Supplementary Information

Specific Assembly of Dihydrobenzofuran Frameworks via Rh(III)-Catalyzed C-H Coupling of *N*-Phenoxyacetamides with 2-Alkenylphenols

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I. General

NMR spectra were recorded on JEOL 400 NMR (^{1}H 400 MHz; ^{13}C 100 MHz) in $CDCl_3$. 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 ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm; CD_3OD: δ_H = 3.31 ppm, δ_C = 49.00 ppm; DMSO-d_6: δ_H = 2.50 ppm, δ_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. The enantiomeric excess (ee) of the products was determined by high-performance liquid chromatography (HPLC) with a chiral stationary phase in comparison with the authentic racemate sample. All the chiral stationary phases including Chiralcel IC-3 used in this study were purchased from Daicel Chirsal Technologies. $[Cp^*IrCl_2]_2$, $[Cp^*RhCl_2]_2$, $[Ru(p\text{-cymene})Cl_2]_2$, and $Cp^*Co(CO)I_2$ were purchased from Aldrich and used without further purification. Other chemicals were purchased from commercial suppliers and were dried and purified when necessary. Chiral rhodium catayst,[S1] *N*-phenoxy amides[S2] and the 2-alkenylphenols[S3] were prepared according to published procedures. Alternatively, these chiral rhodium catalysts can be also purchased from Daicel Chiral Technologies (China) Co., LTD. No attempts were made to optimize yields for substrate synthesis.

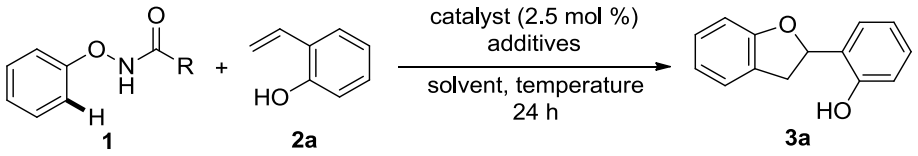
II. Experimental Information and Characterization Data

Optimization studies:

The mixture of *N*-phenoxy amide **1** (0.1 mmol, 1.0 equiv), 2-alkenylphenol **2a**, catalyst (2.5 mol %) and additives in the solvent was stirred at the specified temperature 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 = 0.5) to give the desired dihydrobenzofuran product **3a**.

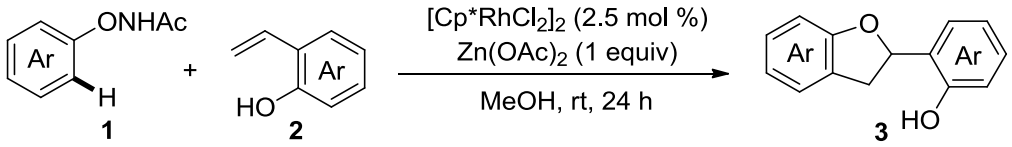
Table S1. Conditions screening for the synthesis of dihydrobenzofuran derivative.[a]



Entry	R	Catalyst (2.5 mol %)	Additive (1 equiv)	*Tem.* (^{o}C)	Solvent	Yield (%)
1	Me	$[Cp^*RhCl_2]_2$	CsOAc	60	MeOH	23
2	Me	$[Cp^*RhCl_2]_2$	CsOAc	60	MeCN	<10
3	Me	$[Cp^*RhCl_2]_2$	CsOAc	60	THF	<10
4	Me	$[Cp^*RhCl_2]_2$	CsOAc	60	dioxane	<10
5	Me	$[Cp^*RhCl_2]_2$	CsOAc	60	toluene	<10
6	Me	$[Cp^*RhCl_2]_2$	CsOAc	60	DCM	17
7	Me	$[Cp^*RhCl_2]_2$	CsOAc	60	DMF	<10
8	Me	$[Cp^*RhCl_2]_2$	CsOAc	60	EtOH	<10
9	Me	$[Cp^*RhCl_2]_2$	CsOAc	60	acetone	18
10	Me	$[Cp^*RhCl_2]_2$	CsOAc	40	MeOH	31
11	Me	$[Cp^*RhCl_2]_2$	CsOAc	rt	MeOH	46
12	Me	$[Cp^*RhCl_2]_2$	NaOAc	rt	MeOH	32
13	Me	$[Cp^*RhCl_2]_2$	Cs_2CO_3	rt	MeOH	<10
14	Me	$[Cp^*RhCl_2]_2$	KOPiv	rt	MeOH	20
15	Me	$[Cp^*RhCl_2]_2$	K_3PO_4	rt	MeOH	30
16	Me	$[Cp^*RhCl_2]_2$	$Zn(OAc)_2$	rt	MeOH	57
17	Me	$[Cp^*RhCl_2]_2$	AgOAc	rt	MeOH	30
18	Me	$[Cp^*RhCl_2]_2$	$Cu(OAc)_2$	rt	MeOH	24
19	Me	$[Cp^*RhCl_2]_2$	Et_3N	rt	MeOH	<10
20	Me	$[Cp^*IrCl_2]_2$	$Zn(OAc)_2$	rt	MeOH	<10
21	Me	$[Ru(p\text{-cymene})Cl_2]_2$	$Zn(OAc)_2$	rt	MeOH	n.d.
22[b]	Me	$Cp^*Co(CO)I_2$	$Zn(OAc)_2$	rt	MeOH	n.d.
23	Et	$[Cp^*RhCl_2]_2$	$Zn(OAc)_2$	rt	MeOH	55
24	^{i}Pr	$[Cp^*RhCl_2]_2$	$Zn(OAc)_2$	rt	MeOH	21
25	Piv	$[Cp^*RhCl_2]_2$	$Zn(OAc)_2$	rt	MeOH	n.d.
26	Ts	$[Cp^*RhCl_2]_2$	$Zn(OAc)_2$	rt	MeOH	n.d.
27[c]	Me	$[Cp^*RhCl_2]_2$	$Zn(OAc)_2$	rt	MeOH	79
28[c,d]	Me	$[Cp^*RhCl_2]_2$	$Zn(OAc)_2$	rt	MeOH	87
29[c,d,e]	Me	$[Cp^*RhCl_2]_2$	$Zn(OAc)_2$	rt	MeOH	60
30[c,d,f]	Me	$[Cp^*RhCl_2]_2$	$Zn(OAc)_2$	rt	MeOH	35
31[g]	Me	$[Cp^*RhCl_2]_2$	$Zn(OPiv)_2$	0	MeOH	85

[a]Reaction Conditions: **1** (0.1 mmol), **2a** (0.1 mmol), catalyst (2.5 mol %) and additive (1 equiv) in solvent (0.2 M) at specified temperature for 24 h without exclusion of air or moisture, isolated yield. [b]The reaction was conducted with 5 mol % of Cp*Co(CO)I_2 under an atmosphere of N_2. [c]**2a** (1.3 equiv). [d]MeOH (0.1 M). [e]K_2CO_3 (1 equiv) was used as an additive. [f]HOAc (1 equiv) was used as an additive. [g]20 mol % of $AgSbF_6$ was used as an additive.

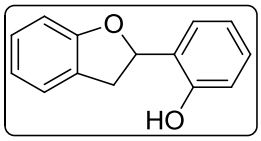
General procedure for the synthesis of dihydrobenzofuran derivatives:



The mixture of *N*-aryloxyacetamides **1** (0.2 mmol, 1.0 equiv), 2-alkenylphenols **2** (0.26 mmol, 1.3 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol %) and $Zn(OAc)_2$ (0.2 mmol, 1.0 equiv) in MeOH (2.0 mL) was stirred at room temperature for 24 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduced pressure, and the resulted mixture was purified by preparative TLC to afford the corresponding dihydrobenzofuran derivatives **3.**

Characterization of products 3:

2-(2,3-dihydrobenzofuran-2-yl)phenol (3a)



This compound was obtained in 87% yield (36.8 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.5.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24-7.14 (m, 4H), 6.95-6.86 (m, 4H), 6.56 (s, 1H), 5.96-5.91 (m, 1H), 3.58 (dd, *J* = 15.5, 8.9 Hz, 1H), 3.33 (dd, *J* = 15.5, 9.9 Hz, 1H).

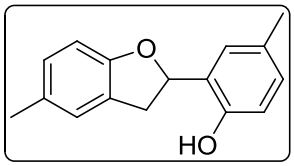
^{13}C NMR (100 MHz, $CDCl_3$): δ 158.7, 154.2, 129.4, 128.3, 127.1, 127.0, 126.0, 125.1, 121.5, 120.6, 116.9, 110.0, 83.4, 37.1.

HRMS (ESI) calculated for $C_{14}H_{13}O_2$ ($[M+H]^+$): 213.0910; found: 213.0909.

Scale-up synthesis of compound 3a: The mixture of *N*-phenoxyacetamides **1a** (2 mmol, 1.0 equiv), 2-alkenylphenol **2a** (2.6 mmol, 1.3 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol %)

and $Zn(OAc)_2$ (2 mmol, 1.0 equiv) in MeOH (20.0 mL) was stirred at room temperature for 24 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduced pressure, and the resulted mixture was purified with silica gel column chromatography (eluent: PE/EA = 10/1) to afford the corresponding dihydrobenzofuran derivative **3a** in 75% (0.3180 g) isolated yield.

4-methyl-2-(5-methyl-2,3-dihydrobenzofuran-2-yl)phenol (3b)



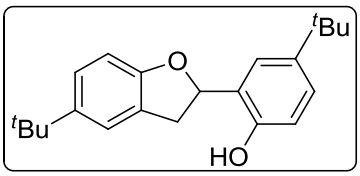
This compound was obtained in 76% yield (37.0 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.6.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.05-6.94 (m, 4H), 6.81-6.76 (m, 2H), 6.43 (s, 1H), 5.88-5.82 (m, 1H), 3.50 (dd, *J* = 15.5, 8.9 Hz, 1H), 3.28 (dd, *J* = 15.4, 10.1 Hz, 1H), 2.30 (s, 3H), 2.27 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 156.6, 152.1, 130.9, 129.8, 129.7, 128.6, 127.4, 127.2, 125.68, 125.65, 116.8, 109.6, 83.8, 37.3, 21.0, 20.7.

HRMS (ESI) calculated for $C_{16}H_{17}O_2$ ($[M+H]^+$): 241.1223; found: 241.1222.

4-(*tert*-butyl)-2-(5-(*tert*-butyl)-2,3-dihydrobenzofuran-2-yl)phenol (3c)



This compound was obtained in 80% yield (51.8 mg) as yellow oil. Eluent: PE/EA = 5/1, R_f = 0.7.

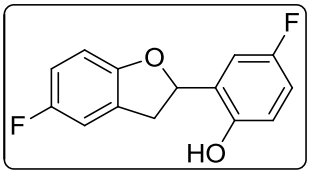
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28-7.17 (m, 4H), 6.85-6.81 (m, 2H), 6.55 (s, 1H), 5.90-5.84 (m, 1H), 3.53 (dd, *J* = 15.4, 8.7 Hz, 1H), 3.35 (dd, *J* = 15.1, 10.8 Hz, 1H), 1.31 (s, 9H), 1.29 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 156.4, 152.2, 144.7, 143.2, 127.0, 126.3, 125.1,

124.8, 124.0, 122.1, 116.6, 109.3, 84.8, 37.5, 34.5, 34.3, 31.9, 31.7.

HRMS (ESI) calculated for $C_{22}H_{29}O_2$ ($[M+H]^+$): 325.2162; found: 325.2166.

4-fluoro-2-(5-fluoro-2,3-dihydrobenzofuran-2-yl)phenol (3d)



This compound was obtained in 81% yield (40.1 mg) as yellow oil. Eluent: PE/EA = 5/1, R_f = 0.5.

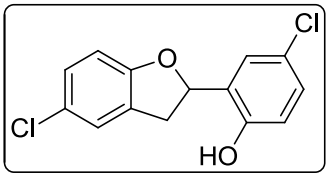
^{1}H NMR (400 MHz, $CDCl_3$): δ 6.97 (dd, *J* = 9.0, 2.8 Hz, 1H), 6.94-6.76 (m, 5H), 6.17 (brs, 1H), 5.94-5.89 (m, 1H), 3.60 (dd, *J* = 15.8, 9.1 Hz, 1H), 3.24 (dd, *J* = 15.8, 9.2 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 158.1 (d, *J* = 236.8 Hz), 157.1 (d, *J* = 237.2 Hz), 154.7, 149.6, 128.1 (d, *J* = 9.0 Hz), 127.8 (d, *J* = 6.8 Hz), 117.5 (d, *J* = 7.9 Hz), 115.6 (d, *J* = 23.0 Hz), 114.6 (d, *J* = 24.2 Hz), 113.3 (d, *J* = 24.5 Hz), 112.3 (d, *J* = 24.8 Hz), 110.1 (d, *J* = 8.1 Hz), 82.6, 37.3.

^{19}F NMR (376 MHz, $CDCl_3$): δ -123.05, -123.34.

HRMS (ESI) calculated for $C_{14}H_{10}F_2O_2Na$ ($[M+Na]^+$): 271.0541; found: 271.0536.

4-chloro-2-(5-chloro-2,3-dihydrobenzofuran-2-yl)phenol (3e)



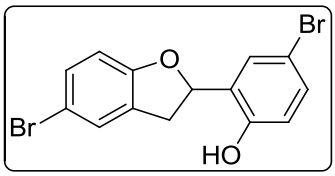
This compound was obtained in 70% yield (39.0 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.5.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21 (s, 1H), 7.19-7.10 (m, 3H), 6.84-6.77 (m, 2H), 5.94-5.89 (m, 1H), 3.61 (dd, *J* = 15.9, 9.2 Hz, 1H), 3.22 (dd, *J* = 15.8, 9.1 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 157.4, 129.1, 128.6, 128.3, 128.2, 126.6, 126.3, 125.6, 125.3, 117.8, 110.8, 82.3, 37.0.

HRMS (ESI) calculated for $C_{14}H_{10}Cl_2O_2Na$ ([M+Na]$^+$): 302.9950; found: 302.9949.

4-bromo-2-(5-bromo-2,3-dihydrobenzofuran-2-yl)phenol (3f)



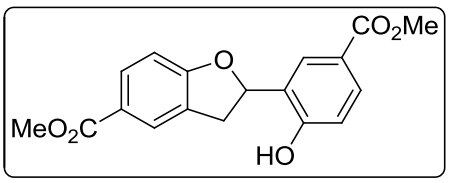
This compound was obtained in 76% yield (55.7 mg) as yellow oil. Eluent: PE/EA = 5/1, R_f = 0.4.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 (d, *J* = 2.0 Hz, 1H), 7.30-7.25 (m, 3H), 6.78 (d, *J* = 8.4 Hz, 1H), 6.73 (d, *J* = 8.5 Hz, 1H), 5.93-5.88 (m, 1H), 3.61 (dd, *J* = 15.9, 9.2 Hz, 1H), 3.21 (dd, *J* = 15.9, 9.1 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 157.9, 152.7, 132.1, 131.2, 129.5, 129.1, 128.6, 128.1, 118.3, 113.4, 112.9, 111.4, 82.1, 36.9.

HRMS (ESI) calculated for $C_{14}H_9Br_2O_2$ ([M-H]$^-$): 366.8975; found: 366.8973.

Methyl 2-(2-hydroxy-5-(methoxycarbonyl)phenyl)-2,3-dihydrobenzofuran-5-carboxylate (3g)



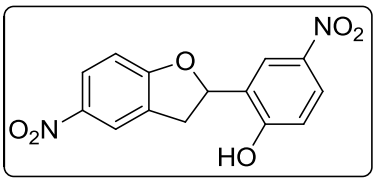
This compound was obtained in 47% yield (30.8 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.4.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (s, 1H), 7.96-7.90 (m, 3H), 6.96-6.86 (m, 3H), 6.09-6.04 (m, 1H), 3.90 (s, 3H), 3.88 (s, 3H), 3.71 (dd, *J* = 15.8, 9.3 Hz, 1H), 3.31 (dd, *J* = 15.7, 9.3 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-*d_6*): δ 166.0, 165.9, 163.3, 158.7, 130.8, 130.7, 128.0, 127.8, 127.3, 126.6, 122.3, 120.2, 115.4, 109.0, 80.5, 51.8, 51.7, 35.8.

HRMS (ESI) calculated for $C_{18}H_{17}O_6$ ([M+H]$^+$): 329.1020; found: 329.1015.

4-nitro-2-(5-nitro-2,3-dihydrobenzofuran-2-yl)phenol (3h)



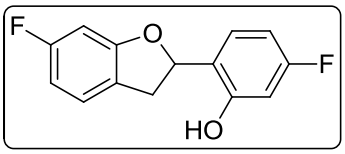
This compound was obtained in 37% yield (22.4 mg) as yellow solid. Eluent: PE/EA = 10/1, R_f = 0.4.

^{1}H NMR (400 MHz, CD_3OD): δ 8.18-8.09 (m, 4H), 7.06 (d, *J* = 9.4 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 1H), 6.19-6.13 (m, 1H), 3.87 (dd, *J* = 16.5, 10.0 Hz, 1H), 3.17 (dd, *J* = 16.6, 7.3 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-*d_6*): δ 164.6, 161.0, 141.6, 139.3, 129.0, 128.1, 125.7, 122.1, 121.4, 115.9, 109.3, 81.6, 35.3.

HRMS (ESI) calculated for $C_{14}H_9N_2O_6$ ($[M-H]^-$): 301.0466; found: 301.0465.

5-fluoro-2-(6-fluoro-2,3-dihydrobenzofuran-2-yl)phenol (3i)



This compound was obtained in 62% yield (30.7 mg) as yellow oil. Eluent: PE/EA = 5/1, R_f = 0.6.

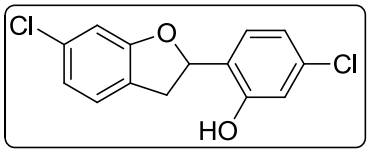
^{1}H NMR (400 MHz, CD_3OD): δ 7.17-7.09 (m, 2H), 6.64 (d, *J* = 8.2 Hz, 1H), 6.60-6.48 (m, 2H), 6.44 (dd, *J* = 9.8, 2.0 Hz, 1H), 6.27-6.23 (m, 1H), 3.47-3.32 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 163.1 (d, *J* = 243.2 Hz), 160.4 (d, *J* = 244.3 Hz), 158.8 (d, *J* = 12.8 Hz), 156.2 (d, *J* = 5.8 Hz), 130.0 (d, *J* = 11.1 Hz), 125.3 (d, *J* = 8.0 Hz), 122.8 (d, *J* = 2.6 Hz), 113.4 (d, J = 2.8 Hz), 112.6 (d, *J* = 15.5 Hz), 108.8 (d, *J* = 22.4 Hz), 107.2 (d, *J* = 21.8 Hz), 99.1 (d, *J* = 26.6 Hz), 81.8 (d, *J* = 5.7 Hz), 36.7.

^{19}F NMR (376 MHz, $CDCl_3$): δ -117.15, -117.40.

HRMS (ESI) calculated for $C_{14}H_{11}F_2O_2$ ($[M+H]^+$): 249.0722; found: 249.0720.

5-chloro-2-(6-chloro-2,3-dihydrobenzofuran-2-yl)phenol (3j)



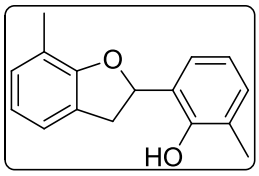
This compound was obtained in 73% yield (40.8 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.6.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.14 (d, *J* = 8.2 Hz, 1H), 7.10 (d, *J* = 8.3 Hz, 1H), 6.92-6.87 (m, 3H), 6.87 (d, *J* = 1.7 Hz, 1H), 6.38 (brs, 1H), 5.96-5.91 (m, 1H), 3.56 (dd, *J* = 15.7, 9.1 Hz, 1H), 3.19 (dd, *J* = 15.7, 9.2 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 154.4, 134.6, 133.7, 127.8, 125.6, 125.5, 125.0, 121.7, 121.0, 117.0, 110.7, 83.1, 36.5.

HRMS (ESI) calculated for $C_{14}H_9Cl_2O_2$ ($[M-H]^-$): 278.9985; found: 278.9984.

2-methyl-6-(7-methyl-2,3-dihydrobenzofuran-2-yl)phenol (3k)



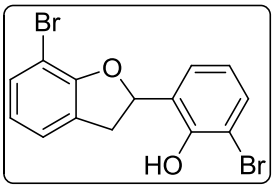
This compound was obtained in 72% yield (34.6 mg) as yellow oil. Eluent: PE/EA = 10/1, R_f = 0.5.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.10 (d, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 7.3 Hz, 1H), 7.02-6.96 (m, 3H), 6.86-6.79 (m, 2H), 5.90-5.84 (m, 1H), 3.52 (dd, *J* = 15.4, 8.8 Hz, 1H), 3.36 (dd, *J* = 15.3, 10.7 Hz, 1H), 2.26 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 156.8, 153.0, 130.8, 129.6, 126.5, 125.8, 124.8, 124.7, 122.4, 121.7, 120.4, 120.0, 84.5, 37.4, 16.0, 15.4.

HRMS (ESI) calculated for $C_{16}H_{17}O_2$ ($[M+H]^+$): 241.1223; found: 241.1221.

2-bromo-6-(7-bromo-2,3-dihydrobenzofuran-2-yl)phenol (3l)



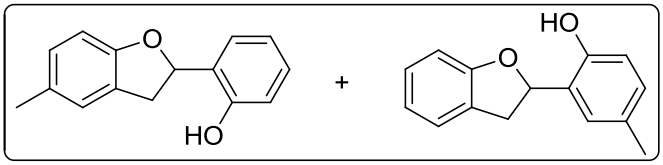
This compound was obtained in 79% yield (57.9 mg) as yellow oil. Eluent: PE/EA = 5/1, R_f = 0.6.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.08 (dd, *J* = 7.3, 1.1 Hz, 1H), 6.82 (t, *J* = 8.0 Hz, 1H), 6.76 (t, *J* = 8.0 Hz, 1H), 6.11-6.04 (m, 1H), 5.84 (s, 1H), 3.81 (dd, *J* = 15.9, 9.7 Hz, 1H), 3.21 (dd, *J* = 15.9, 7.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 156.8, 148.8, 131.4, 131.3, 129.3, 128.0, 125.7, 124.1, 122.4, 121.8, 110.7, 102.7, 80.5, 38.2.

HRMS (ESI) calculated for $C_{14}H_{10}Br_2O_2Na$ ($[M+Na]^+$): 390.8940; found: 390.8948.

2-(5-methyl-2,3-dihydrobenzofuran-2-yl)phenol (3m) & 2-(2,3-dihydrobenzofuran-2-yl)-4-methylphenol (3m')



This compound was obtained in 90% yield (40.6 mg) as white solid by using 4-methyl substituted *N*-phenoxyacetamide with 2-alkenylphenol **2a**. An inseparable mixture of two isomers was obtained, and the ratio was determined to be 1/0.6 by ^{1}H-NMR analysis. Eluent: PE/EA = 5/1, R_f = 0.6.

^{1}H NMR (400 MHz, CD_3OD): δ 7.27 (d, *J* = 7.6 Hz, 0.6H), 7.16-7.06 (m, 3.6H), 6.96 (s, 0.6H), 6.92-6.89 (m, 1.6H), 6.85-6.74 (m, 3.2H), 6.70-6.67 (m, 1.6H), 5.97-5.92 (m, 1.6H), 3.67-3.57 (m, 1.6H), 3.05-2.95 (m, 1.6H), 2.25 (s, 1.8H), 2.19 (s, 3H).

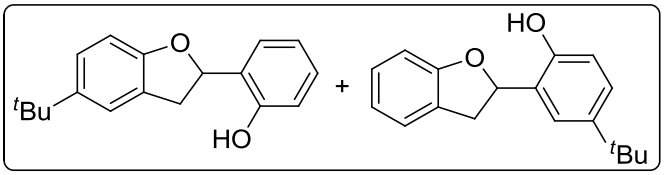
^{13}C NMR (100 MHz, CD_3OD): δ 161.1, 159.0, 152.9, 130.3, 129.84, 129.81, 129.5, 129.4, 129.2, 128.9, 128.21, 128.17, 127.1, 126.6, 126.0, 121.6, 120.3, 115.9, 109.9, 109.5, 80.9, 38.52, 38.48, 20.9, 20.7.

HRMS (ESI) calculated for $C_{15}H_{15}O_3$ ($[M+H]^+$): 227.1067; found: 227.1063.

Another batch of reaction was conducted by using 4-methyl substituted 2-alkenylphenol with *N*-phenoxyacetamide **1a**, the desired compound was obtained in

81% yield (36.6 mg) as white solid, and the ratio was determined to be **3m**/**3m'** = 0.8/1 by ^{1}H-NMR analysis.

2-(5-(*tert*-butyl)-2,3-dihydrobenzofuran-2-yl)phenol (3n) & 4-(*tert*-butyl)-2-(2,3-dihydrobenzofuran-2-yl)phenol (3n')



This compound was obtained in 86% yield (46.0 mg) as white solid by using 4-^{t}Bu substituted *N*-phenoxyacetamide with 2-alkenylphenol **2a**. Eluent: PE/EA = 5/1, R_f = 0.6. An inseparable mixture of two regioisomers was obtained, and the ratio was determined to be 1/0.75 by ^{1}H-NMR analysis.

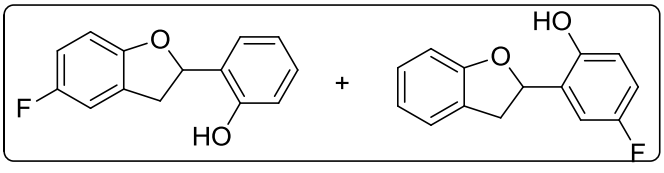
^{1}H NMR (400 MHz, CD_3OD): δ 7.35 (d, *J* = 2.2 Hz, 1H), 7.27 (d, *J* = 7.6 Hz, 0.75H), 7.20 (s, 0.75H), 7.16-7.06 (m, 4.5H), 6.85-6.70 (m, 5.25H), 5.98-5.93 (m, 1.75H), 3.66-3.59 (m, 1.75H), 3.07-2.97 (m, 1.75H), 1.28 (s, 6.75H), 1.22 (s, 9H).

^{13}C NMR (100 MHz, CD_3OD): δ 161.1, 158.8, 155.2, 152.9, 144.7, 143.0, 130.3, 129.4, 129.1, 128.9, 128.3, 127.8, 126.7, 126.2, 126.0, 125.6, 123.5, 123.0, 121.6, 120.4, 115.9, 115.6, 109.9, 109.1, 81.4, 81.0, 38.7, 38.5, 35.1, 34.9, 32.2, 32.1.

HRMS (ESI) calculated for $C_{18}H_{21}O_2$ ($[M+H]^+$): 269.1536; found: 269.1532.

Another batch of reaction was conducted by using 4-^{t}Bu substituted 2-alkenylphenol with *N*-phenoxyacetamide **1a**, the desired compound was obtained in 72% yield (38.6 mg) as white solid, and the ratio was determined to be **3n**/**3n'** = 0.5/1 by ^{1}H-NMR analysis.

2-(5-fluoro-2,3-dihydrobenzofuran-2-yl)phenol (3o) & 2-(2,3-dihydrobenzofuran-2-yl)-4-fluorophenol (3o')



This compound was obtained in 66% yield (30.3 mg) as yellow solid by using 4-F substituted *N*-phenoxyacetamide with 2-alkenylphenol **2a**. Eluent: PE/EA = 5/1, R_f = 0.7. An inseparable mixture of two regioisomers was obtained, and the ratio was determined to be 1/1 by ^{1}H-NMR analysis.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26-7.15 (m, 4H), 6.98-6.77 (m, 10H), 6.39 (brs, 2H), 5.99-5.93 (m, 1H), 5.92-5.87 (m, 1H), 3.65-3.53 (m, 2H), 3.35-3.21 (m, 2H).

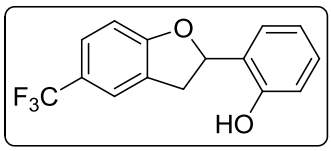
^{13}C NMR (100 MHz, $CDCl_3$): δ 158.6, 158.1 (d, *J* = 236.8 Hz), 157.0 (d, *J* = 236.9 Hz), 154.7, 154.0, 149.8, 129.6, 128.6 (d, *J* = 8.9 Hz), 128.4, 127.9 (d, *J* = 6.5 Hz), 126.9, 126.6, 125.9, 125.2, 121.6, 120.7, 117.5 (d, *J* = 7.9 Hz), 116.8, 115.5 (d, *J* = 23.0 Hz), 114.4 (d, *J* = 24.0 Hz), 113.4 (d, *J* = 24.6 Hz), 112.3 (d, J = 24.8 Hz), 110.12, 110.04, 109.97, 83.8, 82.2, 37.3, 37.1.

^{19}F NMR (376 MHz, $CDCl_3$): δ -123.15, -123.48.

HRMS (ESI) calculated for $C_{14}H_{12}FO_2$ ($[M+H]^+$): 231.0816; found: 231.0816.

Another batch of reaction was conducted by using 4-F substituted 2-alkenylphenol with *N*-phenoxyacetamide **1a**, the desired compound was obtained in 82% yield (37.7 mg) as white solid, and the ratio was determined to be **3o**/**3o'** = 1/1 by ^{1}H-NMR analysis.

2-(5-(trifluoromethyl)-2,3-dihydrobenzofuran-2-yl)phenol (3p)



This compound was obtained in 36% yield (20.0 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.65.

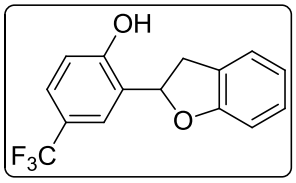
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46-7.44 (m, 2H), 7.29-7.25 (m, 1H), 7.24-7.19 (m, 1H), 6.96-6.92 (m, 2H), 6.85 (d, *J* = 8.1 Hz, 1H), 6.09-6.03 (m, 1H), 5.86 (brs, 1H), 3.66 (dd, *J* = 15.9, 9.3 Hz, 1H), 3.32 (dd, *J* = 15.9, 9.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 161.7, 153.5, 129.6, 128.0, 126.8, 126.33, 126.29, 124.6 (q, *J* = 269.9 Hz), 123.7 (q, *J* = 32.2 Hz), 123.3, 122.5 (d, *J* = 3.4 Hz), 121.0, 116.5, 109.7, 83.1, 36.5.

^{19}F NMR (376 MHz, $CDCl_3$): δ -61.01.

HRMS (ESI) calculated for $C_{15}H_{10}F_3O_2$ ([M-H]$^-$): 279.0638; found: 279.0635.

2-(2,3-dihydrobenzofuran-2-yl)-4-(trifluoromethyl)phenol (3p')



This compound was obtained in 25% yield (14.0 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.55.

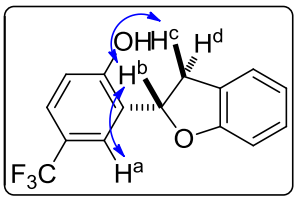
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 (s, 1H), 7.46 (d, *J* = 8.3 Hz, 1H), 7.26-7.17 (m, 2H), 6.97-6.92 (m, 3H), 5.98-5.92 (m, 1H), 3.65 (dd, *J* = 15.5, 9.1 Hz, 1H), 3.28 (dd, *J* = 15.5, 9.7 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 158.5, 157.0, 128.5, 126.9, 126.8, 126.6, 125.2, 124.4 (q, *J* = 269.4 Hz), 124.3 (q, *J* = 3.5 Hz), 122.8 (q, *J* = 32.5 Hz), 121.8, 116.9, 110.1, 82.5, 37.2.

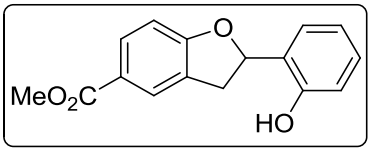
^{19}F NMR (376 MHz, $CDCl_3$): δ -61.32.

HRMS (ESI) calculated for $C_{15}H_{10}F_3O_2$ ([M-H]$^-$): 279.0638; found: 279.0637.

^{1}H-^{1}H NOESY:



methyl 2-(2-hydroxyphenyl)-2,3-dihydrobenzofuran-5-carboxylate (3q)



This compound was obtained in 36% yield (19.5 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.45.

^{1}H NMR (400 MHz, CD_3OD): δ 7.87 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.83 (d, *J* = 1.2 Hz,

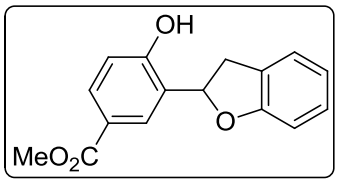
1H), 7.24 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.11 (td, *J* = 7.9, 1.7 Hz, 1H), 6.87 (d, *J* = 8.4 Hz, 1H), 6.83-6.76 (m, 2H), 6.08 (dd, *J* = 9.6, 7.8 Hz, 1H), 3.84 (s, 3H), 3.69 (dd, *J* = 16.0, 9.7 Hz, 1H), 3.09 (dd, *J* = 16.0, 7.7 Hz, 1H).

^{13}C NMR (100 MHz, CD_3OD): δ 168.6, 165.5, 155.4, 132.1, 129.8, 129.3, 129.2, 127.8, 126.7, 123.7, 120.4, 116.0, 109.8, 82.7, 52.3, 37.6.

HRMS (ESI) calculated for $C_{16}H_{15}O_4$ ($[M+H]^+$): 271.0965; found: 271.0959.

Another batch of reaction was conducted by using 4-CO_2Me substituted 2-alkenylphenol with *N*-phenoxyacetamide **1a**, the desired compound was obtained in 44% yield (24.0 mg) as white solid.

methyl 3-(2,3-dihydrobenzofuran-2-yl)-4-hydroxybenzoate (3q')



This compound was obtained in 24% yield (13.0 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.4.

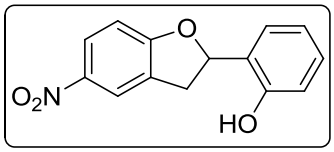
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95-7.85 (m, 2H), 7.24-7.15 (m, 2H), 6.97-6.92 (m, 3H), 5.98-5.93 (m, 1H), 3.87 (s, 3H), 3.62 (dd, *J* = 15.5, 8.9 Hz, 1H), 3.32 (dd, *J* = 15.5, 10.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 158.8, 158.4, 131.4, 129.1, 128.5, 126.7, 125.8, 125.2, 122.5, 121.9, 117.0, 110.1, 83.3, 52.2, 37.2.

HRMS (ESI) calculated for $C_{16}H_{15}O_4$ ($[M+H]^+$): 271.0965; found: 271.0961.

Another batch of reaction was conducted by using 4-CO_2Me substituted 2-alkenylphenol with *N*-phenoxyacetamide **1a**, the desired compound was obtained in 13% yield (7.0 mg) as white solid.

2-(5-nitro-2,3-dihydrobenzofuran-2-yl)phenol (3r)



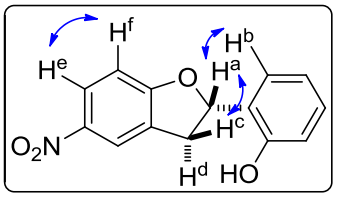
This compound was obtained in 31% yield (16.0 mg) as yellow solid. Eluent: PE/EA = 5/1, R_f = 0.4.

^{1}H NMR (400 MHz, CD_3OD): δ 8.12 (d, *J* = 8.8 Hz, 1H), 8.08 (s, 1H), 7.24 (d, *J* = 7.6 Hz, 1H), 7.13 (t, *J* = 7.7 Hz, 1H), 6.93 (d, *J* = 8.8 Hz, 1H), 6.84-6.77 (m, 2H), 6.19-6.10 (m, 1H), 3.74 (dd, *J* = 16.3, 9.7 Hz, 1H), 3.19 (dd, *J* = 16.3, 7.7 Hz, 1H).

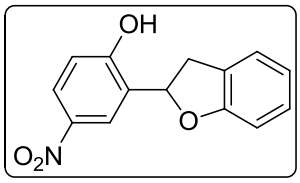
^{13}C NMR (100 MHz, CD_3OD): δ 166.8, 155.6, 143.2, 130.5, 130.2, 128.6, 127.0, 126.6, 122.2, 120.4, 116.2, 109.9, 84.1, 37.3.

HRMS (ESI) calculated for $C_{14}H_{12}NO_4$ ($[M+H]^+$): 258.0761; found: 258.0760.

^{1}H-^{1}H NOESY:



2-(5-nitro-2,3-dihydrobenzofuran-2-yl)phenol (3r')



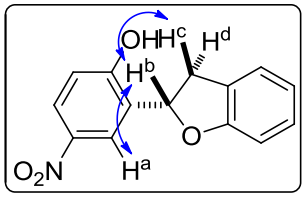
This compound was obtained by using 4-NO_2 substituted 2-alkenylphenol with *N*-phenoxyacetamide **1a**, affording the desired product **3r'** in 64% yield (32.8 mg) as yellow solid. Eluent: PE/EA = 5/1, R_f = 0.4.

^{1}H NMR (400 MHz, CD_3OD): δ 8.19 (d, *J* = 2.3 Hz, 1H), 8.05 (dd, *J* = 8.9, 2.6 Hz, 1H), 7.17-7.12 (m, 2H), 6.92-6.89 (m, 2H), 6.85 (t, *J* = 7.4 Hz, 1H), 5.99-5.89 (m, 1H), 3.74 (dd, *J* = 15.9, 9.6 Hz, 1H), 2.99 (dd, *J* = 15.8, 7.3 Hz, 1H).

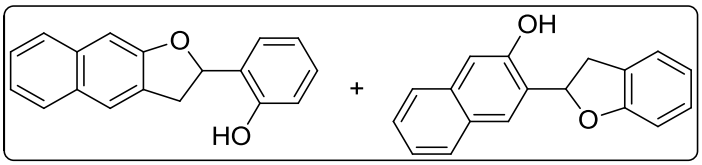
^{13}C NMR (100 MHz, CD_3OD): δ 162.4, 160.7, 141.2, 131.8, 129.2, 127.5, 126.1, 125.9, 122.8, 122.0, 116.3, 110.2, 80.0, 38.2.

HRMS (ESI) calculated for $C_{14}H_{12}NO_4$ ($[M+H]^+$): 258.0761; found: 258.0759.

^{1}H-^{1}H NOESY:



2-(2,3-dihydronaphtho[2,3-*b*]furan-2-yl)phenol (3s) & 3-(2,3-dihydrobenzofuran-2-yl)naphthalen-2-ol (3s')



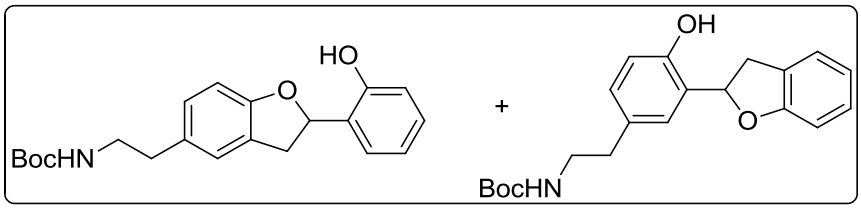
This compound was obtained in 57% yield (29.9 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.3. An inseparable mixture of two regioisomers was obtained, and the ratio was determined to be **3s**/**3s'** = 1/0.33 by ^{1}H-NMR analysis.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78-7.71 (m, 2.66H), 7.68 (s, 0.33H), 7.65 (s, 1H), 7.39 (t, *J* = 7.2 Hz, 1.33H), 7.31 (t, *J* = 7.5 Hz, 1.33H), 7.27-7.16 (m, 4H), 6.98-6.86 (m, 2.66H), 6.11-6.05 (m, 0.33H), 6.04-5.98 (m, 1H), 3.77-3.65 (m, 1.33H), 3.50-3.34 (m, 1.33H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 158.9, 157.5, 154.1, 152.1, 134.5, 130.1, 129.6, 129.4, 128.8, 128.7, 128.4, 128.0, 127.8, 127.1, 127.0, 126.7, 126.3, 126.2, 126.1, 126.0, 125.2, 124.0, 123.83, 123.82, 121.5, 120.7, 116.9, 111.1, 110.0, 104.5, 83.5, 82.8, 37.2, 36.7.

HRMS (ESI) calculated for $C_{18}H_{15}O_2$ ($[M+H]^+$): 263.1067; found: 263.1063.

***tert*-butyl (2-(2-(2-hydroxyphenyl)-2,3-dihydrobenzofuran-5-yl)ethyl)carbamate (3t) & *tert*-butyl 3-(2,3-dihydrobenzofuran-2-yl)-4-hydroxyphenethylcarbamate (3t')**



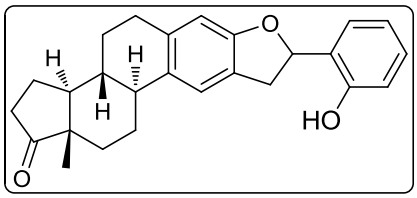
This compound was obtained in 72% yield (50.9 mg) as white solid. Eluent: PE/EA = 10/1, R_f = 0.4. An inseparable mixture of two regioisomers was obtained, and the ratio was determined to be 1/1 by ^{1}H-NMR analysis.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26 (d, *J* = 7.4 Hz, 0.5H), 7.19-7.13 (m, 1.5H), 7.09 (s, 0.5H), 7.00-6.93 (m, 1.5H), 6.91-6.86 (m, 2H), 6.82 (d, *J* = 3.0 Hz, 0.5H), 6.80 (d, *J* = 3.3 Hz, 0.5H), 6.00-5.89 (m, 1H), 4.65 (brs, 1H), 3.63-3.52 (m, 1H), 3.36-3.15 (m, 3H), 2.74-2.67 (m, 2H), 1.44 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.1, 157.8, 156.4, 154.0, 152.6, 131.5, 130.4, 129.9, 129.2, 129.0, 128.5, 128.2, 127.5, 127.2, 127.1, 126.8, 126.5, 125.4, 125.1, 121.1, 120.2, 116.4, 116.2, 115.6, 109.7, 109.5, 82.2, 82.0, 79.7, 42.3, 42.1, 37.2, 35.8, 35.4, 28.5.

HRMS (ESI) calculated for $C_{21}H_{25}NNaO_4$ ($[M+Na]^+$): 378.1676; found: 378.1668.

(*3aR,3bS,10bR,12aR*)-8-(2-hydroxyphenyl)-12*a*-methyl-2,3,3*a*,3b,4,5,7,8,10*b*,11,12,12*a*-dodecahydro-1*H*-cyclopenta[7,8]phenanthro[3,2-*b*]furan-1-one (3u)



This compound was obtained in 36% yield (27.9 mg) as white solid. Eluent: PE/EA = 10/1, R_f = 0.45. An inseparable mixture of two diastereoisomers was obtained, and the *dr* = 1/1 was determined by ^{1}H-NMR analysis.

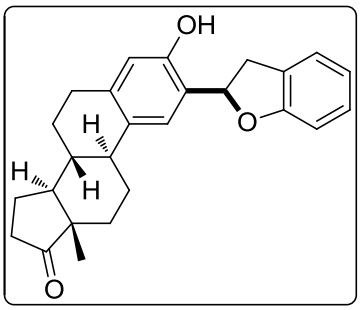
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21 (d, *J* = 7.3 Hz, 1H), 7.16 (t, *J* = 7.8 Hz, 1H), 7.13 (s, 1H), 6.94-6.89 (m, 2H), 6.64 (s, 1H), 5.91-5.85 (m, 1H), 3.59-3.47 (m, 1H), 3.32 (dd, *J* = 15.4, 10.2 Hz, 1H), 2.91-2.80 (m, 2H), 2.50 (dd, *J* = 18.9, 8.5 Hz, 1H), 2.41-2.35 (m, 1H), 2.27-1.89 (m, 5H), 1.69-1.36 (m, 6H), 0.91 (s, 1.5H), 0.90 (s,

1.5H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 221.4, 158.8, 152.24, 152.18, 137.99, 137.95, 131.9, 128.3, 127.22, 127.18, 125.1, 124.0, 121.4, 116.9, 110.0, 83.8, 83.7, 50.5, 48.2, 44.1, 38.4, 37.2, 36.0, 31.6, 29.3, 26.59, 26.57, 26.10, 26.06, 21.7, 14.0.

HRMS (ESI) calculated for $C_{26}H_{29}O_3$ ($[M+H]^+$): 389.2111; found: 389.2106.

(*8R,9S,13S,14S*)-2-((*R*)-2,3-dihydrobenzofuran-2-yl)-3-hydroxy-13-methyl-7,8,9,11,12,13,15,16-octahydro-6*H*-cyclopenta[*a*]phenanthren-17(14*H*)-one (3u')



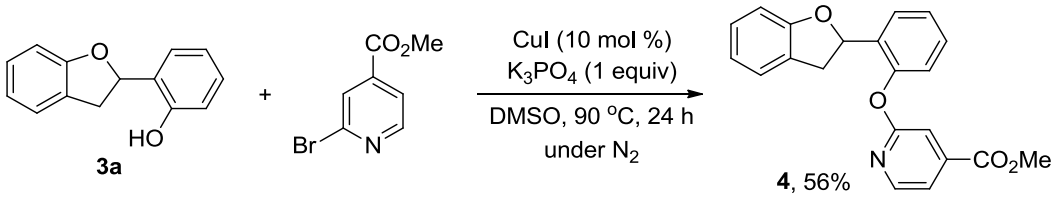
This compound was obtained in 26% yield (20.1 mg) as white solid. Eluent: PE/EA = 10/1, R_f = 0.4. An inseparable mixture of two diastereoisomers was obtained, and the *dr* = 1/1 was determined by ^{1}H-NMR analysis.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24-7.15 (m, 3H), 6.95-6.77 (m, 3H), 6.66 (s, 1H), 5.93-5.88 (m, 1H), 3.60-3.47 (m, 1H), 3.31-3.21 (m, 1H), 2.95-2.85 (m, 2H), 2.51 (dd, *J* = 18.9, 8.5 Hz, 1H), 2.42-2.36 (m, 1H), 2.28-2.23 (m, 1H), 2.20-1.94 (m, 4H), 1.67-1.40 (m, 6H), 0.92 (s, 1.5H), 0.91 (s, 1.5H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 221.6, 157.0, 156.9, 154.28, 154.25, 136.8, 132.9, 129.3, 126.9, 126.3, 124.8, 124.7, 122.0, 121.9, 120.4, 116.8, 109.9, 83.6, 83.5, 50.5, 48.2, 44.4, 44.3, 38.51, 38.48, 37.23, 37.16, 36.0, 31.7, 30.0, 26.64, 26.63, 26.4, 26.2, 21.7, 14.0.

HRMS (ESI) calculated for $C_{26}H_{29}O_3$ ($[M+H]^+$): 389.2111; found: 389.2106.

Derivatization of compound 3a:

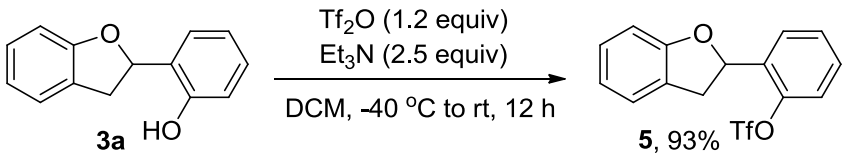


The mixture of dihydrobenzofuran **3a** (0.2 mmol), methyl 2-bromoisonicotinate (0.3 mmol), CuI (10 mol %) and K_3PO_4 (1 equiv) in DMSO (2.0 mL) was stirred at 90 ^oC in an oil bath for 24 h under an atmosphere of N_2. Afterwards, the solvent was removed under reduced pressure, and the resulted mixture was purified by preparative TLC (Eluent: PE/EA = 5/1, R_f = 0.5) to afford the corresponding product **4** in 56% yield (38.8 mg) as yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29 (d, *J* = 5.2 Hz, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.53 (dd, *J* = 5.1, 0.8 Hz, 1H), 7.38 (s, 1H), 7.37-7.32 (m, 1H), 7.27-7.23 (m, 1H), 7.12-7.09 (m, 3H), 6.86-6.79 (m, 2H), 5.93-5.86 (m, 1H), 3.96 (s, 3H), 3.51 (dd, *J* = 15.7, 9.8 Hz, 1H), 3.15 (dd, *J* = 15.8, 7.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.2, 164.2, 159.6, 150.5, 148.6, 141.2, 134.9, 129.1, 128.2, 127.1, 126.6, 125.8, 125.0, 122.1, 120.8, 117.9, 111.3, 109.4, 79.6, 52.9, 37.8.

HRMS (ESI) calculated for $C_{21}H_{18}NO_4$ ($[M+H]^+$): 348.1231; found: 348.1225.



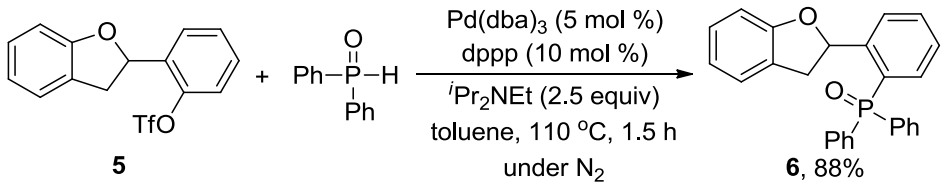
To the mixture of **3a** (1.0 mmol) in DCM (10.0 mL) was added Et_3N (2.5 equiv), and the resulted mixture was cooled to -40 ^oC, then Tf_2O (1.2 equiv) was added slowly. The resulted mixture was allowed to warm to room temperature and monitored by TLC. Afterwards, the solvent was removed under reduced pressure, and the resulted mixture was purified by preparative TLC (Eluent: PE/EA = 20/1, R_f = 0.7) to give the desired product **5** in 93% yield (0.3201 g) as yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66-7.60 (m, 1H), 7.41-7.35 (m, 2H), 7.35-7.30 (m, 1H), 7.20-7.16 (m, 2H), 6.92-6.89 (m, 2H), 6.08-5.97 (m, 1H), 3.77 (dd, *J* = 15.8, 9.7 Hz, 1H), 3.13 (dd, *J* = 15.8, 7.7 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.3, 146.1, 135.6, 129.7, 128.9, 128.5, 127.8, 125.8, 125.2, 121.3, 118.7 (q, *J* = 318.5 Hz), 109.6, 78.0, 38.2.

^{19}F NMR (376 MHz, $CDCl_3$): δ -73.61.

HRMS (ESI) calculated for $C_{15}H_{12}F_3O_4S$ ([M+H]$^+$): 345.0403; found: 345.0402.



