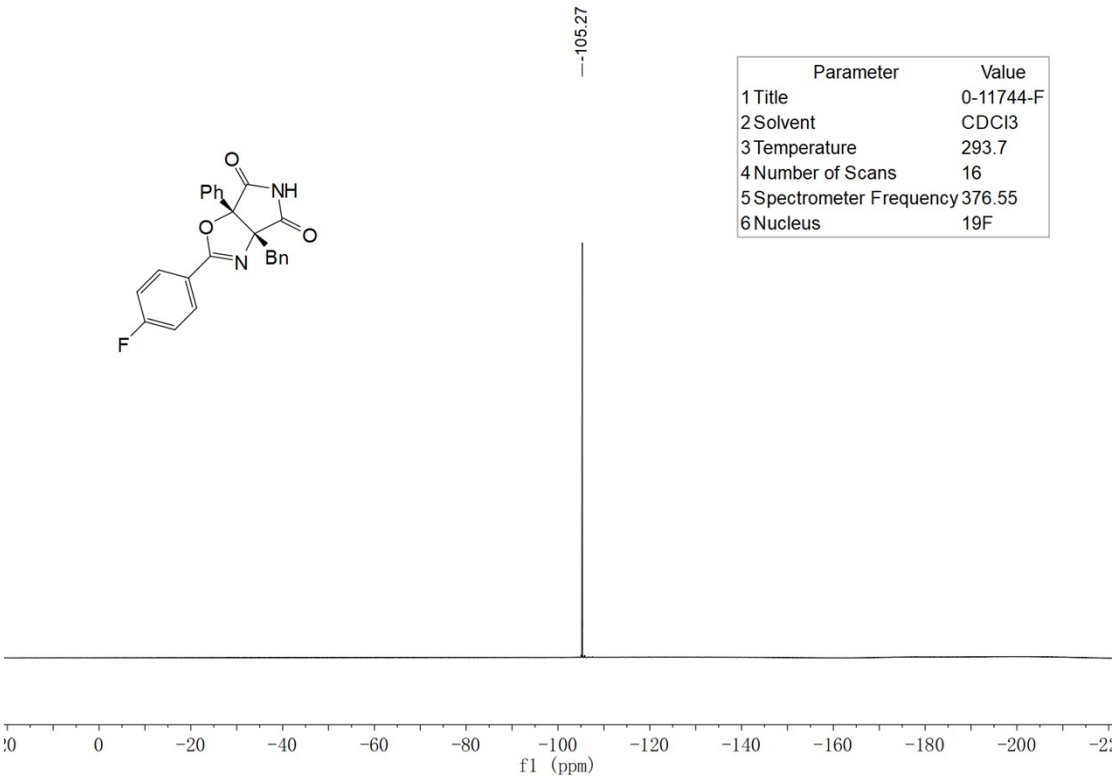
174.26
164.16
156.59
133.65
132.02
130.45
129.29
128.98
128.73
127.56
126.42
126.27
125.79
122.88
91.23
83.14
77.48
77.16
76.84
36.67
35.25
31.22
Parameter Value
1 Title Bn-4tBuPh
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
O
Ph
NH
O
O
N
Bn
H3C
H3C
CH3
f1 (ppm)

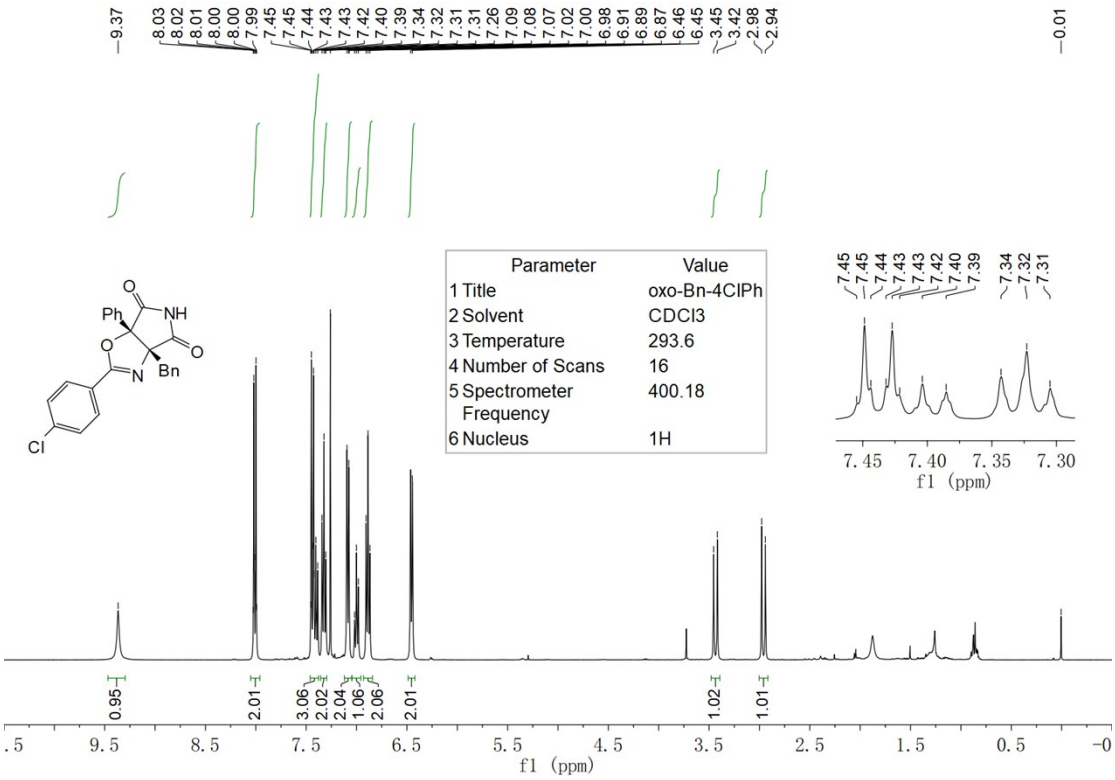
4da

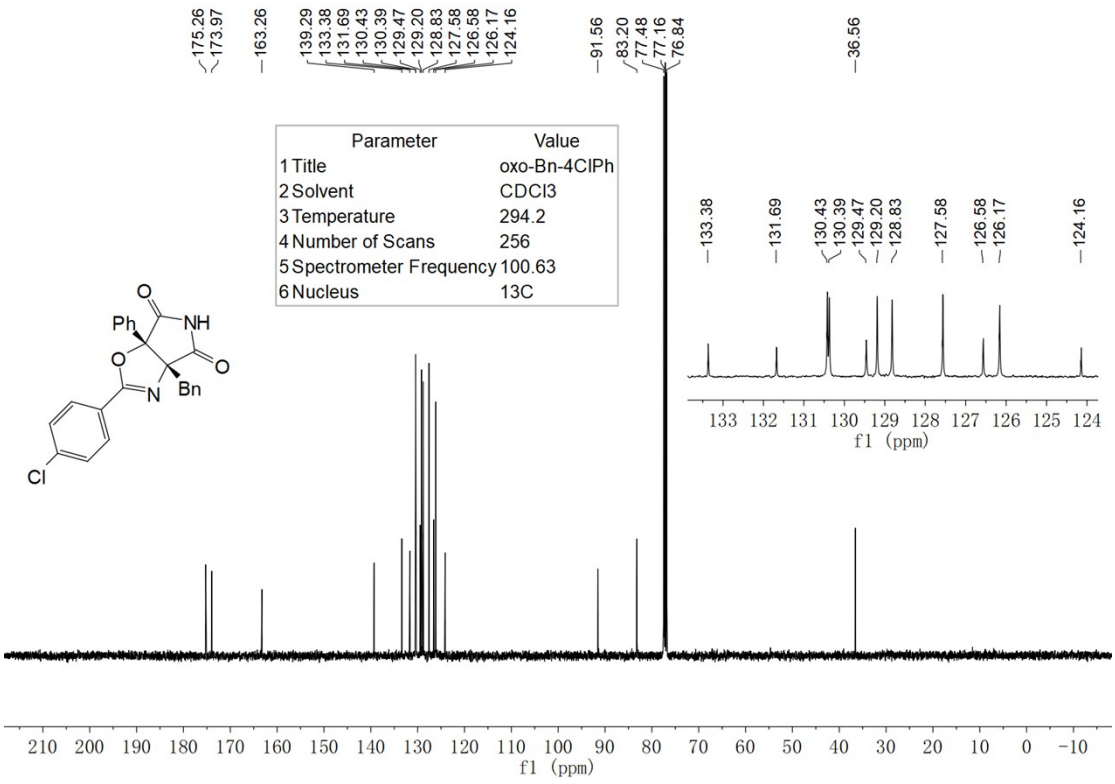

Parameter Value
1 Title C11771
2 Solvent CDCl3
3 Temperature 293.4
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)


Parameter Value
1 Title C11771
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

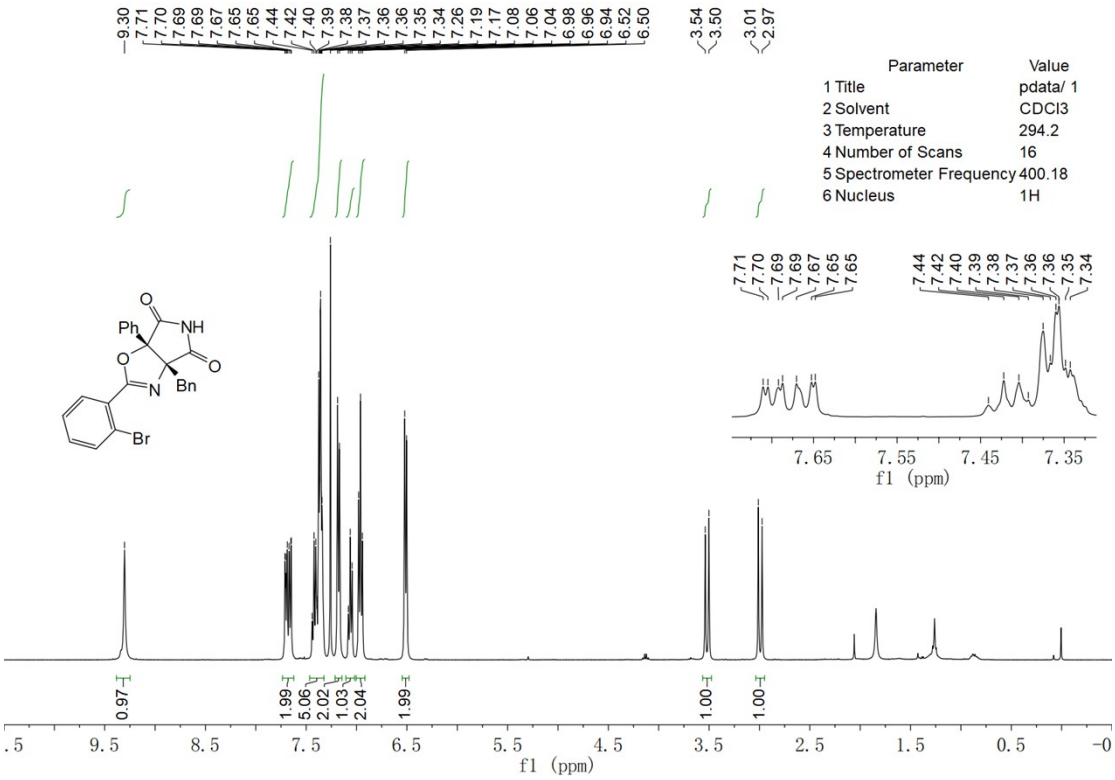

-105.27
Parameter Value
1 Title 0-11744-F
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 376.55
6 Nucleus 19F
O
NH
Ph
O
O
N
Bn
F
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

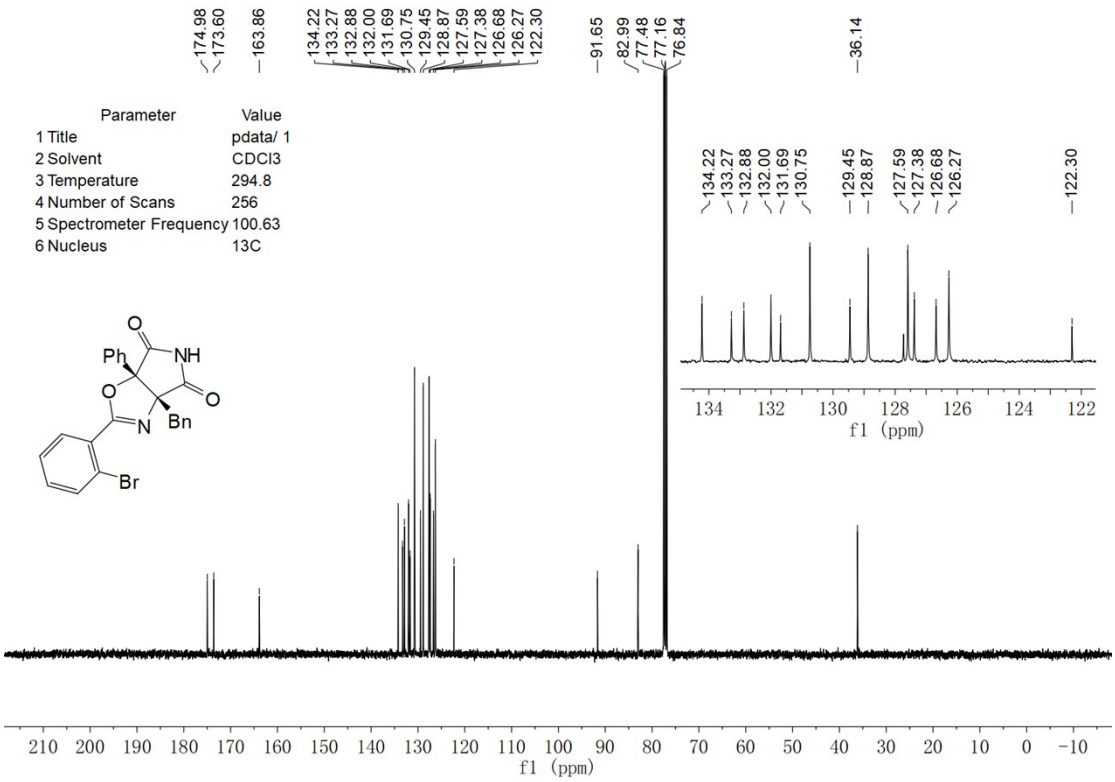
4ea


Parameter Value
1 Title oxo-Bn-4ClPh
2 Solvent CDCl3
3 Temperature 293.6
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

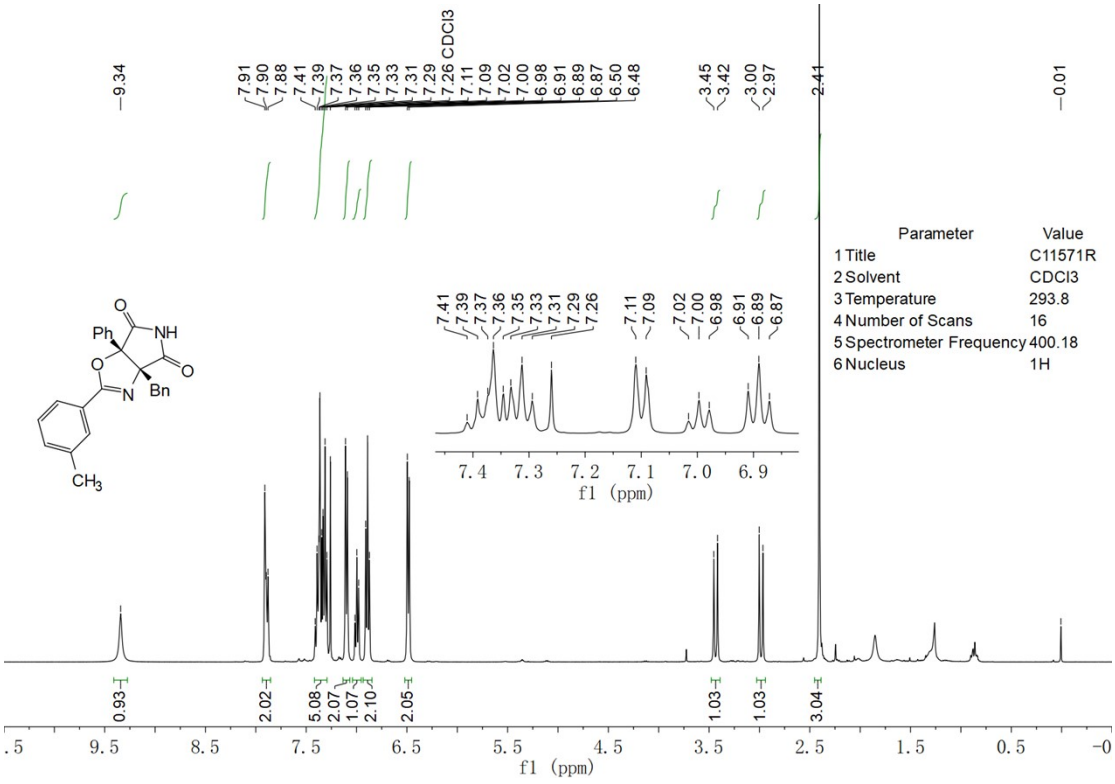

Parameter Value
1 Title oxo-Bn-4ClPh
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

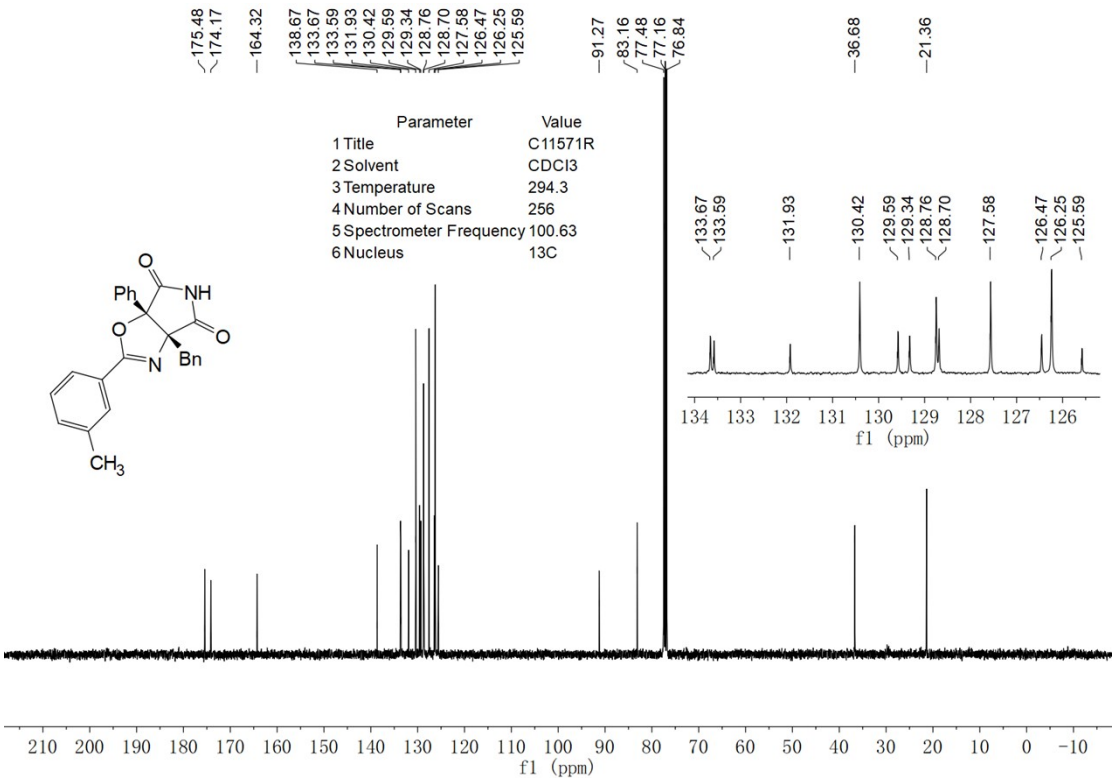
4fa


9.30 7.71 7.70 7.69 7.69 7.67 7.65 7.65 7.44 7.42 7.40 7.39 7.38 7.37 7.36 7.36 7.35 7.34 7.26 7.19 7.17 7.08 7.06 7.04 6.98 6.96 6.94 6.52 6.50
3.54 3.50 3.01 2.97
Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
O NH O Ph O N Bn Br
0.97 1.99 5.06 2.02 1.03 2.04 1.99 1.00 1.00
f1 (ppm)

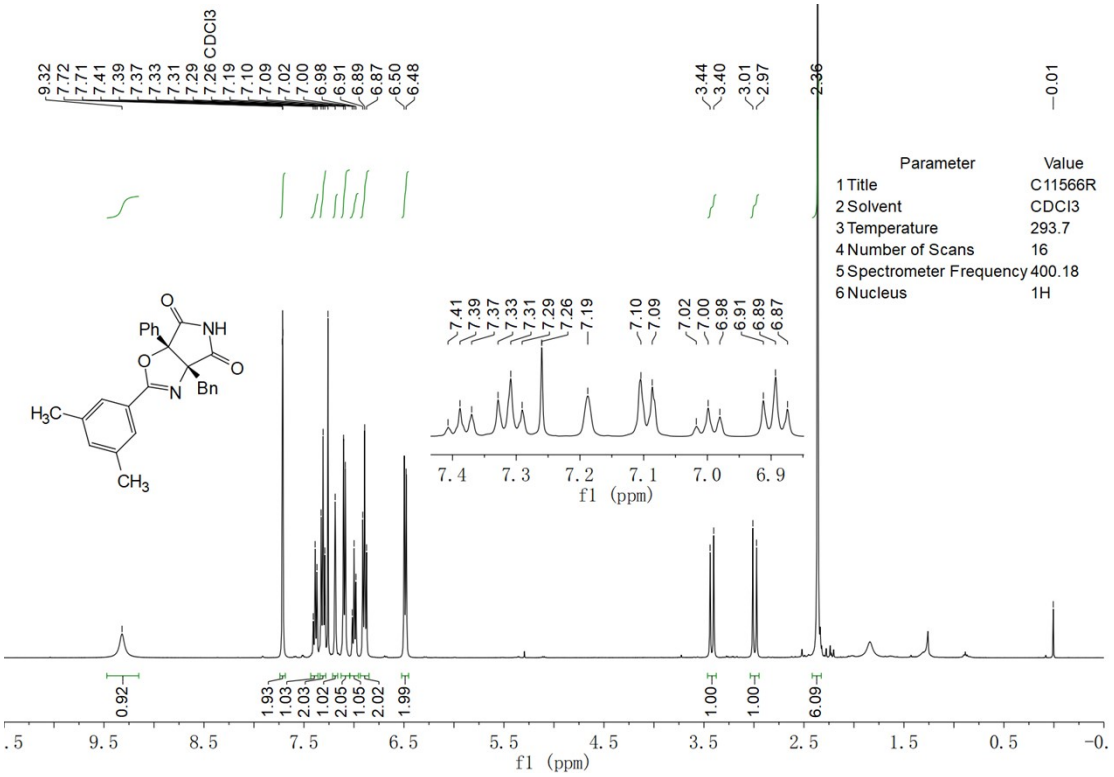

174.98 173.60 163.86 134.22 133.27 132.88 132.00 131.69 130.75 129.45 128.87 127.59 127.38 126.68 126.27 122.30 91.65 82.99 77.48 77.16 76.84 36.14
Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 294.8
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
O NH O Ph O N Bn Br
f1 (ppm)

