

Redox-Neutral [4+2] Annulation of *N*-methoxybenzamides with Alkynes Enabled by an Osmium(II)/HOAc Catalytic System

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Supporting Information

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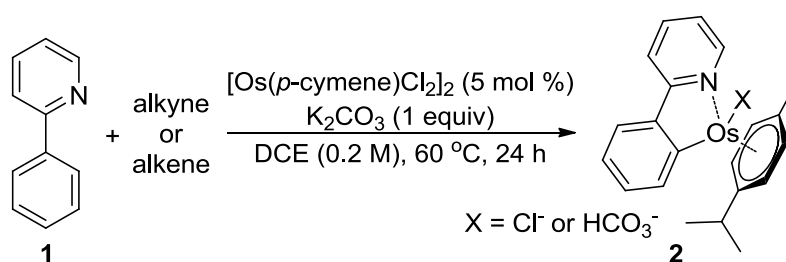
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I. General

NMR spectra were recorded on JEOL 400 NMR (^1H 400 MHz; ^{13}C 100 MHz) or Bruker 500 NMR in either CDCl_3 or $\text{DMSO-}d_6$. Abbreviations for data quoted are s, singlet; brs, broad singlet; d, doublet; t, triplet; dd, doublet of doublets; m, multiplet. The residual solvent signals were used as references and the chemical shifts converted to the TMS scale (CDCl_3 : $\delta_{\text{H}} = 7.26$ ppm, $\delta_{\text{C}} = 77.16$ ppm; d_6 -DMSO: $\delta_{\text{H}} = 2.50$ ppm, $\delta_{\text{C}} = 39.52$ ppm). Mass spectra and high-resolution mass spectra were measured on an agilent TOF-G6230B mass spectrometer and Thermo-DFS mass spectrometer. Thin-layer chromatographies were done on pre-coated silica gel 60 F254 plates (Merck). Silica gel 60H (200-300 mesh) and preparative TLC (200x200 mm, 0.2-0.25 mm in thickness) manufactured by Qingdao Haiyang Chemical Group Co. (China) were used for general chromatography. $[\text{Os}(p\text{-cymene})\text{Cl}_2]_2$ ^{S1} and *N*-methoxybenzamides^{S2} were synthesized according to published procedures. Other chemicals were purchased from commercial suppliers and were dried and purified when necessary. No attempts were made to optimize yields for substrate synthesis.

II. Experimental Information and Characterization Data

General procedure for Os(II)-mediated C-H activation of 2-phenylpyridine:



The mixture of 2-phenylpyridine **1** (0.2 mmol, 1 equiv), toluene (0.2 mmol, 1 equiv) or styrene (0.2 mmol, 1 equiv), $[\text{Os}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol %) and K_2CO_3 (1 equiv) in DCE (1 mL) was stirred at 60 °C in the oil bath for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC (eluent: PE/EA = 3/1, $R_f = 0.3$) to give the desired

osmacycle species **2** (9.7 mg).

Control experiment revealed that the osmacycle species **2** could also be generated in the absence of either toluene or styrene under the above mentioned osmium(II)-catalyzed conditions.

¹H NMR (400 MHz, CDCl₃): δ 9.11 (d, *J* = 8.0 Hz, 1H), 8.02 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.69-7.61 (m, 2H), 7.13 (td, *J* = 7.3, 1.3 Hz, 1H), 7.03-6.98 (m, 2H), 5.59 (d, *J* = 5.5 Hz, 1H), 5.49 (d, *J* = 5.6 Hz, 1H), 5.34 (d, *J* = 5.9 Hz, 1H), 5.17 (d, *J* = 5.5 Hz, 1H), 2.40-2.30 (m, 1H), 2.31 (s, 3H), 0.96 (d, *J* = 7.2 Hz, 3H), 0.84 (d, *J* = 6.9 Hz, 3H).

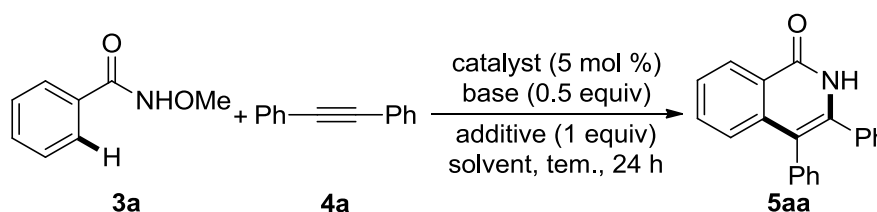
¹³C NMR (100 MHz, CDCl₃): δ 167.0, 166.8, 155.2, 144.0, 139.3, 136.8, 130.5, 124.1, 122.5, 122.2, 118.9, 94.2, 90.9, 81.3, 80.1, 75.0, 71.8, 31.1, 23.0, 22.0, 18.7.

HRMS (ESI) calculated for C₂₁H₂₂NO₂ ([M-X]⁺): 480.1367; found: 480.1355.

Optimization studies:

The mixture of *N*-methoxybenzamide **3a** (0.24 mmol, 1.2 equiv), diphenylacetylene **4a** (0.2 mmol, 1.0 equiv), catalyst (5 mol %), base (0.5 equiv) and additive (1.0 equiv) in the solvent (1.0 mL) was stirred at corresponding temperature in the oil bath for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC (eluent: PE/EA = 3/1) to give the desired 3,4-diphenylisoquinolin-1(2*H*)-one **5aa**.

Table S1. Conditions Screening for the Synthesis of **5aa**.^a

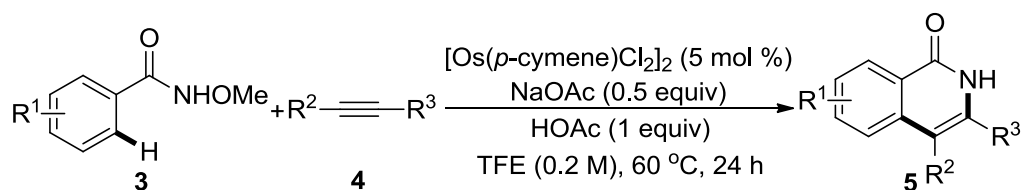


entry	catalyst	base	additive	tem. (°C)	solvent	yield ^b (%)
1	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	/	60	MeOH	21
2	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	/	60	CH ₃ CN	<5

3	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	/	60	THF	<5
4	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	/	60	DCM	<5
5	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	/	60	toluene	<5
6	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	/	60	TFE	57
7	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	/	60	HFIP	26
8	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	/	rt	TFE	18
9	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	/	80	TFE	53
10	[Os(<i>p</i> -cymene)Cl ₂] ₂	CsOAc	/	60	TFE	45
11	[Os(<i>p</i> -cymene)Cl ₂] ₂	AgOAc	/	60	TFE	16
12	[Os(<i>p</i> -cymene)Cl ₂] ₂	K ₂ CO ₃	/	60	TFE	<5
13	[Os(<i>p</i> -cymene)Cl ₂] ₂	Cu(OAc) ₂	/	60	TFE	8
14	[Os(<i>p</i> -cymene)Cl ₂] ₂	Zn(OAc) ₂	/	60	TFE	10
15	[Os(<i>p</i> -cymene)Cl ₂] ₂	KOPiv	/	60	TFE	11
16 ^c	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	HOAc	60	TFE	85
17 ^c	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	HOPiv	60	TFE	59
18 ^c	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	TsOH	60	TFE	15
19 ^c	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	K ₂ CO ₃	60	TFE	10
20 ^c	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	2-phenylpyridine	60	TFE	NR
21 ^c	/	NaOAc	HOAc	60	TFE	NR
22 ^{c,d}	OsCl ₃ ·H ₂ O	NaOAc	HOAc	60	TFE	NR
23 ^{c,d}	Os(PPh ₃) ₃ Cl ₂	NaOAc	HOAc	60	TFE	NR
24 ^e	[Os(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	HOAc	60	TFE	n.d.

^aReaction conditions: **3a** (0.24 mmol), **4a** (0.2 mmol), [Os(*p*-cymene)Cl₂]₂ (5 mol %), base (0.5 equiv) and additive (1.0 equiv) in the solvent (1 mL) at corresponding temperature for 24 h under air. ^bIsolated yields were reported. ^c**1a** (1.2 equiv). ^d10 mol % of catalyst was used. ^e *N*-pivaloyloxybenzamide or *N*-acetoxybenzamide was used as the substrate. TFE: 2,2,2-trifluoroethanol; HFIP: hexafluoroisopropanol; NR: no reaction; n.d.: not detected.

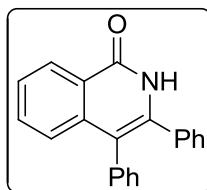
General procedure for C-H annulations:



The mixture of *N*-methoxyamide **3** (0.24 mmol, 1.2 equiv), alkyne **4** (0.2 mmol, 1.0 equiv), [Os(*p*-cymene)Cl₂]₂ (5 mol %), NaOAc (0.5 equiv) and HOAc (1 equiv) in TFE (1 mL) was stirred at 60 °C in the oil bath for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC to give the desired quinolin-2(*1H*)-one derivative **5**.

Characterization of products:

3,4-diphenylisoquinolin-1(*2H*)-one (**5aa**)



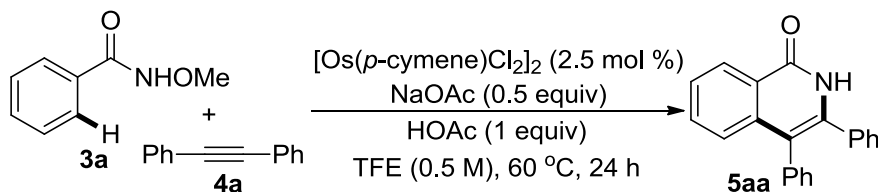
This compound was obtained in 85% yield (50.3 mg) as white solid. Eluent: PE/EA = 3/1, *R_f* = 0.4.

¹H NMR (400 MHz, CDCl₃): δ 9.16 (s, 1H), 8.48 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 7.0 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.31 (d, *J* = 7.0 Hz, 2H), 7.27-7.22 (m, 6H), 7.18 (dd, *J* = 7.4, 1.9 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃): δ 162.8, 138.8, 137.1, 135.8, 135.2, 132.8, 132.0, 129.3, 128.8, 128.5, 127.6, 127.5, 126.8, 125.8, 125.2, 117.4.

HRMS (ESI) calculated for C₂₁H₁₆NO ([M+H]⁺): 298.1226; found: 298.1227.

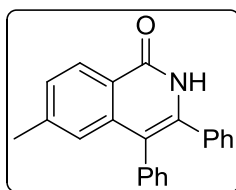
Scale-up synthesis of **5aa**:



The mixture of *N*-methoxyamide **3a** (5.5 mmol, 1.1 equiv), alkyne **4a** (4 mmol, 1.0

equiv), $[\text{Os}(p\text{-cymene})\text{Cl}_2]_2$ (2.5 mol %), NaOAc (0.5 equiv) and HOAc (1 equiv) in TFE (10 mL) was stirred at 60 °C in the oil bath for 24 h without exclusion of air or moisture. Afterwards, the mixture was transferred to a round bottom flask and diluted with EA. Then, the reaction mixture was concentrated and purified by silica column chromatography (eluent: PE/EA = 3/1) to give the desired quinolin-2(1*H*)-one derivative **5aa** (1.0692 g, 72%).

6-methyl-3,4-diphenylisoquinolin-1(2*H*)-one (**5ba**)



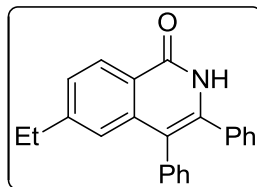
This compound was obtained in 83% yield (51.6 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.3$.

^1H NMR (400 MHz, CDCl_3): δ 9.07 (s, 1H), 8.37 (d, $J = 8.2$ Hz, 1H), 7.35-7.32 (m, 1H), 7.32-7.29 (m, 3H), 7.25-7.20 (m, 5H), 7.19-7.16 (m, 2H), 7.12 (s, 1H), 2.37 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 162.7, 143.5, 138.9, 137.2, 135.9, 135.3, 132.0, 129.3, 128.7, 128.5, 128.4, 127.6, 127.4, 125.5, 123.0, 117.3, 22.3.

HRMS (ESI) calculated for $\text{C}_{22}\text{H}_{18}\text{NO}$ ($[\text{M}+\text{H}]^+$): 312.1383; found: 312.1386.

6-ethyl-3,4-diphenylisoquinolin-1(2*H*)-one (**5ca**)



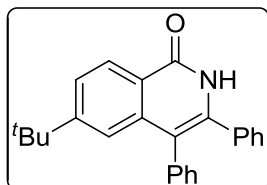
This compound was obtained in 78% yield (50.6 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.3$.

^1H NMR (400 MHz, CDCl_3): δ 10.35 (s, 1H), 8.36 (d, $J = 8.2$ Hz, 1H), 7.34 (dd, $J = 8.2, 1.5$ Hz, 1H), 7.32-7.27 (m, 3H), 7.25-7.22 (m, 5H), 7.20-7.15 (m, 3H), 2.65 (q, $J = 7.6$ Hz, 2H), 1.18 (t, $J = 7.6$ Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.7, 149.7, 138.9, 137.1, 135.9, 135.4, 132.0, 129.3, 128.7, 128.5, 127.8, 127.4, 127.2, 124.5, 123.2, 117.4, 29.5, 15.5.

HRMS (ESI) calculated for C₂₃H₂₀NO ([M+H]⁺): 326.1539; found: 326.1544.

6-(*tert*-butyl)-3,4-diphenylisoquinolin-1(2*H*)-one (5da)



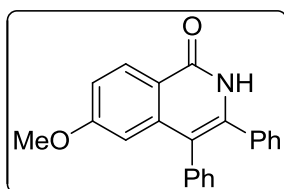
This compound was obtained in 72% yield (51.0 mg) as white solid. Eluent: PE/EA = 3/1, R_f = 0.20.

¹H NMR (400 MHz, CDCl₃): δ 8.79 (s, 1H), 8.42 (d, *J* = 8.5 Hz, 1H), 7.58 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.35 (d, *J* = 1.9 Hz, 1H), 7.32-7.30 (m, 1H), 7.31-7.28 (m, 2H), 7.26-7.22 (m, 3H), 7.22-7.19 (m, 3H), 7.18-7.17 (m, 1H), 1.25 (s, 9H).

¹³C NMR (100 MHz, CDCl₃): δ 162.6, 156.4, 138.7, 136.9, 135.9, 135.5, 131.9, 129.2, 128.7, 128.6, 128.4, 127.4, 125.0, 123.0, 122.0, 117.8, 35.5, 31.1.

HRMS (ESI) calculated for C₂₅H₂₄NO ([M+H]⁺): 354.1852; found: 354.1854.

6-methoxy-3,4-diphenylisoquinolin-1(2*H*)-one (5ea)



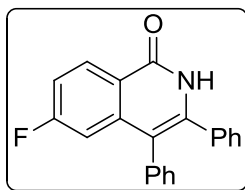
This compound was obtained in 56% yield (36.6 mg) as white solid. Eluent: PE/EA = 3/1, R_f = 0.15.

¹H NMR (400 MHz, DMSO-*d*₆): δ 11.36 (s, 1H), 8.25 (d, *J* = 8.9 Hz, 1H), 7.32-7.25 (m, 3H), 7.22-7.20 (m, 5H), 7.16-7.12 (m, 3H), 6.51 (d, *J* = 2.4 Hz, 1H), 3.67 (s, 3H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.3, 161.4, 140.1, 139.2, 135.9, 134.6, 131.7, 129.8, 129.1, 128.3, 128.2, 127.7, 127.1, 118.9, 115.1, 114.5, 107.2, 55.2.

HRMS (ESI) calculated for C₂₂H₁₈NO₂ ([M+H]⁺): 328.1332; found: 328.1328.

6-fluoro-3,4-diphenylisoquinolin-1(2*H*)-one (5fa)



This compound was obtained in 50% yield (31.5 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.3$.

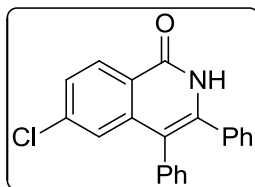
$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 9.49 (s, 1H), 8.46 (dd, $J = 8.9, 6.0$ Hz, 1H), 7.34-7.30 (m, 3H), 7.28-7.26 (m, 1H), 7.26-7.24 (m, 4H), 7.21-7.15 (m, 3H), 6.98 (dd, $J = 10.7, 2.5$ Hz, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 165.7 (d, $J = 250.7$ Hz), 162.3, 141.4 (d, $J = 9.8$ Hz), 138.7, 135.4, 134.8, 131.9, 130.8 (d, $J = 10.0$ Hz), 129.4, 129.0, 128.7, 128.5, 127.7, 121.8, 116.9 (d, $J = 2.4$ Hz), 115.3 (d, $J = 23.5$ Hz), 111.0 (d, $J = 23.5$ Hz).

$^{19}\text{F NMR}$ (376 MHz, CDCl_3): δ -104.8.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{15}\text{FNO}$ ($[\text{M}+\text{H}]^+$): 316.1132; found: 316.1127.

6-chloro-3,4-diphenylisoquinolin-1(2H)-one (5ga)



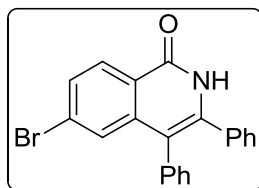
This compound was obtained in 51% yield (34.0 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.3$.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 9.13 (s, 1H), 8.40 (d, $J = 8.5$ Hz, 1H), 7.48-7.42 (m, 1H), 7.35-7.31 (m, 4H), 7.27-7.24 (m, 3H), 7.23-7.19 (m, 2H), 7.19-7.13 (m, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 162.2, 140.2, 139.7, 138.6, 135.1, 134.8, 131.8, 129.5, 129.3, 129.1, 128.8, 128.6, 127.8, 127.4, 125.2, 123.6, 116.6.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{15}\text{ClNO}$ ($[\text{M}+\text{H}]^+$): 332.0837; found: 332.0832.

6-bromo-3,4-diphenylisoquinolin-1(2H)-one (5ha)



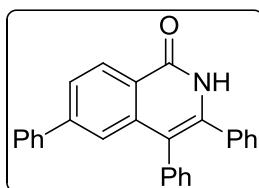
This compound was obtained in 55% yield (41.3 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.25$.

^1H NMR (400 MHz, CDCl_3): δ 8.85 (s, 1H), 8.34 (dd, $J = 8.5, 0.4$ Hz, 1H), 7.61 (dd, $J = 8.5, 1.9$ Hz, 1H), 7.49 (d, $J = 1.9$ Hz, 1H), 7.35-7.31 (m, 3H), 7.27-7.26 (m, 1H), 7.26-7.25 (m, 1H), 7.25-7.24 (m, 1H), 7.21-7.18 (m, 2H), 7.18-7.14 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3): δ 162.2, 140.3, 138.5, 134.9, 131.8, 130.2, 129.5, 129.2, 129.1, 128.8, 128.7, 128.5, 128.3, 127.8, 124.0, 116.5.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{15}\text{BrNO}$ ($[\text{M}+\text{H}]^+$): 376.0332; found: 376.0323.

3,4,6-triphenylisoquinolin-1(2H)-one (5ia)



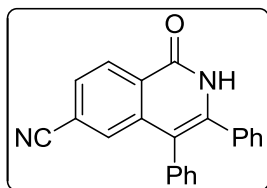
This compound was obtained in 67% yield (50.1 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.2$.

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 11.57 (s, 1H), 8.40 (d, $J = 8.3$ Hz, 1H), 7.81 (dd, $J = 8.4, 1.7$ Hz, 1H), 7.52-7.48 (m, 2H), 7.47-7.42 (m, 2H), 7.41-7.36 (m, 1H), 7.34 (d, $J = 1.7$ Hz, 1H), 7.32 (d, $J = 1.7$ Hz, 1H), 7.30 (s, 1H), 7.29-7.26 (m, 1H), 7.26-7.22 (m, 6H), 7.21 (t, $J = 1.4$ Hz, 1H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 161.5, 144.0, 139.5, 139.2, 138.6, 135.7, 134.5, 131.8, 129.8, 129.2, 128.3, 128.2, 127.7, 127.2, 126.9, 125.1, 124.0, 122.7, 115.5.

HRMS (ESI) calculated for $\text{C}_{27}\text{H}_{20}\text{NO}$ ($[\text{M}+\text{H}]^+$): 374.1539; found: 374.1542.

1-oxo-3,4-diphenyl-1,2-dihydroisoquinoline-6-carbonitrile (5ja)



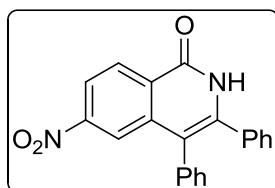
This compound was obtained in 59% yield (37.9 mg) as yellow solid. Eluent: PE/EA = 3/1, $R_f = 0.2$.

^1H NMR (400 MHz, CDCl_3): δ 9.83 (s, 1H), 8.51 (d, $J = 8.7$ Hz, 1H), 7.69-7.65 (m, 2H), 7.37-3.34 (m, 3H), 7.31-7.29 (m, 1H), 7.28 (s, 1H), 7.27-7.23 (m, 3H), 7.15 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3): δ 161.9, 139.4, 139.0, 134.4, 134.3, 131.7, 130.7, 129.3, 129.0, 128.8, 128.6, 128.3, 128.2, 118.4, 116.5, 116.4.

HRMS (ESI) calculated for $\text{C}_{22}\text{H}_{15}\text{N}_2\text{O}$ ($[\text{M}+\text{H}]^+$): 323.1179; found: 323.1175.

6-nitro-3,4-diphenylisoquinolin-1(2H)-one (5ka)



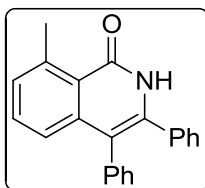
This compound was obtained in 53% yield (36.3 mg) as yellow solid. Eluent: PE/EA = 3/1, $R_f = 0.20$.

^1H NMR (400 MHz, CDCl_3): δ 9.84 (s, 1H), 8.60 (d, $J = 9.3$ Hz, 1H), 8.25-8.21 (m, 2H), 7.37 (d, $J = 1.7$ Hz, 1H), 7.36 (d, $J = 2.0$ Hz, 2H), 7.32-7.30 (m, 1H), 7.29-7.27 (m, 1H), 7.27 (d, $J = 2.7$ Hz, 1H), 7.27-7.24 (m, 2H), 7.20-7.16 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3): δ 161.7, 150.8, 139.8, 139.7, 134.4, 134.3, 131.7, 129.8, 129.4, 129.3, 129.1, 128.8, 128.7, 128.3, 121.3, 120.3, 117.3.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{15}\text{N}_2\text{O}_3$ ($[\text{M}+\text{H}]^+$): 343.1077; found: 343.1076.

8-methyl-3,4-diphenylisoquinolin-1(2H)-one (5la)



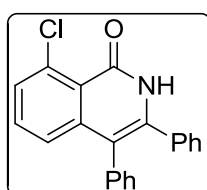
This compound was obtained in 92% yield (57.4 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.5$.

^1H NMR (400 MHz, CDCl_3): δ 8.88 (s, 1H), 8.31-8.29 (m, 1H), 7.41 (d, $J = 8.3$ Hz, 1H), 7.33-7.28 (m, 3H), 7.27-7.21 (m, 6H), 7.19-7.16 (m, 2H), 2.50 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 162.7, 137.0, 136.5, 136.03, 135.95, 135.3, 134.3, 131.9, 129.3, 128.7, 128.53, 128.49, 127.4, 127.2, 125.8, 125.1, 117.4, 21.5.

HRMS (ESI) calculated for $\text{C}_{22}\text{H}_{18}\text{NO}$ ($[\text{M}+\text{H}]^+$): 312.1383; found: 312.1385.

8-chloro-3,4-diphenylisoquinolin-1(2H)-one (5ma)



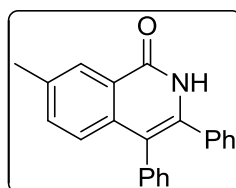
This compound was obtained in 86% yield (56.9 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.4$.

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 11.55 (s, 1H), 7.55-7.49 (m, 2H), 7.32-7.26 (m, 3H), 7.23-7.20 (m, 5H), 7.16-7.12 (m, 2H), 7.05 (dd, $J = 7.2, 2.1$ Hz, 1H).

^{13}C NMR (100 MHz, CDCl_3): δ 161.3, 142.0, 138.4, 135.9, 135.7, 134.6, 132.2, 132.0, 129.8, 129.2, 129.0, 128.7, 128.5, 127.7, 125.1, 121.9, 116.8.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{15}\text{ClNO}$ ($[\text{M}+\text{H}]^+$): 332.0837; found: 332.0840.

7-methyl-3,4-diphenylisoquinolin-1(2H)-one (5na)



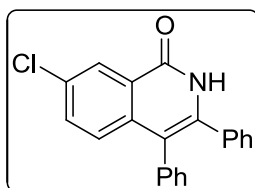
This compound was obtained in 79% yield (49.4 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.25$.

^1H NMR (400 MHz, CDCl_3): δ 9.70 (s, 1H), 7.41-7.36 (m, 1H), 7.32-7.26 (m, 3H), 7.26 (s, 1H), 7.25-7.21 (m, 4H), 7.22-7.20 (m, 1H), 7.18-7.13 (m, 3H), 2.91 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 164.1, 142.0, 140.6, 137.4, 136.7, 135.2, 132.1, 131.8, 129.7, 129.4, 128.6, 128.5, 128.4, 127.3, 124.1, 123.7, 117.3, 24.0.

HRMS (ESI) calculated for $C_{22}H_{18}NO$ ($[M+H]^+$): 312.1383; found: 312.1382.

7-chloro-3,4-diphenylisoquinolin-1(2H)-one (5oa)



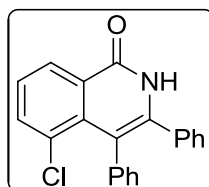
This compound was obtained in 45% yield (30.1 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.4$.

1H NMR (400 MHz, $CDCl_3$): δ 8.93 (s, 1H), 8.45 (d, $J = 2.3$ Hz, 1H), 7.52 (dd, $J = 8.7, 2.3$ Hz, 1H), 7.34-7.29 (m, 4H), 7.29-7.26 (m, 2H), 7.25 (s, 1H), 7.22-7.20 (m, 2H), 7.17-7.15 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 161.7, 137.4, 137.2, 135.3, 134.9, 133.3, 133.0, 131.8, 129.2, 129.0, 128.7, 128.7, 127.7, 127.6, 127.1, 126.4, 117.0.

HRMS (ESI) calculated for $C_{22}H_{15}NO$ ($[M+H]^+$): 332.0837; found: 332.0834.

5-chloro-3,4-diphenylisoquinolin-1(2H)-one (5oa')



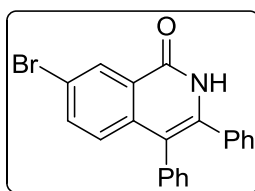
This compound was obtained in 34% yield (22.4 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.25$.

1H NMR (400 MHz, $CDCl_3$): δ 8.91 (s, 1H), 8.50 (dd, $J = 7.9, 1.3$ Hz, 1H), 7.66 (dd, $J = 7.7, 1.3$ Hz, 1H), 7.42 (t, $J = 7.8$ Hz, 1H), 7.25-7.20 (m, 3H), 7.19-7.15 (m, 3H), 7.15-7.10 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 161.8, 139.6, 137.3, 136.8, 135.4, 134.8, 132.3, 131.4, 129.4, 128.7, 128.3, 128.0, 127.6, 127.4, 127.2, 115.8.

HRMS (ESI) calculated for $C_{22}H_{18}NO$ ($[M+H]^+$): 332.0837; found: 332.0834.

7-bromo-3,4-diphenylisoquinolin-1(2H)-one (5pa)



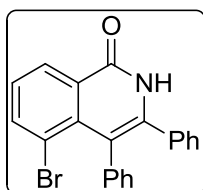
This compound was obtained in 36% yield (27.0 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.45$.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.80 (s, 1H), 8.62 (d, $J = 2.2$ Hz, 1H), 7.66 (dd, $J = 8.7, 2.3$ Hz, 1H), 7.33-7.29 (m, 3H), 7.28-7.26 (m, 2H), 7.25-7.22 (m, 2H), 7.21-7.19 (m, 2H), 7.17-7.13 (m, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 161.7, 137.7, 137.6, 135.9, 135.3, 134.8, 131.8, 130.2, 129.3, 129.0, 128.7, 128.6, 127.7, 126.6, 120.8, 117.0.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{15}\text{BrNO}$ ($[\text{M}+\text{H}]^+$): 376.0332; found: 376.0330.

5-bromo-3,4-diphenylisoquinolin-1(2H)-one (5pa')



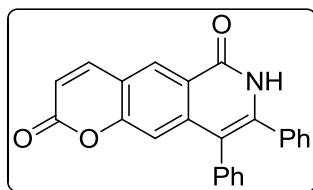
This compound was obtained in 21% yield (15.8 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.35$.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 9.89 (s, 1H), 8.47 (dd, $J = 7.9, 1.2$ Hz, 1H), 7.90 (dd, $J = 7.7, 1.3$ Hz, 1H), 7.29 (t, $J = 7.8$ Hz, 1H), 7.23-7.12 (m, 8H), 7.09 (dd, $J = 7.7, 1.6$ Hz, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 162.0, 140.8, 140.0, 136.7, 135.9, 135.4, 133.1, 129.5, 128.6, 128.1, 128.1, 128.0, 127.7, 127.3, 119.7, 116.5.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{15}\text{BrNO}$ ($[\text{M}+\text{H}]^+$): 376.0332; found: 376.0327.

8,9-diphenyl-2H-pyrano[2,3-g]isoquinoline-2,6(7H)-dione (5qa)



This compound was obtained in 55% yield (40.2 mg) as yellow solid. Eluent: PE/EA

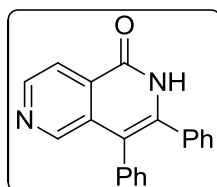
= 1/1, $R_f = 0.3$.

^1H NMR (400 MHz, CDCl_3): δ 9.30 (s, 1H), 8.61 (s, 1H), 7.84 (d, $J = 9.6$ Hz, 1H), 7.34 (d, $J = 1.7$ Hz, 1H), 7.33 (d, $J = 1.9$ Hz, 2H), 7.28 (m, 3H), 7.25 (m, 2H), 7.21 (s, 1H), 7.18-7.14 (m, 2H), 6.45 (d, $J = 9.6$ Hz, 1H).

^{13}C NMR (100 MHz, CDCl_3): δ 162.1, 160.0, 156.3, 143.1, 141.7, 139.6, 134.9, 134.6, 131.7, 129.3, 129.2, 128.9, 128.8, 128.7, 128.0, 122.0, 118.2, 117.2, 117.0, 112.7.

HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{16}\text{NO}_3$ ($[\text{M}+\text{H}]^+$): 366.1125; found: 366.1119.

3,4-diphenyl-2,6-naphthyridin-1(2H)-one (5ra)



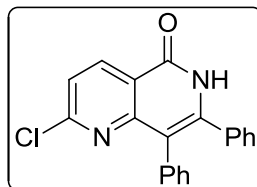
This compound was obtained in 51% yield (30.4 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.2$.

^1H NMR (400 MHz, CDCl_3): δ 10.38 (s, 1H), 8.78-8.74 (m, 1H), 8.72-8.68 (m, 1H), 8.16 (m, 1H), 7.34 (m, 3H), 7.27 (m, 5H), 7.19 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3): δ 163.3, 162.1, 149.5, 146.1, 139.2, 134.3, 134.1, 132.8, 131.8, 129.9, 129.5, 129.2, 128.8, 128.5, 127.9, 119.4, 115.7.

HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{15}\text{N}_2\text{O}$ ($[\text{M}+\text{H}]^+$): 299.1179; found: 299.1176.

2-chloro-7,8-diphenyl-1,6-naphthyridin-5(6H)-one (5sa)



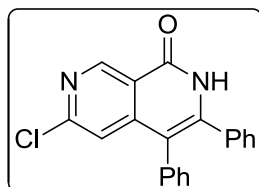
This compound was obtained in 36% yield (23.9 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.25$.

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 12.00 (s, 1H), 8.59 (d, $J = 8.3$ Hz, 1H), 7.56 (d, $J = 8.3$ Hz, 1H), 7.28-7.20 (m, 8H), 7.14-7.09 (m, 2H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 161.2, 154.5, 153.9, 144.5, 139.0, 134.6, 134.0, 132.1, 129.8, 128.7, 127.8, 127.5, 126.7, 122.1, 119.7, 116.4.

HRMS (ESI) calculated for C₂₀H₁₄ClN₂O ([M+H]⁺): 333.0789; found: 333.0785.

6-chloro-3,4-diphenyl-2,7-naphthyridin-1(2H)-one (5sa')



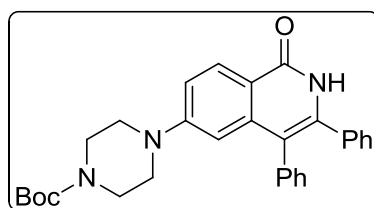
This compound was obtained in 28% yield (18.6 mg) as white solid. Eluent: PE/EA = 3/1, R_f = 0.15.

¹H NMR (400 MHz, DMSO-*d*₆): δ 12.06 (s, 1H), 9.23 (s, 1H), 7.33-7.31 (m, 2H), 7.30-7.29 (m, 1H), 7.28-7.26 (m, 1H), 7.26-7.24 (m, 4H), 7.17-7.15 (m, 2H), 6.93 (s, 1H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 160.9, 152.9, 151.1, 146.1, 145.3, 133.9, 133.5, 131.5, 129.6, 129.0, 128.6, 127.8, 127.7, 119.2, 117.1, 113.4.

HRMS (ESI) calculated for C₂₀H₁₄ClN₂O ([M+H]⁺): 333.0789; found: 333.0785.

***tert*-butyl 4-(1-oxo-3,4-diphenyl-1,2-dihydroisoquinolin-6-yl)piperazine-1-carboxylate (5ta)**



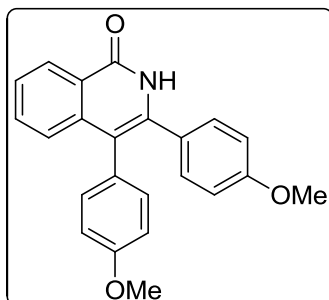
This compound was obtained in 61% yield (58.7 mg) as white solid. Eluent: PE/EA = 3/1, R_f = 0.3.

¹H NMR (400 MHz, CDCl₃): δ 8.74 (s, 1H), 8.35 (d, *J* = 9.0 Hz, 1H), 7.32-7.27 (m, 3H), 7.24-7.16 (m, 7H), 7.09 (dd, *J* = 9.0, 2.5 Hz, 1H), 6.60 (d, *J* = 2.4 Hz, 1H), 3.54-3.49 (m, 4H), 3.18-3.13 (m, 4H), 1.46 (s, 9H).

¹³C NMR (100 MHz, CDCl₃): δ 162.4, 154.7, 154.1, 140.5, 137.7, 136.1, 135.5, 131.9, 129.3, 129.2, 128.7, 128.5, 127.4, 117.4, 117.1, 115.8, 108.9, 80.2, 47.8, 28.6.

HRMS (ESI) calculated for $C_{30}H_{32}N_3O_3$ ($[M+H]^+$): 482.2438; found: 482.2434.

3,4-bis(4-methoxyphenyl)isoquinolin-1(2H)-one (5ab)



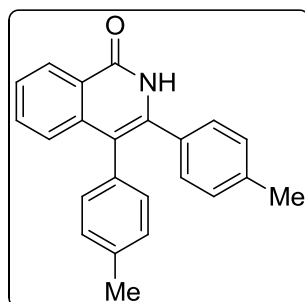
This compound was obtained in 68% yield (48.6 mg) as yellow solid. Eluent: PE/EA = 3/1, $R_f = 0.1$.

1H NMR (400 MHz, $CDCl_3$): δ 9.06 (s, 1H), 8.46 (dd, $J = 8.0, 0.8$ Hz, 1H), 7.61-7.56 (m, 1H), 7.51-7.46 (m, 1H), 7.36 (d, $J = 8.2$ Hz, 1H), 7.15 (d, $J = 8.9$ Hz, 2H), 7.09 (d, $J = 8.8$ Hz, 2H), 6.87 (d, $J = 8.8$ Hz, 2H), 6.77 (d, $J = 8.9$ Hz, 2H), 3.82 (s, 3H), 3.78 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 162.9, 159.7, 158.8, 139.3, 137.0, 133.0, 132.7, 130.6, 128.1, 127.7, 127.6, 126.5, 125.7, 125.0, 116.6, 114.0, 114.0, 55.36, 55.35.

HRMS (ESI) calculated for $C_{23}H_{20}NO_3$ ($[M+H]^+$): 358.1438; found: 358.1429.

3,4-di-*p*-tolylisoquinolin-1(2H)-one (5ac)



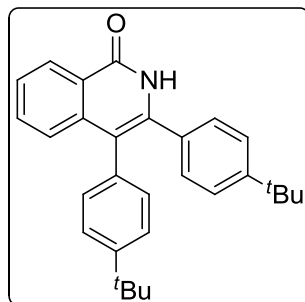
This compound was obtained in 65% yield (42.3 mg) as yellow solid. Eluent: PE/EA = 3/1, $R_f = 0.15$.

1H NMR (400 MHz, $CDCl_3$): δ 9.05 (s, 1H), 8.47 (d, $J = 7.9$ Hz, 1H), 7.57 (t, $J = 7.6$ Hz, 1H), 7.48 (t, $J = 7.5$ Hz, 1H), 7.35 (d, $J = 8.2$ Hz, 1H), 7.16-7.09 (m, 4H), 7.08-7.03 (m, 4H), 2.36 (s, 3H), 2.30 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.9, 139.1, 138.7, 137.0, 132.9, 132.7, 132.5, 131.7, 129.28, 129.25, 129.1, 127.6, 126.6, 125.8, 125.1, 117.1, 21.41, 21.39.

HRMS (ESI) calculated for C₂₃H₂₀NO ([M+H]⁺): 326.1539; found: 326.1533.

3,4-bis(4-(*tert*-butyl)phenyl)isoquinolin-1(2*H*)-one (5ad)



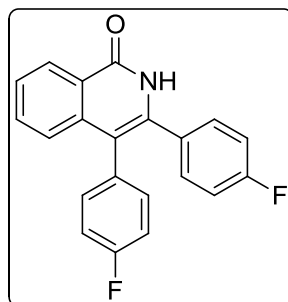
This compound was obtained in 46% yield (37.6 mg) as light yellow solid. Eluent: PE/EA = 3/1, R_f = 0.33.

¹H NMR (400 MHz, CDCl₃): δ 8.80 (s, 1H), 8.48 (d, *J* = 7.8 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 8.1 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.27-7.22 (m, 2H), 7.14-7.08 (m, 4H), 1.32 (s, 9H), 1.26 (s, 9H).

¹³C NMR (100 MHz, CDCl₃): δ 162.8, 151.8, 150.4, 139.1, 137.0, 132.8, 132.7, 132.4, 131.6, 128.8, 127.6, 126.6, 126.0, 125.4, 125.3, 125.2, 117.2, 34.8, 34.7, 31.5, 31.3.

HRMS (ESI) calculated for C₂₉H₃₂NO ([M+H]⁺): 410.2478; found: 410.2468.

3,4-bis(4-fluorophenyl)isoquinolin-1(2*H*)-one (5ae)



This compound was obtained in 84% yield (55.8 mg) as white solid. Eluent: PE/EA = 3/1, R_f = 0.15.

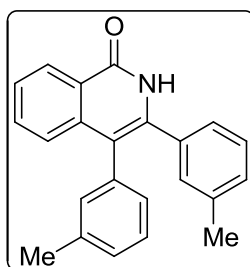
¹H NMR (400 MHz, CDCl₃): δ 9.95 (s, 1H), 8.46-8.42 (m, 1H), 7.65-7.57(m, 1H), 7.55-7.48 (m, 1H), 7.33-7.29 (m, 1H), 7.25-7.21 (m, 2H), 7.16-7.12 (m, 2H), 7.06-7.01 (m, 2H), 7.00-6.95 (m, 2H).

¹³C NMR (100 MHz, CDCl₃): δ 163.4, 162.7 (d, *J* = 248.3 Hz), 162.2 (d, *J* = 245.7 Hz), 138.6, 136.8, 133.5 (d, *J* = 8.1 Hz), 133.0, 131.6 (d, *J* = 3.6 Hz), 131.6, 131.5, 130.9 (d, *J* = 3.4 Hz), 127.7, 126.9, 125.5, 125.2, 116.5, 115.8 (d, *J* = 8.4 Hz), 115.6 (d, *J* = 8.8 Hz).

¹⁹F NMR (376 MHz, CDCl₃): δ -112.9, -114.9.

HRMS (ESI) calculated for C₂₁H₁₃F₂NO ([M+H]⁺): 334.1038; found: 334.1042.

3,4-di-*m*-tolylisoquinolin-1(2*H*)-one (5af)



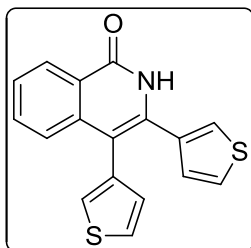
This compound was obtained in 69% yield (44.9 mg) as yellow solid. Eluent: PE/EA = 3/1, R_f = 0.25.

¹H NMR (400 MHz, CDCl₃): δ 9.14 (s, 1H), 8.47 (ddd, *J* = 7.9, 1.5, 0.5 Hz, 1H), 7.61-7.56 (m, 1H), 7.51-7.46 (m, 1H), 7.36 (dd, *J* = 8.2, 0.6 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.13-7.05 (m, 4H), 7.02 (s, 1H), 7.00-6.95 (m, 2H), 2.30 (s, 3H), 2.26 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.9, 139.0, 138.2, 138.0, 137.1, 135.8, 135.1, 132.7, 132.5, 129.8, 129.5, 129.0, 128.3, 128.2, 128.1, 127.5, 126.60, 126.56, 125.9, 125.1, 117.4, 21.52, 21.45.

HRMS (ESI) calculated for C₂₁H₁₃F₂NO ([M+H]⁺): 326.1539; found: 326.1530.

3,4-di(thiophen-3-yl)isoquinolin-1(2*H*)-one (5ag)



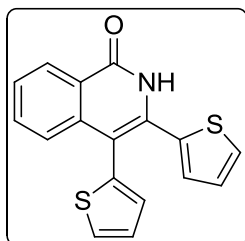
This compound was obtained in 52% yield (32.1 mg) as yellow solid. Eluent: PE/EA = 3/1, $R_f = 0.25$.

^1H NMR (400 MHz, CDCl_3): δ 9.98 (s, 1H), 8.46 (d, $J = 6.7$ Hz, 1H), 7.60 (t, $J = 6.9$ Hz, 1H), 7.49 (dd, $J = 11.0, 4.0$ Hz, 1H), 7.43-7.37 (m, 3H), 7.21 (dd, $J = 5.1, 3.0$ Hz, 1H), 7.12 (dd, $J = 2.9, 1.2$ Hz, 1H), 7.00 (dd, $J = 4.9, 1.2$ Hz, 1H), 6.81 (dd, $J = 5.1, 1.3$ Hz, 1H).

^{13}C NMR (100 MHz, CDCl_3): δ 163.2, 139.1, 136.0, 135.6, 133.2, 132.9, 130.5, 127.6, 127.6, 126.8, 126.5, 125.8, 125.8, 125.7, 125.1, 111.8.

HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{12}\text{NOS}_2$ ($[\text{M}+\text{H}]^+$): 310.0355; found: 310.0353.

3,4-di(thiophen-2-yl)isoquinolin-1(2H)-one (5ah)



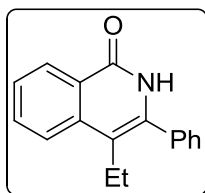
This compound was obtained in 45% yield (27.9 mg) as yellow solid. Eluent: PE/EA = 3/1, $R_f = 0.25$.

^1H NMR (400 MHz, CDCl_3): δ 10.06 (s, 1H), 8.44 (d, $J = 7.9$ Hz, 1H), 7.61 (t, $J = 7.6$ Hz, 1H), 7.50 (m, 3H), 7.35 (dd, $J = 11.8, 6.6$ Hz, 2H), 7.19-7.16 (m, 1H), 7.07 (d, $J = 3.2$ Hz, 1H), 7.06-7.02 (m, 1H).

^{13}C NMR (100 MHz, CDCl_3): δ 163.0, 139.5, 136.1, 136.0, 133.4, 133.1, 131.2, 129.3, 128.1, 128.0, 127.7, 127.4, 126.9, 126.8, 125.9, 124.8, 109.1.

HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{12}\text{NOS}_2$ ($[\text{M}+\text{H}]^+$): 310.0355; found: 310.0353.

4-ethyl-3-phenylisoquinolin-1(2H)-one (5ai)



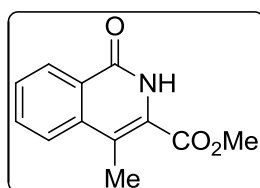
This compound was obtained in 88% yield (43.6 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.32$.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 9.49 (s, 1H), 8.42 (dd, $J = 8.2, 1.4$ Hz, 1H), 7.80-7.76 (m, 1H), 7.75-7.70 (m, 1H), 7.52-7.45 (m, 6H), 2.67 (q, $J = 7.4$ Hz, 2H), 1.20 (t, $J = 7.5$ Hz, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 162.3, 137.9, 136.6, 135.6, 132.9, 129.4, 129.0, 128.9, 128.2, 126.5, 126.0, 123.9, 115.8, 20.7, 15.4.

HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{16}\text{NO}$ ($[\text{M}+\text{H}]^+$): 250.1226; found: 250.1219.

methyl 4-methyl-1-oxo-1,2-dihydroisoquinoline-3-carboxylate (5aj)



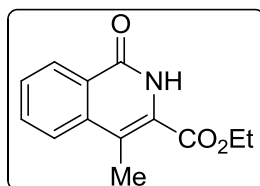
This compound was obtained in 85% yield (37.1 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.14$.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 9.30 (s, 1H), 8.50 (d, $J = 7.9$ Hz, 1H), 7.94 (d, $J = 8.2$ Hz, 1H), 7.79 (t, $J = 7.3$ Hz, 1H), 7.65 (t, $J = 7.5$ Hz, 1H), 4.00 (s, 3H), 2.74 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 163.0, 161.1, 137.9, 133.0, 129.2, 128.1, 128.0, 125.4, 124.5, 120.7, 53.1, 13.3.

HRMS (ESI) calculated for $\text{C}_{12}\text{H}_{12}\text{NO}_3$ ($[\text{M}+\text{H}]^+$): 218.0812; found: 218.0813.

ethyl 4-methyl-1-oxo-1,2-dihydroisoquinoline-3-carboxylate (5ak)



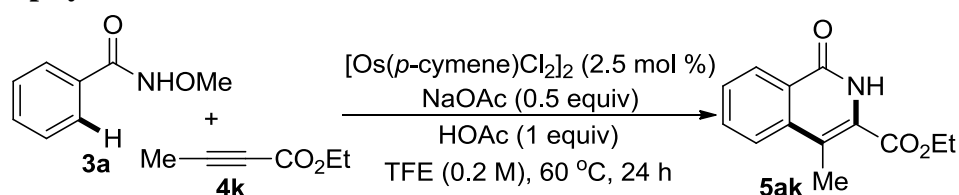
This compound was obtained in 90% yield (41.4 mg) as white solid. Eluent: PE/EA = 3/1, $R_f = 0.20$.

¹H NMR (400 MHz, CDCl₃): δ 9.36 (s, 1H), 8.50 (d, *J* = 7.9 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.78 (t, *J* = 7.6 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 4.46 (q, *J* = 7.1 Hz, 2H), 2.74 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.4, 161.1, 137.9, 132.9, 129.0, 128.04, 127.96, 125.3, 124.6, 120.5, 62.6, 14.3, 13.2.

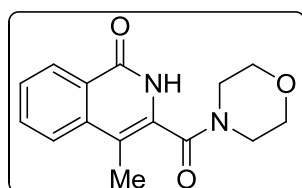
HRMS (ESI) calculated for C₁₃H₁₄NO₃ ([M+H]⁺): 232.0968; found: 232.0963.

Scale-up synthesis of **5ak**:



The mixture of *N*-methoxyamide **3a** (4.4 mmol, 1.1 equiv), alkyne **4k** (4 mmol, 1.0 equiv), [Os(*p*-cymene)Cl₂]₂ (2.5 mol %), NaOAc (0.5 equiv) and HOAc (1 equiv) in TFE (20 mL) was stirred at 60 °C in the oil bath for 24 h without exclusion of air or moisture. Afterwards, the mixture was transferred to a round bottom flask and diluted with EA. Then, the reaction mixture was concentrated and purified by silica column chromatography (eluent: PE/EA = 3/1) to give the desired quinolin-2(1*H*)-one derivative **5ak** (0.8039 g, 87%).