5 **6**, 88%

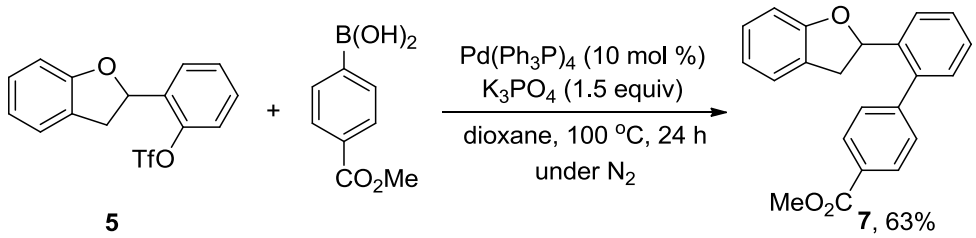
The mixture of 5 (0.2 mmol), diphenylphosphine oxide (0.3 mmol), $Pd(dba)_3$ (5 mol %), dppp (10 mol %) and ^{i}Pr$_2$NEt (2.5 equiv) in toluene (1.0 mL) was stirred at 100 ^{o}C in an oil bath for 1.5 h under an atmosphere of N_2. Afterwards, the reaction was cooled to room temperature, diluted with EA and transferred to a round bottom flask, the solvent was removed under reduced pressure, and the resulted mixture was purified by preparative TLC (Eluent: PE/EA = 3/1, R_f = 0.3) to give the desired product **6** in 88% yield (70.0 mg) as yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (dd, *J* = 7.6, 3.8 Hz, 1H), 7.70-7.61 (m, 4H), 7.59-7.44 (m, 7H), 7.24 (t, *J* = 6.7 Hz, 1H), 7.14-7.02 (m, 3H), 6.86-6.76 (m, 2H), 6.44-6.39 (m, 1H), 3.65 (dd, *J* = 16.1, 9.6 Hz, 1H), 3.00 (dd, *J* = 16.1, 8.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.8, 148.1 (d, *J* = 7.1 Hz), 148.1, 133.4, 133.3, 133.14, 133.06, 132.88, 132.87, 132.4, 132.3, 132.23, 132.20, 132.17, 132.0, 131.9, 131.8, 129.5, 128.9, 128.8, 128.7, 128.5, 128.0, 127.3, 127.2, 127.1, 127.0, 126.6, 125.1, 120.8, 109.1, 81.7 (d, *J* = 5.4 Hz), 39.7.

^{31}P NMR (162 MHz, $CDCl_3$): δ 32.22.

HRMS (ESI) calculated for $C_{26}H_{22}O_2P$ ([M+H]$^+$): 397.1352; found: 397.1348.



5 **7**, 63%

The mixture of 5 (0.2 mmol), arylboronic acid (0.3 mmol), $Pd(Ph_3P)_4$ (5 mol %)

and K_3PO_4 (1 equiv) in dioxane (1.0 mL) was stirred at 100 ^oC in an oil bath for 24 h under an atmosphere of N_2. Afterwards, the reaction was cooled to room temperature, diluted with EA and transferred to a round bottom flask, the solvent was removed under reduced pressure, and the resulted mixture was purified by preparative TLC (Eluent: PE/EA = 1/0, R_f = 0.3) to afford the desired product **7** in 63% yield (36.8 mg) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.2 Hz, 2H), 7.63 (d, *J* = 7.4 Hz, 1H), 7.44 (d, *J* = 8.2 Hz, 2H), 7.41-7.33 (m, 2H), 7.27-7.24 (m, 1H), 7.15-7.07 (m, 2H), 6.88-6.79 (m, 2H), 5.77-5.71 (m, 1H), 3.94 (s, 3H), 3.34 (dd, *J* = 15.7, 9.5 Hz, 1H), 3.15 (dd, *J* = 15.6, 8.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 159.6, 145.5, 139.7, 139.6, 129.73, 129.69, 129.5, 129.2, 128.7, 128.3, 127.9, 126.4, 126.0, 124.9, 120.8, 109.4, 107.2, 81.0, 52.3, 38.9.

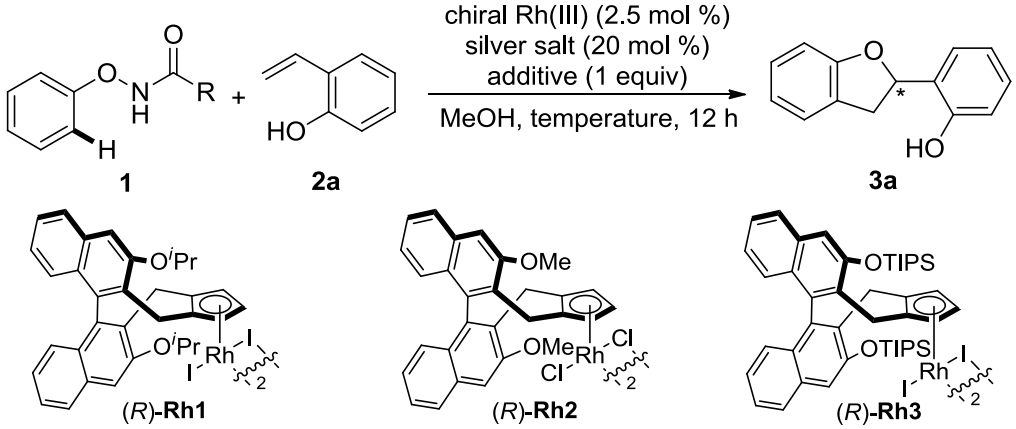
HRMS (ESI) calculated for $C_{22}H_{19}O_3$ ($[M+H]^+$): 331.1329; found: 331.1323.

Asymmetric synthesis of 3a:

Optimization studies:

The mixture of *N*-phenoxy amide **1** (0.1 mmol, 1.0 equiv), 2-alkenylphenol **2a** (1.3 equiv), chiral Rh(III) catalyst (2.5 mol %) and additives in the MeOH (1.0 mL) was stirred for 12 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 dihydrobenzofuran product **3a**. The ee was analyzed by HPLC using an IC-3 column.

Table S2. Chiral Cp^XRh(III) enabled enantioselective synthesis of dihydrobenzofuran 3a:



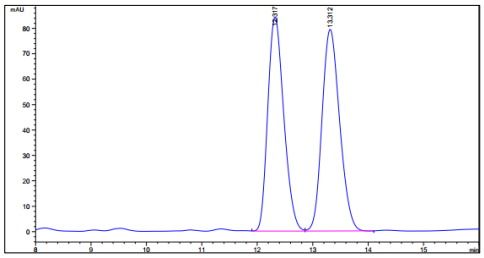
Entry	R	Rh(III)	Silver salt (20 mol %)	Zinc salt (1 equiv)	Additive (10 mol %)	Yields (%)	e.r.[b]
1	Me	(*R*)-**Rh1**	-	$Zn(OAc)_2$	-	n.d.	-
2	Me	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OAc)_2$	-	77	20:80
3	Me	(*R*)-**Rh2**	$AgSbF_6$	$Zn(OAc)_2$	-	57	42:58
4	Me	(*R*)-**Rh3**	$AgSbF_6$	$Zn(OAc)_2$	-	24	33:67
5	Me	(*R*)-**Rh1**	$AgBF_4$	$Zn(OAc)_2$	-	66	20:80
6	Me	(*R*)-**Rh1**	AgOTf	$Zn(OAc)_2$	-	14	18:82
7	Me	(*R*)-**Rh1**	AgOAc	$Zn(OAc)_2$	-	10	18:82
8	Me	(*R*)-**Rh1**	$AgNTf_2$	$Zn(OAc)_2$	-	49	17:83
9	Me	(*R*)-**Rh1**	AgF	$Zn(OAc)_2$	-	46	16:84
10	Me	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OAc)_2$	$CuCl_2$	68	24:76
11	Me	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OAc)_2$	$ZnCl_2$	92	21:79
12	Me	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OAc)_2$	KOPiv	80	22:78
13	Me	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OPiv)_2$	-	93	18:82
14	Et	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OPiv)_2$	-	71	20:80
15	^{i}Pr	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OPiv)_2$	-	9	33:67
16	Piv	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OPiv)_2$	-	n.d.	-
17	cyclopentyl	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OPiv)_2$	-	61	28:72
18	cyclohexyl	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OPiv)_2$	-	33	31:69
19	Ts	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OPiv)_2$	-	n.d.	-
20[c]	Me	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OPiv)_2$	-	61	19:81
21[d]	Me	(*R*)-**Rh1**	$AgSbF_6$	$Zn(OPiv)_2$	-	64	18:82

[a]Reaction Conditions: **1** (0.1 mmol), **2a** (0.13 mmol), chiral Rh(III) catalyst (2.5 mol %), silver salt (20 mol %), zinc salt (1 equiv) and additive in MeOH (0.1 M) at 0 ^{o}C for 12 h without exclusion of air or moisture, isolated yield were reported. [b]Determined by HPLC analysis with a

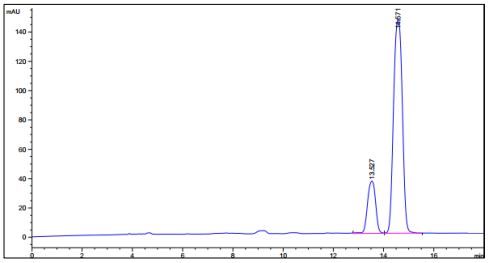
chiral stationary phase. [c]The reaction was conducted at -20 °C. [d]1 mol % of (*R*)-**Rh1** catalyst was used.

General procedure for the enantioselective synthesis of dihydrobenzofuran derivative 3a: The mixture of *N*-phenoxyacetamide **1a** (0.1 mmol, 1.0 equiv), 2-alkenylphenol **2a** (1.3 equiv), *(R)*-**Rh1** (2.5 mol %), $AgSbF_6$ (20 mol %) and $Zn(OPiv)_2$ (1.0 equiv) in MeOH (1.0 mL) was stirred at 0 °C for 12 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduced pressure, and the resulted mixture was purified by preparative TLC to afford the corresponding enantioenriched dihydrobenzofuran derivative **3a**.

HPLC conditions: Daicel Chiralpak IC-3 column (98:2 hexane: 2-propanol, 1.0 mL/min, 30 °C, 254 nm); tr (minor) = 13.53 min, tr (major) = 14.57 min, 18:82 er.



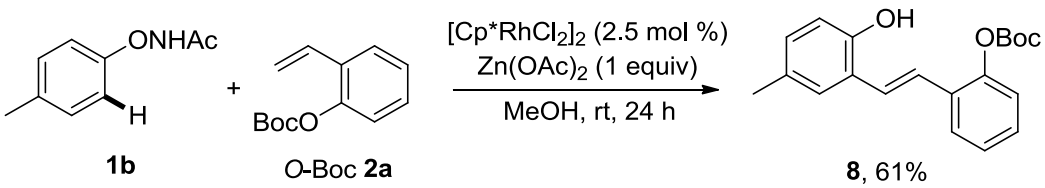
No.	Time	Area	Area(%)
1	12.317	1690.9946	49.0824
2	13.312	1754.2058	50.9176



No.	Time	Area	Area(%)
1	13.527	795.86792	18.3716
2	14.571	3536.17920	81.6284

III. Experimental Mechanistic Studies

Defining the role of -OH:



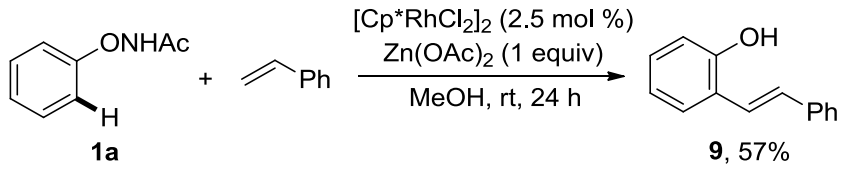
The mixture of *N*-aryloxyacetamide **1b** (0.1 mmol), *O*-Boc **2a** (1.3 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol %) and $Zn(OAc)_2$ (1.0 equiv) in MeOH (1.0 mL) was stirred at room temperature for 24 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduced pressure, and the resulted mixture was purified

by preparative TLC (Eluent: PE/EA = 10/1, R_f = 0.30) to afford the *ortho* C-H alkenylation product **8** in 61% (20.0 mg) isolated yield as white solid.

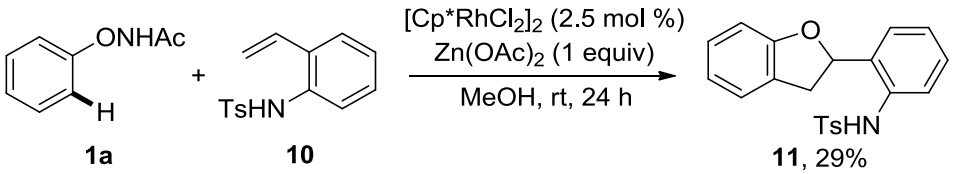
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (dd, *J* = 7.4, 2.0 Hz, 1H), 7.38-7.34 (m, 1H), 7.31 (d, *J* = 1.9 Hz, 1H), 7.29-7.21 (m, 2H), 7.19-7.12 (m, 2H), 6.93 (d, *J* = 8.9 Hz, 1H), 6.67 (dd, *J* = 8.1, 1.3 Hz, 1H), 5.28 (brs, 1H), 2.29 (s, 3H), 1.55 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 152.1, 151.3, 148.5, 130.6, 130.1, 129.7, 128.4, 127.6, 126.8, 126.4, 125.7, 124.3, 122.8, 122.5, 116.0, 84.0, 27.8, 20.7.

HRMS (ESI) calculated for $C_{20}H_{21}O_4$ ([M-H]$^-$): 325.1445; found: 325.1445.



The mixture of *N*-phenoxyacetamide **1a** (0.1 mmol), styrene (1.3 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol %) and $Zn(OAc)_2$ (1.0 equiv) in MeOH (1.0 mL) was stirred at room temperature for 24 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduced pressure, and the resulted mixture was purified by preparative TLC to afford the *ortho* C-H alkenylation product **9** in 57% (11.2 mg) isolated yield as white solid. **9** is a known compound and the characteristic data is in agreement with literature precedent.[S4]



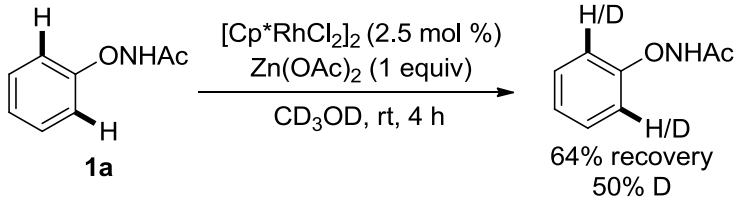
The mixture of *N*-phenoxyacetamide **1a** (0.2 mmol), 2-vinylaniline **10** (1.3 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol %) and $Zn(OAc)_2$ (1.0 equiv) in MeOH (2.0 mL) was stirred at room temperature for 24 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduced pressure, and the resulted mixture was purified by preparative TLC (Eluent: PE/EA = 5/1, R_f = 0.5) to afford the C-H annulation product **11** in 29% (21.2 mg) isolated yield as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.1 Hz, 1H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.29-7.21 (m, 1H), 7.18 (d, *J* = 8.1 Hz, 2H), 7.14 (d, *J* = 7.5 Hz, 2H), 7.09-7.06 (m, 2H), 6.87 (d, *J* = 8.4 Hz, 1H), 6.81 (t, *J* = 7.5 Hz, 1H), 5.56 (dd, *J* = 9.7, 2.7 Hz, 1H), 3.12 (dd, *J* = 16.4, 9.7 Hz, 1H), 2.91 (dd, *J* = 16.4, 2.6 Hz, 1H), 2.37 (s, 3H).

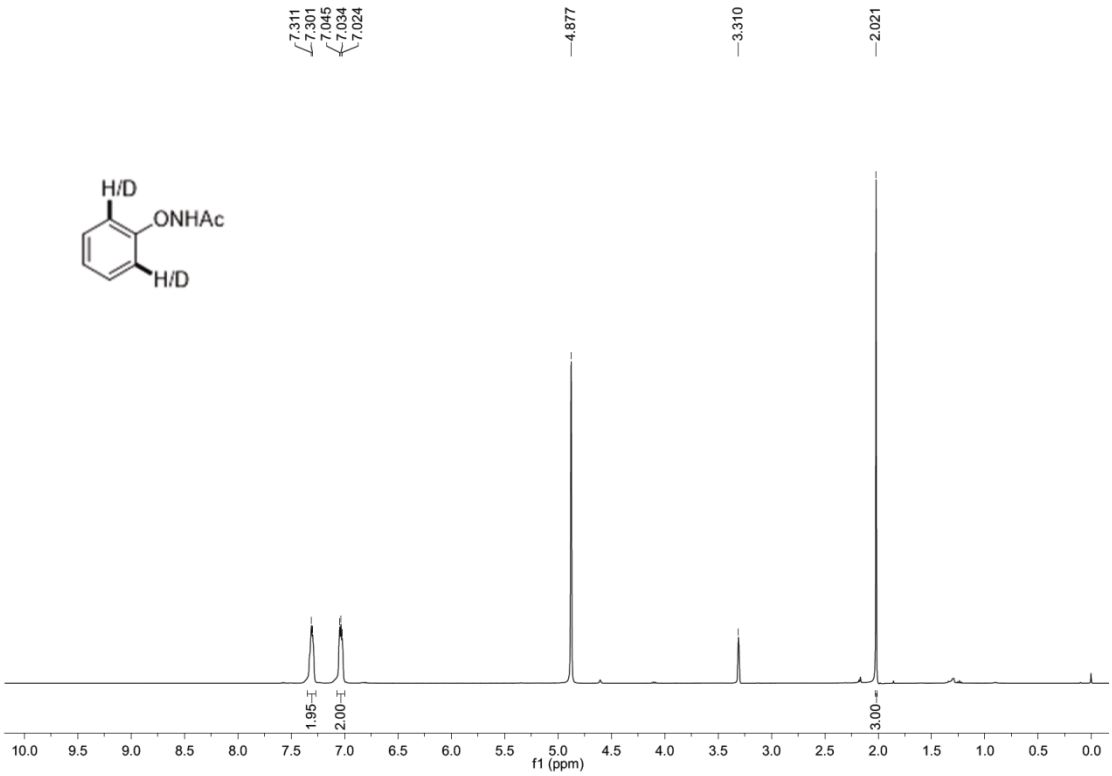
^{13}C NMR (100 MHz, $CDCl_3$): δ 153.2, 144.4, 141.3, 134.6, 132.6, 129.8, 129.2, 128.6, 128.1, 127.3, 126.9, 125.3, 125.0, 121.1, 117.7, 117.2, 60.3, 36.3, 21.7.

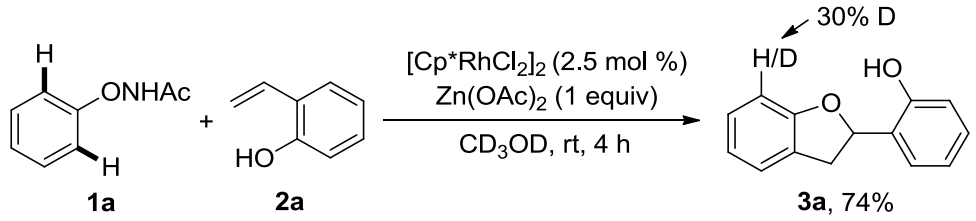
HRMS (ESI) calculated for $C_{21}H_{20}NSO_3$ ($[M+H]^+$): 366.1159; found: 366.1150.

Deuterium-labeling experiments:

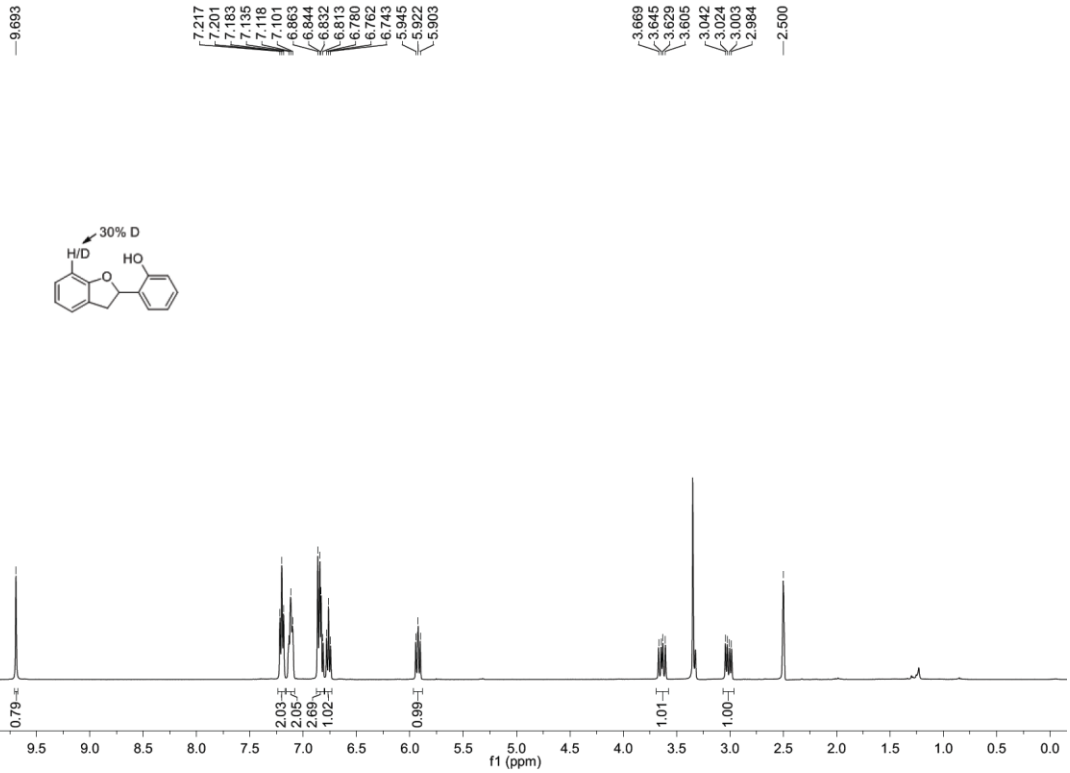


N-phenoxyacetamide **1a** (0.1 mmol) was dissolved in CD_3OD (1.0 mL) in the presence of $[Cp^*RhCl_2]_2$ (2.5 mol %) and $Zn(OAc)_2$ (0.1 mmol). The reaction was conducted under the standard condition for 4 h, afterwards, **1a** was recovered by flash column chromatography on silica gel (Eluent: PE/EA = 2/1) and was analyzed by ^{1}H-NMR spectroscopy. 50% deuteration was detected by ^{1}H-NMR analysis.



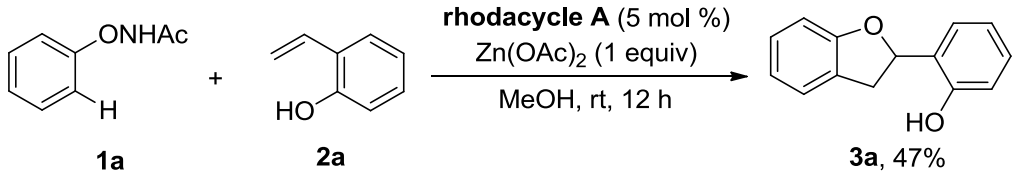


The mixture of *N*-phenoxyacetamide **1a** (0.1 mmol), **2a** (1.3 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol %) and $Zn(OAc)_2$ (1 equiv) in MeOH (1.0 mL) was stirred at room temperature for 4 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduce pressure, and **3a** was purified by preparative TLC in 74% yield (15.7 mg). ^{1}H-NMR analysis showed that 30% deuterium incorporation at the *ortho*-position of the -ONHAc ODG (see the multiplet at δ 6.87-6.81 ppm).



Defining the five-membered rhodacycle as the active intermediate:

The rhodacycle complex A is a known compound and synthesized according to a known procedure.[S5]



The mixture of *N*-phenoxyacetamide **1a** (0.1 mmol), 2-alkenylphenol **2a** (1.3 equiv), rhodacycle A (5 mol %) and $Zn(OAc)_2$ (1.0 equiv) in MeOH (1.0 mL) was stirred at room temperature for 12 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduced pressure, and the resulted mixture was purified by preparative TLC to afford the corresponding products **3a** in 47% yield.

IV. X-Ray Crystallographic Data

Experimental: The sample was dissolved in appropriate amount of EtOAc followed by the addition of PE to furnish a saturated solution. Afterwards, the mixture was allowed to stand at -20 ^{o}C to form the crystals. A suitable crystal was selected and

measured on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. The crystal was kept at 150.00(10) K during data collection.

Crystal structure determination: Crystal Data for $C_{15}H_{11}F_3O_2$ (*M* =280.24 g/mol): monoclinic, space group Pc (no. 7), *a* = 5.6437(5) Å, *b* = 9.0829(10) Å, *c* = 25.058(2) Å, *β* = 92.384(9) °, *V* = 1283.4(2) Å^3, *Z* = 4, *T* = 150.00(10) K, μ(Cu Kα) = 1.078 mm^{-1}, *Dcalc* = 1.450 g/cm^3, 4025 reflections measured (7.062° ≤ 2Θ ≤ 133.134 °), 3116 unique (R_{int} = 0.0331, R_{sigma} = 0.0483) which were used in all calculations. The final R_1 was 0.1165 (I > 2σ(I)) and wR_2 was 0.3677 (all data). The crystallographic data have already been deposited at the Cambridge Crystallographic Data Centre (CCDC numbers: 2117606), which can be acquired from www.ccdc.cam.ac.uk/data_request/cif.

The ellipsoid contour percent probability level is 50% for the image of the structure.

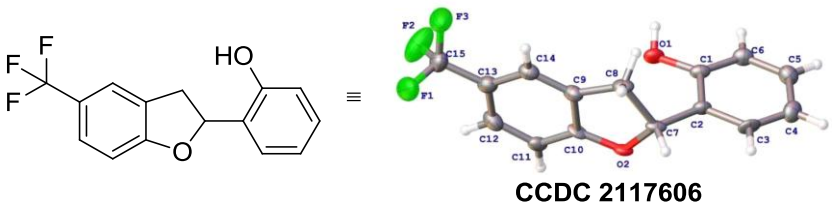


Table S3. Crystal data and structure refinement for **3p**

Identification code	cf3
Empirical formula	$C_{15}H_{11}F_3O_2$
Formula weight	280.24
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	Pc
a/Å	5.6437(5)
b/Å	9.0829(10)
c/Å	25.058(2)
α/°	90
β/°	92.384(9)
γ/°	90
Volume/Å^3	1283.4(2)
Z	4

ρ_{calc}g/cm^3	1.450
μ/mm^{-1}	1.078
F(000)	576.0
Crystal size/mm^3	0.13 × 0.11 × 0.09
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.062 to 133.134
Index ranges	-6 ≤ h ≤ 6, -6 ≤ k ≤ 10, -29 ≤ l ≤ 29
Reflections collected	4025
Independent reflections	3116 [R_{int} = 0.0331, R_{sigma} = 0.0483]
Data/restraints/parameters	3116/242/420
Goodness-of-fit on F^2	1.636
Final R indexes [I>=2σ (I)]	R_1 = 0.1165, wR_2 = 0.3613
Final R indexes [all data]	R_1 = 0.1212, wR_2 = 0.3677
Largest diff. peak/hole / e Å^{-3}	0.54/-0.53
Flack parameter	-0.2(4)

V. DFT Calculations

Computational details:

Density functional theory (DFT) calculations were performed by using Gaussian 09 quantum chemical package.[S6] Unless otherwise specified, the geometries of all reported reactants, intermediates, transition states and products were optimized using the B3LYP functional[S7] with the standard 6-31G(d) basis set (Lanl2dz[S8] basis set for Rh) (denoted as B3LYP/BS1). Frequency analysis was conducted at the same level of theory to verify the stationary points to be real minima or saddle points and to obtain the thermodynamic energy corrections. Intrinsic reaction coordinate (IRC) calculations[S9] were carried out to confirm that all transition state structures connect the corresponding reactants and products. Solvent effects in methanol were estimated by using the SMD[S10] solvation method at the B3LYP level of theory with the DFT-D3(BJ) dispersion corrections.[S11] Herein, SDD[S12] was used for Rh and the 6-311++G(d,p) basis set was used for all other atoms. This combination is named B3D3 SMD/BS2. If not noted, the energies presented in this paper are the B3D3-calculated single point energies with B3LYP-calculated thermodynamic

corrections which were calculated under standard conditions (1 atm and 298.15 K) (denoted as ΔG_{sol} (B3D3 SMD/BS2//B3LYP/BS1) or ΔG for clarity). Computed structures are illustrated using CYLVIEW.[S13]

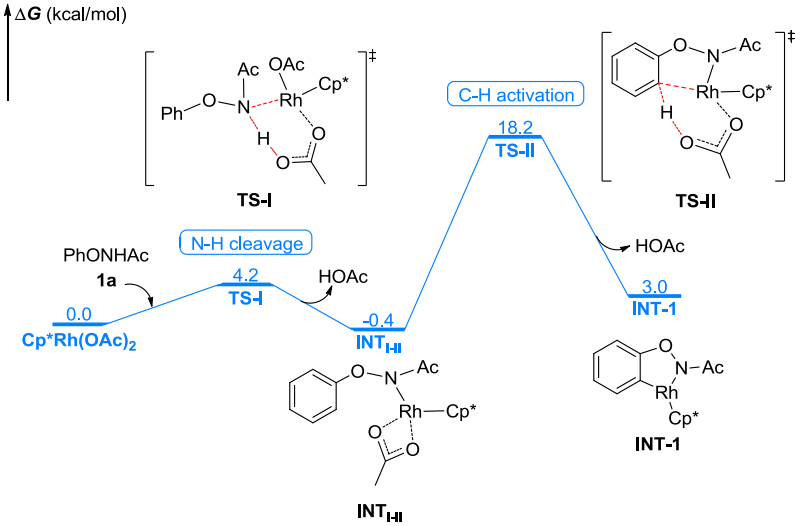


Figure S1. Computed Gibbs free energy changes of N-H/C-H bond cleavage.

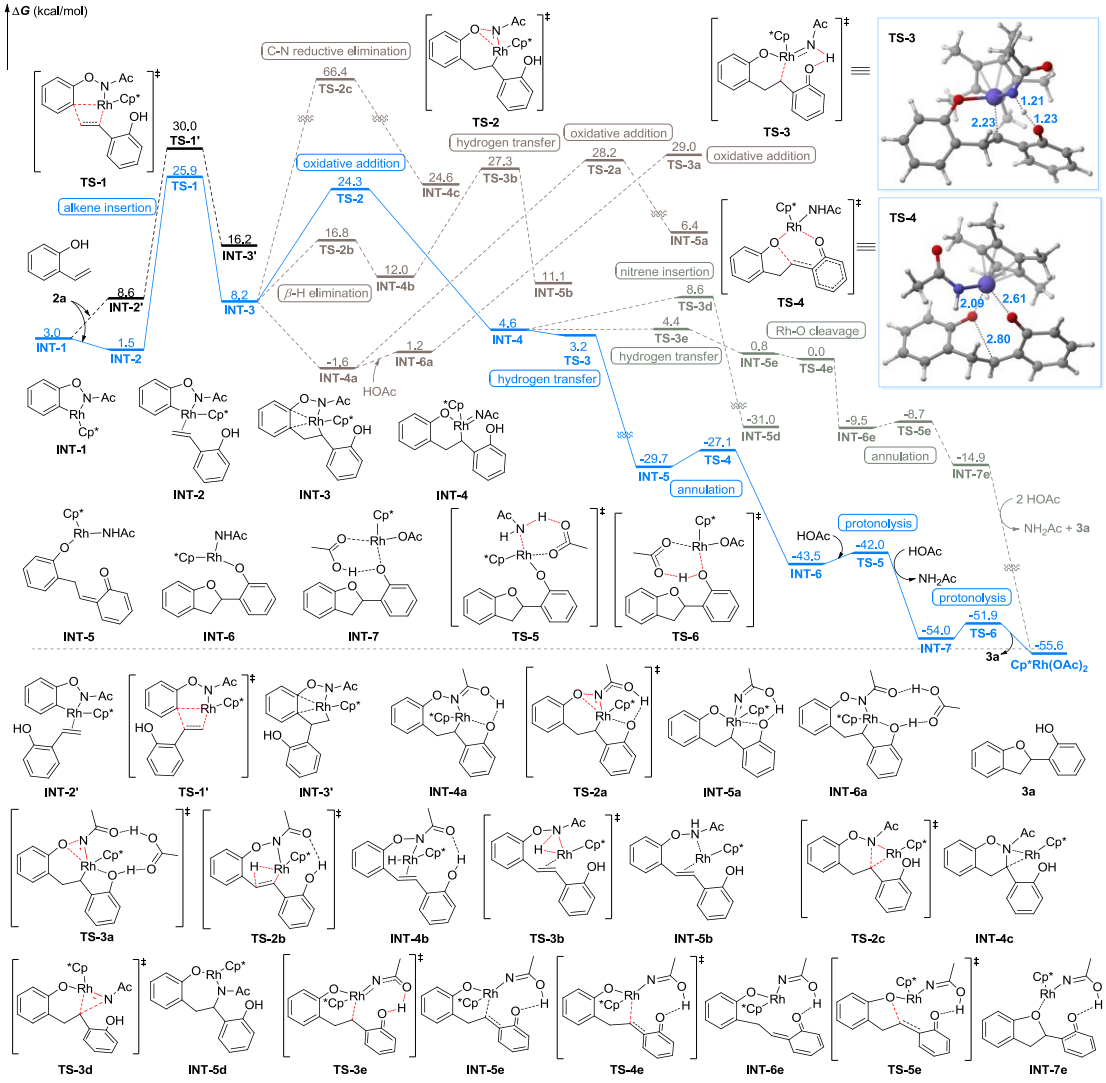


Figure S2. Computed Gibbs free energy changes of the reaction pathways from **INT-1**.

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

Table S4. Energy, enthalpy and free energy corrections of the structures calculated at B3LYP/BS1, single point energies at the B3D3 SMD/BS2//B3LYP/BS1 level (in Hartree) and imaginary frequencies of the transition states.

Structures	corr. to ZPE	corr. to *E*	corr. to *H*	corr. to *G*	SP_{SMD}	Imaginary frequency
Cp*Rh(OAc)$_2$	0.327264	0.351500	0.352444	0.272969	-958.087430	—
1a	0.159145	0.169346	0.170290	0.121710	-515.620930	—

2a	0.137981	0.145871	0.146815	0.105342	-385.021147	—
3a	0.226737	0.238719	0.239663	0.187851	-691.423730	—
HOAc	0.062073	0.066618	0.067562	0.034930	-229.182762	—
NH_2Ac	0.073793	0.079015	0.079960	0.045935	-209.313613	—
TS-I	0.482650	0.518171	0.519116	0.412537	-1473.719454	-815.13
INT_{I-II}	0.423746	0.453682	0.454626	0.361568	-1244.528056	—
TS-II	0.418779	0.447852	0.448796	0.359906	-1244.496748	-932.47
INT-1	0.360731	0.384546	0.385491	0.308455	-1015.321623	—
INT-2	0.501062	0.533344	0.534289	0.438748	-1400.370196	—
TS-1	0.500706	0.532112	0.533056	0.440471	-1400.332991	-337.85
INT-3	0.502393	0.534241	0.535185	0.440777	-1400.361572	—
TS-2	0.499655	0.531597	0.532541	0.437491	-1400.332640	-198.13
INT-4	0.500786	0.533033	0.533977	0.438248	-1400.364783	—
TS-3	0.495570	0.527402	0.528346	0.434138	-1400.362859	-1069.94
INT-5	0.500667	0.534184	0.535128	0.432538	-1400.413740	—
TS-4	0.500526	0.533129	0.534074	0.435970	-1400.413001	-35.38
INT-6	0.504297	0.536282	0.537226	0.440341	-1400.443495	—
TS-5	0.563914	0.601101	0.602045	0.493620	-1629.642211	-594.56
INT-7	0.554908	0.592655	0.593599	0.483722	-1649.531560	—
TS-6	0.553624	0.591368	0.592312	0.480005	-1649.524536	-29.77
INT-2'	0.501192	0.533824	0.534768	0.438845	-1400.358944	—
TS-1'	0.500683	0.532449	0.533393	0.439730	-1400.325798	-346.64
INT-3'	0.502622	0.534512	0.535456	0.440789	-1400.348733	—
INT-4a	0.503002	0.533994	0.534938	0.442843	-1400.379196	—
TS-2a	0.499514	0.531284	0.532228	0.437449	-1400.326388	-100.85
INT-5a	0.501036	0.532920	0.533864	0.439431	-1400.363028	—
INT-6a	0.566089	0.603729	0.604673	0.494578	-1629.574277	—
TS-3a	0.561684	0.599392	0.600336	0.490909	-1629.526313	-32.92
TS-2b	0.498357	0.529520	0.530465	0.438458	-1400.345506	-726.65

INT-4b	0.499979	0.531390	0.532334	0.439874	-1400.354648	—
TS-3b	0.497457	0.529174	0.530118	0.435668	-1400.325991	-1093.17
INT-5b	0.503627	0.535219	0.536163	0.443074	-1400.359180	—
TS-2c	0.500603	0.532290	0.533234	0.438359	-1400.266401	-329.80
INT-4c	0.504273	0.535383	0.536327	0.442916	-1400.337491	—
TS-3d	0.500363	0.532193	0.533138	0.438896	-1400.359074	-132.91
INT-5d	0.503993	0.535580	0.536525	0.442215	-1400.425450	—
TS-3e	0.496906	0.528671	0.529615	0.435757	-1400.362501	-687.92
INT-5e	0.501361	0.533796	0.534740	0.439550	-1400.372135	—
TS-4e	0.500685	0.532691	0.533635	0.439021	-1400.372880	-58.97
INT-6e	0.500606	0.533835	0.534779	0.435375	-1400.384341	—
TS-5e	0.500948	0.532917	0.533861	0.438611	-1400.386361	-197.29
INT-7e	0.501213	0.533486	0.534430	0.437848	-1400.395391	—
TS-3d	0.500363	0.532193	0.533138	0.438896	-1400.359074	-132.91
INT-5d	0.503993	0.535580	0.536525	0.442215	-1400.425450	—

Cartesian coordinates of the optimized structures:

Cp*Rh(OAc)$_2$

Rh	0.01372600	0.21666800	-0.09621600
C	1.23328100	-1.17366900	1.07994900
C	1.11966400	-1.70457500	-0.25047500
C	1.65512800	-0.73313700	-1.16495800
C	2.19585200	0.37308200	-0.37896300
C	1.93494300	0.10322300	0.99348200
C	-1.24029000	2.42134500	0.08235600
O	-0.64724900	2.10927300	-0.99912500
O	-1.09123200	1.67632500	1.10439300
C	-2.13899200	3.62948600	0.14275800
H	-3.15448400	3.32531500	-0.13689600
H	-2.16956700	4.03403000	1.15733600
H	-1.80333500	4.39180400	-0.56453000
O	-1.87683200	-0.38196200	-0.67763700
C	-2.51624400	-1.31118000	-0.02238100
O	-2.07184700	-2.00067800	0.89858800

C	-3.95687700	-1.47672000	-0.50383800
H	-4.55949500	-0.64217000	-0.12663200
H	-4.00934700	-1.45107200	-1.59632400
H	-4.37245200	-2.41297700	-0.12494700
C	2.87932100	1.57564400	-0.95588500
H	3.90605600	1.32666200	-1.25549700
H	2.35051800	1.94324000	-1.84021100
H	2.92784900	2.39543000	-0.23520900
C	2.28590700	0.96147800	2.17108600
H	3.11792300	0.51693400	2.73268100
H	2.58620600	1.96640700	1.86476600
H	1.43522800	1.05943300	2.85205900
C	1.76711700	-0.87040700	-2.65302100
H	1.68033000	0.10046500	-3.14934700
H	2.73907200	-1.30215400	-2.92965700
H	0.98504600	-1.52009400	-3.05381200
C	0.54299200	-3.03967500	-0.60657800
H	0.23245900	-3.07554600	-1.65403000
H	1.30135700	-3.82016700	-0.45458900
H	-0.32609200	-3.26105400	0.01565300
C	0.80633300	-1.86502300	2.33767800
H	-0.19957900	-2.27310200	2.21230300
H	1.50043500	-2.68099300	2.58253000
H	0.79145800	-1.17312100	3.18409000

1a

C	-2.23365700	1.49434800	0.06491700
C	-0.94789300	1.02004200	-0.21048500
C	-0.73980300	-0.35567600	-0.28105400
C	-1.79055600	-1.25472600	-0.08000300
C	-3.06522500	-0.76452600	0.19317800
C	-3.29521500	0.61263300	0.26668800
H	-2.39835900	2.56712900	0.12268800
H	-0.12194000	1.70363200	-0.36406000
H	-1.59118700	-2.32022000	-0.13643900
H	-3.88155400	-1.46417000	0.35134700
H	-4.29008600	0.99169000	0.48149500
O	0.48132400	-0.95642600	-0.56075800
N	1.53907300	-0.05959900	-0.74606100
H	1.88368900	-0.14985500	-1.69716100
C	2.48695100	-0.02984900	0.28078300
O	2.25532600	-0.41386100	1.40643000
C	3.80331900	0.59892800	-0.15163700
H	3.75147800	1.09823700	-1.12454000

H	4.10797700	1.32443700	0.60674500
H	4.57239300	-0.18048400	-0.19409500

2a

C	-2.65893300	0.85326200	0.07609300
C	-1.25426300	0.85560000	0.04716600
C	-0.61080100	2.11208900	-0.00843500
C	-1.34909500	3.29879600	-0.04368700
C	-2.74187700	3.26012200	-0.02271500
C	-3.40163800	2.03049600	0.03814800
H	-3.17666200	-0.09892100	0.14575700
H	-0.82689900	4.25334100	-0.09032100
H	-3.30598500	4.18830200	-0.04885800
H	-4.48658300	1.99019700	0.06480400
C	-0.44670900	-0.37388300	0.08607000
C	-0.88616200	-1.62617000	-0.09873500
H	0.61207600	-0.22019100	0.27641300
H	-0.20433600	-2.46896900	-0.03657700
H	-1.92263900	-1.86325900	-0.32475800
O	0.75924800	2.12195500	-0.03296500
H	1.06427700	3.04214000	-0.04860600

3a

C	-0.70143100	12.63329600	-2.87737200
C	-0.40651900	11.31985800	-3.22352500
C	0.77188600	11.04095200	-3.91891900
C	1.68057300	12.02341100	-4.28618600
C	1.37016300	13.34296400	-3.93251300
C	0.19476500	13.64852700	-3.24060800
H	-1.61145600	12.87243900	-2.33304200
H	2.58548400	11.77337800	-4.83036000
H	2.05490800	14.14013700	-4.20857200
H	-0.02683900	14.68009600	-2.98288800
O	0.93183700	9.69340900	-4.17954400
C	-0.38478900	9.06631800	-3.96002700
H	-0.90578000	9.12040400	-4.92431400
C	-0.24184800	7.62571100	-3.54530400
C	0.73457500	7.20803700	-2.61710500
C	-1.15771200	6.68163500	-4.02549600
C	0.75428100	5.88158300	-2.17078500
C	-1.14323400	5.36072900	-3.58077900
H	-1.90039500	6.99725400	-4.75567800
C	-0.18417700	4.96786300	-2.64335300
H	1.52092300	5.59180700	-1.45887700

H	-1.86684100	4.64739200	-3.96369400
H	-0.15648200	3.94088900	-2.28877600
O	1.67635400	8.05804400	-2.11994900
C	-1.09983000	10.00545100	-2.95030800
H	-0.92789500	9.66968800	-1.91895600
H	-2.18053000	10.01749400	-3.12155100
H	1.73029400	8.82094100	-2.72924300

HOAc

C	-3.21269700	0.01353000	-0.04836400
O	-2.01617200	0.00790700	-0.22983200
O	-3.91600300	1.16019500	0.14023200
H	-3.26340000	1.88432800	0.09308200
C	-4.11158700	-1.19696400	0.00089600
H	-4.62031900	-1.24704100	0.96931800
H	-4.88545300	-1.12106700	-0.77017800
H	-3.51768600	-2.09782000	-0.15487700

NH_2Ac

N	2.51304600	9.69551600	0.08311100
C	3.16830400	10.24655700	1.15367800
O	4.37457900	10.13502500	1.30722300
H	1.54267100	9.88675000	-0.11289800
C	2.28552600	11.00630400	2.13572200
H	2.46439700	12.08093600	2.01790400
H	1.21596300	10.81284700	2.00571700
H	2.57978800	10.73424800	3.15242400
H	3.07341100	9.27157200	-0.64330400

TS-I

C	3.05835200	0.55201900	-0.48617500
C	2.35213200	0.44276300	-1.73389700
C	1.82184800	-0.89072400	-1.83431500
C	2.31037400	-1.64829000	-0.68696500
C	3.04668600	-0.76283400	0.14563200
C	2.12081700	-3.11727200	-0.46041400
H	1.89833700	-3.34118300	0.58576500
H	1.30511900	-3.51457200	-1.07045100
H	3.03455500	-3.65744000	-0.74229300
C	3.69213800	-1.09288700	1.45625000
H	3.33327200	-2.04833200	1.84617700
H	4.78297000	-1.15233400	1.34626500
H	3.46649600	-0.32258500	2.19993200
C	3.77750900	1.76619200	0.01501400

H	4.01311700	1.67042700	1.07801900
H	4.72219000	1.90557400	-0.52899900
H	3.15160900	2.65233800	-0.11601200
C	2.20258900	1.53727700	-2.74386500
H	2.07610900	2.50254300	-2.25065400
H	3.09994100	1.57403600	-3.37746900
H	1.34098800	1.36888800	-3.39486400
C	1.05352000	-1.45576400	-2.99152200
H	1.72628800	-1.95437600	-3.70282600
H	0.31171700	-2.18752100	-2.66005200
H	0.51689700	-0.67046800	-3.52930300
Rh	0.97817700	0.03965000	-0.02559600
C	-0.19100400	2.75234800	-0.45659500
O	0.92436600	3.27073500	-0.37721100
O	-0.46241700	1.47644200	-0.43095400
C	-0.06246500	0.87734200	2.70494000
O	-1.20397800	0.40468900	2.40798100
O	0.97186600	0.80236800	1.97722300
C	0.06567900	1.61653900	4.02084300
H	1.10856200	1.66114500	4.34007700
H	-0.30051900	2.64092000	3.88427500
H	-0.55138900	1.13576100	4.78393600
C	-1.45281100	3.60472800	-0.58678900
H	-2.12288500	3.19387800	-1.34775100
H	-1.99705100	3.58864800	0.36454200
H	-1.18467500	4.63516200	-0.83013200
C	-5.03035700	0.05434400	0.62548000
C	-3.71837700	-0.42955700	0.62630000
C	-3.02878300	-0.51533700	-0.58462900
C	-3.64312400	-0.13191000	-1.78269400
C	-4.95355000	0.33756300	-1.76580000
C	-5.65613000	0.43546200	-0.56055700
H	-5.56151300	0.12902000	1.57063100
H	-3.24709600	-0.70542500	1.56130400
H	-3.07880400	-0.20456400	-2.70707800
H	-5.42451700	0.63635000	-2.69866800
H	-6.67583800	0.80915200	-0.54832400
O	-1.75258200	-1.02741100	-0.73913200
N	-0.92231600	-1.07785300	0.42240500
H	-1.14809800	-0.28820700	1.33223100
C	-0.80662800	-2.39237300	0.93019700
O	-0.05865300	-2.59465500	1.87337500
C	-1.62694100	-3.48707500	0.27753100
H	-2.69677100	-3.26172000	0.33521100

H	-1.38137100	-3.58431000	-0.78481700
H	-1.41700500	-4.42277800	0.79821700

INT_{I-II}

C	3.05858200	0.08735000	-0.57522700
C	2.27864600	0.01442200	-1.75351900
C	1.35772500	-1.11522100	-1.61430400
C	1.64724800	-1.77702500	-0.37253000
C	2.64162200	-0.99761800	0.31324600
C	1.00167300	-3.03973700	0.11114700
H	1.13032200	-3.17963800	1.18632800
H	-0.07325600	-3.03505600	-0.08295200
H	1.44856200	-3.90248800	-0.40103200
C	3.30208500	-1.32640300	1.61799800
H	2.67700100	-1.97655100	2.23412200
H	4.25402400	-1.84682900	1.44310400
H	3.52011900	-0.42275000	2.19505100
C	4.11953200	1.09026300	-0.23616100
H	3.95368700	1.51741000	0.75813000
H	5.10968200	0.61569400	-0.23456900
H	4.14392100	1.91448300	-0.95300300
C	2.33027100	0.92254300	-2.94427500
H	2.92414800	1.81778800	-2.74528300
H	2.77783400	0.40354100	-3.80216000
H	1.32653500	1.24599200	-3.23726200
C	0.39543500	-1.58644100	-2.66053500
H	0.88387400	-2.29581800	-3.34318900
H	-0.46151600	-2.08501800	-2.20281300
H	0.01788600	-0.75225800	-3.25846000
Rh	0.88759300	0.28214700	-0.00387800
C	0.01469700	2.64491000	0.35510300
O	-0.32034300	1.98405000	-0.67658100
O	0.86768700	2.13793100	1.15860300
C	-0.61117100	3.98321000	0.64730500
H	-1.53292100	3.82369900	1.21913900
H	0.06312700	4.60091000	1.24522700
H	-0.87398100	4.49127500	-0.28367100
C	-4.73012600	0.92901200	0.11867100
C	-3.44779600	0.51673900	0.48661600
C	-2.86089100	-0.56293200	-0.17854300
C	-3.55905900	-1.22651700	-1.19640800
C	-4.83870500	-0.80489600	-1.54857900
C	-5.43376500	0.27853600	-0.89606100
H	-5.18309100	1.76906500	0.63990200

H	-2.90166800	1.01569000	1.27641900
H	-3.09287800	-2.07463700	-1.68950300
H	-5.37325300	-1.32839600	-2.33742300
H	-6.43189500	0.60651600	-1.17217400
O	-1.61415700	-1.06873400	0.10071000
N	-0.84700300	-0.29770200	1.03473900
C	-0.74500900	-0.99163200	2.23401900
O	-1.30500600	-2.05271900	2.48287700
C	0.06352300	-0.25064400	3.29378900
H	0.45416600	0.70817000	2.94939700
H	-0.59211400	-0.08746800	4.15611300
H	0.88646900	-0.88778400	3.63653600

TS-II

C	1.51214200	-1.72558700	-1.20668400
C	0.30207800	-2.29318100	-0.71605200
C	0.26892200	-2.09629100	0.72191800
C	1.54243500	-1.52248300	1.11265400
C	2.29009900	-1.25329900	-0.06842400
C	1.96869400	-1.29969400	2.53276800
H	2.92612900	-0.77698800	2.59060100
H	1.23565600	-0.71804900	3.10107600
H	2.08769100	-2.26791100	3.03706800
C	3.66102900	-0.65519500	-0.17478500
H	3.96989300	-0.18003100	0.75925000
H	4.40493200	-1.42471200	-0.42263300
H	3.69449300	0.10519100	-0.96177500
C	1.97952200	-1.66402700	-2.63045500
H	2.33313200	-0.65801800	-2.87871500
H	2.80947700	-2.36326300	-2.79909700
H	1.17985200	-1.92063400	-3.33020500
C	-0.72220700	-3.04335800	-1.51336900
H	-0.73738200	-2.72850200	-2.56040700
H	-0.49045600	-4.11732500	-1.49378000
H	-1.72813000	-2.91022300	-1.10934900
C	-0.76661800	-2.62563000	1.67063400
H	-0.51545600	-3.64541000	1.99502500
H	-0.83806000	-1.99790800	2.56343400
H	-1.75670000	-2.65597800	1.20775200
Rh	0.32621500	-0.09683200	-0.19088300
C	0.35589600	2.38796100	-1.93195200
O	-0.90429800	2.41632300	-1.82671300
O	1.10621500	1.49095300	-1.43442900
C	1.02726400	3.52204100	-2.68368700