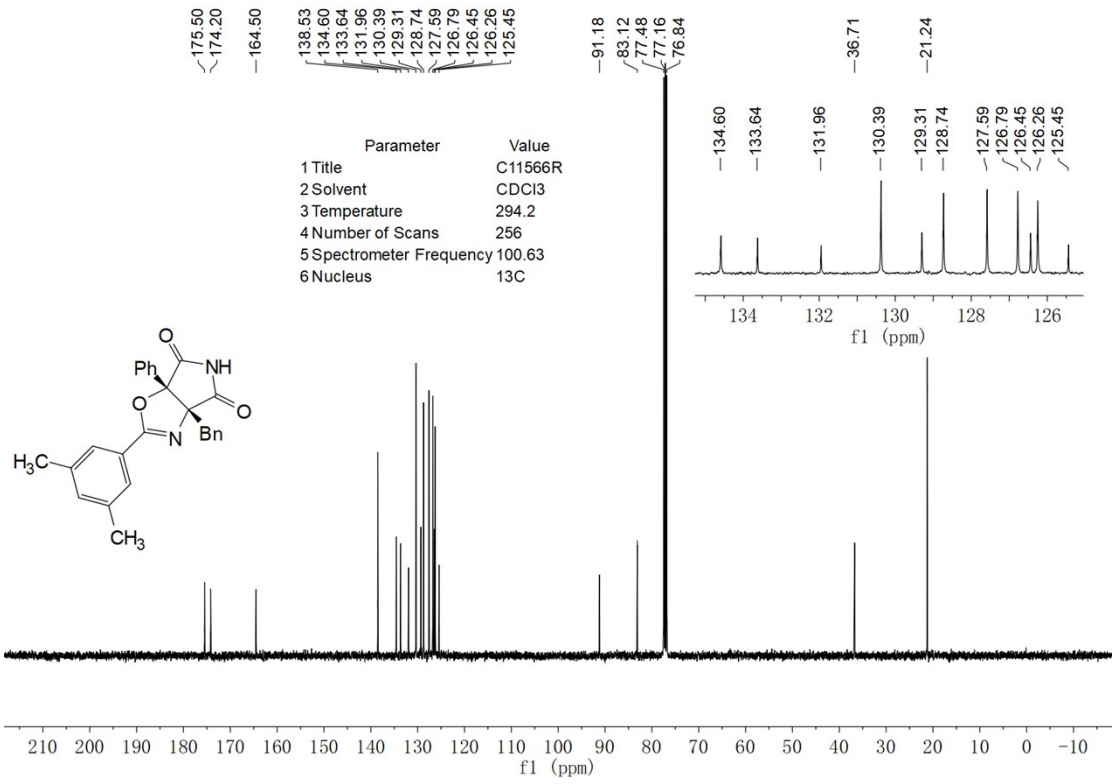
4ga


9.34
7.91
7.90
7.88
7.41
7.39
7.37
7.36
7.35
7.33
7.31
7.29
7.26 CDCl3
7.11
7.09
7.02
7.00
6.98
6.91
6.89
6.87
6.50
6.48
3.45
3.42
3.00
2.97
2.41
0.01
Parameter Value
1 Title C11571R
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph
NH
O
O
N
Bn
CH3
f1 (ppm)
0.93
2.02
5.08
2.07
1.07
2.10
2.05
1.03
1.03
3.04

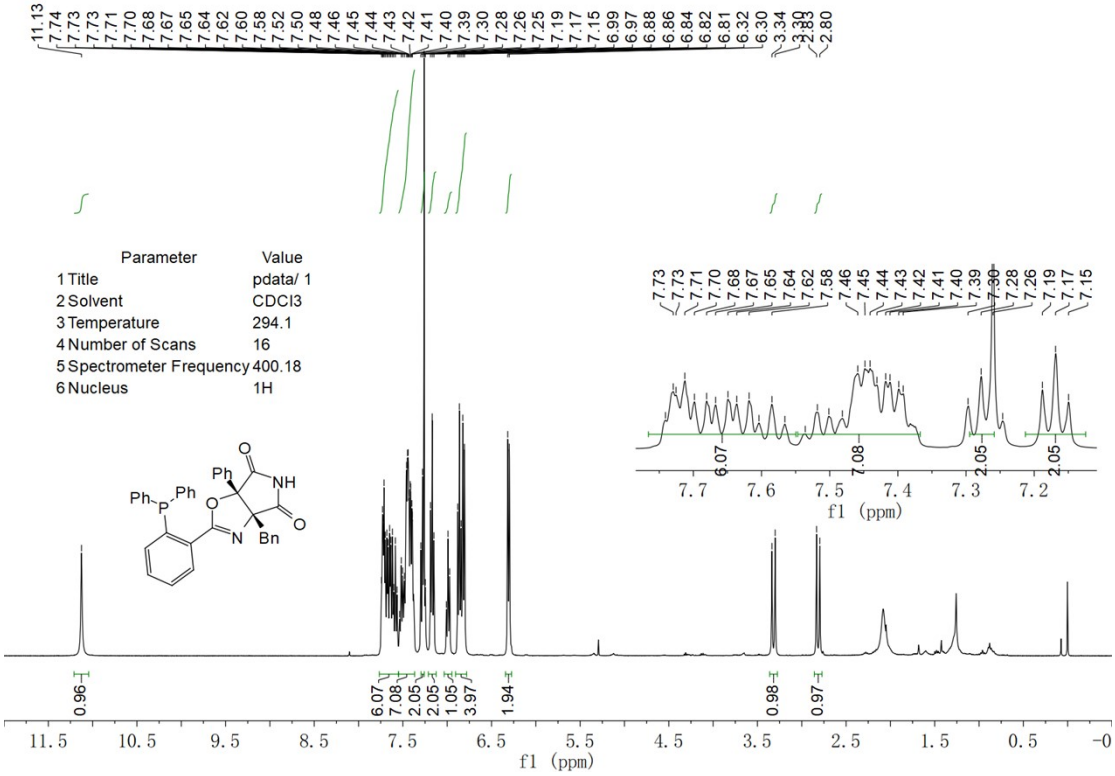

175.48
174.17
164.32
138.67
133.67
133.59
131.93
130.42
129.59
129.34
128.76
128.70
127.58
126.47
126.25
125.59
91.27
83.16
77.48
77.16
76.84
36.68
21.36
Parameter Value
1 Title C11571R
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Ph
NH
O
O
N
Bn
CH3
f1 (ppm)

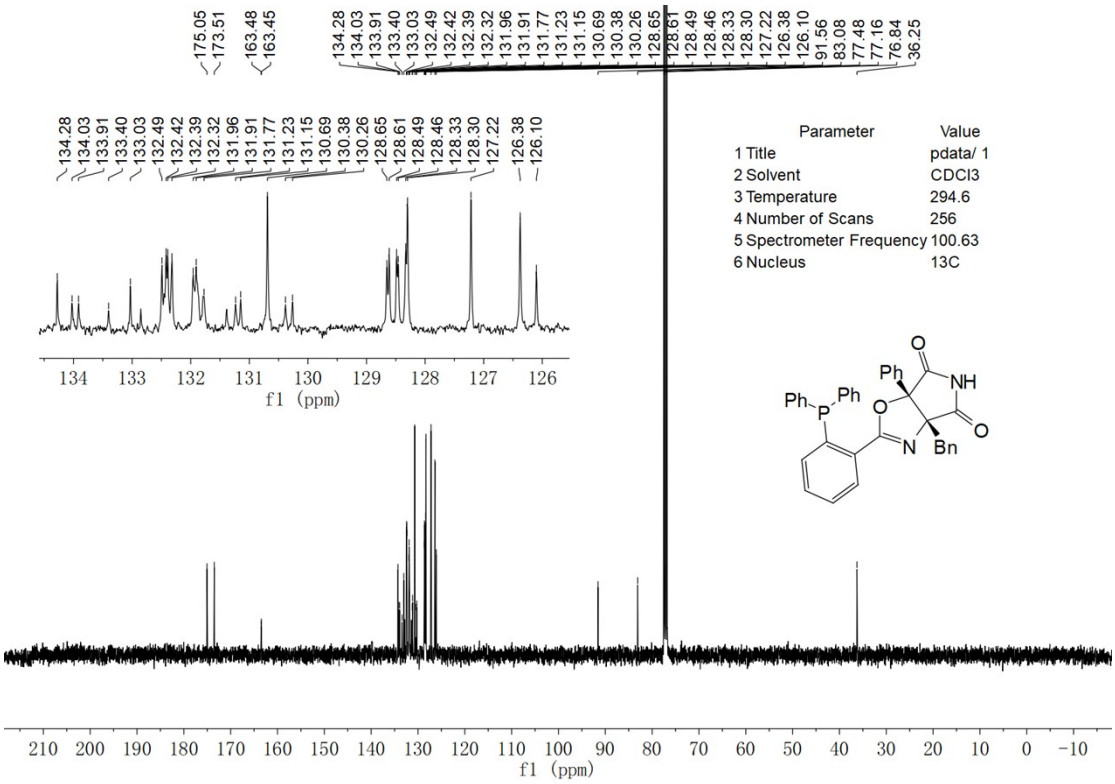
4ha

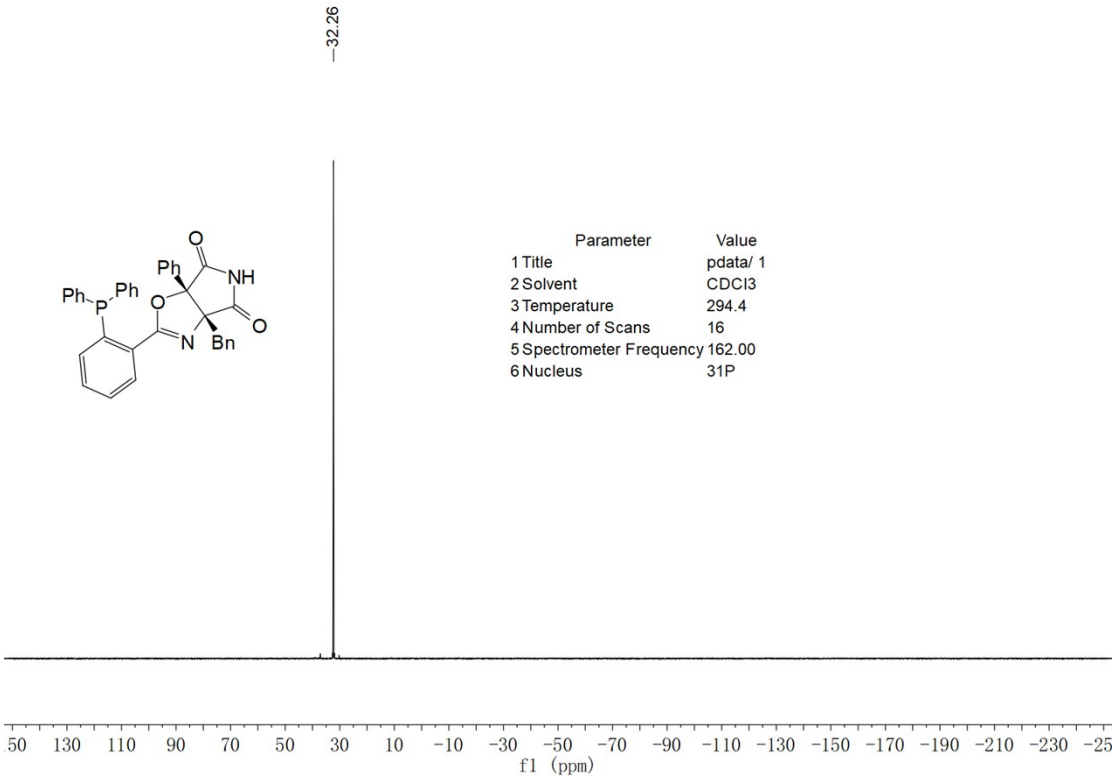

9.32 7.72 7.71 7.41 7.39 7.37 7.33 7.31 7.29 7.26 CDCl3 7.19 7.10 7.09 7.02 7.00 6.98 6.91 6.89 6.87 6.50 6.48
3.44 3.40 3.01 2.97 2.36 0.01
Parameter Value
1 Title C11566R
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph NH O N Bn H3C CH3
7.41 7.39 7.37 7.33 7.31 7.29 7.26 7.19 7.10 7.09 7.02 7.00 6.98 6.91 6.89 6.87
7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
0.92 1.93 1.03 2.03 1.02 2.05 1.05 2.02 1.99 1.00 1.00 6.09
.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.
f1 (ppm)


175.50 174.20 164.50 138.53 134.60 133.64 131.96 130.39 129.31 128.74 127.59 126.79 126.45 126.26 125.45
91.18 83.12 77.48 77.16 76.84
36.71 21.24
Parameter Value
1 Title C11566R
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
134.60 133.64 131.96 130.39 129.31 128.74 127.59 126.79 126.45 126.26 125.45
134 132 130 128 126
f1 (ppm)
Ph NH O N Bn H3C CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

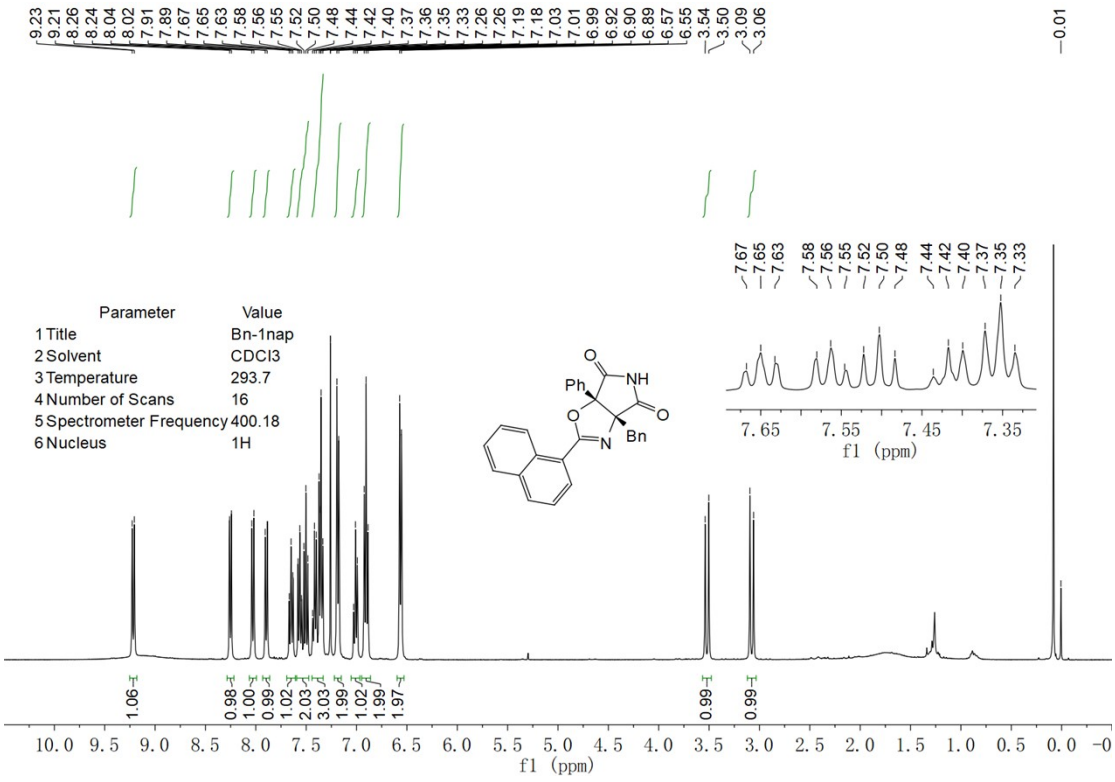
4ia

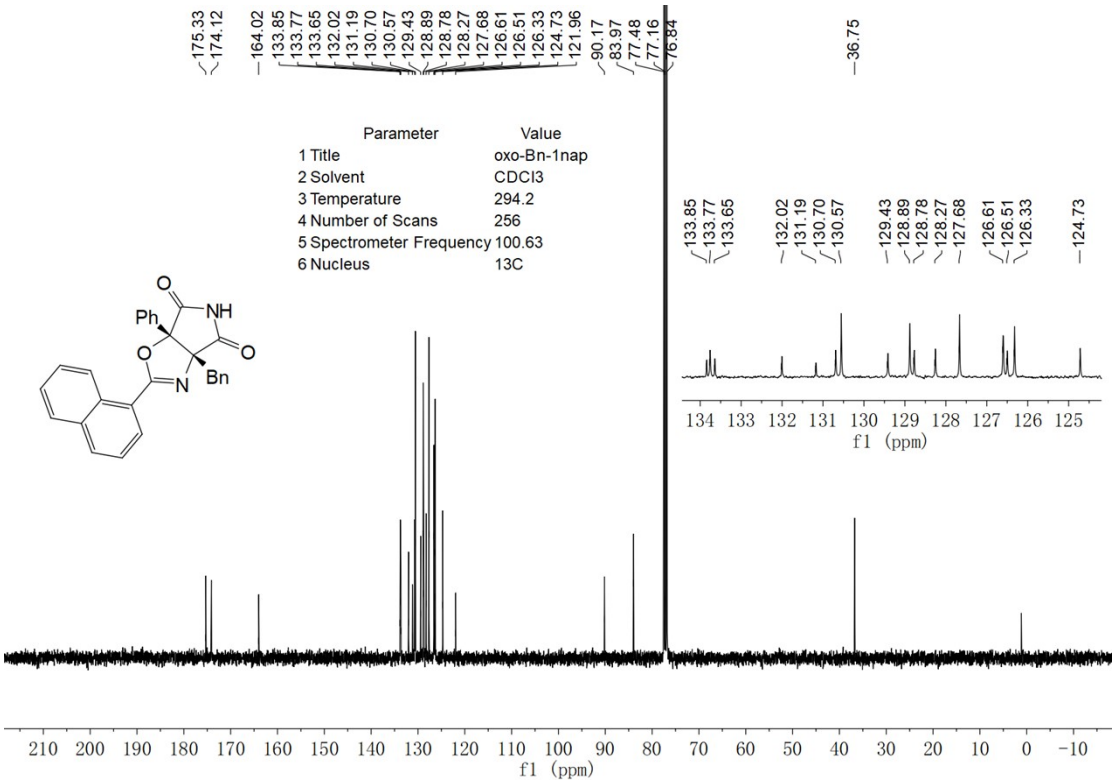

Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 294.1
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)


Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 294.6
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

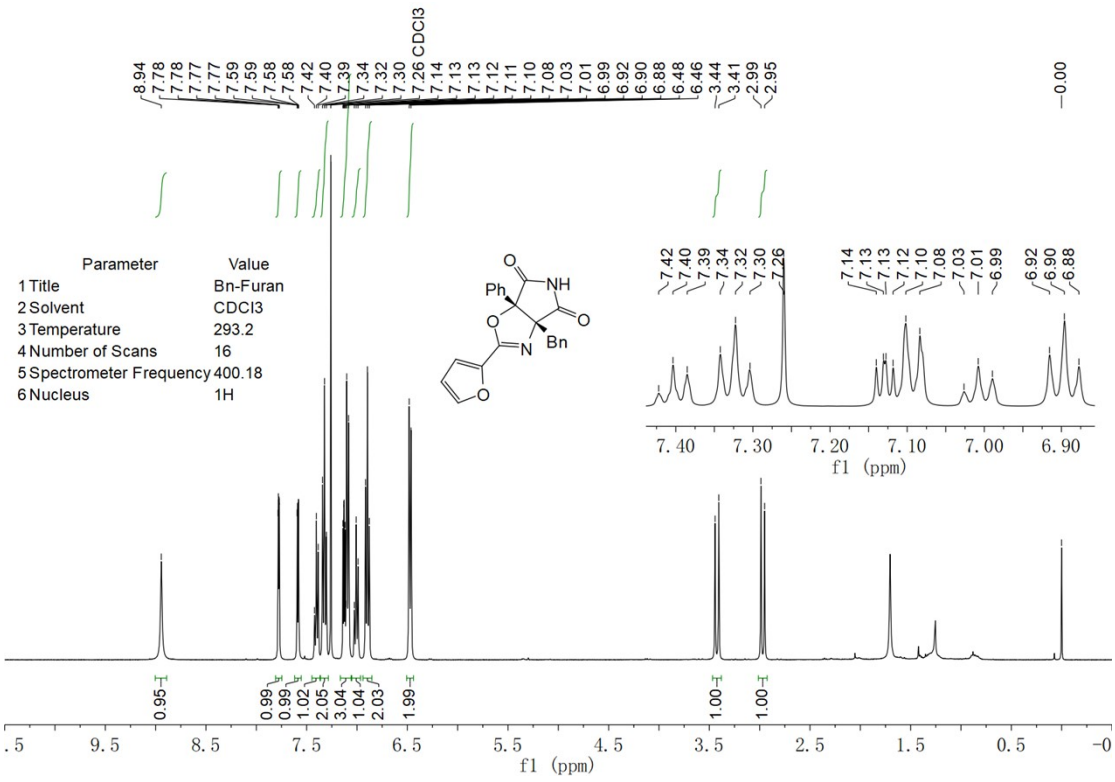

32.26
Ph
Ph
P
O
Ph
NH
O
N
Bn
O
Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 294.4
4 Number of Scans 16
5 Spectrometer Frequency 162.00
6 Nucleus 31P
50 130 110 90 70 50 30 10 −10 −30 −50 −70 −90 −110 −130 −150 −170 −190 −210 −230 −25
f1 (ppm)

