

Electronic Supplementary Information (ESI)

Visible-light-induced Markovnikov addition of olefin for construction of deuterated α -tertiary amino acid derivatives

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1 General information

1.1 Solvents and Reagent

Dry solvents and deuterated solvents were purchased from *J&K*[®] (Extra Dry, H₂O < 30 ppm) stored under molecular sieves. All reagents were purchased from Adamas, TCI, Aldrich and Alfa and used without further purification, unless otherwise stated.

1.2 Experimental chemicals

All reactions were performed under a positive pressure of N₂ ($\geq 99.99\%$) in oven-dried glassware using standard Schlenk techniques, unless otherwise stated. In the process of reaction, Schlenk tube was heated by circulating water to ensure that transformation process was around 40 °C. For thin layer chromatography (TLC) analysis throughout this work, HuangHai- HSGF254 TLC plates (0.2 \pm 0.03 mm thickness, F254 indicator) were employed. Flash column chromatography was performed with glass columns and the purification of products was accomplished using forced-flow chromatography on Silica Gel (300-400 mesh). Organic solvents were concentrated under reduced pressure on an EYELA N-1300 rotary evaporator (in *vacuo* at 30-45 °C). Yields refer to isolated materials of >95% purity, as determined by ¹H NMR analysis. Deuterated ratio ([D] or D/H) and diastereoselectivity ratio (*d.r.*) also determined by ¹H NMR analysis. Regioisomeric ratio (*r.r.*) was determined by ¹H NMR or HPLC analysis using C18 column.

1.3 Analytical Instrumentation

¹H NMR and ¹³C NMR data were recorded on Bruker AVANCE III HD-400, spectrometers using CDCl₃ or DMSO-*d*₆ as solvents, typically at 20–23 °C. Chemical shifts (δ) are reported in ppm relative to the residual solvent signal (δ 7.26 for ¹H NMR, δ 77.00 for ¹³C NMR in CDCl₃, δ 2.50 for ¹H NMR, δ 39.52 for ¹³C NMR in DMSO-*d*₆, δ 4.79 for ¹H NMR in D₂O). ¹⁹F NMR spectra were taken on a Bruker AVANCE III HD (400 MHz) instrument. Data for ¹H NMR are reported as follows: chemical shift (δ ppm), integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), and coupling constant (Hz). Data for ¹³C NMR are reported in terms of chemical shift and no special nomenclature is used for equivalent carbons. High-resolution mass spectra (HRMS) were recorded on a UPLC of Thermo Q Exactive Focus. UV-Vis absorption spectra were recorded using 1 cm quartz cuvettes on a Thermo Scientific NanoDrop 2000C spectrophotometer. Regioisomeric ratio was recorded on Bruker AVANCE III HD-400 or Waters e2695 HPLC.

1.4 Light Sources and Standard Reaction Setup

The setup (shown below) is employed to photochemical organic synthesis reaction, which is made up of separable base and reaction hole (PhotoSyn 3.0 reactor). The integrated light panel with certain wavelength can be embedded into the sliding groove of the base. Due to the hollow design, the reaction can be kept at an ideal temperature through cold or hot medium. In a typical reaction, Schlenk tube was inserted into the hole and the reaction mixture is irradiated under 10 W LEDs with 1.0 cm distance.

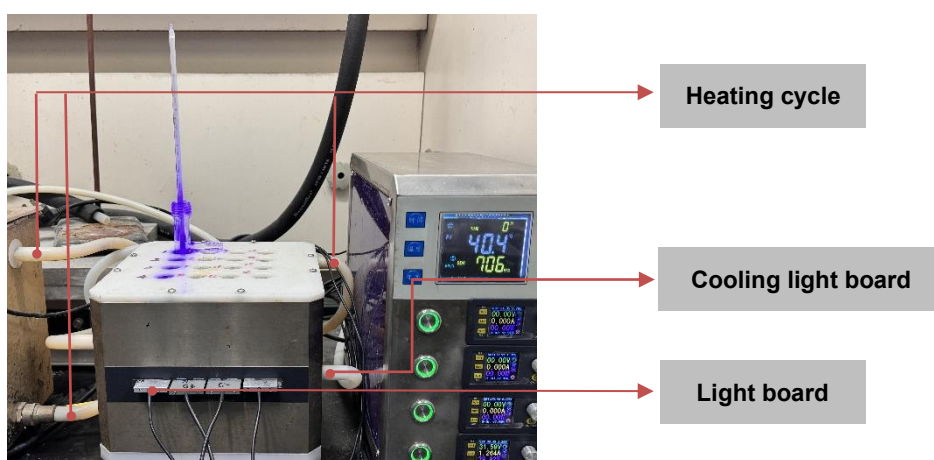


Figure S1. The detailed set-up of the photoreaction.

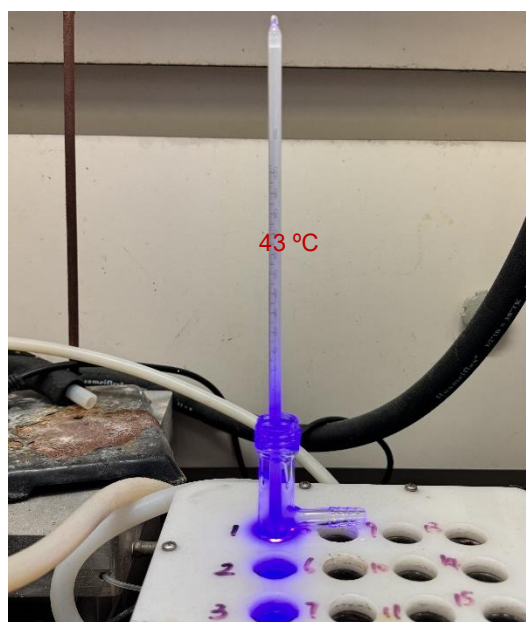


Figure S2. Reaction temperature

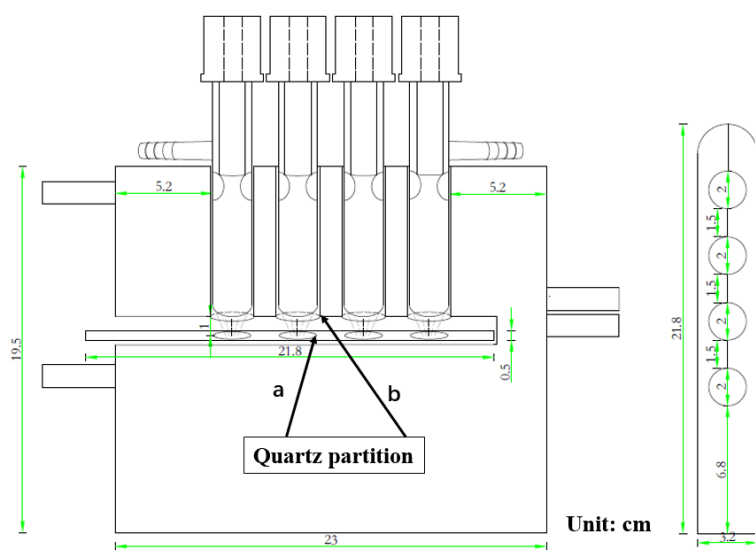


Figure S3. Schematic photoreactor

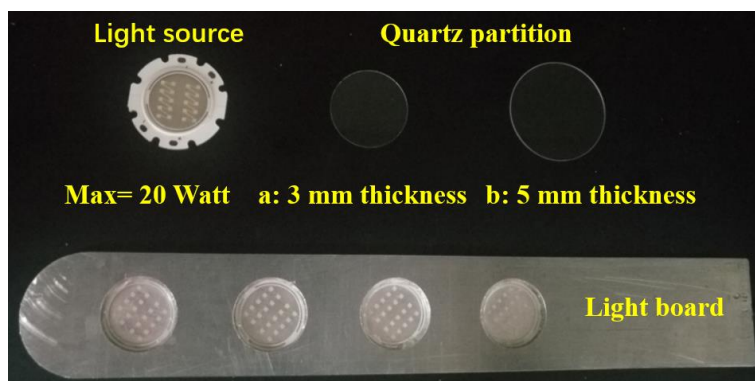
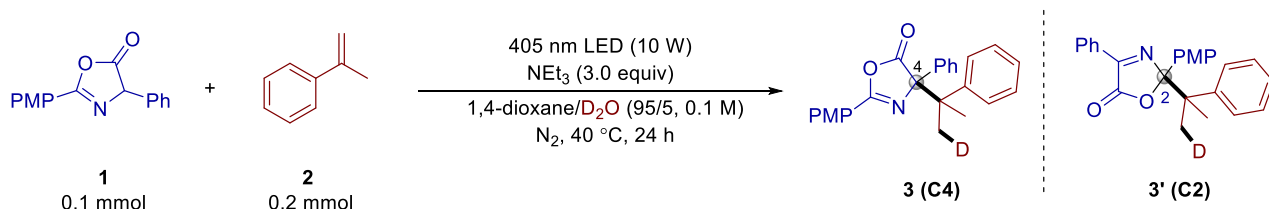


Figure S4. The detail of LEDs board

2 Reaction Optimization

2.1 General procedure



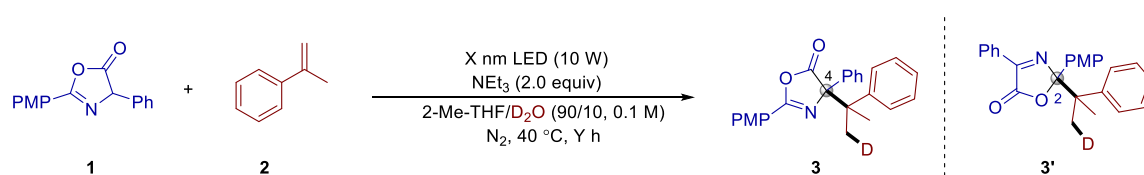
A 10 mL Schlenk tube was equipped with a magnetic stir bar, the 2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one **1** (0.1 mmol) was added. In glove box, α -methyl-styrene **2** (0.2 mmol, 2.0 equiv), NEt₃ (triethylamine) additive (0.3 mmol, 3.0 equiv) and super dry 1,4-dioxane (0.95 mL) and deuterium oxide (D₂O) (0.05 mL) were added. The tube was sealed and removed from the glove box. The reaction mixture was irradiated under 10 W LEDs (405 nm), continuous circulating water was introduced to ensure that the reaction was carried out at 40 °C. Monitored by TLC until the completely consumption of 2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one **1**, and analysed by HPLC until the regioisomers were completely converted (**C2** to **C4**), the mixture was concentrated and purified by column chromatography (PE/EtOAc = 50/1) to afford pure product **3**.

2.2 Evaluation of reaction parameter

For optimization studies, 2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one **1**, α -methyl-styrene **2**, D₂O and NEt₃ was selected as the standard substrate and the reaction conditions, such as light sources, solvents, temperature, concentration, as well as base additives were investigated.

Note: the polarities of products **3** and **3'** are very similar, it's difficult to separate them by chromatography column.

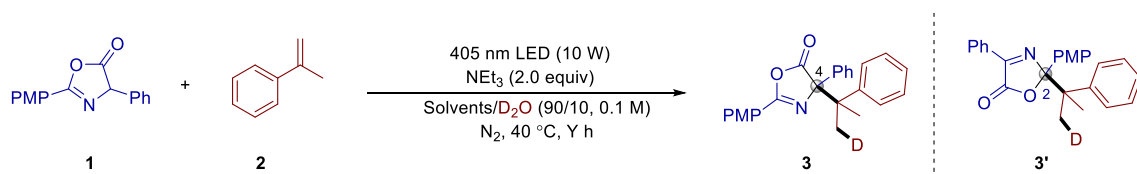
Table S1. Investigation of light sources.^[a]



Entry	Light sources (nm)	Yield ^[b] [%] (<i>r.r.</i> = 3 : 3')		[D]
		1 h	24 h	
1	385	79% (1.2 : 1)	79% (> 20 : 1)	> 20 : 1
2	395	77% (1.1 : 1)	86% (> 20 : 1)	> 20 : 1
3	405	98% (1.1 : 1)	87% (> 20 : 1)	> 20 : 1
4	415	-	84% (> 20 : 1)	> 20 : 1
5	425	76% (1.1 : 1)	95% (1.4 : 1)	> 20 : 1
6	435	-	95% (1.1 : 1)	> 20 : 1
7	445	88% (1 : 1)	97% (1 : 1)	> 20 : 1

[a] Reaction conditions: **1** (0.1 mmol), **2** (0.2 mmol), NEt₃ (0.2 mmol), super dry 1,4-dioxane (0.9 mL), D₂O (0.1 mL), 40 °C. [b] Isolated yield. The regioselectivity of **3/3'** in parentheses. The [D] and *r.r.* were determined by ¹H NMR analysis. [D] = deuterated ratio, *r.r.* = regioselectivity.

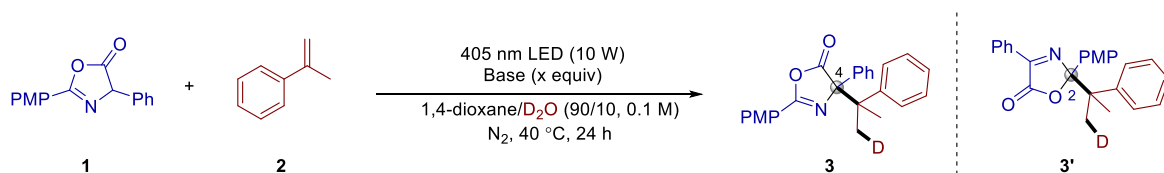
Table S2. Investigation of solvents.^[a]



Entry	Solvent	Yield ^[b] [%] (<i>r.r.</i> = 3 : 3')		[D]
		1 h	24 h	
1	2-Me-THF	98% (1.1 : 1)	87% (> 20 : 1)	> 20 : 1
2	THF	96% (1.1 : 1)	97% (10 : 1)	> 20 : 1
3	MeCN	91% (1.1 : 1)	89% (> 20 : 1)	> 20 : 1
4	1,4-dioxane	98% (1.2 : 1)	92% (> 20 : 1)	> 20 : 1
5	DCM	trace	trace	-
6	DMA	86% (0.42 : 1)	n. d.	-
7	DMF	89% (0.48 : 1)	n. d.	-
8	EA	94% (0.9 : 1)	82% (> 20 : 1)	> 20 : 1

[a] Reaction conditions: **1** (0.1 mmol), **2** (0.2 mmol), NEt₃ (0.2 mmol), super dry 1,4-dioxane (0.9 mL), D₂O (0.1 mL), 40 °C, irradiation with a 10 W purple LED (405 nm). [b] Isolated yield. The regioselectivity of **3/3'** in parentheses. The [D] and *r.r.* were determined by ¹H NMR analysis. n. d. = not detected. [D] = deuterated ratio, *r.r.* = regioselectivity.

Table S3. Investigation of base additives.^[a]

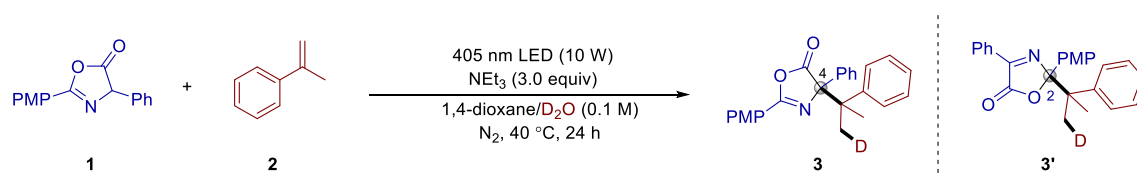


Entry	Base (x equiv)	Yield ^[b] [%] (<i>r.r.</i> = 3 : 3')	[D]
1	K ₂ CO ₃	70% (> 20 : 1)	> 20 : 1
2	Cs ₂ CO ₃	72% (> 20 : 1)	> 20 : 1
3	K ₃ PO ₄	66% (> 20 : 1)	> 20 : 1

4	DIPEA	88% (> 20 : 1)	> 20 : 1
5	DBU	28% (> 20 : 1)	> 20 : 1
6	NEt ₃ (0.2 equiv)	90% (15 : 1)	> 20 : 1
7	NEt ₃ (0.5 equiv)	80% (> 20 : 1)	> 20 : 1
8	NEt ₃ (1.0 equiv)	84% (> 20 : 1)	> 20 : 1
9	NEt ₃ (3.0 equiv)	94% (> 20 : 1)	> 20 : 1
10	NEt ₃ (5.0 equiv)	86% (> 20 : 1)	> 20 : 1
11	No base	69% (12 : 1)	> 20 : 1

[a] Reaction conditions: **1** (0.1 mmol), **2** (0.2 mmol), base additive (0.1x mmol), super dry 1,4-dioxane (0.9 mL), D₂O (0.1 mL), 40 °C, irradiation with a 10 W purple LED (405 nm) for 24 h. [b] Isolated yield. The regioselectivity of **3/3'** in parentheses. The [D] and *r.r.* were determined by ¹H NMR analysis. [D] = deuterated ratio, *r.r.* = regioselectivity.

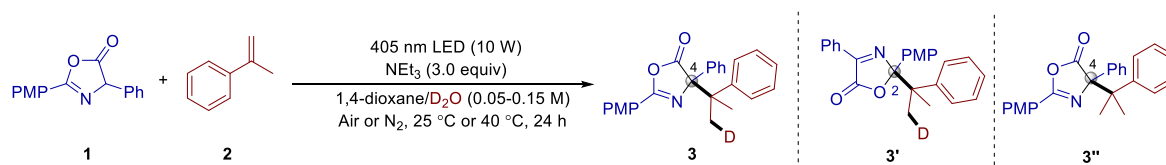
Table S4. Investigation of dosage of deuterium oxide.^[a]



Entry	D ₂ O (x μL)	Yield ^[b] [%] (<i>r.r.</i> = 3 : 3')	[D]
1	80 μL	94% (> 20 : 1)	> 20 : 1
2	60 μL	93% (> 20 : 1)	> 20 : 1
3	50 μL	96% (> 20 : 1)	> 20 : 1
4	40 μL	89% (> 20 : 1)	> 20 : 1
5	30 μL	88% (> 20 : 1)	9 : 1

[a] Reaction conditions: **1** (0.1 mmol), **2** (0.2 mmol), base additive (0.1x mmol), super dry 1,4-dioxane, D₂O, 40 °C, irradiation with a 10 W purple LED (405 nm) for 24 h. [b] Isolated yield. The regioselectivity of **3/3'** in parentheses. The [D] and *r.r.* were determined by ¹H NMR analysis. [D] = deuterated ratio, *r.r.* = regioselectivity.

Table S5. Investigation of temperature and concentration.^[a]



Entry	Concentration	Temperature [°C]	Yield ^[b] [%] (<i>r.r.</i> = 3 : 3')	[D]
1	0.15 M	40	90% (> 20 : 1)	> 20 : 1
2	0.05 M	40	91% (11 : 1)	> 20 : 1
3	2 (1.5 equiv)	40	88% (> 20 : 1)	> 20 : 1
4	0.1 M	25	92% (> 20 : 1)	> 20 : 1
5	No base	40	69% (12 : 1)	> 20 : 1

7	No D ₂ O	40	90% ^[c]	-
8	Air instead of N ₂	40	46%	-
9	In dark	40	n. d.	-

[a] Reaction conditions: **1** (0.1 mmol), **2** (0.2 mmol), NEt₃ (0.3 mmol), super dry 1,4-dioxane (0.62–1.95 mL), D₂O. [b] Isolated yield. n. d. = not detected. The regioselectivity of **3/3'** in parentheses. The [D] and *r.r.* were determined by ¹H NMR analysis. n. d. = not detected. [D] = deuterated ratio, *r.r.* = regioselectivity. [c] At this time, it is a standard product without deuterium substitution **3''**.

3 The Application of the Reaction

3.1 General Procedures for the continuous circulation flow photoreactions.

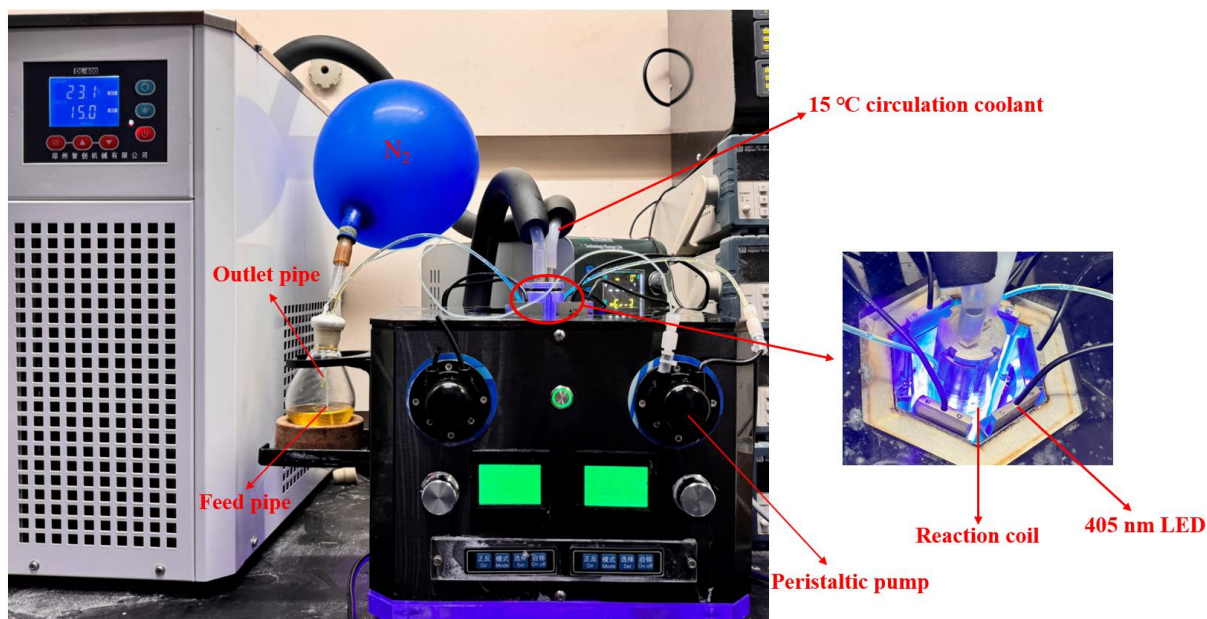
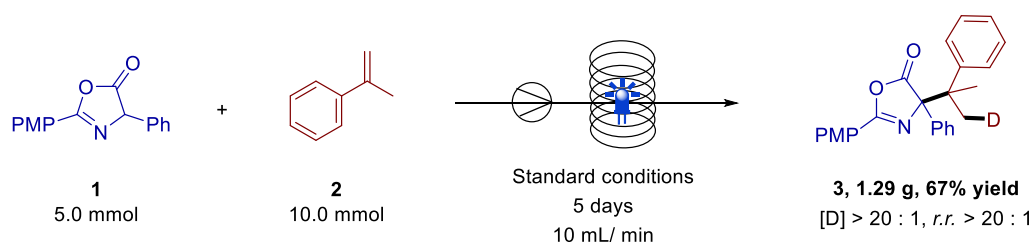


Figure S5: Process of gram-scale synthesis by continuous circulation flow reactor

A 100 mL oven-dried eggplant type flask was charged with the oxazolone **1** (5.0 mmol, 1.34 g). Then, anhydrous 1,4-dioxane (47.5 mL) and D₂O (2.5 mL) were added in glove box, followed by alkene **2** (10 mmol, 1.3 mL, 2.0 equiv) and NEt₃ (15 mmol, 2.1 mL, 3.0 equiv). The eggplant type flask was taken out of the glove box and continuous circulation flow reactor pipeline was degassed by N₂ sparging for 10 min. Both feed and outlet pipes

were inserted into the eggplant type reaction flask and kept under an N₂ atmosphere. The solution was delivered to the flow reactor through a peristaltic pump (Chuang Rui) set at 10 mL/min. The solution was irradiated with 405 nm LED (10 W x 20) at 25 ~ 35 °C and flow back into the reaction flask. After complete consumption of oxazolone and regioisomers were completely converted (**C2** to **C4**), the volatiles were removed in *vacuo*, then the residue purified by flash column chromatography on silica (PE/EtOAc = 50/1) to afford the product **3** (1.29 g, 67% yield) as a colorless oil.

3.2 Gram-scale synthesis

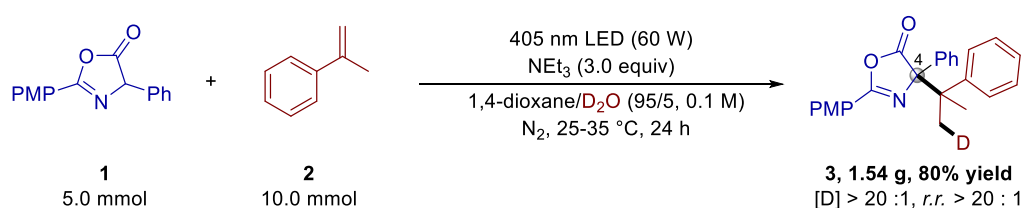


Figure S6: Process of gram-scale synthesis by batch reactor

A 250 mL Schlenk tube was equipped with a magnetic stir bar, the 2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one **1** (5.0 mmol) was added. In glove box, α -methylstyrene **2** (10 mmol, 2.0 equiv), NEt₃ (triethylamine) additive (30 mmol, 3.0 equiv) and super dry 1,4-dioxane (47.5 mL) and deuterium oxide (D₂O) (2.5 mL) were added. The tube was sealed and removed from the glove box. The Schlenk tube was irradiated under 60 W LEDs (405 nm) for 24 h. Monitored by TLC until the completely consumption of 2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one **1**, and analysed by HPLC until the regioisomers were completely converted (**C2** to **C4**), the mixture was concentrated and purified by column chromatography (PE/EtOAc = 50/1) to afford pure product **3** (1.54 g, 80% yield).

3.3 Derivatization reaction

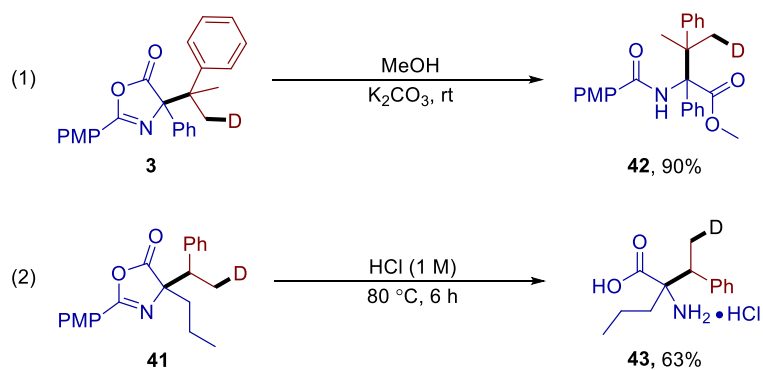


Figure S7

- (1) To a solution of product **3** (53.4 mg, 0.2 mmol) in methanol (4 mL) was added anhydrous K_2CO_3 (14 mg, 0.1 mmol). The mixture was stirred for 1 h at room temperature. After removing solvent, the crude mixture was purified by flash column chromatography (PE/EtOAc = 3/1) to give the title compound **42** (75.2 mg, 90% yield).¹
- (2) The oxazolone **41** (67.6 mg, 0.2 mmol, 1.0 equiv.) was stirred in aq. HCl (1 M, 15 mL) at 80 °C for 6 h. The mixture was subsequently filtered and after dilution with demineralized water the filtrate was washed twice with CH_2Cl_2 . All volatiles were removed under reduced pressure to yield **43** as a colorless solid (28.0 mg, 63%).²

3.4 Unsuccessful substrates

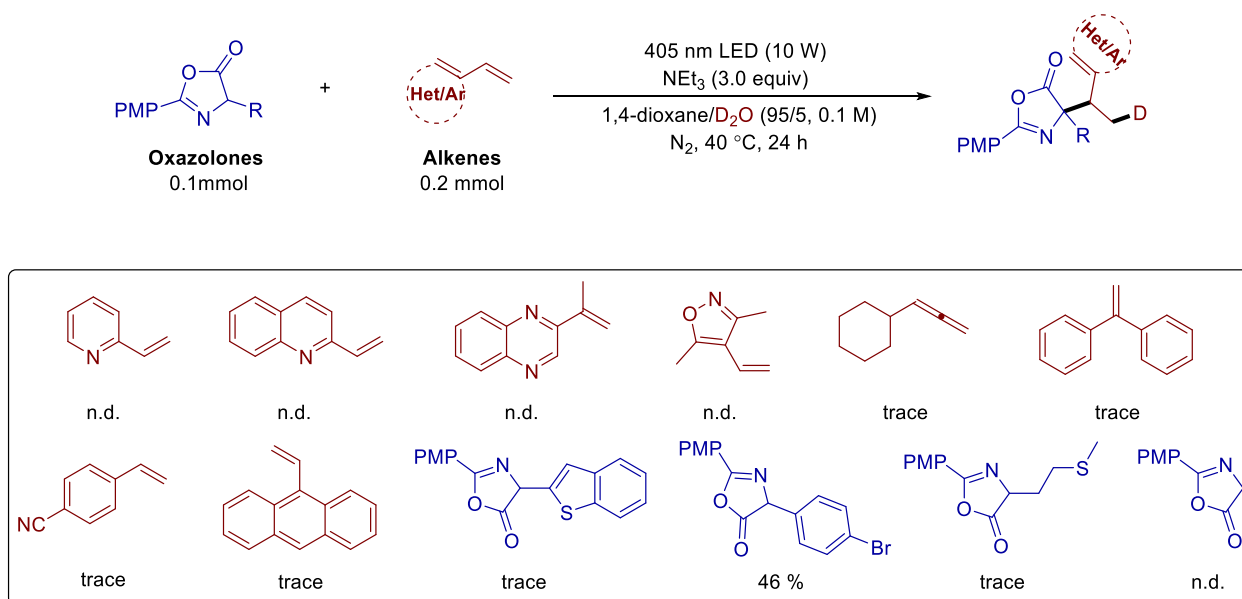


Figure S8

Pyridine, quinoline and quinoxaline-substituted alkene and cyclohexyl-substituted allene are not compatible due to

reduction potential reason. Isoxazole-substituted alkene and 1,1-diphenylethylene are not compatible due to steric hindrance; 9-vinylanthracene and 4-vinylbenzotrile are not compatible due to low reduction potentials of phenyl and cyano groups. Bromo-substituted oxazolone yield debrominated standard **C4** products with 46% yield due to the low reduction potential of bromobenzene. Benzothiophene, alkyl sulfide substituted oxazolone and unsubstituted oxazolone are not compatible due to reduction potential reason.

4 Mechanistic studies

4.1 UV-Vis absorption spectrum

UV-Vis spectra experiment was measured on a Thermo Scientific NanoDrop 2000C spectrophotometer.

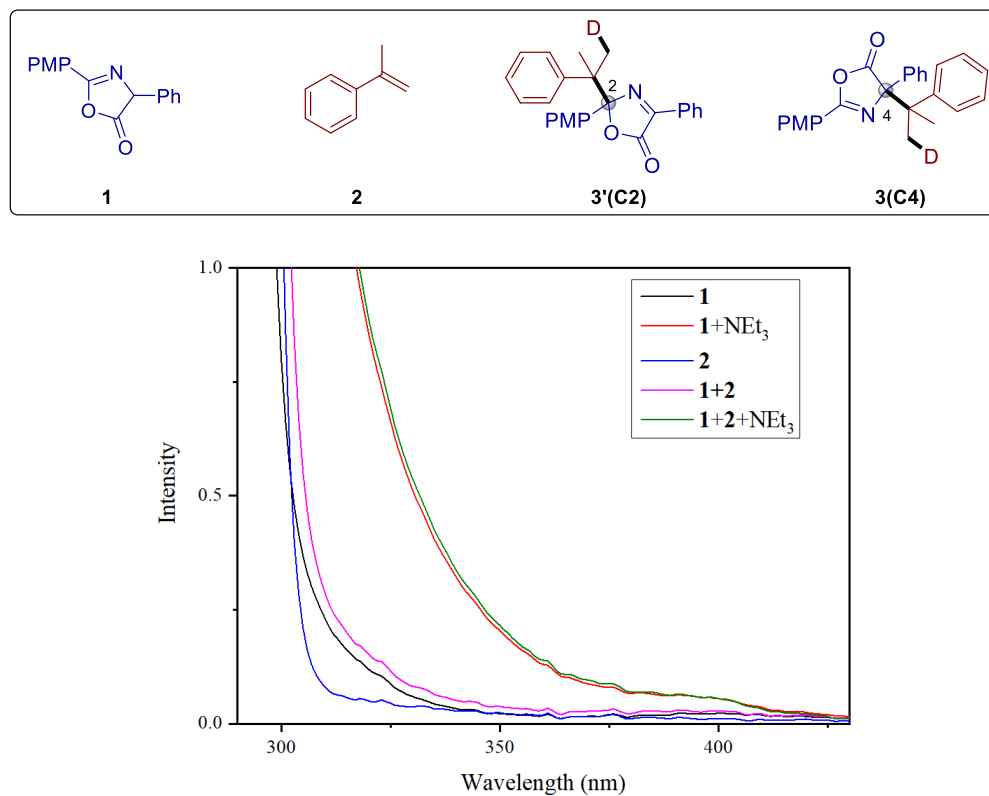


Figure S9. UV-Vis absorption spectra of oxazolone **1** (10^{-3} M), alkene **2** (10^{-3} M) and NEt₃ (10^{-3} M)

were measured in super dry 1,4-dioxane

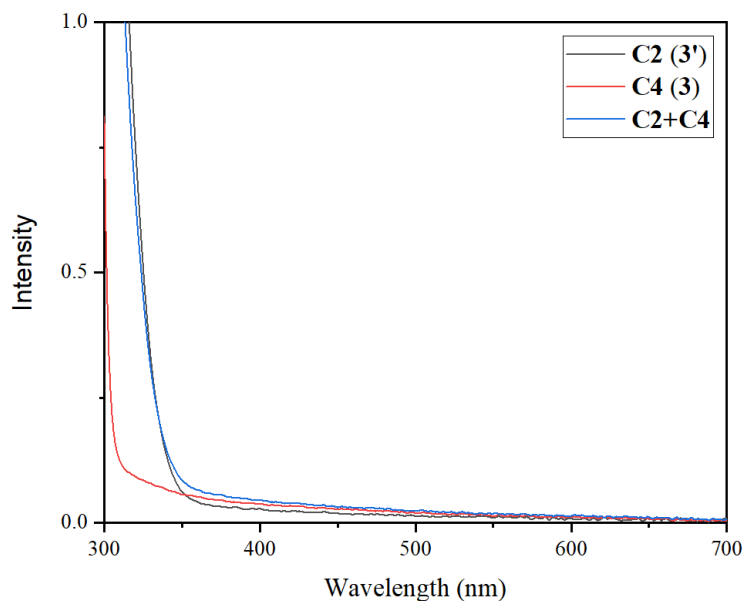


Figure S10. UV-Vis absorption spectra of **C2** (10^{-3} M) and **C4** (10^{-3} M) were measured in super dry 1,4-dioxane

4.2 Time variation curve

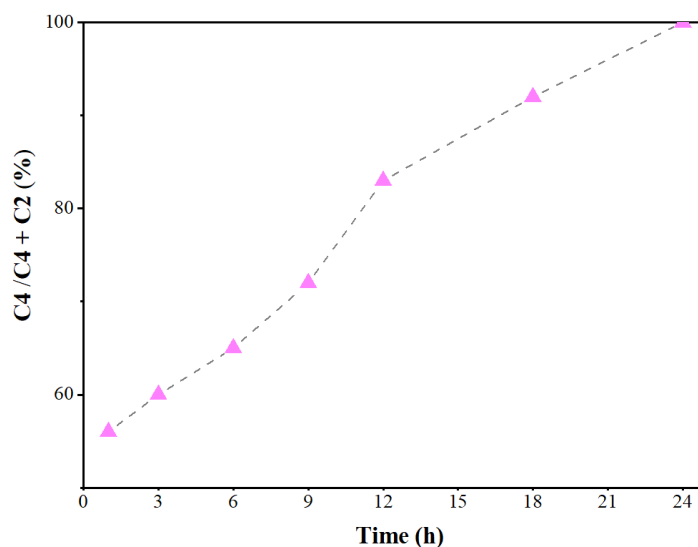


Figure S11. Time variation curve of regioisomers conversion (**C2** to **C4**)

Procedure: Seven oven-dried 10 mL Schlenk tubes were equipped with a magnetic stir bar, the oxazolone **1** (0.1 mmol) was added, respectively. In glove box, α -methyl-styrene **2** (0.2 mmol, 2.0 equiv), NEt_3 (triethylamine) additive (0.3 mmol, 3.0 equiv) and super dry 1,4-dioxane (0.95 mL) and deuterium oxide (D_2O) (0.05 mL) were added, respectively. The tubes were sealed and removed from the glove box. Each reaction solution was irradiated under 10 W LEDs (405 nm), continuous circulating water was introduced to ensure that the reaction was carried out at 40 °C. Seven identical reactions represent different reaction times, and when a certain time was reached, the corresponding reaction was removed. The mixture was concentrated and purified by column chromatography to

afford pure product. The yields first increased and then slowly decreased with the increase of time. The proportion of regioisomers (**C4/C4+C2**) was determined by ¹H NMR.

4.3 Control experiments of regioisomers conversion

Procedure: Six oven-dried 10 mL Schlenk tubes equipped with a magnetic stir bar were charged with **C2** (38.6 mg, 0.1 mmol), respectively. In glove box, NEt₃ (0.3 mmol, 3.0 equiv) and super dry 1,4-dioxane (0.95 mL) and deuterium oxide (D₂O) (0.05 mL) were added for tube 1. Similar to tube 1, without D₂O for tube 2, without NEt₃ for tube 3, without D₂O and NEt₃ for tube 4. And without D₂O and NEt₃, but **C4** (7.72 mg, 20 mol %) was added for tube 5. Under standard conditions, the light-shielded reaction was conducted in tube number 6. The preceding five reaction Schlenk tubes were sealed and removed from the glove box, and the reaction mixture was irradiated using 10 W 405 nm LEDs at 40 °C. The proportion of regioisomers (**C4/C2**) was determined by ¹H NMR.

Table S6. Investigation of conversion of **C2** to **C4**

entry	Conditions	C4/C2
1	None	1 : 1.2
2	w/o D ₂ O	1 : 1.5
3	w/o NEt ₃	1.1 : 1
4	w/o D ₂ O and NEt ₃	1 : 1.5 or > 20 : 1 ^a
5	C4 (20 mol %), w/o D ₂ O and NEt ₃	> 20 : 1
6	No light	0

^a Reaction was performed for 48 h

Table S7. Investigation of conversion of **C4** to **C2**

entry	Conditions	C2 (%)
1	None	0
2	w/o D ₂ O	0
3	w/o NEt ₃	0
4	w/o D ₂ O and NEt ₃	0

Procedure: Four oven-dried 10 mL Schlenk tubes equipped with a magnetic stir bar were charged with **C4** (38.6 mg, 0.1 mmol), respectively. Similar to Table S6. The reaction mixture was irradiated using 10 W 405 nm LEDs for 24 h at 40 °C. During the reaction, HPLC analysis of crude sample from reaction mixture was taken to monitor the reaction.

These control experiments (Table S6, S7) showed: (1) Under standard conditions, it takes 2 days for **C2** to fully convert to **C4**, while **C4** cannot convert to **C2**; (2) D₂O has a slightly promoting effect on the conversion of **C2** to **C4**, while NEt₃ has a slightly inhibitory effect, adding a small amount of **C4** can greatly promote the conversion of **C2** to **C4** within 24 hours. (3) **C4** is stable, which can't be converted to **C2** under any conditions.

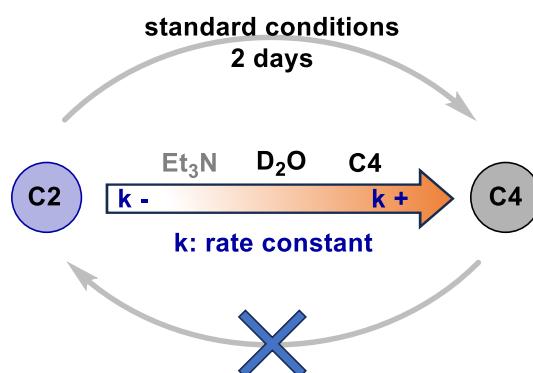


Figure S12. A view of the transformation of regioisomers

4.4 Crossover experiments

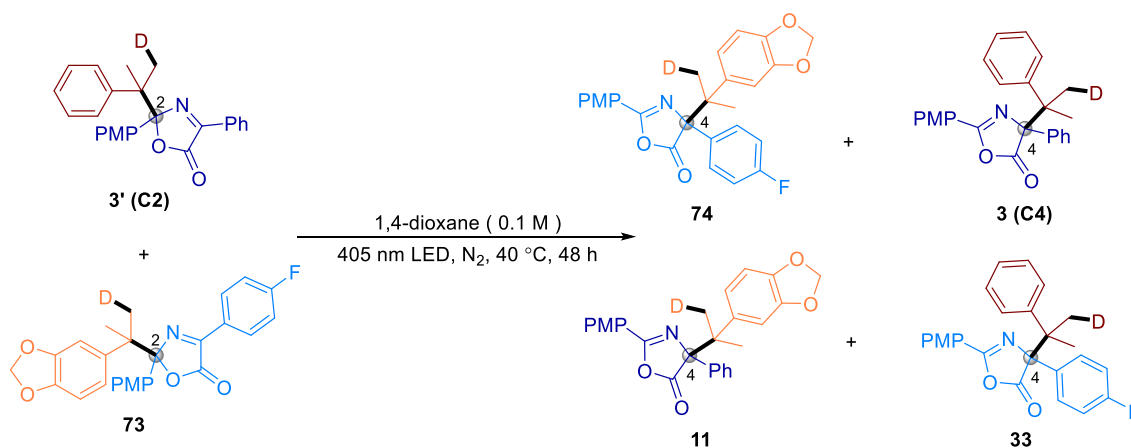


Figure S13
S13

Procedure: A oven-dried 10 mL Schlenk tube was equipped with a magnetic stir bar, the **3'** (19.3 mg, 0.05 mmol) and **73** (22.4 mg, 0.05 mmol) were added. In glove box, super dry 1,4-dioxane (0.5 mL) was added. The tube was sealed and removed from the glove box. The reaction mixture was irradiated under 10 W LEDs (405 nm) at 40 °C for 48 h. After completion, the total ratio of products (**74:3:11:33** =6:42:18:34, due to the different structures of the substrates, the corresponding absorbance values differ as well. The use of this ratio is for reference purposes only) were obtained by HPLC analysis of crude reaction mixture, which revealed that the conversion of regioisomers is a process of C-C bond cleavage followed by intermolecular reaction, rather than intramolecular rearrangement.

4.5 Radical clock experiment

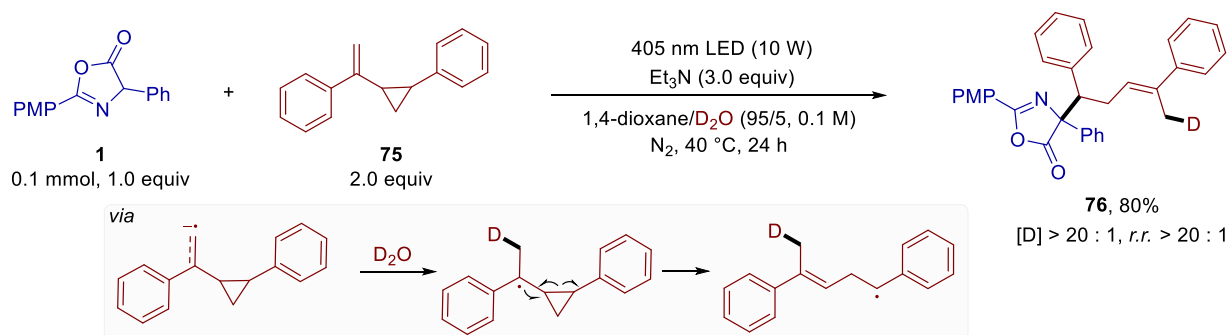


Figure S14

Procedure: An oven-dried 10-mL Schlenk tube equipped with a stirrer was charged with the oxazolone **1** (0.1 mmol, 1.0 equiv). Then, super dry 1,4-dioxane (0.95 mL) and D₂O (0.05 mL) were added in glove box, followed by alkene (0.2 mmol, 44 μL, 2.0 equiv) and NEt₃ (0.3 mmol, 42 μL, 3.0 equiv). The tube was sealed with a screw cap and took out form glove box. The reaction mixture was inserted into the PhotoSyn 3.0 reactor and irradiated using a 10W LED lamp (405 nm) at 40 °C for 24 h. After complete consumption of oxazolone and regioisomers were completely converted (**C-2** to **C-4**), the volatiles were removed in *vacuo*. Then, the crude product was purified by flash chromatography (PE/EtOAc = 50/1) to afford the ring-opening product **76** in 80% yield.

4.6 β -elimination experiment

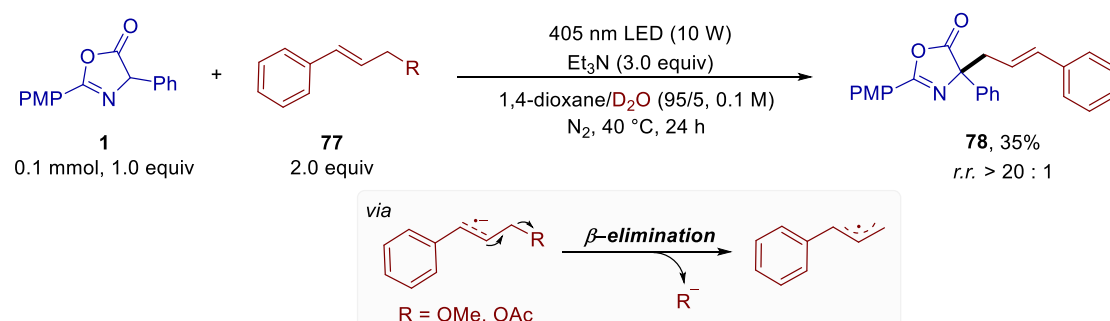


Figure S15

Procedure: An oven-dried 10-mL Schlenk tubes equipped with a stirrer were charged with the oxazolone **1** (0.1 mmol, 1.0 equiv), respectively. Then, super dry 1,4-dioxane (0.95 mL) and D_2O (0.05 mL) were added in glove box, followed by alkene **77** (0.2 mmol, 2.0 equiv) and NEt_3 (0.3 mmol, 42 μL , 3.0 equiv). Two tubes were sealed with a screw cap and took out form glove box. One reaction mixture was inserted into the PhotoSyn 3.0 reactor and irradiated using a 10W LED lamp (405 nm) at 40 °C for 24 h. After complete consumption of oxazolone and regioisomers were completely converted (**C-2** to **C-4**), the volatiles were removed in *vacuo*. Then, the crude product was purified by flash chromatography (PE/EtOAc = 50/1) to afford the non-deuterated product **78** in 35% yield. Other reaction mixture was allowed to react in the dark for one hour, the result revealed that the desired product was not obtained, and indicate it is not a $\text{S}_{\text{N}}2$ reaction.

4.7 Radical anion trapping experiment

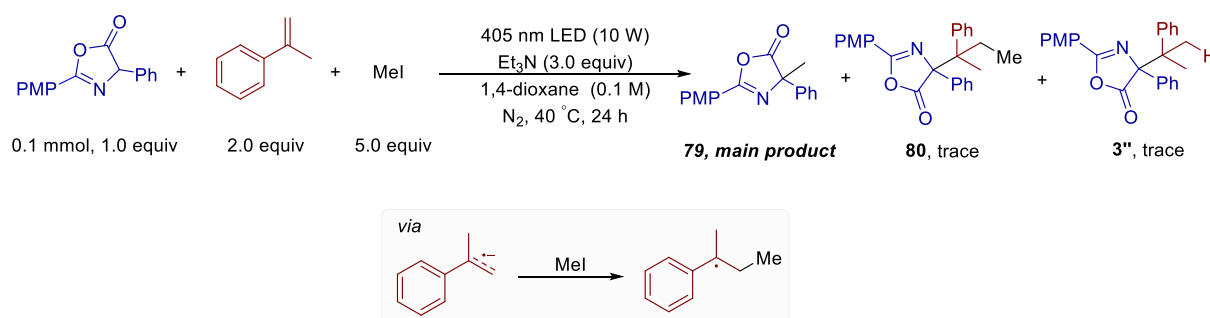
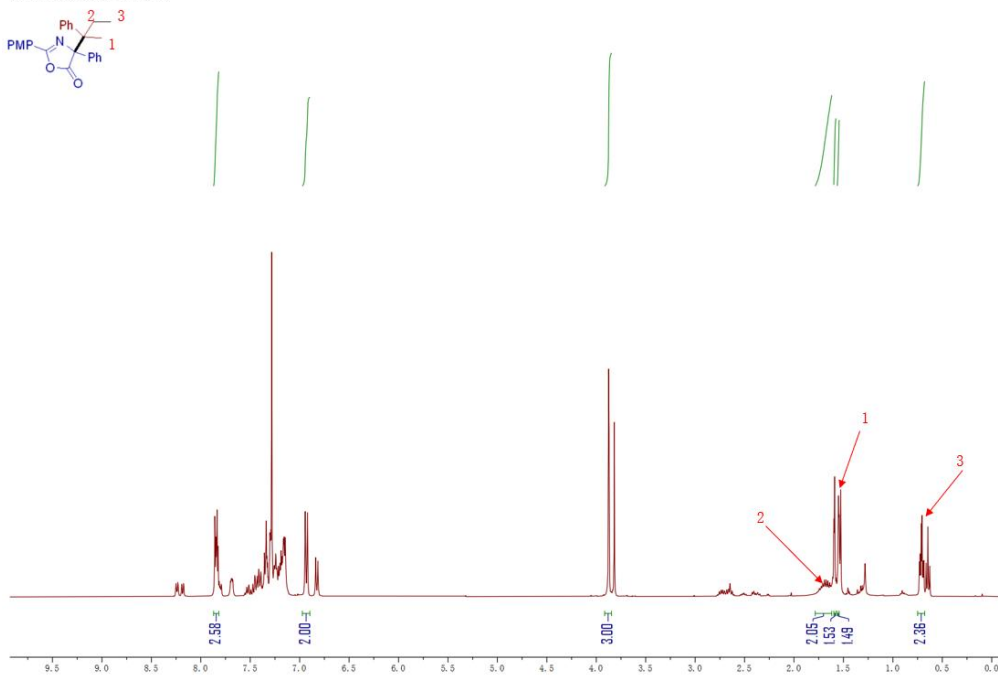
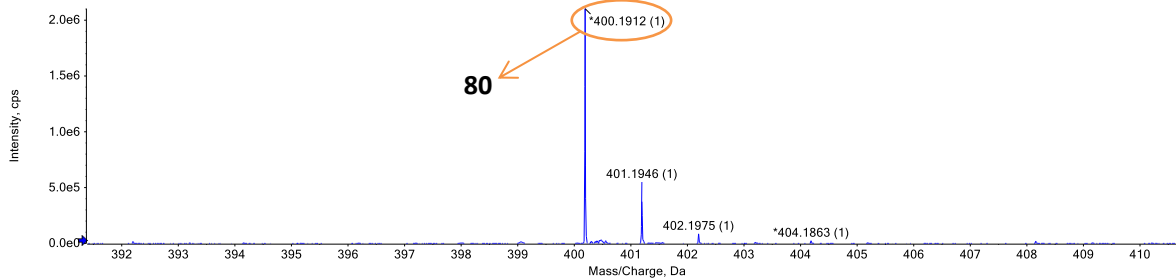


Figure S16

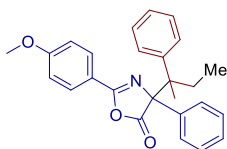
ZK-20240222-CR-58-1-1.1.Fid



Spectrum from 20240410.wiff2 (sample 33) - 12, +TOF MS (100 - 500) from 0.036 to 0.095 min, noise filters... - 500) from 1.603 to 1.769 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



2-(4-methoxyphenyl)-4-phenyl-4-(2-phenylbutan-2-yl)oxazol-5(4H)-one (80)



HRMS (ESI) calcd for C₂₆H₂₅NO₃ (M + H)⁺ 400.1907, found 400.1912

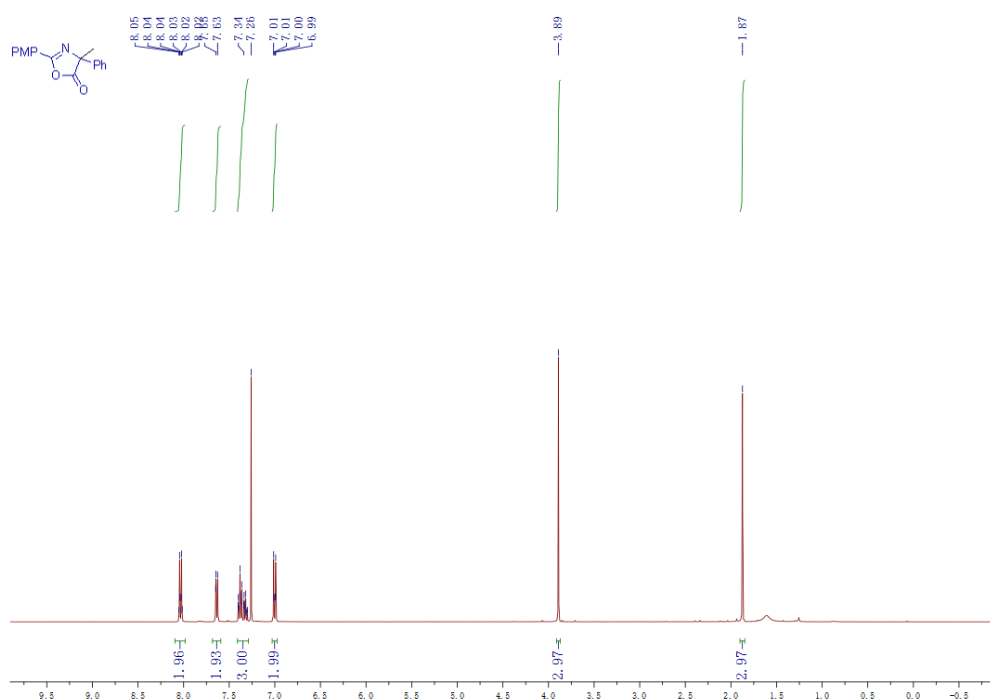
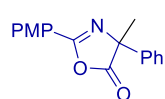


Figure S19

2-(4-methoxyphenyl)-4-methyl-4-phenyloxazol-5(4H)-one (79)



¹H NMR (400 MHz, CDCl₃) δ 8.09 – 7.99 (m, 2H), 7.68 – 7.60 (m, 2H), 7.42 – 7.29 (m, 3H), 7.04 – 6.97 (m, 2H), 3.89 (s, 3H), 1.87 (s, 3H).

Procedure: A 10 mL Schlenk tube was equipped with a magnetic stir bar, the 2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one **1** (0.1 mmol) was added. In glove box, α -methyl-styrene **2** (0.2 mmol, 2.0 equiv), NEt₃ (triethylamine) additive (0.3 mmol, 3.0 equiv) and super dry 1,4-dioxane (1.0 mL) and Mel (5.0 equiv) were added. The tube was sealed and removed from the glove box. The reaction mixture was irradiated under 10 W LEDs (405 nm), continuous circulating water was introduced to ensure that the reaction was carried out at 40 °C. Monitored by TLC until the completely consumption of 2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one **1**, and analysed by HPLC until the regioisomers were completely converted (**C2** to **C4**). Column chromatography and ¹HNMR analysis confirmed the presence of the three-component product, but due to its low polarity and yield, it was not possible to obtain the pure three-component product (**Figure S17**). The main product is oxazolone, which undergoes a two-component SN₂ reaction with Mel to afford the pure product **79** (**Figure S19**).

The ¹HNMR spectrum of the mixture product (**Figure S17**) shows that product **80** has obvious characteristic peaks. And we speculate that the reason why the integral of the methyl at position 3 is less than 3 is because there is a hydrogenated product **3''** generated in the system, and the peak of **3''** is very close to that of **80**. In addition, the

molecular weight of the product **80** was also detected by HRMS analysis (**Figure S18**). The above data all indicate that the alkene generated a radical anion intermediate during the reaction.

4.8 Light on/off experiments

The light on/off experiments showed that no further conversion after initial irradiation in the dark, the fluctuation of yields in the dark are within the range of flash column chromatography error.

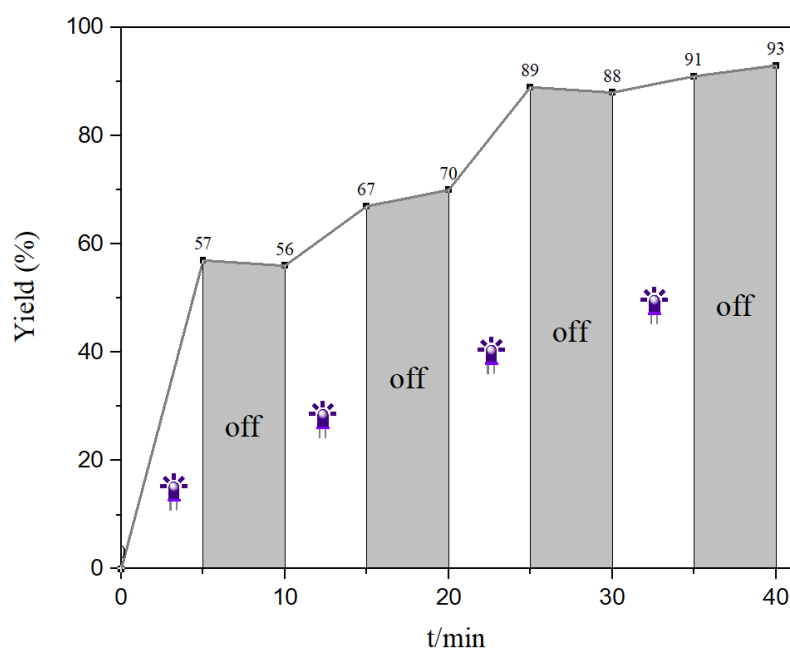


Figure S20 Light on/off experiments

Procedure: Eight oven-dried round bottom flasks (25 ml) with eight stir bars were charged with the oxazolone **1** (1.0 mmol, 26.7 mg), respectively. In glove box, α -methyl-styrene **2** (0.2 mmol, 2.0 equiv), NEt_3 (triethylamine) additive (0.3 mmol, 3.0 equiv) and super dry 1,4-dioxane (0.95 mL) and deuterium oxide (D_2O) (0.05 mL) were added. Eight tubes were sealed and removed from the glove box. The reaction mixture was irradiated under 10 W LEDs (405 nm), continuous circulating water was introduced to ensure that the reaction was carried out at 40 °C. After reaching the corresponding time, the volatiles were removed in *vacuo*, the mixture was concentrated and purified by flash column chromatography to afford pure products and record yield.

4.9 Quantum yield measurement

The photon flux set by the LED ($\lambda = 400$ nm, 10 W) was determined using the standard potassium ferricoxalate photometric method, following a modified literature procedure.

A ferrioxalate actinometer solution was prepared by following the Hammond variation of the Hatchard and Parker procedure outlined in the Handbook of Photochemistry.

1. Potassium ferrioxalate solution: 294.8 mg of potassium ferrioxalate and 139 μL of sulfuric acid (96%) were added to a 50 mL volumetric flask, and filled to the mark with water.

2. Buffer solution with Phenanthroline: 20 mg 1,10-phenanthroline, 2.5 g of NaOAc and 400 μL of sulfuric acid (96%) were added to a 50 mL volumetric flask, and filled to the mark with water.

Both solutions were stored in the dark.

1.0 mL of the 0.0156 M potassium ferric oxalate solution was added to a flask containing a stirring bar. Then, the solution was irradiated for 0 s, 2 s, 5 s. Immediately after irradiation, the buffer solution with Phenanthroline (2.5 mL) was added to the cuvette and the mixture and stirred in the dark for 1 h to allow the ferrous ions to completely coordinate to the phenanthroline. Take 100 μL the mixture and add water to obtain 1 mL solution. The solution was transferred to a quartz cuvette (1.0 cm path length) and the absorbance at $\lambda = 510 \text{ nm}$ was measured by UV/Vis spectroscopy (**Figure S21**).

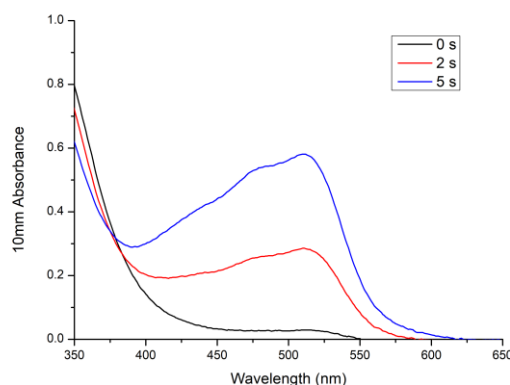


Figure S21. UV/Vis spectra of potassium ferric oxalate/1,10-phenanthroline solutions

The number of moles of Fe^{2+} produced by light irradiation was calculated using:

$$\text{mol Fe}^{2+} = \frac{V_1 V_3 \Delta A (510 \text{ nm})}{V_2 l \varepsilon (510 \text{ nm})}$$

Where

V_1 = the volume of potassium ferric oxalate solution irradiated ($1.0 \times 10^{-3} \text{ L}$).

V_2 = the volume of the solution taken for measurement of the Fe^{2+} ions (100 μL = $1.0 \times 10^{-4} \text{ L}$).

V_3 = the final volume of solution after complexation with 1,10-phenanthroline ($3.5 \times 10^{-3} \text{ L}$).

$\Delta A (510 \text{ nm})$ = the absorbance difference at $\lambda = 510 \text{ nm}$ between the irradiated solution and the solution kept in

dark.

l = the optical path length of the cuvette (1.0 cm).

ϵ (510 nm) = the molar absorption coefficient of the $\text{Fe}(\text{phen})_3^{2+}$ complex at $\lambda = 510 \text{ nm}$ ($1.11 \times 10^4 \text{ L mol}^{-1} \text{ cm}^{-1}$).

t	ΔA	mol Fe^{2+}
2s	0.257	8.18×10^{-6}
5s	0.552	1.76×10^{-5}

The moles of Fe^{2+} were plotted as a function of time (**Figure. S22**)

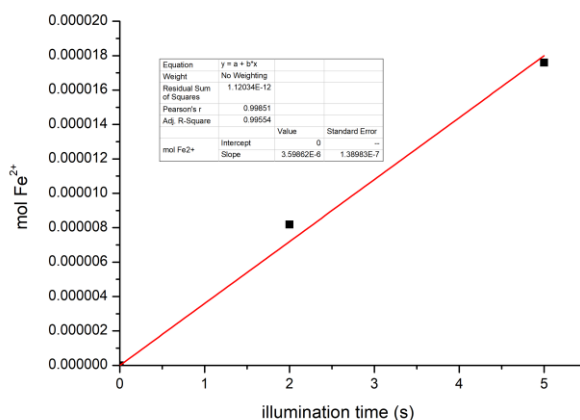


Figure S22. The molar number of Fe^{2+} as a function of time

The photon flux was then calculated using:

$$\text{photon flux} = \frac{\text{mol Fe}^{2+}}{\phi t (1 - 10^{-A})}$$

Where

ϕ the quantum yield of the potassium ferric oxalate in room temperature at 400 nm is 1.13.

t = the irradiated time (s).

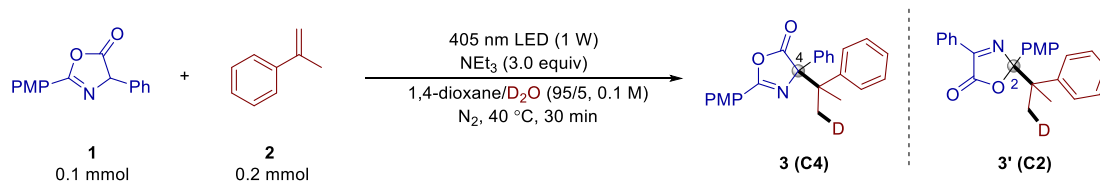
A = the potassium ferric oxalate absorbance at 400 nm, which was measured placing 1 mL of the solution in a cuvette which path length is 1 cm by UV/Vis spectrophotometry.

We obtained an absorbance value of 2.055.

$$\text{photon flux} = \frac{3.6 \times 10^{-6}}{1.13 \times (1 - 10^{-2.055})} = 3.2 \times 10^{-6}$$

The average photon flux was thus calculated to be 3.6×10^{-6} einsteins s^{-1} .

Determination of the reaction quantum yield:



To an oven-dried 10-mL Schlenk tube equipped with a stirrer bar were added oxazolone **1** (0.1 mmol, 26.7 mg). In glove box, α -methylstyrene **2** (0.2 mmol, 2.0 equiv), NEt_3 (0.3 mmol, 3.0 equiv) and super dry 1,4-dioxane (0.95 mL) and deuterium oxide (D_2O) (50 μL) were added. Continuous circulating water was introduced to ensure that the reaction is carried out at 40 $^\circ\text{C}$. The reaction mixture was irradiated using 1 W LEDs ($\lambda \text{ max} = 405 \text{ nm}$) for 30 min, the volatiles were removed in *vacuo*, then the residue purified by flash column chromatography on silica (PE/EtOAc = 50/1) to afford the mixture product **3** and **3'** (48% yield) as a colorless oil.

$$\Phi = \frac{\text{Mol product}}{\text{flux} \cdot t \cdot f}$$

An absorption spectrum gave an $A(400 \text{ nm})$ value of > 3 , indicating that the fraction of absorbed light (f) is > 0.999 .

$$\Phi = \frac{4.8 \times 10^{-5}}{3.2 \times 10^{-6} \times 30 \times 60 \times 1} = 0.0083$$

The reaction quantum yield (Φ) was thus determined to be $\Phi = 0.0083$.

4.10 Proposed mechanism for the radical-radical coupling.

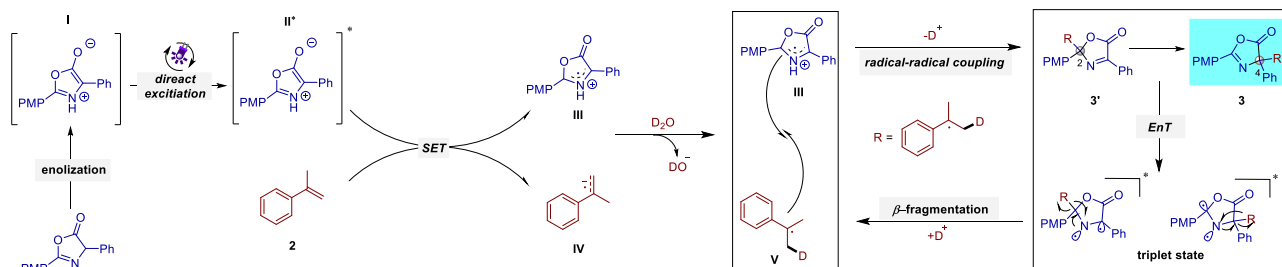
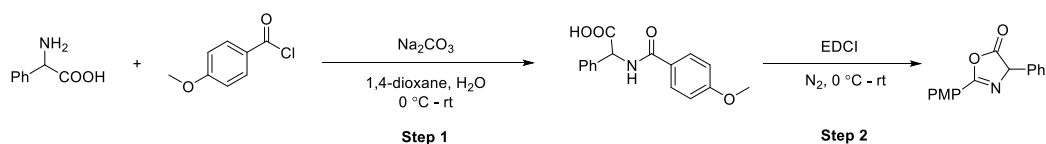


Figure S23. Proposed mechanism

5 Preparation of Starting Materials

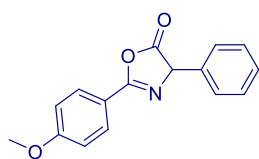
5.1 Synthesis route to oxazolone 1



Step 1: 2-amino-2-phenylacetic acid (1.0 equiv) and Na_2CO_3 (3.4 equiv) was added to round bottom flask equipped with a stirring bar. The reaction mixture was dissolved in 1,4-dioxane (0.50 M) and H_2O (0.18 M). After cooled to $0\text{ }^\circ\text{C}$, 4-methoxybenzoyl chloride (1.1 equiv) was added dropwise. The cooling bath was removed and the reaction mixture was stirred at room temperature. After 1 h, the reaction mixture was diluted with H_2O and CH_2Cl_2 . The aqueous layer was separated, and 1 M HCl aq was added to it until cloudy. It was extracted twice with EA, the combined organic layer was dried over Na_2SO_4 , filtered and concentrated to obtain the crude product. The crude product was purified by flash chromatography (PE/EA = 3/1) to afford the product.

Step 2: To a solution of 2-(4-methoxybenzamido)-2-phenylacetic acid in CH_2Cl_2 (0.072 M) under argon atmosphere was added 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.2 equiv) at $0\text{ }^\circ\text{C}$. The cooling bath was removed and the reaction mixture was stirred at room temperature. After stirring for 1 h, the reaction mixture was washed with H_2O , sat. NaHCO_3 aq and brine. The combined organic layers were dried over Na_2SO_4 and filtered. After removal of solvent under reduced pressure. The crude product was purified by flash chromatography.³

2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (1)

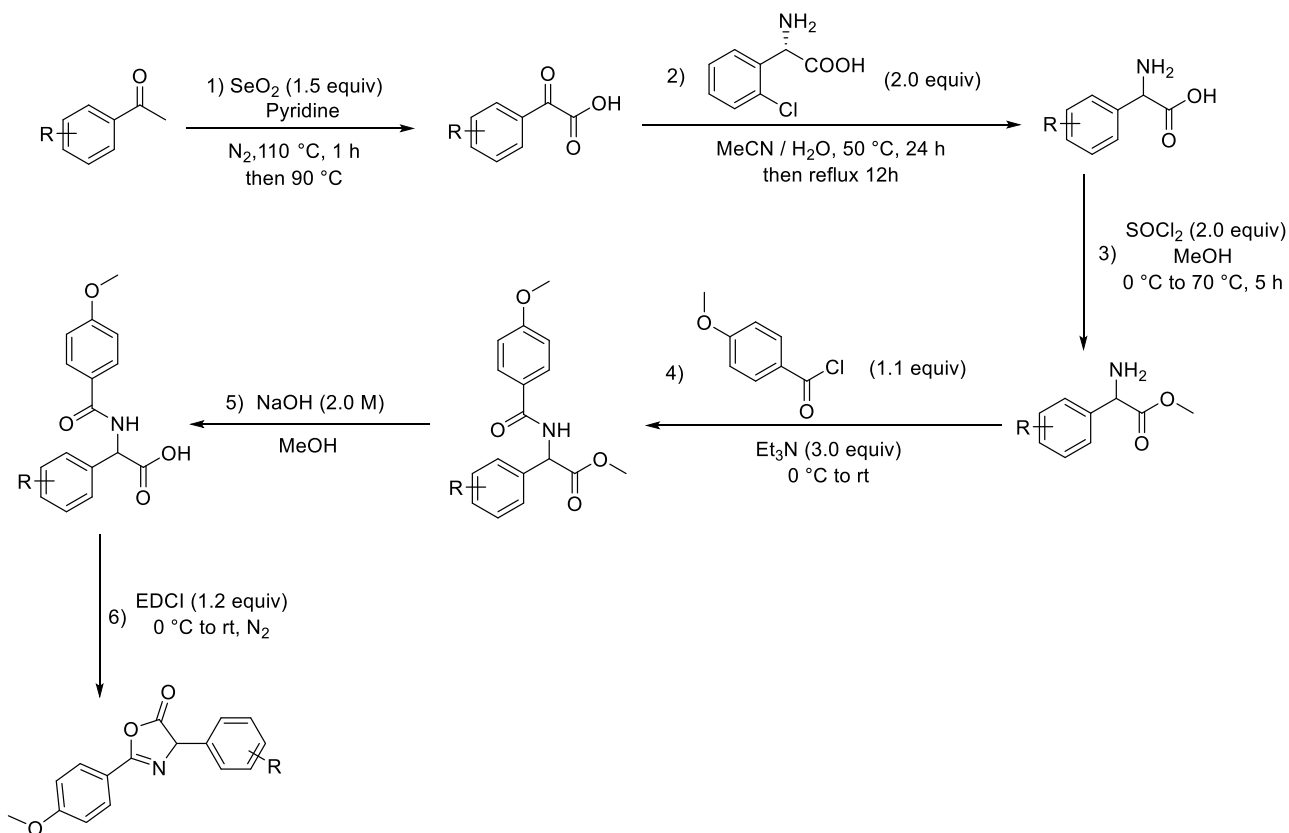


$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.08 – 8.01 (m, 2H), 7.46 – 7.35 (m, 5H), 7.04 – 6.98 (m, 2H), 5.49 (s, 1H), 3.89 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ = 176.53, 163.47, 162.31, 133.79, 130.06, 129.01, 128.69, 126.88, 117.94, 114.33, 68.14, 55.56.

HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{14}\text{NO}_3$ ($\text{M} + \text{H}$)⁺ 268.0968, found 268.0969.

Note: The temperature of the water bath is lower than $40\text{ }^\circ\text{C}$ when the solvent was vacuumed in step2. The crude product was purified by flash chromatography (operation time is less than 15 minutes).

5.2 Synthesis of oxazolones



Step 1: Substituted aryl-methyl ketone (1.0 equiv.) and selenium dioxide (SeO_2 , 1.5 equiv.) were added to a dry, three-necked round-bottomed flask. The flask was then flushed with nitrogen, followed by adding anhydrous pyridine (0.5 M) via a syringe. The reaction mixture was heated in an oil bath to 110 °C for 1 h, and then the bath temperature was reduced to 90 °C for several hours. After completion of the reaction, as determined by TLC, the solution containing precipitated selenium was filtered, and the residue was washed with ethyl acetate. The combined filtrate was concentrated and dissolved in 50 mL ethyl acetate. The organic layer was treated with 1 M HCl in a separating funnel to wash away the remaining pyridine. Then 1 M NaOH was added and the aqueous layer was separated, followed by acidification using 1 M HCl to about pH 1.0. The mixture was extracted with ethyl acetate for several times, and the combined organic layers were dried (anhydrous Na_2SO_4) and concentrated on a rotary evaporator. The crude product was used in the next step without further purification.⁴

Step 2: To a flask charged with aryl glyoxylic acid (1.0 equiv.) and *L*-2-(2-chlorophenyl) glycine (2.0 equiv.) were added MeCN (0.14 M) and H_2O (0.34 M) at room temperature. After the reaction mixture was stirred for 24 h at 50 °C, then it was refluxed for 12 h. Then, it was cooled to room temperature, and Et_2O (10 mL) was added. The reaction mixture was stirred until the product was fully precipitated. After filtration, the precipitate was washed with

Et₂O. Arylglycine was obtained as a white solid.⁵

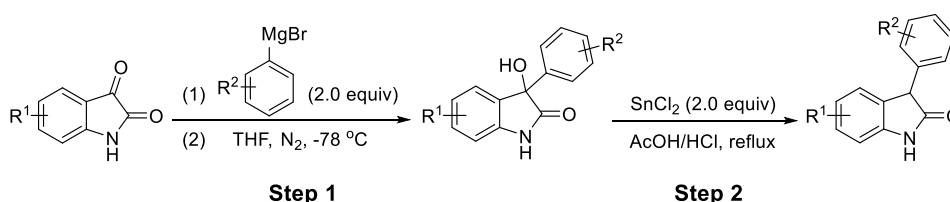
Step 3: To a solution of arylglycine (1.0 equiv.) in MeOH (0.25 M) was added SOCl₂ (2.0 equiv.) slowly at 0 °C. The cooling bath was removed and the reaction mixture was refluxed for 5 h. When cooled to room temperature, the reaction mixture was concentrated on a rotary evaporator. The crude product was used in the next step without further purification.

Step 4: To a solution of Amino acid methyl ester (1.0 equiv.) and Et₃N (3.0 equiv.) in CH₂Cl₂ (0.25 M) was added dropwise 4-methoxybenzoyl chloride (1.1 equiv.) at 0 °C. The cooling bath was removed and the reaction mixture was stirred at room temperature. After 5 h, the reaction mixture was washed with 1 M HCl, sat. NaHCO₃ aq and brine. The combined organic layers were dried over Na₂SO₄, filtered and concentrated to obtain the crude product, which was purified by flash column chromatography (PE/EtOAc = 3/1) to give the amide as white solid.

Step 5: To a solution of amide (1.0 equiv.) in MeOH (0.57 M) was added 2.0 M NaOH (1.9 M) and stirred for 0.5 h. After volatile was removed, H₂O was added to the residue and washed with CH₂Cl₂. The aqueous layer was acidified with 1 M HCl until precipitate was generated. The white precipitate was filtered and washed with diethyl ether. It was used in the next step without further purification.

Step 6: To a solution of acid (1.0 equiv.) in CH₂Cl₂ (0.1 M) was added EDCI (1.2 equiv. in DCM) at 0 °C under argon atmosphere. The cooling bath was removed and the reaction mixture was stirred for 1 h. The reaction mixture was washed with H₂O, sat. NaHCO₃ aq and brine. The organic layers were dried over Na₂SO₄, filtered and concentrated. The pure oxazolones were obtained by recrystallization (diethyl ether/*n*-hexane) or flash column chromatography (PE/EtOAc = 6/1) as white solid.⁶

5.3 Synthesis of 3-Arylindolin-2-one Derivatives



Step 1:

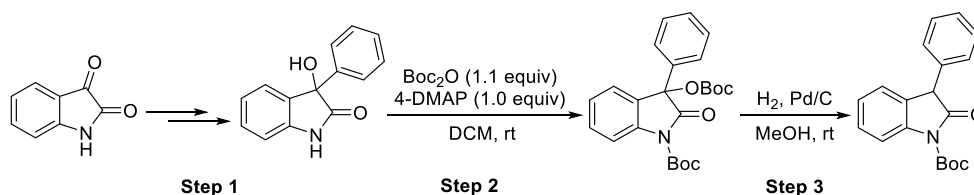
(1) Preparation for Aryl Grignard reagent: a 50 mL round-bottomed flask was equipped with a magnetic stir bar, to a stirring mixture of magnesium (1.2 equiv) and a small piece of iodine in dry THF (1.0 M). A solution of aryl bromide (1.0 equiv) in 2 mL of dry THF was added dropwise to the round-bottom flask and stirred for 3 h under

N₂ atmosphere. After the formation of Grignard reagent (colorless to brownish-green), the reaction mixture was cooled to 0 °C.

(2) Another 50 mL round-bottomed flask was equipped with a magnetic stir bar, to a stirring isatin (10.0 mmol) in dried THF (20 mL), then cooled to -40 °C for 30 min. Previously obtained Grignard reagent in THF (2.0 equiv) was added dropwise to the reaction mixture under N₂ atmosphere, then the mixture was allowed to warm to room temperature and stirred until isatin was consumed completely. The reaction mixture was diluted with ether, cooled in an ice-bath, and then quenched with HCl (2 M). The aqueous layer was extracted with ether, combined organic layers and washed with water and brine, then dried over with Na₂SO₄, filtered and concentrated in *vacuo*, 3-hydroxy-3-arylindolin-2-one was obtained as solid and no purification was necessary for further transformation.

Step 2: A 50 mL round-bottomed flask was equipped with a magnetic stir bar, to a stirring the crude product (5.0 mmol) obtained above in AcOH/HCl (30 mL/2 ml), then SnCl₂ (10.0 mmol) was added at room temperature. The mixture was heated to reflux, monitored by TLC until the completely consumption of the starting material. Next, the solution was cooled to room temperature, concentrated in *vacuo*, and diluted with EtOAc. The residue was washed with water (3x), saturated aqueous NaHCO₃, and brine. The organic layer was dried with anhydrous Na₂SO₄, filtered and concentrated in *vacuo*. The residue was recrystallized (PE/EtOAc) to afford corresponding product as white solid.⁷

5.4 Synthesis of N-Boc-3-Arylindolin-2-one



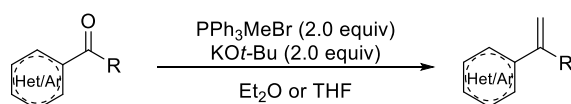
Step 1: Same as above (5.3-step 1);

Step 2: A 25 mL round-bottomed flask was equipped with a magnetic stir bar, to stirring mixture of 3-hydroxy-3-arylindolin-2-one (1125 mg, 5.0 mmol) and 4-DMAP (560 mg, 5.0 mmol, 1.0 equiv) in DCM (10 mL), (Boc)₂O (1.3 mL, 5.5 mmol, 1.1 equiv) was added at room temperature and stirred until starting material was consumed completely. The reaction mixture was diluted with DCM, quenched with saturated aqueous NH₄Cl. The aqueous layer was extracted with DCM (3x), combined organic layers and dried over with Na₂SO₄ and concentrated in *vacuo*.

The residue was purified by flash chromatography to afford provide the desired product.

Step 3: A 25 mL round-bottomed flask was equipped with a magnetic stir bar, put the product obtained above (2.0 mmol) and Pd/C (400 mg) into flask and seal, and then replaced with hydrogen (3x), MeOH (8 mL) was added and stirred under hydrogen atmosphere (balloon) for 6 h at room temperature. The reaction mixture was filtered to remove Pd/C, and the residue washed with DCM, dried over with Na₂SO₄, filtered and concentrated in *vacuo*. The crude product was purified by flash column chromatography (PE/EtOAc = 10/1) to afford *N*-Boc-3-Arylindolin-2-one.⁷

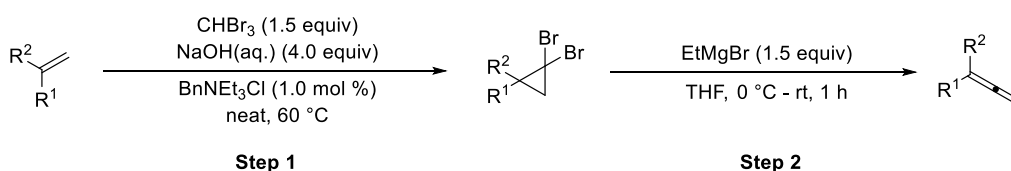
5.5 Synthesis of terminal alkenes Derivatives



According to the reported literature^[8]: In glove box, a 50 mL round-bottomed flask was equipped with a magnetic stir bar, to suspending PPh₃MeBr (10.0 mmol, 2.0 equiv) in dry Et₂O or THF (30 mL), then KO^t-Bu (10.0 mmol, 2.0 equiv) was added in batched. The resulting yellow suspension was stirred for 1 h and the specified ketone (5.0 mmol) was added. The reaction mixture was monitored by TLC until the completely consumption of the starting material or after stirring overnight. The reaction mixture quenched with saturated aqueous NH₄Cl, the organic layer was washed with water (3x), dried over with Na₂SO₄, filtered and concentrated in *vacuo*. The crude product was purified by flash column chromatography (*n*-Pentane) to afford the terminal alkene.⁸

Note: due to the volatility of most of the terminal alkenes, filtered and concentrated must under low temperature.

5.6 Synthesis of 1,1-disubstituted allenes

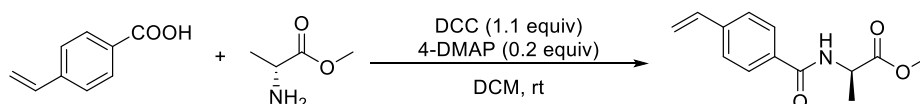


Step 1: To a mixture of alkene (5 mmol, 1.0 equiv), bromoform (7.5 mmol, 1.5 equiv), and triethylbenzylammonium chloride (0.05 mmol, 1.0 mol %) was added dropwise a solution of NaOH (0.8 g) in water (0.8 mL) over 1 h. The resulting mixture was stirred vigorously at 60 °C for 24 h, then cooled to room temperature, and quenched with

water (5.0 mL). The mixture was extracted with dichloromethane and the organic phase was separated, dried over sodium sulfate, and concentrated. The residue was purified by column chromatography over silica gel with hexane as eluent to give the 1,1-Dibromocyclopropane.

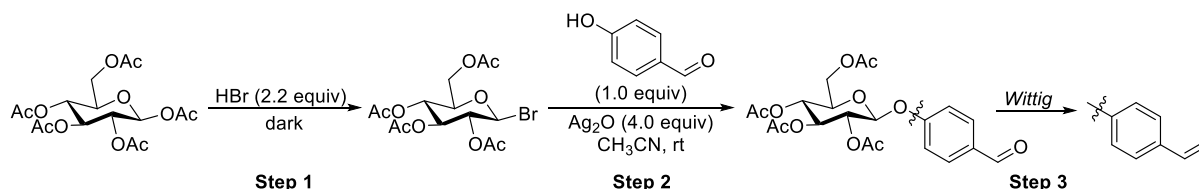
Step 2: To a stirred solution of 1,1-Dibromocyclopropane (4.5 mmol, 1.0 equiv) in dry THF (5.0 mL) at 0 °C was added dropwise ethylmagnesium bromide (6.75 mL, 6.75 mmol, 1.0 M in THF) under nitrogen over 0.5 h. After stirred at 0 °C for 1 h, the mixture was quenched with 3 M hydrochloric acid solution (2.0 mL) and diluted with ethyl ether (20 mL). The organic phase was washed with water (5.0 mL), dried over magnesium sulfate, and concentrated. The residue was purified by column chromatography over silica gel with *n*-pentane as eluent to give 1,1-disubstituted allene.⁹

5.7 L-Alanine esterified derivative



A 50 mL round-bottomed flask was equipped with a magnetic stir bar, to stirring mixture of 4-Vinylbenzoic acid (296 mg, 2.0 mmol), methyl D-alaninate (227 mg, 2.2 mmol, 1.1 equiv), DMAP (24.4 mg, 0.4 mmol, 0.2 equiv) and DCC (453 mg, 2.2 mmol, 1.1 equiv) in DCM (20 mL), the reaction mixture stirred at air atmosphere and monitored by TLC until the completely consumption of the starting material, filtered and concentrated in *vacuo*. The crude product was purified by flash column chromatography (PE/EtOAc = 10/1) to afford the *L*-Alanine esterified derivative.

5.8 Synthesis of α -D-glucopyranosyl derivative



According to the reported literature^[10-11]:

Step 1: In glove box, a 100 mL round-bottomed flask was equipped with a magnetic stir bar and covered with tin foil, to stirring beta-D-galactose pentaacetate (9.8 g, 25 mmol) in dry DCM (40 mL) under dark. The flask was sealed and removed from the glove box, and then equipped with a N₂ balloon, cooled to 0 °C in an ice bath. The hydrogen bromide 33 wt% in acetic acid (9.8 mL, 2.2 equiv) was added dropwise. The reaction mixture was stirred

for 45 minutes at 0 °C and allowed to room temperature. Stirred and monitored by TLC (PE/EtOAc = 1/1). The reaction mixture was diluted with DCM, and then washed with saturated aqueous NaHCO₃ (2x), the aqueous layer was extracted with DCM (2x), and the combined organic layers dried over with Na₂SO₄, filtered, and concentrated in *vacuo*. The 2,3,4,6-tetra-O-acetyl- α -D-galactopyranosyl bromide was obtained and no purification was necessary for further transformation.¹⁰

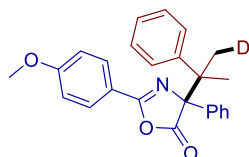
Step 2: In glove box, a 500 mL round-bottomed flask was equipped with a magnetic stir bar, to stirring mixture of the crude product obtained above, 4-hydroxybenzaldehyde (1.22 g, 25 mmol) and silver(I) oxid (23.2 g, 100 mmol) in dry CH₃CN (200 mL), the flask was sealed and removed from the glove box, and then equipped with a N₂ balloon. The reaction mixture was stirred at room temperature for 5 h. Monitored by TLC until the completely consumption of the starting material. The reaction mixture concentrated under reduced pressure, the residue was dissolved in DCM and filtered through a thin Celite layer, and the Celite was washed with DCM (2x). The filtrate was concentrated in *vacuo*. The crude product was purified by flash column chromatography to afford the desired product.¹¹

Step 3: Same as part 5.5

6 Characterization Data

Note: When we tested the melting point of products, and found that most compounds will decompose before melting (190 - 210 °C), so we did not mark the melting point of these compounds. Around 1.56 ppm (water peak) and 1.00 ppm – 1.42 ppm in NMR are respectively from the CDCl₃ and eluent (petroleum ether), which do not affect the yield of the product (background correction of yield was done for each compounds). Due to the influence of deuterium atoms, the carbon connected by deuterium atom will shatter in the carbon spectrum, resulting in unclear performance. Affected by different structures, the range of the carbon connected by deuterium atom chemical shift is between 14 – 30.

2-(4-methoxyphenyl)-4-phenyl-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (3)

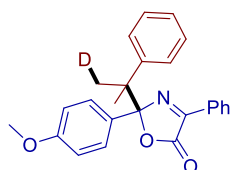


Isolated yield 96% (37.0 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). ¹H NMR (400 MHz, CDCl₃) δ 7.90 – 7.83 (m, 2H), 7.83 – 7.76 (m, 2H), 7.42 – 7.30 (m, 5H), 7.21 – 7.11 (m, 3H), 6.99 – 6.88 (m, 2H), 3.88 (s, 3H), 1.62 – 1.52 (m, 5H). ¹³C NMR (101 MHz, CDCl₃)

δ 177.49, 162.92, 158.62, 142.74, 135.35, 129.66, 128.32, 128.17, 127.90, 127.46, 127.18, 126.73, 118.32, 114.00, 79.34, 55.42, 46.08, 23.99, 23.34.

HRMS (ESI) calcd for C₂₅H₂₂DNO₃ (M + H)⁺ 387.1813, found 387.1811.

2-(4-methoxyphenyl)-4-phenyl-2-(2-phenylpropan-2-yl-1-d)oxazol-5(2H)-one (3')



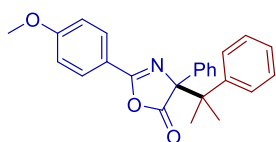
Separation by *prep*-HPLC (Waters E600) (MeOH : H₂O = 90 : 10), [D] > 20 : 1.

¹H NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 7.2 Hz, 2H), 7.54 – 7.48 (m, 1H), 7.47 – 7.36 (m, 4H), 7.30 (d, *J* = 7.1 Hz, 2H), 7.22 – 7.10 (m, 3H), 6.80 (d, *J* = 8.9 Hz, 2H), 3.79 (s, 3H), 1.53 – 1.49 (m, 5H). ¹³C

NMR (101 MHz, CDCl₃) δ 163.86, 159.63, 155.84, 141.73, 132.13, 129.67, 128.74, 128.56, 128.46, 127.33, 126.83, 112.67, 109.34, 55.26, 47.14, 24.36, 24.26.

HRMS (ESI) calcd for C₂₅H₂₂DNO₃ (M + Na)⁺ 409.1633, found 409.1624.

2-(4-methoxyphenyl)-4-phenyl-4-(2-phenylpropan-2-yl)oxazol-5(4H)-one (3'')



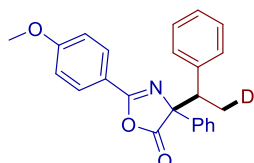
Isolated yield 90% (34.6 mg, 0.1 mmol scale, *r.r.* > 20 : 1), colorless oil, eluent (PE : EA = 50 : 1).

¹H NMR (400 MHz, CDCl₃) δ 7.87 – 7.73 (m, 4H), 7.38 – 7.28 (m, 5H), 7.20 – 7.10 (m, 3H), 6.95 – 6.87 (m, 2H), 3.85 (s, 3H), 1.58 (s, 3H), 1.52 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 177.60, 162.86,

158.54, 142.75, 135.37, 129.62, 128.33, 128.18, 127.90, 127.46, 127.18, 126.74, 118.37, 113.99, 79.35, 55.42, 46.12, 24.02, 23.38.

HRMS (ESI) calcd for $C_{25}H_{23}NO_3$ ($M + H$)⁺ 386.1751, found 386.1752.

2-(4-methoxyphenyl)-4-phenyl-4-(1-phenylethyl-2-d)oxazol-5(4H)-one (4)



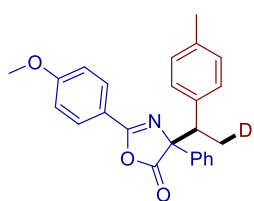
Isolated yield 56% (20.8 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). **¹H NMR** (400 MHz, $CDCl_3$) δ 8.08 – 7.98 (m, 1H), 7.94 – 7.86 (m, 1H), 7.86 – 7.80 (m, 1H), 7.60 – 7.53 (m, H), 7.46 – 7.38 (m, 1H), 7.37 – 7.31 (m, 0.5H), 7.31 – 7.06 (m, 6.5H), 7.04

– 6.88 (m, 2H), 3.94 – 3.78 (m, 3H), 3.68 (t, *J* = 7.1 Hz, 0.5H), 3.61 (t, *J* = 7.0 Hz, 0.5H), 1.36 – 1.21 (m, 2H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 179.04, 178.59, 163.19, 163.06, 159.74, 159.55, 140.20, 139.67, 137.88, 137.67, 129.92, 129.79, 129.09, 129.06, 128.53, 128.09, 127.95, 127.74, 127.60, 127.39, 126.79, 126.29, 126.14, 118.29, 118.25, 114.18, 114.10, 78.13, 77.88, 55.52, 55.47, 50.05, 49.91, 16.4 – 15.0 (m, 2C).

HRMS (ESI) calcd for $C_{24}H_{20}DNO_3$ ($M + H$)⁺ 373.1657, found 373.1656.

2-(4-methoxyphenyl)-4-phenyl-4-(1-(p-tolyl)ethyl-2-d)oxazol-5(4H)-one (5)



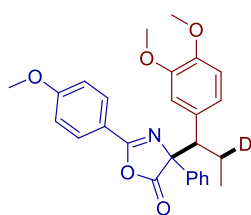
Isolated yield 67% (25.9 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). **¹H NMR** (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.9 Hz, 1H), 7.95 – 7.88 (m, 1H), 7.86 – 7.80 (m, 1H), 7.63 – 7.53 (m, 1H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.37 – 7.31 (m, 0.5H), 7.26 – 7.11 (m, 2.5H), 7.04 (d, *J* = 8.0 Hz, 1H), 7.02 – 6.87 (m, 4H), 3.93 – 3.83 (m, 3H), 3.65 (t, *J* = 7.1 Hz, 0.5H),

3.59 (t, *J* = 7.0 Hz, 0.5H), 2.27 – 2.17 (m, 3H), 1.32 – 1.22 (m, 2H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 178.07, 177.59, 162.09, 161.97, 158.65, 158.45, 136.94, 136.70, 136.05, 135.89, 135.60, 135.21, 128.87, 128.76, 127.87, 127.81, 127.63, 127.46, 127.27, 127.04, 127.00, 126.65, 125.22, 125.11, 117.30, 117.23, 113.10, 113.02, 77.17, 76.91, 54.47, 54.42, 48.51, 20.00, 15.5 – 14.3 (m, 2C).

HRMS (ESI) calcd for $C_{25}H_{22}DNO_3$ ($M + Na$)⁺ 409.1633, found 409.1643.

4-(1-(3,4-dimethoxyphenyl)propyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (6)



Isolated yield 41% (18.3 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 8.09 – 7.98 (m, 2H), 7.57 (d, *J* = 7.4 Hz, 2H), 7.26 –

7.13 (m, 3H), 6.99 (d, *J* = 9.0 Hz, 2H), 6.77 (s, 1H), 6.74 – 6.61 (m, 2H), 3.89 (s, 3H), 3.79 (s, 3H),

3.76 (s, 3H), 3.33 – 3.23 (m, 1H), 1.90 – 1.50 (m, 1H), 0.70 (d, *J* = 7.3 Hz, 3H). **¹³C NMR** (101 MHz,

CDCl₃) δ 178.38, 163.21, 163.17, 159.99, 148.22, 148.18, 137.99, 129.85, 129.75, 128.57, 128.09, 126.32, 122.80, 118.22,

114.20, 111.58, 110.45, 78.43, 57.20, 55.64, 55.53, 55.45, 12.18.

Note: Due to the influence of the water peak in the ¹H NMR spectrum (CDCl₃), the deuterated ratio is determined by the ¹H NMR spectrum in DMSO-*d*₆.

HRMS (ESI) calcd for C₂₇H₂₆DNO₅ (M + Na)⁺ 469.1844, found 469.1852.