4-methyl-3-(morpholine-4-carbonyl)isoquinolin-1(2*H*)-one (**5al**)



This compound was obtained in 79% yield (43.0 mg) as white solid. Eluent: DCM/EA = 1/1, *R_f* = 0.25.

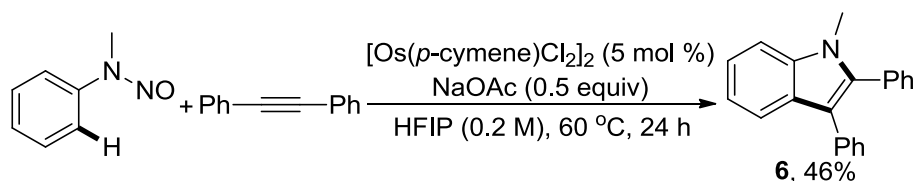
¹H NMR (400 MHz, CDCl₃): δ 12.08 (s, 1H), 8.43 (d, *J* = 7.9 Hz, 1H), 7.78-7.69 (m, 2H), 7.56 (m, 1H), 4.08-3.69 (m, 5H), 3.65-3.35 (m, 3H), 2.31 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.8, 163.6, 137.9, 133.0, 130.8, 127.8, 127.4, 125.9, 123.8, 109.8, 66.8, 66.7, 47.4, 42.6, 13.2.

HRMS (ESI) calculated for C₁₅H₁₇N₂O₃ ([M+H]⁺): 273.1234; found: 273.1228.

NOESY (400 MHz, CDCl₃). The copy of NOESY spectrum is shown in page 116.

III. Divergent C-H Functionalizations under Osmium(II) Catalysis

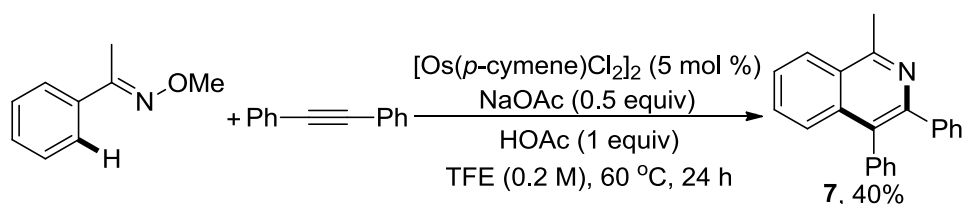


The mixture of *N*-methyl-*N*-phenylnitrous amide (0.2 mmol, 1 equiv), toluene (0.2 mmol, 1 equiv), $[\text{Os}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol %) and NaOAc (0.5 equiv) in HFIP (1 mL) was stirred at 60 °C in the oil bath for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC (Eluent: PE/EA = 5/1, R_f = 0.8) to give the desired 1-methyl-2,3-diphenyl-1H-indole **6** (26.0 mg, 46%) as yellow solid.

^1H NMR (400 MHz, CDCl_3): δ 7.79 (d, J = 7.9 Hz, 1H), 7.41 (d, J = 8.2 Hz, 1H), 7.39-7.35 (m, 3H), 7.35-7.27 (m, 6H), 7.27-7.23 (m, 1H), 7.21-7.15 (m, 2H), 3.67 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 137.9, 137.5, 135.4, 132.1, 131.3, 130.0, 128.5, 128.3, 128.2, 127.1, 125.6, 122.3, 120.3, 119.8, 115.3, 109.7, 31.1.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{18}\text{N}$ ($[\text{M}+\text{H}]^+$): 284.1434; found: 284.1430.



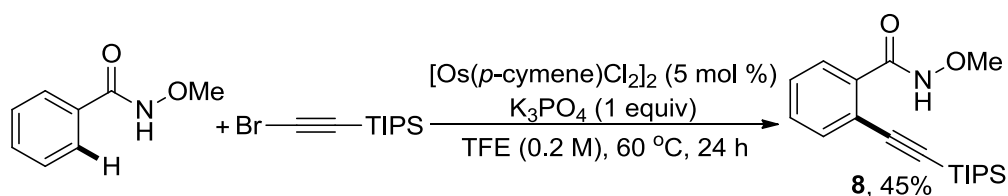
The mixture of acetophenone *O*-methyl oxime (0.2 mmol, 1 equiv), toluene (0.2 mmol, 1 equiv), $[\text{Os}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol %) NaOAc (0.5 equiv) and HOAc (0.2 mmol, 1 equiv) in TFE (1 mL) was stirred at 60 °C in the oil bath for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC (Eluent: PE/EA = 3/1, R_f =

0.8) to give the desired 1-methyl-3,4-diphenylisoquinoline **7** (23.6 mg, 40%) as yellow solid.

¹H NMR (400 MHz, CDCl₃): δ 8.21-8.15 (m, 1H), 7.67-7.63 (m, 1H), 7.59-7.54 (m, 2H), 7.41-7.32 (m, 2H), 7.34-7.29 (m, 3H), 7.23-7.16 (m, 5H), 3.07 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 157.83, 149.54, 141.13, 137.70, 136.11, 131.52, 130.38, 130.01, 129.28, 128.30, 127.71, 127.23, 127.03, 126.63, 126.34, 126.26, 125.63, 22.86.

HRMS (ESI) calculated for C₂₂H₁₈N ([M+H]⁺): 296.1434; found: 296.1427.

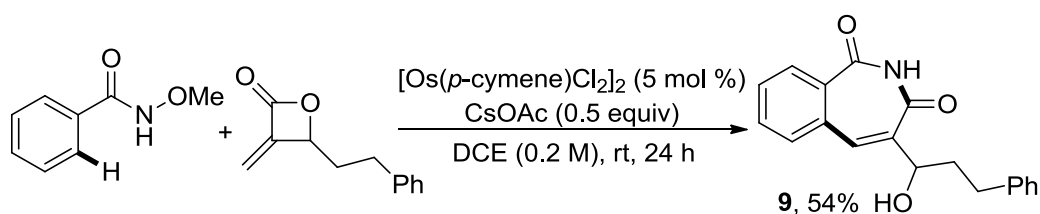


The mixture of *N*-methoxybenzamide (0.2 mmol, 1 equiv), (bromoethynyl)triisopropylsilane (0.2 mmol, 1 equiv), [Os(*p*-cymene)Cl₂]₂ (5 mol %) and K₃PO₄ (0.2 mmol, 1 equiv) in TFE (1 mL) was stirred at 60 °C in the oil bath for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC (PE/EA = 10/1, R_f = 0.25) to give the desired *N*-methoxy-2-((triisopropylsilyl)ethynyl)benzamide **8** (29.8 mg, 45%) as colorless solid.

¹H NMR (400 MHz, CDCl₃): δ 10.50 (s, 1H), 8.13-8.07 (m, 1H), 7.55 (m, 1H), 7.46-7.43 (m, 2H), 3.88 (s, 3H), 1.18-1.14 (m, 21H).

¹³C NMR (100 MHz, CDCl₃): δ 164.5, 134.2, 133.0, 131.2, 130.3, 129.3, 119.6, 105.8, 99.3, 64.6, 18.7, 11.3.

HRMS (ESI) calculated for C₁₉H₃₀NO₂Si ([M+H]⁺): 332.2040; found: 332.2039.



The mixture of *N*-methoxybenzamide (0.2 mmol, 1 equiv), 3-methylene-4-phenethyloxetan-2-one (0.2 mmol, 1 equiv), [Os(*p*-cymene)Cl₂]₂ (5 mol %) and CsOAc (0.1 mmol, 0.5 equiv) in DCE (1 mL) was stirred at room temperature in the oil bath for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC (PE/EA = 1/1, R_f = 0.3) to give the desired 4-(1-hydroxy-3-phenylpropyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione **9** (33.2 mg, 54%) as white solid.

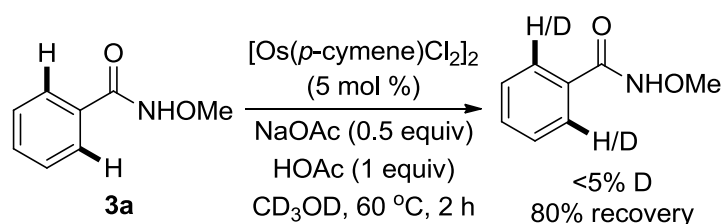
¹H NMR (400 MHz, DMSO-*d*₆): δ 8.03 (s, 1H), 7.64 (s, 1H), 7.62-7.59 (m, 1H), 7.57 (d, *J* = 1.7 Hz, 1H), 7.55-7.50 (m, 2H), 7.50-7.45 (m, 1H), 7.25 (t, *J* = 7.3 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.11 (d, *J* = 6.9 Hz, 2H), 5.71 (dt, *J* = 4.5, 2.5 Hz, 1H), 2.66 (t, *J* = 8.1 Hz, 2H), 2.23-2.13 (m, 1H), 1.96-1.86 (m, 1H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 169.6, 164.3, 140.6, 137.8, 136.2, 130.19, 130.15, 129.9, 128.9, 128.5, 128.4, 128.2, 126.1, 79.5, 32.6, 30.0.

HRMS (ESI) calculated for C₁₉H₁₈NO₃ ([M+H]⁺): 308.1281; found: 308.1280.

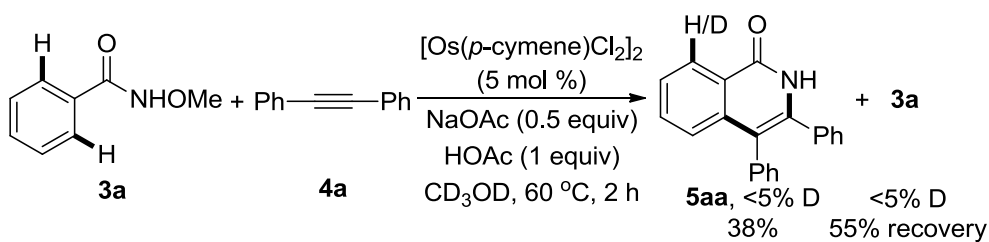
IV. Experimental Mechanistic Studies

Deuterium incorporation:



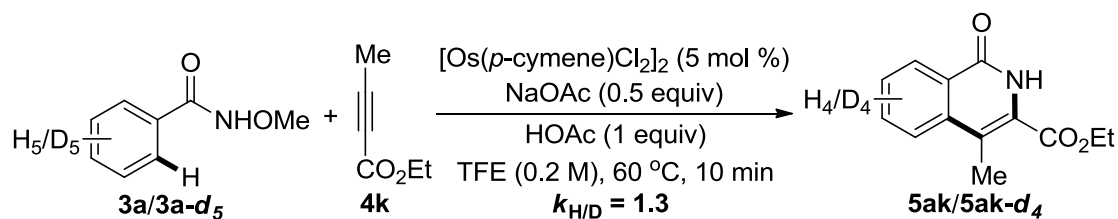
The mixture of *N*-methoxybenzamide **3a** (0.1 mmol, 1 equiv), [Os(*p*-cymene)Cl₂]₂ (5 mol %), NaOAc (0.05 mmol, 0.5 equiv) and HOAc (0.1 mmol, 1 equiv) in CD₃OD (0.5 mL) was stirred at 60 °C in the oil bath for 2 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC (PE/EA = 3/1, R_f = 0.2) to recover the

N-methoxybenzamide (12.0 mg, 80%) and no obvious deuterium incorporation was observed by $^1\text{H-NMR}$ analysis.



The mixture of *N*-methoxybenzamide **3a** (0.2 mmol, 1 equiv), toluene **4a** (0.2 mmol, 1 equiv), $[\text{Os}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol %), NaOAc (0.1 mmol, 0.5 equiv) and HOAc (0.2 mmol, 1 equiv) in CD_3OD (1 mL) was stirred at 60 °C in the oil bath for 2 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC (PE/EA = 3/1, $R_f = 0.2$) to give the desired product **5aa** (22.7 mg, 38%) together with the recovery of **3a** (16.0 mg, 55%). $^1\text{H-NMR}$ analysis revealed no obvious deuterium incorporation at both the *ortho*-position of **5aa** and the recovered **3a**.

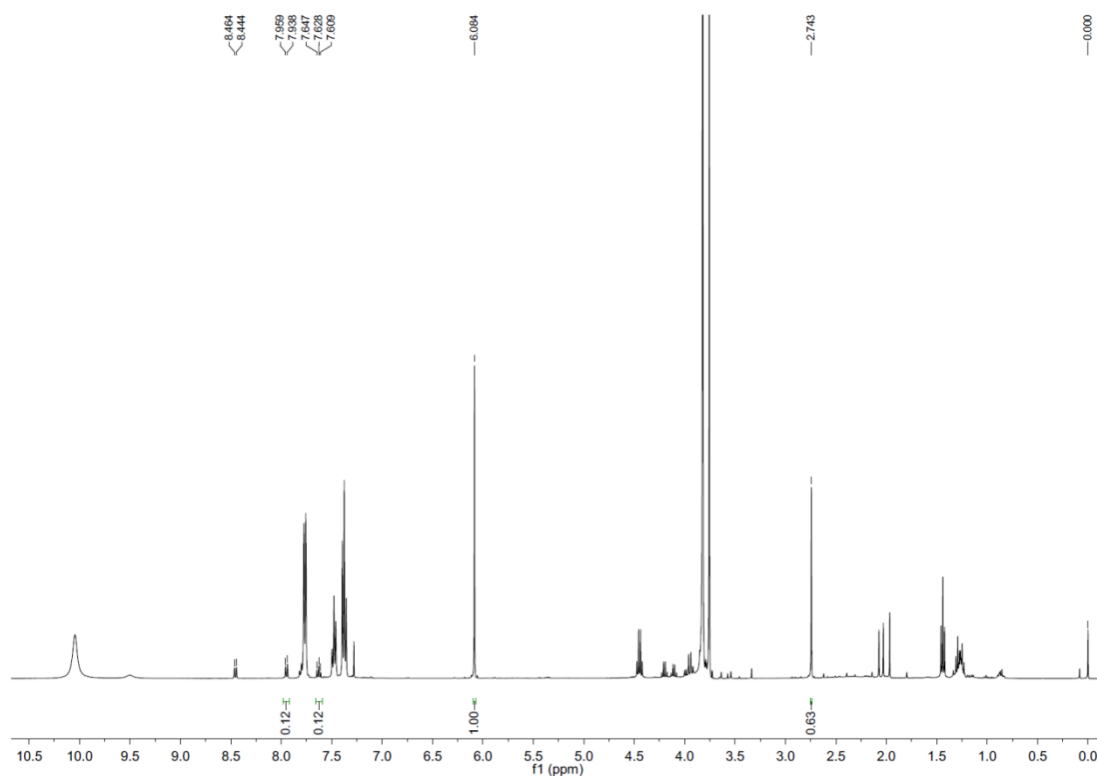
Kinetic isotope study:



In the oil bath, an equimolar mixture of **3a** (0.1 mmol, 1 equiv) and **3a-d₅** (0.1 mmol, 1 equiv) was allowed to react with **4k** (0.1 mmol, 1 equiv) in TFE (0.5 mL) in the presence of $[\text{Os}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol %), NaOAc (0.05 mmol, 0.5 equiv) and HOAc (0.1 mmol, 1 equiv). The reaction was stopped after 10 min, and the crude product was analyzed by $^1\text{H-NMR}$ spectroscopy by employing 1,3,5-trimethoxybenzene as internal standard. The singlet and double doublet at δ : 2.74, 7.93 were used for calculation, and the result revealed that the yield was determined to be 21%, among which **5ak** was obtained in 12% while **5ak-d₄** in 9%

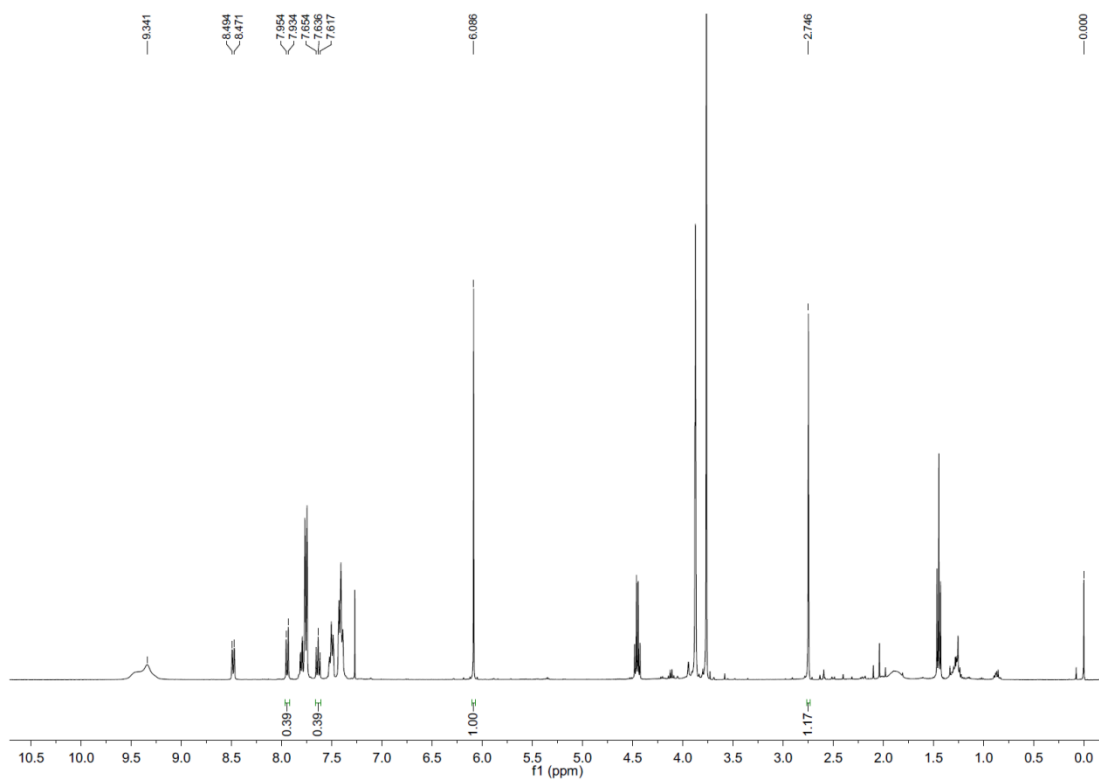
yield, thus giving an average value of $k_H/k_D = 12/9 = 1.3$.

Crude $^1\text{H-NMR}$ of the synthesis for **5ak** and **5ak-d₄** for 10 min

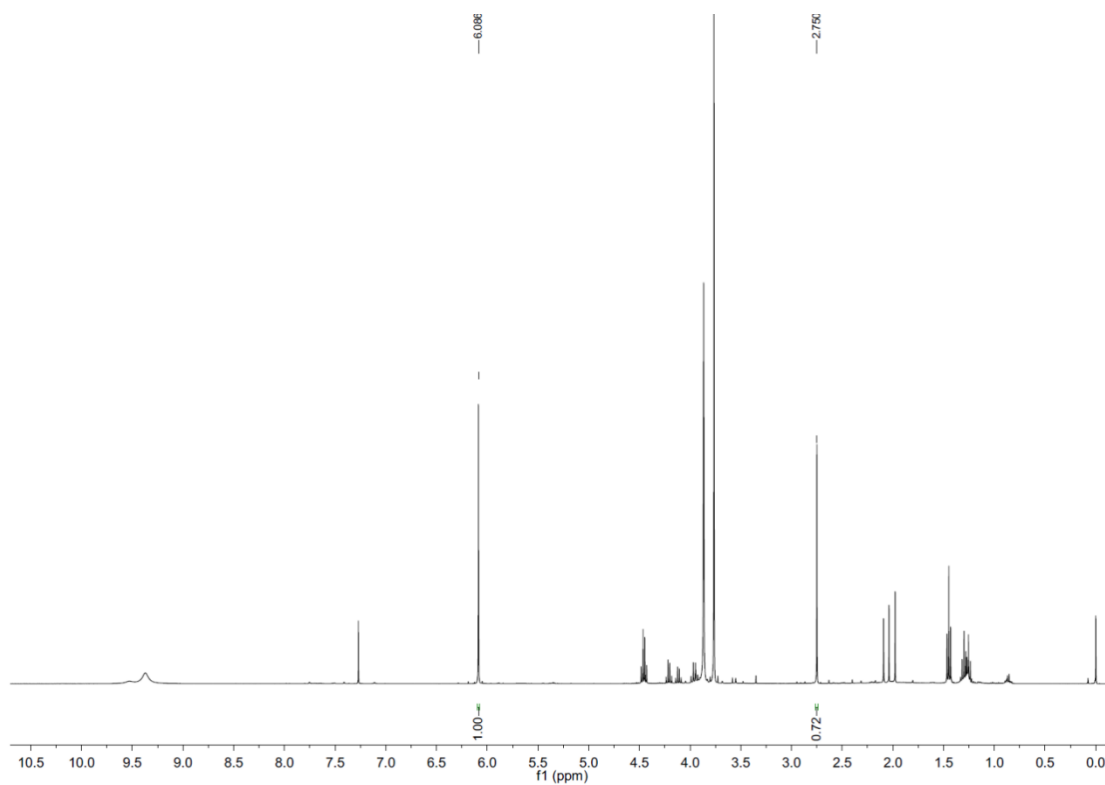


Another two parallel KIE experiments were performed by treating 1 equiv of **3a** or 1 equiv of **3a-d₅** with 1 equiv of **4k** separately under the standard conditions in the oil bath for 10 min. Afterwards, the yield was analyzed by $^1\text{H-NMR}$ with 1,3,5-trimethoxybenzene as the internal standard. The singlet at δ : 2.75 was used for calculation of $^1\text{H-NMR}$ yields, which were determined as 39% and 28%, respectively. Thus the KIE was determined to be $k_H/k_D = 1.6$.

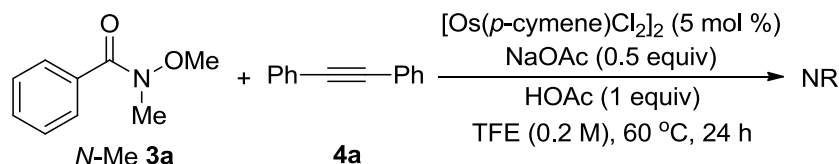
Crude $^1\text{H-NMR}$ of the synthesis for **5ak** under standard condition for 10 min



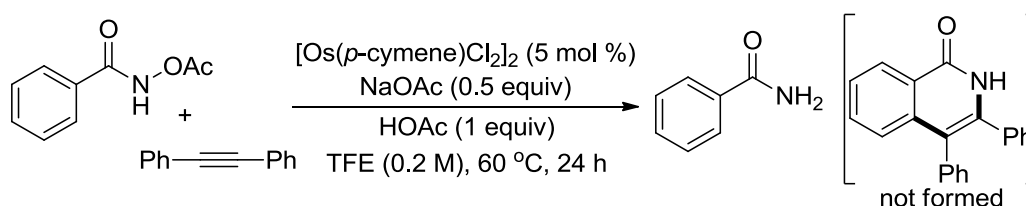
Crude $^1\text{H-NMR}$ of the synthesis for **5ak- d_4** under standard condition for 10 min



Control experiment:



The mixture of *N*-methoxy-*N*-methylbenzamide (0.2 mmol, 1 equiv), tolane **4a** (0.2 mmol, 1 equiv), [Os(*p*-cymene)Cl₂]₂ (5 mol %), NaOAc (0.1 mmol, 0.5 equiv) and HOAc (0.2 mmol, 1 equiv) in TFE (1 mL) was stirred at 60 °C in the oil bath for 24 h without exclusion of air or moisture. The reaction was monitored by TLC and no reaction was detected.



The mixture of *N*-acetoxybenzamide (0.2 mmol, 1 equiv), tolane (0.2 mmol, 1 equiv), [Os(*p*-cymene)Cl₂]₂ (5 mol %), NaOAc (0.1 mmol, 0.5 equiv) and HOAc (0.2 mmol, 1 equiv) in TFE (1 mL) was stirred at 60 °C in the oil bath for 24 h without exclusion of air or moisture. The reaction was monitored by TLC and no desired isoquinolone product was detected, while the decomposition of *N*-acetoxybenzamide was observed to yield the corresponding benzamide.

V. DFT Studies

Computational details

Calculations were performed by using Gaussian 09 quantum chemical package.^{S3} The geometries of all reported reactants, intermediates, transition states, and products were optimized using the B3LYP functional^{S4} with the LANL2DZ basis set^{S5} and corresponding Hay–Wadt effective core potential (ECP) for Os in conjunction with a standard 6-31G(d) basis set for all other atoms. Frequency analysis was conducted at the same level of theory to obtain the thermodynamic energy corrections and to ensure that the optimized structures were at either a minimum or transition state. The located transition structures were reconfirmed by intrinsic reaction coordinate (IRC)^{S6}

calculations. Single point energies were calculated at the level of M06L^{S7}/6-311++G(d,p) (SDD^{S8} basis set for Os) using SMD^{S9} solvation model (solvent = 2,2,2-TriFluoroEthanol, $\epsilon=26.726$). The energies presented in this paper are the M06L-calculated single point energies combined with B3LYP-calculated thermodynamic corrections.

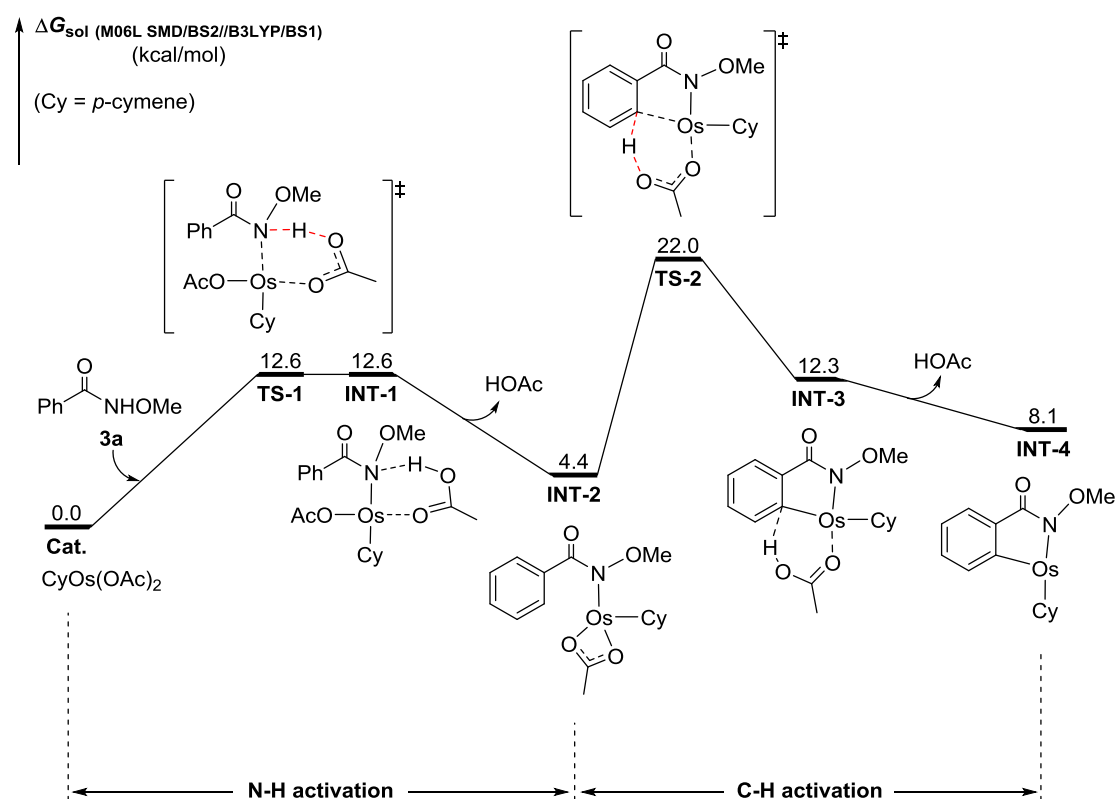


Figure S1. Computed Gibbs free energy changes for N-H/C-H activation process.

Various energy values for the reported species and imaginary frequencies for the transition states

Table S2 Energies, enthalpies, and free energies corrections of the structures calculated at the B3LYP/LANL2DZ-6-31G(d) and single point energies at the M06L/SDD-6-311++G(d,p)(SMD^{TFE})// B3LYP/LANL2DZ-6-31G(d) (in Hartree).

Structures	ZPE	ΔE	ΔH	ΔG	SP _{SMD}	Imaginary frequency
Cat.	0.318984	0.341112	0.342056	0.266016	-937.451654	—

3a	0.160314	0.170372	0.171316	0.124026	-515.497139	—
4a	0.191906	0.202975	0.203919	0.153515	-539.525712	—
5aa	0.303158	0.320432	0.321376	0.256913	-939.413720	—
HOAc	0.062015	0.066603	0.067548	0.034623	-229.135701	—
HOMe	0.051473	0.054763	0.055707	0.028753	-115.745966	—
INT-1	0.480110	0.513405	0.514349	0.413778	-1452.952486	—
INT-2	0.416961	0.444325	0.445269	0.358234	-1223.808894	—
INT-3	0.416049	0.443991	0.444935	0.357016	-1223.795090	—
INT-4	0.352692	0.374740	0.375684	0.300576	-994.644192	—
INT-5	0.546495	0.580770	0.581714	0.479295	-1534.194487	—
INT-6	0.547828	0.581498	0.582442	0.481316	-1534.193078	—
INT-7	0.555025	0.591500	0.592444	0.484432	-1647.609183	—
INT-8	0.555512	0.591636	0.592580	0.485741	-1647.605731	—
INT-9	0.559321	0.594464	0.595408	0.490868	-1647.723040	—
INT-5'	0.546954	0.581049	0.581993	0.480072	-1534.185810	—
INT-7'	0.547594	0.580760	0.581704	0.483157	-1534.161181	—
INT-7a'	0.548575	0.581512	0.582456	0.483889	-1534.190460	—
INT-7''	0.545744	0.580286	0.581230	0.477906	-1534.204253	—
INT-8'	0.620896	0.662471	0.663415	0.544549	-1876.771320	—
INT-9'	0.619637	0.662219	0.663164	0.535461	-1876.785499	—
TS-1	0.475770	0.509014	0.509958	0.407950	-1452.946578	-851.03
TS-2	0.410945	0.438242	0.439187	0.352754	-1223.775308	-817.43
TS-3	0.545172	0.578878	0.579823	0.478403	-1534.165730	-300.55
TS-4	0.609618	0.648470	0.649414	0.538068	-1763.345692	-261.23
TS-5	0.554680	0.590344	0.591288	0.485727	-1647.602626	-131.21
TS-6	0.555041	0.590485	0.591429	0.486738	-1647.604668	-126.32
TS-7	0.618238	0.658787	0.659731	0.543084	-1876.850560	-782.32
TS-3'	0.544645	0.578542	0.579486	0.477746	-1534.153866	-147.05
TS-4'	0.546150	0.579089	0.580033	0.482127	-1534.154827	-291.48

TS-4''	0.543477	0.577365	0.578309	0.478156	-1534.163141	-287.39
TS-5'	0.615928	0.657239	0.658184	0.539801	-1876.756082	-947.97
TS-6'	0.620574	0.661184	0.662128	0.545118	-1876.745729	-402.96

Cartesian coordinates of the optimized structures

Cat.

C	1.81890800	-1.89933500	-0.66108700
O	0.76388000	-1.59568700	-1.30917100
O	1.94852000	-1.38887800	0.49966900
C	2.87443900	-2.78858000	-1.25135400
H	3.59202900	-2.16602000	-1.79855800
H	3.41201900	-3.31928500	-0.46211300
H	2.42824500	-3.49617800	-1.95409900
O	1.55424200	0.91505000	-0.81821600
C	1.63500300	2.22765400	-0.88796800
O	0.88439400	3.03337800	-0.34560700
C	2.81255400	2.67650000	-1.74518800
H	3.75001500	2.31211000	-1.31086200
H	2.73284500	2.24688500	-2.74949600
H	2.83591200	3.76599600	-1.80836300
Os	0.16196800	-0.16001900	0.22380800
C	-0.44185700	0.16472200	2.32564700
C	-1.07501000	-1.03989000	1.85461400
C	-1.82824300	-1.03693100	0.65462400
C	-2.01699100	0.17418700	-0.10749100
C	-1.42814100	1.36676600	0.39214200
C	-0.64577600	1.36854700	1.59479500
H	-0.86740800	-1.98092700	2.35292500
H	-2.17833300	-1.98194000	0.25643300
H	-1.44018600	2.26700200	-0.20836600
H	-0.10180100	2.26630200	1.85658200
C	0.45644900	0.12883800	3.53353400
H	1.01514200	-0.81078900	3.57991800
H	1.17418500	0.95350500	3.51180400
H	-0.14083100	0.21791900	4.45025400
C	-2.81036800	0.20175000	-1.40440500
H	-2.43896100	1.06276500	-1.97499400
C	-4.29947300	0.45104000	-1.08701100
H	-4.43926700	1.37340000	-0.51257700
H	-4.87718800	0.53636600	-2.01439600

H	-4.72082900	-0.37714500	-0.50398100
C	-2.62982300	-1.04918600	-2.27878600
H	-3.12530200	-0.89759200	-3.24427400
H	-1.57245100	-1.26293500	-2.46078900
H	-3.08572000	-1.93542400	-1.82025300

3a

C	-3.41612700	-0.33763700	-0.03232500
C	-2.52441500	-1.40487900	-0.15845500
C	-1.14876800	-1.17200300	-0.14856100
C	-0.65564500	0.13447800	-0.01106900
C	-1.55690400	1.20273200	0.09601300
C	-2.92966600	0.96690600	0.09179600
H	-4.48722700	-0.52091900	-0.03928700
H	-2.89905700	-2.41816000	-0.27453300
H	-0.46395100	-2.00410500	-0.28469300
H	-1.15762700	2.20819500	0.18008900
H	-3.62172400	1.79965400	0.18212000
C	0.80782600	0.46663500	0.01589400
O	1.24595000	1.57238900	-0.25500400
N	1.63787700	-0.61381800	0.31535700
H	1.28740800	-1.28974600	0.98566300
O	2.95857400	-0.29211900	0.66150300
C	3.78908800	-0.31749500	-0.50090200
H	4.79609200	-0.11144500	-0.12907600
H	3.76234100	-1.30195700	-0.98427500
H	3.49007800	0.46063300	-1.20985200

4a

C	-0.00002300	0.60825900	0.00006100
C	0.00002300	-0.60825900	0.00006100
C	0.00002300	-2.03321100	0.00002200
C	0.00002100	-2.75093400	1.21364100
C	0.00002200	-2.75087700	-1.21362300
C	0.00002000	-4.14328400	1.20874500
H	0.00002100	-2.20318700	2.15101900
C	0.00002300	-4.14323300	-1.20878900
H	0.00002300	-2.20309700	-2.15098300
C	0.00002000	-4.84467700	-0.00004000
H	0.00001800	-4.68364900	2.15158900
H	0.00002300	-4.68354800	-2.15166100
H	0.00001900	-5.93122100	-0.00006000
C	-0.00002300	2.03321100	0.00002200
C	-0.00002100	2.75093400	1.21364100

C	-0.00002200	2.75087700	-1.21362300
C	-0.00002000	4.14328400	1.20874500
H	-0.00002100	2.20318700	2.15101900
C	-0.00002300	4.14323300	-1.20878900
H	-0.00002300	2.20309700	-2.15098300
C	-0.00002000	4.84467700	-0.00004000
H	-0.00001800	4.68364900	2.15158900
H	-0.00002300	4.68354800	-2.15166100
H	-0.00001900	5.93122100	-0.00006000

5aa

C	-3.98994800	1.49451000	0.12761600
C	-2.60343500	1.48690600	0.10071300
C	-1.88231000	0.27324400	0.00678200
C	-2.63419100	-0.93087500	-0.03381800
C	-4.03758200	-0.90881600	-0.00951100
C	-4.71873400	0.29530500	0.06703400
H	-4.51561700	2.44325700	0.20015100
H	-2.06137600	2.42398500	0.15704100
H	-4.55834900	-1.86009900	-0.04781200
H	-5.80464800	0.31286600	0.08731300
C	-1.96374300	-2.23654500	-0.09566300
O	-2.52120800	-3.32942400	-0.15340500
N	-0.57502500	-2.15343800	-0.08838800
C	0.19209100	-0.99777200	-0.06516000
C	-0.42348600	0.22789600	-0.01795100
C	0.36534600	1.49385100	0.06736100
C	1.13733000	1.78590100	1.20232800
C	0.33862600	2.42993600	-0.98044300
C	1.87061400	2.97044000	1.28383500
H	1.16129100	1.07502300	2.02330400
C	1.06997300	3.61581100	-0.89954800
H	-0.25642300	2.21990400	-1.86562700
C	1.83972700	3.88940600	0.23329300
H	2.46363200	3.17629100	2.17107900
H	1.04033800	4.32451400	-1.72313600
H	2.40965200	4.81247100	0.29699400
C	1.65866500	-1.24751700	-0.08798000
C	2.50093600	-0.59413500	-1.00174200
C	2.21743500	-2.19822800	0.78411800
C	3.86477400	-0.87969000	-1.03544900
H	2.08215100	0.13263800	-1.68906200
C	3.58334600	-2.47918400	0.75079100
H	1.58227500	-2.70181000	1.50856700

C	4.41128800	-1.82132900	-0.16024900
H	4.50134400	-0.36885300	-1.75268200
H	3.99938200	-3.20930300	1.43963600
H	5.47492400	-2.04132400	-0.18921800
H	-0.10407100	-3.04480100	-0.18872200
HOAc			
C	-0.09248900	0.12563500	0.00002500
O	-0.64566500	1.20201800	-0.00008500
O	-0.77869500	-1.04665400	0.00001000
H	-1.72373000	-0.80289700	-0.00004000
C	1.39753800	-0.10984100	0.00004800
H	1.68547200	-0.69134400	0.88211000
H	1.68545700	-0.69176700	-0.88173700
H	1.91738700	0.84833700	-0.00017300
HOMe			
O	-0.74856200	-0.12249200	0.00000100
H	-1.13602900	0.76526500	0.00000800
C	0.66188000	0.01964700	0.00000200
H	1.03679700	0.54354700	0.89334600
H	1.07971000	-0.99088900	-0.00034500
H	1.03673900	0.54413100	-0.89302800
INT-1			
N	-0.96754000	-0.54520100	0.36187300
O	1.47901100	-0.70017700	1.58252300
O	3.14702300	0.72071600	2.17932000
C	2.42559200	-0.25368000	2.37613700
C	2.55035000	-1.08625500	3.64989800
H	1.68232300	-0.90516000	4.29504000
H	2.56432100	-2.15529300	3.41538400
H	3.45713200	-0.80816300	4.19052600
H	-0.47940000	-2.10968400	0.55495700
O	1.42498900	-2.02244900	-0.78491900
C	0.90165700	-3.05788700	-0.33259000
O	-0.13886800	-3.07449700	0.44968000
C	1.44779400	-4.41224600	-0.69189500
H	0.70955200	-4.94854100	-1.29819800
H	2.37897800	-4.31090400	-1.24969800
H	1.61308400	-4.99659100	0.21843500
Os	1.00632800	0.07351800	-0.29055000
C	2.51907200	0.62504600	-1.88423000
C	2.82034900	1.34004000	-0.70410000

C	1.80111100	2.10704000	-0.03470000
C	0.48936000	2.23233400	-0.56732400
C	0.19474300	1.49479900	-1.77304500
C	1.17706900	0.70077000	-2.41082700
H	3.77370200	1.20742300	-0.20978200
H	2.04222200	2.52073100	0.93413400
H	-0.82466500	1.45771600	-2.14096100
H	0.89251500	0.07813600	-3.25179700
C	3.53063200	-0.27950800	-2.53441800
H	3.07617600	-1.23760700	-2.80381700
C	-0.58845700	3.09523700	0.06701900
H	-1.54163400	2.57146800	-0.08059500
H	3.91791700	0.18477200	-3.45043000
H	4.37330700	-0.47321600	-1.86500700
C	-0.40586000	3.31907500	1.57374900
H	0.48149700	3.92583200	1.78973900
H	-1.27173400	3.85925600	1.97328500
H	-0.32115100	2.36525000	2.10086700
C	-0.66787700	4.43834400	-0.68963100
H	-0.84924000	4.29133700	-1.76039900
H	-1.48273700	5.05247600	-0.28953800
H	0.26595500	5.00293500	-0.57999700
C	-1.97981700	-0.71885900	-0.57597400
O	-1.67270700	-1.16897500	-1.68412200
C	-3.43820400	-0.47570200	-0.26434500
C	-3.94655600	0.55354500	0.54522600
C	-4.34428100	-1.31248300	-0.93877200
C	-5.32571700	0.72879300	0.67799900
H	-3.26846000	1.21247000	1.07017500
C	-5.71851000	-1.15101700	-0.78387100
H	-3.94618400	-2.08249300	-1.59080100
C	-6.21495000	-0.12593400	0.02562700
H	-5.70402100	1.53683800	1.29892000
H	-6.40268800	-1.81837900	-1.30135000
H	-7.28730200	0.00817400	0.14250100
O	-1.38648200	0.08446900	1.57675300
C	-1.51394000	-0.86910500	2.62906200
H	-1.80820900	-0.29092900	3.51028400
H	-2.29577700	-1.60765800	2.40540100
H	-0.55869500	-1.36795500	2.81354600
INT-2			
N	1.19897400	0.04917000	-0.27402700
O	-0.80752300	1.63890100	-1.60064100

O	-0.73887600	1.94768900	0.55222500
C	-0.67915500	2.44338400	-0.61759300
C	-0.44348700	3.90993200	-0.83503300
H	0.63388100	4.09706100	-0.76083700
H	-0.78712400	4.21506700	-1.82584000
H	-0.94302800	4.49655900	-0.05969600
O _s	-0.85663400	-0.11089000	-0.27731300
C	-1.16161600	-2.19338900	-0.97948200
C	-2.20294200	-1.34242700	-1.47162100
C	-3.04611600	-0.58663800	-0.59651000
C	-2.78500500	-0.55222200	0.79698800
C	-1.71964600	-1.39178000	1.30075100
C	-0.96556100	-2.22609100	0.44326200
H	-2.32108200	-1.22274000	-2.54415100
H	-3.76487300	0.09816700	-1.02946700
H	-1.45880400	-1.34126800	2.35287600
H	-0.10458800	-2.74876700	0.83600100
C	-0.30516100	-3.01541600	-1.90446300
H	0.69618100	-3.12829000	-1.48317100
C	-3.57161200	0.30116000	1.77791100
H	-2.85819300	0.62302600	2.54791600
H	-0.74363500	-4.01205400	-2.04826600
H	-0.22205600	-2.53846000	-2.88662500
C	-4.19241400	1.56537100	1.16930600
H	-4.96380600	1.32689300	0.42698000
H	-4.67482300	2.15402500	1.95729600
H	-3.42882200	2.19035300	0.69816400
C	-4.64640800	-0.57123100	2.46164600
H	-4.20740500	-1.45199100	2.94350100
H	-5.17387300	0.00640300	3.22922000
H	-5.38733400	-0.92125100	1.73276400
C	2.13560300	-0.83508800	0.19778300
O	1.87492700	-2.03450100	0.37222300
C	3.53091200	-0.35801600	0.52959700
C	3.80212000	0.83685100	1.21278400
C	4.58709900	-1.23584100	0.24757400
C	5.10810000	1.14748700	1.59221800
H	2.99112200	1.51590200	1.44835300
C	5.89570900	-0.91130000	0.60327400
H	4.36346500	-2.17780700	-0.24316900
C	6.15935000	0.28211900	1.27899700
H	5.30563500	2.06989500	2.13255900
H	6.70684900	-1.59420100	0.36391900
H	7.17710900	0.53364800	1.56666500

O	1.76124300	1.30755300	-0.64540700
C	2.20051300	1.26372700	-2.00185700
H	2.56979900	2.27049800	-2.22147000
H	3.01815800	0.54314300	-2.12962700
H	1.36875800	1.01894400	-2.67032200

INT-3

N	-0.26092700	0.64188300	1.49419700
O	-1.45114000	-1.78851700	0.56543800
O	-3.32698700	-0.78863700	-0.20484500
C	-2.68030100	-1.72246800	0.46263100
C	-3.58771500	-2.73150600	1.11246900
H	-4.15163600	-2.24052000	1.91345500
H	-3.00102200	-3.55050600	1.52885400
H	-4.31278200	-3.10951600	0.38545800
Os	0.29427200	-0.47041400	-0.12941700
C	1.18061300	-2.34457300	-1.06864000
C	1.30307400	-1.27911100	-1.99651100
C	1.86017400	-0.02853700	-1.57417200
C	2.38013600	0.15595400	-0.24999400
C	2.38511500	-1.00039300	0.62367700
C	1.80312500	-2.21248300	0.23082600
H	0.85720200	-1.36602400	-2.98128400
H	1.81429000	0.81552800	-2.25188900
H	2.71274600	-0.87429300	1.64978800
H	1.69785600	-3.01692200	0.95132600
C	0.48275300	-3.62708700	-1.44044000
H	-0.10435800	-4.00937800	-0.59981900
C	3.01838200	1.44909600	0.23379900
H	2.72976200	1.55402400	1.28749500
H	1.21408100	-4.39699400	-1.71948400
H	-0.19167200	-3.47667500	-2.28888200
C	2.53436100	2.70332900	-0.50628500
H	2.87496900	2.71836200	-1.54942900
H	2.94123000	3.59692100	-0.02084800
H	1.44324400	2.78056400	-0.49676500
C	4.55498000	1.32869400	0.16433300
H	4.92126400	0.46591700	0.73256300
H	5.02709800	2.22783100	0.57641100
H	4.89257800	1.21564000	-0.87343500
C	-0.99007300	1.79836300	1.36515700
O	-1.22309900	2.61744800	2.25439400
C	-1.47943100	1.91474100	-0.04608600
C	-1.02069700	0.92884000	-0.95334000

C	-2.31651200	2.96066400	-0.43319200
C	-1.47371200	1.03952800	-2.28362000
H	-2.67650300	-0.13577000	-0.57462200
C	-2.73675200	3.05081600	-1.76174300
H	-2.61955000	3.68762100	0.31565400
C	-2.31743100	2.08605200	-2.68172600
H	-1.17001300	0.30143500	-3.02439800
H	-3.39029900	3.85989700	-2.07739100
H	-2.64635400	2.14625900	-3.71702400
O	0.51472800	0.57875200	2.67783700
C	-0.26450000	0.07472800	3.75862700
H	0.42404300	-0.00090100	4.60654100
H	-0.66846600	-0.91964200	3.52253000
H	-1.07740500	0.76520200	4.00429900

INT-4

N	0.78673300	1.56027500	-0.08512100
Os	-0.22756700	-0.06849000	-0.31206700
C	-1.30525500	-1.17453000	-1.92778400
C	-1.32105600	-2.02349700	-0.78618700
C	-1.73650300	-1.52754400	0.47358600
C	-2.23237200	-0.18036600	0.60607100
C	-2.43025100	0.59339600	-0.58647100
C	-1.91594600	0.13171500	-1.81194100
H	-0.85260000	-2.99949900	-0.84688700
H	-1.59092900	-2.13650600	1.35710300
H	-2.78798000	1.61356900	-0.50383700
H	-1.91368700	0.78871200	-2.67607200
C	-0.76562900	-1.65061100	-3.25151000
H	-0.34860500	-0.81908200	-3.82790700
C	-2.69333800	0.38144100	1.94290100
H	-2.64834700	1.47433900	1.85059100
H	-1.56510000	-2.10869500	-3.84936200
H	0.02374100	-2.39444900	-3.11110500
C	-1.80753200	-0.01602600	3.13298800
H	-1.85952200	-1.09100600	3.34280100
H	-2.14620600	0.50588100	4.03472600
H	-0.76074400	0.24876500	2.95483400
C	-4.16482100	-0.01476000	2.18587000
H	-4.81092000	0.30909300	1.36215100
H	-4.53546900	0.44520800	3.10892600
H	-4.26769200	-1.10205600	2.28678200
C	2.13398400	1.54239500	0.35797200
O	2.79565000	2.54430400	0.56414300

C	2.59385400	0.13333200	0.51328200
C	1.62326900	-0.85316600	0.24380300
C	3.89717300	-0.16539100	0.90094400
C	2.03095300	-2.18783700	0.38345000
C	4.27289000	-1.50482800	1.03468400
H	4.59528400	0.64459400	1.09472200
C	3.33788600	-2.50960800	0.77454800
H	1.33166200	-2.99910100	0.18993500
H	5.28390100	-1.76286700	1.33869000
H	3.62715900	-3.55350700	0.87651700
O	0.22810900	2.85263800	-0.15061500
C	0.60936400	3.51631800	-1.35609200
H	0.07712900	4.47138200	-1.33911400
H	0.29863100	2.93496000	-2.23554400
H	1.68817600	3.69547300	-1.38389100