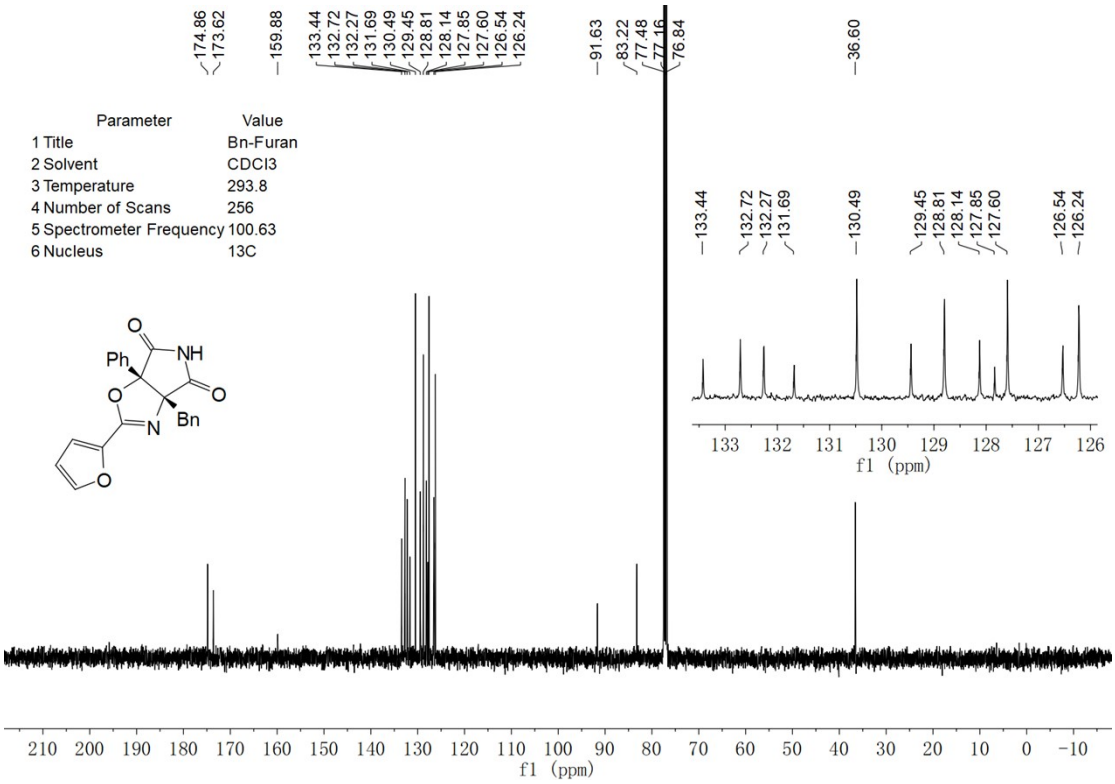
4ja


Parameter Value
1 Title Bn-1nap
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

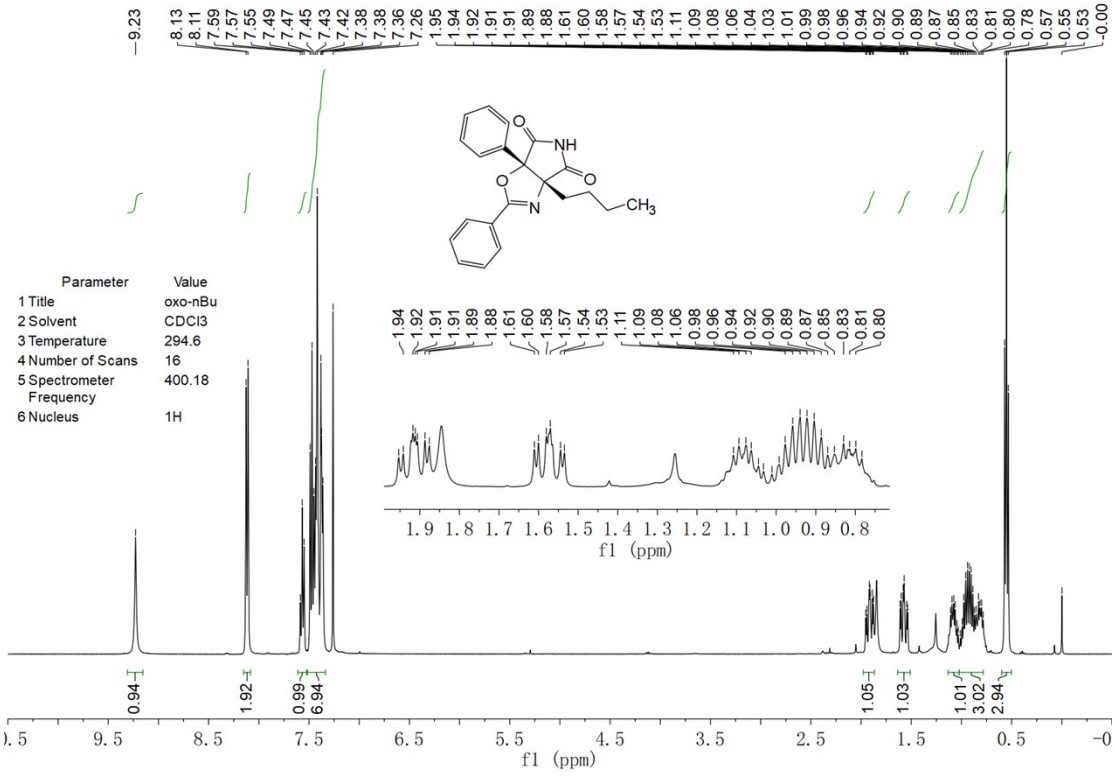

Parameter Value
1 Title oxo-Bn-1nap
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

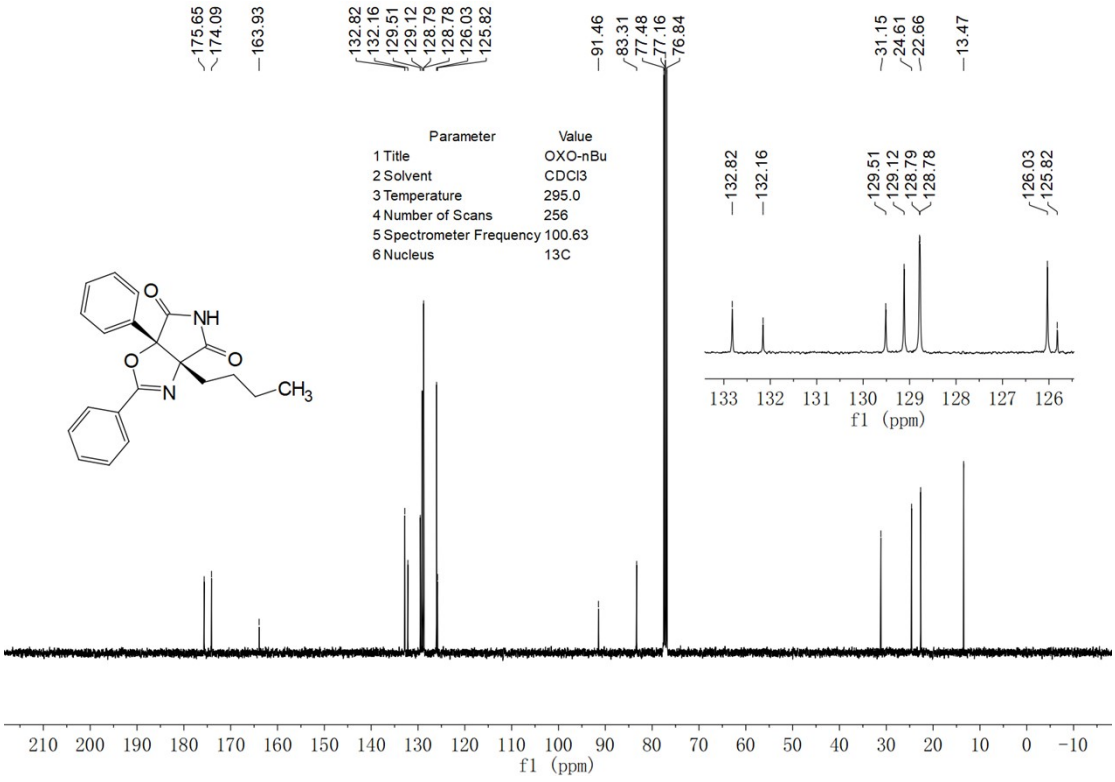
4ka


Parameter Value
1 Title Bn-Furan
2 Solvent CDCl3
3 Temperature 293.2
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

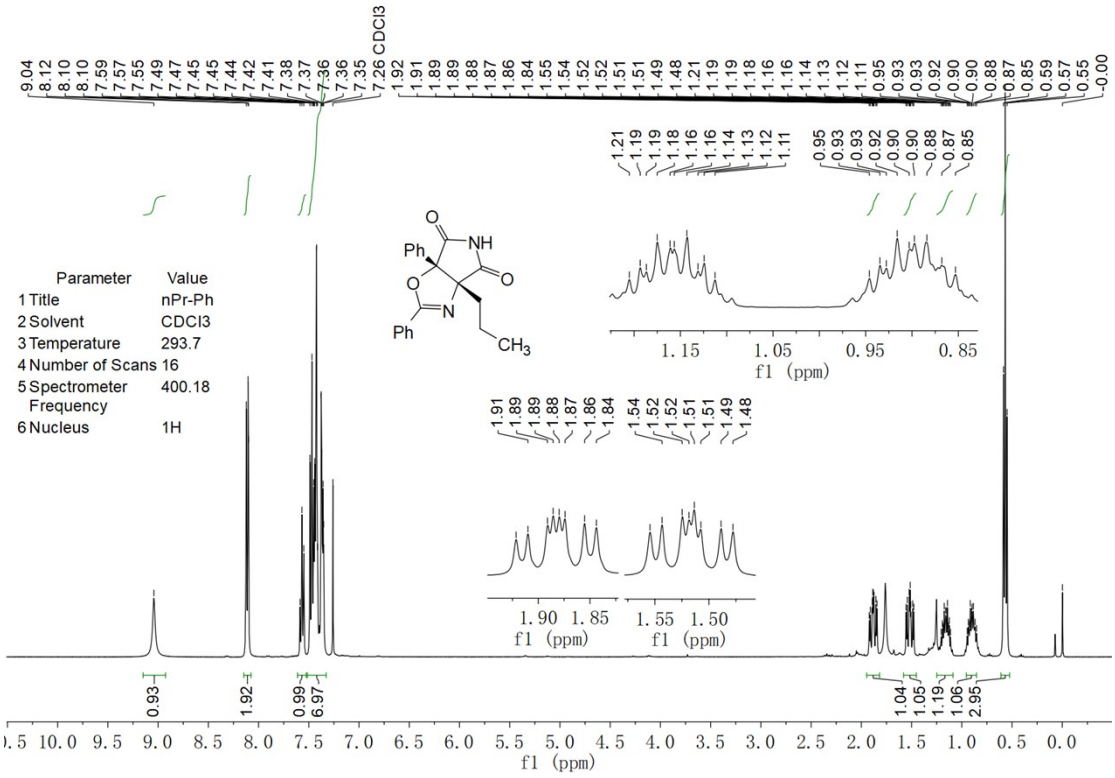

Parameter Value
1 Title Bn-Furan
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

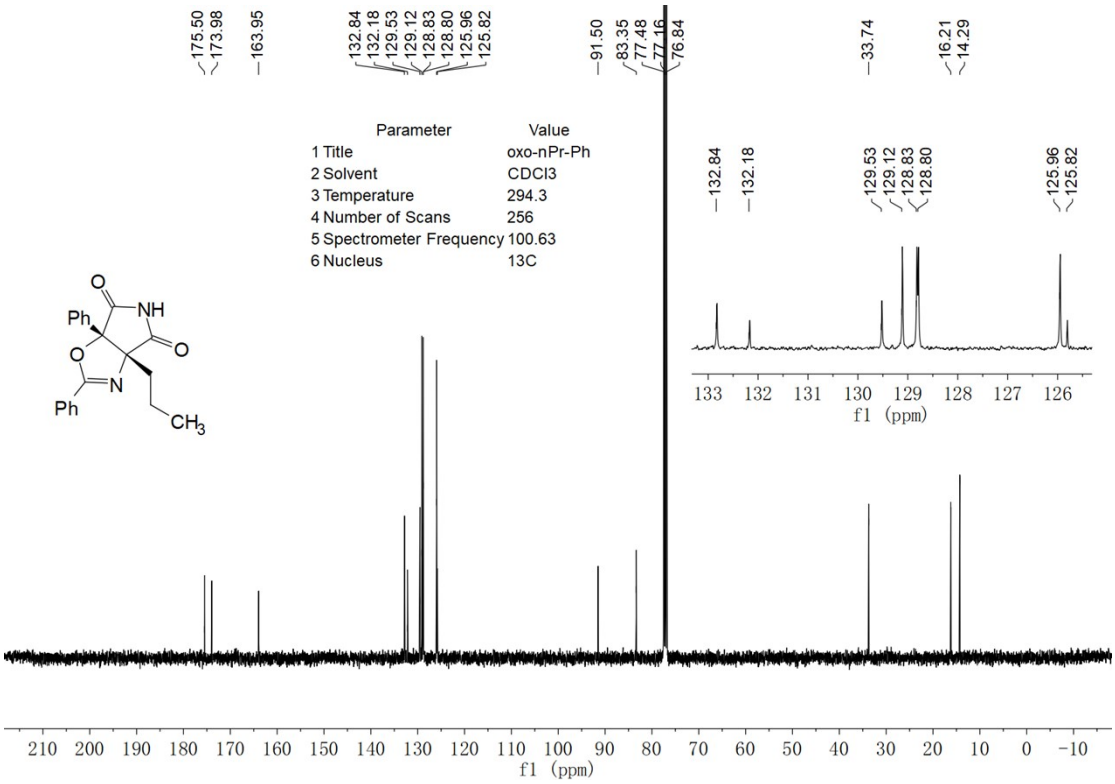
4la


Parameter Value
1 Title oxo-nBu
2 Solvent CDCl3
3 Temperature 294.6
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

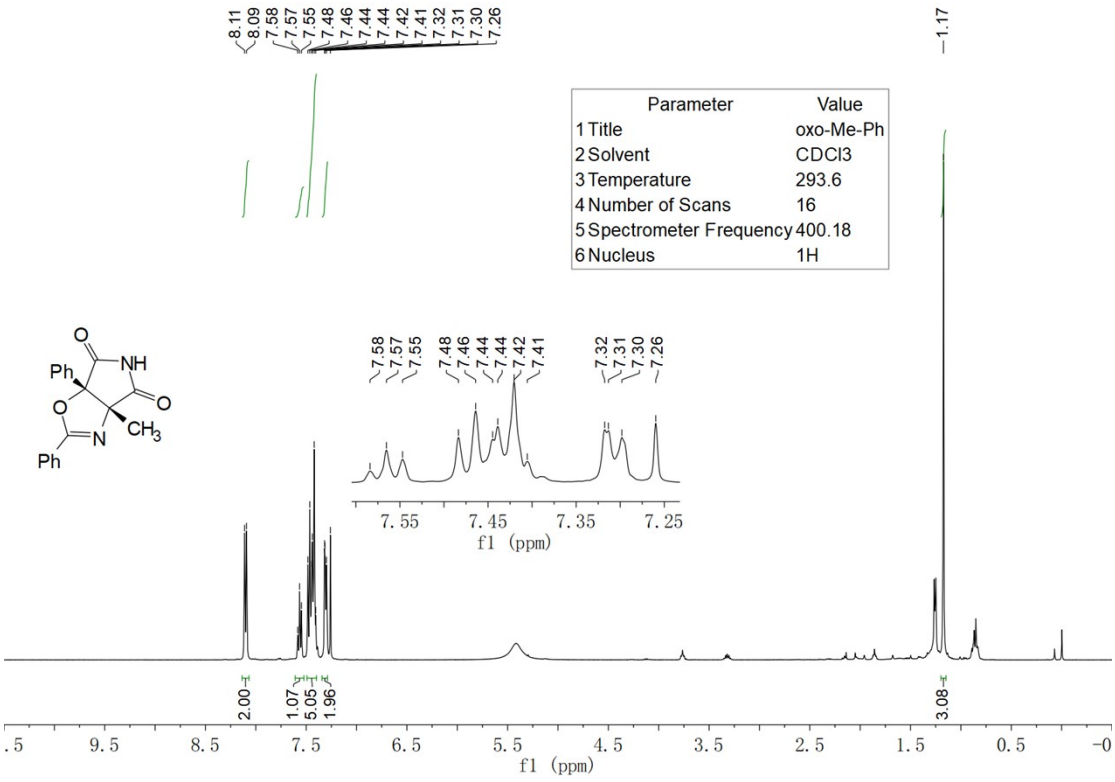

Parameter Value
1 Title OXO-nBu
2 Solvent CDCl3
3 Temperature 295.0
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

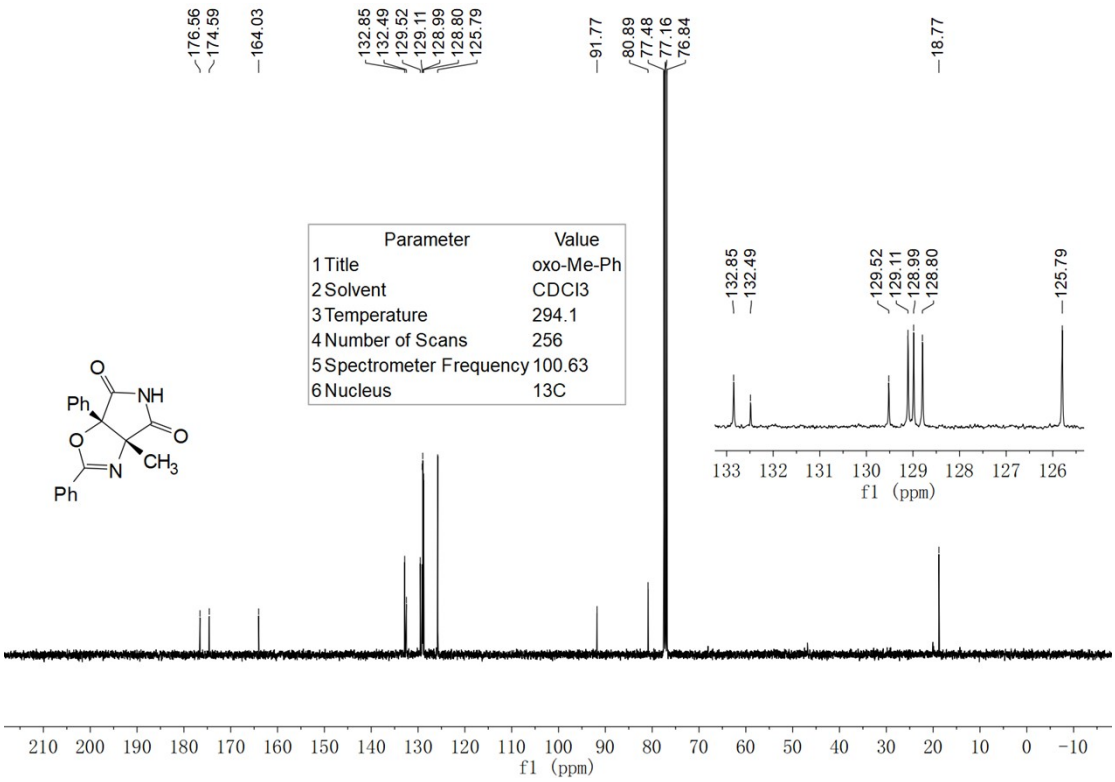
4ma


Parameter Value
1 Title nPr-Ph
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

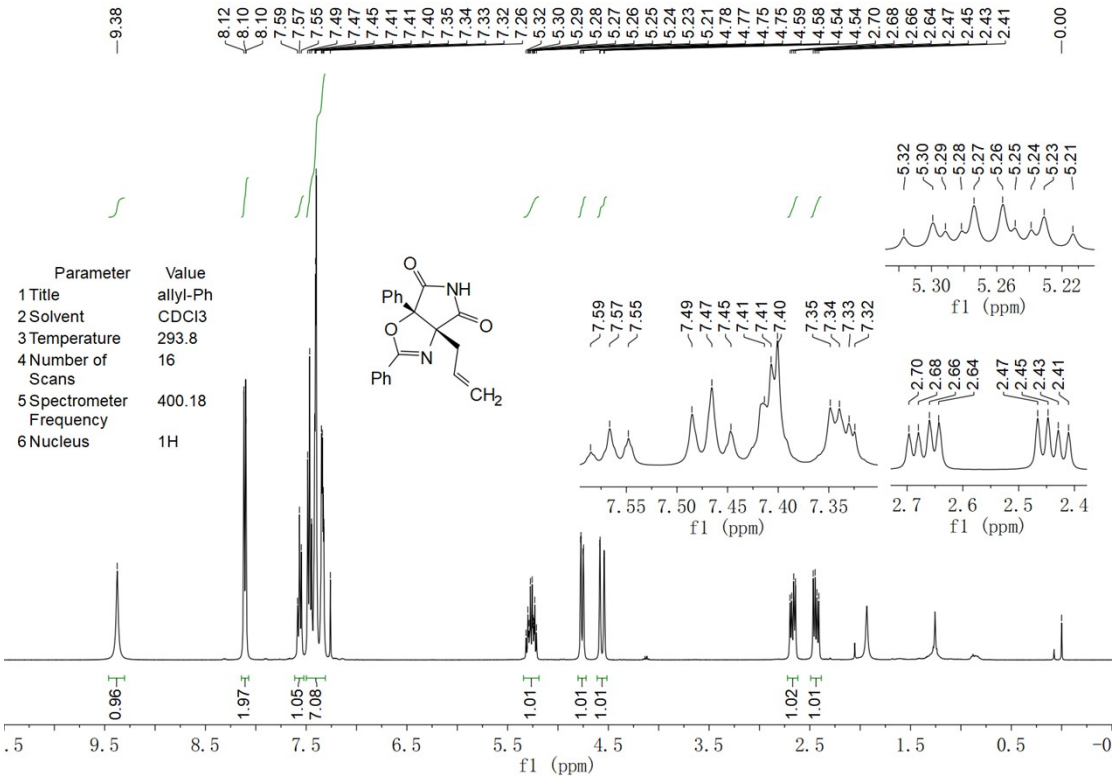

Parameter Value
1 Title oxo-nPr-Ph
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

