Supporting Information

Highly Enantioselective Synthesis of Both Enantiomers of Tetrahydroquinoxaline Derivatives via Ir-catalyzed Asymmetric Hydrogenation

Ana Xu,[a] Lanxing Ren,[a,e] Junrong Huang,[a] Yuxiang Zhu,[d] Gang Wang,[a] Chaoyi Li,[a] Yongqiang Sun,[a] Lijuan Song, [a]* Hengzhi You,[a,b]* Fen-Er Chen[a,b,c]*

[a] School of Science, Harbin Institute of Technology (Shenzhen), Shenzhen, 518055, China; [b] Green Pharmaceutical Engineering Research Center, Harbin Institute of Technology (Shenzhen), Shenzhen, 518055, China; [c] Engineering Center of Catalysis and Synthesis for Chiral Molecules, Department of Chemistry, Fudan University, Shanghai, 200433,China; [d]School of Pharmaceutical Sciences (Shenzhen), Shenzhen Campus of Sun Yat-sen University, Shenzhen, 518107, China; [e] School of Chemistry and Chemical Engineering, Hunan Province Key Laboratory for the Design and Application of Actinide Complexes, University of South China, Hengyang City, Hunan Province, 421001, P.R. China.

* Corresponding authors

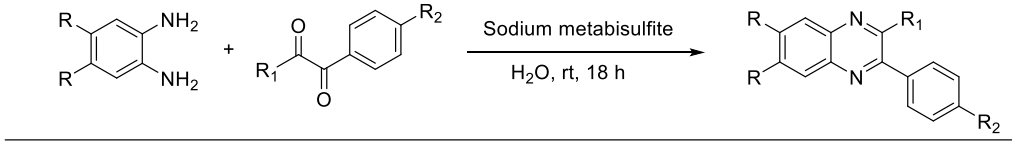
songlijuan@hit.edu.cn; youhengzhi@hit.edu.cn; rfchen@fudan.edu.cn;

Table of contents

1. General remarks

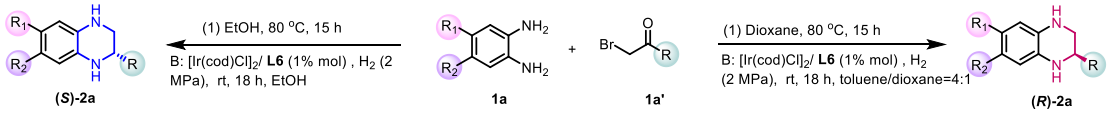
All the reactions dealing with air-or moisture-sensitive compounds were carried out in a dry reaction vessel under a positive pressure of argon or in the argon-filled glovebox. ^{1}H NMR and ^{13}C NMR spectra were recorded using Q. One Instruments Quantum-I 400M spectrometer. ^{1}H NMR and ^{13}C NMR chemical shifts were reported in parts per million (ppm) downfield from tetramethylsilane. Coupling constants (*J*) are reported in Hertz (Hz). The residual solvent peak was used as an internal reference: ^{1}H NMR (chloroform δ 7.26) and ^{13}C NMR (chloroform δ 77.0). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. HRMS were obtained on Waters Xevo G2-XS QTof. All *substrates* were prepared according to the published procedures. Other reagents were received from commercial sources. Solvents were freshly dried and degassed according to the published procedures prior to use. Column chromatography purifications were performed by flash chromatography using Merck silica gel 60. Enatioselectivities were measured by HPLC (Thermo Ultimate 3000).

2. General procedure for the synthesis of di-substituted quinoxaline substrates



Sodium metabisulfite (6 mmol) was added to a solution of pyruvaldehyde (2.4 mmol) in water, then, 1,2-phenylenediamine (2 mmol) was added and the solution was stirred at room temperature. After 18 h the solution was adjusted to pH 10 by the addition of sodium carbonate (Na_2CO_3), the mixture was extracted with ether (3 × 30 mL). The organic phase was dried over magnesium sulfate ($MgSO_4$), filtered, and concentrated under reduced pressure.

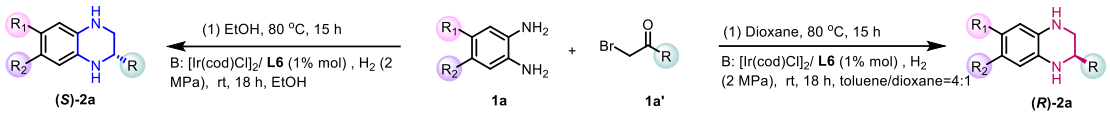
3. General procedure for the synthesis of (*R*)-tetrahydroquinoxaline derivatives via one pot