H	1.16194300	4.36427500	-1.99470800
H	2.00808100	3.21637300	-3.05388500
H	0.39203500	3.85922500	-3.50616000
C	-2.66498800	-0.31886800	-1.40799600
C	-1.78250000	0.31414500	-0.49203700
C	-2.29979300	0.59688900	0.80337300
C	-3.63664300	0.32314600	1.14493100
C	-4.45652700	-0.28272900	0.20438900
C	-3.97914800	-0.61189100	-1.08050200
H	-2.30109500	-0.52615200	-2.41214400
H	-1.28986100	1.34911600	-1.09927100
H	-3.99372900	0.56757400	2.14029700
H	-5.48912100	-0.50123000	0.46570800
H	-4.64422700	-1.06869900	-1.80789600
O	-1.51280900	1.09521400	1.75893400
N	-0.17972000	1.36726000	1.24214200
C	0.62485900	1.74320100	2.29183800
O	0.29533700	1.77217600	3.47458200
C	1.99136600	2.24225100	1.83115200
H	2.15856600	2.12046100	0.75912600
H	2.05261500	3.30802400	2.07947900
H	2.77724900	1.73566700	2.40065700

INT-1

C	1.37062900	-1.97579100	-0.06397600
C	1.67071300	-1.27687800	1.15284100
C	2.35839200	-0.03331100	0.81388400
C	2.40442900	0.06711900	-0.59016000
C	1.74538500	-1.11273700	-1.14745000
C	3.01670000	1.19150700	-1.37037600
H	2.73248500	1.15039400	-2.42565100
H	2.69590900	2.15610300	-0.96661600
H	4.11343300	1.14203800	-1.32208200
C	1.63887200	-1.43571800	-2.60694800
H	1.47492900	-0.53457700	-3.20451500
H	2.56401500	-1.90917900	-2.96605800
H	0.81202800	-2.12267300	-2.80529000
C	0.87998700	-3.38831000	-0.18082800
H	0.31005900	-3.54592700	-1.10082300
H	1.72816100	-4.08681200	-0.19660800
H	0.24103000	-3.66849400	0.66140800
C	1.47170700	-1.80296100	2.54194100
H	0.65866800	-2.53256100	2.58189700
H	2.38598200	-2.29782600	2.89988800

H	1.23464800	-0.99930300	3.24473700
C	2.91244100	0.96532600	1.78579200
H	4.01086200	0.93686200	1.78465200
H	2.59187600	1.97639500	1.51855000
H	2.57950700	0.75936200	2.80697700
Rh	0.17799100	-0.09196000	0.02604600
C	-2.33554500	-1.93768900	-0.22937500
C	-1.75091400	-0.66057400	-0.10447700
C	-2.64823600	0.42857200	-0.06289000
C	-4.04235400	0.28402200	-0.13921100
C	-4.56809400	-0.99361300	-0.26173000
C	-3.71429100	-2.10915200	-0.30695600
H	-1.69985000	-2.81691200	-0.26671100
H	-4.67950100	1.16259600	-0.10190000
H	-5.64487000	-1.12821400	-0.32237200
H	-4.13414300	-3.10745300	-0.40262800
O	-2.16361000	1.68862400	0.05548500
N	-0.74886500	1.66771600	0.12218700
C	-0.24242100	2.94722700	0.23381100
O	0.97465700	3.12086400	0.30603500
C	-1.21837100	4.11033500	0.26332800
H	-1.82393300	4.13703200	-0.64823300
H	-1.91156200	4.01992000	1.10570900
H	-0.64019700	5.03116600	0.35365500

INT-2

Rh	2.58685400	8.55367000	-2.38575900
C	2.67883800	11.00627400	-4.30399000
C	2.32788700	10.46804500	-3.06350200
C	1.77094300	11.33454800	-2.11054800
C	1.58901700	12.69756400	-2.36660200
C	1.96535900	13.21110300	-3.60759100
C	2.50676000	12.36956800	-4.58118000
H	3.08693000	10.36087000	-5.07822800
H	1.15496800	13.33193700	-1.59930000
H	1.82522400	14.26902600	-3.81324900
H	2.79038100	12.76491200	-5.55322500
O	1.40287400	10.86768300	-0.88384700
N	1.53100900	9.44099000	-0.83701100
C	1.07073300	8.91068800	0.29384700
O	1.14503500	7.66503500	0.49698700
C	3.83824400	6.71099800	-1.50694500
C	3.97410200	6.74076800	-2.92785600
C	4.58452200	7.99150700	-3.32034700

C	4.82628300	8.74478300	-2.11976400
C	4.34358200	7.95746100	-1.00769900
C	5.57823700	10.04009300	-2.02581300
H	6.66062100	9.85542100	-1.98458700
H	5.37671200	10.68388400	-2.88605700
H	5.30381900	10.59910600	-1.12717600
C	4.44996500	8.32614100	0.44086000
H	5.38230400	7.92474900	0.86226500
H	4.46257300	9.41035300	0.57994900
H	3.61227400	7.91535500	1.00854000
C	5.08173700	8.33595300	-4.69462600
H	5.19179700	9.41602800	-4.81920200
H	6.06502300	7.88088800	-4.87924400
H	4.40596000	7.97891700	-5.47868500
C	3.64971900	5.60216400	-3.85022100
H	3.58759400	5.92291600	-4.89367300
H	4.43611300	4.83763900	-3.79200800
H	2.70604400	5.11409600	-3.58529800
C	3.34300600	5.56584700	-0.67258700
H	2.77970000	4.84610900	-1.27444000
H	4.18175600	5.02245200	-0.21510200
H	2.68561000	5.92626200	0.12173500
C	0.43427900	7.53043800	-2.96552400
H	0.66034100	6.53171500	-2.60156700
C	-0.81233200	8.08272000	-2.43850100
C	-1.44832700	7.41926400	-1.35672700
C	-1.47772800	9.17182600	-3.03664400
C	-2.73586000	7.80274300	-0.96007400
C	-2.74121500	9.56690200	-2.61609800
H	-1.00367600	9.70290600	-3.85635300
C	-3.37989400	8.86636200	-1.58467500
H	-3.19831100	7.25926000	-0.14207400
H	-3.23560400	10.40537500	-3.09819800
H	-4.37532900	9.15999400	-1.26135200
O	-0.84684900	6.38677600	-0.70643600
H	-0.01087100	6.73631000	-0.28358600
C	1.16068600	8.02172300	-4.04521300
H	0.84602100	8.91742600	-4.56676100
H	1.77192900	7.34287400	-4.62968000
C	0.45935900	9.82783900	1.33922400
H	1.18019400	10.58123000	1.67406500
H	-0.40102500	10.36543800	0.92823900
H	0.14421500	9.21381100	2.18441800

TS-1

Rh	2.52108200	8.65588700	-2.29532900
C	3.04606400	11.24274700	-4.14655500
C	2.26553300	10.63959300	-3.14030500
C	1.77961200	11.48520400	-2.11203600
C	2.02526600	12.86156100	-2.11872000
C	2.77707100	13.42465300	-3.14805200
C	3.30434800	12.61196500	-4.15805100
H	3.41334100	10.62971500	-4.96622800
H	1.64026100	13.46570900	-1.30288700
H	2.96331800	14.49504700	-3.15286400
H	3.89911800	13.04499000	-4.95751900
O	1.05631800	10.98909100	-1.08033000
N	1.38974200	9.60346300	-0.82563900
C	0.79565100	9.13388700	0.27609700
O	0.90898300	7.92190100	0.59188400
C	3.59830500	6.89121000	-1.28901700
C	3.58719700	6.65386700	-2.69209800
C	4.30640400	7.72827300	-3.32568200
C	4.88076700	8.56718400	-2.28336200
C	4.40538700	8.08806500	-1.04422800
C	5.81763800	9.71579400	-2.51101300
H	6.81107000	9.35303100	-2.80858900
H	5.46054700	10.38667000	-3.29899300
H	5.94272100	10.31419300	-1.60467000
C	4.70254300	8.62693800	0.32314300
H	5.48709500	8.03290400	0.81203700
H	5.04299200	9.66539000	0.28708300
H	3.81210300	8.58404400	0.95681200
C	4.65201300	7.80624400	-4.78646500
H	4.92788700	8.82219700	-5.08296000
H	5.50896500	7.15760700	-5.01698800
H	3.82210200	7.48178800	-5.42279600
C	2.95351100	5.47467200	-3.37033100
H	2.77084800	5.66800800	-4.43246800
H	3.60933200	4.59550000	-3.30904100
H	1.99914200	5.22021400	-2.89888800
C	3.15586600	5.93156900	-0.22484700
H	2.39239100	5.24395700	-0.59567900
H	4.01559700	5.33051800	0.10672600
H	2.74284900	6.45395300	0.63919700
C	0.66087200	8.21890600	-3.31200600
H	0.98855900	7.30182500	-3.79906900
C	-0.67187000	8.06788400	-2.66708400

C	-0.90733600	7.00656900	-1.76350600
C	-1.77010600	8.87035200	-3.02592000
C	-2.19282500	6.75011700	-1.28117300
C	-3.05061800	8.62517000	-2.53153900
H	-1.63684300	9.68122800	-3.73650200
C	-3.26638000	7.55297400	-1.66393300
H	-2.32102200	5.92363000	-0.58881500
H	-3.87819300	9.25819500	-2.84029400
H	-4.26257700	7.34773400	-1.28065100
O	0.13411300	6.22301800	-1.33732900
H	0.61522400	6.77300700	-0.65515200
C	1.04376700	9.45094900	-3.97870100
H	0.28764000	10.23062200	-4.00890300
H	1.54565600	9.33492500	-4.93551700
C	-0.00455200	10.08177800	1.15256400
H	0.56531100	10.98169800	1.40210100
H	-0.91204700	10.40528300	0.63088900
H	-0.28163900	9.54616900	2.06199400

INT-3

Rh	2.50017600	8.79113300	-2.07260500
C	1.41956300	11.79986700	-4.42892000
C	1.22377100	11.35086300	-3.11063100
C	2.08591800	11.87337400	-2.12299500
C	3.07005900	12.81901400	-2.44738100
C	3.21972900	13.25762800	-3.75896100
C	2.39496900	12.73681400	-4.76162300
H	0.75745400	11.41694300	-5.20289500
H	3.69738600	13.19893200	-1.64675100
H	3.97961800	13.99650600	-3.99894000
H	2.50188200	13.07036200	-5.79006500
O	1.99013200	11.56247400	-0.78947900
N	1.85243100	10.14242600	-0.56929000
C	1.50897600	9.85092900	0.68268600
O	1.30001000	8.64416100	0.99439700
C	3.09170400	6.83565100	-1.39782700
C	3.19064100	6.81861400	-2.84502900
C	4.14618400	7.81221500	-3.18831600
C	4.81875900	8.27767300	-1.95810500
C	4.19424400	7.66871000	-0.87192800
C	5.94779700	9.26379500	-1.94579500
H	6.86224300	8.81864800	-2.36124400
H	5.71348600	10.14744100	-2.55019800
H	6.17308200	9.60439200	-0.93220300

C	4.50397700	7.82246200	0.58523700
H	4.98063900	6.90987300	0.96937100
H	5.18620100	8.65688800	0.76882500
H	3.58737800	7.98892900	1.15807200
C	4.57263200	8.21055100	-4.56905900
H	4.75293100	9.28848500	-4.63516200
H	5.50922800	7.70398800	-4.84175400
H	3.82056300	7.94705600	-5.31692500
C	2.48737900	5.87547400	-3.77118300
H	2.41225100	6.28195200	-4.78402100
H	3.04490000	4.93053700	-3.83607000
H	1.47512700	5.64579700	-3.43151800
C	2.24896600	5.92495400	-0.56203600
H	1.35472900	5.60181000	-1.10148400
H	2.82353700	5.02665700	-0.29114300
H	1.93338700	6.43027800	0.35301200
C	0.60682300	8.91656800	-3.02501000
H	0.94835700	8.83659500	-4.06684400
C	-0.40360000	7.83480800	-2.80154400
C	-1.12459000	7.63891500	-1.59495500
C	-0.73430000	6.99435300	-3.88522100
C	-2.12408400	6.65787200	-1.52387000
C	-1.72211800	6.01419200	-3.80906400
H	-0.20968400	7.14271300	-4.82708400
C	-2.42817900	5.84928800	-2.61614100
H	-2.65422400	6.55614400	-0.58161000
H	-1.94762100	5.39995000	-4.67683200
H	-3.20880000	5.09717000	-2.53502200
O	-0.95167700	8.41403000	-0.48675900
H	-0.03619000	8.36776800	-0.10844900
C	0.11067000	10.35942700	-2.81581700
H	-0.28001900	10.48572600	-1.80553500
H	-0.72011200	10.55584400	-3.51070200
C	1.34666600	10.96086800	1.70295400
H	2.24645900	11.58108000	1.76815800
H	0.52081800	11.62192500	1.41824000
H	1.13150200	10.50620100	2.67131000

TS-2

Rh	2.36113300	8.60212000	-1.77978000
C	0.39520000	12.32906100	-4.16856600
C	0.83377900	11.38126300	-3.23886500
C	2.06911700	11.60882500	-2.58458800
C	2.78360500	12.80160800	-2.83665500

C	2.32316000	13.72104500	-3.77327700
C	1.12512900	13.48570900	-4.45221100
H	-0.55409800	12.15934800	-4.67253700
H	3.71310600	12.96260400	-2.29813000
H	2.89893000	14.62215300	-3.96950000
H	0.75407300	14.19981200	-5.18180700
O	2.62648900	10.74977700	-1.72587700
N	1.46179800	9.57669500	-0.33100500
C	1.96872800	9.76003000	0.91954300
O	1.50581800	8.99684800	1.77785700
C	2.95213400	6.45693400	-1.62291700
C	3.24621800	6.85791400	-2.97543300
C	4.20248800	7.90831000	-2.90326000
C	4.65917400	8.02728700	-1.51390600
C	3.90588400	7.13257100	-0.73631400
C	5.73851700	8.96714200	-1.06511700
H	6.70957000	8.68550500	-1.49408300
H	5.52570500	9.99374200	-1.38395600
H	5.84478500	8.97002200	0.02286700
C	4.00950100	6.87478000	0.73805000
H	4.21598000	5.81362500	0.92670100
H	4.81786600	7.45528400	1.19094300
H	3.08287500	7.13086500	1.26481900
C	4.81356300	8.64856300	-4.05721700
H	4.96841100	9.70508300	-3.81687500
H	5.79250800	8.22146900	-4.31636400
H	4.18325400	8.59750500	-4.94905900
C	2.71198500	6.22431200	-4.22318100
H	2.60847100	6.94506000	-5.04061500
H	3.40007900	5.43900800	-4.56582400
H	1.73865700	5.75994900	-4.05459700
C	2.04732700	5.33549900	-1.20480100
H	1.16608900	5.26946800	-1.84812300
H	2.57597000	4.37221900	-1.25192600
H	1.69828900	5.47369900	-0.17755500
C	0.56577500	8.81060200	-2.96395800
H	0.98504800	8.68966700	-3.96846100
C	-0.40596800	7.70569400	-2.70681600
C	-1.15675900	7.56419200	-1.50751000
C	-0.66825300	6.77178800	-3.73266800
C	-2.08690900	6.52137800	-1.37020200
C	-1.59759000	5.74410400	-3.60023700
H	-0.14457300	6.89343600	-4.67729900
C	-2.31155300	5.61993800	-2.40333800

H	-2.62694200	6.45264700	-0.43081400
H	-1.77662800	5.06073900	-4.42566600
H	-3.04320800	4.82606600	-2.27822300
O	-1.05480400	8.40231900	-0.45020100
H	-0.20677200	8.90462600	-0.46409100
C	-0.04527100	10.21531100	-2.85621200
H	-0.43638900	10.38614000	-1.84828200
H	-0.92461700	10.22765700	-3.51677900
C	2.93105400	10.88197100	1.22182100
H	3.82411800	10.81433400	0.59582100
H	2.45945800	11.84480900	1.00111700
H	3.19576000	10.83241600	2.28113600

INT-4

Rh	2.39078200	8.73687500	-1.56386400
C	0.43325600	12.34087000	-4.15315500
C	0.94696400	11.45521000	-3.20451800
C	2.33897800	11.47055700	-2.93560800
C	3.16694000	12.38022200	-3.63061600
C	2.62423400	13.27227300	-4.55085600
C	1.25308500	13.25441100	-4.82206100
H	-0.63449700	12.32237100	-4.36269600
H	4.22908400	12.38775600	-3.40099700
H	3.27344300	13.97924300	-5.06165000
H	0.82552900	13.94231700	-5.54595700
O	2.88595300	10.68026900	-2.01322200
N	1.30858100	8.96585500	-0.03440700
C	1.65513100	8.63286100	1.24473300
O	1.65574000	7.48390000	1.69796800
C	3.23886900	6.63156200	-1.38385900
C	3.22755000	6.97209500	-2.79337500
C	4.13922700	8.04581500	-2.98173900
C	4.80121600	8.30345600	-1.71526700
C	4.28123300	7.41179200	-0.74580000
C	5.81296900	9.38604600	-1.51992200
H	6.63553500	9.29317600	-2.23982300
H	5.33355600	10.36050700	-1.68315900
H	6.23847300	9.37420300	-0.51352600
C	4.73653500	7.23105400	0.66930200
H	5.32711200	6.30866900	0.75884900
H	5.36611500	8.06008800	1.00401100
H	3.88697200	7.13735700	1.35393000
C	4.47958000	8.73383000	-4.26933000
H	4.47500600	9.82175600	-4.14995700

H	5.48042400	8.43937800	-4.61374900
H	3.77045100	8.48307500	-5.06263500
C	2.53070200	6.18864500	-3.86032600
H	2.40107400	6.76959800	-4.77720800
H	3.13341400	5.30517600	-4.11401800
H	1.54761100	5.83867900	-3.53972200
C	2.51128100	5.48092300	-0.75337900
H	1.63115600	5.19895800	-1.33718800
H	3.17219500	4.60379000	-0.69578300
H	2.17983200	5.73846700	0.25564800
C	0.57211400	9.00951500	-2.76251100
H	1.04782000	8.97579900	-3.74697500
C	-0.45930100	7.94116000	-2.69499500
C	-1.34681200	7.75558600	-1.59909100
C	-0.67758500	7.13959100	-3.83787000
C	-2.38197200	6.80949200	-1.67853700
C	-1.70242400	6.20336800	-3.91493500
H	-0.04045300	7.29893500	-4.70374500
C	-2.56138900	6.04111000	-2.82125800
H	-3.03143200	6.70260500	-0.81528300
H	-1.84261800	5.62013800	-4.82050000
H	-3.37039700	5.31640100	-2.86206400
O	-1.26923000	8.46815300	-0.45926500
H	-0.34741100	8.82859900	-0.32703100
C	0.08595800	10.45093900	-2.48841600
H	0.05045600	10.65539500	-1.41412400
H	-0.94567900	10.53741500	-2.85464000
C	1.93771200	9.84486300	2.13076100
H	2.21423800	10.72884900	1.54925500
H	1.03770100	10.07681300	2.71178500
H	2.73766200	9.58724100	2.83186600

TS-3

Rh	0.04712400	-0.60407600	0.06242500
C	3.29179100	2.96309600	0.64734400
C	2.38137800	1.91238900	0.77462100
C	2.83596600	0.57814400	0.60251300
C	4.20410400	0.35115800	0.31999500
C	5.09559100	1.41460200	0.22937300
C	4.64407800	2.73000800	0.38520500
H	2.93516200	3.98376700	0.77294100
H	4.54267900	-0.67568400	0.20891400
H	6.14669400	1.21918700	0.03042000
H	5.33686000	3.56302900	0.30646000

O	2.01872600	-0.45826100	0.73277300
N	-0.80876800	-0.37200300	1.78025800
C	-1.51899700	-1.39526900	2.38734500
O	-2.72672300	-1.56704200	2.23549100
C	-1.38617800	-1.73257800	-1.27250000
C	-0.45947600	-1.02407000	-2.13949800
C	0.83930800	-1.55024400	-1.90980700
C	0.71812200	-2.64331900	-0.96286600
C	-0.65454400	-2.78857600	-0.61320000
C	1.87989500	-3.43725400	-0.45881100
H	2.43203900	-3.89710700	-1.28806400
H	2.56688800	-2.76804800	0.07491000
H	1.56876800	-4.23157600	0.22412600
C	-1.27150500	-3.86993200	0.22012300
H	-1.70032300	-4.64316900	-0.43239700
H	-0.53784500	-4.35643700	0.86820000
H	-2.08210400	-3.48546900	0.84572600
C	2.11345800	-1.15371900	-2.59265200
H	2.94234400	-1.09218900	-1.88151700
H	2.38501700	-1.88890200	-3.36277400
H	2.02381500	-0.18039200	-3.08240700
C	-0.84896800	-0.05595300	-3.21107600
H	-0.03182700	0.62409600	-3.46744900
H	-1.11144700	-0.61108600	-4.12262700
H	-1.71525000	0.54399200	-2.92714400
C	-2.87503300	-1.55084700	-1.22706300
H	-3.16373600	-0.55526800	-1.57333800
H	-3.37167400	-2.29105900	-1.87059600
H	-3.25263000	-1.67163300	-0.20735600
C	0.05588600	1.61897700	-0.12576900
H	0.61669900	1.70028700	-1.06129300
C	-1.29093300	2.16355500	-0.28925300
C	-2.23420400	2.23361000	0.80003900
C	-1.68097600	2.71825600	-1.53382300
C	-3.50843000	2.82768900	0.57344900
C	-2.91708300	3.31224100	-1.72341200
H	-0.95813200	2.71961700	-2.34536000
C	-3.83811600	3.36238500	-0.65432800
H	-4.19799300	2.85000800	1.41142800
H	-3.16917100	3.75514200	-2.68280900
H	-4.81026400	3.82662800	-0.80056000
O	-1.95653100	1.76239700	1.98130500
H	-1.28355500	0.73237900	1.94782900
C	0.92232300	2.13213100	1.04918600

H	0.62200300	1.67050300	1.99200100
H	0.73073400	3.20864400	1.15510500
C	-0.68983600	-2.25251300	3.33478300
H	0.26892400	-2.52835600	2.88467600
H	-0.46485000	-1.67107500	4.23674400
H	-1.25651600	-3.14296700	3.61923500

INT-5

Rh	3.69677000	9.30604100	-1.69973900
C	-1.20939700	11.36668600	-2.11658800
C	-0.27044800	10.33675600	-2.21585800
C	1.06627300	10.64437200	-2.59392300
C	1.39401500	11.99467700	-2.85579800
C	0.43714800	13.00361100	-2.75142900
C	-0.87249600	12.69765100	-2.37567600
H	-2.22888300	11.12026500	-1.82233800
H	2.41251900	12.22414600	-3.15810400
H	0.71749300	14.03229700	-2.96646200
H	-1.62027000	13.48046200	-2.28526500
O	1.95621200	9.66221700	-2.73332600
N	3.40521600	10.94765000	-0.60826300
C	4.19926600	11.54573900	0.32141100
O	5.31418900	11.12531400	0.65391800
C	4.12076700	7.18220700	-1.34077000
C	4.13324100	7.38060000	-2.76300600
C	5.13289800	8.36395200	-3.04536000
C	5.81653300	8.71130500	-1.79732300
C	5.19241800	7.97923900	-0.74788400
C	6.99640000	9.62126300	-1.65168500
H	6.86318300	10.26778400	-0.77958600
H	7.91585000	9.03351100	-1.52188200
H	7.12826400	10.25215800	-2.53526600
C	5.61662500	7.96573400	0.68848600
H	6.51715000	7.34780500	0.81101100
H	5.83122900	8.98209300	1.02774000
H	4.83783700	7.54584100	1.33076800
C	5.47214000	8.89384200	-4.40395600
H	4.60221700	8.87142400	-5.06529400
H	5.83509100	9.92408600	-4.35346300
H	6.26388900	8.28451200	-4.86231100
C	3.17316500	6.79451400	-3.75717000
H	2.38718000	7.52084200	-4.00059000
H	3.68831800	6.51688800	-4.68315700
H	2.68873700	5.90026300	-3.35833700

C	3.22412000	6.24791400	-0.59095900
H	2.24783800	6.12956400	-1.06803000
H	3.69773000	5.25702300	-0.52899800
H	3.05909700	6.59445300	0.43290500
C	-1.21317000	8.25525700	-3.22519800
H	-1.73921900	8.94408900	-3.88950300
C	-1.15521100	6.95441400	-3.63924400
C	-0.45704000	5.87825100	-2.86378000
C	-1.77179200	6.60270700	-4.90899300
C	-0.39908200	4.56150800	-3.50055400
C	-1.70226700	5.34795100	-5.41899500
H	-2.29205300	7.39041300	-5.44981300
C	-0.99715300	4.31652100	-4.69579400
H	0.12077600	3.78494400	-2.94727400
H	-2.16690000	5.10745200	-6.37042700
H	-0.95252600	3.31858200	-5.12723500
O	0.04398600	6.06909600	-1.74561800
H	2.54177100	11.45065500	-0.80092600
C	-0.65797800	8.89050700	-1.98568400
H	0.17886400	8.29991800	-1.61308200
H	-1.44166900	8.83069500	-1.21121900
C	3.62864300	12.79641800	0.99310900
H	2.94568400	13.35345700	0.34326100
H	3.07376900	12.50298300	1.89291600
H	4.45240400	13.44409400	1.30220000

TS-4

Rh	3.08109700	8.65228400	-1.82383600
C	-0.60240700	12.27487500	-2.26068500
C	0.00078300	11.02812800	-2.44927100
C	1.34697700	10.94921200	-2.88964700
C	2.05318000	12.15489400	-3.09265800
C	1.44016400	13.38802200	-2.89098900
C	0.10651000	13.45811900	-2.47385500
H	-1.64045000	12.31853900	-1.93519200
H	3.08752400	12.09298600	-3.41911200
H	2.00425900	14.30203800	-3.06195800
H	-0.37445600	14.41974900	-2.31890000
O	1.89776900	9.76545000	-3.14483300
N	2.45386000	9.86482300	-0.32147900
C	3.11591300	10.67644100	0.52942500
O	4.34720400	10.69479000	0.68750500
C	4.27538900	6.75770600	-1.67183700
C	4.04995100	7.05254500	-3.08266100

C	4.64341700	8.30817100	-3.36378600
C	5.19761600	8.83643600	-2.11932300
C	5.02233100	7.82283400	-1.09111400
C	5.99191300	10.09351800	-1.95852000
H	5.73783300	10.57002800	-1.00662500
H	7.06729500	9.86450200	-1.96716200
H	5.79197200	10.80051000	-2.76848100
C	5.60208800	7.86597500	0.29025400
H	6.65566900	7.55281600	0.26210200
H	5.53364700	8.87505300	0.70042200
H	5.07309500	7.18808400	0.96592900
C	4.62289200	8.99431800	-4.69641900
H	3.59459200	9.24742000	-4.97803900
H	5.20193700	9.92071100	-4.67842200
H	5.04894400	8.34442200	-5.47020200
C	3.37639600	6.15759000	-4.07980900
H	2.87033600	6.73929600	-4.85571100
H	4.11259800	5.50867300	-4.57527100
H	2.63310600	5.51074600	-3.60752800
C	3.83911400	5.50216700	-0.98500500
H	2.82905700	5.21720000	-1.28867100
H	4.51560500	4.67519000	-1.24207500
H	3.84297300	5.61756500	0.10105000
C	-0.71996300	8.78830500	-3.34202700
H	-1.13342500	9.20442100	-4.26335400
C	-0.41572000	7.45240700	-3.36727600
C	0.23418000	6.74264600	-2.23341700
C	-0.83090400	6.67495400	-4.51800600
C	0.10505900	5.29241900	-2.23525100
C	-0.82330700	5.31443500	-4.50172000
H	-1.20705100	7.21554900	-5.38397600
C	-0.38178100	4.62343400	-3.32075600
H	0.45637200	4.76846600	-1.35135300
H	-1.17442200	4.74432000	-5.35618700
H	-0.42847600	3.53646600	-3.30483500
O	0.88865100	7.33031200	-1.34169000
H	1.46623600	10.08724900	-0.39478200
C	-0.74265500	9.72927000	-2.18359600
H	-0.37015300	9.22362200	-1.29067600
H	-1.80208800	9.97935100	-2.01270000
C	2.24634600	11.66198200	1.31945900
H	2.07676400	12.56129400	0.71463000
H	1.26848000	11.24410500	1.58306900
H	2.77472900	11.95257900	2.23022800

INT-6

Rh	3.10448700	8.33073300	-1.32735600
C	-0.49990800	12.63416500	-2.74403200
C	-0.31323000	11.31922400	-3.15032800
C	0.72849700	11.00491300	-4.02992100
C	1.58691000	11.97662400	-4.53498000
C	1.38743100	13.29922000	-4.11767100
C	0.35847600	13.63038800	-3.23273800
H	-1.30364800	12.89173200	-2.05821900
H	2.36983000	11.71760300	-5.24041100
H	2.04089200	14.07930500	-4.49987000
H	0.21802600	14.66325500	-2.92697700
O	0.79582000	9.67291800	-4.33439500
N	2.48374000	9.49835900	0.16502700
C	3.13648800	10.16630900	1.14783600
O	4.36616900	10.15398200	1.29872400
C	4.42992400	6.60946700	-1.73473100
C	4.05862700	7.15708000	-3.00188100
C	4.48849500	8.52890800	-3.01271800
C	5.21461800	8.80531400	-1.77968500
C	5.16456600	7.62677400	-0.98142700
C	5.93614600	10.07260600	-1.43869100
H	5.75811200	10.33770100	-0.39334400
H	7.01568300	9.94556500	-1.60043800
H	5.60226000	10.90342000	-2.06617400
C	5.81211100	7.44529700	0.35689100
H	6.89628600	7.30998600	0.23907100
H	5.62923200	8.32524000	0.98062900
H	5.42213900	6.56473300	0.87504300
C	4.29334100	9.48018200	-4.14894600
H	3.33409400	9.30866400	-4.64313600
H	4.31788800	10.51880000	-3.81108800
H	5.09427600	9.34635600	-4.89030700
C	3.34546200	6.46197400	-4.12258900
H	2.62093600	7.12529200	-4.60292500
H	4.06473100	6.13440200	-4.88545700
H	2.79776700	5.58467300	-3.77286700
C	4.19772300	5.20451300	-1.27278300
H	3.34066100	4.75193600	-1.77618000
H	5.08184000	4.58829500	-1.48809800
H	4.02190900	5.16270200	-0.19407900
C	-0.46336800	9.06352300	-3.87120000
H	-1.13064700	9.09076900	-4.74320800

C	-0.27603600	7.62684000	-3.46591800
C	0.48201900	7.25422900	-2.32055400
C	-0.91918300	6.62842300	-4.20833000
C	0.52875900	5.88797900	-1.96522500
C	-0.85356500	5.28058600	-3.85472400
H	-1.49180000	6.92284100	-5.08603400
C	-0.12848600	4.91731900	-2.71688400
H	1.07948200	5.62195000	-1.06685700
H	-1.36716200	4.53091000	-4.44949400
H	-0.08065900	3.87493200	-2.40915300
O	1.08050900	8.17362600	-1.56380400
H	1.47011100	9.57011100	0.18030800
C	-1.01981600	10.03375000	-2.79404500
H	-0.74679500	9.69444700	-1.79009600
H	-2.11146800	10.09699600	-2.85448200
C	2.27802100	10.98919100	2.11057100
H	2.47829200	12.05306100	1.94000500
H	1.20307600	10.81491700	2.00320700
H	2.57967600	10.76120400	3.13733200

TS-5

Rh	1.16241300	-0.26713000	0.11360000
C	-4.35194400	-1.34364200	-1.26205600
C	-3.79685700	-0.21378700	-0.67313700
C	-3.51552600	-0.21098000	0.69883700
C	-3.79170800	-1.31072300	1.50858600
C	-4.35483100	-2.44167200	0.90278600
C	-4.63311200	-2.46571600	-0.46698300
H	-4.57473500	-1.35723400	-2.32649500
H	-3.59414800	-1.27758100	2.57515600
H	-4.58919400	-3.30894000	1.51503800
H	-5.07834500	-3.34936400	-0.91531800
O	-2.96776100	0.95216300	1.14156600
N	0.04840000	-1.57066400	-1.17406300
C	0.25556900	-2.94206700	-1.26239600
O	1.37910600	-3.43400400	-1.24530900
C	2.84001800	0.30646700	1.46597300
C	1.61830100	0.62835000	2.12019600
C	0.84982400	-0.59803900	2.25839700
C	1.67100400	-1.68656000	1.77820500
C	2.86690800	-1.13400500	1.22507100
C	1.35381100	-3.14419700	1.89492100
H	1.70822800	-3.70507400	1.02861600
H	1.84325300	-3.54588600	2.79313900

H	0.27968900	-3.31795500	2.00087100
C	3.99788400	-1.90023000	0.60733200
H	4.69738100	-2.25657100	1.37657100
H	3.62216500	-2.76237400	0.05038800
H	4.55946700	-1.27176300	-0.08969200
C	-0.45803600	-0.70717300	2.97970200
H	-1.13089100	0.10793200	2.70020000
H	-0.96524200	-1.64696200	2.74878700
H	-0.30106900	-0.66788900	4.06701400
C	1.18309000	1.96312700	2.63943100
H	0.11225100	2.12342300	2.48844000
H	1.38339300	2.01892500	3.71864000
H	1.70732100	2.78632700	2.15172200
C	3.93515100	1.24894600	1.07177000
H	3.65048800	2.28999100	1.24129100
H	4.84356100	1.04479500	1.65316400
H	4.17749500	1.13365500	0.01028700
C	-3.03942100	1.93649300	0.04287200
H	-3.89643700	2.57450200	0.29194100
C	-1.80608000	2.79325400	-0.01932500
C	-0.53506300	2.23108800	-0.34507600
C	-1.92252200	4.17442800	0.16824900
C	0.55901700	3.11710800	-0.49392500
C	-0.83000300	5.03271600	0.03785600
H	-2.89945300	4.58448700	0.41981700
C	0.41147000	4.48872300	-0.30252400
H	1.51843900	2.69534700	-0.77815800
H	-0.94750200	6.10171800	0.18986800
H	1.27386400	5.14073700	-0.42821800
O	-0.43937400	0.92526500	-0.54616900
H	-0.93302300	-1.30892600	-1.07431800
C	-3.36721000	1.11636700	-1.24071500
H	-2.48071700	1.01461000	-1.87379000
H	-4.15072300	1.60982200	-1.82632600
C	-0.99011200	-3.79941800	-1.44852700
H	-0.70845700	-4.85417200	-1.44848000
H	-1.72713100	-3.60796500	-0.66009900
H	-1.47444400	-3.55794500	-2.40240900
C	1.93818400	0.30587000	-2.83510900
O	0.98104000	-0.45715600	-3.21496100
O	2.28649200	0.47441000	-1.63758700
C	2.66475000	1.06809000	-3.92027100
H	3.66110200	1.36048400	-3.58321400
H	2.72595800	0.46783000	-4.83105200

H	2.09416500	1.97603500	-4.14983400
H	0.51453400	-0.98085300	-2.28826400

INT-7

Rh	-1.15784500	-0.57966100	-0.09346300
C	4.81575500	-0.71902000	1.10350100
C	3.97578900	0.22262100	0.52152000
C	3.53586700	0.04378100	-0.79458300
C	3.93558300	-1.04672600	-1.56274800
C	4.78349600	-1.98793700	-0.96576200
C	5.22086400	-1.83358600	0.35292900
H	5.16328800	-0.59037700	2.12592100
H	3.61350000	-1.14908500	-2.59414600
H	5.11413100	-2.84581500	-1.54574100
H	5.88791600	-2.56974300	0.79275000
O	2.70755000	1.03431700	-1.23073100
C	-2.52202800	0.14903600	-1.63611700
C	-1.21949200	-0.03569100	-2.25379600
C	-0.85614300	-1.40460800	-2.11351200
C	-1.96169400	-2.10307300	-1.45725200
C	-2.99370900	-1.15427300	-1.19934900
C	-1.96985400	-3.56961200	-1.15211100
H	-2.81340400	-3.84304900	-0.51392200
H	-2.04133500	-4.15466400	-2.07860000
H	-1.04905400	-3.86162200	-0.63722200
C	-4.33817000	-1.42155800	-0.59710000
H	-5.09503000	-1.47704800	-1.39175500
H	-4.35494000	-2.36885100	-0.05203000
H	-4.61436100	-0.62107800	0.09253800
C	0.40461100	-2.05542000	-2.58990100
H	1.20054000	-1.32061200	-2.72269200
H	0.75723900	-2.80366300	-1.87440800
H	0.23716500	-2.55863100	-3.55232200
C	-0.39869000	1.03274400	-2.90722800
H	-0.66945300	2.02500900	-2.54012300
H	0.66916400	0.89506000	-2.72001200
H	-0.56825400	1.01668500	-3.99266300
C	-3.34045300	1.40190700	-1.64174300
H	-2.71030800	2.28874100	-1.73906700
H	-4.04275900	1.38808500	-2.48750000
H	-3.89968100	1.48915800	-0.70844700
C	2.74925600	2.12024400	-0.23583800
H	3.47130300	2.84209900	-0.63820700
C	1.42180200	2.81762300	-0.09457500

C	0.24181300	2.15222500	0.33812600
C	1.36863700	4.19479600	-0.34729200
C	-0.93613300	2.90625600	0.51025600
C	0.19791400	4.93303700	-0.18047500
H	2.27395100	4.69609900	-0.68520300
C	-0.95566400	4.27588300	0.25359000
H	-1.83269400	2.39250500	0.84557600
H	0.18768200	5.99974400	-0.38555300
H	-1.87950200	4.83121300	0.39882600
O	0.26829900	0.83199300	0.58465500
C	3.35049800	1.48844300	1.05266400
H	2.57997700	1.27053800	1.79731300
H	4.07184500	2.17114200	1.51461700
C	-2.90309300	0.21064700	2.24379600
O	-1.90010200	-0.52109600	1.86226100
O	-3.59219800	0.94586500	1.52663700
C	-3.17495100	0.10435700	3.74407100
H	-4.10017800	0.62616900	3.99696700
H	-3.23904900	-0.94493100	4.04981700
H	-2.34239400	0.55378500	4.29725800
C	0.89991600	-1.83473300	1.93594100
O	1.06375400	-0.65612800	2.47538800
O	0.23814100	-2.05346700	0.90740700
C	1.62353700	-2.94849800	2.64653500
H	1.23693100	-3.91715000	2.32721400
H	2.68925400	-2.88389200	2.39742900
H	1.52334100	-2.83262700	3.72916400
H	0.66304800	0.05650200	1.85384200

TS-6

Rh	-1.80285700	-0.44661800	0.18910300
C	4.11850100	-2.33592500	1.25394800
C	3.96978600	-1.10344100	0.63052700
C	3.92306100	-1.03391400	-0.76577600
C	4.03453900	-2.16654700	-1.56780500
C	4.18815600	-3.40263400	-0.92632400
C	4.22990500	-3.49312600	0.46792000
H	4.15146300	-2.40522200	2.33869100
H	4.01251600	-2.08266400	-2.64989800
H	4.28617900	-4.30316800	-1.52763800
H	4.35650500	-4.46090600	0.94511300
O	3.75525100	0.23011600	-1.24367000
C	-1.84872300	-0.33154000	-2.03089800
C	-1.01606700	-1.47622400	-1.63016000

C	-1.82274500	-2.37792100	-0.88767400
C	-3.14284900	-1.77868300	-0.76340200
C	-3.16680900	-0.55017400	-1.55519100
C	-4.31499000	-2.41505300	-0.08644600
H	-5.02377400	-1.66720600	0.27800600
H	-4.84679000	-3.06725700	-0.79374400
H	-3.99625900	-3.02662800	0.76164500
C	-4.36843500	0.30005600	-1.82406600
H	-4.78175900	0.05363800	-2.81182400
H	-5.15422400	0.12852200	-1.08332100
H	-4.10536200	1.35885800	-1.79911200
C	-1.40954900	-3.66904700	-0.24816800
H	-0.35272900	-3.88013200	-0.42453700
H	-1.56345100	-3.62929100	0.83551600
H	-1.99618600	-4.50382900	-0.65104800
C	0.42233800	-1.63471600	-1.99992400
H	1.00089700	-0.75834500	-1.69330700
H	0.87221700	-2.51390300	-1.53494600
H	0.51115600	-1.74116300	-3.08963800
C	-1.37998800	0.82600400	-2.85277400
H	-0.30995300	0.99429100	-2.71399000
H	-1.56278700	0.63172000	-3.91906800
H	-1.90706200	1.73615100	-2.56030500
C	3.90277200	1.15810700	-0.11618600
H	4.92785700	1.54321500	-0.18981900
C	2.95570000	2.32334800	-0.26114900
C	1.55468700	2.16650700	-0.25707300
C	3.48012100	3.61404800	-0.40252500
C	0.72046400	3.27939900	-0.40136900
C	2.65222000	4.72980600	-0.52882500
H	4.56064200	3.74177700	-0.41442600
C	1.26812100	4.55688900	-0.53119900
H	-0.35485400	3.12828700	-0.42199100
H	3.08554900	5.72054800	-0.63456300
H	0.60848900	5.41409300	-0.63983500
O	1.00572500	0.90525700	-0.16974300
C	3.78580200	0.29323500	1.17504700
H	2.81578400	0.40543500	1.66864700
H	4.55735100	0.58020600	1.89822200
C	-2.77824200	2.27855800	0.80863200
O	-2.43332000	1.12534500	1.32169200
O	-2.75259100	2.57424100	-0.38883400
C	-3.19377400	3.29099600	1.86897600
H	-3.61911300	4.17849600	1.39617400

H	-3.91454800	2.84758800	2.56287300
H	-2.31356000	3.57986700	2.45462100
C	-0.33445900	-0.69216000	2.72190600
O	0.43779500	0.19357400	2.31173900
O	-1.25210400	-1.27318700	2.02169800
C	-0.24973500	-1.16016300	4.16590900
H	-0.39584100	-2.24189000	4.23198500
H	0.71082500	-0.87785900	4.60121600
H	-1.05289600	-0.68129000	4.73833000
H	0.75738400	0.67901700	0.77371400

INT-2'

Rh	2.76556500	8.80567800	-2.35914600
C	3.63770000	11.05362400	-4.35813300
C	3.05676000	10.68525100	-3.14357000
C	2.68612500	11.71006900	-2.25732500
C	2.90742100	13.05865400	-2.55148100
C	3.50758400	13.39732600	-3.76513700
C	3.86905100	12.40065200	-4.67250500
H	3.91060000	10.29188100	-5.08359700
H	2.60784500	13.81929100	-1.83618700
H	3.68102500	14.44383500	-4.00190600
H	4.32188700	12.66298800	-5.62516900
O	2.11120700	11.40582000	-1.05553200
N	1.78551800	10.00573500	-1.01205200
C	1.02284000	9.65253300	0.04090400
O	0.71354300	8.45937000	0.23688900
C	0.53840000	10.75732000	0.97094700
H	1.38245800	11.25011700	1.46598300
H	-0.00459900	11.53180600	0.42027500
H	-0.11368300	10.30361500	1.71927000
C	3.41118900	6.72560900	-1.39792400
C	3.81093500	6.73129800	-2.79104200
C	4.73038200	7.80564800	-3.00819800
C	4.86635500	8.51423600	-1.75345700
C	4.07918800	7.80052800	-0.75900100
C	5.84326600	9.61797100	-1.47078800
H	6.82453500	9.20490100	-1.19842200
H	5.97628100	10.26456500	-2.34150300
H	5.50518000	10.24808700	-0.64366800
C	4.00868900	8.11981600	0.70336600
H	4.69716600	7.46757200	1.25872000
H	4.29760100	9.15426900	0.90554000
H	2.99829400	7.96148900	1.08805200

C	5.54268300	8.04729600	-4.24819600
H	5.81346900	9.10131700	-4.34744200
H	6.47551500	7.46698700	-4.21386900
H	5.00372500	7.75609400	-5.15441500
C	3.47101800	5.65316600	-3.77901200
H	3.52998800	5.99519300	-4.81408100
H	4.17729200	4.81942100	-3.66156200
H	2.46830800	5.24888900	-3.61326000
C	2.50989300	5.73560400	-0.71798800
H	1.93350000	5.15170900	-1.44140700
H	3.08900300	5.02460800	-0.11273600
H	1.80351400	6.25457600	-0.06343300
C	0.52632400	9.17099900	-3.61659600
C	0.52454300	9.48090800	-5.05396400
C	-0.38049700	10.46029800	-5.50581800
C	1.33830800	8.84614000	-6.01752600
C	-0.53840500	10.74275400	-6.85838700
H	-0.98720300	10.98253600	-4.77012000
C	1.18905200	9.13044900	-7.37710200
C	0.24331100	10.06212400	-7.79698700
H	-1.26011700	11.48811900	-7.17841600
H	1.83534100	8.61976700	-8.08428400
H	0.13217600	10.27266800	-8.85720800
H	0.18195100	9.98881900	-2.98986200
O	2.31395800	7.95810900	-5.66443900
H	2.54280700	8.10964400	-4.72245500
C	0.66757200	7.94995200	-2.99660400
H	0.84411000	7.05016400	-3.57946400
H	0.33660500	7.82461400	-1.96916200

TS-1'

Rh	2.77275100	8.67824400	-2.26221800
C	3.33286100	10.99999900	-4.37127100
C	2.58632800	10.61250900	-3.24073800
C	2.37401900	11.58913700	-2.23785800
C	2.84515600	12.90084900	-2.37503600
C	3.56817200	13.24638800	-3.51276200
C	3.83194200	12.29222100	-4.50637200
H	3.50739300	10.28217700	-5.16653300
H	2.65803100	13.61649400	-1.58027900
H	3.93827500	14.26237900	-3.62208000
H	4.40578700	12.56405900	-5.38783000
O	1.69914400	11.27885700	-1.11193200
N	1.77130000	9.84773400	-0.83560700

C	0.90915600	9.47954400	0.14087500
O	0.79147100	8.28315000	0.45285300
C	0.12263100	10.56494100	0.86653200
H	0.78696000	11.32005800	1.29879900
H	-0.55252400	11.08763400	0.18004800
H	-0.45725700	10.08425800	1.65625400
C	3.51451000	6.76529600	-1.32003500
C	3.83130000	6.69855200	-2.71586500
C	4.75767700	7.76478700	-3.01319200
C	5.06661400	8.45898500	-1.78796400
C	4.28660700	7.85997300	-0.75585900
C	6.05129200	9.58357100	-1.64339900
H	7.08402500	9.20899600	-1.60942800
H	5.98473100	10.28851700	-2.47877900
H	5.87744500	10.14893000	-0.72357300
C	4.27715900	8.23231700	0.69573000
H	4.97162400	7.58751300	1.25249600
H	4.58645400	9.26917900	0.85130500
H	3.27835800	8.10548600	1.11956500
C	5.45618300	7.98880700	-4.32467600
H	5.70510200	9.04377300	-4.47093100
H	6.39812700	7.42280300	-4.34980700
H	4.85443900	7.66482800	-5.17759800
C	3.40004800	5.60970400	-3.65812400
H	3.39192900	5.93514400	-4.70131000
H	4.08686000	4.75497600	-3.58521600
H	2.39821000	5.24294500	-3.41632200
C	2.68832500	5.79006000	-0.53226400
H	2.06773700	5.17550500	-1.19118800
H	3.33250700	5.10951400	0.04298000
H	2.02234800	6.31543100	0.15665700
C	0.88141500	9.63998300	-3.66436100
C	0.71884300	9.75953400	-5.13980100
C	-0.17664300	10.71883700	-5.64066500
C	1.37734600	8.92532900	-6.06701300
C	-0.44933100	10.82678100	-7.00143100
H	-0.67783800	11.37876700	-4.93653600
C	1.11247400	9.03190700	-7.43522300
C	0.19684800	9.97245500	-7.89925300
H	-1.15816100	11.56820000	-7.35746800
H	1.63999700	8.36987800	-8.11495800
H	-0.00547700	10.04298600	-8.96448700
H	0.31796800	10.40293100	-3.13438200
O	2.31242600	8.00103100	-5.69114300

H	2.51001100	8.09373600	-4.73809800
C	0.83650400	8.33511900	-3.01313200
H	0.80627800	7.46241000	-3.66496300
H	0.18668900	8.24087000	-2.14772500

INT-3'

Rh	2.94775500	8.76636300	-2.04138000
C	2.74354600	11.76283000	-4.69778200
C	1.94535000	11.16714100	-3.70896500
C	2.07503900	11.65422700	-2.39397100
C	2.96890700	12.67610600	-2.07009700
C	3.76334300	13.23933100	-3.06783900
C	3.64695400	12.77969100	-4.38190700
H	2.64056700	11.44526300	-5.72993100
H	3.01964100	13.01608000	-1.04031700
H	4.45899000	14.03770400	-2.82395100
H	4.24931800	13.22410600	-5.16974400
O	1.24390800	11.14073000	-1.41437200
N	1.90453800	10.01770900	-0.76434600
C	1.30683700	9.72524300	0.42181500
O	1.61336300	8.70074100	1.05331400
C	0.27230400	10.69785300	0.96954600
H	0.66342700	11.71868400	1.01180500
H	-0.61531500	10.72356500	0.32769300
H	-0.00849500	10.36037700	1.96877800
C	3.40392900	6.82676200	-1.24802300
C	3.69137200	6.78590600	-2.67876300
C	4.74874500	7.70297900	-2.90459600
C	5.23635100	8.18470200	-1.59916600
C	4.45988800	7.61447100	-0.59151000
C	6.38400900	9.13678900	-1.44740300
H	7.33020200	8.65805800	-1.73416700
H	6.25928600	10.01534500	-2.09095100
H	6.48360100	9.48746400	-0.41758400
C	4.62379900	7.75411200	0.89189900
H	5.04204800	6.82947000	1.31439600
H	5.30649900	8.57022500	1.14542800
H	3.65979900	7.95128700	1.36470200
C	5.46122900	7.97597400	-4.19746600
H	5.72608700	9.03401600	-4.29683800
H	6.39945400	7.40370900	-4.23306800
H	4.86628300	7.69613900	-5.06869700
C	3.03883100	5.88628700	-3.68578100
H	3.04005100	6.32809700	-4.68575000