¹H NMR (400 MHz, CDCl₃) δ 7.98 – 7.87 (m, 2H), 7.81 (d, *J* = 7.3 Hz, 2H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 1H), 6.95

(d, *J* = 9.0 Hz, 2H), 6.82 (dd, *J* = 8.2, 1.9 Hz, 1H), 6.78 – 6.69 (m, 2H), 3.87 (s, 3H), 3.80 (s, 3H), 3.55 (s, 3H), 3.36 – 3.28 (m,

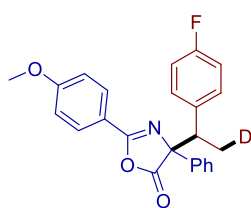
1H), 1.95 – 1.82 (m, 0.5H), 1.68 – 1.50 (m, 0.5H), 0.60 (d, *J* = 7.4 Hz, 3H). **¹³C NMR** (101 MHz, CDCl₃) δ 178.31, 163.25, 163.21,

160.05, 148.22, 148.18, 137.95, 129.89, 129.80, 128.58, 128.10, 126.31, 122.80, 118.14, 114.26, 114.21, 111.56, 110.45, 78.41,

57.21, 55.64, 55.53, 55.46, 12.18.

HRMS (ESI) calcd for C₂₇H₂₆DNO₅ (M + Na)⁺ 469.1844, found 469.1853.

4-(1-(4-fluorophenyl)ethyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (7)



Isolated yield 91% (35.5 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 8.03 (d, *J* = 8.9 Hz, 1H), 7.93 – 7.87 (m, 1H), 7.84 –

7.78 (m, 1H), 7.54 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.38 – 7.30 (m, 0.5H), 7.26 –

7.15 (m, 2.5H), 7.16 – 7.08 (m, 1H), 7.00 (d, *J* = 8.9 Hz, 1H), 6.95 (d, *J* = 8.9 Hz, 1H), 6.89 – 6.77 (m,

2H), 3.92 – 3.84 (m, 3H), 3.67 (t, *J* = 7.1 Hz, 0.5H), 3.59 (t, *J* = 7.0 Hz, 0.5H), 1.32 – 1.20 (m, 2H, containing petroleum ether

peak). **¹³C NMR** (101 MHz, CDCl₃) δ 177.91, 177.52, 162.23, 161.00 (d, *J* = 237.35 Hz), 160.66 (d, *J* = 245.83 Hz), 158.81,

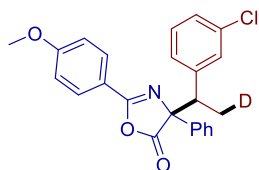
158.69, 136.60, 136.52, 134.89 (d, *J* = 3.5 Hz), 134.38 (d, *J* = 3.2 Hz), 129.54 (d, *J* = 7.8 Hz), 129.47 (d, *J* = 7.0 Hz), 128.90,

128.76, 127.54, 127.14, 126.80, 125.19, 125.00, 117.06, 117.01, 113.66 (d, *J* = 39.3 Hz), 113.45 (d, *J* = 39.2 Hz), 113.18, 113.13,

76.98, 76.69, 54.49, 54.45, 48.24, 48.01. **¹⁹F NMR** (377 MHz, CDCl₃) δ -115.21, -116.05.

HRMS (ESI) calcd for C₂₄H₁₉DFNO₃ (M + H)⁺ 391.1563, found 391.1571.

4-(1-(3-chlorophenyl)ethyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (8)



Isolated yield 69% (28.0 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 8.10 – 8.01 (m, 1H), 7.97 – 7.87 (m, 1H), 7.84 – 7.76

(m, 1H), 7.55 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.45 – 7.38 (m, 1H), 7.38 – 7.32 (m, 0.5H), 7.27 – 7.18 (m,

2.5H), 7.17 – 6.92 (m, 5H), 3.92 – 3.84 (m, 3H), 3.64 (t, *J* = 7.1 Hz, 0.5H), 3.58 (t, *J* = 7.0 Hz, 0.5H),

1.30 – 1.20 (m, 2H, containing petroleum ether peak). **¹³C NMR** (101 MHz, CDCl₃) δ 178.87, 178.40, 163.33, 163.21, 160.04,

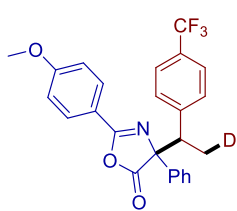
159.88, 142.36, 141.80, 137.47, 137.37, 133.71, 133.39, 130.02, 129.86, 129.26, 129.22, 128.82, 128.62, 128.27, 128.23,

127.96, 127.58, 127.33, 127.29, 126.97, 126.25, 126.03, 118.04, 117.99, 114.26, 114.17, 77.78, 77.49, 55.55, 55.49, 49.69,

49.50, 16.41, 16.22, 16.03, 15.45, 15.23, 15.03.

HRMS (ESI) calcd for C₂₄H₁₉DCINO₃ (M + H)⁺ 407.1267, found 407.1280.

2-(4-methoxyphenyl)-4-phenyl-4-(1-(4-(trifluoromethyl)phenyl)ethyl-2-d)oxazol-5(4H)-one (9)



Isolated yield 38% (16.7 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 8.07 (d, *J* = 8.8 Hz, 2H), 7.55 (dd, *J* = 7.9, 1.5 Hz, 2H),

7.38 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 7.25 – 7.17 (m, 3H), 7.01 (d, *J* = 9.0 Hz, 2H), 3.90 (s,

3H), 3.71 (t, *J* = 7.0 Hz, 1H), 1.30 (d, *J* = 7.0 Hz, 2H). **¹³C NMR** (101 MHz, CDCl₃) δ 177.87, 163.53,

160.41, 143.79, 137.19, 130.08, 129.47, 128.69, 128.42, 126.23, 124.95 (q, *J* = 3.8 Hz), 124.90, 117.49, 114.31, 77.60, 55.54,

49.58. **¹⁹F NMR** (376 MHz, DMSO-*d*₆) δ -60.88.

HRMS (ESI) calcd for C₂₅H₁₉DF₃NO₃ (M + H)⁺ 441.1531, found 441.1535.

¹H NMR (400 MHz, CDCl₃) δ 8.00 – 7.90 (m, 2H), 7.87 – 7.78 (m, 2H), 7.48 – 7.33 (m, 7H), 6.96 (d, *J* = 8.9 Hz, 2H), 3.88 (s,

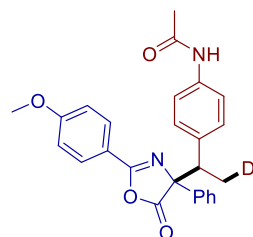
3H), 3.74 (t, *J* = 7.1 Hz, 1H), 1.30 (d, *J* = 7.2 Hz, 2H). **¹³C NMR** (101 MHz, CDCl₃) δ 163.56, 160.26, 144.27, 137.05, 130.17,

129.42, 128.31, 128.10, 125.98, 124.56 (q, *J* = 3.7 Hz), 117.64, 114.33, 78.14, 55.59, 49.61. **¹⁹F NMR** (376 MHz, DMSO-*d*₆) δ -

60.96.

HRMS (ESI) calcd for C₂₅H₁₉DF₃NO₃ (M + H)⁺ 441.1531, found 441.1534.

N-(4-(1-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)ethyl-2-d)phenyl)acetamide (10)



Isolated yield 66% (28.3 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). **¹H NMR** (600 MHz, CDCl₃) δ 8.02 (d, *J* = 8.6 Hz, 1H), 7.89 (d, *J* = 8.6 Hz, 1H),

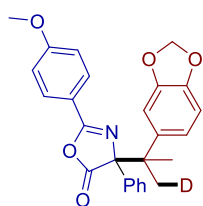
7.81 (d, *J* = 7.9 Hz, 1H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.3 Hz, 0.5H),

7.30 (d, *J* = 8.4 Hz, 1H), 7.27 – 7.24 (m, 1H), 7.23 – 7.20 (m, 2.5H), 7.17 (t, *J* = 6.8 Hz, 1H), 7.10 (d,

$J = 8.3$ Hz, 1H), 6.99 (d, $J = 8.7$ Hz, 1H), 6.94 (d, $J = 8.7$ Hz, 1H), 3.91 – 3.83 (m, 3H), 3.64 (t, $J = 7.0$ Hz, 0.5H), 3.58 (t, $J = 7.0$ Hz, 0.5H), 2.12 – 2.06 (m, 3H), 1.28 – 1.22 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 178.01, 177.58, 167.14, 167.11, 162.17, 162.07, 158.72, 158.57, 136.77, 136.59, 136.03, 135.47, 135.14, 134.56, 128.90, 128.78, 128.58, 127.50, 127.10, 126.74, 125.19, 125.06, 118.11, 117.83, 117.11, 113.16, 113.11, 77.08, 76.80, 54.49, 54.44, 48.39, 48.27, 23.56, 23.55, 15.5 – 14.0 (m, 2C).

HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{23}\text{DN}_2\text{O}_4$ ($\text{M} + \text{Na}$) $^+$ 452.1691, found 452.1694.

4-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (11)

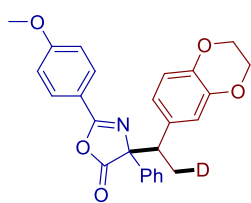


Isolated yield 74% (31.8 mg, 0.1 mmol scale, $r.r. > 20 : 1$), $[\text{D}] > 20 : 1$, colorless oil, eluent (PE : EA = 50 : 1). ^1H NMR (400 MHz, CDCl_3) δ 7.86 (d, $J = 8.9$ Hz, 2H), 7.82 – 7.73 (m, 2H), 7.38 – 7.28 (m, 3H), 7.00 – 6.91 (m, 2H), 6.87 (d, $J = 1.9$ Hz, 1H), 6.76 (dd, $J = 8.3, 1.6$ Hz, 1H), 6.59 (d, $J = 8.3$ Hz, 1H), 5.87 (d, $J = 1.5$ Hz, 1H), 5.81 (d, $J = 1.5$ Hz, 1H), 3.86 (s, 3H), 1.54 – 1.48 (m, 2.5H), 1.48 – 1.42 (m, 2.5H). ^{13}C NMR

(101 MHz, CDCl_3) δ 177.55, 162.93, 158.67, 146.68, 146.04, 136.84, 135.42, 129.68, 128.29, 127.92, 127.46, 121.68, 118.37, 114.04, 109.17, 106.86, 100.78, 79.42, 55.44, 45.90, 24.36, 23.80.

HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{22}\text{DNO}_5$ ($\text{M} + \text{Na}$) $^+$ 453.1531, found 453.1514.

4-(1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)ethyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (12)

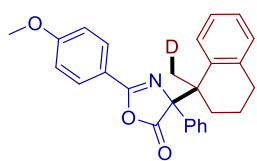


Isolated yield 56% (24.1 mg, 0.1 mmol scale, $r.r. > 20 : 1$, $d.r. = 1 : 1$), $[\text{D}] > 20 : 1$, colorless oil, eluent (PE : EA = 50 : 1). ^1H NMR (400 MHz, CDCl_3) δ 8.09 – 8.00 (m, 1H), 7.97 – 7.88 (m, 1H), 7.83 – 7.76 (m, 1H), 7.60 – 7.54 (m, 1H), 7.40 (t, $J = 7.4$ Hz, 1H), 7.35 – 7.30 (m, 0.5H), 7.26 – 7.15 (m, 1.5H), 7.05 – 6.93 (m, 2H), 6.84 – 6.77 (m, 1H), 6.74 (dd, $J = 8.4, 2.1$ Hz, 0.5H), 6.64 (d, $J = 8.3$ Hz, 0.5H),

6.60 – 6.54 (m, 1H), 4.24 – 4.02 (m, 4H), 3.95 – 3.80 (m, 3H), 3.57 (t, $J = 7.1$ Hz, 0.5H), 3.52 (t, $J = 7.0$ Hz, 0.5H), 1.25 – 1.18 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 178.10, 177.59, 162.13, 161.98, 158.75, 158.53, 141.79, 141.64, 141.58, 141.19, 136.90, 136.65, 132.59, 131.96, 128.93, 128.81, 127.47, 127.08, 127.02, 126.69, 125.21, 125.09, 121.33, 120.80, 117.32, 117.20, 117.02, 116.65, 115.52, 115.12, 113.12, 113.04, 77.13, 76.88, 63.21, 63.11, 54.48, 54.44, 48.24, 48.17, 15.5 – 14.0 (m, 2C).

HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{22}\text{DNO}_5$ ($\text{M} + \text{H}$) $^+$ 431.1712, found 431.1721.

2-(4-methoxyphenyl)-4-(1-(methyl-d)-1,2,3,4-tetrahydronaphthalen-1-yl)-4-phenyloxazol-5(4H)-one (13)



Isolated yield 70% (28.8 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 3 : 2), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). ¹H NMR (400 MHz, CDCl₃) δ 7.97 – 7.91 (m, 1H), 7.84 (dd, *J* = 8.0, 1.6 Hz, 1H),

7.79 (dd, *J* = 7.5, 2.1 Hz, 1H), 7.77 – 7.71 (m, 1H), 7.48 (d, *J* = 7.9 Hz, 0.5H), 7.40 – 7.26 (m, 3.5H),

7.09 – 7.02 (m, 1.5H), 7.01 – 6.78 (m, 3.5H), 3.91 – 3.80 (m, 3H), 2.82 – 2.70 (m, 0.5H), 2.69 – 2.51 (m, 2H), 2.31 – 2.16 (m,

1H), 1.94 – 1.80 (m, 0.5H), 1.64 – 1.38 (m, 3H), 1.33 – 1.18 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 178.92, 177.61, 162.99,

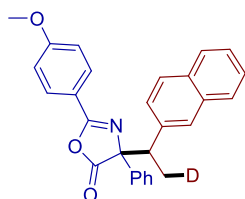
162.76, 158.95, 157.84, 139.88, 139.40, 139.06, 138.90, 136.02, 135.66, 129.79, 129.45, 129.07, 128.73, 128.66, 128.27,

127.97, 127.91, 127.59, 127.37, 126.40, 126.31, 125.43, 124.98, 118.62, 118.32, 114.13, 113.93, 80.36, 80.12, 55.48, 55.41,

46.26, 45.90, 34.52, 34.46, 31.49, 30.61, 20.45, 19.98.

HRMS (ESI) calcd for C₂₇H₂₄DNO₃ (M + Na)⁺ 435.1789, found 435.1789.

2-(4-methoxyphenyl)-4-(1-(naphthalen-2-yl)ethyl-2-d)-4-phenyloxazol-5(4H)-one (14)



Isolated yield 32% (13.5 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). ¹H NMR (400 MHz, CDCl₃) δ 8.09 – 8.01 (m, 1H), 7.92 – 7.82 (m, 2H), 7.79 – 7.66

(m, 2.5H), 7.66 – 7.52 (m, 2.5H), 7.50 – 7.32 (m, 4.5H), 7.24 – 7.08 (m, 1.5H), 7.04 – 6.96 (m, 1H),

6.95 – 6.88 (m, 1H), 3.91 – 3.71 (m, 4H), 1.44 – 1.33 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 179.09,

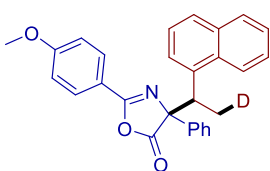
178.52, 163.23, 163.06, 159.92, 159.70, 137.94, 137.92, 137.66, 137.40, 133.11, 133.00, 132.69, 132.39, 129.96, 129.82,

128.57, 128.34, 128.15, 128.13, 127.97, 127.85, 127.79, 127.43, 127.37, 127.01, 126.75, 126.31, 126.13, 125.78, 125.69,

125.58, 125.43, 118.23, 114.21, 114.07, 78.22, 77.97, 55.53, 55.46, 50.04, 49.99, 16.27, 16.26, 16.14, 15.71, 15.69, 15.62.

HRMS (ESI) calcd for C₂₈H₂₂DNO₃ (M + Na)⁺ 445.1633, found 445.1640.

2-(4-methoxyphenyl)-4-(1-(naphthalen-1-yl)ethyl-2-d)-4-phenyloxazol-5(4H)-one (15)



Isolated yield 44% (18.6 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil,

eluent (PE : EA = 50 : 1). ¹H NMR (600 MHz, CDCl₃) δ 8.43 (d, *J* = 8.7 Hz, 1H), 7.96 (d, *J* = 7.4 Hz,

2H), 7.92 (d, *J* = 8.8 Hz, 2H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.66 (d, *J* = 8.1 Hz, 1H), 7.60 (t, *J* = 7.3 Hz,

1H), 7.52 (d, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.23 – 7.19 (m, 1H), 6.96

(d, *J* = 8.8 Hz, 2H), 4.73 (t, *J* = 7.0 Hz, 1H), 3.88 (s, 3H), 1.38 (d, *J* = 6.9 Hz, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 178.14, 163.15,

160.11, 138.41, 136.19, 133.85, 131.79, 129.86, 128.68, 128.58, 128.19, 127.94, 126.46, 126.15, 125.96, 125.48, 124.67,

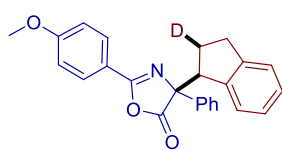
123.43, 118.31, 114.17, 77.51, 55.50, 42.24, 17.00, 16.86, 16.75, 16.72.

HRMS (ESI) calcd for C₂₈H₂₂DNO₃ (M + Na)⁺ 445.1633, found 445.1637.

¹H NMR (600 MHz, **CDCl₃**) δ 8.13 (d, *J* = 8.6 Hz, 1H), 7.96 (d, *J* = 7.1 Hz, 1H), 7.91 (d, *J* = 8.8 Hz, 2H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.65 – 7.59 (m, 3H), 7.45 (t, *J* = 8.2 Hz, 1H), 7.41 – 7.34 (m, 2H), 7.11 (t, *J* = 7.6 Hz, 2H), 7.05 (t, *J* = 7.3 Hz, 1H), 6.94 (d, *J* = 8.8 Hz, 2H), 4.68 (t, *J* = 7.0 Hz, 1H), 3.86 (s, 3H), 1.40 (d, *J* = 7.0 Hz, 2H). **¹³C NMR** (151 MHz, **CDCl₃**) δ 178.26, 162.10, 158.47, 136.35, 135.99, 132.38, 131.06, 128.86, 127.56, 127.03, 126.70, 126.26, 125.09, 124.77, 124.55, 124.16, 123.90, 122.17, 117.06, 113.05, 77.33, 54.46, 41.54.

HRMS (ESI) calcd for C₂₈H₂₂DNO₃ (M + Na)⁺ 445.1633, found 445.1624.

4-(2,3-dihydro-1H-inden-1-yl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (16)



Isolated yield 82% (31.5 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil,

eluent (PE : EA = 50 : 1). **¹H NMR** (400 MHz, **CDCl₃**) δ 7.82 – 7.73 (m, 4H), 7.44 – 7.37 (m, 2H),

7.37 – 7.32 (m, 1H), 7.26 – 7.22 (m, 2H), 7.14 – 7.00 (m, 3H), 6.87 (d, *J* = 9.0 Hz, 1H), 4.15 – 4.05

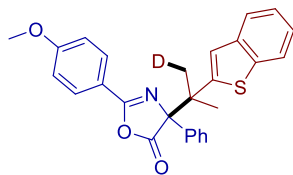
(m, 1H), 3.83 (s, 3H), 3.11 (dd, *J* = 15.7, 8.5 Hz, 1H), 2.73 (ddd, *J* = 15.7, 5.8, 3.2 Hz, 1H), 2.15 (d, *J* = 8.3 Hz, 0.5H), 2.03 (q, *J* = 8.7 Hz, 0.5H). **¹³C NMR** (101 MHz, **CDCl₃**) δ 179.29, 173.61, 162.97, 159.48, 146.01, 140.27, 138.16, 129.63, 129.52, 128.55, 128.15, 127.73, 126.37, 126.09, 124.51, 124.28, 118.07, 113.99, 78.14, 55.44, 54.78, 31.69.

HRMS (ESI) calcd for C₂₅H₂₀DNO₃ (M + Na)⁺ 407.1476, found 407.1477.

¹H NMR (400 MHz, **CDCl₃**) δ 8.04 – 7.93 (m, 2H), 7.69 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.45 – 7.33 (m, 3H), 7.24 – 7.10 (m, 2H), 6.97 (d, *J* = 9.0 Hz, 1H), 6.86 (t, *J* = 7.4 Hz, 1H), 6.32 (d, *J* = 6.4 Hz, 1H), 4.15 – 4.07 (m, 1H), 3.88 (s, 3H), 2.94 (dd, *J* = 15.7, 8.5 Hz, 1H), 2.82 – 2.66 (m, 1H), 2.22 (dd, *J* = 17.6, 8.8 Hz, 0.5H), 1.86 (d, *J* = 8.4 Hz, 0.5H). **¹³C NMR** (101 MHz, **CDCl₃**) δ 159.96, 145.45, 140.76, 137.52, 130.06, 129.95, 128.46, 128.25, 127.48, 127.21, 126.68, 125.81, 125.47, 124.43, 114.21, 78.08, 55.52, 54.25, 31.71.

HRMS (ESI) calcd for C₂₅H₂₀DNO₃ (M + Na)⁺ 407.1476, found 407.1478.

4-(2-(benzo[b]thiophen-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (17)



Isolated yield 69% (30.5 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE :

EA = 50 : 1). **¹H NMR** (400 MHz, **CDCl₃**) δ 7.97 – 7.89 (m, 2H), 7.80 (dd, *J* = 6.3, 2.6 Hz, 2H),

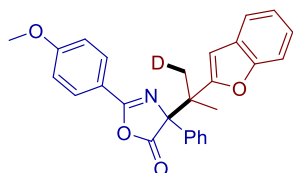
7.70 (d, *J* = 7.4 Hz, 1H), 7.62 (dd, *J* = 6.9, 1.7 Hz, 1H), 7.35 – 7.28 (m, 3H), 7.28 – 7.20 (m, 2H),

7.05 (s, 1H), 6.93 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H), 1.65 – 1.60 (m, 5H). **¹³C NMR** (101 MHz,

CDCl₃) δ 177.31, 163.03, 159.54, 149.29, 139.73, 139.11, 135.05, 129.95, 129.85, 128.31, 128.14, 127.60, 123.77, 123.32, 122.75, 121.75, 118.29, 114.08, 79.21, 55.46, 45.82, 25.20.

HRMS (ESI) calcd for $C_{27}H_{22}DNO_3S$ ($M + H$)⁺ 443.1534, found 443.1530.

4-(2-(benzofuran-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (18)



Isolated yield 84% (35.8 mg, 0.1 mmol scale, *r.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent (PE :

EA = 50 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 8.30 – 8.23 (m, 2H), 7.50 (dd, *J* = 8.4, 6.4 Hz, 1H), 7.47 – 7.39 (m, 5H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.22 – 7.10 (m, 2H), 6.81 (d, *J* = 9.0 Hz, 2H), 6.47 (s, 1H), 3.79 (s, 3H), 1.55 – 1.47 (m, 5H). **¹³C NMR** (101 MHz, CDCl₃) δ 162.88, 158.75, 158.37,

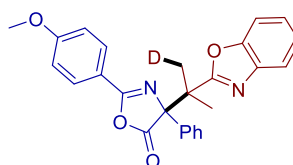
154.94, 153.40, 131.23, 128.40, 127.54, 127.33, 126.96, 122.79, 121.43, 119.64, 111.83, 109.98, 107.67, 104.28, 54.23, 44.91, 21.75, 21.49.

HRMS (ESI) calcd for $C_{27}H_{22}DNO_4$ ($M + Na$)⁺ 449.1582, found 449.1586.

¹H NMR (400 MHz, CDCl₃) δ 7.95 – 7.82 (m, 2H), 7.77 (dd, *J* = 6.5, 3.2 Hz, 2H), 7.50 – 7.40 (m, 1H), 7.40 – 7.28 (m, 4H), 7.22 – 7.08 (m, 2H), 6.89 (d, *J* = 9.0 Hz, 2H), 6.46 (s, 1H), 3.83 (s, 3H), 1.60 – 1.47 (m, 5H). **¹³C NMR** (101 MHz, CDCl₃) δ 176.22, 161.89, 159.62, 158.21, 153.32, 134.10, 128.72, 127.16, 127.11, 127.08, 126.56, 122.60, 121.33, 119.60, 117.23, 112.95, 109.89, 103.07, 77.12, 54.39, 43.84, 21.36, 21.23.

HRMS (ESI) calcd for $C_{27}H_{22}DNO_4$ ($M + Na$)⁺ 449.1582, found 449.1586.

4-(2-(benzo[d]oxazol-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (19)



Isolated yield 50% (21.4 mg, 0.1 mmol scale, *r.r.* = 6 : 1), [D] > 20 : 1, colorless oil, eluent (PE :

EA = 20 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 8.37 – 8.26 (m, 2H), 7.68 – 7.63 (m, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.49 – 7.38 (m, 5H), 7.33 – 7.24 (m, 2H), 6.81 (d, *J* = 9.0 Hz, 2H), 3.78 (s, 3H), 1.70

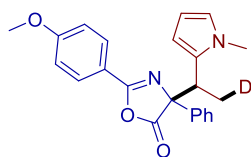
– 1.57 (m, 5H). **¹³C NMR** (101 MHz, CDCl₃) δ 167.33, 163.74, 160.03, 156.59, 150.65, 140.64, 132.55, 129.25, 129.15, 128.74, 128.68, 128.40, 128.03, 125.07, 124.27, 120.10, 113.15, 110.56, 108.01, 55.28, 47.05, 22.49, 22.27.

HRMS (ESI) calcd for $C_{26}H_{21}DN_2O_4$ ($M + Na$)⁺ 450.1535, found 450.1532.

¹H NMR (400 MHz, CDCl₃) δ 7.93 – 7.86 (m, 2H), 7.80 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.65 – 7.58 (m, 1H), 7.43 – 7.38 (m, 1H), 7.37 – 7.32 (m, 3H), 7.27 – 7.21 (m, 3H), 6.88 (d, *J* = 9.1 Hz, 1H), 3.82 (s, 3H), 1.71 – 1.62 (m, 5H). **¹³C NMR** (101 MHz, CDCl₃) δ 177.17, 168.62, 163.08, 160.12, 150.54, 140.78, 134.77, 129.91, 129.81, 128.51, 128.33, 127.83, 124.76, 124.10, 120.08, 114.00, 110.36, 55.45, 45.82, 22.45, 22.05.

HRMS (ESI) calcd for $C_{26}H_{21}DN_2O_4$ ($M + Na$)⁺ 450.1535, found 450.1542.

2-(4-methoxyphenyl)-4-(1-(1-methyl-1H-pyrrol-2-yl)ethyl-2-d)-4-phenyloxazol-5(4H)-one (20)



Isolated yield 55% (20.6 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). ¹H NMR (400 MHz, CDCl₃) δ 8.03 – 7.96 (m, 1H), 7.91 (t, *J* = 4.2 Hz, 1H), 7.79 (d,

J = 7.4 Hz, 1H), 7.69 (d, *J* = 7.0 Hz, 1H), 7.45 – 7.27 (m, 3H), 7.04 – 6.90 (m, 2H), 6.51 – 6.44 (m,

0.5H), 6.36 – 6.25 (m, 0.5H), 6.19 (dd, *J* = 3.4, 1.6 Hz, 0.5H), 6.04 – 5.98 (m, 0.5H), 5.96 – 5.88 (m, 1H), 3.93 – 3.83 (m, 3H),

3.75 (t, *J* = 7.0 Hz, 0.5H), 3.64 – 3.56 (m, 2H), 3.30 (s, 1.5H), 1.26 (t, *J* = 11.1 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 178.91,

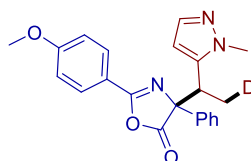
178.02, 163.12, 159.90, 159.34, 137.85, 137.32, 131.28, 130.92, 129.93, 129.82, 129.73, 129.63, 128.48, 128.27, 128.15,

128.00, 126.32, 121.82, 121.39, 118.53, 114.23, 114.19, 114.11, 107.65, 107.45, 106.89, 106.69, 77.70, 77.24, 55.51, 55.48,

41.52, 40.91, 33.95, 33.61, 16.61, 16.42.

HRMS (ESI) calcd for C₂₃H₂₁DN₂O₃ (M + H)⁺ 376.1766, found 376.1765.

2-(4-methoxyphenyl)-4-(1-(1-methyl-1H-pyrazol-5-yl)ethyl-2-d)-4-phenyloxazol-5(4H)-one (21)



Isolated yield 60% (22.6 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent

(PE : EA = 50 : 1). ¹H NMR (400 MHz, CDCl₃) δ 8.02 – 7.91 (m, 2H), 7.81 – 7.73 (m, 1H), 7.70 – 7.61

(m, 1H), 7.45 – 7.26 (m, 4H), 7.07 – 6.89 (m, 2H), 6.31 (d, *J* = 1.9 Hz, 0.5H), 6.04 (d, *J* = 1.9 Hz,

0.5H), 3.91 – 3.85 (m, 3H), 3.84 (s, 1.5H), 3.79 (t, *J* = 7.0 Hz, 0.5H), 3.69 (t, *J* = 7.6 Hz, 0.5H), 3.51 (s, 1.5H), 1.31 – 1.22 (m,

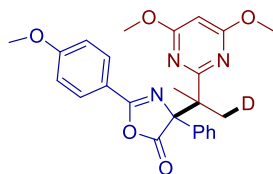
2H). ¹³C NMR (101 MHz, CDCl₃) δ 178.32, 177.83, 163.40, 163.36, 160.39, 160.02, 141.41, 141.23, 138.11, 137.95, 137.06,

136.76, 130.00, 129.90, 128.64, 128.48, 128.41, 126.25, 126.09, 118.06, 117.78, 114.30, 114.26, 105.25, 105.15, 77.50, 55.53,

41.24, 40.58, 36.66, 36.24, 16.25, 16.06, 15.96, 15.86, 15.75, 15.56.

HRMS (ESI) calcd for C₂₂H₂₀DN₃O₃ (M + H)⁺ 377.1718, found 377.1715.

4-(2-(4,6-dimethoxypyrimidin-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (22)



Isolated yield 46% (20.6 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE :

EA = 20 : 1). ¹H NMR (400 MHz, CDCl₃) δ 7.96 – 7.87 (m, 2H), 7.84 (d, *J* = 8.9 Hz, 2H), 7.42 – 7.30

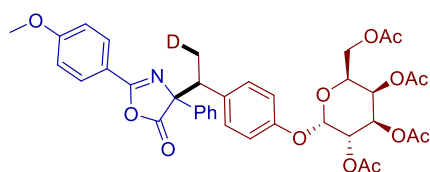
(m, 3H), 6.89 (d, *J* = 8.9 Hz, 2H), 5.73 (s, 1H), 3.90 (s, 6H), 3.83 (s, 3H), 1.57 – 1.51 (m, 3H), 1.49

– 1.43 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 177.05, 171.53, 169.91, 161.77, 158.33, 143.68,

135.86, 128.52, 127.55, 126.97, 126.58, 117.79, 112.97, 86.32, 54.39, 53.08, 50.59, 23.15, 21.31.

HRMS (ESI) calcd for C₂₅H₂₄DN₃O₅ (M + Na)⁺ 471.1749, found 471.1740.

(2S,3R,4R,5S,6S)-2-(acetoxymethyl)-6-(4-(1-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)ethyl-2-d)phenoxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate (23)



Isolated yield 60% (43.1 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1,

colorless oil, eluent (PE : EA = 5 : 1). ¹H NMR (600 MHz, CDCl₃) δ 8.04 – 7.98 (m,

1H), 7.92 – 7.87 (m, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.40 (t, *J*

= 7.6 Hz, 1H), 7.33 (t, *J* = 7.3 Hz, 0.5H), 7.25 – 7.17 (m, 2.5H), 7.08 (dd, *J* = 8.6, 3.2 Hz, 1H), 6.99 (d, *J* = 8.7 Hz, 1H), 6.95 (dd,

J = 11.0, 8.9 Hz, 1H), 6.79 (d, *J* = 8.5 Hz, 1H), 6.76 (d, *J* = 8.3 Hz, 1H), 5.49 – 5.38 (m, 2H), 5.09 – 5.03 (m, 1H), 4.95 – 4.91

(m, 1H), 4.27 – 4.08 (m, 2H), 4.03 – 3.97 (m, 1H), 3.90 – 3.86 (m, 3H), 3.68 – 3.62 (m, 0.5H), 3.61 – 3.55 (m, 0.5H), 2.18 – 2.14

(m, 3H), 2.07 (d, *J* = 8.4 Hz, 1.5H), 2.05 – 1.95 (m, 7.5H), 1.26 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 177.91, 177.55, 169.37,

169.21, 169.09, 168.33, 162.20, 162.09, 158.78, 158.72, 158.62, 155.13, 155.05, 154.68, 136.70, 136.53, 134.25, 134.13,

133.74, 133.60, 129.16, 129.14, 129.12, 128.88, 128.86, 128.76, 127.51, 127.11, 126.77, 125.17, 125.05, 117.09, 115.44,

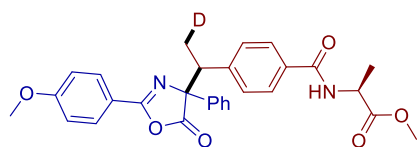
115.14, 115.10, 114.94, 113.16, 113.14, 113.08, 98.77, 98.73, 98.54, 98.39, 77.07, 76.79, 69.88, 69.84, 69.77, 69.74, 67.62,

67.59, 67.54, 65.78, 60.24, 60.21, 54.49, 54.44, 48.12, 48.04, 19.64, 19.56, 15.52, 15.45, 14.66, 14.64.

HRMS (ESI) calcd for C₃₈H₃₈DNO₁₃ (M + Na)⁺ 741.2376, found 741.2387.

Methyl(4-(1-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)ethyl-2-d)benzoyl)-L-alaninate (24)

(24)



Isolated yield 29% (14.5 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1,

colorless oil, eluent (PE : EA = 5 : 1). ¹H NMR (600 MHz, CDCl₃) δ 8.61 (s, 0.5H), 8.19

– 8.11 (m, 1H), 8.07 – 8.02 (m, 0.5H), 7.92 – 7.87 (m, 0.5H), 7.83 – 7.79 (m, 0.5H),

7.76 – 7.72 (m, 1H), 7.65 – 7.59 (m, 1.5H), 7.59 – 7.47 (m, 2H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 8.2 Hz, 1H), 7.25 – 7.15

(m, 1.5H), 7.02 (m, 1H), 6.95 (d, *J* = 9.0 Hz, 0.5H), 6.82 (d, *J* = 6.9 Hz, 0.5H), 6.63 (d, *J* = 6.5 Hz, 0.5H), 4.85 – 4.70 (m, 1H),

3.94 – 3.65 (m, 7H), 2.78 – 2.64 (m, 1H), 1.56 – 1.51 (m, 1H), 1.51 – 1.45 (m, 2H), 1.32 – 1.22 (m, 2H). ¹³C NMR (101 MHz,

CDCl₃) δ 177.86, 177.30, 172.69, 172.64, 172.60, 172.53, 165.41, 165.36, 165.09, 158.92, 158.86, 143.47, 142.92, 137.90,

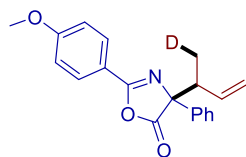
136.54, 136.33, 131.73, 131.11, 130.44, 129.29, 128.95, 128.83, 128.72, 128.29, 127.56, 127.45, 127.21, 126.93, 126.91,

125.72, 125.38, 125.19, 124.95, 123.67, 123.47, 116.85, 113.22, 112.55, 76.69, 76.42, 54.51, 54.46, 54.34, 51.65, 51.55, 48.67,

48.50, 47.64, 47.38, 47.37, 47.35, 17.66, 17.62, 17.55.

HRMS (ESI) calcd for C₂₉H₂₇DN₂O₆ (M + Na)⁺ 524.1902, found 524.1902.

4-(but-3-en-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (26)

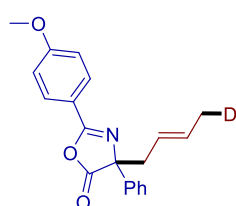


Isolated yield 33% (10.6 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). ¹H NMR (400 MHz, CDCl₃) δ 8.09 – 7.97 (m, 2H), 7.75 – 7.63 (m, 2H), 7.41 – 7.28 (m, 3H), 7.05 – 6.93 (m, 2H), 5.80 – 5.68 (m, 0.2H), 5.67 – 5.53 (m, 0.8H), 5.20 (d, *J* = 17.1 Hz, 0.8H), 5.06

(dd, *J* = 10.2, 1.4 Hz, 0.8H), 4.97 – 4.87 (m, 0.4H), 3.89 (s, 3H), 3.12 – 3.00 (m, 1H), 1.06 – 0.96 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 177.84, 162.16, 158.64, 136.49, 136.15, 128.94, 127.43, 126.99, 125.14, 117.30, 116.14, 113.13, 76.71, 54.49, 46.93.

HRMS (ESI) calcd for C₂₀H₁₈DNO₃ (M + H)⁺ 323.1500, found 323.1500.

(E)-4-(but-2-en-1-yl-4-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (26)

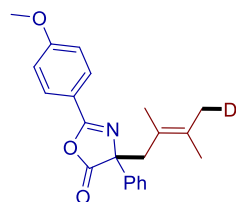


Isolated yield 48% (15.6 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). ¹H NMR (400 MHz, CDCl₃) δ 8.09 – 7.95 (m, 2H), 7.78 – 7.64 (m, 2H), 7.42 – 7.28 (m, 3H), 7.00 (d, *J* = 9.0 Hz, 2H), 5.70 – 5.54 (m, 1H), 5.41 – 5.21 (m, 1H), 3.89 (s, 3H), 2.86 (d, *J* = 7.8 Hz, 2H), 1.56 (d, *J* = 5.2 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 178.56, 163.22, 159.70, 138.29, 131.80, 129.95,

128.60, 128.10, 125.70, 123.02, 118.21, 114.21, 74.88, 55.53, 44.12, 18.00, 17.80, 17.61.

HRMS (ESI) calcd for C₂₀H₁₈DNO₃ (M + H)⁺ 323.1500, found 323.1503.

(E)-4-(2,3-dimethylbut-2-en-1-yl-4-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (28)

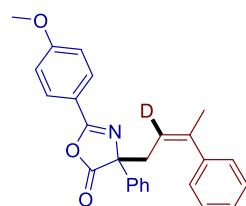


Isolated yield 58% (20.3 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). ¹H NMR (400 MHz, CD₃CN) δ 8.03 – 7.93 (m, 2H), 7.76 – 7.66 (m, 2H), 7.46 – 7.38 (m, 2H), 7.38 – 7.30 (m, 1H), 7.07 (d, *J* = 9.0 Hz, 2H), 3.87 (s, 3H), 3.08 (d, *J* = 13.7 Hz, 1H), 2.94 (d, *J* = 13.7 Hz, 1H), 1.62 (d, *J* = 7.3 Hz, 5.6H), 1.52 (d, *J* = 7.1 Hz, 2.3H). ¹³C NMR (101 MHz, CDCl₃) δ 179.30,

163.04, 158.89, 138.99, 131.59, 129.80, 129.70, 128.47, 127.93, 125.82, 121.54, 118.49, 114.24, 114.19, 75.26, 55.50, 46.64, 21.22, 20.97, 20.91, 20.71, 20.52, 20.26.

HRMS (ESI) calcd for C₂₂H₂₂DNO₃ (M + H)⁺ 351.1813, found 351.1819.

(Z)-2-(4-methoxyphenyl)-4-phenyl-4-(3-phenylbut-2-en-1-yl-2-d)oxazol-5(4H)-one (30)

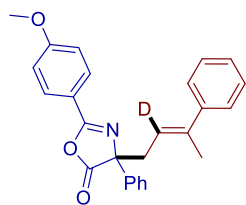


Isolated yield 13% (5.2 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). ¹H NMR (400 MHz, CDCl₃) δ 8.05 (d, *J* = 8.9 Hz, 2H), 7.62 – 7.55 (m, 2H), 7.36 – 7.28 (m, 5H), 7.26 – 7.20 (m, 1H), 7.15 – 7.10 (m, 2H), 7.02 (d, *J* = 9.0 Hz, 2H), 3.90 (s, 3H), 2.93 – 2.77 (m, 2H), 1.95 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 177.61, 162.22, 158.71, 140.80, 140.29, 136.95,

128.98, 127.49, 127.13, 127.01, 126.83, 125.77, 124.80, 117.17, 113.20, 73.16, 54.51, 39.25, 24.94.

HRMS (ESI) calcd for $C_{26}H_{22}DNO_3$ ($M + Na$)⁺ 421.1633, found 421.1639.

(E)-2-(4-methoxyphenyl)-4-phenyl-4-(3-phenylbut-2-en-1-yl-2-d)oxazol-5(4H)-one (30)



Isolated yield 38% (15.1 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA =

50 : 1). **¹H NMR** (400 MHz, $CDCl_3$) δ 8.08 – 7.98 (m, 2H), 7.86 – 7.71 (m, 2H), 7.40 (t, *J* = 7.4 Hz, 2H),

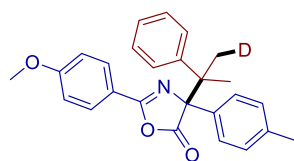
7.37 – 7.30 (m, 1H), 7.26 – 7.15 (m, 5H), 6.98 (d, *J* = 8.9 Hz, 2H), 3.88 (s, 3H), 3.10 (q, *J* = 14.2 Hz,

2H), 2.01 (s, 3H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 177.68, 162.19, 158.78, 142.47, 139.58, 137.16,

128.91, 127.60, 127.16, 127.08, 125.95, 124.86, 124.77, 117.10, 113.19, 73.71, 54.47, 39.21, 15.46.

HRMS (ESI) calcd for $C_{26}H_{22}DNO_3$ ($M + Na$)⁺ 421.1633, found 421.1541.

2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)-4-(p-tolyl)oxazol-5(4H)-one (31)



Isolated yield 89% (35.6 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE :

EA = 50 : 1). **¹H NMR** (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.8 Hz, 2H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.36

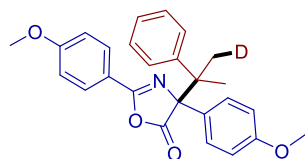
– 7.31 (m, 2H), 7.19 – 7.11 (m, 5H), 6.91 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H), 2.34 (s, 3H), 1.59 –

1.54 (m, 2.5H), 1.54 – 1.48 (m, 2.5H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 176.37, 161.89, 157.64, 141.74, 136.68, 131.13, 128.70,

127.17, 127.15, 127.11, 126.16, 125.68, 117.11, 112.94, 78.16, 54.39, 44.96, 22.97, 22.23, 20.04.

HRMS (ESI) calcd for $C_{26}H_{24}DNO_3$ ($M + K$)⁺ 439.1529, found 439.1530.

2,4-bis(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (32)



Isolated yield 92% (38.3 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE :

EA = 50 : 1). **¹H NMR** (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.8 Hz, 2H), 7.69 (d, *J* = 8.7 Hz, 2H), 7.33

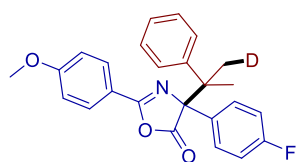
(d, *J* = 6.6 Hz, 2H), 7.21 – 7.11 (m, 3H), 6.91 (d, *J* = 8.9 Hz, 2H), 6.85 (d, *J* = 8.9 Hz, 2H), 3.85

(s, 3H), 3.81 (s, 3H), 1.58 – 1.53 (m, 2.5H), 1.53 – 1.47 (m, 2.5H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 177.83, 162.83, 159.23, 158.45,

142.85, 129.61, 129.52, 128.19, 127.37, 127.18, 126.70, 118.39, 113.98, 112.81, 78.98, 55.44, 55.27, 46.01, 23.93, 23.32.

HRMS (ESI) calcd for $C_{26}H_{24}DNO_4$ ($M + Na$)⁺ 439.1739, found 439.1741.

4-(4-fluorophenyl)-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (33)



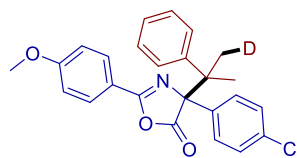
Isolated yield 86% (34.7 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE :

EA = 50 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 7.82 (d, *J* = 8.9 Hz, 2H), 7.72 (dd, *J* = 8.4, 5.6 Hz, 2H),

7.30 (dd, *J* = 7.8, 1.6 Hz, 2H), 7.21 – 7.11 (m, 3H), 7.00 (t, *J* = 8.7 Hz, 2H), 6.92 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H), 1.57 – 1.52 (m, 2.5H), 1.52 – 1.46 (m, 2.5H). **¹³C NMR** (101 MHz, CDCl₃) δ 176.51, 161.43 (d, *J* = 248.3 Hz), 161.92, 157.69, 141.39, 130.00 (d, *J* = 3.0 Hz), 129.03 (d, *J* = 8.1 Hz), 128.62, 127.12, 126.17, 125.79, 117.07, 113.27 (d, *J* = 21.4 Hz), 112.99, 77.81, 54.40, 45.00, 22.75, 22.26. **¹⁹F NMR** (377 MHz, CDCl₃) δ -114.33.

HRMS (ESI) calcd for C₂₅H₂₁DFNO₃ (M + Na)⁺ 427.1539, found 427.1549.

4-(4-chlorophenyl)-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (34)



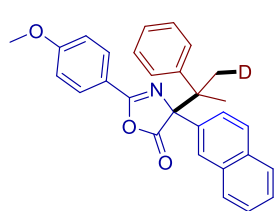
Isolated yield 82% (34.4 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE :

EA = 50 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 7.79 (d, *J* = 8.9 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.30

– 7.22 (m, 4H), 7.17 – 7.07 (m, 3H), 6.89 (d, *J* = 8.9 Hz, 2H), 3.82 (s, 3H), 1.53 – 1.48 (m, 2.5H), 1.48 – 1.43 (m, 2.5H). **¹³C NMR** (101 MHz, CDCl₃) δ 177.41, 163.01, 158.83, 142.34, 134.06, 133.87, 129.71, 129.68, 128.17, 127.62, 127.26, 126.89, 118.08, 114.05, 78.91, 55.46, 46.10, 23.81, 23.30.

HRMS (ESI) calcd for C₂₅H₂₁DCINO₃ (M + H)⁺ 421.1424, found 421.1414.

2-(4-methoxyphenyl)-4-(naphthalen-2-yl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (35)



Isolated yield 20% (8.7 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA

= 50 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 8.87 (s, 0.5H), 8.23 (d, *J* = 8.6 Hz, 0.4H), 7.97 – 7.82 (m,

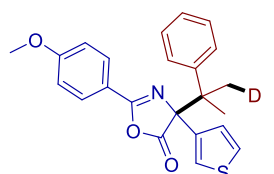
2H), 7.61 – 7.49 (m, 2H), 7.48 – 7.40 (m, 2H), 7.33 (d, *J* = 7.4 Hz, 2H), 7.23 – 7.08 (m, 3H), 6.83

(d, *J* = 8.9 Hz, 2H), 3.80 (s, 3H), 1.59 – 1.54 (m, 5H). **¹³C NMR** (101 MHz, CDCl₃) δ 162.99, 158.60,

154.48, 140.66, 131.63, 129.01, 128.68, 128.47, 128.41, 127.73, 127.70, 127.24, 126.97, 126.72, 126.30, 125.82, 125.63, 123.19, 111.66, 108.37, 54.23, 46.17, 23.40, 23.26.

HRMS (ESI) calcd for C₂₉H₂₄DNO₃ (M + Na)⁺ 459.1789, found 459.1790.

2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)-4-(thiophen-3-yl)oxazol-5(4H)-one (36)



Isolated yield 60% (23.5 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA

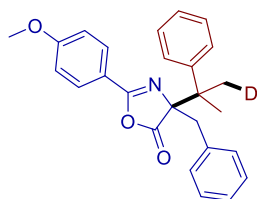
= 50 : 1). **¹H NMR** (600 MHz, CDCl₃) δ 7.80 (d, *J* = 8.7 Hz, 2H), 7.33 (d, *J* = 7.5 Hz, 2H), 7.31 (d, *J* =

4.5 Hz, 1H), 7.24 (d, *J* = 5.0 Hz, 1H), 7.18 – 7.10 (m, 3H), 6.91 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H), 1.59

– 1.55 (m, 2.5H), 1.55 – 1.51 (m, 2.5H). ^{13}C NMR (151 MHz, CDCl_3) δ 176.64, 161.84, 158.03, 141.63, 134.61, 128.59, 126.99, 126.96, 126.20, 125.72, 123.10, 117.21, 112.94, 77.69, 54.39, 44.83, 22.99, 22.21.

HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{20}\text{DNO}_3\text{S}$ ($\text{M} + \text{H}$) $^+$ 393.1378, found 393.1374.

4-benzyl-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (37)

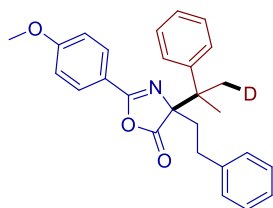


Isolated yield 30% (12.0 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). ^1H NMR (400 MHz, CDCl_3) δ 7.59 (d, J = 8.8 Hz, 2H), 7.44 (d, J = 7.7 Hz, 2H), 7.21 (t, J = 7.4 Hz, 2H), 7.18 – 7.14 (m, 1H), 7.10 – 7.00 (m, 5H), 6.83 (d, J = 8.9 Hz, 2H), 3.81 (s, 3H), 3.28 (d, J = 12.9 Hz, 1H), 3.18 (dd, J = 12.9, 1.5 Hz, 1H), 1.78 – 1.72 (m, 2.5H), 1.72 – 1.68 (m, 2.5H). ^{13}C

NMR (101 MHz, CDCl_3) δ 178.60, 162.67, 158.77, 143.64, 134.87, 130.50, 129.38, 127.98, 127.85, 127.43, 126.81, 126.66, 118.15, 113.86, 79.96, 55.37, 44.10, 38.65, 23.92, 23.62.

HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{24}\text{DNO}_3$ ($\text{M} + \text{Na}$) $^+$ 423.1789, found 423.1792.

2-(4-methoxyphenyl)-4-phenethyl-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (38)

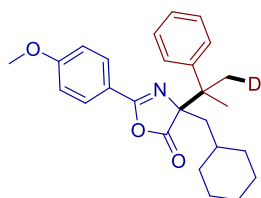


Isolated yield 35% (14.5 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). ^1H NMR (400 MHz, CDCl_3) δ 7.83 (d, J = 8.8 Hz, 2H), 7.37 (d, J = 7.4 Hz, 2H), 7.30 – 7.22 (m, 2H), 7.21 – 7.09 (m, 6H), 6.95 (d, J = 8.9 Hz, 2H), 3.87 (s, 3H), 2.52 – 2.18 (m, 4H), 1.67 – 1.56 (m, 5H). ^{13}C NMR (101 MHz, CDCl_3) δ 178.30, 161.98, 158.53, 142.34, 139.77, 128.68, 127.48,

127.38, 126.79, 126.40, 125.68, 125.10, 116.92, 113.05, 77.81, 54.44, 43.33, 33.42, 29.99, 22.74, 22.14.

HRMS (ESI) calcd for $\text{C}_{27}\text{H}_{26}\text{DNO}_3$ ($\text{M} + \text{Na}$) $^+$ 437.1946, found 437.1956.

4-(cyclohexylmethyl)-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (39)

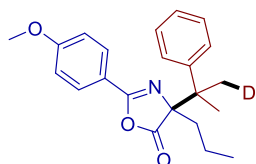


Isolated yield 56% (22.7 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). ^1H NMR (400 MHz, CDCl_3) δ 7.84 – 7.74 (m, 2H), 7.34 (d, J = 7.2 Hz, 2H), 7.20 – 7.08 (m, 3H), 6.93 (d, J = 8.9 Hz, 2H), 3.86 (s, 3H), 1.92 (qd, J = 13.9, 5.8 Hz, 2H), 1.72 – 1.43 (m, 10H), 1.13 – 0.97 (m, 4H), 0.95 – 0.80 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 179.25, 161.78, 157.80, 142.33,

128.51, 126.92, 126.26, 125.55, 117.26, 113.01, 76.91, 54.41, 43.87, 38.61, 33.71, 33.46, 32.58, 25.11, 25.08, 25.05, 22.71, 21.93.

HRMS (ESI) calcd for $\text{C}_{26}\text{H}_{30}\text{DNO}_3$ ($\text{M} + \text{H}$) $^+$ 407.2439, found 407.2442.

2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)-4-propyloxazol-5(4H)-one (40)

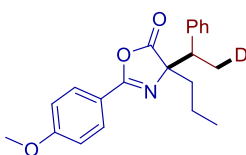


Isolated yield 38% (13.4 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 7.79 (d, *J* = 8.8 Hz, 2H), 7.38 (d, *J* = 7.5 Hz, 2H), 7.18 (t, *J* = 7.4 Hz, 2H), 7.15 – 7.10 (m, 1H), 6.92 (d, *J* = 8.9 Hz, 2H), 3.86 (s, 3H), 2.04 – 1.93 (m, 1H), 1.92 –

1.82 (m, 1H), 1.65 – 1.52 (m, 5H), 1.18 – 1.06 (m, 1H), 1.03 – 0.92 (m, 1H), 0.86 (t, *J* = 7.1 Hz, 3H). **¹³C NMR** (101 MHz, CDCl₃) δ 179.65, 162.89, 159.12, 143.65, 129.57, 127.86, 127.36, 126.60, 118.21, 114.05, 79.12, 55.44, 44.14, 34.32, 23.74, 23.29, 17.87, 13.94.

HRMS (ESI) calcd for C₂₂H₂₄DNO₃ (M + H)⁺ 353.1970, found 353.1971.

2-(4-methoxyphenyl)-4-(1-phenylethyl-2-d)-4-propyloxazol-5(4H)-one (41)



Isolated yield 71% (23.9 mg, 0.1 mmol scale, *r.r.* > 20 : 1, *d.r.* = 1 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 8.02 – 7.90 (m, 2H), 7.44 – 7.35 (m, 2H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.26 – 7.19 (m, 1H), 7.03 – 6.92 (m, 2H), 3.88 (s, 3H), 3.20 (t, *J* = 7.1 Hz, 1H), 1.78 (ddd,

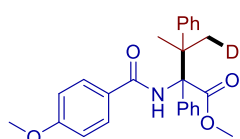
J = 13.6, 11.5, 5.4 Hz, 1H), 1.60 – 1.50 (m, 1H), 1.22 (d, *J* = 6.9 Hz, 2H), 1.17 – 1.00 (m, 2H), 0.78 (t, *J* = 7.3 Hz, 3H). **¹³C NMR** (101 MHz, CDCl₃) δ 181.06, 163.11, 159.68, 141.21, 129.81, 128.96, 128.18, 127.07, 118.09, 114.16, 55.51, 46.90, 38.29, 17.41, 13.79.

HRMS (ESI) calcd for C₂₁H₂₂DNO₃ (M + H)⁺ 339.1813, found 339.1815.

¹H NMR (400 MHz, CDCl₃) δ 7.82 (d, *J* = 8.9 Hz, 2H), 7.19 – 7.10 (m, 5H), 6.93 (d, *J* = 8.9 Hz, 2H), 3.86 (s, 3H), 3.24 (t, *J* = 7.1 Hz, 1H), 2.11 – 2.01 (m, 1H), 1.92 – 1.82 (m, 1H), 1.49 (d, *J* = 7.0 Hz, 2H), 1.27 – 1.13 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H). **¹³C NMR** (101 MHz, CDCl₃) δ 179.95, 162.99, 159.85, 140.46, 129.66, 128.78, 127.94, 127.16, 118.15, 114.10, 55.46, 46.51, 37.62, 27.89, 27.86, 17.56, 13.96.

HRMS (ESI) calcd for C₂₁H₂₂DNO₃ (M + H)⁺ 339.1813, found 339.1813.

methyl 2-(4-methoxybenzamido)-3-methyl-2,3-diphenylbutanoate-4-d (42)



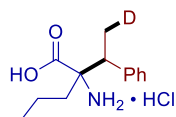
Isolated yield 90% (75.2 mg, 0.2 mmol scale), [D] > 20 : 1, white solid, eluent (PE : EA = 2 : 1). **¹H NMR** (400 MHz, CDCl₃) δ 7.75 – 7.58 (m, 4H), 7.38 – 7.28 (m, 3H), 7.29 – 7.21 (m, 3H), 7.21 – 7.14 (m, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 6.76 (s, 1H), 3.85 (s, 3H), 3.60 (s, 3H), 1.63 – 1.55 (m, 2.5H), 1.47 –

1.40 (m, 2.5H). **¹³C NMR** (101 MHz, CDCl₃) δ 171.03, 166.32, 162.35, 143.46, 136.40, 128.82, 128.72, 128.10, 127.70, 127.52,

127.18, 127.00, 126.90, 113.87, 69.65, 55.47, 51.98, 45.67, 25.52, 25.11.

HRMS (ESI) calcd for $C_{26}H_{26}DNO_4$ ($M + Na$)⁺ 441.1895, found 441.1893.

2-amino-2-(1-phenylethyl-2-d)pentanoic acid (43)

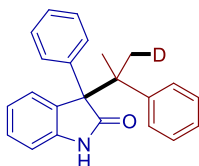


Isolated yield 63% (27.9 mg, 0.2 mmol scale), $[D] > 20 : 1$, white solid.

¹H NMR (400 MHz, D_2O) δ 7.47 – 7.32 (m, 5H), 3.50 (t, $J = 7.3$ Hz, 0.5H), 3.40 (t, $J = 7.2$ Hz, 0.5H), 2.06 – 1.94 (m, 1H), 1.92 – 1.81 (m, 0.5H), 1.76 – 1.56 (m, 0.5H), 1.43 (t, $J = 7.6$ Hz, 2H), 1.39 – 1.12 (m, 2H), 1.05 – 0.80 (m, 3H). **¹³C NMR** (101 MHz, D_2O) δ 173.16, 171.54, 138.61, 138.23, 128.93, 128.87, 128.76, 128.19, 128.16, 67.82, 67.64, 44.57, 43.96, 36.65, 35.03, 16.77, 16.58, 14.71, 14.53, 14.34, 13.23, 13.13.

HRMS (ESI) calcd for $C_{13}H_{18}DNO_2$ ($M + H$)⁺ 223.1551, found 223.1553.

3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (44)

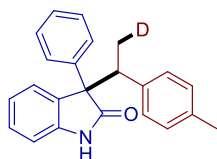


Isolated yield 88% (28.9 mg, 0.1 mmol scale), $[D] > 20 : 1$, white solid, eluent (PE : EA : DCM = 10 : 1 :

7.5). **¹H NMR** (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.92 – 7.76 (m, 2H), 7.36 – 7.27 (m, 3H), 7.24 – 7.05 (m, 4H), 6.94 – 6.76 (m, 4H), 6.54 (d, $J = 7.1$ Hz, 1H), 1.72 – 1.66 (m, 2.5H), 1.45 – 1.34 (m, 2.5H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 178.00, 143.39, 139.82, 134.31, 129.31, 129.15, 127.73, 127.48, 126.81, 126.23, 126.16, 125.81, 125.43, 119.76, 108.20, 61.26, 43.91, 24.47, 23.72.

HRMS (ESI) calcd for $C_{23}H_{20}DNO$ ($M + Na$)⁺ 351.1578, found 351.1571.

3-phenyl-3-(1-(p-tolyl)ethyl-2-d)indolin-2-one. (45)

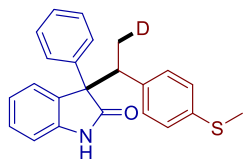


Isolated yield 73% (24.0 mg, 0.1 mmol scale, $d.r. = 1 : 1$), $[D] = 13 : 1$, white solid, eluent (PE : EA :

DCM = 10 : 1 : 7.5). **¹H NMR** (400 MHz, $CDCl_3$) δ 8.25 (s, 0.5H), 7.70 – 7.54 (m, 2.5H), 7.48 (s, 0.5H), 7.41 – 7.33 (m, 1H), 7.33 – 7.23 (m, 2H), 7.23 – 7.15 (m, 1H), 6.98 (td, $J = 7.6, 1.0$ Hz, 0.5H), 6.91 – 6.83 (m, 1.5H), 6.82 – 6.71 (m, 3H), 6.68 (d, $J = 7.3$ Hz, 0.5H), 4.15 – 3.85 (m, 1H), 2.23 (s, 1.3H), 2.16 (s, 1.4H), 1.39 – 1.31 (m, 1.1H), 1.29 – 1.21 (m, 1.1H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 180.01, 179.23, 141.57, 140.87, 138.69, 138.09, 137.35, 137.30, 136.24, 136.17, 129.76, 129.35, 129.17, 128.60, 128.51, 128.42, 128.25, 128.18, 127.97, 127.92, 127.89, 127.87, 127.36, 127.26, 127.16, 121.71, 121.46, 109.91, 109.61, 62.00, 61.32, 46.73, 46.50, 20.97.

HRMS (ESI) calcd for $C_{23}H_{20}DNO$ ($M + Na$)⁺ 351.1578, found 351.1571.

3-(1-(4-(methylthio)phenyl)ethyl-2-d)-3-phenylindolin-2-one. (46)



Isolated yield 86% (31.0 mg, 0.1 mmol scale, *d.r.* = 1 : 1), [D] > 20 : 1, white solid, eluent (PE : EA :

DCM = 10 : 1 : 7.5). ¹H NMR (400 MHz, CDCl₃) δ 8.17 (s, 0.5H), 7.65 – 7.53 (m, 2.5H), 7.42 – 7.33

(m, 1.5H), 7.33 – 7.23 (m, 2.5H), 7.22 – 7.15 (m, 1H), 7.02 – 6.92 (m, 1.5H), 6.88 (d, *J* = 8.2 Hz, 1.5H),

6.83 (d, *J* = 7.7 Hz, 0.5H), 6.81 – 6.75 (m, 2H), 6.69 (d, *J* = 7.7 Hz, 0.5H), 4.10 – 3.88 (m, 1H), 2.40 (s, 1.5H), 2.34 (s, 1.5H),

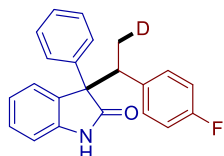
1.37 – 1.31 (m, 1H), 1.27 – 1.21 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 179.78, 179.02, 141.48, 140.84, 138.49, 137.89, 137.29,

137.27, 136.53, 136.48, 129.75, 129.54, 129.22, 129.11, 128.55, 128.32, 128.08, 127.85, 127.42, 127.27, 127.22, 125.51,

125.26, 121.78, 121.55, 110.02, 109.68, 61.90, 61.21, 46.62, 46.44, 15.65, 15.58.

HRMS (ESI) calcd for C₂₃H₂₀DNOS (M + Na)⁺ 383.1299, found 383.1294.

3-(1-(4-fluorophenyl)ethyl-2-d)-3-phenylindolin-2-one. (47)



Isolated yield 84% (27.9 mg, 0.1 mmol scale, *d.r.* = 1 : 1), [D] = 10 : 1, white solid, eluent (PE : EA : DCM

= 10 : 1 : 7.5). ¹H NMR (600 MHz, CDCl₃) δ 7.61 – 7.55 (m, 3H), 7.39 – 7.33 (m, 2H), 7.32 – 7.26 (m,

2H), 7.24 (s, 1H), 7.18 (td, *J* = 7.6, 1.0 Hz, 1H), 6.84 – 6.79 (m, 2H), 6.73 – 6.65 (m, 3H), 4.05 (t, *J* = 7.2

Hz, 1H), 1.36 – 1.31 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 178.87, 161.66 (d, *J* = 164.0 Hz), 141.35, 137.69, 136.02 (d, *J* =

2.0 Hz), 130.20 (d, *J* = 5.1 Hz), 128.93, 128.62, 128.57, 127.82, 127.47, 127.21, 121.85, 114.20 (d, *J* = 14.1 Hz), 109.90, 61.89,

46.24, 16.04, 15.88, 15.76, 15.63. ¹⁹F NMR (565 MHz, CDCl₃) δ -116.05.

HRMS (ESI) calcd for C₂₂H₁₇DFNO (M + Na)⁺ 355.1327, found 355.1318.

¹H NMR (600 MHz, CDCl₃) δ 8.05 (s, 1H), 7.60 – 7.56 (m, 2H), 7.34 – 7.29 (m, 2H), 7.28 – 7.23 (m, 1H), 7.20 (td, *J* = 7.7, 1.1

Hz, 1H), 6.99 (td, *J* = 7.6, 0.9 Hz, 1H), 6.87 (d, *J* = 7.5 Hz, 1H), 6.86 – 6.80 (m, 3H), 6.78 – 6.73 (m, 2H), 3.97 (t, *J* = 7.1 Hz,

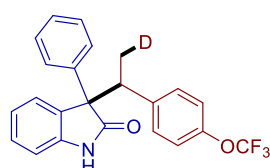
1H), 1.30 – 1.26 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 179.58, 161.66 (d, *J* = 164.1 Hz), 140.66, 138.41, 136.04 (d, *J* = 1.9

Hz), 130.64 (d, *J* = 5.2 Hz), 129.63, 128.39, 128.13, 127.74, 127.34, 126.96, 121.64, 113.99 (d, *J* = 13.4 Hz), 109.65, 61.17,

46.28, 15.51, 15.37, 15.24, 15.11. ¹⁹F NMR (565 MHz, CDCl₃) δ -116.15.

HRMS (ESI) calcd for C₂₂H₁₇DFNO (M + Na)⁺ 355.1327, found 355.1319.

3-phenyl-3-(1-(4-(trifluoromethoxy)phenyl)ethyl-2-d)indolin-2-one. (48)



Isolated yield 55% (21.9 mg, 0.1 mmol scale, *d.r.* = 1 : 1), [D] > 20 : 1, white solid, eluent (PE : EA :

DCM = 10 : 1 : 7.5). ¹H NMR (400 MHz, CDCl₃) δ 7.65 – 7.55 (m, 3H), 7.42 – 7.33 (m, 2H), 7.33 –

7.26 (m, 2H), 7.19 (td, *J* = 7.6, 1.0 Hz, 1H), 7.02 (s, 1H), 6.92 – 6.82 (m, 4H), 6.67 (d, *J* = 7.6 Hz,

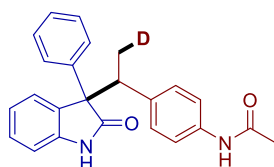
1H), 4.07 (t, $J = 7.2$ Hz, 1H), 1.38 – 1.32 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 178.56, 148.08 (d, $J = 13.1$ Hz), 141.27, 139.07, 137.54, 130.07, 128.74, 128.60, 127.82, 127.54, 127.24, 121.93, 119.77, 109.88, 61.75, 46.44. ^{19}F NMR (376 MHz, CDCl_3) δ -57.88.

HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{17}\text{DF}_3\text{NO}_2$ ($\text{M} + \text{Na}$) $^+$ 421.1245, found 421.1240.

^1H NMR (400 MHz, CDCl_3) δ 7.96 (s, 1H), 7.64 – 7.55 (m, 2H), 7.35 – 7.24 (m, 3H), 7.20 (td, $J = 7.7, 1.1$ Hz, 1H), 7.00 (td, $J = 7.6, 0.8$ Hz, 1H), 6.95 – 6.84 (m, 5H), 6.81 (d, $J = 7.7$ Hz, 1H), 4.00 (t, $J = 7.0$ Hz, 1H), 1.33 – 1.27 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 179.37, 147.98 (d, $J = 16.2$ Hz), 140.63, 139.07, 138.25, 130.50, 129.53, 128.45, 128.23, 127.74, 127.42, 126.88, 121.72, 120.39 (q, $J = 255.5$ Hz), 119.49, 109.68, 61.06, 46.38. ^{19}F NMR (376 MHz, CDCl_3) δ -57.86.

HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{17}\text{DF}_3\text{NO}_2$ ($\text{M} + \text{Na}$) $^+$ 421.1245, found 421.1242.

N-(4-(1-(2-oxo-3-phenylindolin-3-yl)ethyl-2-d)phenyl)acetamide. (49)



Isolated yield 70% (26.0 mg, 0.1 mmol scale, $d.r. = 1 : 1$), $[\text{D}] = 7 : 1$, white solid, eluent (PE : EA =

2 : 1). ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 10.47 (s, 1H), 9.77 (s, 1H), 7.58 (d, $J = 7.5$ Hz, 2H), 7.33 (t, $J = 7.6$ Hz, 2H), 7.29 – 7.21 (m, 3H), 7.18 (d, $J = 7.5$ Hz, 1H), 7.07 (td, $J = 7.6, 1.0$ Hz, 1H), 6.94 –

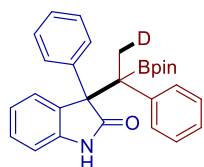
6.88 (m, 1H), 6.85 (d, $J = 8.6$ Hz, 2H), 6.65 (d, $J = 7.6$ Hz, 1H), 3.96 (t, $J = 6.9$ Hz, 1H), 1.97 (s, 3H), 1.21 – 1.15 (m, 2.1H). ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$) δ 178.97, 168.52, 141.82, 140.33, 138.07, 135.86, 131.76, 129.45, 128.79, 128.12, 127.79, 127.28, 126.22, 121.33, 118.12, 109.64, 61.04, 45.53, 24.40, 15.85.

HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{21}\text{DN}_2\text{O}_2$ ($\text{M} + \text{Na}$) $^+$ 394.1636, found 394.1627.

^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 10.03 (s, 1H), 9.76 (s, 1H), 7.59 (d, $J = 7.4$ Hz, 1H), 7.50 (d, $J = 7.5$ Hz, 2H), 7.36 (t, $J = 7.5$ Hz, 2H), 7.32 – 7.17 (m, 4H), 7.13 (td, $J = 7.5, 0.9$ Hz, 1H), 6.72 (d, $J = 8.6$ Hz, 2H), 6.65 (d, $J = 7.5$ Hz, 1H), 3.91 (t, $J = 7.0$ Hz, 1H), 1.97 (s, 3H), 1.24 – 1.18 (m, 2.1H). ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$) δ 178.52, 168.52, 143.06, 139.13, 138.21, 135.70, 129.39, 129.19, 128.90, 128.81, 128.00, 127.50, 127.38, 121.52, 118.20, 110.07, 61.69, 45.97, 24.41, 16.57.

HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{21}\text{DN}_2\text{O}_2$ ($\text{M} + \text{Na}$) $^+$ 394.1636, found 394.1627.

3-phenyl-3-(1-phenyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl-2-d)indolin-2-one. (50)



Isolated yield 61% (19.1 mg, 0.1 mmol scale, $d.r. = 1 : 1$), $[\text{D}] > 20 : 1$, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). ^1H NMR (400 MHz, CDCl_3) δ 7.94 (s, 1H), 7.54 (dd, $J = 6.8, 3.0$ Hz, 2H), 7.24 – 7.13 (m,

6H), 7.09 (td, $J = 7.7, 1.0$ Hz, 1H), 7.04 – 6.97 (m, 2H), 6.81 – 6.71 (m, 2H), 6.54 (d, $J = 7.7$ Hz, 1H), 1.60 – 1.56 (m, 2H), 1.15 (d, $J = 8.6$ Hz, 12H). ^{13}C NMR (101 MHz, CDCl_3) δ 180.90, 142.10, 141.00, 136.09, 132.59, 130.86, 130.13,

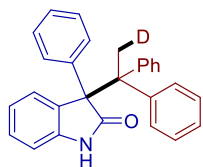
128.32, 127.23, 127.06, 126.84, 126.75, 126.52, 120.42, 108.74, 83.56, 60.63, 24.61, 24.42.

HRMS (ESI) calcd for $C_{28}H_{29}DBNO_3$ ($M + Na$)⁺ 463.2274, found 463.2273.

¹H NMR (400 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.56 – 7.49 (m, 2H), 7.24 – 7.11 (m, 7H), 7.11 – 6.98 (m, 3H), 6.91 (td, $J = 7.6, 1.0$ Hz, 1H), 6.76 (d, $J = 7.7$ Hz, 1H), 1.42 – 1.35 (m, 2H), 1.17 (d, $J = 6.1$ Hz, 12H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 180.26, 140.81, 140.13, 136.06, 132.09, 130.98, 130.85, 127.73, 127.54, 126.82, 126.56, 126.50, 126.26, 121.23, 109.32, 83.36, 63.33, 24.70, 24.55.

HRMS (ESI) calcd for $C_{28}H_{29}DBNO_3$ ($M + Na$)⁺ 463.2274, found 463.2272.

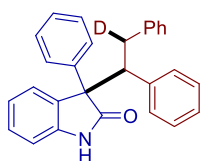
3-(1,1-diphenylethyl-2-d)-3-phenylindolin-2-one. (51)



Isolated yield 42% (16.4 mg, 0.1 mmol scale), $[D] > 20 : 1$, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). **¹H NMR** (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.90 – 7.78 (m, 2H), 7.35 – 7.30 (m, 3H), 7.23 – 7.12 (m, 4H), 7.07 – 6.95 (m, 7H), 6.86 (td, $J = 7.7, 1.0$ Hz, 1H), 6.71 (d, $J = 7.4$ Hz, 1H), 6.56 (d, $J = 7.2$ Hz, 1H), 2.30 – 2.10 (m, 2H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 179.42, 146.41, 143.40, 141.16, 136.29, 132.07, 131.56, 129.69, 129.35, 128.45, 128.08, 127.48, 127.41, 127.25, 127.15, 126.53, 126.49, 121.24, 110.04, 63.45, 53.50, 28.10 – 27.58 (m, 1C).

HRMS (ESI) calcd for $C_{28}H_{22}DNO$ ($M + Na$)⁺ 413.1735, found 413.1738.

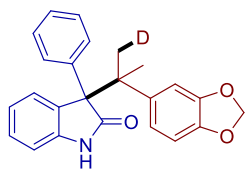
3-(1,2-diphenylethyl-2-d)-3-phenylindolin-2-one. (52)



Isolated yield 85% (33.2 mg, 0.1 mmol scale, $d.r. = 1 : 1$), $[D] = 2 : 1$, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). **¹H NMR** (400 MHz, $CDCl_3$) δ 8.46 (s, 0.5H), 7.82 – 7.59 (m, 3H), 7.45 (t, $J = 7.6$ Hz, 1H), 7.40 – 7.31 (m, 2H), 7.31 – 7.24 (m, 1.5H), 7.14 – 6.85 (m, 9H), 6.85 – 6.78 (m, 1H), 6.78 – 6.68 (m, 2H), 4.19 – 4.01 (m, 1H), 3.36 – 3.24 (m, 0.3H), 3.19 – 3.01 (m, 1H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 179.99, 178.85, 141.86, 140.52, 140.49, 140.48, 140.08, 140.05, 140.03, 140.00, 139.06, 138.06, 137.50, 137.49, 131.72, 130.03, 129.57, 129.26, 128.88, 128.79, 128.75, 128.71, 128.04, 127.94, 127.84, 127.69, 127.36, 127.32, 127.27, 127.25, 126.92, 126.66, 125.87, 125.83, 125.64, 121.96, 110.19, 109.69, 62.21, 61.80, 55.52, 55.16, 36.36, 35.20.

HRMS (ESI) calcd for $C_{28}H_{22}DNO$ ($M + Na$)⁺ 413.1735, found 413.1729.

3-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-3-phenylindolin-2-one. (53)



Isolated yield 86% (32.0 mg, 0.1 mmol scale), [D] > 20 : 1, white solid, eluent (PE : EA : DCM = 10 :

1 : 7.5). **¹H NMR** (400 MHz, CDCl₃) δ 8.27 (s, 1H), 7.84 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.33 – 7.27 (m, 3H),

7.19 (td, *J* = 7.7, 1.1 Hz, 1H), 6.93 (td, *J* = 7.7, 1.1 Hz, 1H), 6.87 – 6.76 (m, 1H), 6.68 (d, *J* = 7.2 Hz,

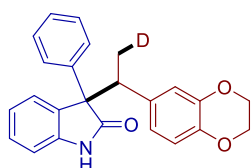
1H), 6.58 (d, *J* = 8.3 Hz, 1H), 6.33 (dd, *J* = 8.3, 1.9 Hz, 1H), 6.24 (d, *J* = 1.4 Hz, 1H), 5.89 (dd, *J* = 9.2, 1.5 Hz, 2H), 1.68 – 1.60

(m, 2.5H), 1.38 – 1.30 (m, 2.5H). **¹³C NMR** (101 MHz, CDCl₃) δ 179.09, 146.37, 145.81, 140.90, 138.67, 135.32, 130.35, 130.16,

128.76, 127.92, 127.32, 127.29, 121.80, 120.89, 109.49, 109.35, 106.57, 100.82, 62.46, 44.92, 25.93, 25.18.

HRMS (ESI) calcd for C₂₄H₂₀DNO₃ (M + Na)⁺ 395.1476, found 395.1470.

3-(1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)ethyl-2-d)-3-phenylindolin-2-one. (54)



Isolated yield 74% (27.5 mg, 0.1 mmol scale, *d.r.* = 1 : 1), [D] > 20 : 1, white solid, eluent (PE : EA :

DCM = 10 : 1 : 7.5). **¹H NMR** (400 MHz, CDCl₃) δ 7.91 (s, 1H), 7.63 – 7.56 (m, 2H), 7.33 – 7.27 (m,

2H), 7.27 – 7.16 (m, 2H), 7.00 (td, *J* = 7.5, 1.0 Hz, 1H), 6.94 (d, *J* = 7.4 Hz, 1H), 6.83 (d, *J* = 7.7 Hz,

1H), 6.54 (d, *J* = 8.4 Hz, 1H), 6.42 (d, *J* = 2.1 Hz, 1H), 6.33 (dd, *J* = 8.4, 2.2 Hz, 1H), 4.26 – 4.07 (m, 4H), 3.90 (t, *J* = 7.0 Hz,

1H), 1.25 – 1.18 (m, 2.5H). **¹³C NMR** (101 MHz, CDCl₃) δ 179.69, 142.31, 142.15, 140.75, 138.62, 133.76, 129.66, 128.29,

128.00, 127.83, 127.28, 127.23, 122.48, 121.59, 118.14, 115.74, 109.53, 64.30, 64.22, 61.27, 46.23.

HRMS (ESI) calcd for C₂₄H₂₀DNO₃ (M + Na)⁺ 395.1476, found 395.1472.

¹H NMR (400 MHz, CDCl₃) δ 7.64 – 7.48 (m, 3H), 7.36 – 7.30 (m, 2H), 7.29 – 7.25 (m, 2H), 7.24 (s, 1H), 7.15 (td, *J* = 7.6, 1.0

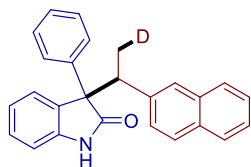
Hz, 1H), 6.68 (d, *J* = 7.7 Hz, 1H), 6.48 (d, *J* = 8.3 Hz, 1H), 6.39 – 6.26 (m, 2H), 4.15 – 4.01 (m, 4H), 3.93 (t, *J* = 7.2 Hz, 1H),

1.32 – 1.25 (m, 2.5H). **¹³C NMR** (101 MHz, CDCl₃) δ 179.00, 142.44, 142.18, 141.49, 138.07, 133.81, 129.26, 128.50, 128.48,

127.84, 127.34, 127.21, 121.77, 117.61, 116.00, 109.89, 64.22, 64.12, 61.88, 46.47.

HRMS (ESI) calcd for C₂₄H₂₀DNO₃ (M + Na)⁺ 395.1476, found 395.1472.

3-(1-(naphthalen-2-yl)ethyl-2-d)-3-phenylindolin-2-one. (55)



Isolated yield 85% (31.0 mg, 0.1 mmol scale, *d.r.* = 1 : 1), [D] > 20 : 1, white solid, eluent (PE : EA :

DCM = 10 : 1 : 7.5). **¹H NMR** (400 MHz, CDCl₃) δ 8.23 (s, 0.5H), 7.76 – 7.54 (m, 4H), 7.54 – 7.44 (m,

1H), 7.44 – 7.15 (m, 8H), 6.99 – 6.77 (m, 2H), 6.62 – 6.49 (m, 0.5H), 4.35 – 4.05 (m, 1H), 1.49 – 1.41

(m, 1H), 1.37 – 1.29 (m, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 179.86, 178.95, 141.52, 140.90, 138.54, 138.10, 138.05, 137.93,

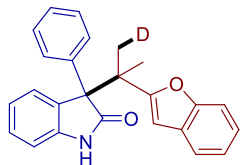
132.92, 132.69, 132.40, 132.29, 129.55, 129.21, 128.58, 128.31, 128.12, 128.08, 127.94, 127.93, 127.90, 127.88, 127.44,

127.33, 127.29, 127.27, 126.83, 126.72, 126.35, 125.63, 125.55, 125.52, 125.47, 121.79, 121.50, 109.99, 109.72, 62.00, 61.29,

47.30, 47.06, 16.20, 15.57.

HRMS (ESI) calcd for C₂₆H₂₀DNO (M + Na)⁺ 387.1578, found 387.1571.

3-(2-(benzofuran-2-yl)propan-2-yl-1-d)-3-phenylindolin-2-one. (56)



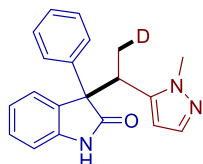
Isolated yield 86% (31.6 mg, 0.1 mmol scale), [D] > 20 : 1, white solid, eluent (PE : EA : DCM = 10 :

1 : 7.5). ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.62 (s, 1H), 7.84 – 7.74 (m, 2H), 7.56 – 7.48 (m, 1H), 7.35 – 7.24 (m, 4H), 7.23 – 7.11 (m, 3H), 6.94 – 6.83 (m, 2H), 6.77 (d, *J* = 7.6 Hz, 1H), 6.29 (s, 1H), 1.60 –

1.52 (m, 2.5H), 1.40 – 1.34 (m, 2.5H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 177.77, 162.74, 153.75, 142.37, 135.78, 130.37, 129.97, 128.51, 128.25, 127.90, 127.75, 127.57, 124.18, 123.09, 121.29, 120.99, 111.16, 109.75, 104.03, 61.14, 43.12, 24.23, 23.69.

HRMS (ESI) calcd for C₂₅H₂₀DNO₂ (M + Na)⁺ 391.1527, found 391.1521.

3-(1-(1-methyl-1H-pyrazol-5-yl)ethyl-2-d)-3-phenylindolin-2-one. (57)



Isolated yield 59% (18.8 mg, 0.1 mmol scale, *d.r.* = 1 : 1), [D] > 20 : 1, white solid, eluent (PE : EA = 5 : 1).

¹H NMR (400 MHz, CDCl₃) δ 8.21 (s, 1H), 7.58 – 7.50 (m, 2H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 1.6 Hz, 1H), 7.31 – 7.18 (m, 4H), 7.06 (td, *J* = 7.6, 1.0 Hz, 1H), 6.88 (d, *J* = 7.7 Hz, 1H), 6.19 (d, *J* = 1.8 Hz,

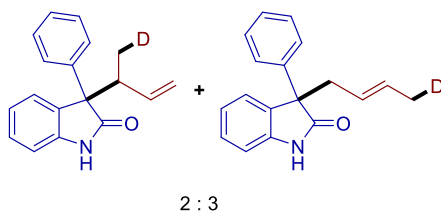
1H), 3.89 (t, *J* = 6.9 Hz, 1H), 3.10 (s, 3H), 1.23 – 1.15 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 179.11, 142.60, 140.66, 137.76, 137.41, 129.56, 128.53, 128.43, 127.60, 127.57, 126.91, 121.99, 109.83, 105.91, 60.09, 39.09, 36.10.

HRMS (ESI) calcd for C₂₀H₁₈DN₃O (M + Na)⁺ 341.1483, found 341.1484.

¹H NMR (400 MHz, CDCl₃) δ 7.66 – 7.58 (m, 2H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.43 – 7.29 (m, 5H), 7.21 (td, *J* = 7.6, 1.0 Hz, 1H), 7.09 (d, *J* = 1.7 Hz, 1H), 6.79 (d, *J* = 7.8 Hz, 1H), 4.98 (d, *J* = 1.9 Hz, 1H), 4.18 (t, *J* = 7.1 Hz, 1H), 3.95 (s, 3H), 1.34 – 1.27 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 178.54, 142.47, 141.84, 137.63, 137.25, 128.91, 128.66, 127.73, 127.68, 127.33, 121.94, 110.14, 103.96, 60.16, 38.00, 36.78.

HRMS (ESI) calcd for C₂₀H₁₈DN₃O (M + Na)⁺ 341.1483, found 341.1481.

3-(but-3-en-2-yl-1-d)-3-phenylindolin-2-one and (E)-3-(but-2-en-1-yl-4-d)-3-phenylindolin-2-one. (58)



2 : 3

Isolated yield 66% (17.4 mg, 0.1 mmol scale, *d.r.* = 1 : 1, *Z* / *E* = 3 : 1), [D] > 20 : 1,

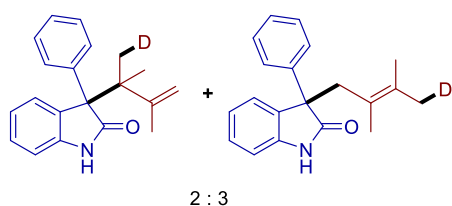
white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). ¹H NMR (400 MHz, CDCl₃) δ 8.70 – 8.20 (m, 1H), 7.49 – 7.13 (m, 7H), 7.12 – 7.00 (m, 1H), 6.95 – 6.87 (m, 1H), 5.80

(ddd, *J* = 17.2, 10.6, 5.9 Hz, 0.2H), 5.52 – 5.36 (m, 0.6H), 5.29 (ddd, *J* = 17.1, 10.1,

8.2 Hz, 0.2H), 5.14 – 4.81 (m, 1.4H), 3.53 – 3.37 (m, 0.4H), 3.17 – 2.90 (m, 1.2H), 1.54 – 1.40 (m, 1.2H), 1.10 – 1.02 (m, 0.4H),

0.87 – 0.79 (m, 0.4H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 180.74, 180.57, 180.15, 179.98, 141.33, 140.93, 139.62, 139.56, 138.51, 138.31, 138.10, 138.06, 132.76, 132.68, 130.12, 130.09, 129.82, 129.42, 128.61, 128.58, 128.51, 128.46, 128.31, 128.26, 128.13, 128.05, 127.82, 127.69, 127.66, 127.39, 127.34, 127.32, 127.08, 127.06, 126.65, 126.52, 125.41, 125.22, 124.43, 123.83, 122.46, 122.39, 122.01, 121.97, 116.82, 116.60, 110.05, 109.97, 109.92, 60.91, 60.40, 57.21, 56.82, 45.32, 43.53, 40.59, 34.79, 17.92, 17.84, 17.64, 17.45. **HRMS** (ESI) calcd for $\text{C}_{18}\text{H}_{16}\text{DNO}$ ($\text{M} + \text{Na}$) $^+$ 287.1265, found 287.1263.

3-(2,3-dimethylbut-3-en-2-yl-1-d)-3-phenylindolin-2-one and (E)-3-(2,3-dimethylbut-2-en-1-yl-4-d)-3-phenylindolin-2-one. (59)



Isolated yield 73% (21.3 mg, 0.1 mmol scale), $[\text{D}] > 20 : 1$, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.01 – 7.88 (m, 2H), 7.81 (s, 1H), 7.75 (d, $J = 7.7$ Hz, 1H), 7.33 – 7.19 (m, 4H), 7.07 (td, $J = 7.7, 1.0$ Hz, 1H), 6.84 (d, $J = 7.7$ Hz, 1H), 4.82 (s, 1H), 4.55 (s, 1H), 1.45 – 1.37 (m, 5H), 1.23 – 1.16

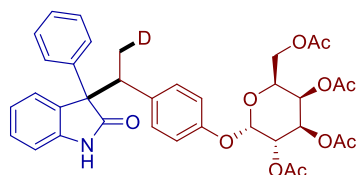
(m, 2.5H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 178.83, 149.25, 140.75, 135.81, 130.95, 129.86, 128.69, 127.88, 127.44, 127.03, 121.03, 114.55, 109.36, 61.44, 46.11, 24.73, 24.65, 22.16.

HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{20}\text{DNO}$ ($\text{M} + \text{Na}$) $^+$ 315.1578, found 315.1570.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.31 (s, 1H), 7.50 – 7.43 (m, 2H), 7.35 – 7.28 (m, 2H), 7.28 – 7.20 (m, 2H), 7.17 (d, $J = 7.4$ Hz, 1H), 7.06 – 6.99 (m, 1H), 6.90 (d, $J = 7.7$ Hz, 1H), 3.29 (d, $J = 13.6$ Hz, 1H), 3.07 (d, $J = 13.6$ Hz, 1H), 1.53 – 1.43 (m, 5H), 1.30 – 1.23 (m, 2.5H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 181.10, 140.88, 140.63, 132.10, 129.21, 128.45, 127.97, 127.21, 127.03, 126.44, 123.42, 121.87, 109.69, 57.14, 42.66, 21.08, 20.78, 19.05.

HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{20}\text{DNO}$ ($\text{M} + \text{Na}$) $^+$ 315.1578, found 315.1575.

(2S,3R,4R,5S,6S)-2-(acetoxymethyl)-6-(4-(1-(2-oxo-3-phenylindolin-3-yl)ethyl-2-d)phenoxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate. (60)



Isolated yield 56% (37.0 mg, 0.1 mmol scale, $d.r. = 1 : 1$), $[\text{D}] > 20 : 1$, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.75 (d, $J = 12.3$ Hz, 1H), 7.57 (d, $J = 8.3$ Hz, 2H), 7.32 – 7.27 (m, 2H), 7.26 – 7.16 (m, 2H), 7.00 – 6.94 (m, 1H), 6.92 –

6.77 (m, 4H), 6.74 – 6.68 (m, 2H), 5.48 – 5.41 (m, 2H), 5.07 (dd, $J = 10.5, 3.4$ Hz, 1H), 4.95 (dd, $J = 7.9, 4.2$ Hz, 1H), 4.26 – 4.08 (m, 2H), 4.04 – 3.93 (m, 2H), 2.20 – 2.14 (m, 3H), 2.06 (s, 1.5H), 2.04 (s, 3H), 2.02 – 1.99 (m, 4.5H), 1.30 – 1.22 (m, 2H).

$^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 179.40, 179.37, 170.41, 170.40, 170.29, 170.27, 170.25, 170.17, 169.40, 169.37, 155.55, 140.73,

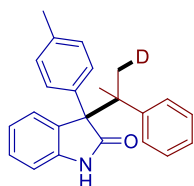
140.68, 138.49, 135.35, 135.32, 130.36, 129.57, 129.37, 128.32, 128.30, 128.11, 128.09, 127.87, 127.81, 127.29, 127.28, 127.24, 127.10, 121.55, 115.59, 115.53, 109.58, 99.54, 99.49, 70.96, 70.89, 70.82, 70.79, 68.63, 68.60, 66.83, 61.35, 61.30, 61.17, 61.14, 46.24, 46.08, 20.75, 20.71, 20.67, 20.60.

HRMS (ESI) calcd for $C_{36}H_{36}DNO_{11}$ ($M + Na$)⁺ 683.2322, found 683.2332.

¹H NMR (600 MHz, $CDCl_3$) δ 7.64 – 7.53 (m, 3H), 7.35 (t, $J = 7.6$ Hz, 2H), 7.32 – 7.28 (m, 1H), 7.28 – 7.22 (m, 1H), 7.20 – 7.14 (m, 1H), 7.01 (d, $J = 3.7$ Hz, 1H), 6.83 – 6.74 (m, 2H), 6.72 – 6.60 (m, 3H), 5.51 – 5.35 (m, 2H), 5.06 (ddd, $J = 10.4, 7.0, 3.5$ Hz, 1H), 4.93 (dd, $J = 23.3, 8.0$ Hz, 1H), 4.23 (dd, $J = 11.4, 6.9$ Hz, 0.5H), 4.19 – 4.09 (m, 1.5H), 4.06 – 3.96 (m, 2H), 2.16 (d, $J = 3.0$ Hz, 3H), 2.07 (s, 1.5H), 2.03 (s, 3H), 2.02 (s, 1.5H), 2.00 (d, $J = 1.0$ Hz, 3H), 1.36 – 1.27 (m, 2H). **¹³C NMR** (151 MHz, $CDCl_3$) δ 178.66, 170.51, 170.40, 170.27, 170.25, 170.16, 169.39, 169.37, 155.62, 155.51, 141.42, 141.39, 137.83, 137.80, 135.47, 135.27, 129.90, 129.82, 129.06, 128.98, 128.56, 128.50, 127.81, 127.44, 127.25, 121.76, 116.03, 115.70, 109.88, 99.71, 99.30, 71.03, 70.90, 70.84, 70.78, 68.56, 66.86, 61.87, 61.84, 61.37, 61.30, 46.34, 46.31, 20.75, 20.74, 20.72, 20.66, 20.59.

HRMS (ESI) calcd for $C_{36}H_{36}DNO_{11}$ ($M + Na$)⁺ 683.2322, found 683.2321.

3-(2-phenylpropan-2-yl-1-d)-3-(p-tolyl)indolin-2-one. (61)



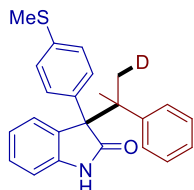
Isolated yield 89% (30.4 mg, 0.1 mmol scale), $[D] > 20 : 1$, white solid, eluent (PE : EA : DCM = 10 : 1 :

7.5). **¹H NMR** (600 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.70 (d, $J = 8.2$ Hz, 2H), 7.19 – 7.13 (m, 2H), 7.14 – 7.05 (m, 4H), 6.90 – 6.81 (m, 3H), 6.79 (d, $J = 7.6$ Hz, 1H), 6.51 (s, 1H), 2.34 (s, 3H), 1.71 – 1.66 (m, 2.5H), 1.44 – 1.34 (m, 2.5H). **¹³C NMR** (151 MHz, $CDCl_3$) δ 179.34, 144.62, 140.92, 136.87, 132.33, 130.60,

130.11, 128.69, 128.56, 128.03, 127.77, 126.85, 126.43, 120.76, 109.25, 62.13, 44.84, 25.55, 24.79, 20.95.

HRMS (ESI) calcd for $C_{24}H_{22}DNO$ ($M + Na$)⁺ 365.1735, found 365.1729.

3-(4-(methylthio)phenyl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (62)



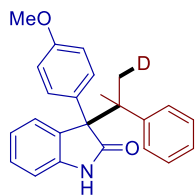
Isolated yield 46% (17.2 mg, 0.1 mmol scale), $[D] > 20 : 1$, white solid, eluent (PE : EA : DCM = 10 : 1 :

7.5). **¹H NMR** (600 MHz, $CDCl_3$) δ 7.78 – 7.71 (m, 3H), 7.21 – 7.10 (m, 6H), 6.88 – 6.82 (m, 3H), 6.76 (d, $J = 7.6$ Hz, 1H), 6.46 (s, 1H), 2.47 (s, 3H), 1.69 – 1.64 (m, 2.5H), 1.41 – 1.36 (m, 2.5H). **¹³C NMR** (151 MHz, $CDCl_3$) δ 178.66, 144.39, 140.70, 137.52, 132.06, 130.65, 130.23, 128.70, 128.54, 127.92, 126.93,

126.53, 125.06, 120.88, 109.18, 61.86, 44.97, 25.43, 24.72, 15.53.

HRMS (ESI) calcd for $C_{24}H_{24}DNOS$ ($M + Na$)⁺ 397.1455, found 397.1453

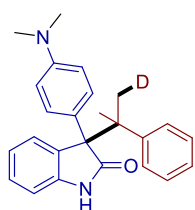
3-(4-methoxyphenyl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (63)



Isolated yield 74% (26.5 mg, 0.1 mmol scale), [D] > 20 : 1, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). **¹H NMR** (400 MHz, DMSO-*d*₆) δ 10.44 (s, 1H), 7.68 (d, *J* = 8.9 Hz, 2H), 7.20 – 7.06 (m, 4H), 6.92 – 6.75 (m, 5H), 6.72 – 6.59 (m, 2H), 3.73 (s, 3H), 1.60 – 1.50 (m, 2.5H), 1.35 – 1.26 (m, 2.5H). **¹³C NMR** (101 MHz, DMSO-*d*₆) δ 178.59, 158.59, 144.92, 142.38, 131.40, 130.75, 128.38, 128.32, 128.25, 127.88, 127.27, 126.73, 120.54, 113.02, 109.57, 61.21, 55.47, 44.45, 25.88, 24.96.

HRMS (ESI) calcd for C₂₄H₂₂DNO₂ (M + Na)⁺ 381.1684, found 381.1676.

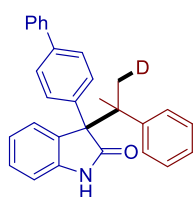
3-(4-(dimethylamino)phenyl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (64)



Isolated yield 77% (28.6 mg, 0.1 mmol scale), [D] > 20 : 1, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). **¹H NMR** (400 MHz, DMSO-*d*₆) δ 10.36 (s, 1H), 7.54 (d, *J* = 8.9 Hz, 2H), 7.20 – 7.05 (m, 4H), 6.87 – 6.75 (m, 3H), 6.73 – 6.52 (m, 4H), 2.86 (s, 6H), 1.60 – 1.50 (m, 2.5H), 1.34 – 1.24 (m, 2.5H). **¹³C NMR** (101 MHz, DMSO-*d*₆) δ 178.84, 149.52, 145.26, 142.33, 131.10, 130.92, 128.32, 128.29, 128.01, 127.23, 126.62, 122.92, 120.37, 111.38, 109.43, 61.13, 44.42, 40.37, 26.00, 24.98.