To a solution of benzene-1,2-diamine **1a** (27 mg, 0.25 mmol) in dioxane (1 mL) was added 2-bromo-1-phenylethan-1-one **1a'** (50 mg, 0.25 mmol) in a 10 mL schlenk tube at room temperature. Then the reaction mixture was stirred at 80 °C for 15 h. After the completion (as indicated by TLC), the mixture was cooled to room temperature. Next,

this mixture was delivered to a nitrogen-filled glovebox, and anhydrous toluene (4 mL) was added. This mixture will be proceeded a simple purification by a silicone column made from glass-tipped droppers and the organic layer (substrate) was collected. The solution of $[Ir(cod)Cl]_2$ (3.4 mg, 0.005 mmol) and ligand (9.8 mg, 0.011 mmol) in 2.0 mL anhydrous toluene was stirred at room temperature for 2 h. 500 μL of the resulting solution was transferred by syringe into a vial charged with substrate. The vials were transferred to an autoclave, which were then charged with 2 MPa of H_2 and stirred at room temperature for 18 h. After release of H_2, the resulting mixture was concentrated under vacuum. The residue was purified by column chromatography to give the product (*R*)-**2a**. The enantiomeric excess was determined by HPLC analysis of the crude product. The other (*R*)- tetrahydroquinoxaline derivatives were prepared with the same procedure.

4. General procedure for the synthesis of (*S*)-tetrahydroquinoxaline derivatives via one pot



To a solution of benzene-1,2-diamine **1a** (27 mg, 0.25 mmol) in EtOH (1 mL) was added 2-bromo-1-phenylethan-1-one **1a**' (50 mg, 0.25 mmol) in a 10 mL schlenk tube at room temperature. Then the reaction mixture was stirred at 80 °C for 15 h. After the completion (as indicated by TLC), the mixture was cooled to room temperature. The solvent was removed under reduced pressure and the residue (substrate) was purified by a silicone column made from glass-tipped droppers. Next, this substrate was delivered to a nitrogen-filled glovebox, and anhydrous EtOH (4 mL) was added. The solution of $[Ir(cod)Cl]_2$ (3.4 mg, 0.005 mmol) and ligand (9.8 mg, 0.011 mmol) in 2.0 mL anhydrous EtOH was stirred at room temperature for 30 min. 500 μL of the resulting solution was transferred by syringe into a vial charged with substrate. The vials were transferred to an autoclave, which were then charged with 2 MPa of H_2 and stirred at room temperature for 18 h. After release of H_2, the resulting mixture was concentrated under vacuum. The residue was purified by column chromatography to give the product (*S*)-**2a**. The enantiomeric excess was determined by HPLC analysis of the crude product. The other (*S*)- tetrahydroquinoxaline derivatives were prepared with the same procedure.

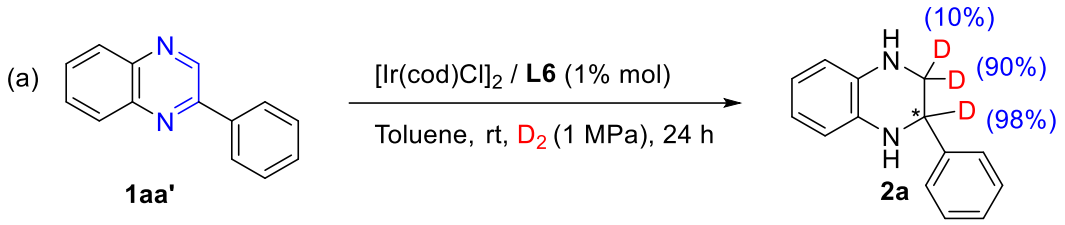
5. General procedure for the asymmetric hydrogenation of di-substituted quinoxaline derivatives

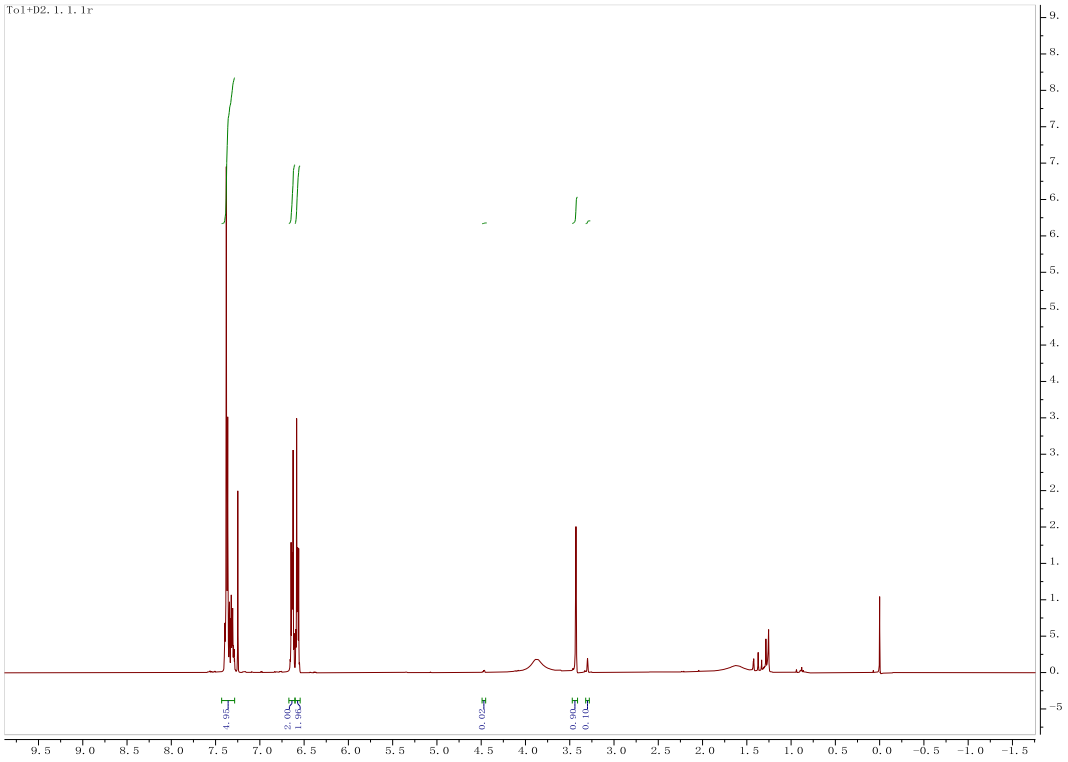
In the nitrogen-filled glovebox, solution of $[Ir(cod)Cl]_2$ (3.4 mg, 0.005 mmol) and ligand (9.8 mg, 0.011 mmol) in 2.0 mL anhydrous solvent was stirred at room temperature for 2 h. 500 μL of the resulting solution was transferred by syringe to a Score-Break ampule charged with substrate (0.25 mmol) and (***R***)-4-