H	3.57026400	4.92620300	-3.73748300
H	2.00007700	5.67167300	-3.41802000
C	2.40521000	5.99219300	-0.51183700
H	1.64630200	5.58319700	-1.18455100
H	2.90691400	5.14855100	-0.01594800
H	1.91116600	6.60028600	0.25309300
C	0.89314300	10.07785400	-3.97610600
C	0.63452100	9.81329600	-5.45379800
C	-0.56483100	10.23084400	-6.04660400
C	1.55573800	9.12828900	-6.27091900
C	-0.85166000	9.98730100	-7.38988700
H	-1.28900400	10.75932000	-5.43058700
C	1.28160400	8.87795900	-7.61834400
C	0.07956100	9.30684200	-8.17660200
H	-1.79251600	10.32395900	-7.81546800
H	2.02358200	8.34736800	-8.20755800
H	-0.12726500	9.10712000	-9.22461000
H	-0.03969300	10.48666400	-3.57239000
O	2.76516700	8.68153200	-5.79821100
H	2.84178400	8.88521900	-4.84966000
C	1.18137800	8.75662900	-3.18043900
H	1.19617500	7.89486000	-3.85313300
H	0.38799900	8.58678300	-2.44954000

INT-4a

Rh	2.68784100	8.65617600	-1.93906600
C	0.94795500	12.07593100	-4.42709500
C	1.04543900	11.43449600	-3.18007300
C	1.90477900	12.02703100	-2.23658700
C	2.58693200	13.21698500	-2.52222300
C	2.44759900	13.83471400	-3.76073400
C	1.62973500	13.25270500	-4.73088500
H	0.28913300	11.63410400	-5.17154300
H	3.22443400	13.63996000	-1.75165000
H	2.98065600	14.75915500	-3.96525800
H	1.51199400	13.71566600	-5.70645600
O	2.13649900	11.59081800	-0.94087900
N	1.89267600	10.21445400	-0.67284000
C	1.35373400	10.07581400	0.50818500
O	1.08046000	8.88206200	0.97856800
C	4.58650200	7.31670200	-1.64118600
C	3.99827000	7.25168100	-2.98513500
C	4.19376000	8.53343500	-3.60837300
C	4.71667700	9.41584700	-2.61223800

C	5.01657600	8.63130500	-1.41186500
C	5.16275000	10.83155500	-2.82814000
H	6.23101900	10.86005600	-3.08787500
H	4.60720600	11.31564100	-3.63437000
H	5.02682500	11.43494100	-1.92620100
C	5.66534700	9.18911100	-0.17801100
H	6.73401800	9.38283000	-0.34497700
H	5.20715200	10.13860800	0.11952400
H	5.58158900	8.50195200	0.66836200
C	3.93452800	8.87812800	-5.04476700
H	3.57370400	9.90498800	-5.15633400
H	4.85761200	8.78108500	-5.63291200
H	3.19163500	8.21145900	-5.49197300
C	3.53497600	5.98800400	-3.65093200
H	2.84285500	6.19749800	-4.47131000
H	4.38242000	5.42114400	-4.06244600
H	3.01206000	5.33953300	-2.94199300
C	4.60256300	6.15840500	-0.68955500
H	3.58107800	5.80546300	-0.50324800
H	5.17781400	5.31971600	-1.10234100
H	5.04669500	6.42870400	0.27232300
C	1.00022700	8.86423100	-3.17325400
H	1.35250800	8.85827300	-4.21221900
C	0.12189300	7.65986900	-2.89602800
C	0.35137300	6.95158200	-1.70321900
C	-0.92312900	7.25254900	-3.73317100
C	-0.47822200	5.88050100	-1.34049900
C	-1.74471300	6.17570800	-3.38735900
H	-1.09773700	7.78740100	-4.66576500
C	-1.52226700	5.49967800	-2.18421500
H	-0.28101600	5.35050000	-0.41242500
H	-2.55031900	5.86880000	-4.04896300
H	-2.15765100	4.66240900	-1.90516100
O	1.41489000	7.30314300	-0.93735400
H	1.19523700	8.15074100	0.23958700
C	0.22798100	10.18020600	-2.94500500
H	-0.21107000	10.17905500	-1.94397300
H	-0.62474100	10.20472400	-3.64096100
C	1.01293800	11.22891300	1.41017300
H	1.91076200	11.79796600	1.67032200
H	0.32981900	11.91903000	0.90595000
H	0.54572000	10.84009900	2.31603400

TS-2a

Rh	2.57865400	8.23008000	-1.80692500
C	0.50828600	12.59496200	-3.75704600
C	1.09488300	11.67538600	-2.88536300
C	2.26089900	12.09094100	-2.13446400
C	2.66637700	13.46531500	-2.21493300
C	2.06378100	14.33900400	-3.10054800
C	0.98517000	13.90241000	-3.88831500
H	-0.36497200	12.28837000	-4.33006400
H	3.51473100	13.76392500	-1.60576300
H	2.42102800	15.36216200	-3.18856100
H	0.50117300	14.58775600	-4.57866500
O	2.97621900	11.25286700	-1.47043700
N	2.18207800	9.45469800	-0.34998500
C	1.40684800	9.48202600	0.66558200
O	0.77084100	8.38191100	1.10461300
C	4.50466400	6.95081600	-1.31066600
C	3.80847300	6.40534400	-2.46259200
C	3.84527800	7.36324700	-3.52278700
C	4.47355500	8.55155900	-3.00528100
C	4.89816800	8.27488100	-1.64176200
C	4.81887700	9.77928200	-3.79456600
H	5.71689800	9.60630100	-4.40509800
H	4.00975700	10.06387200	-4.47517000
H	5.00539900	10.63040000	-3.13764100
C	5.63914000	9.24559800	-0.77069600
H	6.67503200	9.36148100	-1.11692800
H	5.15589700	10.22658300	-0.79224700
H	5.67129800	8.90637100	0.26801400
C	3.39297200	7.14689500	-4.93758600
H	3.15358500	8.09369100	-5.43046900
H	4.18419600	6.66406400	-5.52744600
H	2.50317700	6.51303000	-4.99058600
C	3.21049900	5.03222900	-2.51711100
H	2.61811000	4.88681100	-3.42341100
H	3.99680500	4.26608600	-2.49704700
H	2.55022100	4.86511100	-1.65973700
C	4.76918800	6.20551400	-0.03477500
H	3.92696500	5.55852200	0.23097400
H	5.65689700	5.56363400	-0.12735200
H	4.94226300	6.88631900	0.80338700
C	1.11204300	9.01847700	-3.10227700
H	1.59303900	9.19966500	-4.07041400
C	0.08102100	7.91259900	-3.20197000
C	0.01071900	6.99976100	-2.13175600

C	-0.83769200	7.80294700	-4.25239000
C	-1.00771200	6.03405800	-2.09464500
C	-1.83652300	6.82573200	-4.23444600
H	-0.77558300	8.49936600	-5.08742600
C	-1.92234600	5.95327200	-3.14490300
H	-1.05050400	5.34478000	-1.25563400
H	-2.54122700	6.74858700	-5.05775300
H	-2.69869100	5.19222300	-3.11868500
O	0.96463900	7.04324400	-1.17637900
H	0.78295100	7.71720800	0.34716900
C	0.42945100	10.35146900	-2.62923200
H	0.20319300	10.25879900	-1.56300600
H	-0.54003400	10.37697200	-3.14677500
C	1.15860500	10.72049300	1.47975300
H	1.39184900	10.51581500	2.53079200
H	1.77352700	11.54240800	1.11317300
H	0.09830300	10.99161400	1.42284500

INT-5a

Rh	2.31481500	8.67015800	-1.87840100
C	0.88902800	12.91464100	-3.83058200
C	1.19895800	11.82432300	-3.01803600
C	2.48103300	11.73358300	-2.42249500
C	3.40800700	12.77461800	-2.65904900
C	3.06580100	13.86949500	-3.45212300
C	1.80804600	13.94430600	-4.05286000
H	-0.09889200	12.96594600	-4.28540700
H	4.38037000	12.73025200	-2.17738500
H	3.79055300	14.66671600	-3.60149900
H	1.54275900	14.79126700	-4.67924200
O	2.78769700	10.72755500	-1.60423200
N	1.33645300	9.08164500	-0.15398300
C	1.09367600	8.20814300	0.74100300
O	1.25903200	6.85744100	0.66329400
C	4.57578400	7.75886200	-1.08784400
C	3.88188700	6.86115100	-1.94179200
C	3.79510600	7.45241500	-3.29660100
C	4.41691400	8.69739700	-3.24176000
C	4.91488100	8.88593000	-1.86661000
C	4.66314500	9.65863300	-4.36309700
H	5.72591100	9.66221000	-4.64275700
H	4.09077500	9.38902700	-5.25477900
H	4.39203000	10.68206200	-4.08440200
C	5.61423500	10.09618900	-1.38524100

H	6.20301300	10.57407200	-2.17399300
H	4.81943600	10.80301100	-1.08342900
H	6.25671600	9.89183700	-0.52476100
C	3.25411000	6.72655700	-4.49030300
H	3.08421800	7.40404800	-5.33141600
H	3.95790200	5.95197600	-4.82528400
H	2.30715300	6.23227900	-4.25385000
C	3.52918800	5.45013200	-1.62463700
H	2.53902500	5.20329800	-2.01590000
H	4.25879800	4.78211500	-2.10536200
H	3.54427000	5.25698700	-0.54957800
C	4.89687900	7.52848200	0.36275300
H	4.06617000	7.03162800	0.87269700
H	5.79054600	6.90125700	0.48274200
H	5.08048300	8.47283400	0.88179600
C	0.77614500	9.33824500	-3.17252600
H	1.34381300	9.42361700	-4.11016600
C	-0.28060800	8.26493200	-3.25862200
C	-0.01175200	7.06334200	-2.59966200
C	-1.48197200	8.39578800	-3.96543800
C	-0.92462200	5.99900900	-2.63452900
C	-2.39817100	7.34254100	-4.01316800
H	-1.70174700	9.32168800	-4.49120300
C	-2.11604700	6.14859700	-3.34292500
H	-0.69251400	5.07843100	-2.10622300
H	-3.32647700	7.45534600	-4.56578000
H	-2.82853500	5.32794800	-3.36885900
O	1.16387700	6.94491700	-1.94484700
H	1.25011000	6.65275000	-0.30881100
C	0.23612400	10.70737400	-2.74778900
H	-0.03027800	10.65712400	-1.68429900
H	-0.69352400	10.89323200	-3.30398500
C	0.56065300	8.63887200	2.08784000
H	1.22556400	8.27044800	2.87829100
H	0.49461600	9.72606900	2.14227500
H	-0.42822500	8.19669400	2.25491800

INT-6a

Rh	2.32773200	8.71109600	-2.36320300
C	0.95166800	12.81658200	-4.47254100
C	1.16288800	11.98155900	-3.36035000
C	2.23616300	12.32032700	-2.51510400
C	3.03435700	13.44441100	-2.78377000
C	2.78651000	14.25146900	-3.88726100

C	1.73442000	13.93435400	-4.74863300
H	0.12433600	12.57136700	-5.13531100
H	3.84641500	13.66541500	-2.09725500
H	3.41393400	15.11937900	-4.07196300
H	1.52228800	14.55018300	-5.61797100
O	2.63307900	11.68022500	-1.36181600
N	2.11665100	10.37890900	-1.09069700
C	1.92553800	10.20294900	0.21746100
O	1.77293600	9.02723800	0.66213100
C	3.86187600	6.96601800	-1.82705100
C	3.23001400	6.81073200	-3.14737300
C	3.64054600	7.89834500	-3.96930600
C	4.35057600	8.83066100	-3.12032800
C	4.55751000	8.17781400	-1.81669900
C	5.05721600	10.07746500	-3.56578400
H	6.09983600	9.85871800	-3.83815800
H	4.57043000	10.52821300	-4.43458400
H	5.06833200	10.82905700	-2.77194100
C	5.33796900	8.77997300	-0.68648300
H	6.41692300	8.63000400	-0.83103300
H	5.16345800	9.85819100	-0.62026100
H	5.06039300	8.34034700	0.27474000
C	3.40186100	8.04011800	-5.44282500
H	3.42615300	9.08702700	-5.75794500
H	4.18193300	7.50868300	-6.00515000
H	2.43593400	7.62068700	-5.74033400
C	2.47300100	5.59250600	-3.59083600
H	1.79374800	5.81999800	-4.41680600
H	3.16276500	4.80530300	-3.92720800
H	1.87333100	5.17611300	-2.77593900
C	3.70337300	5.98528400	-0.70337600
H	2.64640400	5.78167100	-0.49766100
H	4.18222500	5.02775500	-0.94918500
H	4.15080900	6.35857600	0.22066400
C	0.86212700	9.46470400	-3.68264300
H	1.30769000	9.63228600	-4.66886100
C	-0.17455300	8.36736200	-3.75557900
C	-0.44705300	7.65128500	-2.57863300
C	-0.91190900	8.04221300	-4.89765700
C	-1.43087100	6.67024700	-2.50763000
C	-1.89790900	7.04721900	-4.85934200
H	-0.71855200	8.57943800	-5.82408000
C	-2.15899200	6.37316000	-3.66655700
H	-1.60396500	6.14167700	-1.57515200

H	-2.45889100	6.80492900	-5.75780900
H	-2.92343100	5.60138600	-3.63154400
O	0.37476300	7.99410100	-1.52998100
H	0.82959900	8.41142200	1.68063600
C	0.24373600	10.78865000	-3.18890100
H	-0.08679700	10.67841200	-2.15331100
H	-0.66211200	10.98581700	-3.78264100
C	1.91516100	11.39244300	1.15995800
H	1.45939000	11.08421700	2.10373700
H	2.93979400	11.72710100	1.36028000
H	1.37345400	12.24322900	0.73931000
C	-0.30455700	6.83087000	1.79854900
O	0.24201000	7.89046400	2.34740200
O	-0.20460900	6.51272600	0.60891900
H	0.24614400	7.46977400	-0.68858300
C	-1.09333700	5.99546000	2.78054500
H	-1.86003000	6.61292800	3.25982900
H	-1.55783700	5.15186500	2.26896600
H	-0.42946000	5.63187800	3.57216100

TS-3a

Rh	2.08664000	8.52672400	-2.08776000
C	0.96020000	13.19962700	-4.27520600
C	1.42002100	12.21767300	-3.39513600
C	2.77233700	12.30094100	-2.87502300
C	3.56274900	13.44306100	-3.25251300
C	3.07025700	14.39415800	-4.12296000
C	1.76551000	14.27756200	-4.64546500
H	-0.05536100	13.13014900	-4.66205700
H	4.56655200	13.51142000	-2.84165600
H	3.68899300	15.24127100	-4.41111200
H	1.38236300	15.03507100	-5.32377100
O	3.23051100	11.36600800	-2.13671500
N	1.96296500	9.71389500	-0.57255400
C	2.05923200	9.66599800	0.72099800
O	2.07059200	8.57225400	1.39983000
C	3.57661000	6.82535500	-1.47281600
C	2.82781800	6.40028900	-2.63716900
C	3.12185700	7.27481900	-3.73311600
C	3.98512400	8.31141300	-3.23284500
C	4.26525700	8.02120300	-1.83040700
C	4.66933700	9.36429800	-4.04898900
H	5.59016900	8.95476800	-4.48912300
H	4.03948100	9.71460300	-4.87230000

H	4.92017500	10.23044800	-3.43622200
C	5.17854300	8.82652800	-0.95723900
H	6.22754400	8.59732400	-1.19084000
H	5.01169600	9.89560300	-1.11514000
H	5.00933200	8.60368400	0.09914800
C	2.68355500	7.09717300	-5.15724300
H	2.68540700	8.04815500	-5.69757700
H	3.36285100	6.41762500	-5.69000900
H	1.67508200	6.67987100	-5.22670000
C	1.93701300	5.19519500	-2.69422100
H	1.21712200	5.26753200	-3.51376100
H	2.53553700	4.28785200	-2.85425200
H	1.37663200	5.06527700	-1.76380400
C	3.64048200	6.11983200	-0.14936100
H	2.84662000	5.37255600	-0.06434500
H	4.59964600	5.59641700	-0.03405200
H	3.51891800	6.82462300	0.67733200
C	0.96695600	9.68392000	-3.49338000
H	1.59052300	9.81476200	-4.38141300
C	-0.23209700	8.81974500	-3.80186200
C	-0.73356000	8.00891000	-2.77288100
C	-0.89868900	8.79150400	-5.03116400
C	-1.85892200	7.20725500	-2.92544700
C	-2.03214400	7.98997400	-5.21504500
H	-0.53006700	9.40702500	-5.84854400
C	-2.50895900	7.20426800	-4.16538400
H	-2.20061500	6.58679600	-2.10223600
H	-2.53556800	7.97773400	-6.17759700
H	-3.38415100	6.57608800	-4.30670300
O	-0.00274200	8.07450900	-1.60225700
H	0.96328600	7.58673700	1.62191200
C	0.55666600	11.09736100	-2.92075700
H	0.56846000	11.04233300	-1.82715100
H	-0.47562600	11.28621000	-3.24605900
C	2.15471400	10.99069500	1.45928600
H	1.27692900	11.10695800	2.10549500
H	3.04137200	10.96651200	2.10270700
H	2.22376100	11.83387500	0.76937800
C	-0.32497100	6.08087400	1.29811600
O	0.32777400	6.89617200	2.07635800
O	-0.34829300	6.11517700	0.05763600
H	-0.14853700	7.32041700	-0.94799300
C	-1.09504600	5.02546800	2.05969400
H	-0.40268900	4.42000100	2.65397200

H	-1.78368900	5.50817300	2.76078000
H	-1.64941600	4.38885200	1.36937000

TS-2b

Rh	-1.00254100	-0.36608200	-0.16919100
C	2.90692500	-2.36908400	-1.37784100
C	1.94760000	-1.69719500	-0.59912300
C	2.08655600	-1.75986400	0.80366700
C	3.16289800	-2.45589600	1.37409800
C	4.10489700	-3.09361100	0.57642500
C	3.98020900	-3.05158000	-0.81496100
H	2.79642900	-2.34549200	-2.46017700
H	3.23057500	-2.48375200	2.45707800
H	4.93368100	-3.62143500	1.04005800
H	4.70436500	-3.54999300	-1.45240800
O	1.18538800	-1.28908100	1.72708200
N	0.42053400	-0.14435600	1.34360700
C	0.50894700	0.85222000	2.23717800
O	-0.16178200	1.90131800	2.08482100
C	-2.89039600	0.94487500	0.27101900
C	-2.86807700	0.68637600	-1.12429600
C	-2.89967300	-0.74487100	-1.31463500
C	-3.05779400	-1.36977200	-0.01340900
C	-2.98561500	-0.33882700	0.96153100
C	-3.30614900	-2.83002900	0.24148800
H	-4.38308600	-3.04899500	0.21910600
H	-2.82892800	-3.46310500	-0.51235300
H	-2.92786700	-3.13776800	1.22032900
C	-3.11246300	-0.49100000	2.44882400
H	-4.14735600	-0.30838500	2.77066700
H	-2.83375000	-1.49610000	2.77755400
H	-2.47244900	0.22670000	2.96956200
C	-3.00077700	-1.45513800	-2.63584600
H	-2.44939700	-0.93049700	-3.42227700
H	-2.60764400	-2.47485300	-2.57657300
H	-4.04696600	-1.52667900	-2.96460000
C	-2.81640000	1.72876800	-2.20277900
H	-2.51078900	1.30195700	-3.16307900
H	-3.80566900	2.18323900	-2.34998800
H	-2.11055000	2.52279700	-1.94166100
C	-3.02948500	2.28486300	0.92857500
H	-2.69258700	3.08921400	0.27027700
H	-4.08451000	2.47235000	1.17674100
H	-2.44279300	2.34025700	1.84770900

C	0.59678700	0.37429200	-1.46017700
H	-0.00015600	0.65350400	-2.32956700
C	1.58745200	1.43090700	-1.09967900
C	1.16899100	2.71189100	-0.67490100
C	2.95868400	1.24301400	-1.35202800
C	2.09280400	3.75163600	-0.53613400
C	3.88010900	2.27900300	-1.20335900
H	3.30702900	0.27557100	-1.69514400
C	3.44470000	3.54256200	-0.80191600
H	1.72246800	4.71667200	-0.20382000
H	4.93068800	2.09940600	-1.41542100
H	4.15336100	4.35896000	-0.68799000
O	-0.14867300	2.96445600	-0.39183800
H	-0.33833800	2.51251100	0.47765500
C	0.80391600	-1.05348700	-1.33274600
H	0.51574500	-1.62611800	-2.21524800
H	-0.24876500	-1.75953000	-0.45990000
C	1.43571400	0.70973000	3.43331300
H	1.16787100	-0.15832800	4.04420700
H	2.47226100	0.57190900	3.10912900
H	1.35793900	1.62104900	4.02831500

INT-4b

Rh	-0.94627600	-0.48981500	-0.04695700
C	2.72311600	-2.52565600	-1.43892000
C	1.89800600	-1.70806000	-0.63903500
C	2.16744800	-1.68706000	0.74808900
C	3.23252500	-2.44017000	1.27074600
C	4.03612100	-3.21729300	0.44866100
C	3.78073200	-3.26624500	-0.92508600
H	2.51452700	-2.56329800	-2.50617600
H	3.39973300	-2.39839400	2.34253000
H	4.85559100	-3.78585900	0.87968700
H	4.39262300	-3.87553100	-1.58359600
O	1.43834500	-1.07266800	1.73324700
N	0.52622300	-0.05272100	1.35070200
C	0.53868200	0.97901200	2.20541700
O	-0.25120100	1.94321100	2.04431300
C	-2.93606100	0.91231600	0.28517100
C	-2.81194400	0.67901400	-1.09948500
C	-2.79003700	-0.76115200	-1.32248800
C	-2.98831900	-1.40304400	-0.05433700
C	-2.96981400	-0.37469800	0.95677600
C	-3.28706800	-2.85979200	0.16909100

H	-4.37004800	-3.03367600	0.09807800
H	-2.80045500	-3.49663900	-0.57447300
H	-2.96229000	-3.19326600	1.15800600
C	-3.18945600	-0.55903800	2.42997100
H	-4.24853600	-0.42097200	2.69033700
H	-2.89211400	-1.55818000	2.76042400
H	-2.60872300	0.17196200	3.00006800
C	-2.82484300	-1.43694600	-2.66460600
H	-2.18916100	-0.92544700	-3.39477800
H	-2.48403000	-2.47436700	-2.59851500
H	-3.84398500	-1.44891500	-3.07596100
C	-2.75091100	1.73239000	-2.16641000
H	-2.41519200	1.31848400	-3.12241900
H	-3.74408600	2.17020200	-2.33628900
H	-2.06564500	2.53697900	-1.88241400
C	-3.11804700	2.23800200	0.96010500
H	-2.83031000	3.06357500	0.30421000
H	-4.17363300	2.37914300	1.23375800
H	-2.51346600	2.30663000	1.86705000
C	0.64180300	0.39003100	-1.48473300
H	-0.07362600	0.71880000	-2.23633200
C	1.60736300	1.44258300	-1.08704600
C	1.16508900	2.71955300	-0.67579800
C	2.98780800	1.24930500	-1.27949700
C	2.07899800	3.76158200	-0.49853900
C	3.89740000	2.28881400	-1.09408200
H	3.34578600	0.27914900	-1.60617800
C	3.44079000	3.55166100	-0.71047800
H	1.69647600	4.72613900	-0.17920100
H	4.95657100	2.11454900	-1.26233000
H	4.14334200	4.36870000	-0.56735900
O	-0.16460900	2.95057500	-0.43759200
H	-0.36987100	2.53464200	0.44926200
C	0.79353200	-0.99859700	-1.35013600
H	0.33307600	-1.60742600	-2.12596400
H	-0.55747400	-1.95147500	0.32592800
C	1.52485600	0.98653700	3.36027900
H	1.38768200	0.11301100	4.00570100
H	2.55521400	0.95856400	2.99183100
H	1.36507000	1.90158900	3.93272400

TS-3b

Rh	-0.89093700	-0.32857300	-0.01536600
C	2.47849800	-2.91745500	-0.68549000

C	1.89997500	-1.68210200	-0.35059500
C	2.42587200	-1.01115500	0.77408700
C	3.50299500	-1.52706600	1.49143100
C	4.08112900	-2.73968000	1.11189000
C	3.55756200	-3.44212200	0.02611500
H	2.08095700	-3.46296800	-1.53847400
H	3.87830900	-0.96369900	2.33984100
H	4.92402000	-3.13591100	1.67092500
H	3.98834200	-4.39428600	-0.27043700
O	1.93914600	0.22435200	1.16378700
N	0.54523100	0.22106000	1.50752600
C	0.28098600	0.75056300	2.74657400
O	-0.87752000	0.81842200	3.15769600
C	-3.06101900	0.65645400	0.41486800
C	-2.88354000	0.63280300	-0.98072100
C	-2.62105900	-0.75324400	-1.36117300
C	-2.79271000	-1.58865900	-0.19846400
C	-2.97565800	-0.71717800	0.91469700
C	-2.83831000	-3.09053000	-0.18778700
H	-3.85428100	-3.45189000	-0.40326400
H	-2.17294700	-3.52504600	-0.94031400
H	-2.54468800	-3.49598200	0.78435400
C	-3.28994000	-1.12489200	2.32567900
H	-4.37498500	-1.08800300	2.50026500
H	-2.95830500	-2.14741900	2.52961300
H	-2.79916300	-0.46138400	3.03921200
C	-2.52055200	-1.25080800	-2.77557100
H	-1.96268400	-0.56240700	-3.41829300
H	-2.03369200	-2.22917600	-2.82781500
H	-3.52172500	-1.35986600	-3.21507500
C	-2.98775900	1.79174800	-1.93147200
H	-2.38879900	1.63065800	-2.83315500
H	-4.02765400	1.93662400	-2.25718100
H	-2.64677300	2.72804400	-1.48108800
C	-3.36840800	1.85101100	1.26950400
H	-3.14632200	2.78694700	0.74823100
H	-4.43435500	1.86719300	1.53829800
H	-2.78533700	1.82463400	2.19308600
C	0.58501700	0.18510700	-1.57406700
H	-0.08612700	0.30620900	-2.42538400
C	1.58035300	1.29148500	-1.47201500
C	1.20042900	2.59710000	-1.09712100
C	2.90384400	1.08640800	-1.89349800
C	2.11580200	3.65219000	-1.15997000

C	3.82125100	2.13378100	-1.95535700
H	3.20583100	0.08695500	-2.19352800
C	3.41942800	3.42178400	-1.59214700
H	1.78459700	4.64113900	-0.85789400
H	4.83660500	1.94738100	-2.29351800
H	4.12325500	4.24879700	-1.63901300
O	-0.05936400	2.88342300	-0.65659200
H	-0.48343900	2.03947300	-0.39510600
C	0.77142900	-1.16553700	-1.16335900
H	0.32659700	-1.92993100	-1.79794900
H	-0.10342100	-1.06274900	1.19638300
C	1.45757900	1.25920200	3.56217200
H	2.14339300	0.44323600	3.81229900
H	2.03037600	2.00789100	3.00716100
H	1.05858200	1.69611000	4.47899100

INT-5b

Rh	-0.84072900	-0.22069400	-0.04711600
C	2.30312600	-3.06648200	-0.72897200
C	1.81327800	-1.80616700	-0.33334200
C	2.36288500	-1.27704500	0.85278200
C	3.35306300	-1.93668300	1.57899600
C	3.84292400	-3.16442700	1.13374100
C	3.30140900	-3.73337600	-0.02065000
H	1.89816700	-3.51458500	-1.63320400
H	3.72912200	-1.46876100	2.48382800
H	4.62379500	-3.67376500	1.69063500
H	3.65902900	-4.69655800	-0.37430600
O	1.95237400	-0.04824400	1.35727100
N	0.52732900	-0.08127600	1.67747400
C	0.20597800	1.01876500	2.57205000
O	-0.61974100	0.79973400	3.43500100
C	-2.97621200	0.51229800	0.62800100
C	-2.86202800	0.66451800	-0.77289900
C	-2.58280400	-0.65181500	-1.32411500
C	-2.72723900	-1.63458900	-0.25820200
C	-2.89386300	-0.92127200	0.94255300
C	-2.70035300	-3.12465800	-0.44384400
H	-3.66965800	-3.49721200	-0.80605900
H	-1.94539400	-3.43062800	-1.17621500
H	-2.48040700	-3.64616800	0.49259100
C	-3.08049800	-1.48704500	2.32182000
H	-4.13786900	-1.45497800	2.62099700
H	-2.75772000	-2.53153500	2.37769900

H	-2.51591200	-0.91731400	3.06654600
C	-2.53202800	-0.97702800	-2.79125500
H	-2.08032900	-0.16606000	-3.37154800
H	-1.95611700	-1.88785500	-2.98545300
H	-3.54223000	-1.13998000	-3.19299300
C	-3.06822700	1.91781300	-1.57667800
H	-2.37925300	1.98064100	-2.42510300
H	-4.08908400	1.95524000	-1.98383600
H	-2.92210100	2.81887000	-0.97430300
C	-3.33192800	1.57560700	1.62711900
H	-3.15312100	2.57870100	1.22798700
H	-4.39593200	1.51486600	1.89863100
H	-2.75596700	1.47499500	2.55237700
C	0.67822500	0.23468300	-1.50921800
H	0.09875100	0.39781800	-2.42129800
C	1.73792200	1.27100400	-1.35248700
C	1.35960600	2.60866900	-1.11182300
C	3.09843400	1.00600600	-1.56851600
C	2.30650700	3.63529400	-1.08684000
C	4.05242200	2.02400500	-1.54257700
H	3.40518400	-0.01472600	-1.77723200
C	3.65161000	3.34167400	-1.30754900
H	1.97163600	4.65063200	-0.89533500
H	5.09892000	1.79120100	-1.71924300
H	4.38548100	4.14345800	-1.29343500
O	0.05063100	2.92888000	-0.87224400
H	-0.42525900	2.07668600	-0.70958200
C	0.75774800	-1.15407100	-1.13561300
H	0.30716900	-1.84881900	-1.84411500
H	0.37300900	-0.94251400	2.21258900
C	0.88817500	2.33297900	2.33346200
H	1.96435500	2.20082000	2.20060400
H	0.49869200	2.79184600	1.41835300
H	0.67856700	2.98149400	3.18572900

TS-2c

Rh	2.78216800	7.96923000	-0.95991300
C	0.10980500	13.03399100	-3.37245200
C	0.78898000	11.93521100	-2.82631700
C	2.14397000	12.10368300	-2.52548200
C	2.81299600	13.30411300	-2.77855200
C	2.11496400	14.37388100	-3.33175100
C	0.75372100	14.24401900	-3.62258100
H	-0.94439700	12.92152800	-3.61627500

H	3.86770200	13.37855500	-2.53198300
H	2.63237100	15.30876700	-3.52778200
H	0.20158300	15.07549800	-4.05041800
O	2.93298600	11.09405400	-1.98328300
N	2.23746000	10.03761900	-1.35220400
C	1.81506000	10.27075600	-0.07717300
O	1.50371500	9.18118100	0.50731400
C	3.58120200	6.06652800	-0.14439100
C	3.48788900	5.89955200	-1.55700700
C	4.31654600	6.92533000	-2.13018100
C	5.16523600	7.48974900	-1.05822300
C	4.71576800	6.97408900	0.15054500
C	6.26600200	8.48076900	-1.29369200
H	7.12047800	8.01502400	-1.80552000
H	5.92943000	9.31152400	-1.92523700
H	6.63577600	8.90672900	-0.35616200
C	5.22209700	7.26607400	1.53174700
H	5.74128100	6.39635500	1.96009800
H	5.92630200	8.10366200	1.53735600
H	4.40381300	7.51665600	2.21698000
C	4.57920800	7.12120400	-3.59693700
H	4.81326300	8.16627100	-3.82731600
H	5.43234300	6.51402900	-3.93535000
H	3.71253300	6.82987500	-4.19879400
C	2.67343400	4.88827700	-2.30469500
H	2.13558900	5.33481900	-3.14710700
H	3.31290100	4.08708700	-2.70469500
H	1.92527300	4.41996300	-1.65860400
C	2.88200500	5.24750200	0.90343200
H	1.93537200	4.84425100	0.53261200
H	3.50342200	4.39994300	1.22842200
H	2.65925100	5.84806200	1.79172000
C	1.00307700	9.40340600	-2.62297400
H	1.72737700	9.43865200	-3.43335900
C	0.28408800	8.10117500	-2.61773600
C	-0.73651800	7.75746800	-1.68986500
C	0.41152200	7.29500800	-3.77287000
C	-1.57775800	6.67259100	-1.93806500
C	-0.43368800	6.21532900	-4.01357400
H	1.17036600	7.55639800	-4.50731200
C	-1.44199200	5.90615200	-3.09687600
H	-2.33896200	6.44641600	-1.19733900
H	-0.31450500	5.62947700	-4.92099600
H	-2.11323400	5.07104500	-3.27652400

O	-0.94049700	8.46992900	-0.54092600
H	-0.07332700	8.65855800	-0.11116000
C	0.08400500	10.61492500	-2.61233000
H	-0.50810000	10.61060100	-1.68864400
H	-0.64376600	10.46550700	-3.42299400
C	1.75882800	11.61350400	0.58551400
H	1.55242300	11.46251200	1.64685300
H	2.70955100	12.14550100	0.46895500
H	0.97666000	12.25021300	0.15489200

INT-4c

Rh	2.81038700	7.94204000	-0.91316900
C	0.23172700	13.41597700	-2.56574100
C	0.74969100	12.11797300	-2.46298800
C	2.12969000	11.98765100	-2.26069400
C	2.97233400	13.09886100	-2.18655900
C	2.43016300	14.37627900	-2.30195100
C	1.05347900	14.53861800	-2.48447900
H	-0.83753600	13.53732900	-2.72498800
H	4.03644200	12.94347400	-2.03653300
H	3.08208700	15.24326000	-2.24180100
H	0.62536300	15.53301900	-2.57044700
O	2.76258800	10.74897600	-2.15453300
N	1.87349600	9.66836300	-1.83482100
C	1.69967100	9.52346700	-0.37346900
O	0.81564800	8.60451100	-0.09681400
C	3.89092900	6.42701500	0.28202100
C	3.58024600	5.70284900	-0.96408400
C	4.19986600	6.37589100	-2.01647500
C	4.90223400	7.54212900	-1.44715700
C	4.82921600	7.46576900	-0.01532300
C	5.78227600	8.47000800	-2.23474000
H	6.77657200	8.02805900	-2.39402500
H	5.35800500	8.68659000	-3.21983400
H	5.92032000	9.42457200	-1.71867600
C	5.57914900	8.31646600	0.96826500
H	6.54984600	7.86579200	1.22220300
H	5.77841200	9.31564600	0.56840800
H	5.02319000	8.43904800	1.90287900
C	4.17050500	6.02217500	-3.47475400
H	4.12830800	6.91682300	-4.10468000
H	5.07179200	5.46397100	-3.76718700
H	3.30178800	5.40539100	-3.72214900
C	2.72308500	4.47324400	-1.03769100

H	2.38761500	4.27616900	-2.05973600
H	3.27277600	3.58654300	-0.69023300
H	1.83050600	4.56670600	-0.41013500
C	3.47397100	5.96746400	1.64947700
H	2.43389800	5.62643900	1.65550300
H	4.09779500	5.12964400	1.99317600
H	3.56213200	6.77097000	2.38668300
C	0.76760200	9.66738400	-2.87641600
H	1.34862100	9.88270700	-3.77722400
C	0.06374500	8.35519600	-3.16833600
C	-1.04888700	7.85270900	-2.45332300
C	0.45720500	7.67176300	-4.33205300
C	-1.75512000	6.74699900	-2.94962400
C	-0.22596100	6.55527100	-4.80760200
H	1.31175200	8.04858500	-4.89038200
C	-1.35369200	6.10470000	-4.11624600
H	-2.61194500	6.40247700	-2.37881100
H	0.10259200	6.06018400	-5.71689100
H	-1.91369100	5.24673000	-4.47973000
O	-1.49028200	8.40716500	-1.29551000
H	-0.68149200	8.58326700	-0.73922900
C	-0.12266000	10.88817100	-2.60683700
H	-0.74129300	10.71863900	-1.71940000
H	-0.81728000	11.01669000	-3.44583000
C	1.98513500	10.65219200	0.58289600
H	2.06503500	10.21737200	1.58283900
H	2.90977600	11.17848000	0.34271100
H	1.16022300	11.37742700	0.59206700

TS-3e

Rh	2.23343000	8.65719200	-1.58581300
C	0.58580300	12.22649000	-4.36806300
C	0.93914900	11.38151200	-3.31384200
C	2.24490300	11.46349800	-2.76729100
C	3.14275400	12.41941700	-3.29423100
C	2.75654600	13.26935000	-4.32810000
C	1.47717700	13.17286600	-4.88112000
H	-0.41832100	12.15273300	-4.78291800
H	4.13044500	12.49649300	-2.84644300
H	3.46126000	14.00637500	-4.70700600
H	1.17485500	13.82650200	-5.69453300
O	2.63403000	10.70623800	-1.74393600
N	1.18842000	9.00093200	-0.05689300
C	0.90228800	8.91745900	1.20956700

O	-0.25255100	8.56732900	1.65149300
C	2.95060500	6.44355800	-1.78090600
C	3.19880900	7.06817000	-3.06199200
C	4.07842200	8.16281800	-2.85595100
C	4.43937100	8.19479400	-1.44798300
C	3.76407300	7.11016100	-0.79864600
C	5.39131500	9.18420600	-0.84966500
H	6.39276000	9.07807800	-1.28690300
H	5.03725500	10.20254900	-1.04718400
H	5.48323500	9.05747800	0.23233000
C	3.90572300	6.68988000	0.63478900
H	4.59234500	5.83641500	0.71552600
H	4.30442300	7.49521600	1.25600800
H	2.94719300	6.38046000	1.06189600
C	4.65420600	9.06610100	-3.90315100
H	4.63846900	10.10959500	-3.57780300
H	5.69696200	8.79129700	-4.11390300
H	4.09696900	9.00363500	-4.84152100
C	2.72898900	6.55957500	-4.39067200
H	2.48415400	7.37263400	-5.08158200
H	3.52230700	5.96256900	-4.86132300
H	1.85076900	5.91984900	-4.29093900
C	2.15324400	5.19337800	-1.55396400
H	1.26056100	5.16039300	-2.18414500
H	2.75968700	4.30562100	-1.78371400
H	1.82860600	5.10961200	-0.51343500
C	0.42884000	8.93304400	-2.92649800
H	0.89728100	8.80882700	-3.90627700
C	-0.48202500	7.82365000	-2.63229900
C	-1.21216900	7.72093900	-1.40373500
C	-0.64358000	6.77675900	-3.57371100
C	-1.94273300	6.54395000	-1.11969400
C	-1.42094500	5.65907000	-3.31184200
H	-0.16115900	6.87764700	-4.54188800
C	-2.05639300	5.53520300	-2.06224300
H	-2.45533500	6.47911000	-0.16399900
H	-1.54694700	4.88987000	-4.06872700
H	-2.65884800	4.65718900	-1.84338600
O	-1.17803700	8.73119100	-0.55589200
H	-0.95008700	8.52578000	0.52263600
C	-0.02122000	10.38478600	-2.72574600
H	-0.19981900	10.57123200	-1.66542400
H	-0.99386100	10.48529300	-3.23215700
C	1.95306200	9.34575800	2.22194800

H	2.88256700	9.66221900	1.74470000
H	1.54320200	10.17723700	2.80418500
H	2.14489500	8.51536700	2.90958100

INT-5e

Rh	0.13733400	0.54414400	0.20225200
C	-3.71457900	-1.87461200	-1.44323200
C	-2.69895900	-1.31919600	-0.66258100
C	-2.84952000	-0.00314300	-0.15753200
C	-4.04247900	0.69778100	-0.44415300
C	-5.05145700	0.11353300	-1.20776800
C	-4.89186500	-1.17480500	-1.72286800
H	-3.58563500	-2.88582800	-1.82660800
H	-4.16481200	1.69452700	-0.02713400
H	-5.96427500	0.67144000	-1.40535700
H	-5.67172900	-1.63139100	-2.32585100
O	-1.92624500	0.56780900	0.61484800
N	0.36919300	-0.44140400	1.83732900
C	-0.11601900	-0.56290100	3.00503000
O	0.16281200	-1.65342000	3.75101700
C	2.05613300	1.64033200	-0.47486900
C	1.13696800	1.71586700	-1.59969200
C	-0.03369400	2.37381900	-1.16451200
C	0.15934000	2.76487800	0.23233800
C	1.47352700	2.35143700	0.62838600
C	-0.84159700	3.54936600	1.02101500
H	-1.01352300	4.53270600	0.56381300
H	-1.79470700	3.00890000	1.04242600
H	-0.51370600	3.71022700	2.05127100
C	2.13878900	2.60074400	1.95020400
H	2.89989800	3.38692000	1.85787800
H	1.41903100	2.92229700	2.70688400
H	2.63316900	1.69949500	2.32511900
C	-1.23705300	2.72591200	-1.98515600
H	-2.16285500	2.44182100	-1.47635600
H	-1.27245200	3.80824800	-2.17056600
H	-1.22343800	2.22258100	-2.95554800
C	1.43848700	1.27847300	-3.00177800
H	0.55777800	0.86459500	-3.50284700
H	1.77973000	2.13603400	-3.59803900
H	2.23005200	0.52734100	-3.02757000
C	3.45583200	1.10395900	-0.52228300
H	3.52348600	0.18708100	-1.11481400
H	4.13413000	1.84346100	-0.97168200

H	3.82820700	0.87986600	0.48079000
C	-0.19204200	-1.46864100	-0.94786100
H	-0.38903400	-1.07285500	-1.94693100
C	1.10695700	-2.04935900	-0.82629100
C	1.58978500	-2.69019300	0.40456200
C	1.98803500	-2.03237700	-1.95492600
C	2.95908400	-3.15631200	0.42503400
C	3.25541400	-2.55835000	-1.90739000
H	1.60547500	-1.63299400	-2.89034700
C	3.75002300	-3.11557300	-0.69031000
H	3.30877300	-3.58824000	1.35834600
H	3.87770700	-2.57129200	-2.79811100
H	4.75941200	-3.51920600	-0.66031400
O	0.85418500	-2.80222000	1.42378300
H	0.62541100	-2.27204800	3.13359900
C	-1.44454600	-2.07560100	-0.31951800
H	-1.30827500	-2.17715100	0.75739300
H	-1.52534700	-3.09906000	-0.71926400
C	-0.98809600	0.44145900	3.71430900
H	-1.42971100	1.13015000	2.99483200
H	-1.78408800	-0.08938400	4.24568900
H	-0.39745700	0.98964400	4.45818100

TS-4e

Rh	0.14147800	0.59204900	0.22482700
C	-3.69760900	-1.88442700	-1.43834900
C	-2.68974100	-1.32824000	-0.64835600
C	-2.83827100	-0.00704300	-0.15379800
C	-4.02545900	0.69586800	-0.46199800
C	-5.02621400	0.11214000	-1.23667500
C	-4.86668600	-1.18038600	-1.74099000
H	-3.56994300	-2.90010000	-1.81048500
H	-4.14992500	1.69502800	-0.05141900
H	-5.93337100	0.67337300	-1.45049000
H	-5.64056000	-1.63742500	-2.35125900
O	-1.92543800	0.56460000	0.62880100
N	0.38290600	-0.41262900	1.84189900
C	-0.11072800	-0.55583500	3.00233400
O	0.14752600	-1.67236100	3.72132000
C	2.05113800	1.66984300	-0.47969000
C	1.12495300	1.74141900	-1.60391100
C	-0.04156200	2.40343800	-1.17061100
C	0.14878000	2.78377500	0.22891500
C	1.47426200	2.38062500	0.62118600

C	-0.84777600	3.57218400	1.02007400
H	-1.00542500	4.56200300	0.57154100
H	-1.80674100	3.04264300	1.03348000
H	-0.52259300	3.71922000	2.05326700
C	2.14184300	2.64456400	1.93880200
H	2.87313400	3.45843000	1.84411500
H	1.41803800	2.93595500	2.70379900
H	2.67097100	1.75946200	2.30427400
C	-1.24959800	2.75018600	-1.98678100
H	-2.17157000	2.44134100	-1.48518200
H	-1.30305100	3.83492900	-2.15213600
H	-1.22624700	2.26540200	-2.96637500
C	1.42368000	1.29052800	-3.00218000
H	0.53514200	0.90015100	-3.50798000
H	1.79477700	2.13492000	-3.59964000
H	2.19393100	0.51711100	-3.01927300
C	3.44942600	1.13005500	-0.53398200
H	3.50971200	0.20584100	-1.11583400
H	4.12522400	1.86213400	-0.99890400
H	3.83099600	0.91718000	0.46807200
C	-0.19554400	-1.56641200	-0.96444600
H	-0.39698900	-1.13320300	-1.94599500
C	1.09798200	-2.11452100	-0.83353700
C	1.57294700	-2.77779400	0.39696400
C	1.99677300	-2.05711200	-1.95379600
C	2.94939600	-3.23533300	0.41538400
C	3.26614400	-2.56656800	-1.90094300
H	1.61910800	-1.63945700	-2.88322300
C	3.75021600	-3.15150900	-0.68734200
H	3.29448500	-3.68748300	1.34064200
H	3.90364500	-2.54895300	-2.78056300
H	4.76500000	-3.54158800	-0.65557400
O	0.83346500	-2.91745100	1.40189300
H	0.59211500	-2.28955300	3.09027700
C	-1.44685800	-2.09412100	-0.28127400
H	-1.29626800	-2.14341900	0.79683900
H	-1.55695300	-3.13745000	-0.62021400
C	-0.97363200	0.43595400	3.74019000
H	-1.37197500	1.17770700	3.04880800
H	-1.80249900	-0.09580900	4.21780400
H	-0.39060500	0.92301400	4.53116700

INT-6e

Rh	0.26661000	1.15685800	0.14200800

C	-4.20133900	-1.42156700	-0.85768100
C	-2.81120200	-1.30483000	-0.78898900
C	-2.18532400	-0.09446200	-1.17738700
C	-2.99763100	0.97619300	-1.60346800
C	-4.38339100	0.84501800	-1.65801900
C	-4.99576700	-0.35557600	-1.28613000
H	-4.67001000	-2.35947400	-0.56417400
H	-2.51322200	1.90367100	-1.89823100
H	-4.98941300	1.68216900	-1.99766400
H	-6.07601600	-0.46240000	-1.33238700
O	-0.85071200	-0.02526100	-1.18635500
N	-0.88461000	0.66610100	1.55702400
C	-1.67074600	0.17180100	2.40862600
O	-1.50287400	-1.04100600	2.99720700
C	2.11579800	2.10800800	0.91237500
C	2.48035700	1.10029800	-0.06599200
C	1.91586500	1.48266900	-1.33183700
C	1.19588400	2.70893500	-1.15104400
C	1.32601700	3.09885200	0.23805400
C	0.49744500	3.47908400	-2.23158400
H	1.18591900	4.18863900	-2.71259800
H	0.11369400	2.81009100	-3.00680700
H	-0.34660100	4.05390700	-1.83892700
C	0.77778800	4.35539600	0.84468300
H	1.48874300	5.18320100	0.71440900
H	-0.16372200	4.65044100	0.37311300
H	0.59508800	4.23797700	1.91592200
C	1.98628400	0.71273700	-2.61771400
H	0.98244700	0.38611400	-2.91414800
H	2.40419500	1.33062300	-3.42177300
H	2.61114300	-0.17795600	-2.51681000
C	3.36074500	-0.08281100	0.19464800
H	3.15738300	-0.90211500	-0.49821700
H	4.41780600	0.19911800	0.08197900
H	3.22690100	-0.46737300	1.20902900
C	2.57416700	2.15464800	2.34013200
H	2.71370900	1.14973600	2.74811300
H	3.53230500	2.68562700	2.42568800
H	1.84948000	2.67081800	2.97595600
C	-0.65795500	-2.57202500	-1.02322500
H	-0.77508500	-2.49482900	-2.10405200
C	0.58556900	-2.97291200	-0.58697100
C	0.96547500	-3.13252300	0.84353800
C	1.57276900	-3.28772000	-1.60027700

C	2.28034100	-3.71329300	1.09242700
C	2.79837800	-3.79610500	-1.29470900
H	1.28916000	-3.13018500	-2.63901200
C	3.14091800	-4.02332500	0.08231000
H	2.53958800	-3.87197600	2.13497100
H	3.50943800	-4.04782300	-2.07580500
H	4.11543700	-4.44757100	0.31637300
O	0.24307500	-2.80117400	1.80639900
H	-0.76981300	-1.53610300	2.55631300
C	-1.93237300	-2.41986700	-0.26194000
H	-1.73058800	-2.30863700	0.80302000
H	-2.47288500	-3.37556200	-0.37426100
C	-2.92862100	0.85494900	2.89148100
H	-2.99343800	1.86796000	2.49172000
H	-3.80184400	0.28054300	2.56242300
H	-2.93987600	0.88437300	3.98676700

TS-5e

Rh	0.32600000	0.99886800	0.15442300
C	-4.33184800	-1.35015500	-0.67922600
C	-2.93962600	-1.35411700	-0.69680800
C	-2.23824400	-0.19463100	-1.06827600
C	-2.93024500	0.96892000	-1.42166300
C	-4.32731300	0.96174600	-1.39519400
C	-5.03116800	-0.18803200	-1.02533200
H	-4.87316400	-2.24977800	-0.39470700
H	-2.37984800	1.85986200	-1.70962900
H	-4.86983500	1.86276800	-1.67109800
H	-6.11746600	-0.18304300	-1.01308300
O	-0.88538700	-0.31681400	-1.08519500
N	-0.80122000	0.56254400	1.58730900
C	-1.66177100	0.06225900	2.37097300
O	-1.55204400	-1.14584000	2.94032300
C	2.08628700	2.05468500	0.90965900
C	2.56205900	1.04883100	-0.02028200
C	2.00542200	1.34692700	-1.30934400
C	1.21532400	2.54144600	-1.20295500
C	1.27134600	2.98633000	0.16834100
C	0.52101900	3.23714300	-2.33572600
H	1.19976100	3.94524900	-2.83210800
H	0.17942400	2.52406500	-3.09135100
H	-0.34924100	3.80333400	-1.99073500
C	0.64541900	4.23582200	0.71063200
H	1.32548800	5.08827900	0.57445400

H	-0.29030000	4.47354500	0.19701700
H	0.43100300	4.14822800	1.77863000
C	2.21507400	0.57077300	-2.57516100
H	1.26510300	0.40647500	-3.09364500
H	2.88117400	1.11867600	-3.25505400
H	2.65860000	-0.40698400	-2.37793500
C	3.51438400	-0.05834000	0.30615700
H	3.36448000	-0.92931400	-0.33490500
H	4.55024700	0.28721500	0.17384900
H	3.40526500	-0.39077500	1.34128700
C	2.48510300	2.17728600	2.35041800
H	2.65894700	1.19597000	2.79941600
H	3.41103400	2.76049400	2.44795000
H	1.71079100	2.67687700	2.93868300
C	-0.69860800	-2.22590400	-1.05029800
H	-0.80769200	-2.24847800	-2.13399400
C	0.58395600	-2.66250700	-0.60611200
C	0.91746600	-2.94821500	0.79025100
C	1.54992700	-2.93517500	-1.62232600
C	2.20972000	-3.56396000	1.01065400
C	2.77685900	-3.49784700	-1.35548600
H	1.27406800	-2.71478900	-2.65298100
C	3.09171200	-3.82362400	-0.00839800
H	2.44714600	-3.81256000	2.04131100
H	3.47564900	-3.72185800	-2.15606400
H	4.04993200	-4.28910400	0.21674100
O	0.16477200	-2.71474500	1.78248700
H	-0.81781200	-1.67382900	2.49187300
C	-2.00781100	-2.48582600	-0.34148000
H	-1.84984400	-2.57523000	0.73495900
H	-2.39592500	-3.44915400	-0.70196300
C	-2.92994000	0.78489900	2.76220100
H	-2.92758700	1.80939600	2.38681000
H	-3.79122700	0.24990600	2.34728700
H	-3.02753000	0.78750500	3.85333800