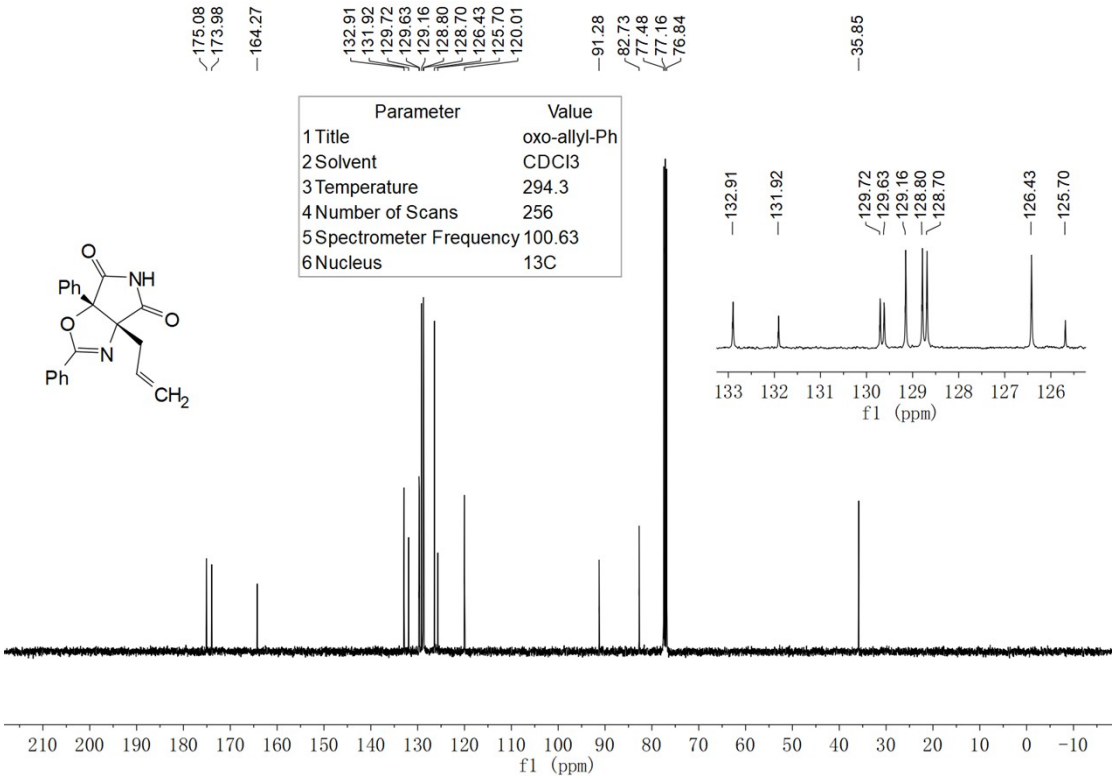
4na


8.11
8.09
7.58
7.57
7.55
7.48
7.46
7.44
7.44
7.42
7.41
7.32
7.31
7.30
7.26
1.17
Parameter Value
1 Title oxo-Me-Ph
2 Solvent CDCl3
3 Temperature 293.6
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph
NH
O
O
O
N
CH3
Ph
7.55
7.45
7.35
7.25
f1 (ppm)
2.00
1.07
5.05
1.96
3.08
f1 (ppm)

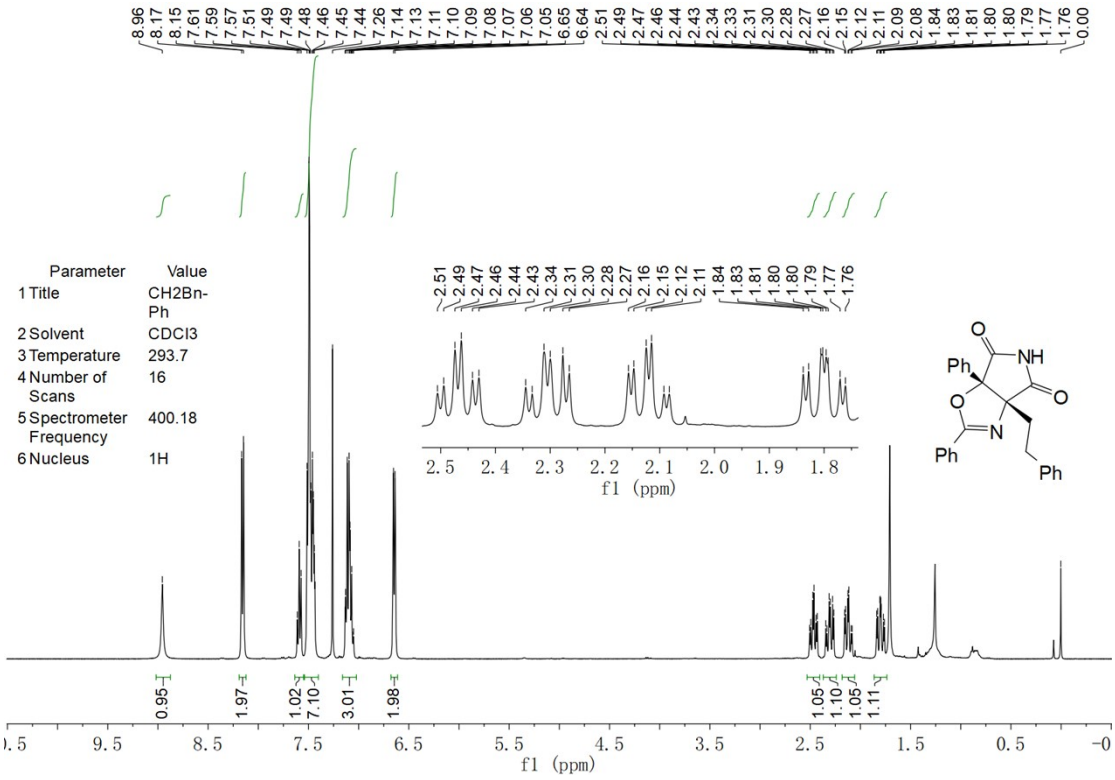

176.56
174.59
164.03
132.85
132.49
129.52
129.11
128.99
128.80
125.79
91.77
80.89
77.48
77.16
76.84
18.77
Parameter Value
1 Title oxo-Me-Ph
2 Solvent CDCl3
3 Temperature 294.1
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Ph
NH
O
O
O
N
CH3
Ph
132.85
132.49
129.52
129.11
128.99
128.80
125.79
133 132 131 130 129 128 127 126
f1 (ppm)
f1 (ppm)

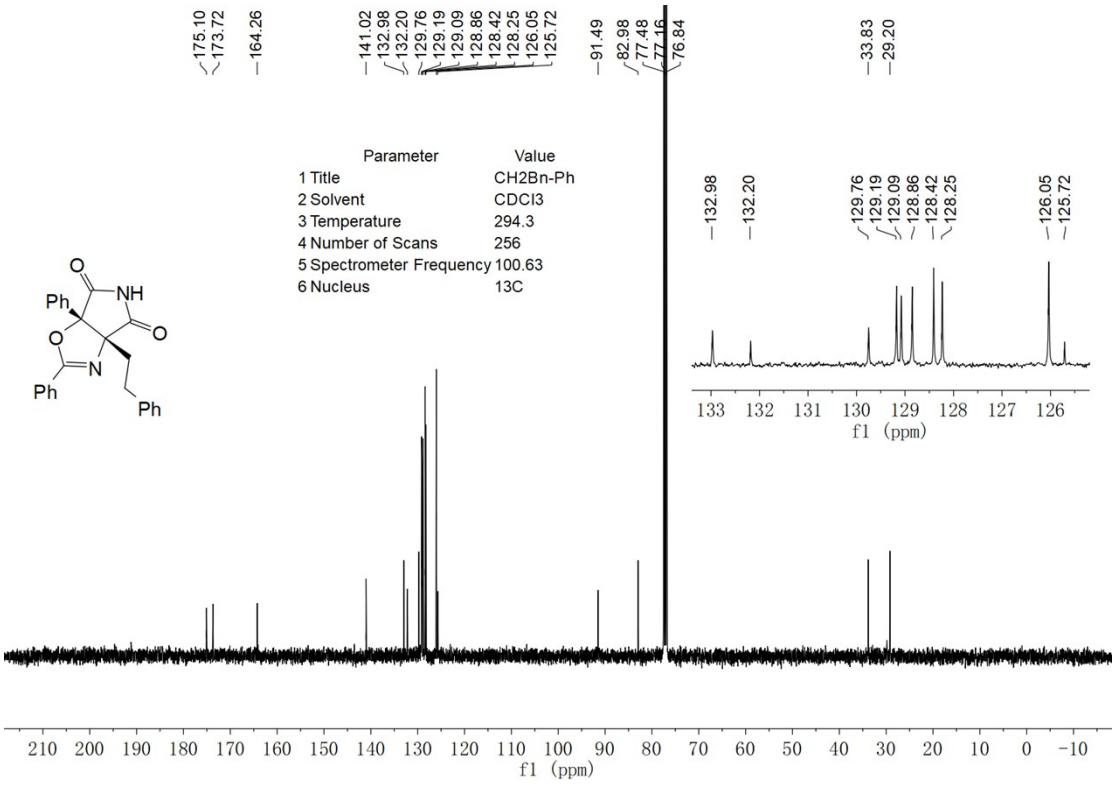
4oa


Parameter Value
1 Title allyl-Ph
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

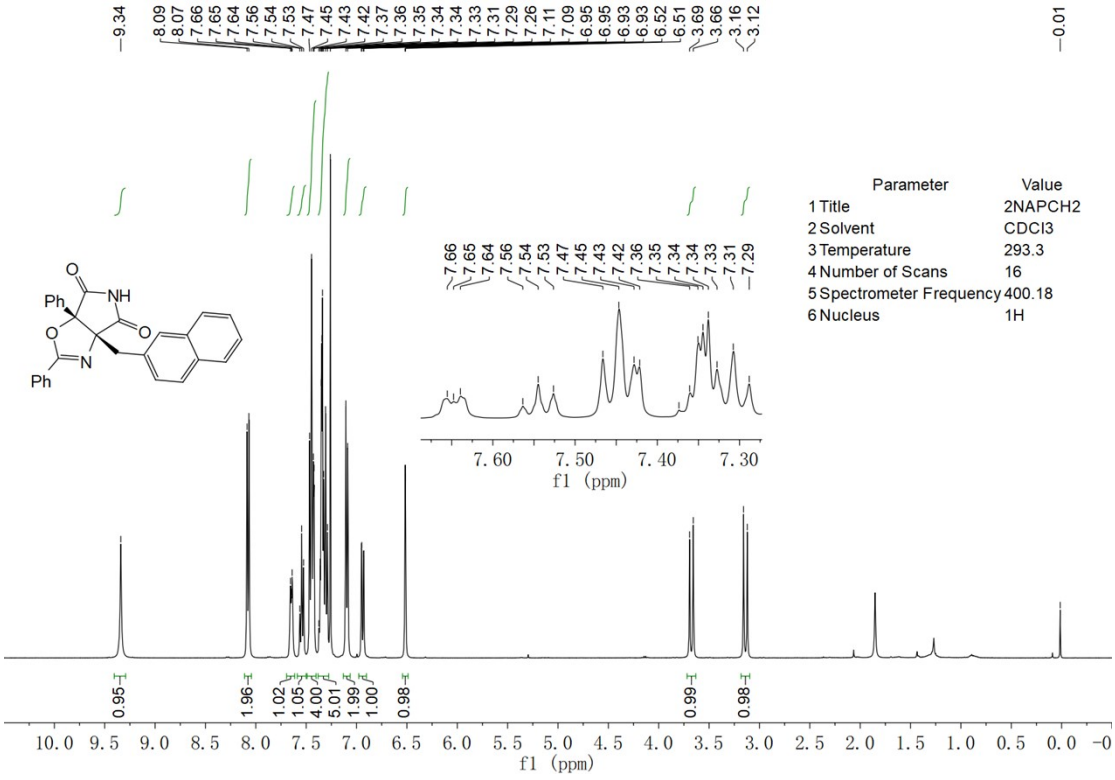

Parameter Value
1 Title oxo-allyl-Ph
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

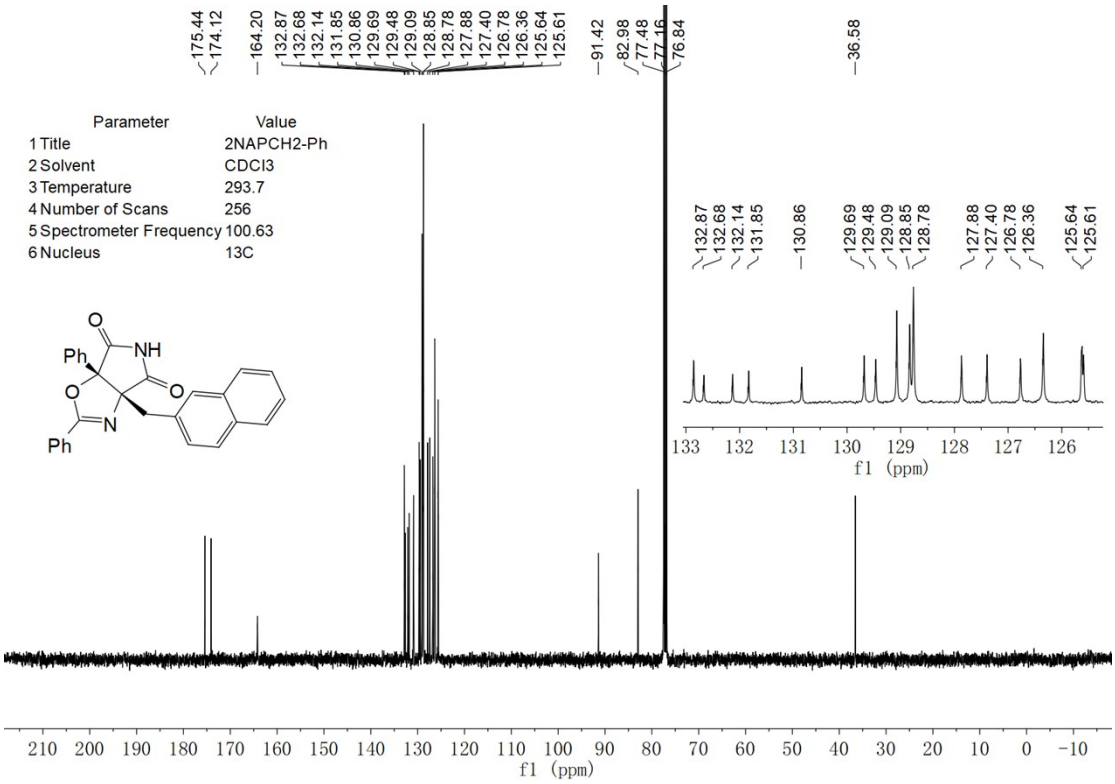
4pa


Parameter Value
1 Title CH2Bn-Ph
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)

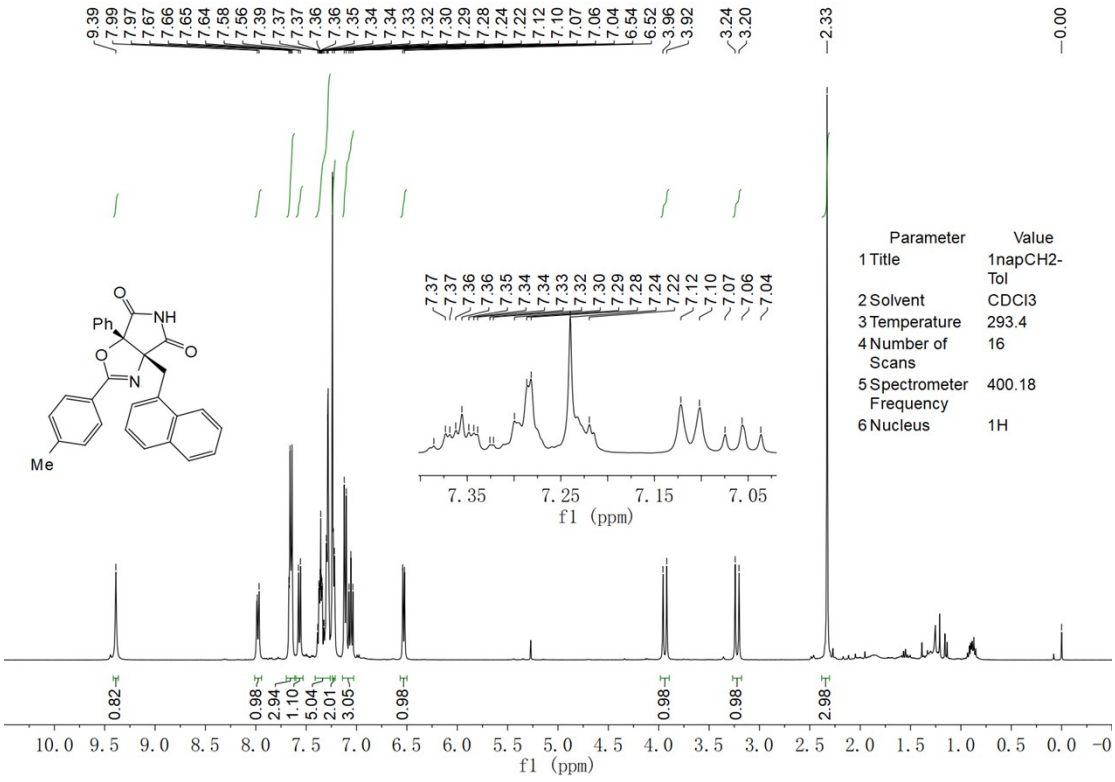

Parameter Value
1 Title CH2Bn-Ph
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

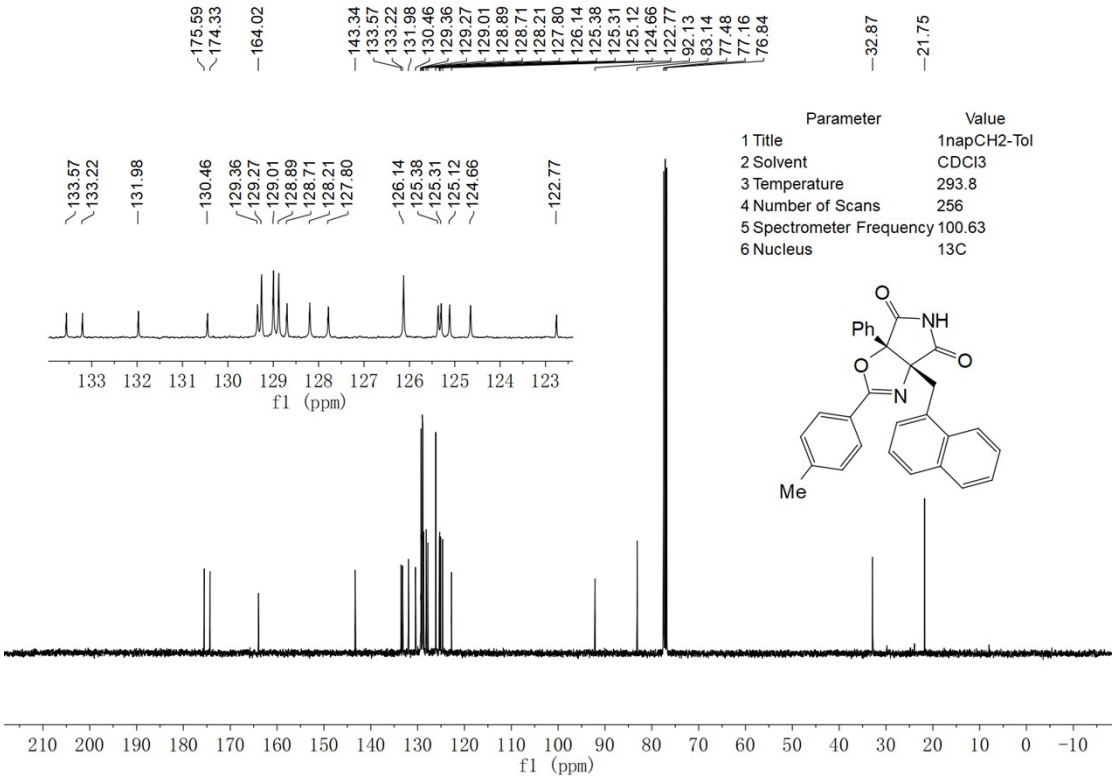
4qa


9.34
8.09
8.07
7.66
7.65
7.64
7.56
7.54
7.53
7.47
7.45
7.43
7.42
7.37
7.36
7.35
7.34
7.34
7.33
7.31
7.29
7.26
7.11
7.09
6.95
6.95
6.93
6.93
6.52
6.51
3.69
3.66
3.16
3.12
0.01
Parameter Value
1 Title 2NAPCH2
2 Solvent CDCl3
3 Temperature 293.3
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)
0.95
1.96
1.02
1.05
4.00
5.01
1.99
1.00
0.98
0.99
0.98