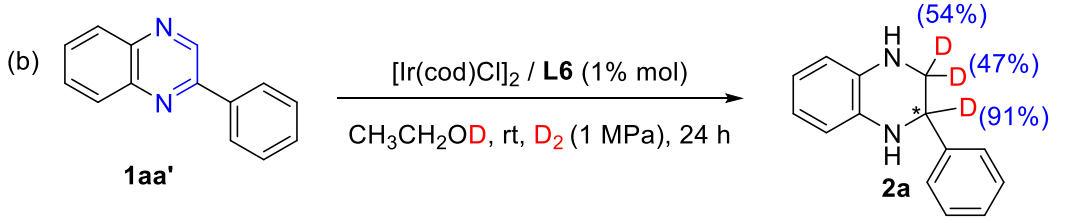
hydroxydinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepine 4-oxide ((***R***)-CPA) (0.5 mmol) solution. The ampule was placed into an autoclave, which was then charged with 2 MPa H_2. The autoclave was stirred at room temperature for the indicated period of time. After release of H_2, the resulting mixture was concentrated under vacuum. The residue was purified by column chromatography to give the product. The enantiomeric excess was determined by HPLC analysis of the crude product.

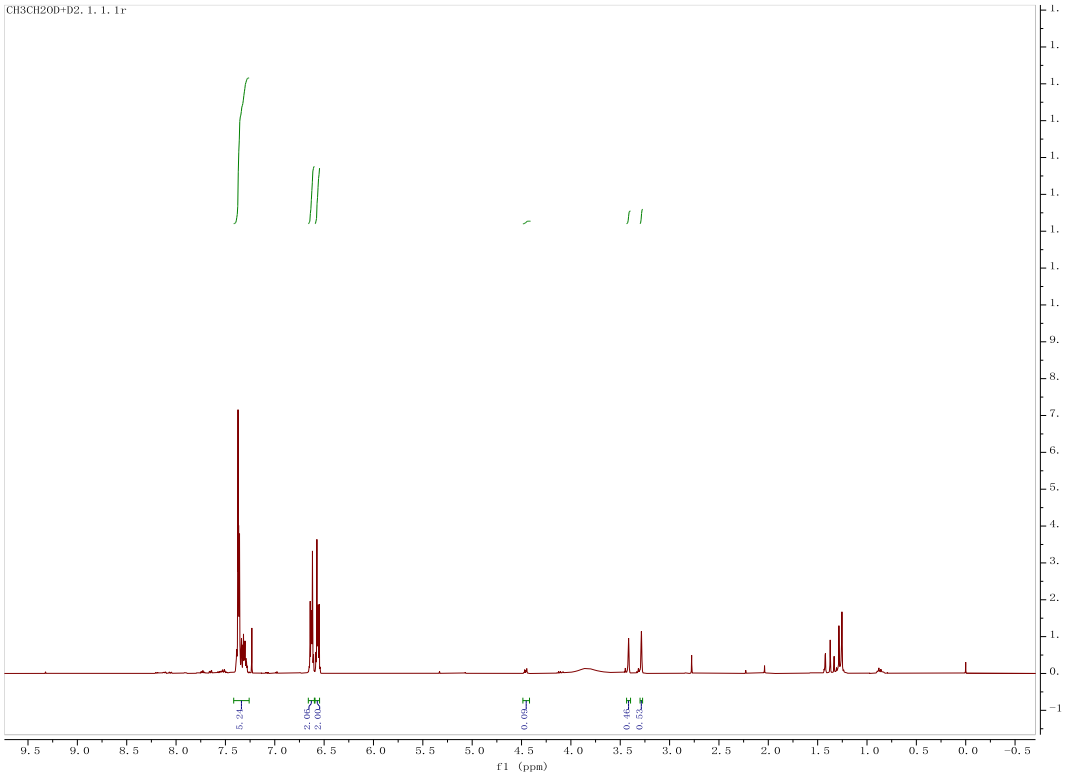
6. Result of deuterium labeling experiments

Following standard hydrogenation procedure, deuterium labeling experiments were conducted with specific modification.