INT-7e

Rh	0.36627700	0.97140300	0.16291100
C	-4.42001100	-1.43460800	-0.64074300
C	-3.02958700	-1.46703100	-0.67924200
C	-2.32606000	-0.29489500	-0.96658600
C	-2.96145600	0.91345400	-1.22441200
C	-4.36098900	0.93184900	-1.18312400
C	-5.08622100	-0.22774300	-0.89437400

H	-4.98381300	-2.33660900	-0.41657300
H	-2.38857300	1.80879000	-1.44405000
H	-4.88640100	1.86202500	-1.38283000
H	-6.17182700	-0.19477500	-0.87098800
O	-0.95541600	-0.48559200	-0.97769400
N	-0.76021900	0.63277000	1.61613300
C	-1.66569900	0.09271900	2.33217300
O	-1.58480600	-1.12177600	2.85380500
C	2.09933600	2.02908700	0.90291100
C	2.61102500	1.02778800	-0.01006700
C	2.07166500	1.31121600	-1.31028000
C	1.26955900	2.49926100	-1.23286500
C	1.28466200	2.95017200	0.13561600
C	0.59290600	3.18319900	-2.38396600
H	1.27897000	3.88757200	-2.87541800
H	0.26417000	2.46520300	-3.14075500
H	-0.28306200	3.75252200	-2.05909600
C	0.64563200	4.20049600	0.66010900
H	1.33911600	5.04726700	0.56084500
H	-0.26469700	4.45163100	0.10875600
H	0.38466900	4.10485500	1.71684900
C	2.35530800	0.54084300	-2.56430600
H	1.48334500	0.51529000	-3.22465600
H	3.17700800	1.01556700	-3.11833600
H	2.64179800	-0.48946400	-2.34545300
C	3.57739200	-0.06069000	0.33358200
H	3.43721600	-0.94417800	-0.29255000
H	4.60833700	0.29726400	0.19462500
H	3.47175000	-0.37882100	1.37331200
C	2.46910900	2.17266600	2.34886500
H	2.67310300	1.20027900	2.80388800
H	3.37084300	2.79122100	2.45494600
H	1.66704600	2.64498300	2.92185800
C	-0.75697100	-2.03139900	-1.08910000
H	-0.82629100	-2.15867400	-2.17460400
C	0.56877400	-2.51406100	-0.62678700
C	0.87135900	-2.82067300	0.75564800
C	1.50917200	-2.82487300	-1.63125800
C	2.15184200	-3.43092200	0.99210400
C	2.74155300	-3.40573400	-1.36098000
H	1.23726400	-2.61974000	-2.66708800
C	3.04654800	-3.71573400	-0.02092300
H	2.37472800	-3.68504600	2.02508200
H	3.43081200	-3.65013700	-2.16421300

H	3.99545300	-4.19283100	0.21978500
O	0.07858200	-2.62733500	1.74750500
H	-0.83578100	-1.66752000	2.38427500
C	-2.04087800	-2.57932100	-0.44235100
H	-1.87623800	-2.77024800	0.62207800
H	-2.32481700	-3.52109100	-0.92413100
C	-2.94260400	0.82426200	2.68176700
H	-2.91233000	1.85960900	2.33820400
H	-3.78978400	0.31084300	2.21434900
H	-3.08813400	0.79670800	3.76713300

TS-3d

Rh	0.69631300	-0.87782700	0.18039700
C	1.95487600	3.75475000	-0.29575000
C	1.55014800	2.55472100	0.29024200
C	2.49562600	1.51832400	0.52245300
C	3.84875900	1.76162500	0.18353500
C	4.23457100	2.97475800	-0.38300500
C	3.29104500	3.97455300	-0.64147800
H	1.21736100	4.53886000	-0.46119000
H	4.58280700	0.99475200	0.41326500
H	5.28218000	3.14361300	-0.62326300
H	3.59409800	4.91803600	-1.08667700
O	2.12070600	0.38577900	1.09953100
N	-0.67984300	-0.40006100	1.45811800
C	-1.77550100	-1.21635500	1.57675000
O	-2.55013400	-1.54823900	0.67087400
C	0.06603900	-2.09607600	-1.59837300
C	1.31445200	-1.40490300	-1.91488900
C	2.33643800	-1.91544400	-1.06026300
C	1.72410900	-2.83473900	-0.14535700
C	0.32374200	-2.99027900	-0.52113700
C	2.43469100	-3.59713800	0.93119500
H	2.91318500	-4.49594200	0.51780700
H	3.21263500	-2.98709500	1.39811500
H	1.74514700	-3.91879700	1.71600900
C	-0.64198700	-3.98954300	0.03572200
H	-0.68891000	-4.87197400	-0.61747200
H	-0.34094400	-4.33198000	1.03012000
H	-1.64682200	-3.56385100	0.10982100
C	3.78290400	-1.53452600	-1.08848300
H	4.25198800	-1.67619200	-0.11187600
H	4.32404200	-2.15479800	-1.81639400
H	3.91981800	-0.48733300	-1.36969000

C	1.52633200	-0.42768000	-3.03269700
H	2.26936200	0.32949000	-2.76578600
H	1.88428500	-0.94534600	-3.93351900
H	0.60114400	0.08959600	-3.30175500
C	-1.23853000	-1.97373100	-2.32696300
H	-1.22995800	-1.14100800	-3.03465400
H	-1.44024800	-2.88961700	-2.89895900
H	-2.05524800	-1.81727200	-1.61648900
C	-0.61238400	1.35687000	-0.18385500
H	-0.09635500	1.19358500	-1.12897500
C	-2.05129800	1.47420000	-0.36217300
C	-2.93184400	1.72856000	0.72425800
C	-2.59699600	1.46445900	-1.66491600
C	-4.27342600	2.04531900	0.48678700
C	-3.93254500	1.75825700	-1.89858500
H	-1.93318200	1.26109000	-2.50182900
C	-4.76682100	2.06202600	-0.81347600
H	-4.91353800	2.24707800	1.33966600
H	-4.32380800	1.76396100	-2.91138100
H	-5.81352900	2.29945600	-0.98411800
O	-2.51094100	1.67117500	2.00659200
H	-1.67834300	1.13769200	2.03982500
C	0.14602400	2.29434900	0.75263100
H	0.17829000	1.88019000	1.76653200
H	-0.41888100	3.23486300	0.80258700
C	-2.04494800	-1.63502200	3.02531200
H	-1.14097600	-1.60899900	3.63966000
H	-2.77640400	-0.94282100	3.45832200
H	-2.47971600	-2.63886000	3.02827300

INT-5d

Rh	0.85820100	-0.94737800	-0.08902600
C	1.48095100	3.85599100	-0.92945500
C	1.24495900	2.69189700	-0.19371100
C	2.23857800	1.68833500	-0.14985800
C	3.45761800	1.90288300	-0.82883400
C	3.67550600	3.07573600	-1.54986800
C	2.68311900	4.05677100	-1.61271700
H	0.71312500	4.62748800	-0.95298100
H	4.23452400	1.14738700	-0.75697000
H	4.62461400	3.22575100	-2.05956800
H	2.84776600	4.97299600	-2.17294000
O	2.04794000	0.58002300	0.57876400
N	-0.84734700	0.15531900	-0.15123600

C	-1.80997900	-0.50409900	-0.97098300
O	-2.02729400	-0.17793900	-2.12782500
C	0.73523600	-2.73219400	-1.49582700
C	2.00533500	-2.00285600	-1.57567100
C	2.71322700	-2.20334000	-0.33477900
C	1.82984000	-2.87316400	0.55287900
C	0.62551500	-3.25442500	-0.18527100
C	2.12972100	-3.24786800	1.97243900
H	2.56707100	-4.25540800	2.02085500
H	2.84117600	-2.55125900	2.42337100
H	1.22545200	-3.25280400	2.58811300
C	-0.42854100	-4.16970600	0.35964000
H	-0.02663500	-5.18887300	0.44256900
H	-0.75103100	-3.86925400	1.36195200
H	-1.31126900	-4.21117600	-0.28039100
C	4.07838800	-1.69778900	0.01754200
H	3.99478900	-0.81435300	0.66171300
H	4.65242100	-2.46886100	0.54314500
H	4.63821400	-1.41339600	-0.87735300
C	2.54743800	-1.33931700	-2.80353600
H	3.09229000	-0.42381400	-2.55286400
H	3.23641500	-2.01276400	-3.33303900
H	1.74350100	-1.07053200	-3.49379800
C	-0.19495100	-2.93625100	-2.65311900
H	-0.53956200	-1.98652900	-3.07541900
H	0.31483700	-3.49535600	-3.44833800
H	-1.08134600	-3.50414800	-2.36154600
C	-1.09835600	1.62753700	-0.16495600
H	-1.14027900	1.95839200	-1.20907000
C	-2.46709900	1.89863500	0.46729200
C	-2.82465700	1.33550400	1.71187000
C	-3.36523900	2.78043500	-0.14384700
C	-4.03732100	1.67928300	2.32079600
C	-4.57562700	3.12683700	0.45823300
H	-3.10138900	3.20429900	-1.11049100
C	-4.90384600	2.57647000	1.69945000
H	-4.27864900	1.22882100	3.27903800
H	-5.25393300	3.81554500	-0.03726000
H	-5.84231400	2.83684400	2.18228500
O	-2.01632800	0.44523900	2.35876000
H	-1.35308400	0.13500700	1.69936000
C	-0.03156900	2.48040400	0.56784200
H	0.17568800	2.03035200	1.54435100
H	-0.49937200	3.45335100	0.75288300

C	-2.63907700	-1.58378800	-0.29783900
H	-2.14307700	-2.03917100	0.55946600
H	-3.54486200	-1.08899300	0.07605100
H	-2.94996300	-2.33979000	-1.02370200

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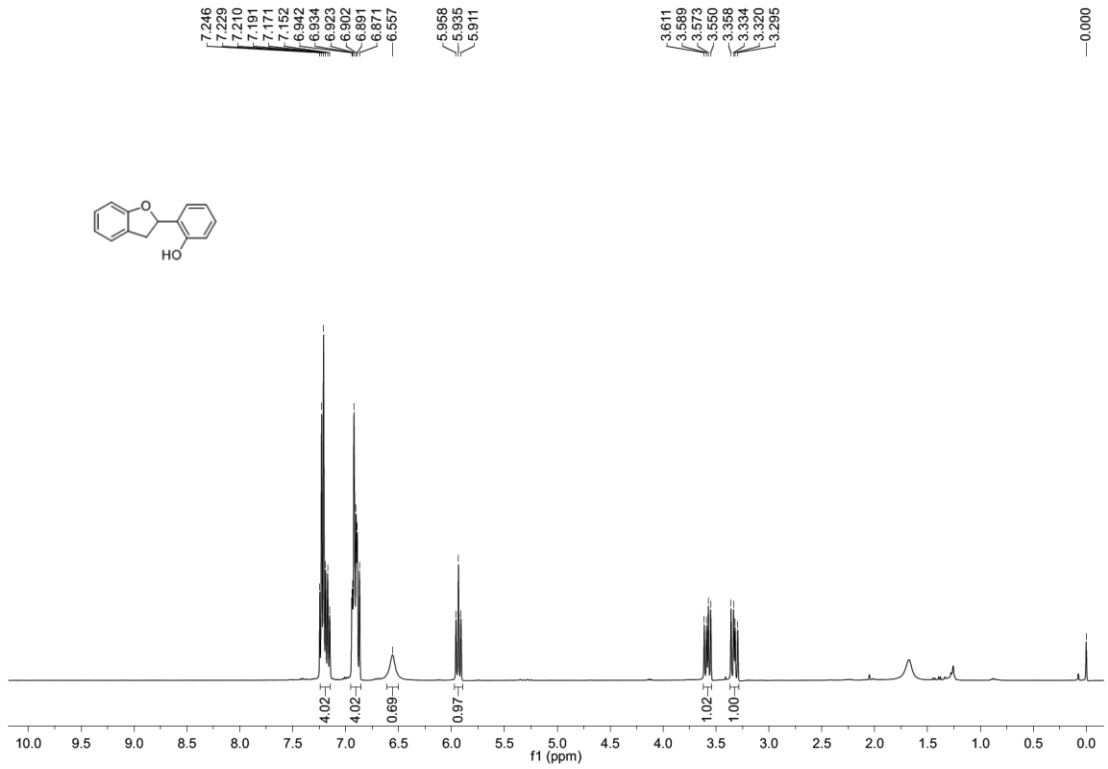
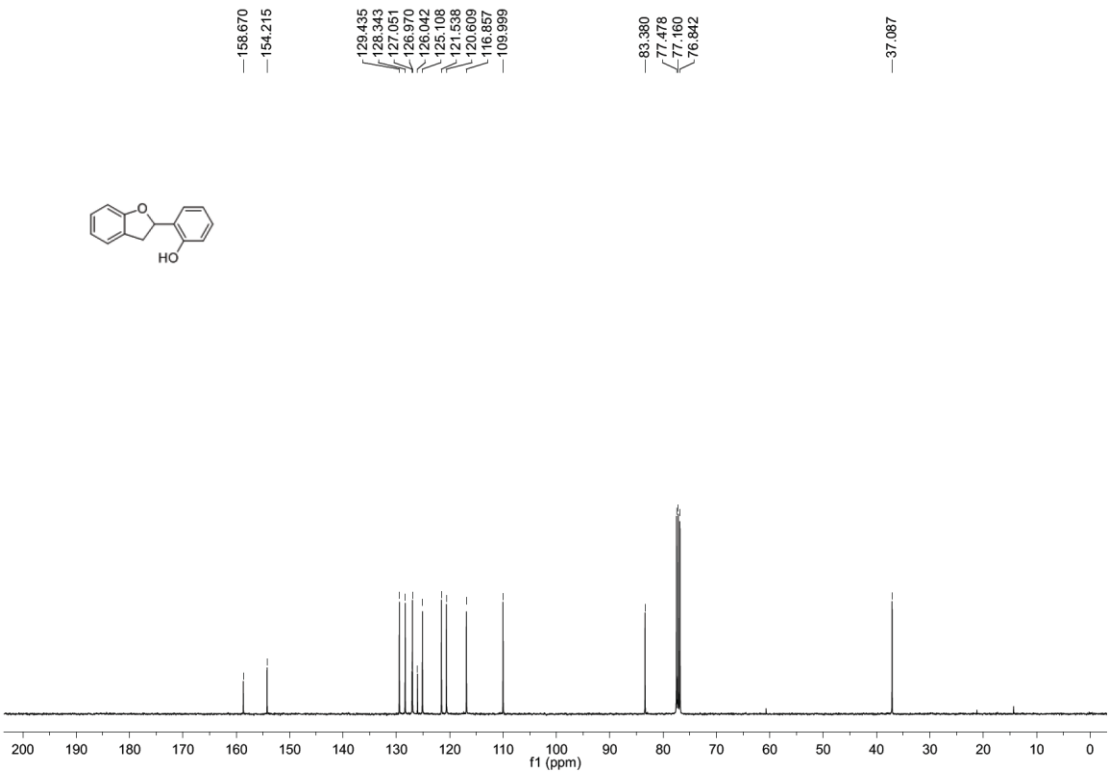
VII. Copies of ^{1}H and ^{13}C NMR Spectra

3a-^{1}H NMR (400 MHz, $CDCl_3$)



3a-^{13}C NMR (100 MHz, $CDCl_3$)



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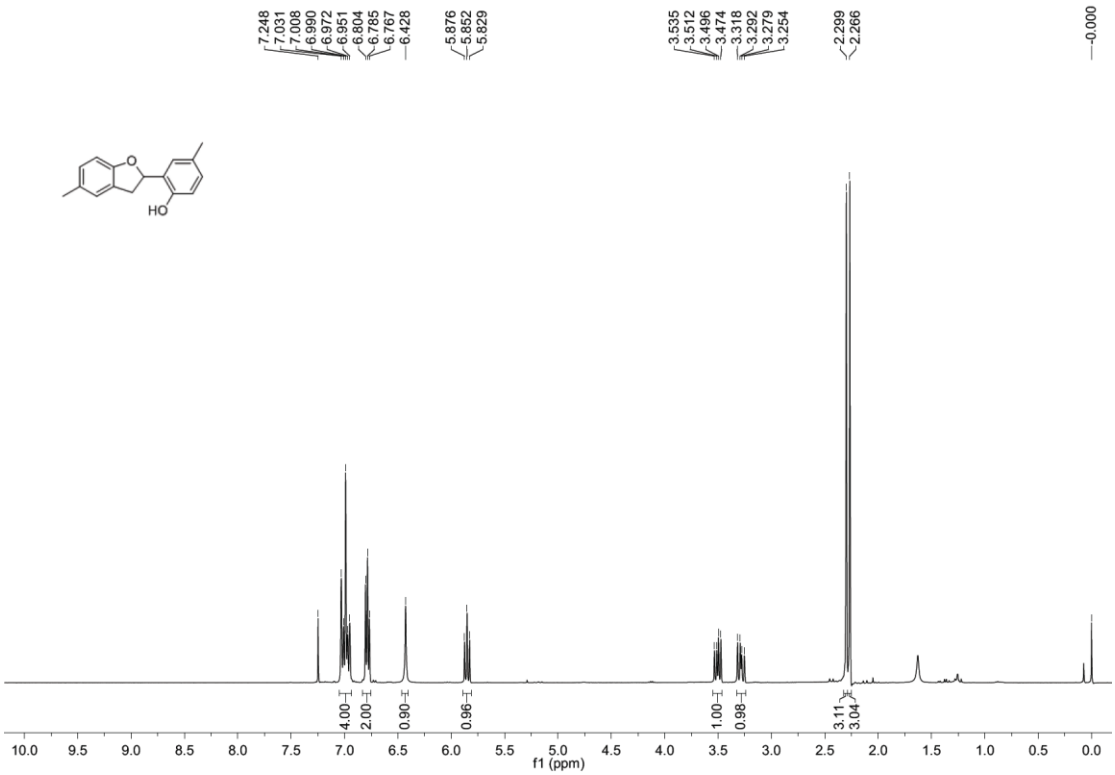

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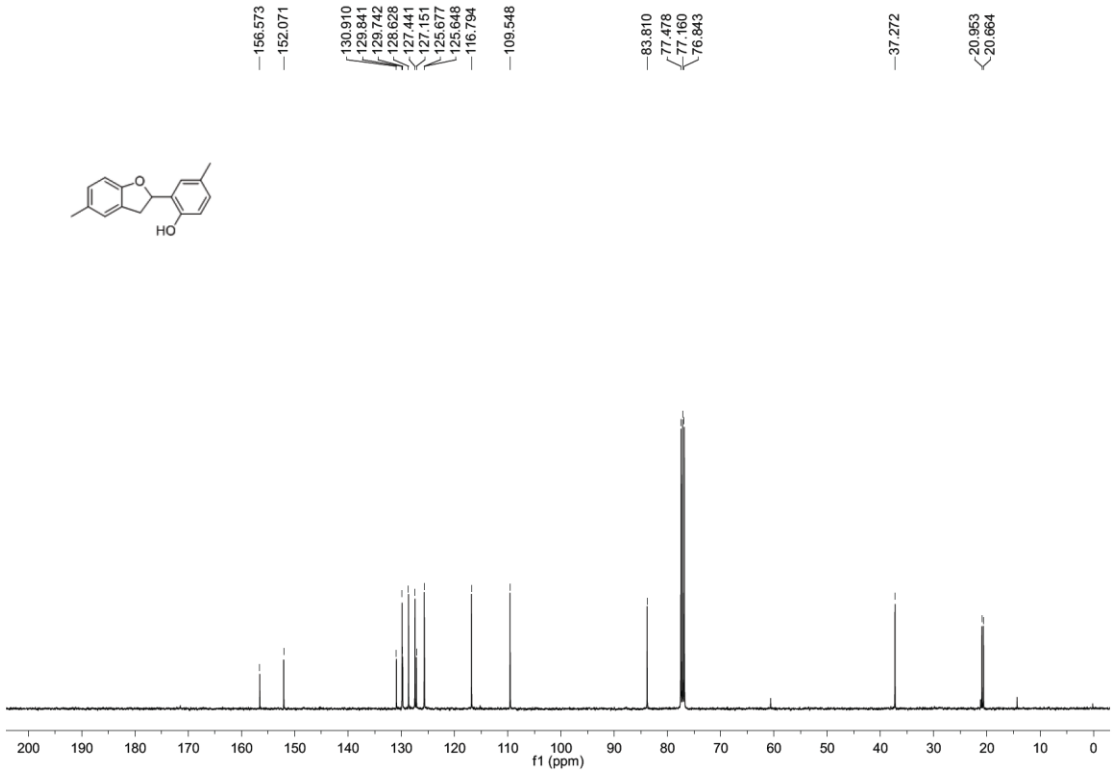

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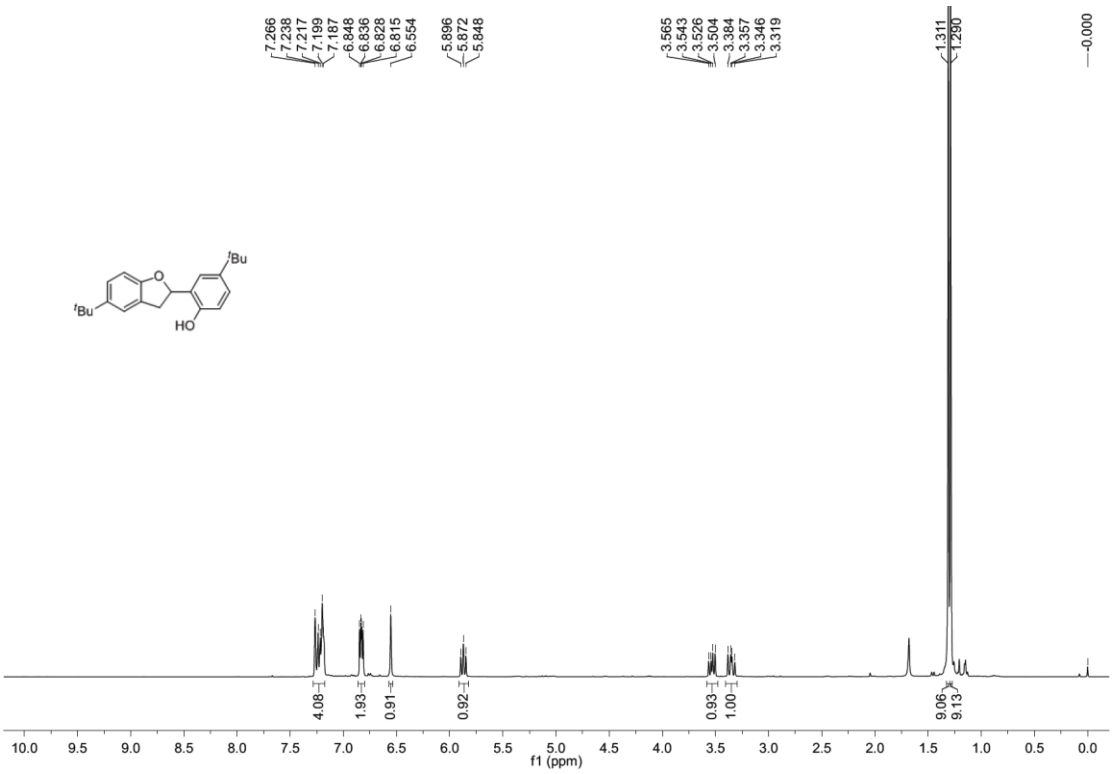

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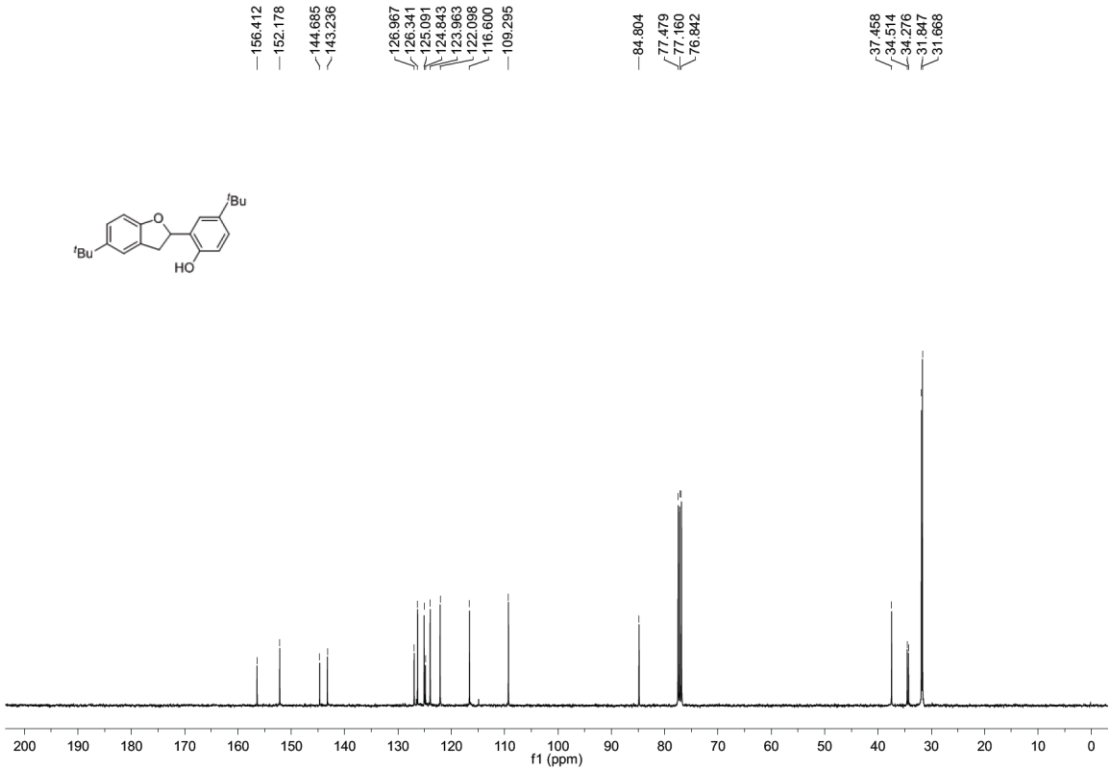

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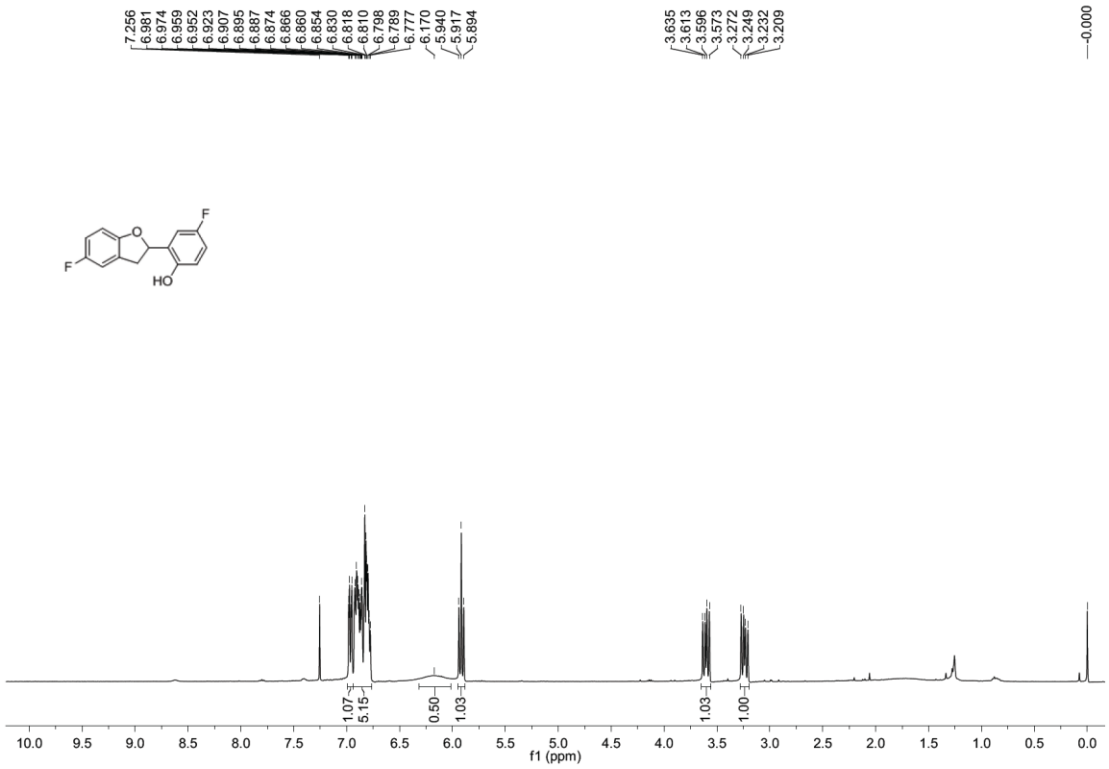

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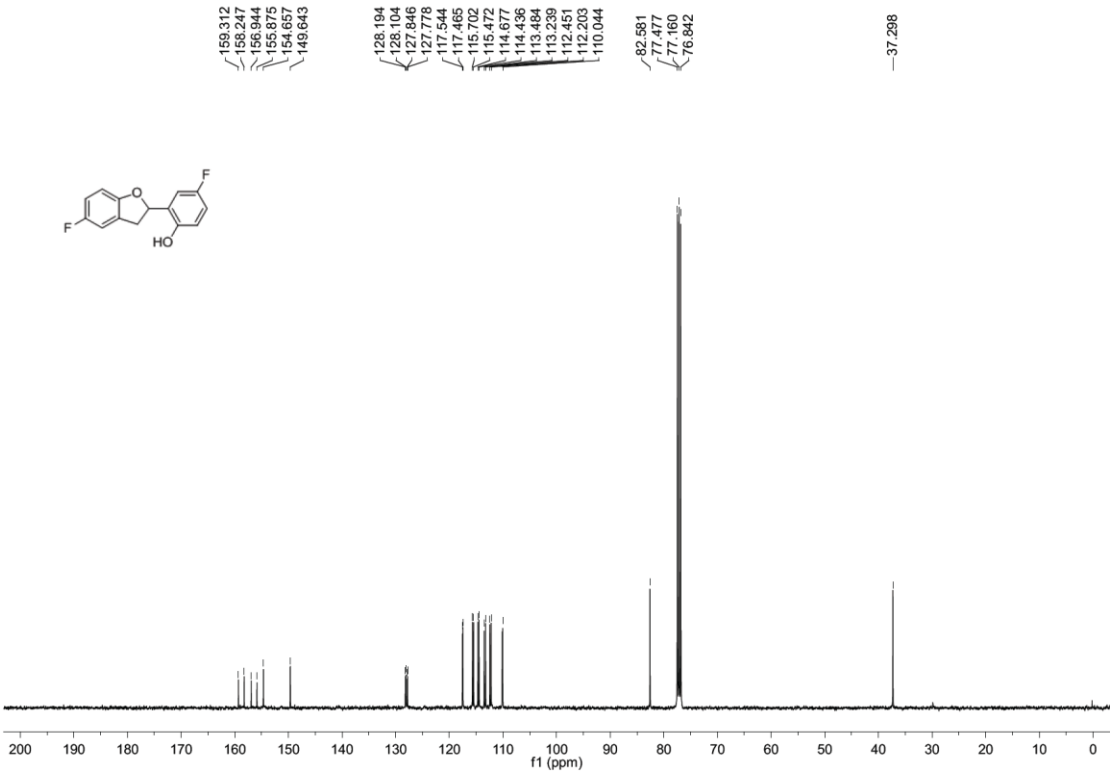
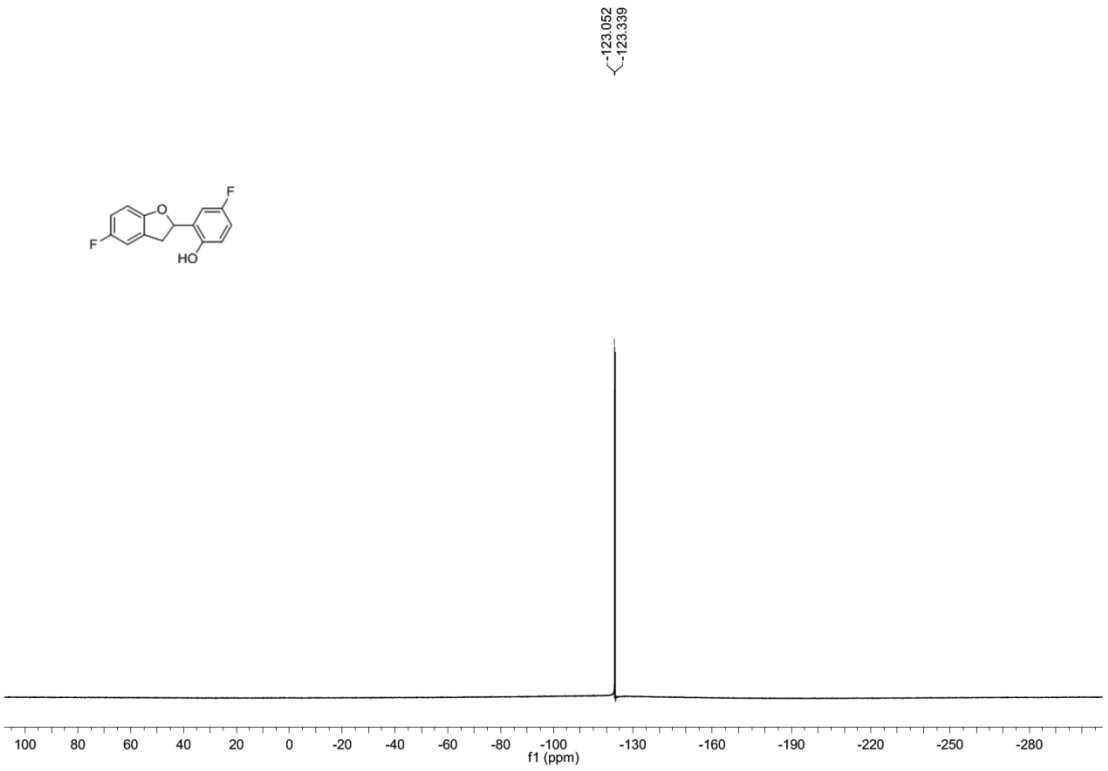


3d-^{19}F NMR (376 MHz, $CDCl_3$)



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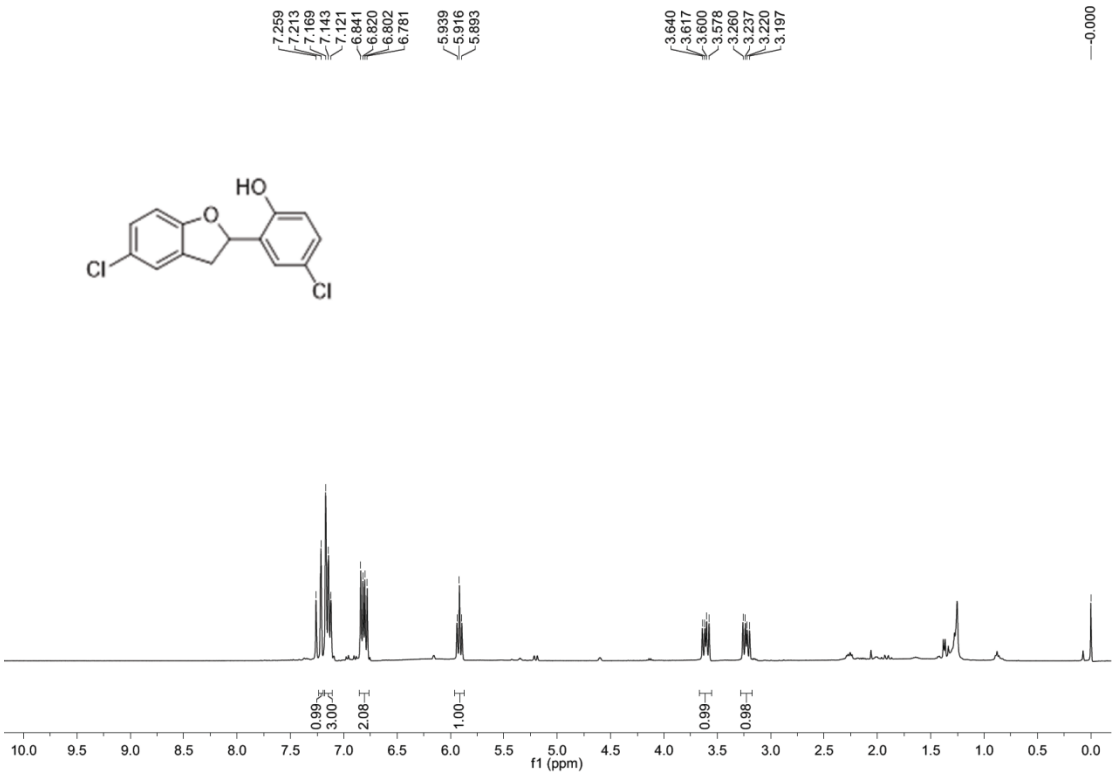
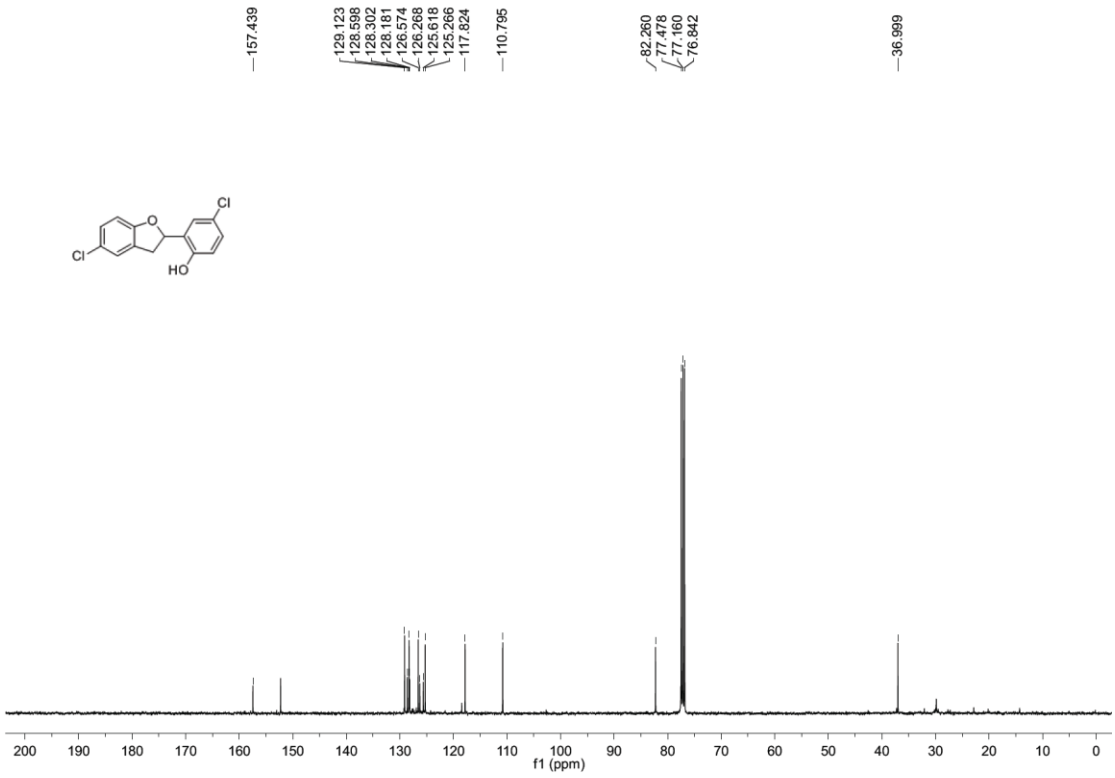


3e-^{13}C NMR (100 MHz, $CDCl_3$)



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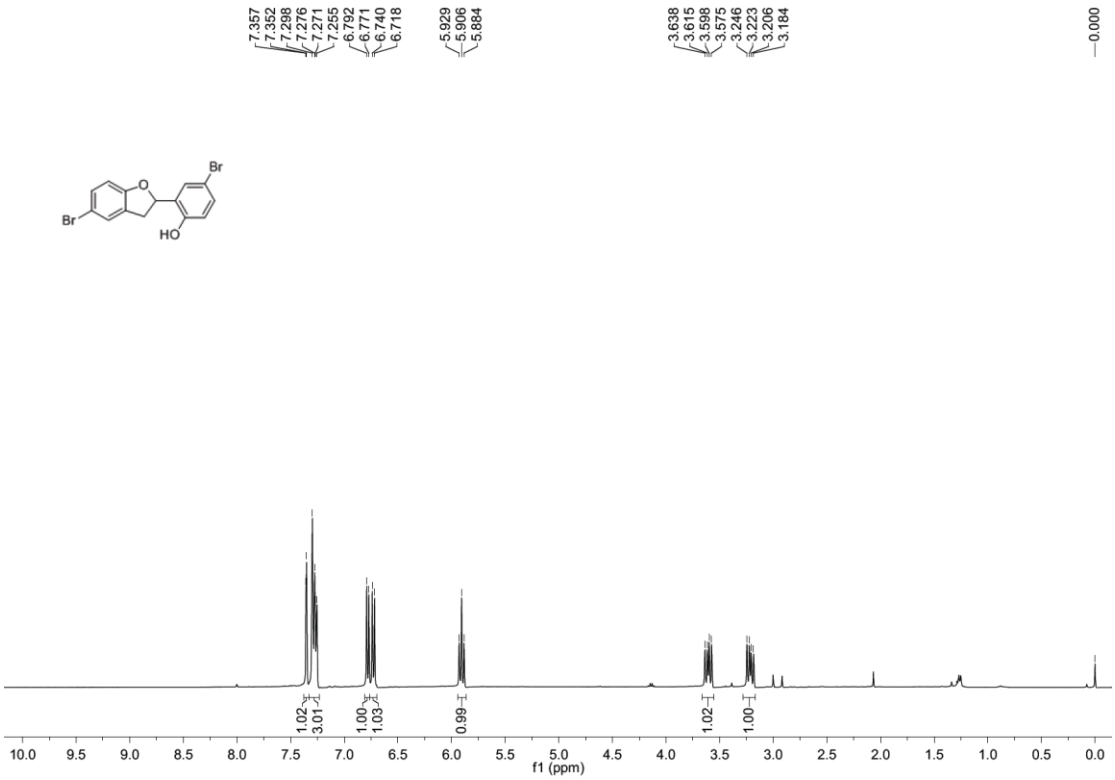

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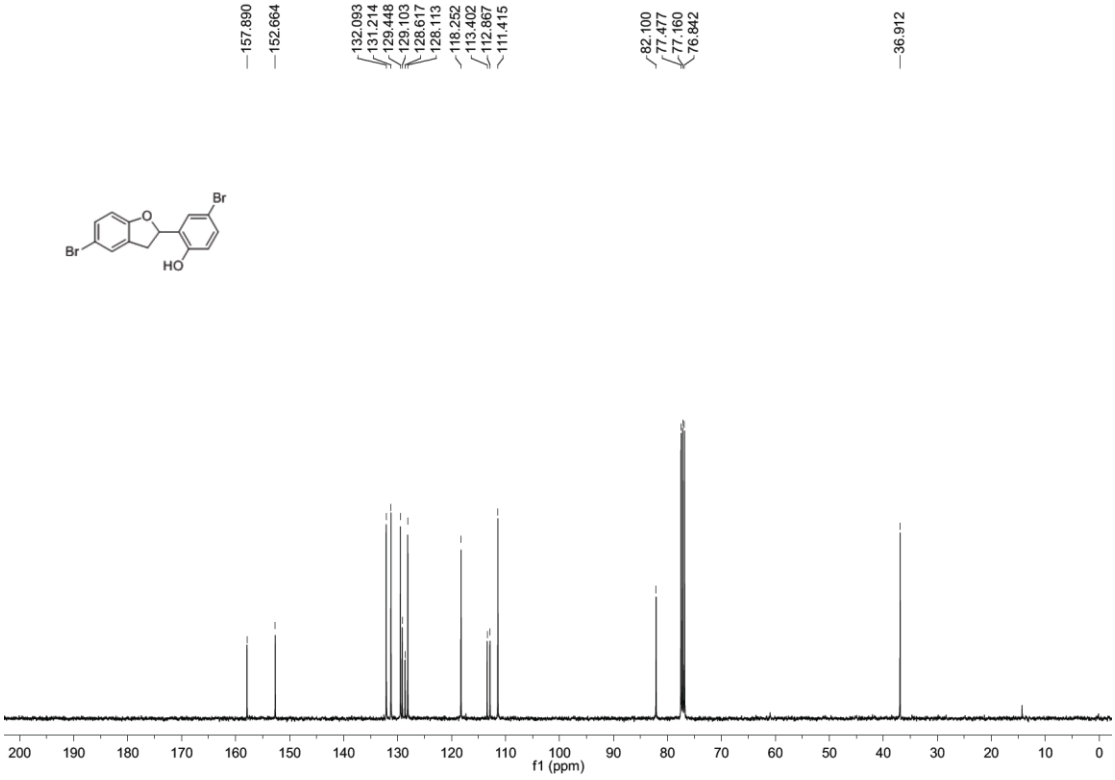

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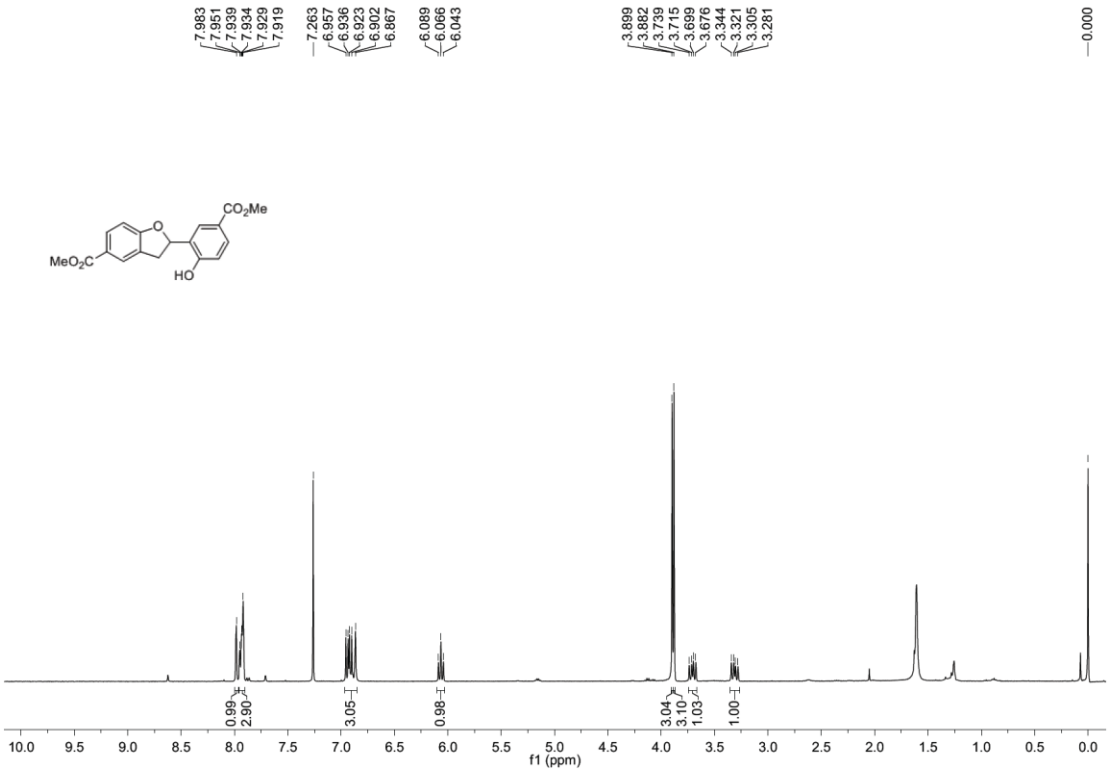