HRMS (ESI) calcd for C₂₅H₂₅DN₂O (M + Na)⁺ 394.2000, found 394.1996.

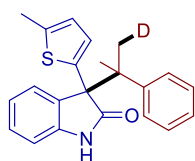
3-([1,1'-biphenyl]-4-yl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (65)



Isolated yield 47% (19.0 mg, 0.1 mmol scale), [D] > 20 : 1, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). **¹H NMR** (400 MHz, CDCl₃) δ 8.02 (s, 1H), 7.91 (d, *J* = 8.5 Hz, 2H), 7.67 – 7.57 (m, 2H), 7.54 (d, *J* = 8.7 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.3 Hz, 1H), 7.24 – 7.16 (m, 2H), 7.13 (t, *J* = 7.4 Hz, 2H), 6.94 – 6.85 (m, 3H), 6.79 (d, *J* = 7.7 Hz, 1H), 6.59 (d, *J* = 7.3 Hz, 1H), 1.78 – 1.69 (m, 2.5H), 1.48 – 1.40 (m, 2.5H). **¹³C NMR** (101 MHz, CDCl₃) δ 178.86, 144.44, 140.83, 140.50, 139.76, 134.51, 130.62, 130.35, 128.79, 128.76, 128.56, 127.93, 127.35, 127.01, 126.91, 126.52, 125.82, 120.90, 109.26, 62.19, 45.08, 25.53, 24.79.

HRMS (ESI) calcd for C₂₉H₂₄DNO (M + Na)⁺ 427.1891, found 427.1891.

3-(5-methylthiophen-2-yl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (66)

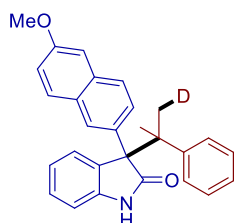


Isolated yield 40% (14.0 mg, 0.1 mmol scale), [D] > 20 : 1, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). **¹H NMR** (400 MHz, CDCl₃) δ 7.84 (s, 1H), 7.21 – 7.06 (m, 4.5H), 7.00 – 6.93 (m, 2H), 6.89 (td, *J* = 7.7, 0.8 Hz, 1H), 6.74 – 6.66 (m, 2H), 6.64 – 6.60 (m, 1H), 2.43 (m, *J* = 0.9 Hz, 3H), 1.77 – 1.73 (m, 2.5H),

1.48 – 1.42 (m, 2.5H). ^{13}C NMR (101 MHz, CDCl_3) δ 178.24, 143.97, 140.57, 139.53, 136.48, 131.31, 128.57, 128.17, 128.15, 127.37, 126.91, 126.48, 124.37, 124.29, 121.13, 109.14, 60.81, 44.89, 25.09, 24.12, 15.15.

HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{20}\text{DNOS}$ ($\text{M} + \text{Na}$) $^+$ 371.1299, found 371.1297.

3-(6-methoxynaphthalen-2-yl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (67)



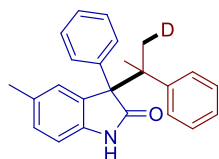
Isolated yield 82% (33.5 mg, 0.1 mmol scale), $[\text{D}] > 20 : 1$, white solid, eluent (PE : EA : DCM = 10 : 1 :

7.5). ^1H NMR (400 MHz, CDCl_3) δ 8.38 (s, 1H), 8.13 (s, 0.2H), 8.05 – 7.97 (m, 0.3H), 7.73 – 7.63 (m, 1.5H), 7.24 – 7.04 (m, 6H), 6.93 (td, $J = 7.7, 0.9$ Hz, 1H), 6.88 – 6.78 (m, 3H), 6.64 (d, $J = 7.4$ Hz, 1H), 3.92 (s, 3H), 1.81 – 1.70 (m, 2.5H), 1.49 – 1.41 (m, 2.5H). ^{13}C NMR (101 MHz, CDCl_3) δ 179.29, 157.97,

144.57, 140.98, 133.46, 130.58, 130.42, 130.17, 130.11, 129.60, 128.76, 128.59, 127.98, 127.90, 126.87, 126.50, 125.21, 120.91, 118.67, 109.36, 105.02, 62.35, 55.33, 45.17, 25.66, 24.87.

HRMS (ESI) calcd for $\text{C}_{28}\text{H}_{24}\text{DNO}_2$ ($\text{M} + \text{Na}$) $^+$ 431.1840, found 431.1841.

5-methyl-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (68)



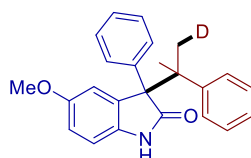
Isolated yield 92% (31.5 mg, 0.1 mmol scale), $[\text{D}] > 20 : 1$, white solid, eluent (PE : EA : DCM = 10 : 1 :

7.5). ^1H NMR (400 MHz, CDCl_3) δ 8.37 (s, 1H), 7.91 – 7.77 (m, 2H), 7.34 – 7.26 (m, 3H), 7.19 (t, $J = 7.2$ Hz, 1H), 7.12 (t, $J = 7.4$ Hz, 2H), 6.98 (d, $J = 7.8$ Hz, 1H), 6.81 (d, $J = 7.5$ Hz, 2H), 6.70 (d, $J = 7.8$ Hz,

1H), 6.20 (s, 1H), 2.22 (s, 3H), 1.73 – 1.67 (m, 2.5H), 1.42 – 1.33 (m, 2.5H). ^{13}C NMR (101 MHz, CDCl_3) δ 179.30, 144.57, 138.51, 135.51, 130.27, 130.25, 129.90, 129.78, 128.64, 128.10, 127.25, 127.16, 126.75, 126.51, 108.88, 62.38, 44.96, 25.50, 24.82, 21.41.

HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{22}\text{DNO}$ ($\text{M} + \text{Na}$) $^+$ 365.1735, found 365.1729.

5-methoxy-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (69)



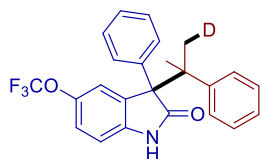
Isolated yield 90% (32.2 mg, 0.1 mmol scale), $[\text{D}] > 20 : 1$, white solid, eluent (PE : EA : DCM = 10 :

1 : 7.5). ^1H NMR (400 MHz, CDCl_3) δ 8.44 (s, 1H), 7.88 – 7.80 (m, 2H), 7.34 – 7.26 (m, 3H), 7.23 – 7.08 (m, 3H), 6.83 (d, $J = 7.3$ Hz, 2H), 6.77 – 6.70 (m, 2H), 6.03 (s, 1H), 3.64 (s, 3H), 1.74 – 1.69 (m,

2.5H), 1.42 – 1.34 (m, 2.5H). ^{13}C NMR (101 MHz, CDCl_3) δ 179.30, 154.05, 144.51, 135.38, 134.57, 131.49, 130.18, 128.63, 127.28, 127.24, 126.92, 126.57, 115.89, 113.04, 109.40, 62.76, 55.68, 45.03, 44.96, 25.65, 24.81.

HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{22}\text{DNO}_2$ ($\text{M} + \text{Na}$) $^+$ 381.1684, found 381.1680.

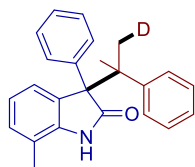
3-phenyl-3-(2-phenylpropan-2-yl-1-d)-5-(trifluoromethoxy)indolin-2-one. (70)



Isolated yield 53% (21.8 mg, 0.1 mmol scale), [D] > 20 : 1, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.31 (s, 1H), 7.85 – 7.68 (m, 2H), 7.37 – 7.28 (m, 3H), 7.20 (t, $J = 7.2$ Hz, 1H), 7.16 – 7.04 (m, 3H), 6.87 – 6.73 (m, 3H), 6.37 (s, 1H), 1.74 – 1.66 (m, 2.5H), 1.44 – 1.36 (m, 2.5H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 179.04, 143.69, 143.08 (d, $J = 1.8$ Hz), 143.07, 143.04, 139.62, 134.45, 131.71, 129.98, 128.34, 127.58, 127.49, 127.14, 126.81, 122.93, 121.34, 120.61 (d, $J = 257.4$ Hz), 109.42, 62.70, 45.11, 25.34, 24.73. $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -58.21.

HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{19}\text{DF}_3\text{NO}_2$ ($\text{M} + \text{Na}$) $^+$ 435.1401, found 435.1396.

7-methyl-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (71)

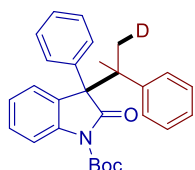


Isolated yield 98% (33.5 mg, 0.1 mmol scale), [D] > 20 : 1, white solid, eluent (PE : EA : DCM = 10 : 1 : 7.5). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.29 (s, 1H), 7.90 – 7.79 (m, 2H), 7.35 – 7.20 (m, 3H), 7.16 (t, $J = 7.2$ Hz, 1H), 7.09 (t, $J = 7.4$ Hz, 2H), 7.02 (d, $J = 7.6$ Hz, 1H), 6.85 – 6.75 (m, 3H), 6.32 (d, $J = 7.5$ Hz, 1H), 2.28 (s, 3H), 1.75 – 1.67 (m, 2.5H), 1.44 – 1.36 (m, 2.5H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 180.07, 144.54,

139.91, 135.58, 130.28, 129.94, 129.11, 128.58, 127.21, 127.16, 126.77, 126.44, 126.20, 120.64, 118.66, 62.80, 44.91, 25.58, 24.88, 16.55.

HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{22}\text{DNO}$ ($\text{M} + \text{Na}$) $^+$ 365.1735, found 365.1730

tert-butyl 2-oxo-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indoline-1-carboxylate. (72)



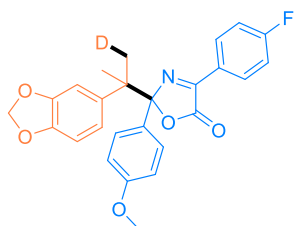
Isolated yield 37% (15.8 mg, 0.1 mmol scale), [D] > 20 : 1, white solid, eluent (PE : EA = 20 : 1). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.80 (dd, $J = 6.6, 2.9$ Hz, 2H), 7.69 (d, $J = 8.0$ Hz, 1H), 7.34 – 7.27 (m, 3H), 7.27 – 7.21 (m, 1H), 7.19 (t, $J = 7.2$ Hz, 1H), 7.10 (t, $J = 7.5$ Hz, 2H), 6.98 (td, $J = 7.7, 0.9$ Hz, 1H), 6.75 (d, $J = 7.5$

Hz, 2H), 6.48 (d, $J = 7.3$ Hz, 1H), 1.74 – 1.68 (m, 2.5H), 1.61 (s, 9H), 1.42 – 1.34 (m, 2.5H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 175.32, 149.00, 144.23, 139.77, 135.19, 130.14, 128.52, 128.36, 128.32, 128.07, 127.47, 127.43, 126.98, 126.64, 122.51, 114.23, 84.24, 61.83, 46.15, 28.12, 25.83, 24.80.

HRMS (ESI) calcd for $\text{C}_{28}\text{H}_{28}\text{DNO}_3$ ($\text{M} + \text{Na}$) $^+$ 451.2102, found 451.2092.

2-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-4-(4-fluorophenyl)-2-(4-methoxyphenyl)oxazol-5(2H)-one

(73)

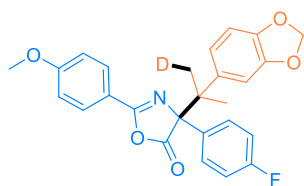


Separation by *prep*-HPLC (Waters E600) (MeOH : H₂O = 90 : 10), [D] > 20 : 1. ¹H NMR (400 MHz, CDCl₃) δ 8.30 (dd, *J* = 8.6, 5.5 Hz, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.13 (t, *J* = 8.7 Hz, 2H), 6.90 – 6.77 (m, 3H), 6.72 (dd, *J* = 8.2, 1.5 Hz, 1H), 6.62 (d, *J* = 8.3 Hz, 1H), 5.97 – 5.66 (m, 2H), 3.80 (s, 3H), 1.52 – 1.40 (m, 5H). ¹³C NMR (101 MHz, CDCl₃) δ 165.30 (d, *J* = 223.9 Hz), 163.82, 159.66, 154.72, 146.93, 146.13, 135.68, 130.92 (d, *J* = 8.9 Hz), 129.62, 128.60, 124.99 (d, *J* = 3.2 Hz), 122.20, 115.91 (d, *J* = 21.9 Hz), 112.72, 109.57, 109.45, 107.00, 100.91, 55.27, 47.00, 24.74, 24.60. ¹⁹F NMR (376 MHz, CDCl₃) δ -106.10.

HRMS (ESI) calcd for C₂₆H₂₁DFNO₅ (M + Na)⁺ 471.1437, found 471.1444.

4-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-4-(4-fluorophenyl)-2-(4-methoxyphenyl)oxazol-5(4H)-one

(74)

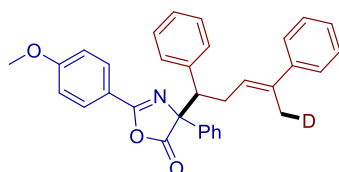


Isolated yield 69% (30.9 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). ¹H NMR (400 MHz, CDCl₃) δ 7.93 – 7.82 (m, 2H), 7.73 (dd, *J* = 8.4, 5.5 Hz, 2H), 7.08 – 6.96 (m, 2H), 6.97 – 6.91 (m, 2H), 6.86 (d, *J* = 1.9 Hz, 1H), 6.74 (dd, *J* = 8.3, 1.6 Hz, 1H), 6.60 (d, *J* = 8.3 Hz, 1H), 5.88 (d, *J* = 1.5 Hz, 1H), 5.82 (d, *J* = 1.4 Hz, 1H), 3.85 (s, 3H), 1.53 –

1.41 (m, 5H). ¹³C NMR (101 MHz, CDCl₃) δ 177.50, 163.06, 162.50 (d, *J* = 248.4 Hz), 158.87, 146.74, 146.14, 136.54, 131.17 (d, *J* = 8.0 Hz), 130.07 (d, *J* = 3.2 Hz), 129.72, 129.62, 121.69, 118.18, 114.32 (d, *J* = 21.4 Hz), 114.10, 109.15, 106.89, 100.83, 78.96, 55.44, 45.92, 24.18, 23.77. ¹⁹F NMR (376 MHz, CDCl₃) δ -114.21.

HRMS (ESI) calcd for C₂₆H₂₁DFNO₅ (M + Na)⁺ 471.1437, found 471.1437.

(*E*)-4-(1,4-diphenylpent-3-en-1-yl-5-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (76)

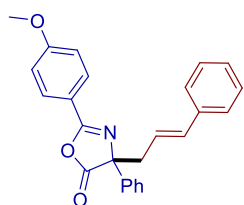


Isolated yield 80% (39.0 mg, 0.1 mmol scale, *r.r.* > 20 : 1), [D] > 20 : 1, colorless oil, eluent (PE : EA = 50 : 1). ¹H NMR (400 MHz, CDCl₃) δ 7.90 (d, *J* = 8.8 Hz, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.71 – 7.64 (m, 1H), 7.55 – 7.43 (m, 1H), 7.37 – 7.24 (m, 2.5H), 7.23 – 7.06 (m, 9H), 6.98 – 6.89 (m, 2.5H), 6.86 (dd, *J* = 6.4, 2.9 Hz, 1H), 5.18 (t, *J* = 7.2 Hz, 0.5H), 5.03 (t, *J* =

7.3 Hz, 0.5H), 3.93 – 3.80 (m, 3H), 3.54 – 3.44 (m, 1H), 2.62 – 2.31 (m, 2H), 1.89 – 1.72 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 185.37, 177.15, 162.05, 162.00, 159.28, 158.77, 140.66, 140.22, 137.47, 137.27, 136.90, 136.74, 136.44, 136.32, 136.32, 128.84, 128.74, 128.69, 127.46, 126.97, 126.95, 126.90, 126.66, 126.55, 126.51, 126.40, 125.65, 125.46, 125.18, 125.16, 125.06, 123.49, 122.98, 117.27, 117.16, 113.04, 113.01, 77.01, 54.96, 54.91, 54.47, 54.42, 29.56, 27.50, 24.37, 24.35.

HRMS (ESI) calcd for $C_{33}H_{28}DNO_3$ ($M + Na$)⁺ 511.2102, found 511.2074.

4-cinnamyl-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (78)



Isolated yield 35% (13.4 mg, 0.1 mmol scale, *r.r.* > 20 : 1), colorless oil, eluent (PE : EA = 50 : 1). **¹H**

NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.9 Hz, 2H), 7.84 – 7.63 (m, 2H), 7.40 (t, J = 7.4 Hz, 2H), 7.37 – 7.30 (m, 1H), 7.26 – 7.15 (m, 5H), 6.98 (d, J = 8.9 Hz, 2H), 6.53 (d, J = 15.8 Hz, 1H), 6.15 – 5.91 (m, 1H), 3.88 (s, 3H), 3.09 (d, J = 7.3 Hz, 2H). **¹³C NMR** (101 MHz, $CDCl_3$) δ 177.35, 162.25, 158.97,

137.05, 135.81, 134.51, 128.99, 127.65, 127.40, 127.21, 126.50, 125.34, 124.69, 121.00, 117.00, 113.19, 73.62, 54.48, 43.40.

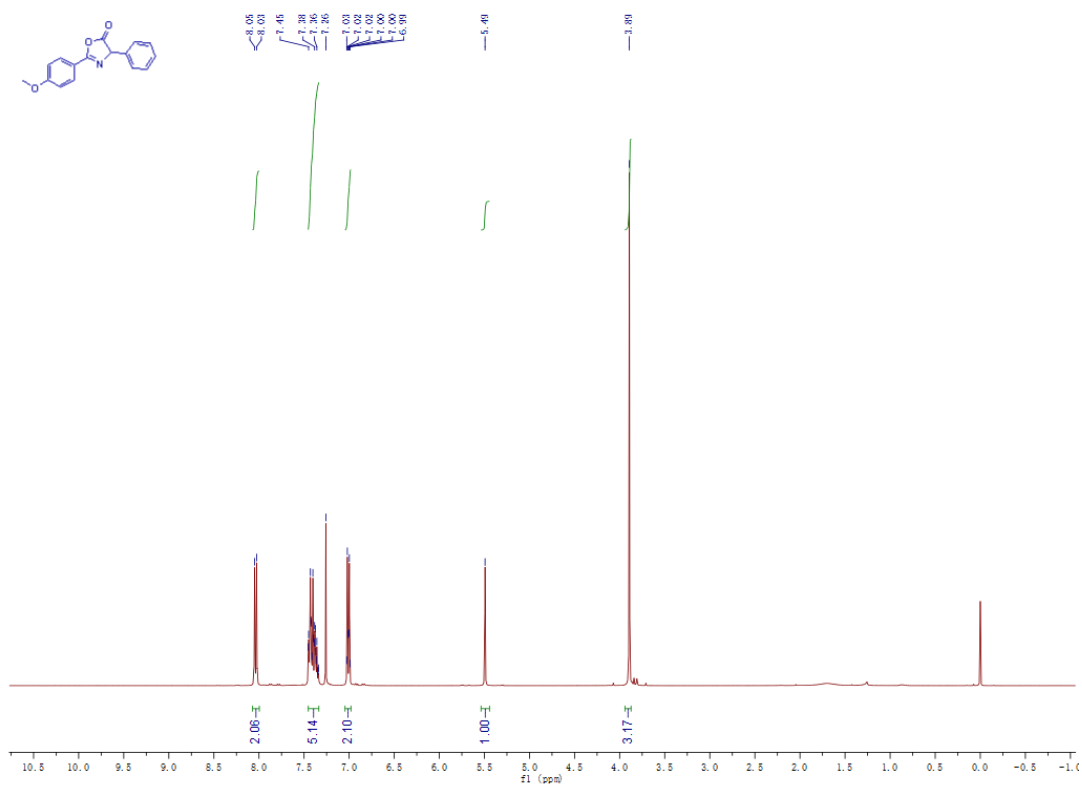
HRMS (ESI) calcd for $C_{25}H_{21}NO_3$ ($M + H$)⁺ 384.1594, found 384.1593.

7 References

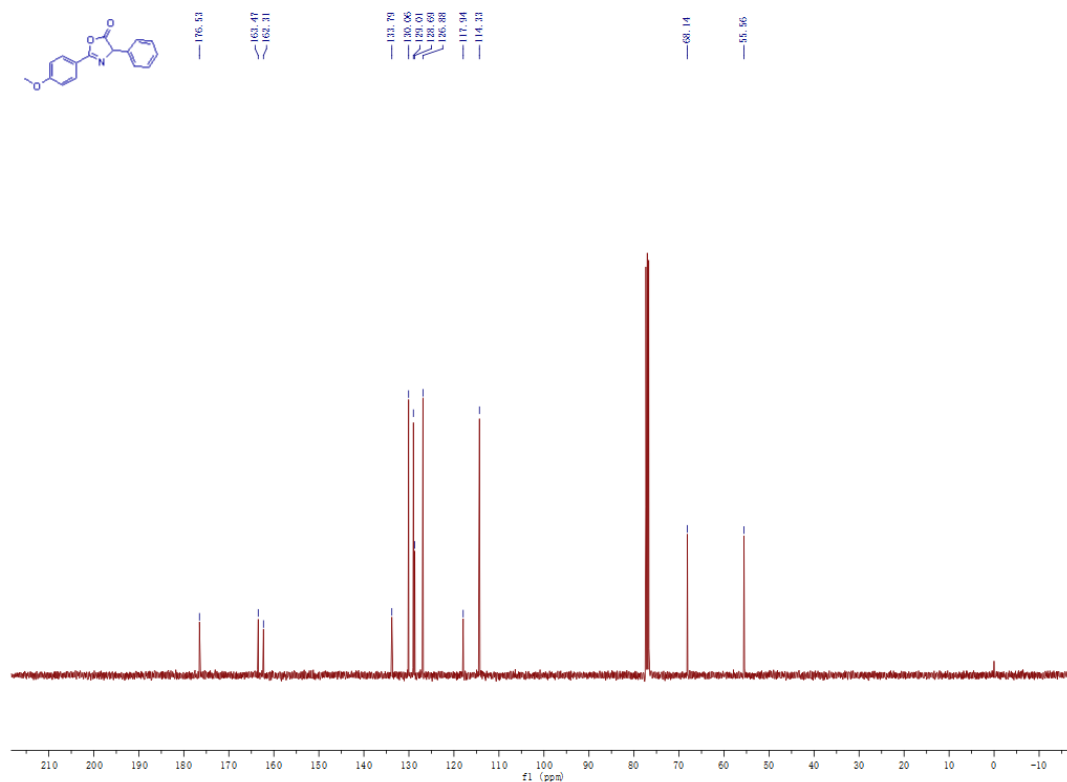
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8 NMR Spectra

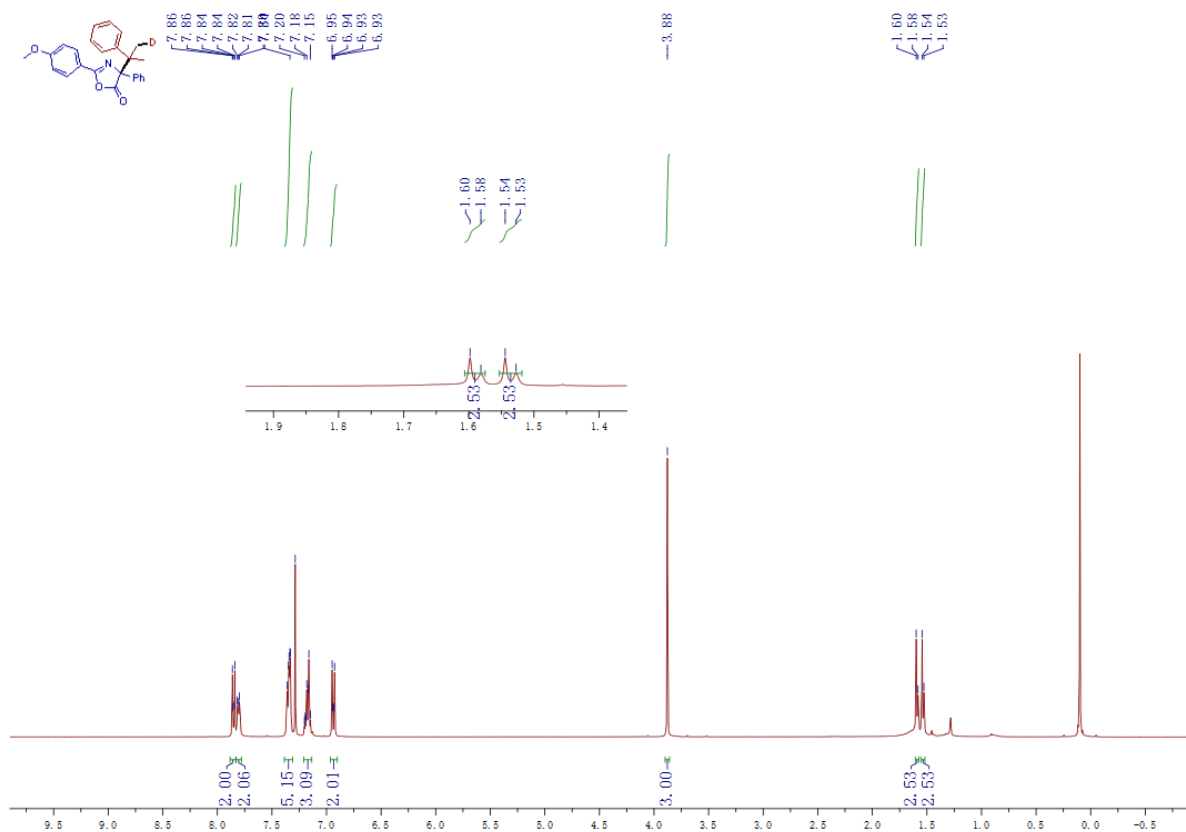
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (1)



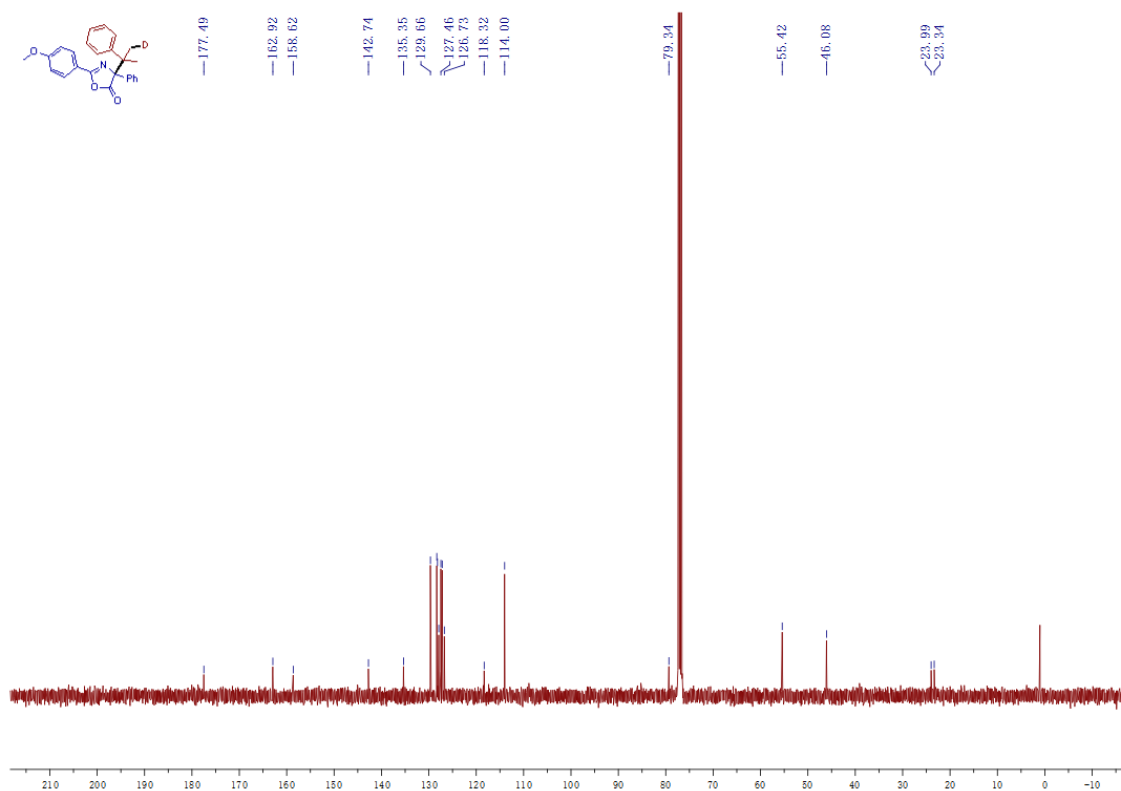
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (1)



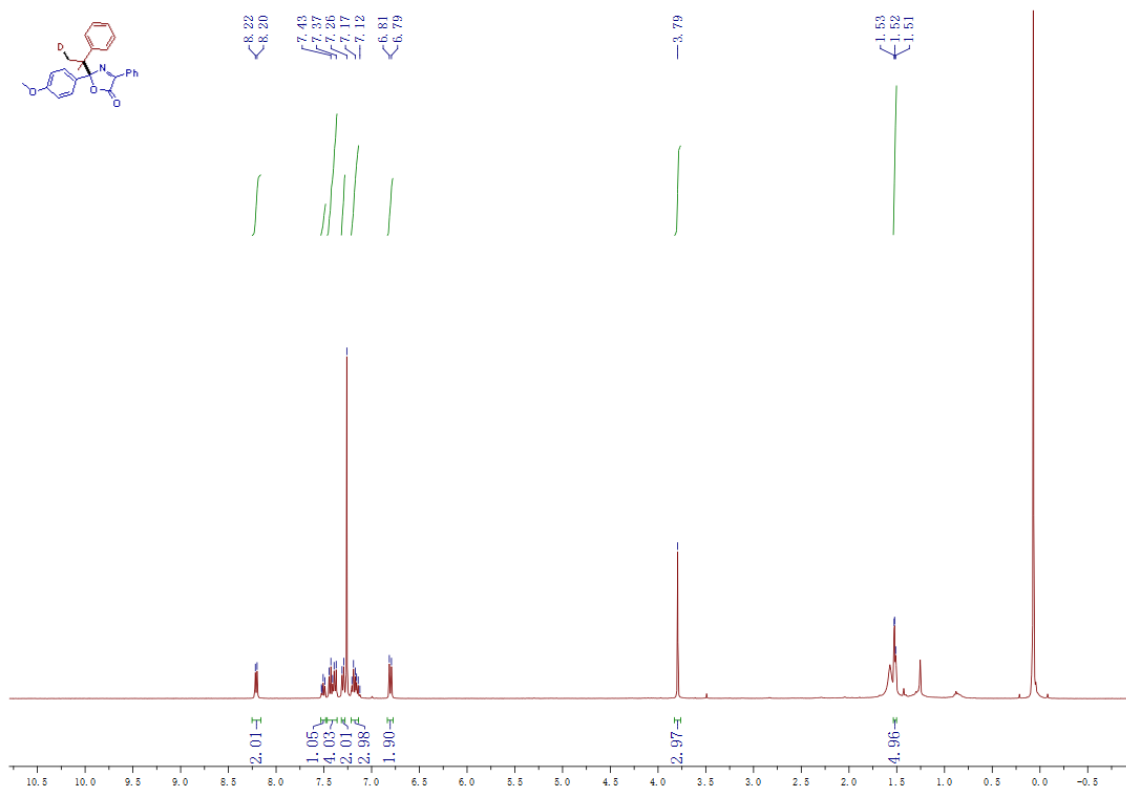
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-phenyl-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (3)



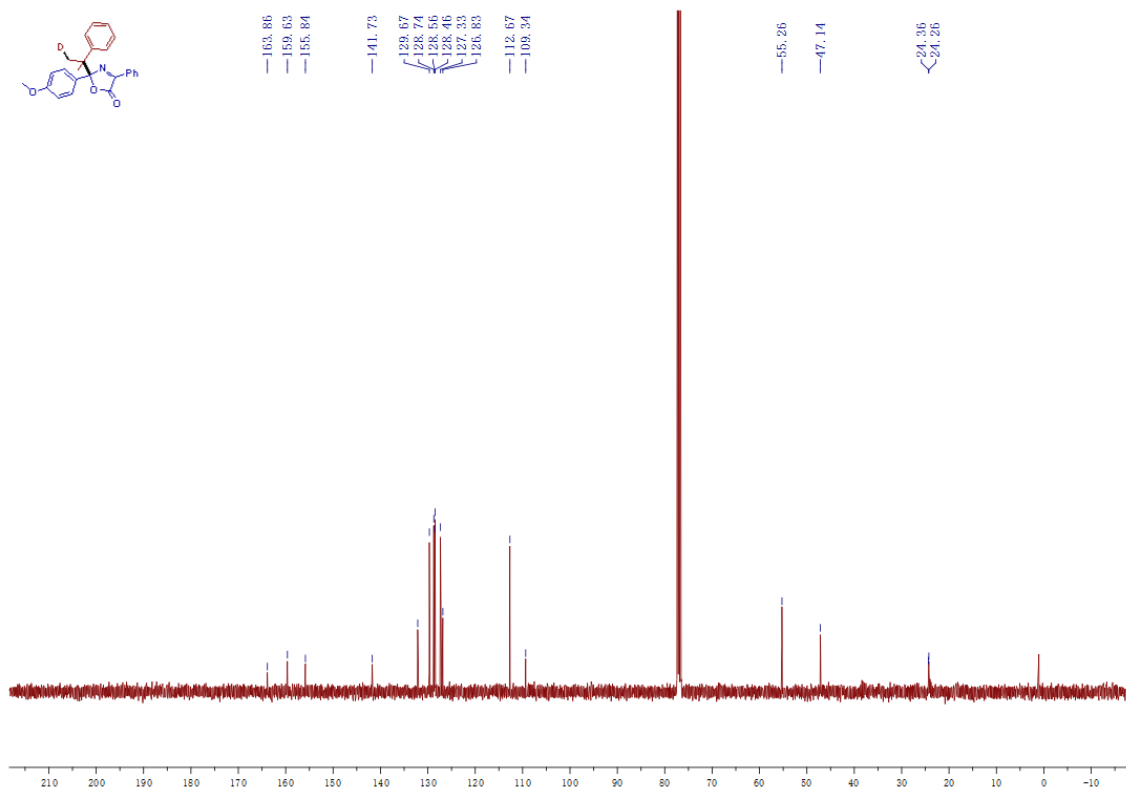
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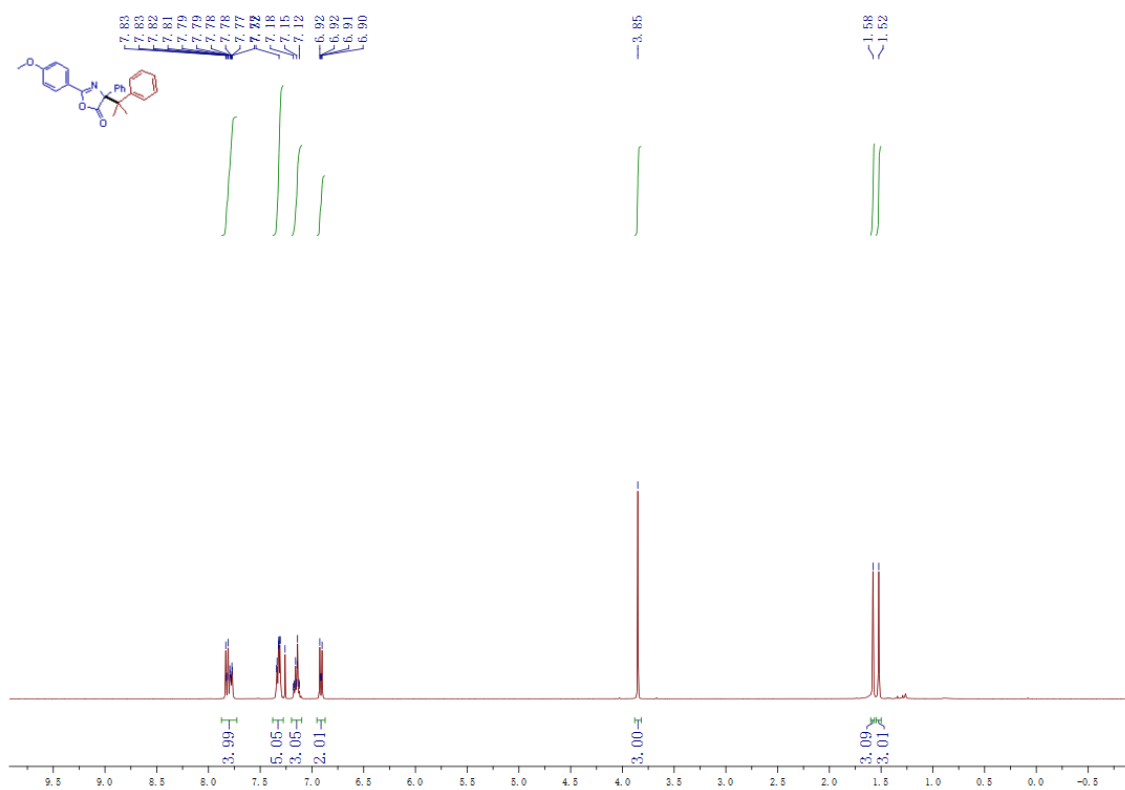
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-phenyl-2-(2-phenylpropan-2-yl-1-d)oxazol-5(2H)-one (3')



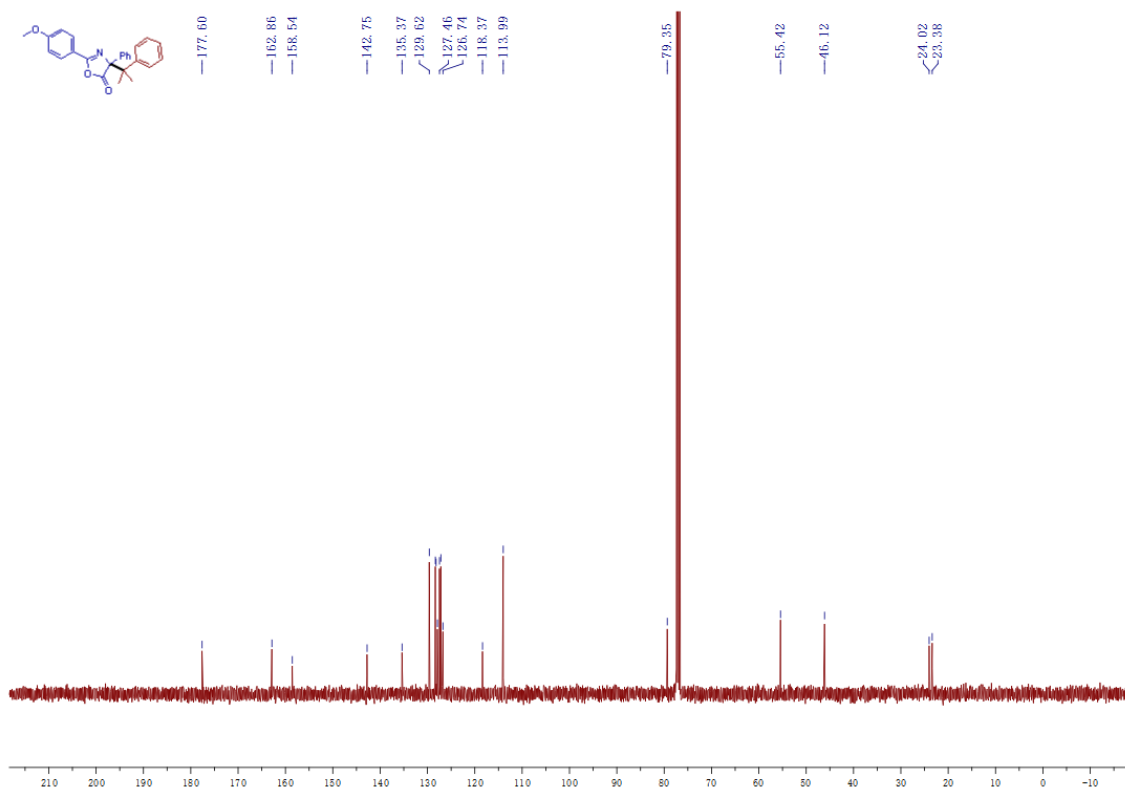
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-phenyl-2-(2-phenylpropan-2-yl-1-d)oxazol-5(2H)-one (3')



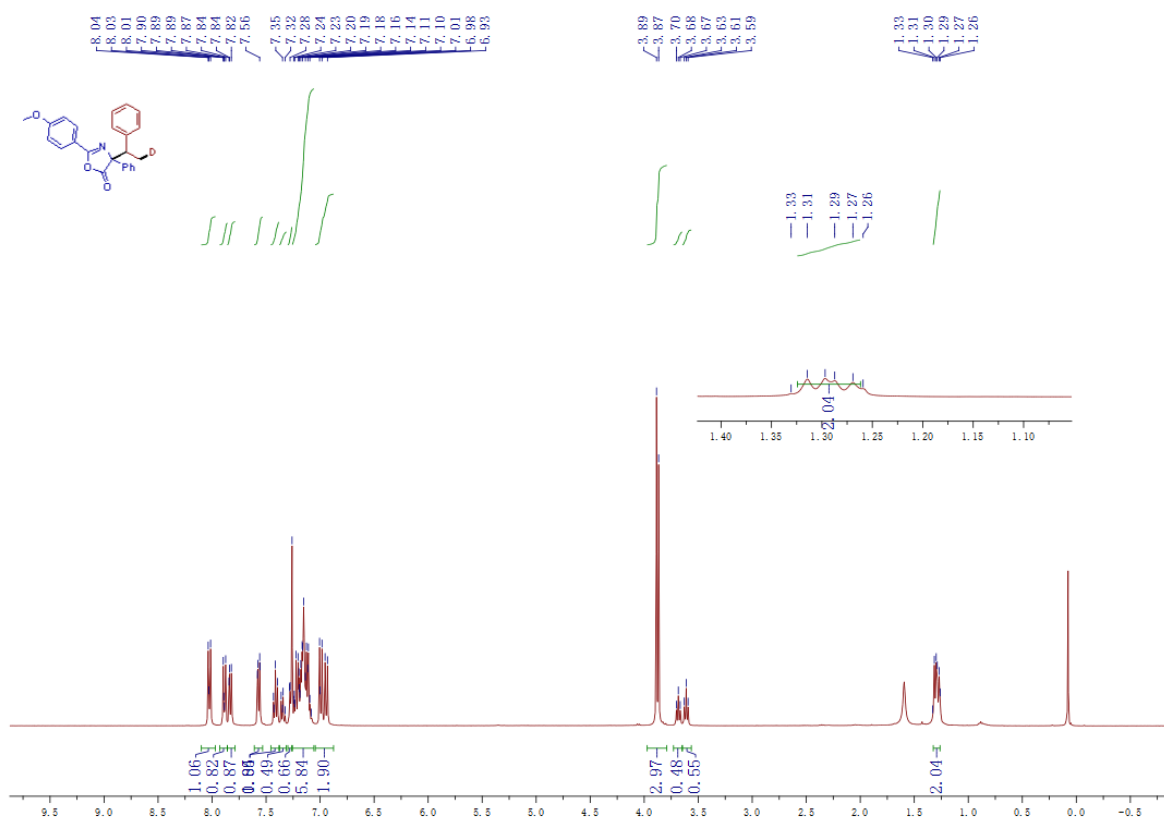
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-phenyl-4-(2-phenylpropan-2-yl)oxazol-5(4H)-one (3'')



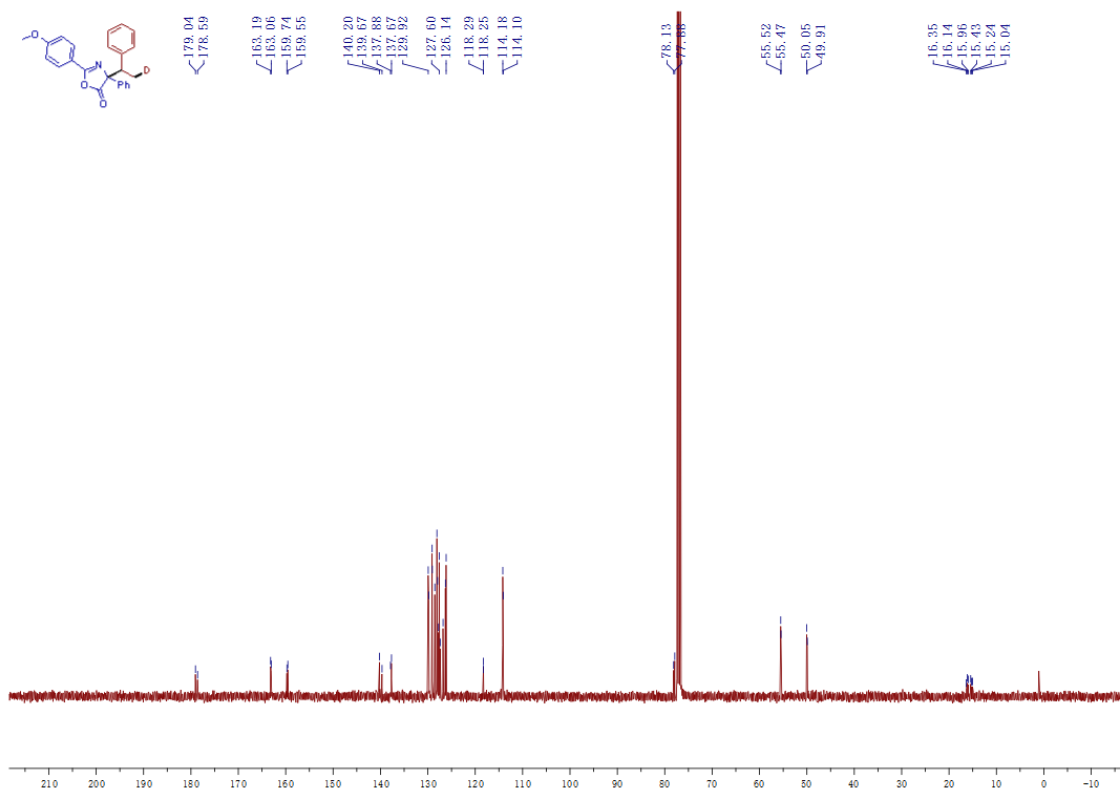
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-phenyl-4-(2-phenylpropan-2-yl)oxazol-5(4H)-one (3'')



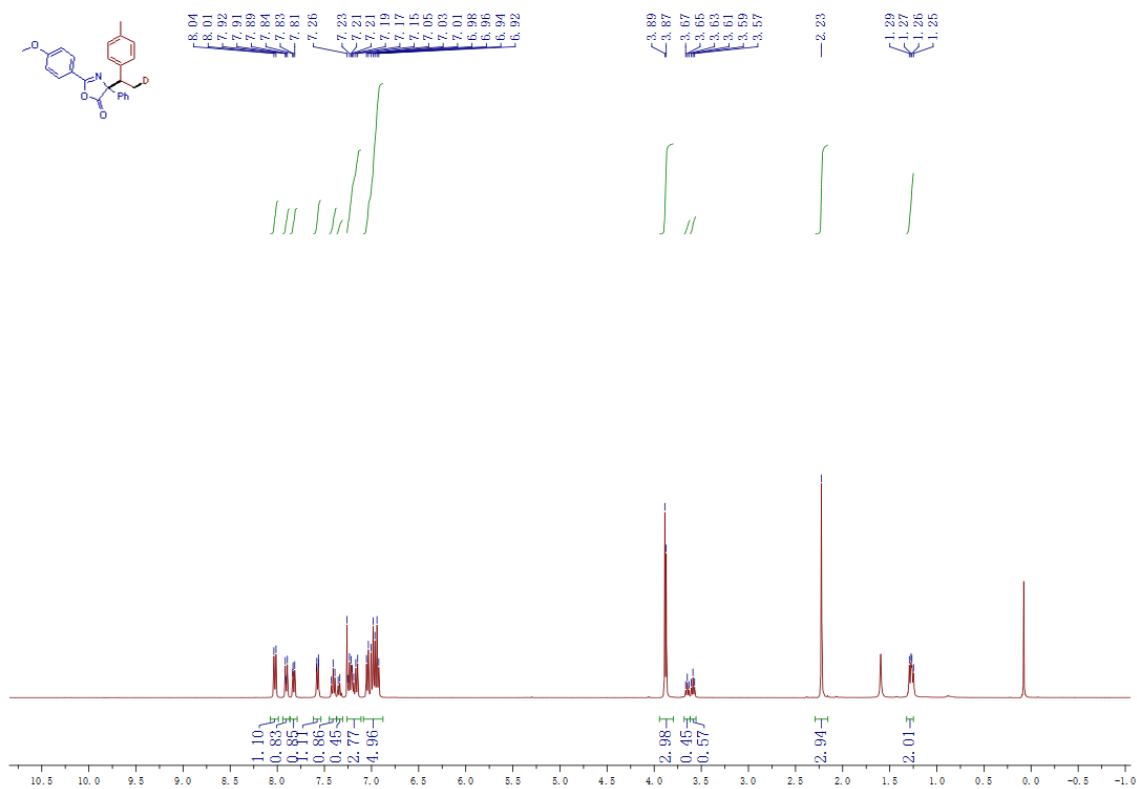
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-phenyl-4-(1-phenylethyl-2-d)oxazol-5(4H)-one (4)



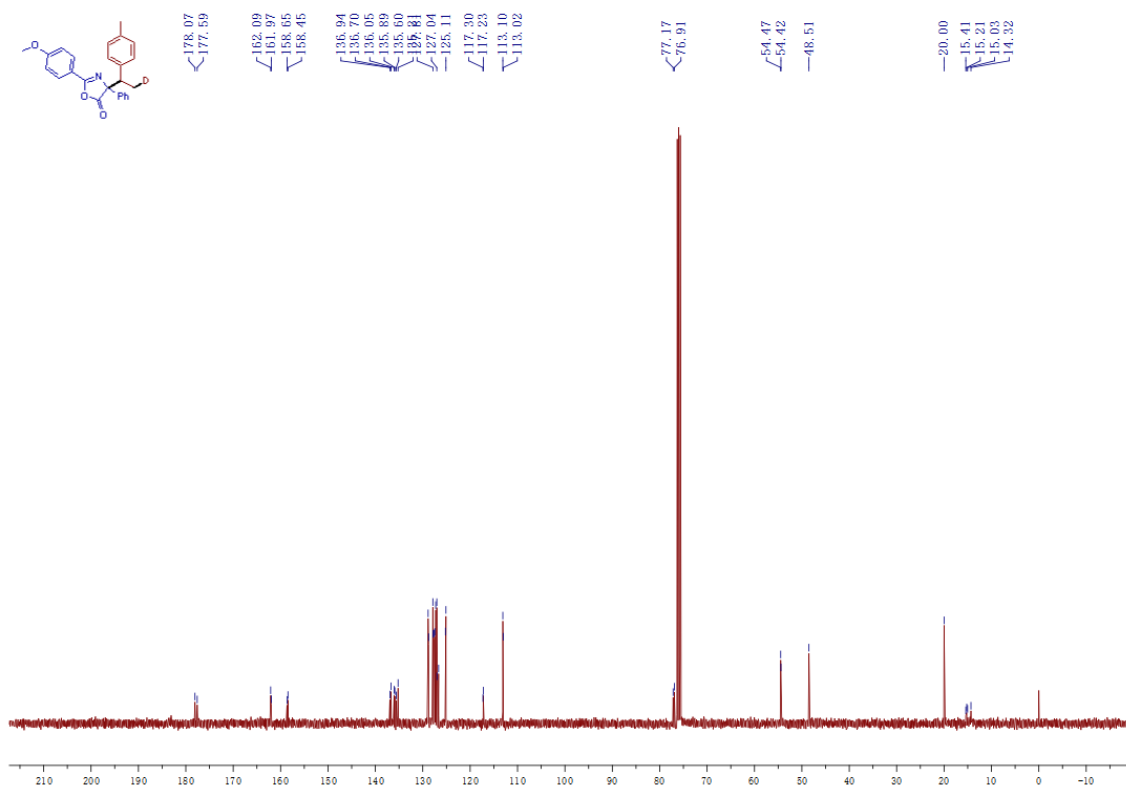
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-phenyl-4-(1-phenylethyl-2-d)oxazol-5(4H)-one (4)



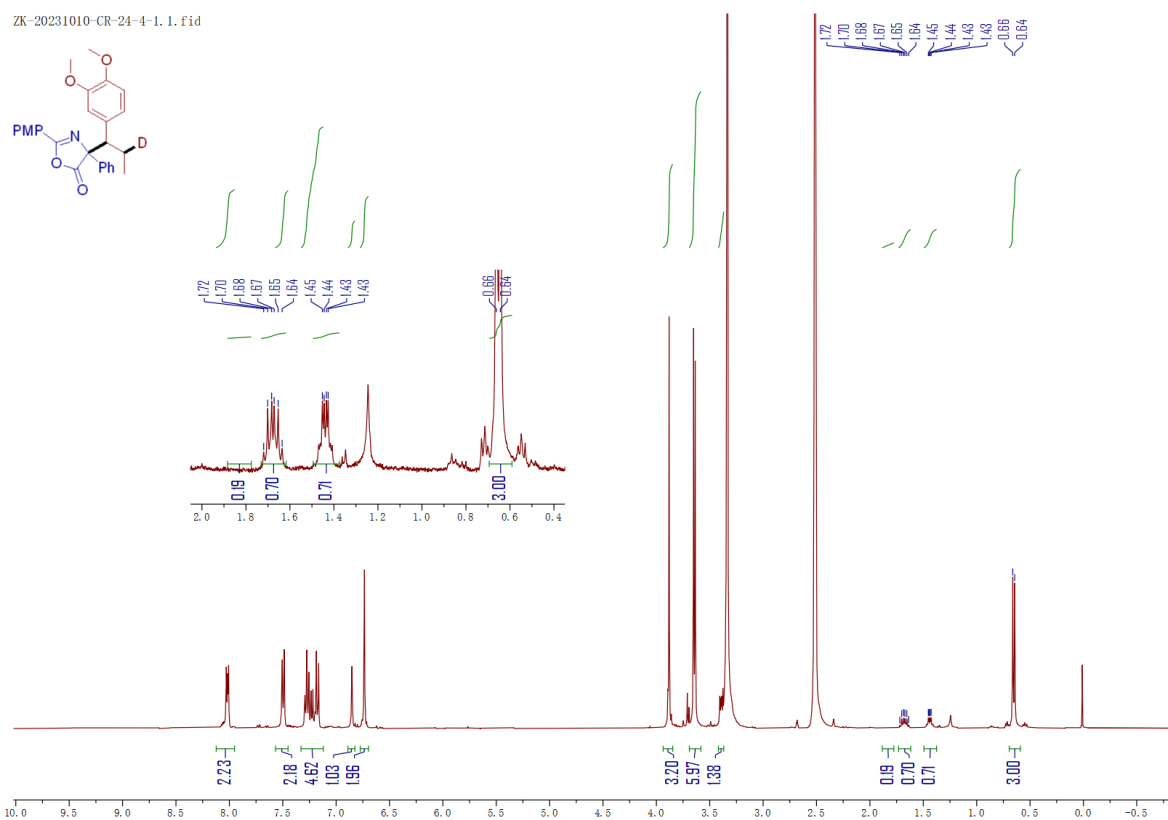
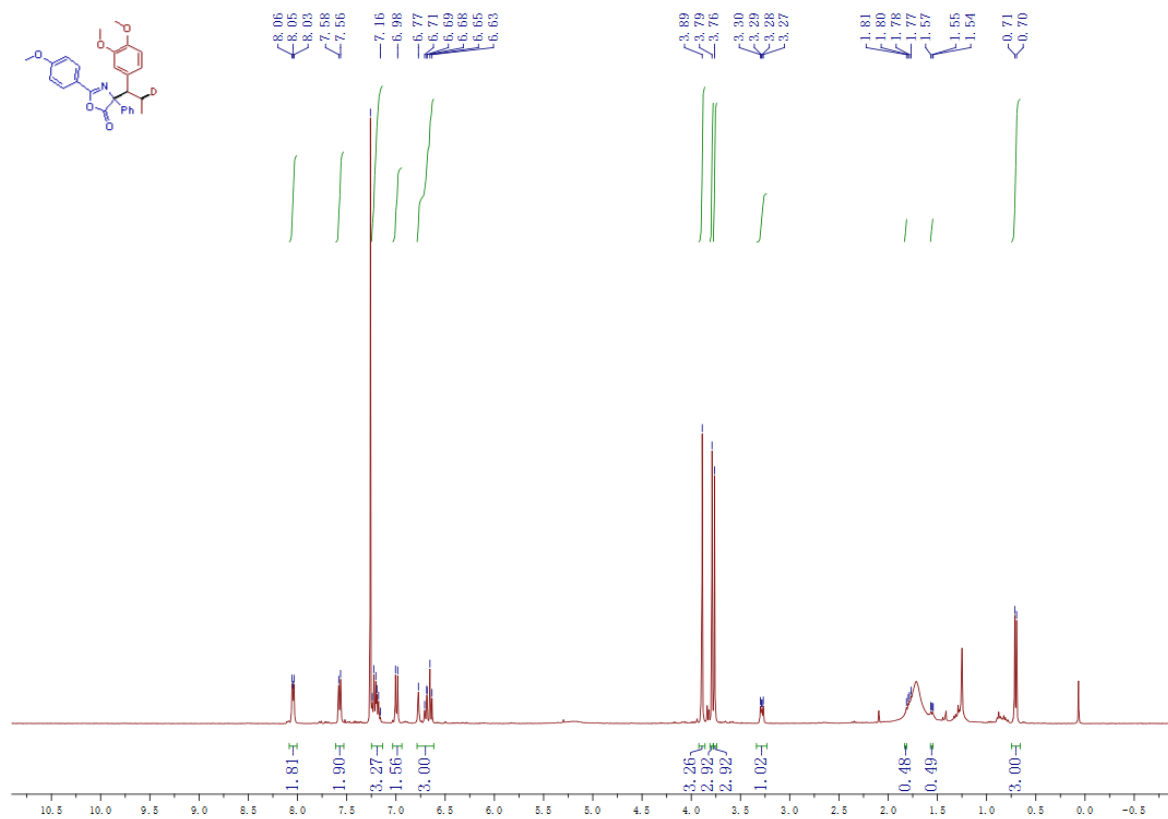
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-phenyl-4-(1-(p-tolyl)ethyl-2-d)oxazol-5(4H)-one (5)



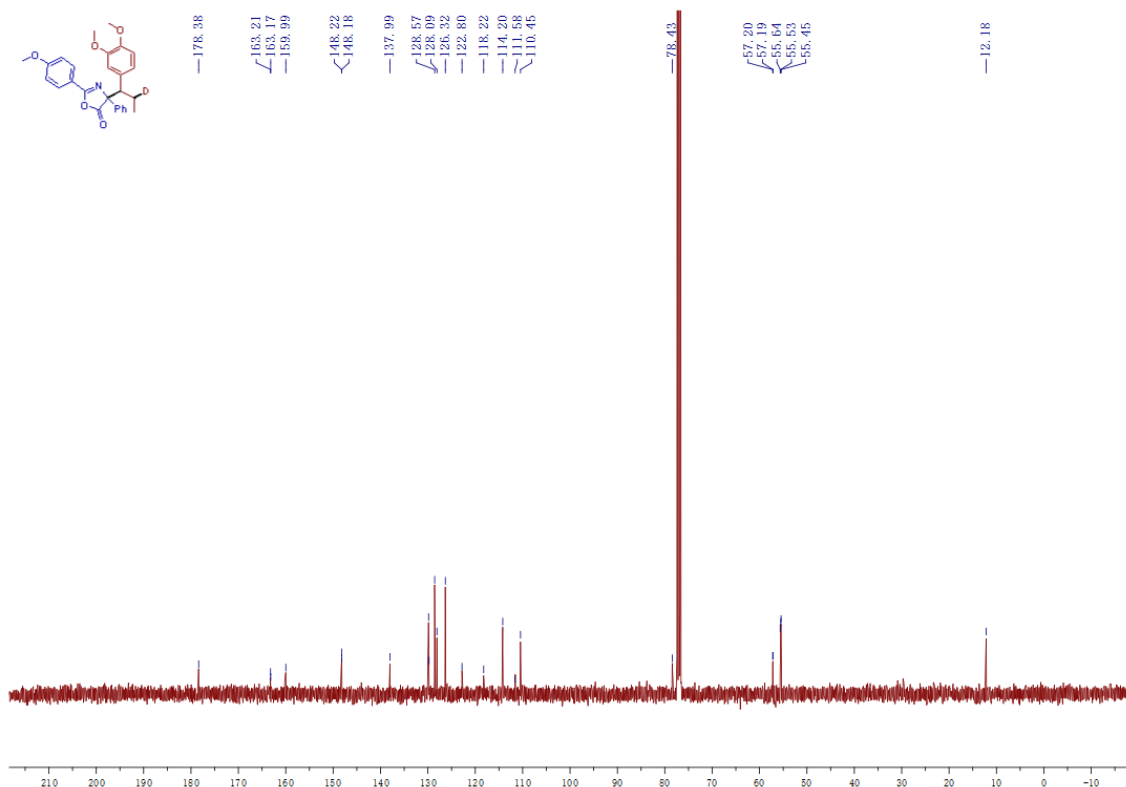
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-phenyl-4-(1-(p-tolyl)ethyl-2-d)oxazol-5(4H)-one (5)



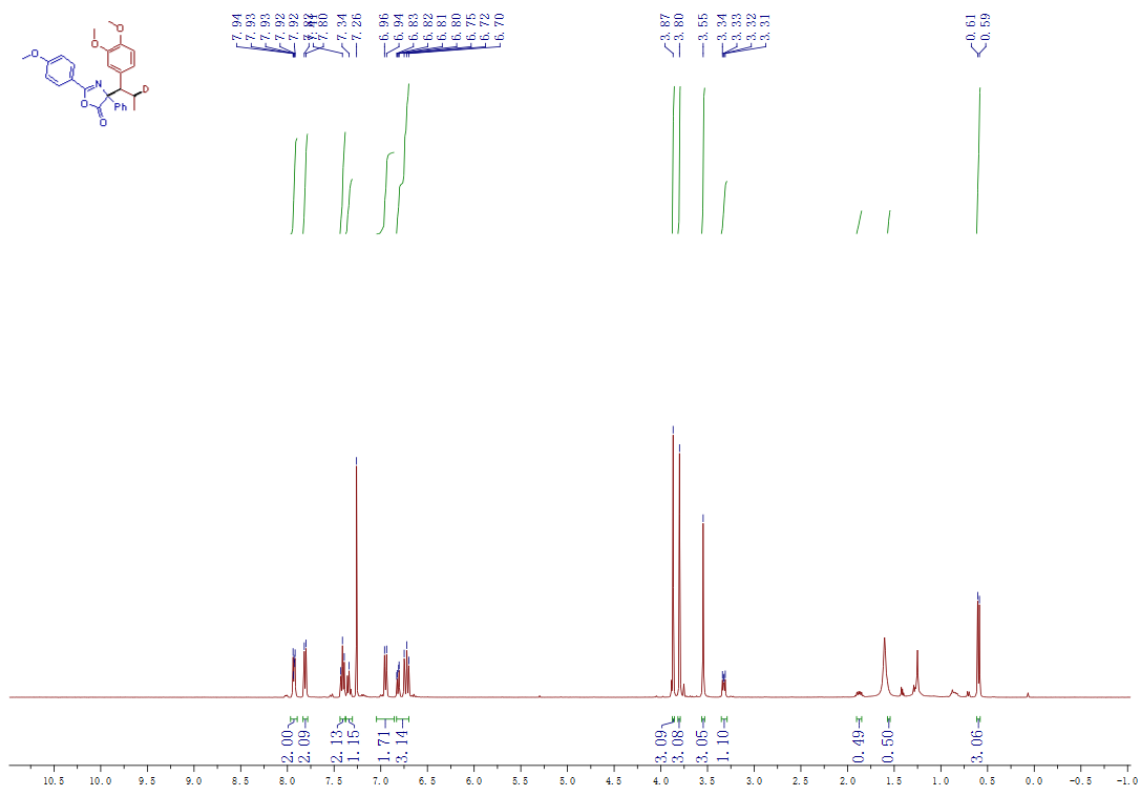
¹H NMR spectrum of 4-(1-(3,4-dimethoxyphenyl)propyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (6)



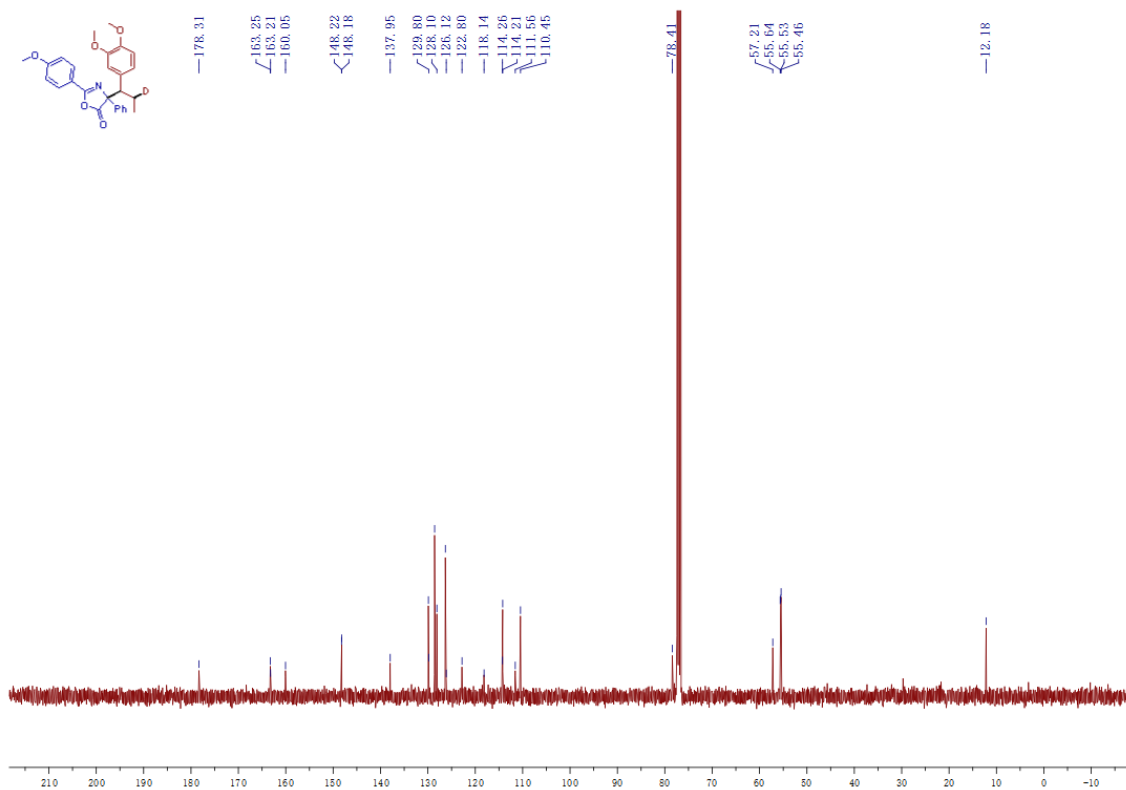
¹³C NMR spectrum of 4-(1-(3,4-dimethoxyphenyl)propyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (6)



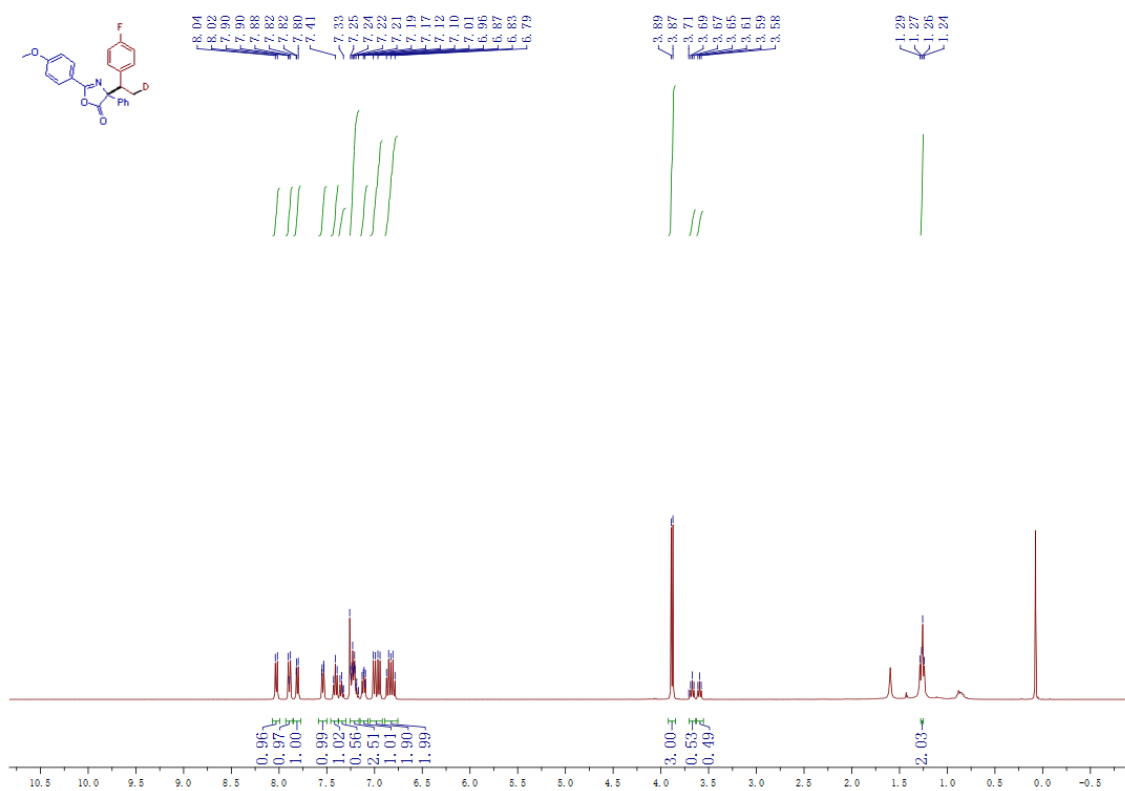
¹H NMR spectrum of 4-(1-(3,4-dimethoxyphenyl)propyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (6)



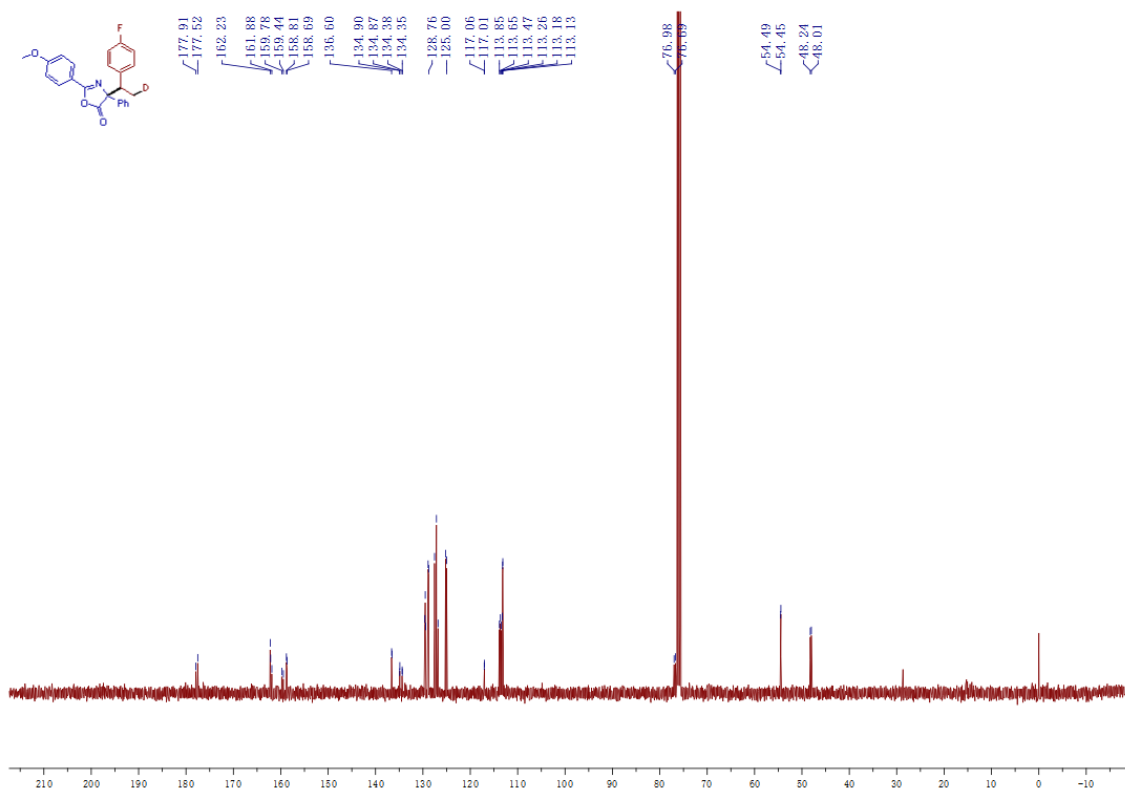
¹³C NMR spectrum of 4-(1-(3,4-dimethoxyphenyl)propyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (6)



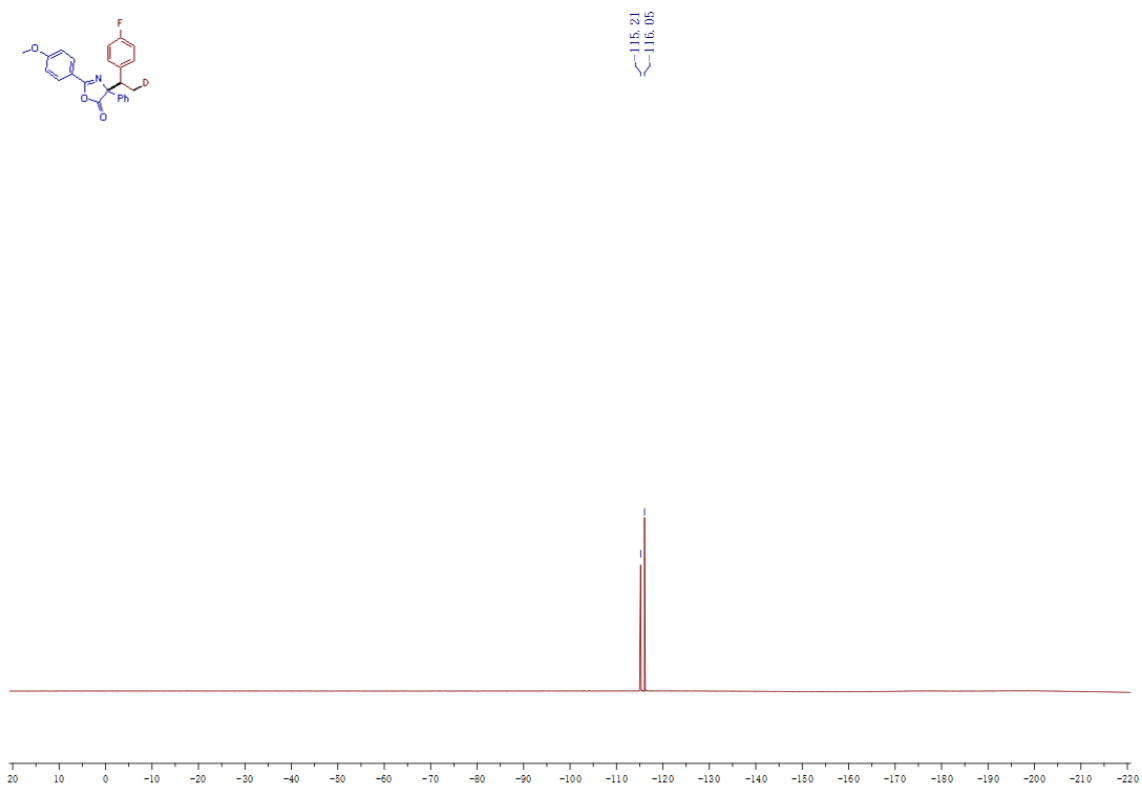
¹H NMR spectrum of 4-(1-(4-fluorophenyl)ethyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (7)



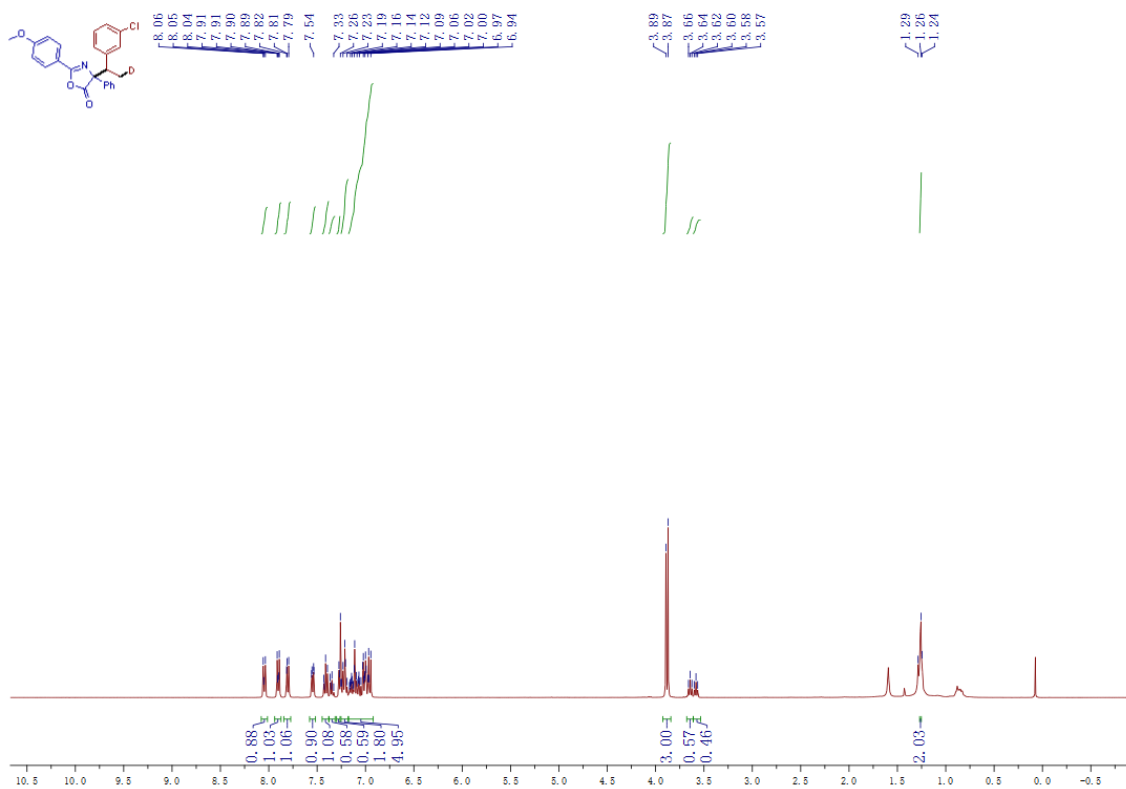
¹³C NMR spectrum of 4-(1-(4-fluorophenyl)ethyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (7)



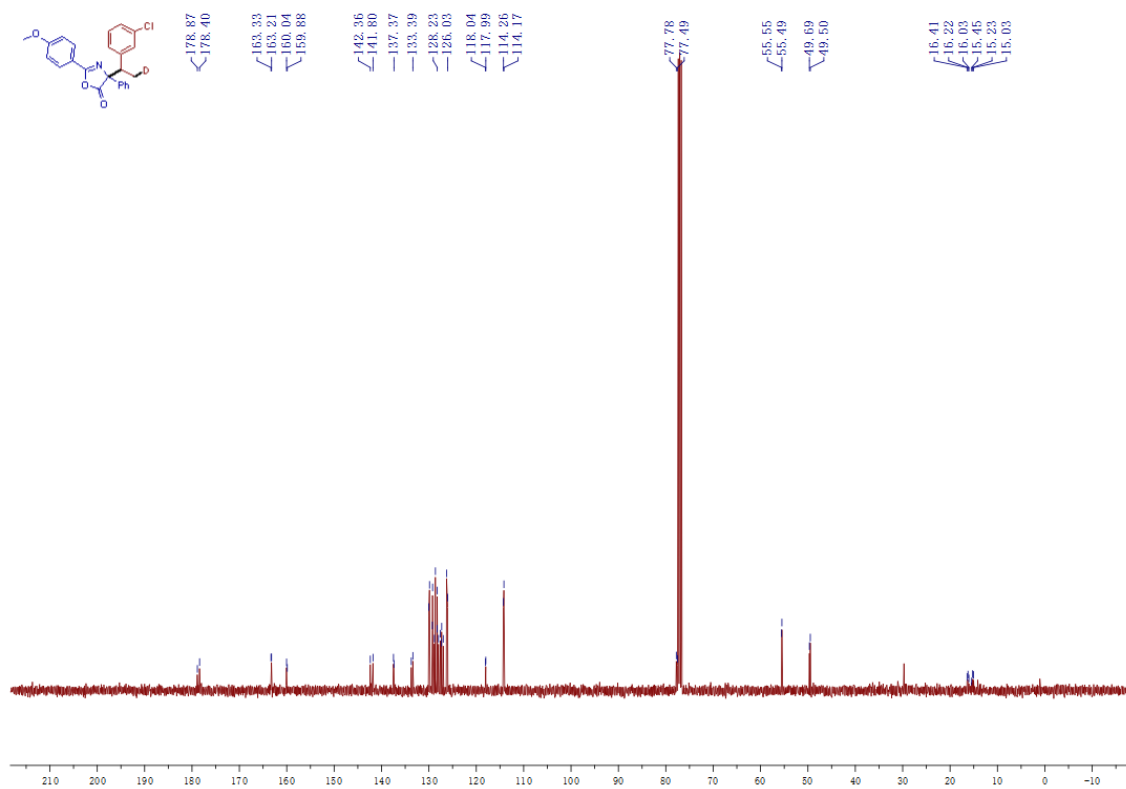
¹⁹F NMR spectrum of 4-(1-(4-fluorophenyl)ethyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (7)



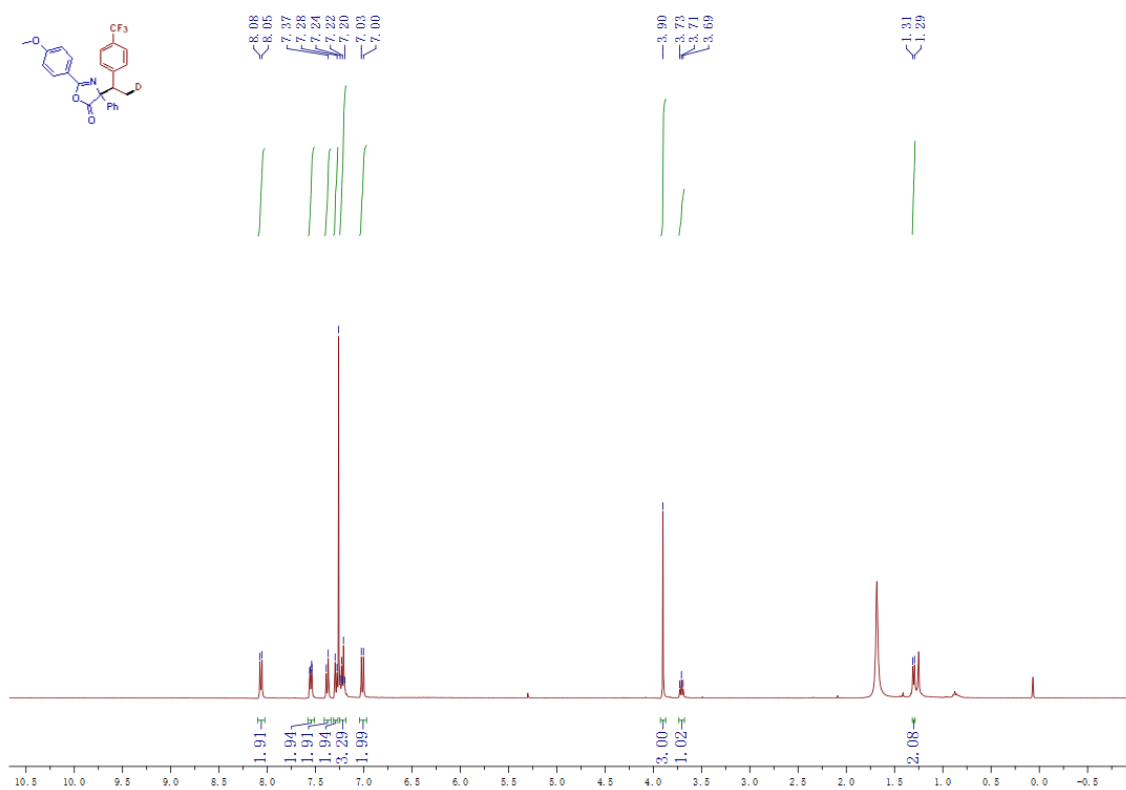
¹H NMR spectrum of 4-(1-(3-chlorophenyl)ethyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (8)



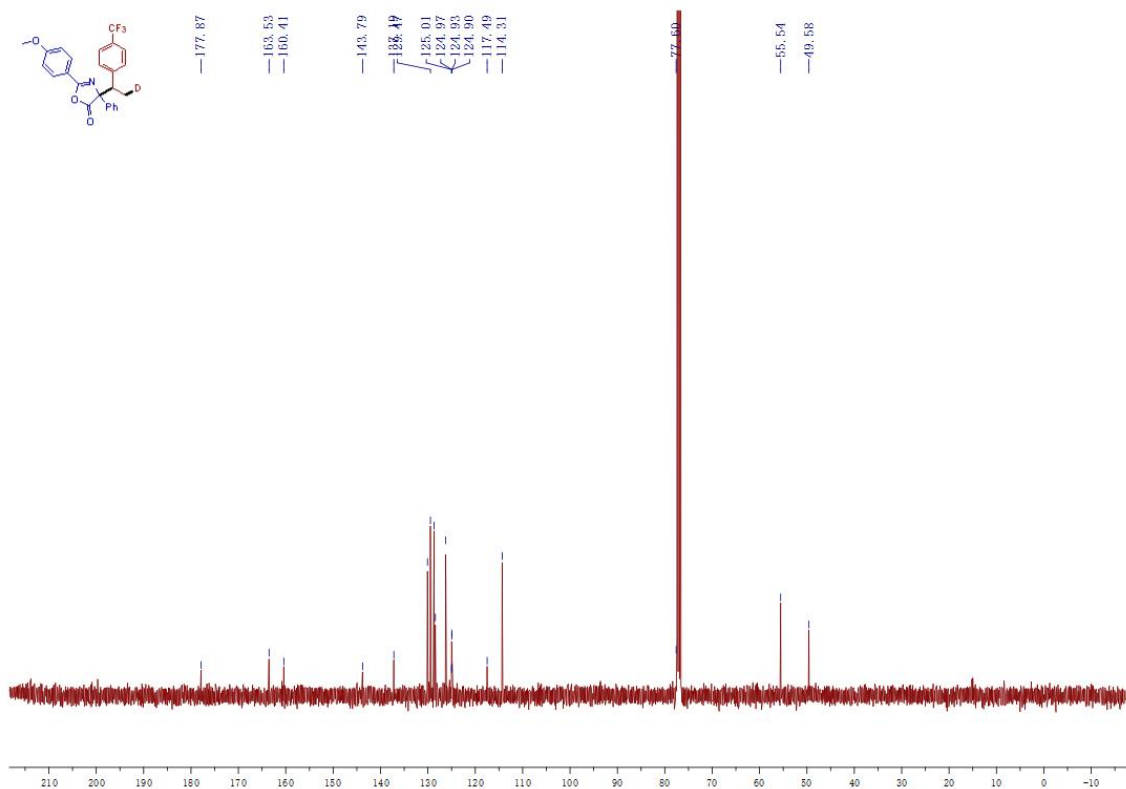
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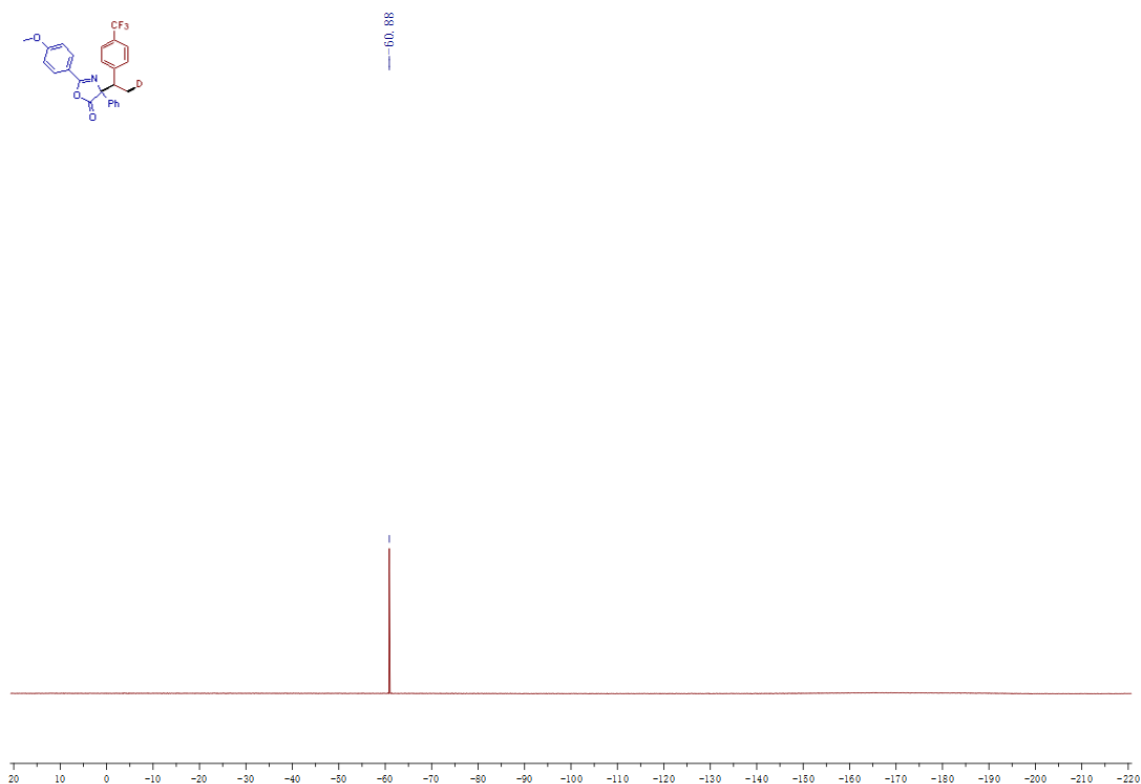
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-phenyl-4-(1-(4-(trifluoromethyl)phenyl)ethyl)-2-d)oxazol-5(4H)-one (9)