INT-5

Os	0.40326200	0.16355300	-0.45668100
C	0.38304100	-0.18189600	-2.81859900
C	0.89151100	1.09315900	-2.43694400
C	2.09911100	1.24564600	-1.66229600
C	2.75258700	0.12558800	-1.11560000
C	2.11596900	-1.14234800	-1.30935000
C	0.98846600	-1.29004800	-2.17496900
H	0.39911100	1.98884500	-2.80046400
H	2.46261600	2.24496000	-1.45551400
H	2.53004200	-2.01964900	-0.82777900
H	0.55831800	-2.27920700	-2.30271500
C	-0.76500000	-0.33915500	-3.77718500
H	-1.38008600	-1.20538500	-3.51451000
C	4.03617400	0.19873800	-0.30738600
C	-1.45212800	4.19469300	-0.13559800
C	-1.12391400	2.92582200	-0.62710400
C	-0.32840300	2.04960600	0.12435600
C	0.09724300	2.48120800	1.39060000
C	-0.22389700	3.74537600	1.89049100
C	-1.00145600	4.61038600	1.12143500
H	-2.06946500	4.85901300	-0.73665000
H	-1.51736300	2.62082300	-1.59437800
H	0.14813900	4.02520600	2.87245200
H	-1.25940400	5.59765400	1.49616500
C	0.93449000	1.52622900	2.16748500
O	1.54180400	1.80154300	3.20659000
N	0.90397300	0.30378800	1.54769400

O	1.83689200	-0.63835900	2.05049500
C	1.39200000	-1.17241200	3.30328400
H	2.12085500	-1.94775100	3.56013400
H	0.39626200	-1.61928500	3.20231200
H	1.38779500	-0.39094100	4.06640000
H	3.94461200	-0.56398500	0.47444900
H	-0.39831300	-0.48720300	-4.80136000
H	-1.40484800	0.54827100	-3.77538300
C	4.27927200	1.54343900	0.39064100
H	4.39542200	2.36582300	-0.32608000
H	5.20899600	1.48632000	0.96688500
H	3.47412900	1.78767400	1.08903900
C	5.22256400	-0.17947800	-1.22251900
H	5.07906700	-1.15850400	-1.69374800
H	6.14804200	-0.21763100	-0.63767100
H	5.35731700	0.56232200	-2.01913800
C	-0.84187400	-1.47589300	0.15886000
C	-1.60759400	-0.46682100	-0.03177700
C	-2.97069500	0.03954000	-0.01626200
C	-3.91962600	-0.52048600	-0.89408100
C	-3.38847900	1.04610200	0.87297000
C	-5.24613300	-0.09145800	-0.87928800
H	-3.60599600	-1.29534500	-1.58859400
C	-4.71803900	1.46494700	0.88836100
H	-2.66953500	1.48654200	1.55386900
C	-5.65097800	0.90291200	0.01374400
H	-5.96329800	-0.53665600	-1.56424800
H	-5.02459700	2.23785200	1.58806800
H	-6.68510200	1.23657700	0.02831600
C	-0.73343700	-2.88182500	0.48969000
C	0.47205700	-3.46900300	0.91716500
C	-1.87636600	-3.70245200	0.37325600
C	0.53197800	-4.82991600	1.21440500
H	1.34227100	-2.83485500	1.04607200
C	-1.80878600	-5.06042500	0.67165700
H	-2.81428000	-3.25910700	0.05192800
C	-0.60352400	-5.63332600	1.08930700
H	1.47019300	-5.26381900	1.55105100
H	-2.70036400	-5.67505300	0.57709400
H	-0.55265300	-6.69420000	1.31870600

INT-6

Os	1.03679600	0.01844200	-0.37123100
C	1.47751400	-0.98641500	-2.40875400

C	2.12132700	0.28697400	-2.25053800
C	3.20486600	0.48187000	-1.31226800
C	3.42759800	-0.44461300	-0.29750800
C	2.48049600	-1.54795900	-0.22956000
C	1.66281600	-1.91317200	-1.36393700
H	1.90551300	1.07545200	-2.96454400
H	3.73865300	1.42477900	-1.32648600
H	2.54615600	-2.24387800	0.60175000
H	1.09001100	-2.83203100	-1.33679700
C	0.55571300	-1.23982900	-3.57203500
H	-0.13782800	-2.05865200	-3.36519200
C	4.50457400	-0.31825900	0.76319400
C	-2.50238100	3.76674700	-1.77336000
C	-2.58710200	2.41162800	-1.47291800
C	-1.80794900	1.82337700	-0.45764800
C	-0.94774800	2.65861700	0.28695600
C	-0.90388300	4.03611200	0.00549100
C	-1.65546700	4.58878900	-1.02518200
H	-3.10759800	4.18320000	-2.57447100
H	-3.27899500	1.77988800	-2.02266800
H	-0.27359400	4.66479800	0.62595600
H	-1.59537600	5.65403500	-1.23123600
C	-0.05670000	2.24978400	1.43571500
O	-0.01661700	2.92765000	2.45553700
N	0.84444000	1.21039200	1.19277000
O	1.96526700	1.30437100	2.06682700
C	1.70748500	0.62052800	3.29319500
H	2.63597600	0.70102200	3.86683000
H	1.47618500	-0.43751200	3.10813300
H	0.89256500	1.09908900	3.84246900
H	4.03495600	-0.58659100	1.71831500
H	1.13791700	-1.50835100	-4.46313400
H	-0.03034700	-0.34689400	-3.81225900
C	5.08908400	1.09138500	0.90904800
H	5.61772200	1.40682600	0.00075900
H	5.81766900	1.10632400	1.72714900
H	4.30455700	1.81772400	1.13784300
C	5.61631900	-1.35287500	0.47838400
H	5.21827800	-2.37150100	0.40994300
H	6.36361500	-1.33509400	1.27966400
H	6.12685900	-1.12705300	-0.46549300
C	-0.96301600	-0.50080800	-0.11512700
C	-2.00082000	0.37224500	-0.16745400
C	-3.43267900	-0.01234900	0.07119800

C	-4.11007200	-0.94429200	-0.72999500
C	-4.14686000	0.60674300	1.11286100
C	-5.44725500	-1.26455800	-0.48653700
H	-3.58676400	-1.41518100	-1.55554700
C	-5.47893300	0.28165900	1.36341600
H	-3.64655600	1.34617600	1.73282200
C	-6.13594700	-0.65712400	0.56383500
H	-5.95076200	-1.98833300	-1.12266400
H	-6.00583400	0.76494500	2.18233000
H	-7.17615900	-0.90765900	0.75495900
C	-1.19299800	-1.92118600	0.30515400
C	-1.43063300	-2.96083900	-0.61073400
C	-1.13650500	-2.25536000	1.67010400
C	-1.60119800	-4.27922500	-0.18419800
H	-1.49713400	-2.72812200	-1.67034500
C	-1.30878600	-3.57198600	2.09994300
H	-0.96386900	-1.46600000	2.39647100
C	-1.53739100	-4.59288100	1.17504000
H	-1.79328700	-5.06082800	-0.91552300
H	-1.26887300	-3.79920800	3.16252100
H	-1.67127100	-5.61825200	1.50905400

INT-7

Os	-1.05408900	-0.14004400	0.03936600
C	-1.06632900	0.02359700	2.51862200
C	-1.26081400	1.25327800	1.79540400
C	-2.46476000	1.48359300	1.04524700
C	-3.40637800	0.46236600	0.81182700
C	-3.00333600	-0.82731900	1.26414000
C	-1.94128700	-1.02074200	2.20713400
H	-0.55364500	2.06358300	1.93275000
H	-2.59464200	2.45721700	0.58619500
H	-3.59022900	-1.68689400	0.96312500
H	-1.76393900	-2.01315300	2.60943900
C	0.05879100	-0.09995300	3.50464600
H	0.18100400	-1.12842100	3.85434600
C	-4.69098300	0.63326300	0.02533200
C	2.00937600	4.47979600	0.46182100
C	2.21858400	3.11854500	0.68258300
C	1.60860800	2.14342900	-0.12697100
C	0.80389200	2.59255100	-1.19433900
C	0.61500800	3.95764300	-1.43430500
C	1.21226300	4.90567800	-0.60425800
H	2.48404500	5.20933400	1.11298000

H	2.87820300	2.79885000	1.48453800
H	0.00606000	4.26647000	-2.27965100
H	1.06665900	5.96589900	-0.79266300
C	0.11337800	1.57267500	-2.06421300
O	0.33998600	1.38862800	-3.25127500
N	-0.93404900	1.00913200	-1.36965600
H	-4.78346900	-0.27357900	-0.58408200
H	-0.13973900	0.53679800	4.37595700
H	0.99948600	0.23442700	3.05482600
C	-4.66837900	1.83744500	-0.92651000
H	-4.65366200	2.79065200	-0.38217500
H	-5.57201900	1.83348100	-1.54516000
H	-3.79947200	1.80038500	-1.59139900
C	-5.89876300	0.69856000	0.98517300
H	-5.94820900	-0.18282600	1.63463800
H	-6.83206000	0.74850400	0.41318500
H	-5.84721400	1.58800700	1.62539700
C	1.02622400	-0.33502600	0.02941800
C	1.92673200	0.69146800	0.05621100
C	3.40634200	0.44522300	0.20121800
C	3.94808400	-0.20224800	1.32237200
C	4.29344900	0.90998400	-0.78585000
C	5.32502000	-0.39354000	1.44802700
H	3.28220000	-0.56851000	2.09806900
C	5.66839000	0.71210300	-0.66716100
H	3.89521500	1.42185100	-1.65788800
C	6.19134800	0.06041800	0.45245800
H	5.71996500	-0.89792600	2.32642800
H	6.33249100	1.06854300	-1.45055900
H	7.26346300	-0.09012900	0.54820700
C	1.54450700	-1.73867700	-0.03156000
C	2.17471700	-2.18518000	-1.20559600
C	1.40851500	-2.64831700	1.02766200
C	2.65616800	-3.48922000	-1.31165300
H	2.28058200	-1.49676100	-2.03873500
C	1.89708800	-3.95117900	0.92896600
H	0.91893500	-2.33105400	1.94387800
C	2.52193600	-4.37967200	-0.24394200
H	3.14017400	-3.80953600	-2.23094800
H	1.79061400	-4.63265400	1.76990700
H	2.90147900	-5.39501400	-0.32400400
O	-1.00492500	-2.00311400	-0.75234200
C	-2.04853600	-2.49914400	-1.41289600
O	-3.16029400	-1.99342900	-1.47891600

C	-1.68786000	-3.79775400	-2.11231700
H	-1.06113300	-3.56842700	-2.98161800
H	-1.10150600	-4.44298500	-1.45225900
H	-2.59464800	-4.30529100	-2.44678800

INT-8

Os	-1.00926000	-0.25235300	0.05035500
C	-0.92930800	-0.12349200	2.56600300
C	-1.08617400	1.10940100	1.84831200
C	-2.22887100	1.33363500	1.01521600
C	-3.22424400	0.30709900	0.85435300
C	-2.88019600	-0.97465500	1.33028600
C	-1.77253200	-1.18637300	2.21988200
H	-0.38764800	1.92090000	2.01777500
H	-2.37921700	2.31411600	0.58027400
H	-3.49205800	-1.82076100	1.04484800
H	-1.60579400	-2.17692100	2.62795000
C	0.18392000	-0.26003500	3.56733100
H	0.26921100	-1.28086900	3.94834000
C	-4.49586200	0.48167000	0.04161600
C	1.93493600	4.48559100	0.51918200
C	2.16366500	3.11647700	0.59034700
C	1.40695200	2.16718900	-0.13596400
C	0.36046200	2.68463600	-0.95880000
C	0.17932400	4.07705900	-1.05946400
C	0.94389100	4.97807300	-0.33183100
H	2.54136700	5.16367000	1.11407000
H	2.96714400	2.75469300	1.22305900
H	-0.60840600	4.42020200	-1.72142700
H	0.76588300	6.04617600	-0.42110400
C	-0.69097100	1.90791400	-1.72768200
O	-1.52454800	2.47386000	-2.43863000
N	-0.67669200	0.54612800	-1.58159600
H	-4.52580300	-0.37813800	-0.63905900
H	-0.00873300	0.40682800	4.41731000
H	1.14257500	0.03466300	3.12849600
C	-4.54882600	1.76683500	-0.79486900
H	-4.58598100	2.66242900	-0.16075300
H	-5.46172300	1.76386000	-1.39991700
H	-3.69803100	1.85716200	-1.47761100
C	-5.71445800	0.39143600	0.98948900
H	-5.72776000	-0.54816000	1.55233400
H	-6.63987600	0.44785200	0.40637300
H	-5.71864600	1.21988100	1.70860500

C	1.10542200	-0.37071600	0.11212600
C	1.87772300	0.74162000	-0.00073700
C	3.38027000	0.61867200	-0.00374500
C	4.08005000	0.02424000	1.05767600
C	4.12200300	1.12889700	-1.08332700
C	5.47218500	-0.07019100	1.03689500
H	3.52713800	-0.37561200	1.90253400
C	5.51233100	1.02718300	-1.11044000
H	3.59908100	1.60306700	-1.90949500
C	6.19439900	0.42801700	-0.04873500
H	5.99199100	-0.53387900	1.87140800
H	6.06358800	1.41792700	-1.96188900
H	7.27834200	0.35239700	-0.06685800
C	1.67970700	-1.74360900	0.06203400
C	2.35188400	-2.17264200	-1.09619700
C	1.54401200	-2.65545400	1.11950000
C	2.88592200	-3.45632100	-1.18136100
H	2.44415400	-1.48900700	-1.93349800
C	2.08657200	-3.93808300	1.04158400
H	1.01080600	-2.35656500	2.01568400
C	2.76044200	-4.34540400	-0.11097400
H	3.39941400	-3.76444900	-2.08852400
H	1.97939600	-4.62091400	1.88098500
H	3.17845700	-5.34645100	-0.17682200
O	-0.80745200	-1.98234500	-1.08684000
C	-1.87605100	-2.55035200	-1.58704800
O	-3.04469600	-2.22552900	-1.36723500
C	-1.53237800	-3.69317100	-2.53329700
H	-1.32710200	-3.27588500	-3.52634700
H	-0.63541500	-4.22248500	-2.20202400
H	-2.37939200	-4.37854300	-2.61306300

INT-9

Os	-1.67433400	-0.16161300	0.03100300
C	-2.07816900	-2.12510400	1.10172500
C	-1.82761300	-1.05603000	2.03693200
C	-2.60318500	0.13325600	2.04386100
C	-3.60231300	0.34343400	1.03314400
C	-3.82739200	-0.68723200	0.07420600
C	-3.06797900	-1.90179800	0.11408800
H	-0.99568000	-1.14895800	2.72776900
H	-2.34600800	0.92936700	2.73087500
H	-4.49213900	-0.51945100	-0.76289300
H	-3.19028500	-2.60707000	-0.69767200

C	-1.31233500	-3.41641300	1.18001900
H	-1.25350800	-3.90389600	0.20410300
C	-4.41353800	1.62762100	0.93774200
C	3.27001200	4.50231800	-0.45252600
C	3.56615400	3.17560900	-0.20357500
C	2.53535300	2.20326700	-0.11069100
C	1.19701000	2.65513400	-0.29770100
C	0.90996900	4.01294900	-0.55216700
C	1.93688400	4.93239300	-0.62682600
H	4.07899500	5.22535500	-0.51941700
H	4.59821000	2.86625500	-0.08338200
H	-0.12583500	4.30682300	-0.68845600
H	1.72439500	5.97949400	-0.82270700
C	0.15809700	1.67449700	-0.20449000
O	-1.11211500	1.89939300	-0.30695500
N	0.42725700	0.38343100	0.04210400
H	-4.55788000	1.81980900	-0.13335700
H	-1.82092700	-4.10127300	1.87240100
H	-0.29381400	-3.26213200	1.54474600
C	-3.72874200	2.86019500	1.54518900
H	-3.64756900	2.78219000	2.63677100
H	-4.32668500	3.75318200	1.33147000
H	-2.72985600	3.00335100	1.12433300
C	-5.80207800	1.39455200	1.57020500
H	-6.32522900	0.55556100	1.09876500
H	-6.42350300	2.29018200	1.45756700
H	-5.71390200	1.17894300	2.64211100
C	1.71232900	-0.08066000	0.14991600
C	2.78772600	0.79741100	0.11064400
C	4.19966000	0.31621700	0.22647600
C	4.96118000	0.60374900	1.37125900
C	4.80491800	-0.40782800	-0.81197700
C	6.28391800	0.17103300	1.47964900
H	4.50725800	1.16760500	2.18256900
C	6.12622100	-0.84343600	-0.70442200
H	4.22984500	-0.63327900	-1.70543800
C	6.87025600	-0.55621500	0.44175700
H	6.85471500	0.40020800	2.37596500
H	6.57535700	-1.40577800	-1.51891100
H	7.89957100	-0.89487200	0.52499400
C	1.87917700	-1.56013700	0.22226700
C	1.37498700	-2.34795400	-0.82596400
C	2.56662300	-2.18505400	1.27277800
C	1.58902400	-3.72668000	-0.83787900

H	0.82147100	-1.86609900	-1.62638300
C	2.76081400	-3.56764100	1.26831000
H	2.96199100	-1.58553000	2.08683200
C	2.28284100	-4.34077400	0.20780100
H	1.21165400	-4.32224700	-1.66529900
H	3.29576100	-4.03828900	2.08902100
H	2.44831000	-5.41491400	0.19764900
O	-1.22223400	-0.27141600	-1.98377800
C	-2.00941500	-0.74609400	-2.92390300
O	-3.10272800	-1.28226600	-2.76326300
C	-1.40909900	-0.55691600	-4.31396400
H	-1.26374300	0.51023400	-4.51389300
H	-0.42349300	-1.03171200	-4.37101900
H	-2.07000600	-0.98620800	-5.06938900

INT-5'

Os	0.27944900	0.35663900	-0.23087700
C	-0.25481700	2.97167300	-1.53142100
C	0.10859700	2.68369100	-0.12745700
C	1.47232200	2.38059500	0.19663200
C	2.21011900	1.66043600	-0.75280600
C	1.41875600	1.29478700	-1.92002900
C	0.43066700	2.24293300	-2.44612700
H	-0.49328500	3.14729000	0.64653300
H	1.86685000	2.58567100	1.18493000
H	1.86182900	0.58181100	-2.60690600
H	0.24771000	2.30484100	-3.51521100
C	-1.34463900	3.95600500	-1.83814200
H	-1.52683200	4.02763100	-2.91469600
C	3.66380500	1.24766100	-0.62545600
C	1.07706300	-0.07231700	4.07287400
C	0.61465500	0.43899200	2.85438600
C	0.96740500	-0.17850200	1.64740100
C	1.79960100	-1.30914000	1.69754200
C	2.26789400	-1.81950800	2.91016800
C	1.90404900	-1.19956100	4.10488500
H	0.78796700	0.41488800	5.00133100
H	-0.02606400	1.31691800	2.85939200
H	2.91360200	-2.69314900	2.88725600
H	2.26100800	-1.58751100	5.05528000
C	2.18448900	-1.92832500	0.39586300
O	2.95572800	-2.88098300	0.27087500
N	1.54055600	-1.25945600	-0.60993300
O	1.89667400	-1.63380300	-1.91527400

C	1.32482300	-2.88431000	-2.31495500
H	1.71125300	-3.05755300	-3.32381500
H	0.23156000	-2.82936300	-2.34232400
H	1.65325700	-3.68582400	-1.64869200
H	3.71324900	0.18384400	-0.88879500
H	-1.09227800	4.95779900	-1.46543000
H	-2.28259900	3.66229700	-1.34943700
C	4.24889600	1.42694600	0.78183400
H	4.26874200	2.48419800	1.07688800
H	5.28202600	1.06373500	0.80048600
H	3.68473900	0.86688600	1.53259700
C	4.50295500	2.02464500	-1.66440300
H	4.12793400	1.87461100	-2.68234400
H	5.54429900	1.68500400	-1.63554400
H	4.49248000	3.10143500	-1.45431600
C	-1.72461900	0.35378700	0.02072600
C	-1.31903000	-0.84339500	-0.37546300
C	-1.77663800	-2.21699900	-0.53259600
C	-1.23571900	-3.24912900	0.25543600
C	-2.77873800	-2.53269100	-1.46852600
C	-1.70354000	-4.55525500	0.12243400
H	-0.45955100	-3.01751700	0.97657000
C	-3.22888500	-3.84477300	-1.60950500
H	-3.18583200	-1.74831900	-2.10059300
C	-2.69758500	-4.85972500	-0.81069300
H	-1.28216700	-5.33920800	0.74569900
H	-3.99818100	-4.07281900	-2.34256900
H	-3.05292200	-5.88096600	-0.91749800
C	-2.92808900	1.04418400	0.46447800
C	-2.90933300	1.97472400	1.51999000
C	-4.16175100	0.76906600	-0.15885600
C	-4.07973700	2.60248600	1.94076500
H	-1.97307400	2.18068600	2.02683500
C	-5.32763800	1.41177300	0.25216900
H	-4.19618700	0.04775800	-0.96865100
C	-5.29296000	2.33104400	1.30341600
H	-4.04427800	3.30657400	2.76786800
H	-6.26720200	1.18902500	-0.24644100
H	-6.20354300	2.82846900	1.62562200

INT-7'

Os	-1.11742900	-0.27072700	-0.32539100
C	-1.86572200	-0.99781200	-2.34330600
C	-2.72292000	-1.49630500	-1.30886100

C	-3.40587900	-0.64503600	-0.40119400
C	-3.16291900	0.76212800	-0.42110400
C	-2.33757400	1.28961300	-1.46391900
C	-1.67884500	0.41529400	-2.37996500
H	-2.80936700	-2.57095400	-1.18348300
H	-4.00084400	-1.08440600	0.38959600
H	-2.12858900	2.35298500	-1.49025000
H	-0.99827600	0.82904600	-3.11741000
C	-1.21038800	-1.92089400	-3.33666300
H	-0.28023600	-1.49082300	-3.72072500
C	-3.81209200	1.71436200	0.57218300
C	1.39867400	-4.35653500	0.28323700
C	2.07076500	-3.17939300	0.19047200
C	1.39056100	-1.91417600	0.35255100
C	-0.06431200	-1.93830800	0.74905000
C	-0.69978000	-3.26236900	0.85750700
C	-0.01437300	-4.40127600	0.61296300
H	1.92367600	-5.29232600	0.10786200
H	3.12268300	-3.16821300	-0.07697200
H	-1.73920600	-3.29284500	1.17227300
H	-0.50666000	-5.36780400	0.68425200
C	-0.38630800	-1.01940300	1.87491200
O	-0.97195000	-1.19923800	2.93078900
N	-0.06147100	0.31170400	1.38084100
O	-0.37681000	1.41443400	2.18810800
C	0.32507400	1.40072000	3.44790200
H	0.13928000	2.39305300	3.86482200
H	1.40037700	1.26382400	3.30025500
H	-0.07349100	0.62215500	4.09876100
H	-3.13780000	2.57622500	0.65598600
H	-1.87487300	-2.10835200	-4.19151900
H	-0.97131300	-2.88539000	-2.87851100
C	-3.98855000	1.12559900	1.98009800
H	-4.73262300	0.31984900	1.99402300
H	-4.34864300	1.90539600	2.66072800
H	-3.04586100	0.73445900	2.37308300
C	-5.15759800	2.21467200	0.00563900
H	-5.03420900	2.68203500	-0.97782700
H	-5.60378900	2.95445400	0.68014500
H	-5.86803600	1.38596800	-0.10206200
C	0.85613900	0.41495800	0.16004300
C	1.91241300	-0.67184700	0.13129400
C	3.35226700	-0.42129000	-0.11786500
C	3.80137100	0.25732500	-1.26715100

C	4.32539500	-0.89307500	0.78440100
C	5.16095300	0.45228500	-1.50357300
H	3.07426700	0.62887600	-1.98221300
C	5.68731300	-0.70116300	0.54728500
H	4.00079100	-1.40817900	1.68449700
C	6.11170400	-0.02598200	-0.59818300
H	5.47969900	0.97599500	-2.40135800
H	6.41590200	-1.07418800	1.26292000
H	7.17153100	0.12777200	-0.78364600
C	1.32851200	1.83245100	-0.06739200
C	2.24647200	2.43243000	0.81234400
C	0.92439900	2.57365300	-1.18395700
C	2.70715000	3.73121900	0.60618100
H	2.62516100	1.86583300	1.65664200
C	1.39329900	3.87101700	-1.40682200
H	0.24589500	2.11881500	-1.89320100
C	2.27876200	4.46020600	-0.50553800
H	3.41150000	4.16981400	1.30829400
H	1.06371600	4.41874100	-2.28630300
H	2.64055100	5.47153100	-0.67143700

INT-7a'

Os	1.57806200	-0.22004300	0.13007000
C	1.52396300	-0.31137700	2.34025000
C	2.52265300	-1.22081500	1.85152400
C	3.54209700	-0.75214400	0.97492800
C	3.73172600	0.64834100	0.67523300
C	2.76338700	1.53289000	1.17766800
C	1.64865300	1.05902100	1.95173200
H	2.44325200	-2.28154500	2.06527600
H	4.19904100	-1.48418500	0.51851800
H	2.79950700	2.58116200	0.89673500
H	0.87855800	1.76253200	2.25016300
C	0.42182500	-0.77654400	3.25515500
H	-0.46034300	-0.13529600	3.16578100
C	4.88490900	1.13642800	-0.18449900
C	-2.47758300	-4.33811900	-0.30548100
C	-2.82963800	-3.00943500	-0.08718100
C	-1.94164600	-1.95943600	-0.39601000
C	-0.65935900	-2.30705100	-0.89029000
C	-0.31894200	-3.64468800	-1.13051400
C	-1.22384800	-4.65950600	-0.83957300
H	-3.18444500	-5.12602300	-0.05965400
H	-3.80480300	-2.78311400	0.32750600

H	0.66754600	-3.86223300	-1.52734300
H	-0.95449600	-5.69715500	-1.01826900
C	0.32725500	-1.25212400	-1.06427400
O	1.48362400	-1.34043500	-1.70139900
N	-0.14809900	0.16417300	-1.13749500
O	0.07974900	0.84516600	-2.40508900
C	-0.63091300	0.21807100	-3.47211800
H	-0.44764500	0.85815200	-4.33917200
H	-1.71048500	0.17809500	-3.27600600
H	-0.24179400	-0.78685600	-3.66646700
H	4.65319700	2.17429700	-0.45984300
H	0.75184200	-0.74974100	4.30269500
H	0.11968200	-1.80202300	3.02160100
C	5.05217600	0.33929200	-1.48993400
H	5.36015400	-0.69496400	-1.29613700
H	5.82804000	0.79854600	-2.11375800
H	4.11548700	0.30943800	-2.05495700
C	6.19387800	1.14794700	0.63187500
H	6.09564200	1.75713100	1.53745900
H	7.01768200	1.55561800	0.03409800
H	6.47392500	0.13269000	0.93853000
C	-1.45925600	0.47139400	-0.62099100
C	-2.29571900	-0.53904600	-0.22589400
C	-3.59325000	-0.21549300	0.44988800
C	-3.60145900	0.38287300	1.71824800
C	-4.82581200	-0.51783200	-0.15302700
C	-4.80309400	0.67869500	2.36292900
H	-2.65573700	0.62472900	2.19478200
C	-6.02843200	-0.22099600	0.48944400
H	-4.83839100	-0.98030400	-1.13664500
C	-6.02117800	0.37889600	1.75070500
H	-4.78650000	1.14415800	3.34493500
H	-6.97119700	-0.45608900	0.00231600
H	-6.95728500	0.61013100	2.25174400
C	-1.78233100	1.92489700	-0.63225400
C	-3.03271200	2.39521400	-1.06792800
C	-0.81370700	2.87250600	-0.25580200
C	-3.31621600	3.76011700	-1.09344700
H	-3.78669600	1.68998200	-1.39716500
C	-1.09918100	4.23582000	-0.27745500
H	0.17070500	2.52846500	0.03885800
C	-2.35418900	4.68769400	-0.69150500
H	-4.29066200	4.09737300	-1.43685900
H	-0.33561300	4.94873700	0.02328700

H	-2.57552600	5.75151400	-0.71136100
INT-7''			
Os	-0.99101600	-0.18296500	0.51539700
C	-1.41680800	-0.68546000	-1.63886500
C	-2.20096400	-1.55001700	-0.78599400
C	-3.57680300	-1.25879700	-0.47680300
C	-4.14809600	-0.05828400	-0.82302400
C	-3.32932000	0.87886200	-1.54585800
C	-2.06090900	0.57146300	-1.97188700
H	-1.85013600	-2.56312200	-0.61337800
H	-4.14147200	-2.01431800	0.05907700
H	-3.75400500	1.84602200	-1.80595400
H	-1.52486200	1.27013600	-2.60812700
C	-0.33756100	-1.22350700	-2.55067400
H	0.41707200	-0.46428800	-2.77291400
C	-5.58807100	0.32341700	-0.51705800
C	3.25735700	-3.82798100	-1.17377700
C	3.00334800	-2.45876300	-1.21768800
C	2.21830800	-1.82508900	-0.23489400
C	1.72452000	-2.62220000	0.81761100
C	2.00790800	-3.99087800	0.88032500
C	2.76663100	-4.60011500	-0.11689200
H	3.85377500	-4.28939400	-1.95661300
H	3.42609100	-1.86181400	-2.02039900
H	1.63070900	-4.56716900	1.72057200
H	2.98205100	-5.66412000	-0.06693700
C	0.86451900	-1.98239000	1.87519200
O	1.17335800	-1.89769600	3.05579200
N	-0.37695100	-1.69008600	1.34382100
O	-1.69500300	1.04568800	1.77232100
C	-1.59811900	2.43517200	2.02919000
H	-0.86369700	2.61528600	2.82157000
H	-2.58337700	2.77124500	2.37627500
H	-1.31297300	3.00298800	1.13779500
H	-5.56792100	1.37162900	-0.18220400
H	-0.78914000	-1.54401900	-3.49946700
H	0.17179000	-2.08096800	-2.10678800
C	-6.23314800	-0.50685700	0.60058600
H	-6.36711800	-1.55315900	0.30074900
H	-7.22546100	-0.10821600	0.83746200
H	-5.63199200	-0.48829100	1.51598000
C	-6.44450400	0.26956900	-1.80169300
H	-6.02290700	0.89185900	-2.59875700

H	-7.46209600	0.62295000	-1.59957800
H	-6.50895100	-0.75820300	-2.17809400
C	0.93249000	0.38740700	0.01997200
C	2.05799900	-0.33815500	-0.25111600
C	3.35489600	0.36722900	-0.56173400
C	3.50725500	1.17827500	-1.69638800
C	4.46966400	0.18004300	0.27384000
C	4.72606500	1.79819600	-1.97897200
H	2.66196600	1.32392000	-2.36246700
C	5.68489500	0.80565400	-0.00080100
H	4.37416500	-0.45793200	1.14841000
C	5.81876700	1.61773000	-1.13004300
H	4.82055600	2.42088600	-2.86515400
H	6.52978100	0.65662000	0.66681000
H	6.76735900	2.10163900	-1.34752200
C	1.05767700	1.87496300	0.16459700
C	1.66471600	2.39738100	1.32237800
C	0.58795000	2.78371200	-0.79865600
C	1.80345500	3.77347500	1.50252400
H	2.03428900	1.70822300	2.07587400
C	0.72917400	4.16105700	-0.62144400
H	0.13065600	2.40671900	-1.70786800
C	1.33576800	4.66296900	0.53238000
H	2.28222800	4.15109300	2.40240300
H	0.37176200	4.84232800	-1.38978000
H	1.44653400	5.73500600	0.67123200

INT-8'

Os	-0.66827600	-0.69574400	-0.22961600
C	-1.45151200	-0.57127300	2.84205500
C	-0.96218100	0.41413000	1.92436300
C	-1.87419200	1.18383600	1.16194700
C	-3.27599200	0.99742100	1.27886100
C	-3.71550200	0.01961600	2.15992200
C	-2.82148100	-0.75274700	2.92559300
H	0.06172200	0.75538300	2.02328400
H	-1.49760100	2.03011400	0.60306600
H	-4.78418200	-0.14275800	2.28234200
H	-3.22009300	-1.49215900	3.61595500
C	-0.48976900	-1.35431200	3.69479800
H	0.02652500	-2.10767300	3.08919600
C	-4.26867900	1.89878800	0.55905500
C	0.87562700	4.64757600	0.74857100
C	1.44677600	3.38374600	0.82864300

C	1.11366600	2.34174400	-0.06528100
C	0.17077400	2.64554300	-1.08030600
C	-0.34839500	3.95125500	-1.19551600
C	-0.02183600	4.94400500	-0.28231500
H	1.14580900	5.40748900	1.47692100
H	2.18590700	3.18284400	1.59758600
H	-1.02206700	4.15898800	-2.02051200
H	-0.45056100	5.93740800	-0.37710600
C	-0.33993700	1.70724400	-2.12035600
O	-0.51173400	2.04991500	-3.28113400
N	-0.76727200	0.41806100	-1.73420000
H	-5.25141900	1.41539100	0.64542600
H	-1.00924300	-1.87012900	4.50848100
H	0.27313200	-0.70087000	4.13579500
C	-3.97115600	2.08442000	-0.93887200
H	-3.04747300	2.65328700	-1.09391500
H	-4.78175900	2.65322600	-1.40913700
H	-3.87182900	1.13059200	-1.46433000
C	-4.36450100	3.26724900	1.26831500
H	-4.62692800	3.15347800	2.32602600
H	-5.12781700	3.89319700	0.79110800
H	-3.40951500	3.80409300	1.21370100
C	1.36596100	-0.19201100	0.01703300
C	1.88895100	1.06939500	0.04617900
C	3.37088800	1.32596900	0.14876200
C	4.10852300	0.99871100	1.29732200
C	4.04346300	1.95332000	-0.91386800
C	5.47452500	1.27464200	1.37612700
H	3.60549700	0.52532600	2.13475100
C	5.41052400	2.21891100	-0.84262900
H	3.48683400	2.22843200	-1.80614500
C	6.13207300	1.88134200	0.30477700
H	6.02457800	1.01390700	2.27677000
H	5.91165400	2.69286100	-1.68273700
H	7.19657100	2.09210000	0.36408000
C	2.34762900	-1.32922400	0.00207600
C	2.91167200	-1.73927800	-1.21753700
C	2.71918100	-2.02386900	1.16456300
C	3.82682000	-2.79243300	-1.27133900
H	2.62871500	-1.22208500	-2.13000400
C	3.63681200	-3.07382000	1.11562100
H	2.28414700	-1.73530600	2.11705900
C	4.19629900	-3.46430100	-0.10412300
H	4.25446700	-3.08332100	-2.22755000

H	3.91609000	-3.58708600	2.03265500
H	4.91365000	-4.27992500	-0.14298600
O	-0.24782100	-2.38637700	-1.40785200
C	-0.07914000	-3.14829200	-0.39260900
O	-0.16481600	-2.57425000	0.74447600
C	0.24622700	-4.59815600	-0.54203500
H	-0.03692000	-4.95263900	-1.53496400
H	1.32764000	-4.72293900	-0.41147600
H	-0.26165700	-5.17817000	0.23295400
O	-2.61622900	-1.50346300	-0.25862600
C	-3.27700300	-1.67875400	-1.37557300
O	-2.98888500	-1.17350700	-2.46352100
C	-4.49714000	-2.57806000	-1.22240100
H	-4.17243200	-3.59966800	-0.99362300
H	-5.11500900	-2.24065500	-0.38405200
H	-5.08303400	-2.58223000	-2.14333200
H	-1.24555600	-0.05296000	-2.52075100

INT-9'

Os	0.87749000	-1.39115300	-0.65907300
C	-3.60938700	-0.11379600	2.62625400
C	-3.57465800	0.56341300	1.39658800
C	-4.71784400	0.68743200	0.60947500
C	-5.94608900	0.13967000	1.01673200
C	-5.97706900	-0.53548300	2.24155400
C	-4.83093000	-0.66016600	3.03214400
H	-2.63872300	0.99337700	1.04817600
H	-4.64744400	1.22263300	-0.33489800
H	-6.91268600	-0.97154400	2.58634100
H	-4.89096700	-1.19157500	3.97979700
C	-2.36059400	-0.24571200	3.46734900
H	-1.54070800	-0.68338200	2.88566000
C	-7.20233000	0.27588400	0.16623400
C	-1.81041200	3.41832500	-0.91941900
C	-0.68849700	2.89083200	-0.29169100
C	0.13968000	1.92539900	-0.90662300
C	-0.20974600	1.51902500	-2.21725800
C	-1.31553700	2.10127800	-2.86504600
C	-2.12363800	3.03156200	-2.22579900
H	-2.42744800	4.14425200	-0.39686100
H	-0.42511200	3.23608500	0.70267600
H	-1.52294700	1.79737200	-3.88584800
H	-2.97899300	3.45866100	-2.74153800
C	0.48720400	0.48927400	-3.04451400

O	0.66837400	0.62446600	-4.24673900
N	0.74998000	-0.75273000	-2.44564100
H	-8.01287500	-0.23508000	0.70411100
H	-2.53383000	-0.87770800	4.34480600
H	-2.01566600	0.73237700	3.82735000
C	-7.05037800	-0.41613300	-1.20204500
H	-6.26001800	0.05338700	-1.80000300
H	-7.98329500	-0.35161100	-1.77487600
H	-6.79560100	-1.47532900	-1.08428100
C	-7.62107200	1.74861900	-0.00542300
H	-7.76994800	2.23326400	0.96566500
H	-8.55712800	1.82182300	-0.57228000
H	-6.85741900	2.31787600	-0.54881600
C	1.84582800	0.26518800	0.00989700
C	1.38304800	1.53760800	-0.17600400
C	2.11382500	2.72465700	0.39174400
C	2.29592500	2.90170300	1.77178300
C	2.59999700	3.71652800	-0.47741500
C	2.95818300	4.02605500	2.26744200
H	1.91063600	2.15546100	2.45903700
C	3.27354400	4.83320100	0.01570800
H	2.45230100	3.60416700	-1.54831400
C	3.45440800	4.99293100	1.39173600
H	3.08513700	4.14515400	3.34037400
H	3.65364800	5.58112300	-0.67536600
H	3.97372600	5.86609100	1.77766100
C	3.18288300	0.06444800	0.66134300
C	4.34850700	0.21264000	-0.10882000
C	3.32031400	-0.29498700	2.01185000
C	5.61115000	0.02156900	0.45428900
H	4.25894700	0.48591400	-1.15668100
C	4.58239900	-0.47994900	2.57819200
H	2.43067700	-0.43361800	2.61836800
C	5.73398400	-0.32347200	1.80190000
H	6.49866900	0.14843500	-0.16036200
H	4.66536800	-0.74545100	3.62920300
H	6.71653400	-0.46584700	2.24424600
O	2.53491500	-2.55320300	-0.95139200
C	2.62970800	-3.00160300	0.26310000
O	1.75412900	-2.58073200	1.06484800
C	3.74647800	-3.91978600	0.64070600
H	4.07551900	-4.50102900	-0.22352800
H	4.58722000	-3.31144300	0.99546700
H	3.43038100	-4.57984000	1.45152700

O	-0.81515200	-1.56379100	0.35077500
C	-1.41621300	-2.59106800	-0.25072900
O	-0.79126900	-3.17542900	-1.14447500
C	-2.79050800	-2.94897000	0.22376700
H	-2.75607000	-3.20100300	1.28873900
H	-3.45445500	-2.08417900	0.12338600
H	-3.17193500	-3.79521700	-0.34930700
H	0.89446500	-1.44402200	-3.18875700

TS-1

N	0.91803900	0.79408600	0.33069600
O	-1.50277000	0.61507800	1.57457900
O	-3.11226800	-0.87651900	2.16074200
C	-2.42419900	0.12018900	2.36752400
C	-2.57323400	0.93285200	3.65144900
H	-1.65662900	0.85832600	4.24796300
H	-2.72391500	1.99207200	3.41854900
H	-3.41457200	0.55637700	4.23631000
H	0.44280200	1.96317300	0.39213100
O	-1.63278800	1.88622800	-0.80064600
C	-1.14952700	2.97412900	-0.36701600
O	-0.07435500	3.07712400	0.30629000
C	-1.89955400	4.25047200	-0.67030600
H	-1.21502600	4.98558200	-1.10406600
H	-2.73311000	4.06266700	-1.34852400
H	-2.28101600	4.66980300	0.26737600
Os	-1.00349500	-0.10952900	-0.30578900
C	-2.41393200	-0.81389500	-1.90631000
C	-2.68753700	-1.51605200	-0.70652600
C	-1.63469300	-2.20221000	-0.00330600
C	-0.30797300	-2.24381900	-0.50476000
C	-0.04408300	-1.51065000	-1.72000300
C	-1.06525500	-0.81722100	-2.41438800
H	-3.65651900	-1.43467500	-0.23213200
H	-1.86861700	-2.60884600	0.97038800
H	0.97857700	-1.41445800	-2.06934700
H	-0.80772200	-0.20470400	-3.27111700
C	-3.47493300	0.00267600	-2.59245500
H	-3.08299900	0.98301300	-2.87803300
C	0.81163400	-3.01900900	0.16973100
H	1.74643200	-2.48658900	-0.05068800
H	-3.81575800	-0.51167100	-3.50005400
H	-4.33778200	0.15520000	-1.93852600
C	0.67569700	-3.11270300	1.69583500

H	-0.19056800	-3.71611700	1.99114900
H	1.56431900	-3.59684500	2.11712500
H	0.57718500	-2.11829100	2.14009300
C	0.91501900	-4.41953200	-0.47045400
H	1.05759400	-4.35838200	-1.55536600
H	1.76310900	-4.97047600	-0.04785400
H	0.00530900	-5.00228000	-0.28227000
C	1.97064900	0.88315000	-0.62331000
O	1.67020500	1.27987800	-1.74202400
C	3.40839200	0.59411200	-0.28714500
C	3.86610000	-0.36595600	0.63167300
C	4.35263300	1.31036800	-1.04499200
C	5.23505300	-0.59169100	0.78675100
H	3.15855500	-0.93211700	1.22094500
C	5.71693400	1.09932100	-0.86839300
H	3.99243500	2.02956000	-1.77258500
C	6.16306200	0.14409000	0.04891800
H	5.57499500	-1.34443600	1.49305000
H	6.43210500	1.67415000	-1.45046200
H	7.22770400	-0.02771500	0.18430100
O	1.33765000	0.30909600	1.60904000
C	1.43082000	1.36765100	2.56438600
H	1.76176700	0.88459900	3.48789600
H	2.17296000	2.11669600	2.25849000
H	0.45593600	1.83730000	2.71509200

TS-2

N	0.10017000	0.67676300	1.52059800
O	-2.37387200	-0.05175000	0.43946000
O	-2.42950400	1.94864500	-0.56875200
C	-2.96368000	1.03398100	0.11036300
C	-4.38566700	1.21995700	0.59437500
H	-4.37519200	1.89219300	1.46019900
H	-4.82631800	0.26732600	0.89373500
H	-4.98675800	1.69425600	-0.18562800
O _s	-0.35553700	-0.48244200	-0.12936300
C	-1.08740400	-2.33591900	-1.24354000
C	-0.05770300	-1.73430200	-2.00092300
C	1.21176200	-1.41692900	-1.40037900
C	1.50513300	-1.73234400	-0.04652900
C	0.44939000	-2.36486200	0.71559600
C	-0.80185700	-2.66687500	0.13522300
H	-0.25625200	-1.41837200	-3.01960100
H	1.93039300	-0.85535600	-1.98463900

H	0.58554600	-2.51017100	1.78168500
H	-1.60279600	-3.04130300	0.76420700
C	-2.45402400	-2.59822400	-1.81638400
H	-3.23121100	-2.29032500	-1.10993300
C	2.83827000	-1.45407300	0.62936800
H	2.60158700	-1.04934100	1.62200200
H	-2.58736000	-3.66766800	-2.02437000
H	-2.60274400	-2.04864600	-2.75061700
C	3.71392500	-0.42748200	-0.10043200
H	4.05600000	-0.80480400	-1.07252200
H	4.60642900	-0.21598600	0.49787300
H	3.18735100	0.51795700	-0.25992600
C	3.60226700	-2.78118300	0.82456400
H	3.01168400	-3.51277300	1.38736500
H	4.53234700	-2.60472000	1.37629600
H	3.86217500	-3.22971100	-0.14221900
C	0.80040700	1.84311400	1.42302500
O	1.29886600	2.48720200	2.34897600
C	0.90784600	2.24386700	-0.02033000
C	0.15608000	1.51808000	-0.98026200
C	1.79937400	3.24491800	-0.39947200
C	0.34834200	1.84557900	-2.34208300
H	-1.11087400	1.54254000	-0.75746800
C	1.97364900	3.53845400	-1.75355100
H	2.35142700	3.76732000	0.37646900
C	1.24903700	2.83711300	-2.72599300
H	-0.25238900	1.34370600	-3.09802500
H	2.66821200	4.31875600	-2.05457000
H	1.37836400	3.07870700	-3.77805100
O	0.12726700	0.07109300	2.79356400
C	-0.85771500	0.65040200	3.65019900
H	-0.79161800	0.08976300	4.58792600
H	-1.86068000	0.53792900	3.22029300
H	-0.63429400	1.70584000	3.83395300

TS-3

Os	0.63651600	-0.47412500	-0.33871800
C	0.46614300	-1.74692500	-2.26904300
C	0.97470100	-0.47943600	-2.63804300
C	2.11286800	0.06750700	-1.96290700
C	2.87096400	-0.67502700	-1.00809100
C	2.32810600	-1.93812400	-0.63212600
C	1.16232700	-2.48009100	-1.24265600
H	0.44750200	0.12007600	-3.37275200

H	2.40233700	1.08620600	-2.19281800
H	2.77658200	-2.48036800	0.19382100
H	0.78679100	-3.44183700	-0.91392800
C	-0.74201800	-2.33342400	-2.95243500
H	-1.37703400	-2.87369600	-2.24561200
C	4.16058500	-0.18376600	-0.36957300
C	1.03893500	3.94879700	0.13044600
C	0.59550700	2.74894900	-0.41515500
C	0.44851100	1.58989200	0.38278200
C	0.79687100	1.69535000	1.75076200
C	1.19976600	2.91237500	2.30634700
C	1.31880500	4.04424100	1.50211300
H	1.15281500	4.82037500	-0.50971600
H	0.32924600	2.70854500	-1.46860300
H	1.45212000	2.92613900	3.36300500
H	1.64049200	4.99031100	1.92945500
C	0.90988700	0.44568900	2.55828400
O	1.12228800	0.42552300	3.77627400
N	0.80146800	-0.62306800	1.72537500
O	1.08897500	-1.88415100	2.27612700
C	0.11013600	-2.30133400	3.23748100
H	0.40850800	-3.31634400	3.51813600
H	-0.89076400	-2.32138500	2.79228300
H	0.12835200	-1.64463000	4.10983900
H	4.15150900	-0.54565100	0.66715700
H	-0.42607700	-3.03763400	-3.73312100
H	-1.34543800	-1.55427800	-3.42756000
C	4.30072400	1.34392700	-0.32556400
H	4.40354000	1.77186800	-1.33079600
H	5.20347100	1.61430200	0.23297500
H	3.44372800	1.81382300	0.16524700
C	5.37012700	-0.82634800	-1.08217800
H	5.30941100	-1.92047100	-1.07467900
H	6.30375400	-0.53586200	-0.58682400
H	5.42678000	-0.49930300	-2.12782500
C	-1.37968700	-0.50985800	0.17004400
C	-1.28738400	0.78569900	0.02120900
C	-2.17583000	1.85663300	-0.45589300
C	-2.85432000	1.70809200	-1.67816200
C	-2.42931400	2.99701400	0.32619700
C	-3.76353400	2.67520800	-2.10810000
H	-2.66476100	0.82616500	-2.28337700
C	-3.34836600	3.95394800	-0.09930400
H	-1.90407200	3.11924600	1.26805600

C	-4.01407300	3.79947900	-1.31899400
H	-4.27763000	2.54836400	-3.05729000
H	-3.54389400	4.82439100	0.52115800
H	-4.72475200	4.55155700	-1.65118700
C	-2.45023600	-1.46959000	0.39255000
C	-2.19946000	-2.85460900	0.41197500
C	-3.77531700	-1.03494900	0.61323100
C	-3.23058900	-3.77130800	0.61374700
H	-1.17775700	-3.19838000	0.29279200
C	-4.80211000	-1.95148600	0.81984200
H	-3.99014400	0.02858100	0.62267400
C	-4.53825400	-3.32485700	0.81411300
H	-3.01007300	-4.83568700	0.62589400
H	-5.81439200	-1.59281400	0.98763200
H	-5.34260000	-4.03765900	0.97435900