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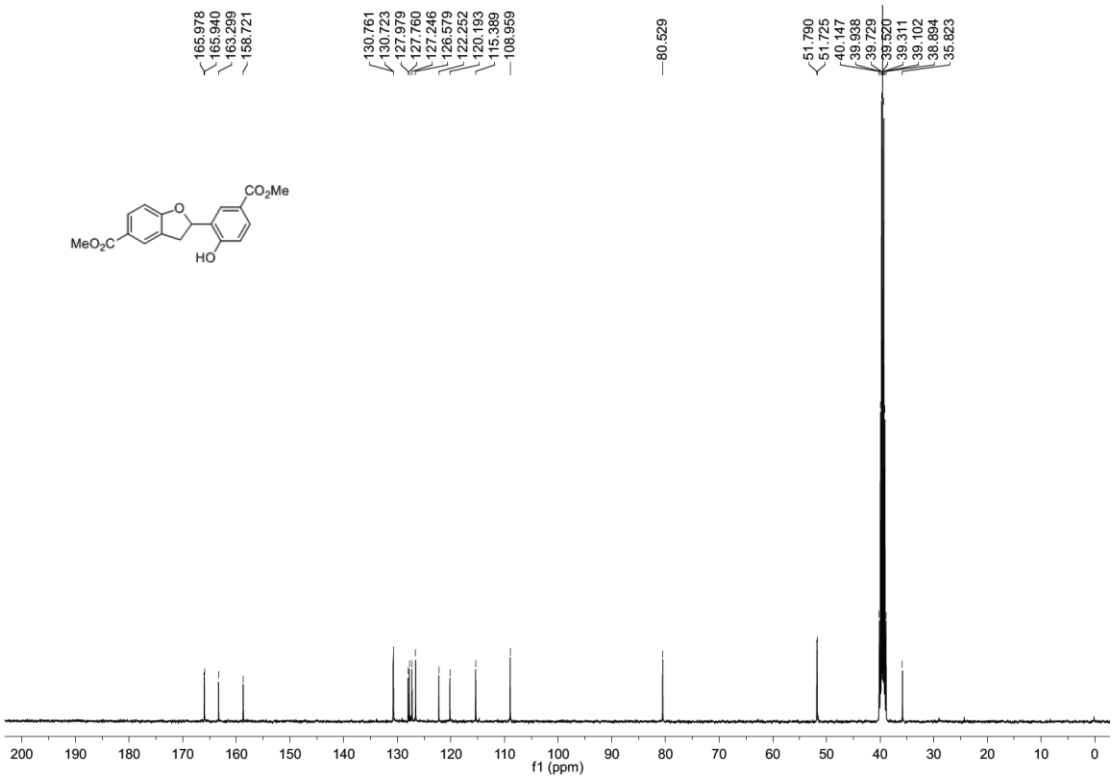
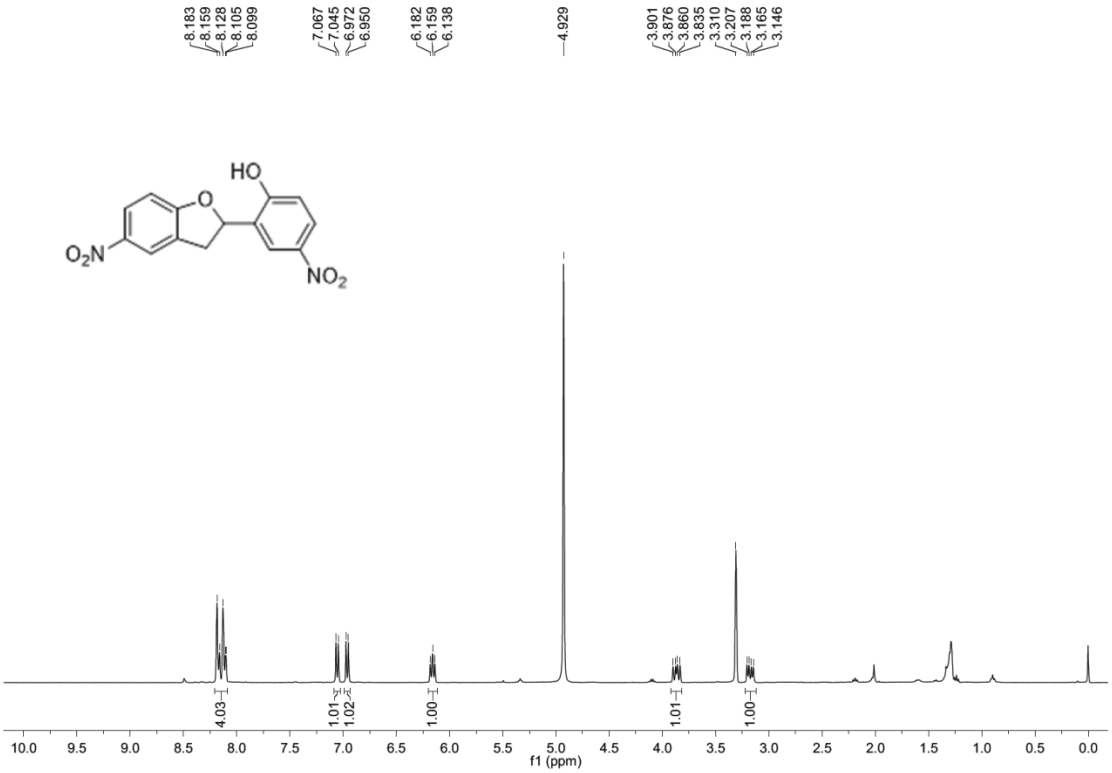
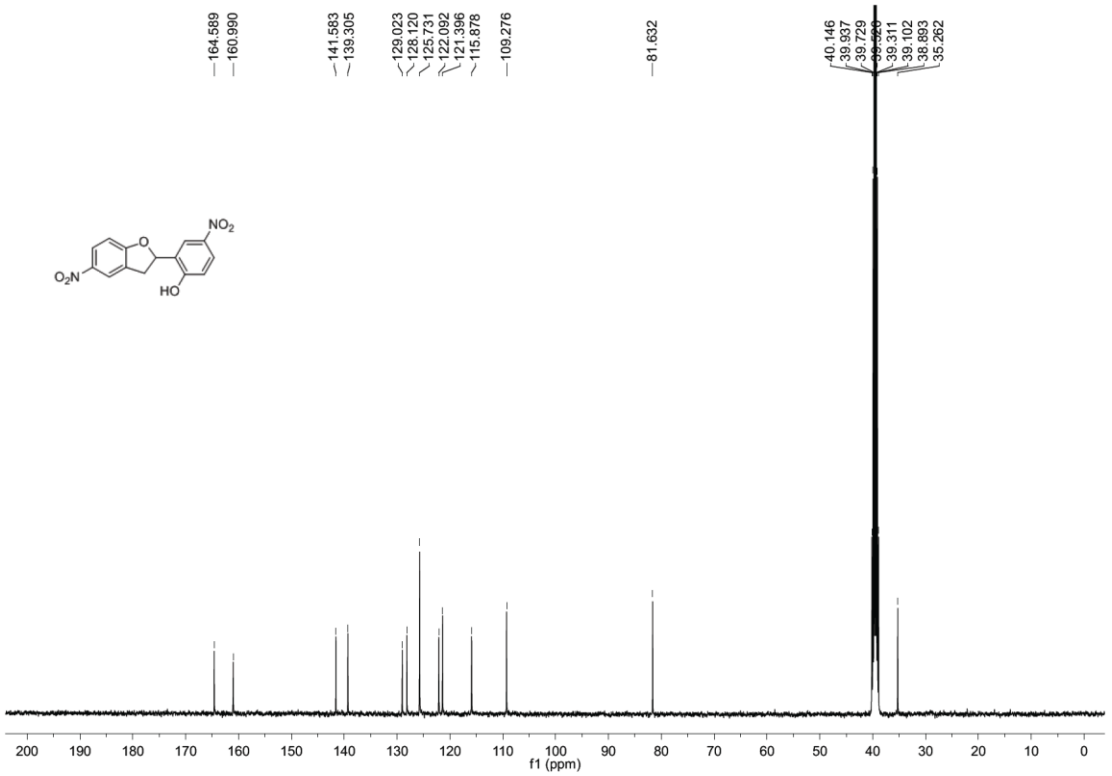


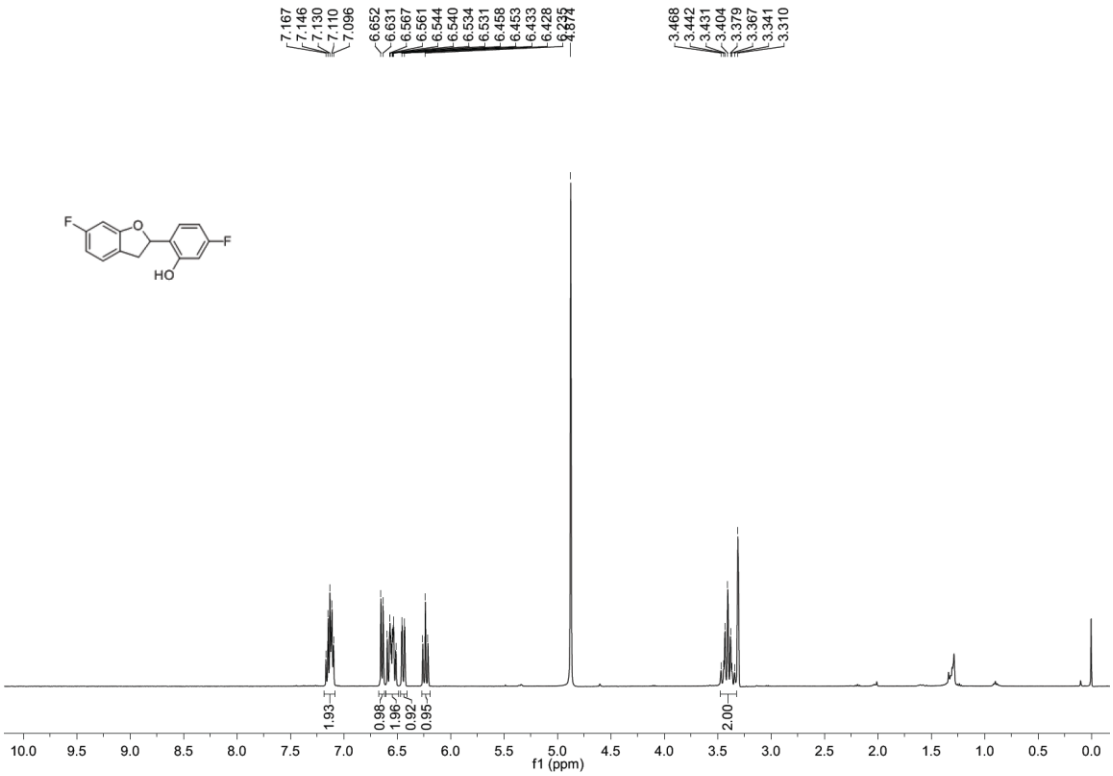
3h-^{1}H NMR (400 MHz, DMSO-d_6)



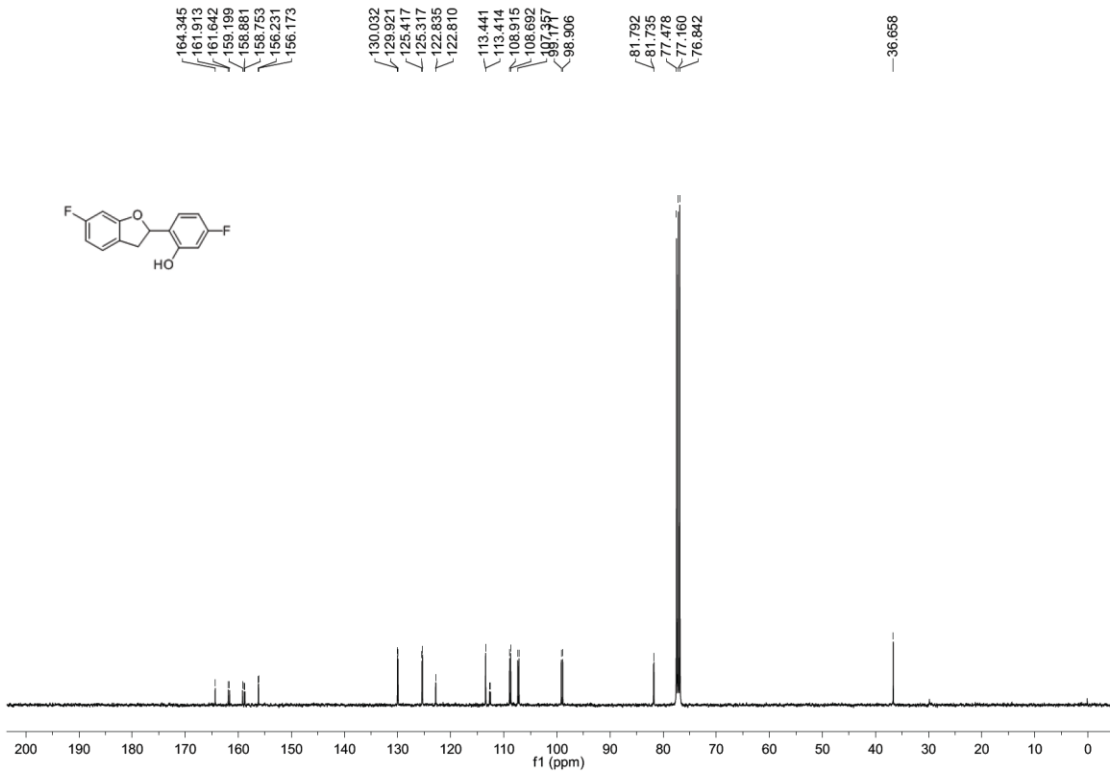
3h-^{13}C NMR (100 MHz, DMSO-d_6)



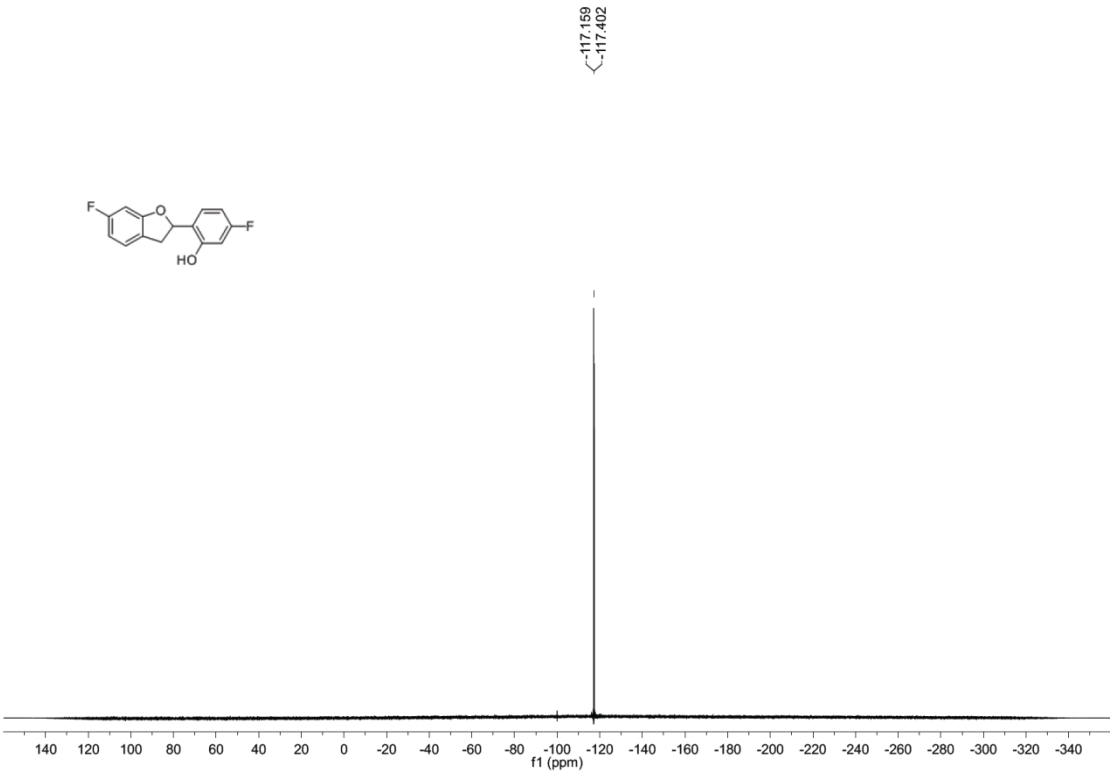
3i-^{1}H NMR (400 MHz, CD_3OD)



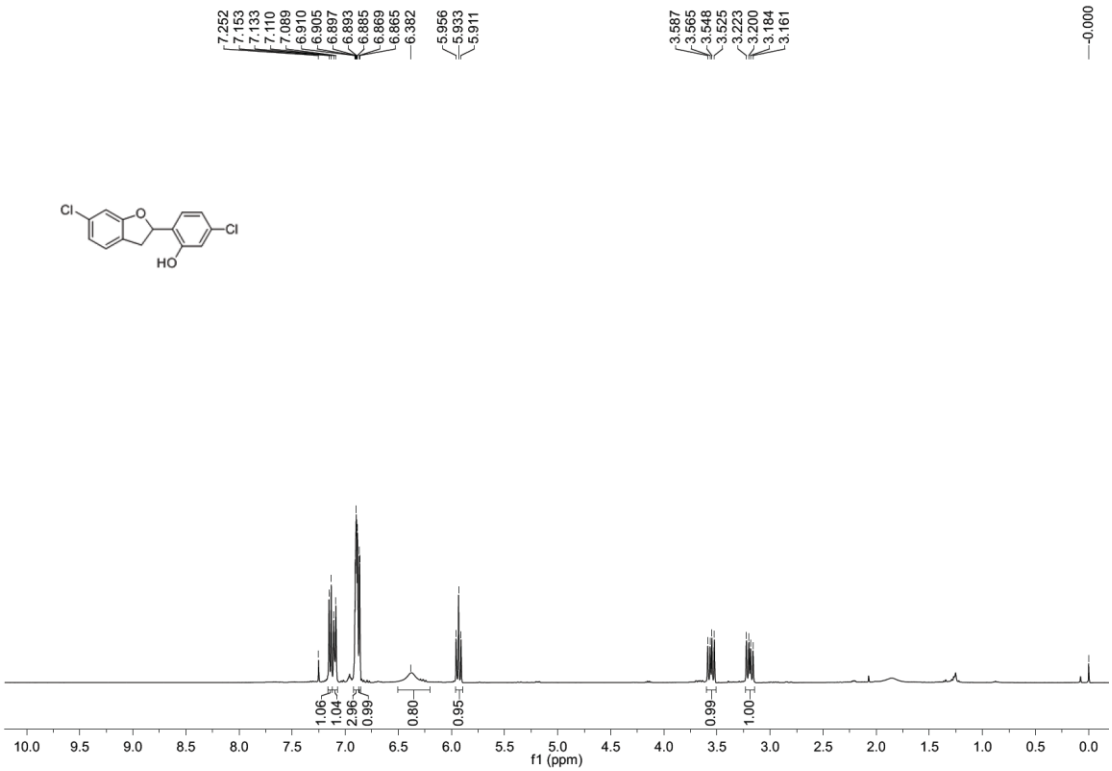
3i-^{13}C NMR (100 MHz, $CDCl_3$)



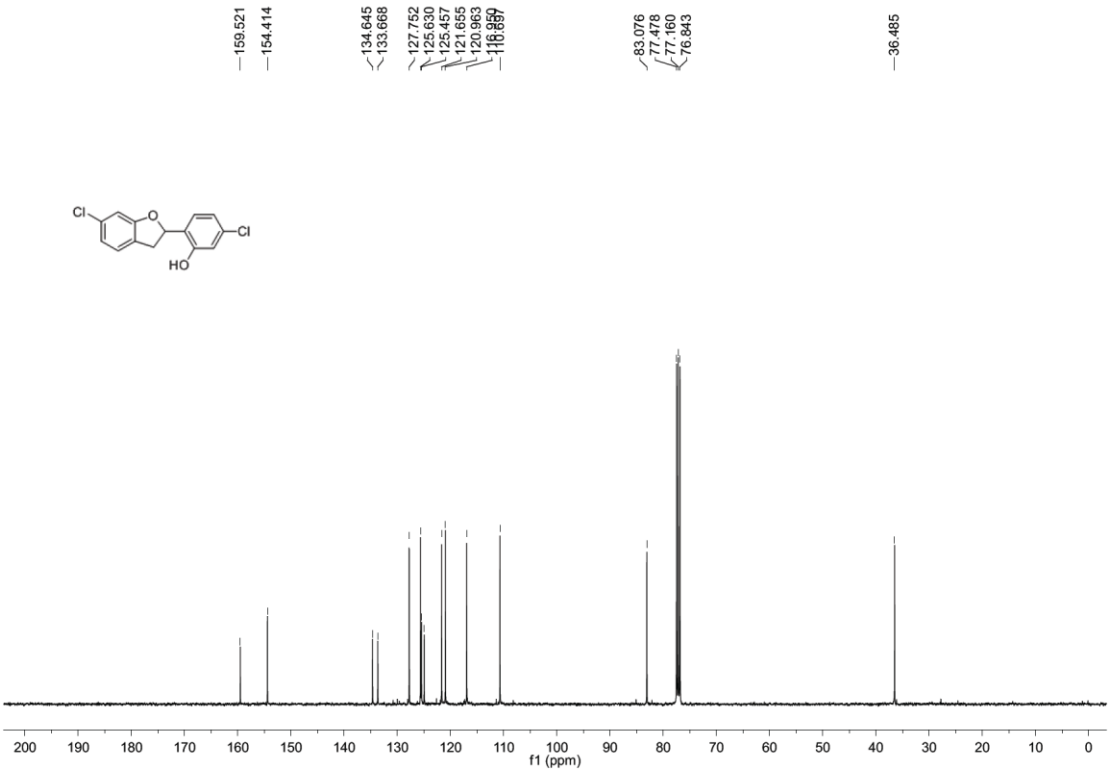
3i-^{19}F NMR (376 MHz, $CDCl_3$)



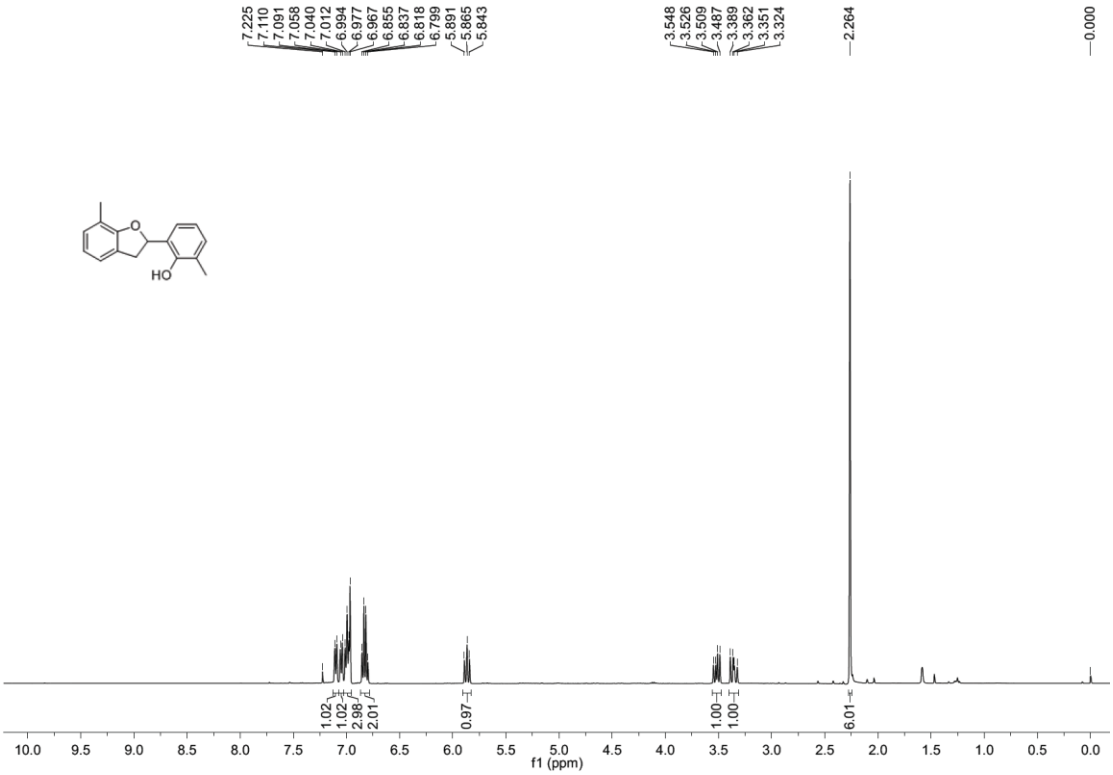
3j-^{1}H NMR (400 MHz, $CDCl_3$)



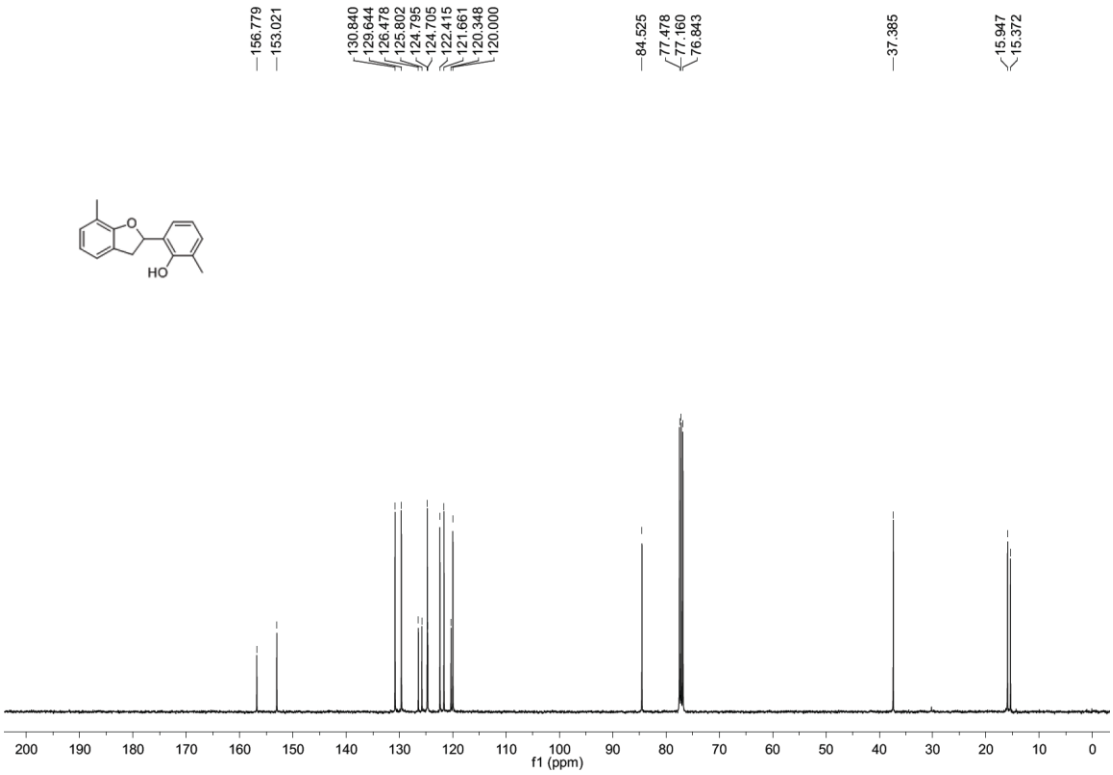
3j-^{13}C NMR (100 MHz, $CDCl_3$)



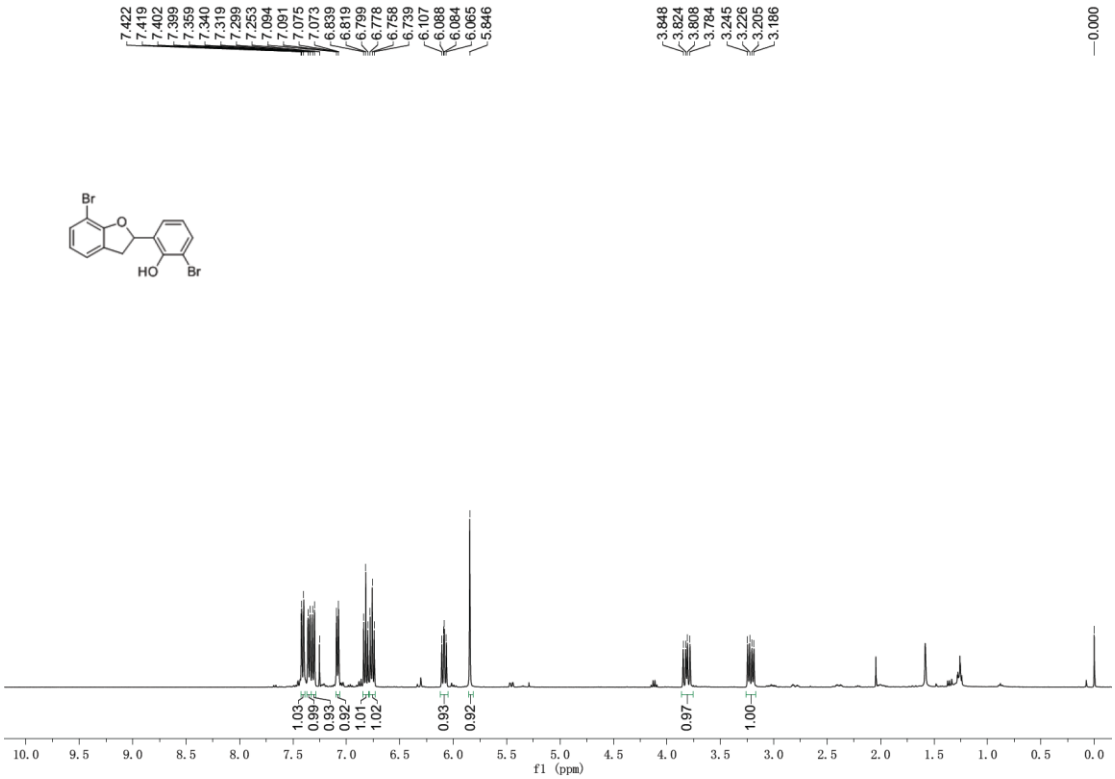
3k-^{1}H NMR (400 MHz, $CDCl_3$)



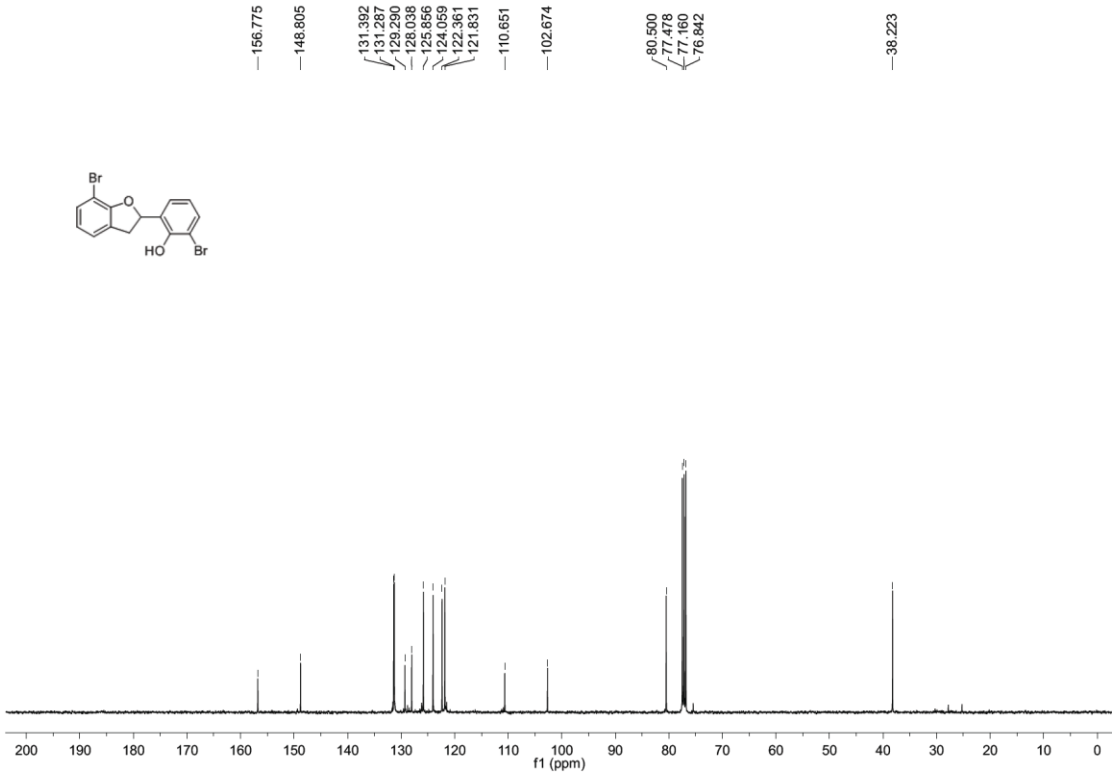
3k-^{13}C NMR (100 MHz, $CDCl_3$)



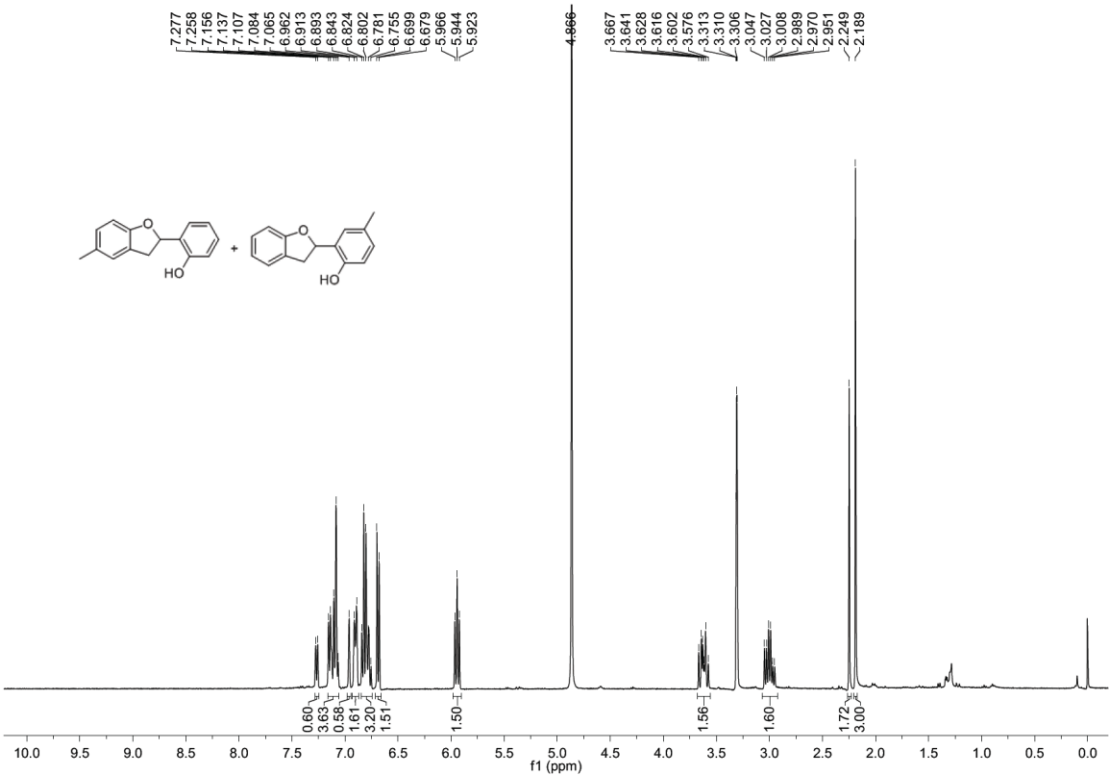
3l-^{1}H NMR (400 MHz, $CDCl_3$)



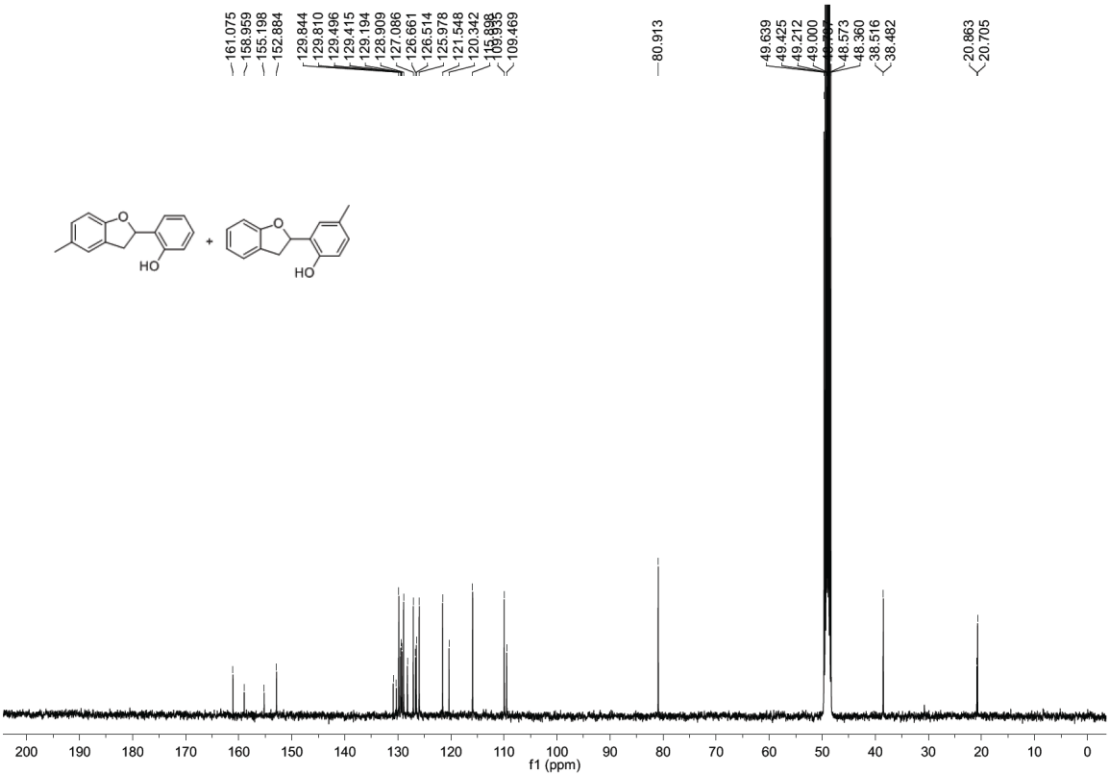
3l-^{13}C NMR (100 MHz, $CDCl_3$)



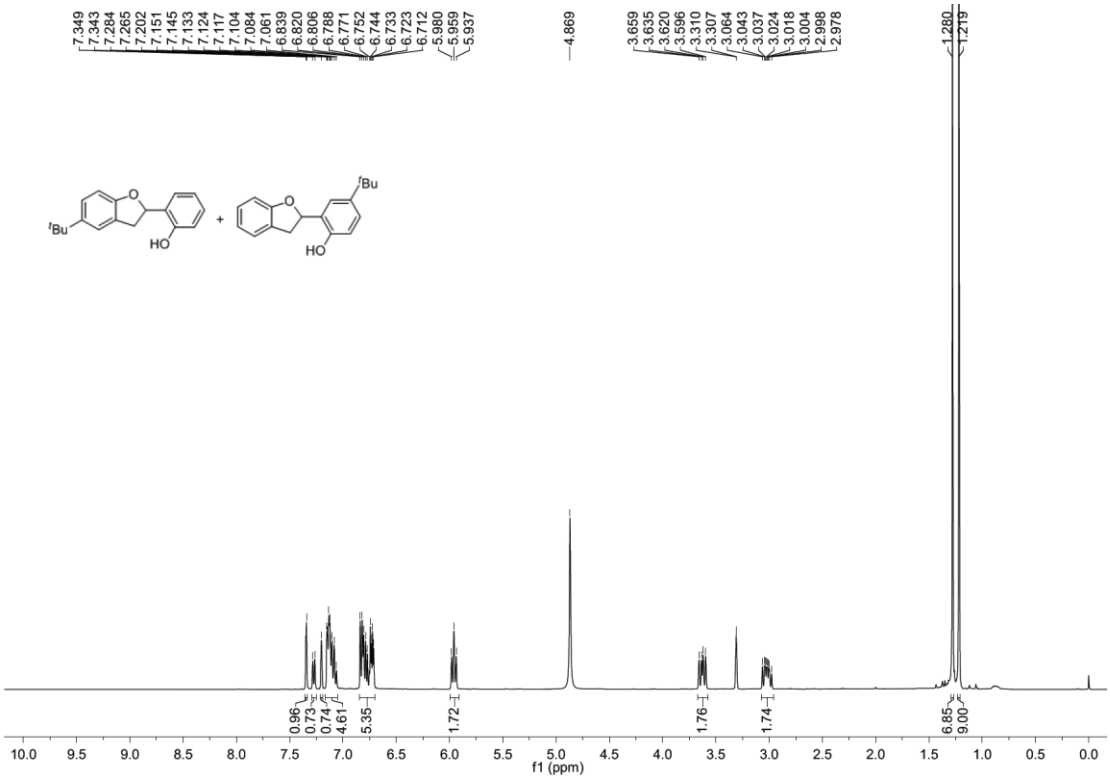
3m-^{1}H NMR (400 MHz, CD_3OD)



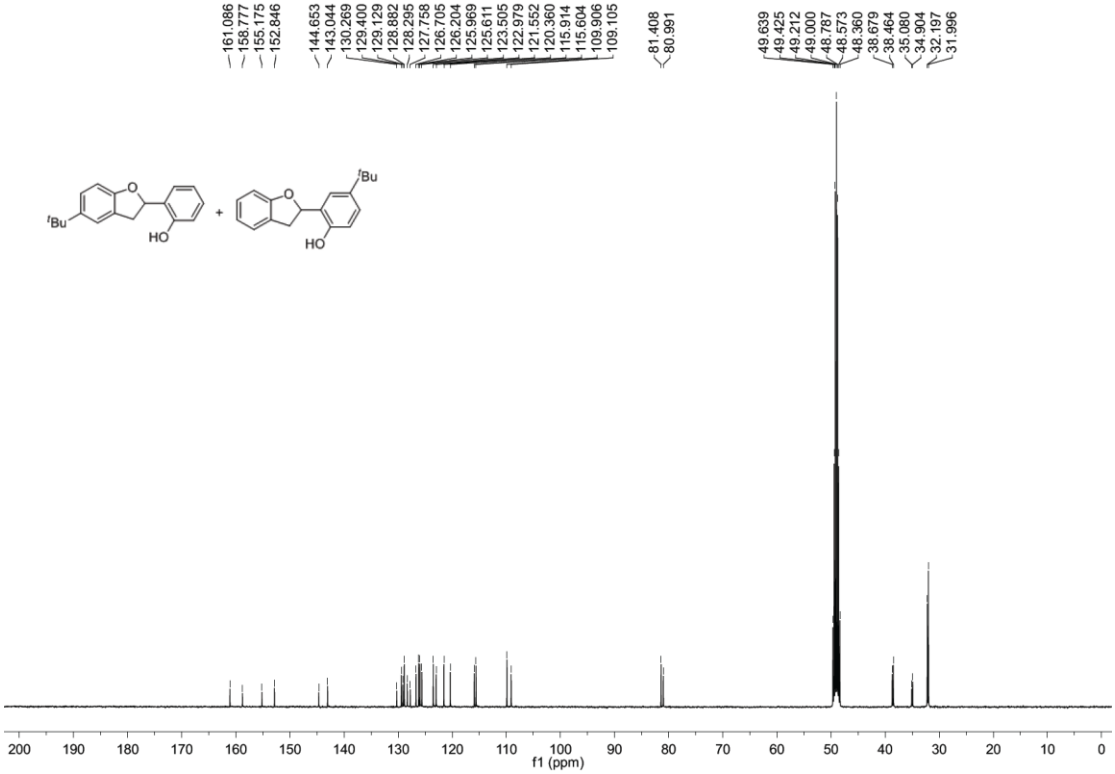
3m-^{13}C NMR (100 MHz, CD_3OD)



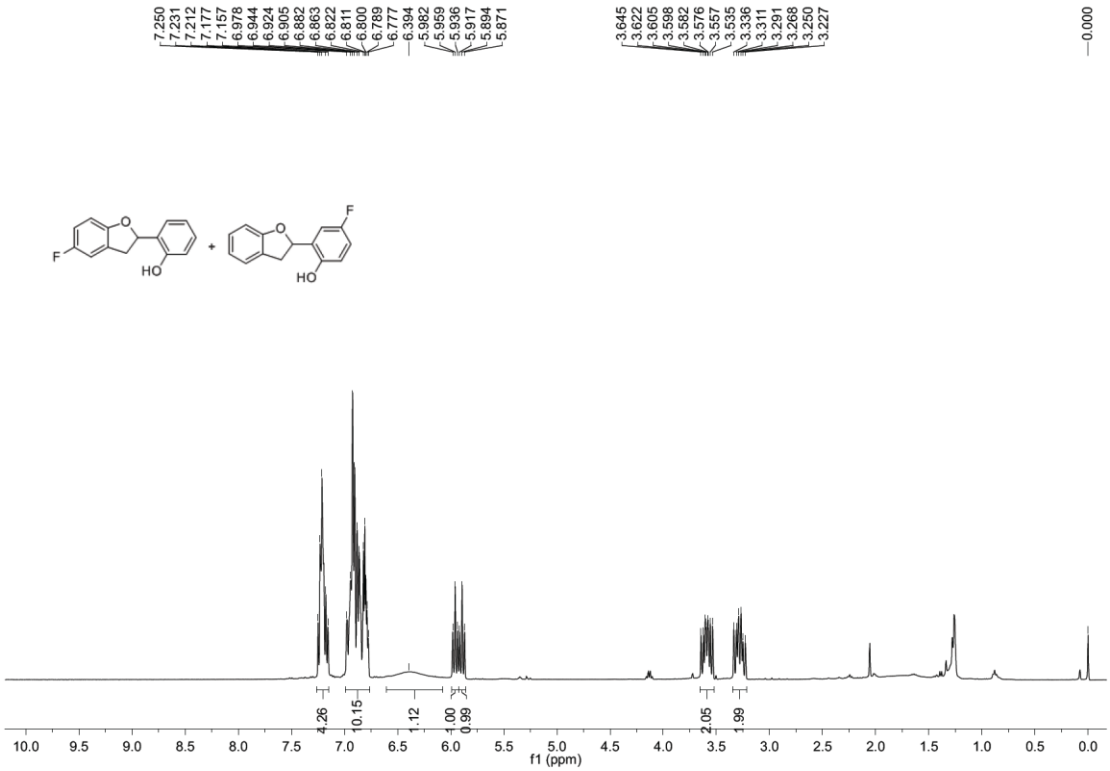
3n-^{1}H NMR (400 MHz, CD_3OD)



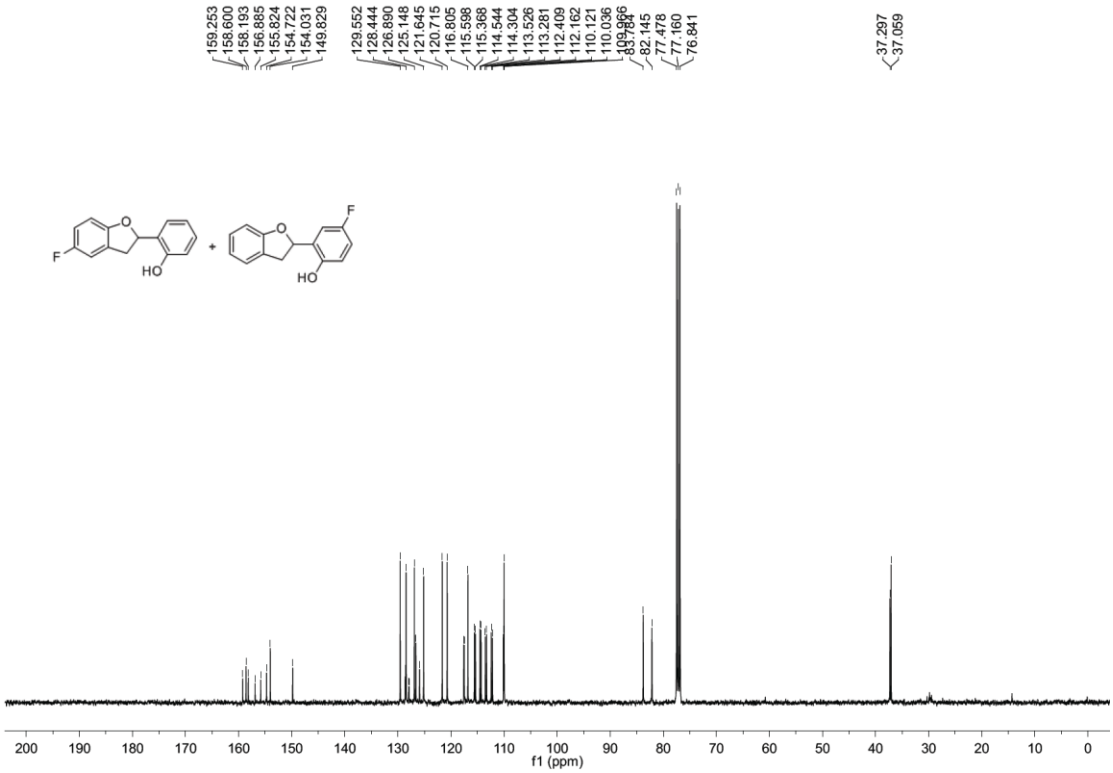
3n-^{13}C NMR (100 MHz, CD_3OD)



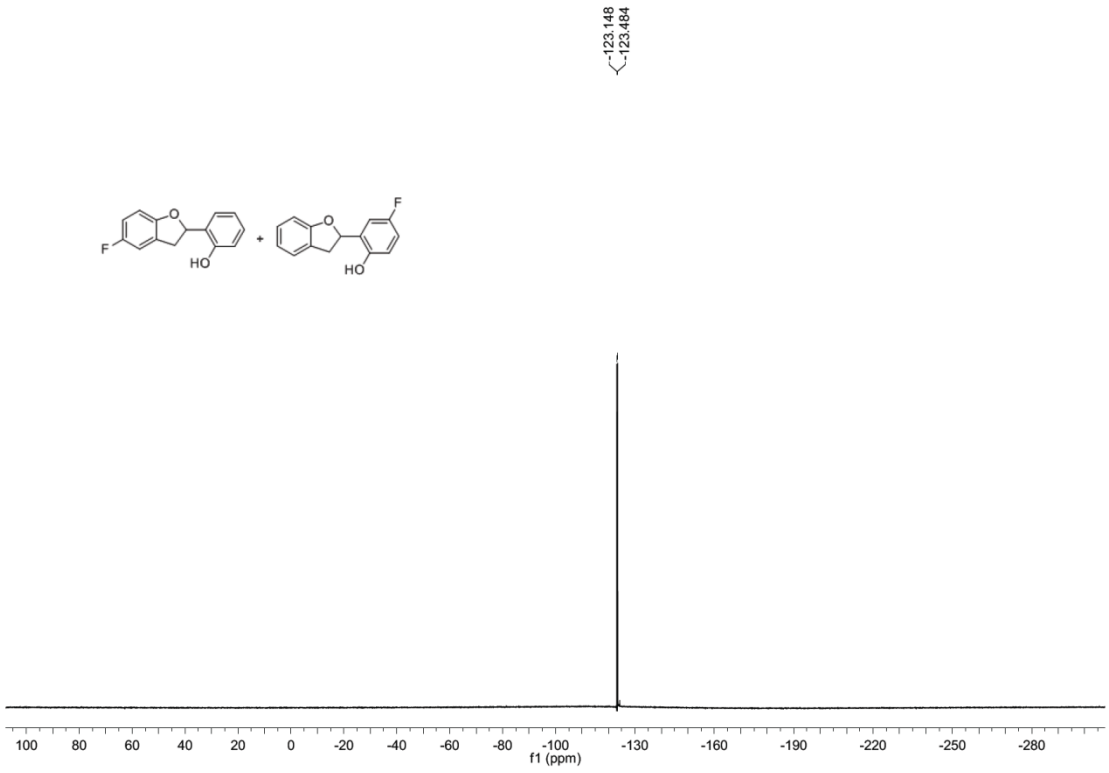
3o-^{1}H NMR (400 MHz, $CDCl_3$)