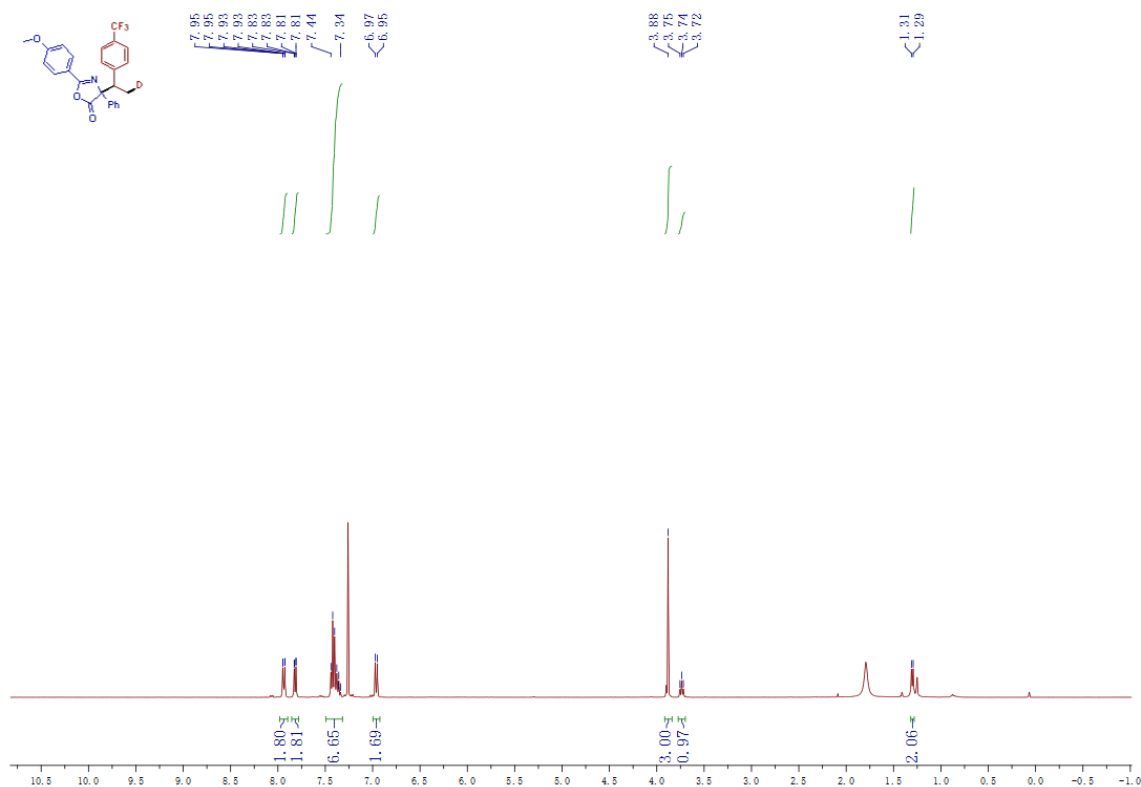
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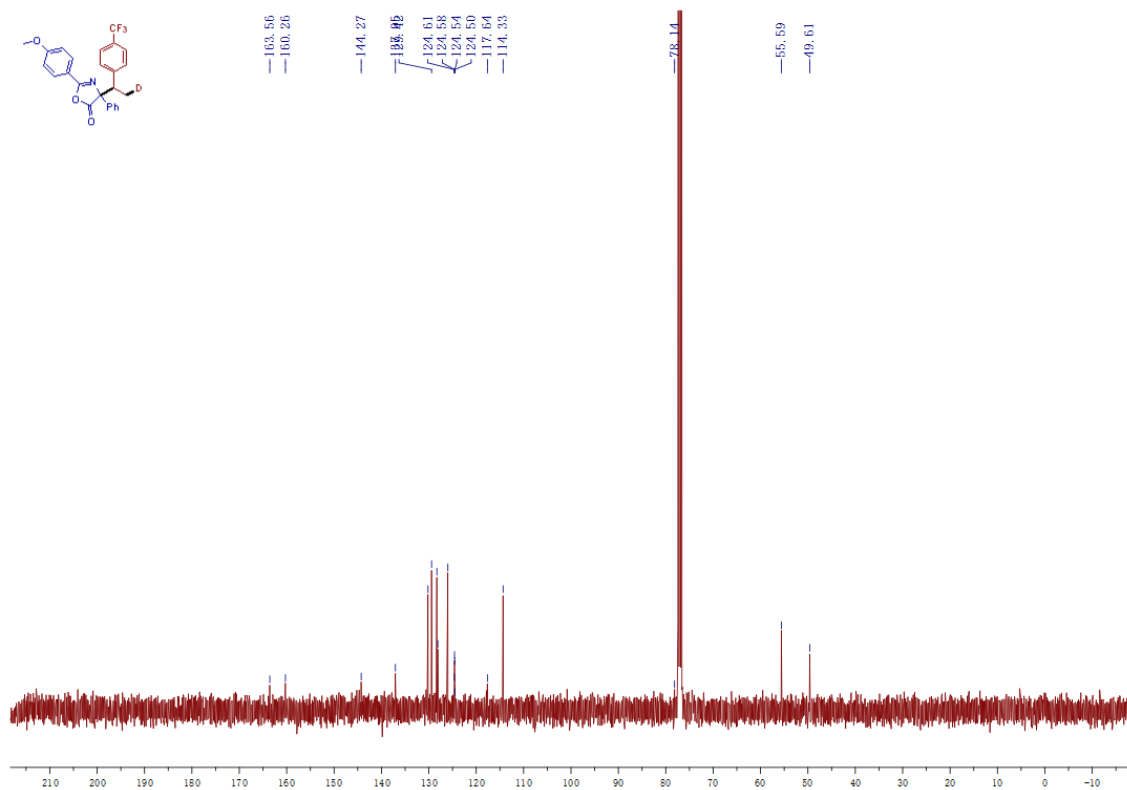
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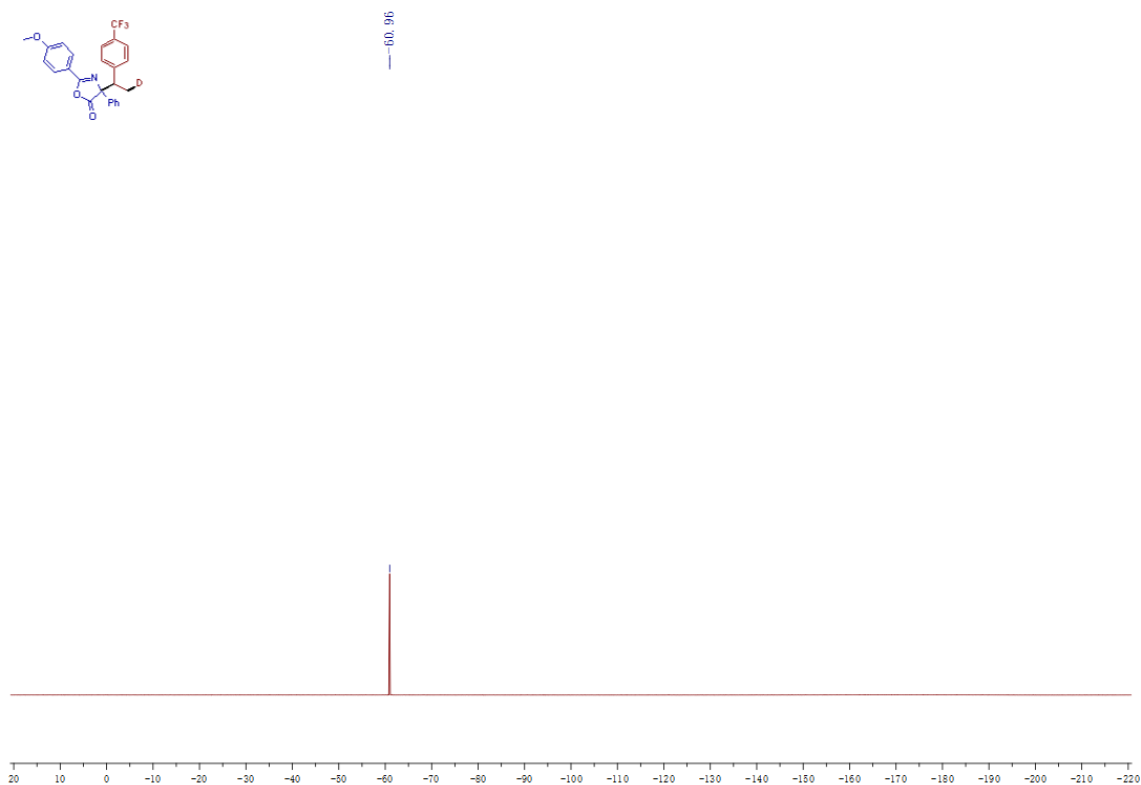
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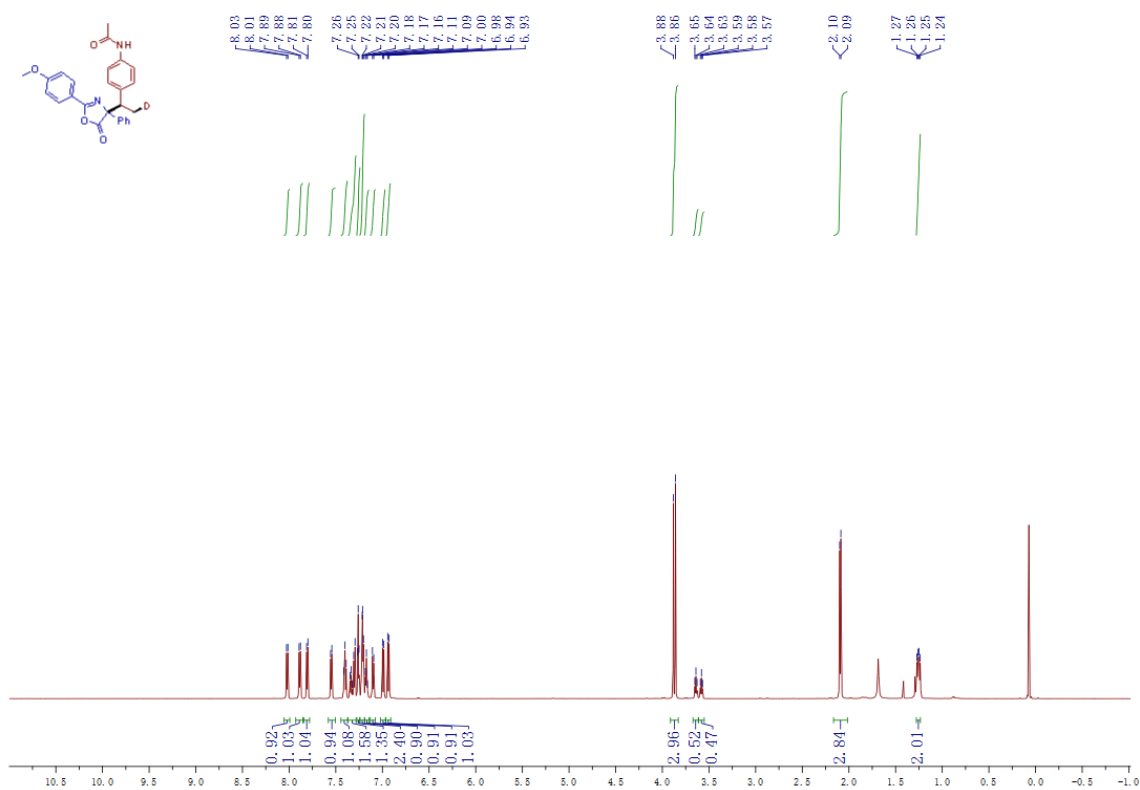
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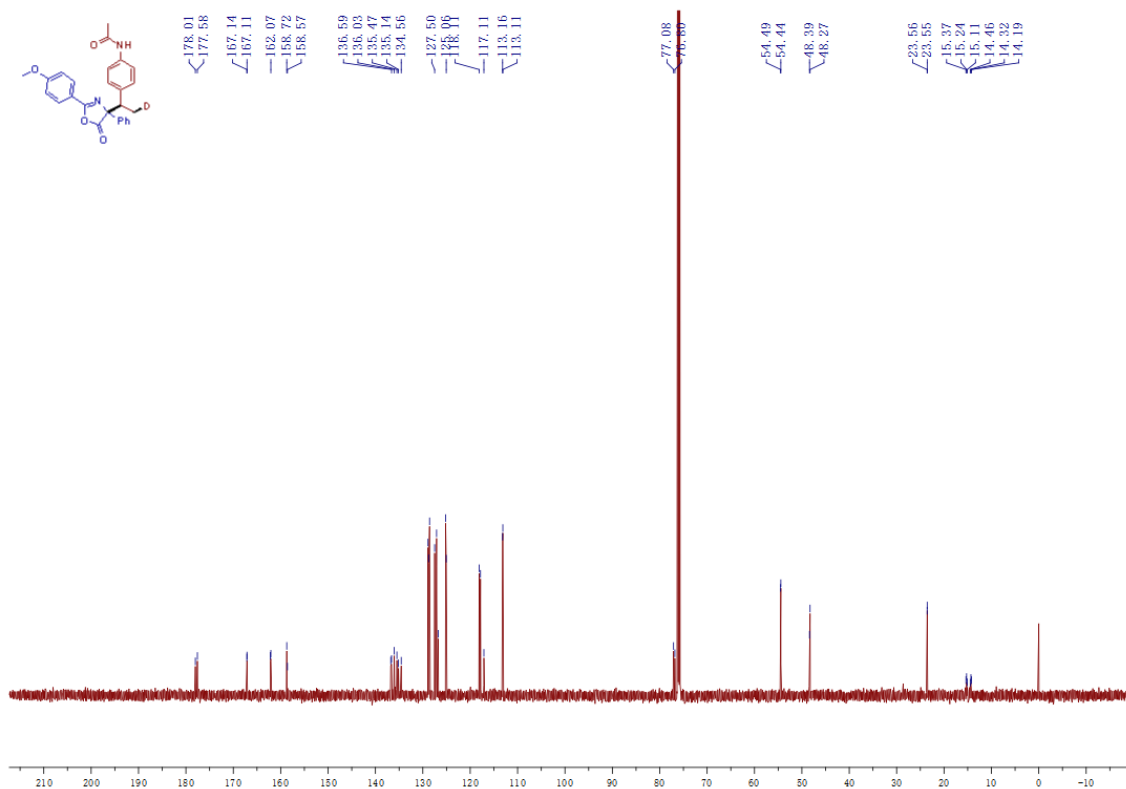
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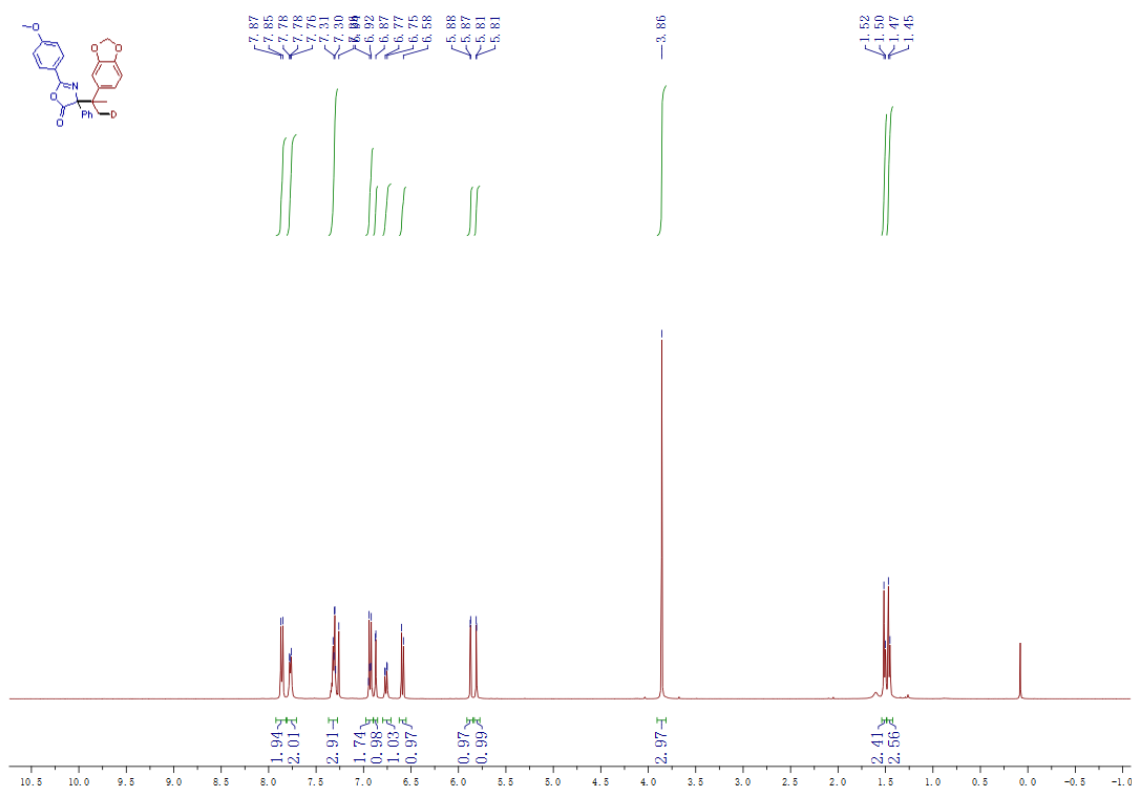
¹H NMR spectrum of *N*-(4-(1-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)ethyl-2-d)phenyl)acetamide (10)



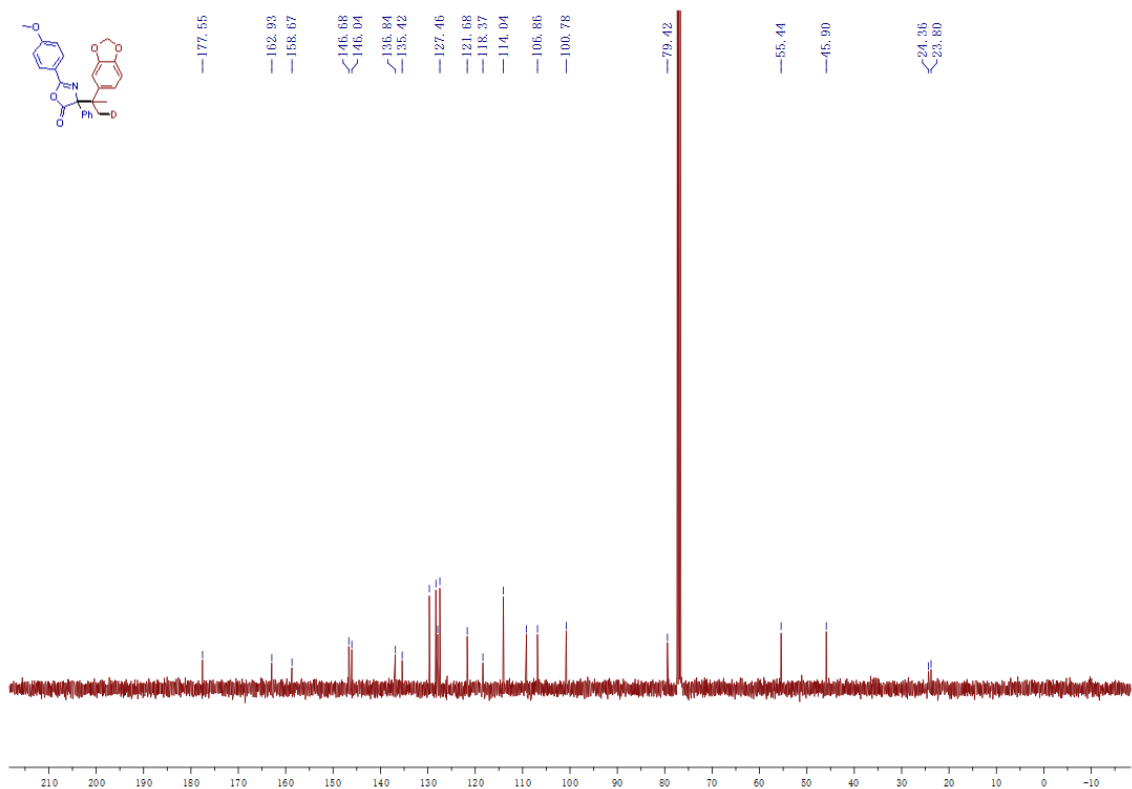
¹³C NMR spectrum of *N*-(4-(1-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)ethyl-2-d)phenyl)acetamide (10)



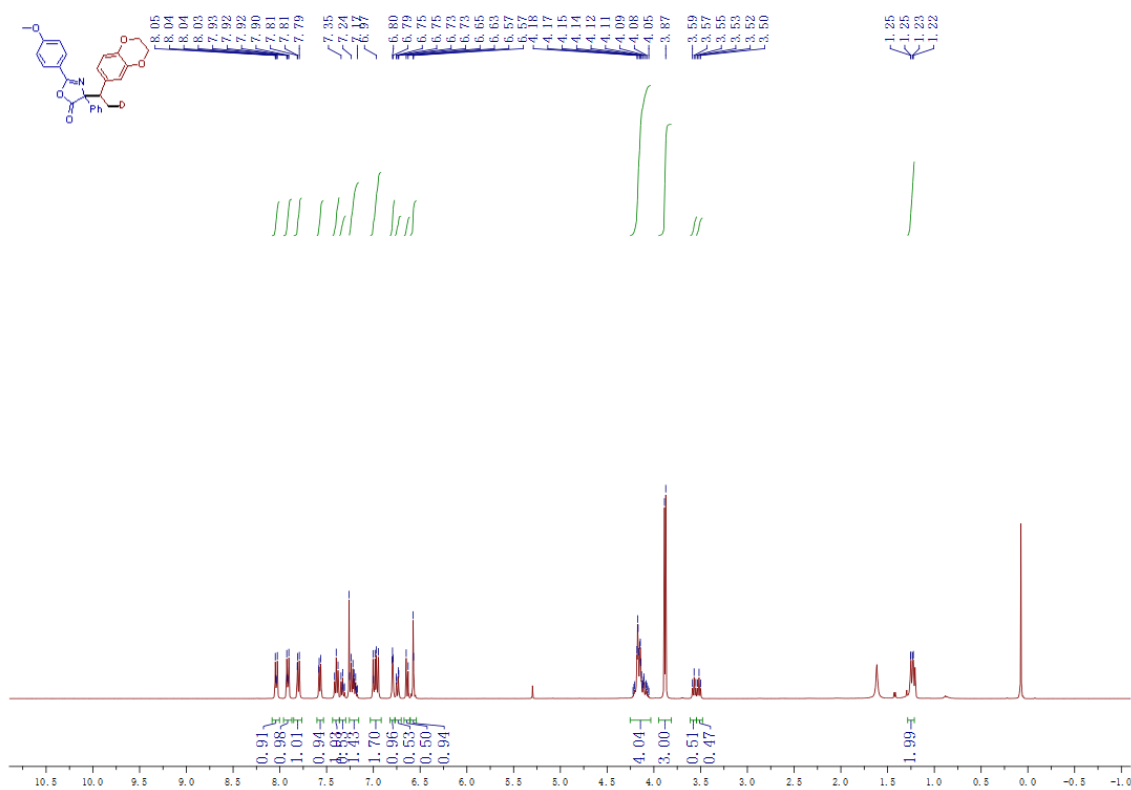
¹H NMR spectrum of 4-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (11)



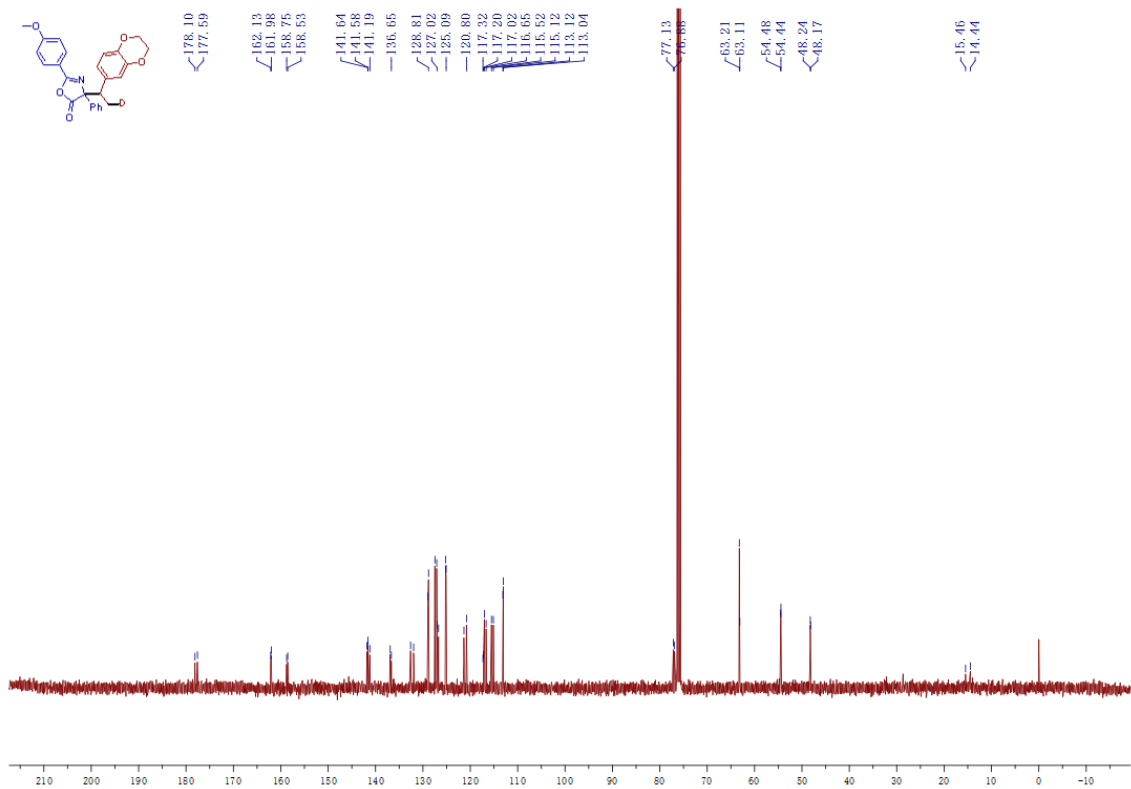
¹³C NMR spectrum of 4-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (11)



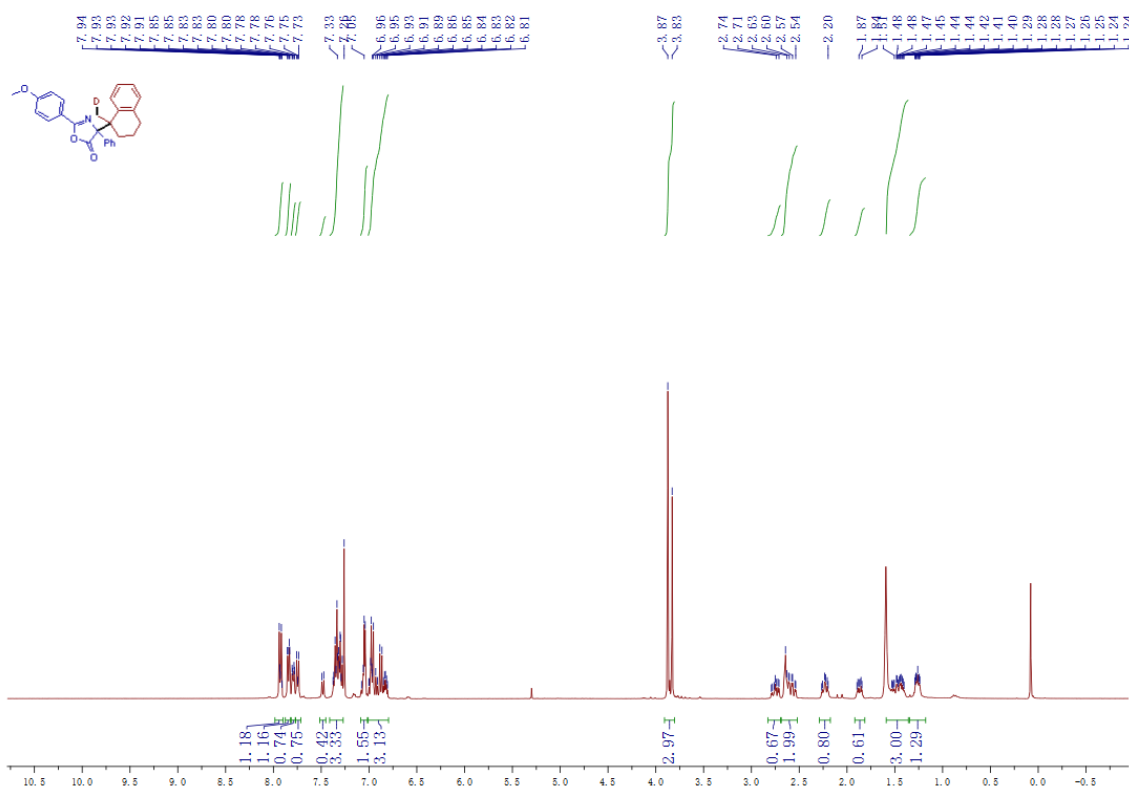
¹H NMR spectrum of 4-(1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)ethyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (12)



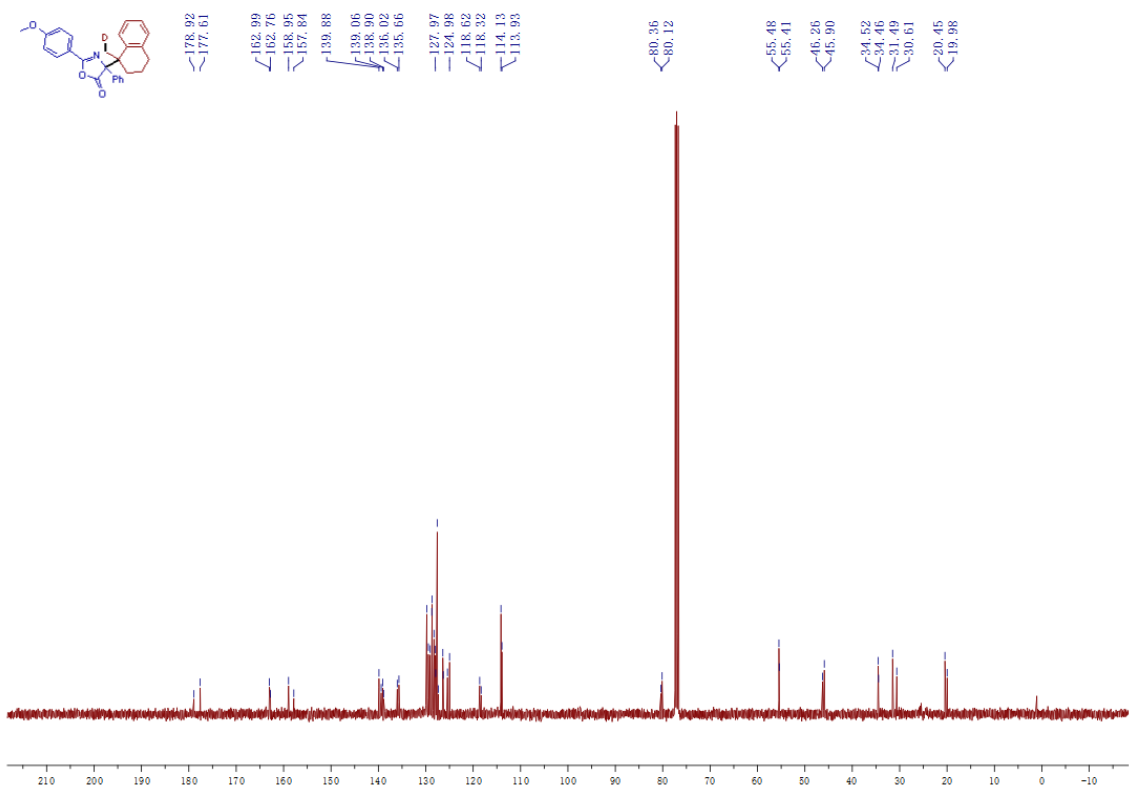
¹³C NMR spectrum of 4-(1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)ethyl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (12)



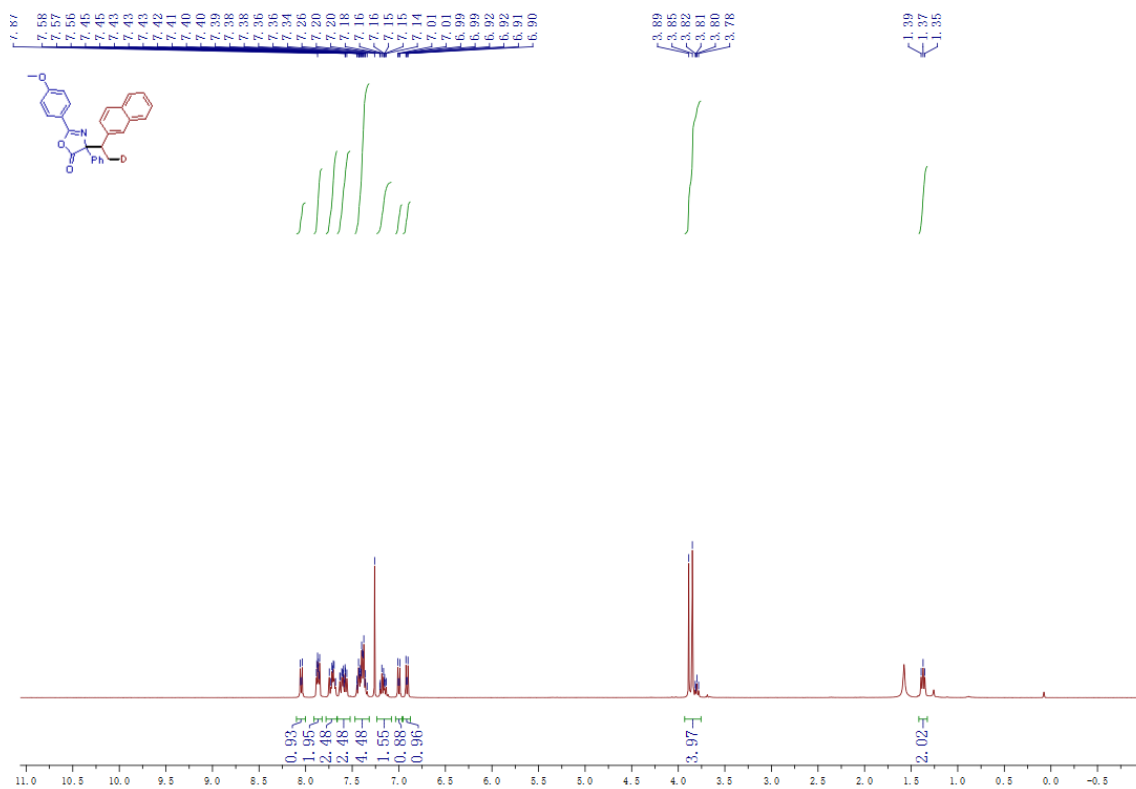
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(1-(methyl-d)-1,2,3,4-tetrahydronaphthalen-1-yl)-4-phenyloxazol-5(4H)-one (13)



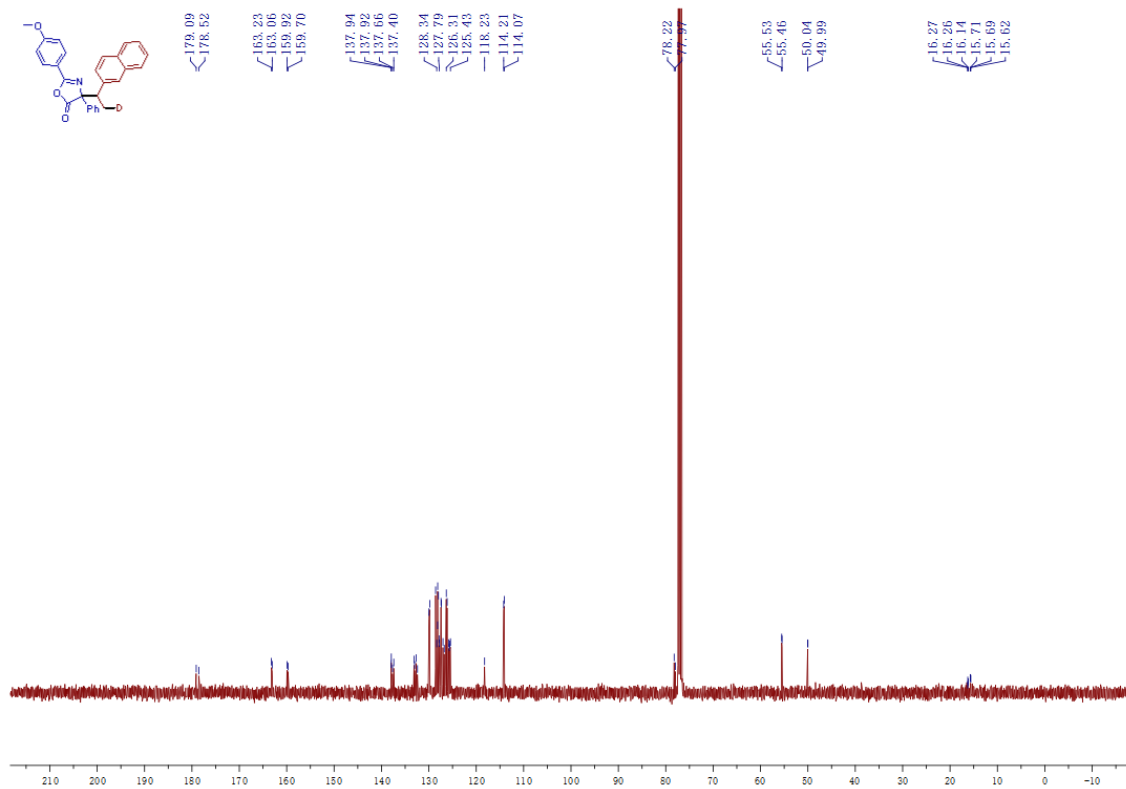
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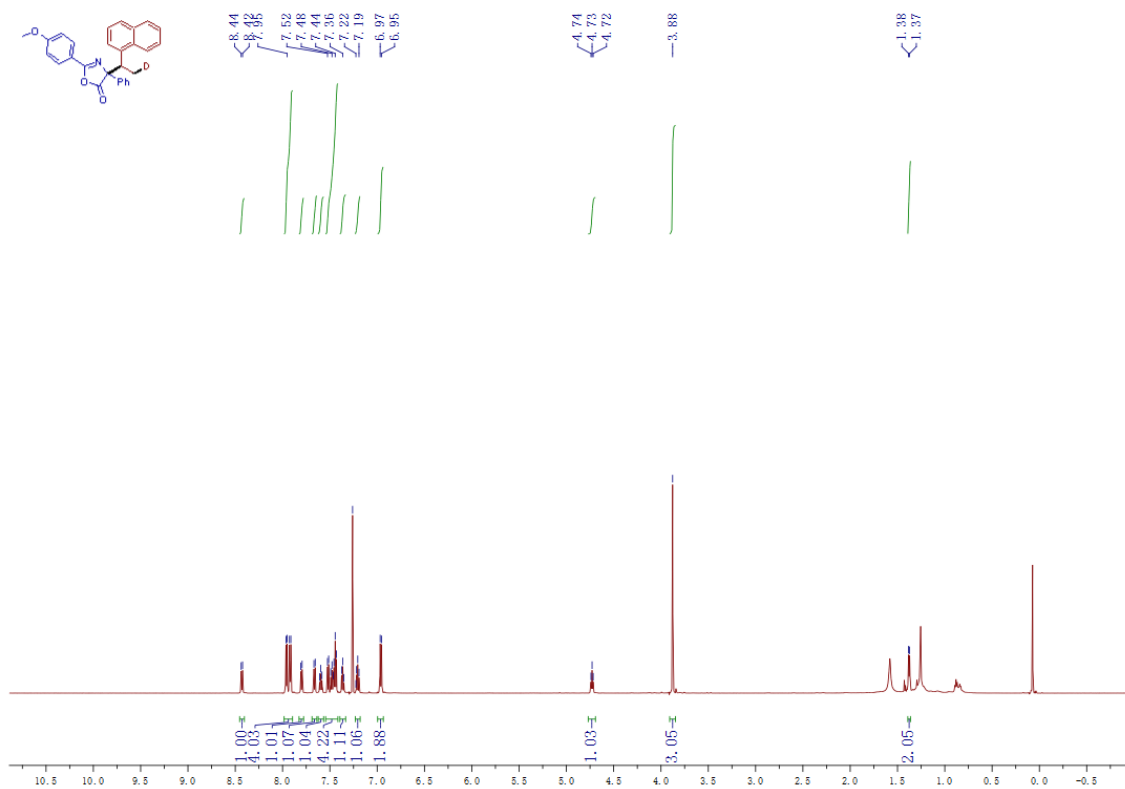
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(1-(naphthalen-2-yl)ethyl-2-d)-4-phenyloxazol-5(4H)-one (14)



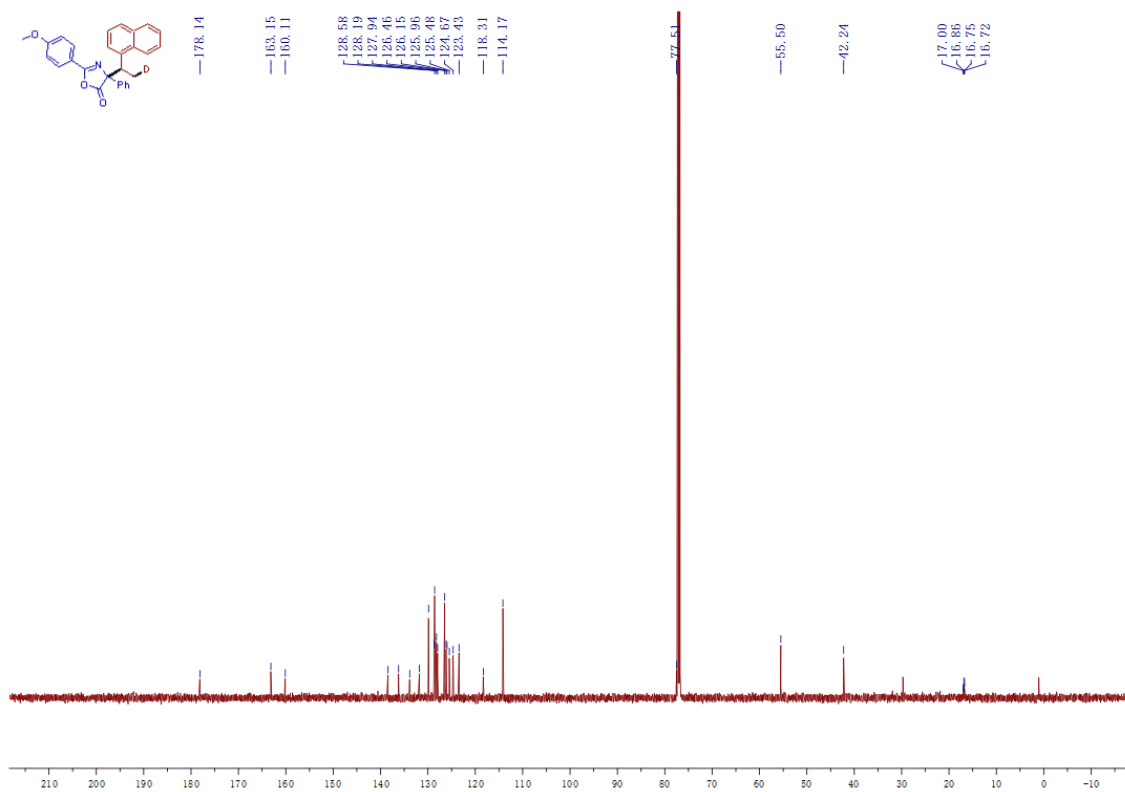
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-(1-(naphthalen-2-yl)ethyl-2-d)-4-phenyloxazol-5(4H)-one (14)



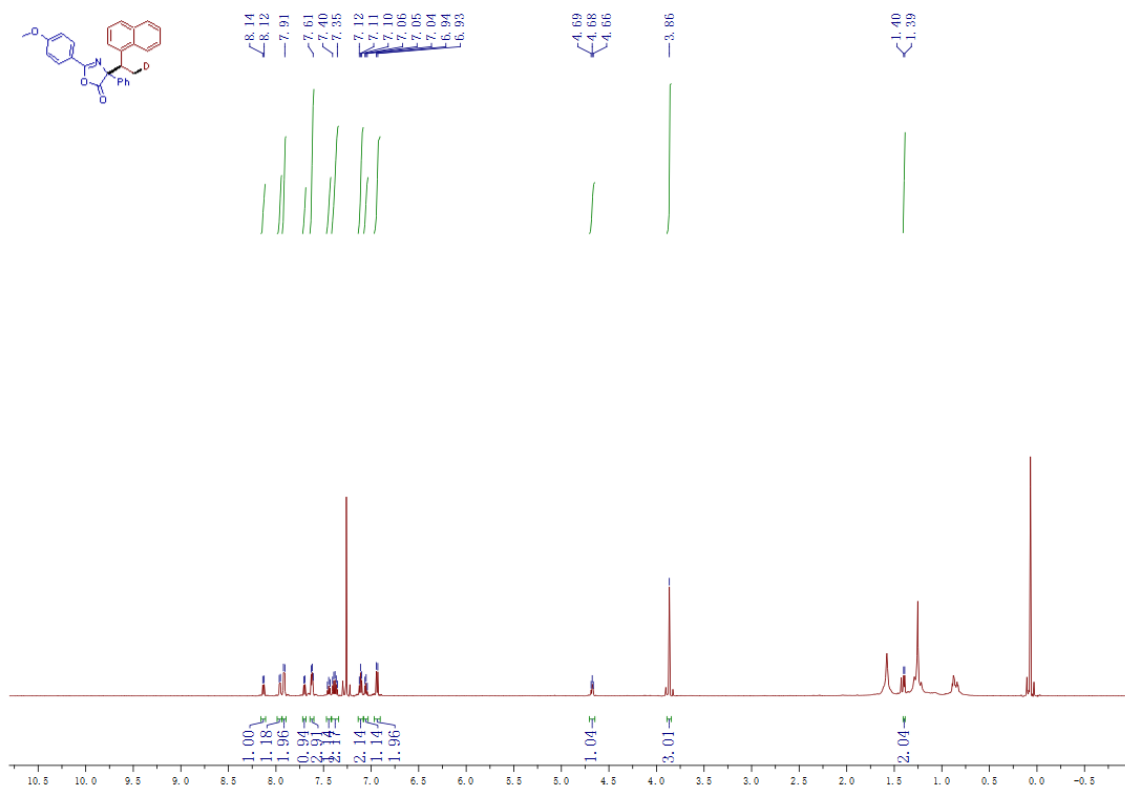
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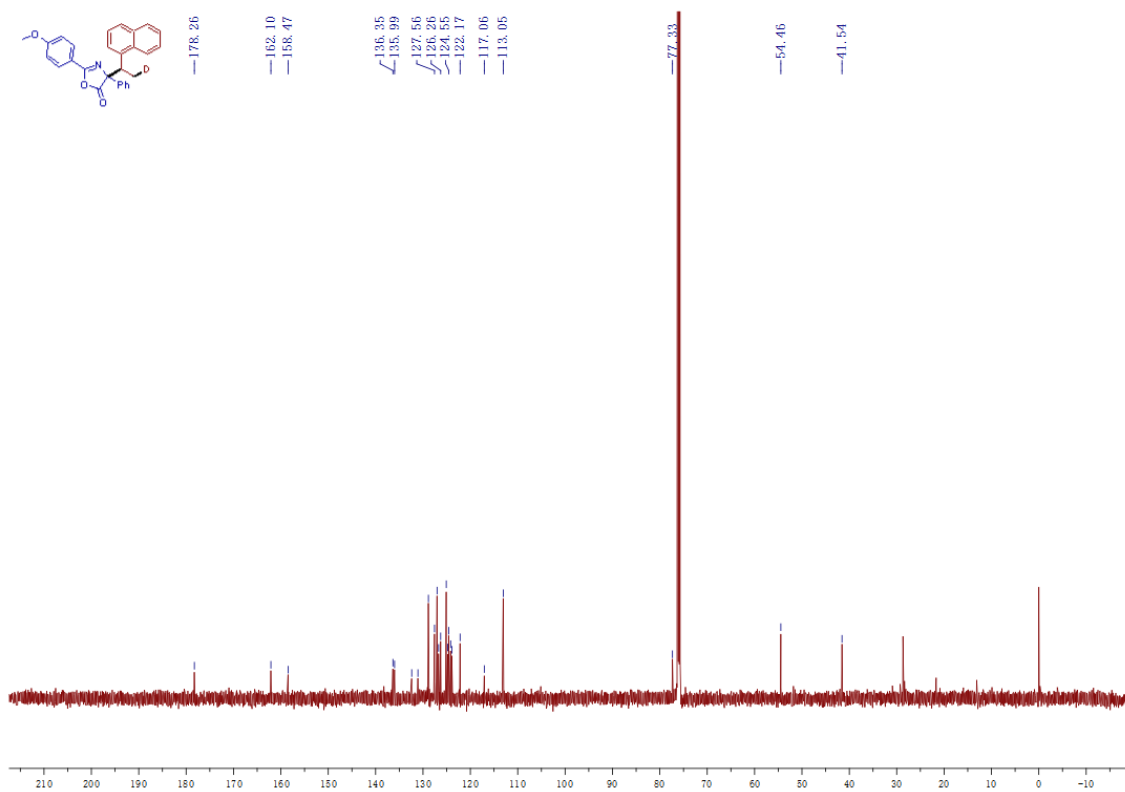
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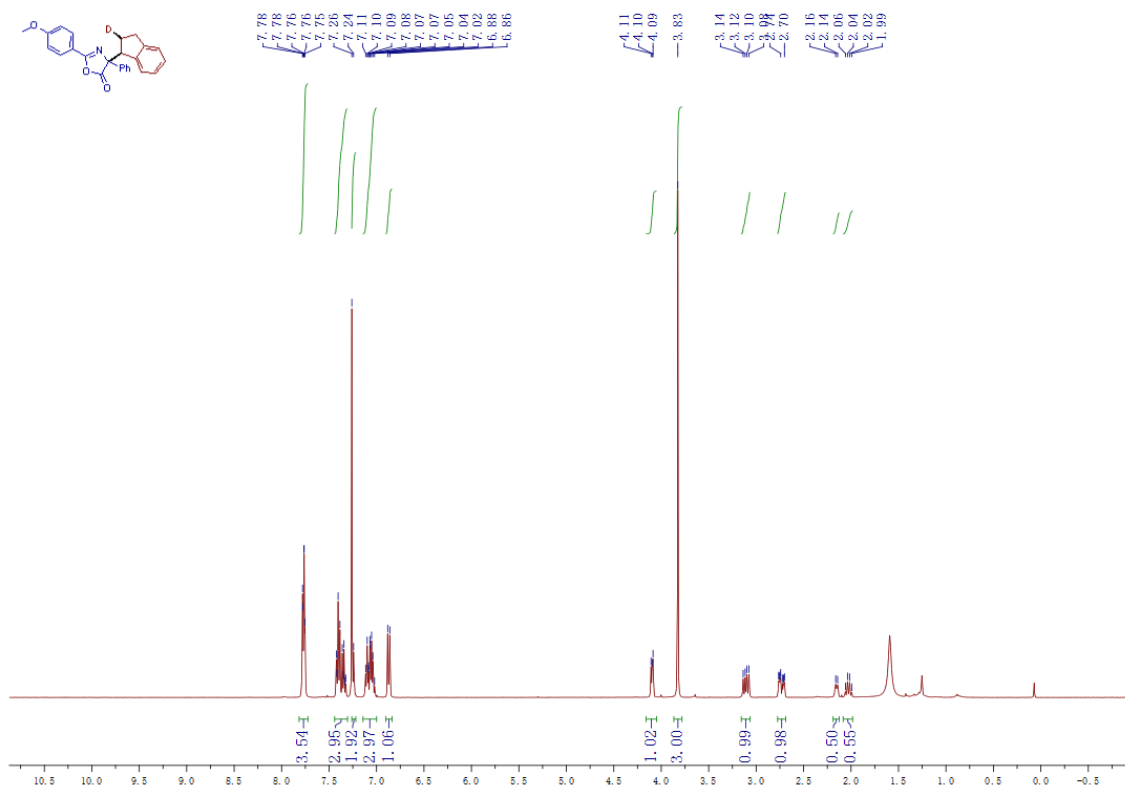
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(1-(naphthalen-1-yl)ethyl-2-d)-4-phenyloxazol-5(4H)-one (15)



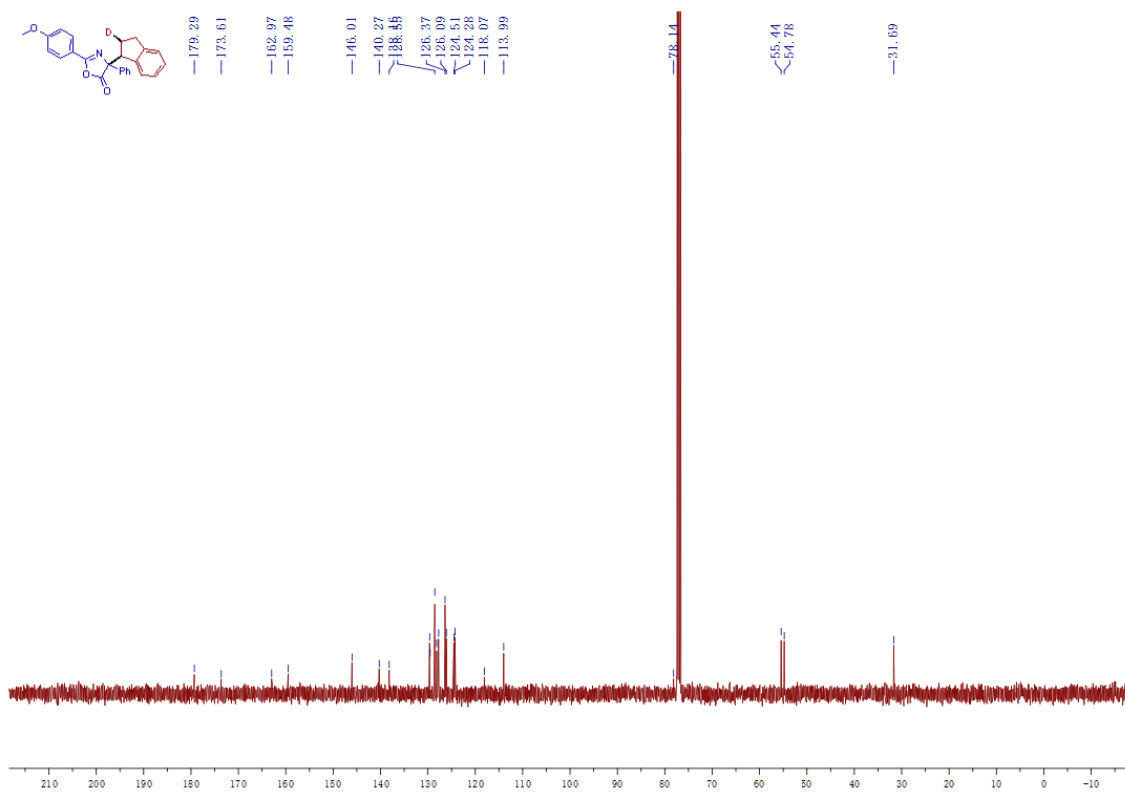
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-(1-(naphthalen-1-yl)ethyl-2-d)-4-phenyloxazol-5(4H)-one (15)



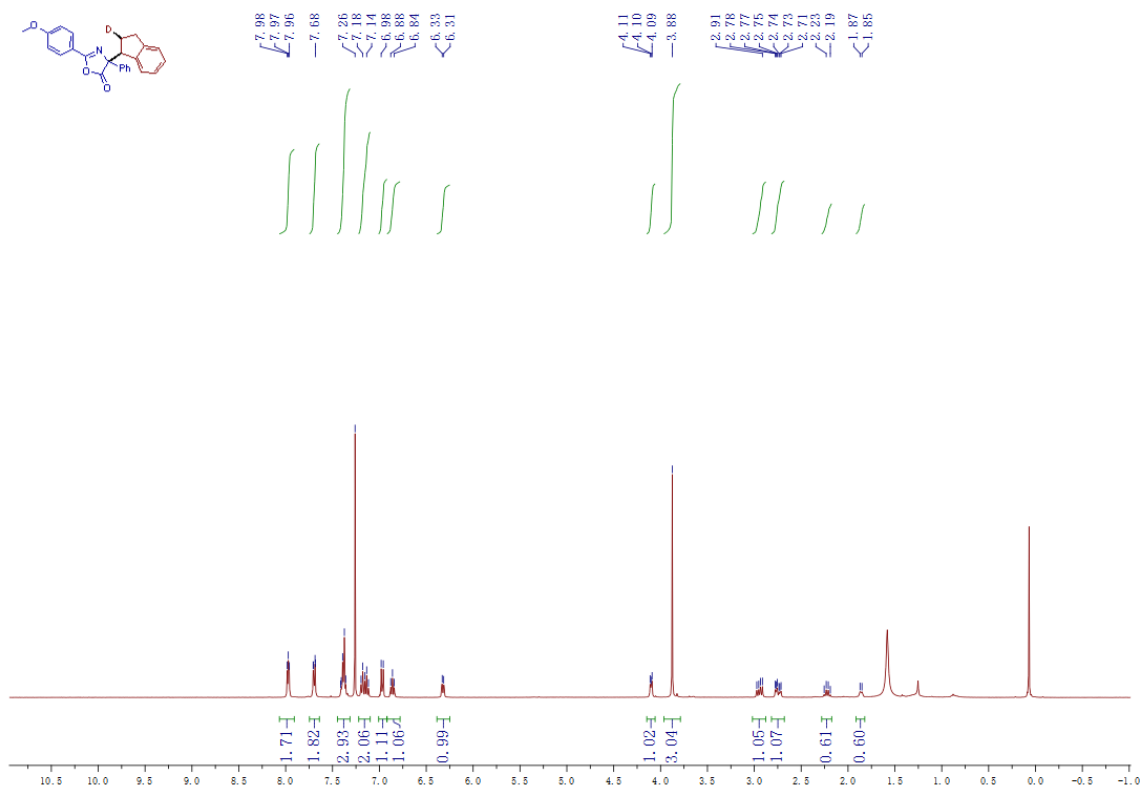
¹H NMR spectrum of 4-(2,3-dihydro-1H-inden-1-yl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (16)



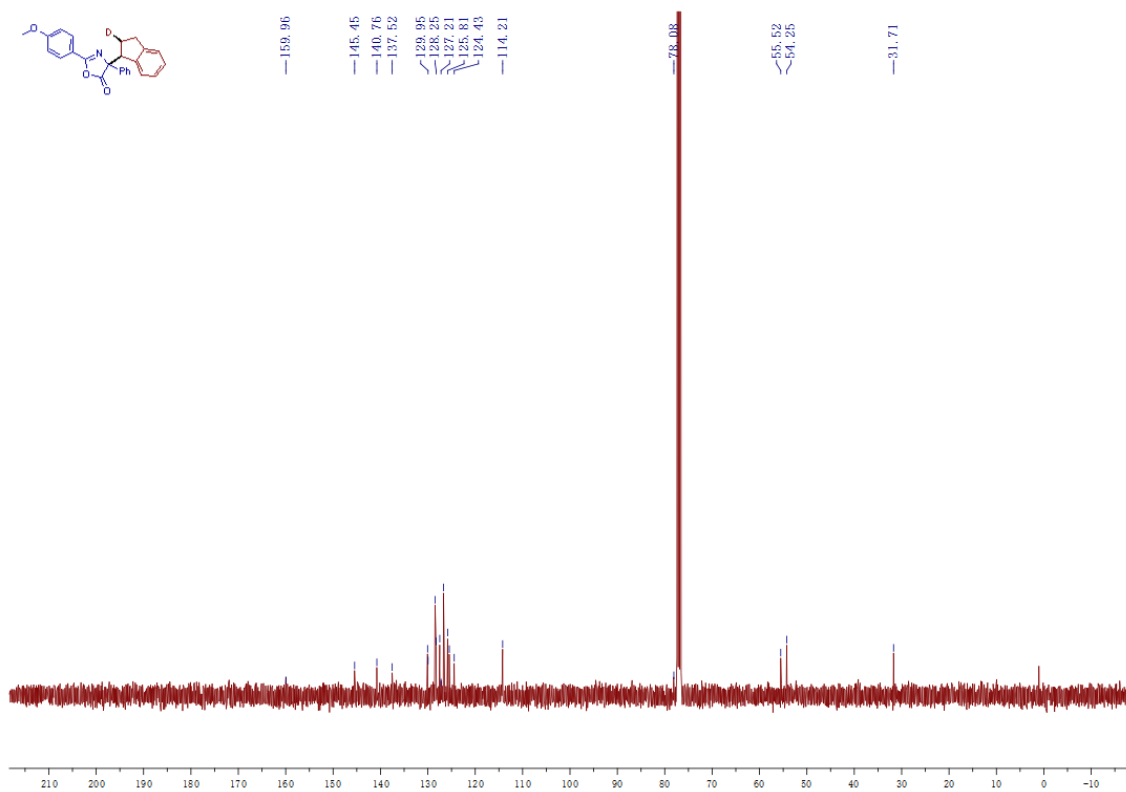
¹³C NMR spectrum of 4-(2,3-dihydro-1H-inden-1-yl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (16)



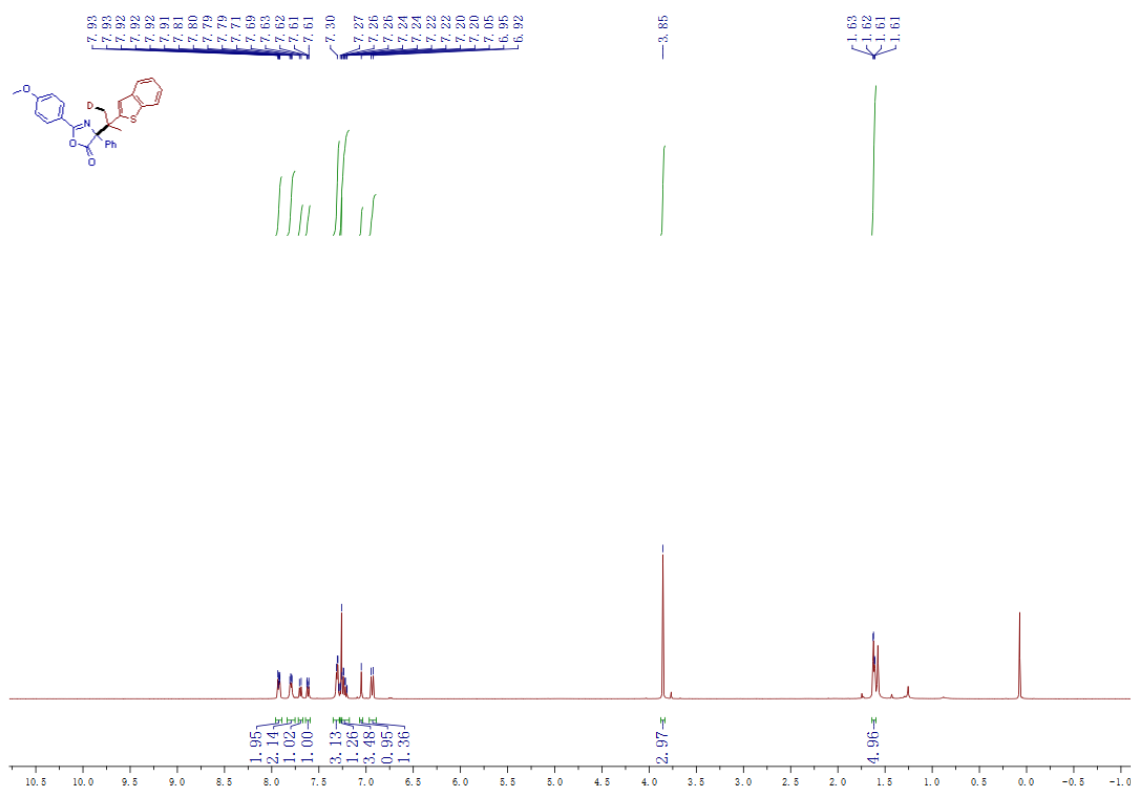
¹H NMR spectrum of 4-(2,3-dihydro-1H-inden-1-yl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (16)



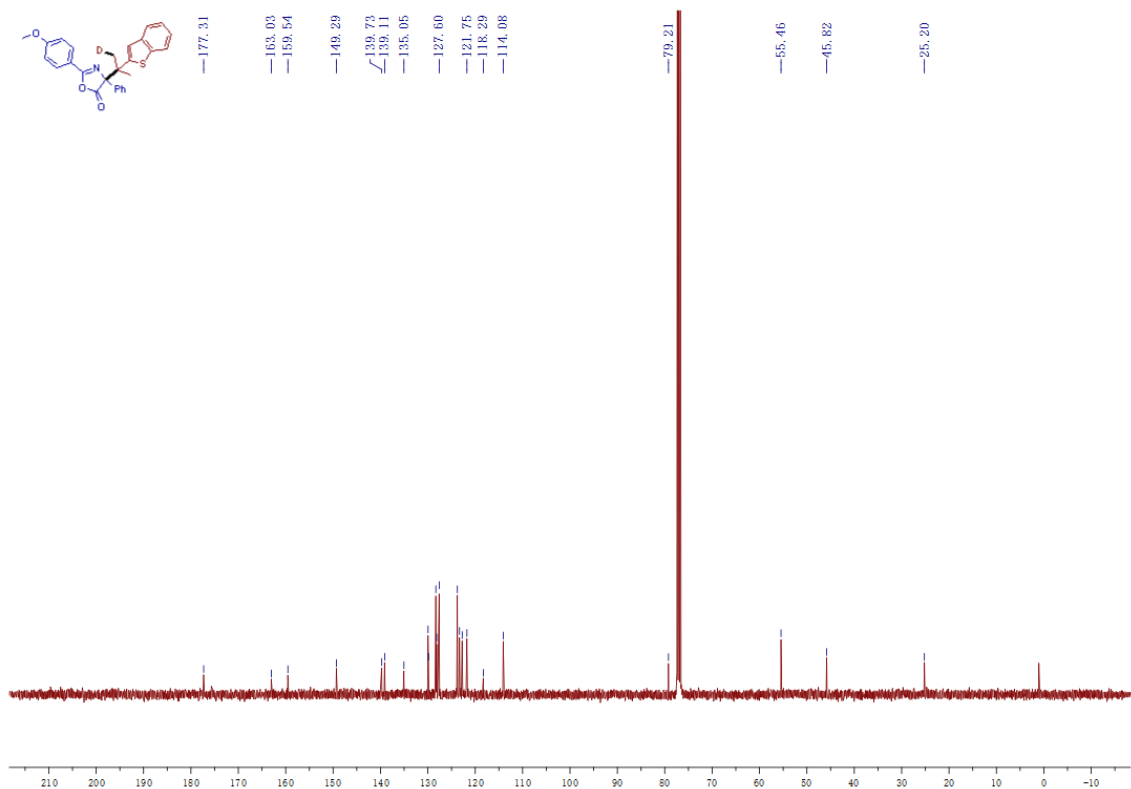
¹³C NMR spectrum of 4-(2,3-dihydro-1H-inden-1-yl-2-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (16)



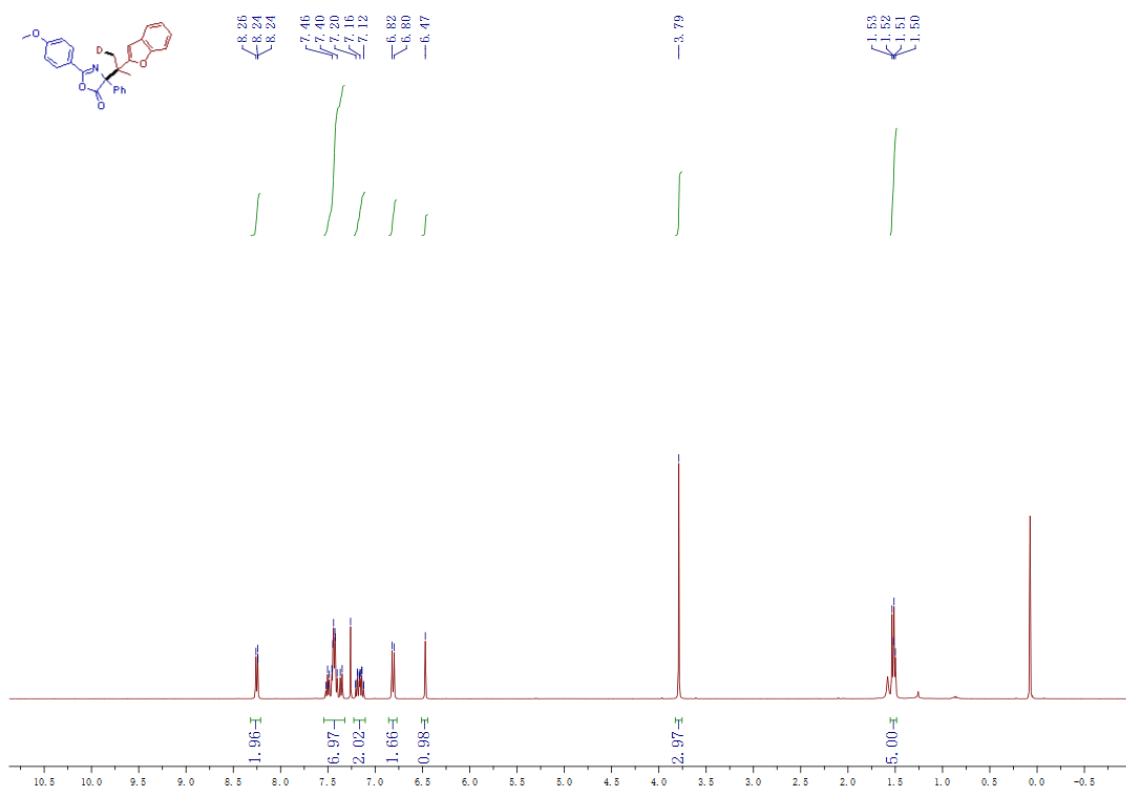
¹H NMR spectrum of 4-(2-(benzo[b]thiophen-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (17)



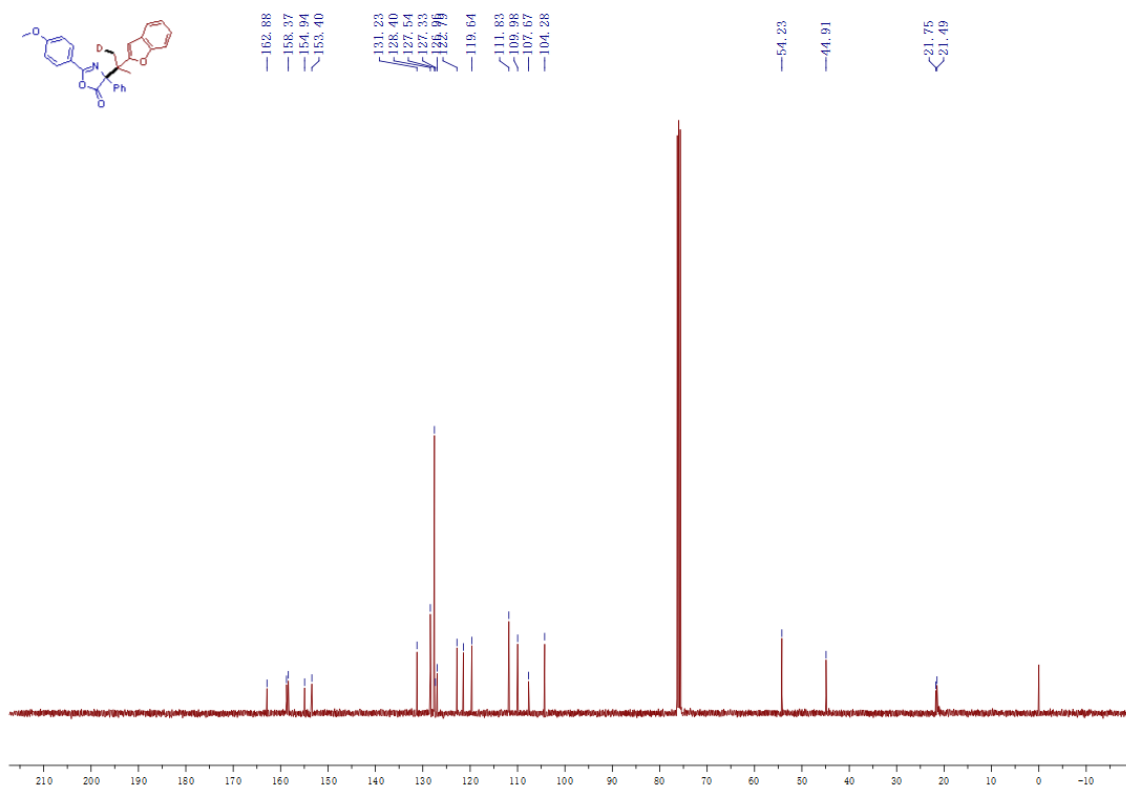
¹³C NMR spectrum of 4-(2-(benzo[b]thiophen-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (17)



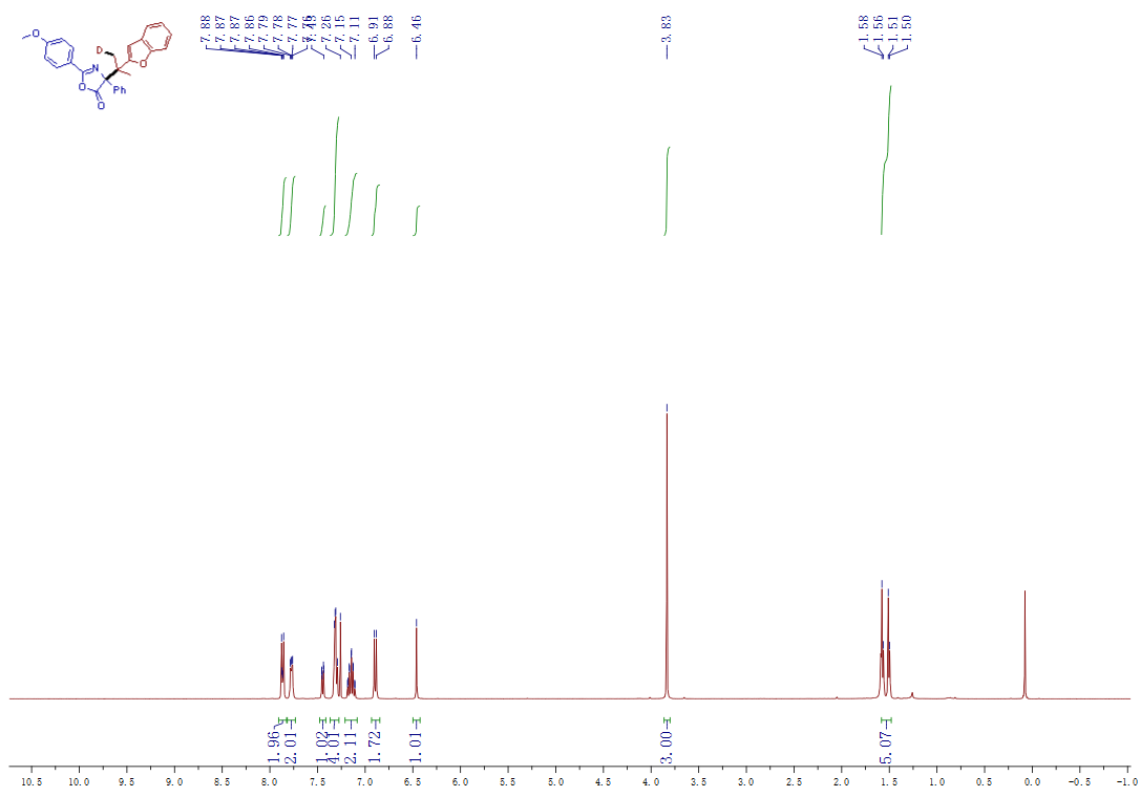
¹H NMR spectrum of 4-(2-(benzofuran-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (18)



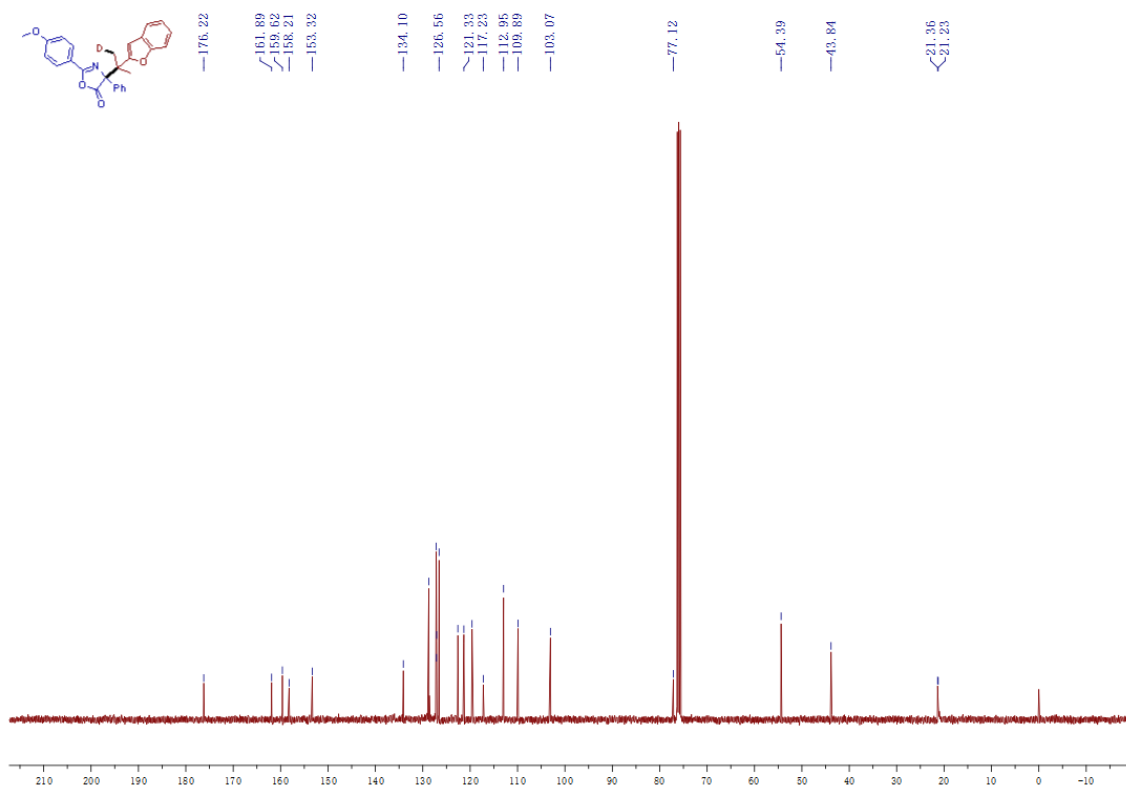
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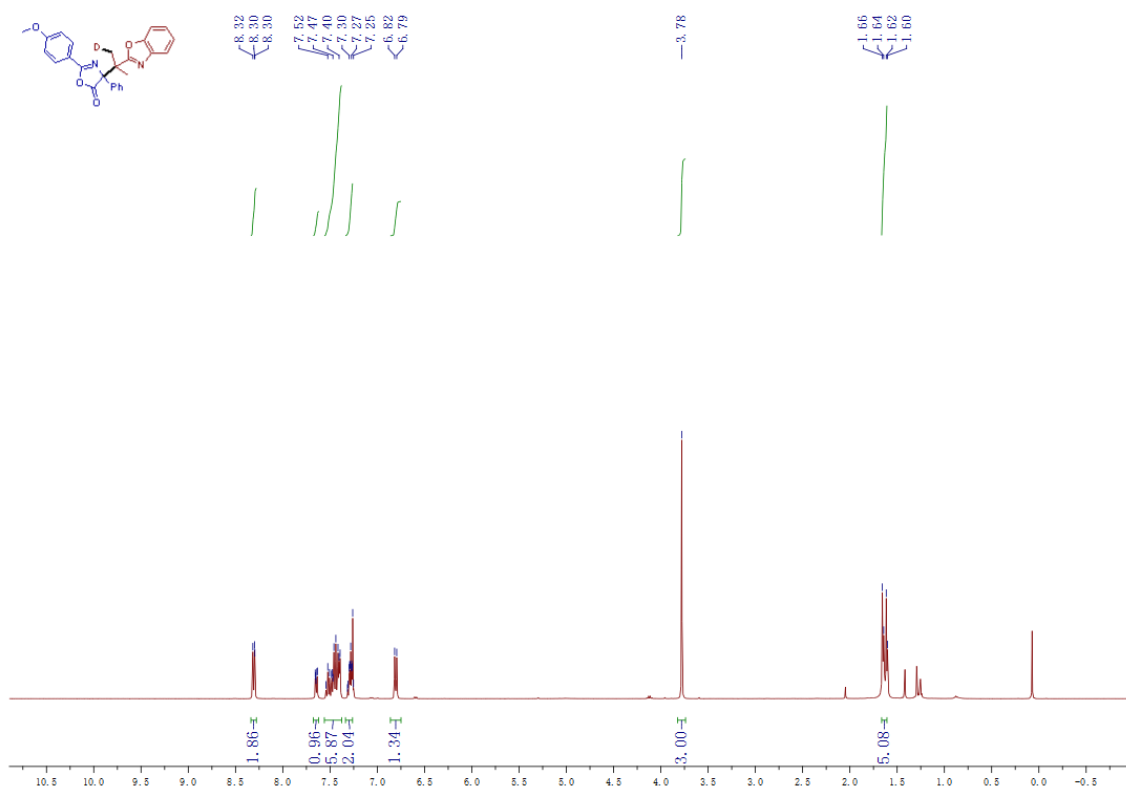
¹H NMR spectrum of 4-(2-(benzofuran-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (18)



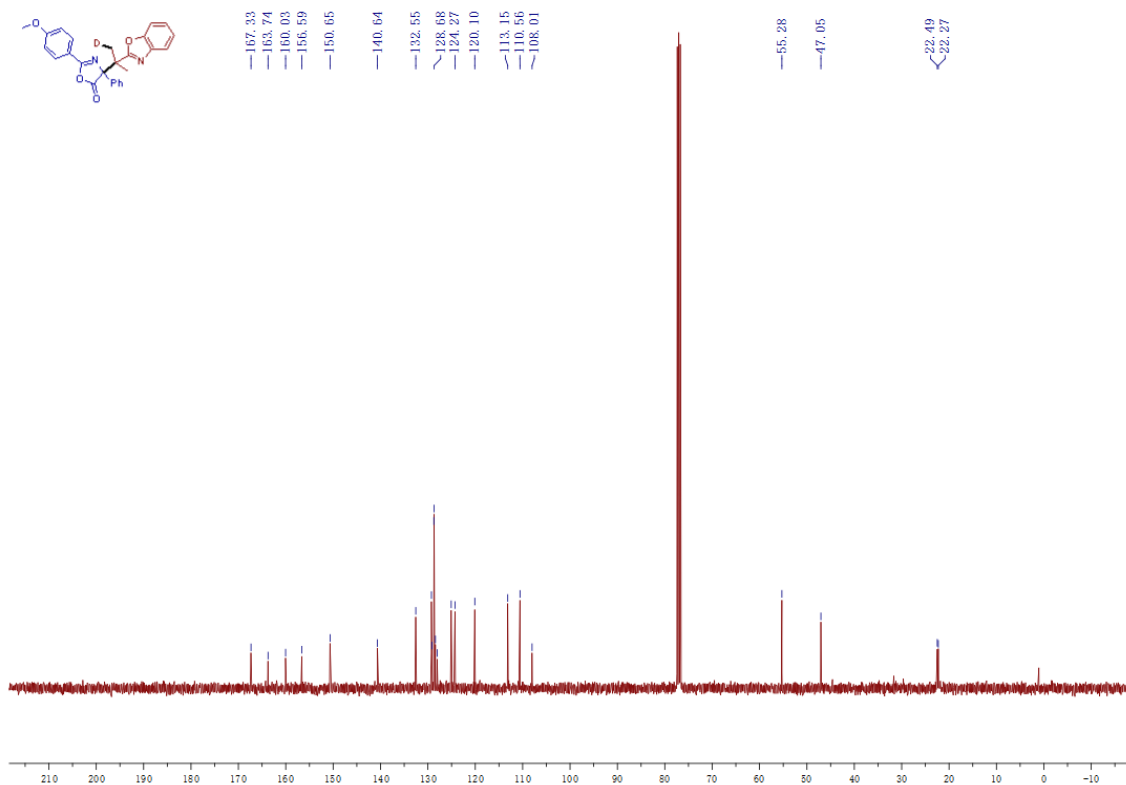
¹³C NMR spectrum of 4-(2-(benzofuran-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (18)



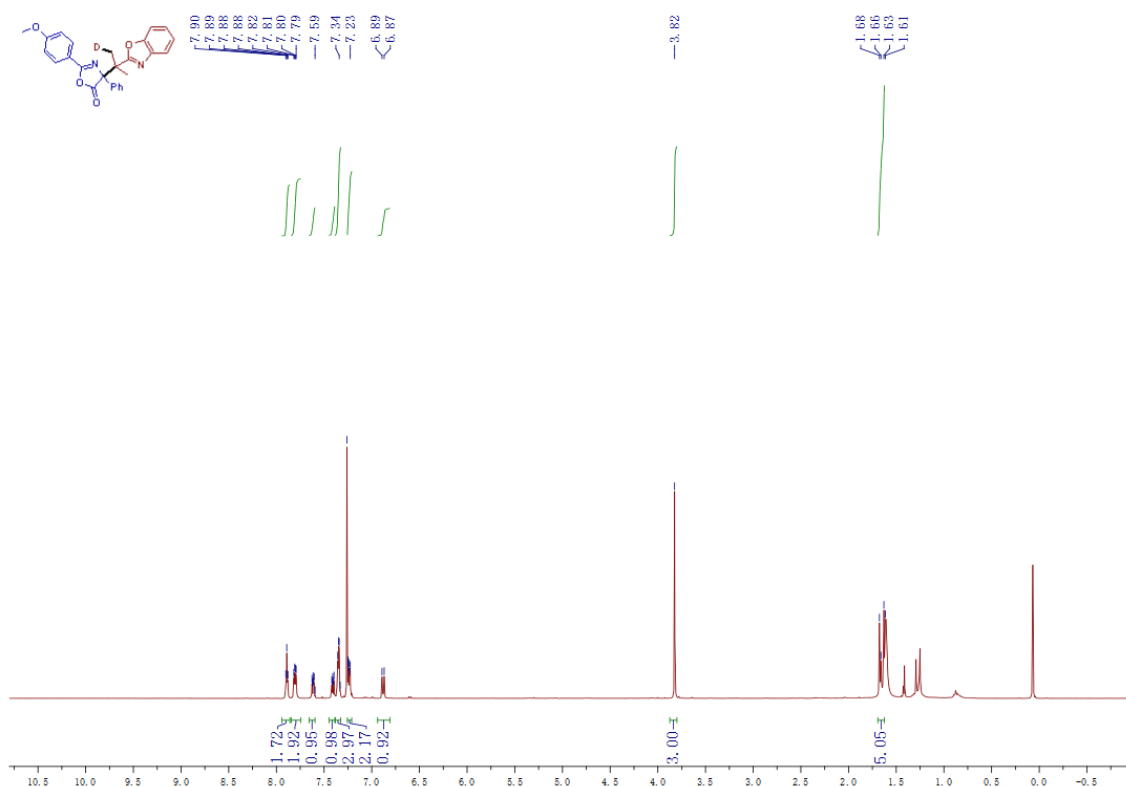
¹H NMR spectrum of 4-(2-(benzo[d]oxazol-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (19)



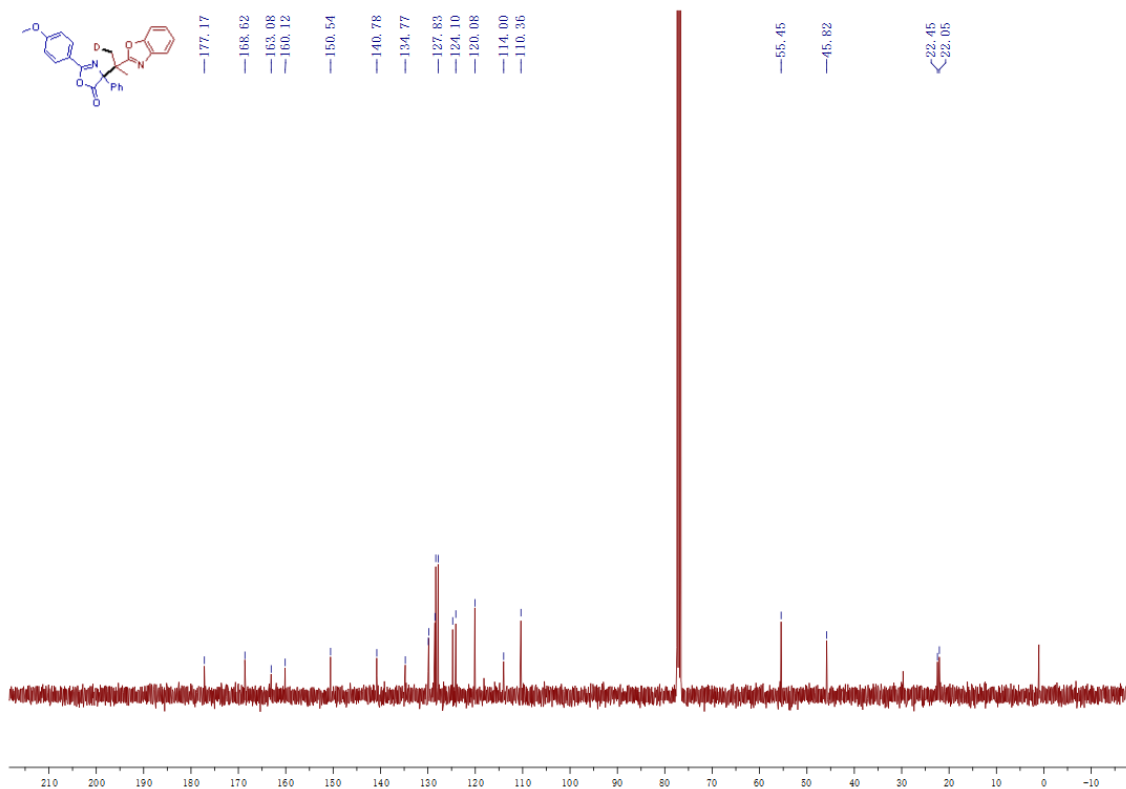
¹³C NMR spectrum of 4-(2-(benzo[d]oxazol-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (19)



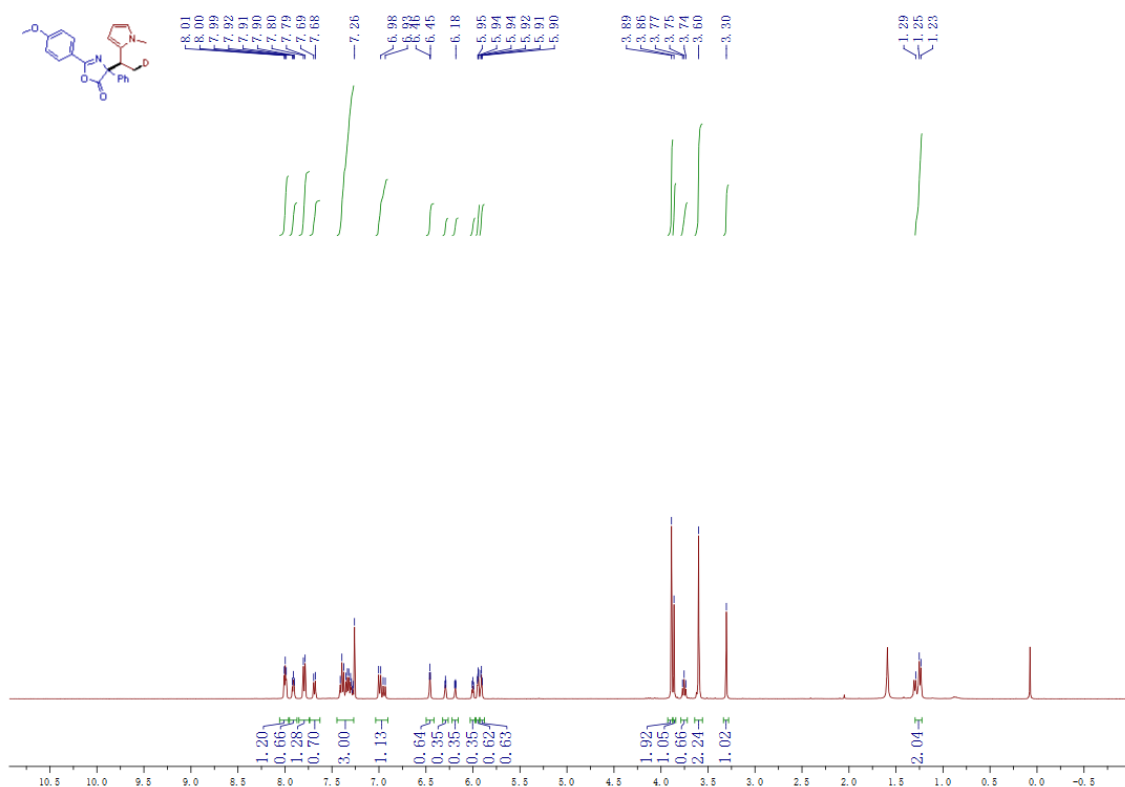
¹H NMR spectrum of 4-(2-(benzo[d]oxazol-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (19)



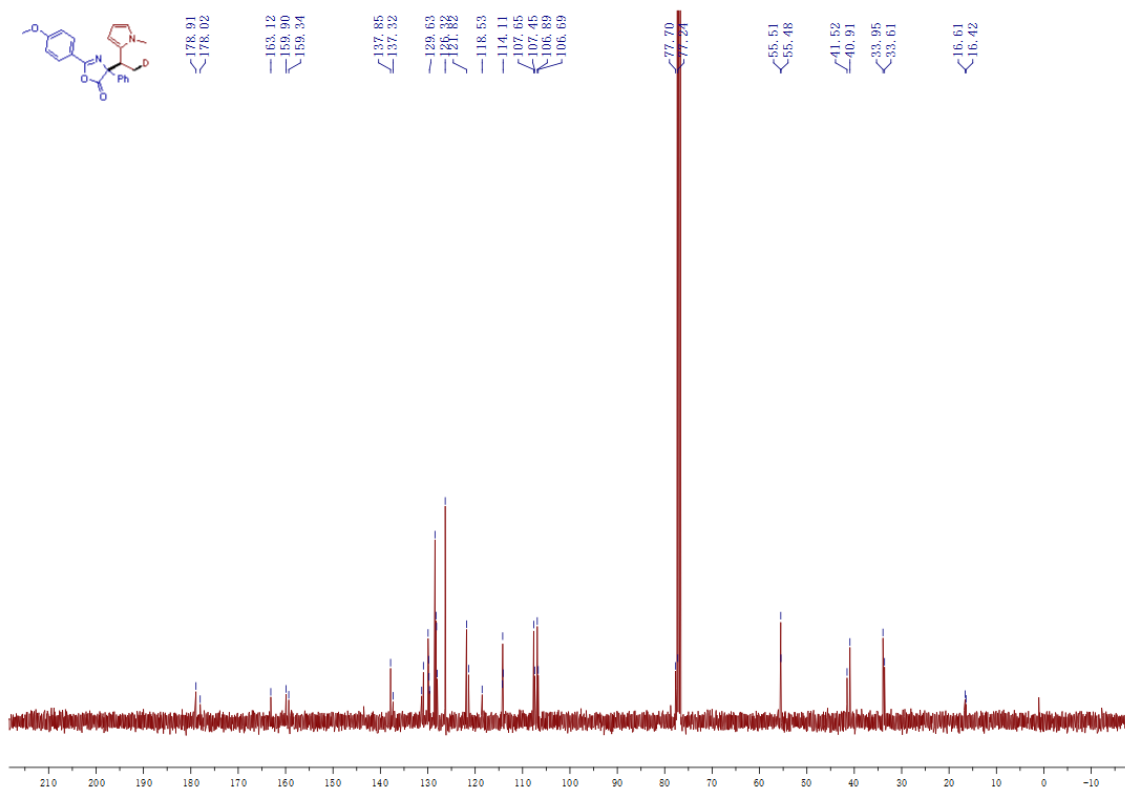
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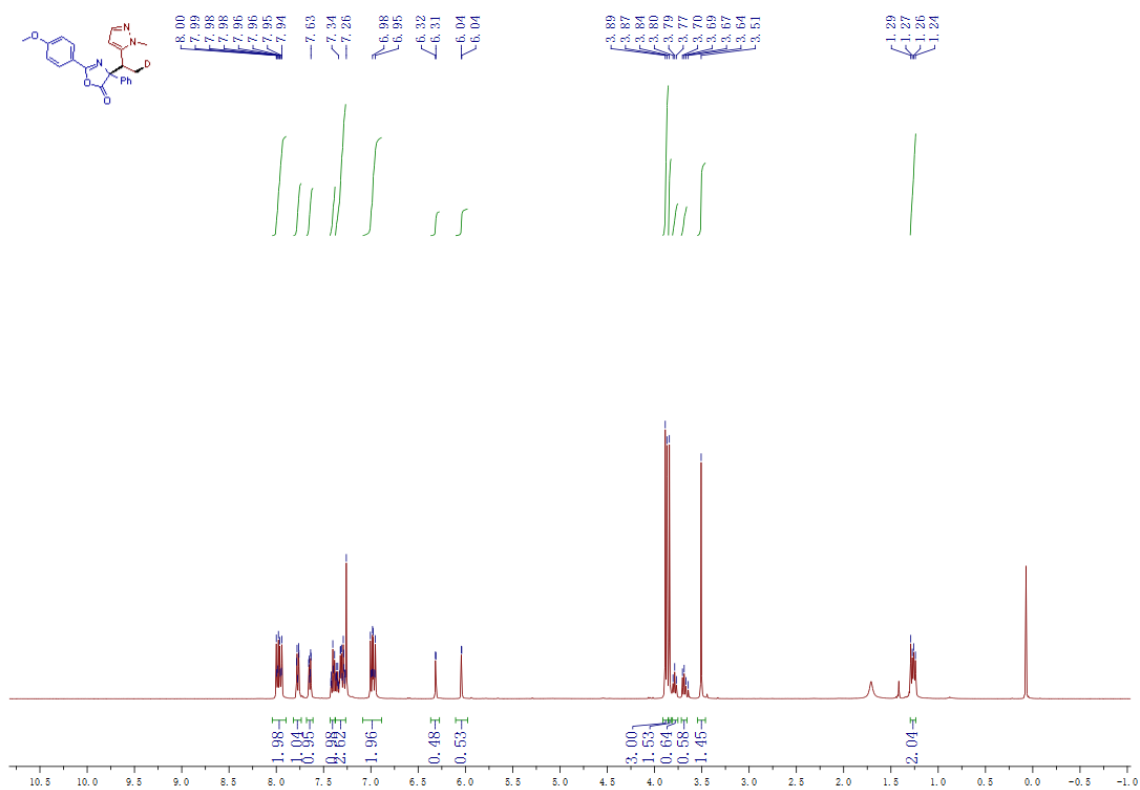
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(1-(1-methyl-1H-pyrrol-2-yl)ethyl)-2-d-4-phenyloxazol-5(4H)-one (20)



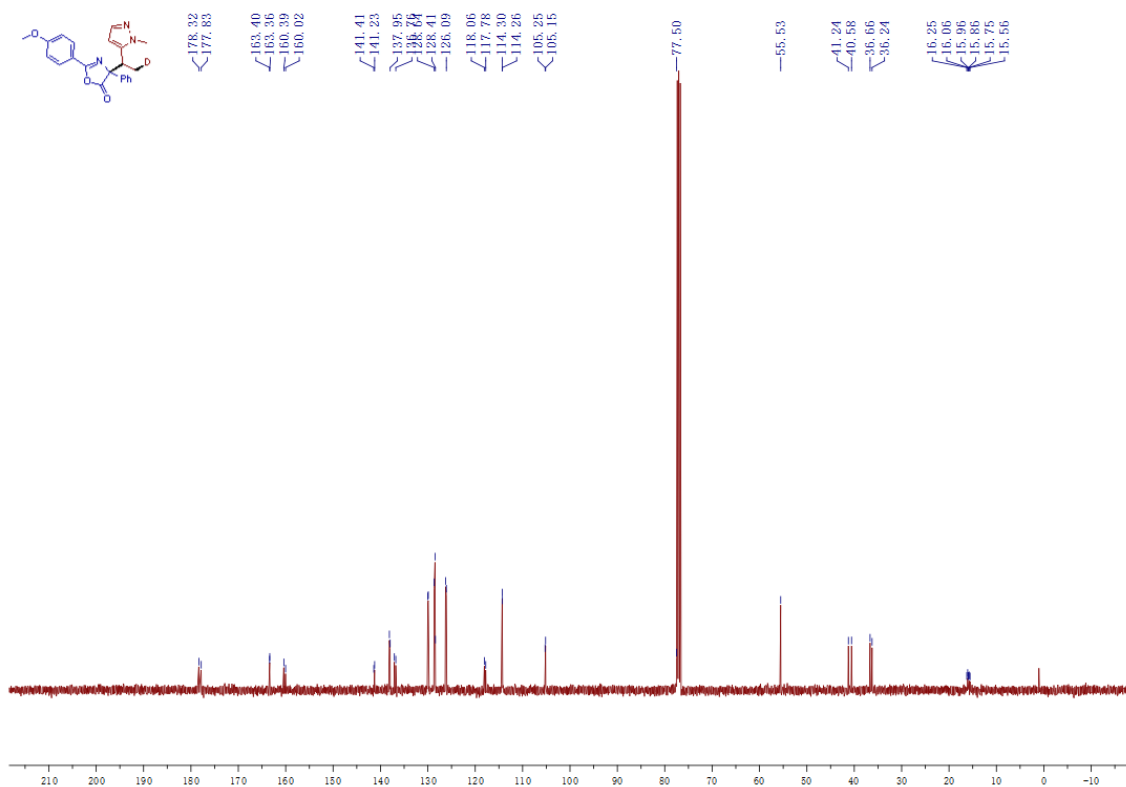
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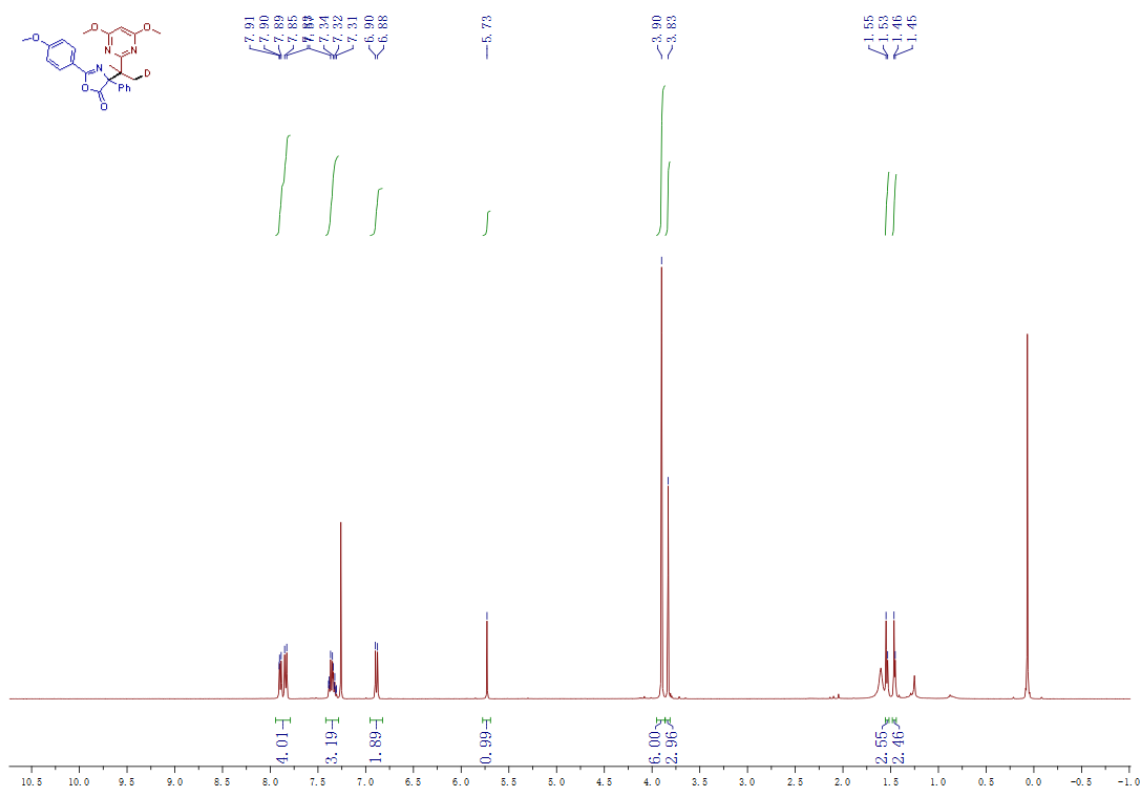
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(1-(1-methyl-1H-pyrazol-5-yl)ethyl)-2-d-4-phenyloxazol-5(4H)-one (21)