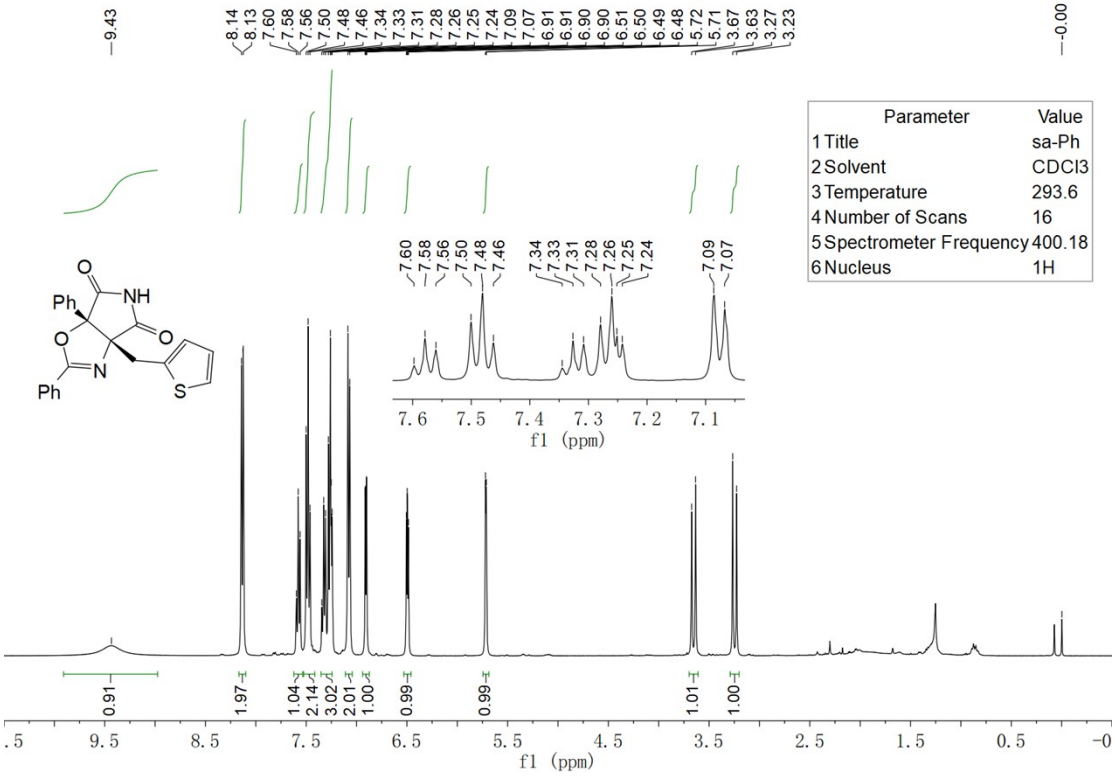

175.44
174.12
164.20
132.87
132.68
132.14
131.85
130.86
129.69
129.48
129.09
128.85
128.78
127.88
127.40
126.78
126.36
125.64
125.61
91.42
82.98
77.48
77.16
76.84
36.58
Parameter Value
1 Title 2NAPCH2-Ph
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

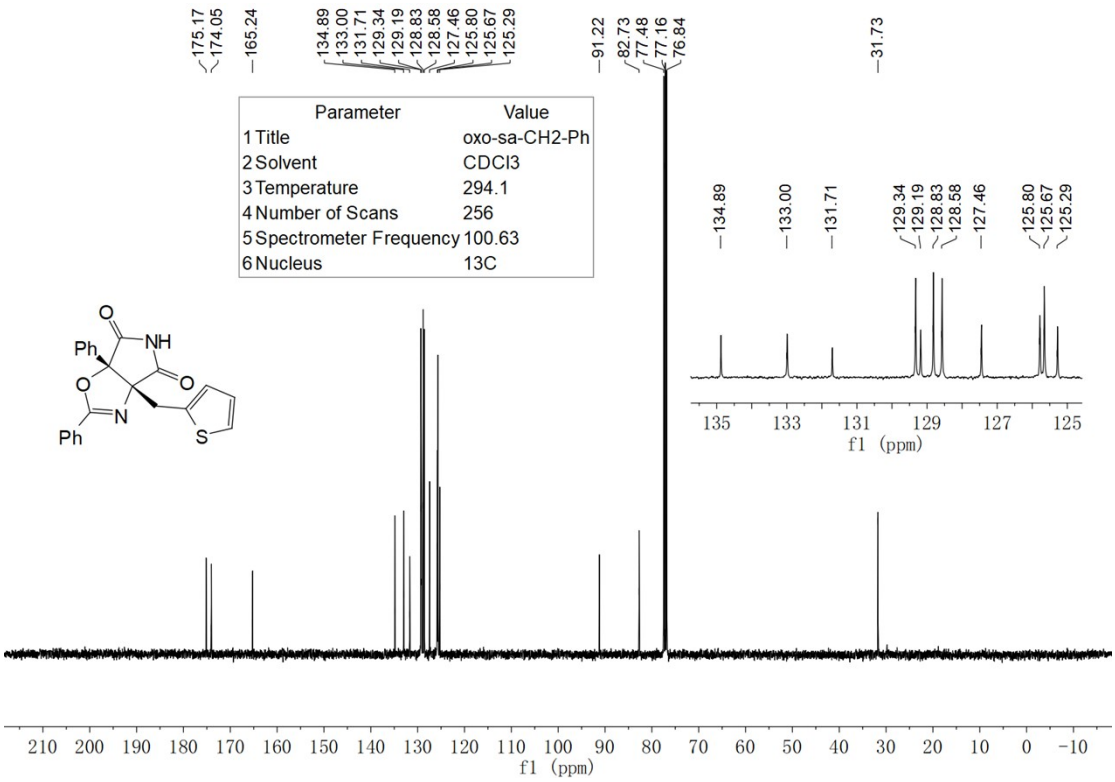
4ra


9.39 7.99 7.97 7.67 7.66 7.65 7.64 7.58 7.56 7.39 7.37 7.37 7.36 7.36 7.35 7.34 7.34 7.33 7.32 7.30 7.29 7.28 7.24 7.22 7.12 7.10 7.07 7.06 7.04 6.54 6.52 3.96 3.92 3.24 3.20 2.33 0.00
Parameter Value
1 Title 1napCH2-Tol
2 Solvent CDCl3
3 Temperature 293.4
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph NH O O N Me
7.37 7.37 7.36 7.36 7.35 7.34 7.34 7.33 7.32 7.30 7.29 7.28 7.24 7.22 7.12 7.10 7.07 7.06 7.04
7.35 7.25 7.15 7.05
f1 (ppm)
0.82 0.98 2.94 1.10 5.04 2.01 3.05 0.98 0.98 0.98 2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0
f1 (ppm)

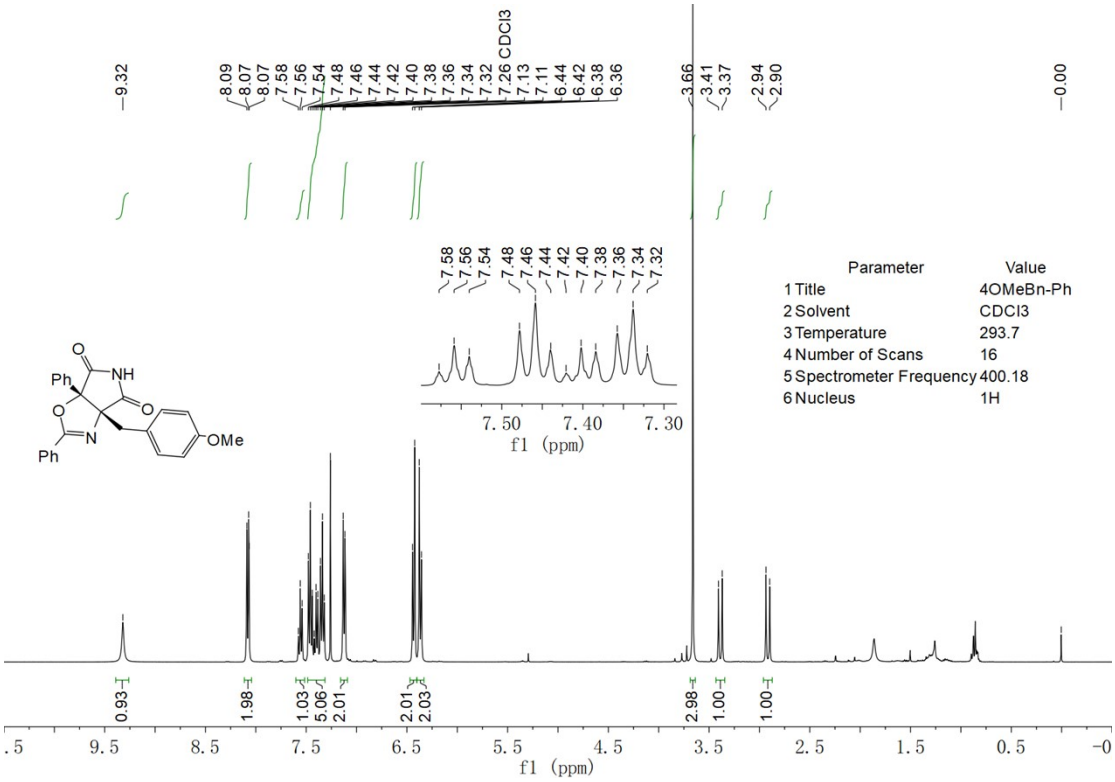

175.59 174.33 164.02 143.34 133.57 133.22 131.98 130.46 129.36 129.27 129.01 128.89 128.71 128.21 127.80 126.14 125.38 125.31 125.12 124.66 122.77 92.13 83.14 77.48 77.16 76.84 32.87 21.75
Parameter Value
1 Title 1napCH2-Tol
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Ph NH O O N Me
133 132 131 130 129 128 127 126 125 124 123
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

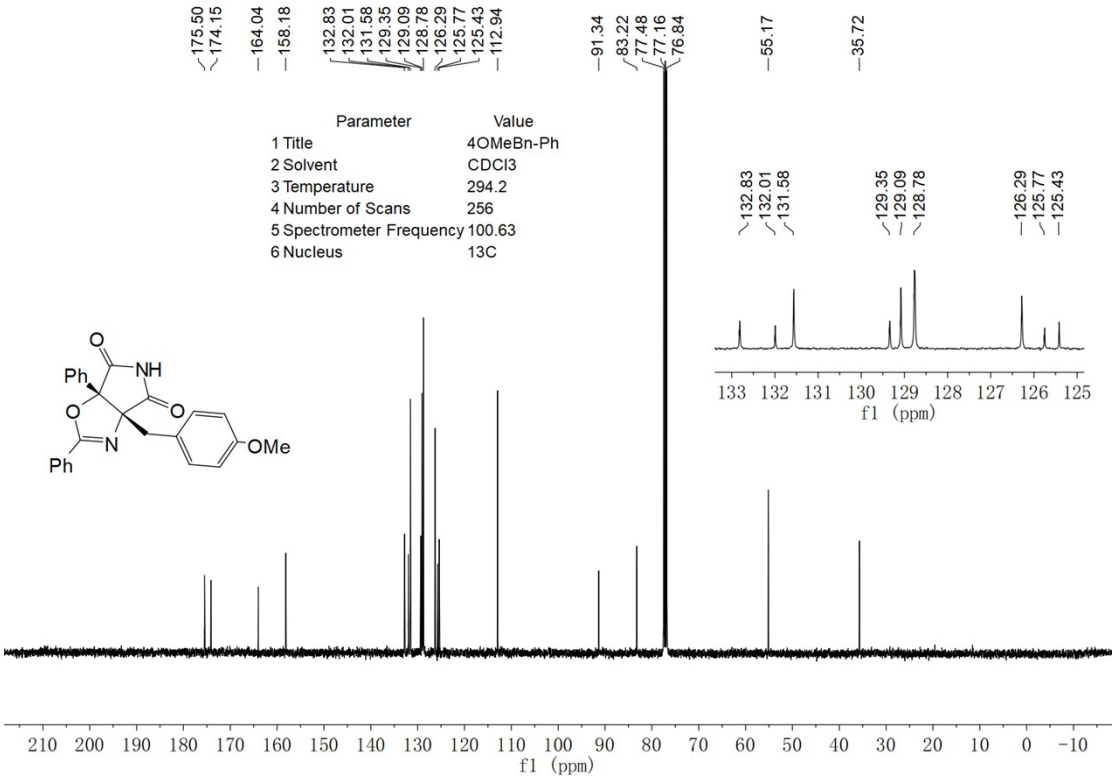
4sa


9.43
8.14
8.13
7.60
7.58
7.56
7.50
7.48
7.46
7.34
7.33
7.31
7.28
7.26
7.25
7.24
7.09
7.07
6.91
6.91
6.90
6.90
6.51
6.50
6.49
6.48
5.72
5.71
3.67
3.63
3.27
3.23
0.00
Parameter Value
1 Title sa-Ph
2 Solvent CDCl3
3 Temperature 293.6
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph
NH
O
O
O
N
Ph
S
f1 (ppm)
0.91
1.97
1.04
2.14
3.02
2.01
1.00
0.99
0.99
1.01
1.00

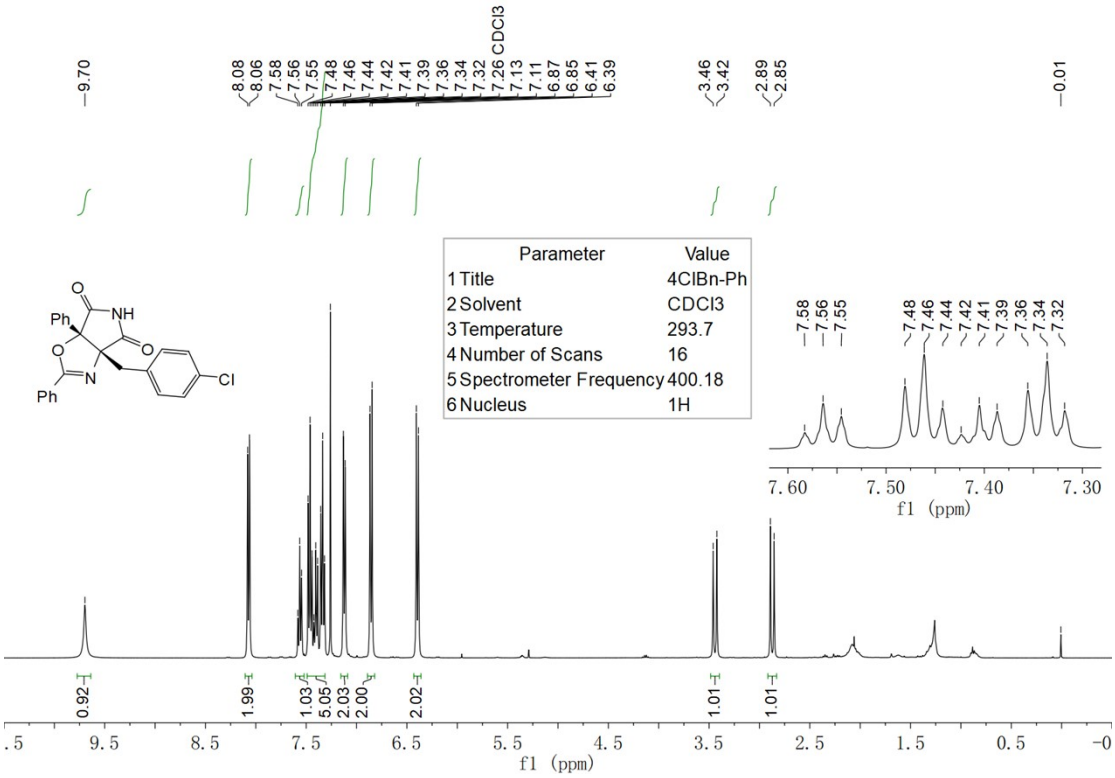

175.17
174.05
165.24
134.89
133.00
131.71
129.34
129.19
128.83
128.58
127.46
125.80
125.67
125.29
91.22
82.73
77.48
77.16
76.84
31.73
Parameter Value
1 Title oxo-sa-CH2-Ph
2 Solvent CDCl3
3 Temperature 294.1
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Ph
NH
O
O
O
N
Ph
S
f1 (ppm)

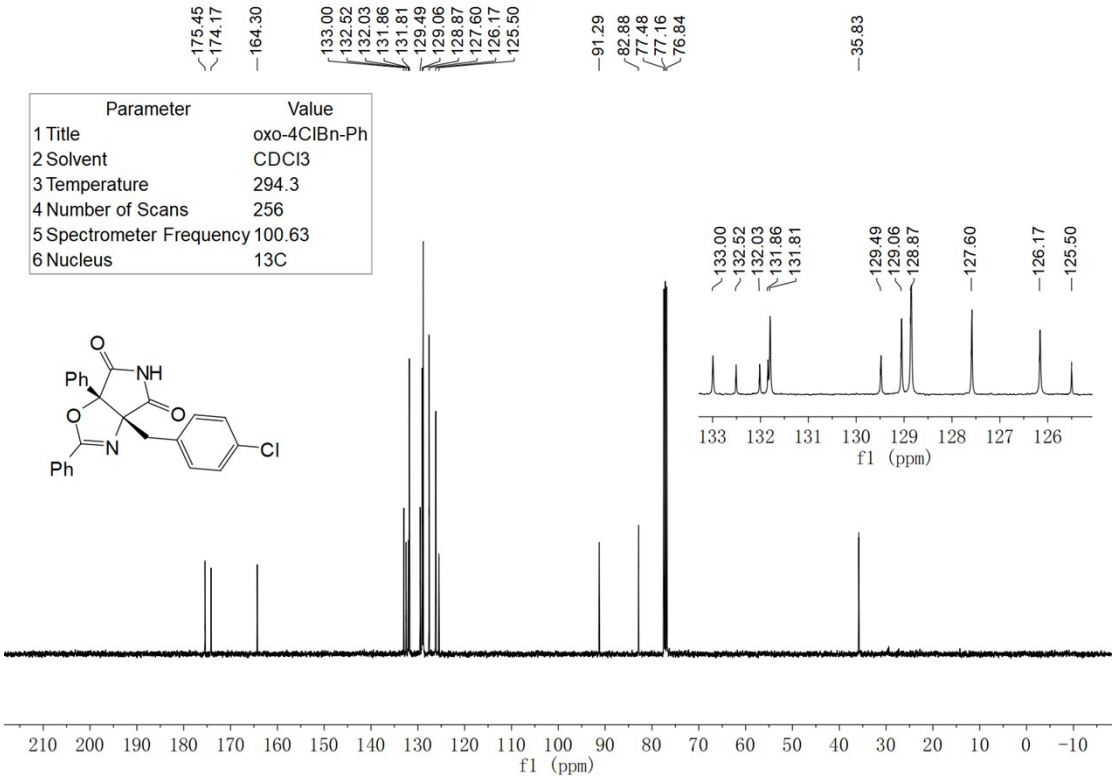
4ta


9.32
8.09
8.07
8.07
7.58
7.56
7.54
7.48
7.46
7.44
7.42
7.40
7.38
7.36
7.34
7.32
7.26 CDCl3
7.13
7.11
6.44
6.42
6.38
6.36
3.66
3.41
3.37
2.94
2.90
0.00
Parameter Value
1 Title 4OMeBn-Ph
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)
0.93
1.98
1.03
5.06
2.01
2.01
2.03
2.98
1.00
1.00

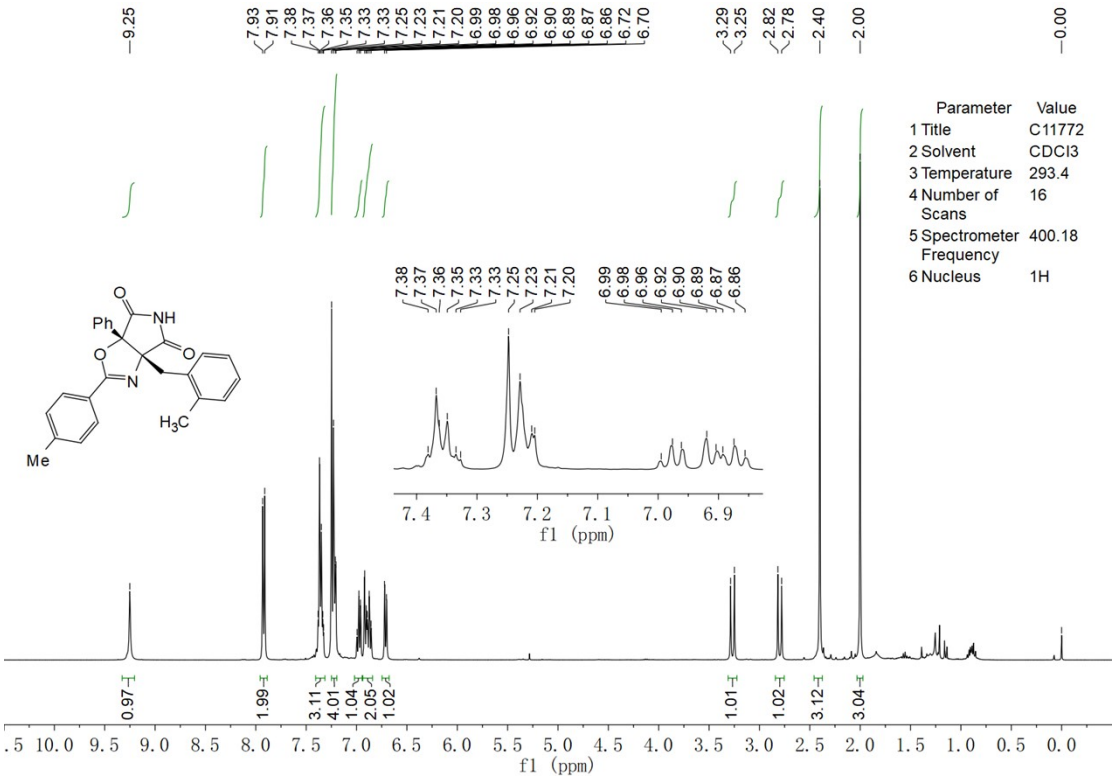

175.50
174.15
164.04
158.18
132.83
132.01
131.58
129.35
129.09
128.78
126.29
125.77
125.43
112.94
91.34
83.22
77.48
77.16
76.84
55.17
35.72
Parameter Value
1 Title 4OMeBn-Ph
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