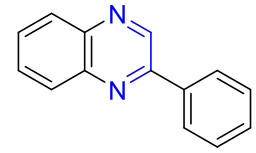








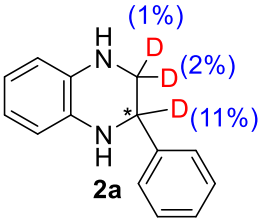
(c)



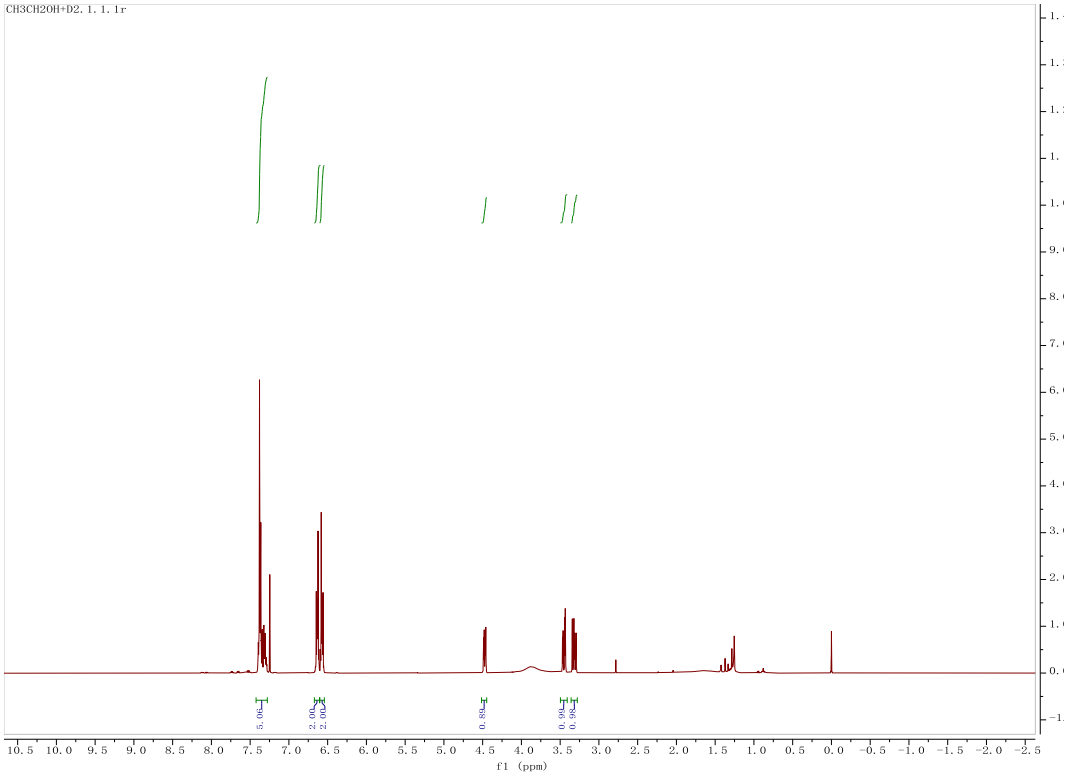
1aa'

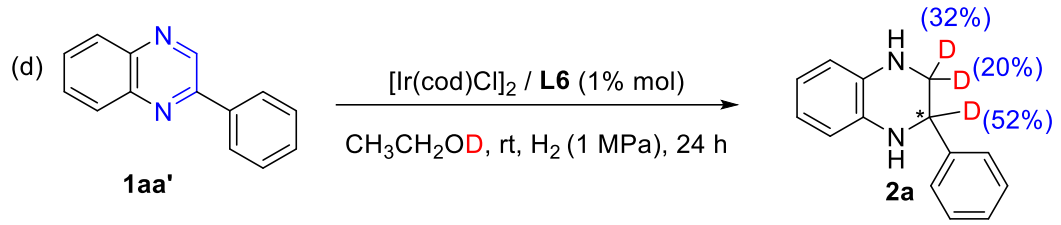
$[Ir(cod)Cl]_2$ / **L6** (1% mol)