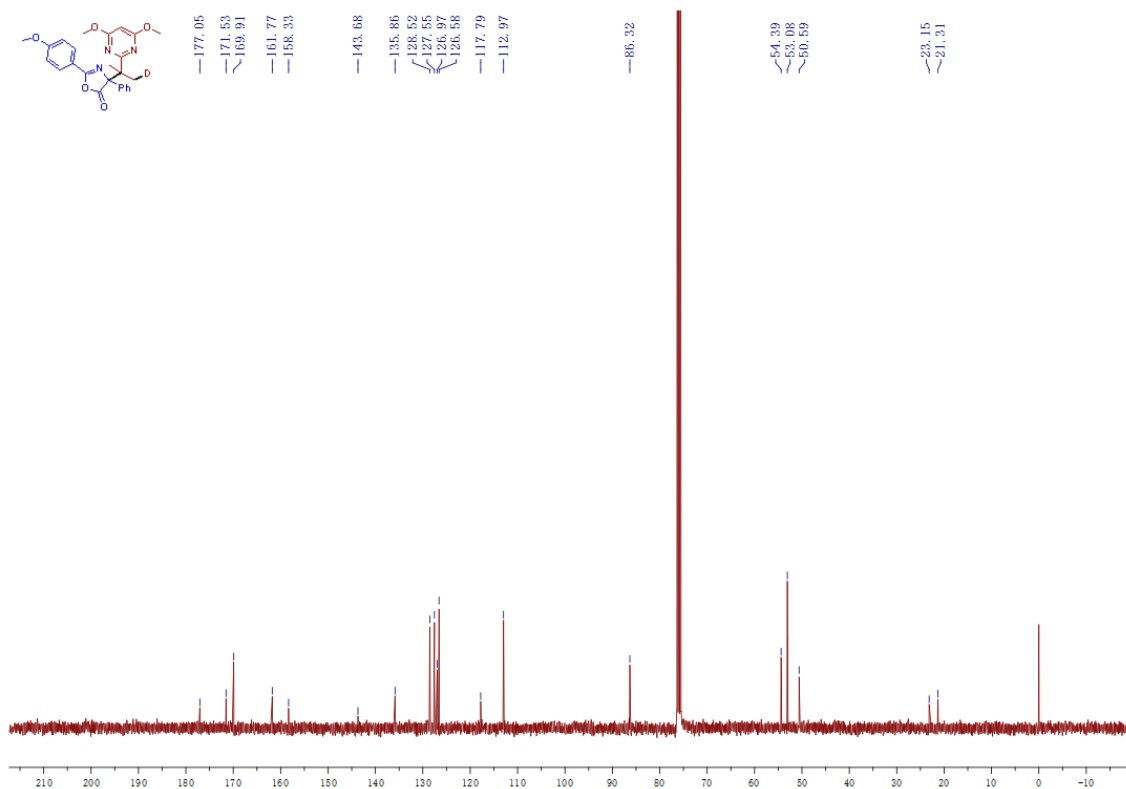
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-(1-(1-methyl-1H-pyrazol-5-yl)ethyl)-2-d-4-phenyloxazol-5(4H)-one (21)



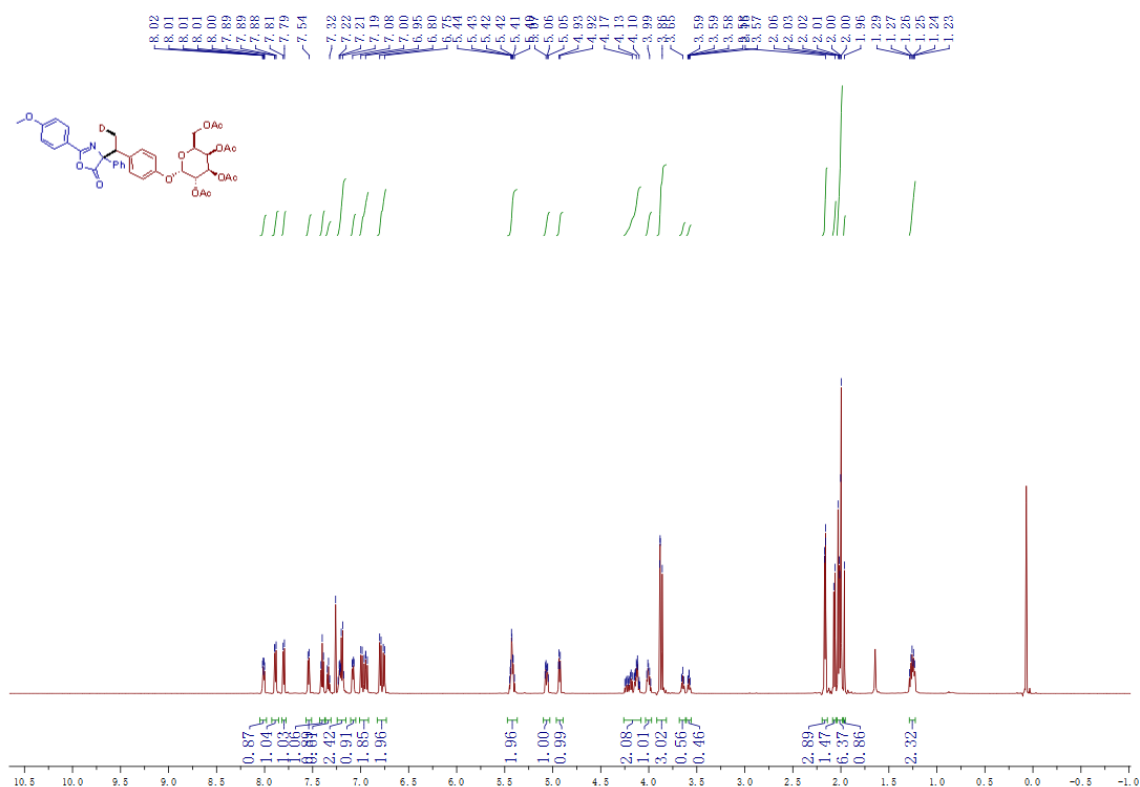
¹H NMR spectrum of 4-(2-(4,6-dimethoxypyrimidin-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (22)



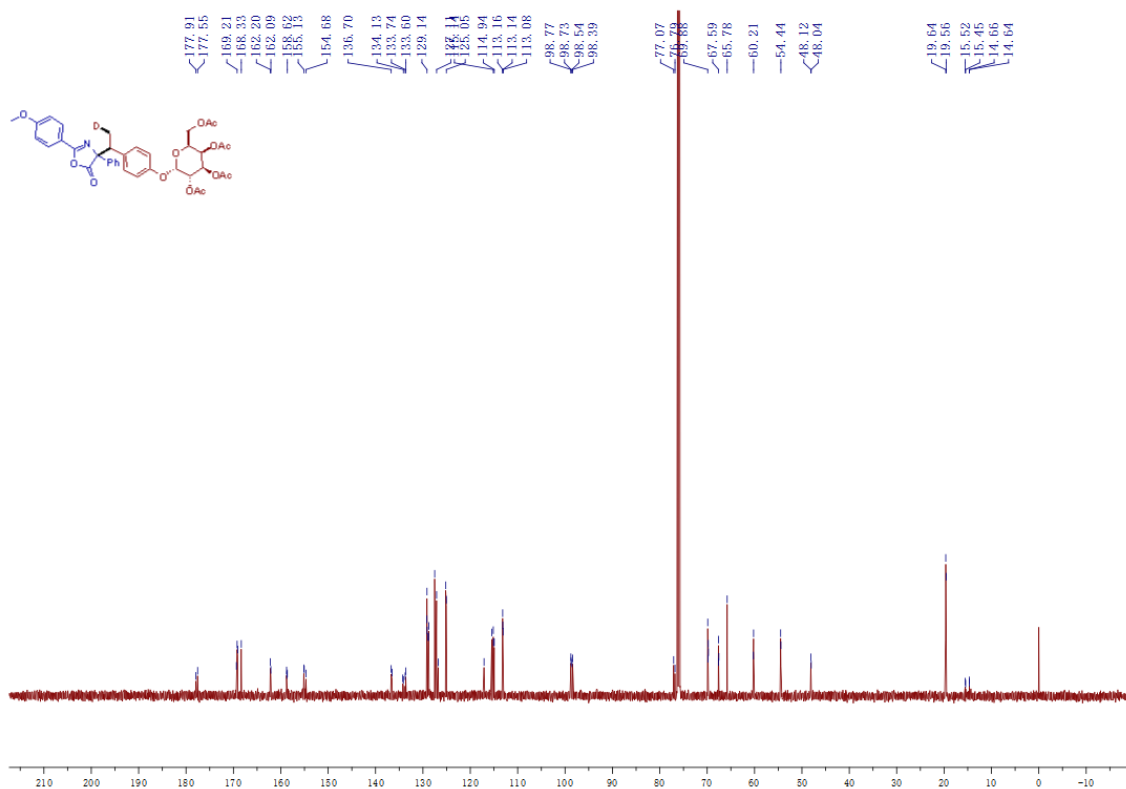
¹³C NMR spectrum of 4-(2-(4,6-dimethoxypyrimidin-2-yl)propan-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (22)



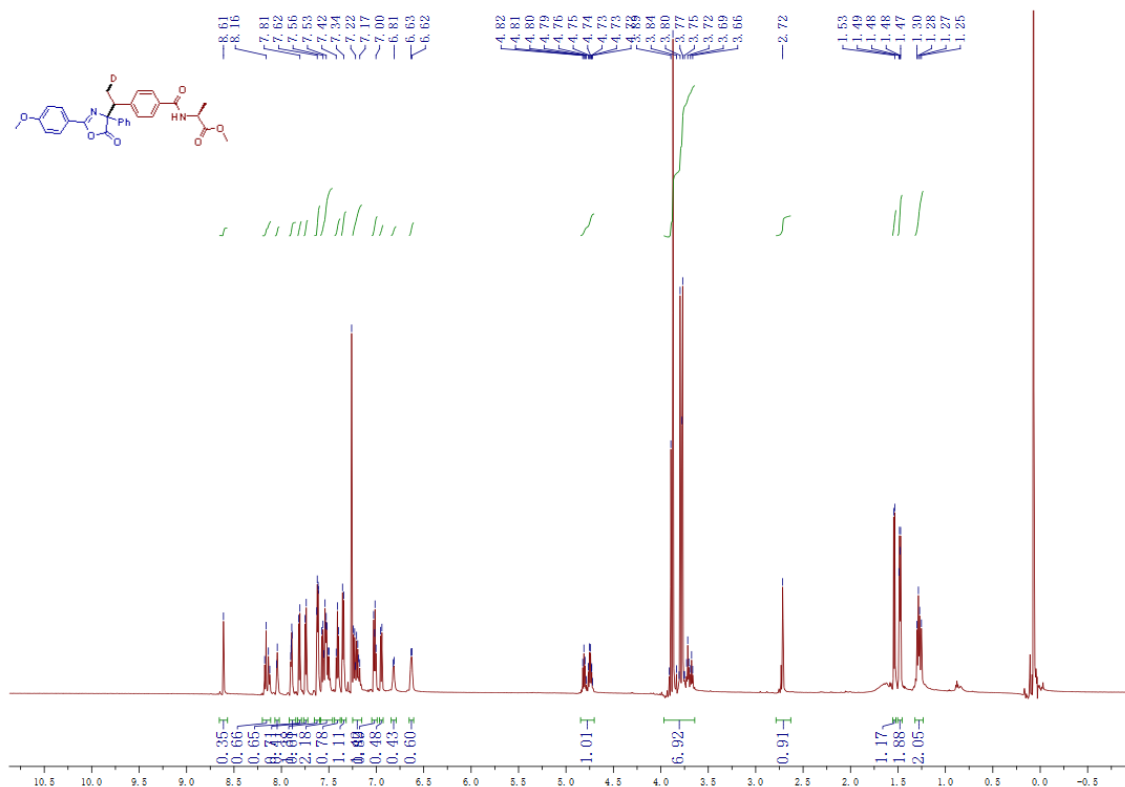
¹H NMR spectrum of (2S,3R,4R,5S,6S)-2-(acetoxymethyl)-6-(4-(1-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)ethyl-2-d)phenoxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate (23)



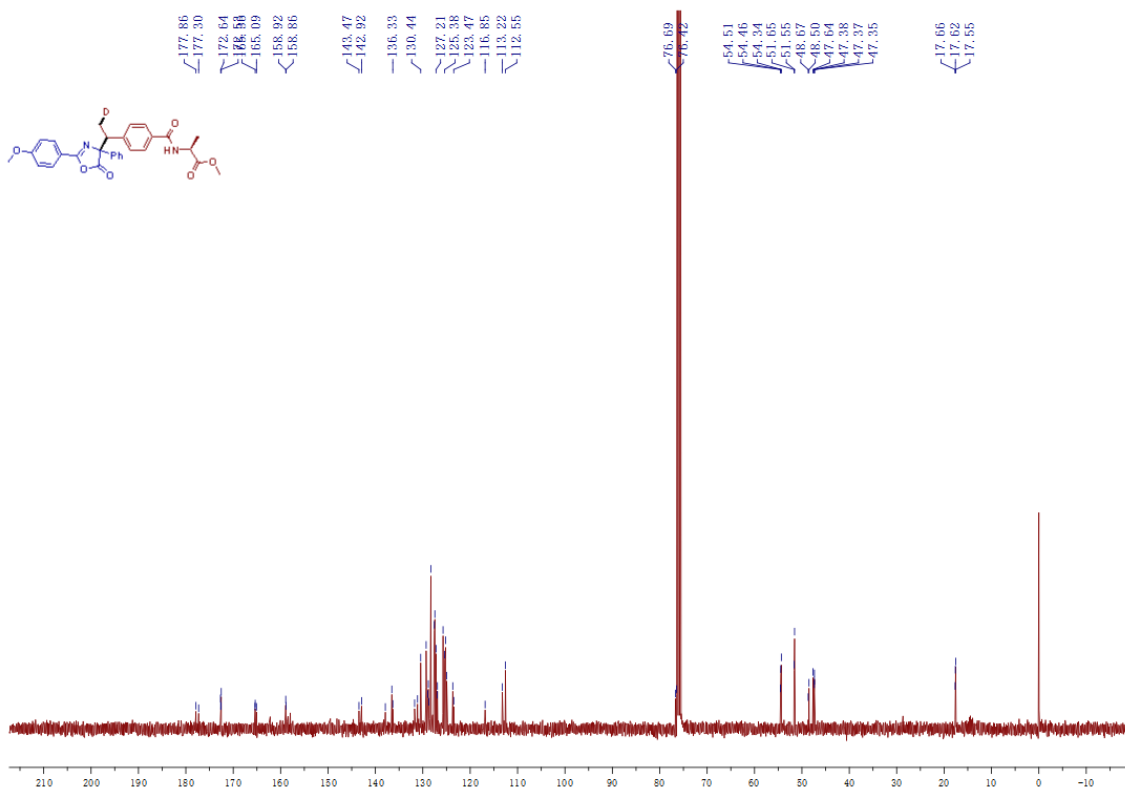
¹³C NMR spectrum of (2S,3R,4R,5S,6S)-2-(acetoxymethyl)-6-(4-(1-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)ethyl-2-d)phenoxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate (23)



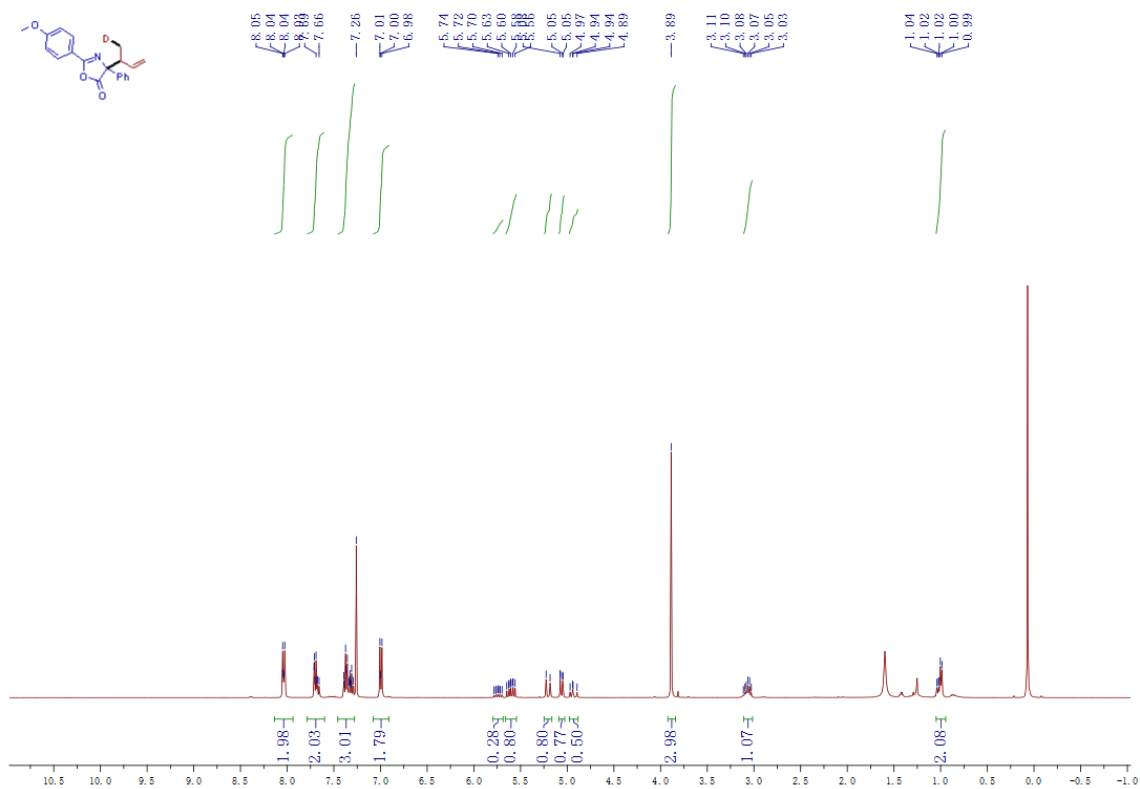
¹H NMR spectrum of Methyl(4-(1-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)ethyl-2-d)benzoyl)-L-alaninate (24)



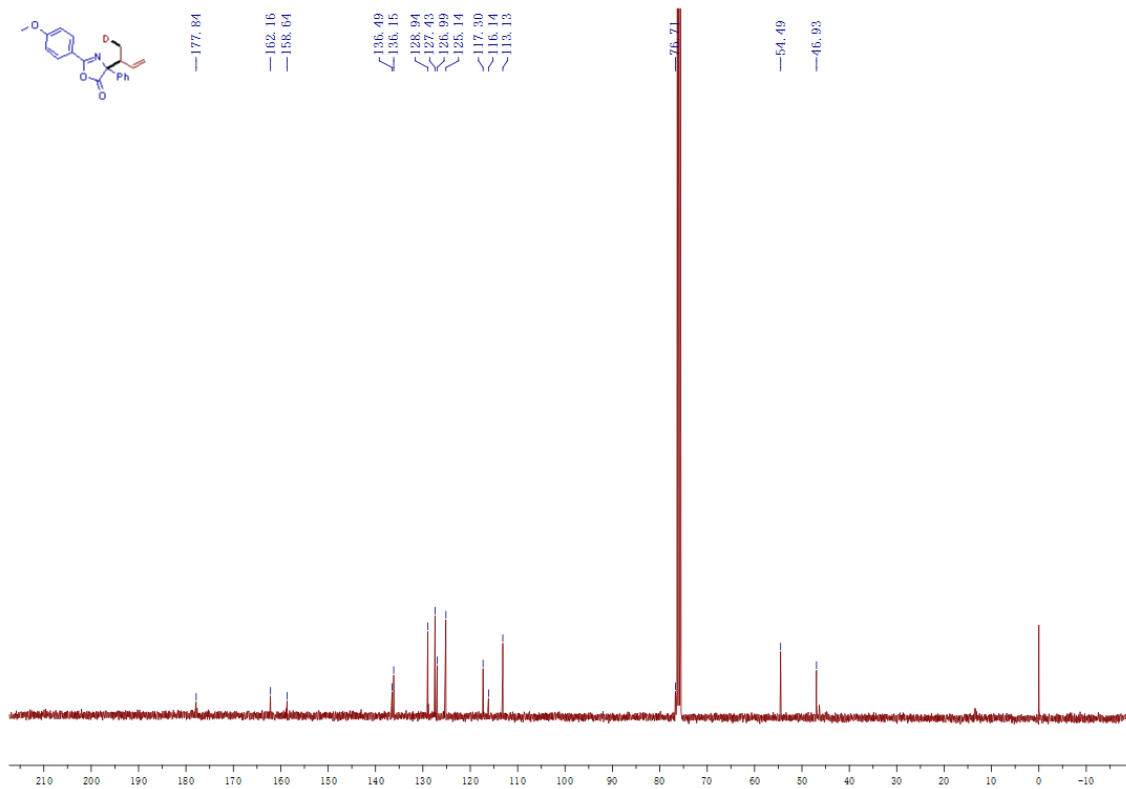
¹³C NMR spectrum of Methyl(4-(1-(2-(4-methoxyphenyl)-5-oxo-4-phenyl-4,5-dihydrooxazol-4-yl)ethyl-2-d)benzoyl)-L-alaninate (24)



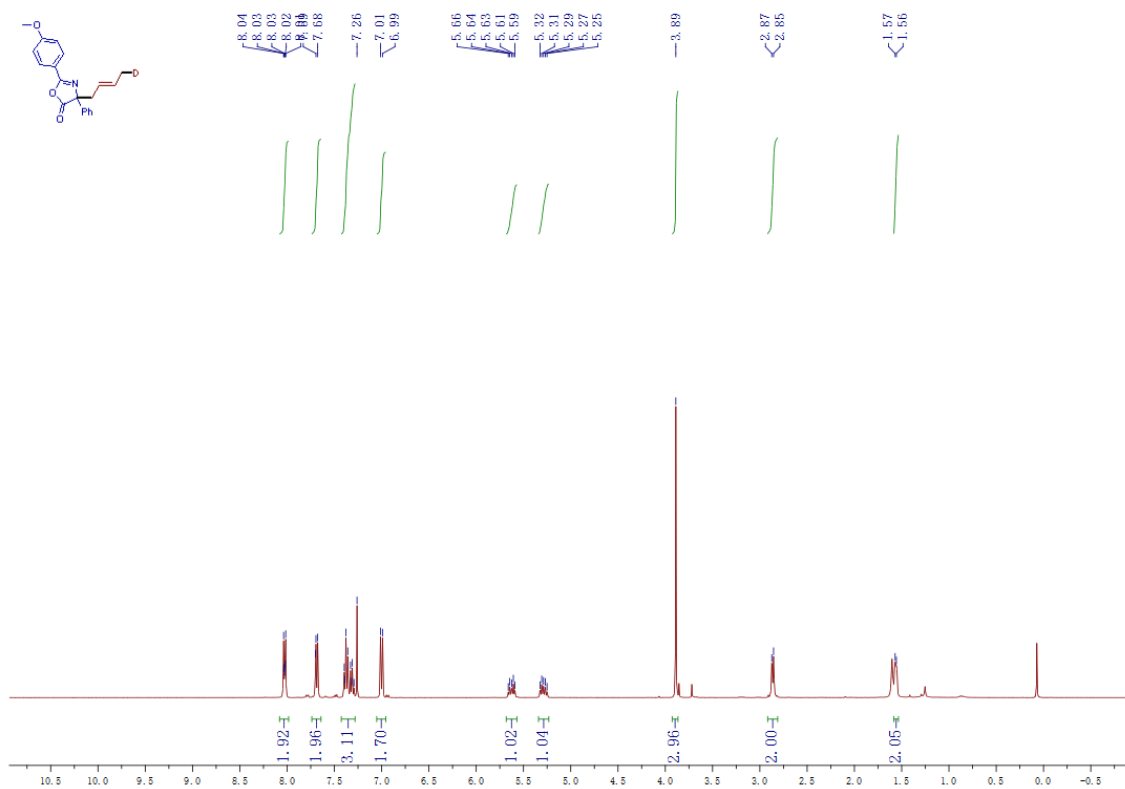
¹H NMR spectrum of 4-(but-3-en-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (26)



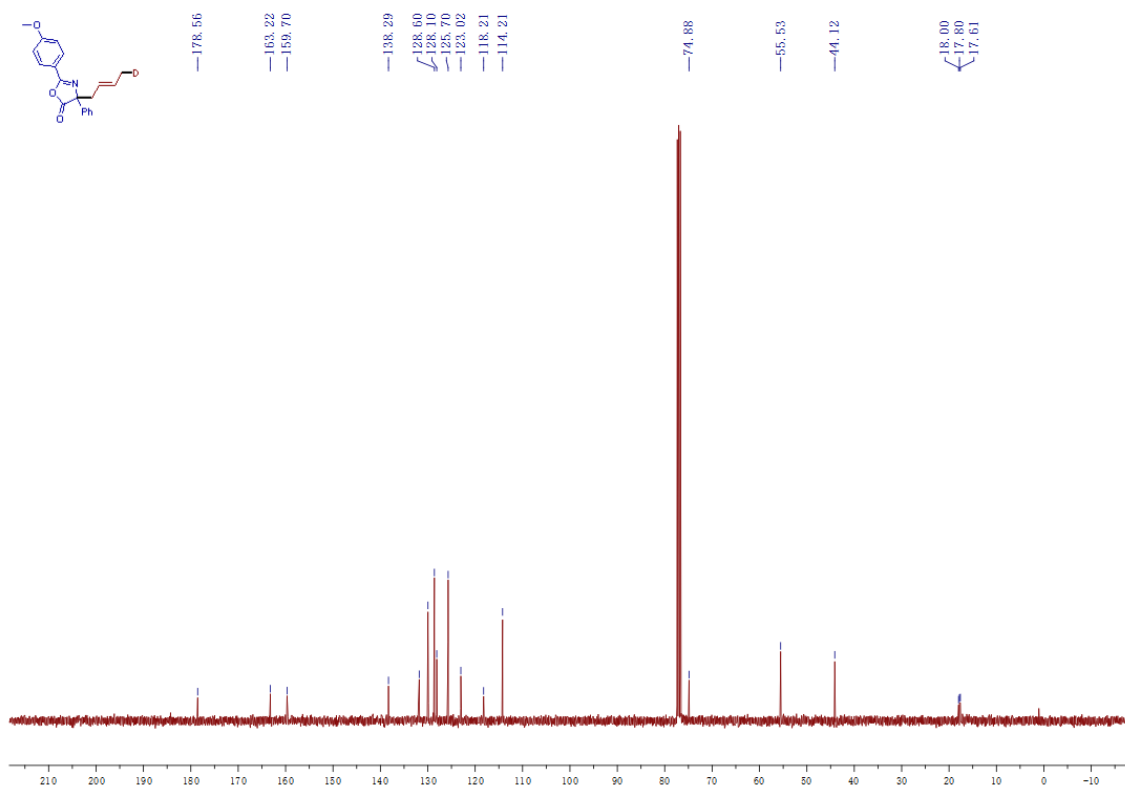
¹³C NMR spectrum of 4-(but-3-en-2-yl-1-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (26)



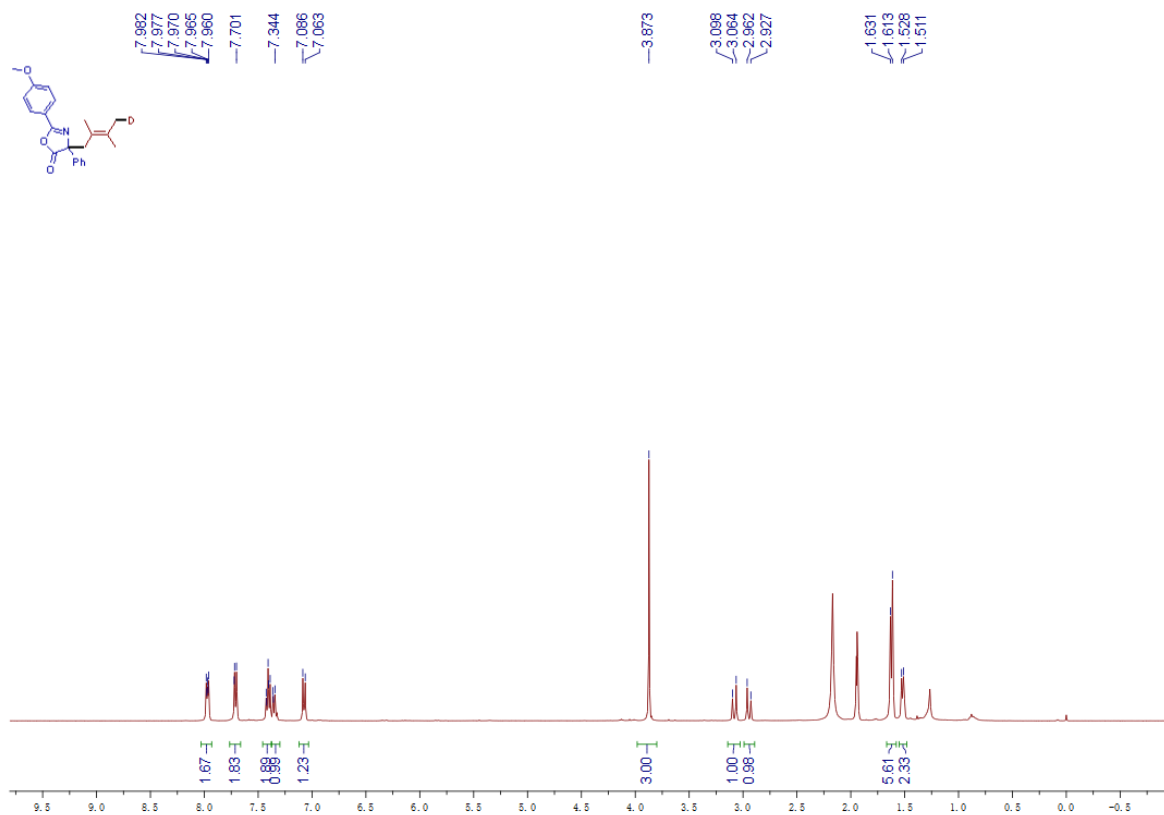
¹H NMR spectrum of (E)-4-(but-2-en-1-yl-4-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (26)



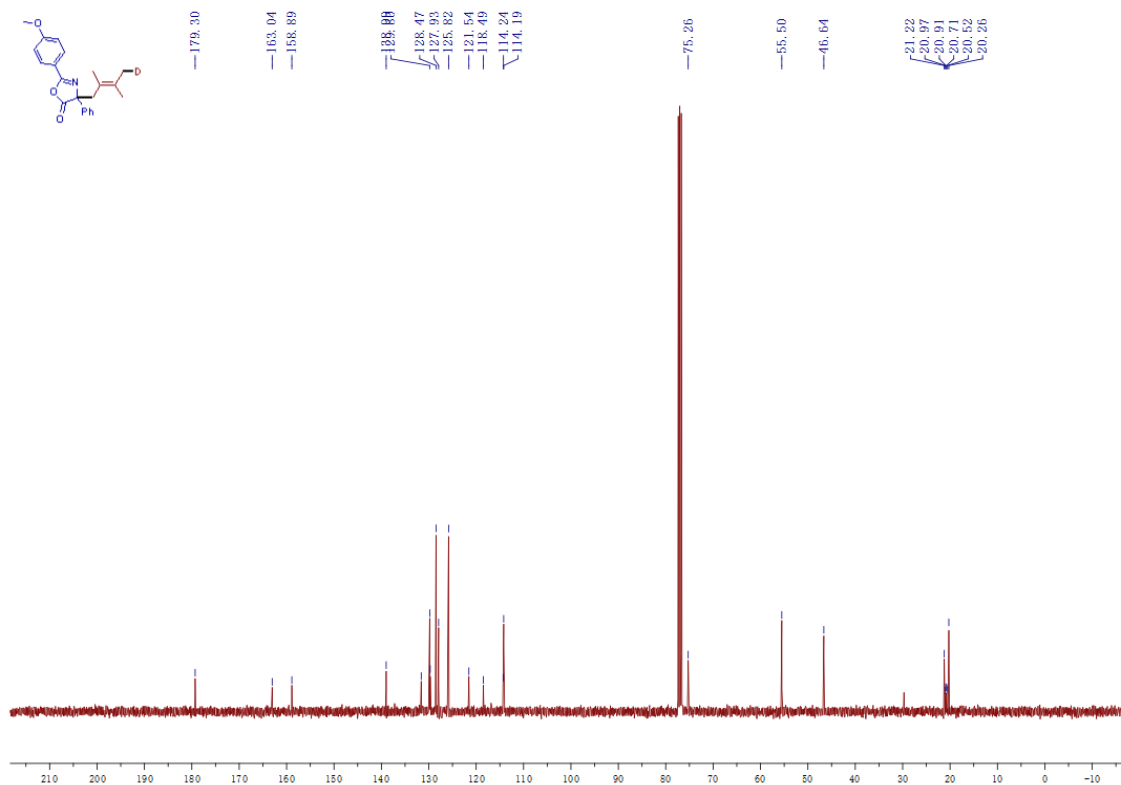
¹³C NMR spectrum of (E)-4-(but-2-en-1-yl-4-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (26)



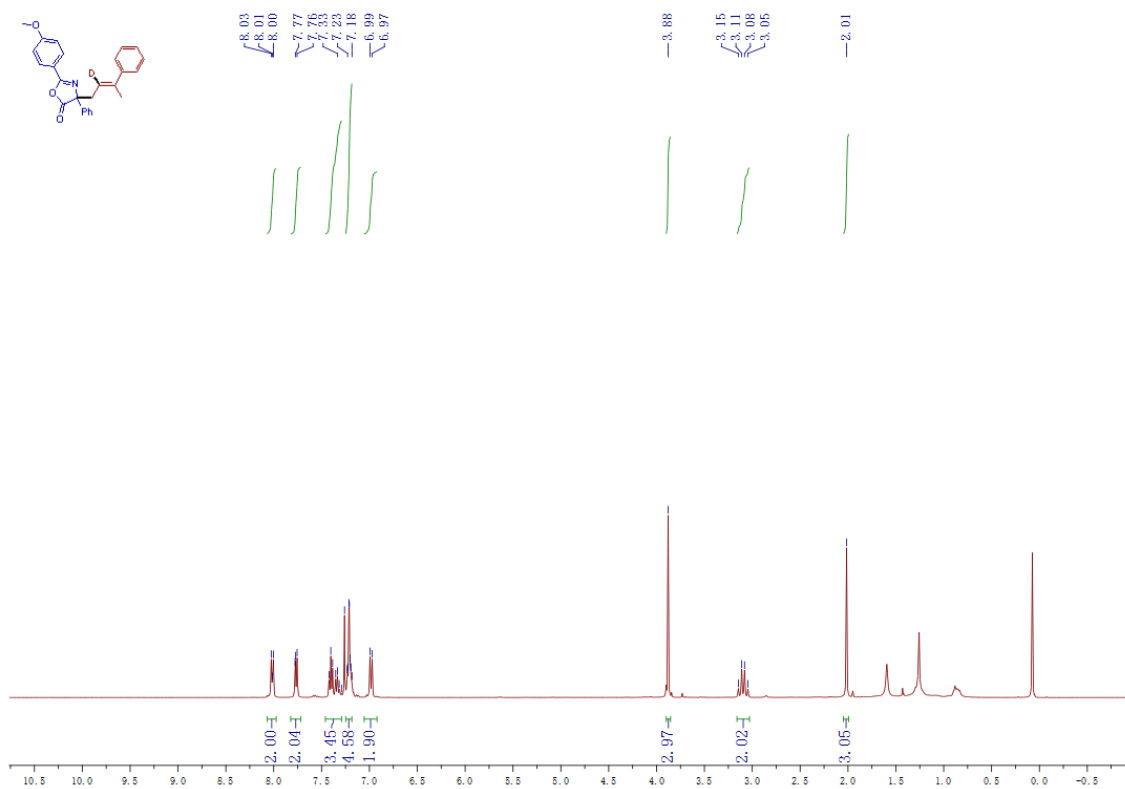
¹H NMR spectrum of (E)-4-(2,3-dimethylbut-2-en-1-yl-4-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (28)



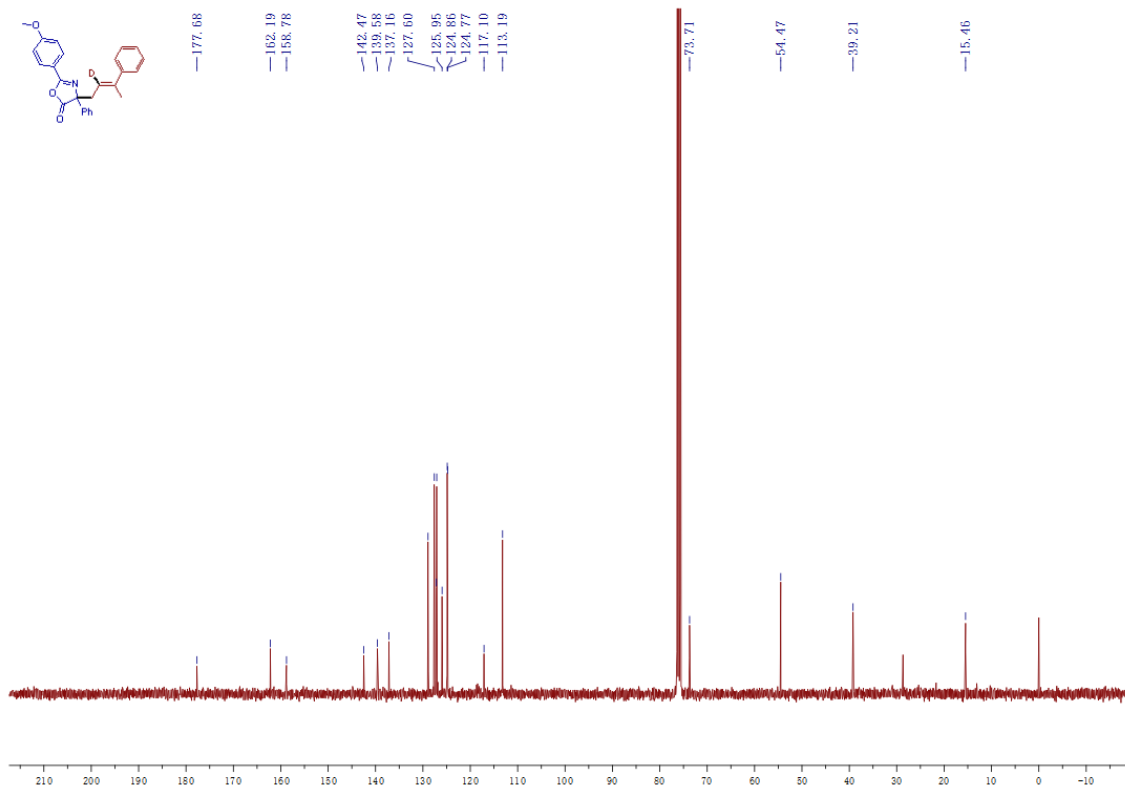
¹³C NMR spectrum of (E)-4-(2,3-dimethylbut-2-en-1-yl-4-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (28)



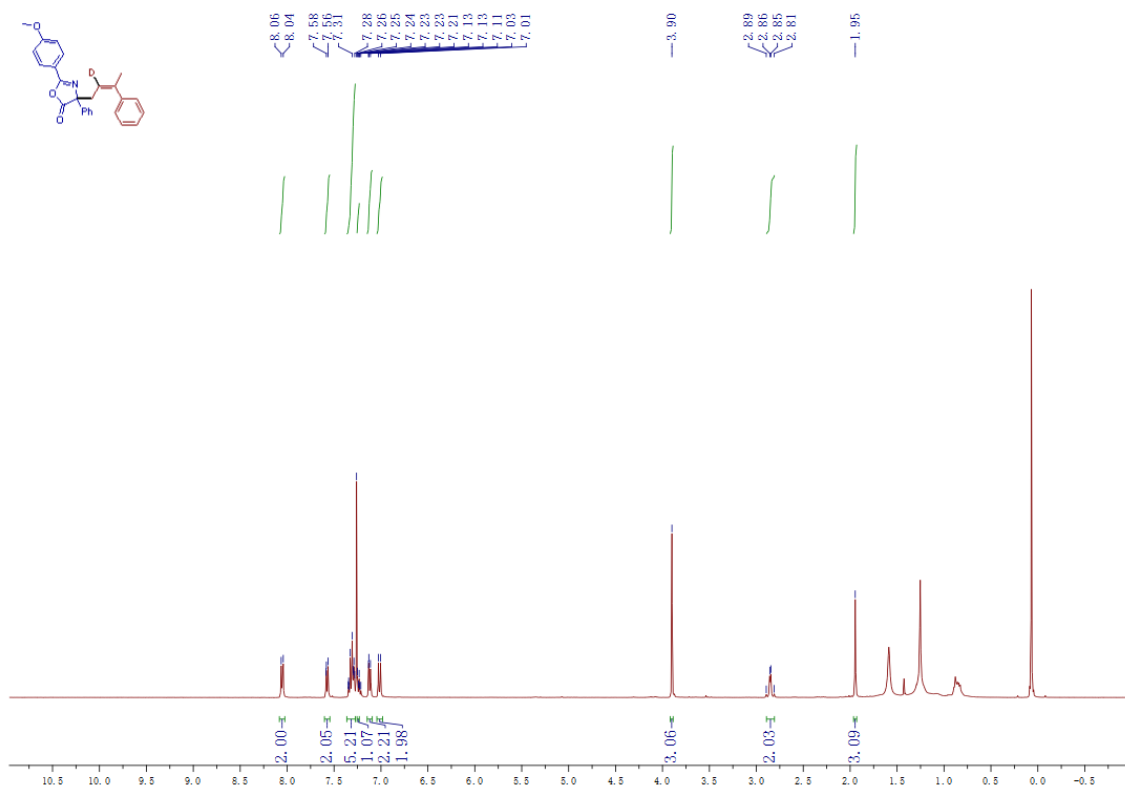
¹H NMR spectrum of (E)-2-(4-methoxyphenyl)-4-phenyl-4-(3-phenylbut-2-en-1-yl-2-d)oxazol-5(4H)-one (30)



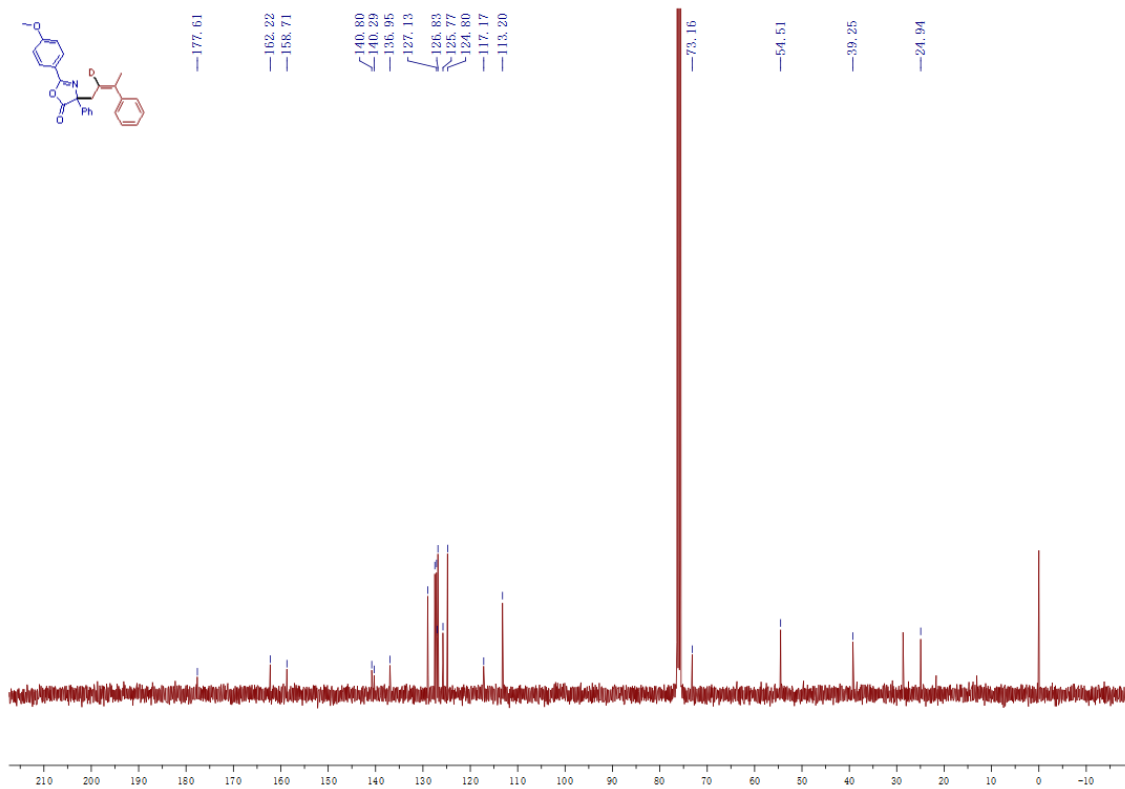
¹³C NMR spectrum of (E)-2-(4-methoxyphenyl)-4-phenyl-4-(3-phenylbut-2-en-1-yl-2-d)oxazol-5(4H)-one (30)



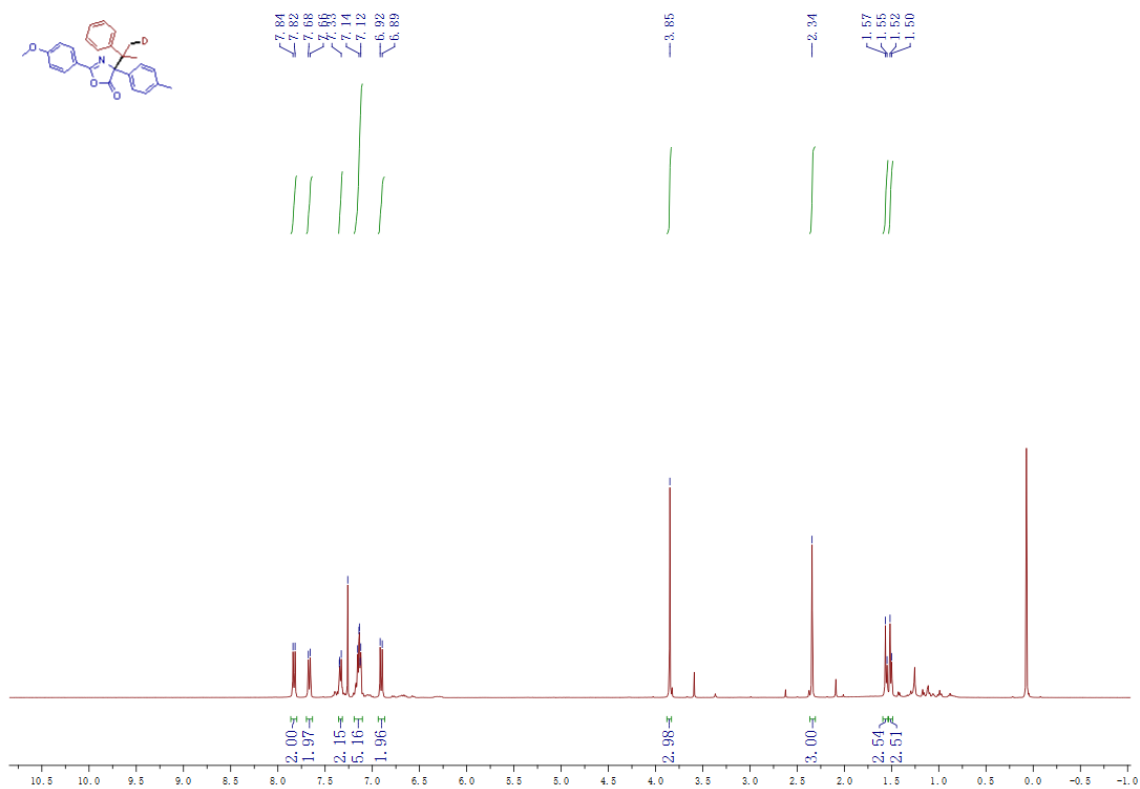
¹H NMR spectrum of (Z)-2-(4-methoxyphenyl)-4-phenyl-4-(3-phenylbut-2-en-1-yl-2-d)oxazol-5(4H)-one (30)



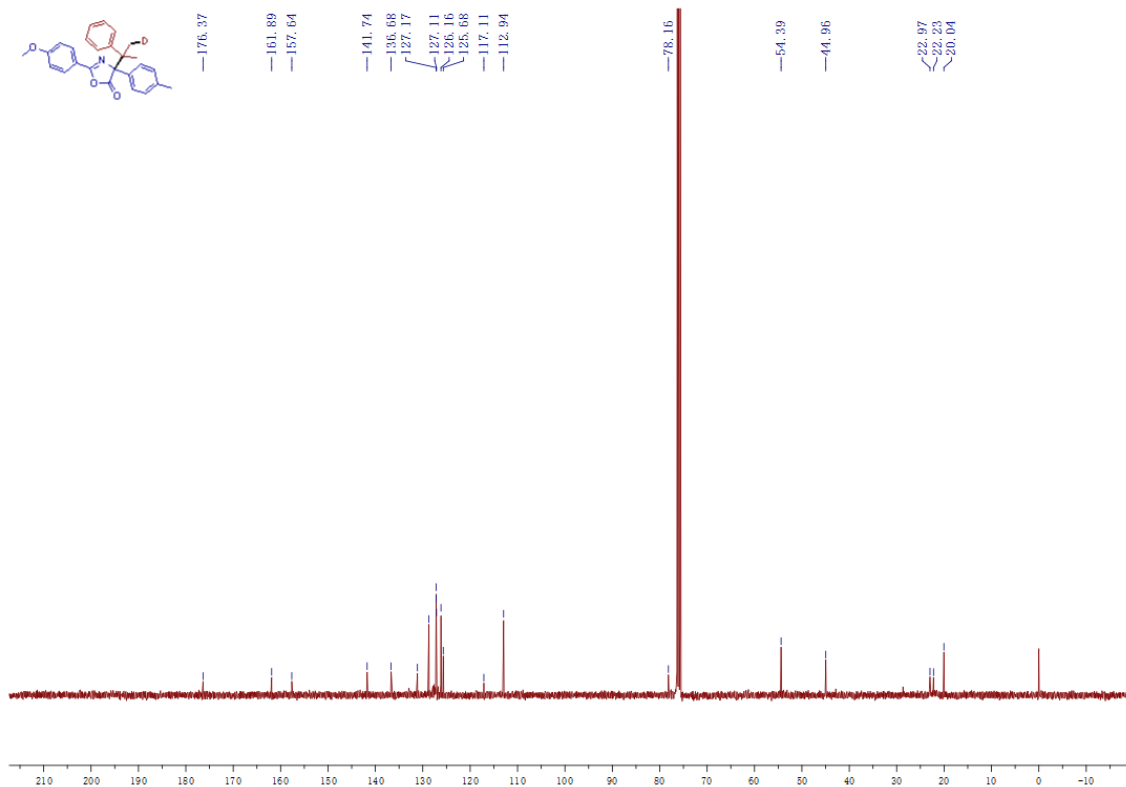
¹³C NMR spectrum of (Z)-2-(4-methoxyphenyl)-4-phenyl-4-(3-phenylbut-2-en-1-yl-2-d)oxazol-5(4H)-one (30)



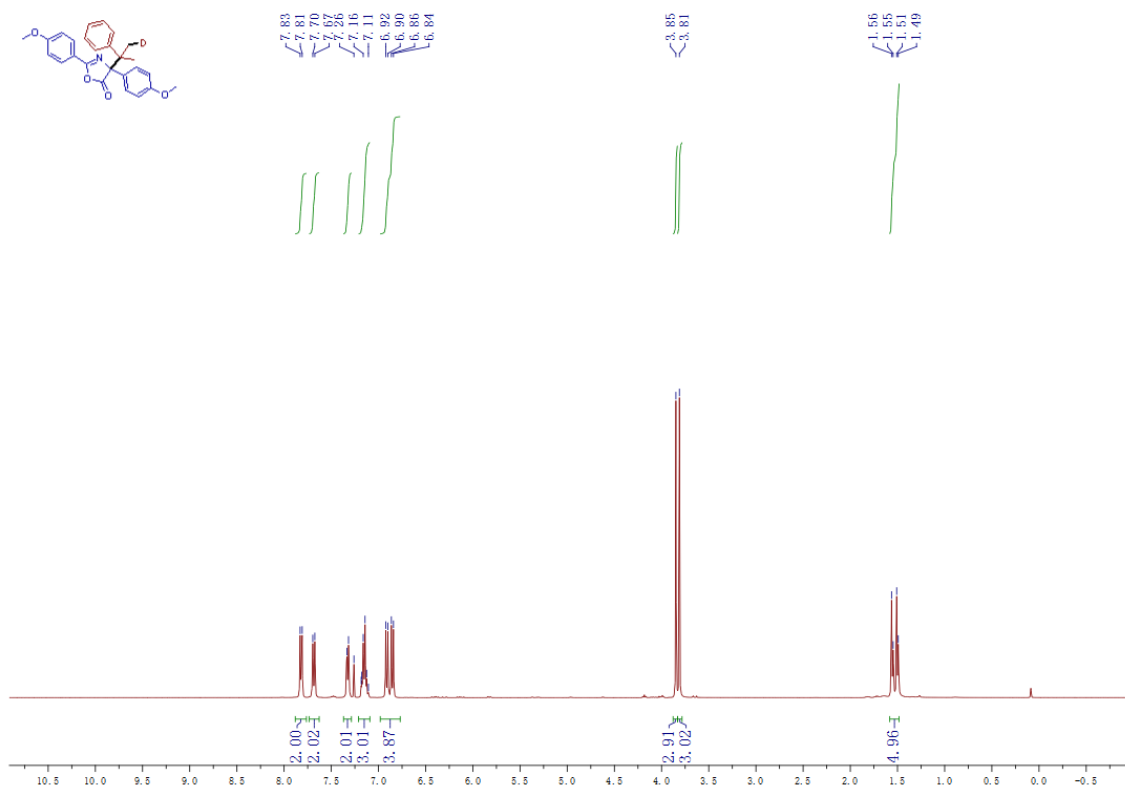
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)-4-(p-tolyl)oxazol-5(4H)-one (31)



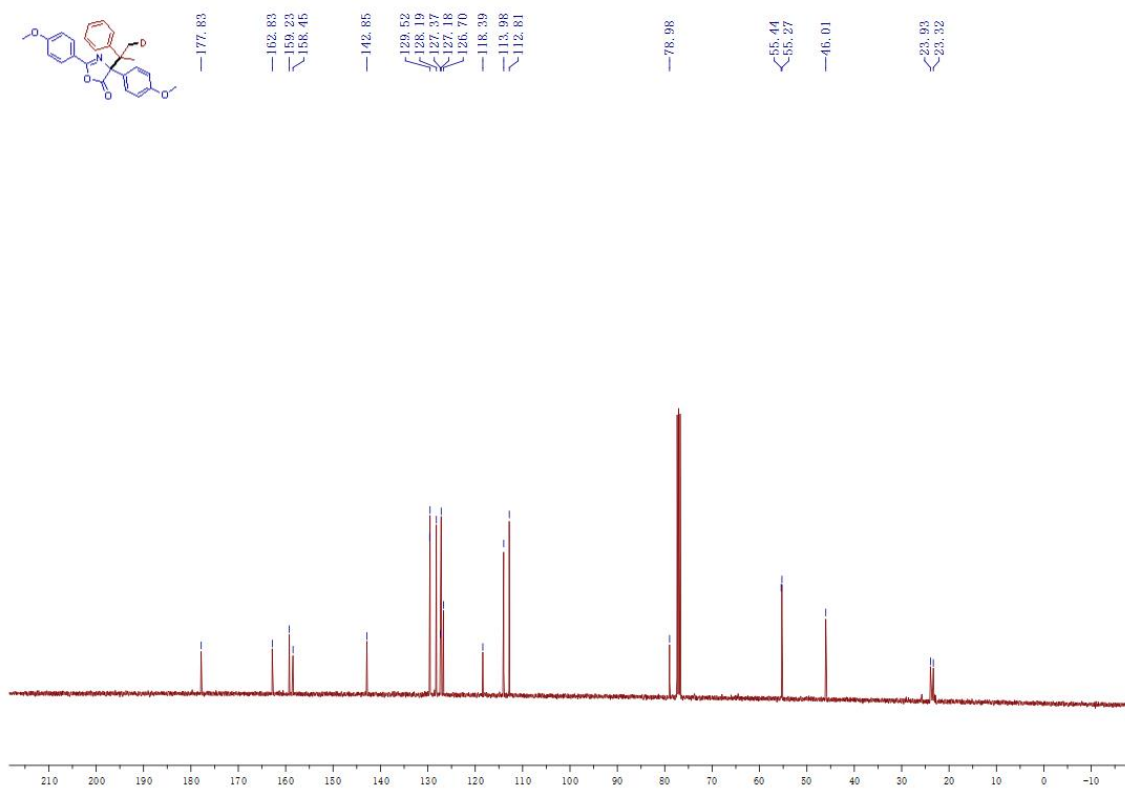
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)-4-(p-tolyl)oxazol-5(4H)-one (31)



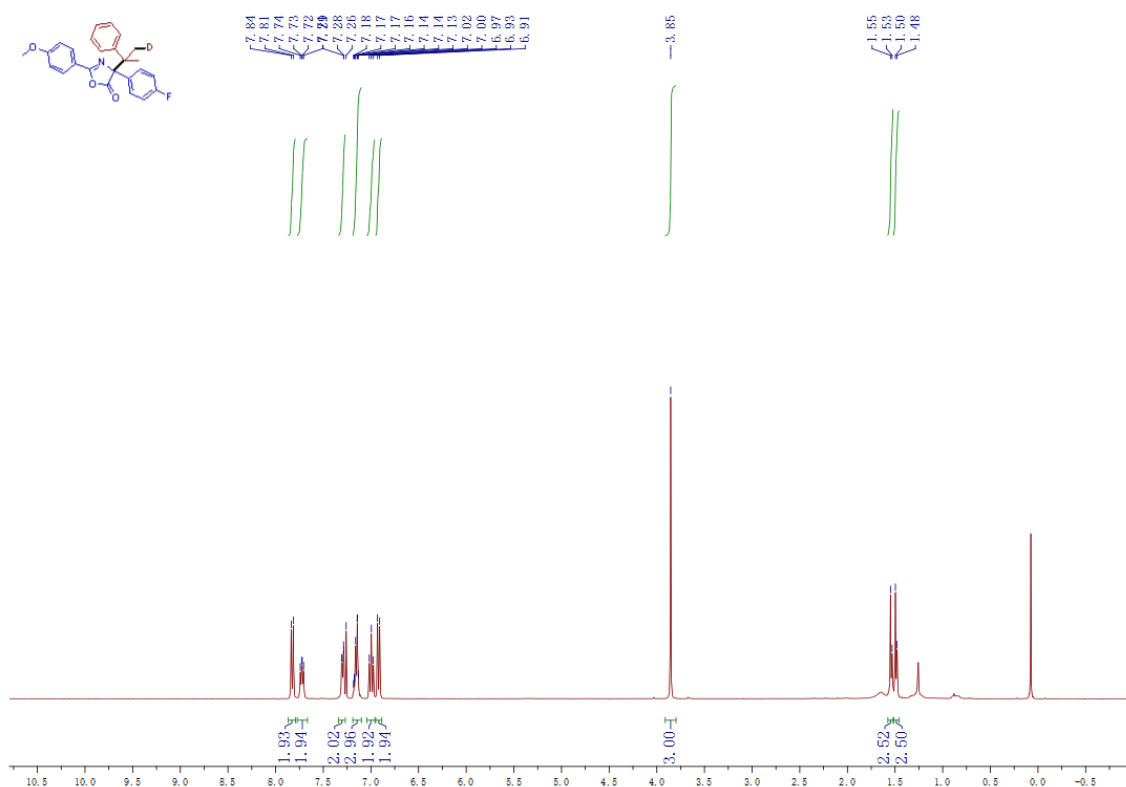
¹H NMR spectrum of 2,4-bis(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (32)



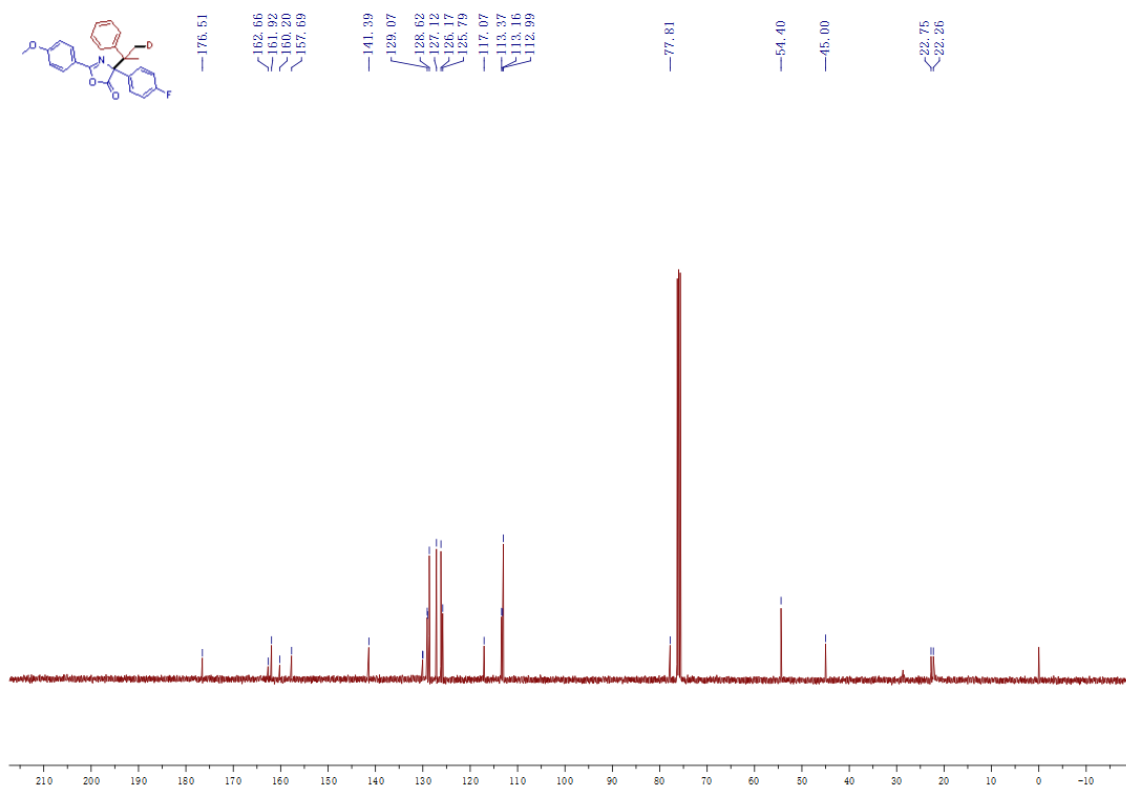
¹³C NMR spectrum of 2,4-bis(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (32)



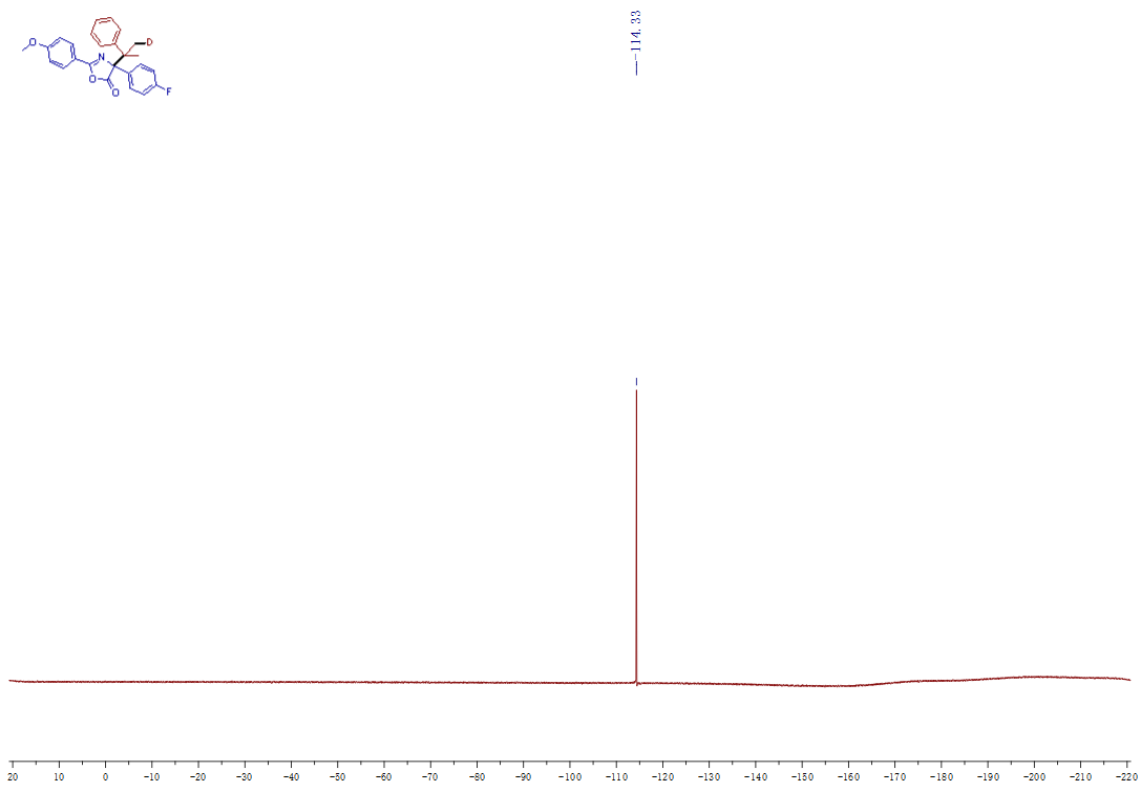
¹H NMR spectrum of 4-(4-fluorophenyl)-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (33)



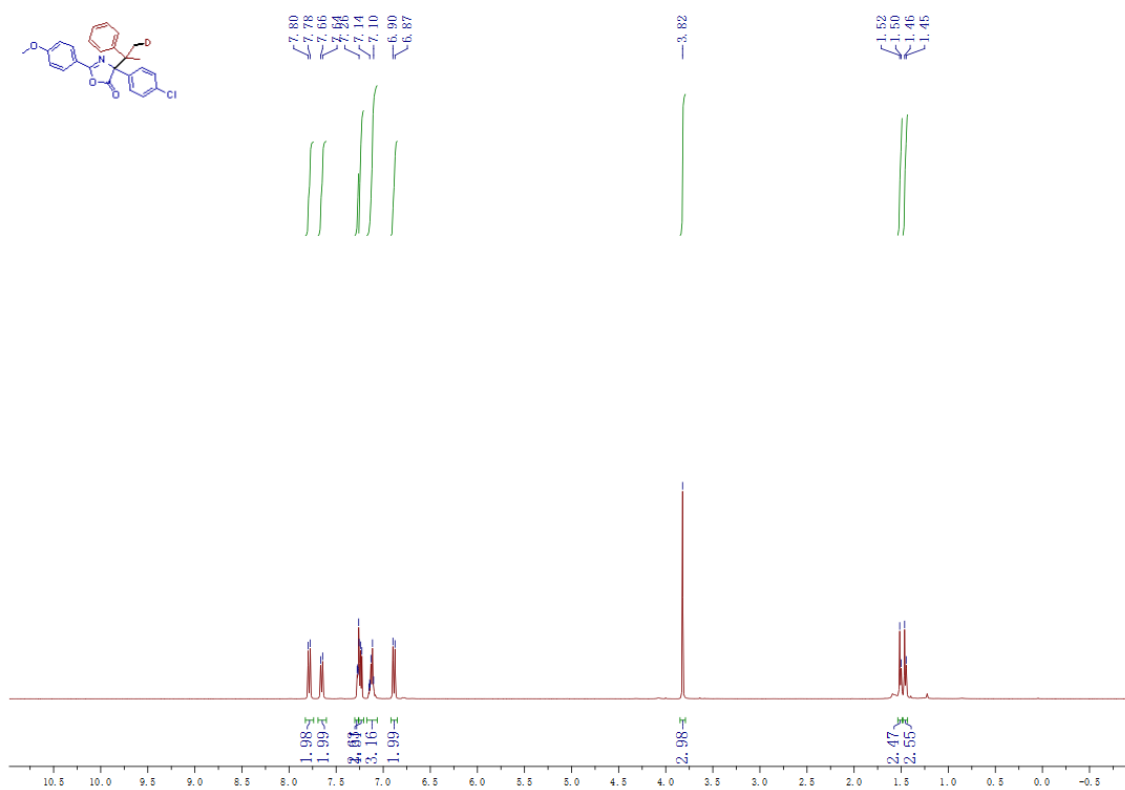
¹³C NMR spectrum of 4-(4-fluorophenyl)-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (33)



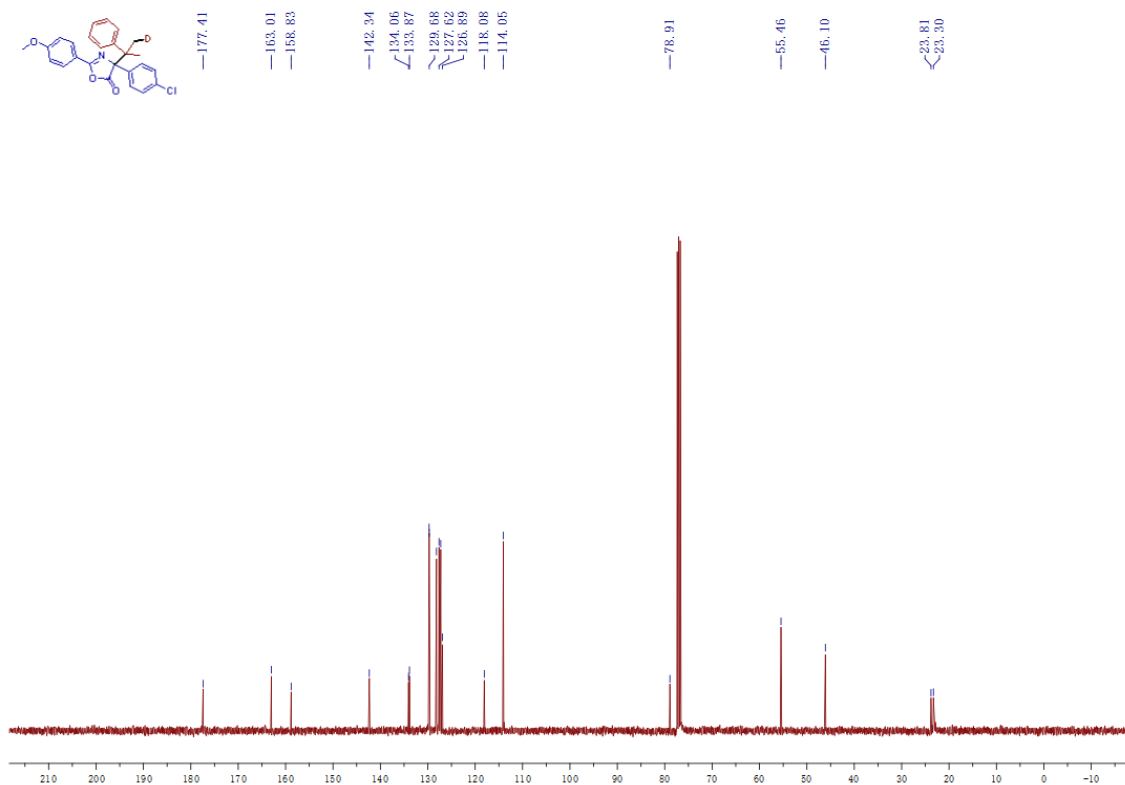
¹⁹F NMR spectrum of 4-(4-fluorophenyl)-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (33)



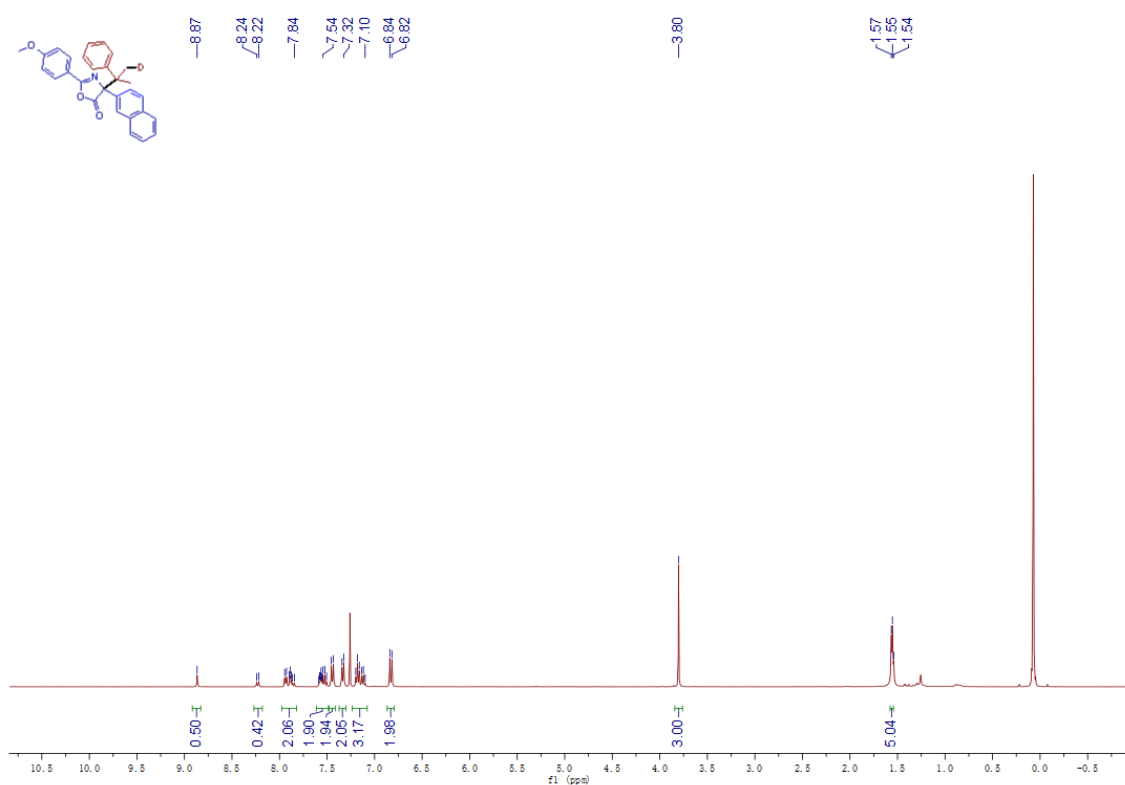
¹H NMR spectrum of 4-(4-chlorophenyl)-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (34)



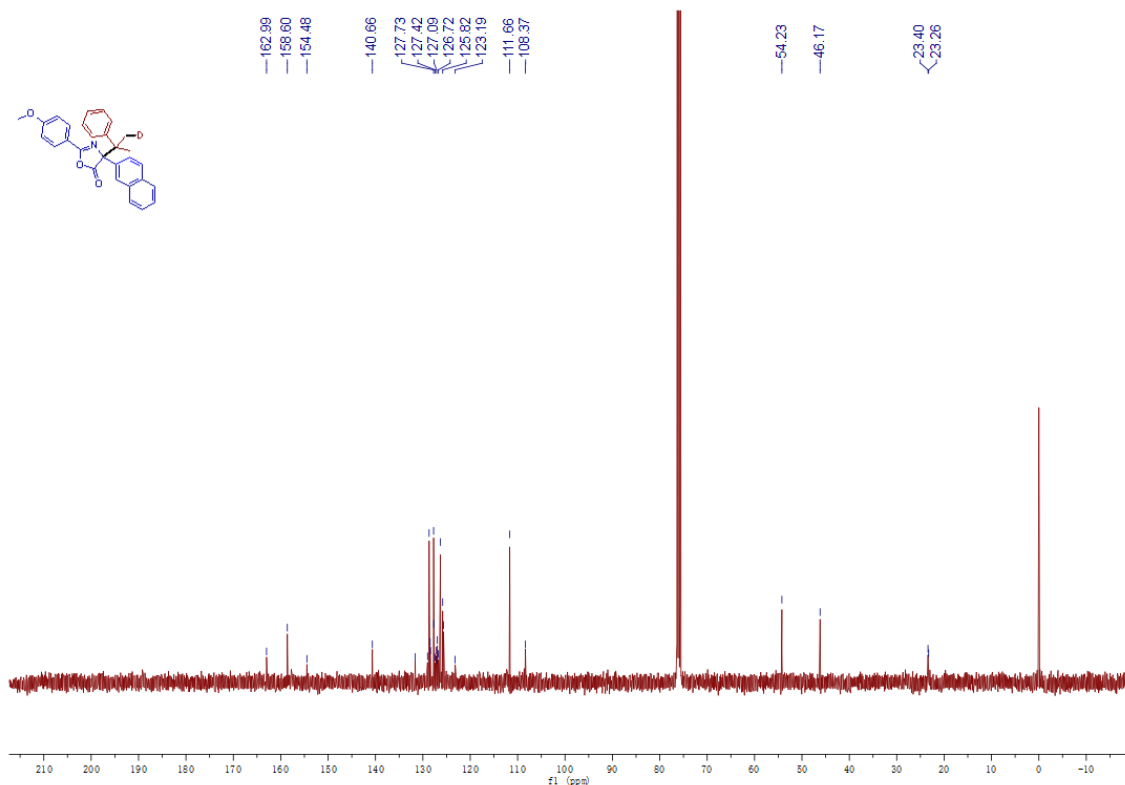
¹³C NMR spectrum of 4-(4-chlorophenyl)-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (34)



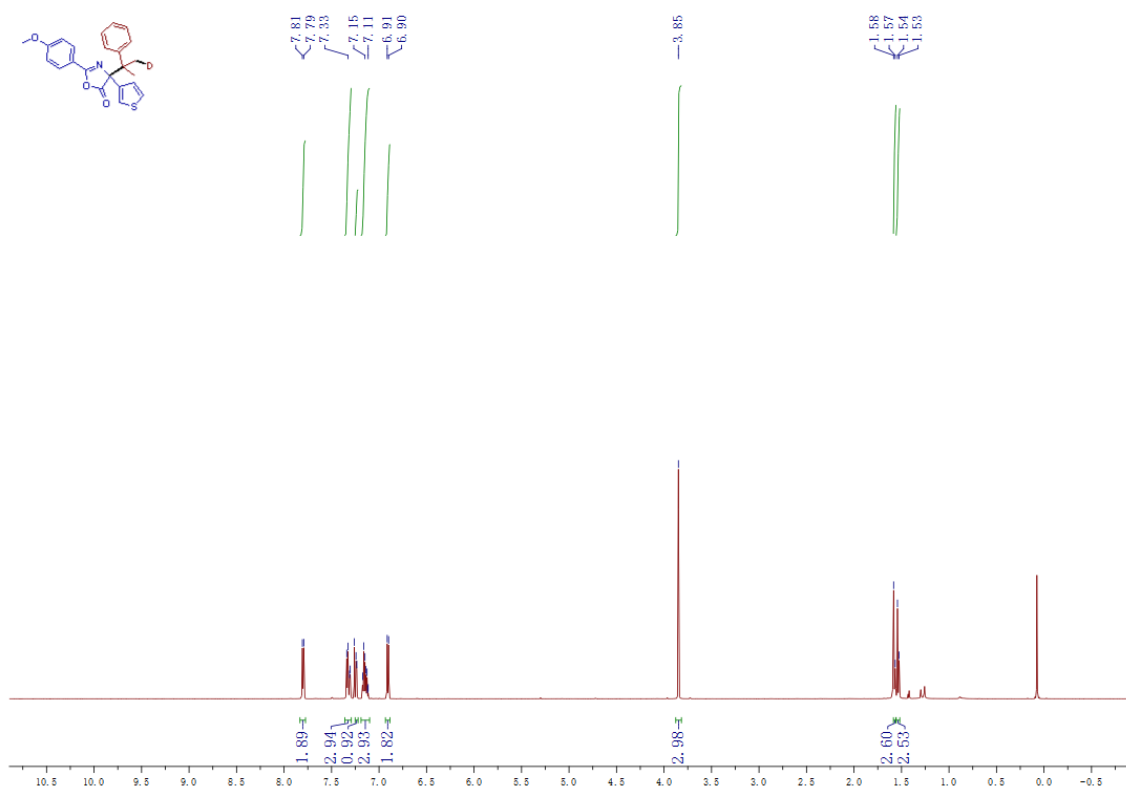
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(naphthalen-2-yl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (35)



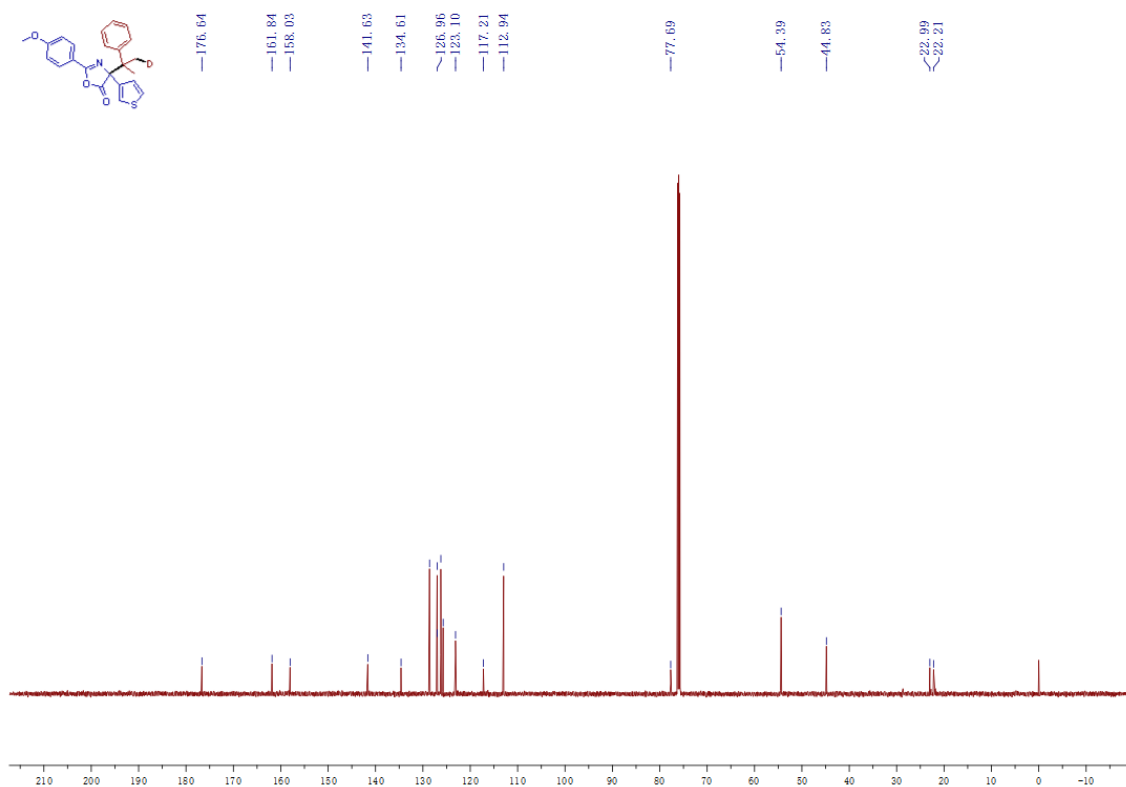
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-(naphthalen-2-yl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (35)



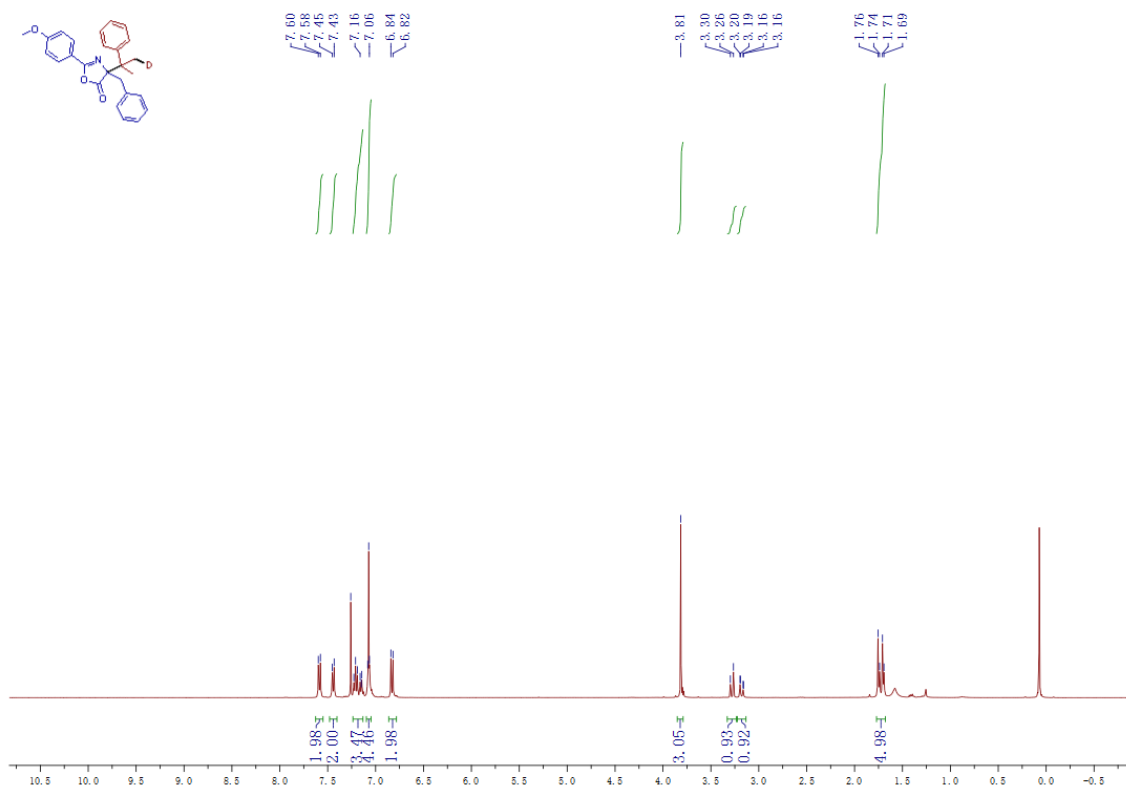
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)-4-(thiophen-3-yl)oxazol-5(4H)-one (36)



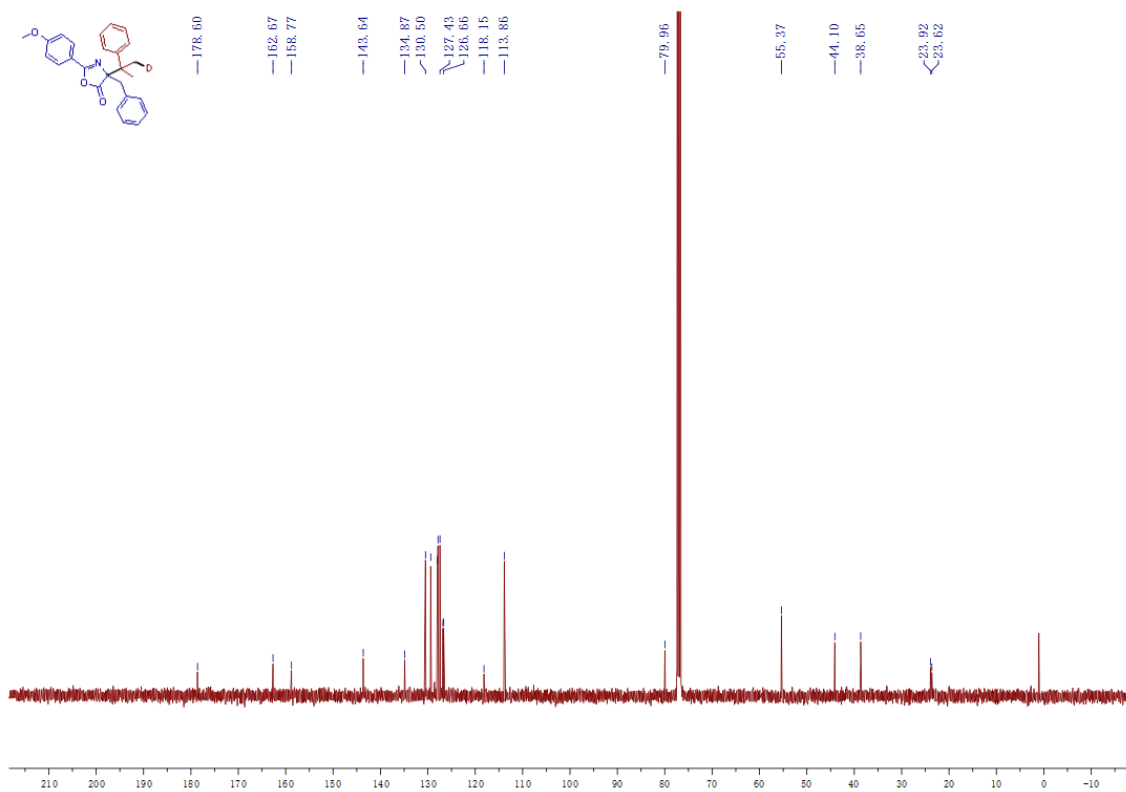
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)-4-(thiophen-3-yl)oxazol-5(4H)-one (36)



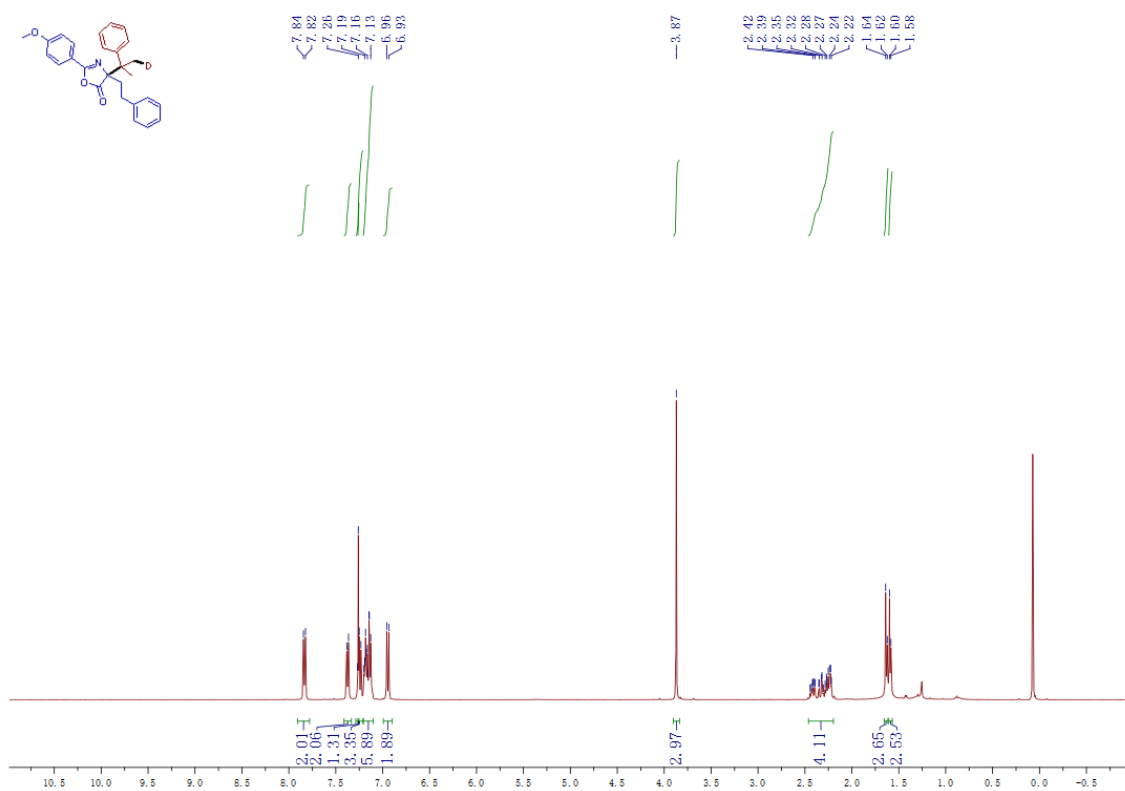
¹H NMR spectrum of 4-benzyl-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (37)



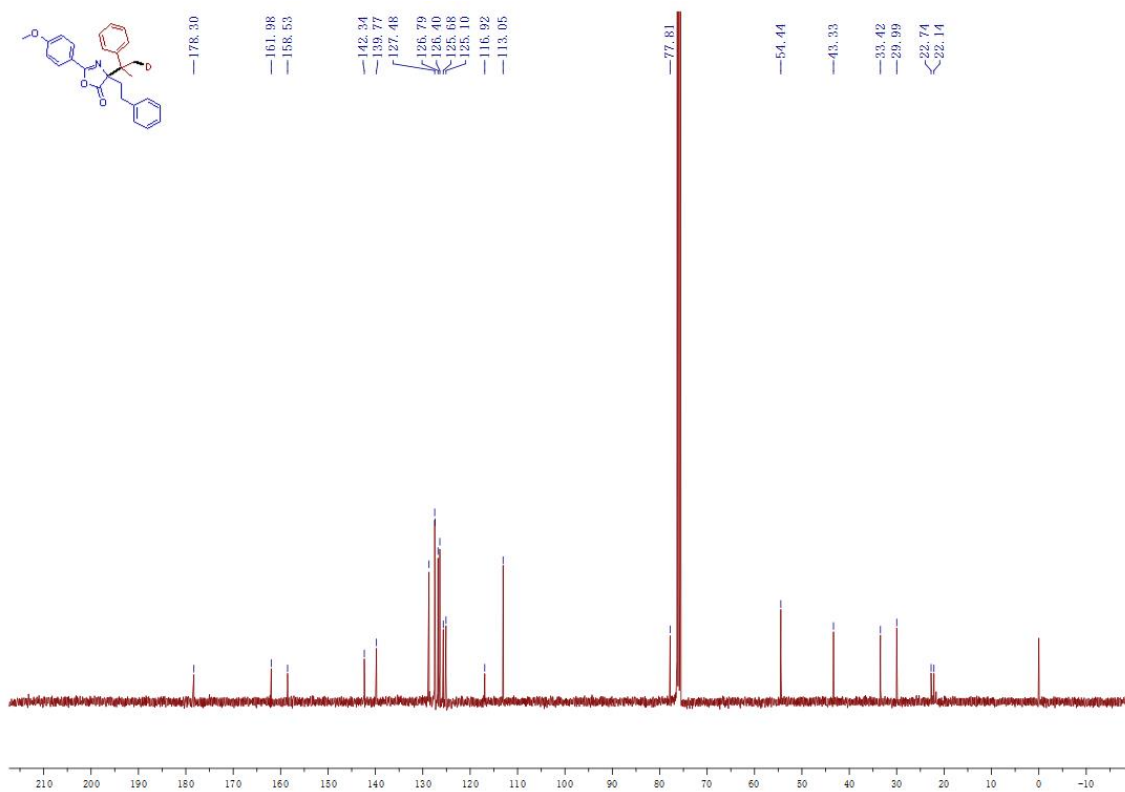
¹³C NMR spectrum of 4-benzyl-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (37)