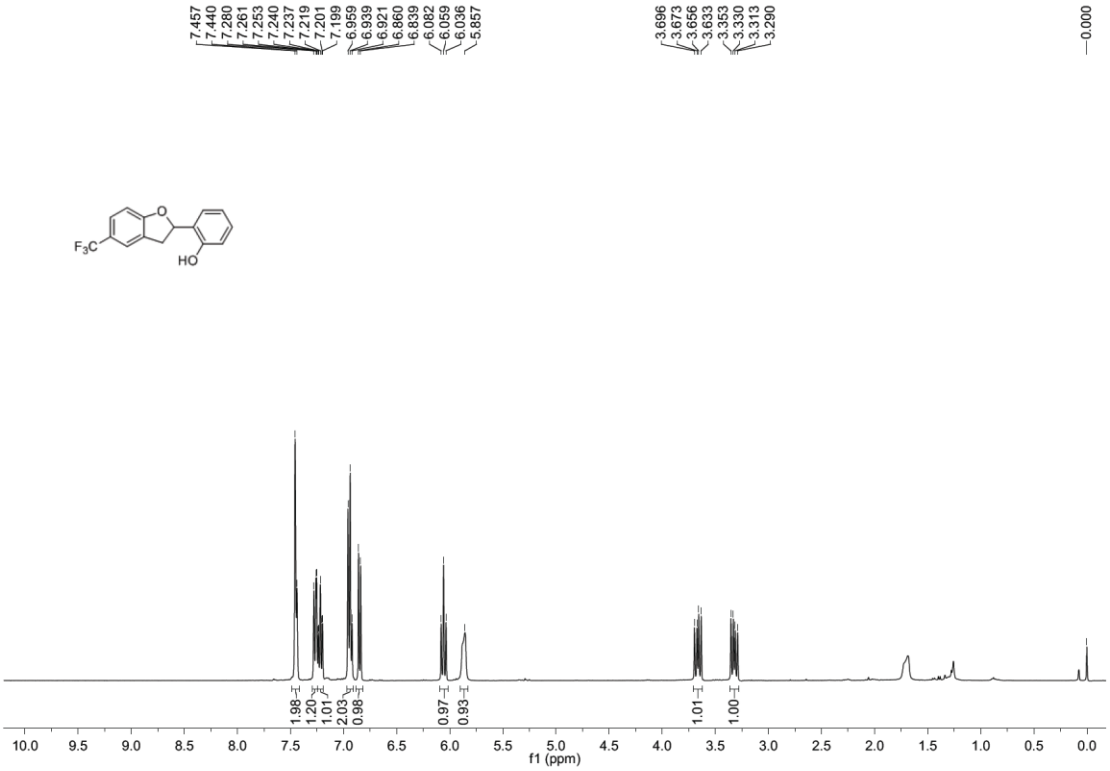
3o-^{13}C NMR (100 MHz, $CDCl_3$)



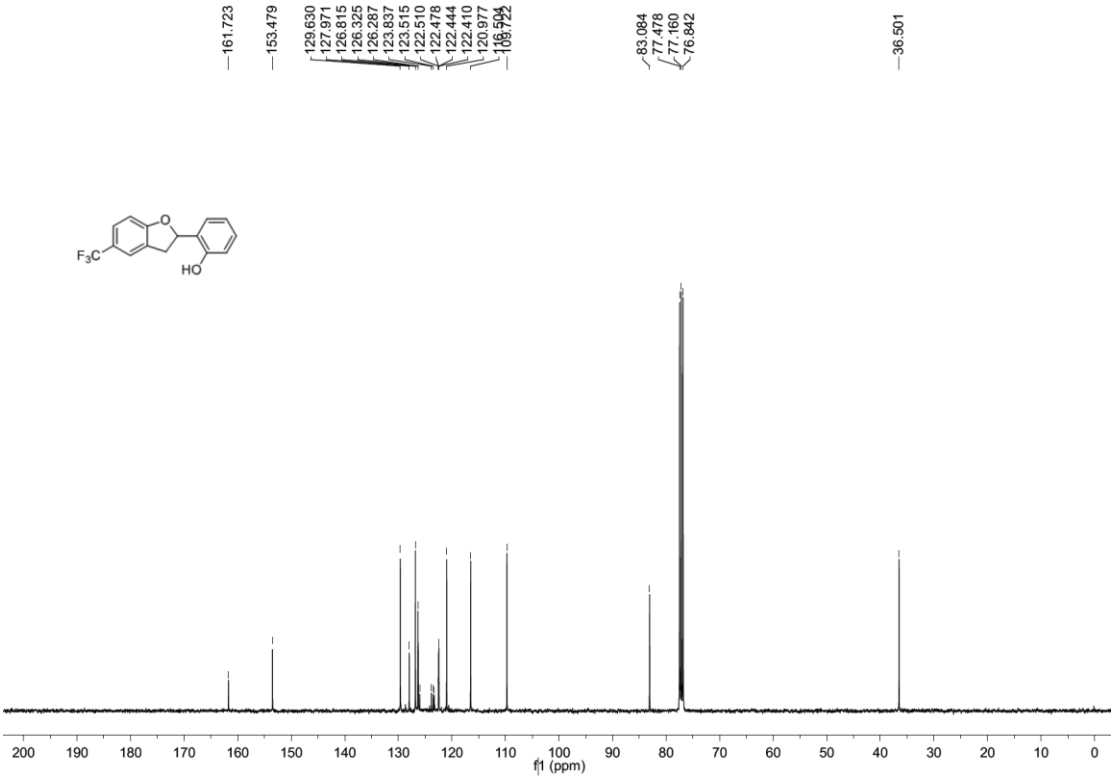
3o-^{19}F NMR (376 MHz, $CDCl_3$)



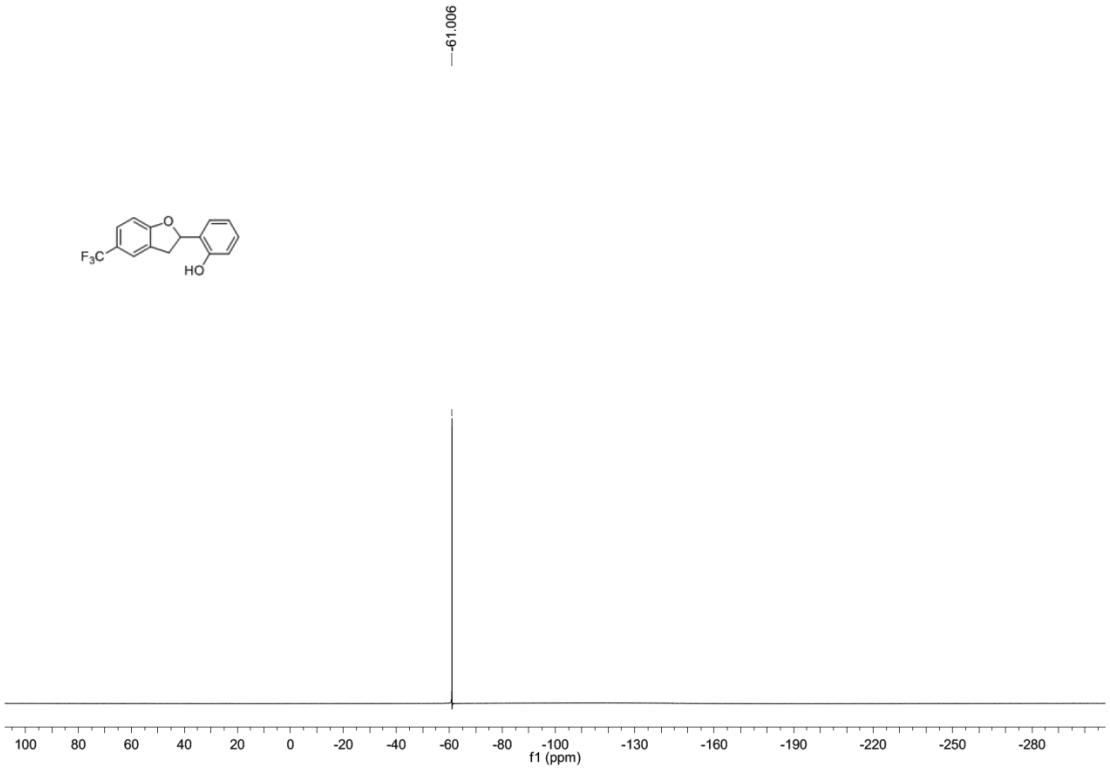
3p-^{1}H NMR (400 MHz, $CDCl_3$)



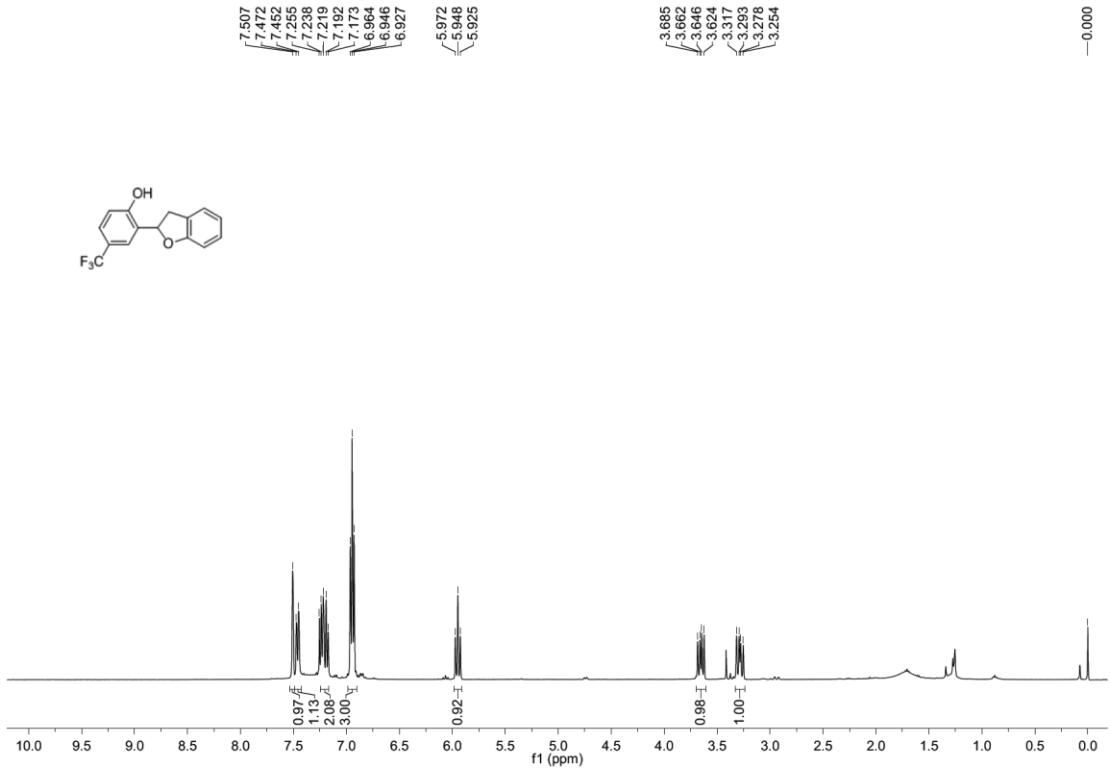
3p-^{13}C NMR (100 MHz, $CDCl_3$)



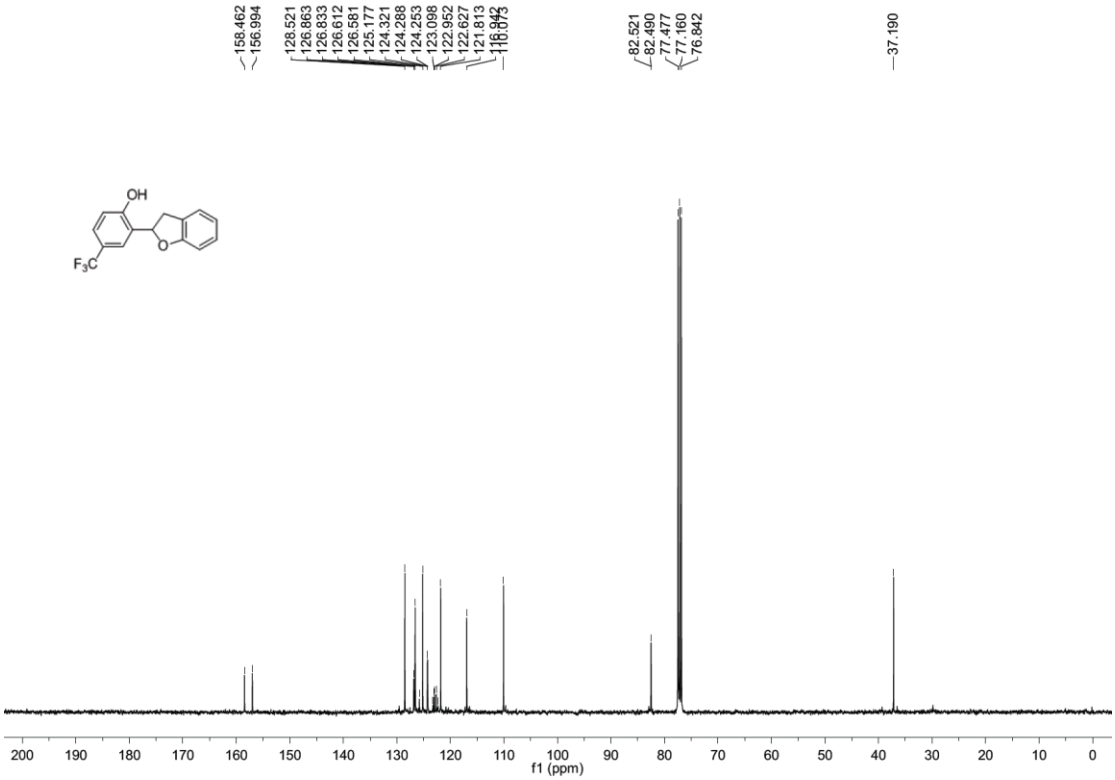
3p-^{19}F NMR (376 MHz, $CDCl_3$)



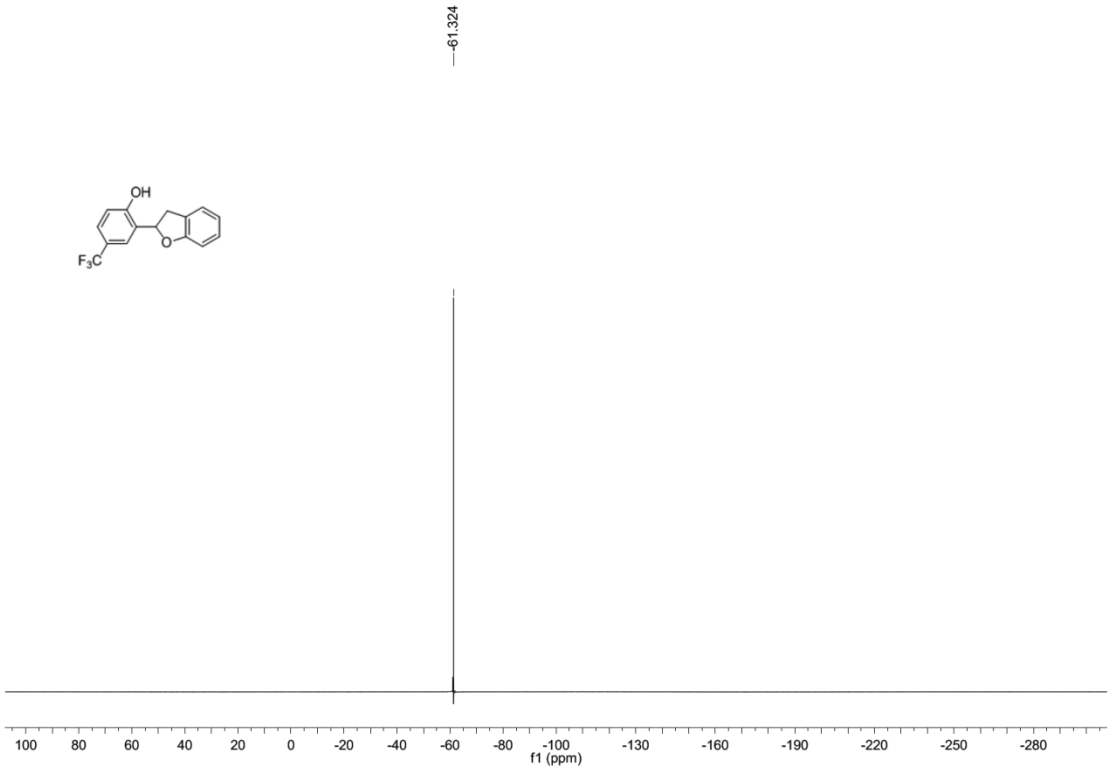
3p'-^{1}H NMR (400 MHz, $CDCl_3$)



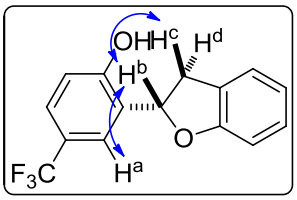
3p'-^{13}C NMR (100 MHz, $CDCl_3$)

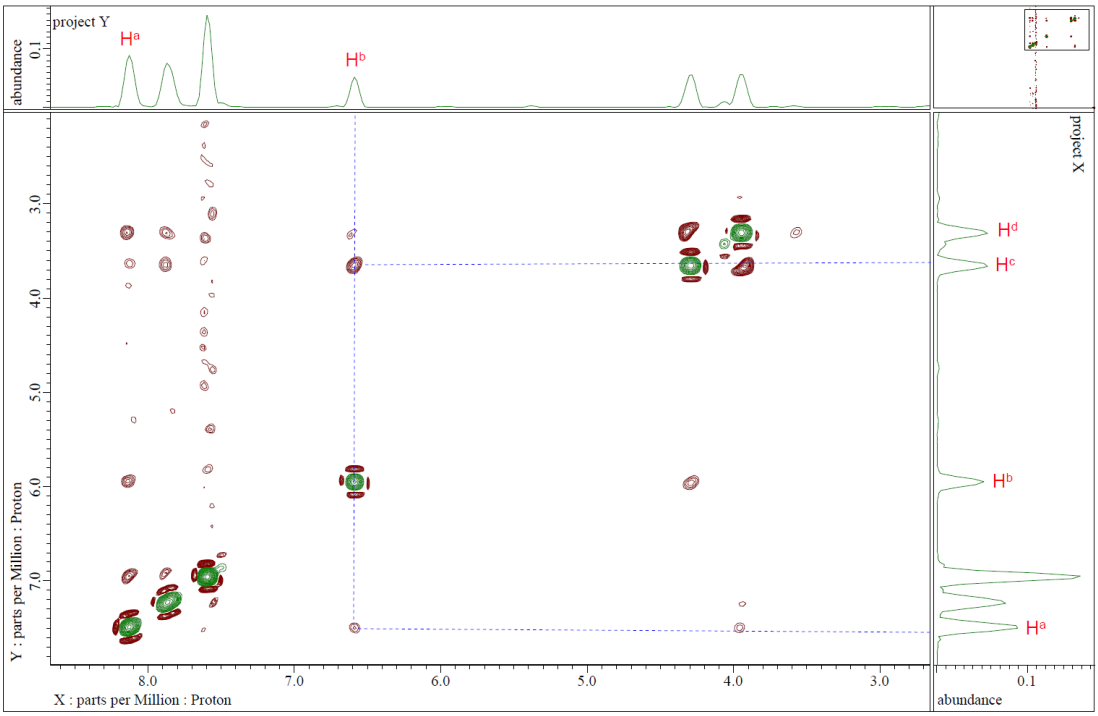


3p'-^{19}F NMR (376 MHz, $CDCl_3$)

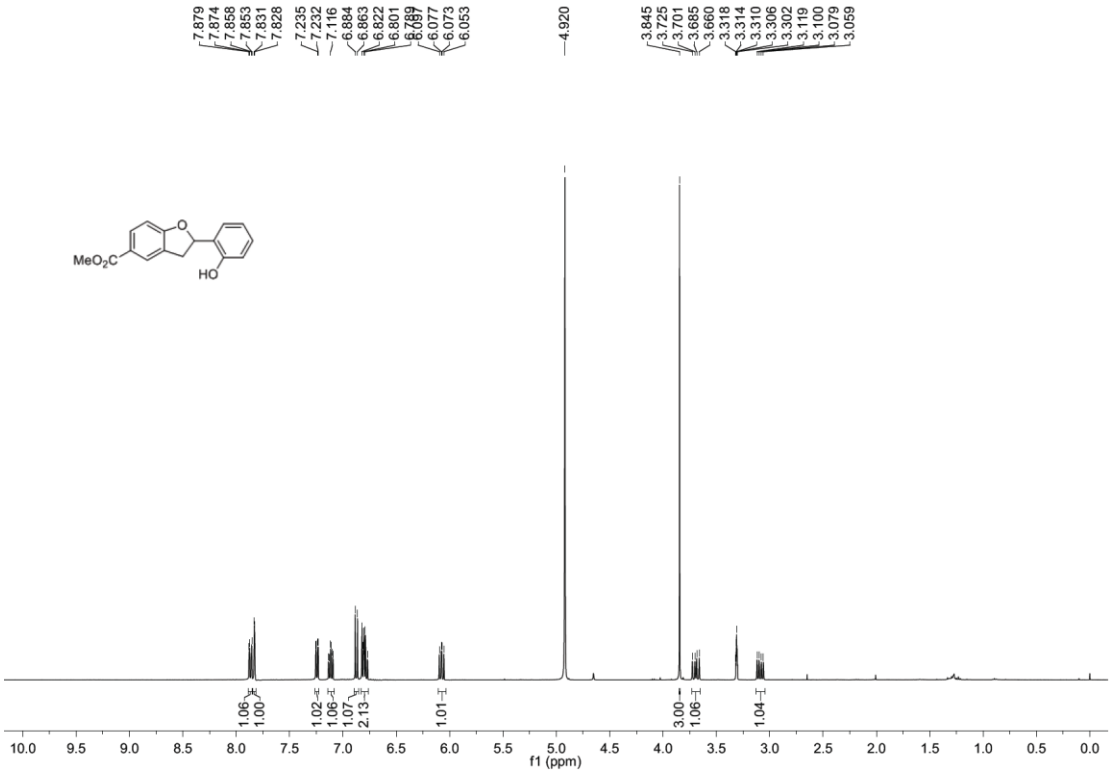


^{1}H-^{1}H NOESY of 3p':

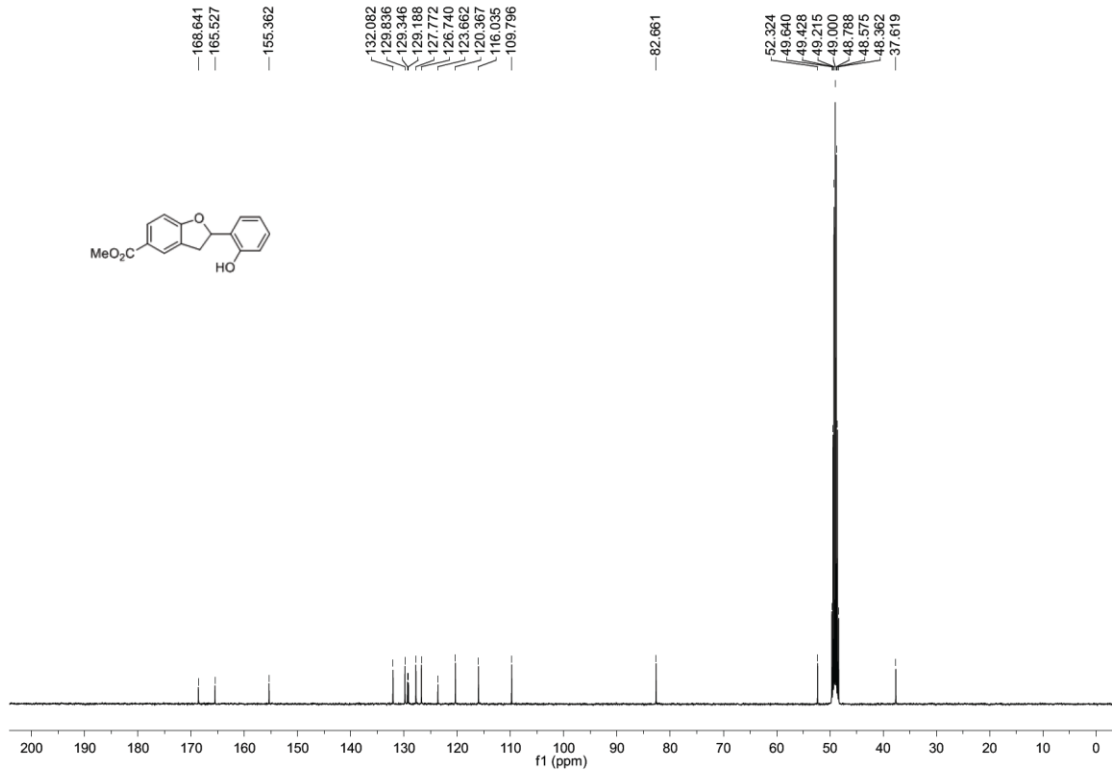




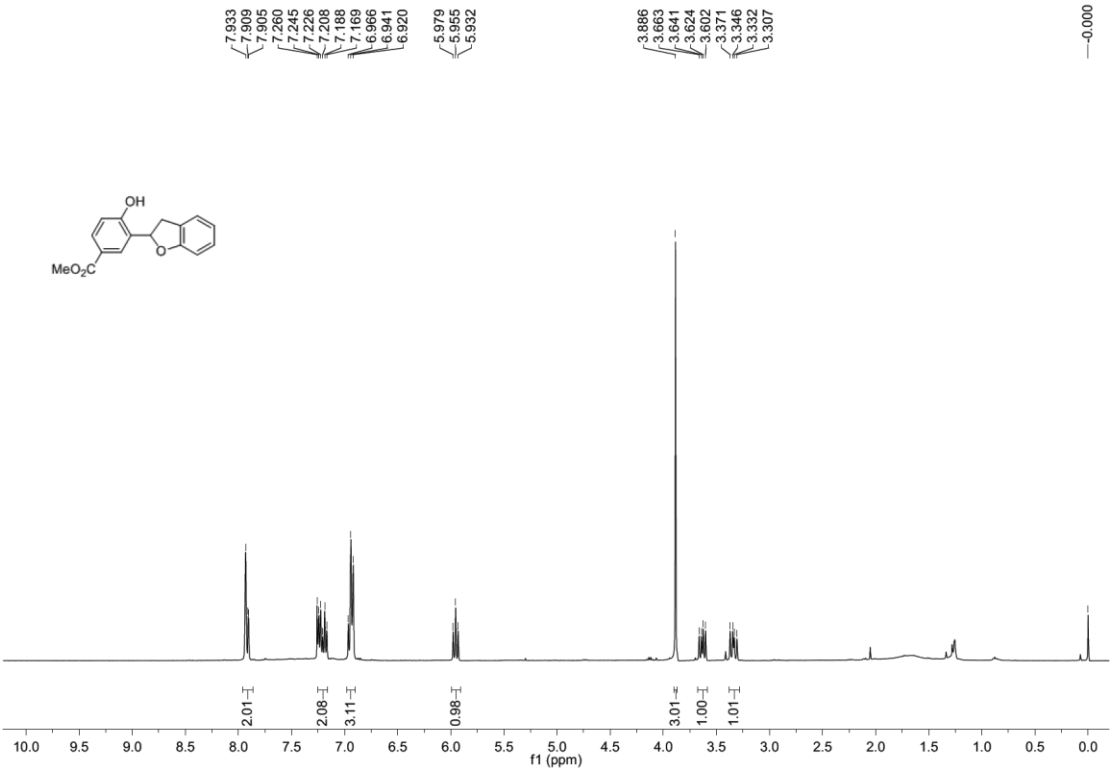
3q-^{1}H NMR (400 MHz, CD_3OD)



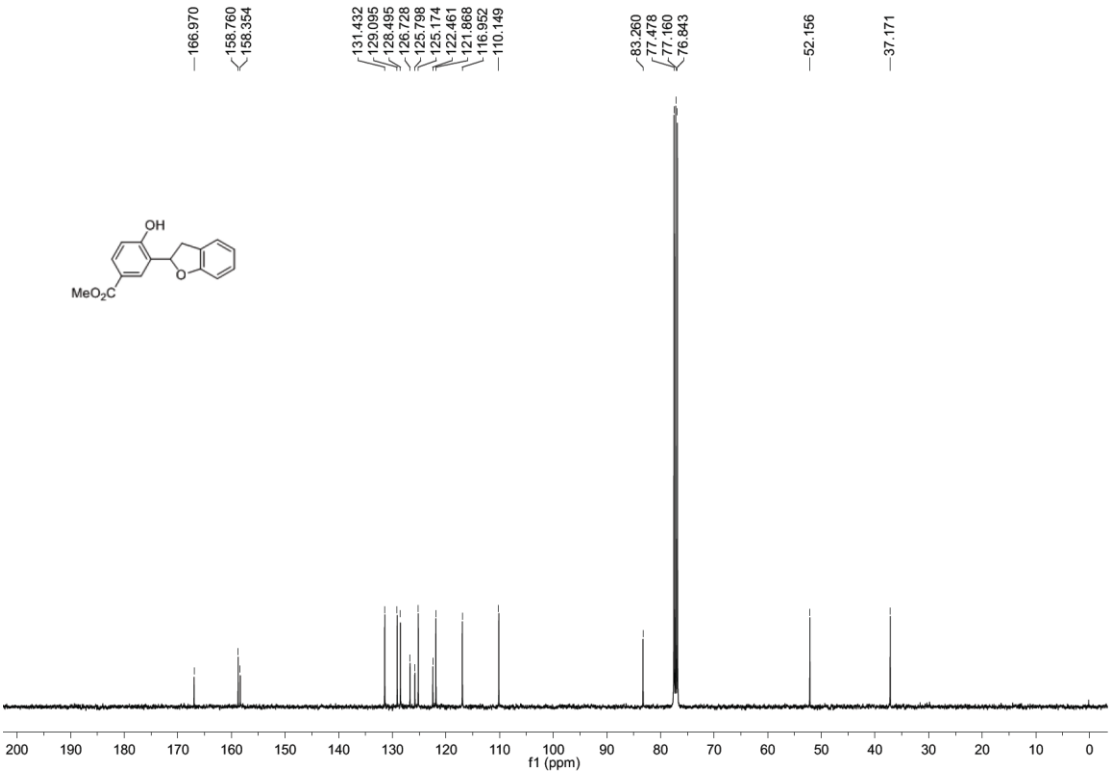
3q-^{13}C NMR (100 MHz, CD_3OD)



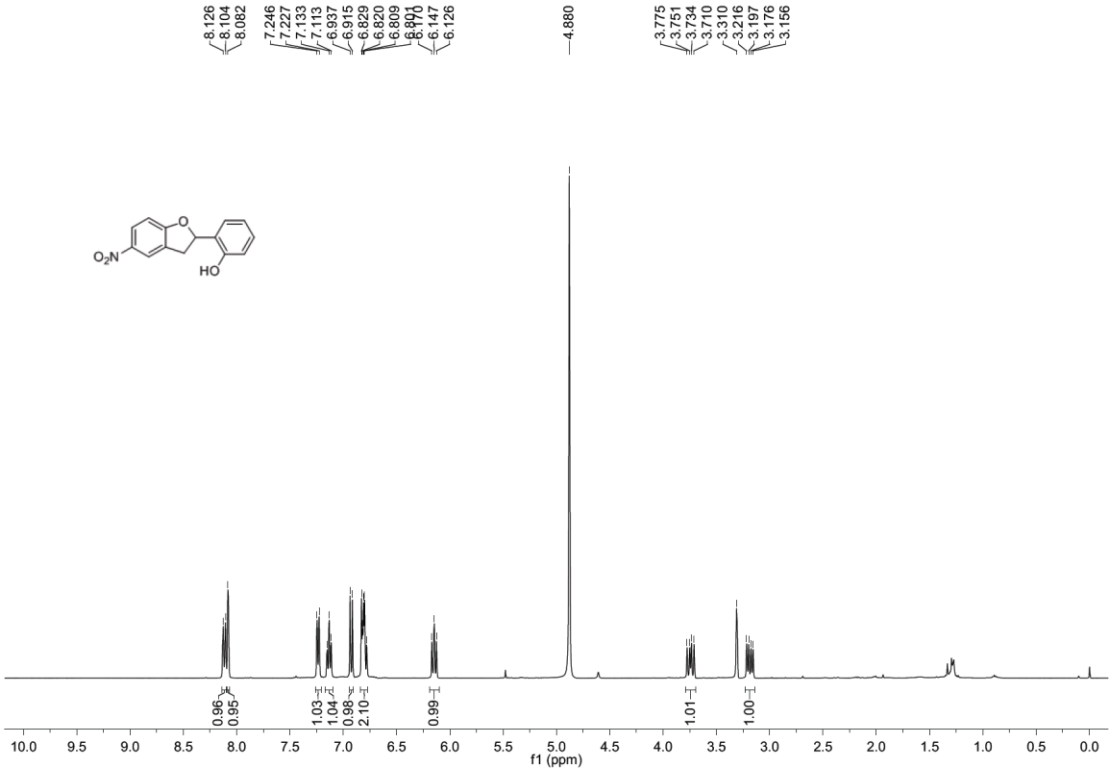
3q'-^{1}H NMR (400 MHz, $CDCl_3$)



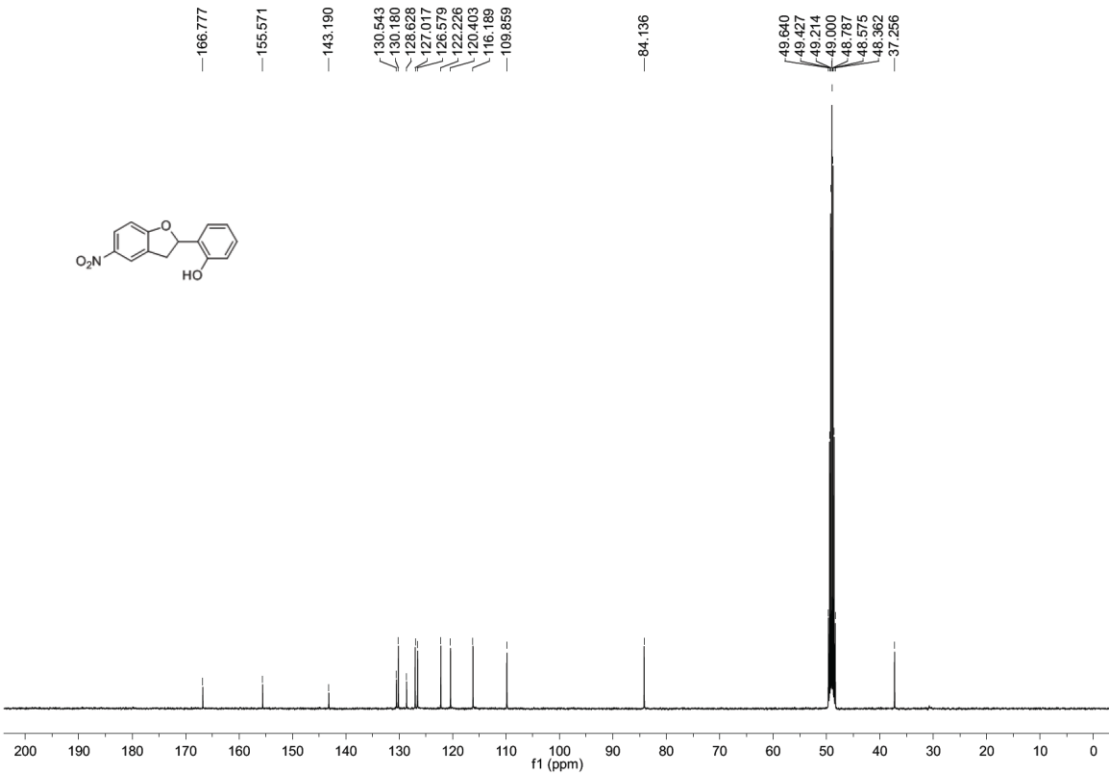
3q'-^{13}C NMR (100 MHz, $CDCl_3$)



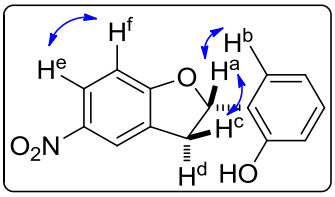
3r-^{1}H NMR (400 MHz, CD_3OD)

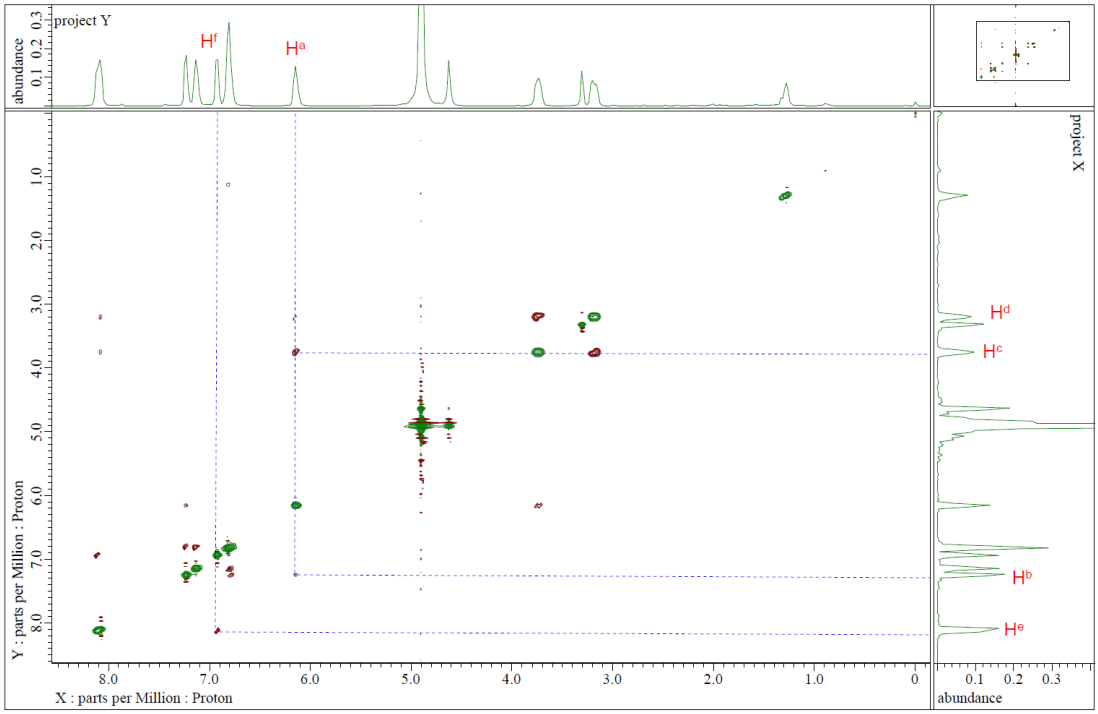


3r-^{13}C NMR (100 MHz, CD_3OD)

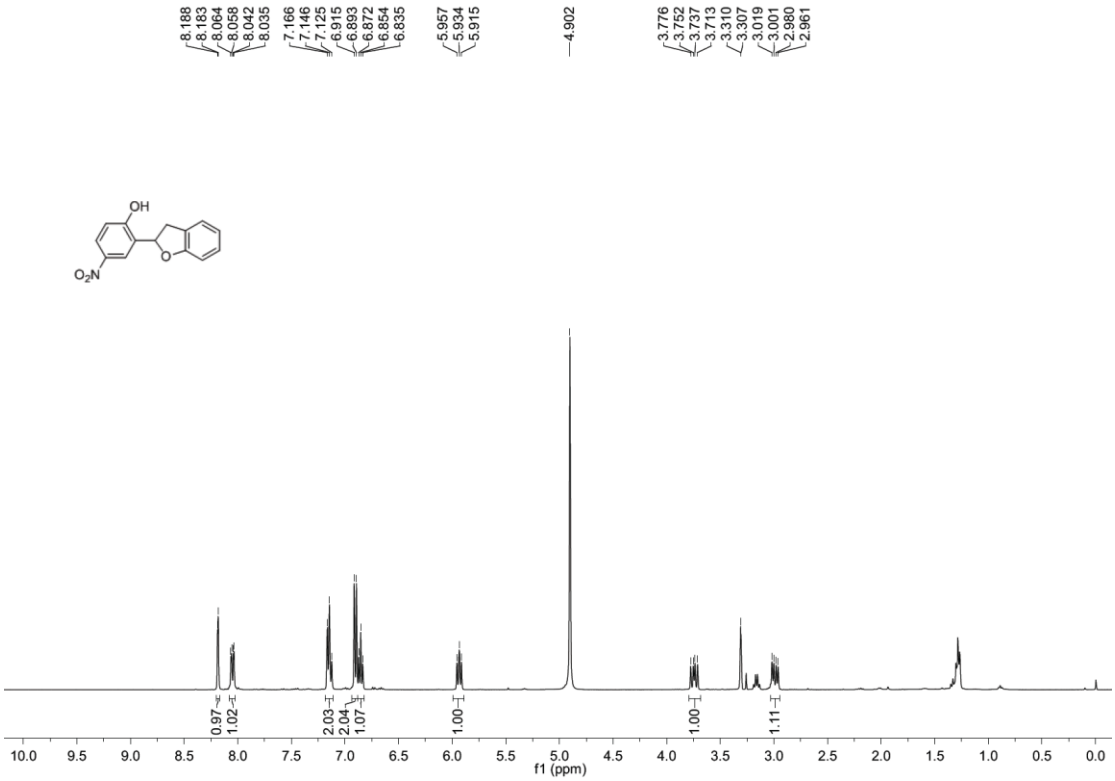


^{1}H-^{1}H NOESY of 3r:

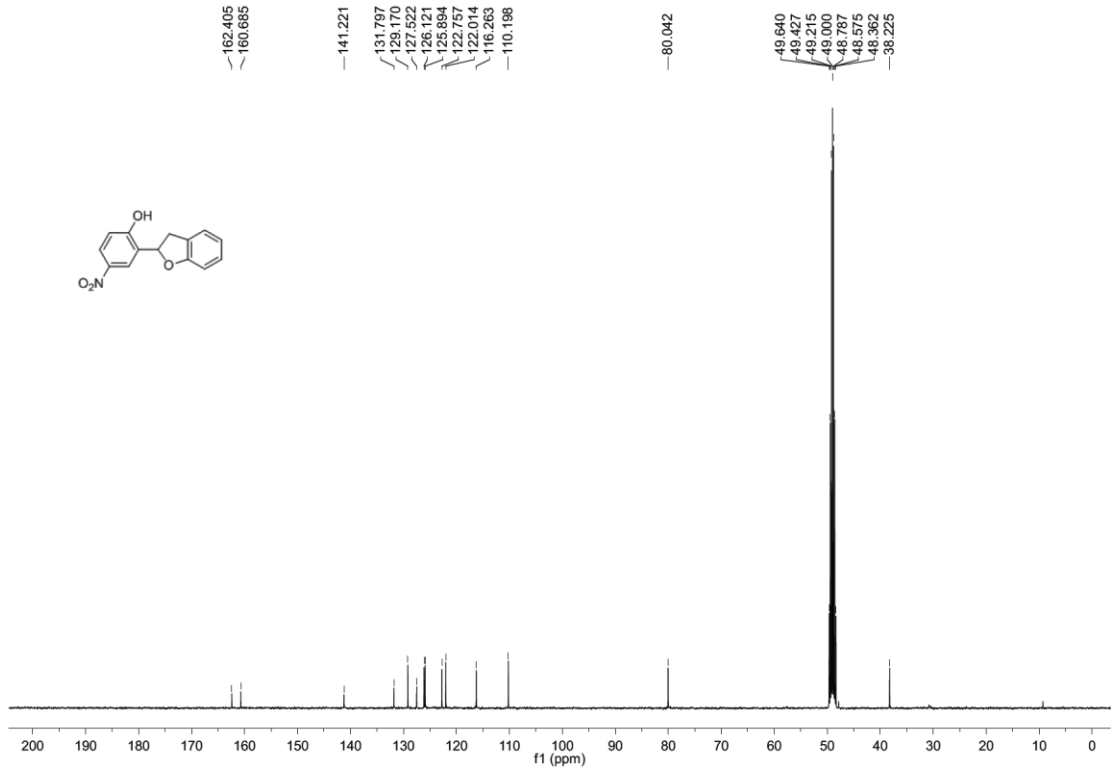




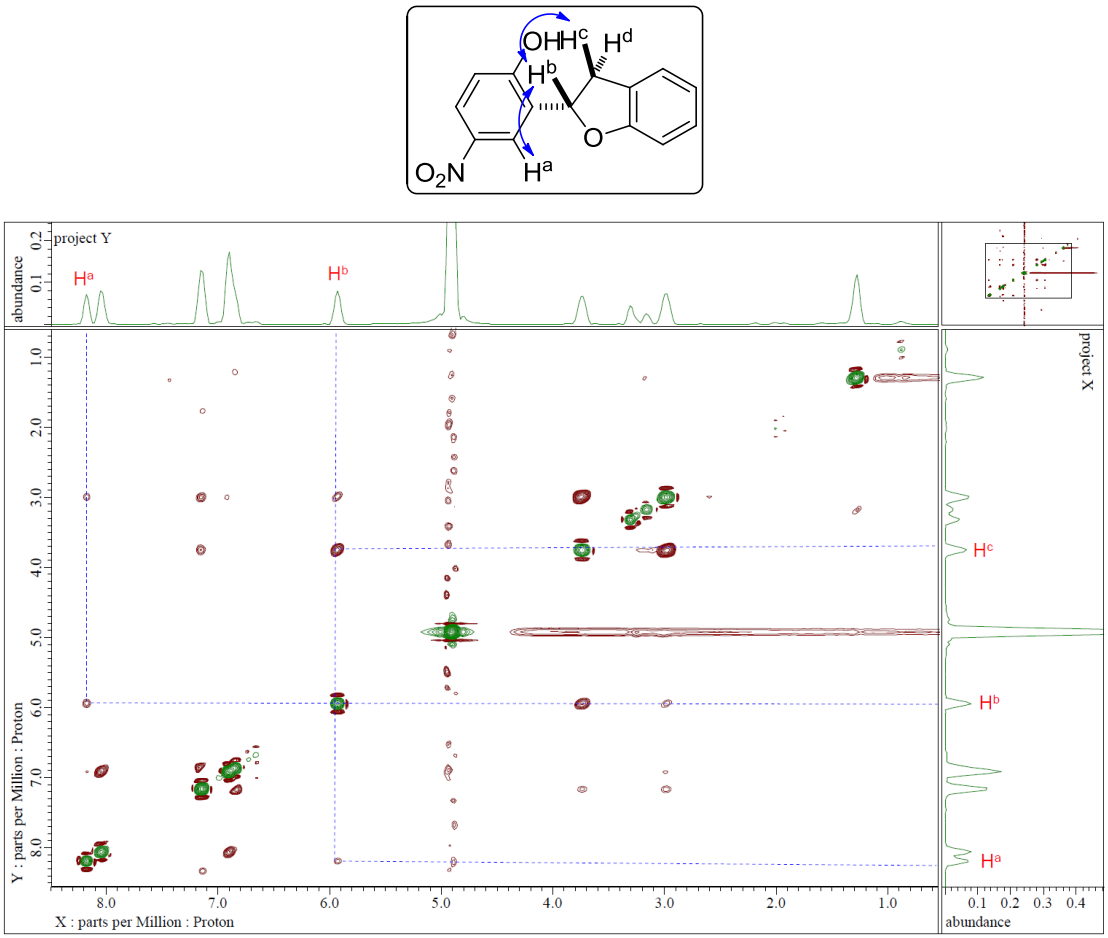
3r'-^{1}H NMR (400 MHz, CD_3OD)



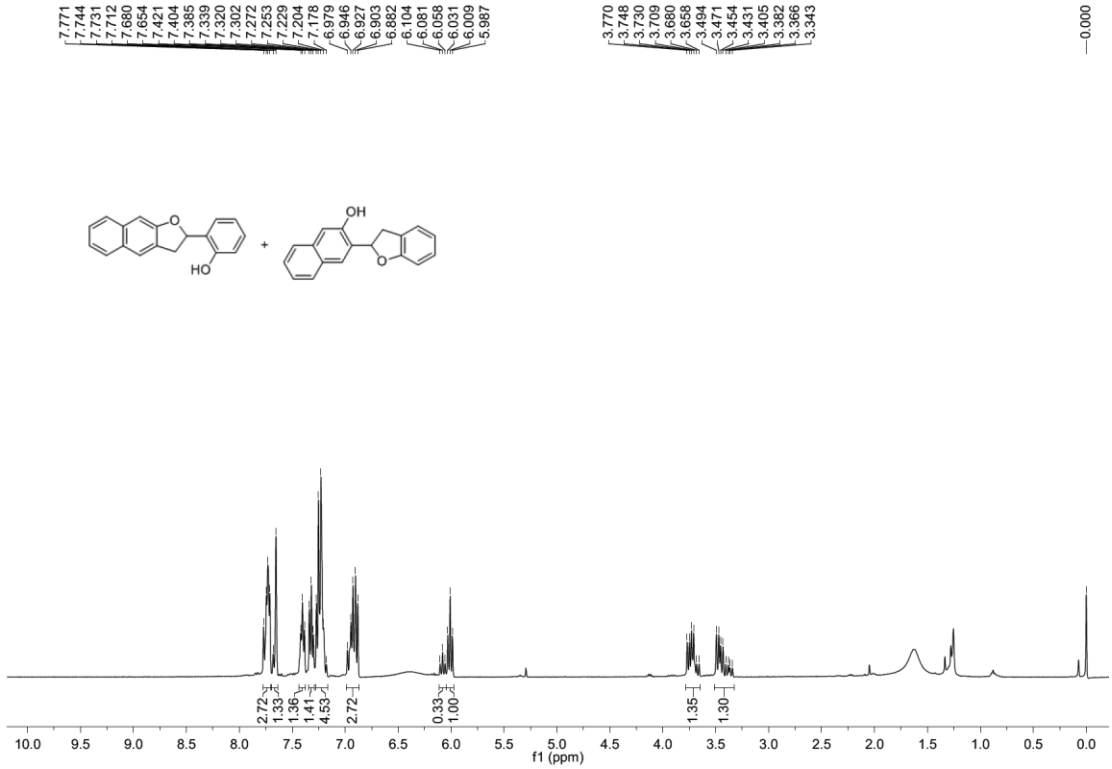
3r'-^{13}C NMR (100 MHz, CD_3OD)



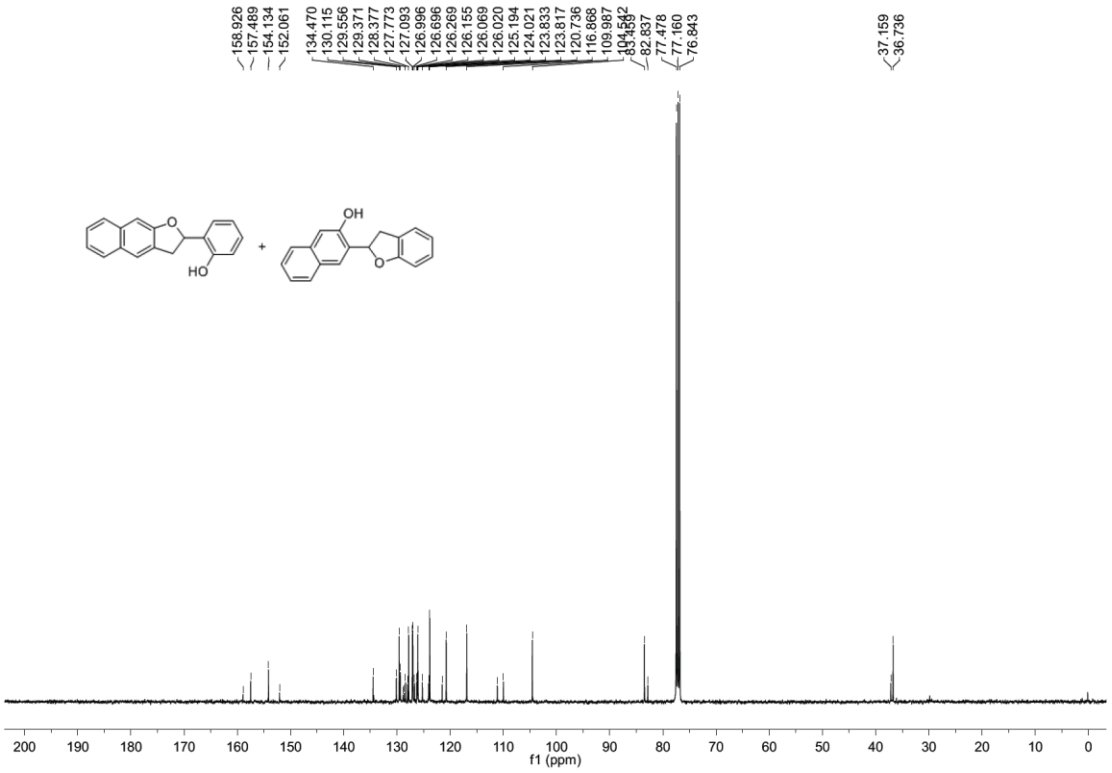
^{1}H-^{1}H NOESY of 3r':