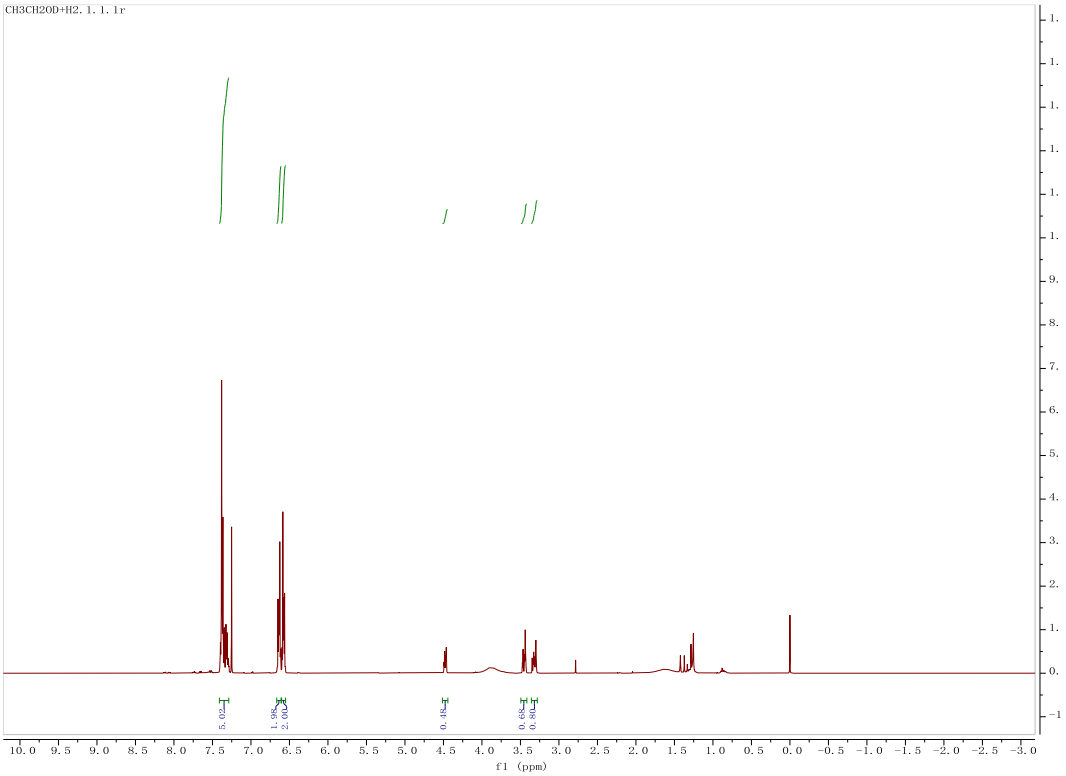
CH_3CH_2OH, rt, D_2 (1 MPa), 24 h



2a







7. General procedure for asymmetric hydrogenation under continuous flow

All process parts, including fittings, tubes, valves and junctions that hold pressure were purchased from Shenzhen Yizheng Technology Co., LTD. The specification of the reaction coil is 0.5 mL/m. The information of other main components is summarized in Table S1.

Table S1 Components details of reactor system

Name	Information
Pump	Sanotac high pressure HPLC pump AP0030（0-10 mL/min; 100 bar)
MFC	Beijing sevenstar flow CO. LTD, D08-1F, (0-100 sccm, 150 bar)
Relief check	X-tec Proportional ReliefValves RV-K2F (1000-1500 psi)
BPR	X-tec General-Purpose Back-PressureRegulators RBG (1000 psi)
Gas liquid separator	Shenzhen yizheng technology CO. LTD, (100 mL, 1000 psi)
Mixer	Shenzhen yizheng technology CO. LTD, (0.6 mL, 1000 psi)

In the nitrogen-filled glovebox, solution of $[Ir(cod)Cl]_2$ (49.5 mg, 0.073 mmol) and ligand (143.1 mg, 0.16 mmol) in 5.0 mL anhydrous EtOH was stirred at room temperature for 1 h. Then the substrate **1aa'** (3 g, 14.6 mmol) was dissolved in 292 mL anhydrous EtOH and mixed with the above solution. The resulting mixture was filtered and the filtrate was added into a flask. The process was washed by anhydrous EtOH at a liquid flow rate of 5 mL/min and gas flow rate of 10 sccm (avoid back flow of liquid to gas flow meter) for 10 minutes and then pressurized the BPR. After the reactor was pressurized to 3 MPa, the aforehand reaction medium was pumped instead of solvent. Liquid flow rate was set at 0.2 mL/min and gas flow rate was 8 sccm. The liquid holding capacity of the reaction coil can be adjusted according to the needs. The crude product (***S***)-2a cloud be collected in gas-liquid separator. Conversion and *ee* value were analyzed by NMR and HPLC. When reaction finished, system was depressurized by releasing the gas of Equilibar BPR slowly, and washed the whole system by pumping EtOH for 10 minutes.

In the nitrogen-filled glovebox, solution of $[Ir(cod)Cl]_2$ (49.5 mg, 0.073 mmol) and ligand (143.1 mg, 0.16 mmol) in 5.0 mL anhydrous dioxane was stirred at room temperature for 2 h. Then the substrate **1aa'** (3 g, 14.6 mmol) and HCl (0.365 mmol) were dissolved in 292 mL anhydrous dioxane and mixed with the above solution. The resulting mixture was filtered and the filtrate was added into a flask. This process was washed by anhydrous dioxane at a liquid flow rate of 5 mL/min and gas flow rate of 10 sccm (avoid back flow of liquid to gas flow meter) for 10 minutes and then pressurized the BPR. After the reactor was pressurized to 3 MPa, the aforehand reaction medium was pumped instead of solvent. Liquid flow rate was set at 0.1 mL/min and gas flow rate was 6 sccm. The liquid holding capacity of the reaction coil can be adjusted according to the needs. The crude product (***R***)-2a cloud be collected in gas-liquid separator. Conversion and *ee* value were analyzed by NMR and HPLC. When reaction finished, system was depressurized by releasing the gas of Equilibar BPR slowly, and washed the whole system by pumping EtOH for 10 minutes.