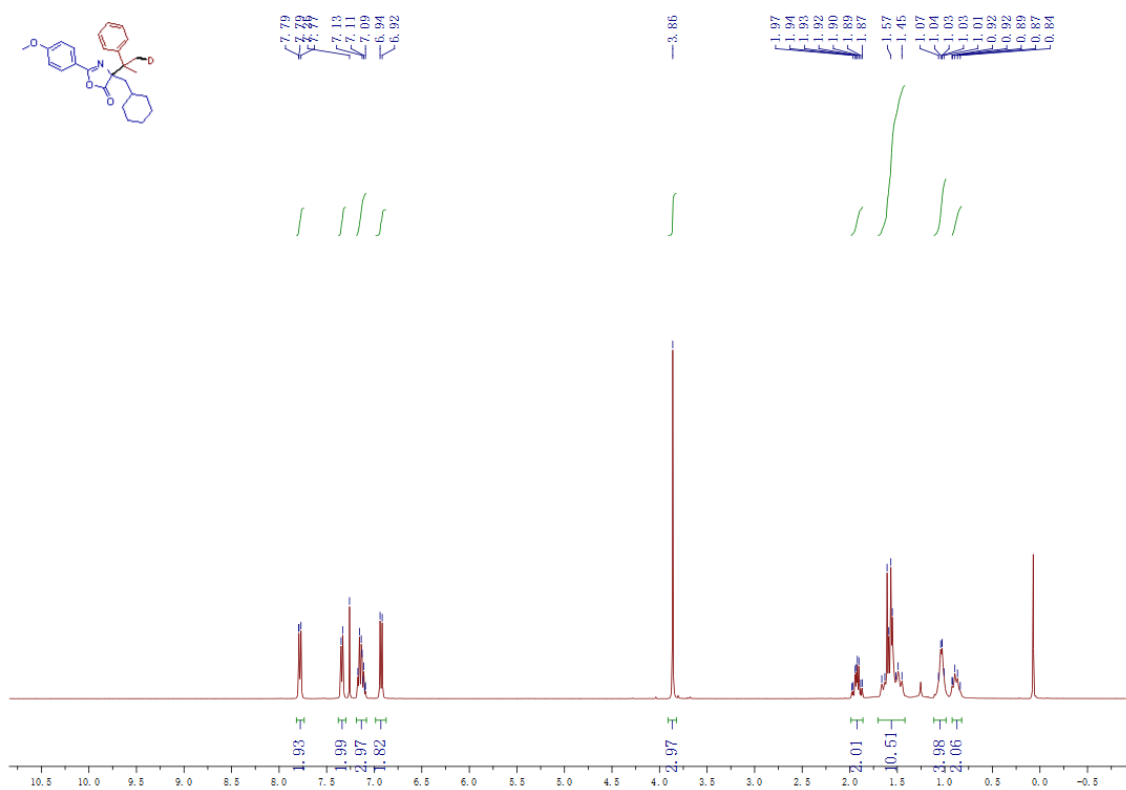
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-phenethyl-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (38)



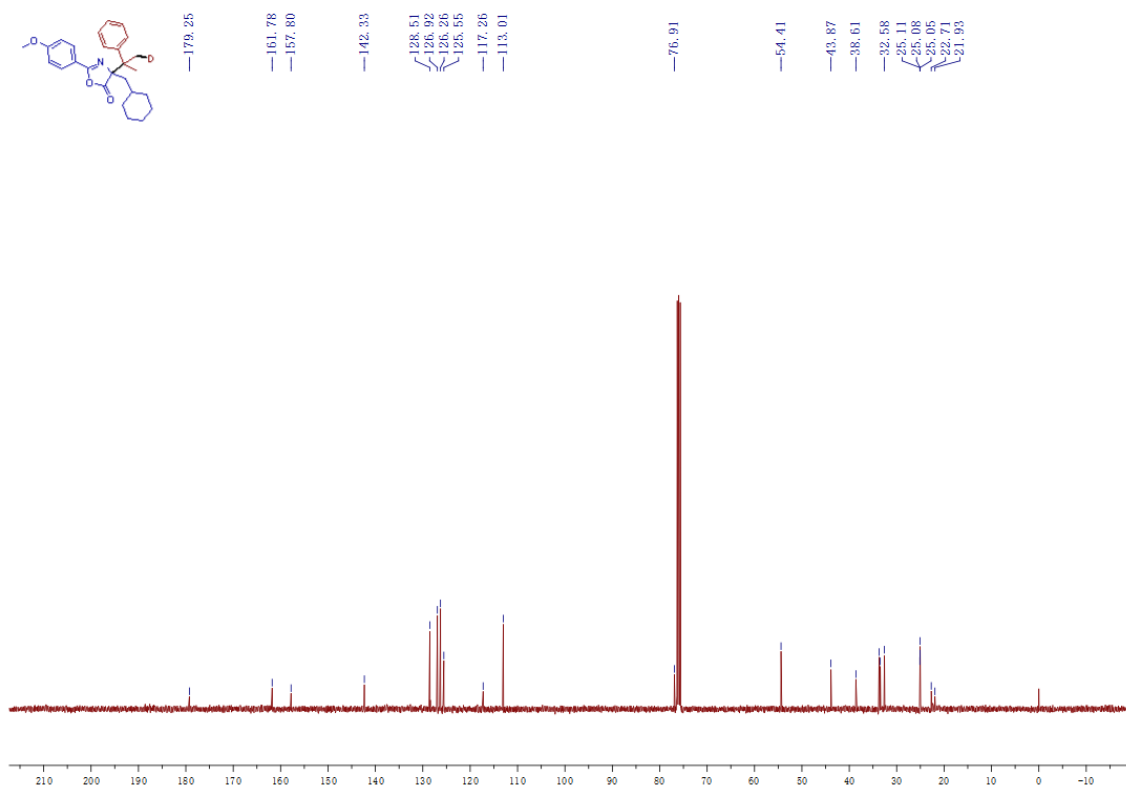
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-phenethyl-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (38)



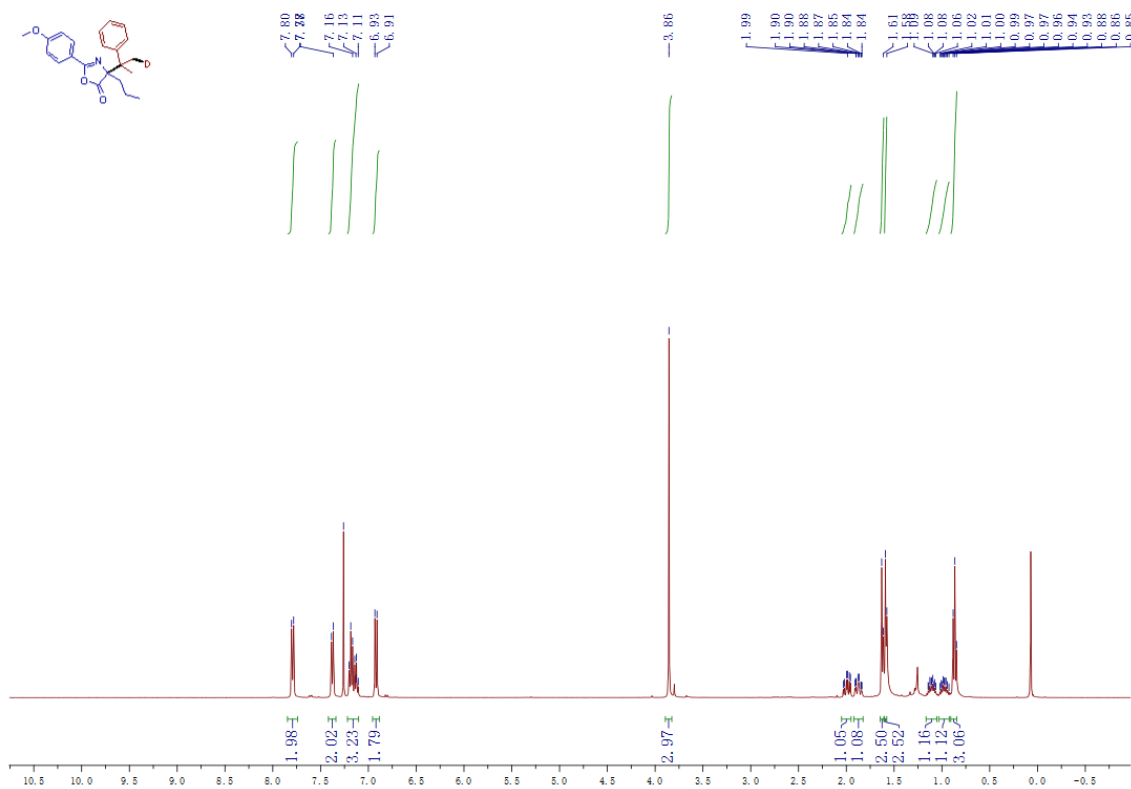
¹H NMR spectrum of 4-(cyclohexylmethyl)-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (39)



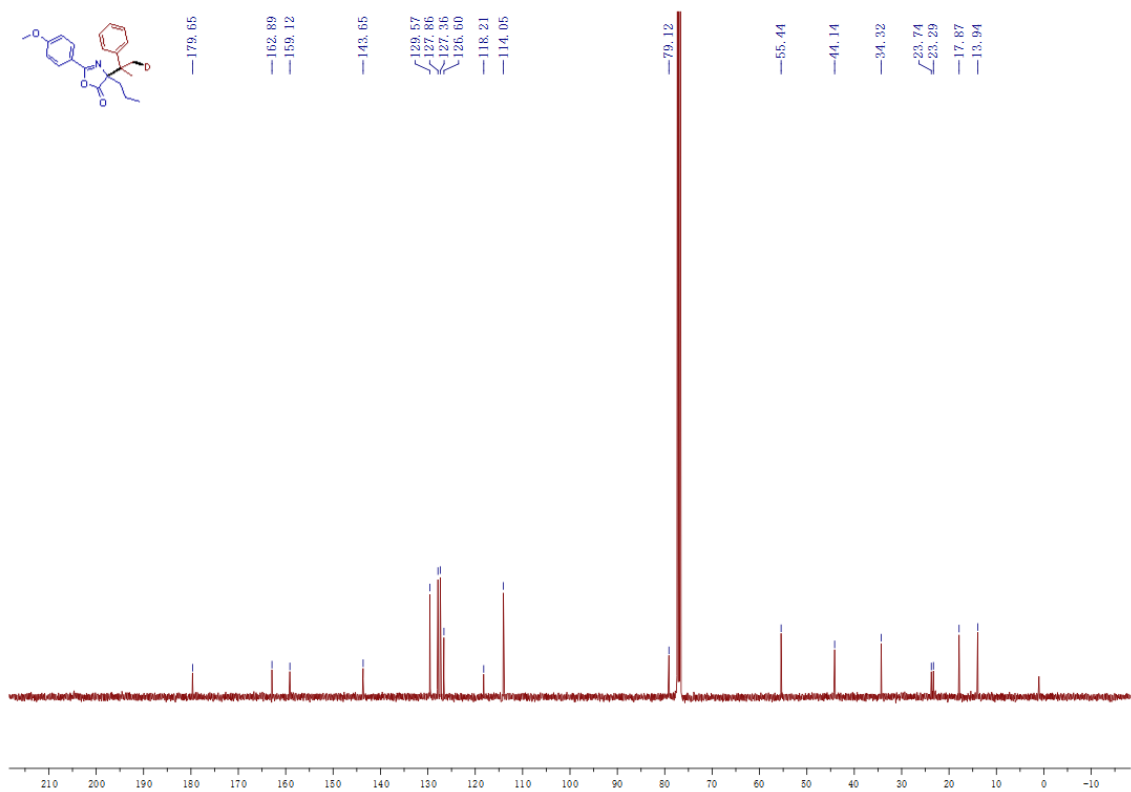
¹³C NMR spectrum of 4-(cyclohexylmethyl)-2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)oxazol-5(4H)-one (39)



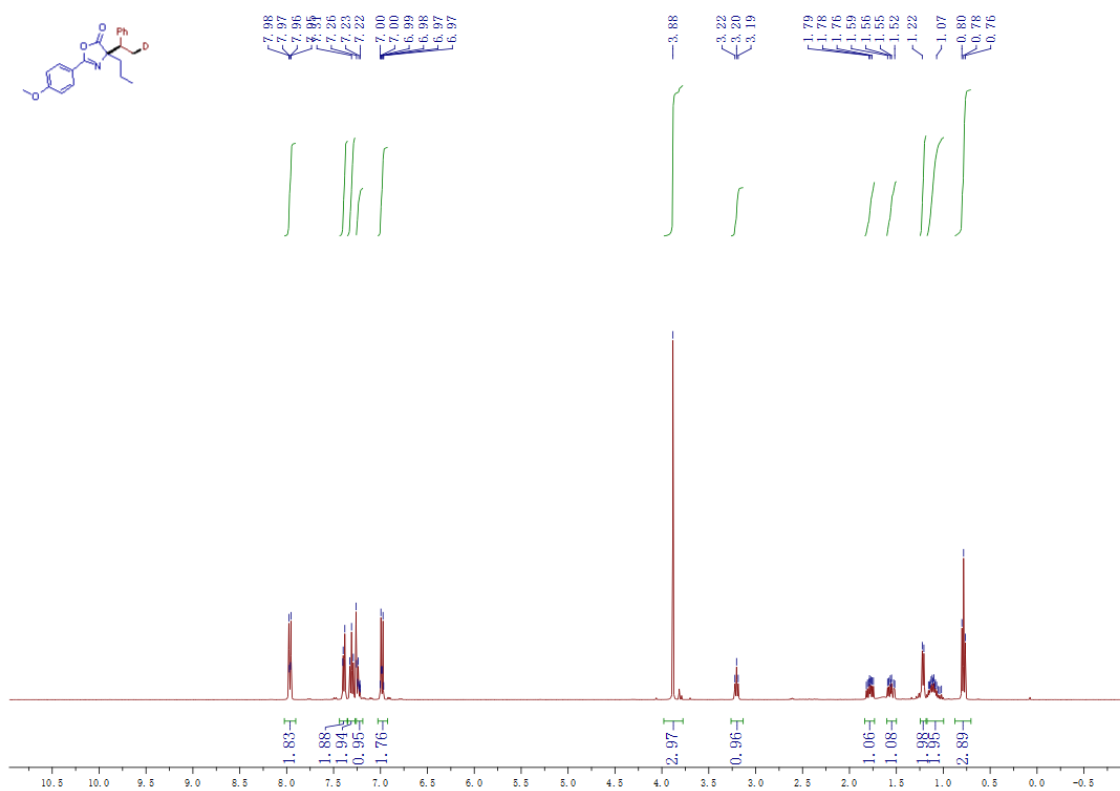
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)-4-propyloxazol-5(4H)-one (40)



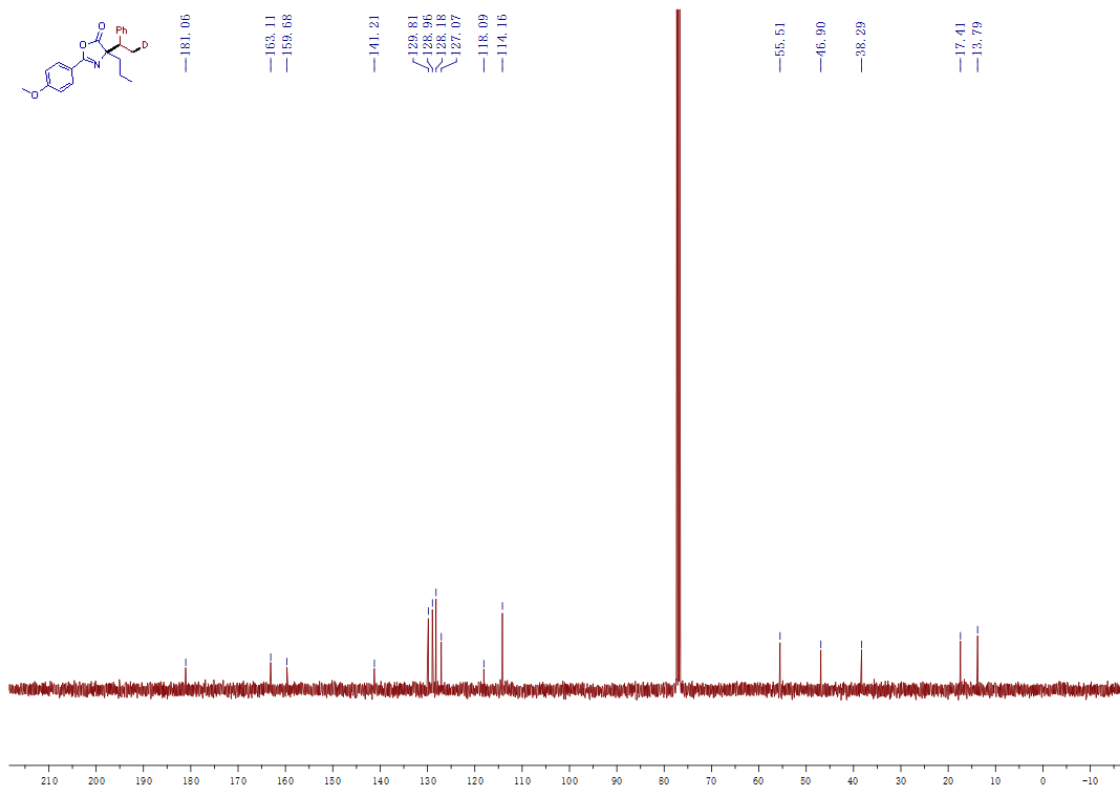
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-(2-phenylpropan-2-yl-1-d)-4-propyloxazol-5(4H)-one (40)



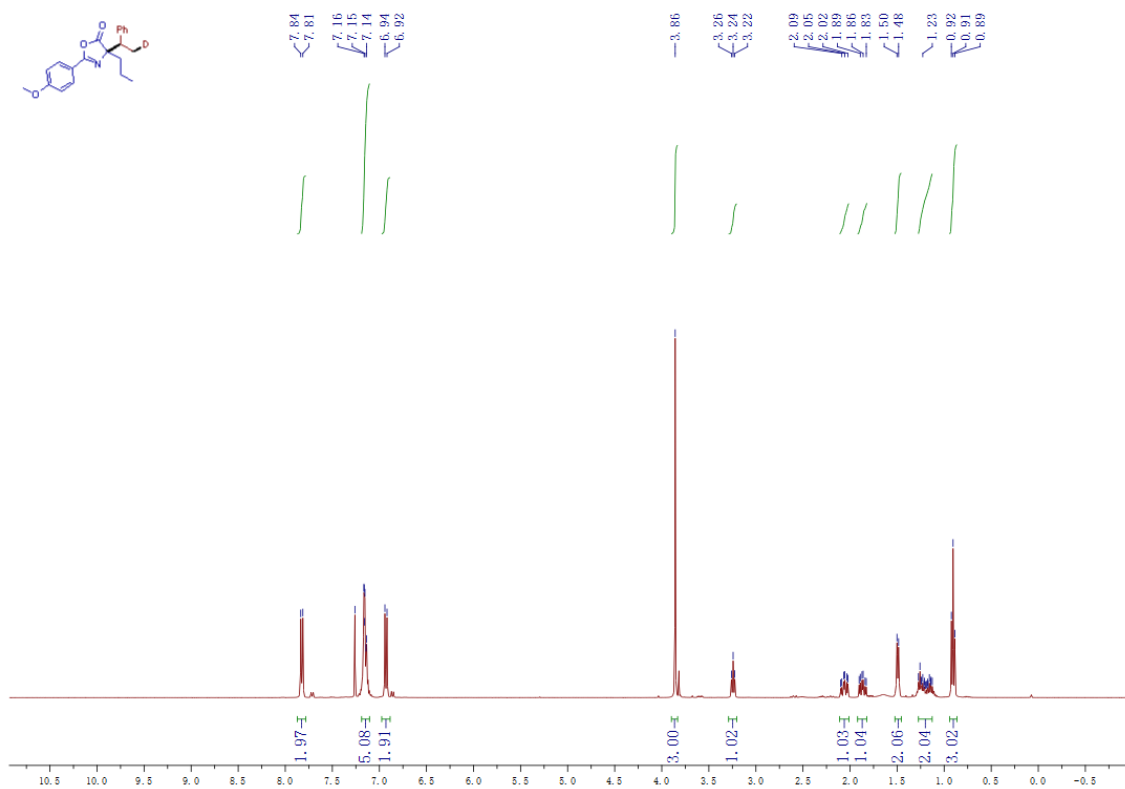
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(1-phenylethyl-2-d)-4-propyloxazol-5(4H)-one (41)



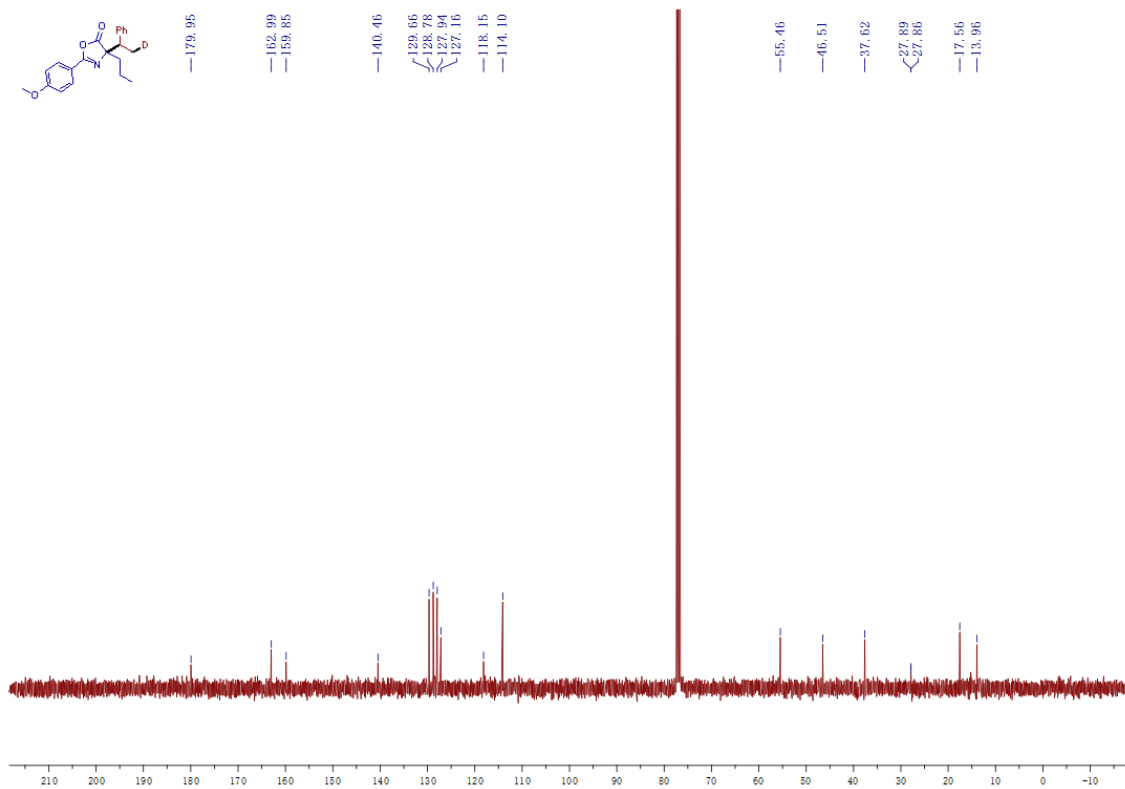
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-(1-phenylethyl-2-d)-4-propyloxazol-5(4H)-one (41)



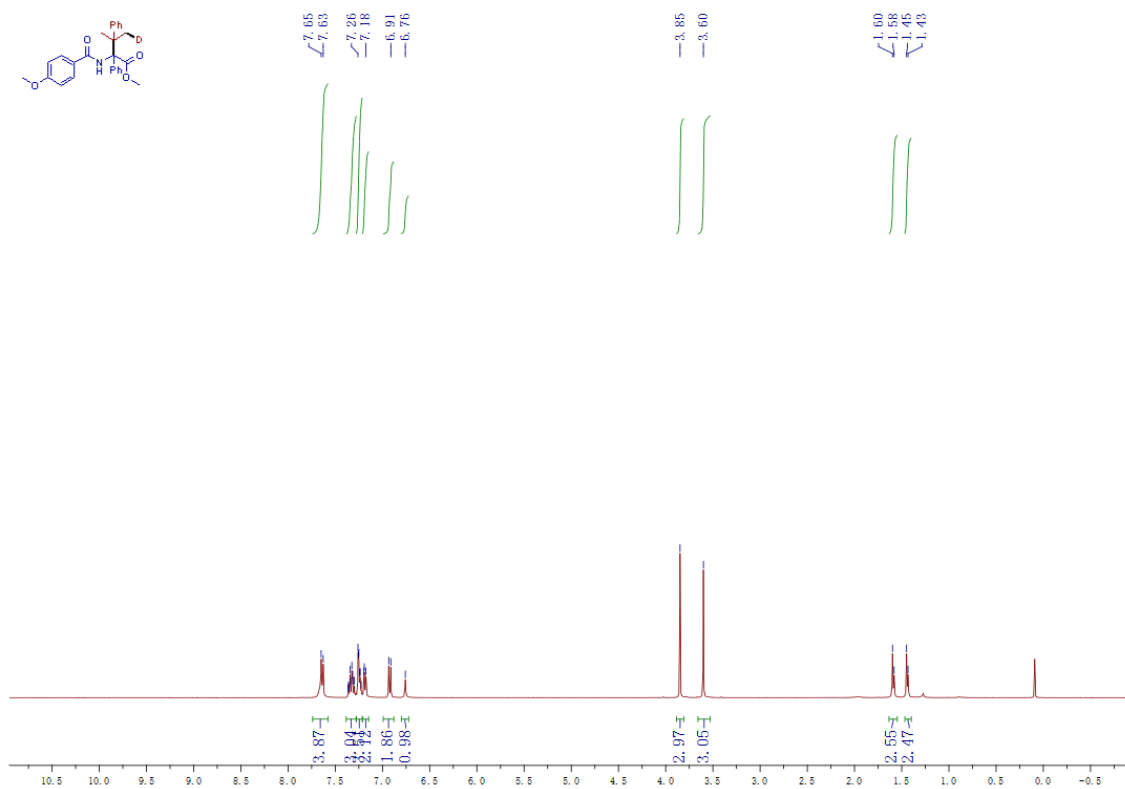
¹H NMR spectrum of 2-(4-methoxyphenyl)-4-(1-phenylethyl-2-d)-4-propyloxazol-5(4H)-one (41)



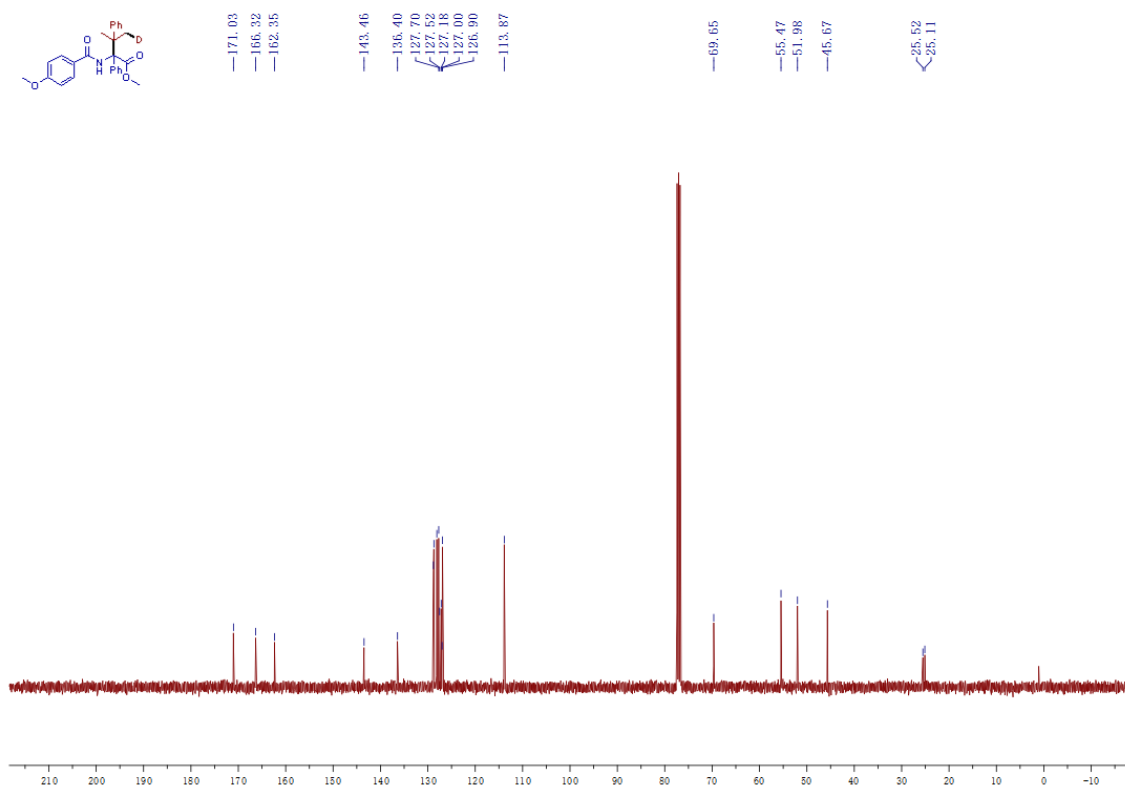
¹³C NMR spectrum of 2-(4-methoxyphenyl)-4-(1-phenylethyl-2-d)-4-propyloxazol-5(4H)-one (41)



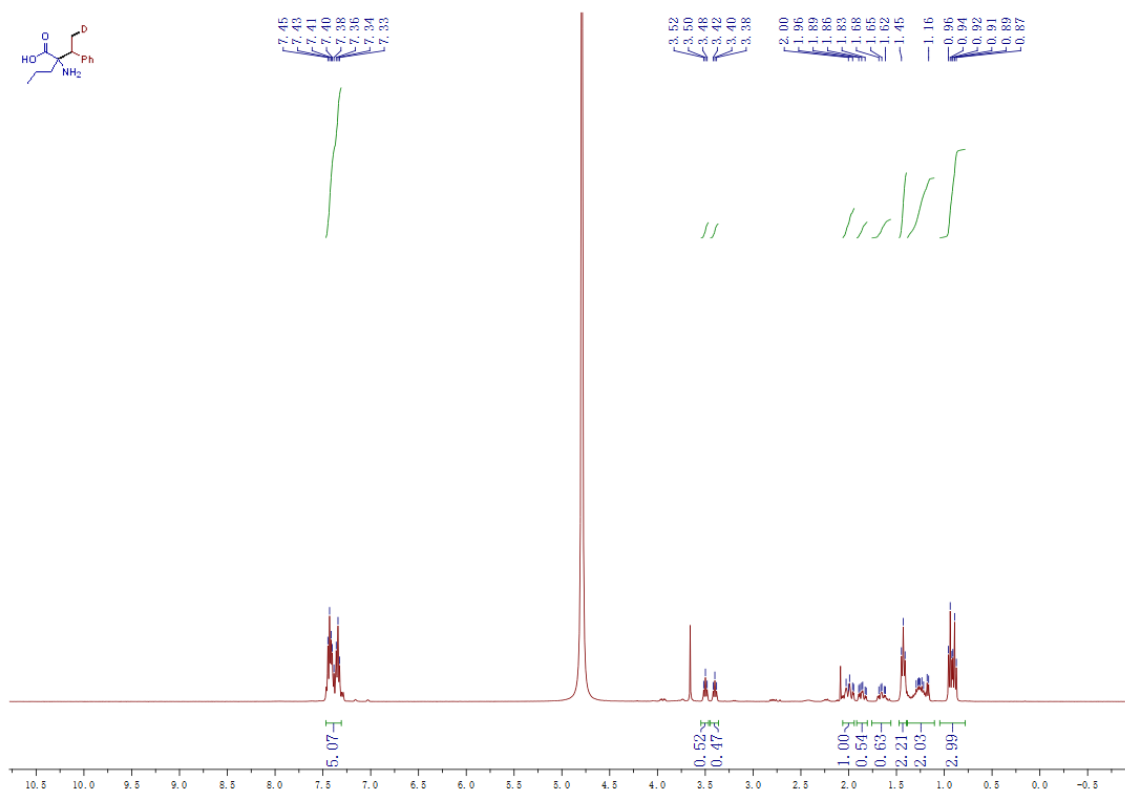
¹H NMR spectrum of methyl 2-(4-methoxybenzamido)-3-methyl-2,3-diphenylbutanoate-4-d (42)



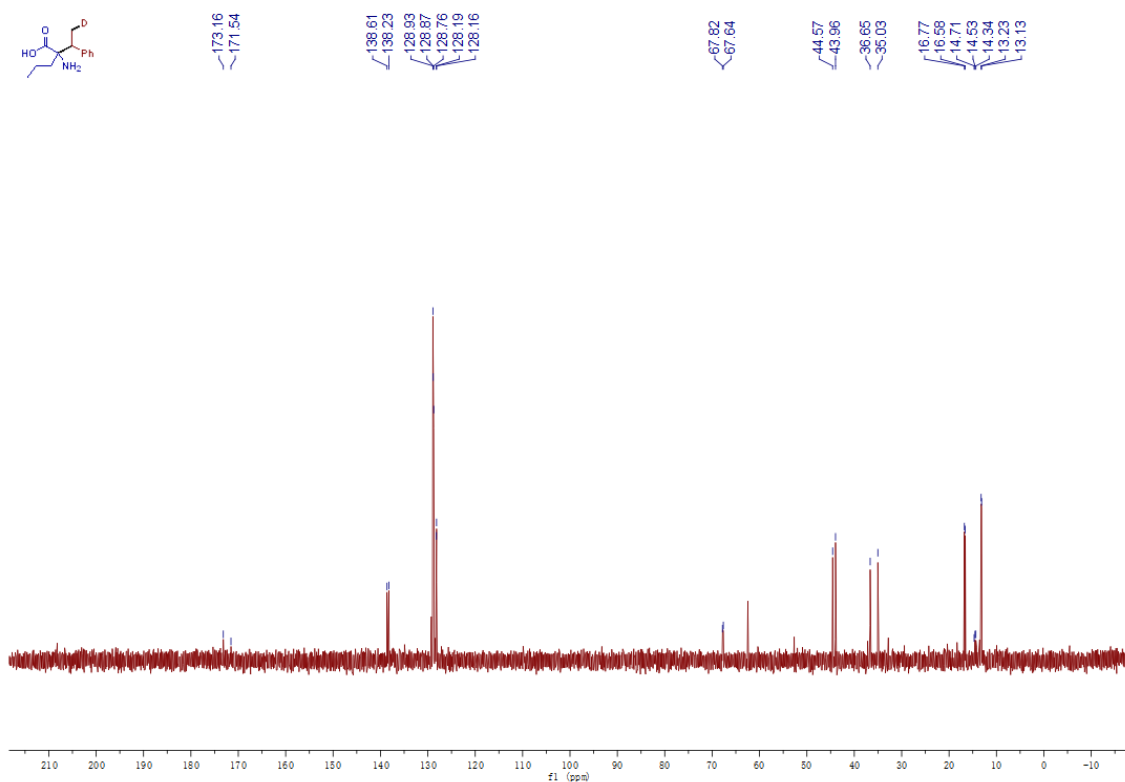
¹³C NMR spectrum of methyl 2-(4-methoxybenzamido)-3-methyl-2,3-diphenylbutanoate-4-d (42)



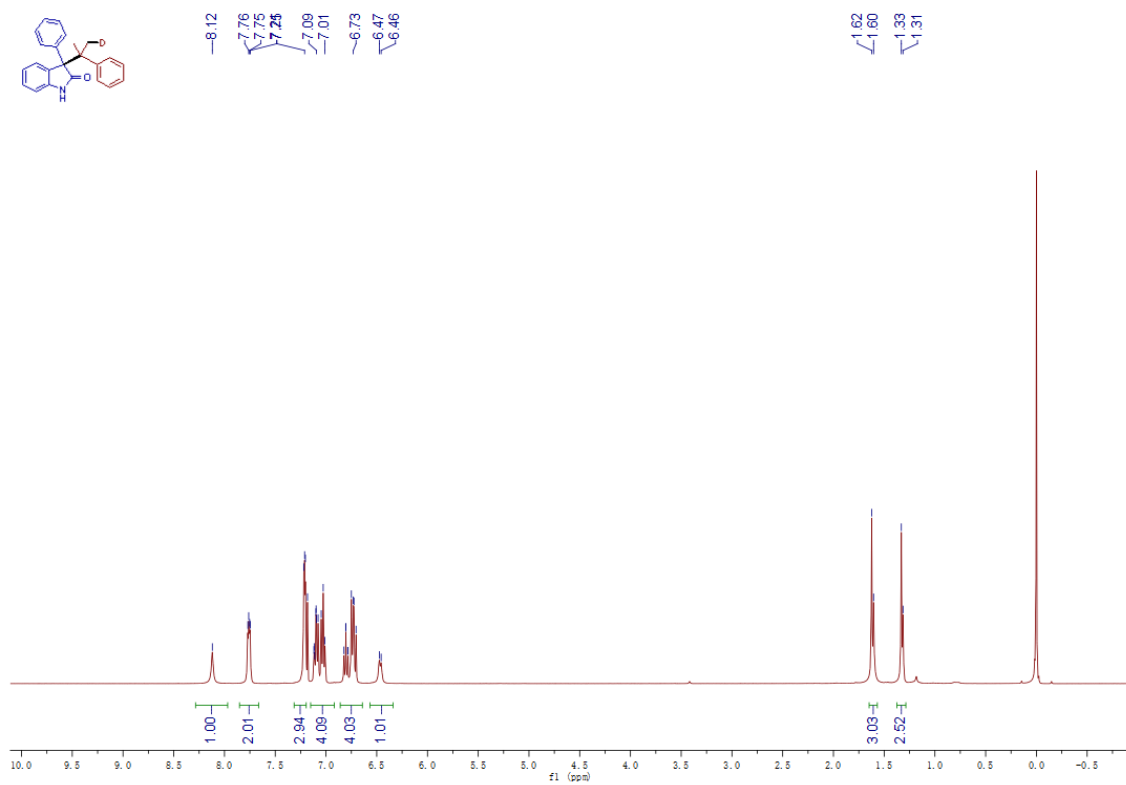
¹H NMR spectrum of 2-amino-2-(1-phenylethyl-2-d)pentanoic acid (43)



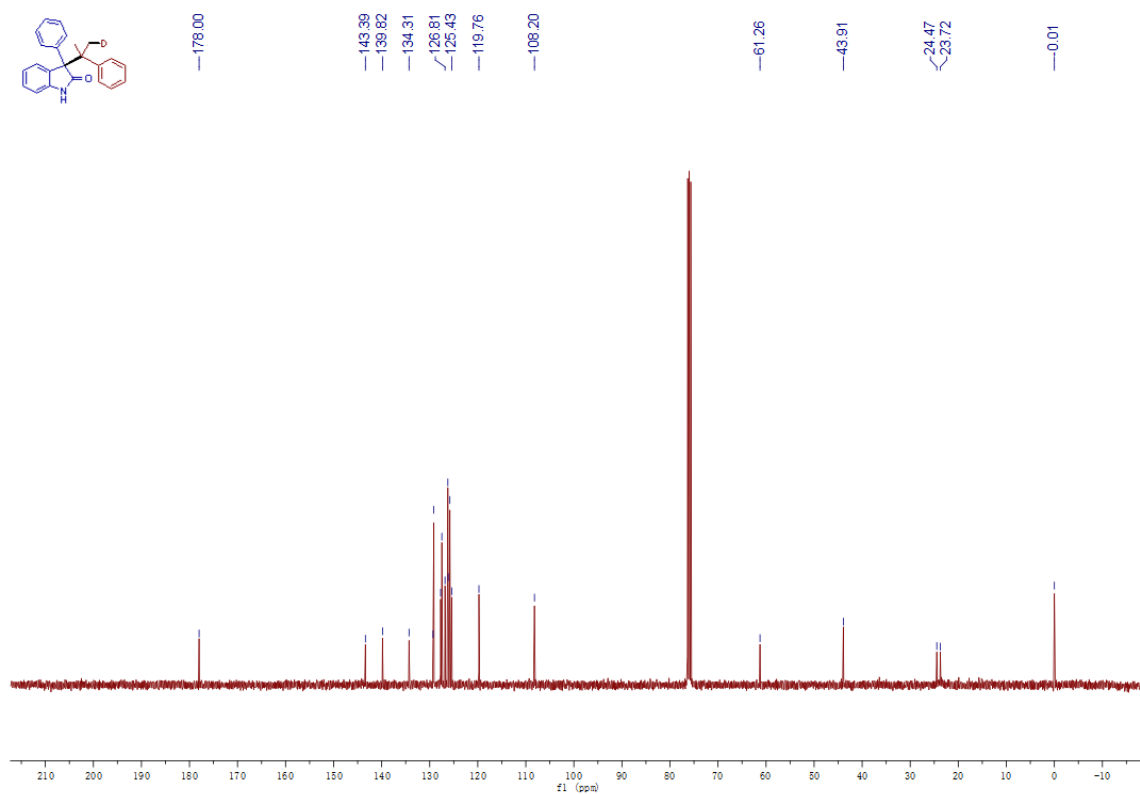
¹³C NMR spectrum of 2-amino-2-(1-phenylethyl-2-d)pentanoic acid (43)



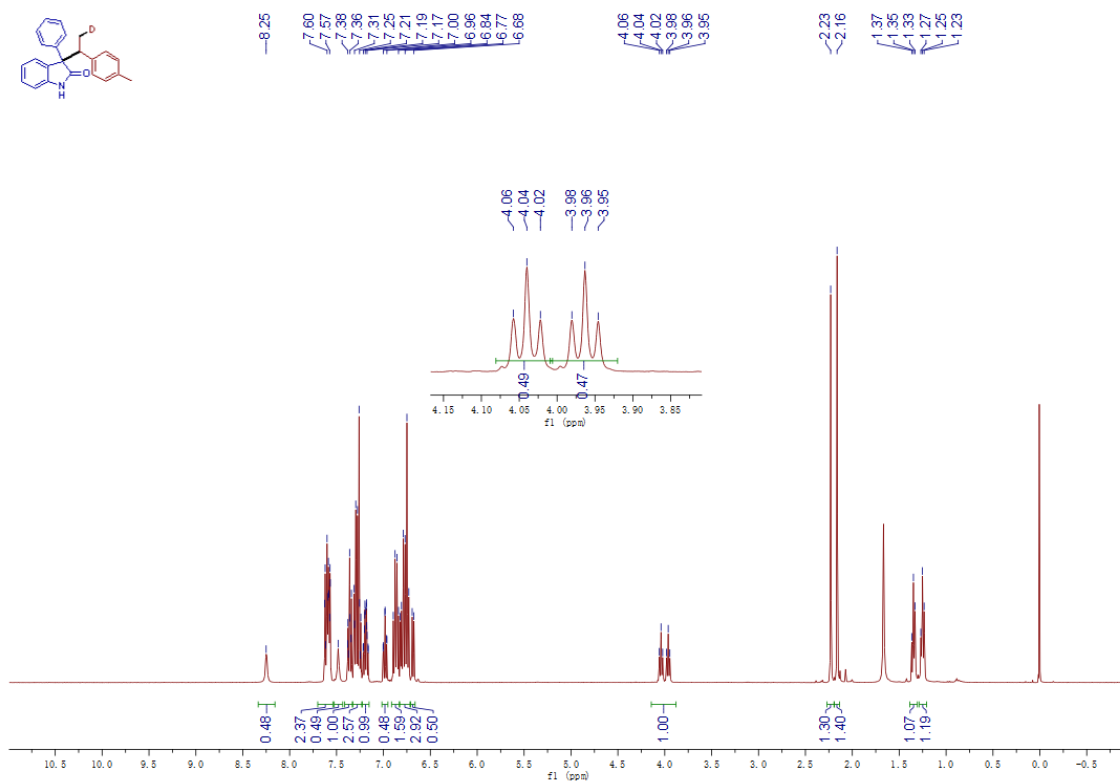
¹H NMR spectrum of 3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (44)



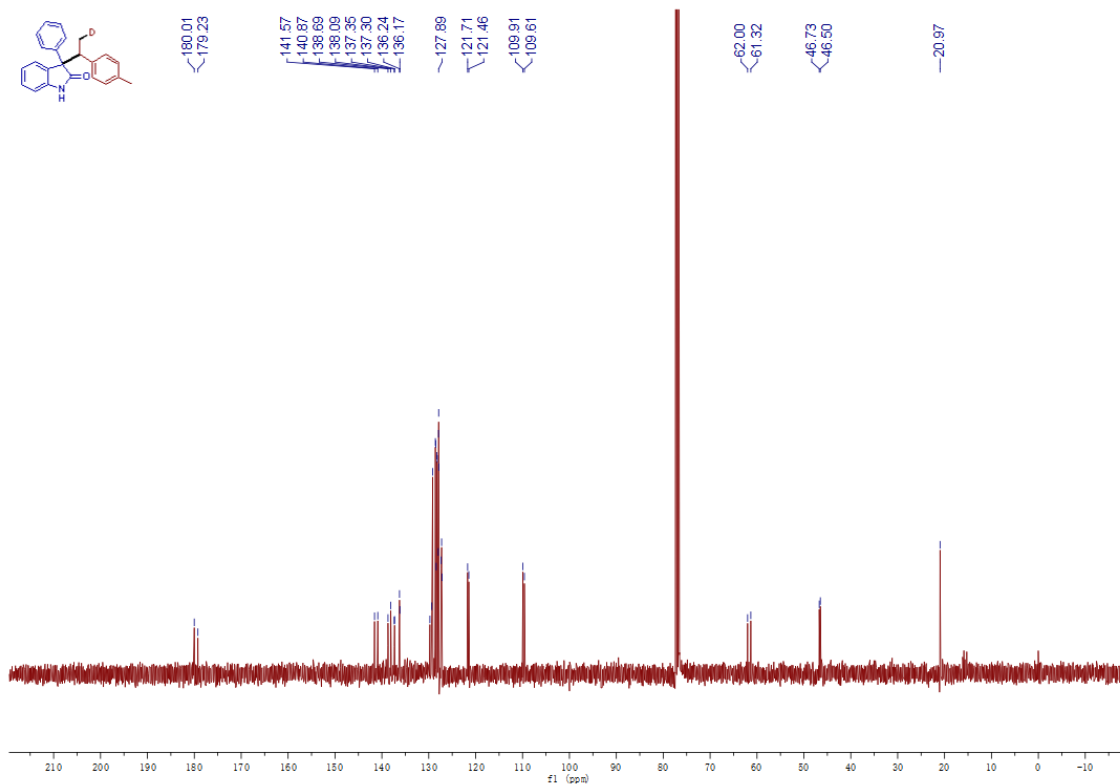
¹³C NMR spectrum of 3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (44)



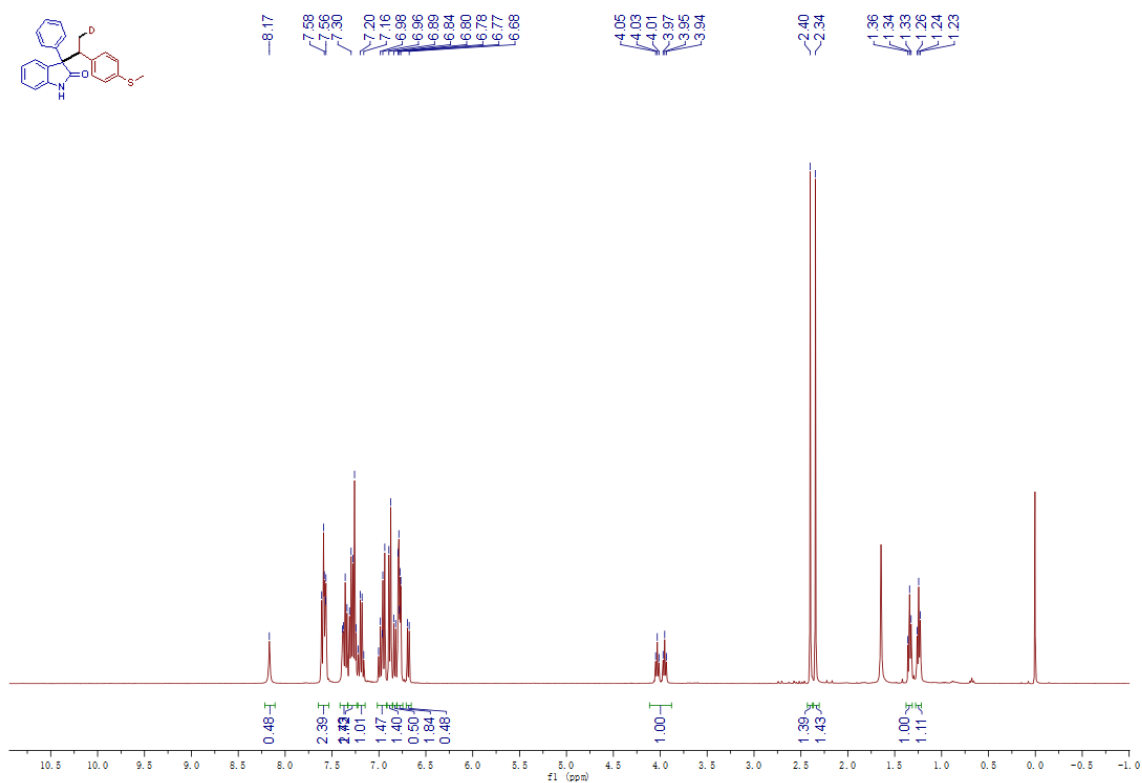
¹H NMR spectrum of 3-phenyl-3-(1-(p-tolyl)ethyl-2-d)indolin-2-one. (45)



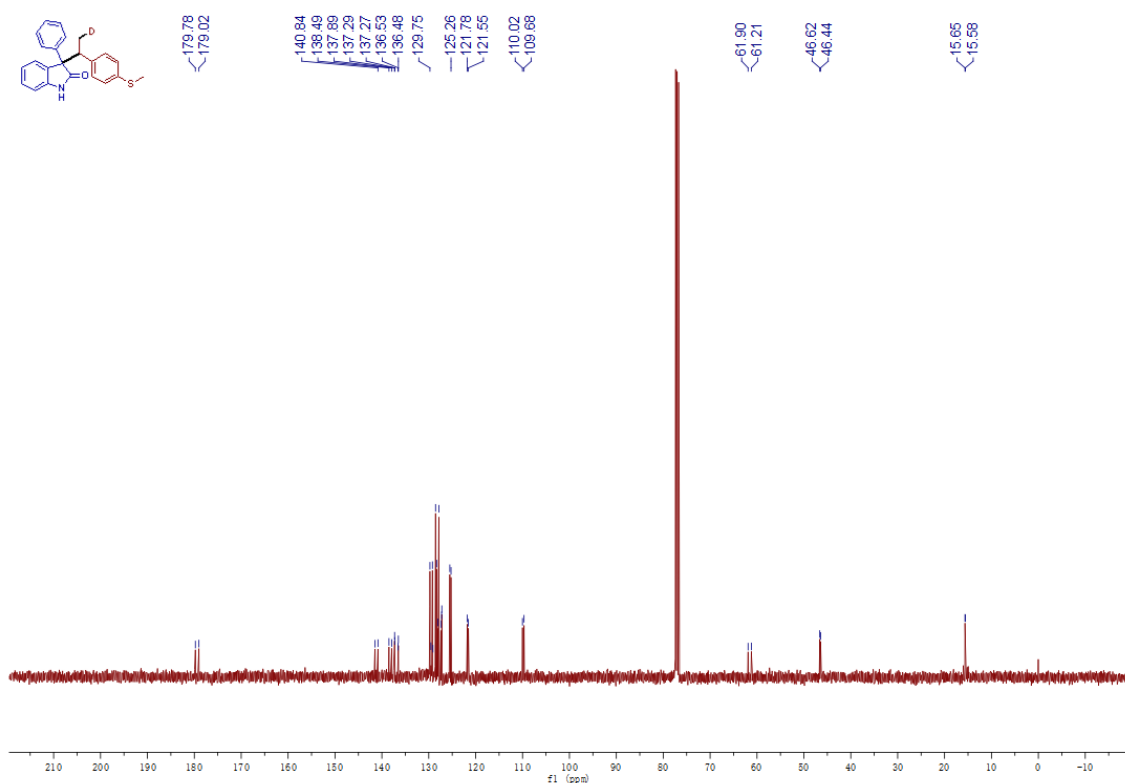
¹³C NMR spectrum of 3-phenyl-3-(1-(p-tolyl)ethyl-2-d)indolin-2-one. (45)



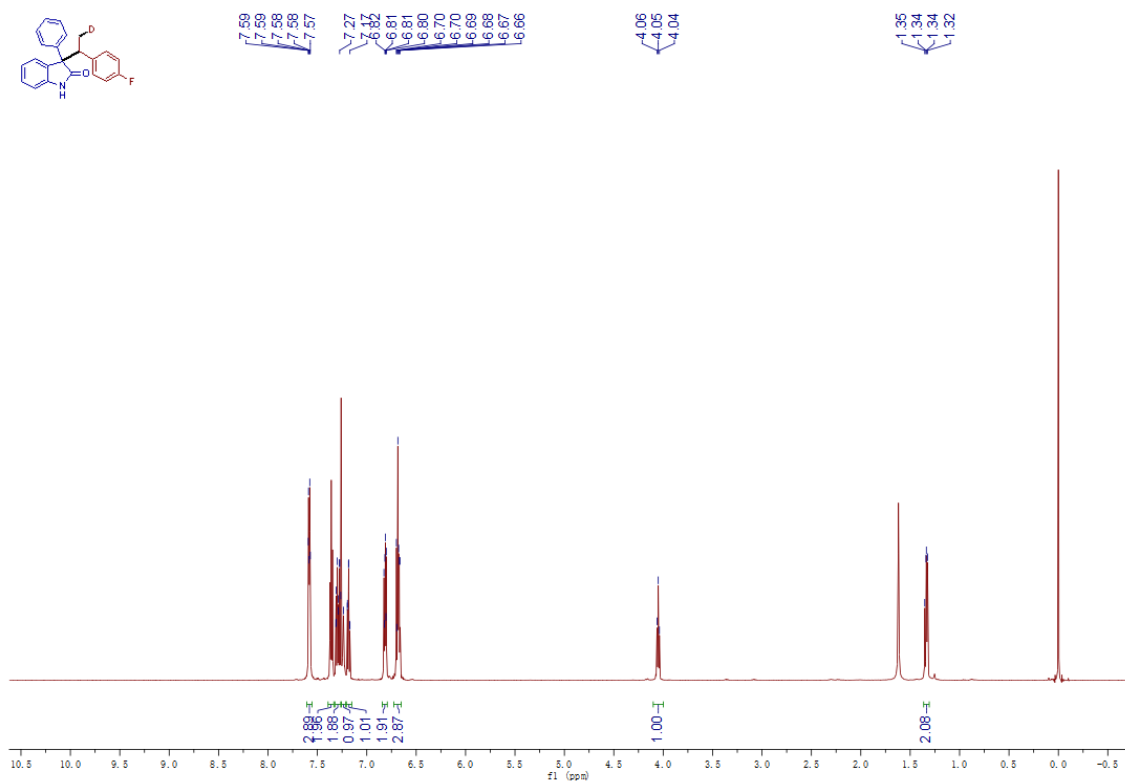
¹H NMR spectrum of 3-(1-(4-(methylthio)phenyl)ethyl-2-d)-3-phenylindolin-2-one. (46)



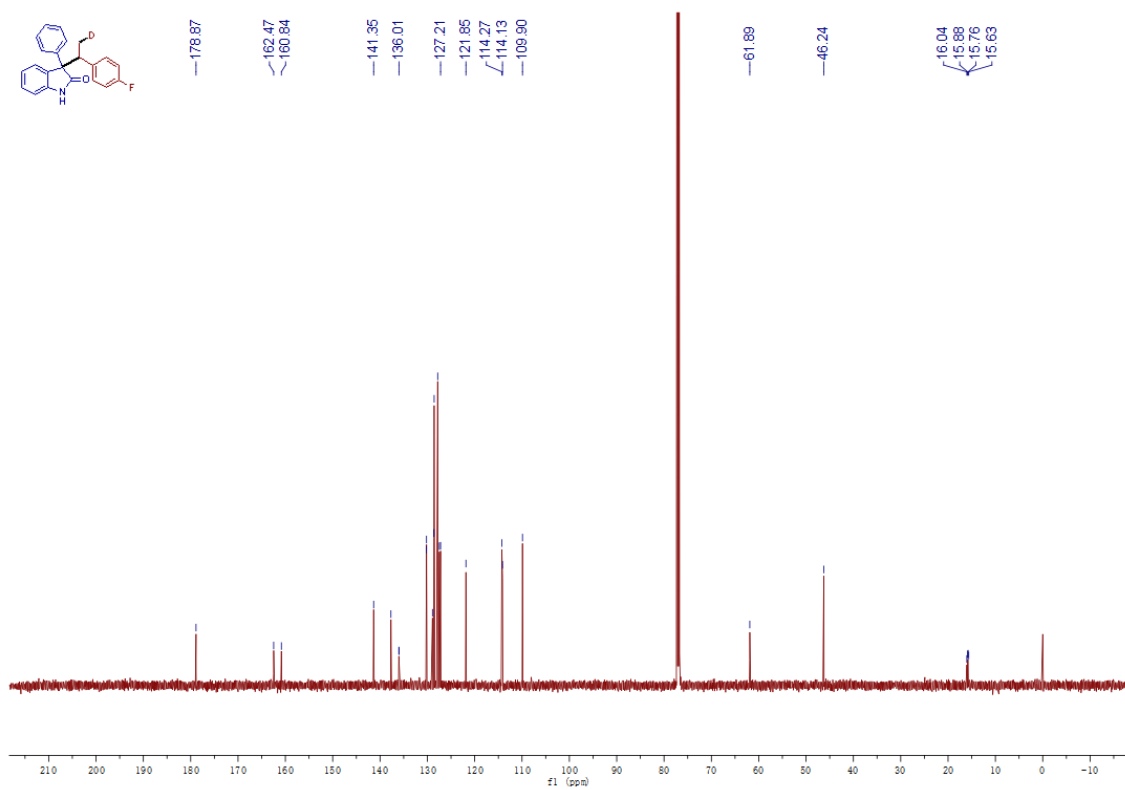
¹³C NMR spectrum of 3-(1-(4-(methylthio)phenyl)ethyl-2-d)-3-phenylindolin-2-one. (46)



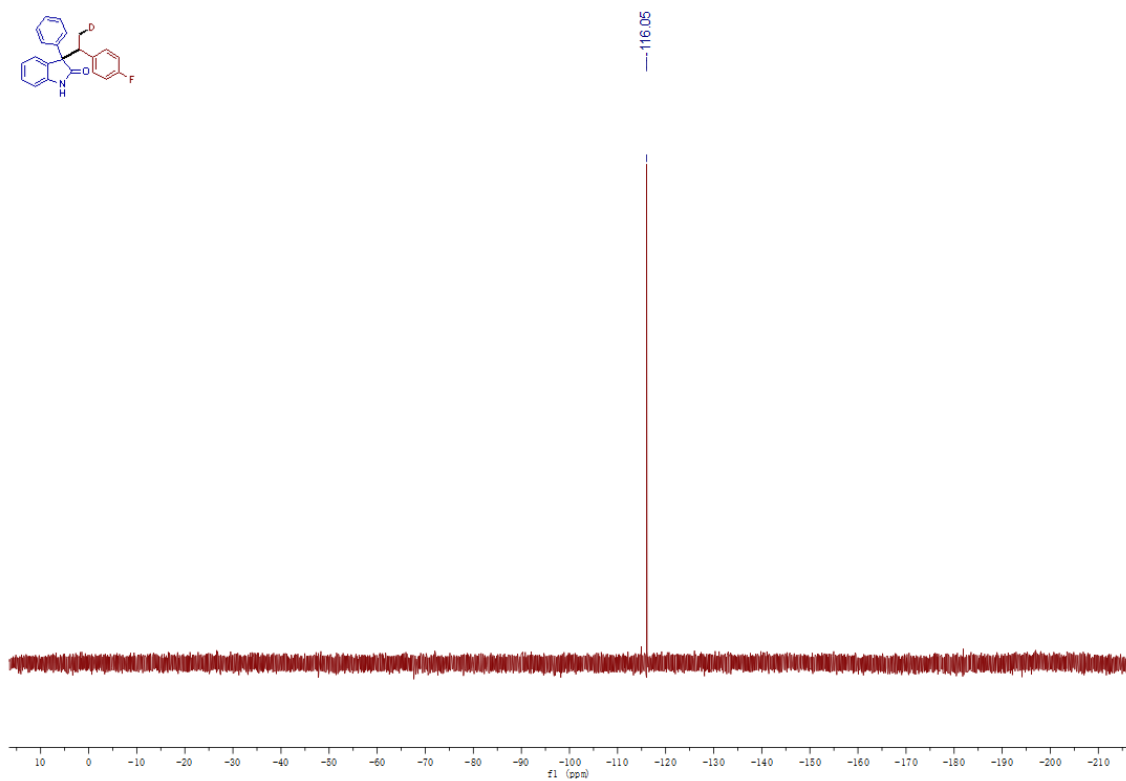
¹H NMR spectrum of 3-(1-(4-fluorophenyl)ethyl-2-d)-3-phenylindolin-2-one. (47)



¹³C NMR spectrum of 3-(1-(4-fluorophenyl)ethyl-2-d)-3-phenylindolin-2-one. (47)



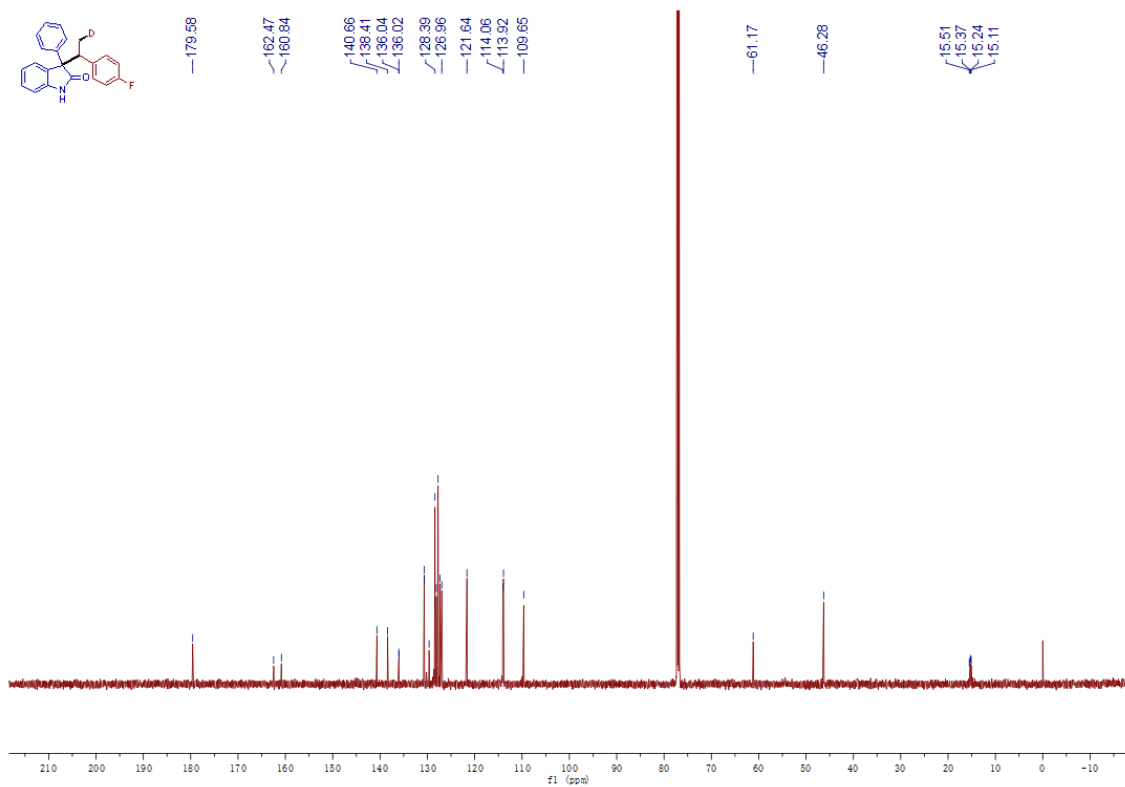
¹⁹F NMR spectrum of 3-(1-(4-fluorophenyl)ethyl-2-d)-3-phenylindolin-2-one. (47)



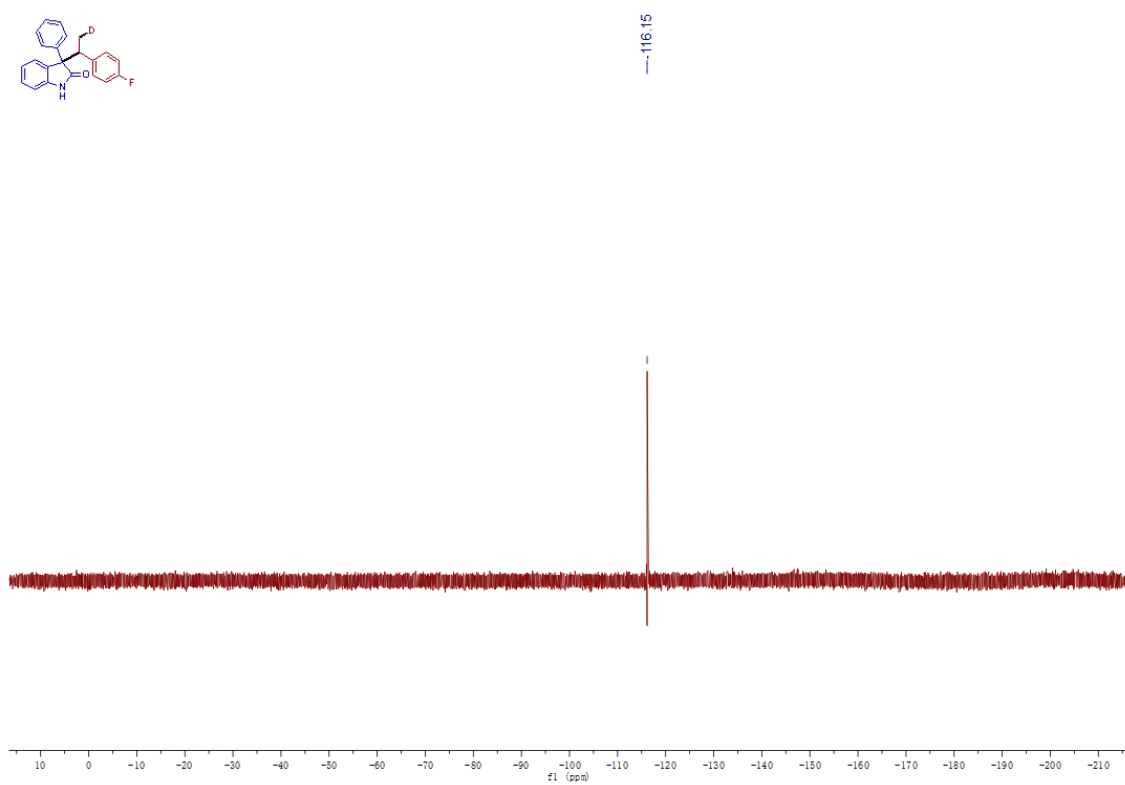
¹H NMR spectrum of 3-(1-(4-fluorophenyl)ethyl-2-d)-3-phenylindolin-2-one. (47)



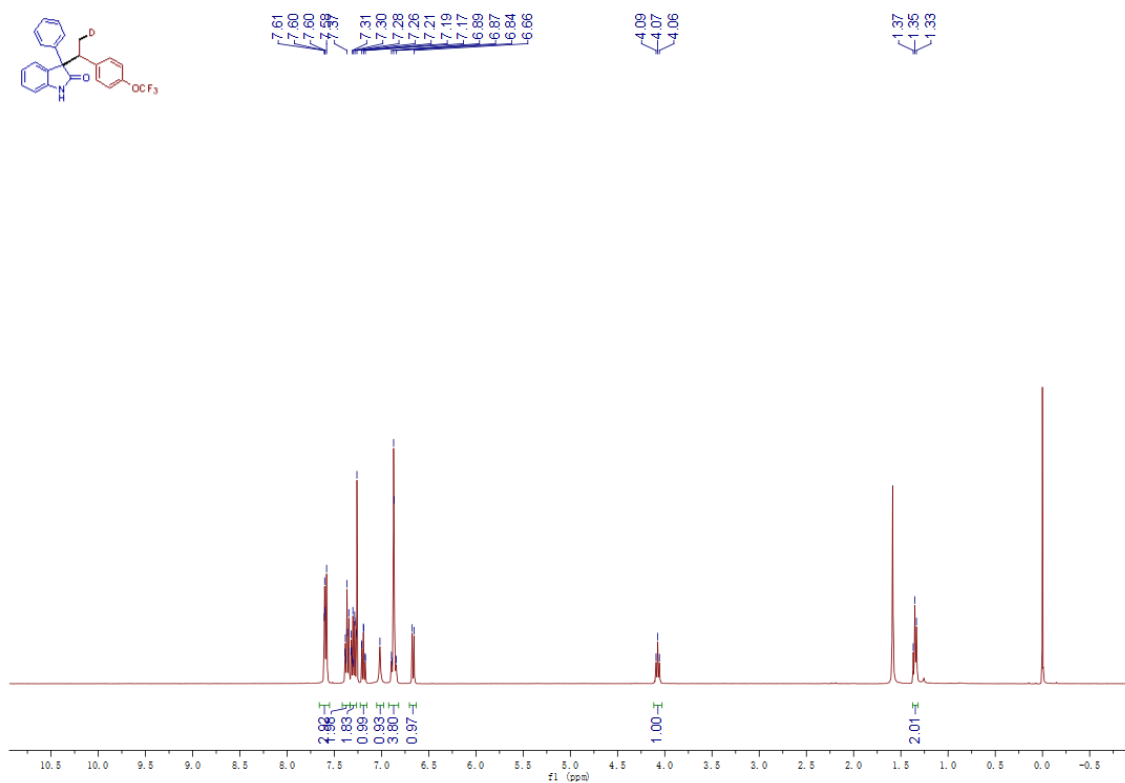
¹³C NMR spectrum of 3-(1-(4-fluorophenyl)ethyl-2-d)-3-phenylindolin-2-one. (47)



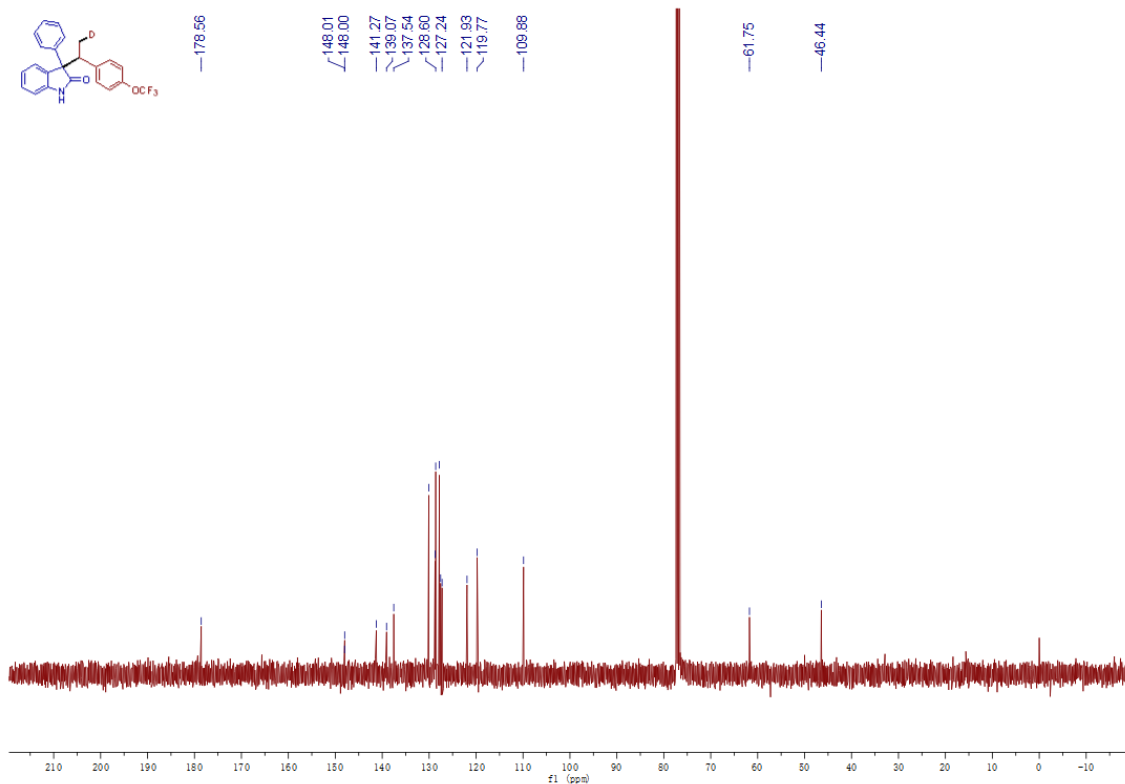
¹⁹F NMR spectrum of 3-(1-(4-fluorophenyl)ethyl-2-d)-3-phenylindolin-2-one. (47)



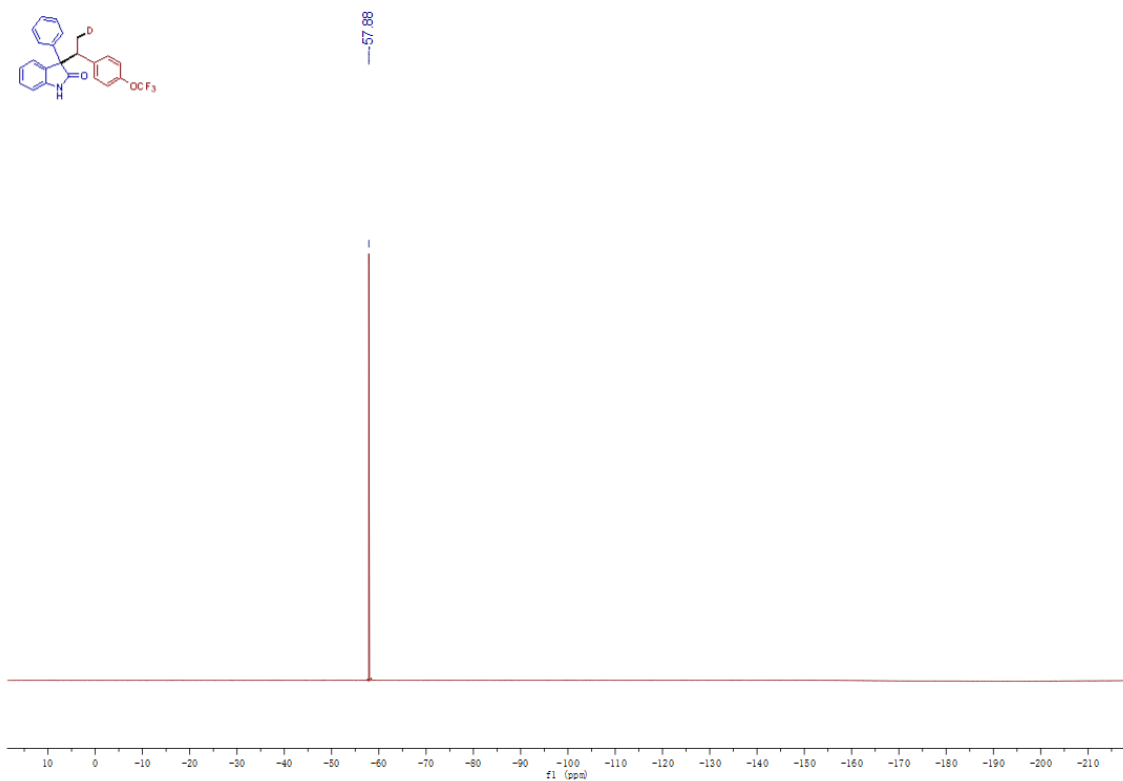
¹H NMR spectrum of 3-phenyl-3-(1-(4-(trifluoromethoxy)phenyl)ethyl-2-d)indolin-2-one. (48)



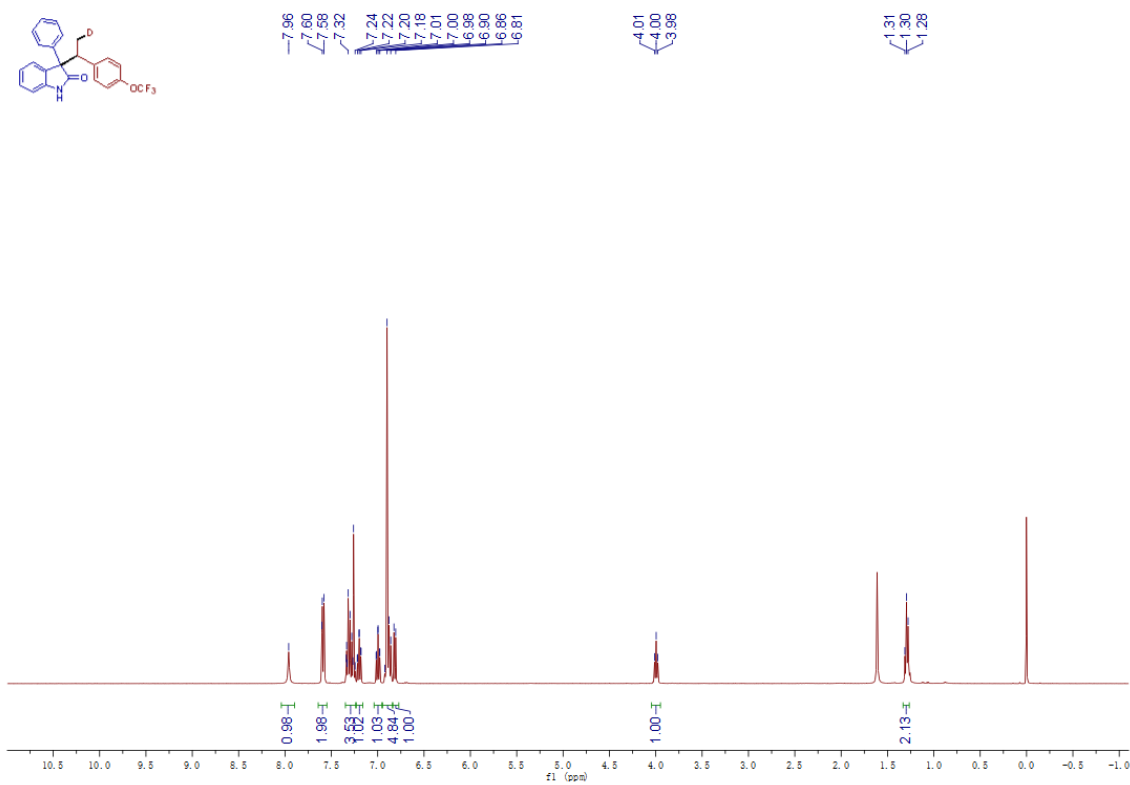
¹³C NMR spectrum of 3-phenyl-3-(1-(4-(trifluoromethoxy)phenyl)ethyl-2-d)indolin-2-one. (48)



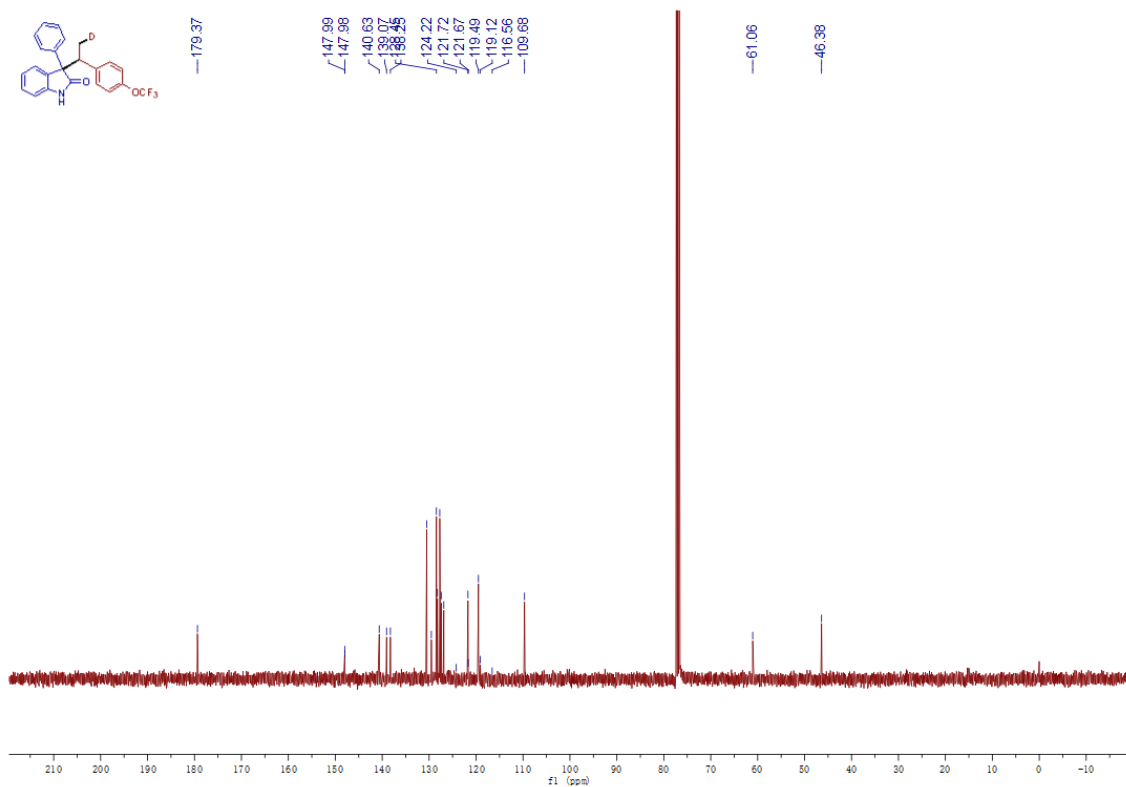
¹⁹F NMR spectrum of 3-phenyl-3-(1-(4-(trifluoromethoxy)phenyl)ethyl-2-d)indolin-2-one. (48)



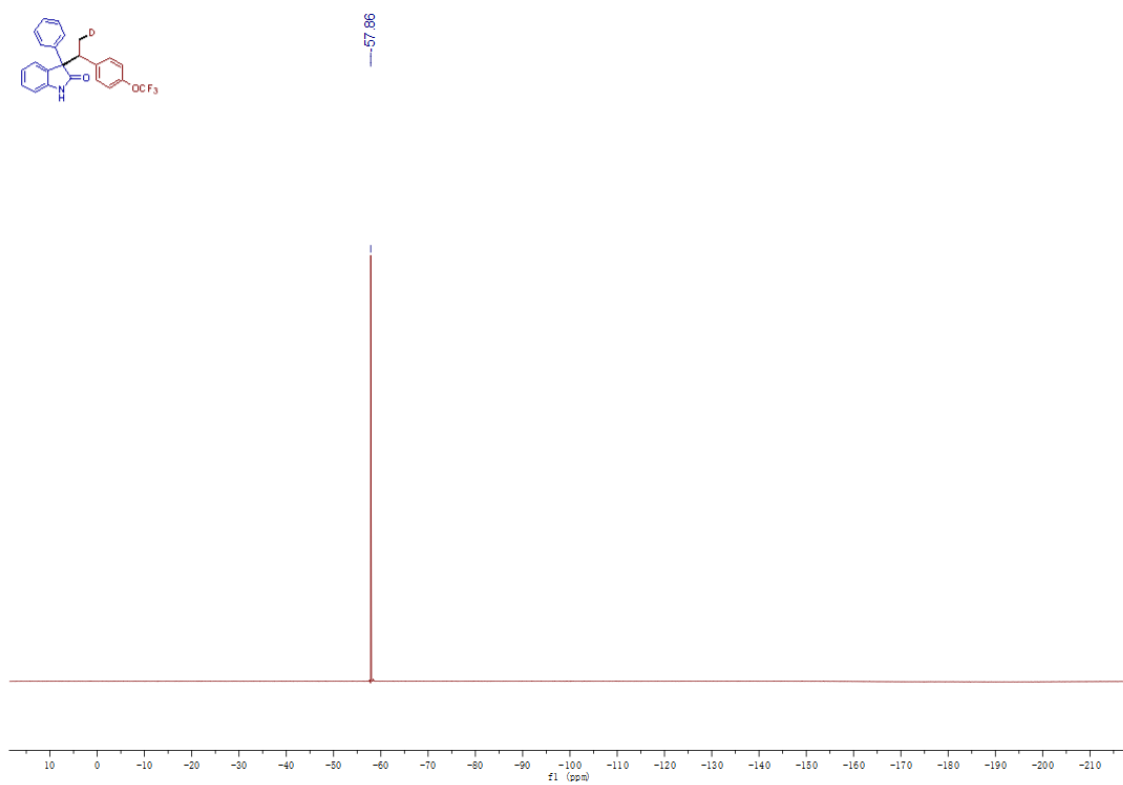
¹H NMR spectrum of 3-phenyl-3-(1-(4-(trifluoromethoxy)phenyl)ethyl-2-d)indolin-2-one. (48)



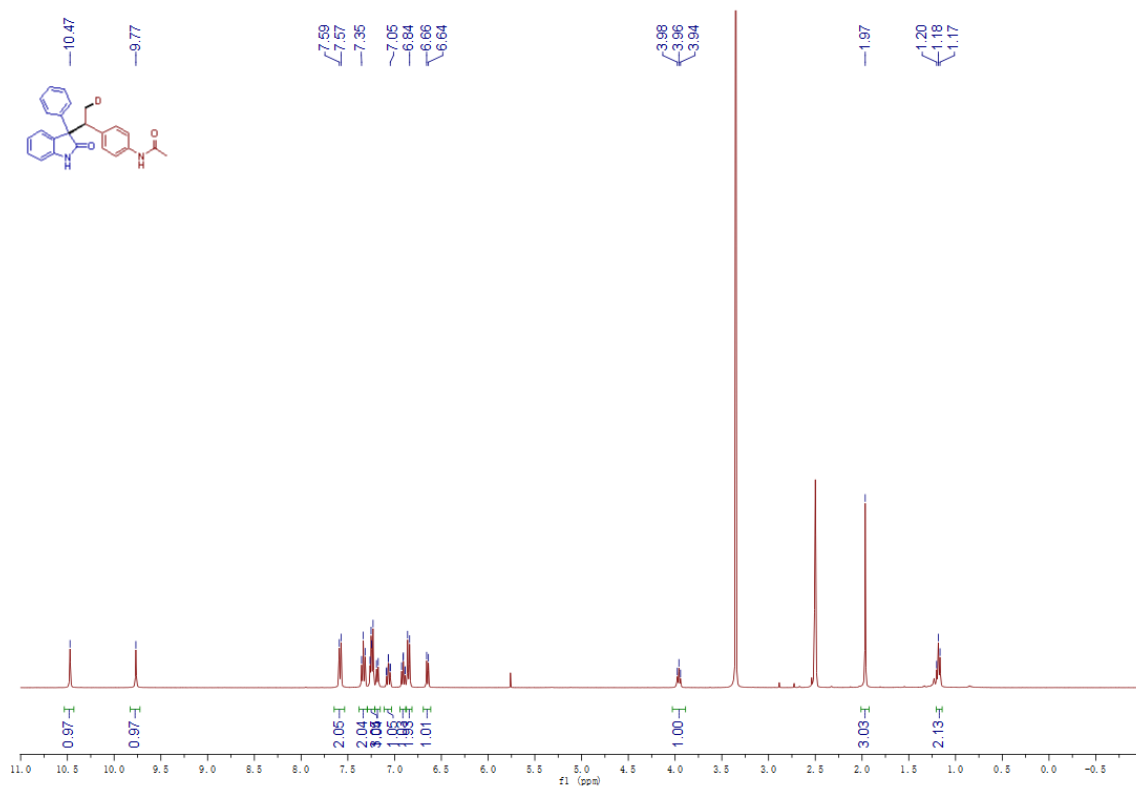
¹³C NMR spectrum of 3-phenyl-3-(1-(4-(trifluoromethoxy)phenyl)ethyl-2-d)indolin-2-one. (48)



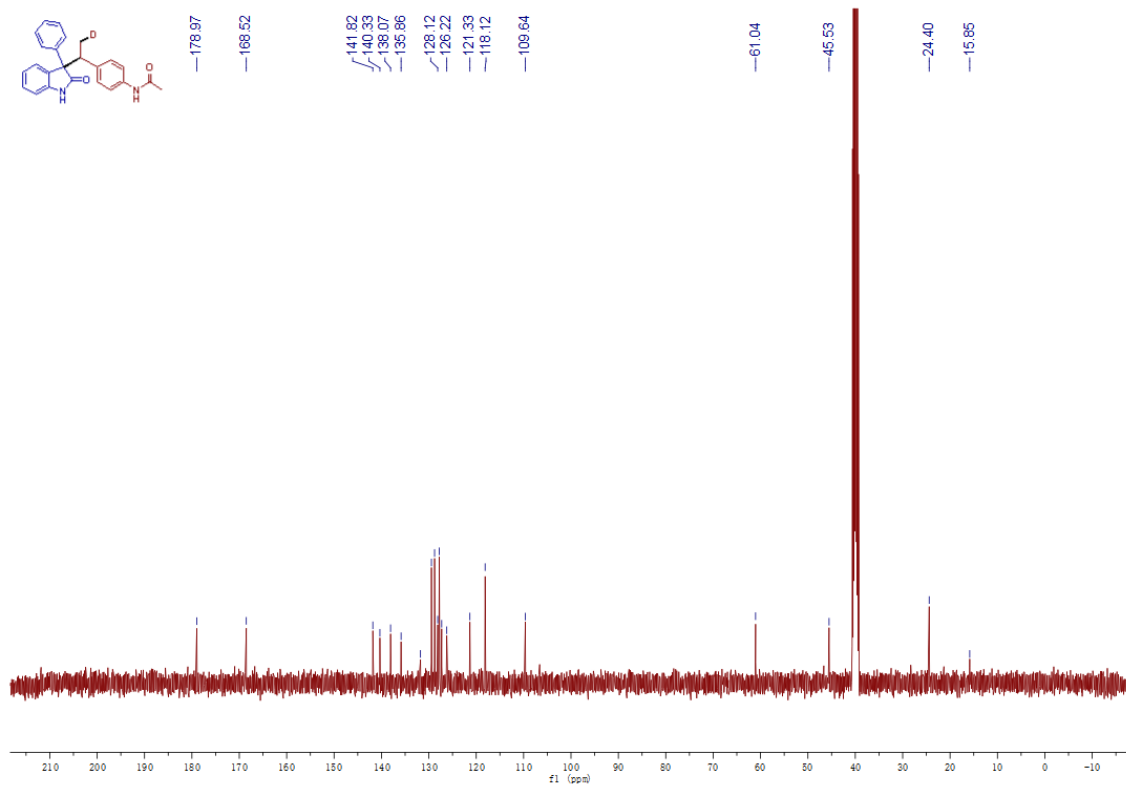
¹⁹F NMR spectrum of 3-phenyl-3-(1-(4-(trifluoromethoxy)phenyl)ethyl-2-d)indolin-2-one. (48)



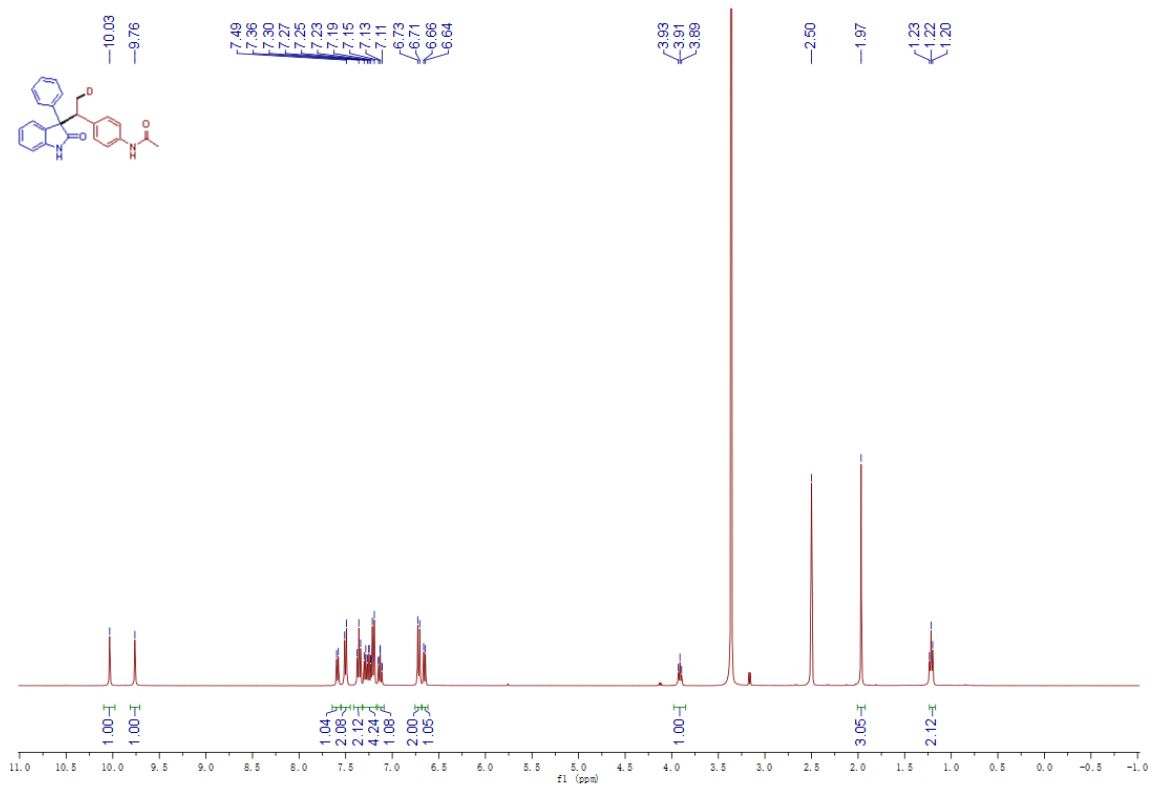
¹H NMR spectrum of N-(4-(1-(2-oxo-3-phenylindolin-3-yl)ethyl)-2-d)phenyl)acetamide. (49)