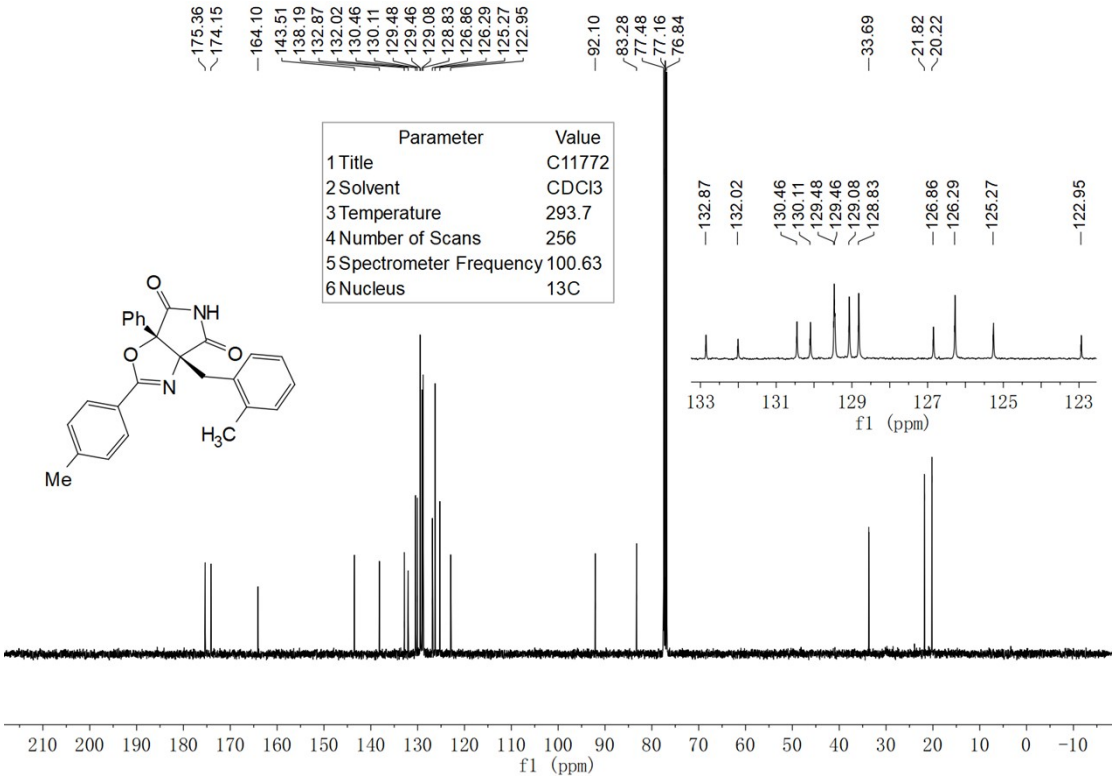
4ua


9.70
8.08
8.06
7.58
7.56
7.55
7.48
7.46
7.44
7.42
7.41
7.39
7.36
7.34
7.32
7.26 CDCl3
7.13
7.11
6.87
6.85
6.41
6.39
3.46
3.42
2.89
2.85
0.01
Parameter Value
1 Title 4ClBn-Ph
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)
0.92
1.99
1.03
5.05
2.03
2.00
2.02
1.01
1.01

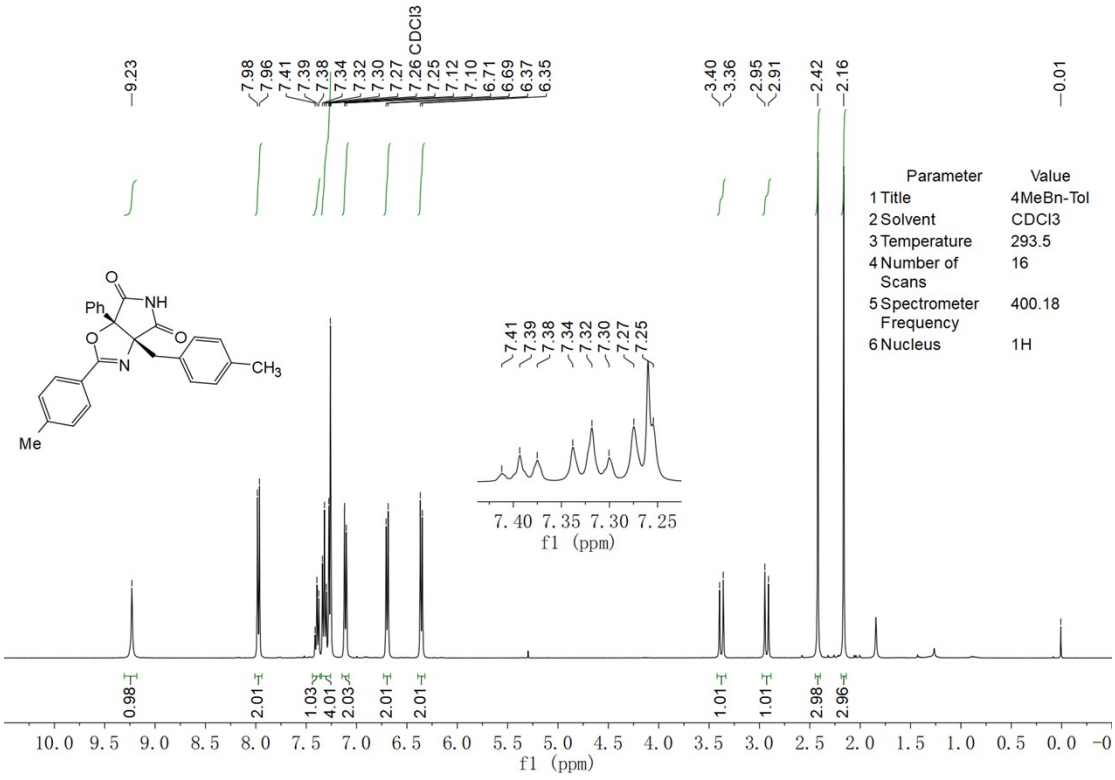

175.45
174.17
164.30
133.00
132.52
132.03
131.86
131.81
129.49
129.06
128.87
127.60
126.17
125.50
91.29
82.88
77.48
77.16
76.84
35.83
Parameter Value
1 Title oxo-4ClBn-Ph
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

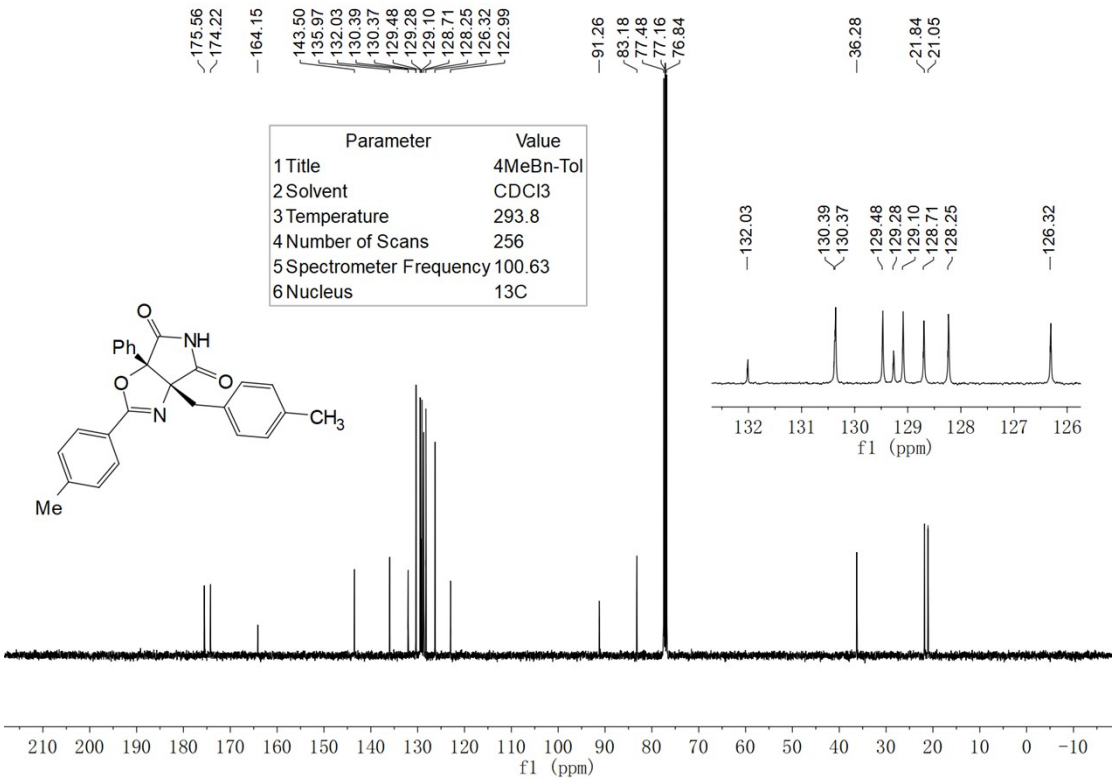
4va


9.25
7.93
7.91
7.38
7.37
7.36
7.35
7.33
7.25
7.23
7.21
7.20
6.99
6.98
6.96
6.92
6.90
6.89
6.87
6.72
6.70
3.29
3.25
2.82
2.78
2.40
2.00
0.00
Parameter Value
1 Title C11772
2 Solvent CDCl3
3 Temperature 293.4
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph
NH
O
O
N
O
H3C
Me
0.97
1.99
3.11
4.01
1.04
2.05
1.02
1.01
1.02
3.12
3.04
f1 (ppm)

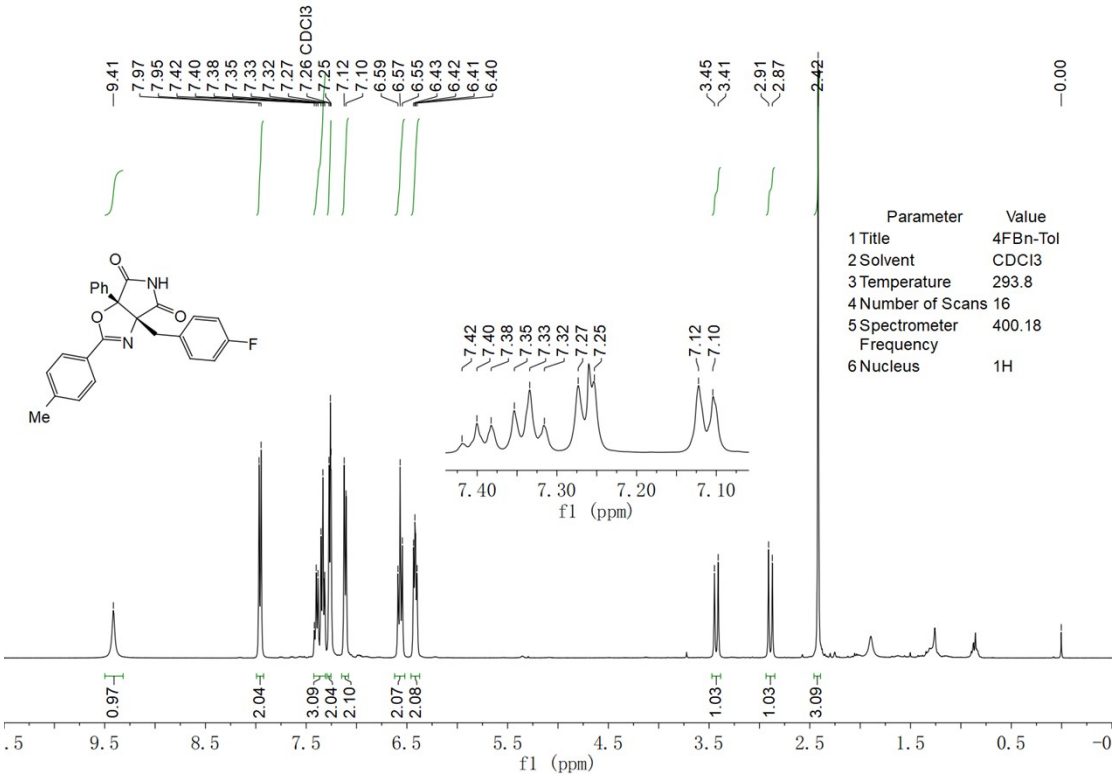

175.36
174.15
164.10
143.51
138.19
132.87
132.02
130.46
130.11
129.48
129.46
129.08
128.83
126.29
125.27
122.95
92.10
83.28
77.48
77.16
76.84
33.69
21.82
20.22
Parameter Value
1 Title C11772
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Ph
NH
O
O
N
O
H3C
Me
f1 (ppm)

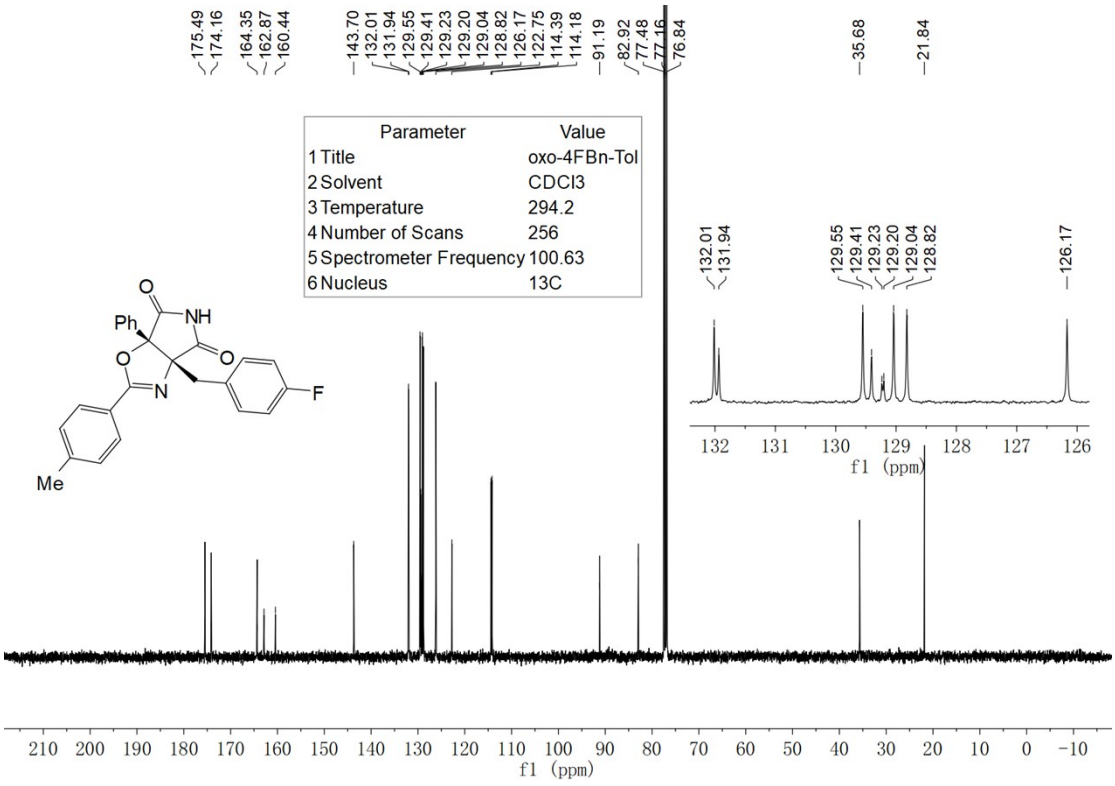
4wa


9.23
7.98
7.96
7.41
7.39
7.38
7.34
7.32
7.30
7.27
7.26 CDCl3
7.25
7.12
7.10
6.71
6.69
6.37
6.35
3.40
3.36
2.95
2.91
2.42
2.16
0.01
Parameter Value
1 Title 4MeBn-Tol
2 Solvent CDCl3
3 Temperature 293.5
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph
NH
O
N
CH3
Me
7.40 7.35 7.30 7.25
f1 (ppm)
0.98
2.01
1.03
4.01
2.03
2.01
2.01
1.01
1.01
2.98
2.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0
f1 (ppm)

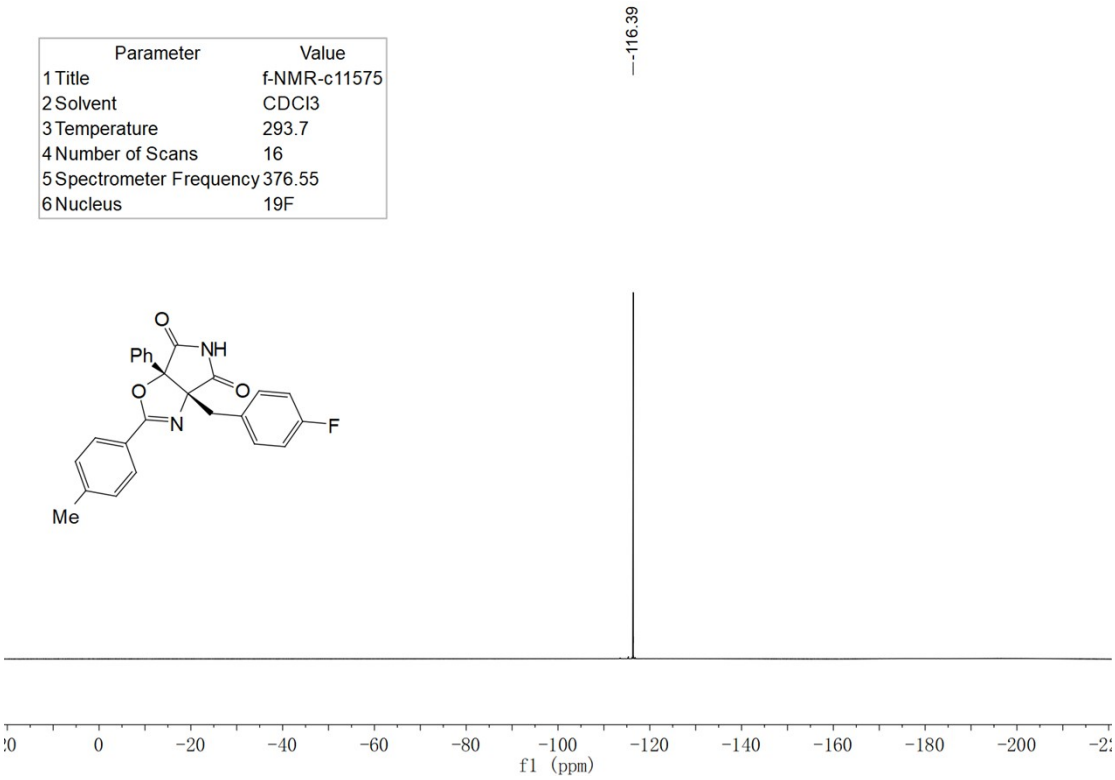

175.56
174.22
164.15
143.50
135.97
132.03
130.39
130.37
129.48
129.28
129.10
128.71
128.25
126.32
122.99
91.26
83.18
77.48
77.16
76.84
36.28
21.84
21.05
Parameter Value
1 Title 4MeBn-Tol
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
132.03
130.39
130.37
129.48
129.28
129.10
128.71
128.25
126.32
132 131 130 129 128 127 126
f1 (ppm)
Ph
NH
O
N
CH3
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

4xa

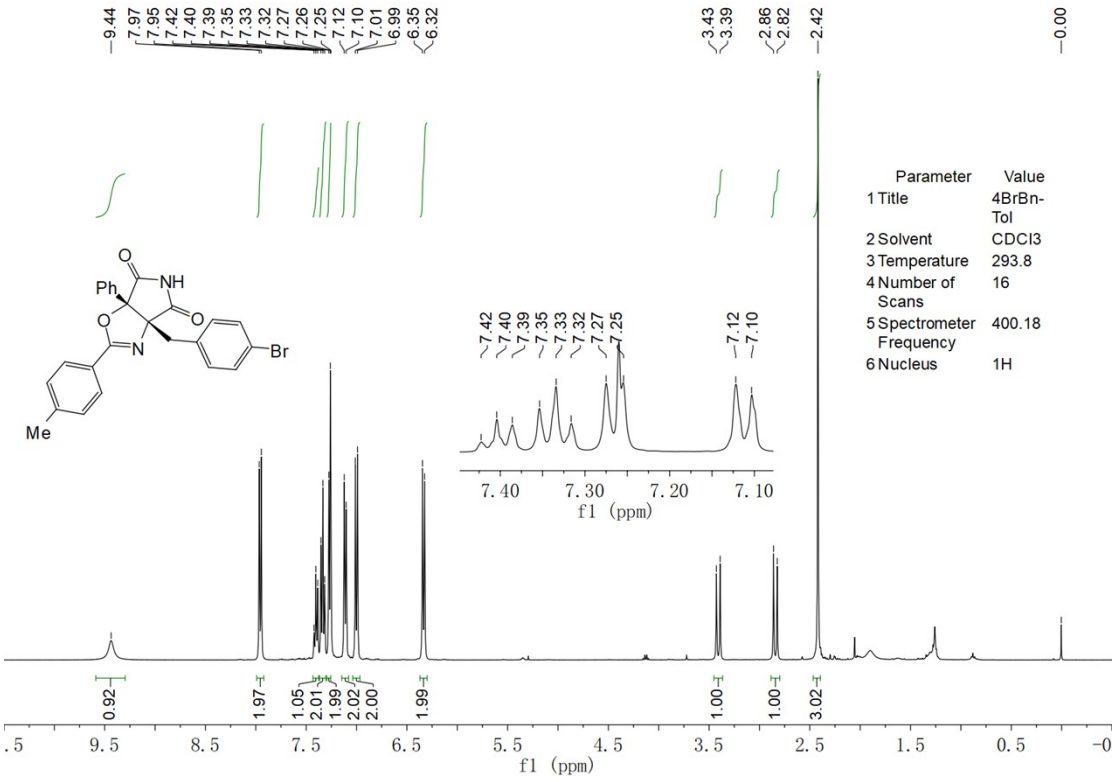

9.41
7.97
7.95
7.42
7.40
7.38
7.35
7.33
7.32
7.27
7.26 CDCl3
7.25
7.12
7.10
6.59
6.57
6.55
6.43
6.42
6.41
6.40
3.45
3.41
2.91
2.87
2.42
0.00
Parameter Value
1 Title 4FBn-Tol
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph
NH
O
N
F
Me
7.40 7.30 7.20 7.10
f1 (ppm)
0.97
2.04
3.09
2.04
2.10
2.07
2.08
1.03
1.03
3.09
f1 (ppm)