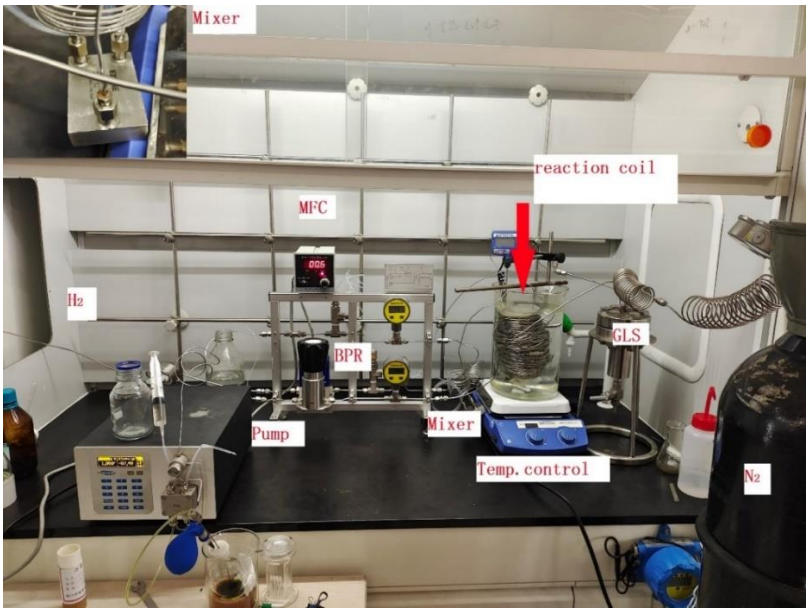
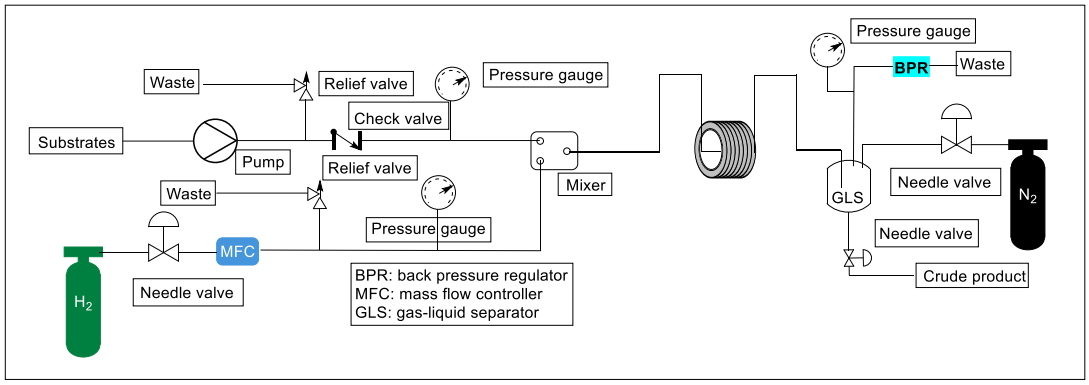
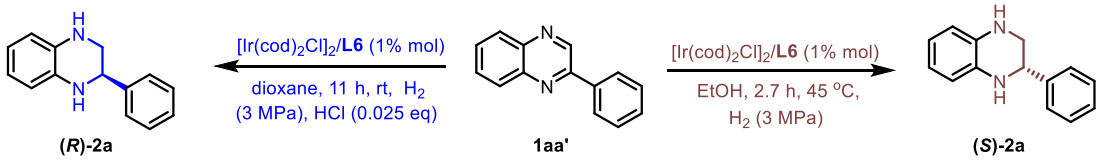


Figure S1. Set-up for asymmetric hydrogenation under continuous flow.



Scheme S1. Process scheme of **3j** under continuous flow.