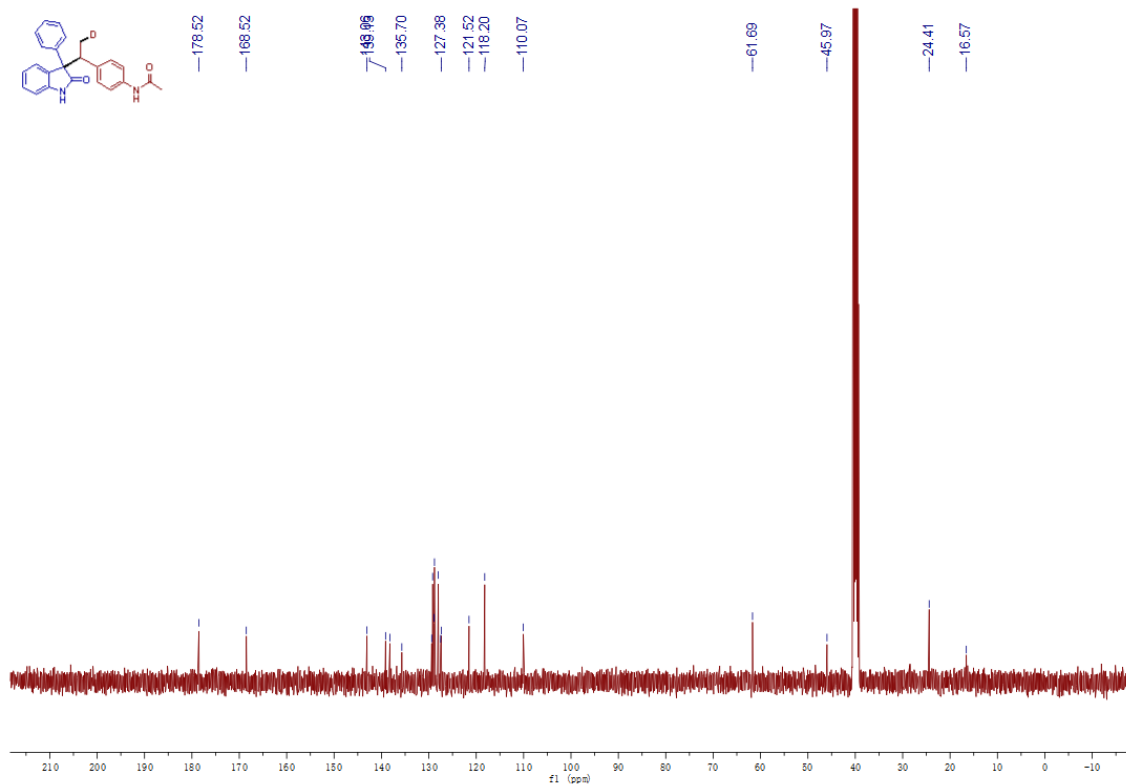
¹³C NMR spectrum of N-(4-(1-(2-oxo-3-phenylindolin-3-yl)ethyl)-2-d)phenyl)acetamide. (49)



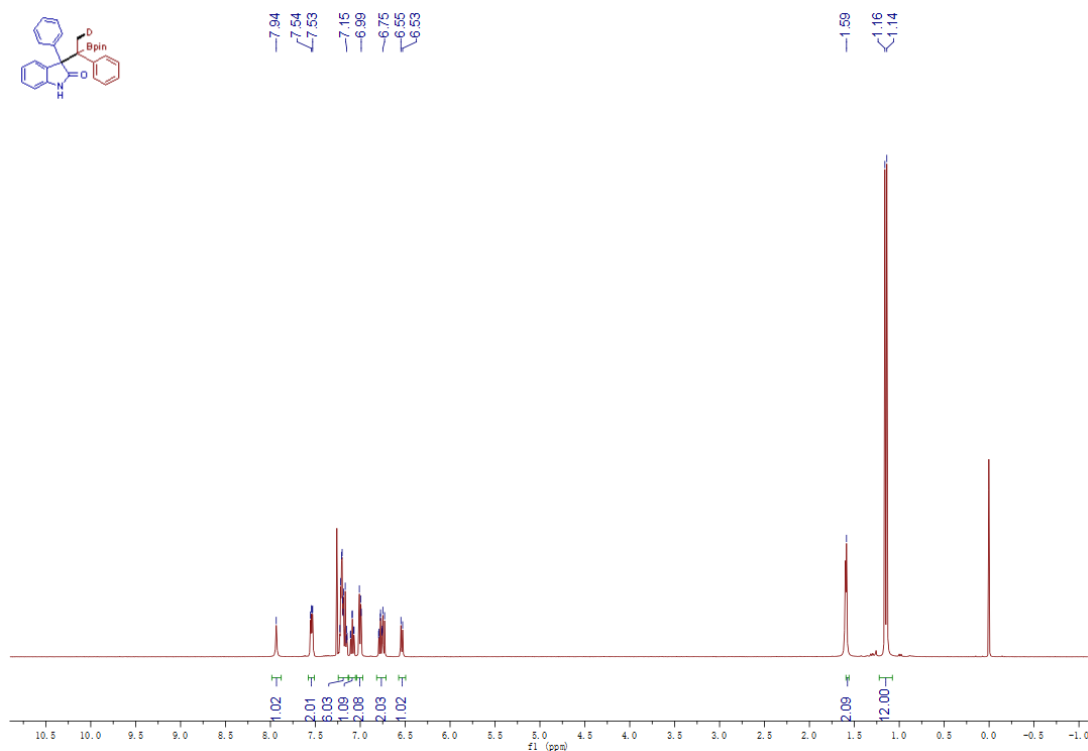
¹H NMR spectrum of N-(4-(1-(2-oxo-3-phenylindolin-3-yl)ethyl-2-d)phenyl)acetamide. (49)



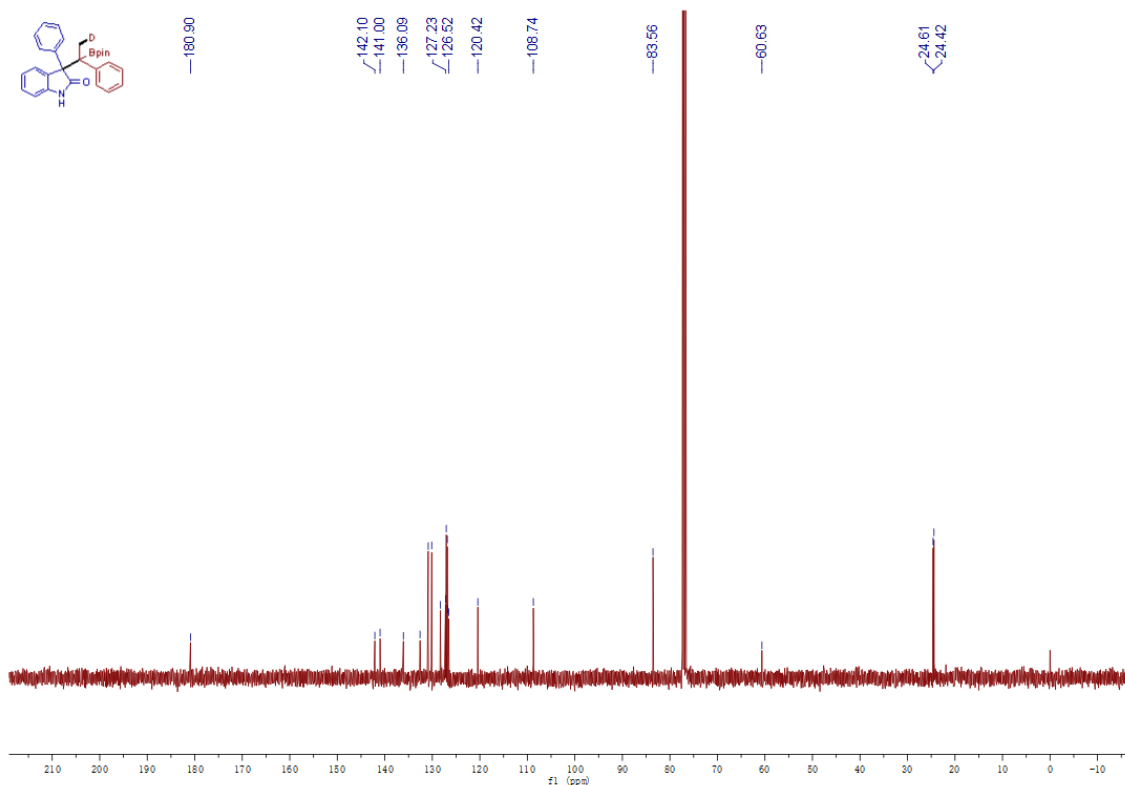
¹³C NMR spectrum of N-(4-(1-(2-oxo-3-phenylindolin-3-yl)ethyl-2-d)phenyl)acetamide. (49)



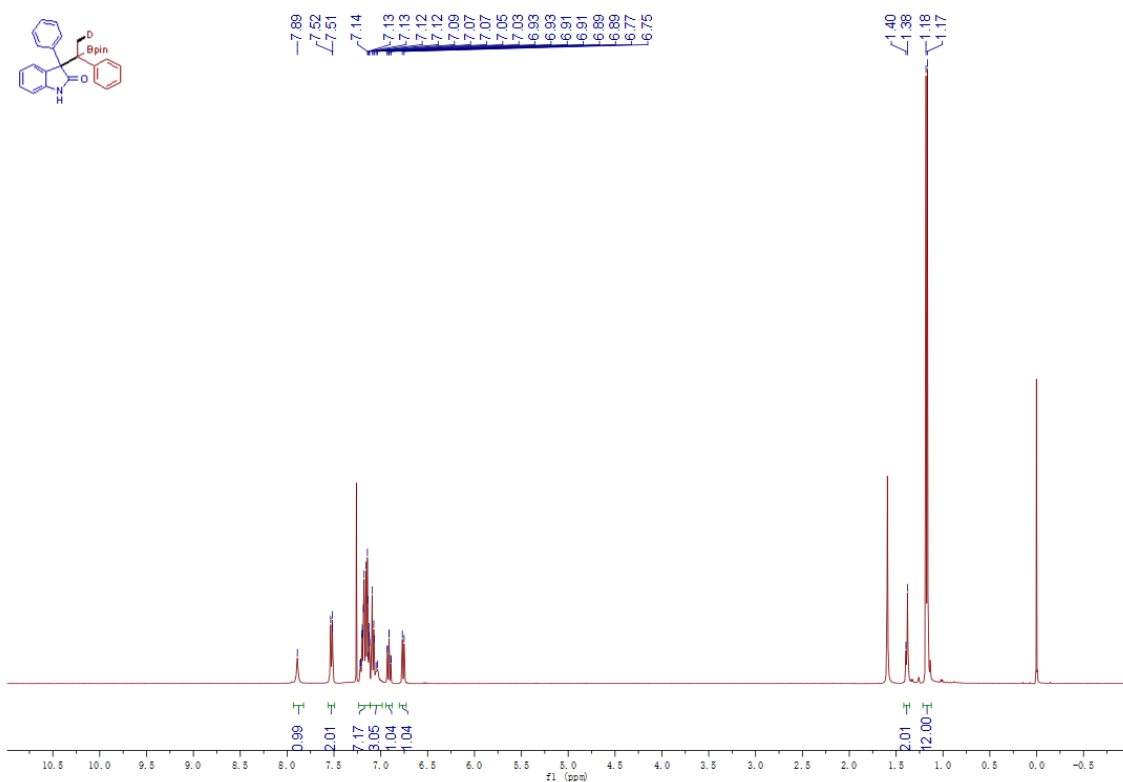
¹H NMR spectrum of 3-phenyl-3-(1-phenyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl-2-d)indolin-2-one. (50)



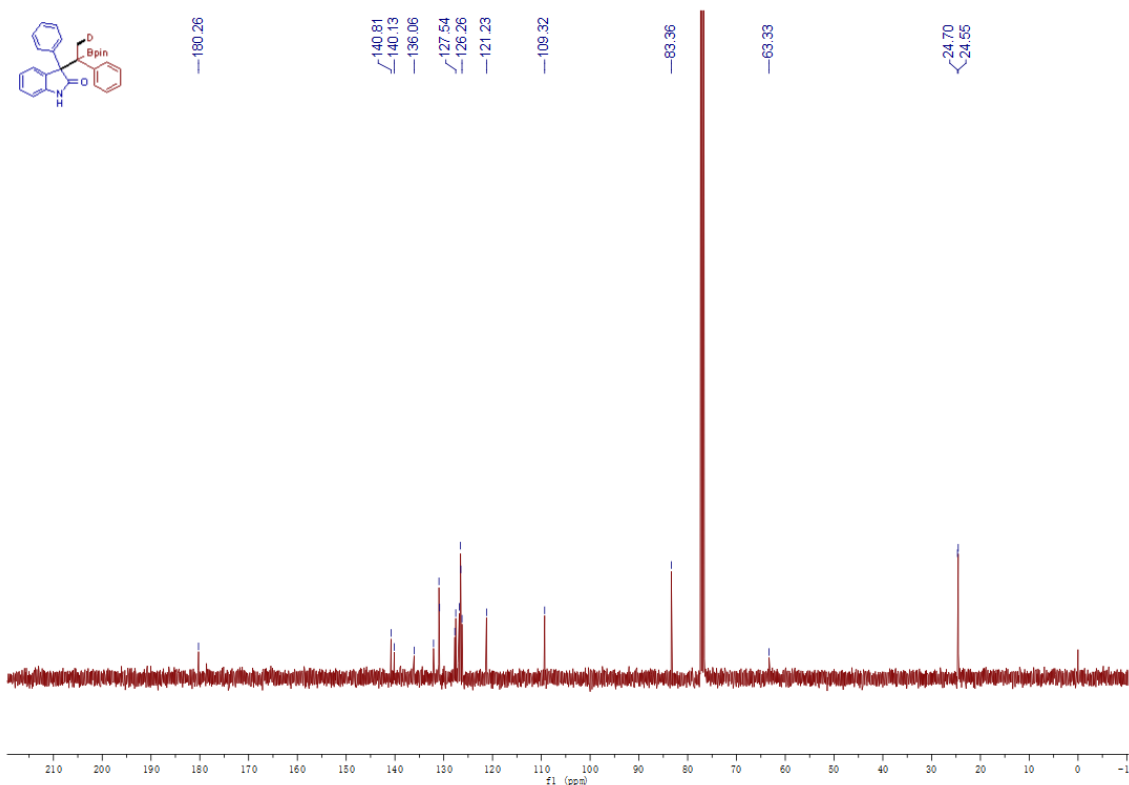
¹³C NMR spectrum of 3-phenyl-3-(1-phenyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl-2-d)indolin-2-one. (50)



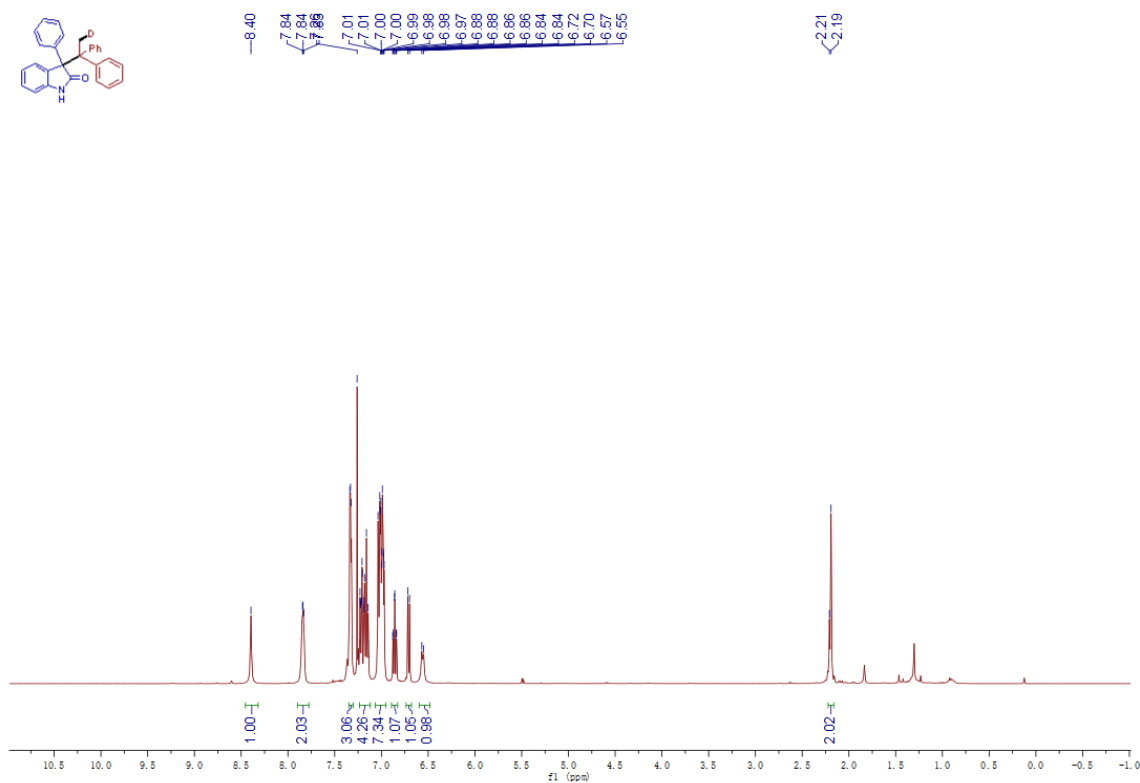
¹H NMR spectrum of 3-phenyl-3-(1-phenyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl-2-d)indolin-2-one. (50)



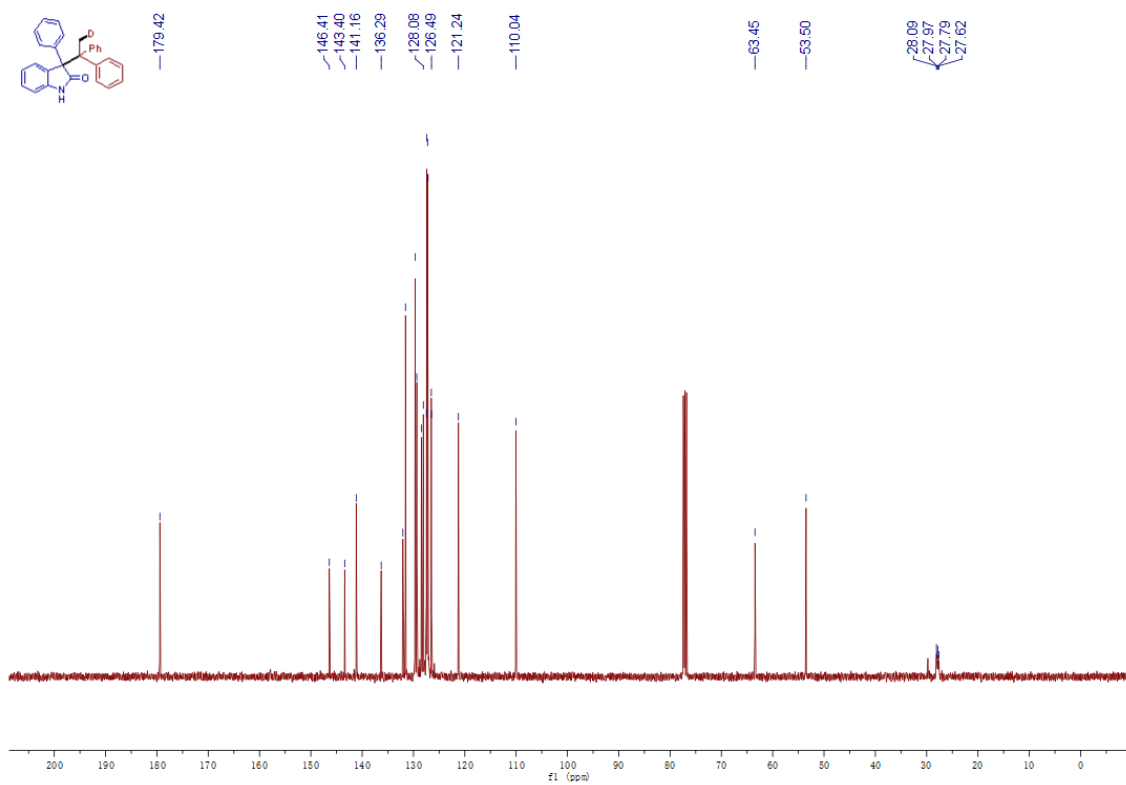
¹³C NMR spectrum of 3-phenyl-3-(1-phenyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl-2-d)indolin-2-one. (50)



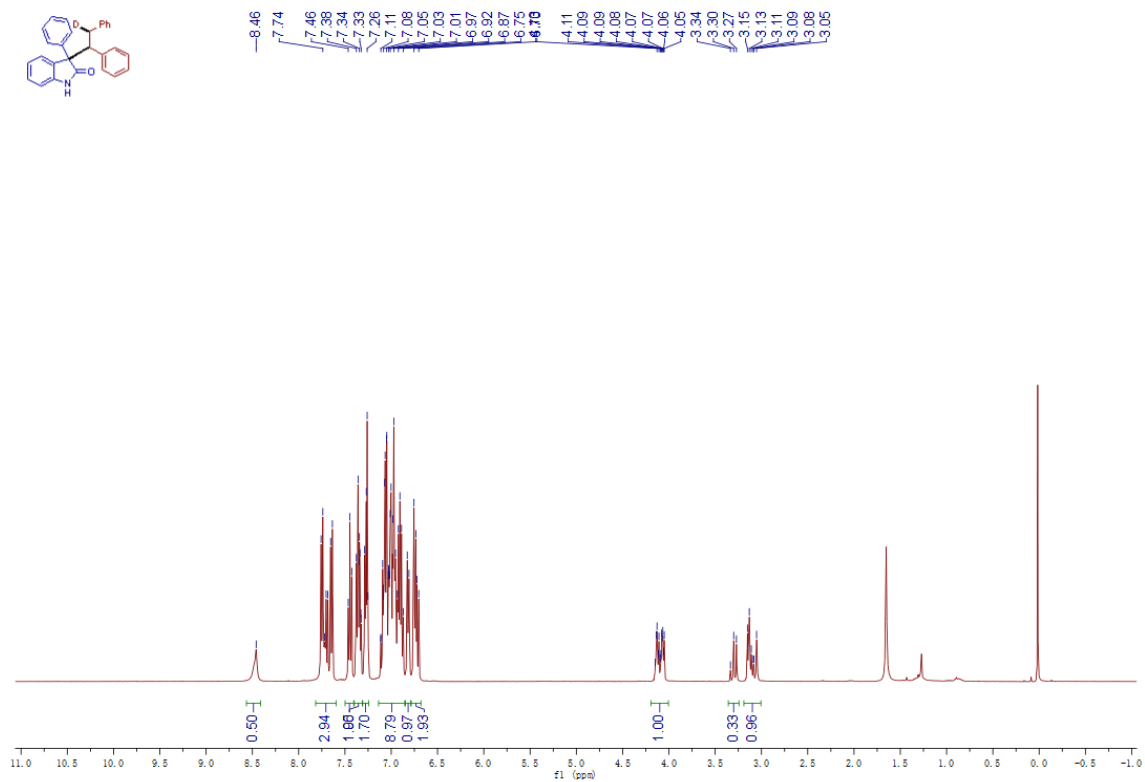
¹H NMR spectrum of 3-(1,1-diphenylethyl-2-d)-3-phenylindolin-2-one. (51)



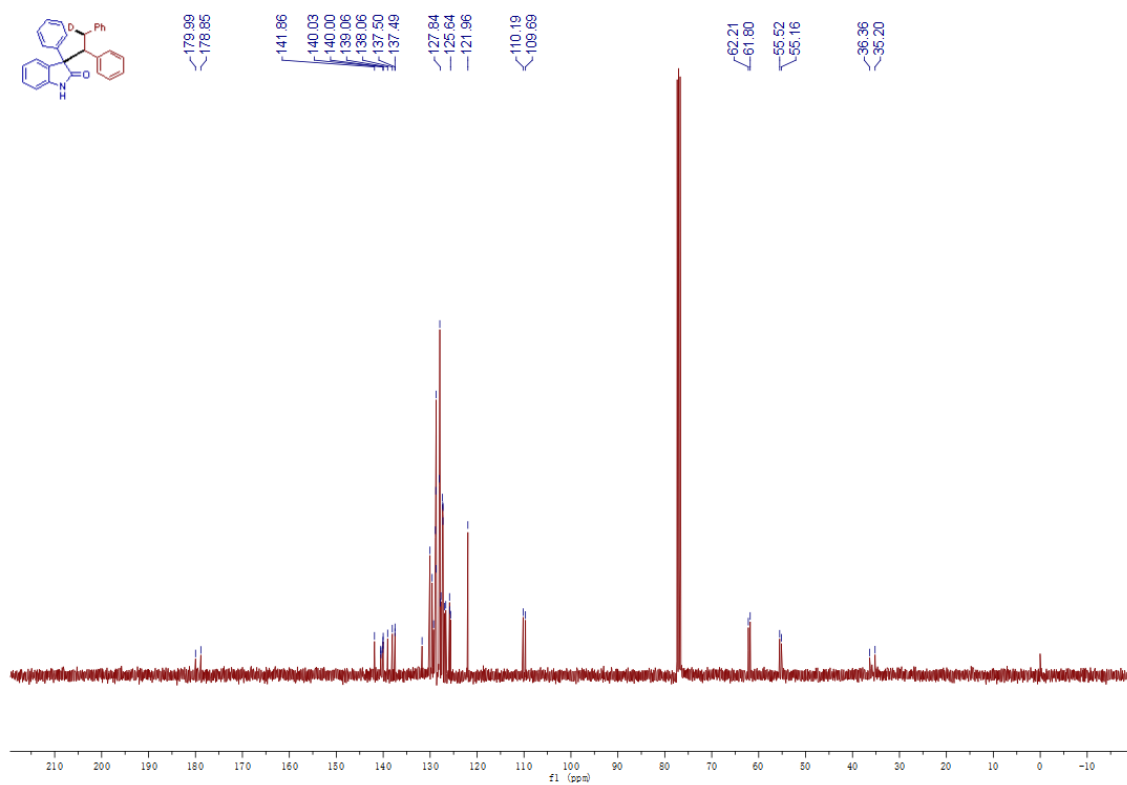
¹³C NMR spectrum of 3-(1,1-diphenylethyl-2-d)-3-phenylindolin-2-one. (51)



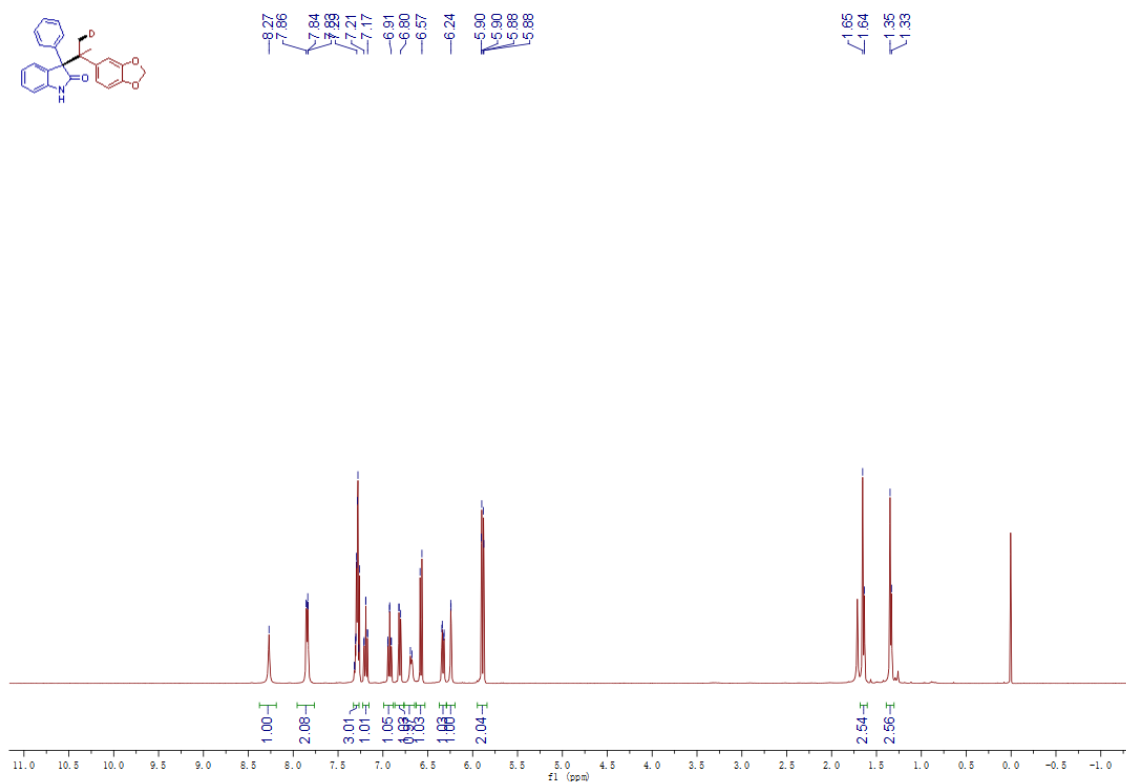
¹H NMR spectrum of 3-(1,2-diphenylethyl-2-d)-3-phenylindolin-2-one. (52)



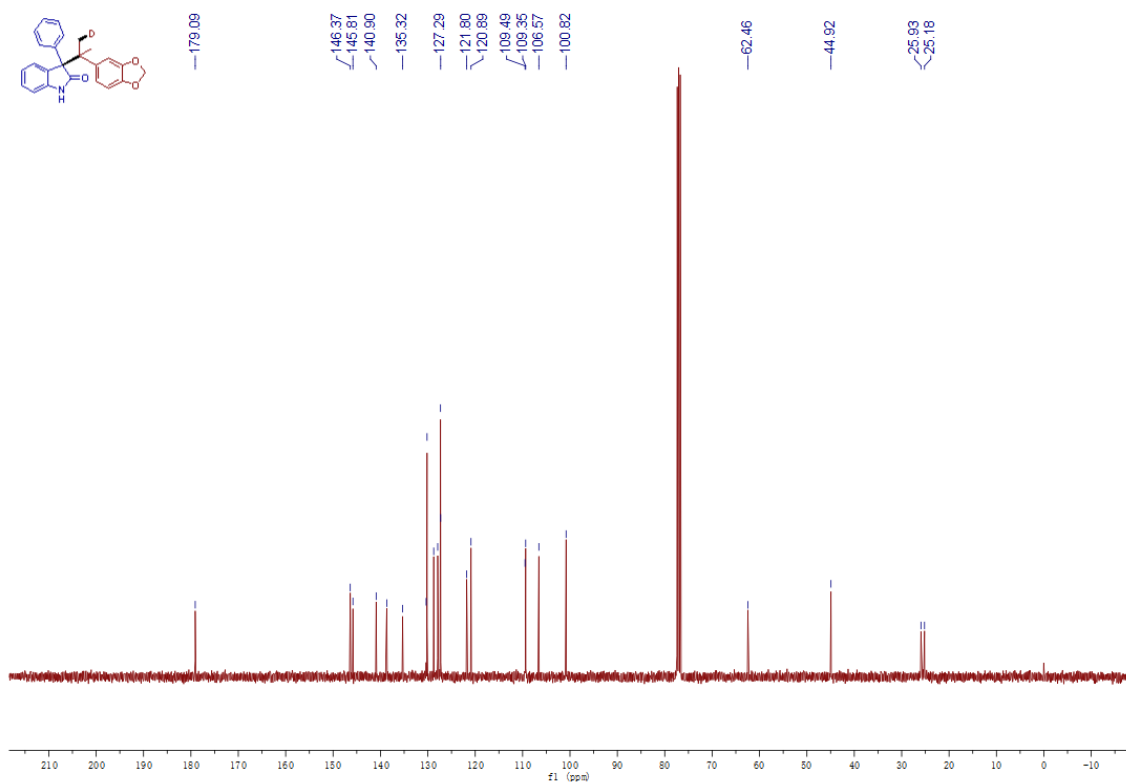
¹³C NMR spectrum of 3-(1,2-diphenylethyl-2-d)-3-phenylindolin-2-one. (52)



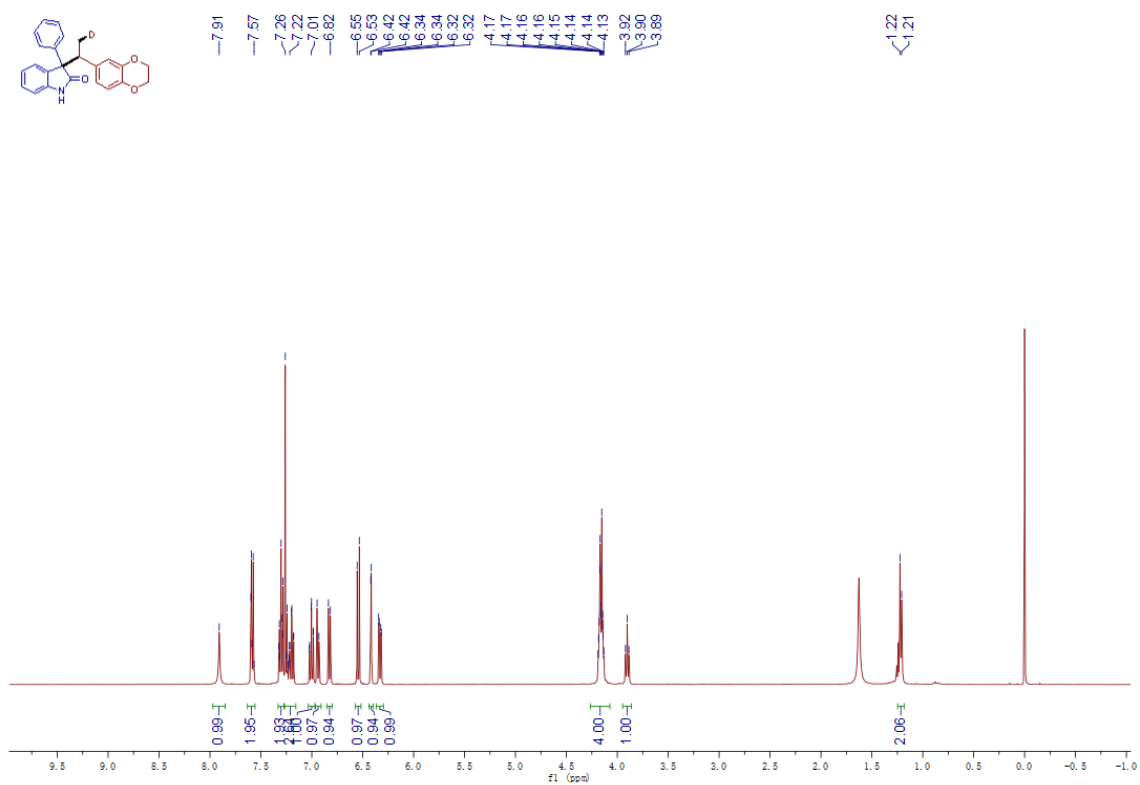
¹H NMR spectrum of 3-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-3-phenylindolin-2-one. (53)



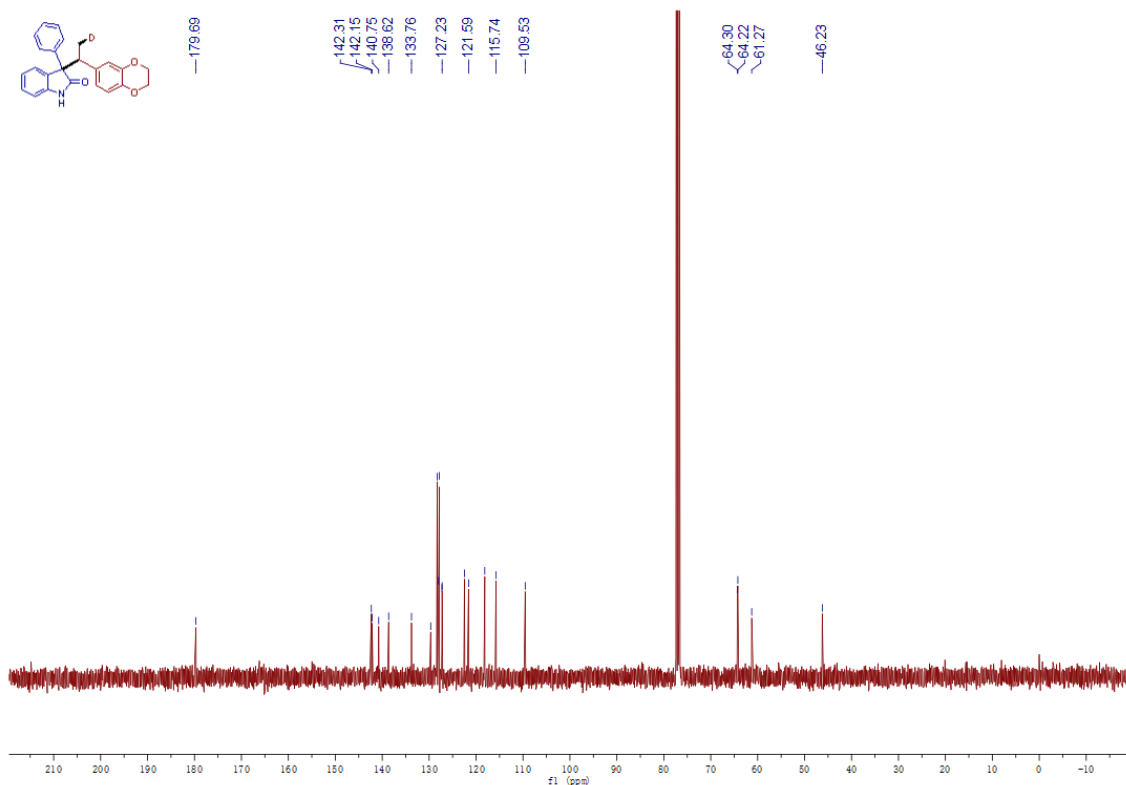
¹³C NMR spectrum of 3-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-3-phenylindolin-2-one. (53)



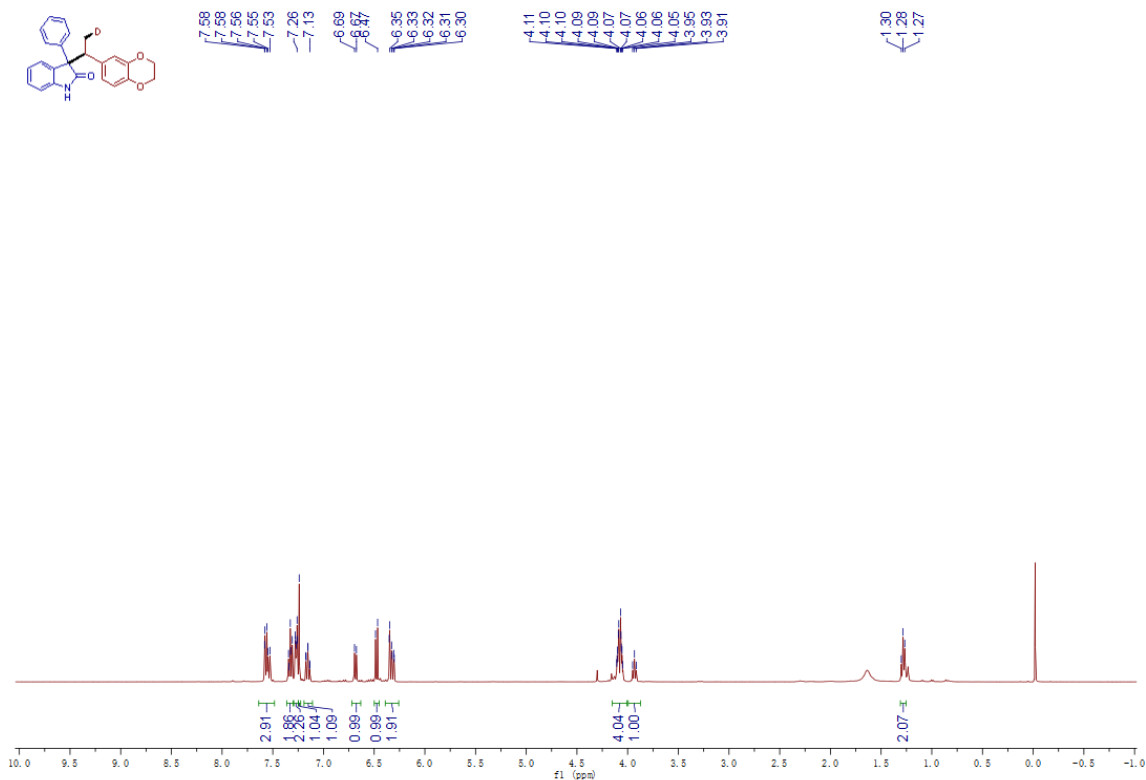
¹H NMR spectrum of 3-(1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)ethyl-2-d)-3-phenylindolin-2-one. (54)



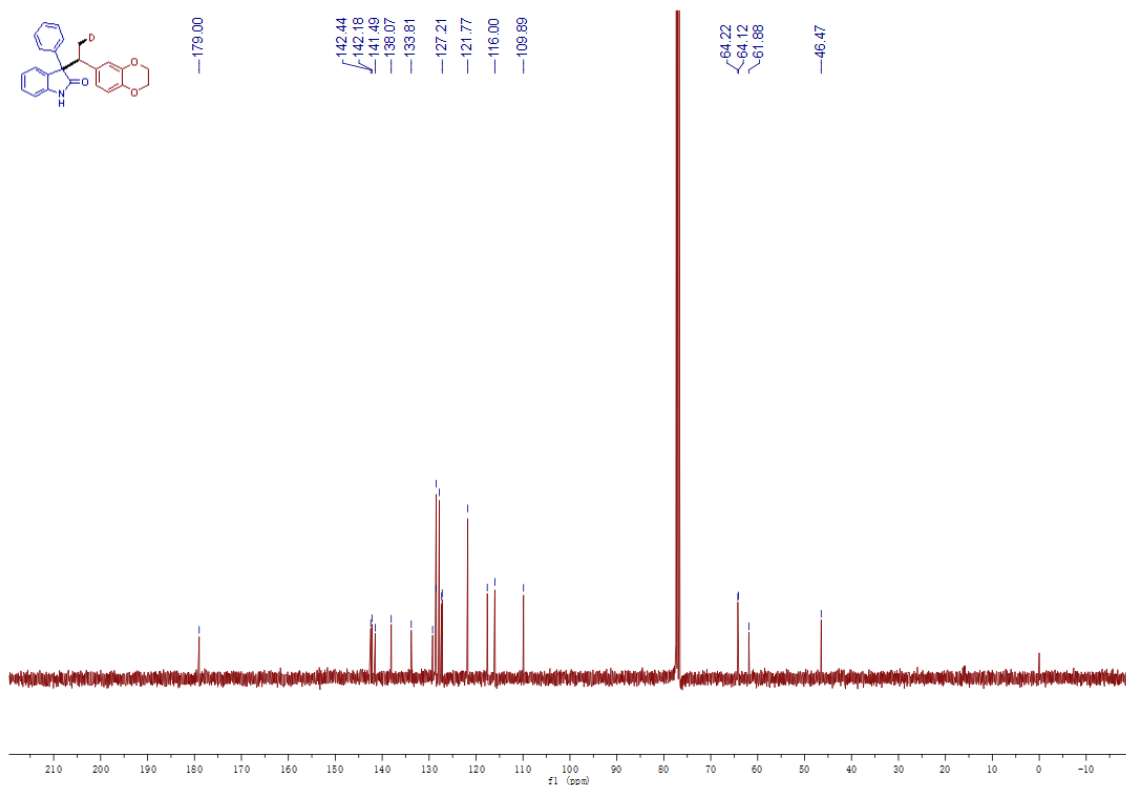
¹³C NMR spectrum of 3-(1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)ethyl-2-d)-3-phenylindolin-2-one. (54)



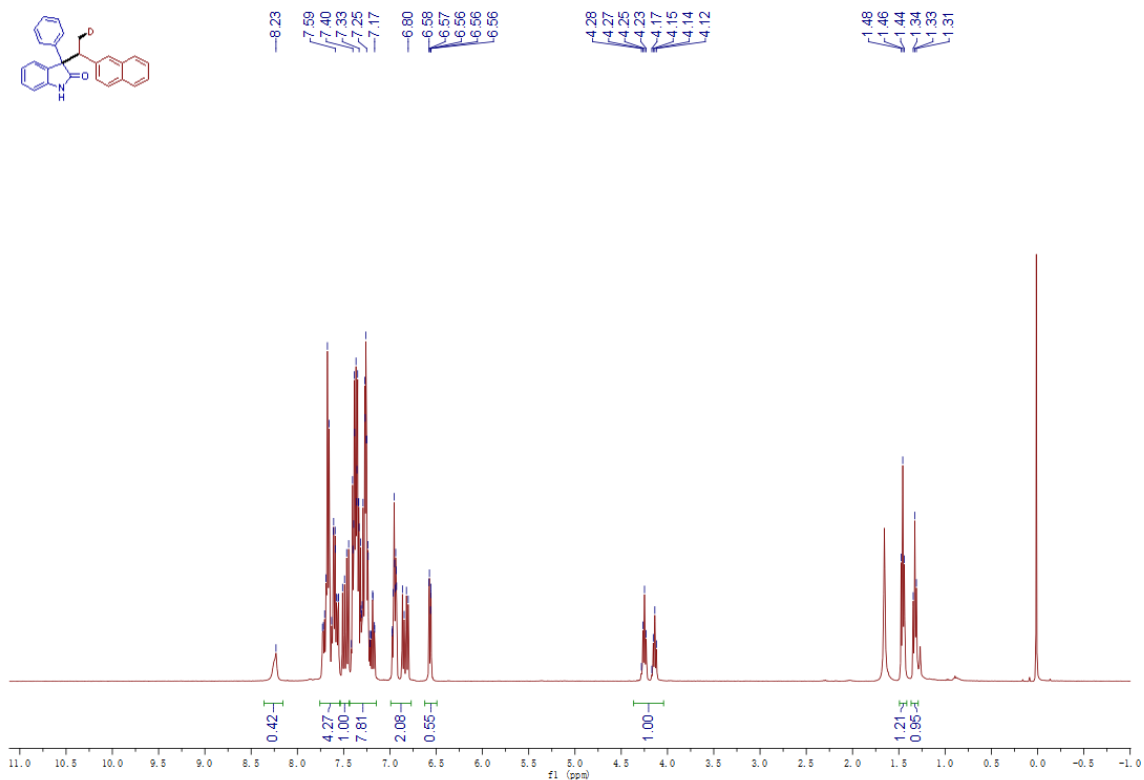
¹H NMR spectrum of 3-(1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)ethyl-2-d)-3-phenylindolin-2-one. (54)



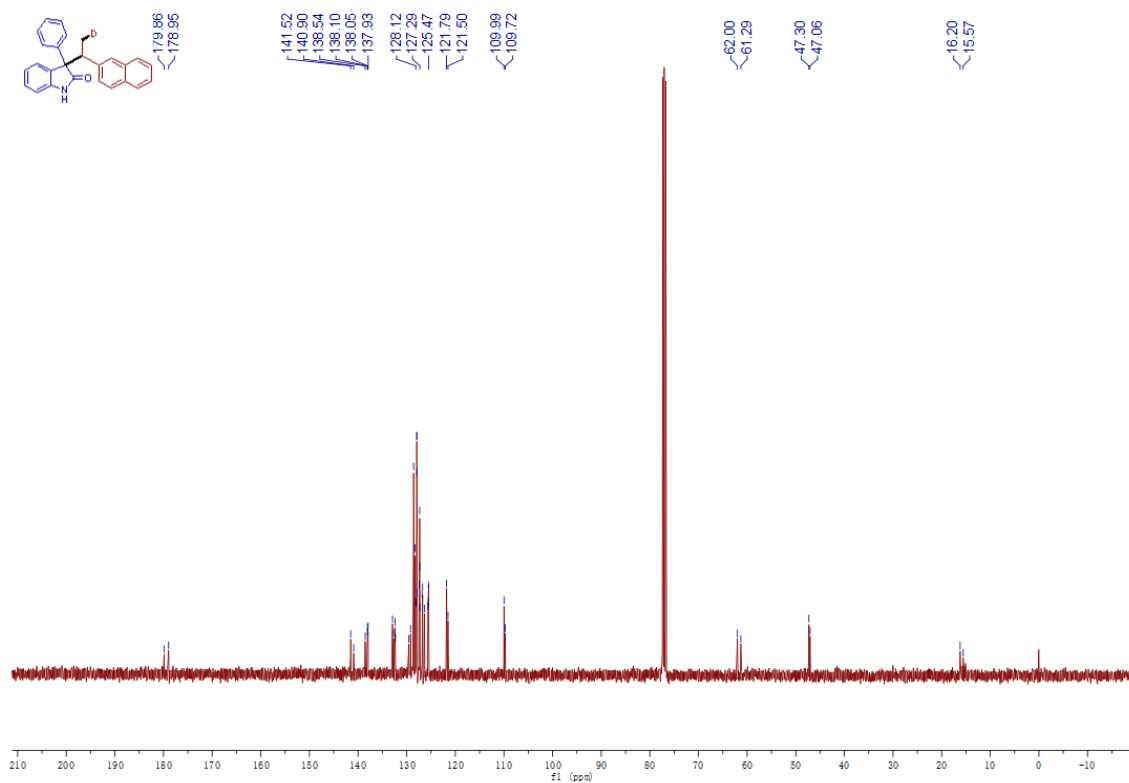
¹³C NMR spectrum of 3-(1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)ethyl-2-d)-3-phenylindolin-2-one. (54)



¹H NMR spectrum of 3-(1-(naphthalen-2-yl)ethyl-2-d)-3-phenylindolin-2-one. (55)



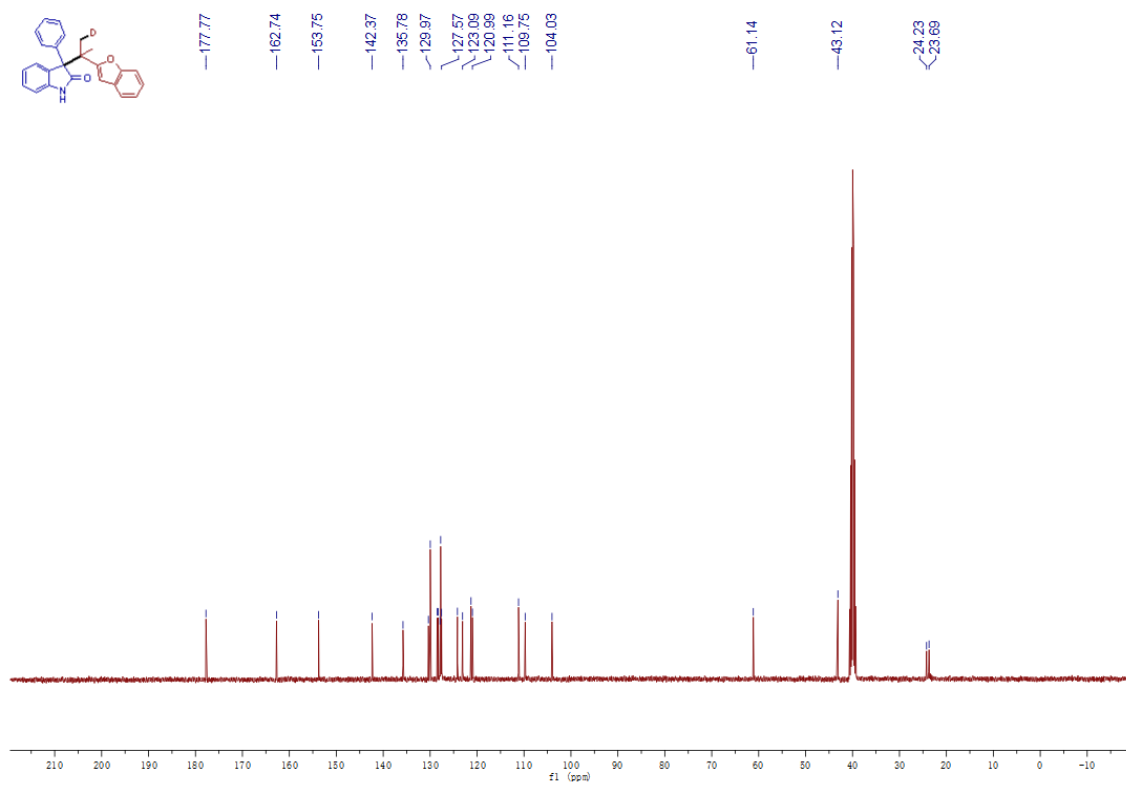
¹³C NMR spectrum of 3-(1-(naphthalen-2-yl)ethyl-2-d)-3-phenylindolin-2-one. (55)



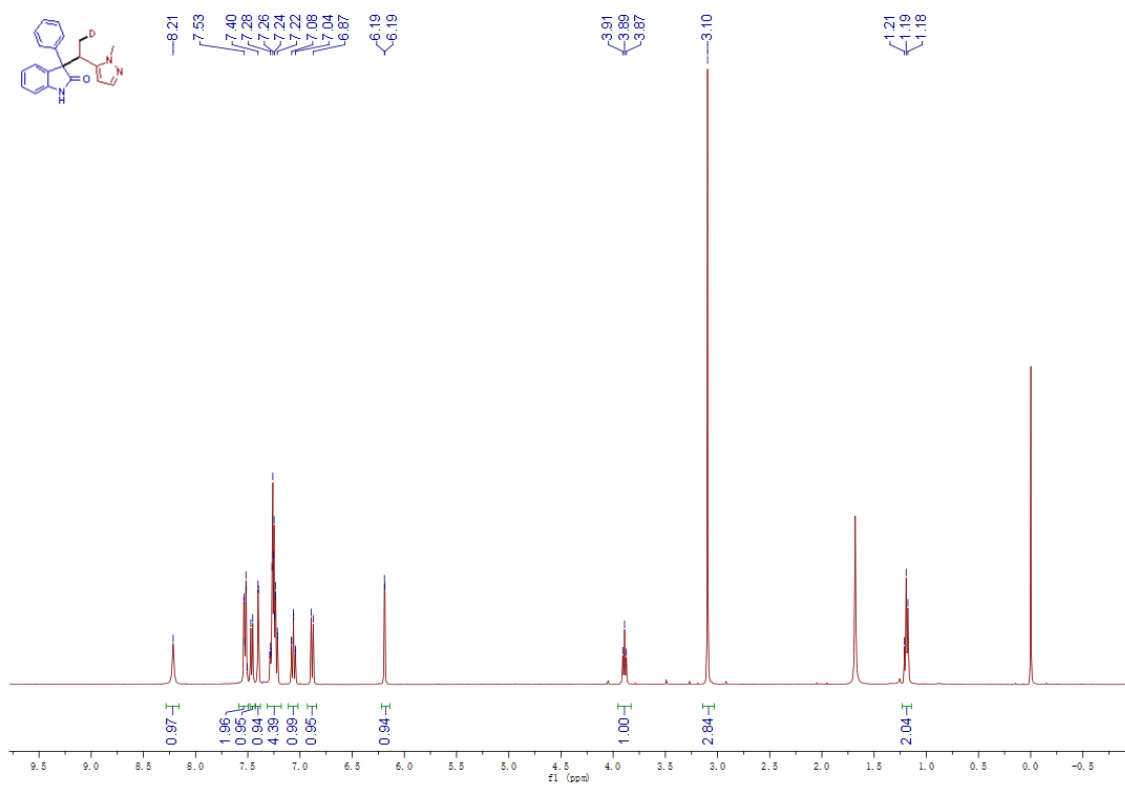
¹H NMR spectrum of 3-(2-(benzofuran-2-yl)propan-2-yl-1-d)-3-phenylindolin-2-one. (56)



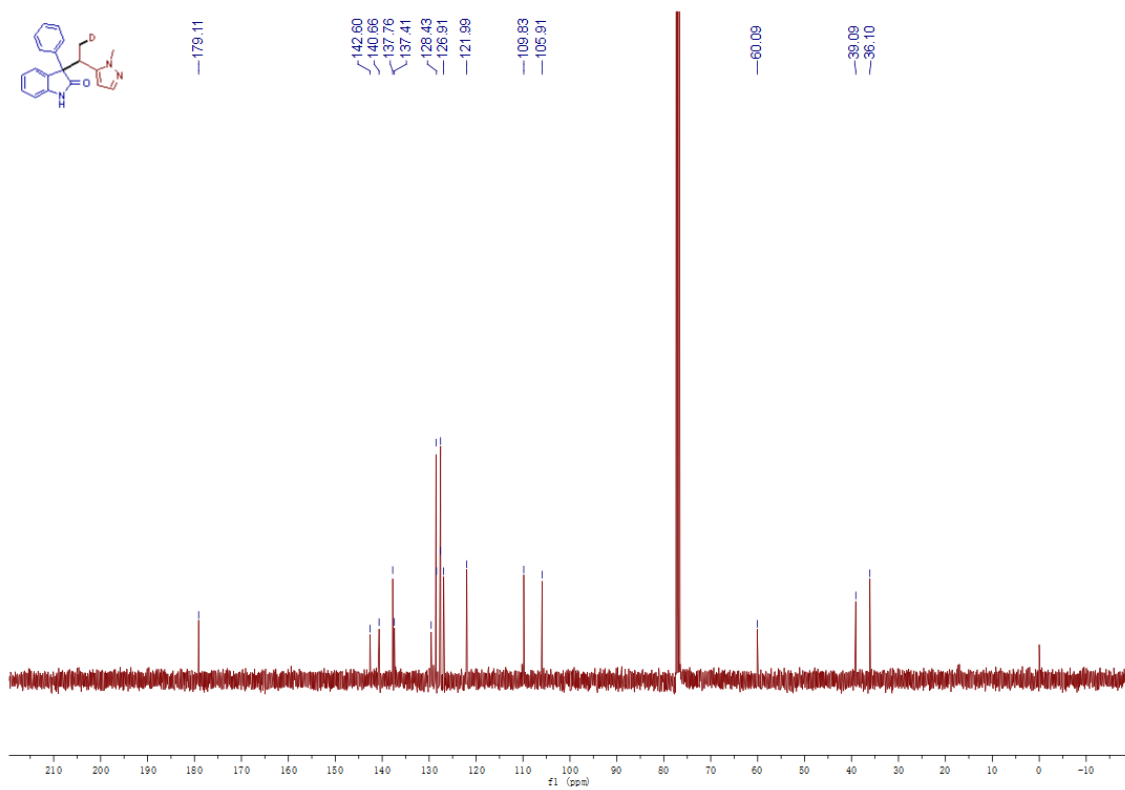
¹³C NMR spectrum of 3-(2-(benzofuran-2-yl)propan-2-yl-1-d)-3-phenylindolin-2-one. (56)



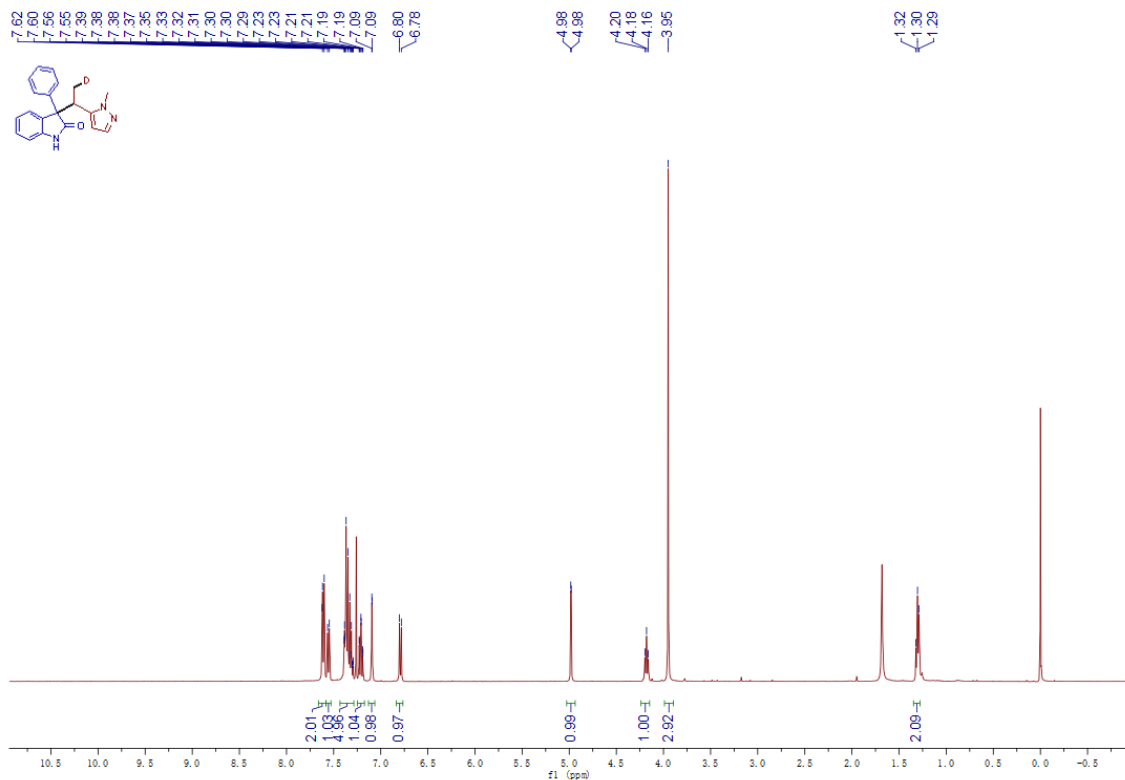
¹H NMR spectrum of 3-(1-(1-methyl-1H-pyrazol-5-yl)ethyl-2-d)-3-phenylindolin-2-one. (57)



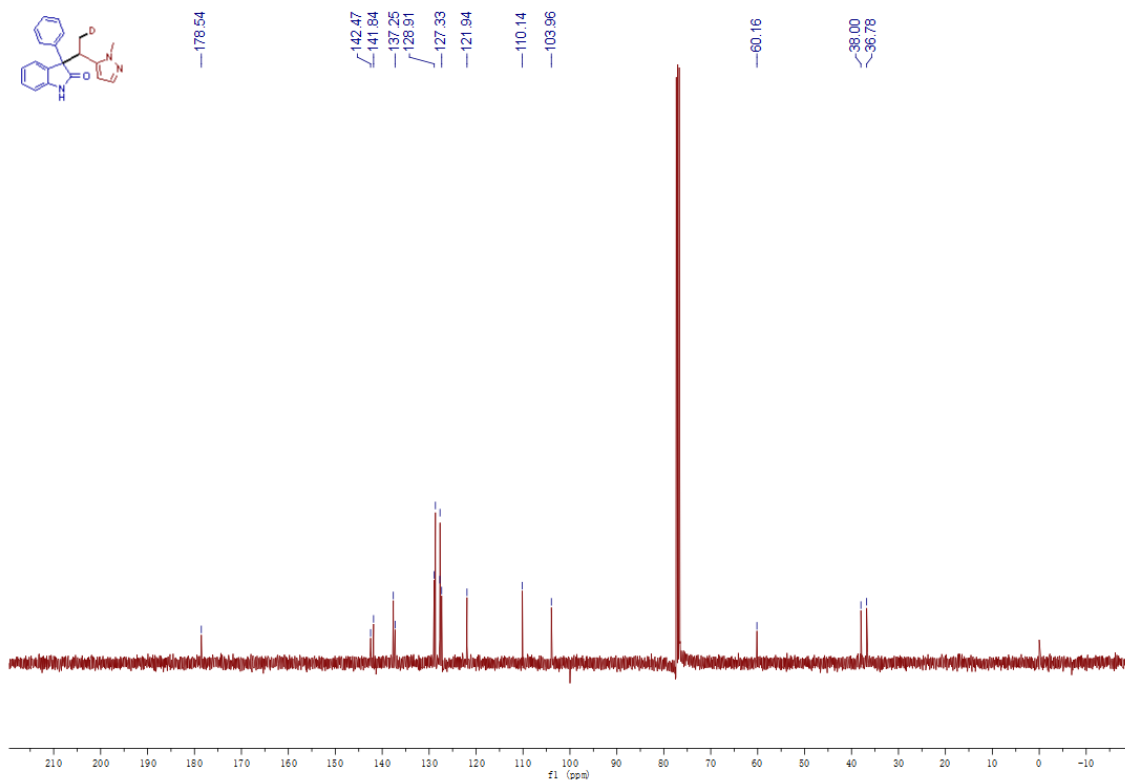
¹³C NMR spectrum of 3-(1-(1-methyl-1H-pyrazol-5-yl)ethyl-2-d)-3-phenylindolin-2-one. (57)



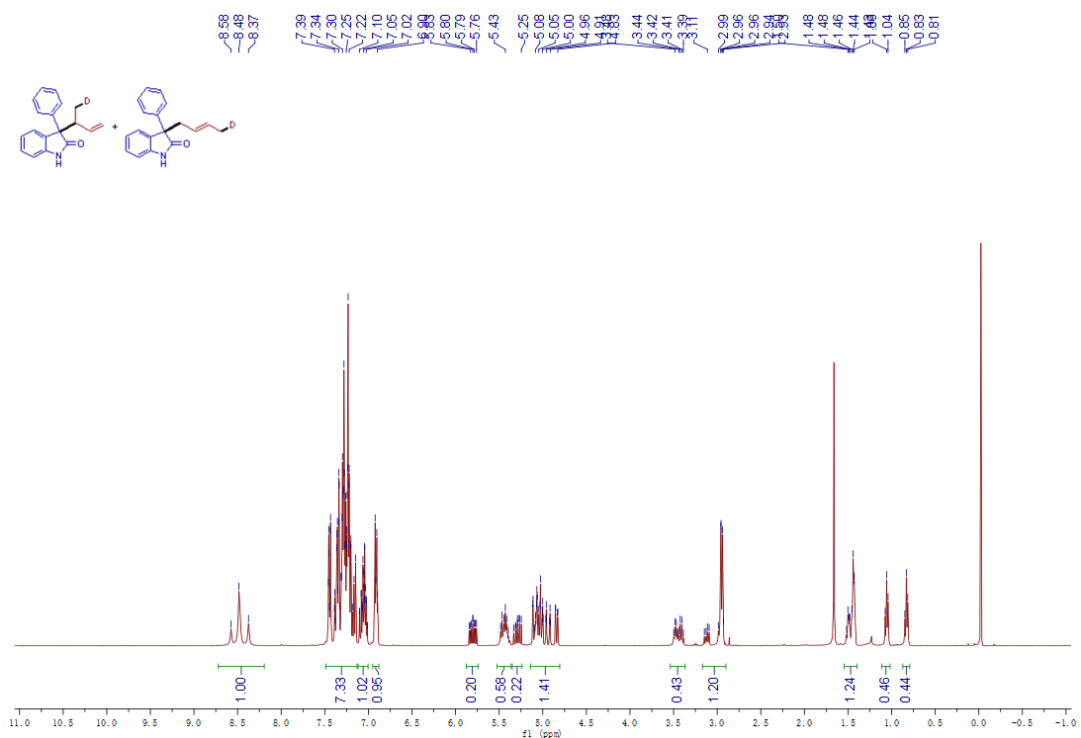
¹H NMR spectrum of 3-(1-(1-methyl-1H-pyrazol-5-yl)ethyl-2-d)-3-phenylindolin-2-one. (57)



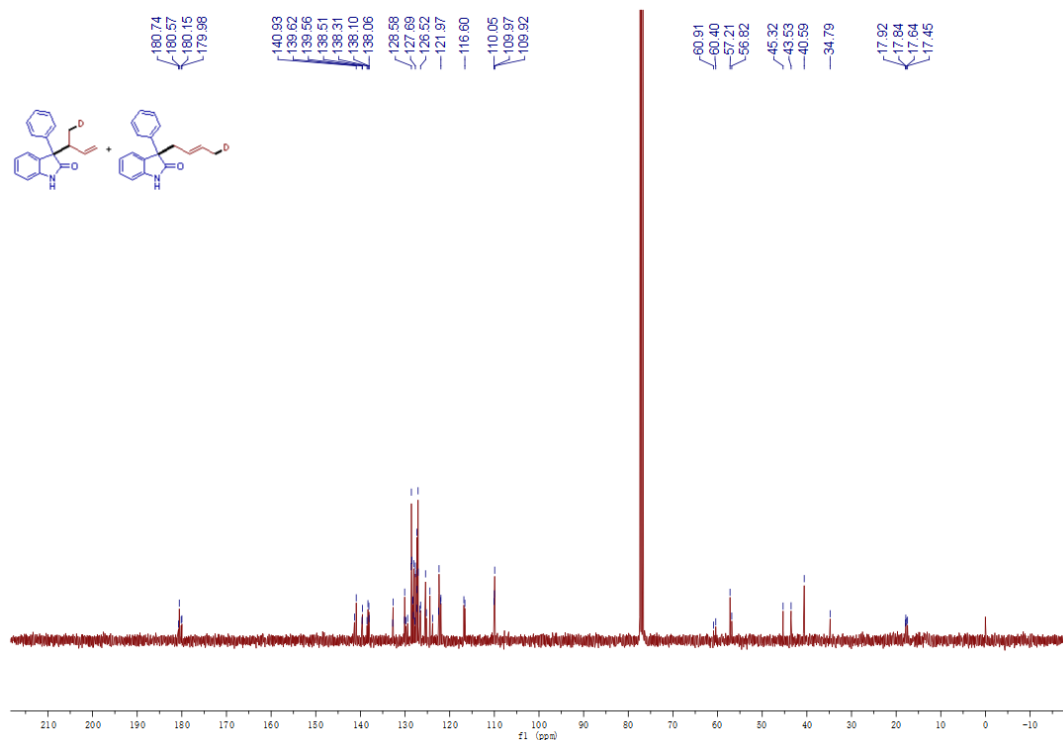
¹³C NMR spectrum of 3-(1-(1-methyl-1H-pyrazol-5-yl)ethyl-2-d)-3-phenylindolin-2-one. (57)



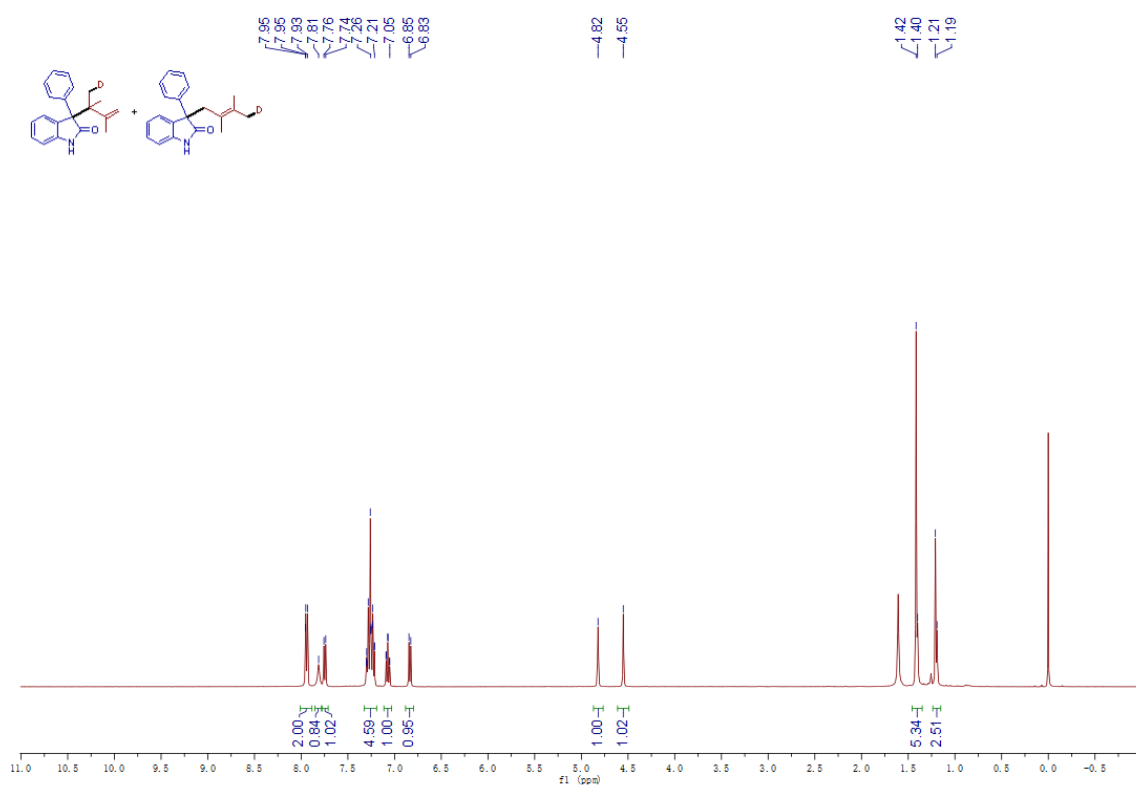
¹H NMR spectrum of 3-(but-3-en-2-yl-1-d)-3-phenylindolin-2-one and (E)-3-(but-2-en-1-yl-4-d)-3-phenylindolin-2-one. (58)



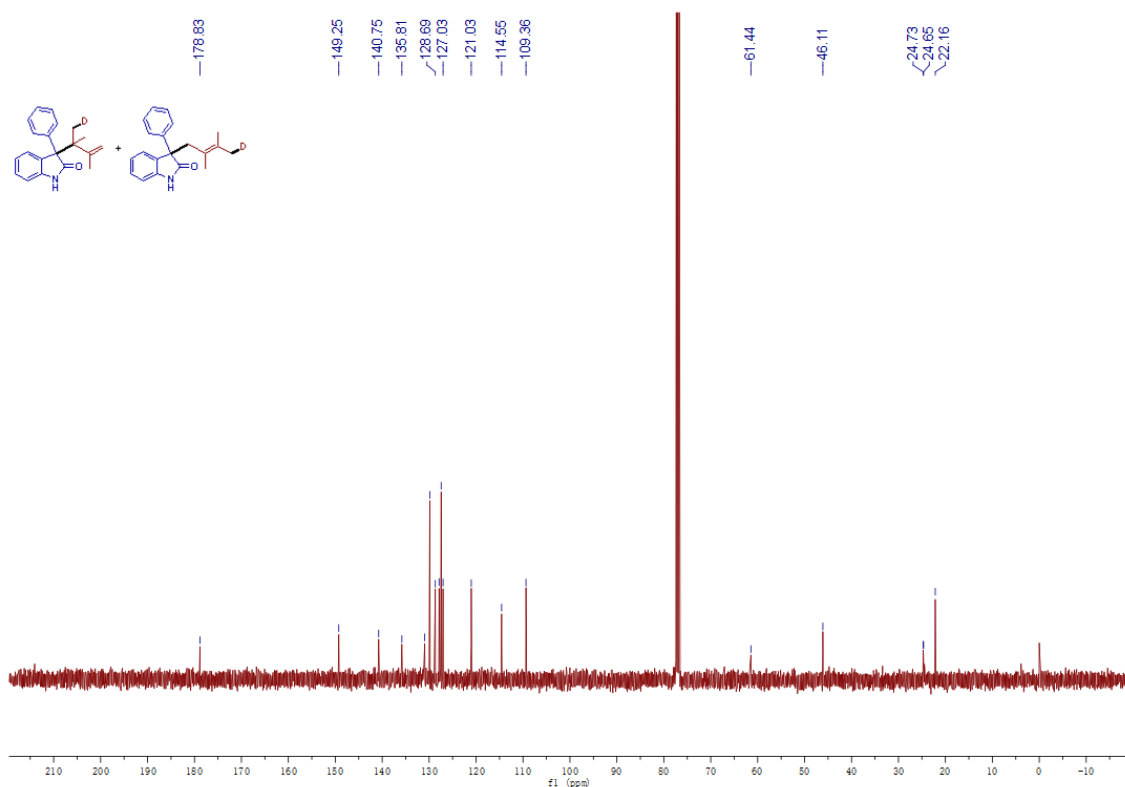
¹³C NMR spectrum of 3-(but-3-en-2-yl-1-d)-3-phenylindolin-2-one and (E)-3-(but-2-en-1-yl-4-d)-3-phenylindolin-2-one. (58)



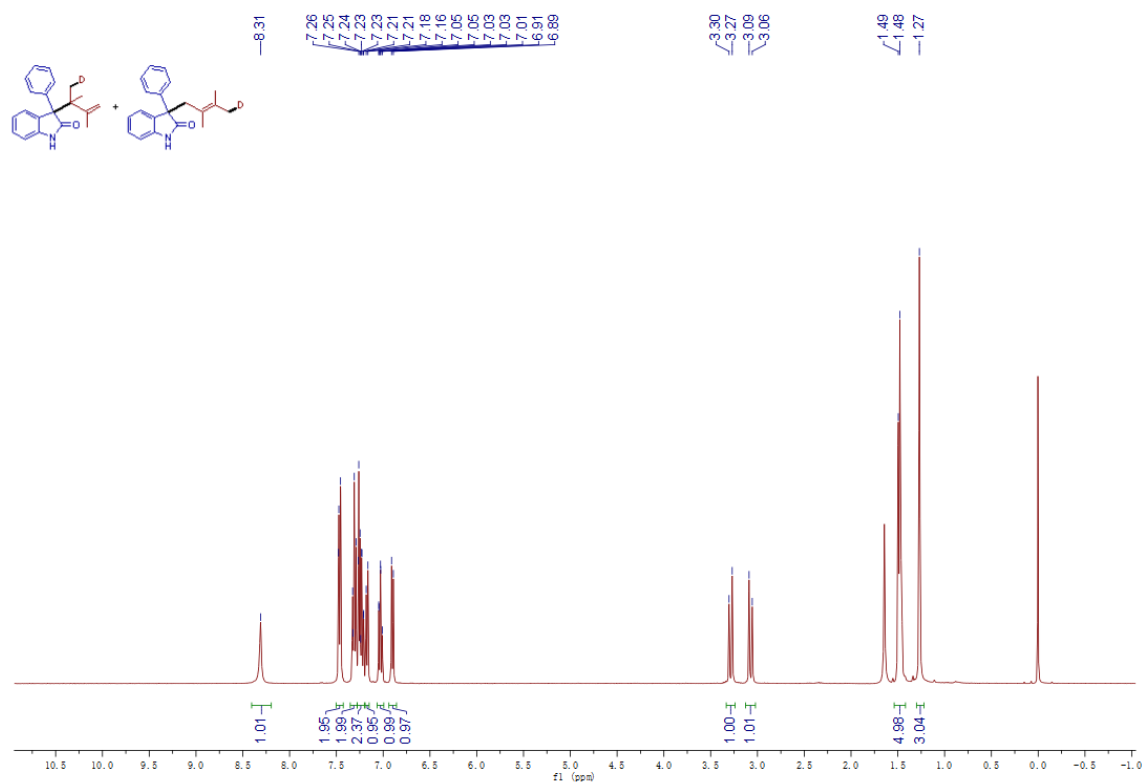
¹H NMR spectrum of 3-(2,3-dimethylbut-3-en-2-yl-1-d)-3-phenylindolin-2-one and (E)-3-(2,3-dimethylbut-2-en-1-yl-4-d)-3-phenylindolin-2-one. (59)



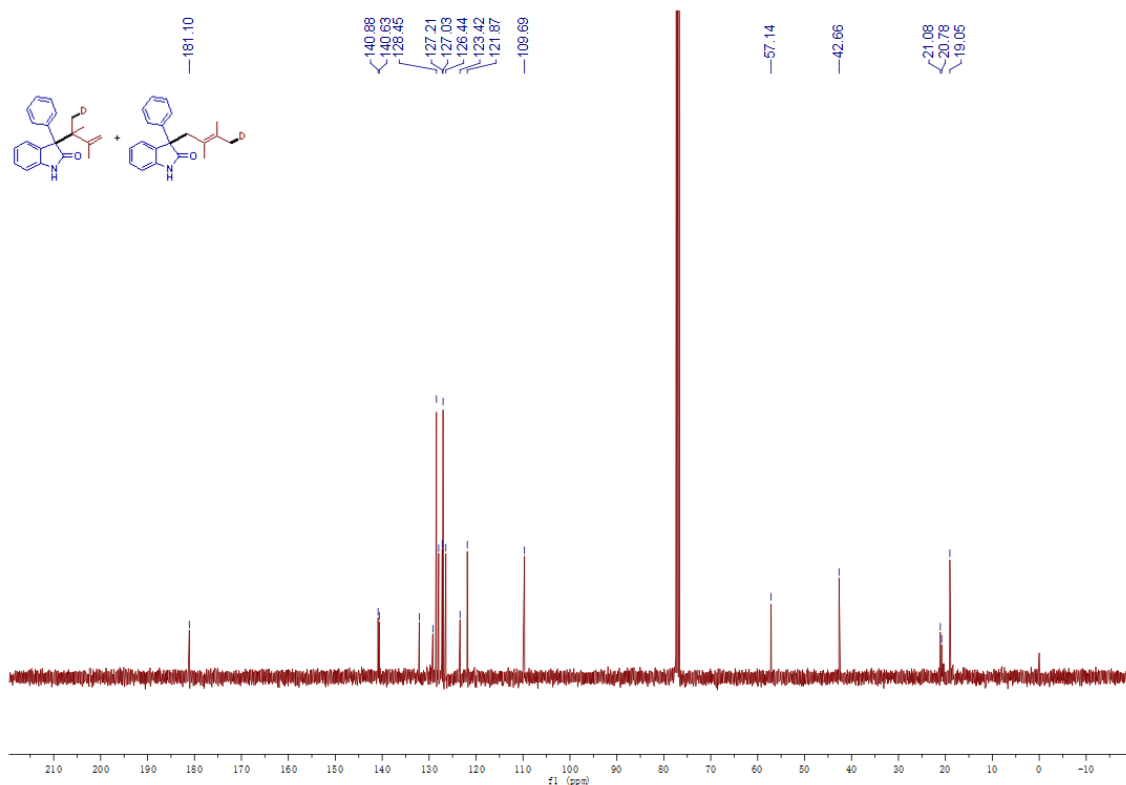
¹³C NMR spectrum of 3-(2,3-dimethylbut-3-en-2-yl-1-d)-3-phenylindolin-2-one and (E)-3-(2,3-dimethylbut-2-en-1-yl-4-d)-3-phenylindolin-2-one. (59)



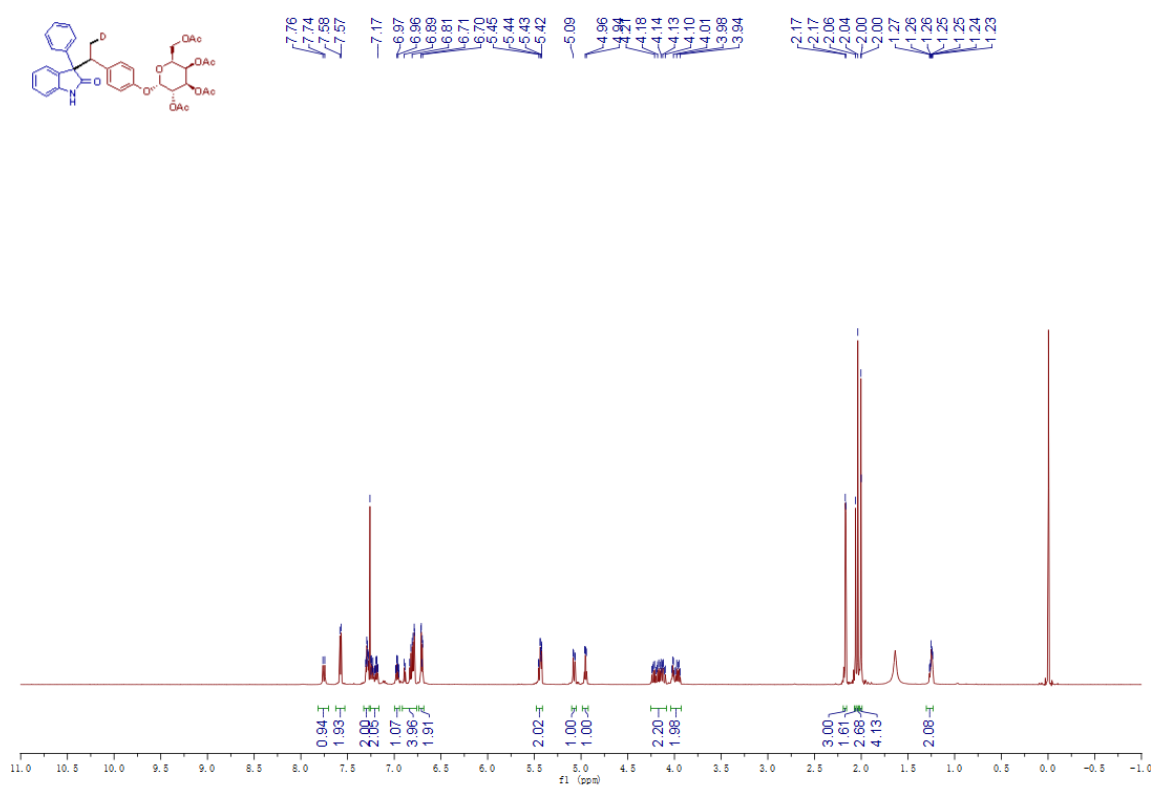
¹H NMR spectrum of 3-(2,3-dimethylbut-3-en-2-yl-1-d)-3-phenylindolin-2-one and (E)-3-(2,3-dimethylbut-2-en-1-yl-4-d)-3-phenylindolin-2-one. (59)



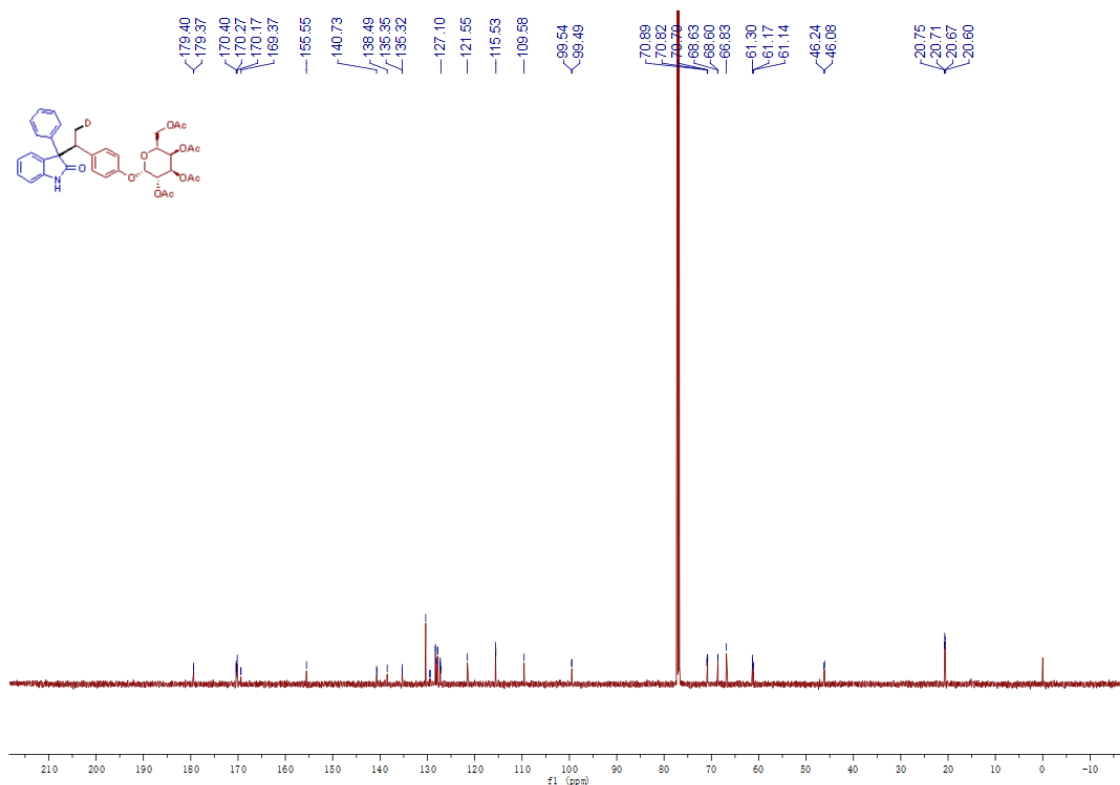
¹³C NMR spectrum of 3-(2,3-dimethylbut-3-en-2-yl-1-d)-3-phenylindolin-2-one and (E)-3-(2,3-dimethylbut-2-en-1-yl-4-d)-3-phenylindolin-2-one. (59)



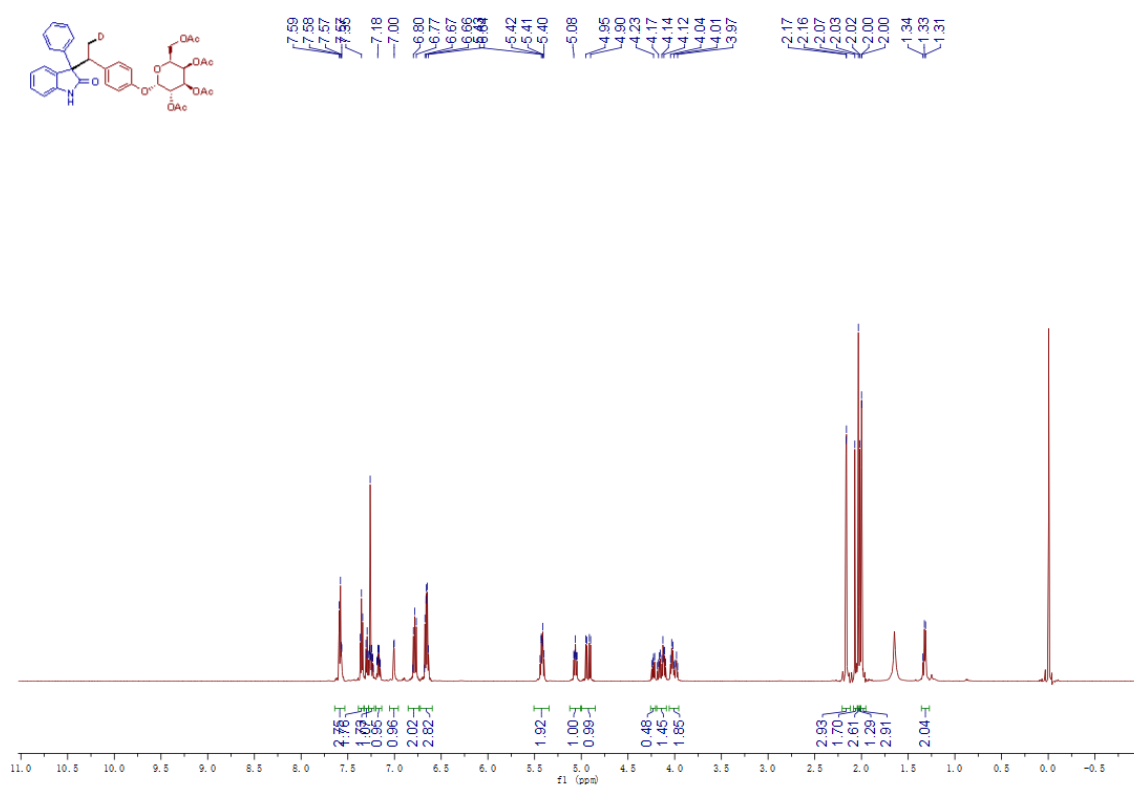
¹H NMR spectrum of (2S,3R,4R,5S,6S)-2-(acetoxymethyl)-6-(4-(1-(2-oxo-3-phenylindolin-3-yl)ethyl-2-d)phenoxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate. (60)



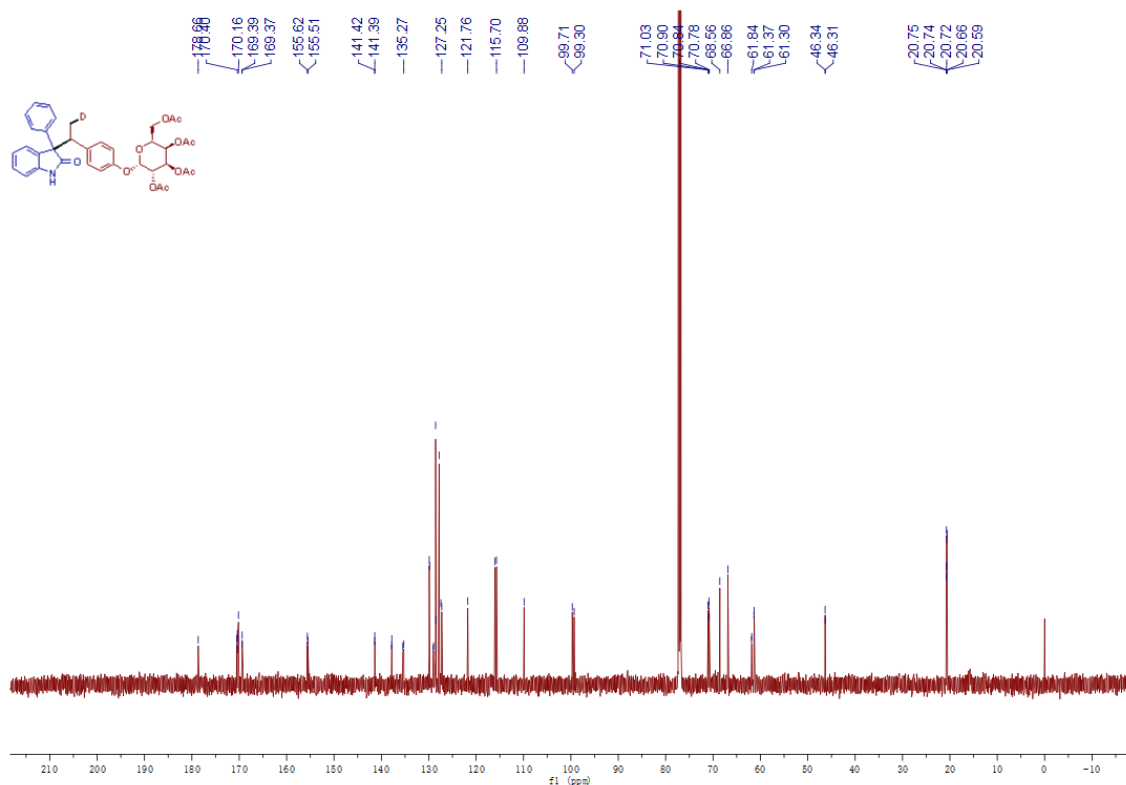
¹³C NMR spectrum of (2S,3R,4R,5S,6S)-2-(acetoxymethyl)-6-(4-(1-(2-oxo-3-phenylindolin-3-yl)ethyl-2-d)phenoxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate. (60)



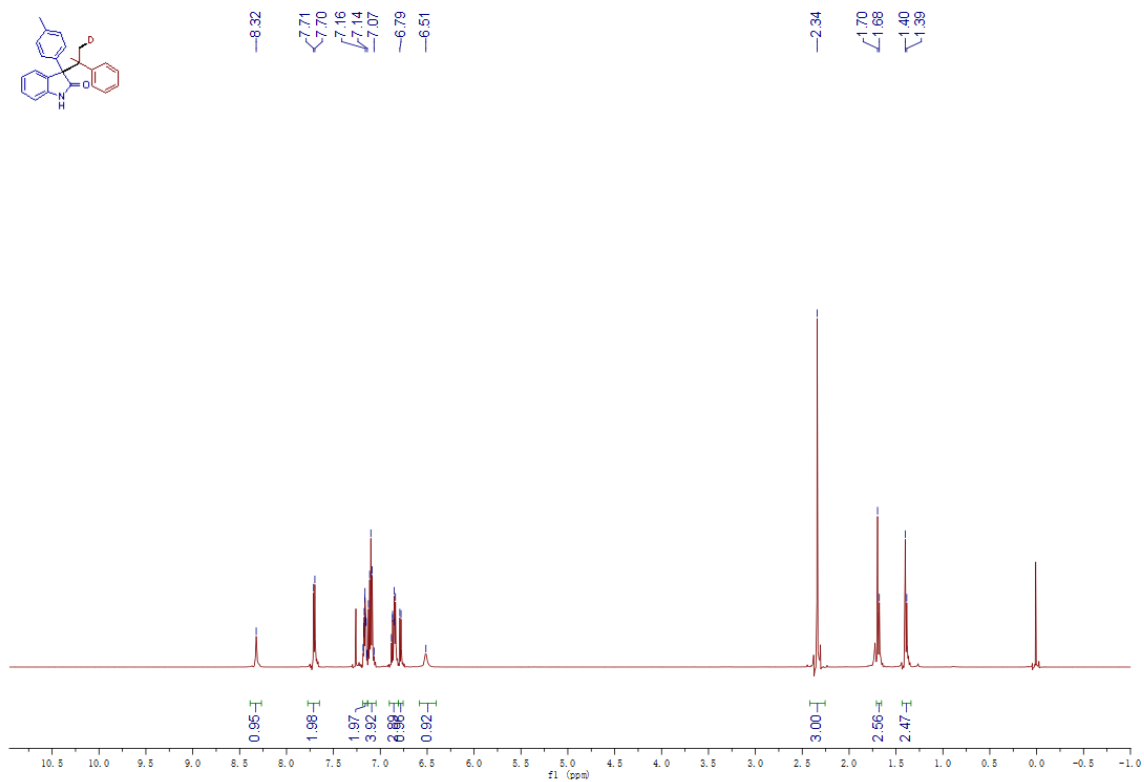
¹H NMR spectrum of (2S,3R,4R,5S,6S)-2-(acetoxymethyl)-6-(4-(1-(2-oxo-3-phenylindolin-3-yl)ethyl-2-d)phenoxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate. (60)