TS-4

Os	-0.97301700	0.15926400	-0.36590600
C	-0.84615700	-0.31533800	-2.67713300
C	-1.04256100	-1.48525200	-1.86476600
C	-2.18966400	-1.59275100	-1.01458500
C	-3.19095500	-0.57319000	-0.93237200
C	-2.86221600	0.63351600	-1.59270600
C	-1.74463900	0.75144100	-2.49596100
H	-0.33482600	-2.30259000	-1.91861200
H	-2.27815300	-2.48004200	-0.39885000
H	-3.49348100	1.50401700	-1.43980800
H	-1.56427900	1.69779200	-2.99483700
C	0.31840000	-0.24206700	-3.62467500
H	0.45827800	0.76924400	-4.01593400
C	-4.46927500	-0.69033400	-0.12006700
C	1.77926600	-4.46258000	-0.64077600
C	2.14519400	-3.12090600	-0.73005800
C	1.53470100	-2.13130700	0.06517200
C	0.57012700	-2.55614800	1.00023300
C	0.22510400	-3.90944300	1.11352200
C	0.81146600	-4.86360600	0.28483900
H	2.25878100	-5.19625300	-1.28378700
H	2.92198800	-2.82144400	-1.42817900
H	-0.48878200	-4.20471300	1.87732000
H	0.53398600	-5.91031400	0.37517900
C	-0.04612900	-1.61063500	2.01420800
O	0.11902600	-1.79238200	3.21895100
N	-0.84893000	-0.70818900	1.39919700

O	-1.53279100	0.21347700	2.79559300
C	-0.59562100	1.00641200	3.55630000
H	-1.18331700	1.66600100	4.20374000
H	0.03847600	1.59940700	2.89097900
H	-0.00375100	0.30848500	4.14189500
H	-4.64073400	0.29816700	0.32518900
H	0.14855700	-0.91644700	-4.47342900
H	1.23973600	-0.55553000	-3.12427000
C	-4.38710400	-1.70917800	1.02654600
H	-4.31209400	-2.73736200	0.65101800
H	-5.29744400	-1.65291500	1.63294700
H	-3.52954000	-1.51494700	1.67773000
C	-5.65630900	-1.00839000	-1.05525300
H	-5.76193200	-0.25668700	-1.84564000
H	-6.59225700	-1.03463100	-0.48544800
H	-5.52670400	-1.98626100	-1.53524500
C	1.11057800	0.34591000	-0.20535400
C	1.97094300	-0.70516600	-0.07052600
C	3.46684800	-0.54744000	-0.05910600
C	4.15871000	0.09830800	-1.09699700
C	4.22157500	-1.09563500	0.99383800
C	5.54954500	0.20975200	-1.07558000
H	3.59838200	0.52486300	-1.92345900
C	5.61082600	-0.97881500	1.02128300
H	3.70737800	-1.61141900	1.80068800
C	6.28243400	-0.32543300	-0.01482900
H	6.06076000	0.71436400	-1.89177700
H	6.16967000	-1.40065000	1.85302100
H	7.36566300	-0.23769700	0.00301900
C	1.65358800	1.73853700	-0.18832400
C	2.30572900	2.22660600	0.95831000
C	1.50491300	2.61562000	-1.27532900
C	2.78842800	3.53422500	1.01504900
H	2.44320900	1.56249400	1.80662700
C	1.99983900	3.91815200	-1.22930400
H	0.99145000	2.26921700	-2.16750400
C	2.64051400	4.38788900	-0.07999200
H	3.28879900	3.88365200	1.91497400
H	1.88192400	4.57039600	-2.09169500
H	3.02225300	5.40480900	-0.04041500
H	-2.13327000	0.85664900	2.26921400
O	-1.03109200	2.17366100	0.30756100
C	-1.99166600	2.70797900	0.97560200
O	-2.84795000	2.08138000	1.64403800

C	-2.04817300	4.22399800	0.90397600
H	-1.04820700	4.63966700	0.76151300
H	-2.66172000	4.51786900	0.04289600
H	-2.51412100	4.62856600	1.80520500

TS-5

Os	-1.00553300	-0.31422900	0.09461600
C	-1.12624200	-0.29129700	2.58908100
C	-1.17367800	0.97224600	1.89528700
C	-2.28029200	1.30937900	1.04104800
C	-3.29036300	0.35836300	0.72606600
C	-3.02492300	-0.96404800	1.16357800
C	-2.02387100	-1.26525600	2.15526000
H	-0.42901400	1.72717600	2.12146100
H	-2.32025700	2.30756600	0.61989100
H	-3.64625800	-1.76981500	0.79242700
H	-1.94450900	-2.28168000	2.52842700
C	-0.10001000	-0.52855100	3.65986500
H	-0.03533900	-1.58528500	3.93243200
C	-4.48886400	0.64560600	-0.15565700
C	1.74377900	4.47379700	0.79249200
C	2.01914600	3.10849600	0.80215600
C	1.36541000	2.19399900	-0.05205900
C	0.40086700	2.73871400	-0.94277700
C	0.16477600	4.12061100	-0.98277400
C	0.82101100	4.99121400	-0.11841000
H	2.26669900	5.13229000	1.48135500
H	2.78021200	2.73015600	1.47790300
H	-0.54744900	4.48241000	-1.71759000
H	0.61734400	6.05804500	-0.15676300
C	-0.49704100	1.93187900	-1.87722100
O	-0.98402200	2.39484100	-2.91450400
N	-0.63608400	0.71295800	-1.36706800
H	-4.59570300	-0.23835300	-0.79636900
H	-0.36770900	0.03980900	4.55996100
H	0.88739500	-0.18553400	3.33494800
C	-4.32568100	1.87503900	-1.06112300
H	-4.28168700	2.80614600	-0.48166900
H	-5.19399000	1.95096200	-1.72395700
H	-3.43136500	1.81218900	-1.68965600
C	-5.75700800	0.76448300	0.72042100
H	-5.91466500	-0.13047500	1.33248600
H	-6.63730400	0.89695900	0.08228700
H	-5.69405200	1.62972100	1.39167600

C	1.10774800	-0.37516200	0.06827900
C	1.85415100	0.76211200	0.00431600
C	3.35999400	0.68252200	0.00942200
C	4.06984100	0.07030600	1.05423700
C	4.09531300	1.25992900	-1.04037400
C	5.46461200	0.01997500	1.04374100
H	3.52201100	-0.37732000	1.87825400
C	5.48835000	1.20279300	-1.05753400
H	3.56481800	1.75217000	-1.85110500
C	6.18021300	0.58278400	-0.01410900
H	5.99149700	-0.45955600	1.86495200
H	6.03441600	1.64539100	-1.88678800
H	7.26622200	0.54207400	-0.02444300
C	1.73075200	-1.72268600	-0.02240700
C	2.39038200	-2.11225200	-1.20131600
C	1.64985300	-2.65432400	1.02475900
C	2.96117100	-3.37843200	-1.31925000
H	2.45166700	-1.40888100	-2.02572200
C	2.22957000	-3.91748000	0.91427300
H	1.13095800	-2.38121100	1.93882800
C	2.88788100	-4.28680800	-0.26080600
H	3.46683900	-3.65552000	-2.24082400
H	2.16607400	-4.61544700	1.74583400
H	3.33707300	-5.27240800	-0.35090200
O	-0.87050300	-2.16821800	-0.75607700
C	-1.87373100	-2.65312600	-1.47315600
O	-2.98574500	-2.15095300	-1.58737900
C	-1.47886700	-3.93832600	-2.18292500
H	-0.88253900	-3.68349900	-3.06662100
H	-0.85750700	-4.56657400	-1.53932300
H	-2.37412100	-4.47515500	-2.50329700

TS-6

Os	-1.08163000	-0.20416300	0.16856400
C	-0.91470300	0.25883800	2.49526300
C	-1.11339400	1.44141500	1.71377700
C	-2.23237100	1.54789600	0.83384000
C	-3.23763400	0.51230300	0.78309900
C	-2.95057200	-0.68700000	1.47023500
C	-1.80598200	-0.82235300	2.32150600
H	-0.39953500	2.25403100	1.77766000
H	-2.35535300	2.45054300	0.24752800
H	-3.58060400	-1.54922900	1.29450800
H	-1.62190400	-1.76650000	2.82064800

C	0.27717200	0.16002400	3.40852800
H	0.46015800	-0.87075300	3.72385400
C	-4.47843500	0.59679500	-0.08776800
C	2.05236800	4.48424200	0.28475700
C	2.30373300	3.12637200	0.45965600
C	1.57600700	2.13580700	-0.23311200
C	0.57626900	2.57882500	-1.13373900
C	0.35244900	3.95084900	-1.32771500
C	1.07760000	4.90554500	-0.62415200
H	2.62725400	5.21325000	0.84992400
H	3.08533200	2.81523900	1.14521500
H	-0.40883800	4.23603300	-2.04660800
H	0.89020200	5.96376800	-0.78332600
C	-0.35565500	1.66979700	-1.87631300
O	-1.10994100	2.07772500	-2.76340800
N	-0.41023300	0.34464600	-1.51329000
H	-4.59296500	-0.40067400	-0.52656500
H	0.10035700	0.76386800	4.30783500
H	1.17844900	0.54197800	2.92021400
C	-4.37700400	1.61342800	-1.23370600
H	-4.36555500	2.64731900	-0.86497700
H	-5.25353000	1.51441900	-1.88290000
H	-3.48457000	1.45494100	-1.84802900
C	-5.70618300	0.88554300	0.80529100
H	-5.82433200	0.13114000	1.59112700
H	-6.61706500	0.88394400	0.19647900
H	-5.62534400	1.86818900	1.28680300
C	1.11402500	-0.35718600	-0.00545600
C	1.96460900	0.70748800	-0.04298500
C	3.44924600	0.49210900	0.08038200
C	4.01344000	-0.18821000	1.17052900
C	4.31491500	0.99921200	-0.90510700
C	5.39373000	-0.36931900	1.26747100
H	3.36329000	-0.58576200	1.94372800
C	5.69316700	0.81032500	-0.81477300
H	3.89942700	1.53735700	-1.75256800
C	6.23938500	0.12615700	0.27382000
H	5.80735700	-0.89864100	2.12194200
H	6.34118400	1.19909400	-1.59603100
H	7.31406400	-0.01722200	0.34729600
C	1.60118600	-1.75034500	-0.13557700
C	2.24880200	-2.15627200	-1.31451300
C	1.43617800	-2.69205200	0.89285100
C	2.73516300	-3.45519500	-1.44980400

H	2.35844100	-1.44429900	-2.12594600
C	1.93992900	-3.98448500	0.76753800
H	0.90711000	-2.40449500	1.79635000
C	2.58984000	-4.37301300	-0.40724000
H	3.22965500	-3.75071700	-2.37144700
H	1.81630000	-4.69382600	1.58204900
H	2.97323600	-5.38468900	-0.51079200
O	-1.03419600	-2.06054400	-0.76503600
C	-2.11281000	-2.70329800	-1.13851500
O	-3.28089000	-2.37494700	-0.92401200
C	-1.77672900	-3.96001000	-1.93322900
H	-1.55119000	-3.67346900	-2.96726700
H	-0.89010700	-4.45426100	-1.52742400
H	-2.63167100	-4.63995200	-1.93648600

TS-7

Os	1.69237000	0.19058000	0.23254800
C	-3.32560300	4.33312500	-0.33417400
C	-3.44773600	2.96683700	-0.11994500
C	-2.42002200	2.07720600	-0.50764700
C	-1.27831900	2.62579500	-1.13635700
C	-1.17394500	4.00780200	-1.36429000
C	-2.18551400	4.86494900	-0.95706300
H	-4.12972400	4.99503700	-0.02264300
H	-4.34677000	2.57451900	0.34119400
H	-0.28694300	4.37327700	-1.87174100
H	-2.10265700	5.93456000	-1.12790800
C	-0.18145100	1.75050200	-1.58142400
O	0.76976200	2.17129400	-2.24039800
N	-0.22552300	0.39126600	-1.17859000
C	-1.44903100	-0.15866100	-0.72401500
C	-2.51850600	0.62711700	-0.36814100
C	-3.84491600	0.04506700	0.01858000
C	-4.66601700	-0.55831700	-0.94641900
C	-4.32389000	0.13643000	1.33522400
C	-5.91675600	-1.07185000	-0.60312800
H	-4.31261100	-0.63172200	-1.97073800
C	-5.57694600	-0.37365000	1.68078900
H	-3.70667700	0.60911900	2.09500400
C	-6.37717800	-0.98188500	0.71217200
H	-6.53342200	-1.54065100	-1.36553400
H	-5.92576100	-0.29681100	2.70751100
H	-7.35201100	-1.38089200	0.97957700
C	-1.57390700	-1.64904300	-0.77633100

C	-1.94817600	-2.39905100	0.34785700
C	-1.41652200	-2.31668000	-2.00160600
C	-2.16537600	-3.77292500	0.25248000
H	-2.08169600	-1.90377500	1.30263400
C	-1.63915100	-3.69038000	-2.09881100
H	-1.13278900	-1.76116600	-2.88879100
C	-2.01699800	-4.42467600	-0.97362400
H	-2.45809000	-4.33299100	1.13691600
H	-1.52298300	-4.18467000	-3.05981700
H	-2.19448900	-5.49417900	-1.05084200
O	1.34699100	-1.82446300	-0.00661700
C	2.21641600	-2.76021100	0.31528600
O	3.29119200	-2.58929200	0.88555400
C	1.75100600	-4.14392900	-0.11742600
H	1.68088900	-4.18514500	-1.20980400
H	2.45482000	-4.90047500	0.23519300
H	0.74805900	-4.34500400	0.27001100
H	0.44197200	-0.29126300	-2.09735000
O	2.78023100	-0.13128800	-1.57534800
C	2.33948300	-0.54067500	-2.68836600
O	1.10973700	-0.73930000	-2.95797500
C	3.33722100	-0.77899600	-3.79439200
H	3.02204500	-1.62660900	-4.40790100
H	3.36395700	0.10963000	-4.43620900
H	4.33421100	-0.95050400	-3.38498500
C	3.02802500	1.94661400	0.61270700
C	3.53804000	0.75296800	1.24745500
C	2.73464500	0.00741700	2.14870100
C	1.38276800	0.39816600	2.45832800
C	0.88416700	1.55227000	1.79266700
C	1.70572200	2.34487900	0.92028600
H	4.50085700	0.35252200	0.95018800
H	3.10711100	-0.94956900	2.49056900
H	-0.16001000	1.82259000	1.89707300
H	1.26184100	3.17480600	0.38399800
C	3.84771400	2.68113600	-0.41264700
H	3.20087400	3.22787900	-1.10325400
C	0.58209900	-0.43150700	3.44943500
H	0.70759500	-1.48232500	3.15697200
H	4.52531000	3.39099100	0.07900800
H	4.44879800	1.97788800	-0.99563800
C	1.17634400	-0.25977500	4.86353100
H	1.09110300	0.78092600	5.19927500
H	0.63955900	-0.89152200	5.58032000

H	2.23474700	-0.53933300	4.89543600
C	-0.91704300	-0.11348100	3.45522000
H	-1.34611900	-0.17920600	2.45144900
H	-1.44740800	-0.82303600	4.09936900
H	-1.11223000	0.89304900	3.84673000

TS-3'

Os	0.84248600	0.18542200	-0.35391600
C	1.42165700	1.97736500	-1.81435900
C	2.02117700	2.11141100	-0.51232000
C	2.82447200	1.06288500	0.02243900
C	3.08872700	-0.14407800	-0.72002400
C	2.36437500	-0.29492400	-1.93290200
C	1.59572500	0.76983300	-2.51550900
H	1.85156600	3.01233000	0.06593500
H	3.25345200	1.18707200	1.00987700
H	2.40051700	-1.24758500	-2.45052700
H	1.08863100	0.60823300	-3.45998600
C	0.61497900	3.10868800	-2.39607200
H	-0.03853700	2.75929000	-3.20126700
C	4.04571400	-1.23890300	-0.27078500
C	0.92454500	-0.80556300	3.97109200
C	1.11599800	-0.12249000	2.76604700
C	0.67787300	-0.65238300	1.53570500
C	0.04369200	-1.91582000	1.59362000
C	-0.14088500	-2.61343500	2.79227100
C	0.29341200	-2.05486300	3.99209600
H	1.27583300	-0.36245800	4.90107800
H	1.62582800	0.83951500	2.79291000
H	-0.61084500	-3.59324500	2.75552300
H	0.15247500	-2.58369200	4.93128700
C	-0.35696000	-2.52741900	0.29812000
O	-0.73616100	-3.69247100	0.15303300
N	-0.25032500	-1.58755000	-0.70999000
O	-0.12297800	-2.13997400	-2.00729600
C	-1.35667800	-2.58496200	-2.56686800
H	-1.07606700	-3.07854100	-3.50273600
H	-2.01983000	-1.74051800	-2.79139900
H	-1.85288000	-3.29889200	-1.90615900
H	3.56774400	-2.19569900	-0.52054400
H	1.28874900	3.86842700	-2.81419800
H	-0.00190400	3.59529400	-1.63581600
C	4.34768400	-1.24758900	1.23359400
H	4.90124200	-0.35054200	1.53950700

H	4.97510700	-2.11206200	1.47782700
H	3.43272100	-1.30981800	1.82854500
C	5.35384200	-1.14072000	-1.08607200
H	5.16327700	-1.19895600	-2.16338000
H	6.03404100	-1.95729200	-0.81678800
H	5.86963600	-0.19307600	-0.88639400
C	-1.11267200	1.00235600	0.06654700
C	-2.00012800	0.12186400	-0.19729200
C	-3.17128000	-0.65813700	-0.32608400
C	-3.51794300	-1.61750700	0.65518500
C	-4.06449600	-0.41091900	-1.39673100
C	-4.71851900	-2.31099900	0.55471000
H	-2.83419400	-1.80330000	1.47561700
C	-5.27213400	-1.09330800	-1.47294900
H	-3.79261000	0.32120300	-2.15091100
C	-5.59624500	-2.04848600	-0.50212400
H	-4.97530000	-3.05360300	1.30407700
H	-5.95932600	-0.89134200	-2.28948700
H	-6.53652200	-2.58887200	-0.57011700
C	-1.39174700	2.37591100	0.56098000
C	-0.69603000	2.90373300	1.65997000
C	-2.37381900	3.16764500	-0.05934400
C	-0.98320800	4.18547500	2.12909000
H	0.04922300	2.29080700	2.15284600
C	-2.64591400	4.45619000	0.40228100
H	-2.91547700	2.77064800	-0.91312500
C	-1.95279400	4.97013300	1.49956500
H	-0.44426400	4.57320300	2.98973900
H	-3.40400700	5.05572200	-0.09502100
H	-2.16632200	5.97218500	1.86147700

TS-4'

Os	1.08062000	0.26871000	-0.35839700
C	1.81805800	0.99443900	-2.39171100
C	2.62912600	1.55203400	-1.35475300
C	3.35520600	0.75461500	-0.42563000
C	3.16415500	-0.65656200	-0.40177400
C	2.35185800	-1.24743400	-1.42758200
C	1.68081700	-0.42534800	-2.38428700
H	2.66342300	2.63208200	-1.25169100
H	3.92186200	1.24136500	0.35754400
H	2.18024900	-2.31775100	-1.42359000
H	1.02483500	-0.88678600	-3.11566400
C	1.13095600	1.85841000	-3.41633100

H	0.19933000	1.39727600	-3.75904300
C	3.81756800	-1.55981400	0.63452700
C	-1.42369600	4.32642700	0.22549000
C	-2.08534000	3.13740900	0.10737900
C	-1.40703000	1.88867700	0.31437200
C	-0.00652100	1.92823200	0.80708100
C	0.62053300	3.24024900	0.94201700
C	-0.04387900	4.38367700	0.63364000
H	-1.94494800	5.25429100	0.00214100
H	-3.11856200	3.11707200	-0.22359700
H	1.63166400	3.27195500	1.33683600
H	0.44413400	5.35035600	0.72435700
C	0.37703300	0.97590100	1.90776400
O	0.93177100	1.24925800	2.96743100
N	0.18512800	-0.33745100	1.42088400
O	0.66613500	-1.40132600	2.19639300
C	-0.04441000	-1.54704700	3.43745500
H	0.37936200	-2.44889600	3.88568500
H	-1.11397300	-1.69678400	3.26159900
H	0.12637100	-0.68285800	4.08174800
H	3.09467000	-2.36071100	0.83511500
H	1.77500800	2.01230700	-4.29313200
H	0.88699100	2.84151100	-3.00229700
C	4.11769200	-0.86860600	1.97228200
H	4.90229800	-0.10828800	1.87199600
H	4.48182200	-1.61064800	2.69169300
H	3.22308200	-0.39978700	2.39220300
C	5.09147300	-2.19440600	0.03804200
H	4.87830700	-2.74054600	-0.88786900
H	5.53599600	-2.89773800	0.75139600
H	5.84126800	-1.42678400	-0.18959600
C	-0.89718300	-0.40077400	-0.05381000
C	-1.92880700	0.62955000	0.04186900
C	-3.38768700	0.39098800	-0.10061400
C	-3.92314600	-0.30710700	-1.20017200
C	-4.29246200	0.89305300	0.85570100
C	-5.29733000	-0.49651500	-1.33528200
H	-3.25080900	-0.70042800	-1.95638600
C	-5.66887600	0.71006500	0.71881500
H	-3.90317800	1.42350400	1.72064600
C	-6.17847700	0.01203000	-0.37745100
H	-5.68249100	-1.03770200	-2.19591300
H	-6.34212300	1.10609800	1.47515900
H	-7.24993700	-0.13548400	-0.48452500

C	-1.32053400	-1.83163400	-0.18886900
C	-2.18419400	-2.41956500	0.75370000
C	-0.89901000	-2.62425700	-1.26568600
C	-2.58415700	-3.74871000	0.63977400
H	-2.55312100	-1.81766600	1.57769700
C	-1.31426900	-3.95137200	-1.39819200
H	-0.25382400	-2.18843300	-2.01752200
C	-2.15020100	-4.52299300	-0.43947600
H	-3.24357700	-4.17852700	1.38933900
H	-0.97827100	-4.53821000	-2.24948000
H	-2.46569300	-5.55876200	-0.53323000

TS-4''

Os	1.19012100	-0.26830500	0.07332200
C	1.26424600	-1.08831900	2.18469300
C	2.12183000	-1.83804200	1.30101400
C	3.26507700	-1.25969400	0.66802600
C	3.42885200	0.14222700	0.69396500
C	2.54654900	0.92608300	1.52506800
C	1.52993400	0.30850200	2.28650800
H	1.91722100	-2.89445100	1.15228000
H	3.89154900	-1.87711400	0.03660800
H	2.65917400	2.00373700	1.55042300
H	0.87435900	0.91853700	2.89935000
C	0.18091400	-1.75241600	2.99136700
H	-0.64726200	-1.06340300	3.18111100
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C	-2.91902400	-3.87976100	0.62649000
C	-2.81010800	-2.49832000	0.78016500
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C	-1.29663200	-2.41967900	-1.08167800
C	-1.39724000	-3.80828000	-1.23863600
C	-2.21549300	-4.54302500	-0.38643000
H	-3.55902100	-4.44375800	1.30019600
H	-3.37855900	-1.99862700	1.55862700
H	-0.85167200	-4.29270800	-2.04344000
H	-2.31154600	-5.61803100	-0.51040900
C	-0.47879500	-1.59539600	-2.07899100
O	-0.79162300	-1.32849100	-3.22650800
N	0.63136100	-1.44714200	-1.34200300
O	1.71179700	0.32265900	-1.96440200
C	1.06519800	1.29338100	-2.74953300
H	-0.00335300	1.09838100	-2.88693000
H	1.53125700	1.26695700	-3.74579700

H	1.17962900	2.30313400	-2.32499500
H	4.09796000	1.82777500	-0.38364200
H	0.57346100	-2.08766600	3.96103100
H	-0.22248900	-2.62307900	2.46794900
C	4.96412800	0.13401800	-1.36056400
H	5.48291900	-0.80646500	-1.13610700
H	5.66857400	0.76413500	-1.91500900
H	4.10160800	-0.07388800	-1.99957700
C	5.71709100	1.13962900	0.85322800
H	5.41542300	1.69967800	1.74574600
H	6.47937100	1.72524000	0.32719300
H	6.18058600	0.20238000	1.18422000
C	-0.75355700	0.50692200	0.03640400
C	-1.90224200	-0.24341200	0.09070500
C	-3.25508100	0.37364700	0.32497300
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C	-4.77018600	1.73118700	1.66910600
H	-2.69534000	1.39794300	2.13422000
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H	-4.93740300	2.35793500	2.54161400
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H	0.05499400	4.97158600	1.29879200
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TS-5'

Os	-0.62901200	-0.72805400	-0.18516100
C	-1.33830500	-0.72353600	2.77793500
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C	-1.87714900	1.13910800	1.25662300
C	-3.25895200	0.90761900	1.40596500
C	-3.64106200	-0.17585500	2.19674100

C	-2.70374500	-0.97989800	2.85790600
H	0.10082700	0.73579900	2.04451700
H	-1.53355300	2.01310300	0.71724400
H	-4.69979400	-0.38832000	2.32798000
H	-3.05419300	-1.79256500	3.48909400
C	-0.35072900	-1.50078000	3.60583100
H	0.01958300	-2.36334100	3.04256100
C	-4.30881800	1.85673100	0.84269200
C	0.65125800	4.72370200	0.44323200
C	1.29276200	3.50638600	0.65514400
C	1.05349700	2.38450100	-0.16478400
C	0.15186900	2.55775000	-1.23965100
C	-0.46053200	3.79764100	-1.47978700
C	-0.22539200	4.87936600	-0.63504900
H	0.84946500	5.55884300	1.11002400
H	2.00859400	3.41269900	1.46642500
H	-1.11586100	3.90143900	-2.34026100
H	-0.70519900	5.83547400	-0.82417400
C	-0.17503000	1.43627600	-2.17162100
O	0.07009100	1.44361900	-3.36376900
N	-0.94757500	0.39296500	-1.60881300
H	-5.25902500	1.30489600	0.83240500
H	-0.81732800	-1.86963100	4.52519800
H	0.50927000	-0.88071100	3.88088300
C	-4.03016400	2.33104700	-0.59260000
H	-3.12627700	2.94817100	-0.64697800
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H	-3.91037200	1.49272100	-1.28450300
C	-4.48878500	3.06251900	1.79105400
H	-4.74012000	2.73971300	2.80754600
H	-5.29170800	3.71669600	1.43142600
H	-3.56873700	3.65725300	1.84477700
C	1.35436900	-0.13593000	-0.01948600
C	1.85231500	1.13743200	0.02556300
C	3.32000200	1.42482800	0.21266900
C	3.99452200	1.10115400	1.40003800
C	4.04336400	2.07771700	-0.80050000
C	5.34784500	1.40228100	1.56494400
H	3.45085800	0.60651100	2.19950600
C	5.39687500	2.37314300	-0.64223000
H	3.53596100	2.34754400	-1.72321600
C	6.05551900	2.03688700	0.54311600
H	5.84822200	1.14078000	2.49409300
H	5.93783700	2.86729800	-1.44543500

H	7.10968800	2.26973200	0.66923600
C	2.36224500	-1.25199600	-0.04301700
C	3.01272600	-1.56688200	-1.24912800
C	2.67295800	-2.02107700	1.08941400
C	3.94558200	-2.60198500	-1.31726500
H	2.77938900	-0.98816900	-2.13836600
C	3.61331100	-3.05145600	1.02786700
H	2.17763600	-1.80389600	2.03066700
C	4.25385300	-3.34895300	-0.17741100
H	4.43680700	-2.82067900	-2.26221500
H	3.84757100	-3.62011400	1.92484200
H	4.98742800	-4.14963800	-0.22651300
O	-0.10075400	-2.39961400	-1.30000000
C	-0.04711600	-3.23080400	-0.31628200
O	-0.27212300	-2.75154700	0.82912300
C	0.31937600	-4.66043200	-0.56087100
H	-0.01421600	-4.97811100	-1.55149400
H	1.41157200	-4.74702100	-0.51725000
H	-0.11328200	-5.29735300	0.21395000
O	-2.70941000	-1.59350800	-0.51567900
C	-3.36554400	-1.42174500	-1.57535900
O	-3.06721900	-0.56669000	-2.48919200
C	-4.59140800	-2.27148000	-1.83019000
H	-4.36085000	-2.99860600	-2.61742700
H	-4.88693700	-2.80522400	-0.92531300
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TS-6'

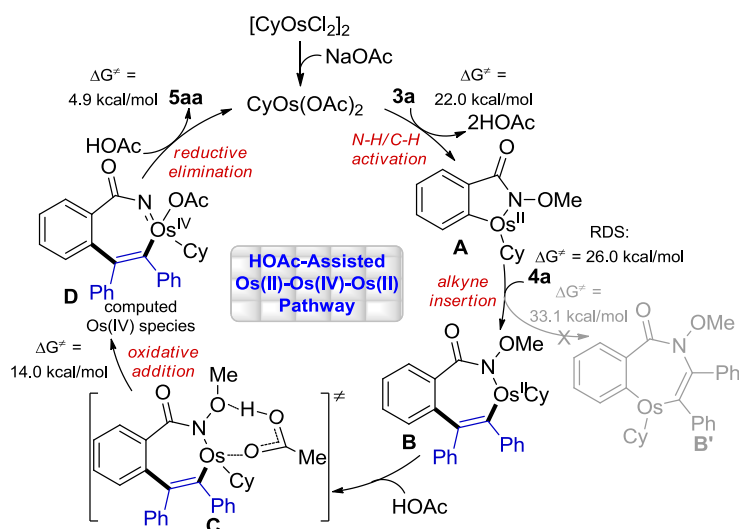
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C	-1.01171500	0.33429400	1.76948100
C	-1.89966200	0.97353000	0.86569500
C	-3.32058200	0.86777200	1.04378800
C	-3.77725000	0.05957500	2.06546200
C	-2.89266000	-0.61024000	2.94771700
H	0.01105100	0.68764500	1.83872300
H	-1.52440000	1.76635500	0.23561900
H	-4.84823700	-0.01762000	2.24537500
H	-3.30921500	-1.20797600	3.75539400
C	-0.57500000	-1.09690600	3.82799300
H	0.03216800	-1.86613200	3.33790900
C	-4.29204400	1.77964000	0.30037300
C	0.24615800	4.77361300	0.08058600

C	0.91961900	3.62377400	0.45957700
C	0.81743100	2.41880100	-0.28209200
C	0.00740500	2.44713900	-1.45517600
C	-0.62671700	3.63900800	-1.85345800
C	-0.53376400	4.79089900	-1.08833000
H	0.33086100	5.66958400	0.69057700
H	1.53919300	3.63432800	1.35051700
H	-1.18858400	3.62178600	-2.78207000
H	-1.04725500	5.69791600	-1.39444700
C	-0.09361000	1.29928400	-2.37341400
O	-0.31677100	1.40580500	-3.58150700
N	0.13313800	0.03956200	-1.83073100
H	-5.29653500	1.36115400	0.45884700
H	-1.11148400	-1.56095300	4.66176200
H	0.11510000	-0.35063600	4.24340100
C	-4.06632500	1.89312800	-1.21562800
H	-3.09839000	2.35008600	-1.44556400
H	-4.84202600	2.53135600	-1.65554400
H	-4.09382600	0.91974100	-1.70937400
C	-4.27910600	3.18348700	0.94776200
H	-4.49354700	3.13053300	2.02083400
H	-5.03226500	3.82739200	0.47779100
H	-3.30196600	3.66466900	0.82050600
C	1.32004100	-0.04141900	-0.30974000
C	1.63896300	1.26077100	0.05298600
C	2.99763200	1.57838200	0.61599500
C	3.33688700	1.26065200	1.94053600
C	3.94979000	2.25834100	-0.16317400
C	4.58677100	1.59545100	2.46679100
H	2.60717000	0.75398500	2.56719700
C	5.20107100	2.58861200	0.35603600
H	3.70118500	2.52453200	-1.18686500
C	5.52490800	2.25792100	1.67454200
H	4.82430000	1.34093300	3.49677100
H	5.92443800	3.10595800	-0.26921000
H	6.49870200	2.51847600	2.08091500
C	2.43983800	-1.01113000	-0.55186300
C	2.95915500	-1.18405200	-1.84732500
C	3.05671600	-1.70657900	0.50216300
C	4.03778400	-2.03650300	-2.08340400
H	2.52727300	-0.63132400	-2.67511700
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C	4.63919600	-2.72204600	-1.02645600

H	4.41699700	-2.15085600	-3.09546900
H	4.61823400	-3.05618900	1.10538200
H	5.48737300	-3.37677800	-1.20802100
O	-0.03447100	-2.74338500	-1.15555300
C	0.37854600	-3.21279500	-0.04108300
O	0.29993100	-2.40644100	0.95705400
C	0.93003500	-4.59337100	0.09462200
H	0.48607400	-5.25056000	-0.65638600
H	2.01353700	-4.55360200	-0.06633500
H	0.74168300	-4.97609000	1.10041300
O	-2.37392200	-2.16807500	0.31584000
C	-3.06453800	-1.80274200	-0.70046300
O	-2.54304800	-0.92523700	-1.46039900
C	-4.42072400	-2.38357700	-0.96383200
H	-4.40225700	-3.46507700	-0.80155600
H	-5.13983300	-1.95017400	-0.25965500
H	-4.73802200	-2.15863300	-1.98387700
H	0.21137200	-0.65542600	-2.57625700

VI. Mechanistic Proposal

Scheme S1. Proposed Catalytic Cycle



On the basis of both DFT calculations and experimental mechanistic studies, a plausible catalytic cycle involving the HOAc-assisted Os(II)-Os(IV)-Os(II) pathway is proposed in Scheme 6. Initially, the active Os(*p*-cymene)(OAc)₂ is generated with the aid of NaOAc, which then coordinates with *N*-methoxybenzamide **3a** via N–H bond cleavage, followed by the irreversible *ortho*-osmation to produce the five-membered osmacycle intermediate **A** (INT-4). Subsequent regioselective

migratory insertion of alkyne **4a** into the C–Os bond with the highest energy barrier of 26.0 kcal/mol is employed as the rate-determining step to generate a seven-membered intermediate **B** (INT-6). Thereafter, a preferable oxidative addition process of osmium into the N–O bond involving a relative low energy barrier ($\Delta G^\ddagger = 14.0$ kcal/mol) occurs with the assistance of HOAc, yielding the key Os(IV) intermediate **D** (INT-7). Further reductive elimination from **D** leads to the intramolecular formation of C–N bond. Finally, the protonolysis and subsequent ligand exchange are involved in the presence of HOAc to deliver the desired isoquinolone product **5aa** together with the regeneration of the active osmium(II) catalyst for the turnover of the next catalytic cycle.

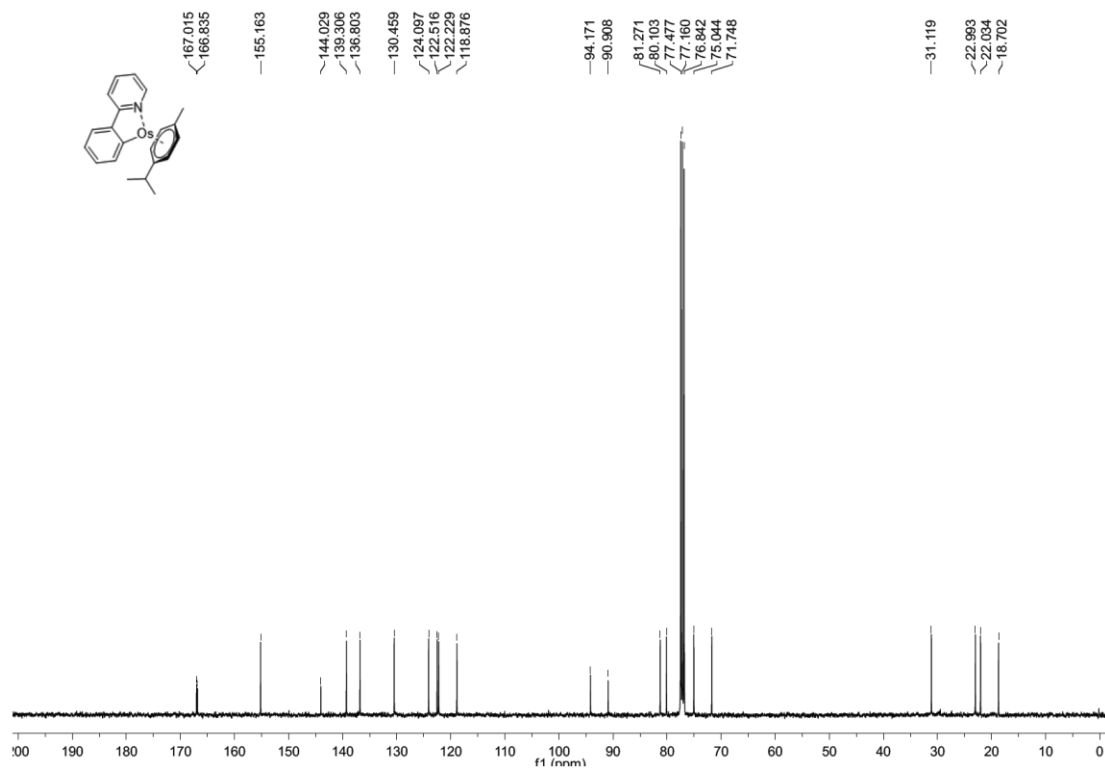
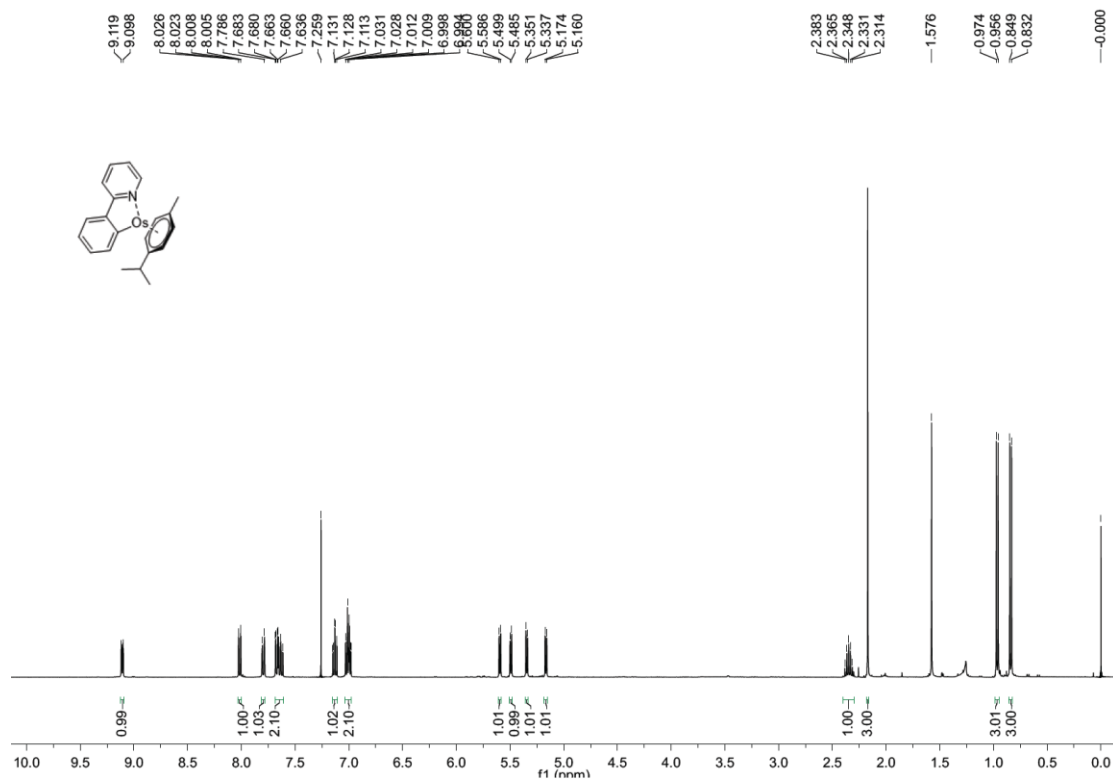
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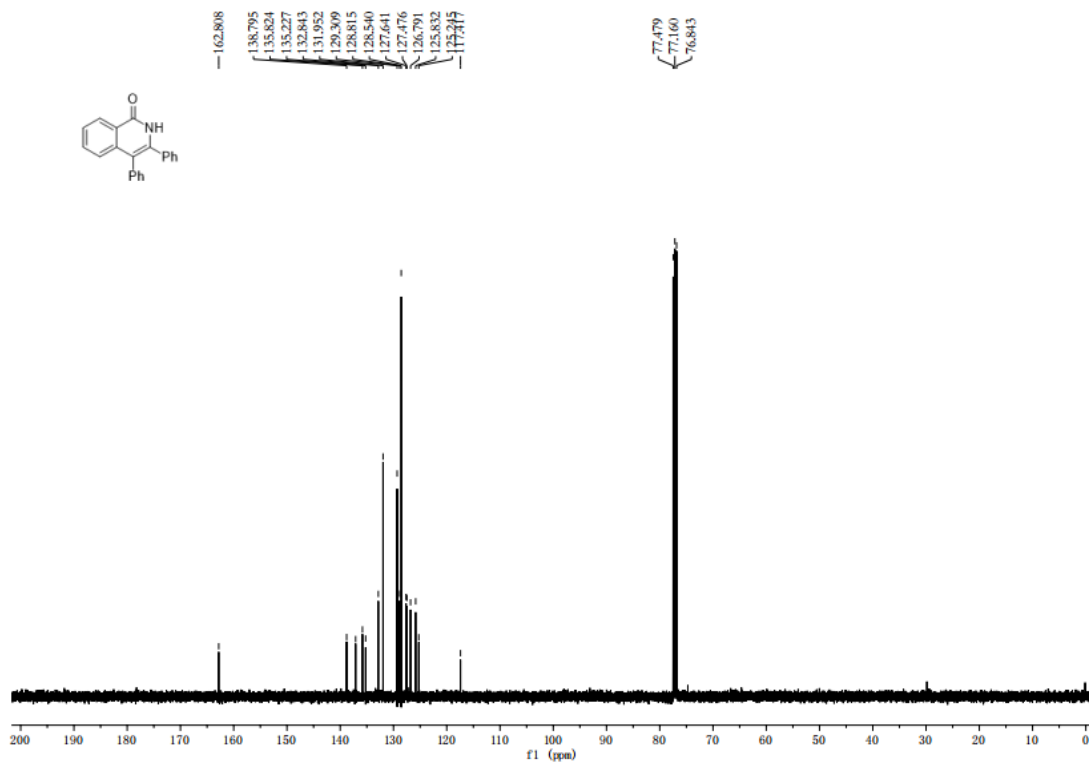
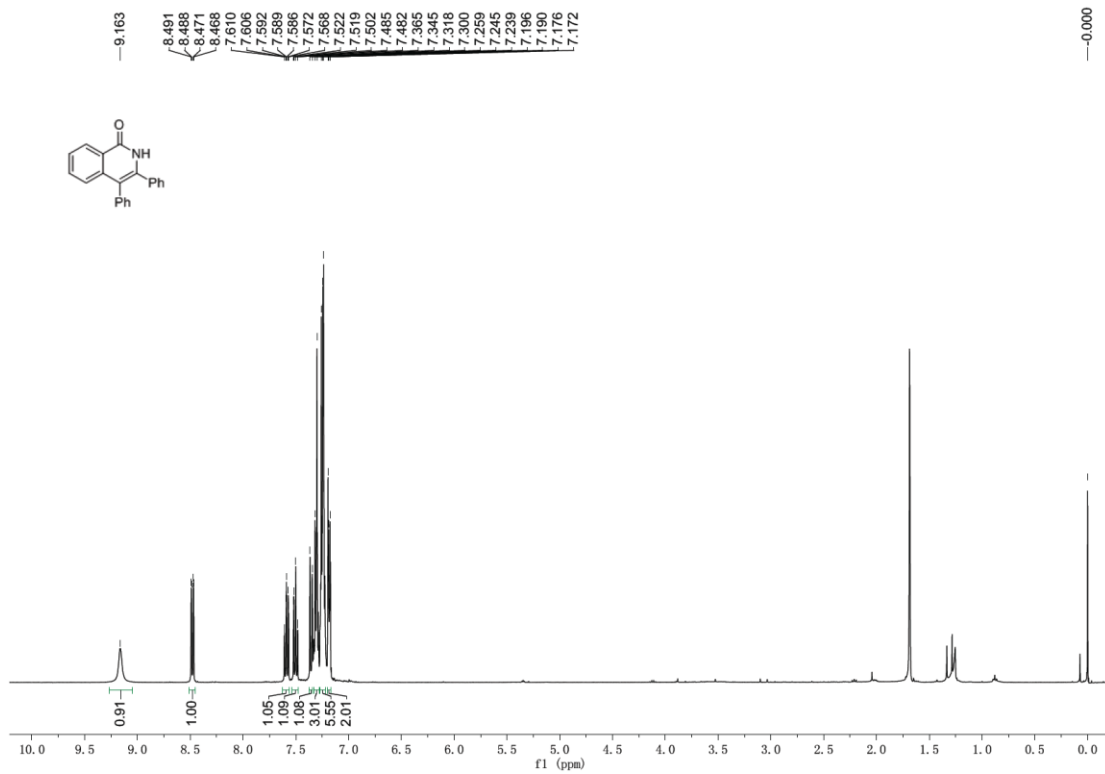
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VIII. Copies of ^1H and ^{13}C NMR Spectra