Table S2. The optimization of **1aa'** under continuous flow



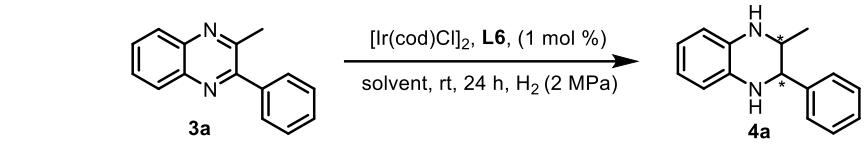
(*R*)-2a　　1aa'　　(*S*)-2a

Conc (M)	Gas (sccm)	Solvent	Liquid (mL/min)	H_2 (MPa)	RetTime (min)	*Conv* (%)[a]	*ee* (%)[b]
0.05	10	EtOH	1	2	35	12	--
0.05	7	EtOH	0.5	2	58	13	
0.075	10	EtOH	0.5	3	46	12	
0.075	10	Tol/Di=2:1	0.5	3	46	0	
0.075	10	Dioxane	0.3	3	53	10	
0.05	10	EtOH	0.5	2.5	66	10	
0.05	15	EtOH	0.3	2.5	55	22	
0.05	18	EtOH	0.2	3	50	35[c]	
0.05	10	EtOH	0.2	3	125	64	
0.05	10	EtOH	0.2	3	125	89[c]	87(*S*)
0.05	**8**	**EtOH**	**0.2**	**3**	**162**	**91[c]**	**87(*S*)**
0.05	8	Dio/tol=4:1	0.2	3	162	11[c]	
0.05	8	Dioxane	0.2	3	162	14[c]	
0.05	8	Dioxane	0.2	3	240	16[c]	
0.05	8	Dioxane	0.2	3	390	15[c]	
0.05 (0.1 eq HCl)	8	Dioxane	0.2	3	390	92[c]	73(*R*)
0.05 (0.05 eq HCl)	8	Dioxane	0.2	3	390	92	87(*R*)
0.05 (0.035 eq HCl)	9	Dioxane	0.2	3	390	93	89(*R*)
0.05 (0.035 eq HCl)	9	Dioxane	0.2	3	390	93	89(*R*)
0.05 (0.025 eq HCl)	9	Dioxane	0.2	3	390	66	90(*R*)
0.05 (0.025 eq HCl)	**6**	**Dioxane**	**0.1**	**3**	**660**	**92**	**93(*R*)**
0.05 (0.03 eq HCl)	6	Dioxane	0.1	3	660	94	90(*R*)

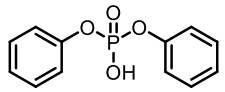
a. conversion was determined by ^{1}HNMR. b. *ee* were determined by HPLC. c. The reaction temperature was 45 °C.

8. Optimization of reaction conditions for Ir-Catalyzed asymmetric hydrogenation of di-substituted quinoxalines

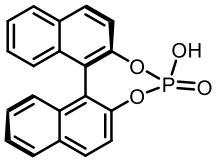
Table S3. The optimization of reaction conditions for di-substituted quinoxalines



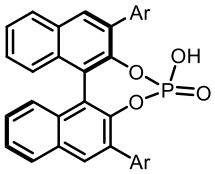
Additives:



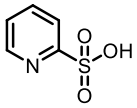
1



CPA



3: Ar=2,4,6-(^{i}Pr)$_3$-Ph



4

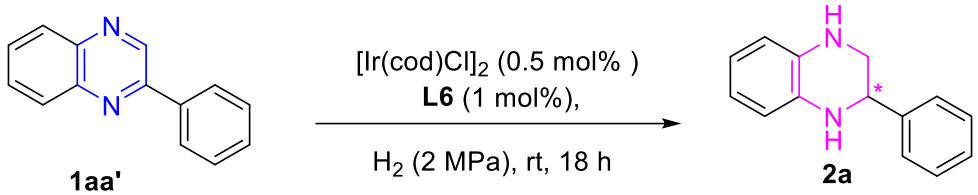
Entry	Solvent	Additive	(x)eq	Conv. (%)	Cis/trans	*ee* (%) of *trans*	*ee* (%) of *cis*
1	EtOH	-	--	20	>25:1	--	81 (2*R*, 3*S*)
2	toluene	-	--	99	1.5：1	99 (2*S*, 3*S*)	41 (2*R*, 3*S*)
3	toluene	$KOC(CH_3)_3$	0.2	0	--	--	--
4	toluene	CH_3CH_2ONa	0.2	0	--	--	--
5	toluene	CH_3COOH	0.2	99	1.5：1	99 (2*S*, 3*S*)	36 (2*R*, 3*S*)
6	EtOH	CH_3COONa	0.2	0	--	--	--
7	EtOH	CH_3COOH	0.2	0	--	--	--
8	Dioxane	HCl	0.2	99	7:93	99 (2*S*, 3*S*)	29 (2*R*, 3*S*)
9	toluene	KCl	0.2	99	1.6:1	99 (2*S*, 3*S*)	47 (2*R*, 3*S*)
10	toluene	NaCl	0.2	99	1.6:1	99 (2*S*, 3*S*)	48 (2*R*, 3*S*)
11	toluene	L-CSA	1.5	99	>20:1	--	71 (2*R*, 3*S*)
12	toluene	$In(OTf)_3$	0.2	0	--	--	--
13	toluene	HCOOH	0.2	99	1:1	99 (2*S*, 3*S*)	31 (2*R*, 3*S*)
14	dioxane	L-CSA	1.5	99	>20:1	--	35 (2*R*, 3*S*)
15	THF	L-CSA	1.5	99	>20:1	--	67 (2*R*, 3*S*)
16	toluene	1	1.5	99	>20:1	--	76 (2*R*, 3*S*)
17	toluene	2	1.5	99	>20:1	--	87 (2*R*, 3*S*)
18	toluene	3	1.5	56	>20:1	--	75 (2*R*, 3*S*)
19	toluene	4	1.5	92	1.5:1	97 (2*S*, 3*S*)	67 (2*R*, 3*S*)
20	toluene	(*R*)-CPA	2	99	>20:1	--	91 (2*R*, 3*S*)
21	toluene	(*S*)-CPA	2	99	>20:1	--	80 (2*S*, 3*R*)

Reaction conditions: 0.25 mmol substrate **3a**, 1.0 mol % [Ir (COD)Cl]$_2$/**L6**, H_2 (2 MPa), 2.0 mL solvent, rt, additives, and 24 h. Conversion and *Cis*/*trans* were determined by ^{1}H NMR. *ee* value was determined by HPLC.