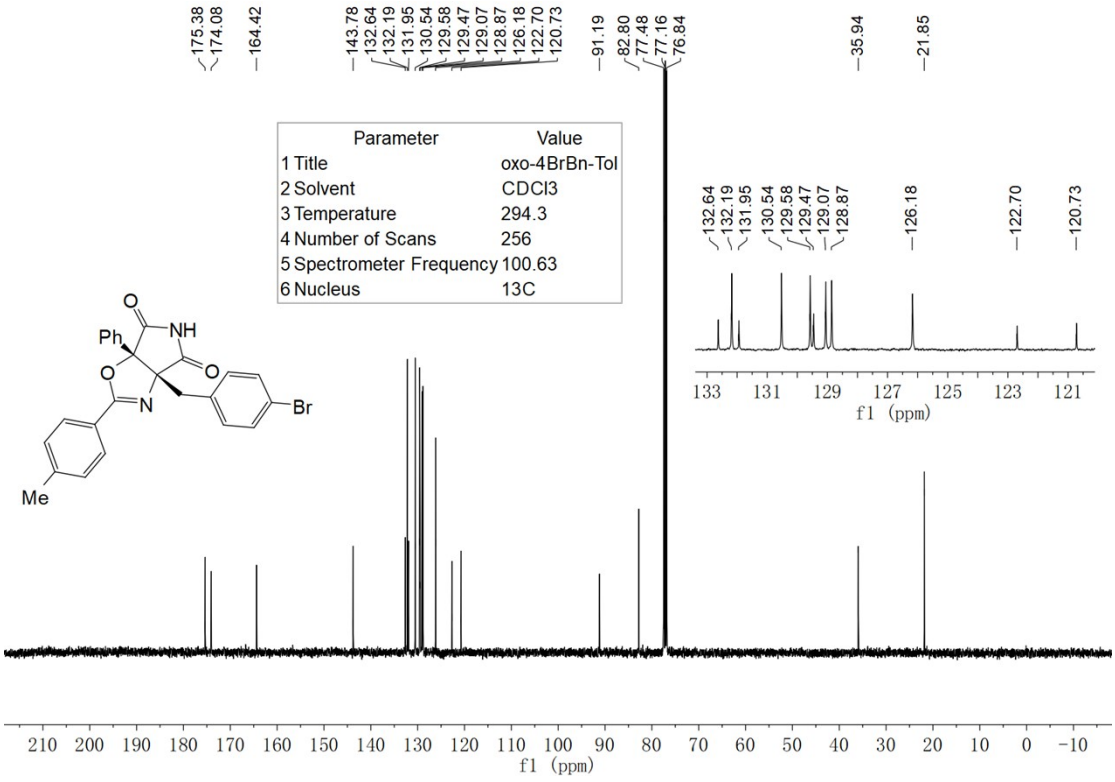

175.49
174.16
164.35
162.87
160.44
143.70
132.01
131.94
129.55
129.41
129.23
129.20
129.04
128.82
126.17
122.75
114.39
114.18
91.19
82.92
77.48
77.16
76.84
35.68
21.84
Parameter Value
1 Title oxo-4FBn-Tol
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Ph
NH
O
N
F
Me
132 131 130 129 128 127 126
f1 (ppm)
f1 (ppm)

Parameter	Value
1 Title	f-NMR-c11575
2 Solvent	CDCl3
3 Temperature	293.7
4 Number of Scans	16
5 Spectrometer Frequency	376.55
6 Nucleus	19F

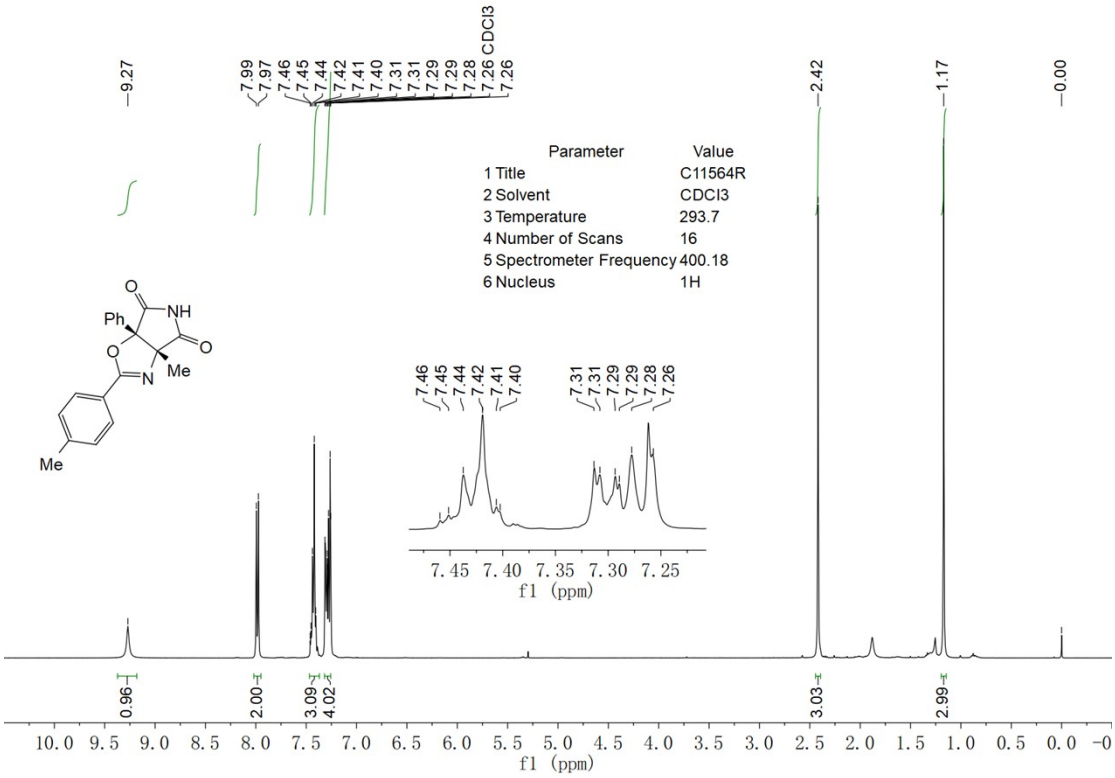


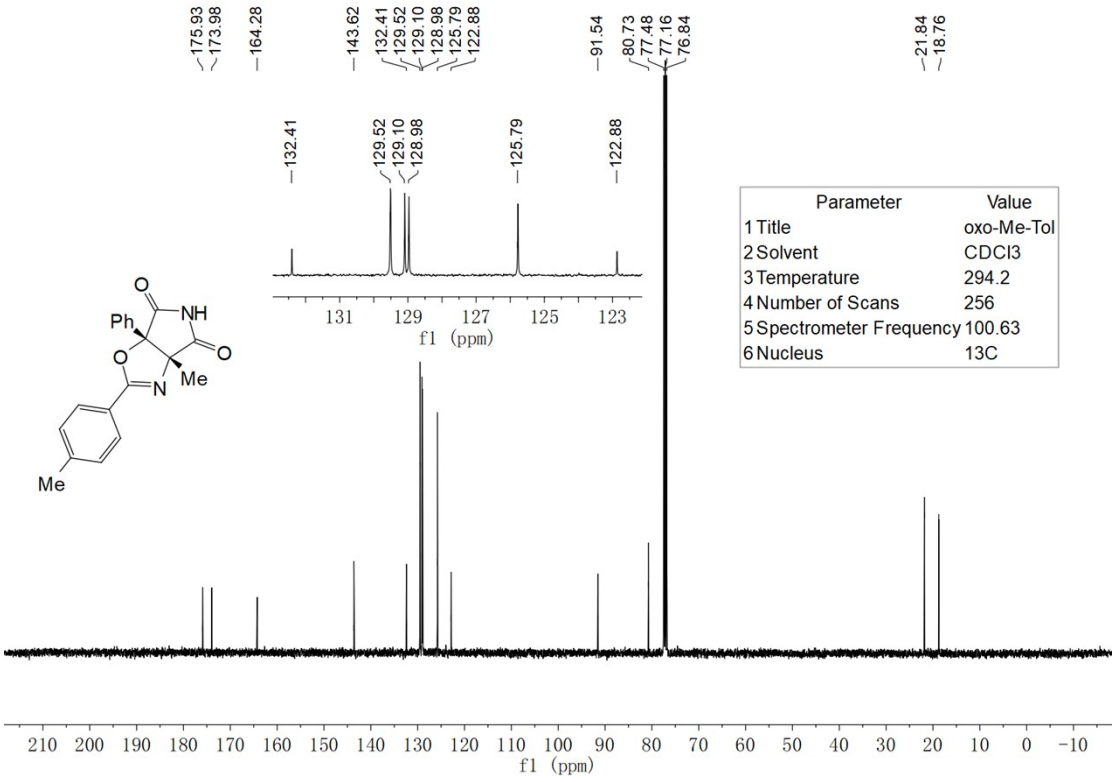
4ya


9.44
7.97
7.95
7.42
7.40
7.39
7.35
7.33
7.32
7.27
7.26
7.25
7.12
7.10
7.01
6.99
6.35
6.32
3.43
3.39
2.86
2.82
2.42
0.00
Parameter Value
1 Title 4BrBn-Tol
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph
NH
O
O
O
N
Br
Me
7.42
7.40
7.39
7.35
7.33
7.32
7.27
7.25
7.12
7.10
7.40
7.30
7.20
7.10
f1 (ppm)
0.92
1.97
1.05
2.01
1.99
2.02
2.00
1.99
1.00
1.00
3.02
f1 (ppm)

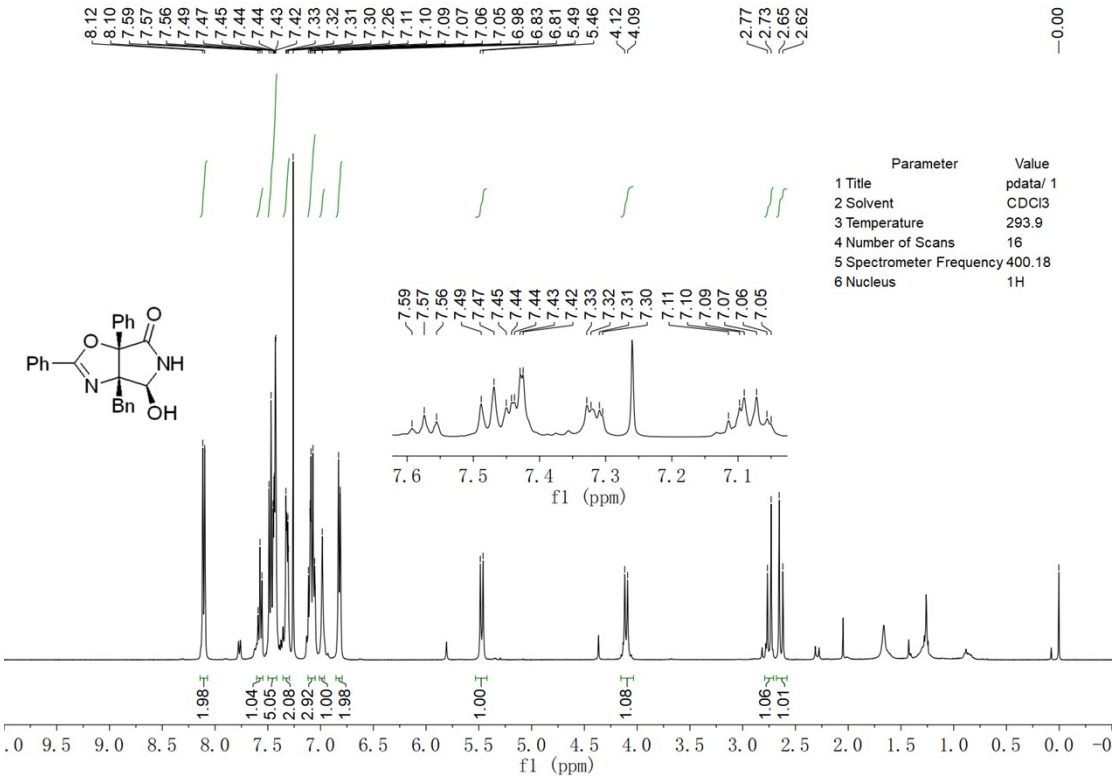

175.38
174.08
164.42
143.78
132.64
132.19
131.95
130.54
129.58
129.47
129.07
128.87
126.18
122.70
120.73
91.19
82.80
77.48
77.16
76.84
35.94
21.85
Parameter Value
1 Title oxo-4BrBn-Tol
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Ph
NH
O
O
O
N
Br
Me
132.64
132.19
131.95
130.54
129.58
129.47
129.07
128.87
126.18
122.70
120.73
133
131
129
127
125
123
121
f1 (ppm)
f1 (ppm)

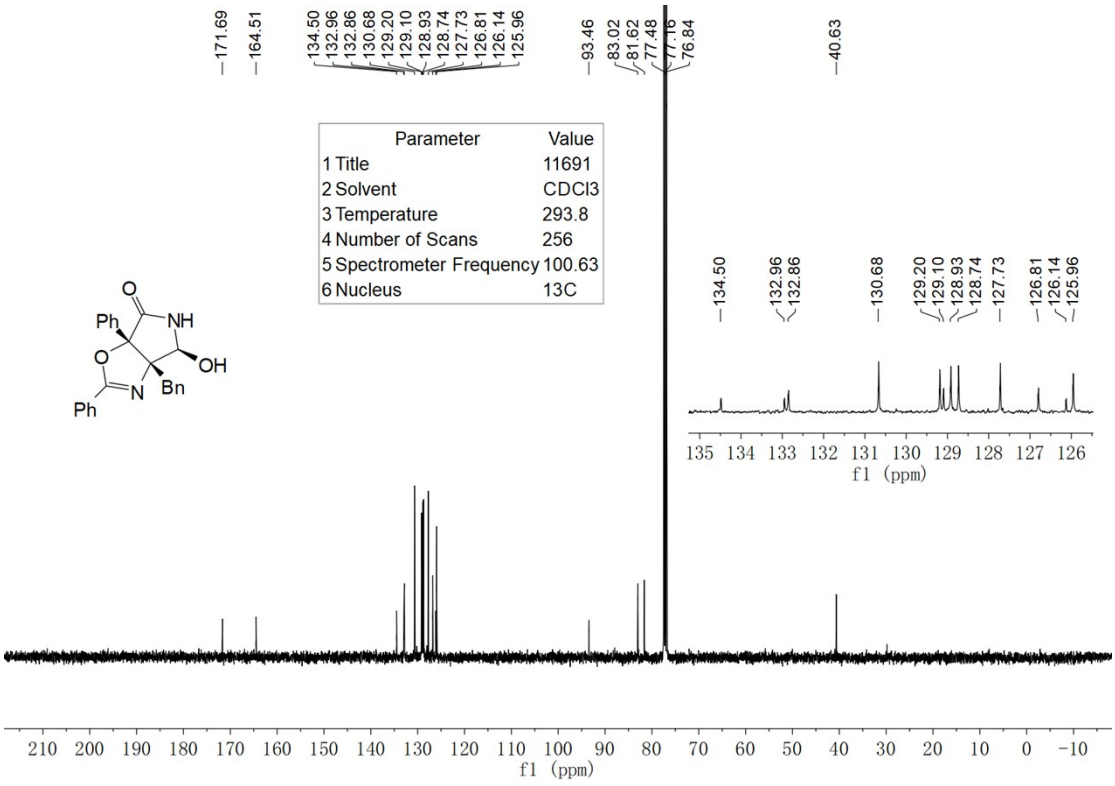
4za


9.27
7.99
7.97
7.46
7.45
7.44
7.42
7.41
7.40
7.31
7.31
7.29
7.29
7.28
7.26 CDCl3
7.26
2.42
1.17
0.00
Parameter Value
1 Title C11564R
2 Solvent CDCl3
3 Temperature 293.7
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph
NH
O
O
O
N
Me
Me
7.45 7.40 7.35 7.30 7.25
f1 (ppm)
0.96
2.00
3.09
4.02
3.03
2.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0
f1 (ppm)

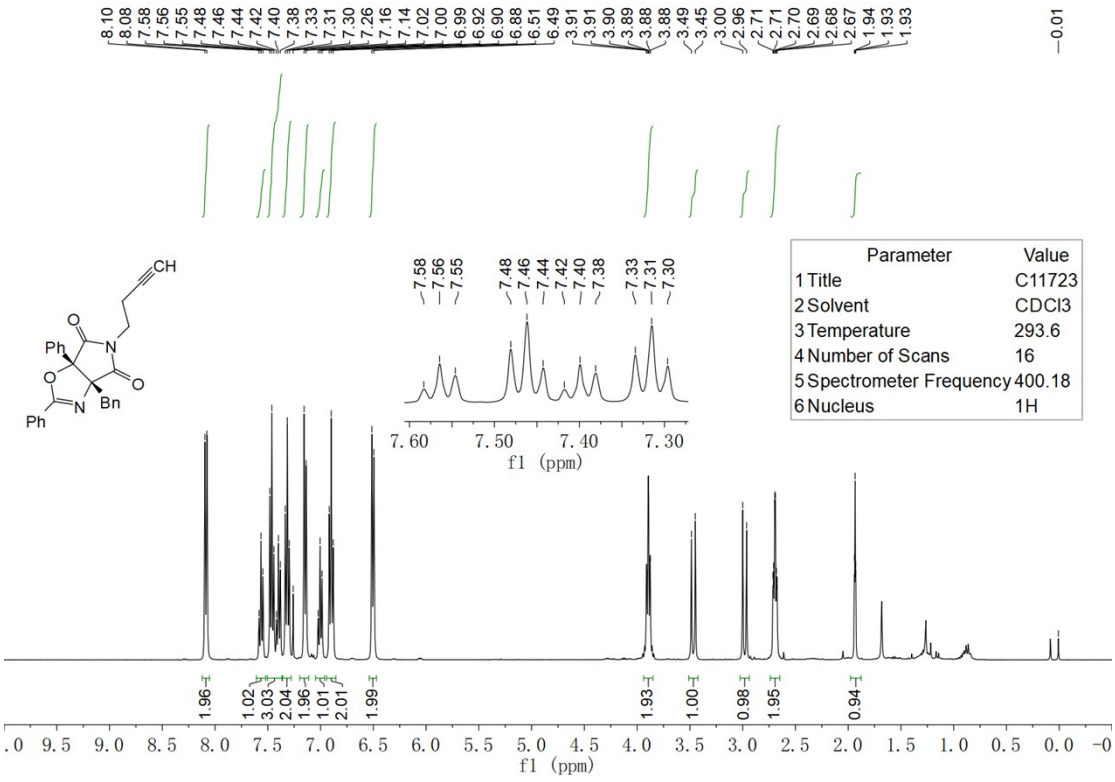

175.93
173.98
164.28
143.62
132.41
129.52
129.10
128.98
125.79
122.88
91.54
80.73
77.48
77.16
76.84
21.84
18.76
131 129 127 125 123
f1 (ppm)
Parameter Value
1 Title oxo-Me-Tol
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
Ph
NH
O
O
O
N
Me
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

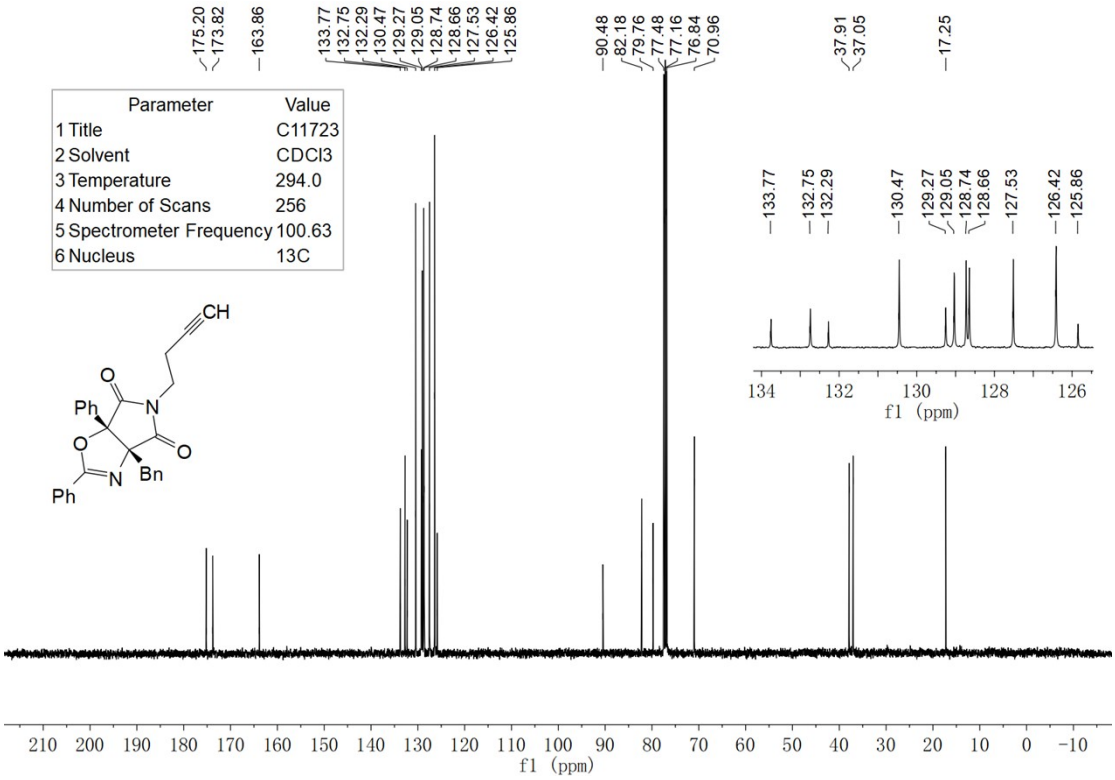
5


8.12 8.10 7.59 7.57 7.56 7.49 7.47 7.45 7.44 7.44 7.43 7.42 7.33 7.32 7.31 7.30 7.26 7.11 7.10 7.09 7.07 7.06 7.05 6.98 6.83 6.81 5.49 5.46 4.12 4.09 2.77 2.73 2.65 2.62 0.00
Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 293.9
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph O NH Ph O N Bn OH
7.59 7.57 7.56 7.49 7.47 7.45 7.44 7.44 7.43 7.42 7.33 7.32 7.31 7.30 7.11 7.10 7.09 7.07 7.06 7.05
7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
1.98 1.04 5.05 2.08 2.92 1.00 1.98 1.00 1.08 1.06 1.01
.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0
f1 (ppm)