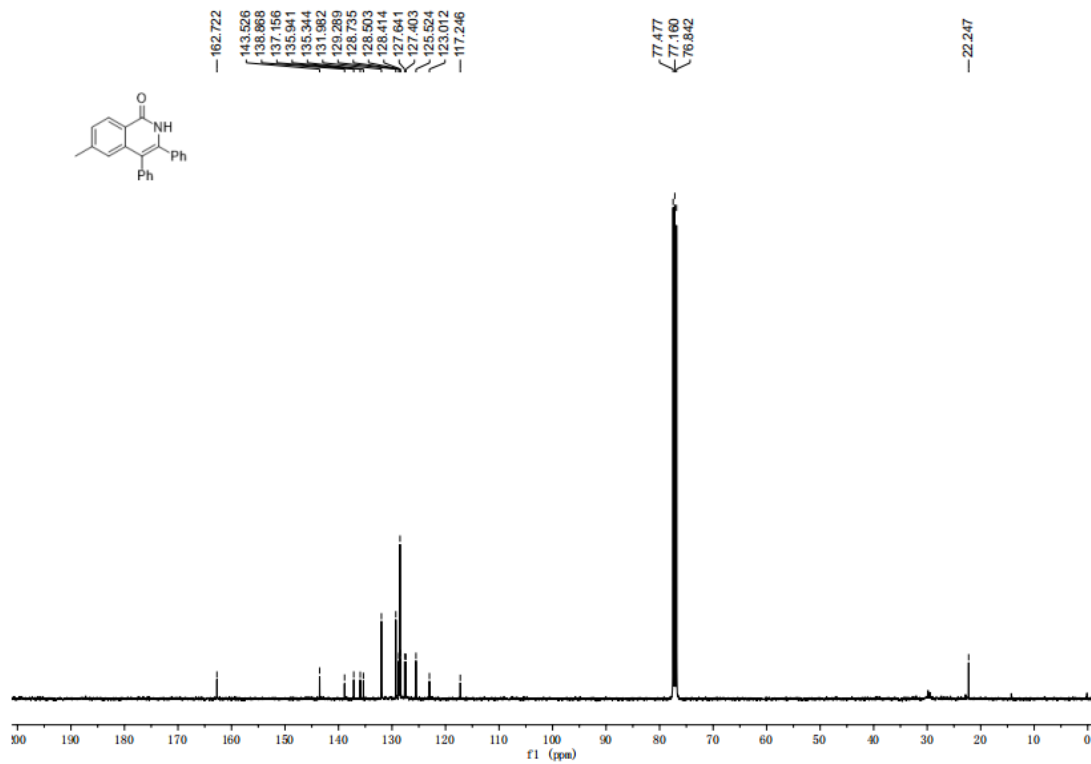
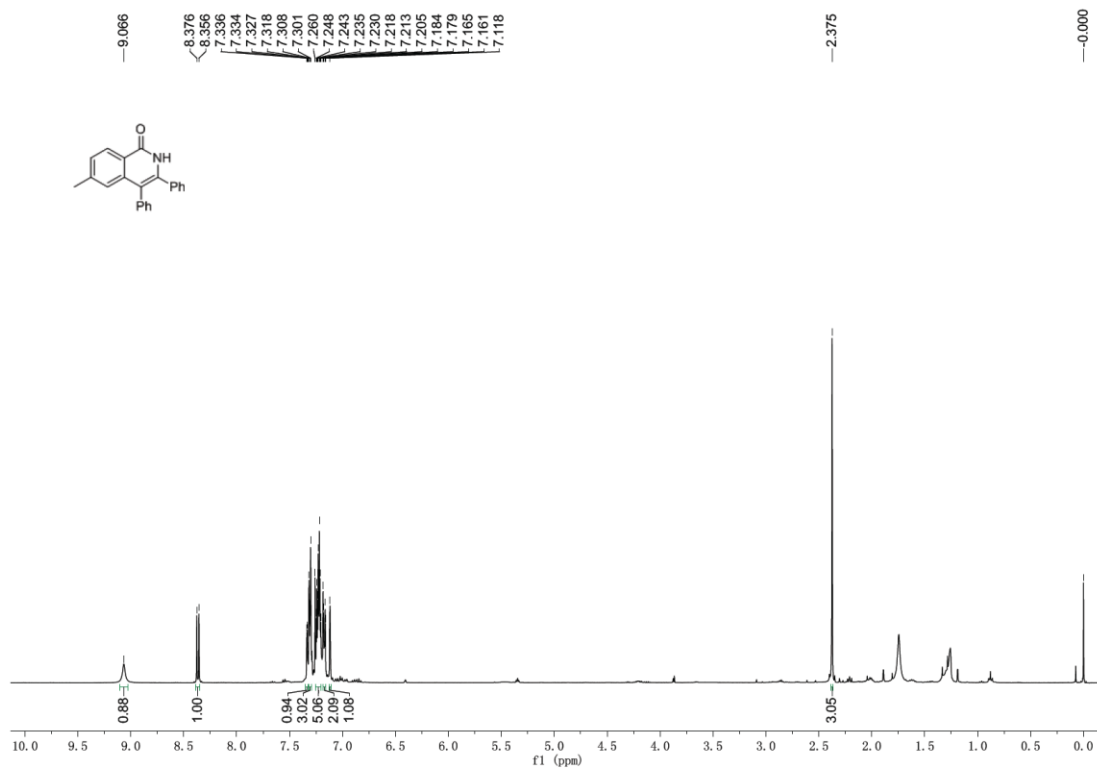
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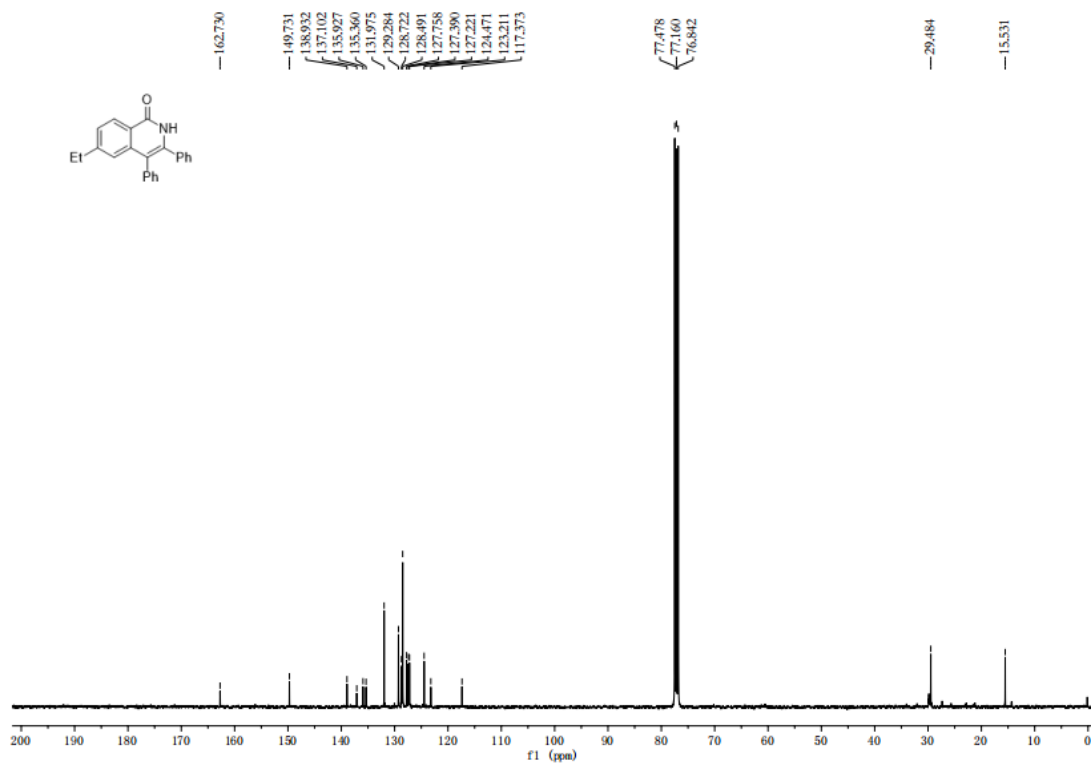
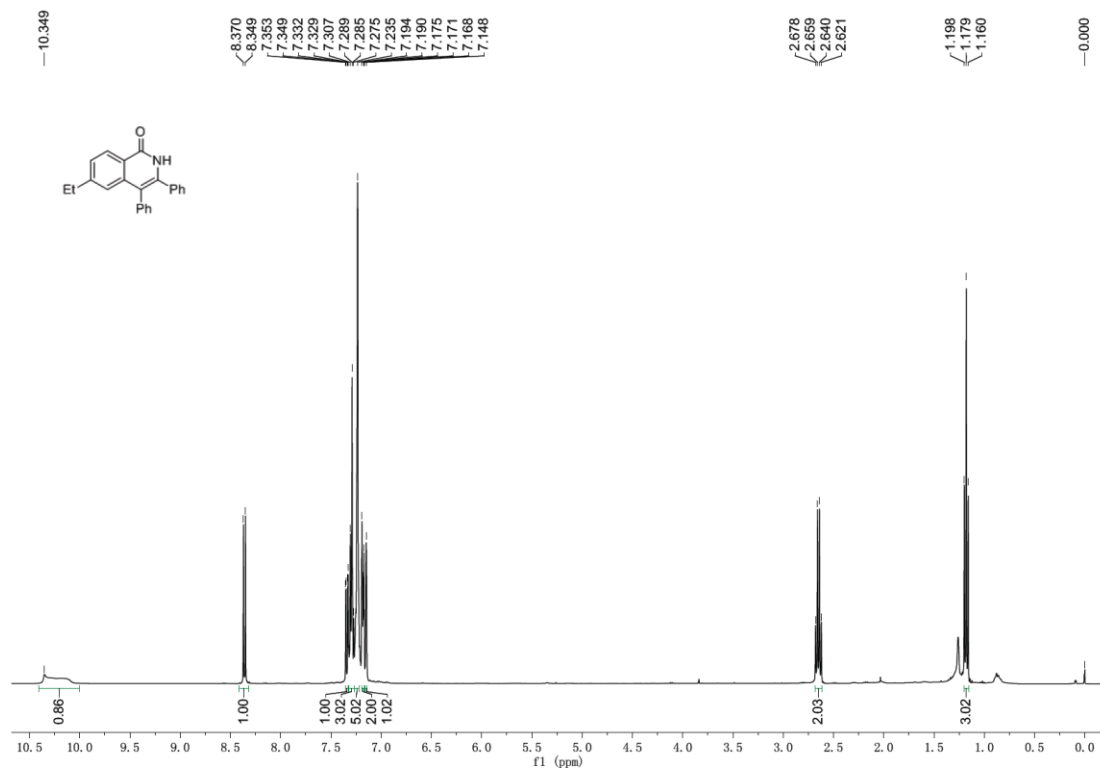
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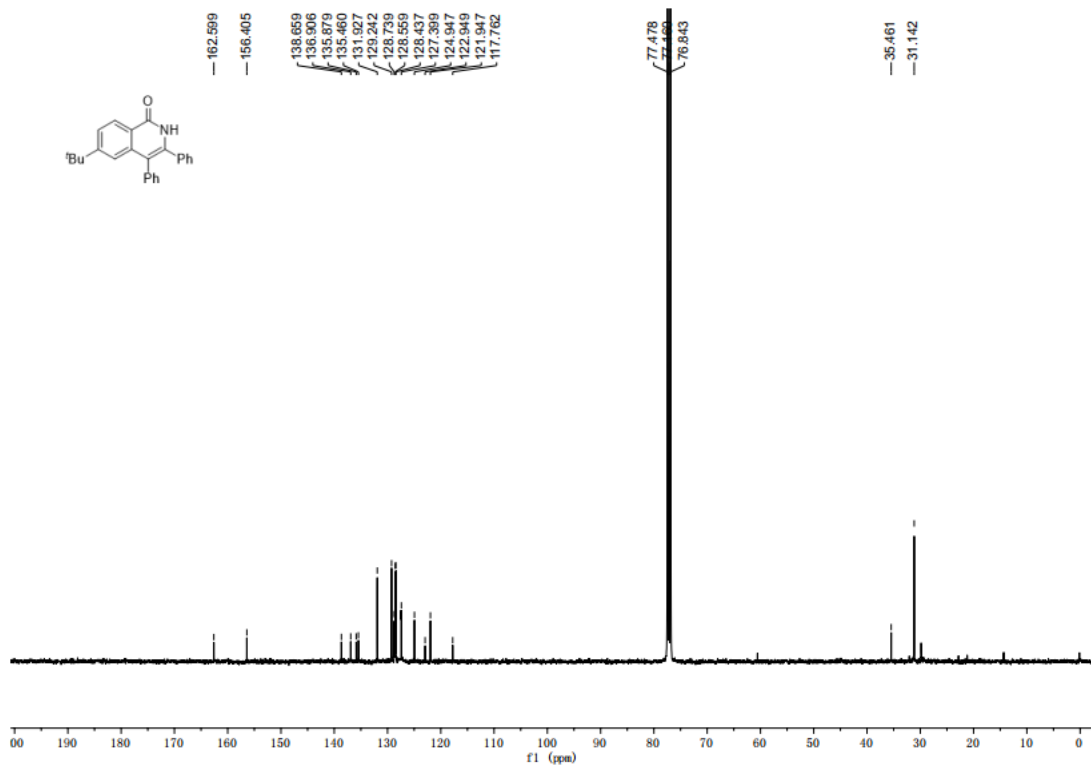
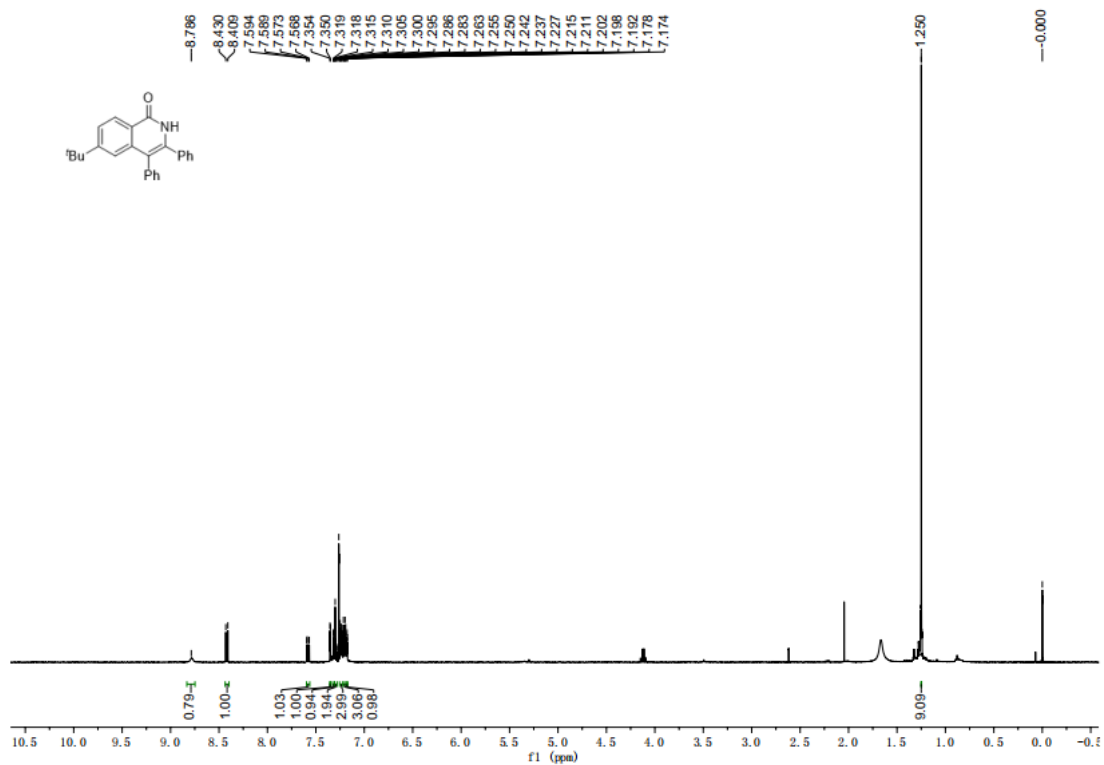
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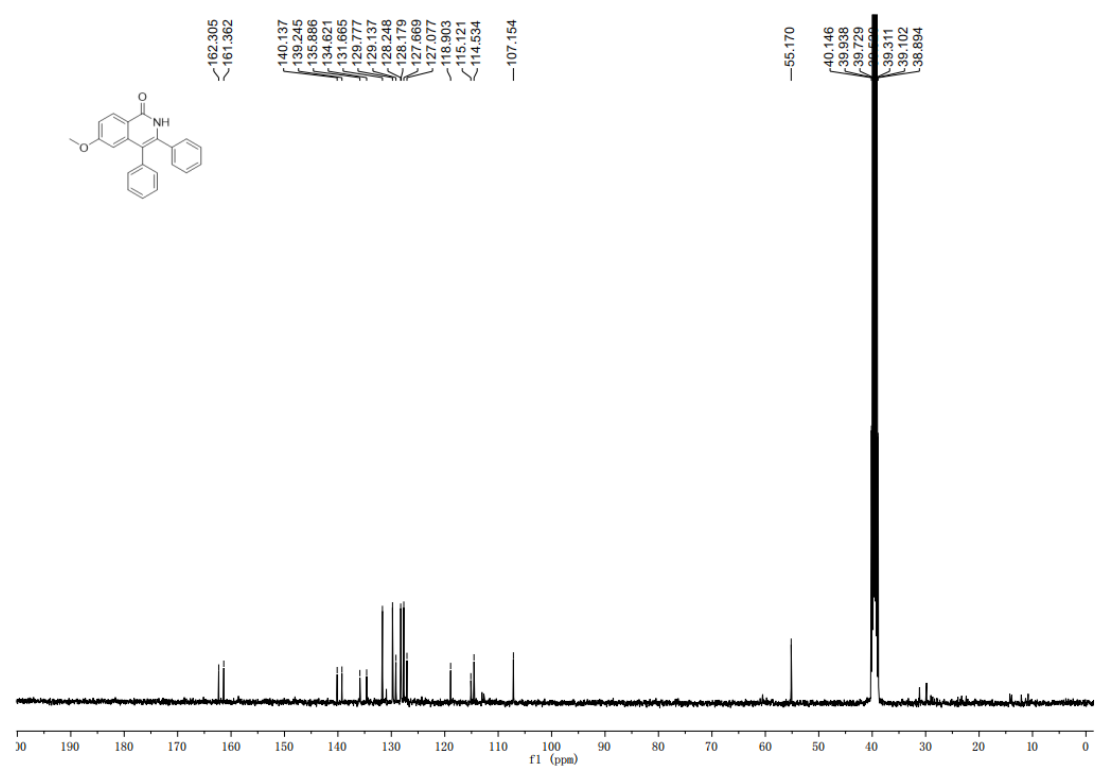
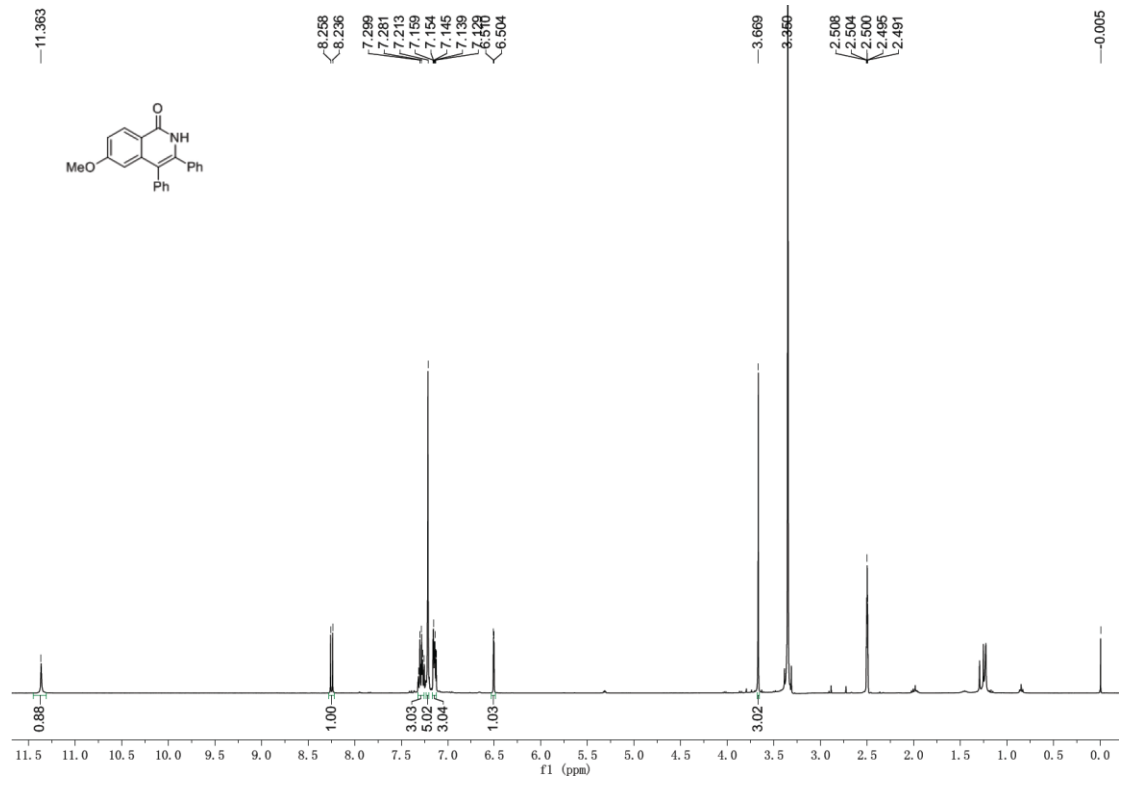
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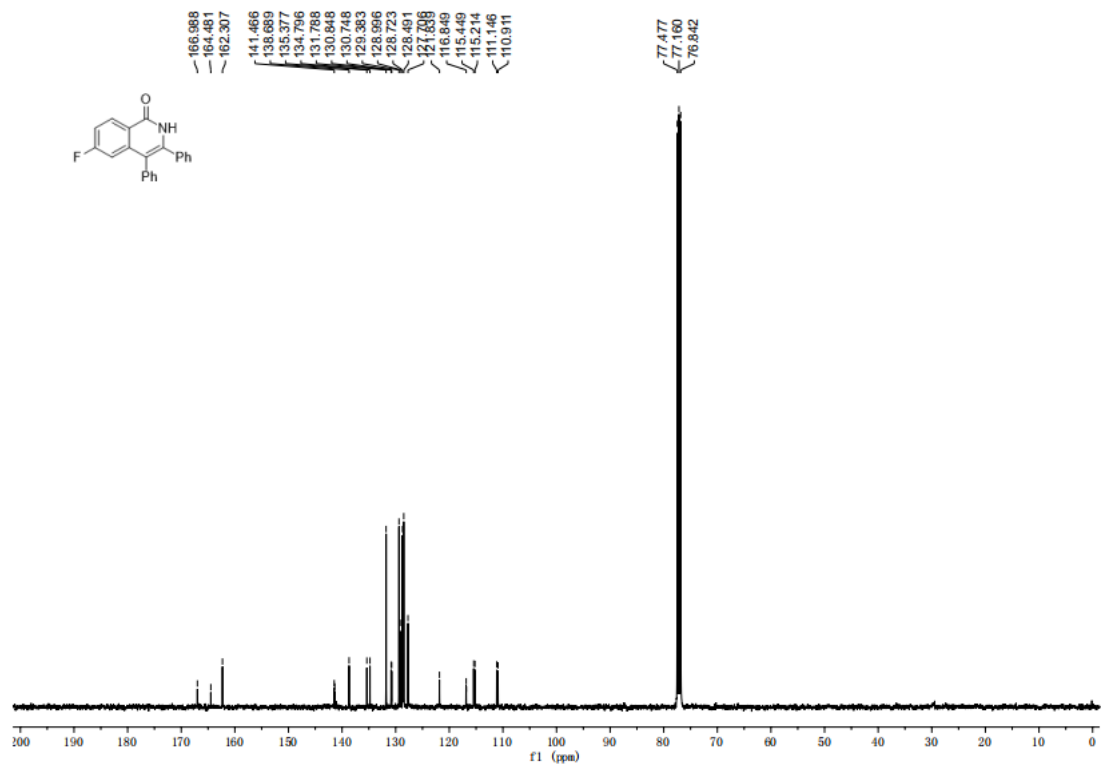
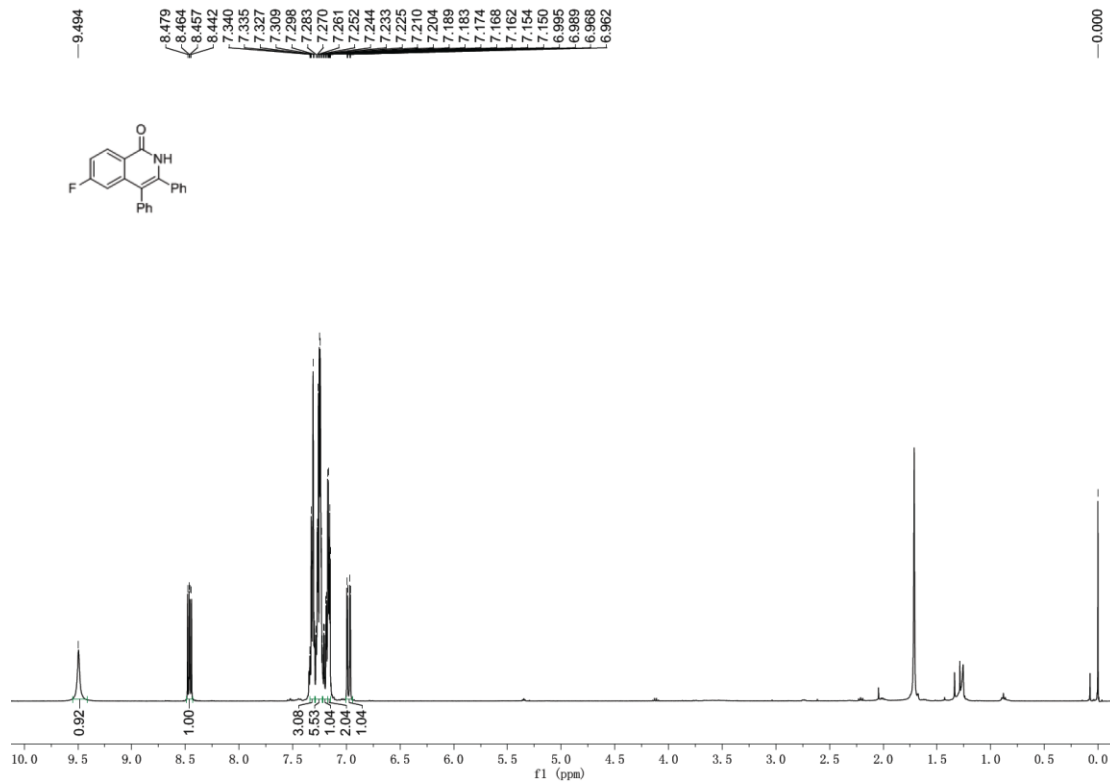
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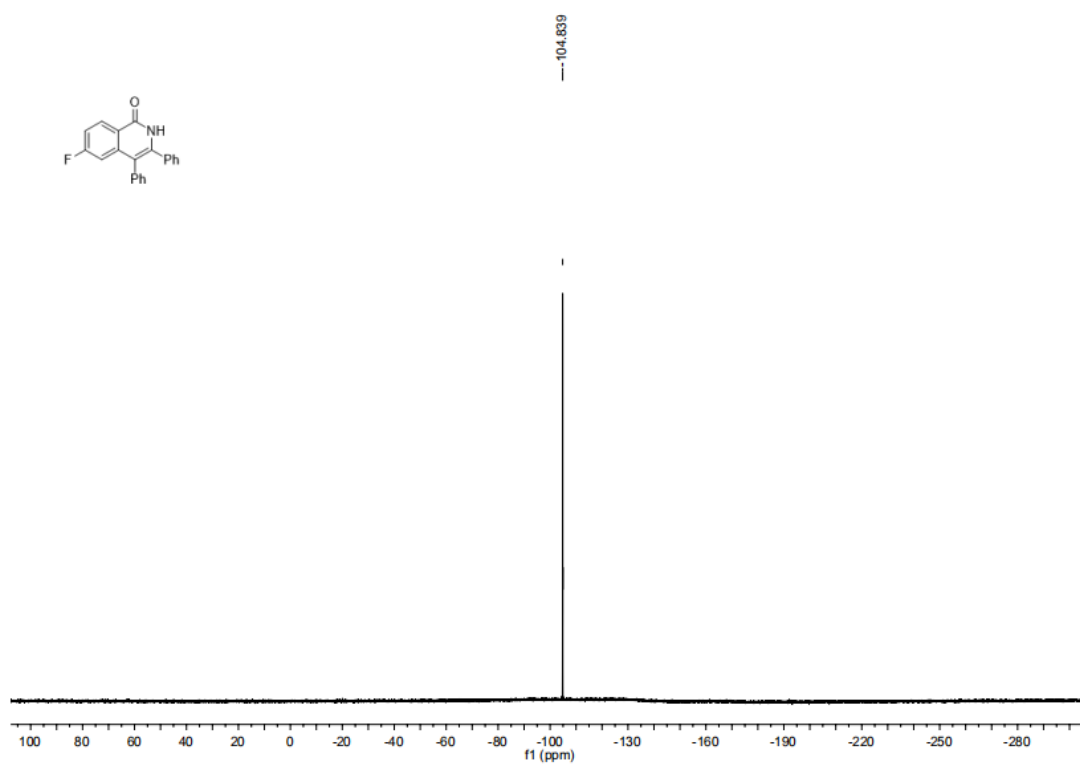
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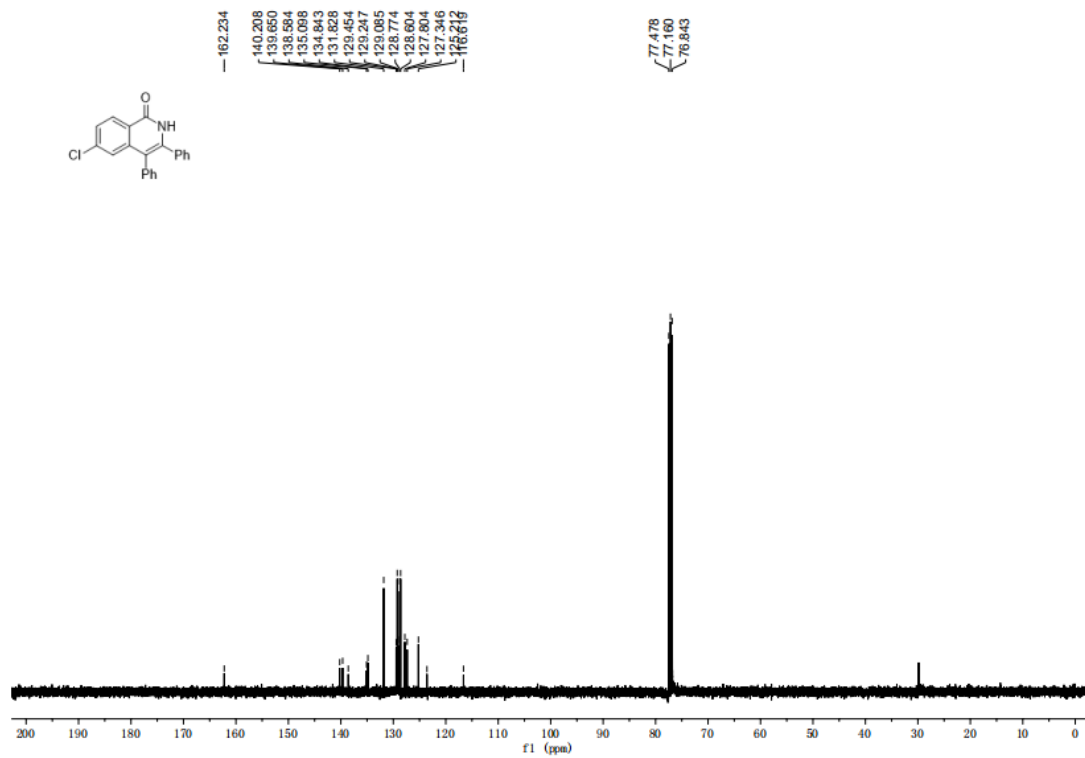
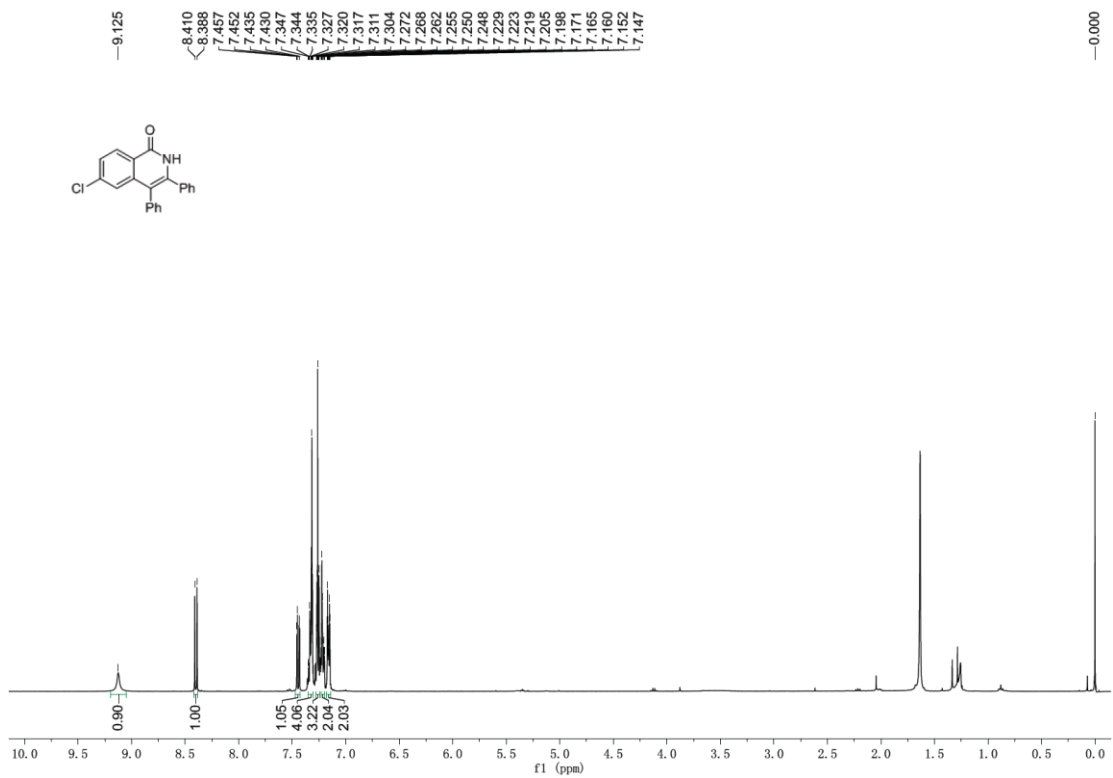
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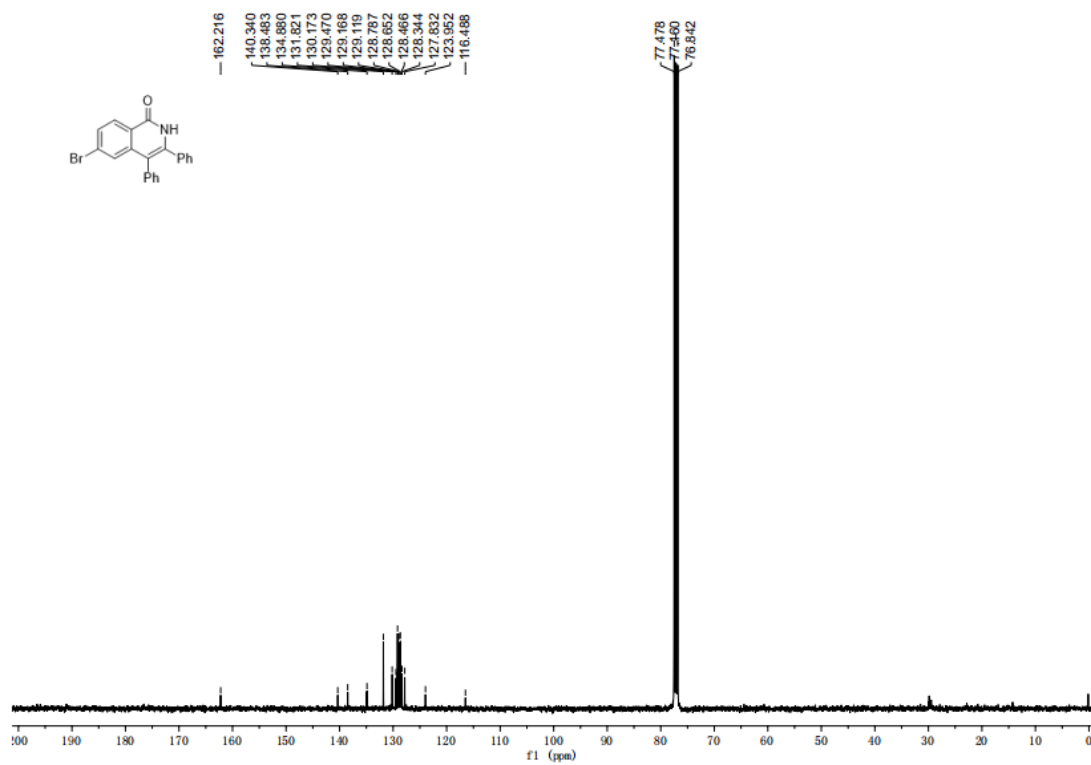
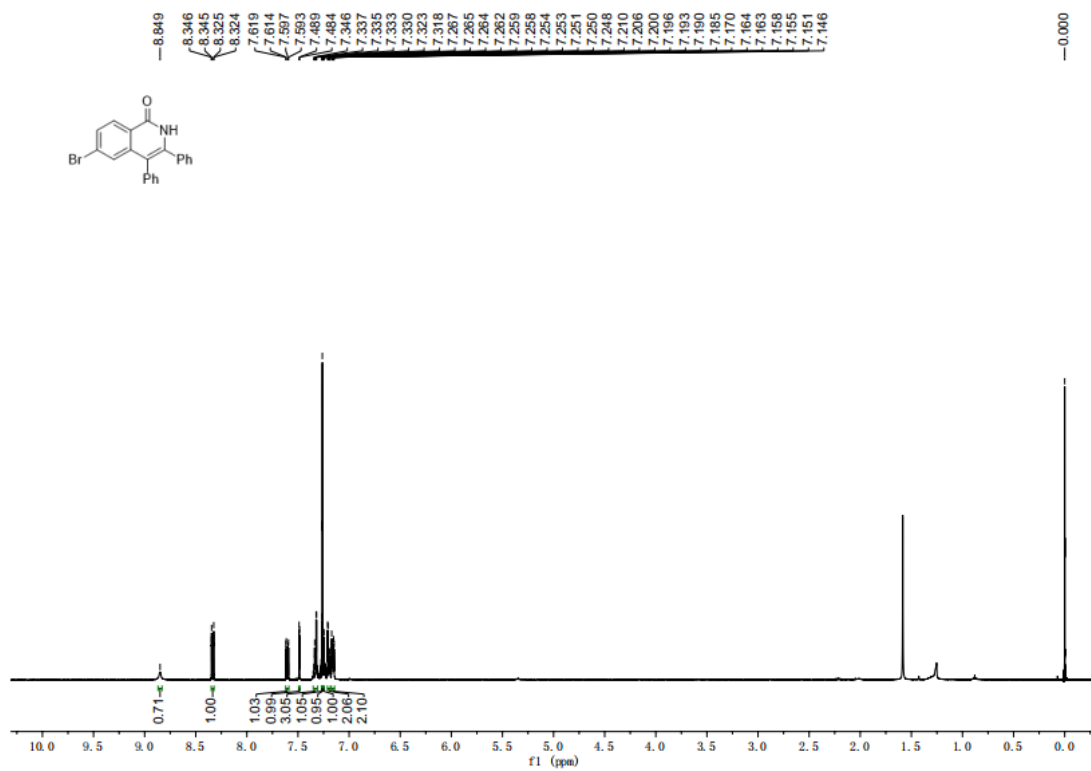
¹⁹F NMR spectrum of 5fa