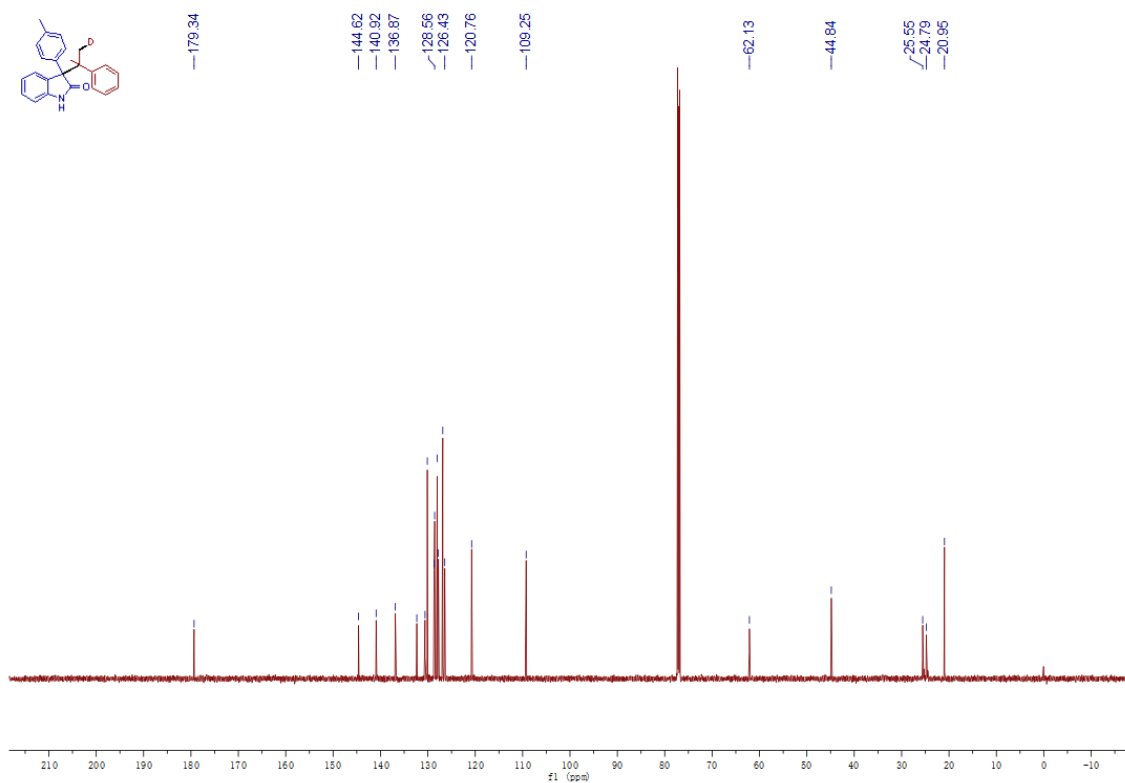
¹³C NMR spectrum of (2S,3R,4R,5S,6S)-2-(acetoxymethyl)-6-(4-(1-(2-oxo-3-phenylindolin-3-yl)ethyl-2-d)phenoxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate. (60)



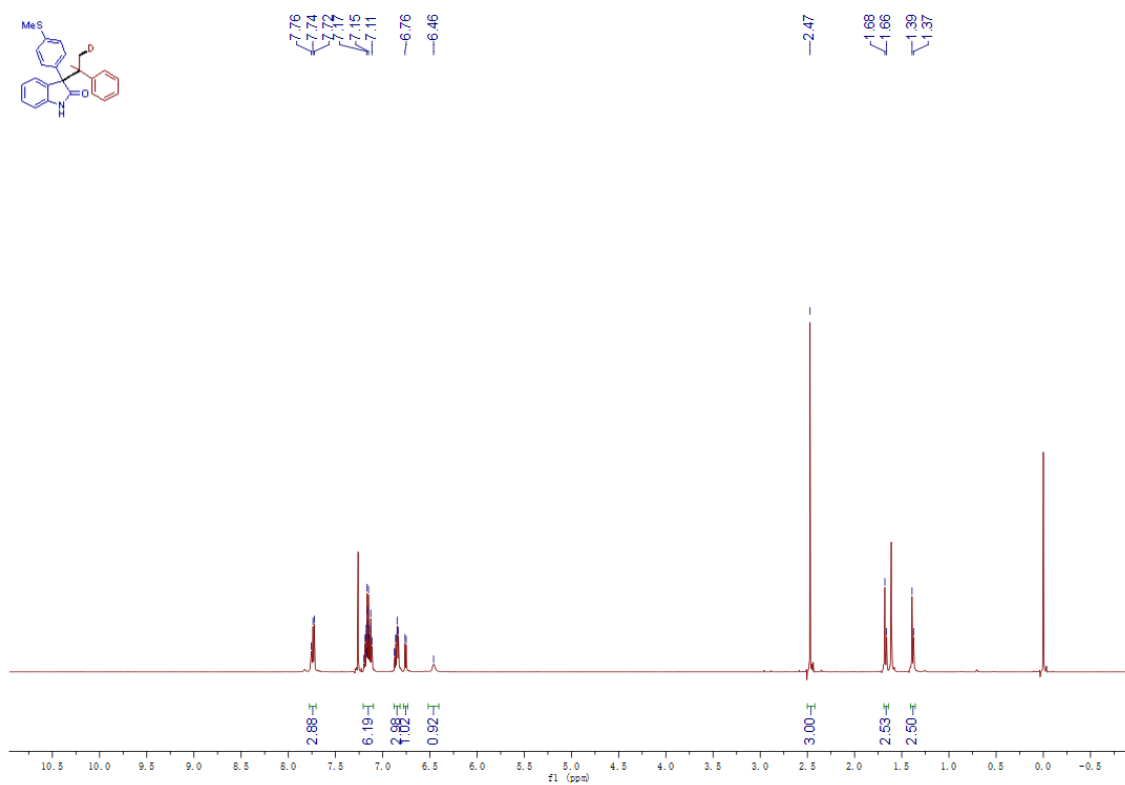
¹H NMR spectrum of 3-(2-phenylpropan-2-yl-1-d)-3-(p-tolyl)indolin-2-one. (61)



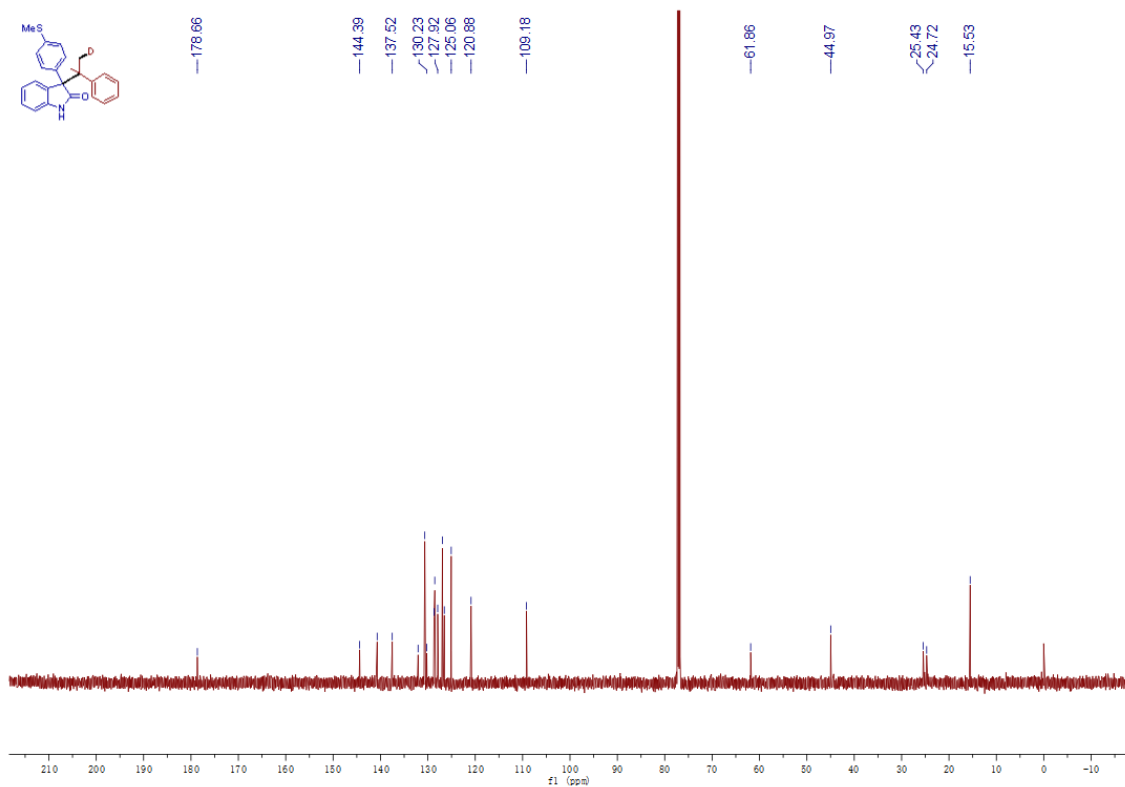
¹³C NMR spectrum of 3-(2-phenylpropan-2-yl-1-d)-3-(p-tolyl)indolin-2-one. (61)



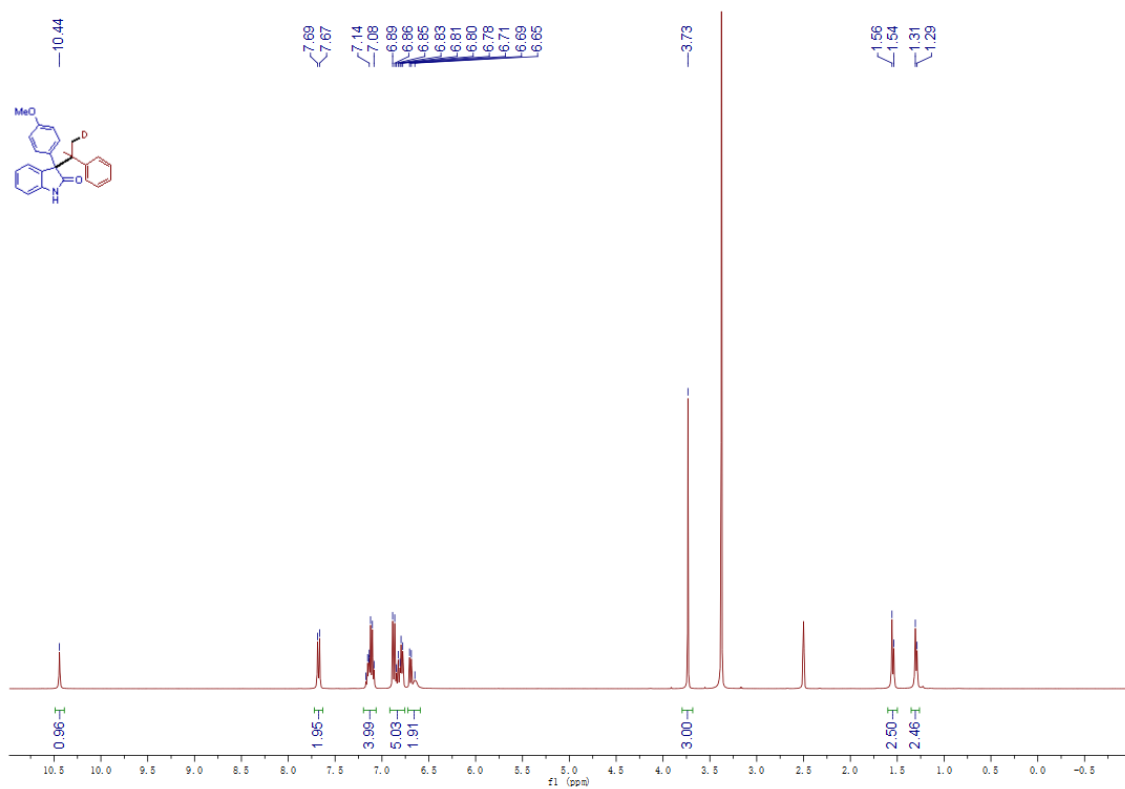
¹H NMR spectrum of 3-(4-(methylthio)phenyl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (62)



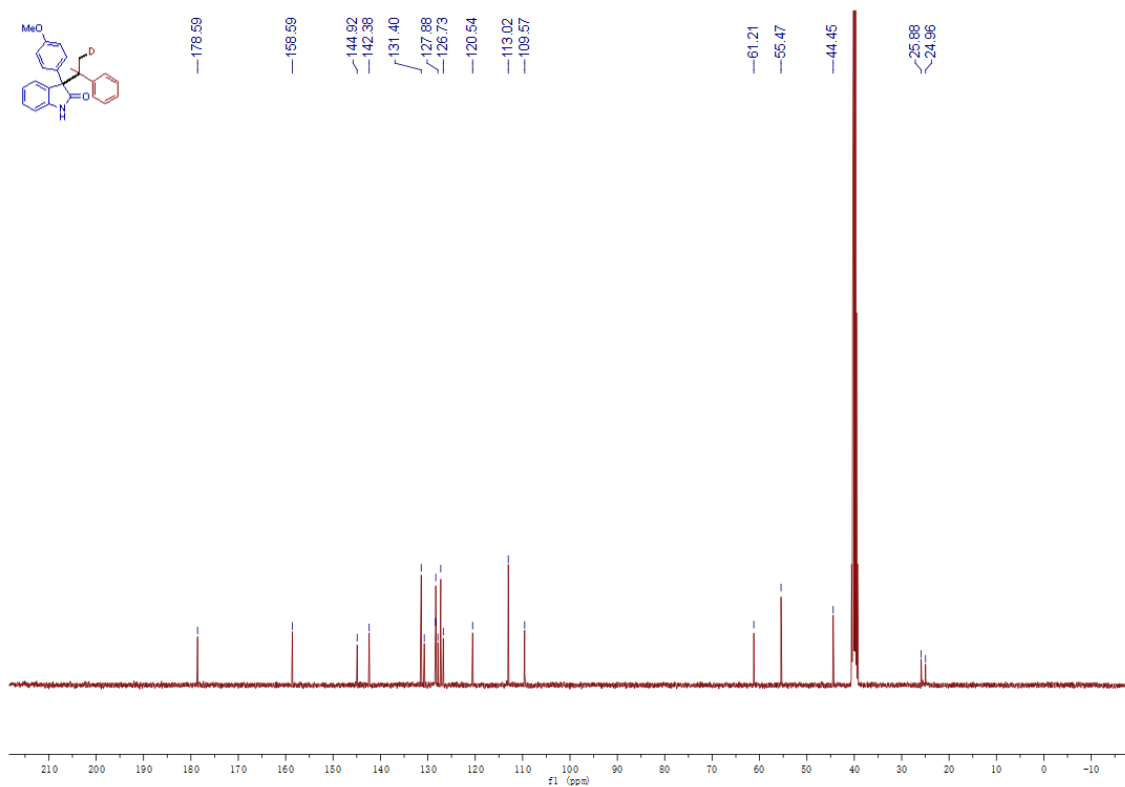
¹³C NMR spectrum of 3-(4-(methylthio)phenyl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (62)



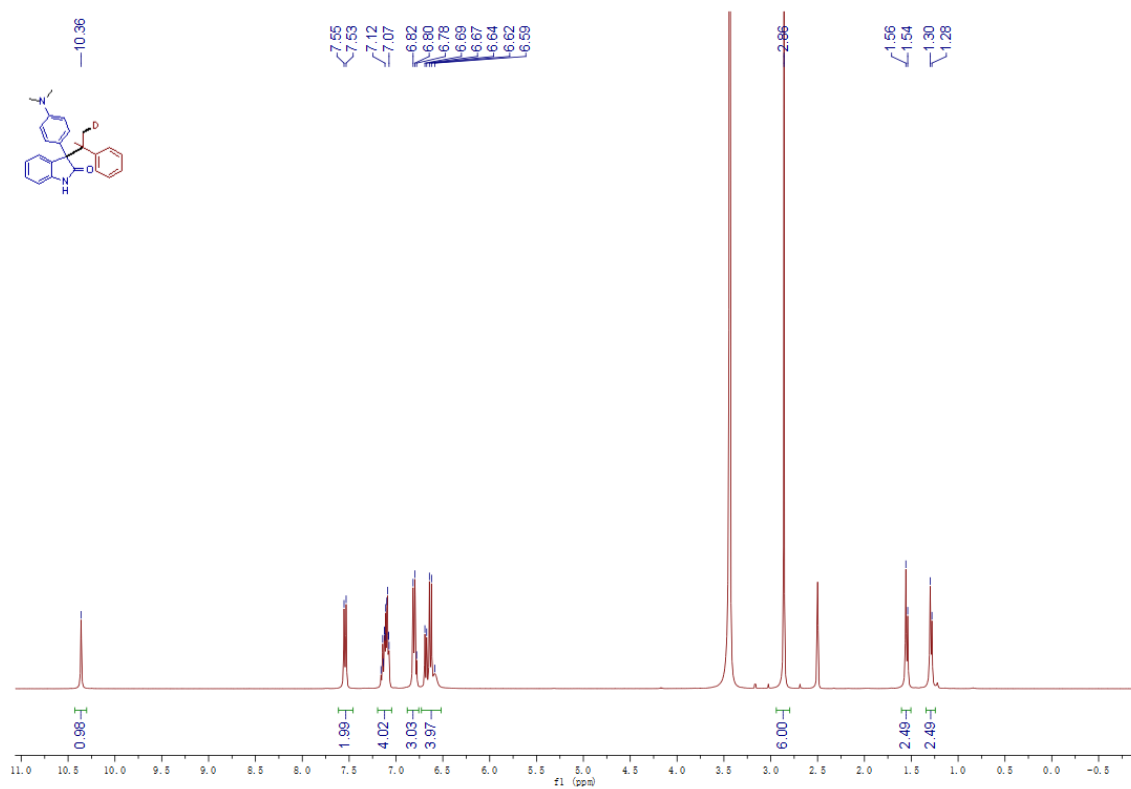
¹H NMR spectrum of 3-(4-methoxyphenyl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (63)



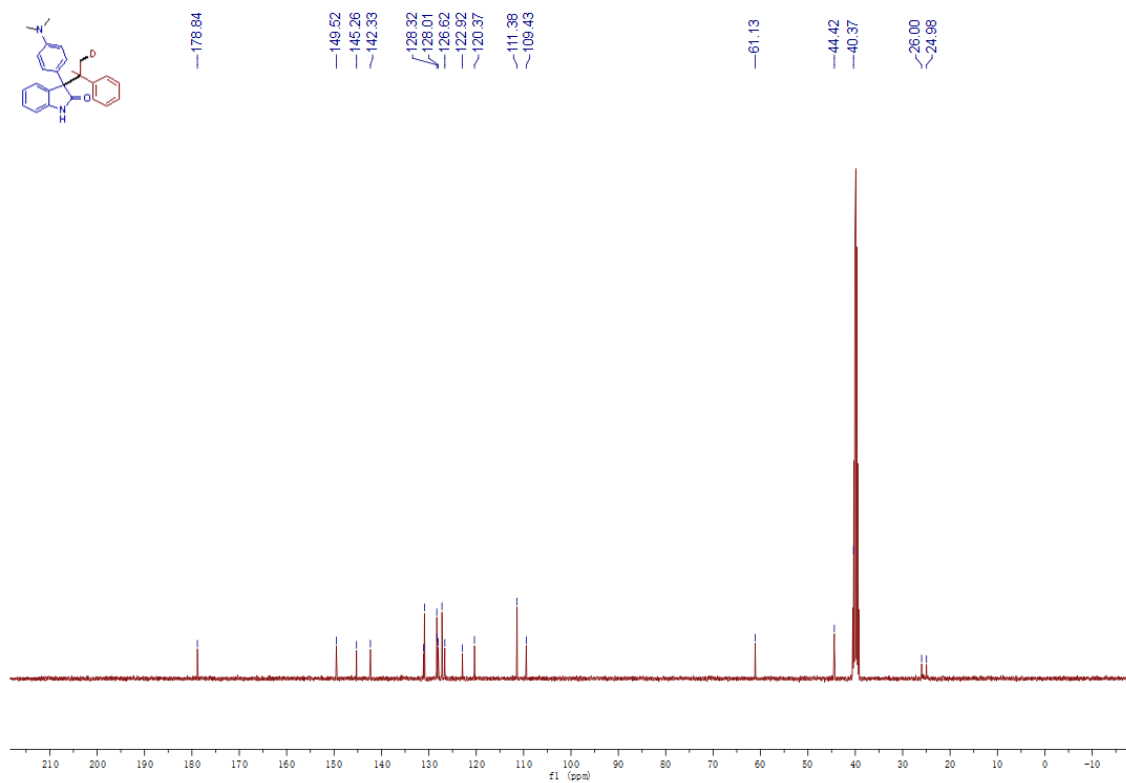
¹³C NMR spectrum of 3-(4-methoxyphenyl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (63)



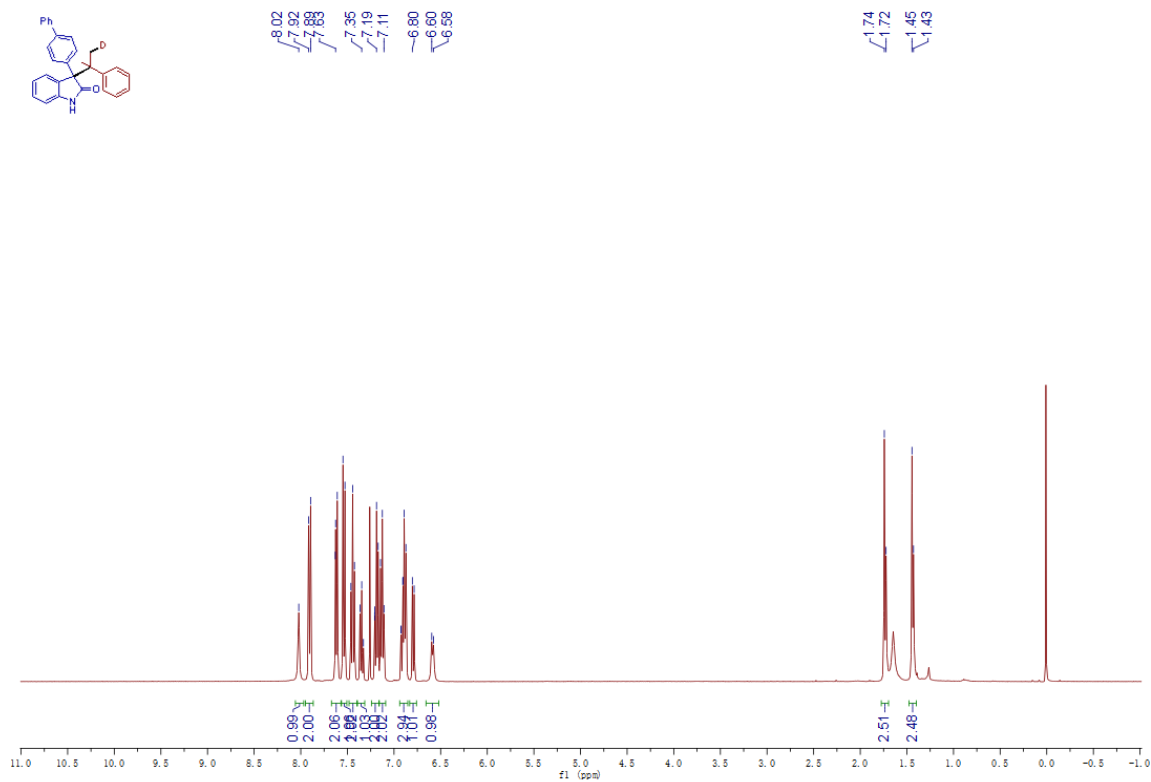
¹H NMR spectrum of 3-(4-(dimethylamino)phenyl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (64)



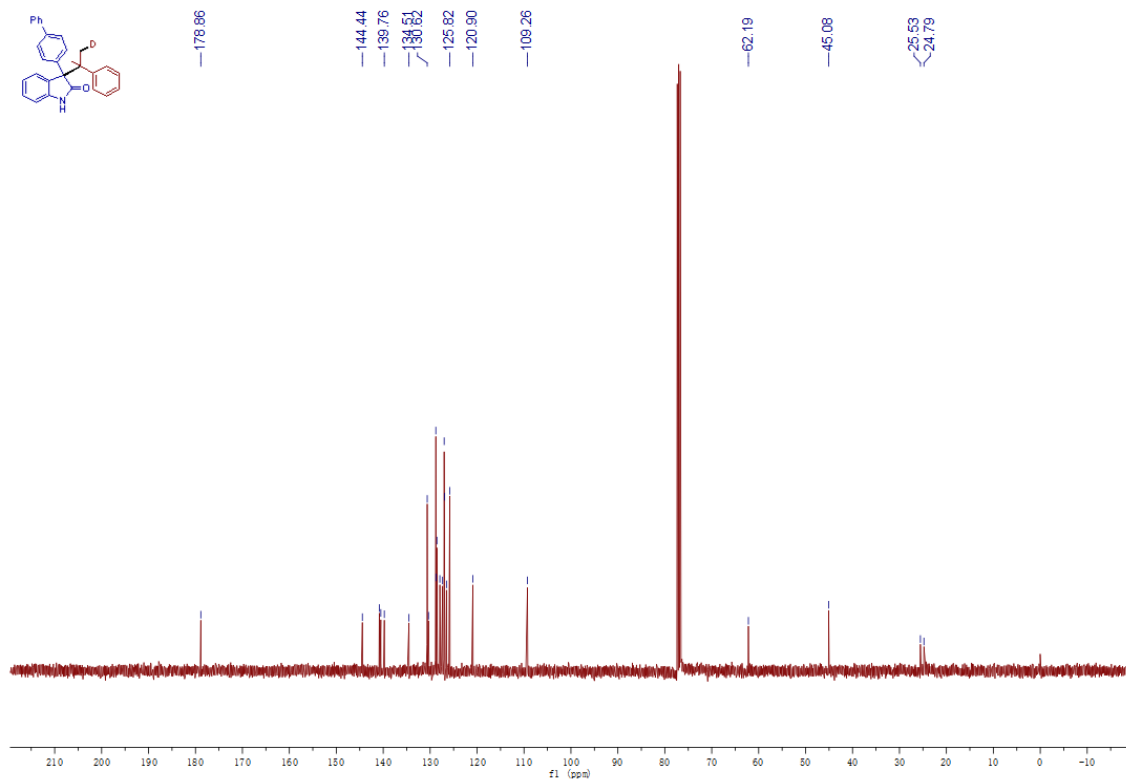
¹³C NMR spectrum of 3-(4-(dimethylamino)phenyl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (64)



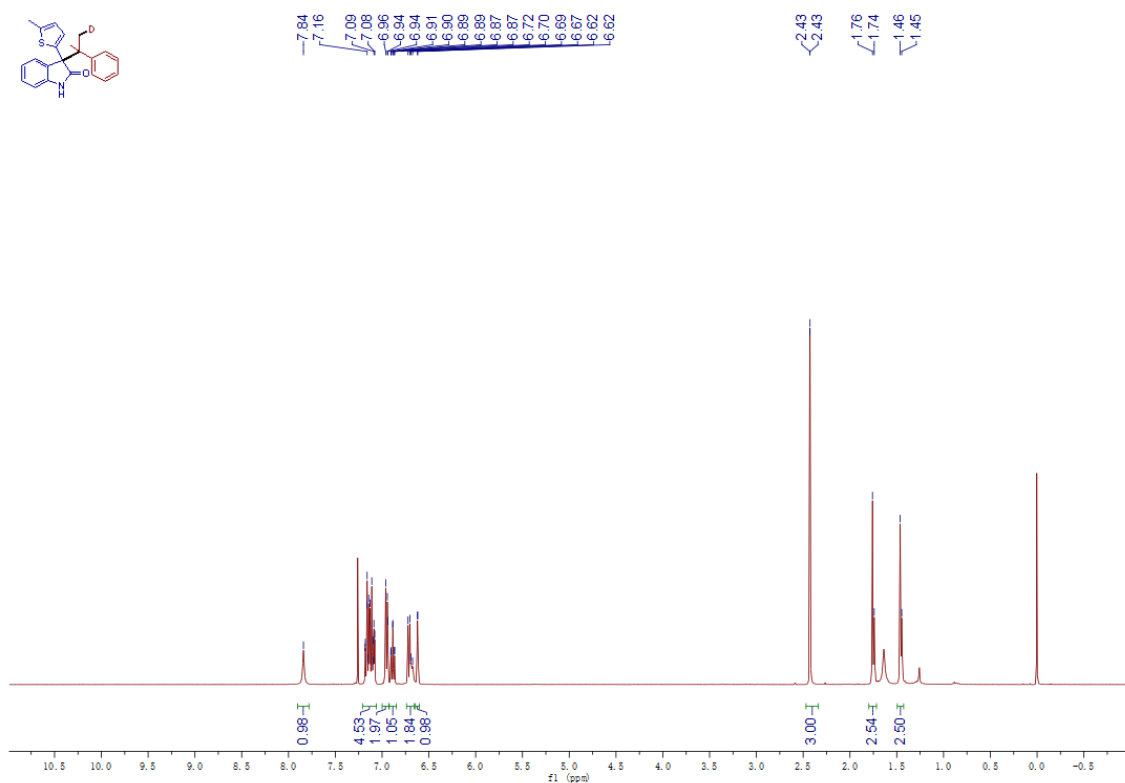
¹H NMR spectrum of 3-([1,1'-biphenyl]-4-yl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (65)



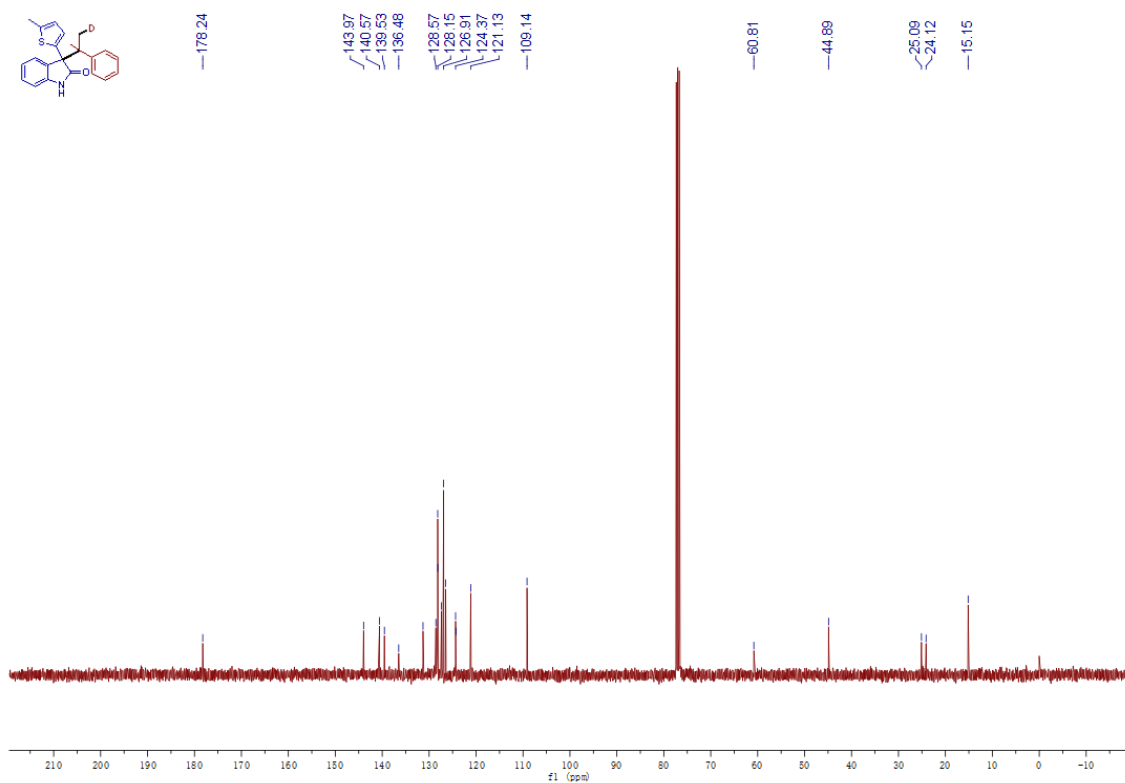
¹³C NMR spectrum of 3-([1,1'-biphenyl]-4-yl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (65)



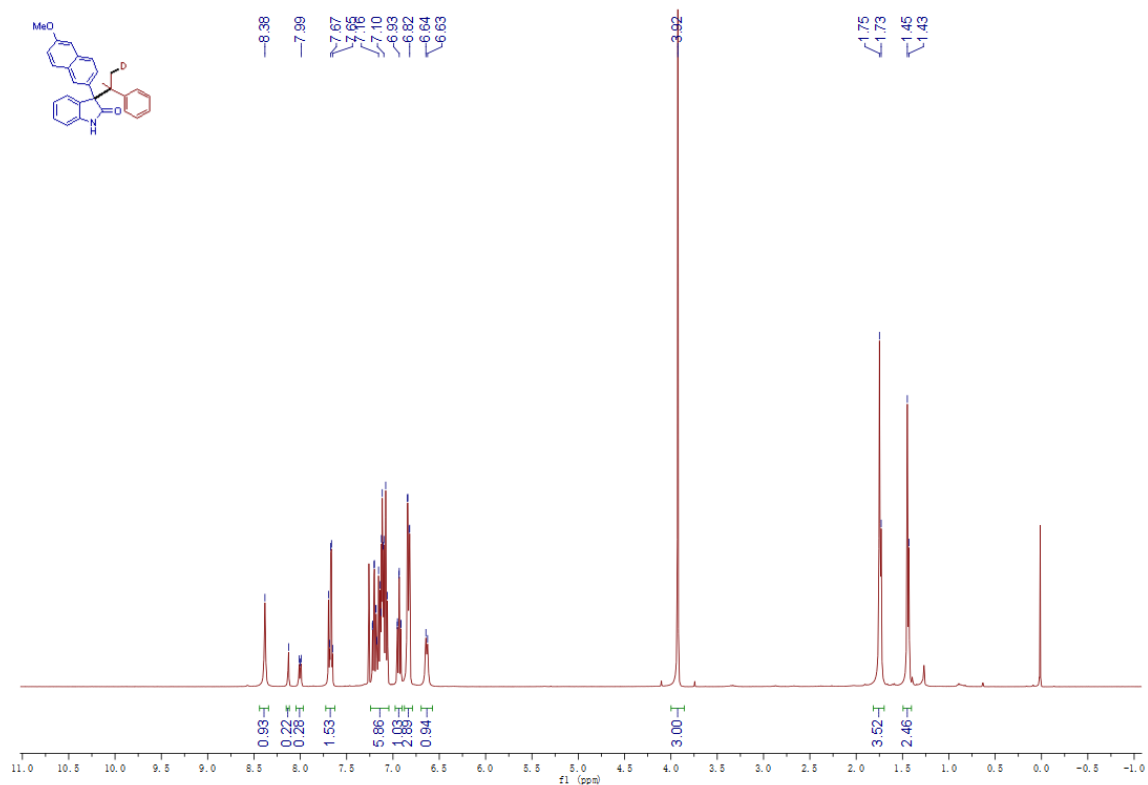
¹H NMR spectrum of 3-(5-methylthiophen-2-yl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (66)



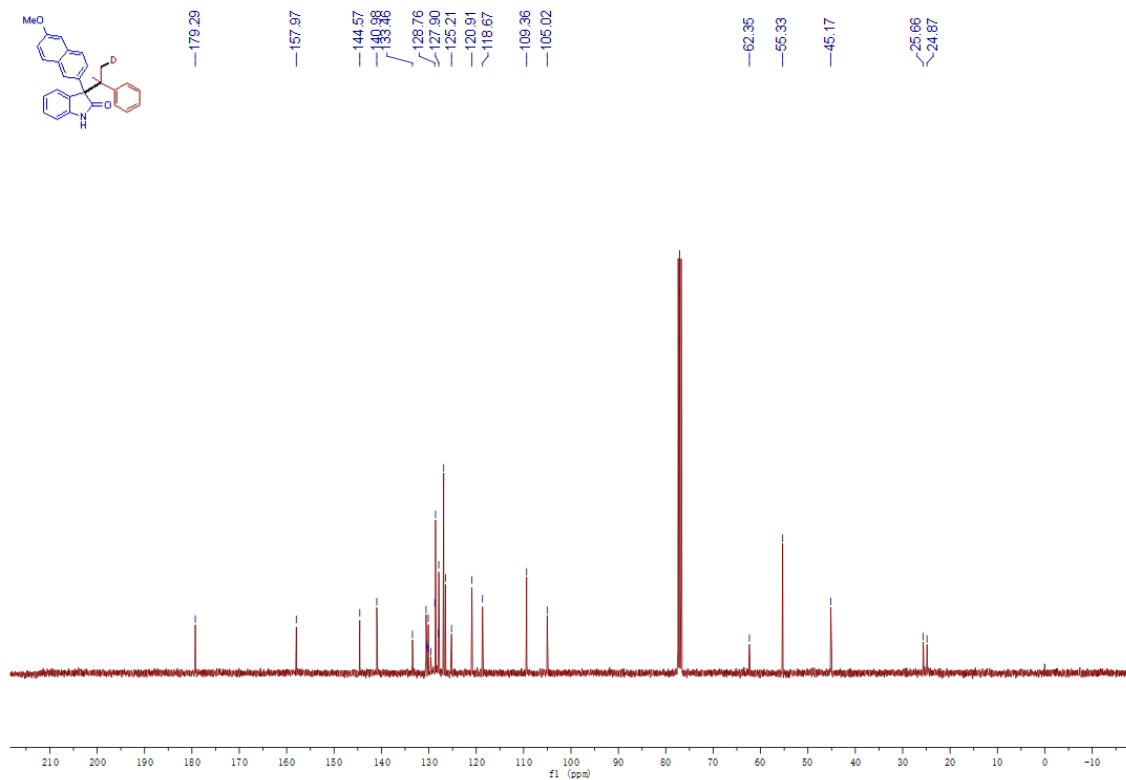
¹³C NMR spectrum of 3-(5-methylthiophen-2-yl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (66)



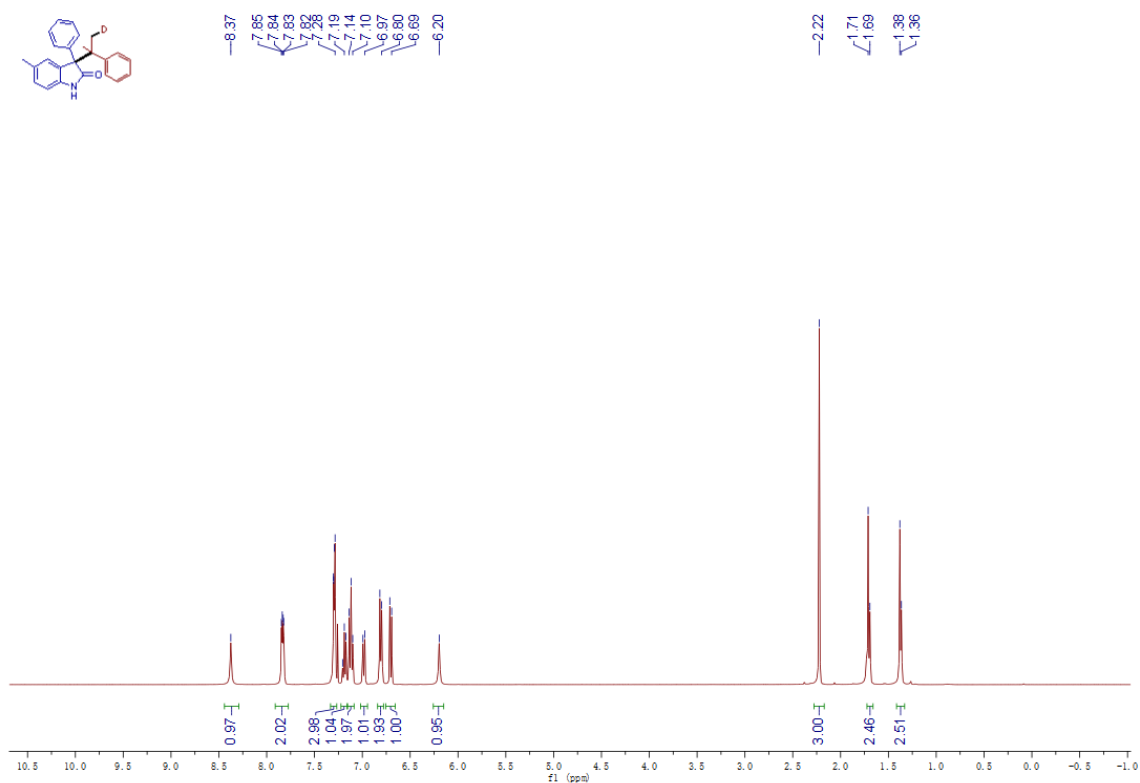
¹H NMR spectrum of 3-(6-methoxynaphthalen-2-yl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (67)



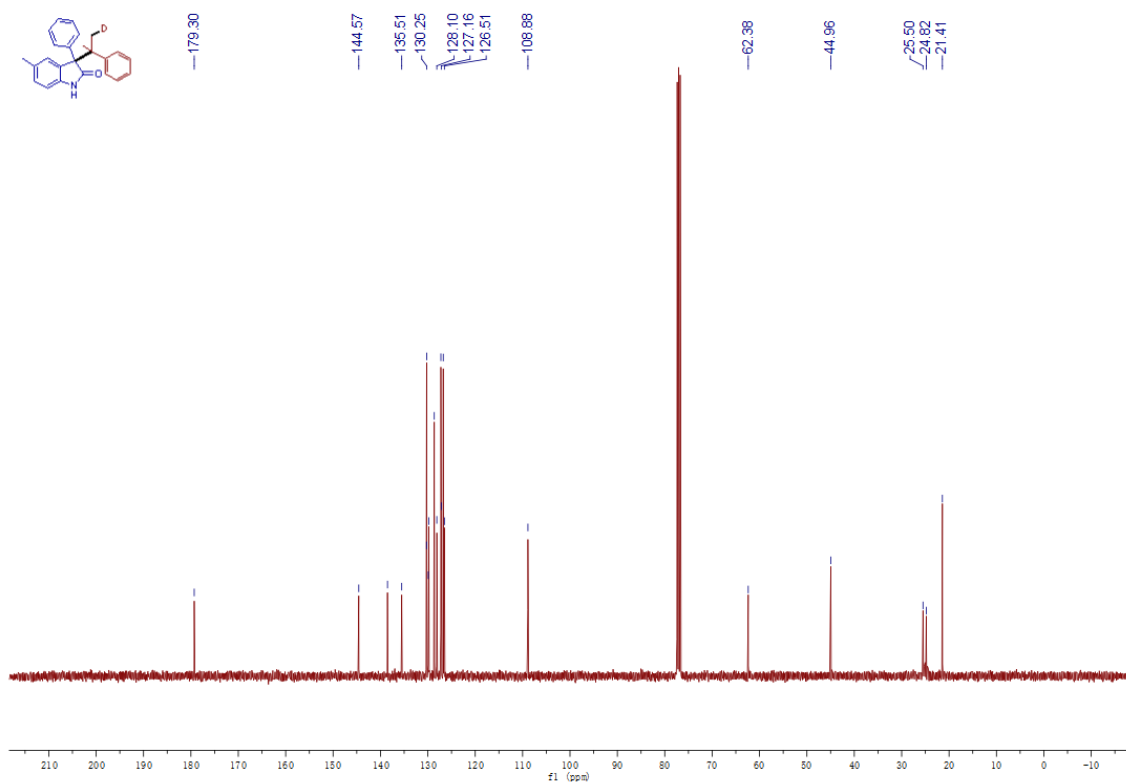
¹³C NMR spectrum of 3-(6-methoxynaphthalen-2-yl)-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (67)



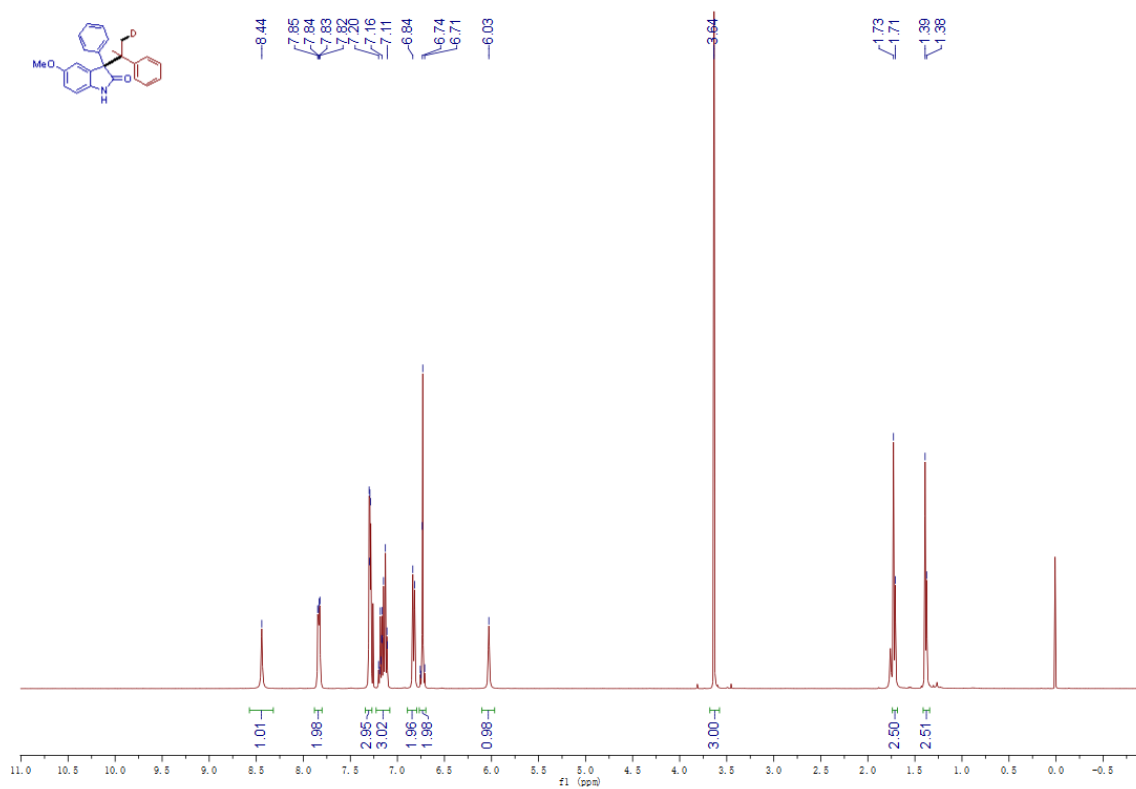
¹H NMR spectrum of 5-methyl-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (68)



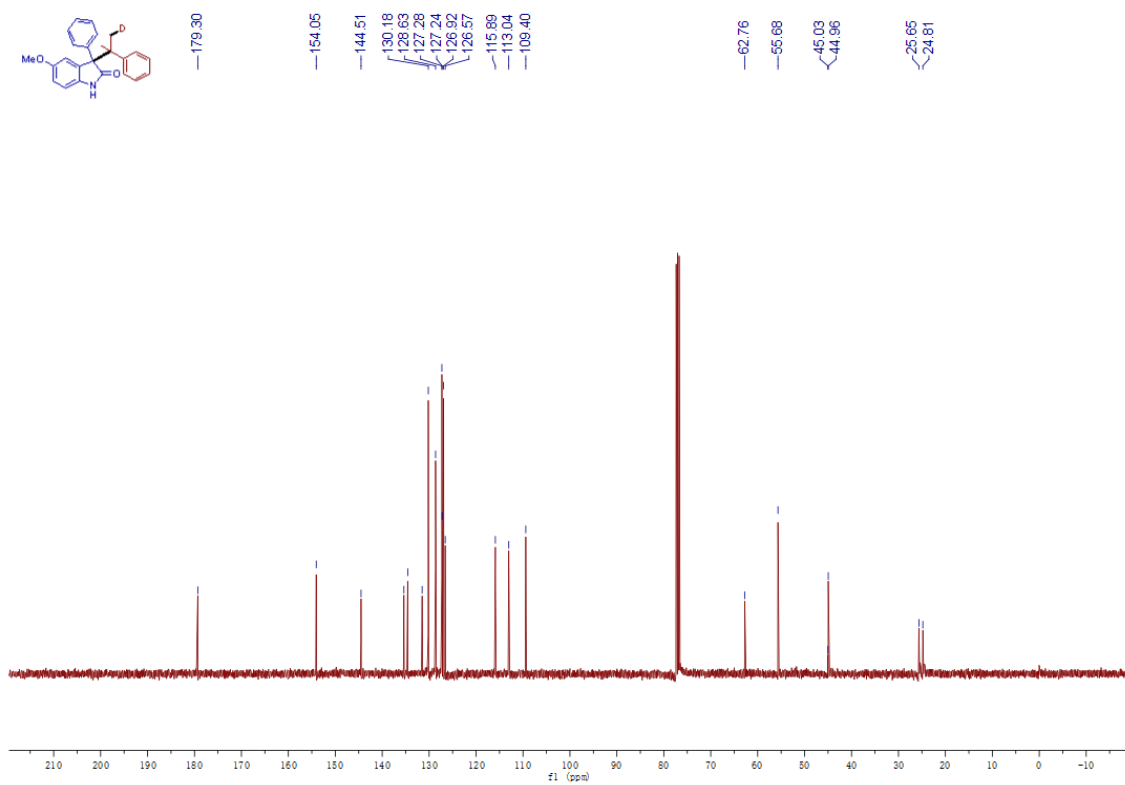
¹³C NMR spectrum of 5-methyl-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (68)



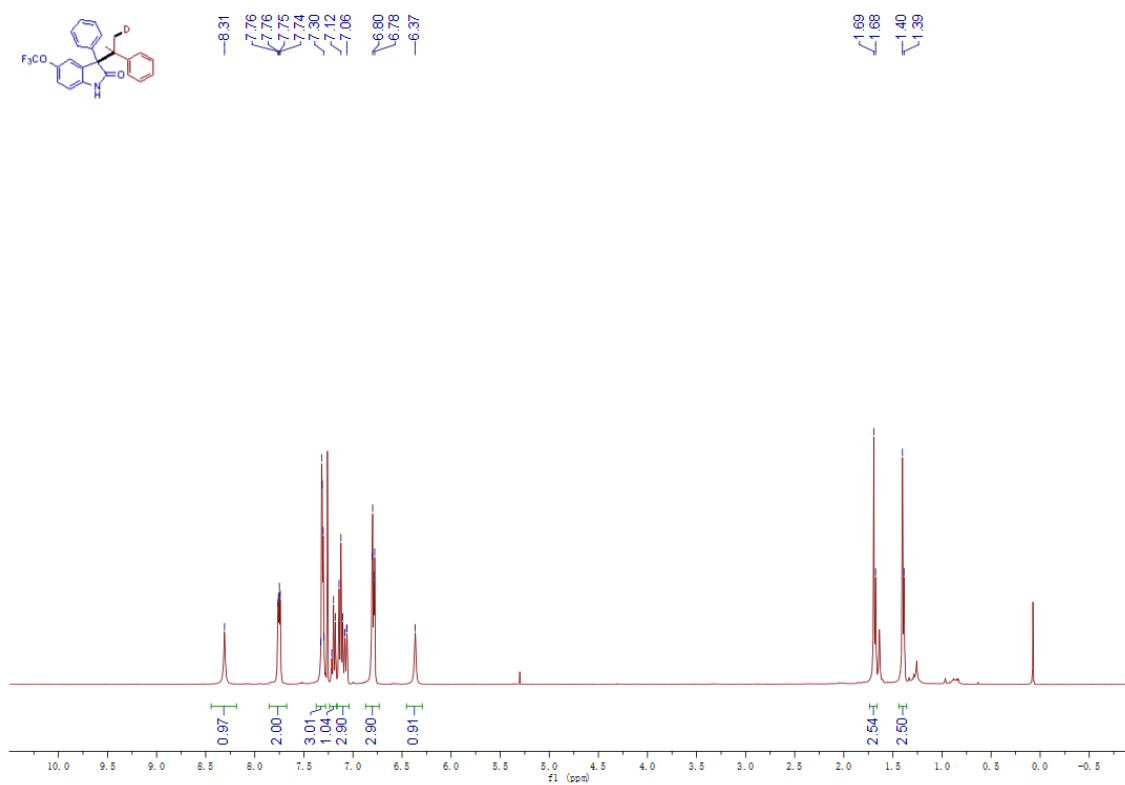
¹H NMR spectrum of 5-methoxy-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (69)



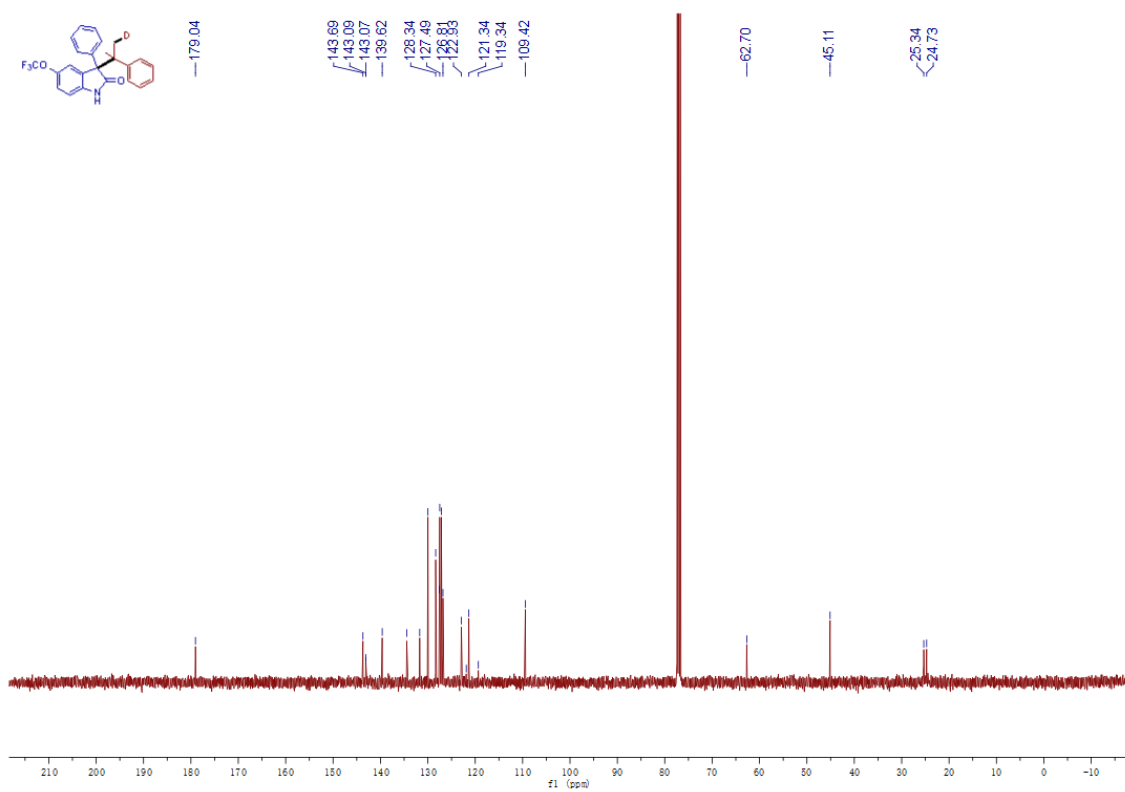
¹³C NMR spectrum of 5-methoxy-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (69)



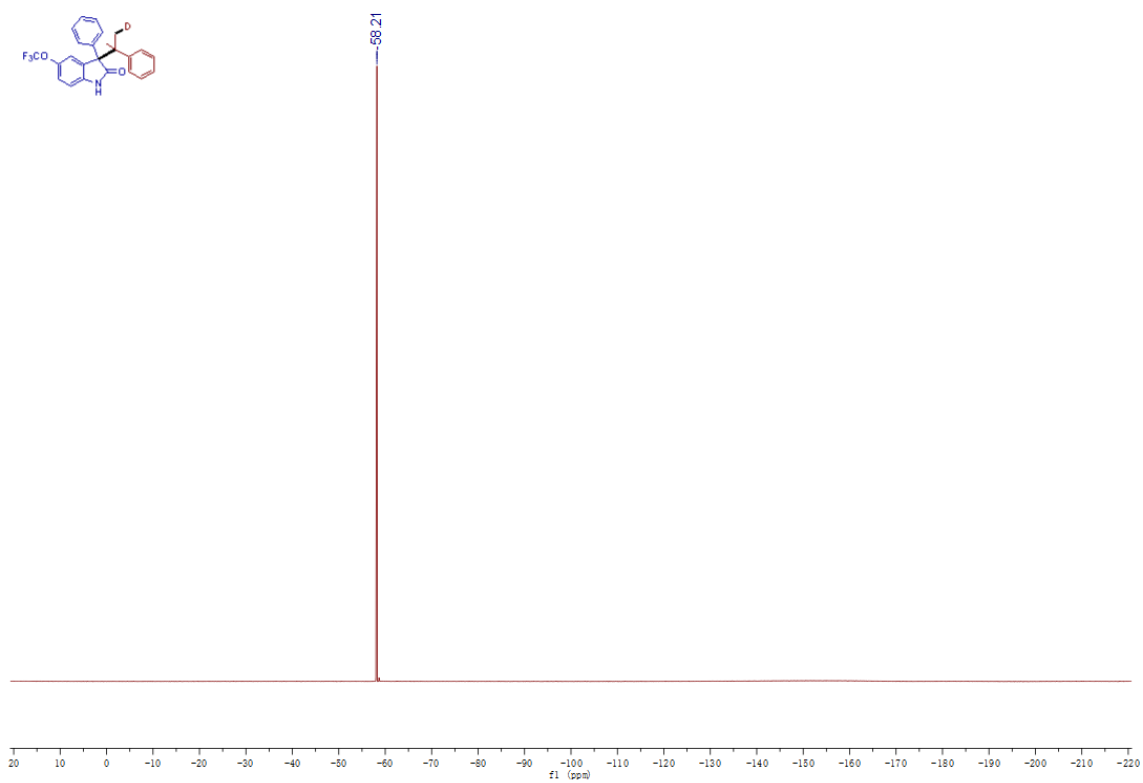
¹H NMR spectrum of 3-phenyl-3-(2-phenylpropan-2-yl-1-d)-5-(trifluoromethoxy)indolin-2-one. (70)



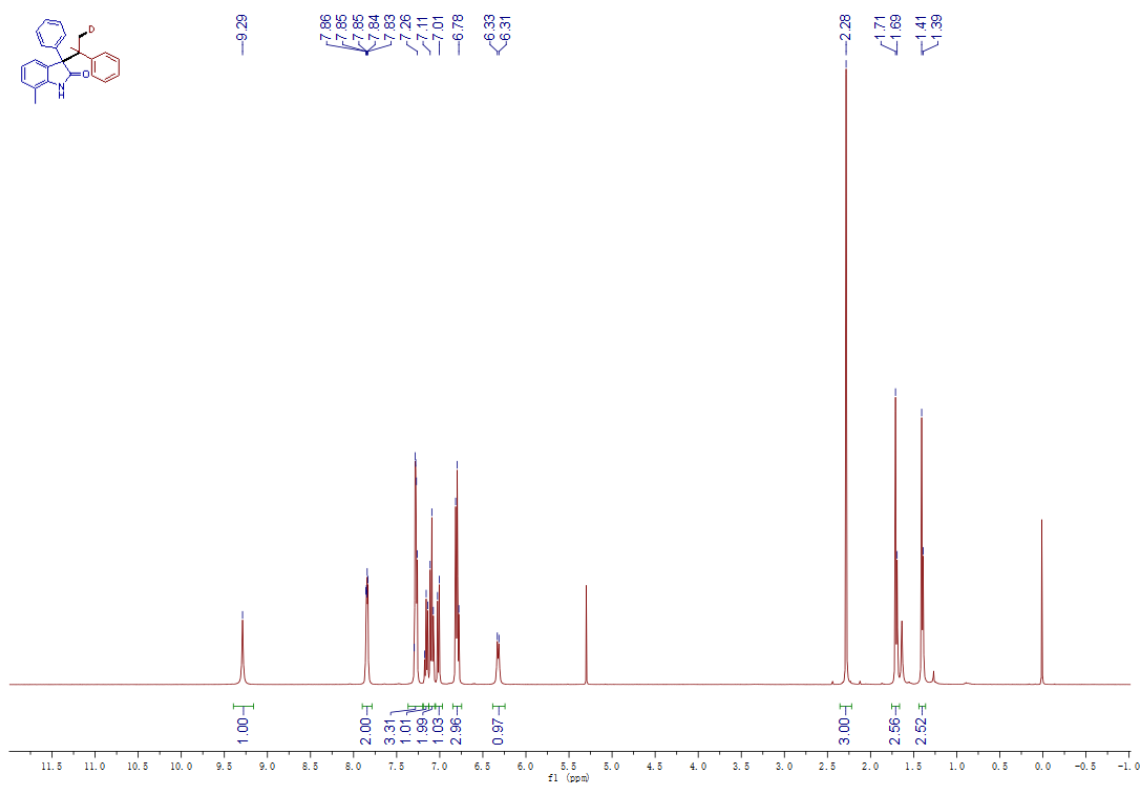
¹³C NMR spectrum of 3-phenyl-3-(2-phenylpropan-2-yl-1-d)-5-(trifluoromethoxy)indolin-2-one. (70)



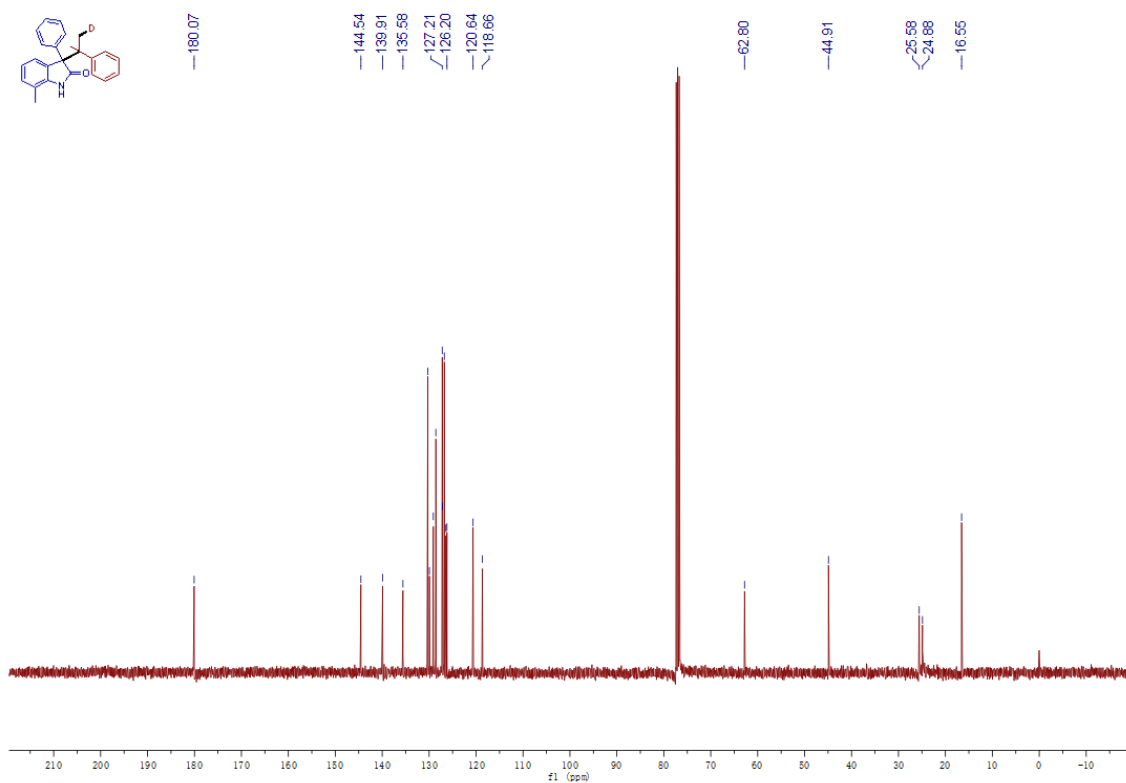
¹⁹F NMR spectrum of 3-phenyl-3-(2-phenylpropan-2-yl-1-d)-5-(trifluoromethoxy)indolin-2-one. (70)



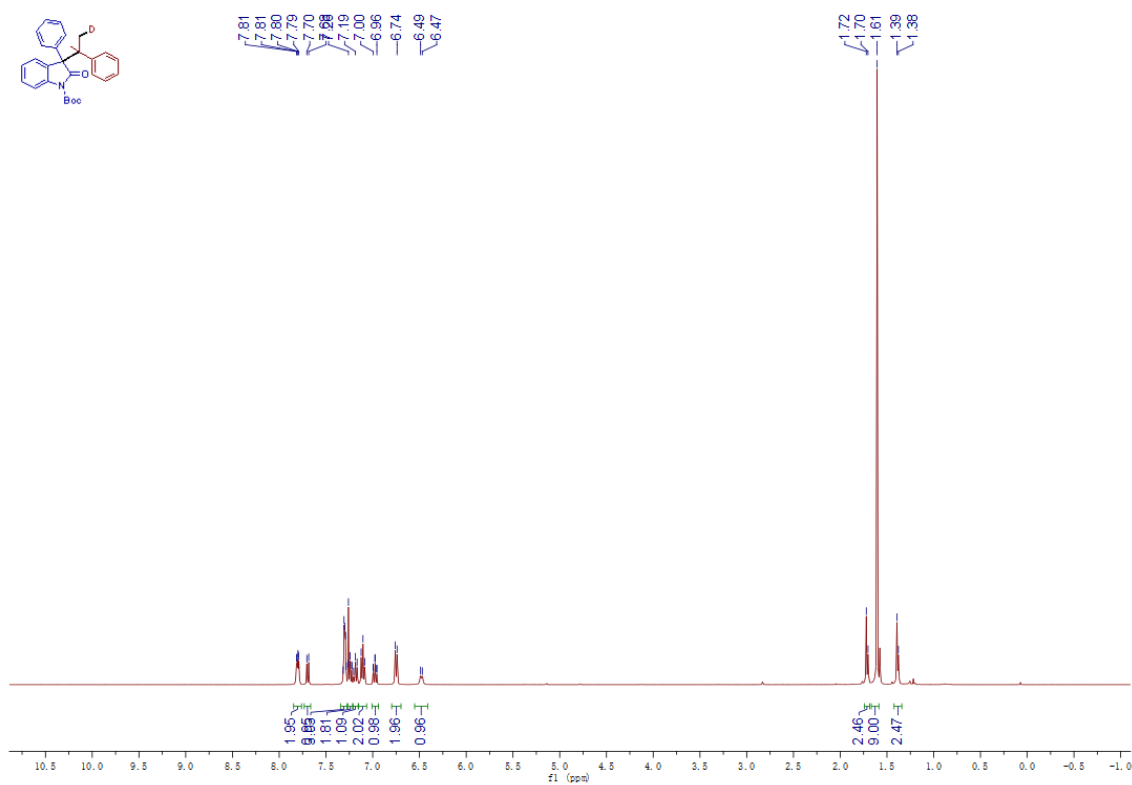
¹H NMR spectrum of 7-methyl-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (71)



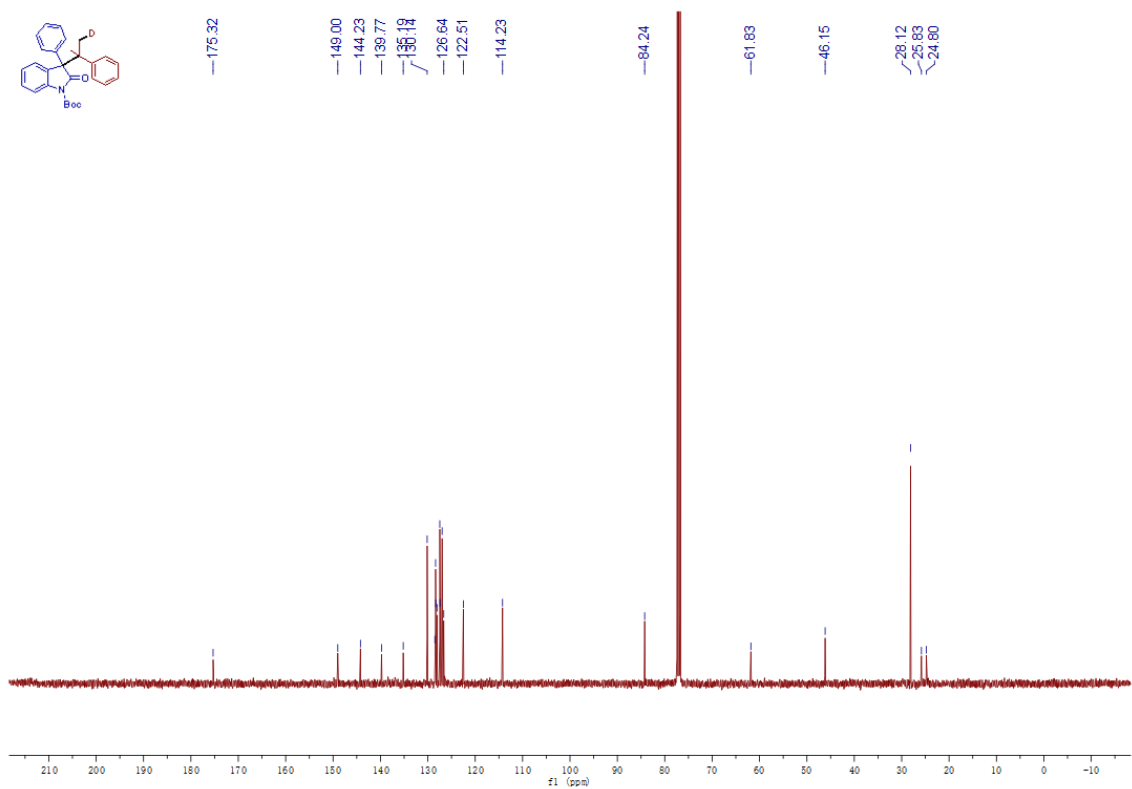
¹³C NMR spectrum of 7-methyl-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indolin-2-one. (71)



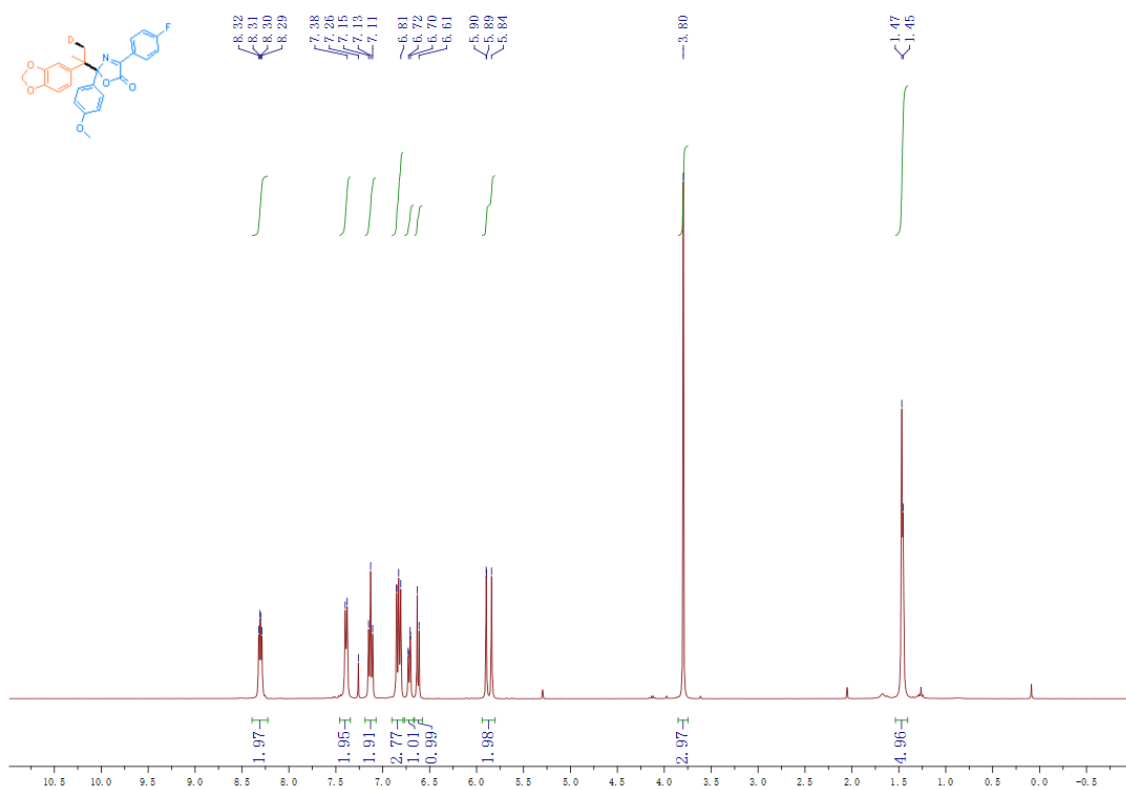
¹H NMR spectrum of tert-butyl 2-oxo-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indoline-1-carboxylate. (72)



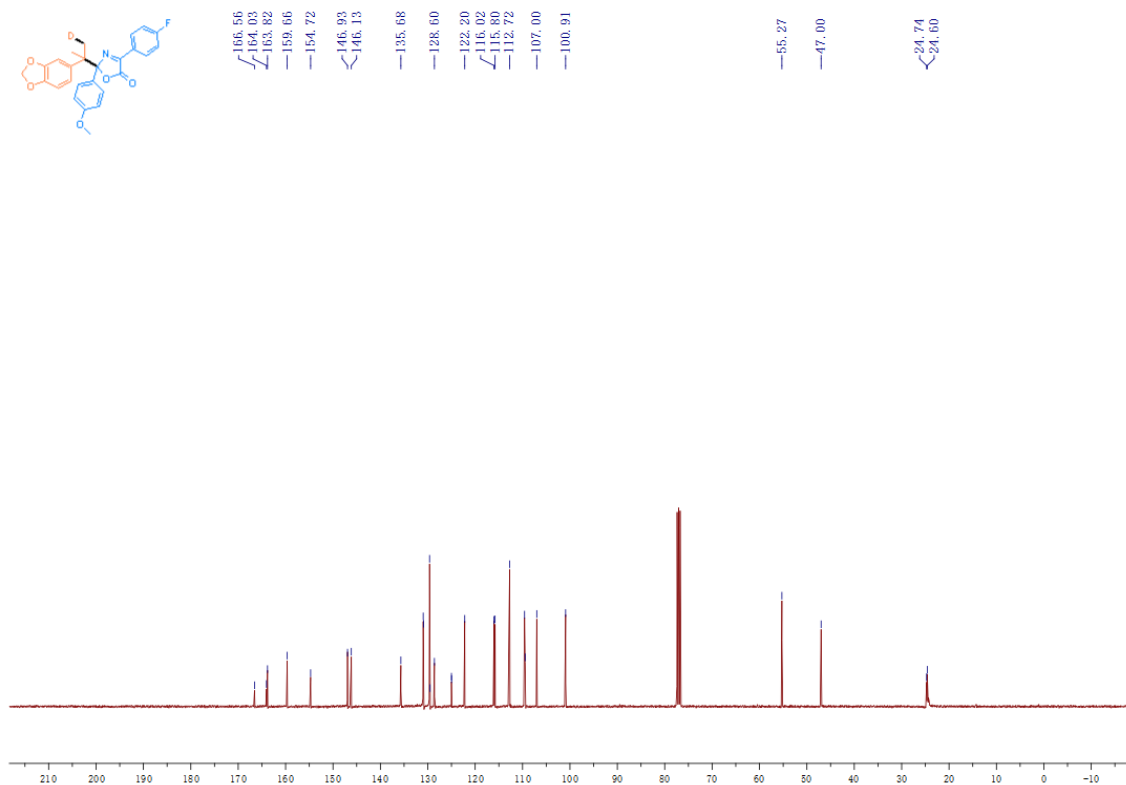
¹³C NMR spectrum of tert-butyl 2-oxo-3-phenyl-3-(2-phenylpropan-2-yl-1-d)indoline-1-carboxylate. (72)



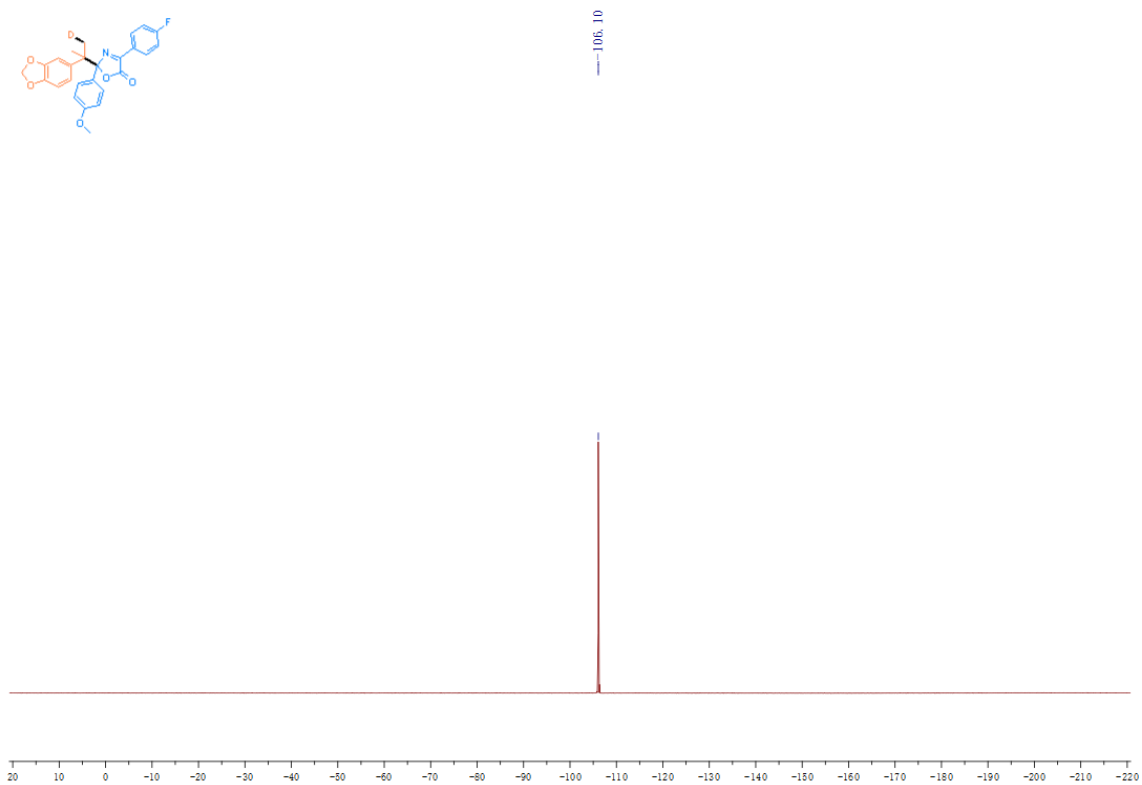
¹H NMR spectrum of 2-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-4-(4-fluorophenyl)-2-(4-methoxyphenyl)oxazol-5(2H)-one (73)



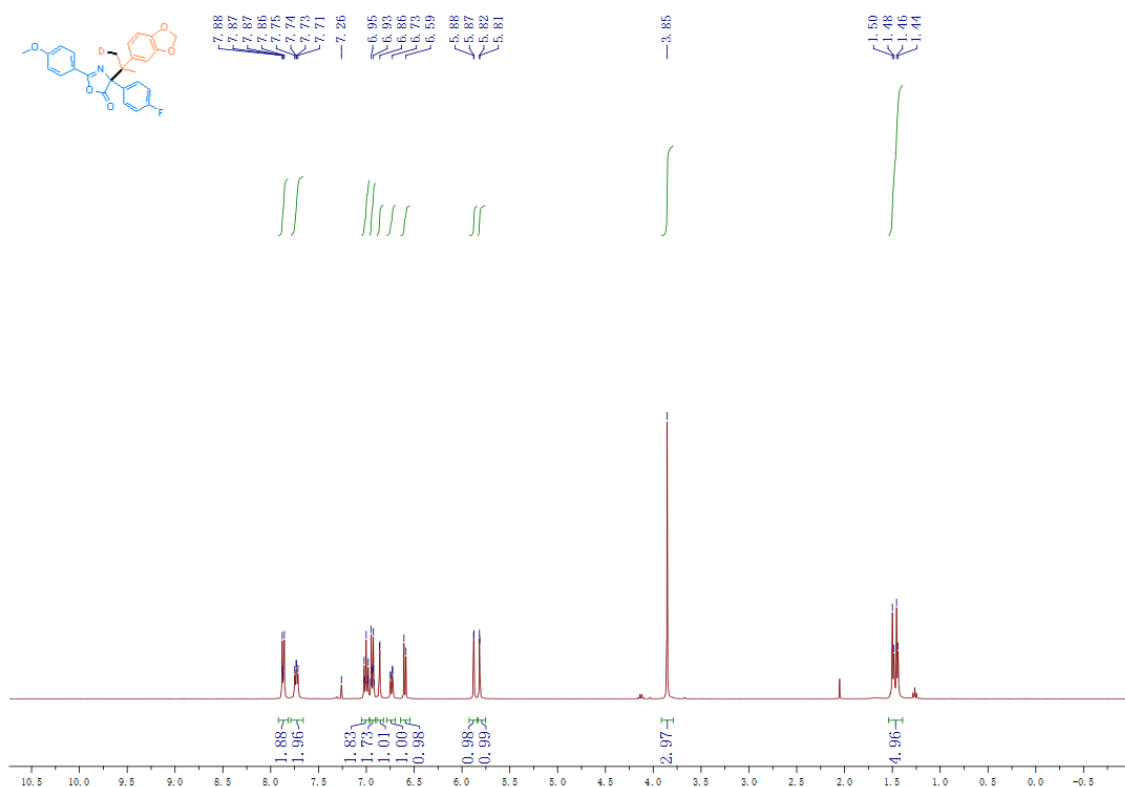
¹³C NMR spectrum of 2-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-4-(4-fluorophenyl)-2-(4-methoxyphenyl)oxazol-5(2H)-one (73)



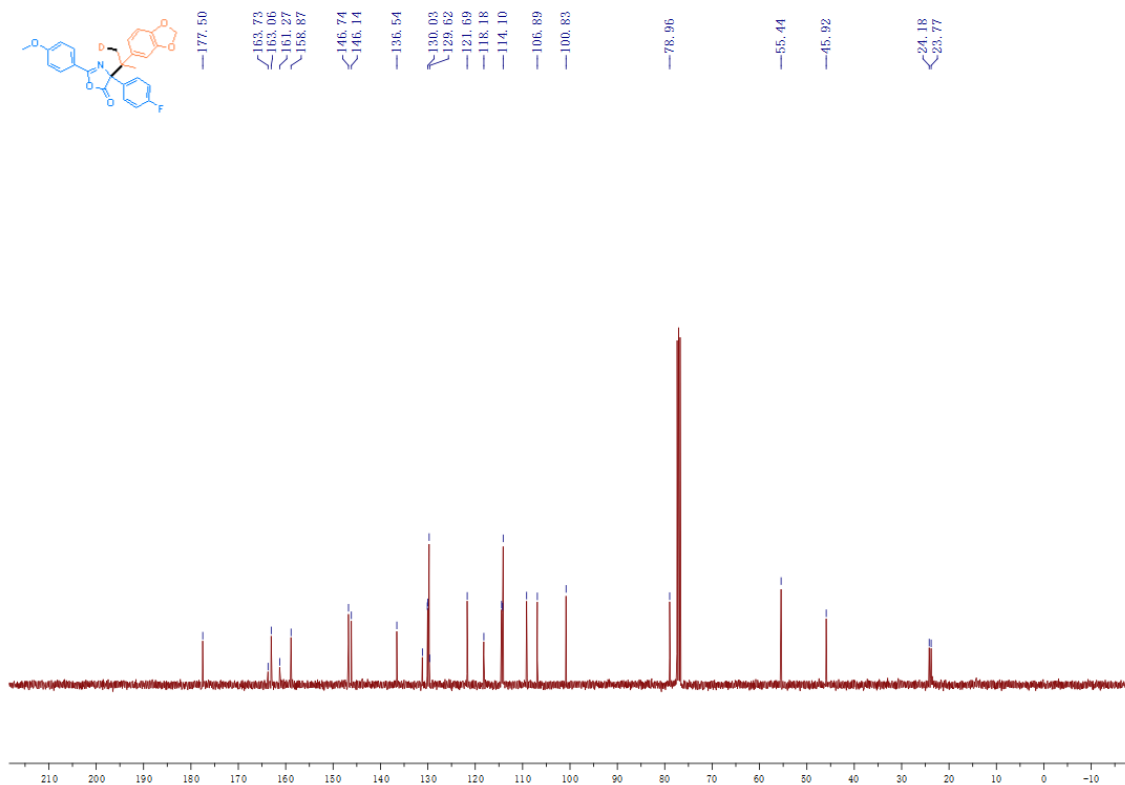
¹⁹F NMR spectrum of 2-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-4-(4-fluorophenyl)-2-(4-methoxyphenyl)oxazol-5(2H)-one (73)



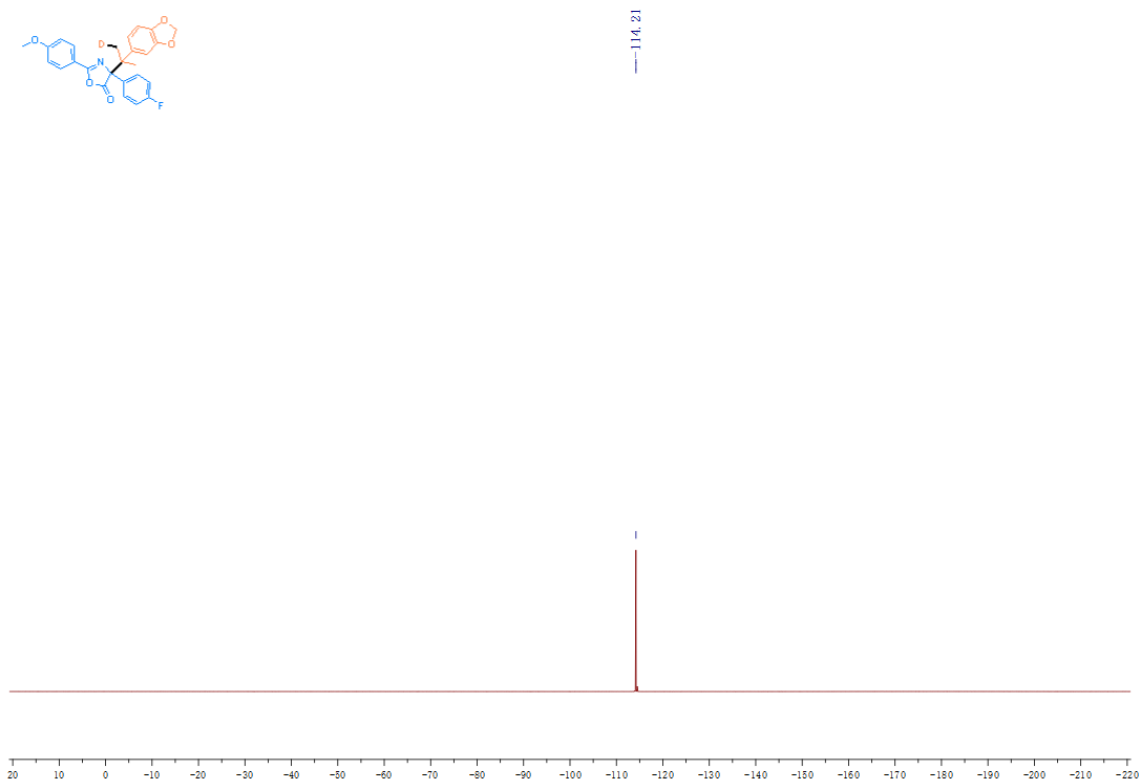
¹H NMR spectrum of 4-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-4-(4-fluorophenyl)-2-(4-methoxyphenyl)oxazol-5(4H)-one (74)



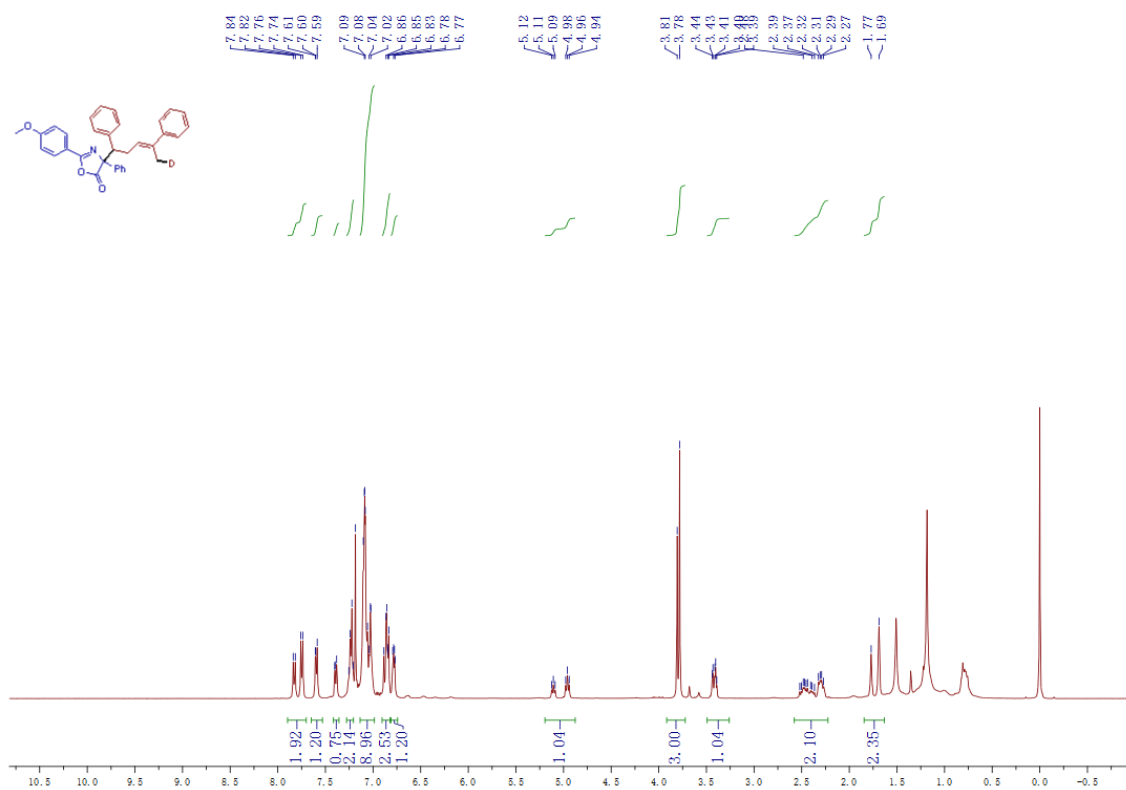
¹³C NMR spectrum of 4-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-4-(4-fluorophenyl)-2-(4-methoxyphenyl)oxazol-5(4H)-one (74)



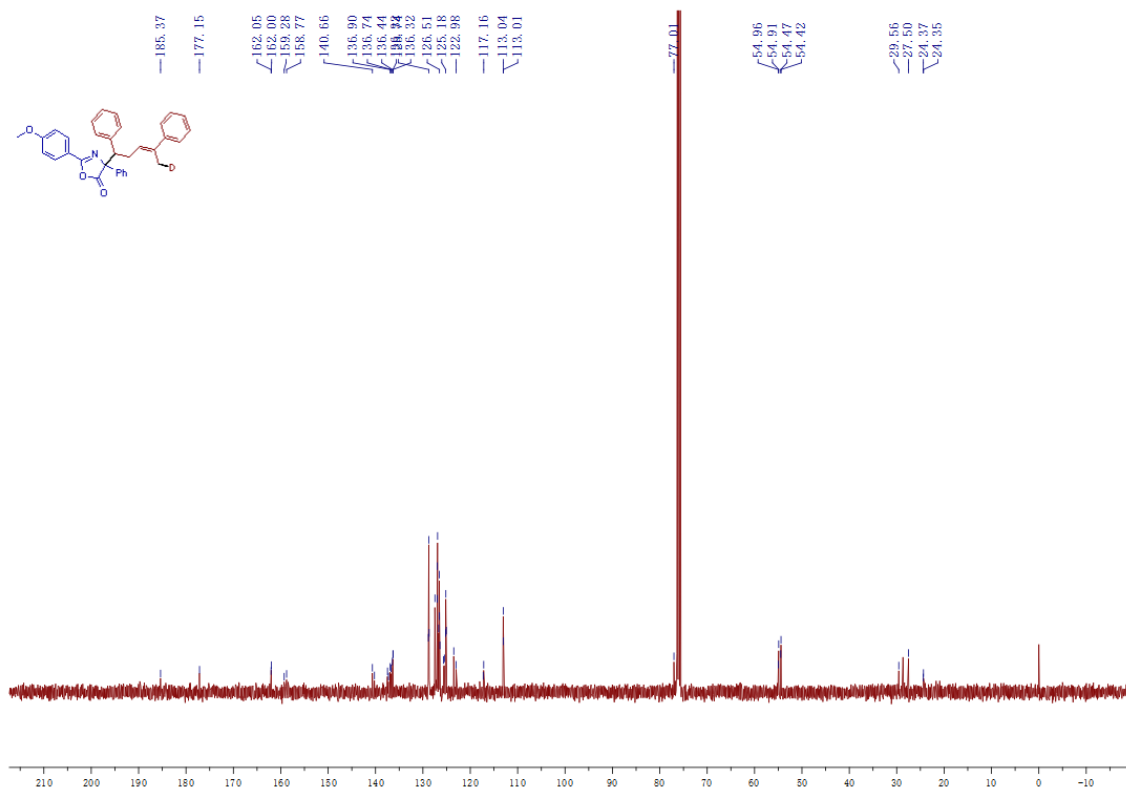
¹⁹F NMR spectrum of 4-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl-1-d)-4-(4-fluorophenyl)-2-(4-methoxyphenyl)oxazol-5(4H)-one (74)



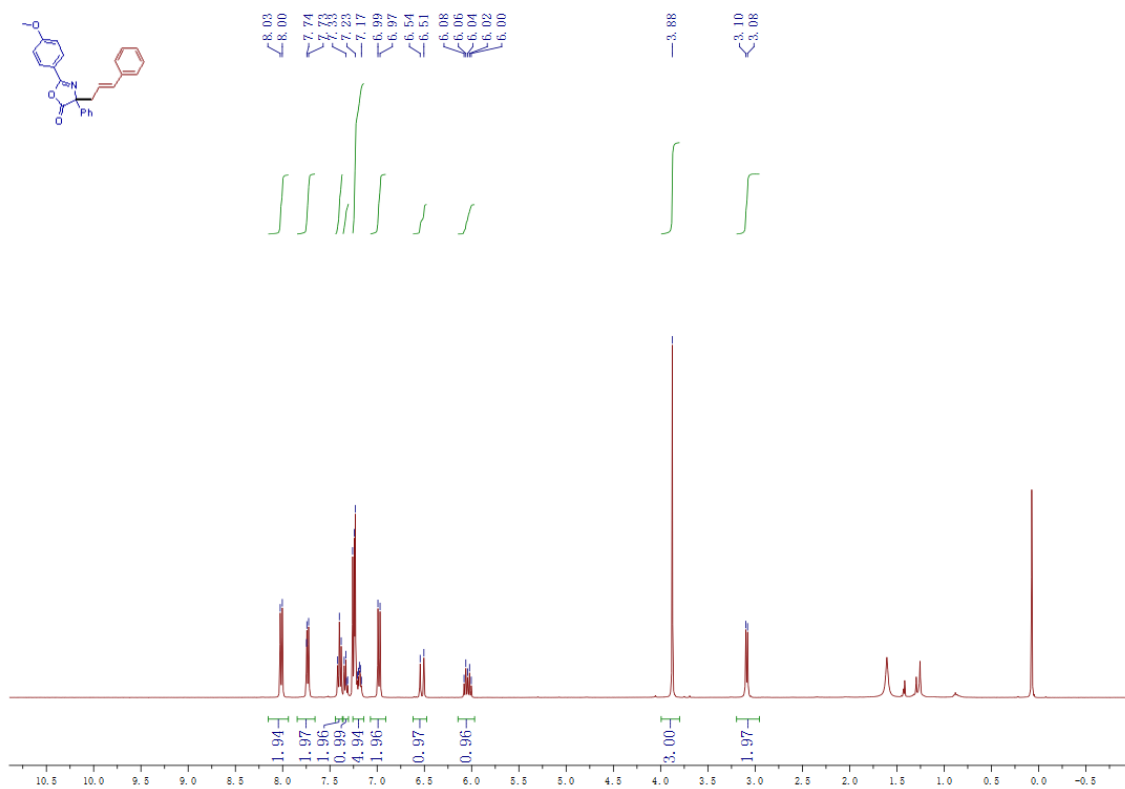
¹H NMR spectrum of (E)-4-(1,4-diphenylpent-3-en-1-yl-5-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (76)



¹³C NMR spectrum of (E)-4-(1,4-diphenylpent-3-en-1-yl-5-d)-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (76)



¹H NMR spectrum of 4-cinnamyl-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (78)



¹³C NMR spectrum of 4-cinnamyl-2-(4-methoxyphenyl)-4-phenyloxazol-5(4H)-one (78)