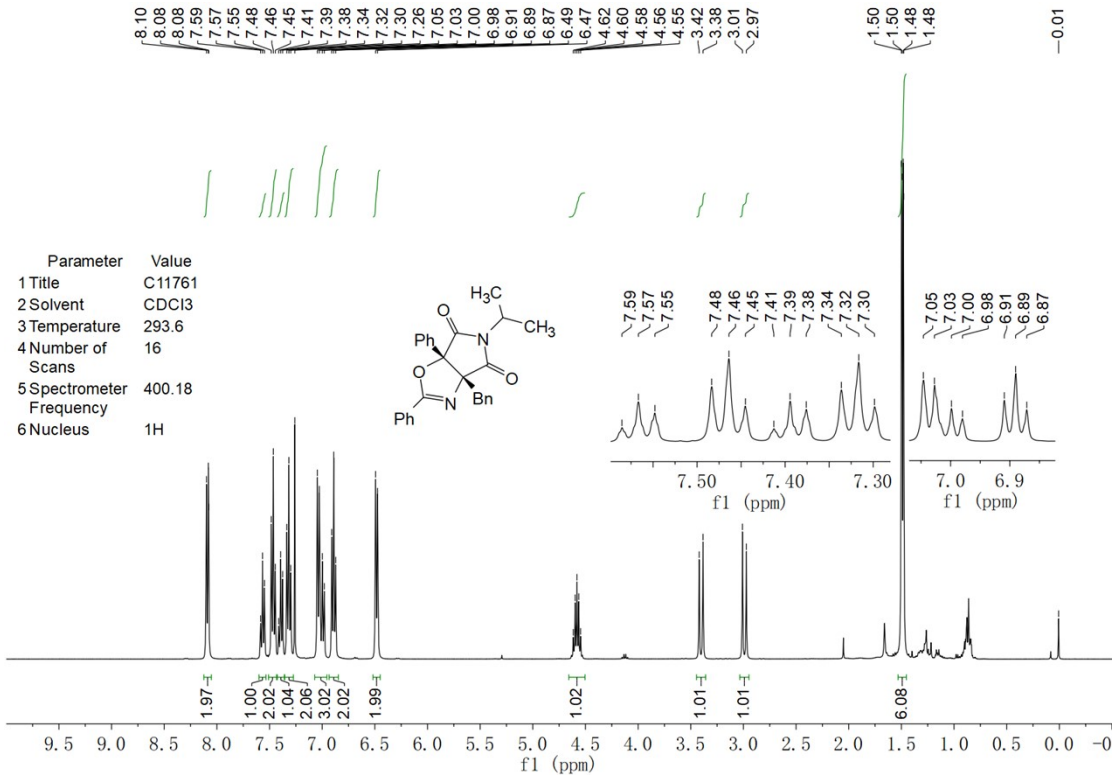

171.69 164.51 134.50 132.96 132.86 130.68 129.20 129.10 128.93 128.74 127.73 126.81 126.14 125.96 93.46 83.02 81.62 77.48 77.16 76.84 40.63
Parameter Value
1 Title 11691
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
O NH Ph O OH N Bn Ph
134.50 132.96 132.86 130.68 129.20 129.10 128.93 128.74 127.73 126.81 126.14 125.96
135 134 133 132 131 130 129 128 127 126
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

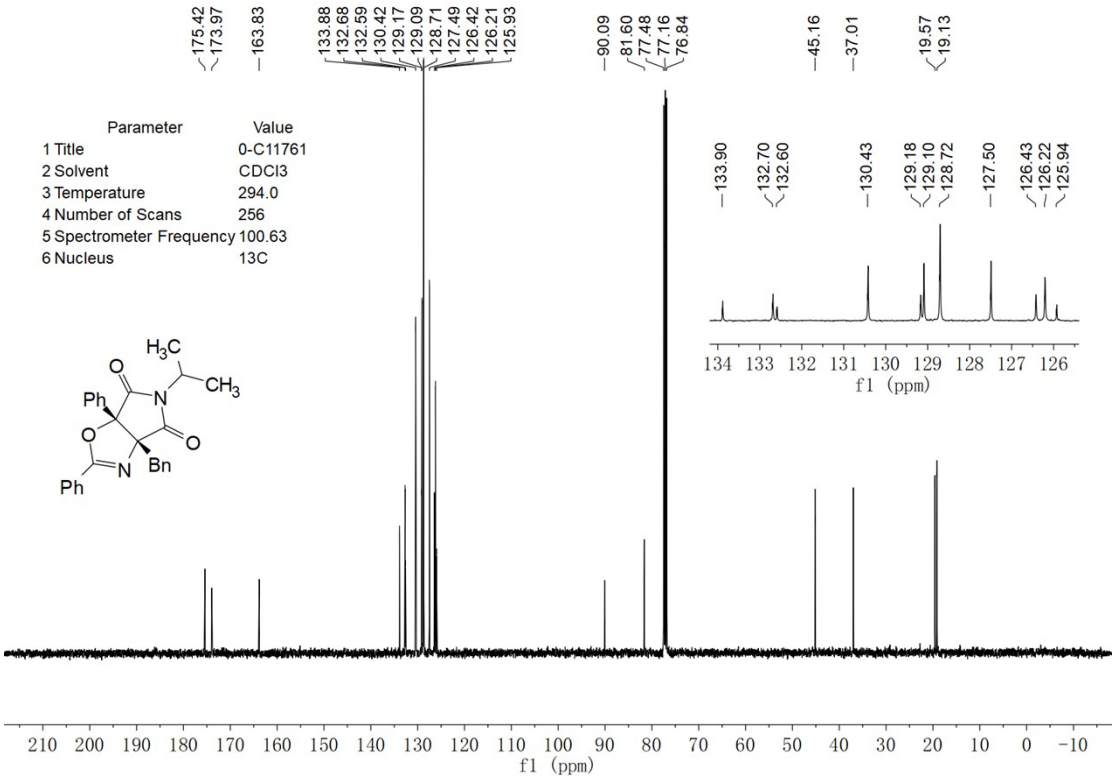
6a


8.10 8.08 7.58 7.56 7.55 7.48 7.46 7.44 7.42 7.40 7.38 7.33 7.31 7.30 7.26 7.16 7.14 7.02 7.00 6.99 6.92 6.90 6.88 6.51 6.49 3.91 3.91 3.90 3.89 3.88 3.88 3.49 3.45 3.00 2.96 2.71 2.71 2.70 2.69 2.68 2.67 1.94 1.93 1.93 0.01
CH
O
N
Ph
O
O
N
Bn
Ph
7.58 7.56 7.55 7.48 7.46 7.44 7.42 7.40 7.38 7.33 7.31 7.30
7.60 7.50 7.40 7.30
f1 (ppm)
Parameter Value
1 Title C11723
2 Solvent CDCl3
3 Temperature 293.6
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
1.96 1.02 3.03 2.04 1.96 1.01 2.01 1.99 1.93 1.00 0.98 1.95 0.94
f1 (ppm)

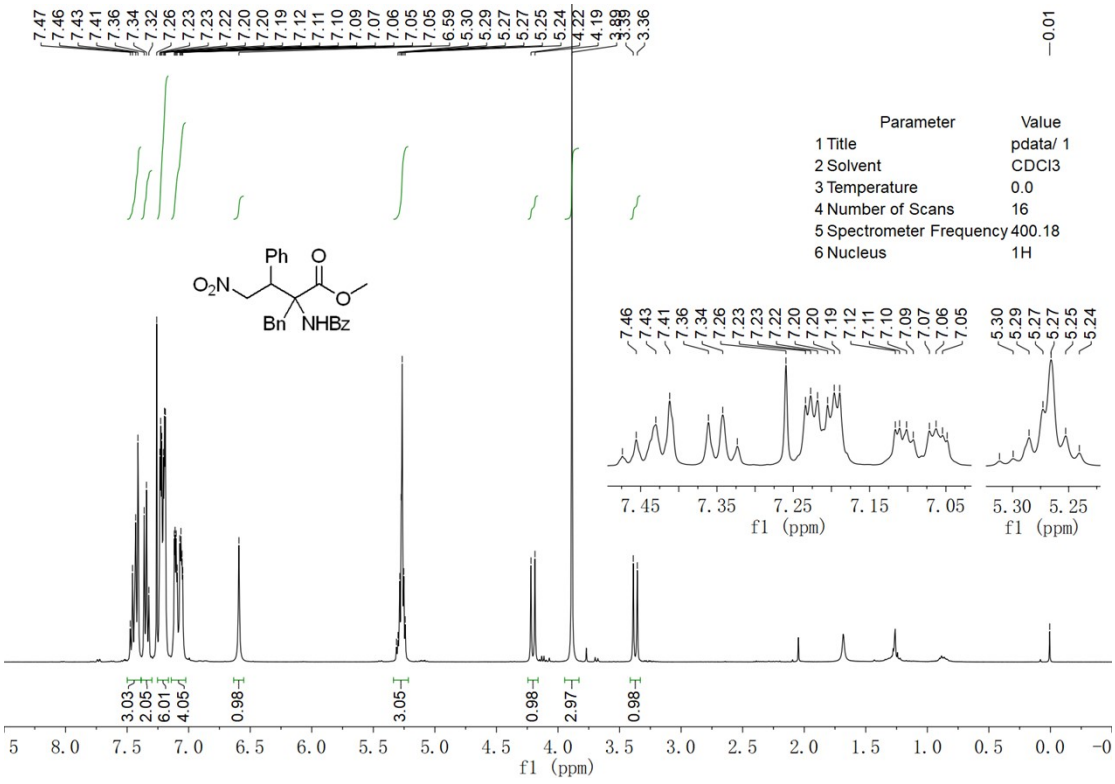

175.20 173.82 163.86 133.77 132.75 132.29 130.47 129.27 129.05 128.74 128.66 127.53 126.42 125.86 90.48 82.18 79.76 77.48 77.16 76.84 70.96 37.91 37.05 17.25
Parameter Value
1 Title C11723
2 Solvent CDCl3
3 Temperature 294.0
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
CH
O
N
Ph
O
O
N
Bn
Ph
133.77 132.75 132.29 130.47 129.27 129.05 128.74 128.66 127.53 126.42 125.86
134 132 130 128 126
f1 (ppm)
f1 (ppm)

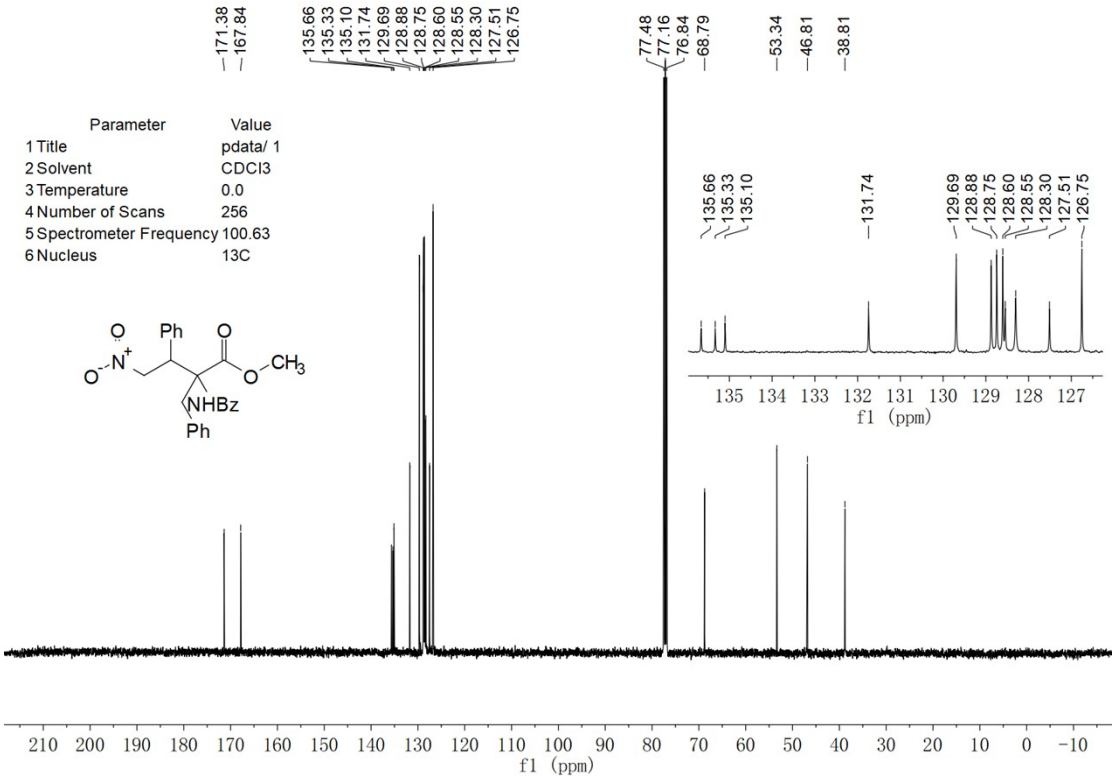
6b


8.10 8.08 8.08 7.59 7.57 7.55 7.48 7.46 7.45 7.41 7.39 7.38 7.34 7.32 7.30 7.26 7.05 7.03 7.00 6.98 6.91 6.89 6.87 6.49 6.47 4.62 4.60 4.58 4.56 4.55 3.42 3.38 3.01 2.97 1.50 1.50 1.48 1.48 0.01
Parameter Value
1 Title C11761
2 Solvent CDCl3
3 Temperature 293.6
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
1.97 1.00 2.02 1.04 2.06 3.02 2.02 1.99 1.02 1.01 1.01 6.08
f1 (ppm)

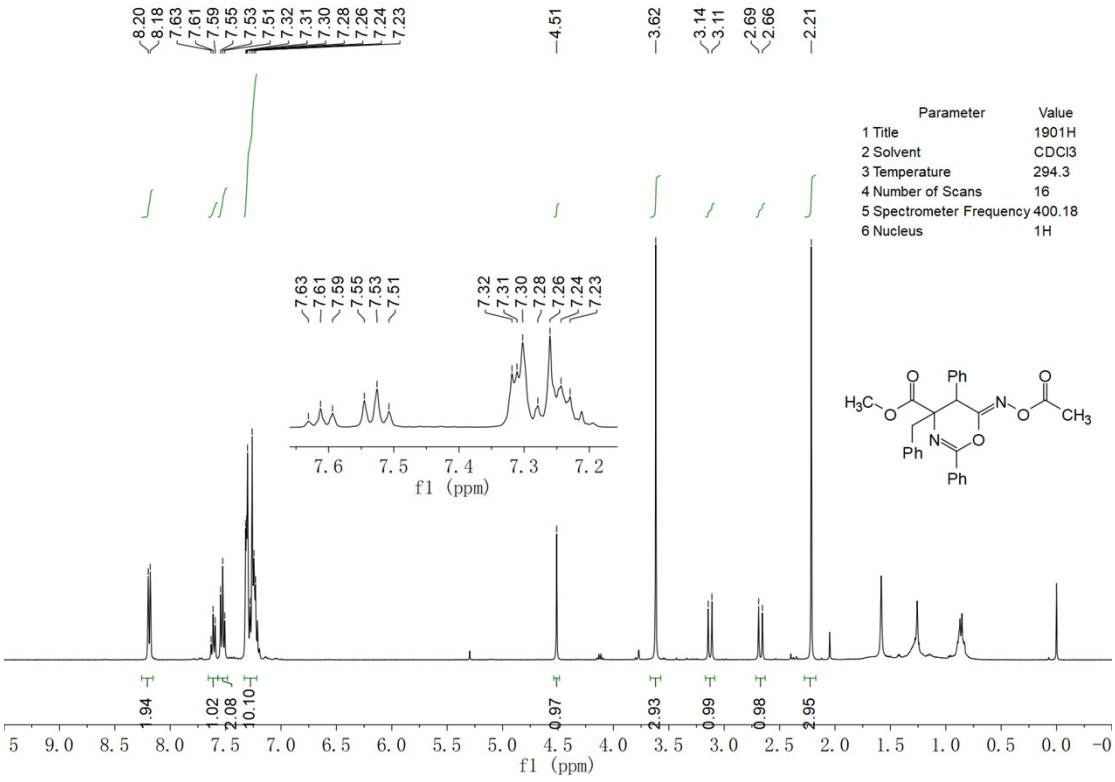

175.42 173.97 163.83 133.88 132.68 132.59 130.42 129.17 129.09 128.71 127.49 126.42 126.21 125.93 90.09 81.60 77.48 77.16 76.84 45.16 37.01 19.57 19.13
Parameter Value
1 Title 0-C11761
2 Solvent CDCl3
3 Temperature 294.0
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)

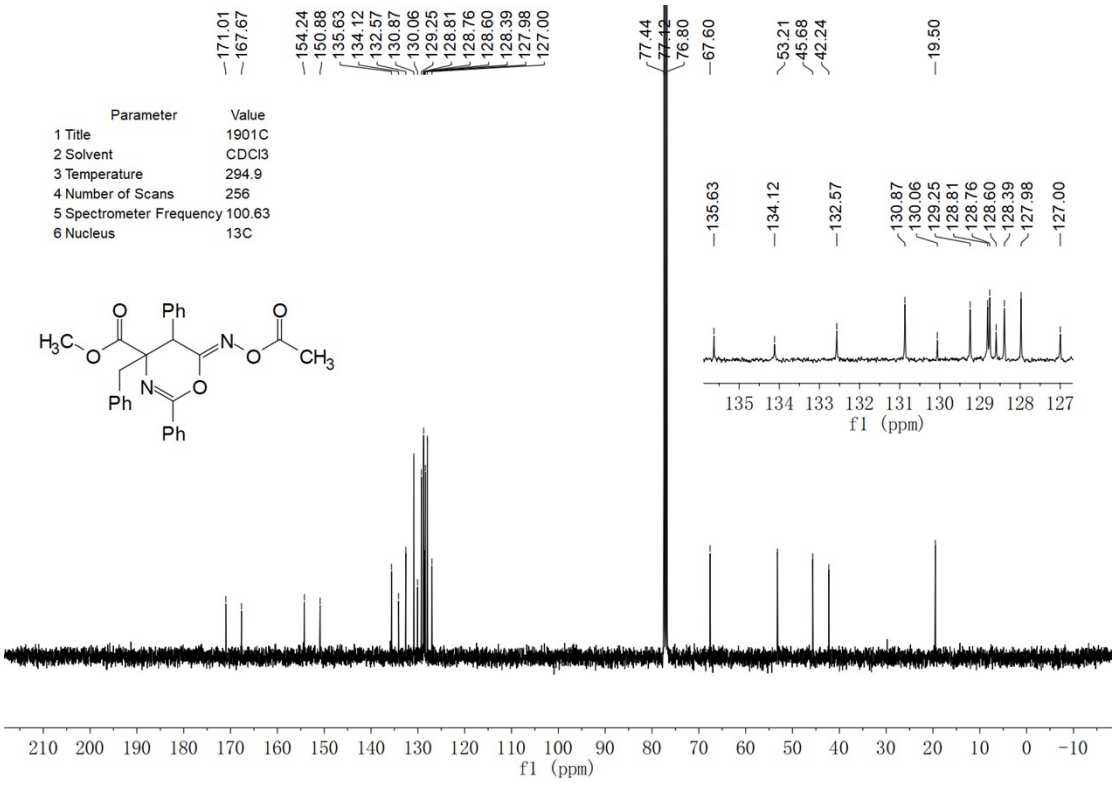
7


Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 0.0
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
Ph O
O2N
Bn NHBz
f1 (ppm)


Parameter Value
1 Title pdata/ 1
2 Solvent CDCl3
3 Temperature 0.0
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
O Ph O
O N+
O CH3
NHBz
Ph
f1 (ppm)

8


8.20
8.18
7.63
7.61
7.59
7.55
7.53
7.51
7.32
7.31
7.30
7.28
7.26
7.24
7.23
4.51
3.62
3.14
3.11
2.69
2.66
2.21
Parameter Value
1 Title 1901H
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 16
5 Spectrometer Frequency 400.18
6 Nucleus 1H
f1 (ppm)
1.94
1.02
2.08
10.10
0.97
2.93
0.99
0.98
2.95


171.01
167.67
154.24
150.88
135.63
134.12
132.57
130.87
130.06
129.25
128.81
128.76
128.60
128.39
127.98
127.00
77.44
77.12
76.80
67.60
53.21
45.68
42.24
19.50
Parameter Value
1 Title 1901C
2 Solvent CDCl3
3 Temperature 294.9
4 Number of Scans 256
5 Spectrometer Frequency 100.63
6 Nucleus 13C
f1 (ppm)