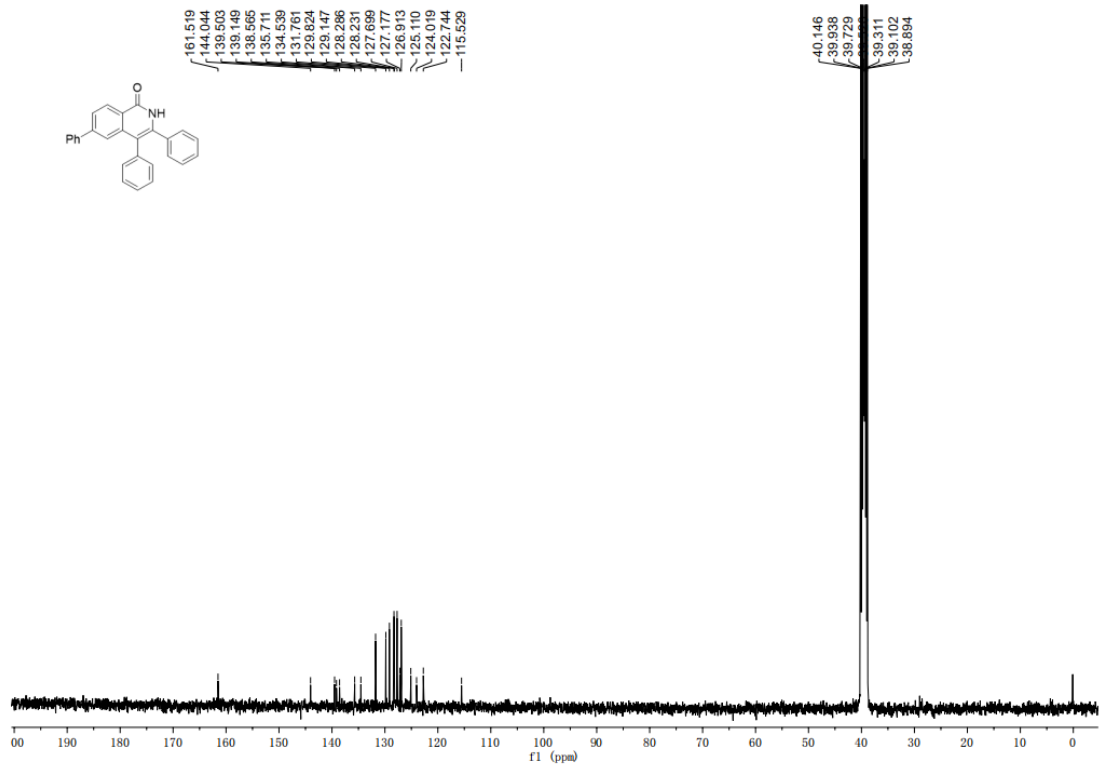
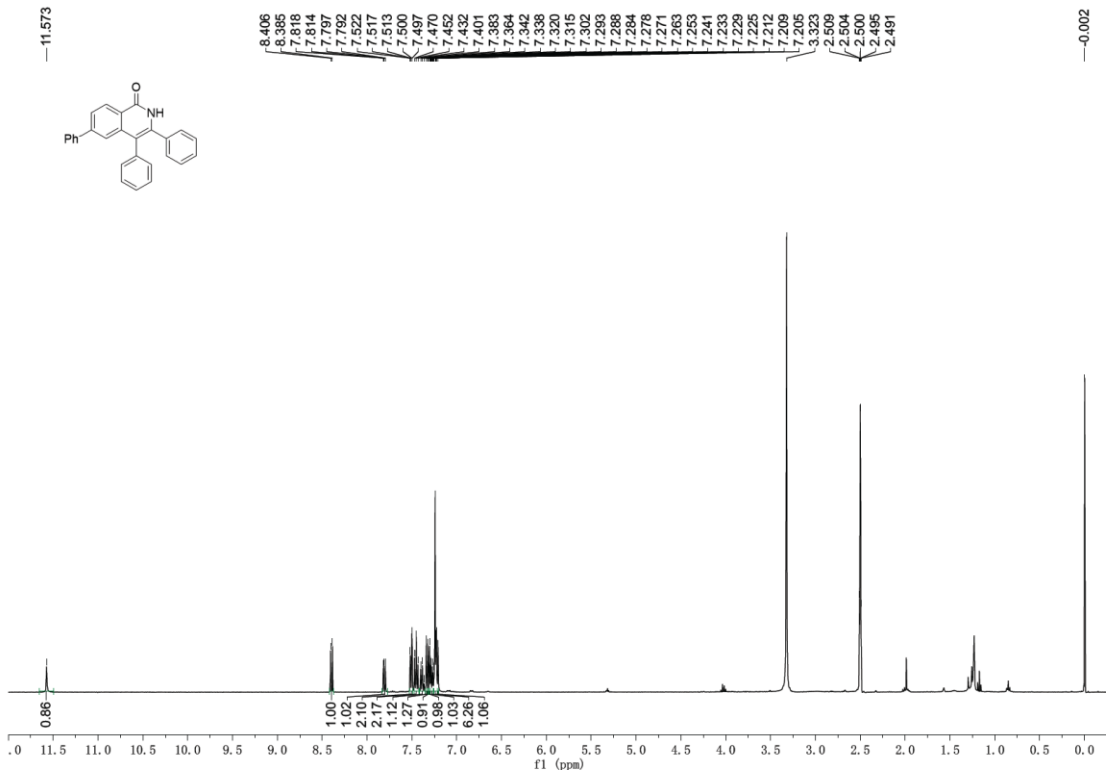
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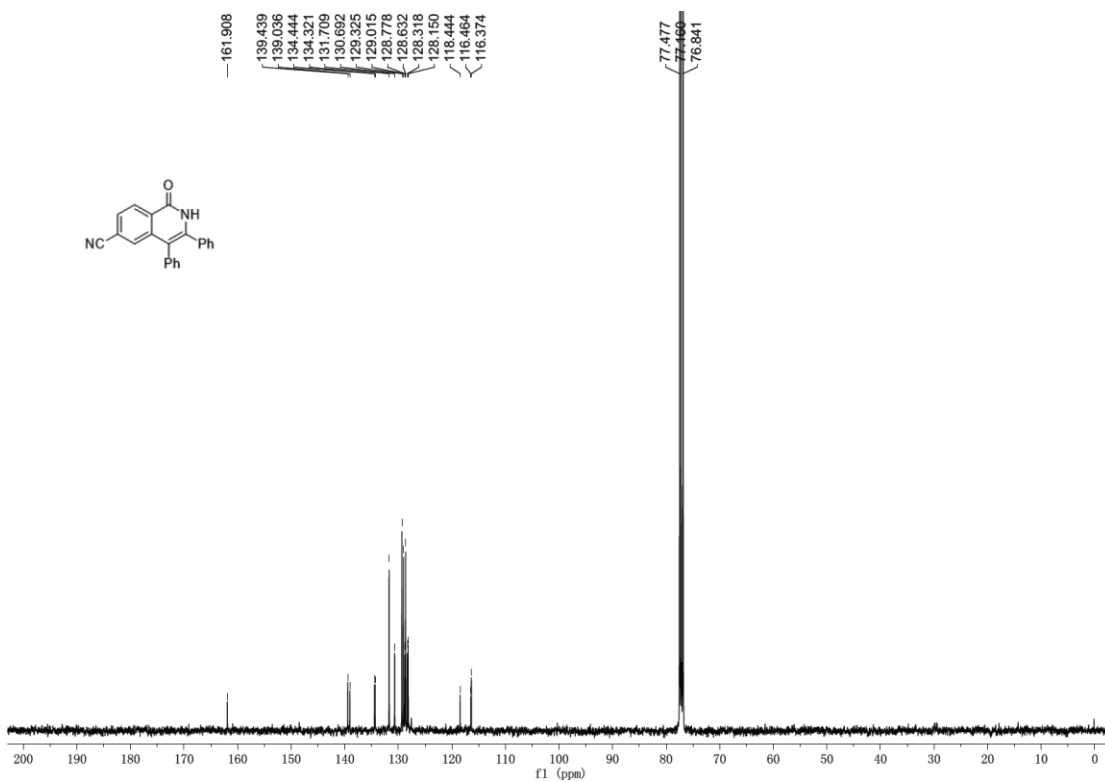
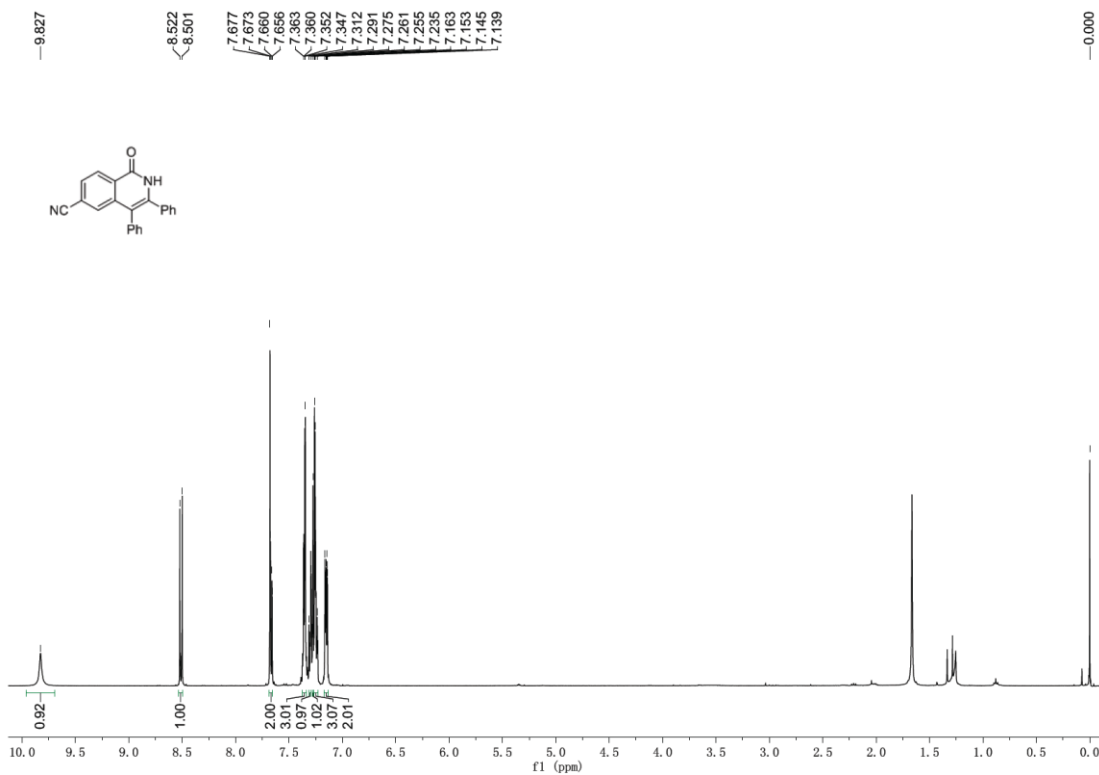
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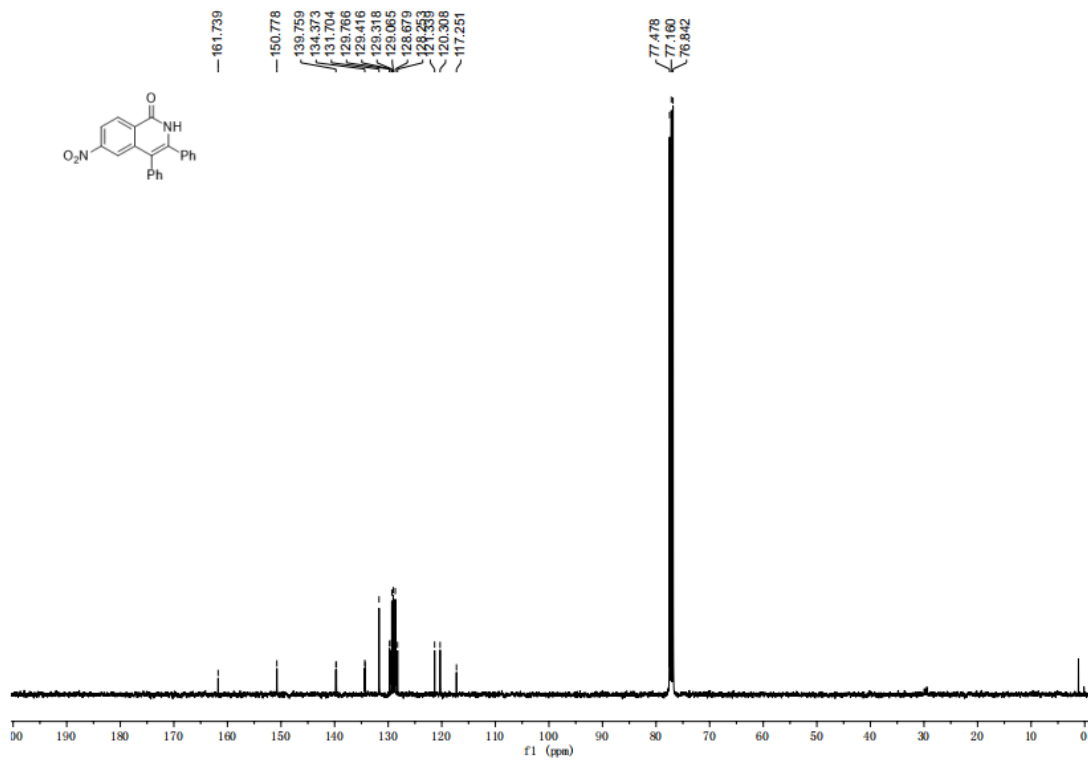
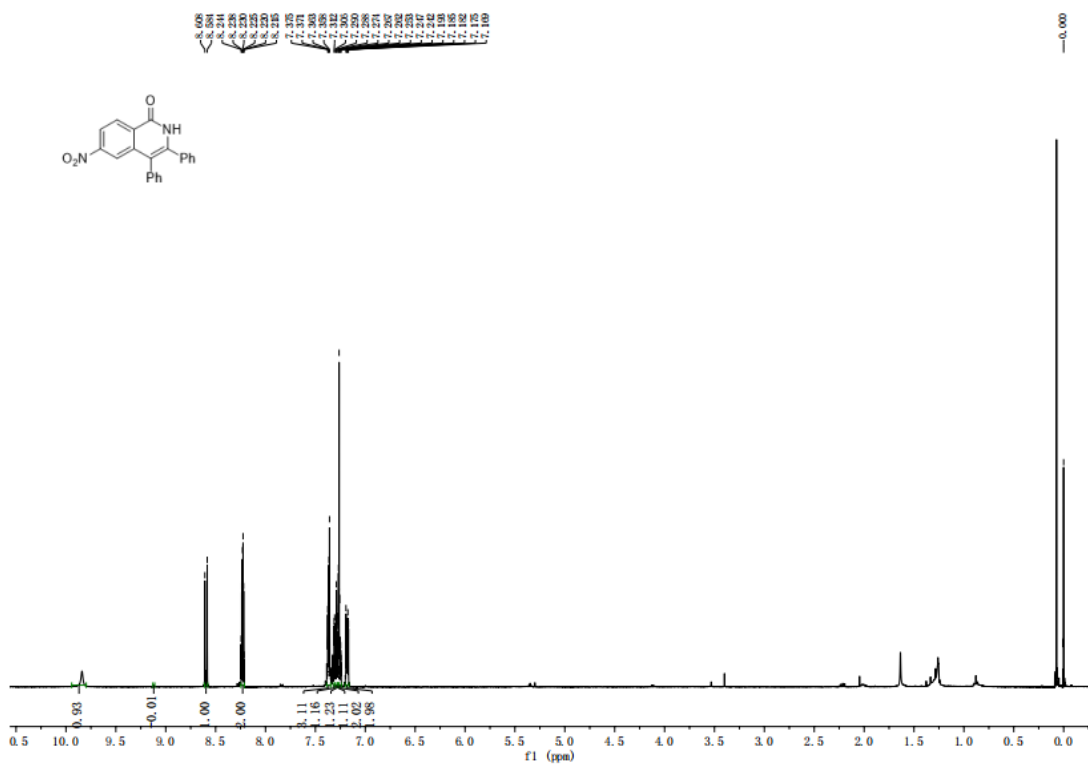
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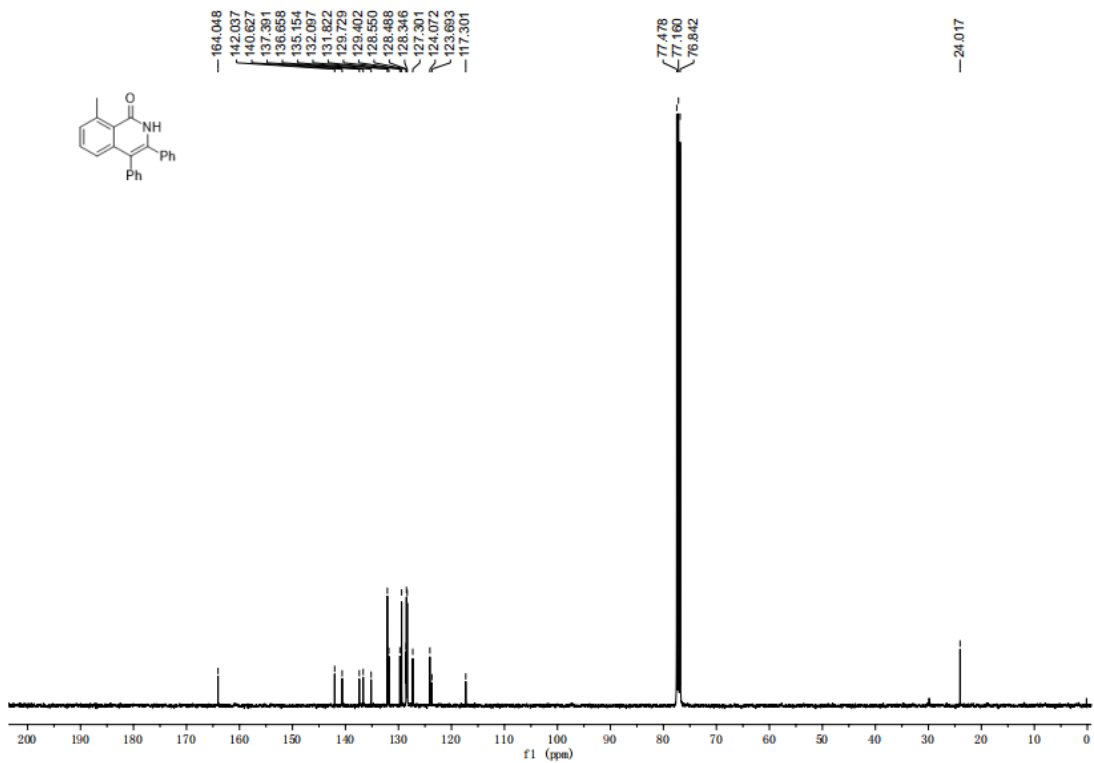
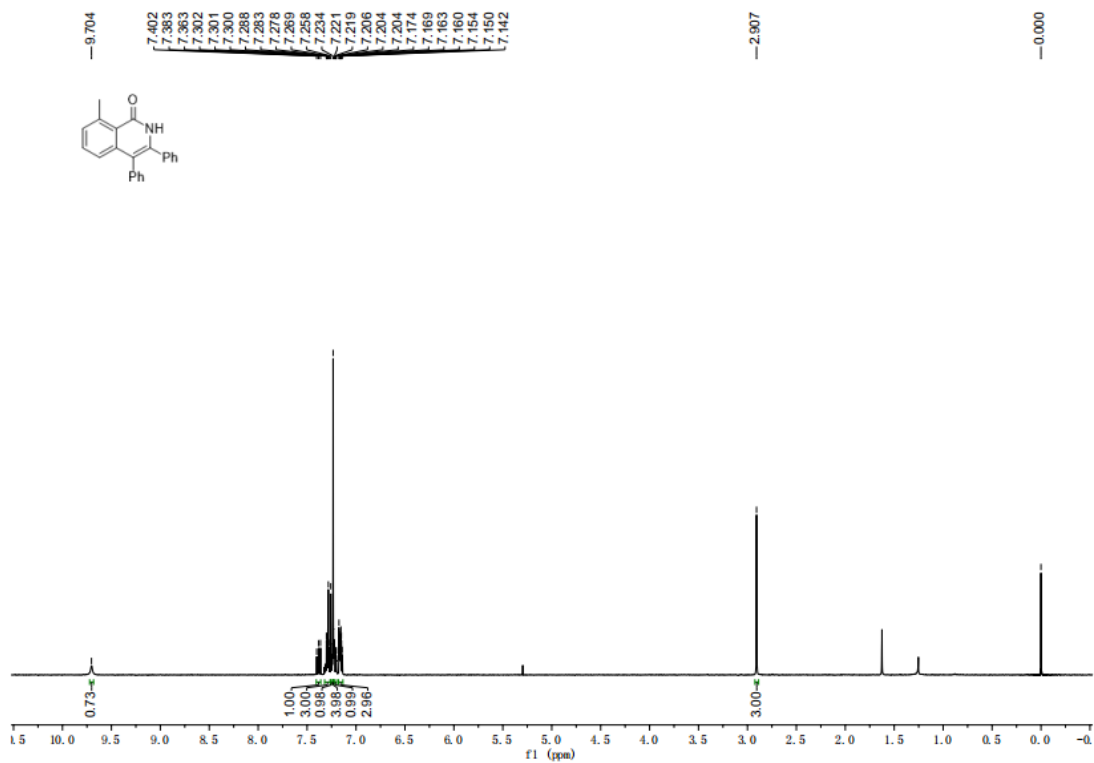
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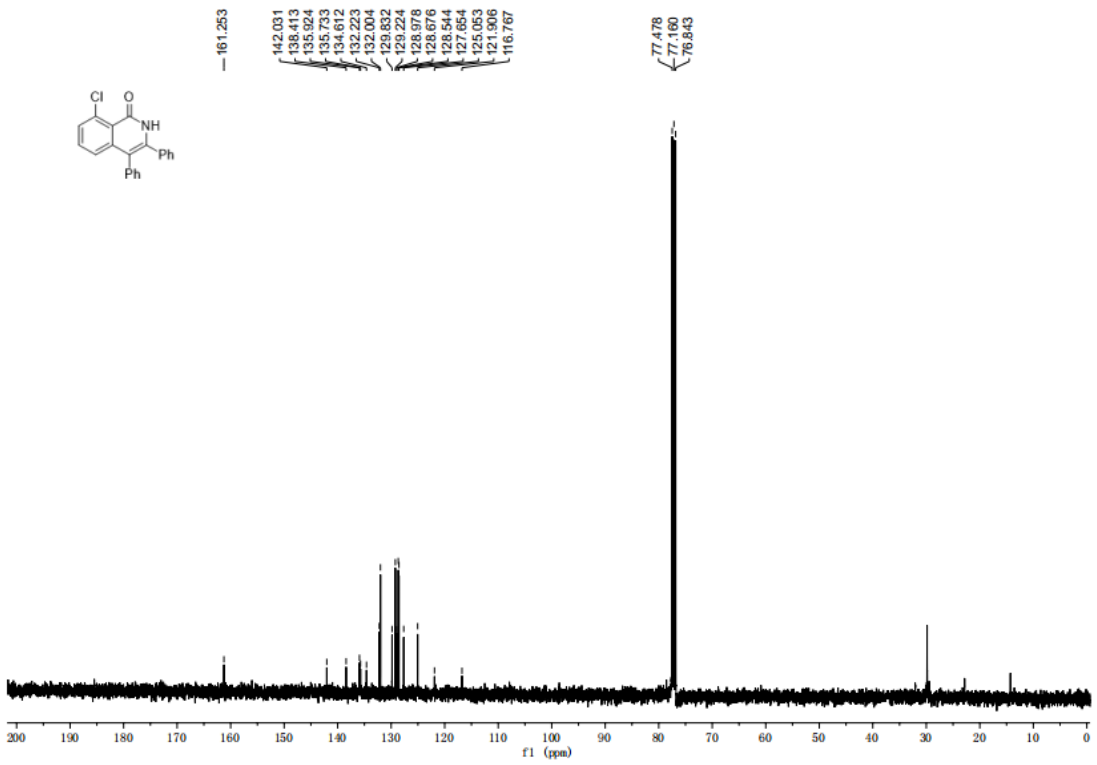
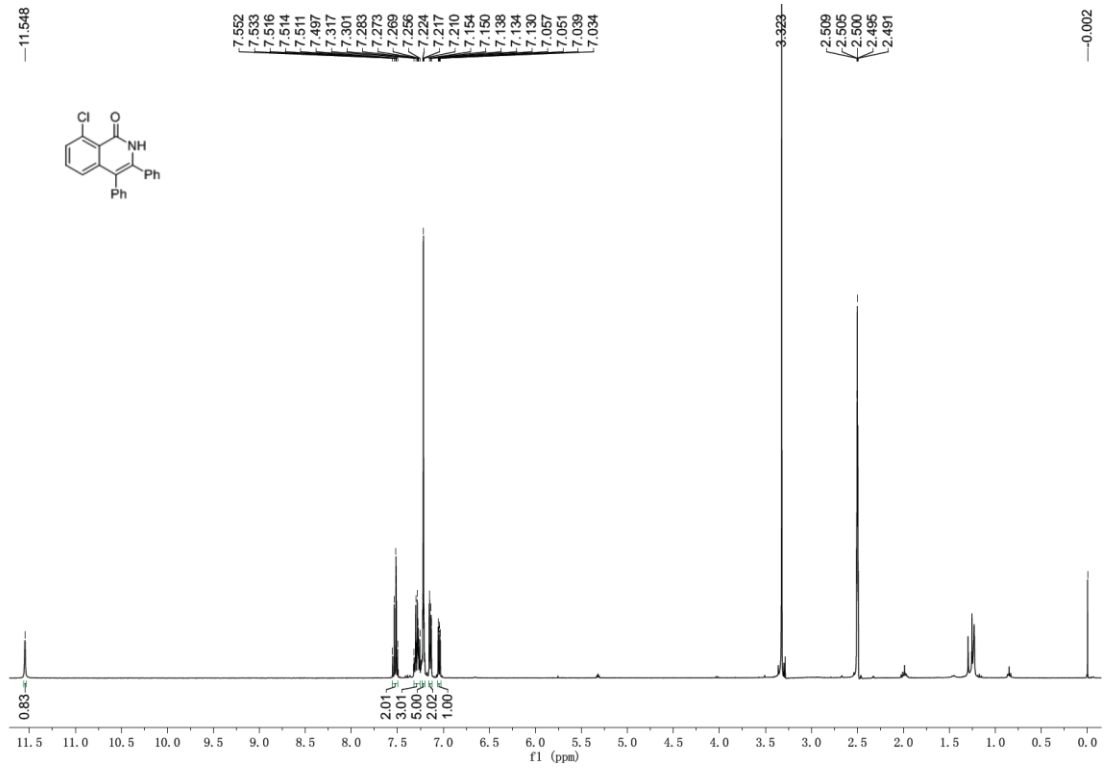
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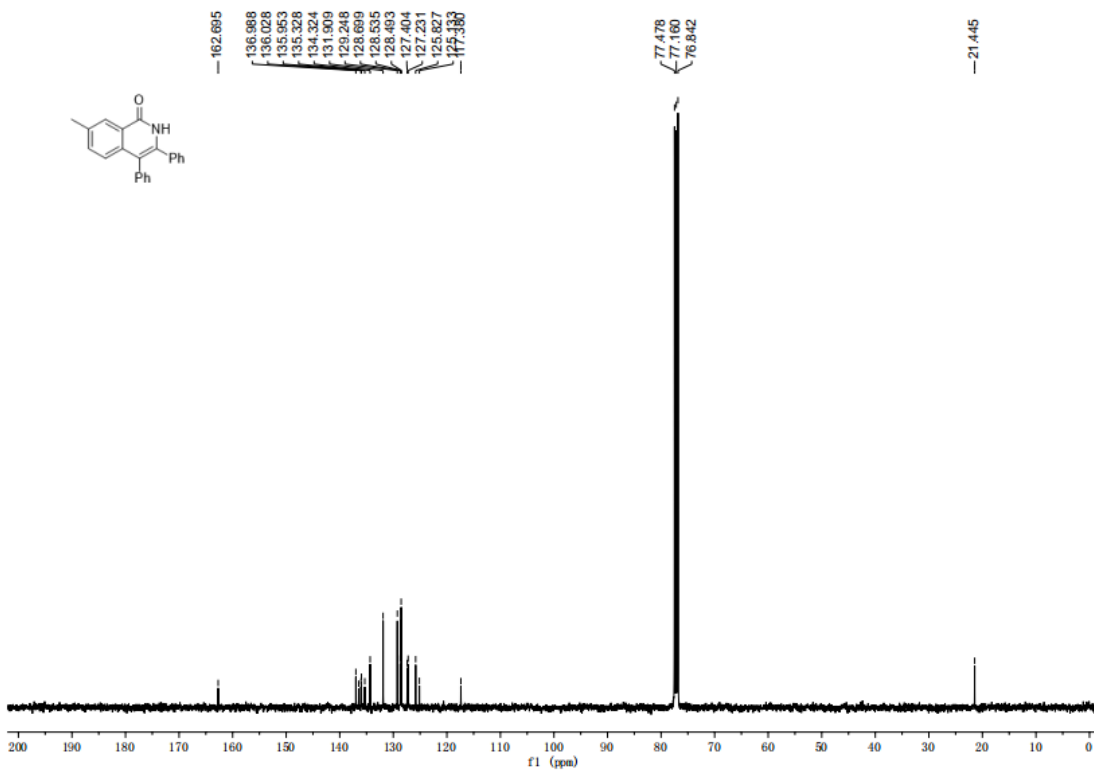
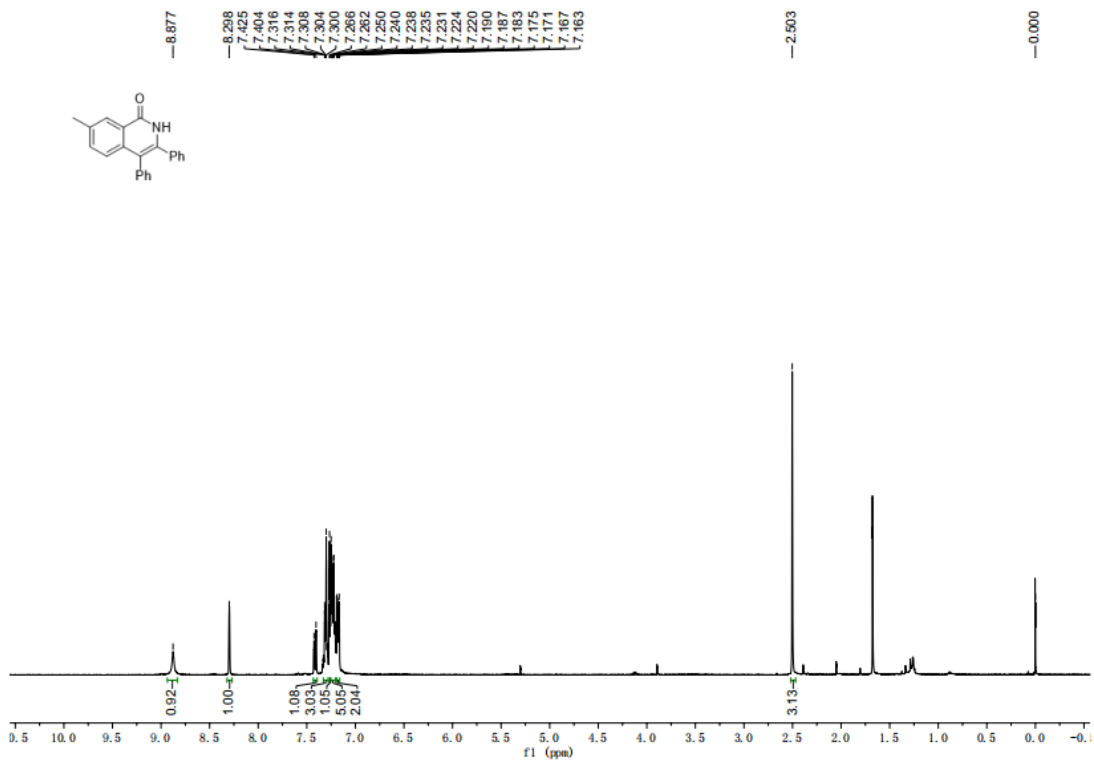
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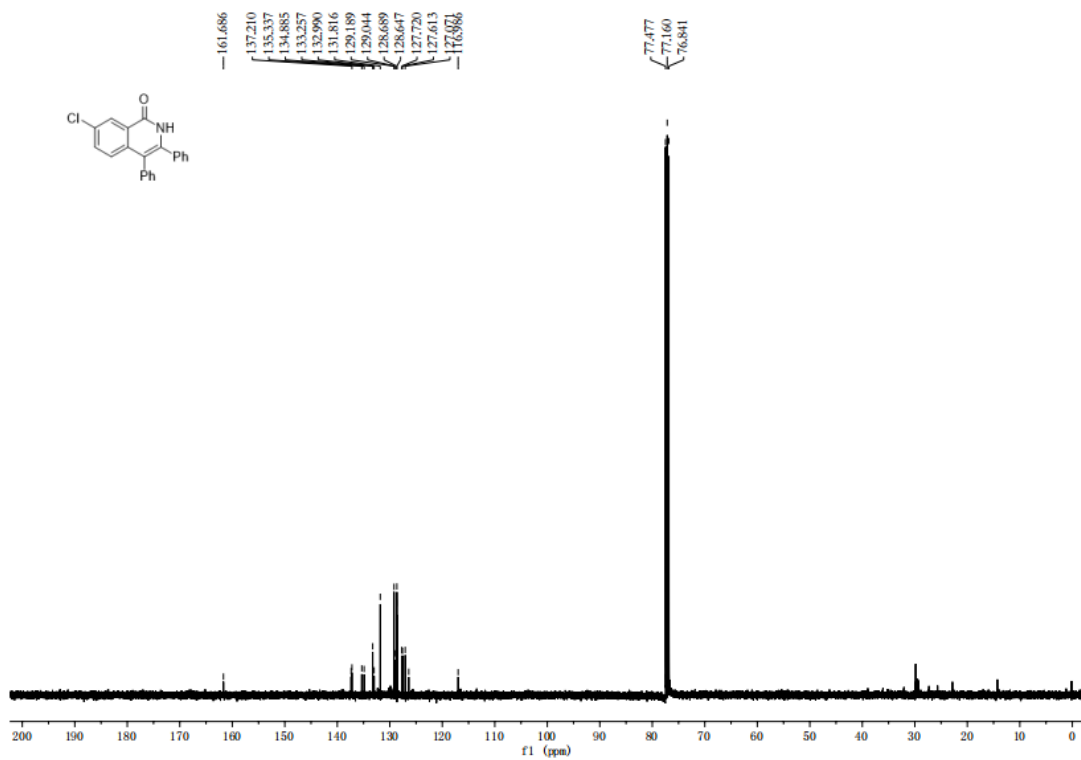
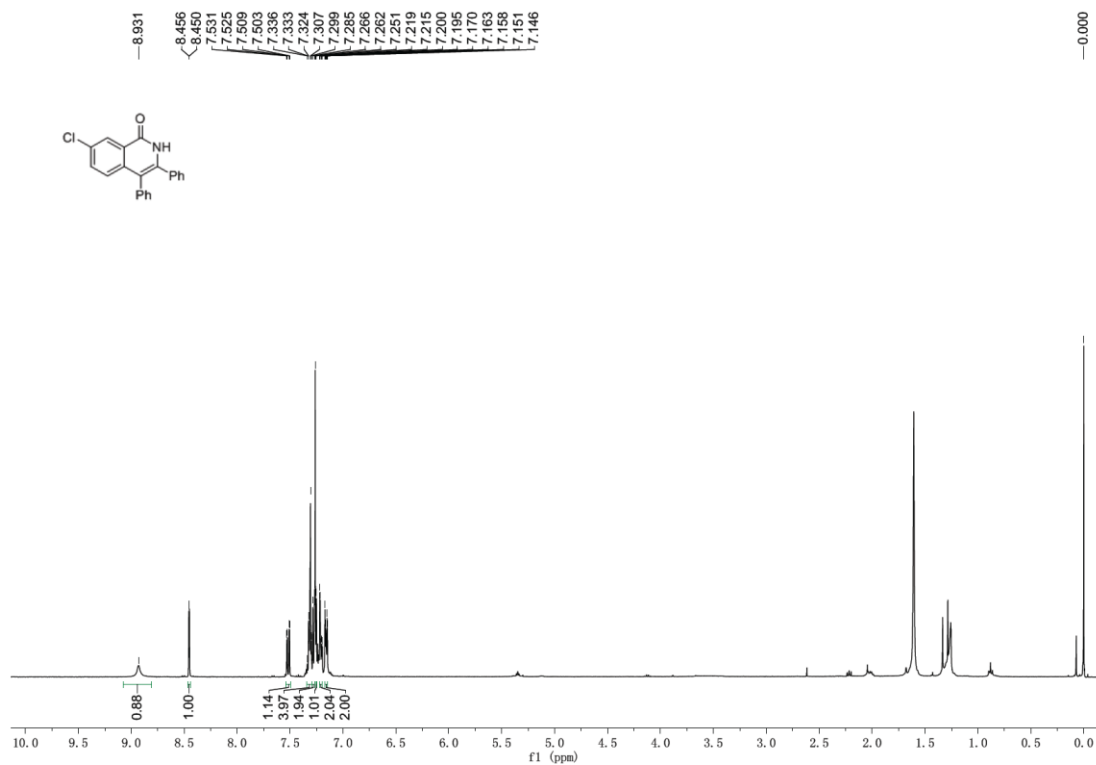
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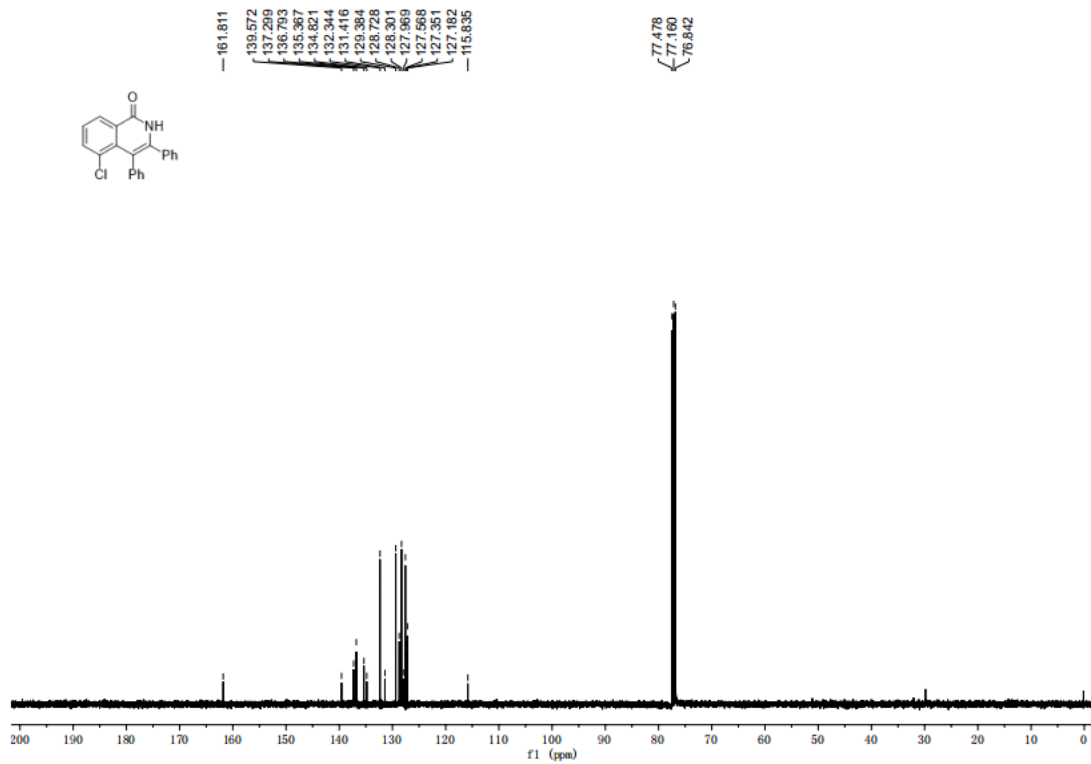
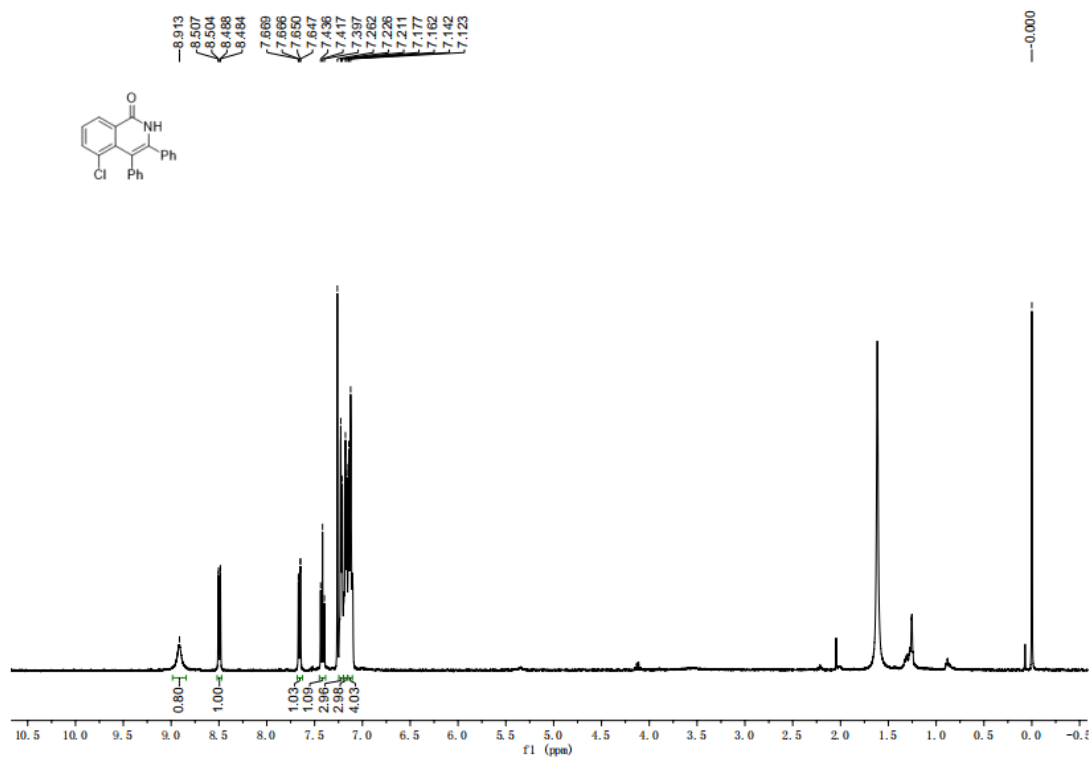
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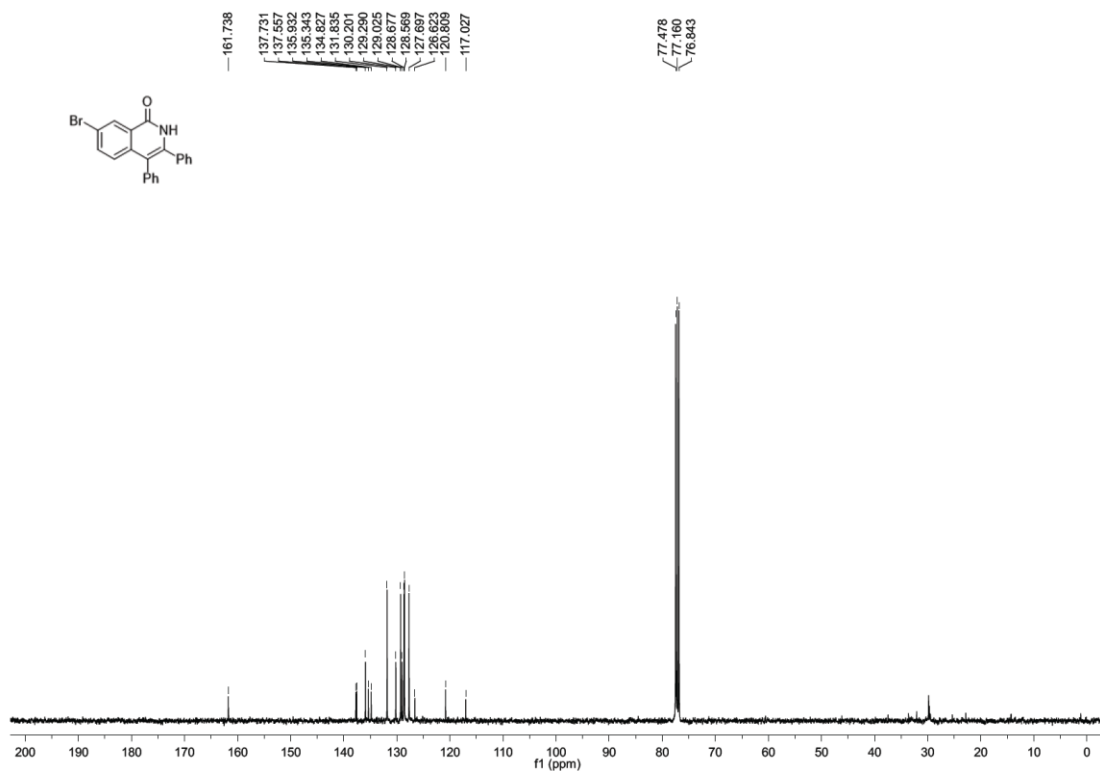
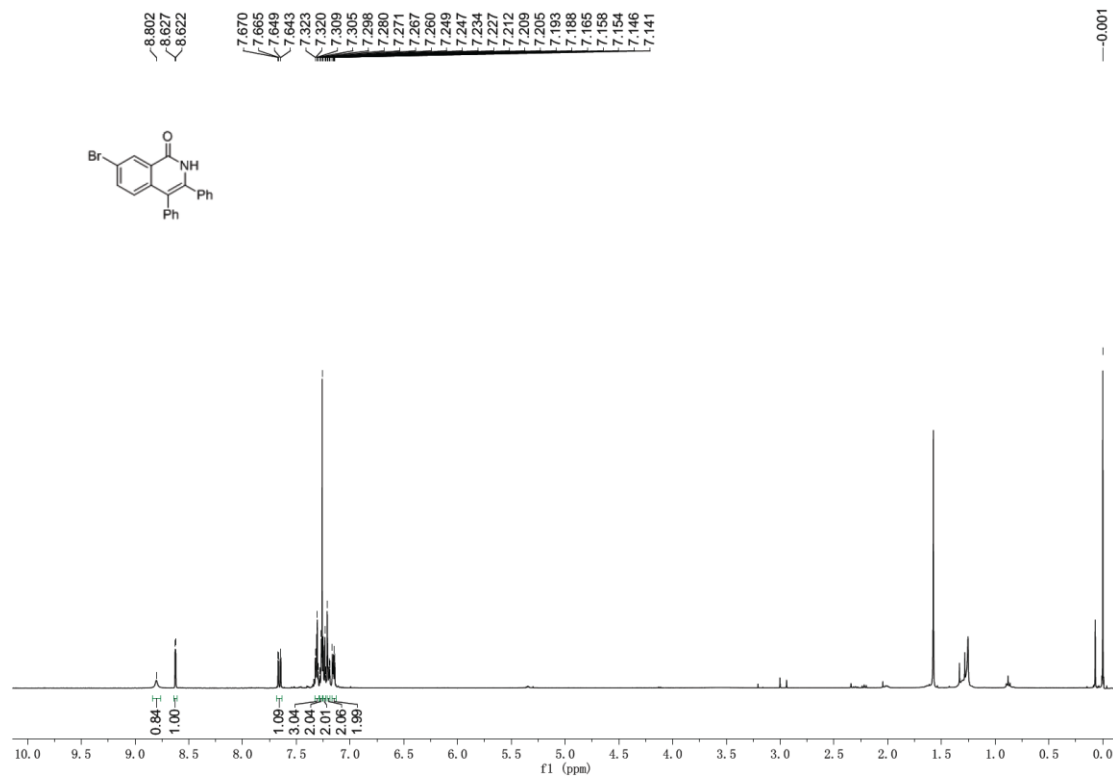
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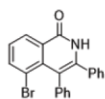
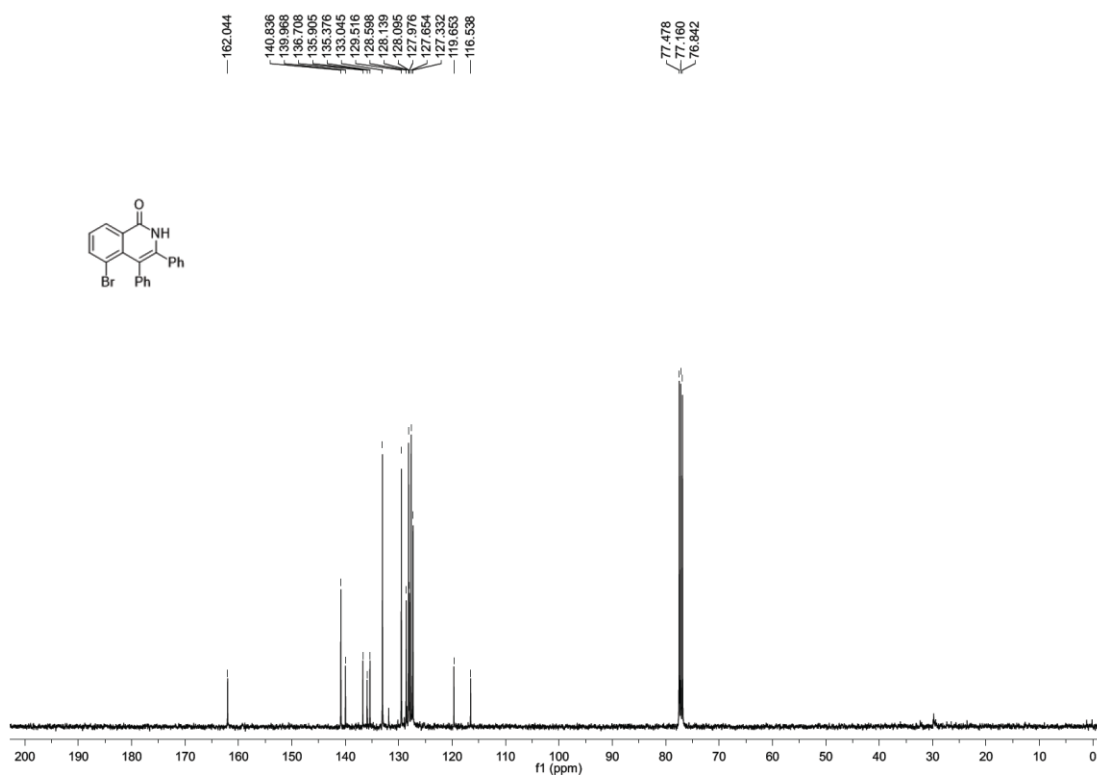
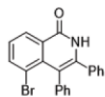
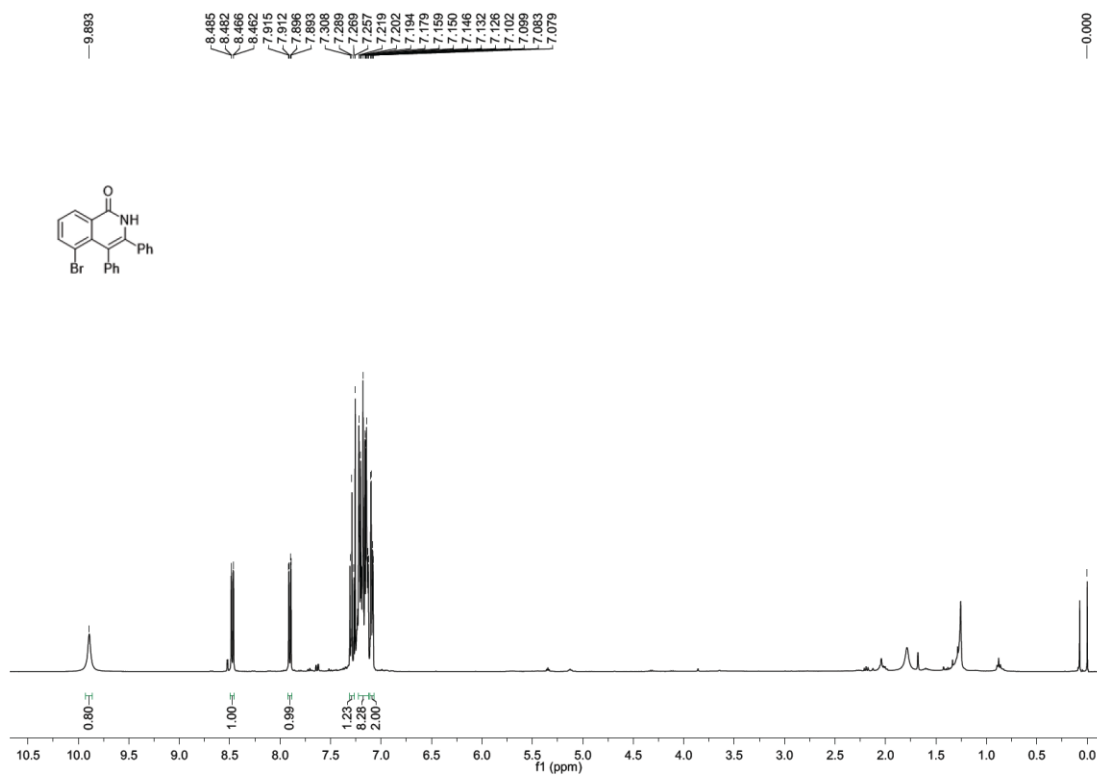
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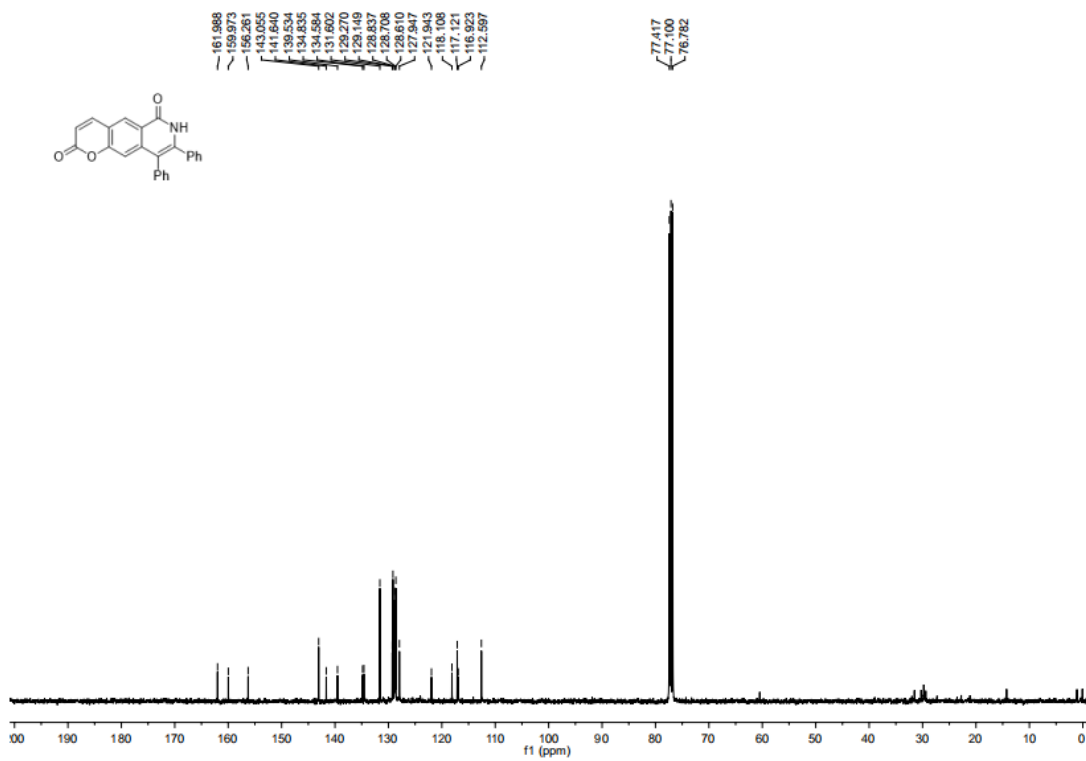
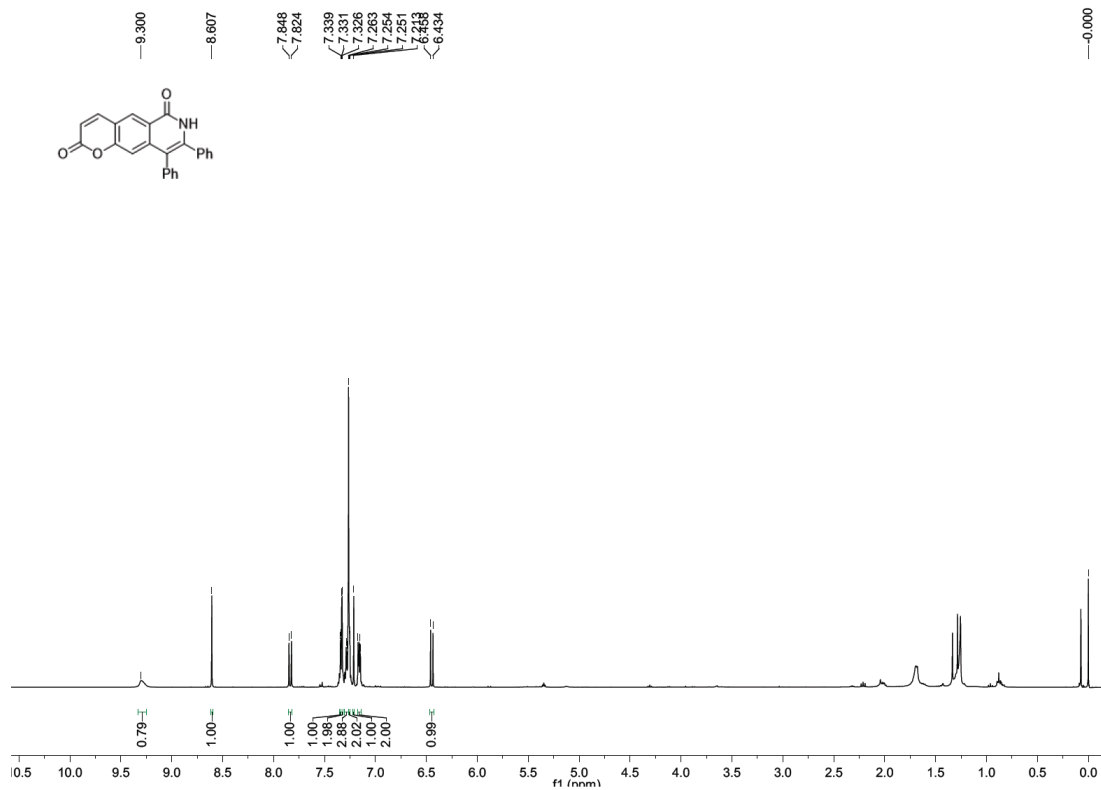
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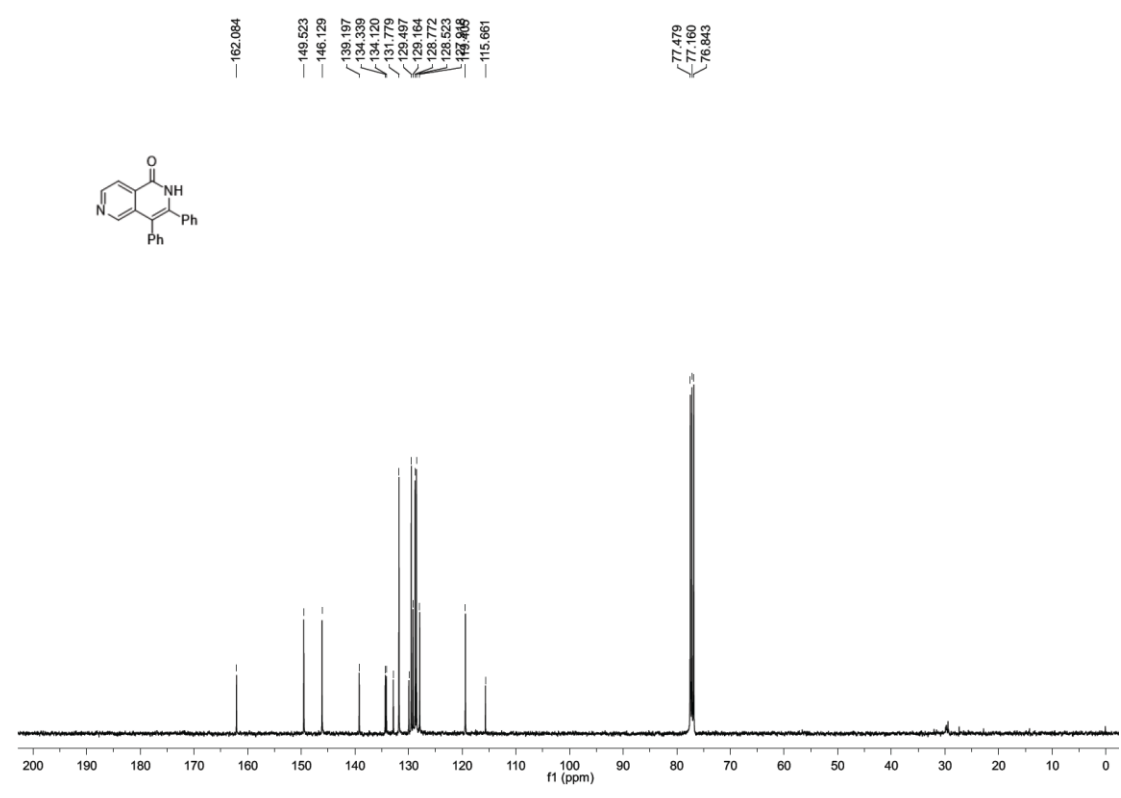
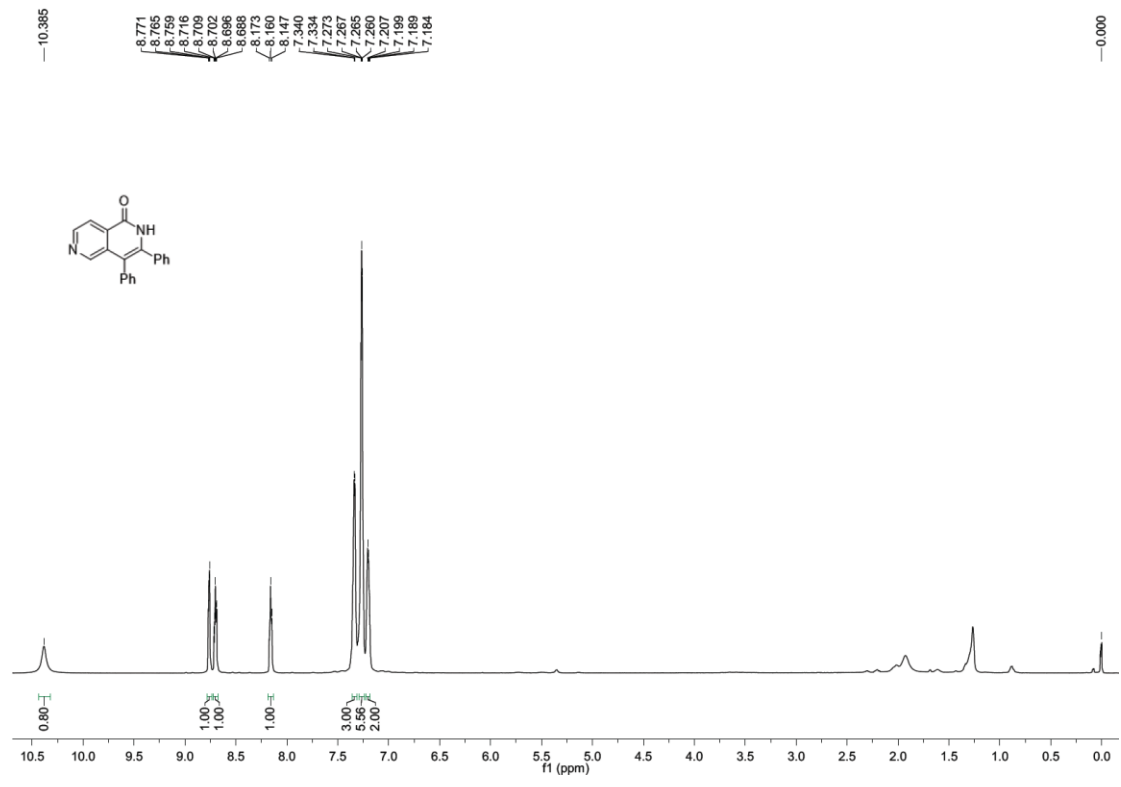
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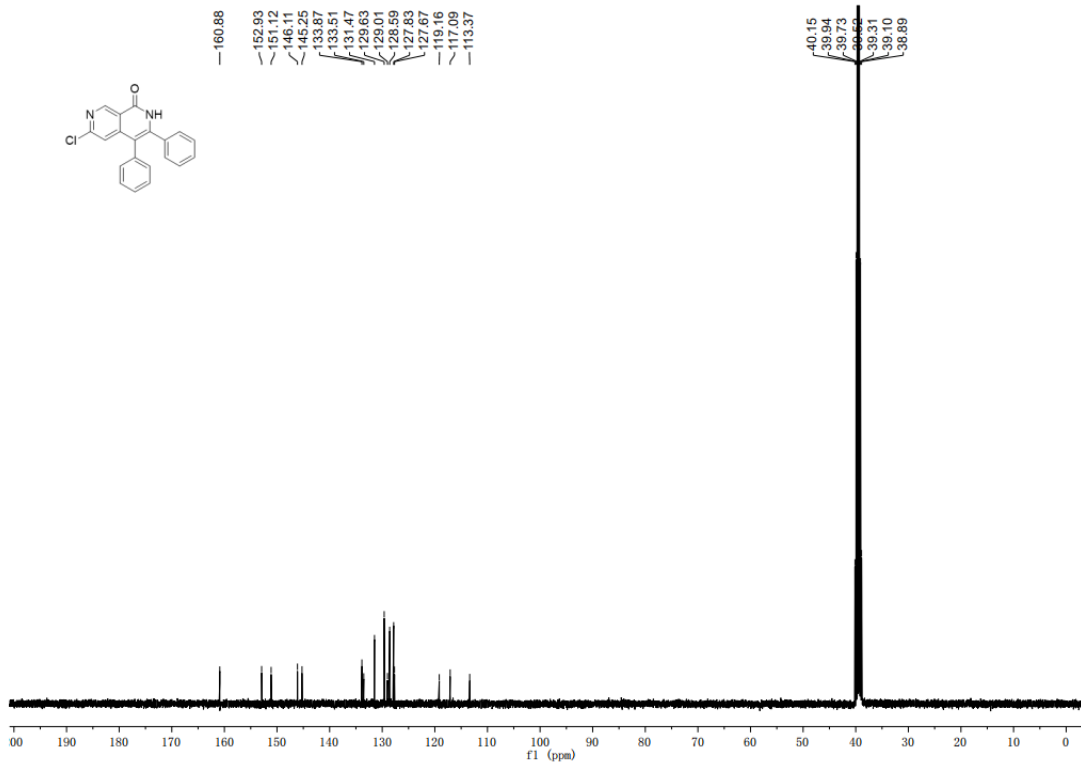
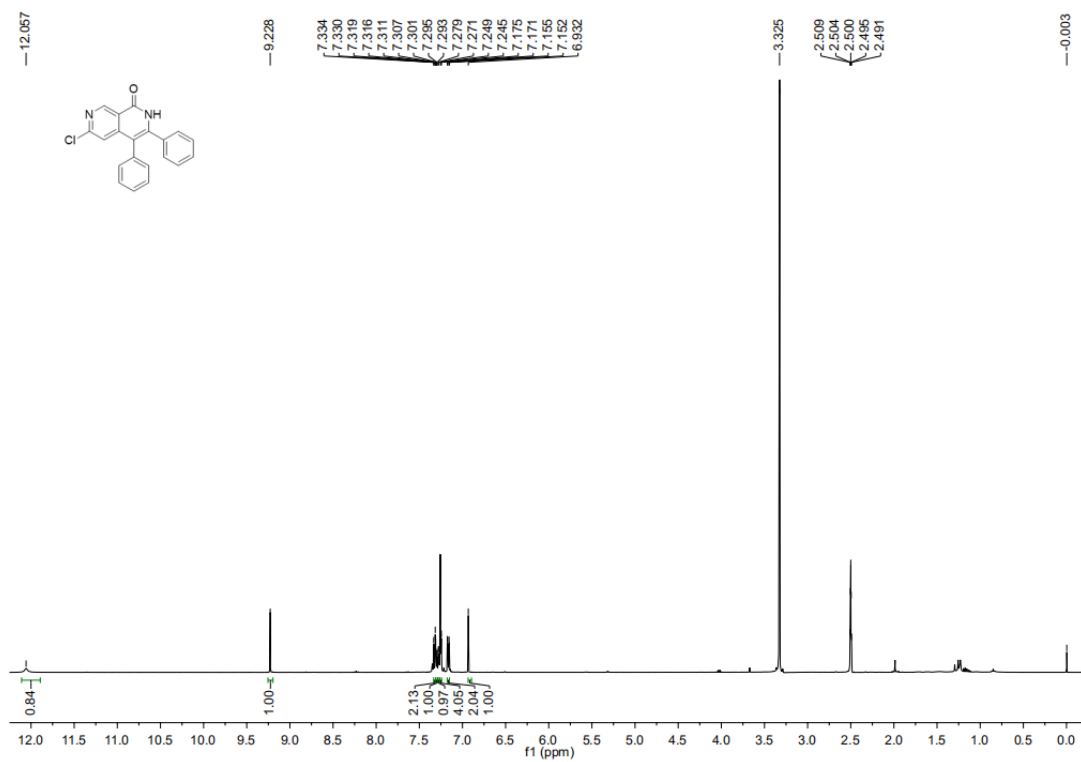
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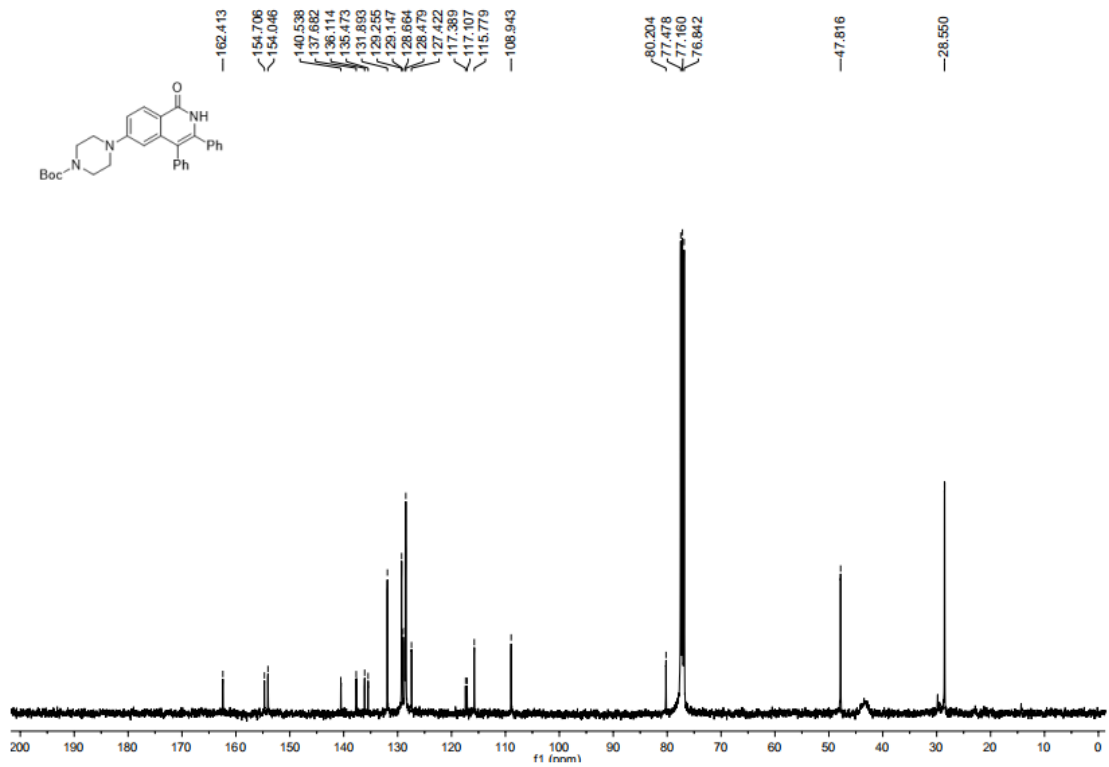
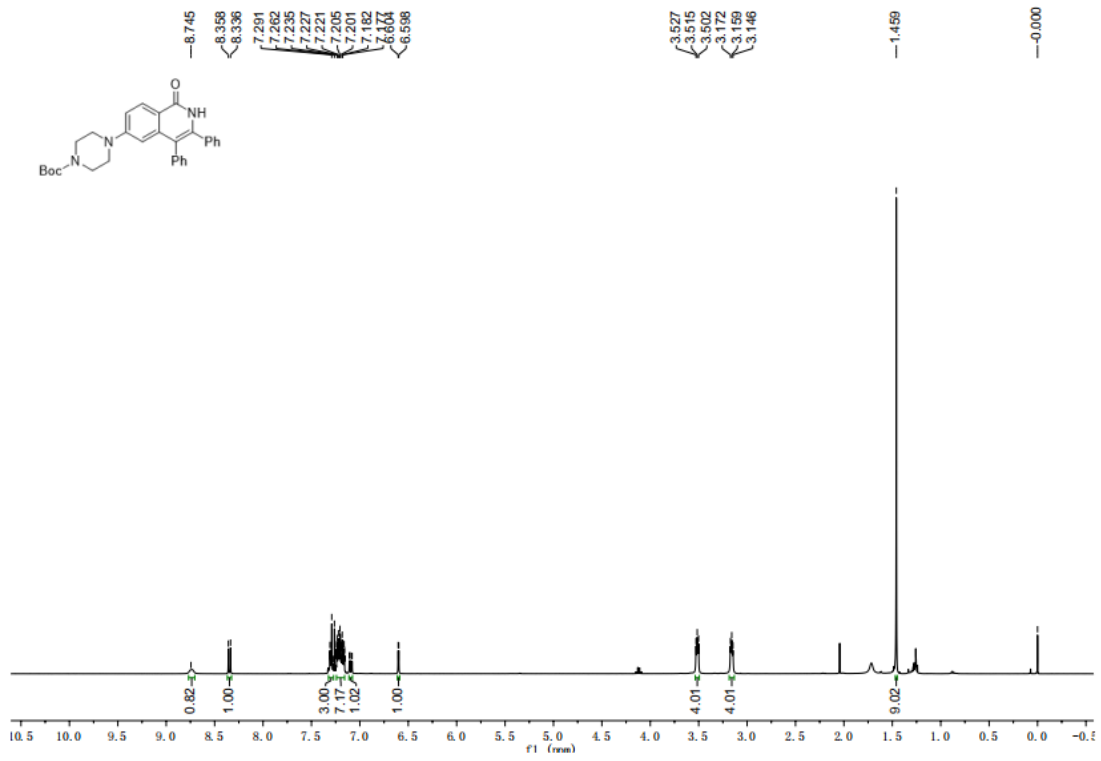
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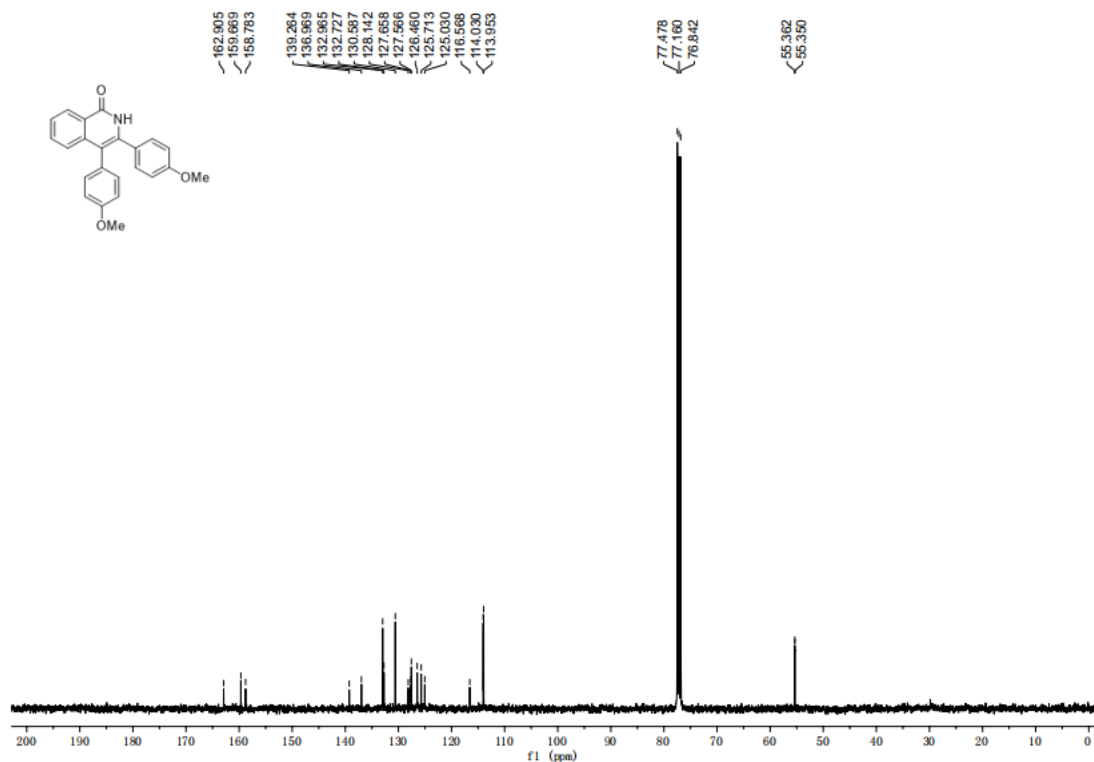
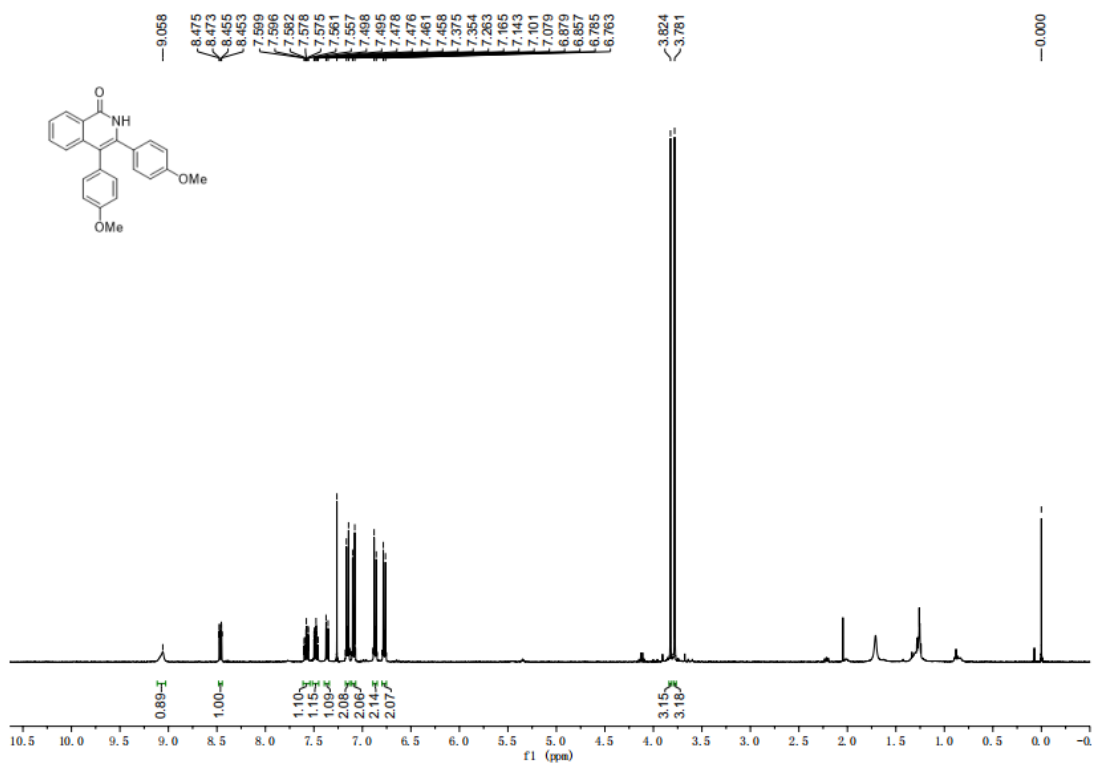
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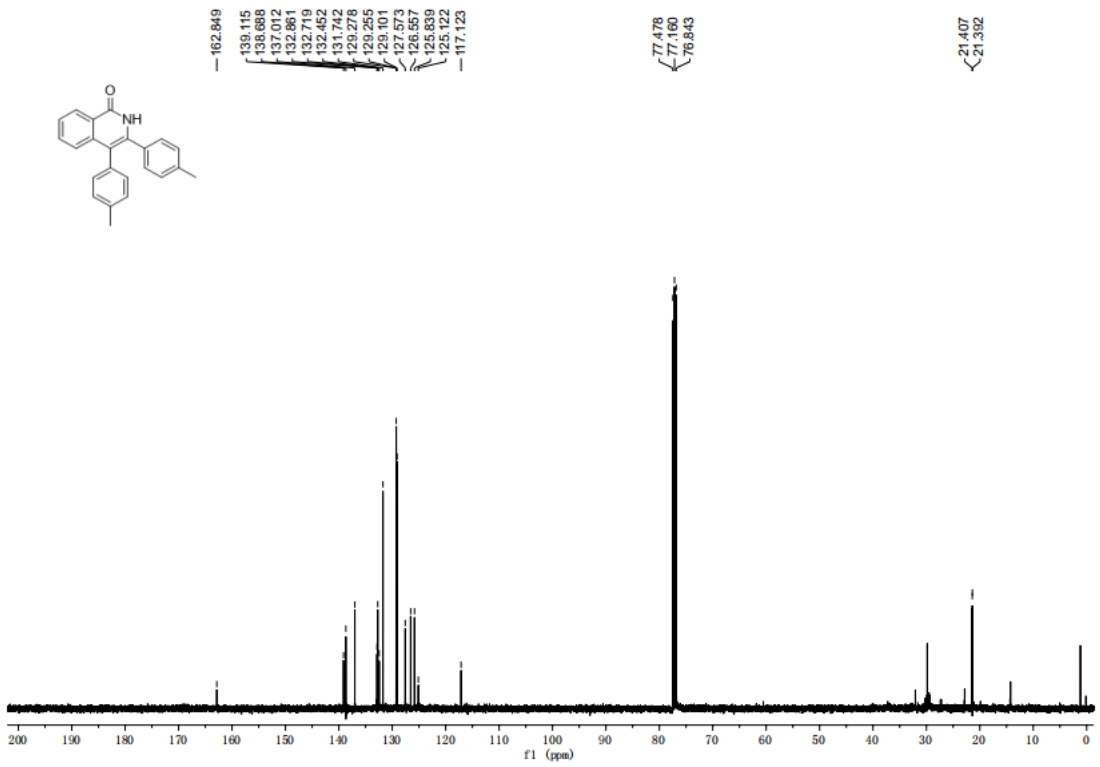
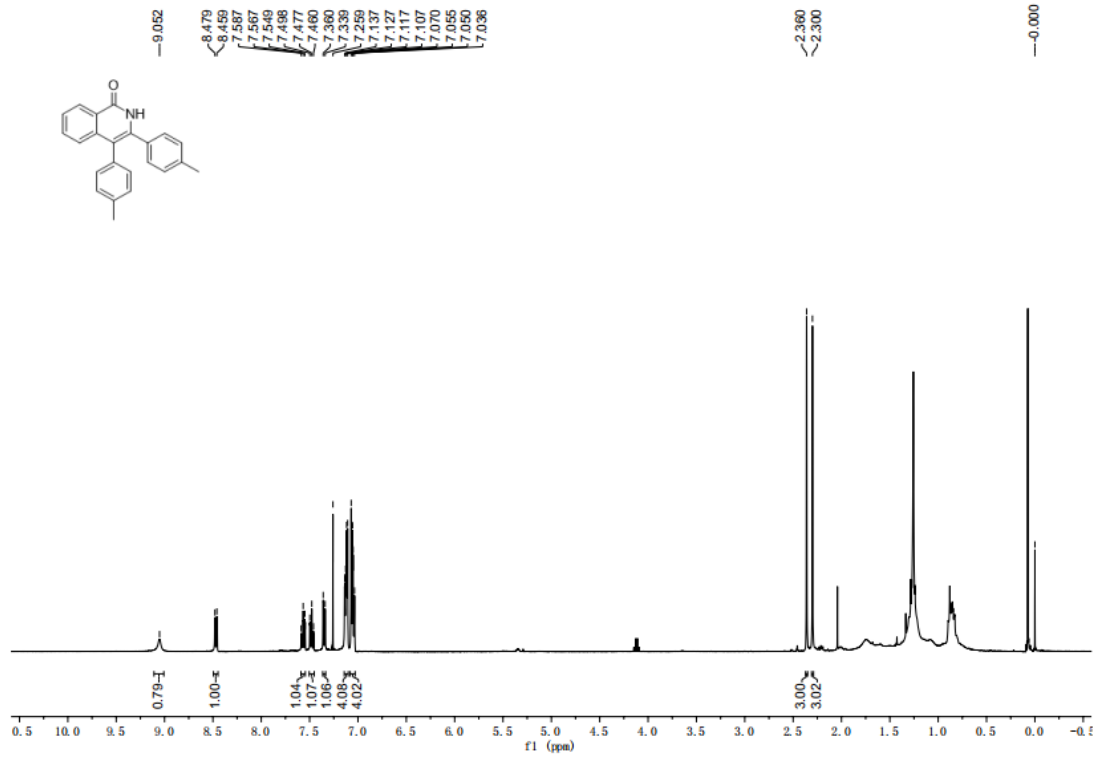
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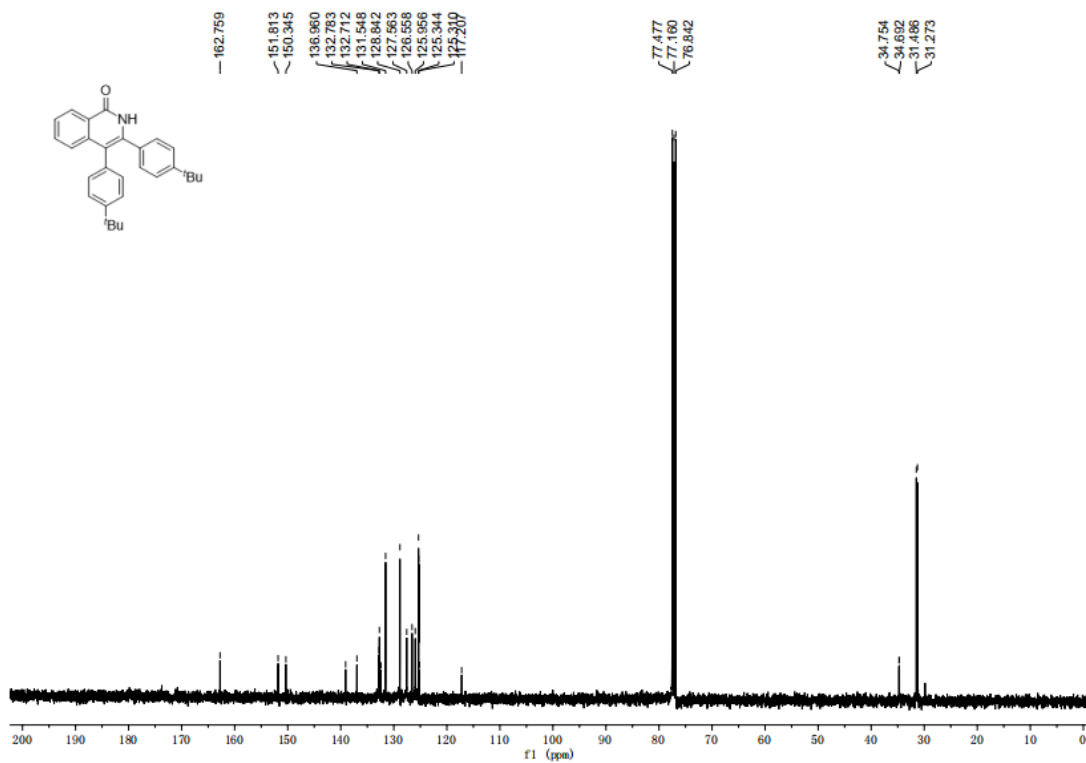
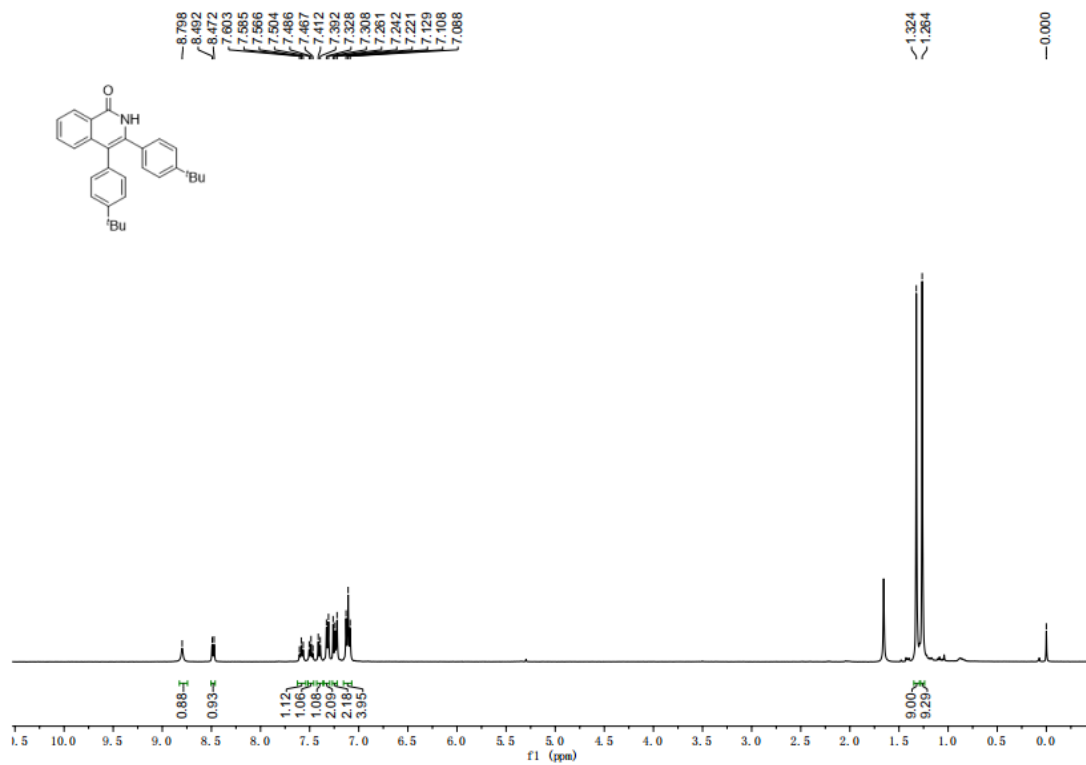
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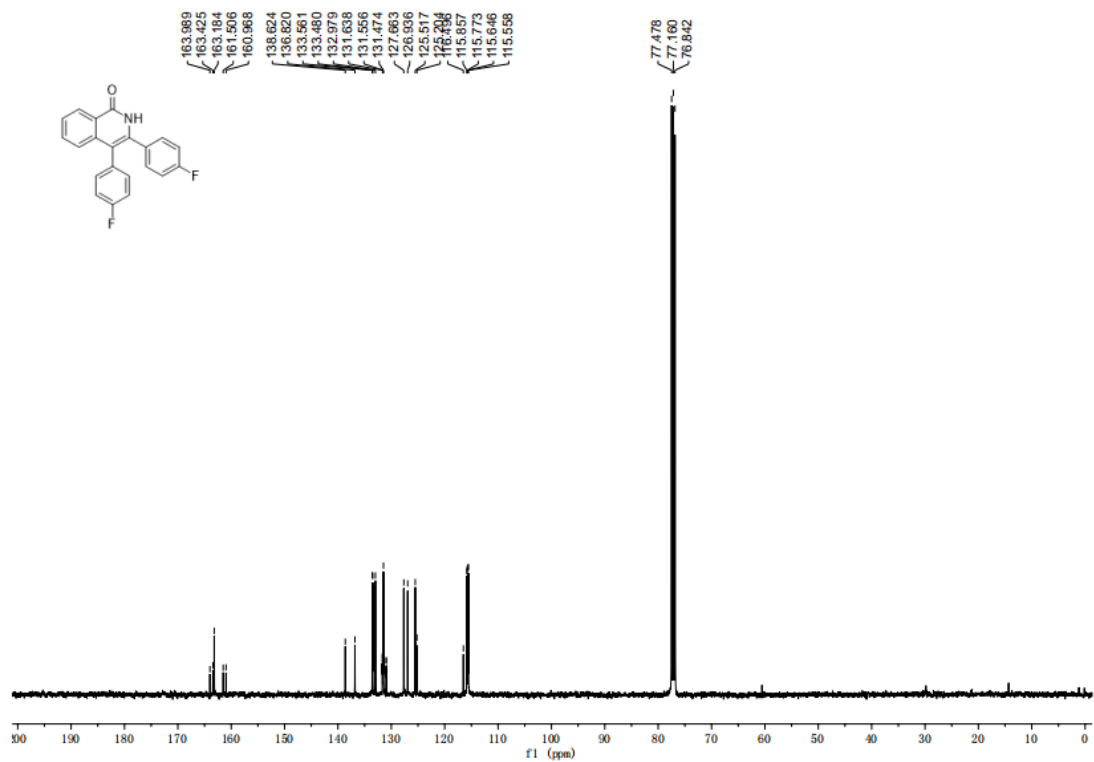
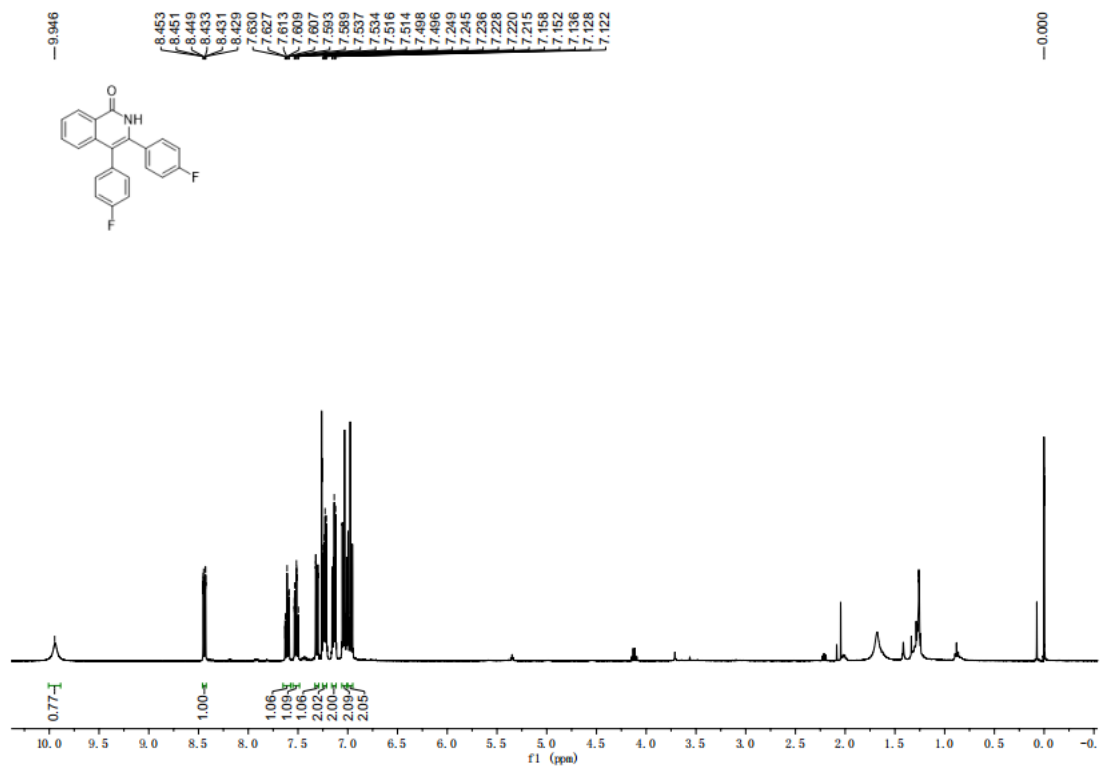
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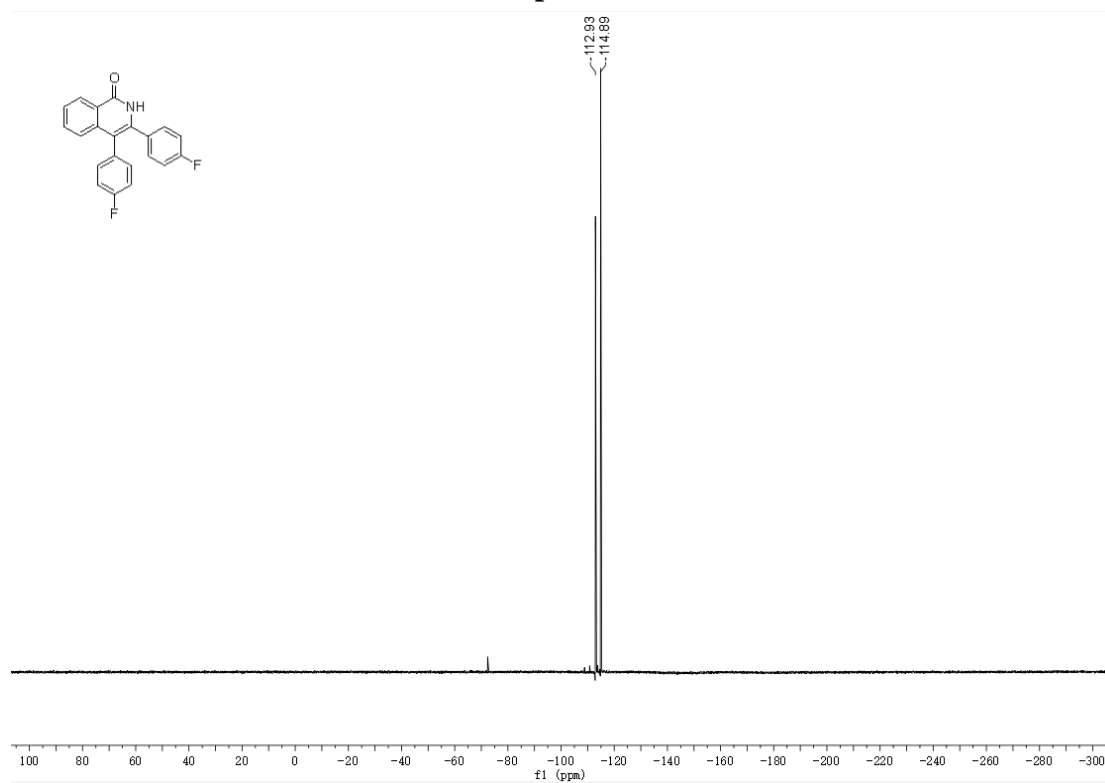
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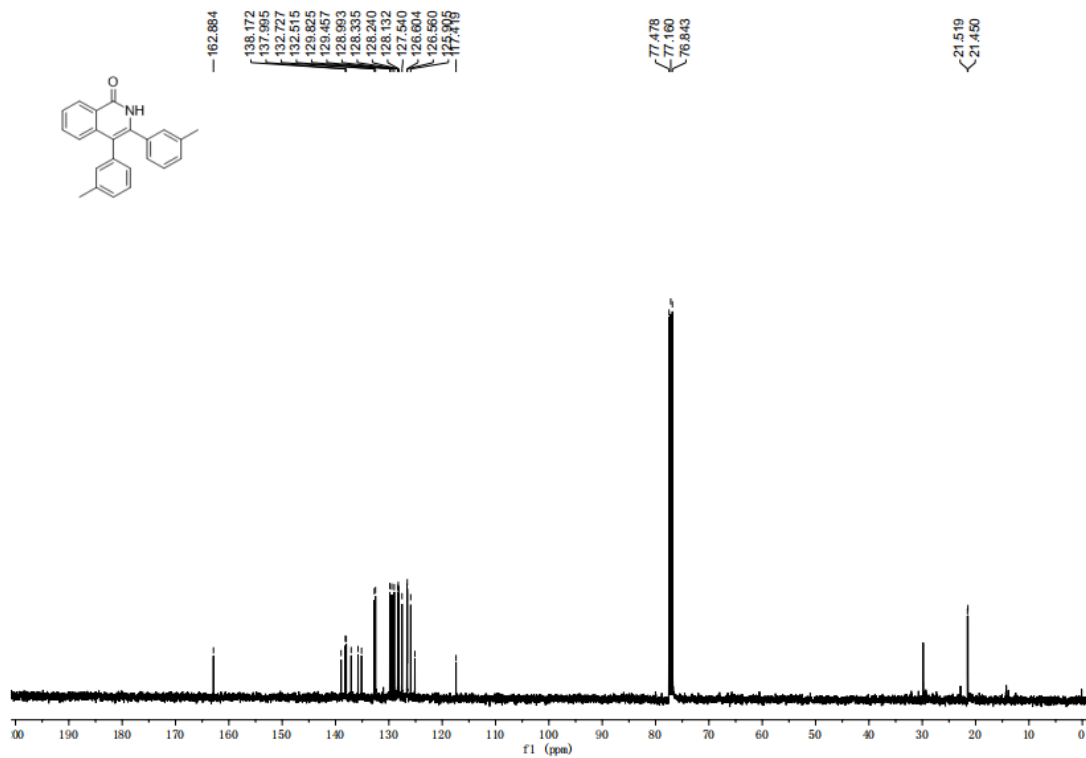
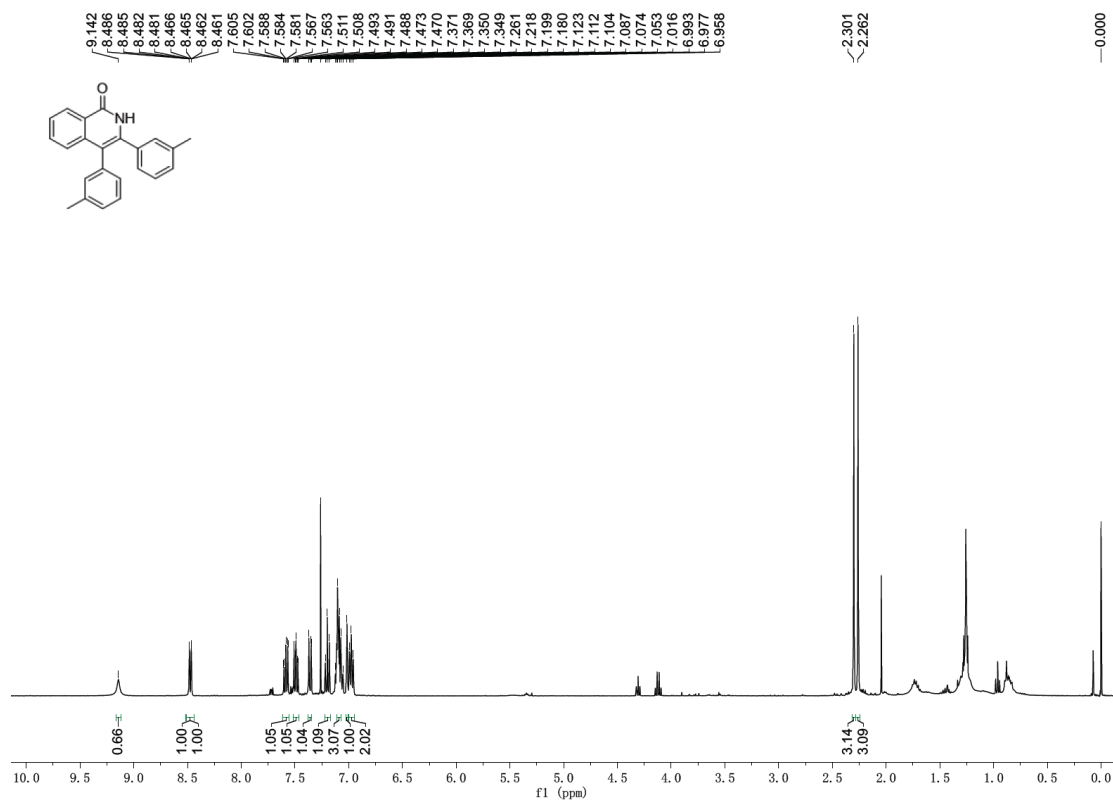
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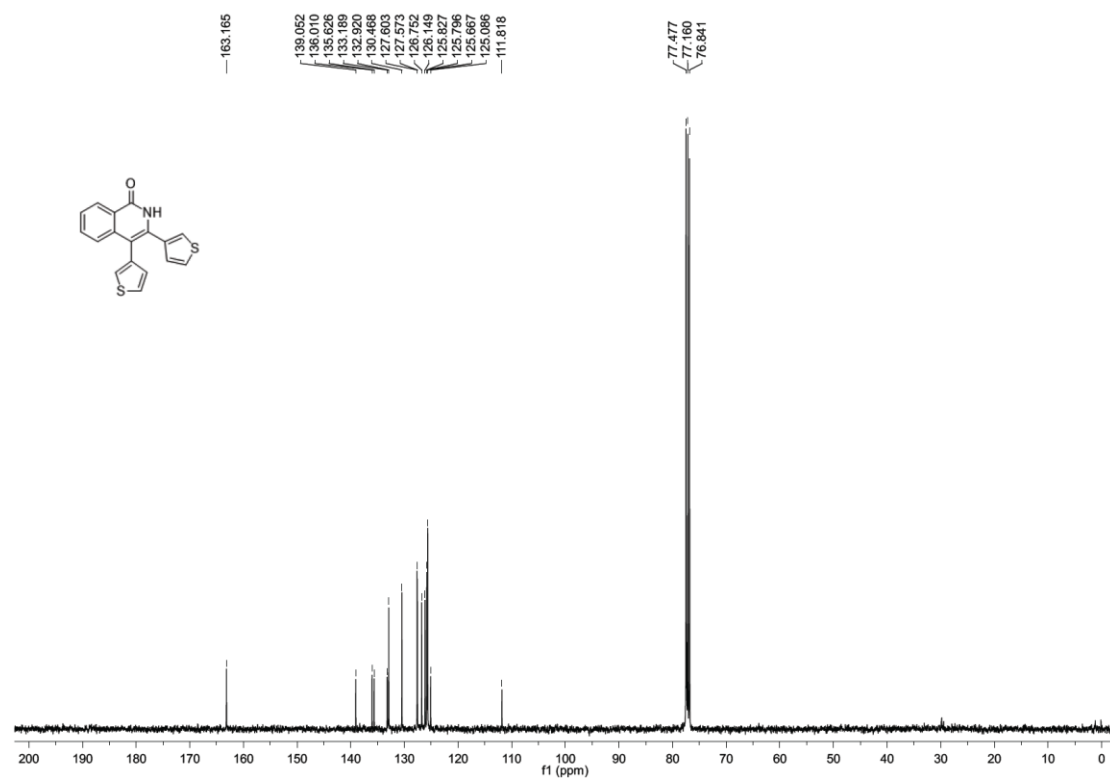
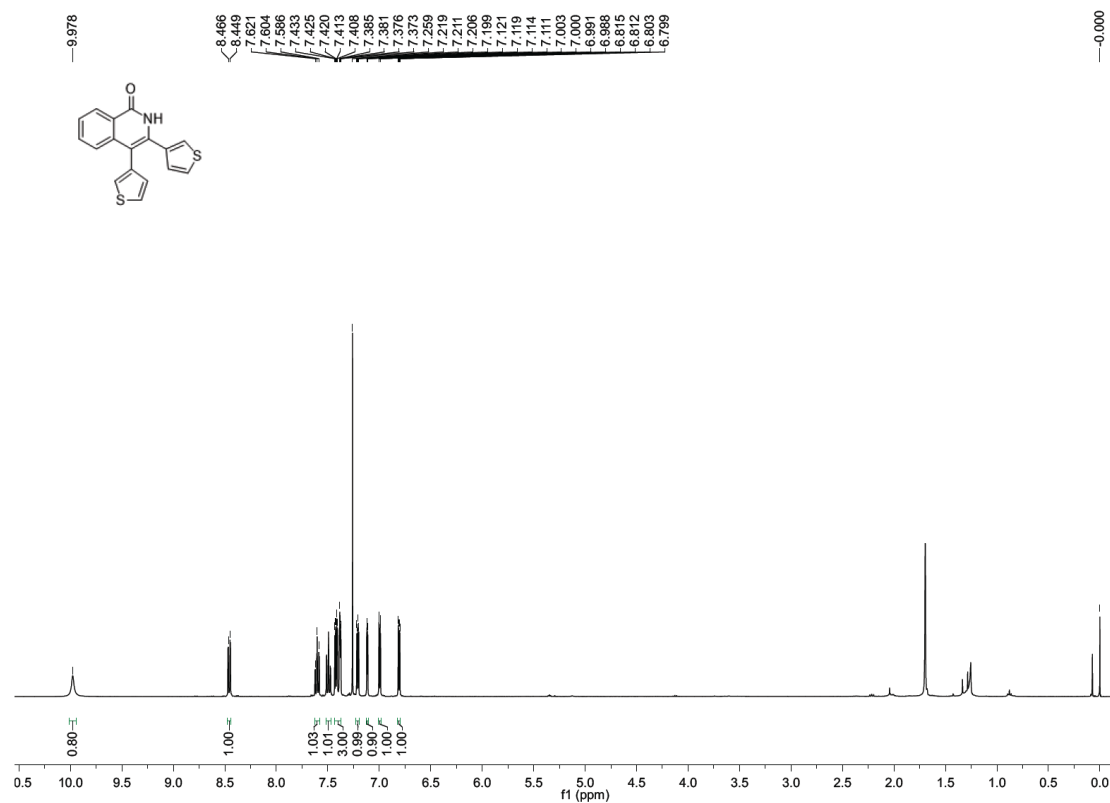
¹⁹F NMR spectrum of 5ae