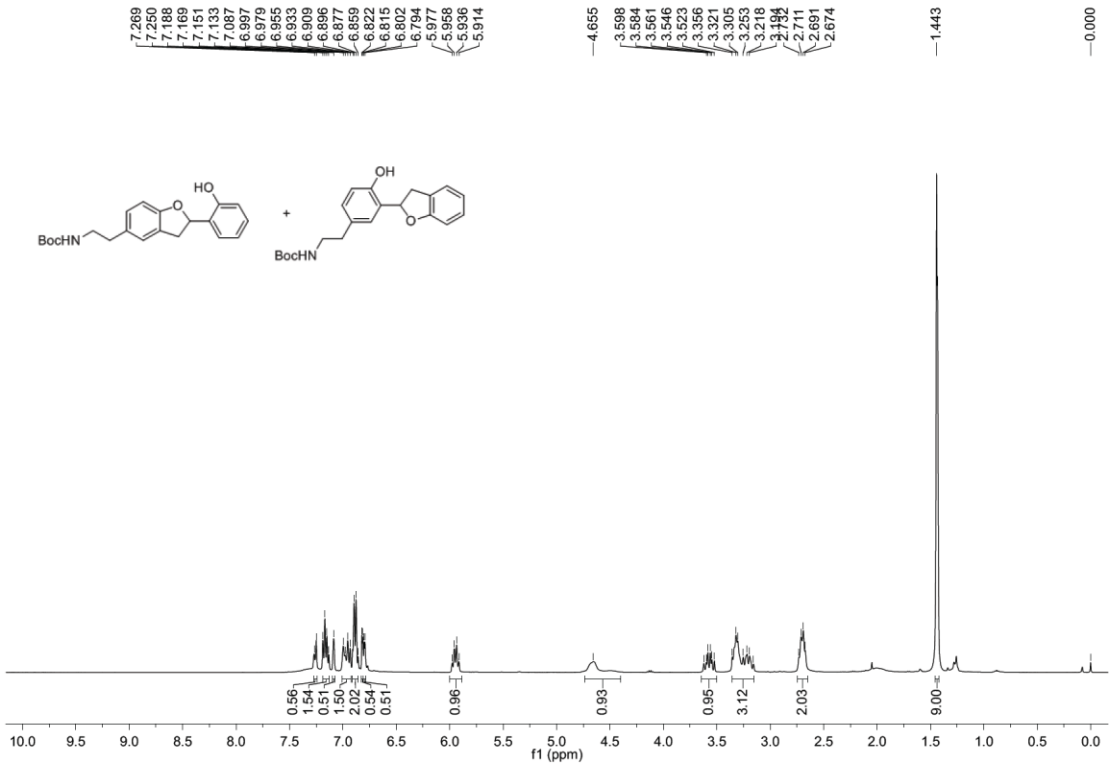
3s-^{1}H NMR (400 MHz, $CDCl_3$)



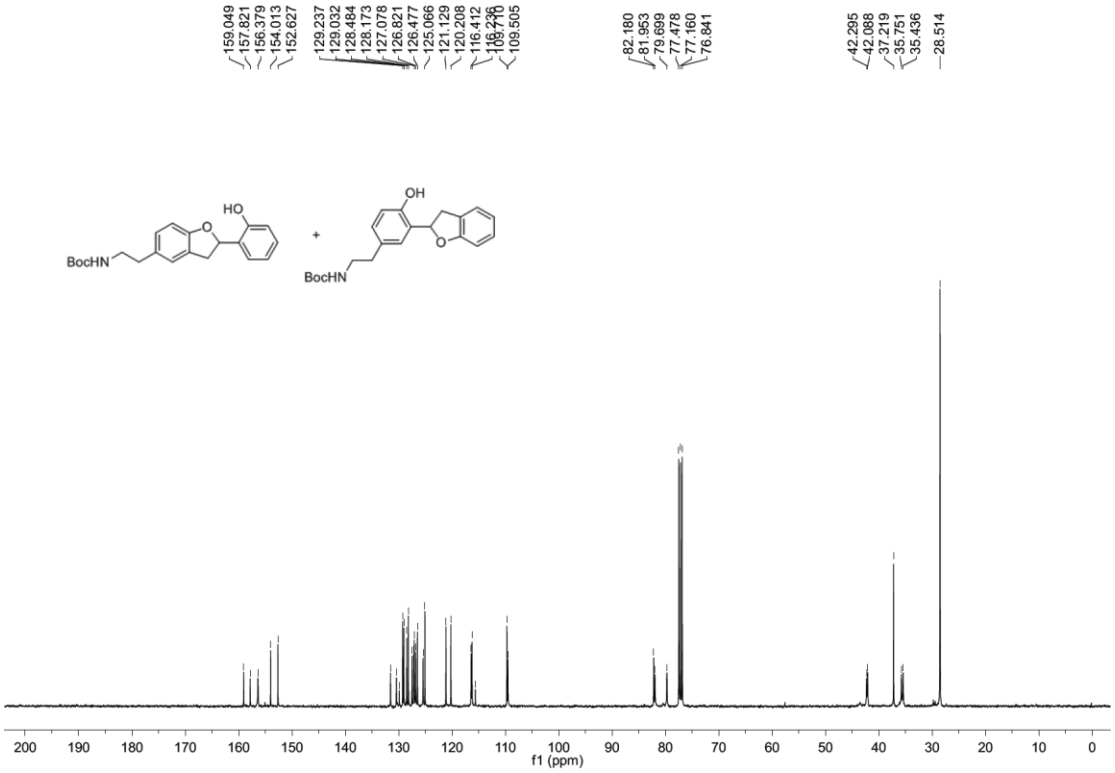
3s-^{13}C NMR (100 MHz, $CDCl_3$)



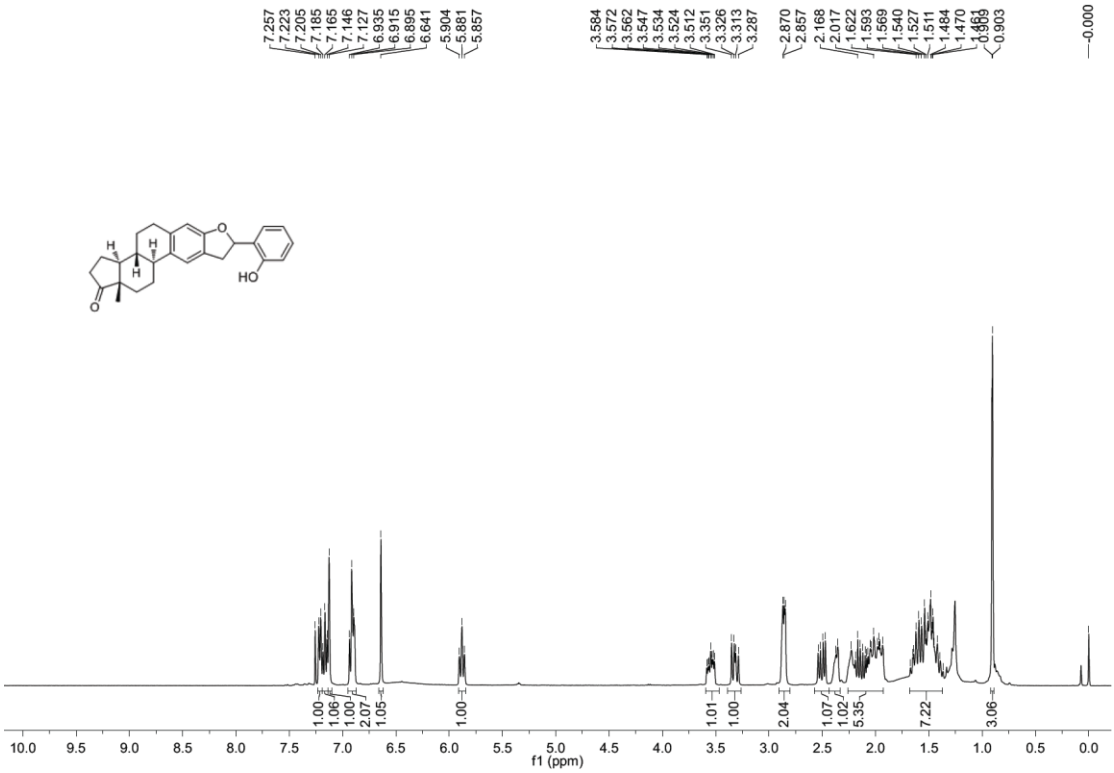
3t-^{1}H NMR (400 MHz, $CDCl_3$)



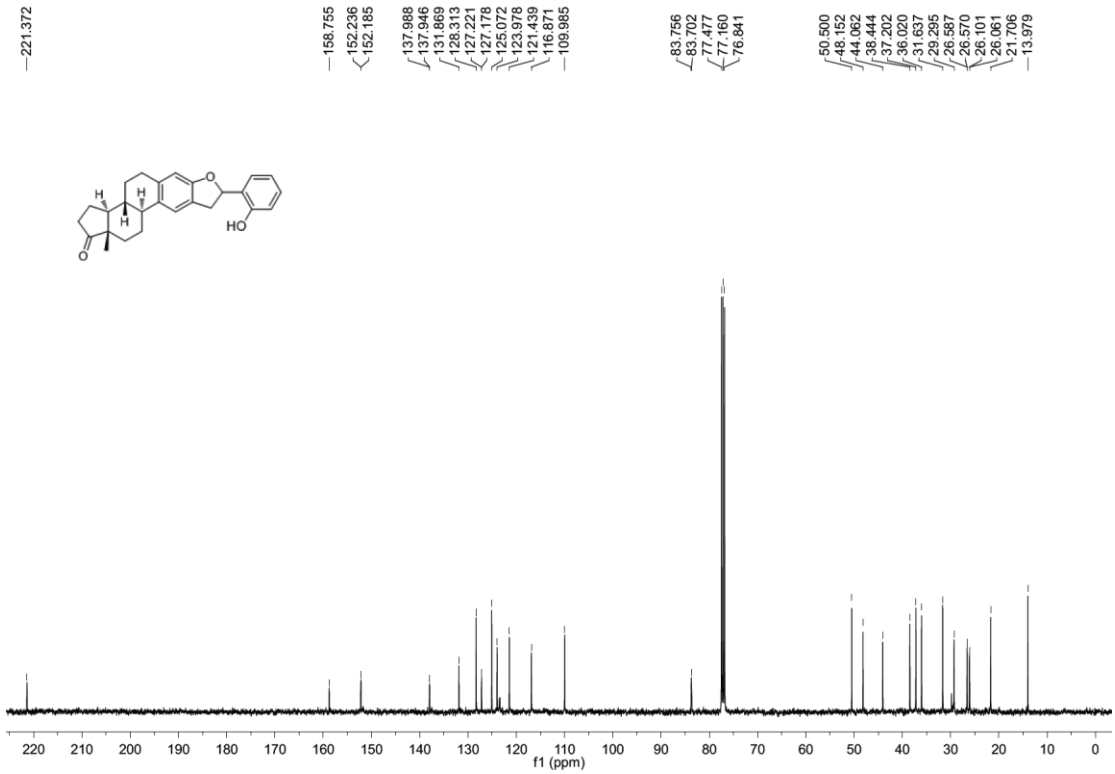
3t-^{13}C NMR (100 MHz, $CDCl_3$)



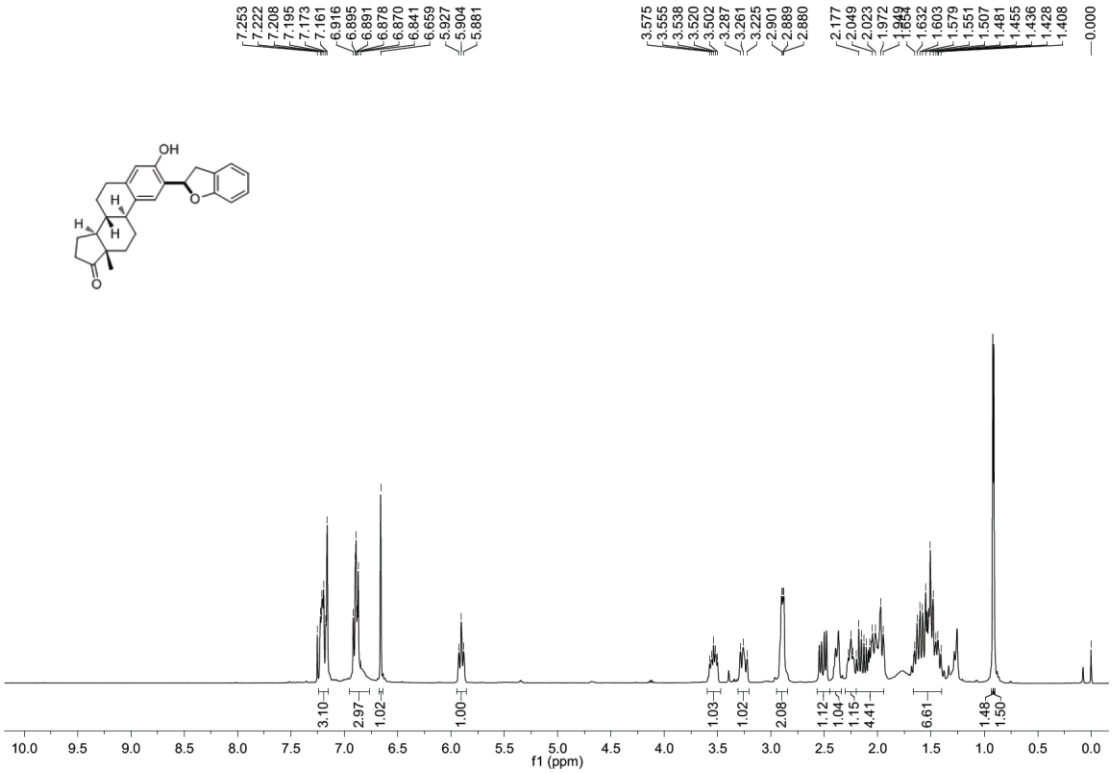
3u-^{1}H NMR (400 MHz, $CDCl_3$)



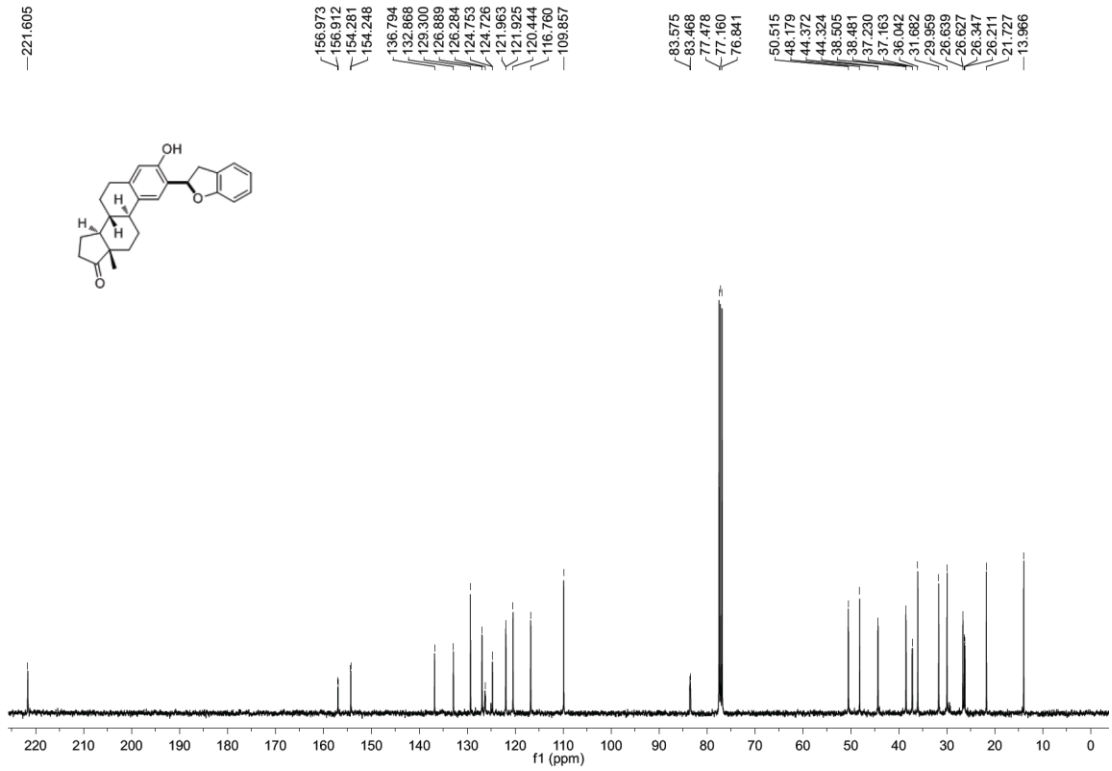
3u-^{13}C NMR (100 MHz, $CDCl_3$)



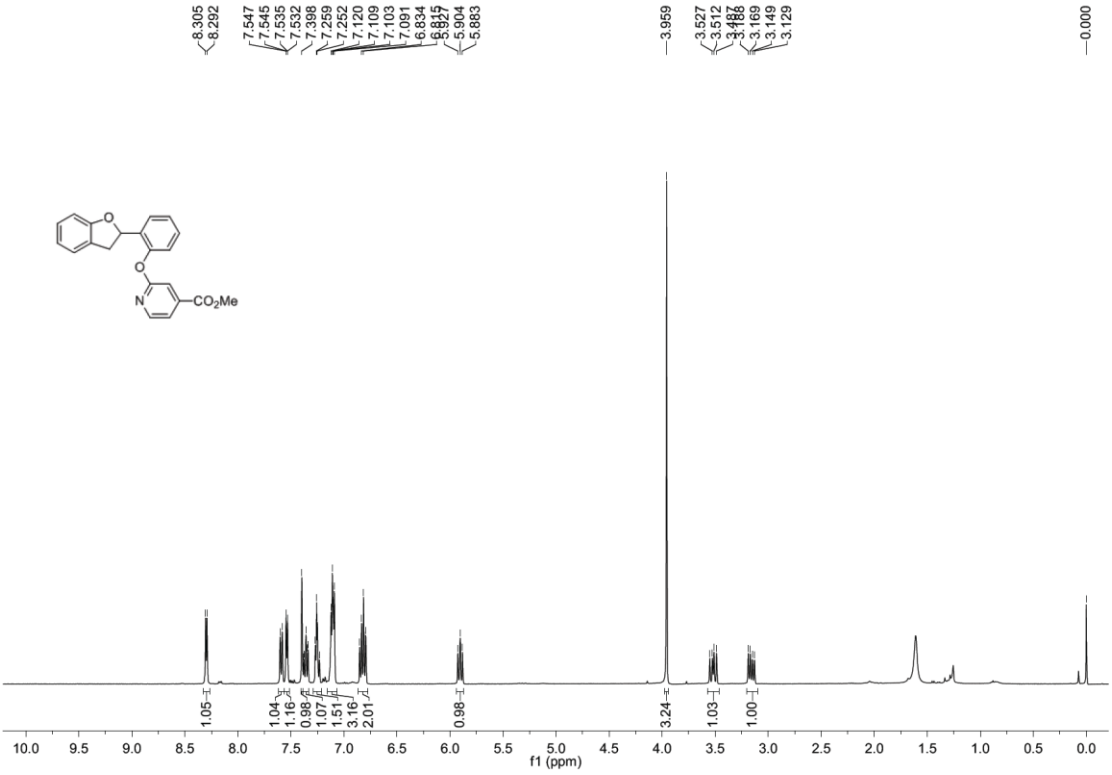
3u'-^{1}H NMR (400 MHz, $CDCl_3$)



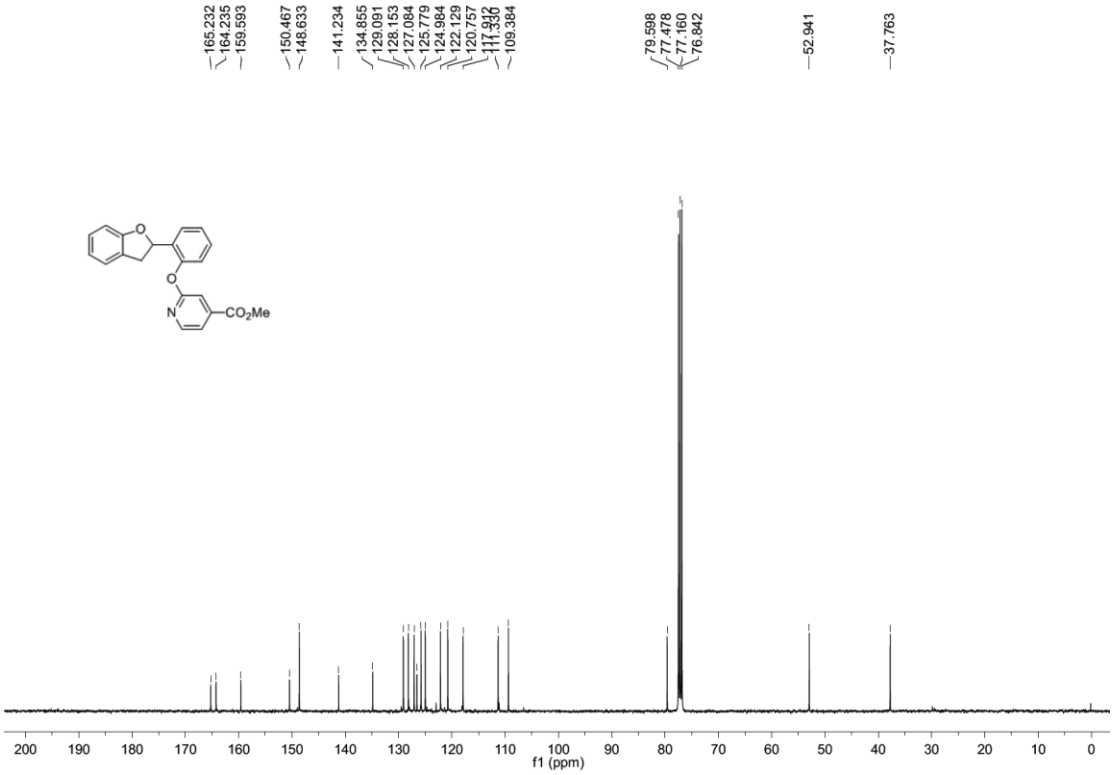
3u'-^{13}C NMR (100 MHz, $CDCl_3$)



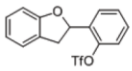
4-^{1}H NMR (400 MHz, $CDCl_3$)

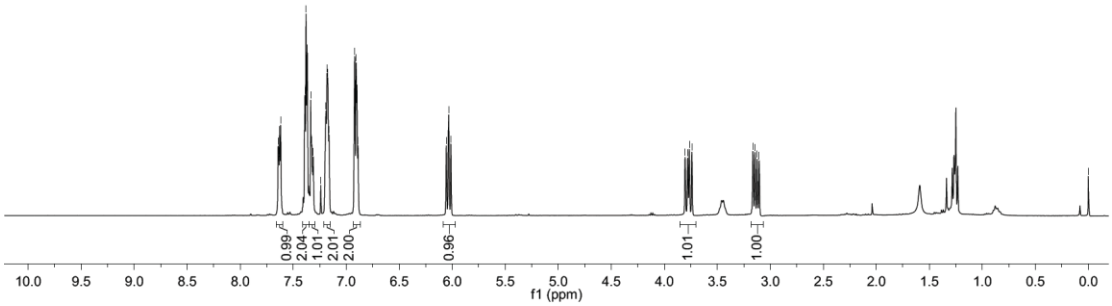


4-^{13}C NMR (100 MHz, $CDCl_3$)

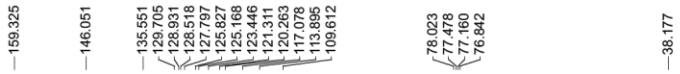


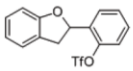
5-^{1}H NMR (400 MHz, $CDCl_3$)

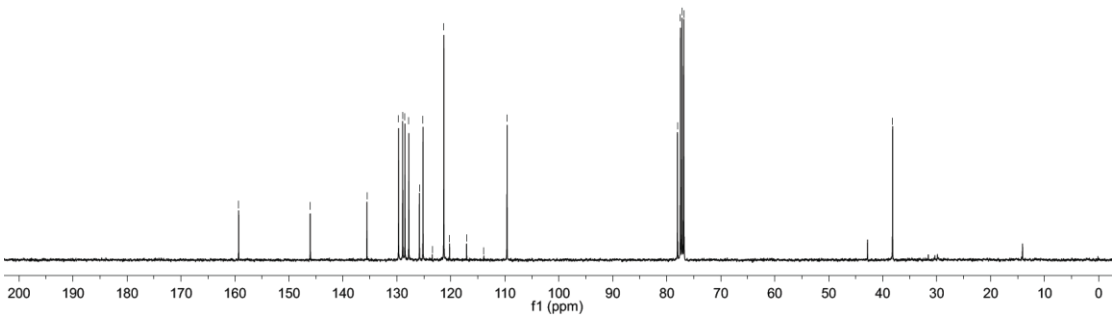




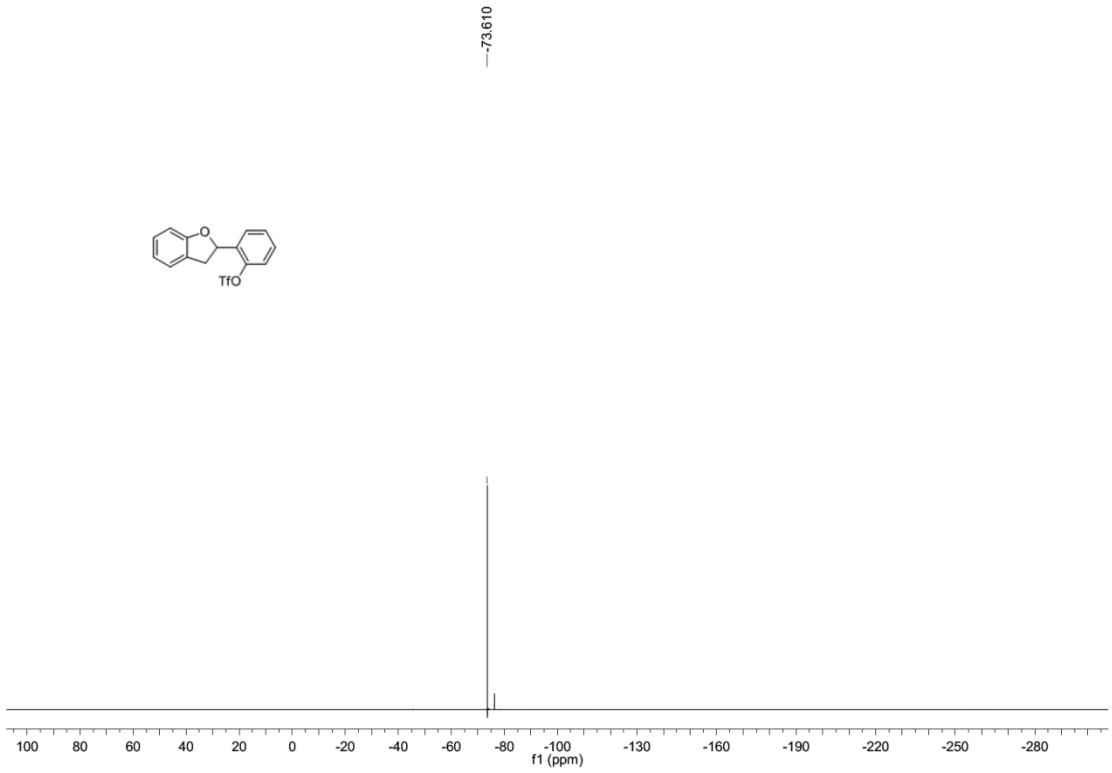
5-^{13}C NMR (100 MHz, $CDCl_3$)



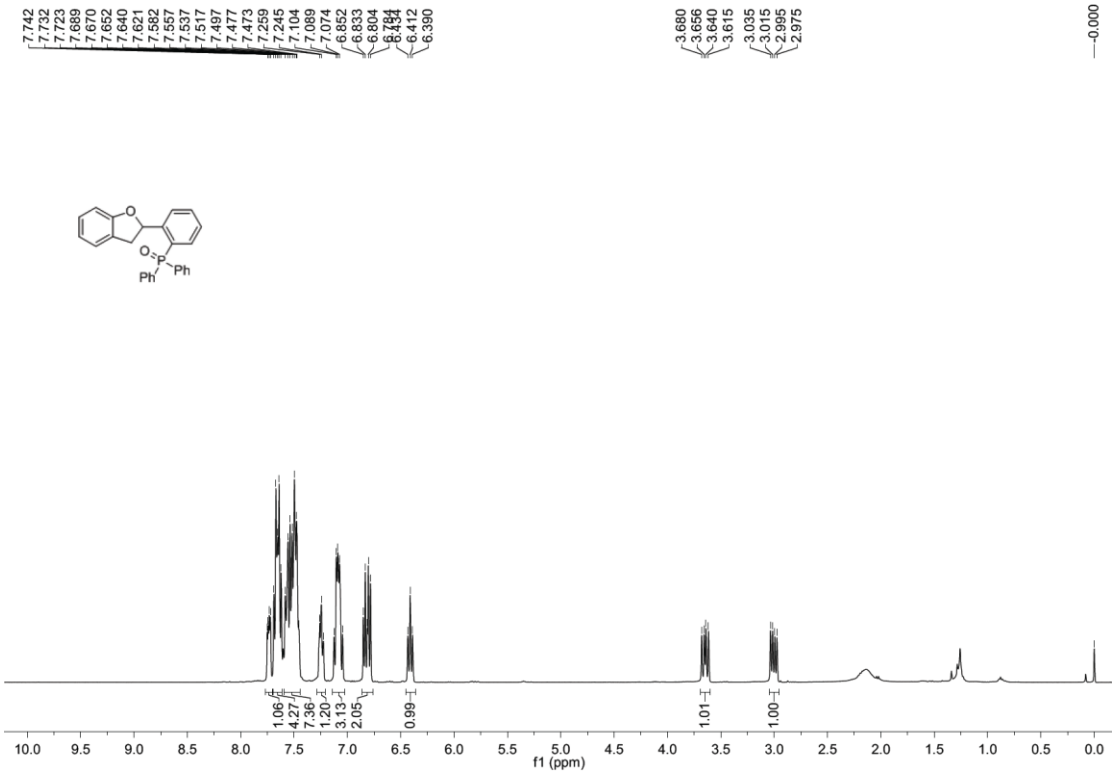




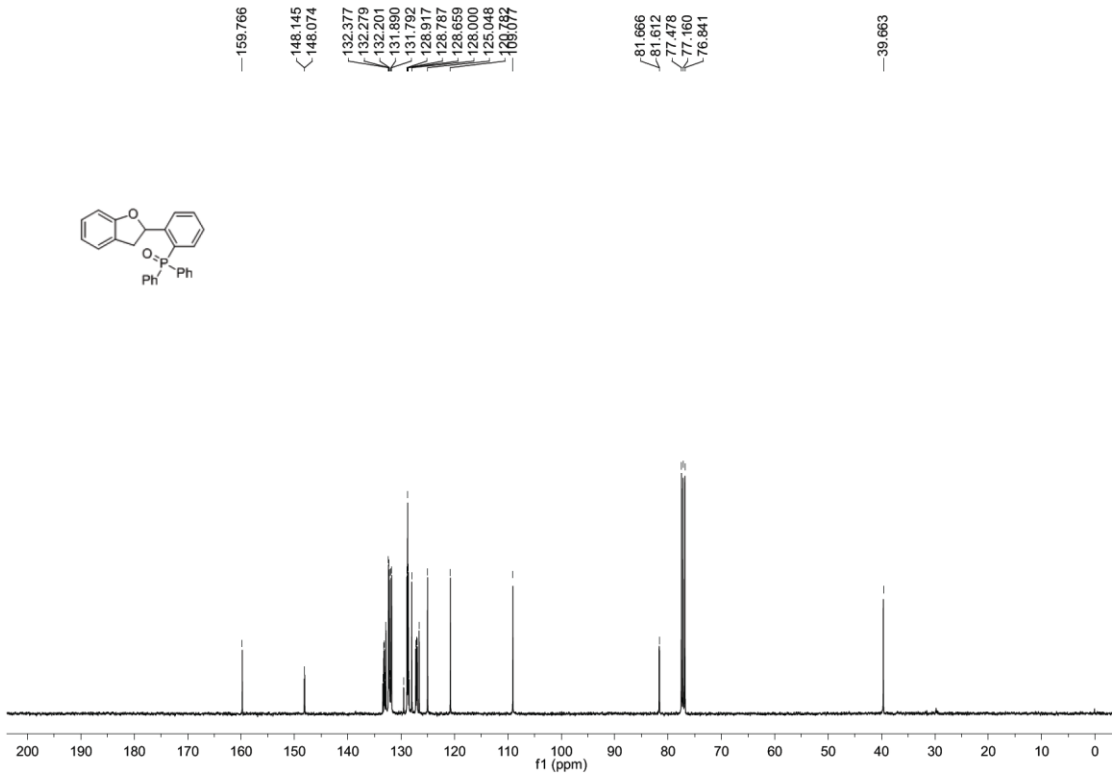
5-^{19}F NMR (376 MHz, $CDCl_3$)



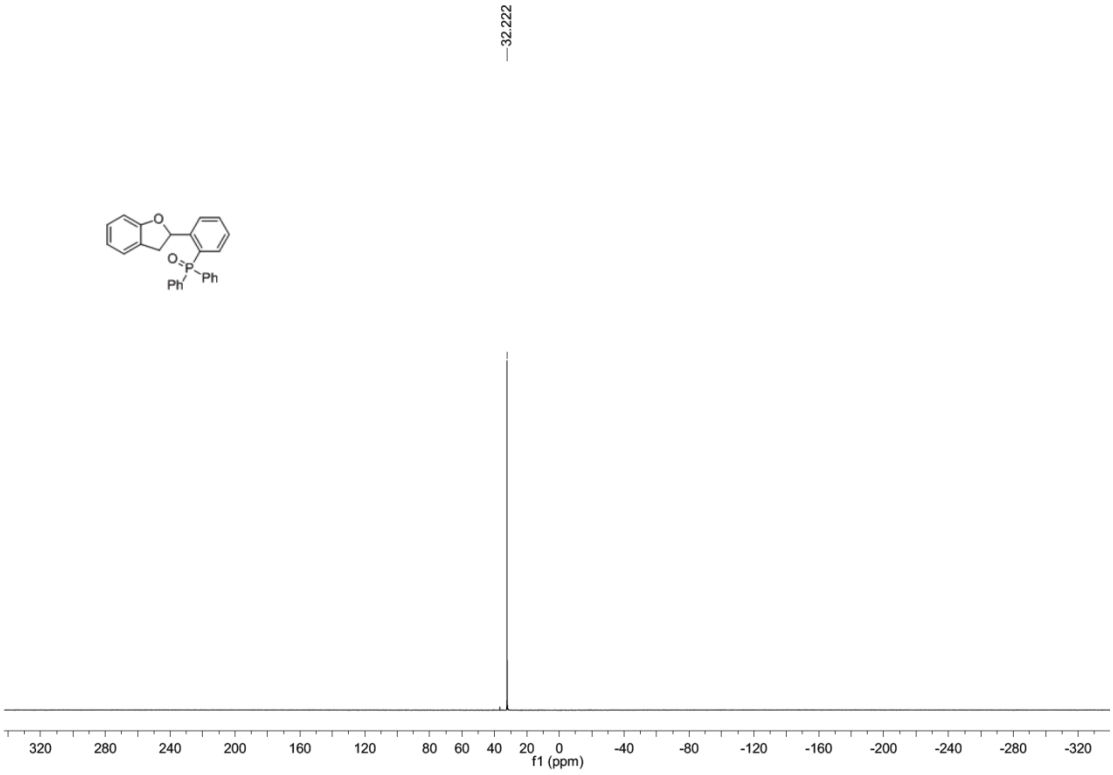
6-^{1}H NMR (400 MHz, $CDCl_3$)



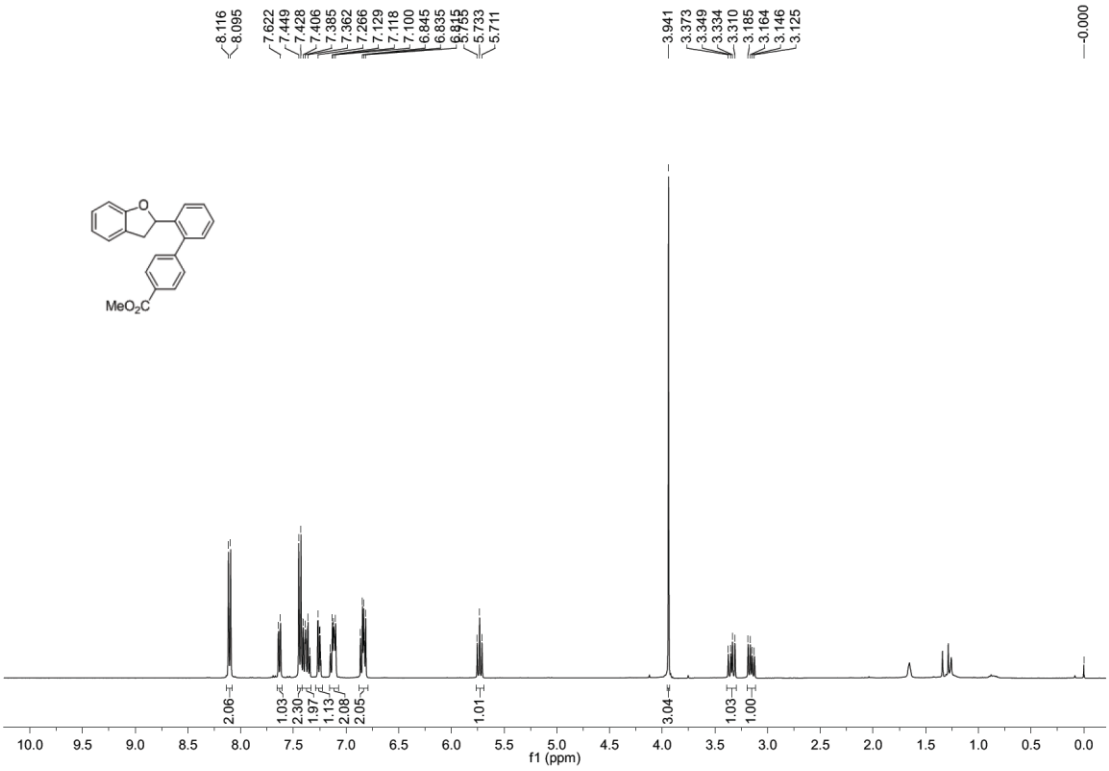
6-^{13}C NMR (100 MHz, $CDCl_3$)



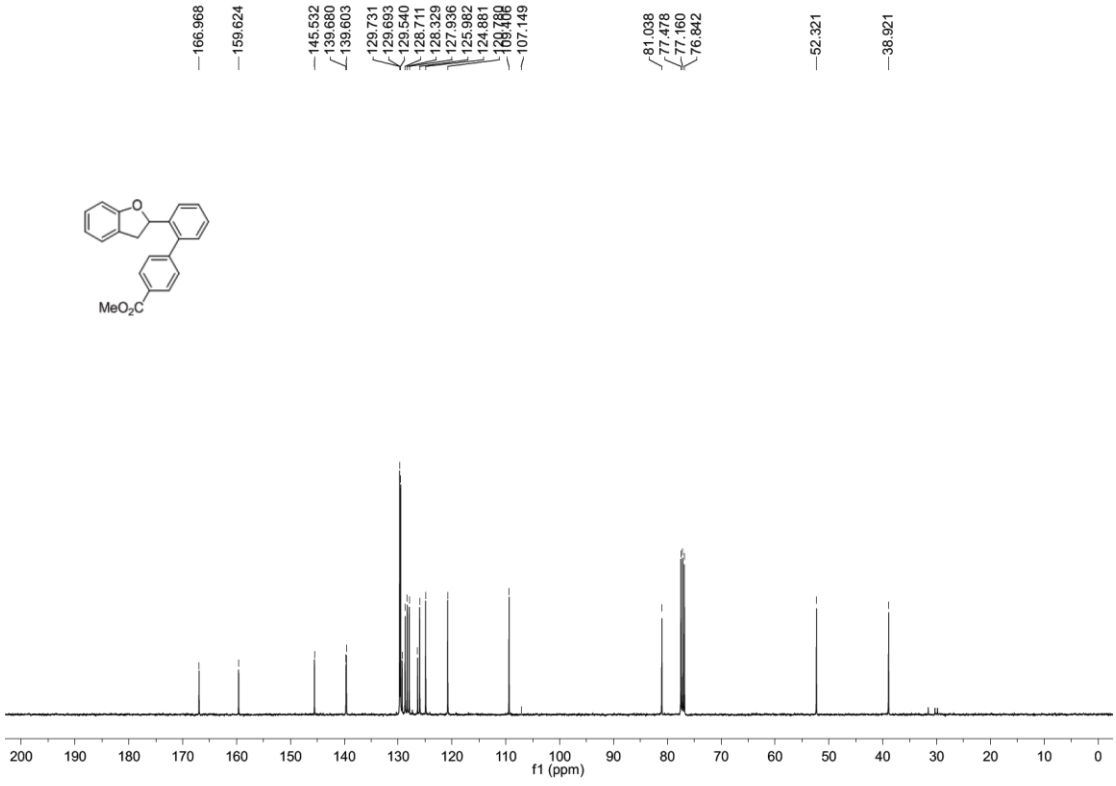
6-^{31}P NMR (162 MHz, $CDCl_3$)



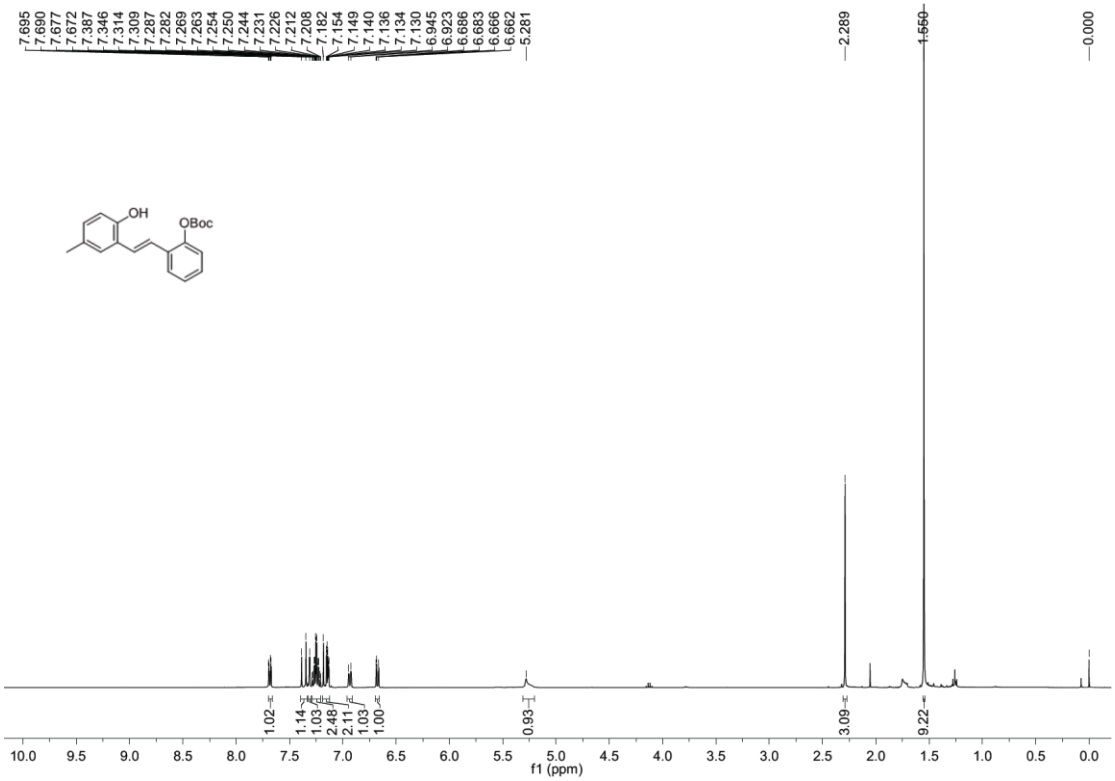
7-^{1}H NMR (400 MHz, $CDCl_3$)



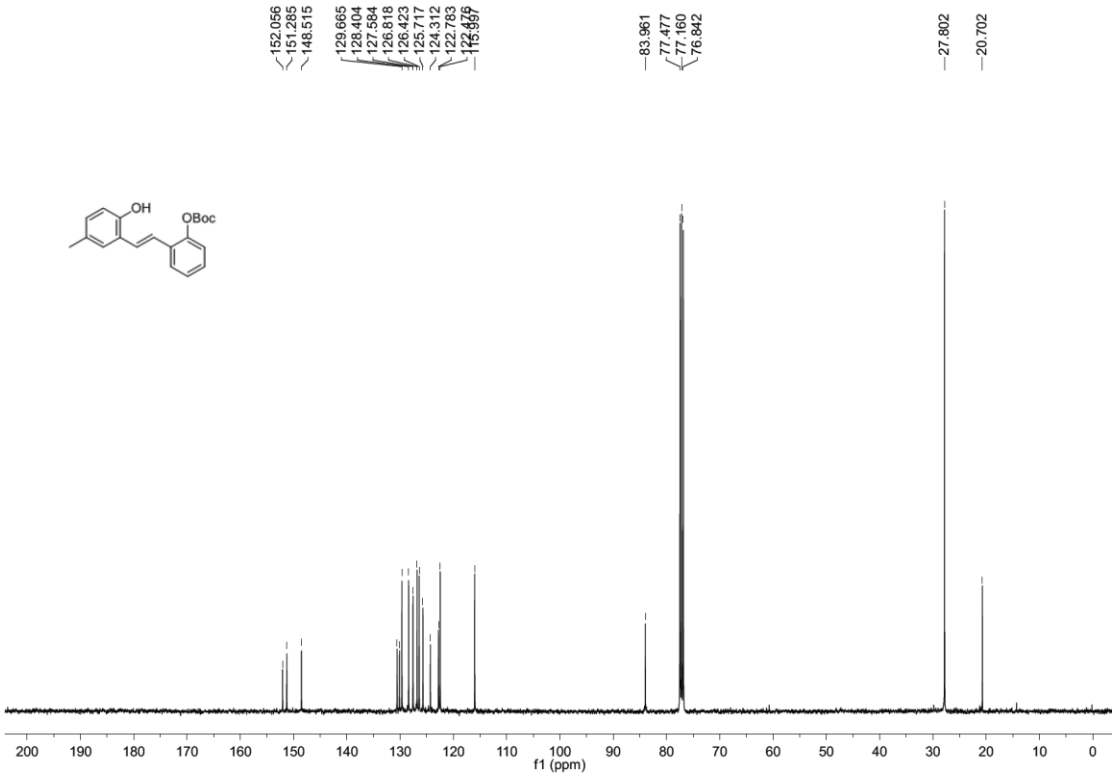
7-^{13}C NMR (100 MHz, $CDCl_3$)



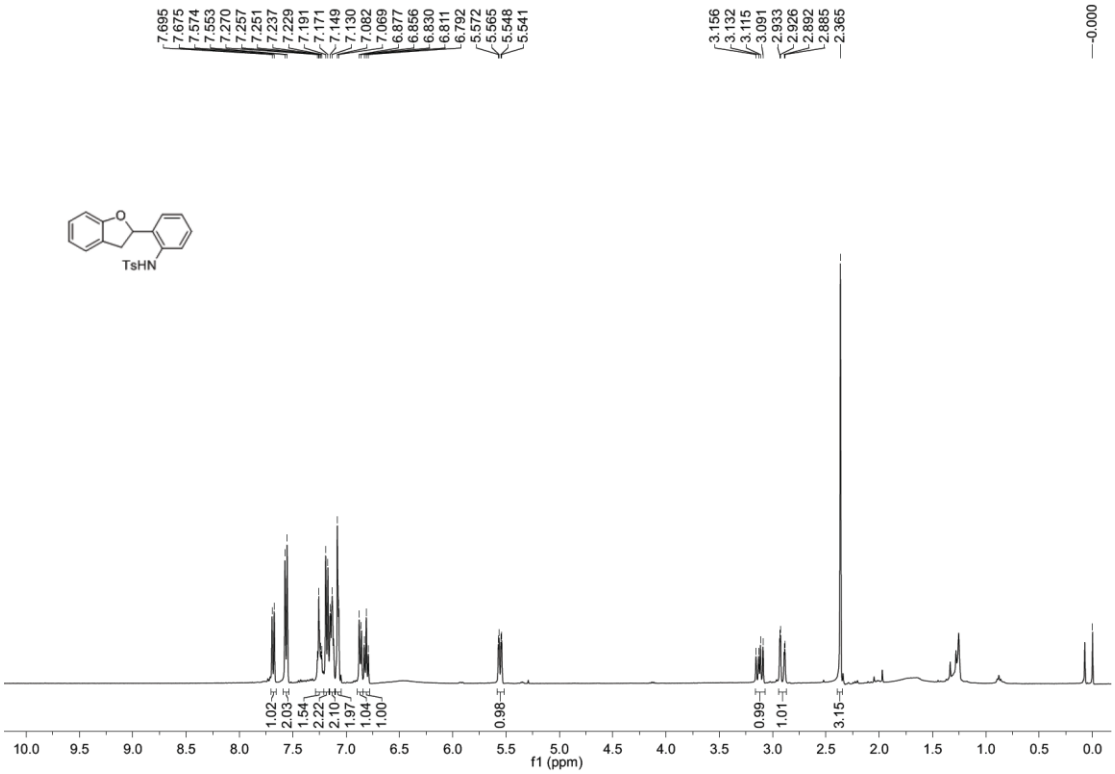
8-^{1}H NMR (400 MHz, $CDCl_3$)



8-^{13}C NMR (100 MHz, $CDCl_3$)



11-^{1}H NMR (400 MHz, $CDCl_3$)



11-^{13}C NMR (100 MHz, $CDCl_3$)