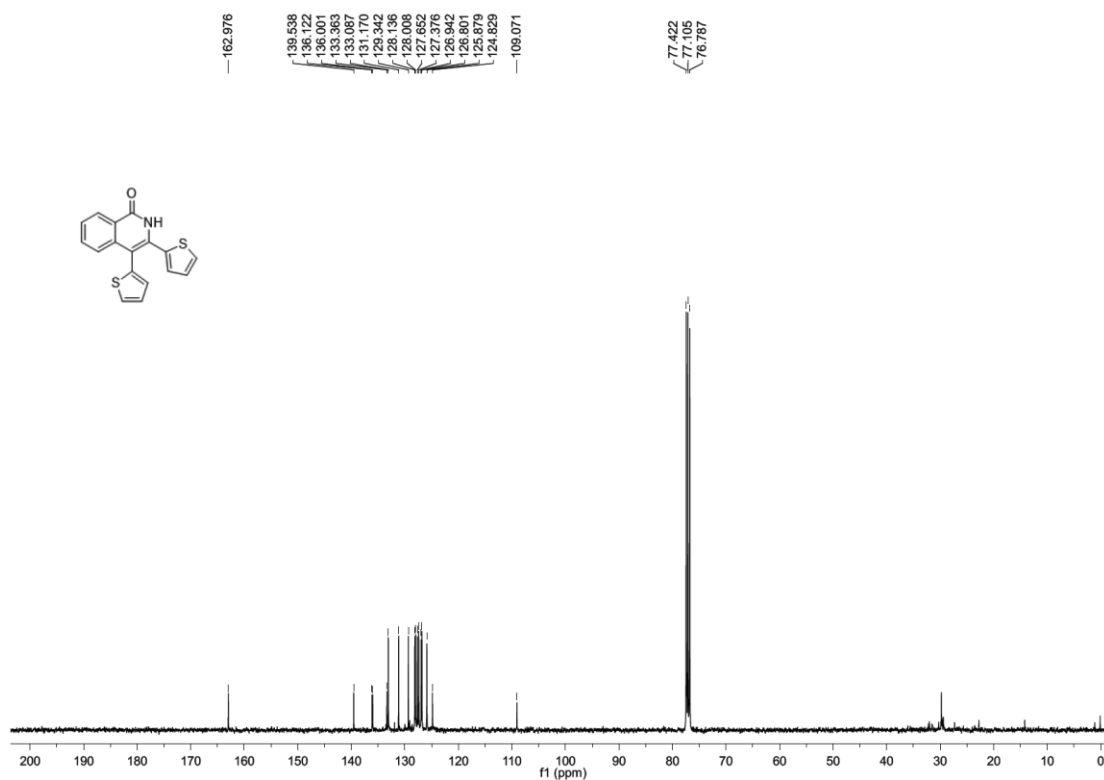
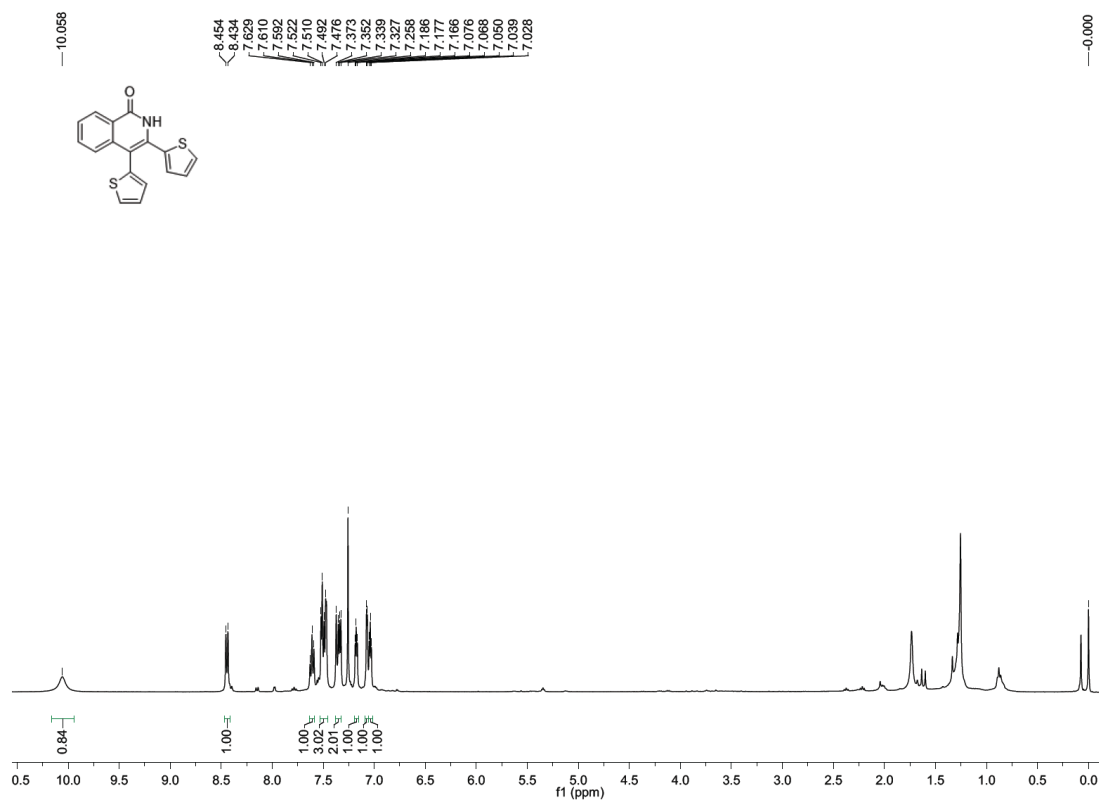
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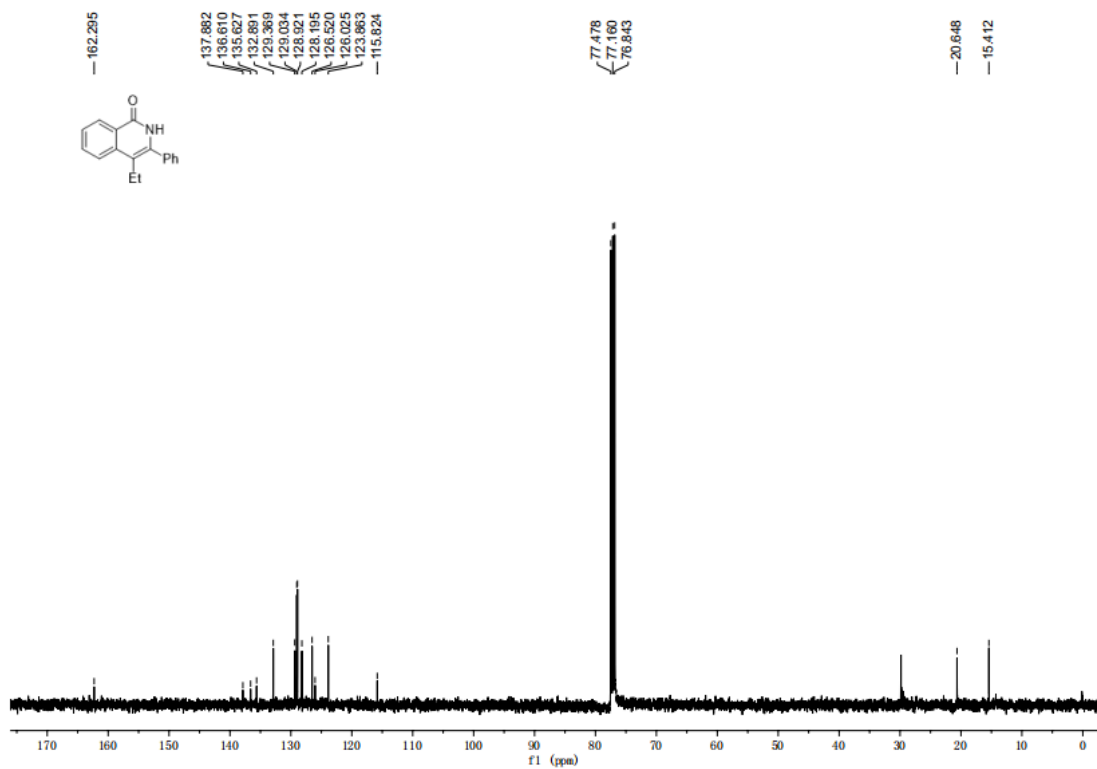
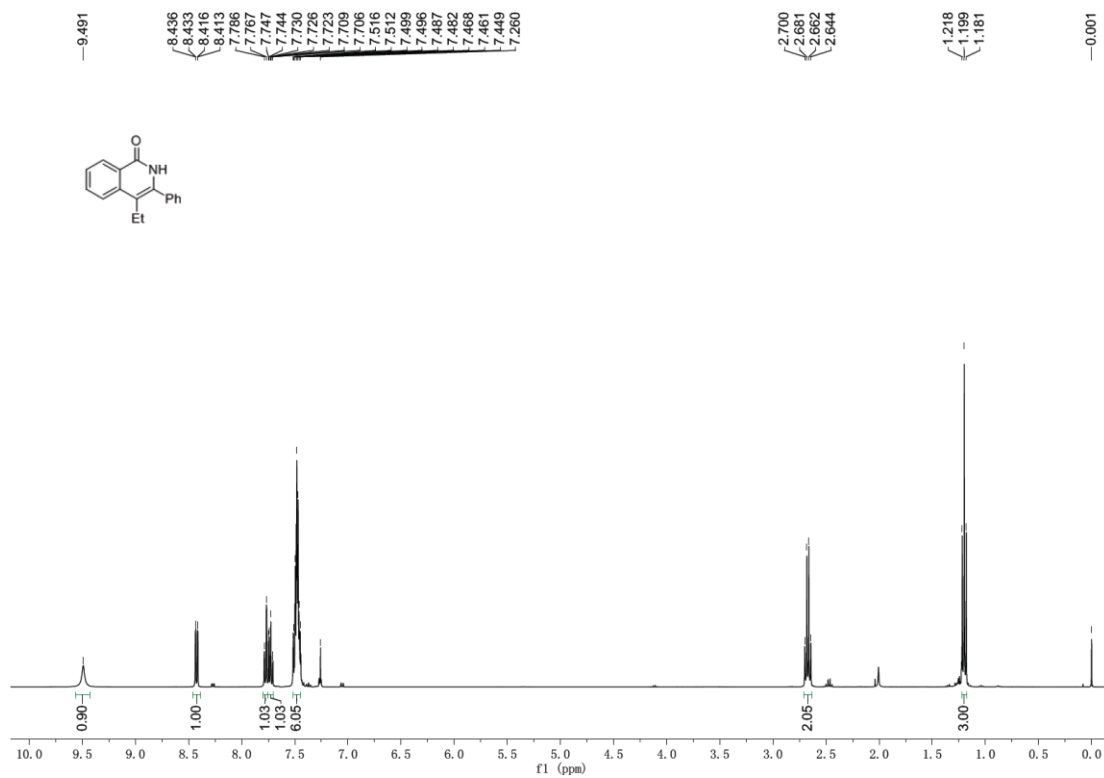
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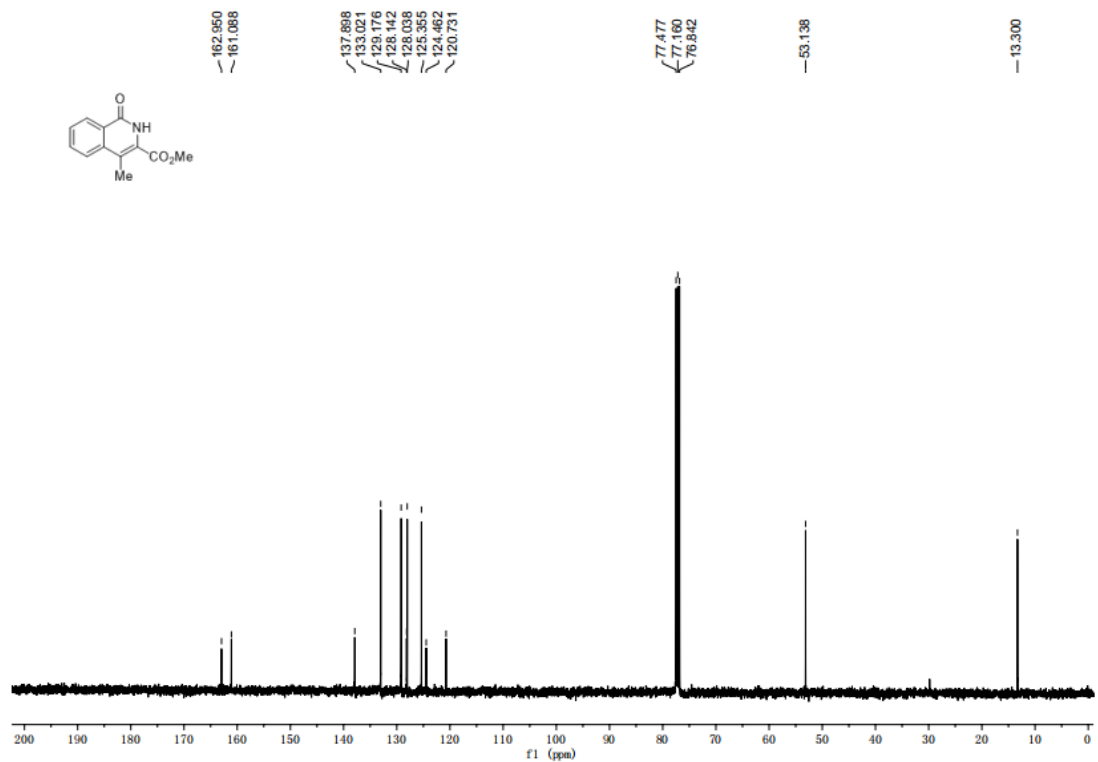
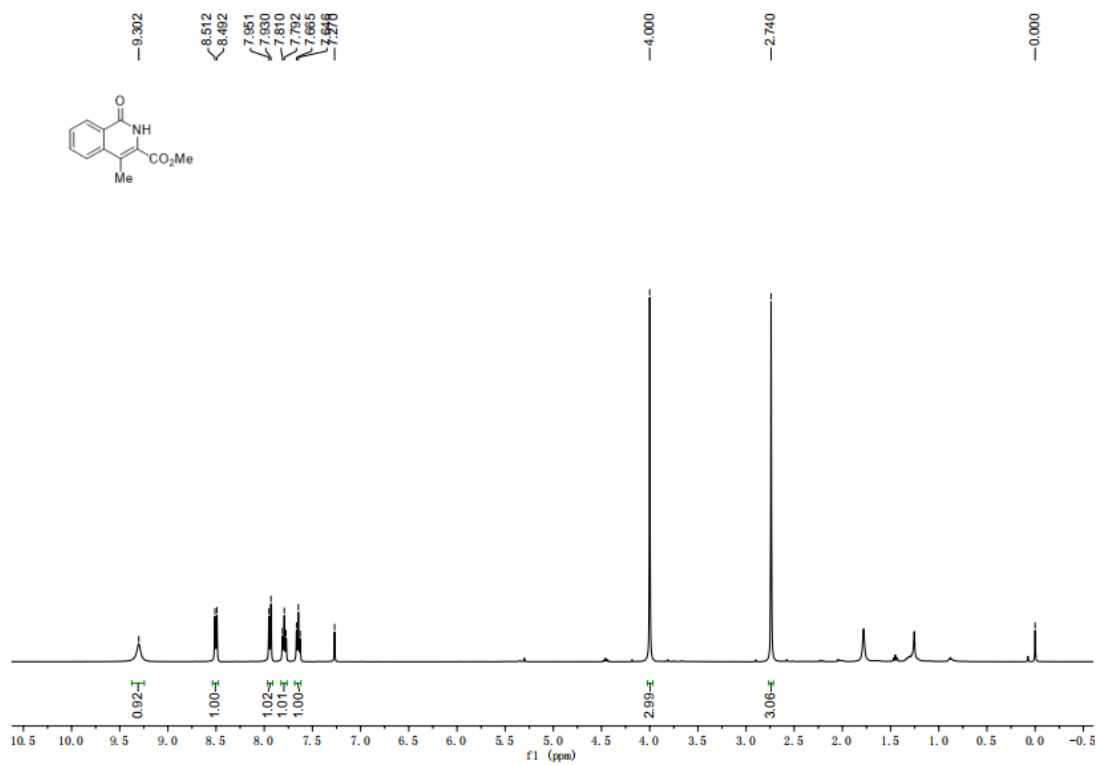
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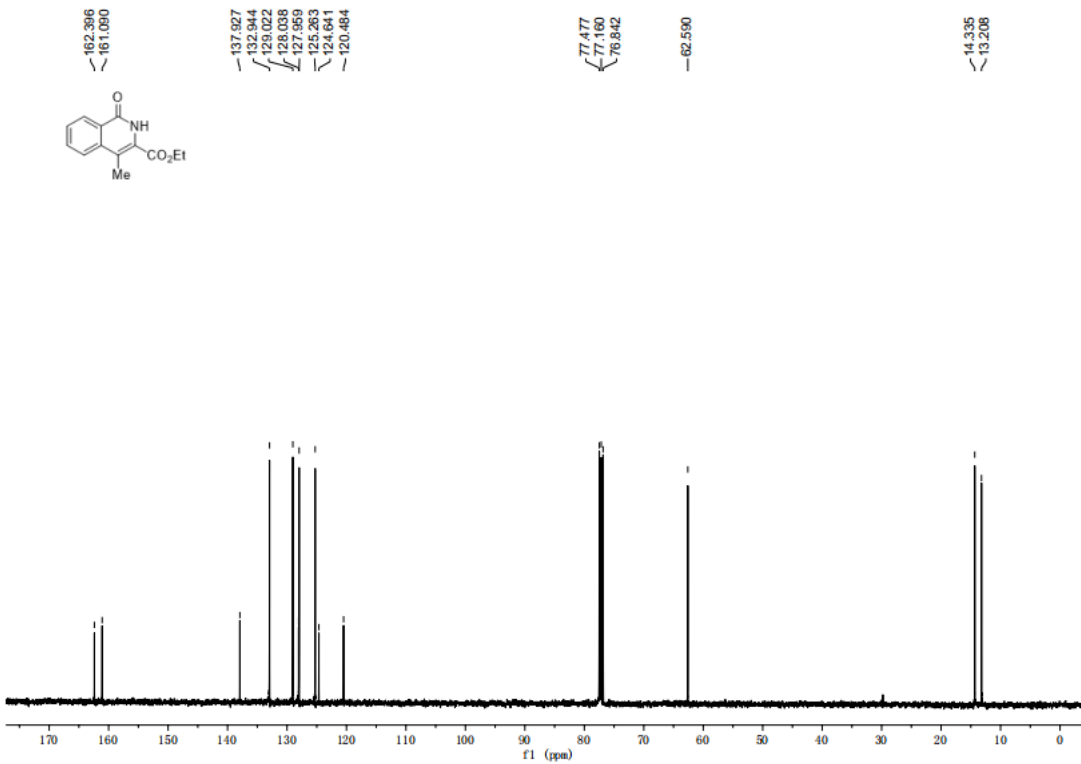
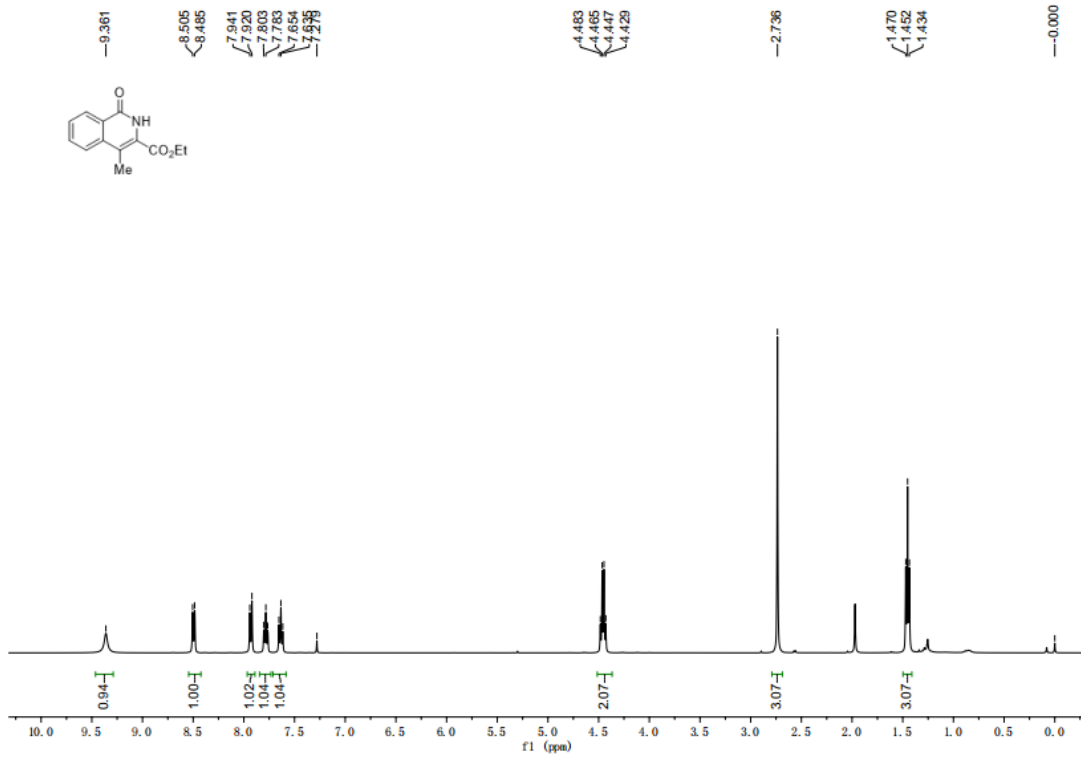
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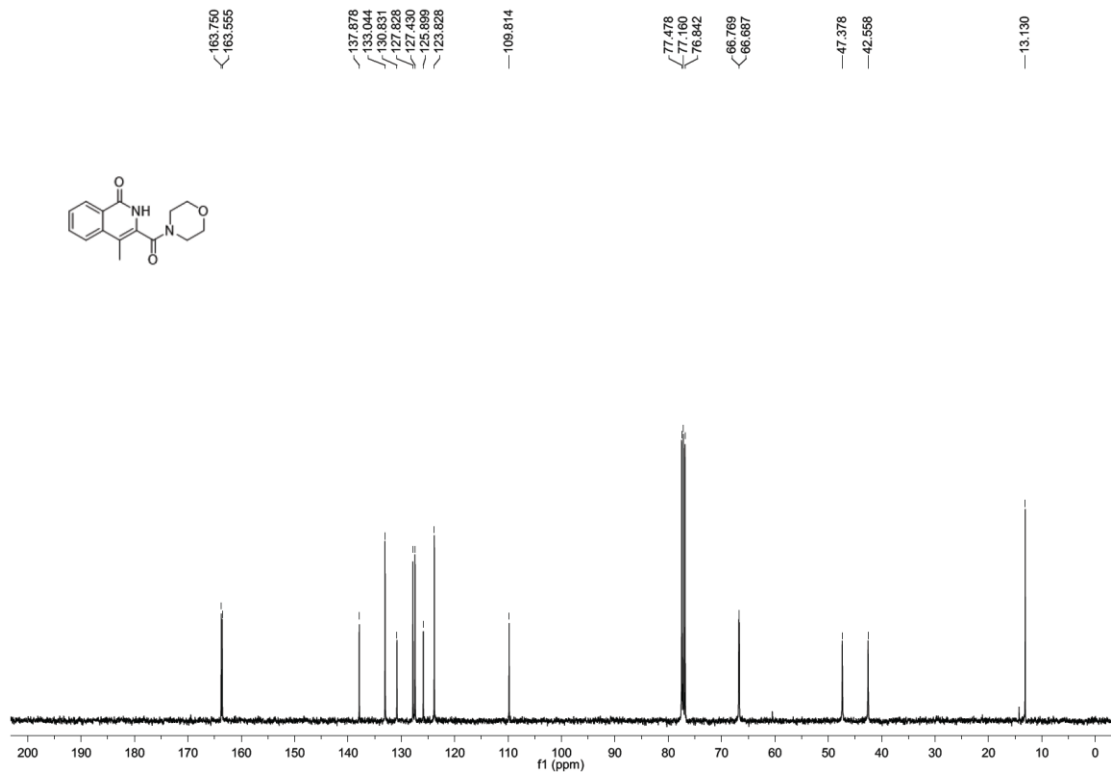
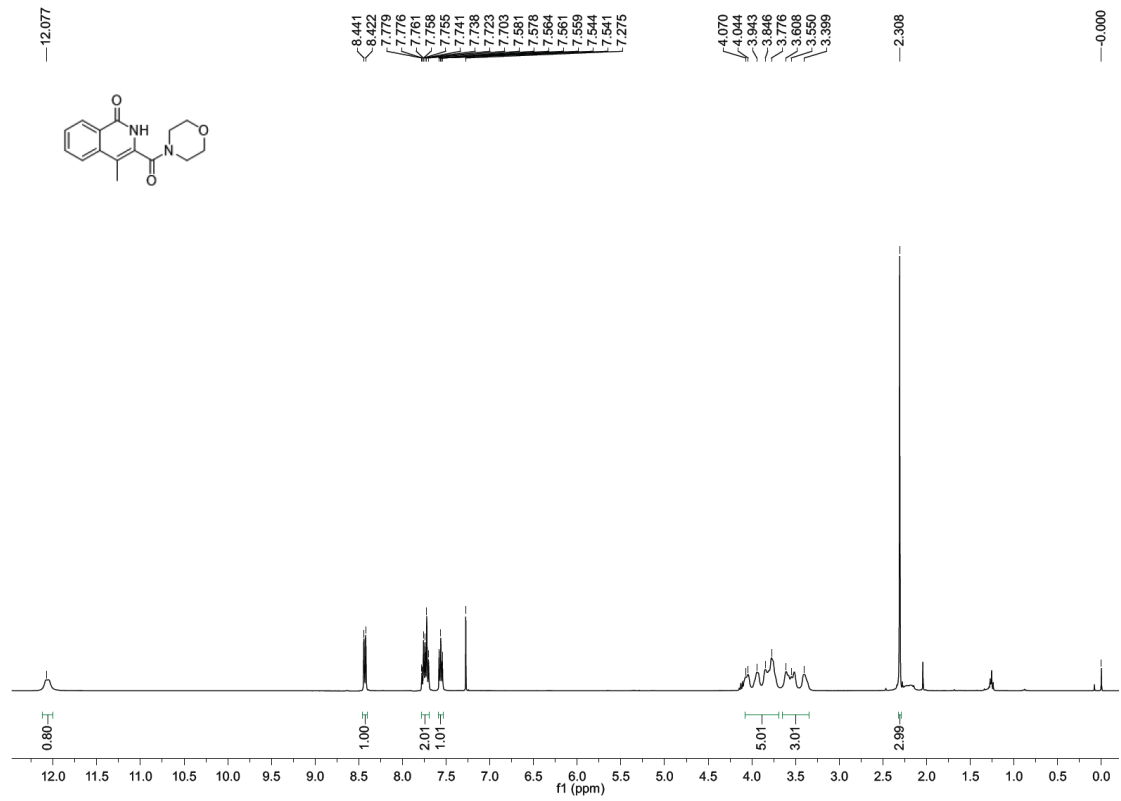
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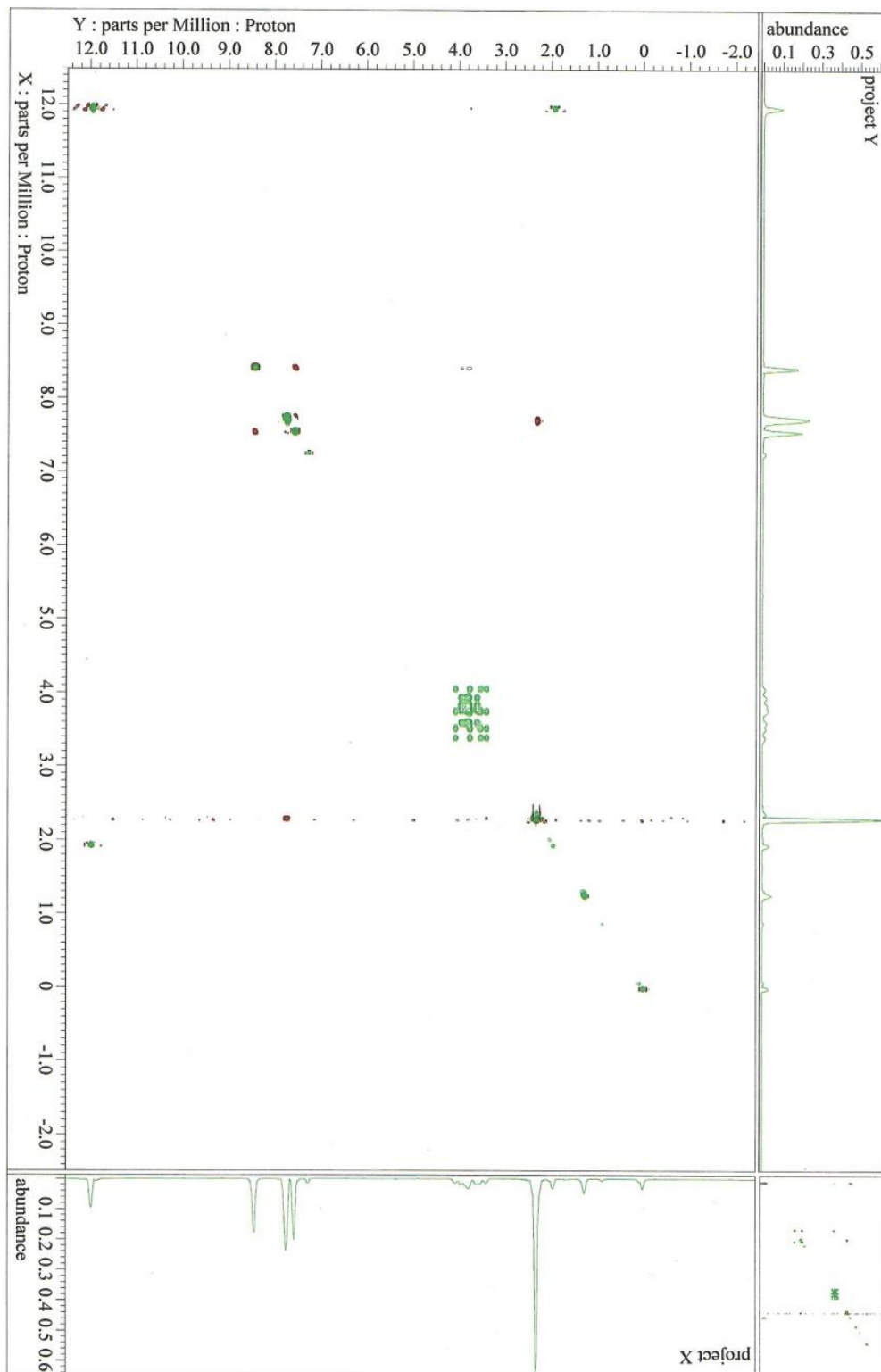
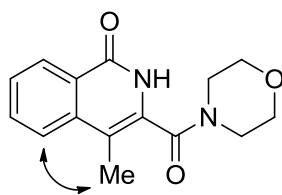
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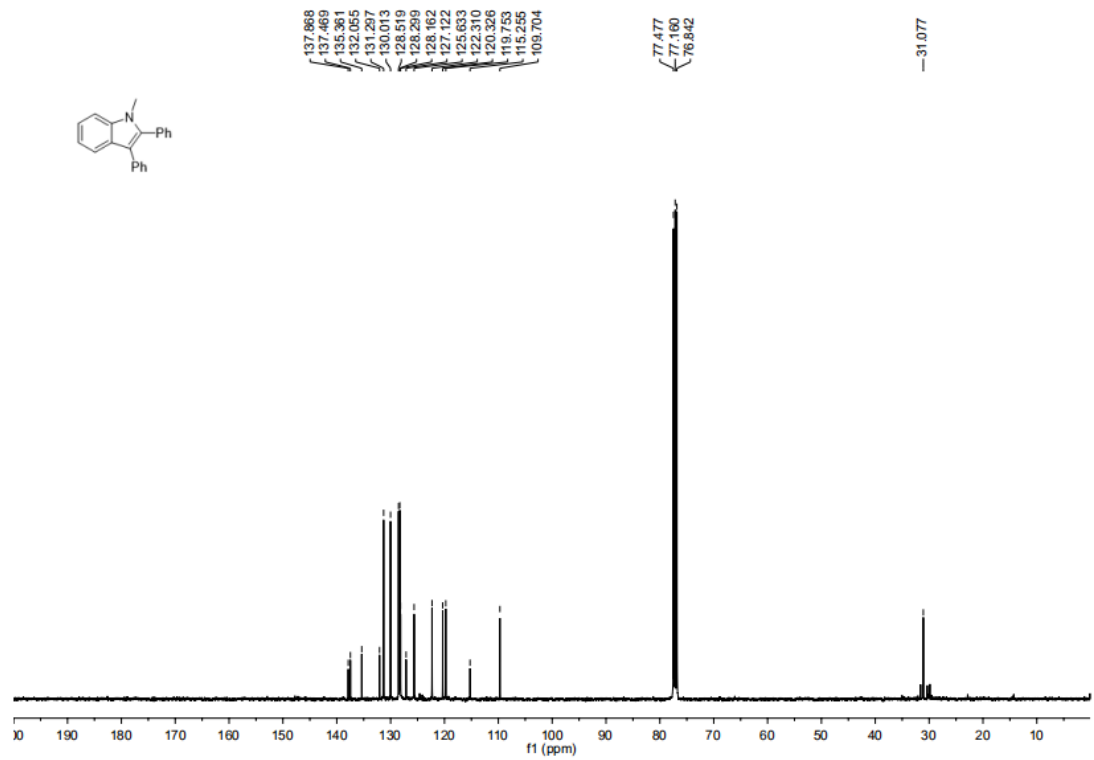
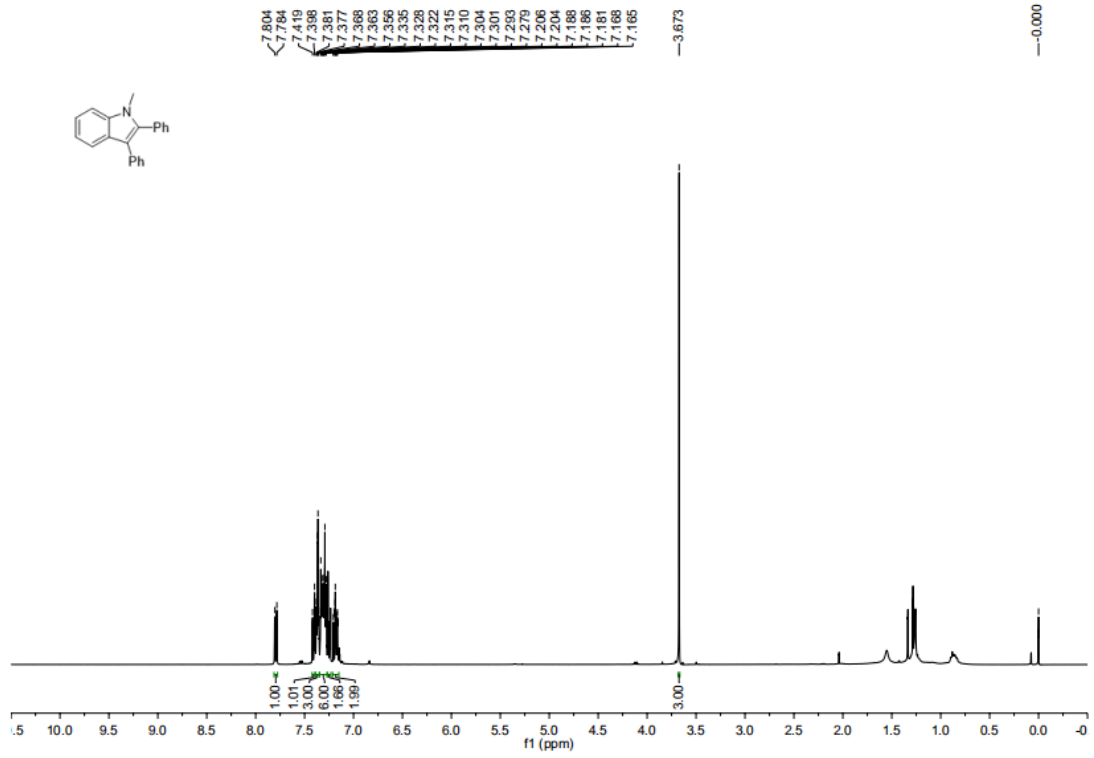
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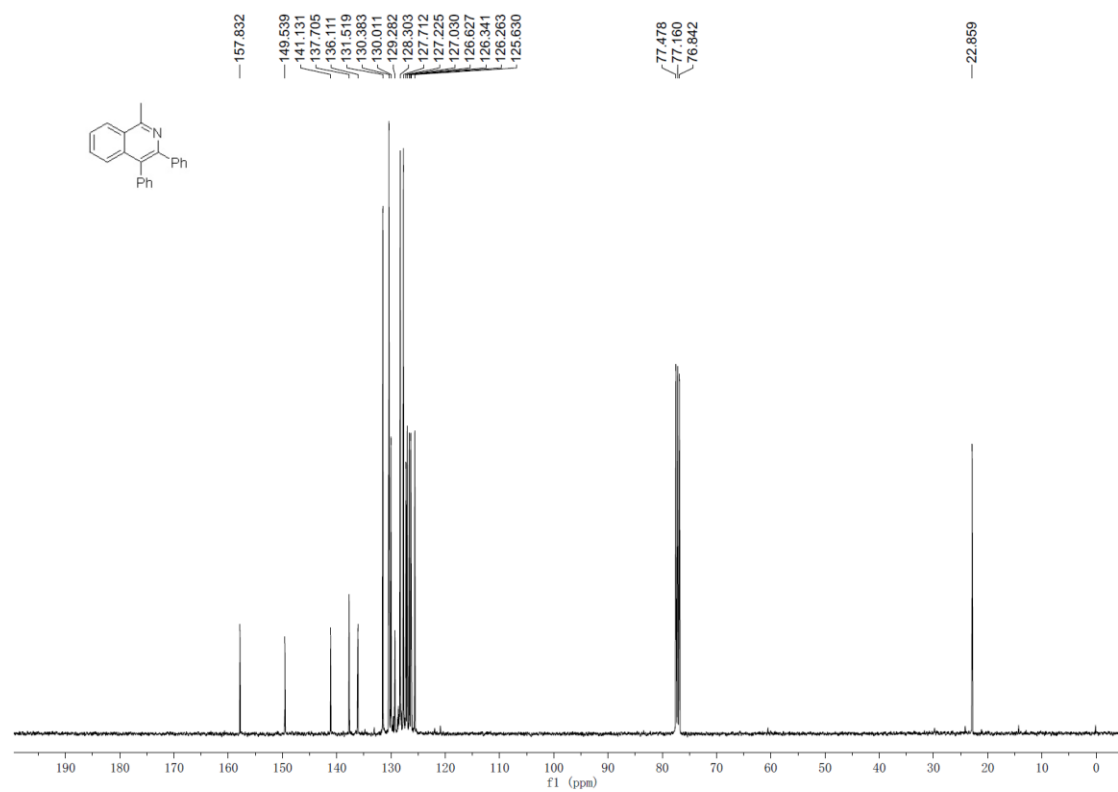
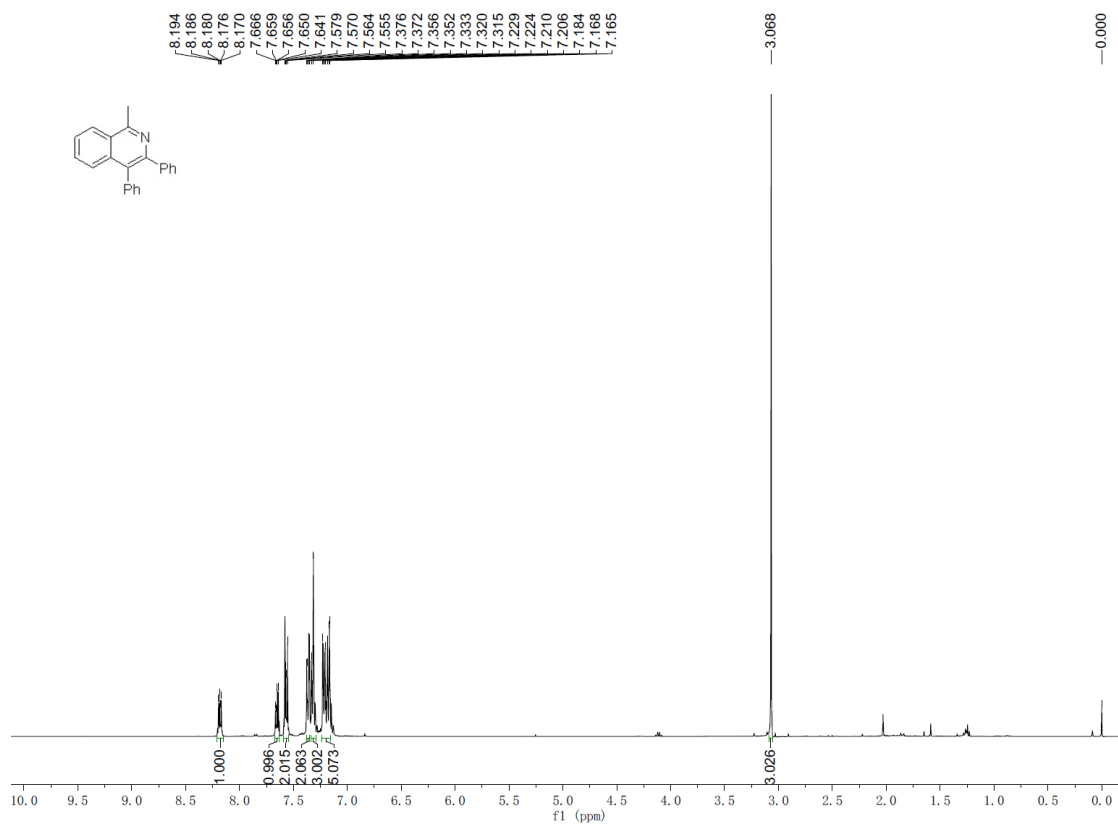
The NOESY spectrum of 5aI:



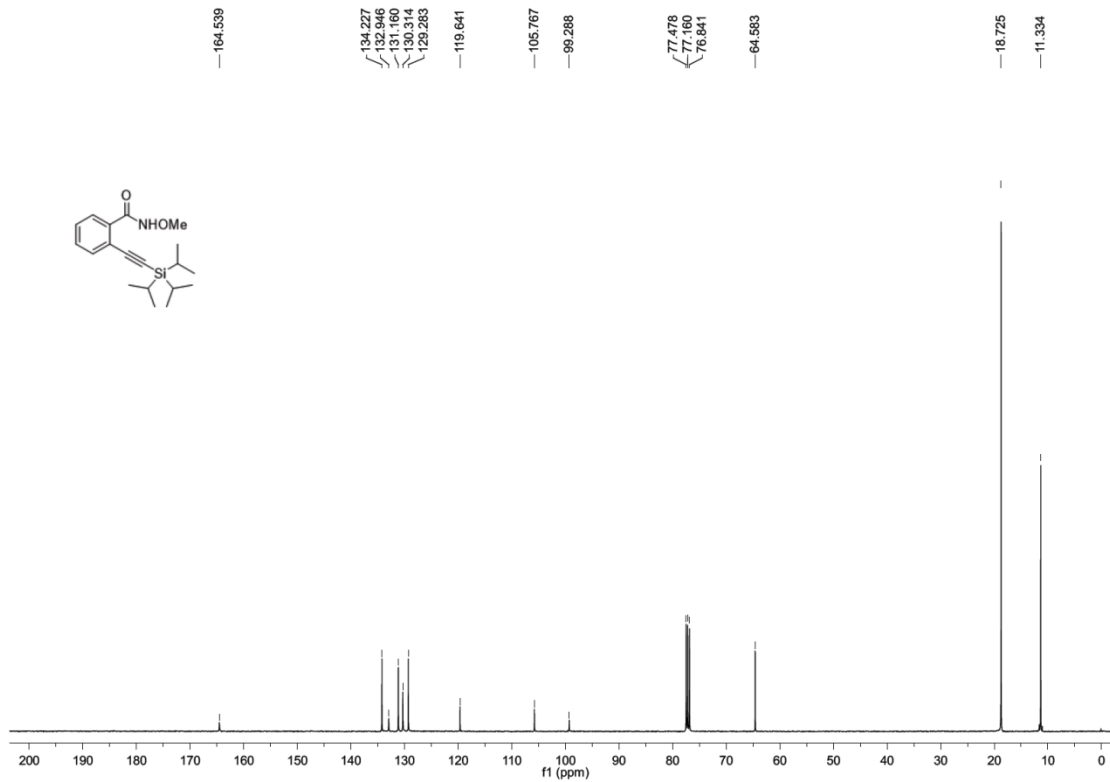
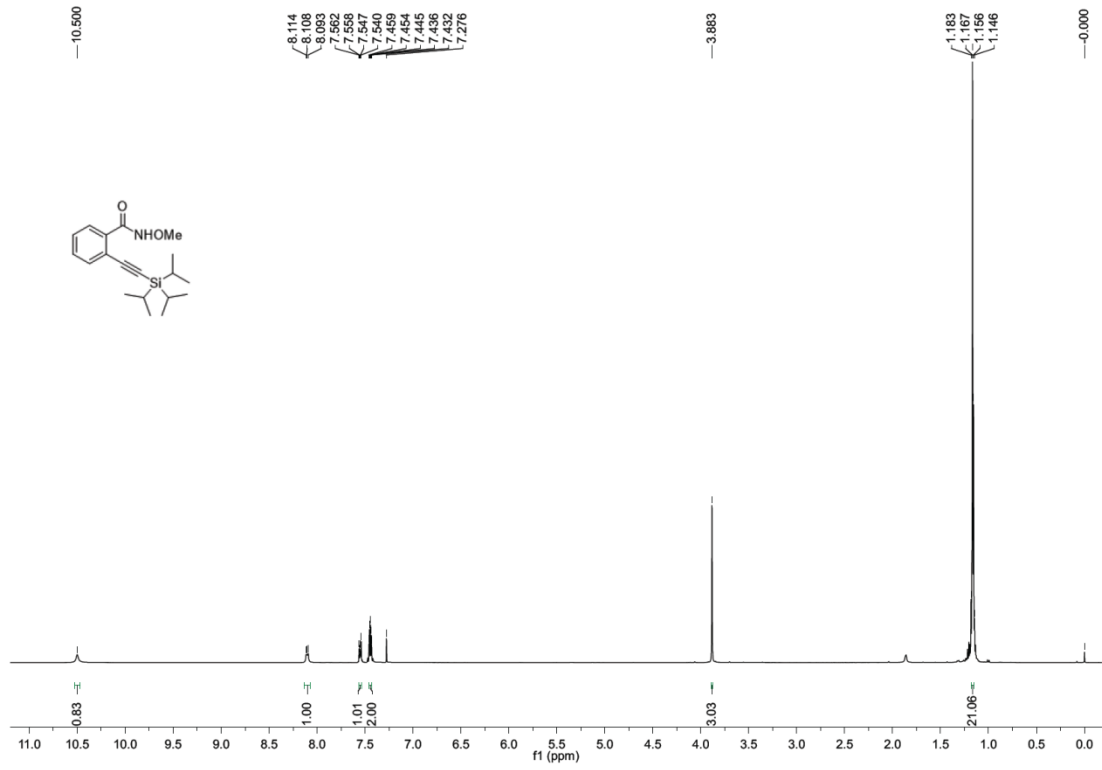
6



7



8



9