9. Studies of the effect of ethanol

In the nitrogen-filled glovebox, solution of $[Ir(cod)Cl]_2$ (3.4 mg, 0.005 mmol) and ligand (9.8 mg, 0.011 mmol) in 2.0 mL anhydrous toluene was stirred at room temperature for 2 h (30 min in EtOH solvent for entries 9-11). 500 μL of the resulting solution was transferred by syringe to a Score-Break ampule charged with substrate (0.25 mmol). And then a relevant amount of ethanol solvent was added and the total volume of solvent was 3 mL. The ampule was placed into an autoclave, which was then charged with 2 MPa H2. The autoclave was stirred at room temperature for the indicated period of time. After release of H_2, the resulting mixture was concentrated under vacuum. The residue was purified by column chromatography to give the product. The enantiomeric excess was determined by HPLC analysis of the crude product.

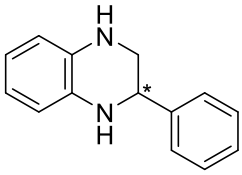
Table S4. Studies of the effect of ethanol for toluene/dioxane catalytic system.



Entry	Solvent	Conv. (%)	*ee* (%)
1	Toluene	99	97 (*R*)
2	EtOH	99	89 (*S*)
3	Toluene (0.2 eq EtOH)	99	94 (*R*)
4	Toluene (1 eq EtOH)	99	94 (*R*)
5	Toluene: EtOH=20:1	99	91 (*R*)
6	Toluene: EtOH=10:1	99	79 (*R*)
7	Toluene: EtOH=5:1	99	56 (*R*)
8	Toluene: EtOH=1:1	99	70 (*S*)
9	EtOH: Toluene=5:1	99	88 (*S*)
10	EtOH: Toluene=10:1	99	90 (*S*)
11	EtOH: Toluene=20:1	99	88 (*S*)

Reaction conditions: 0.25 mmol substrate **1aa'**, 1.0 mol % $[Ir(COD)Cl]_2$/**L6**, H_2 (2 MPa), 2.0 mL solvent, rt, and 18 h. Conversion were determined by ^1H NMR. *ee* value was determined by HPLC.

10. Characterization data of chiral Tetrahydroquinoxalines and Dihydroquinoxalinones



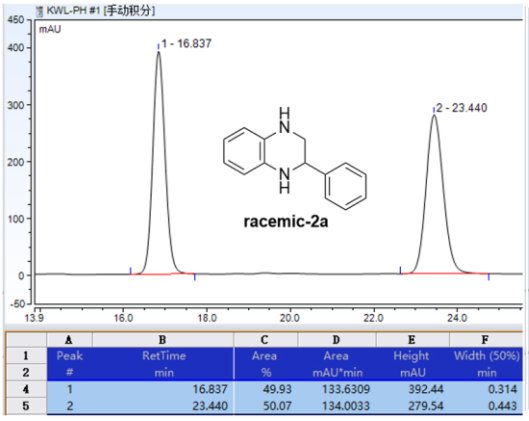
(*R*/*S*)-2-phenyl-1,2,3,4-tetrahydroquinoxaline (2a)[1]

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.48 – 7.30 (m, 5H), 6.73 – 6.66 (m, 2H), 6.66 – 6.60 (m, 2H), 4.53 (dd, *J* = 8.2, 3.1 Hz, 1H), 3.51 (dd, *J* = 11.1, 3.1 Hz, 1H), 3.37 (dd, *J* = 11.0, 8.2 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 141.92, 134.22, 132.89, 128.74, 127.99, 127.09, 119.00, 118.87, 114.81, 114.52, 54.79, 49.22.

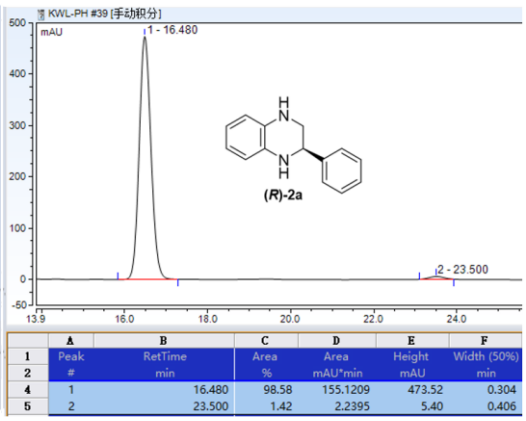
$[\alpha]_D^{25}$ = -94.733 (*c* 0.1, $CHCl_3$) for **(*R*)-2a**. $[\alpha]_D^{25}$ = 86.044 (*c* 0.1, $CHCl_3$) for **(*S*)-2a**.

HRMS (ESI) calcd for $C_{14}H_{14}N_2^+$ [$(M+H)^+$] 211.1230, found 211.1231.

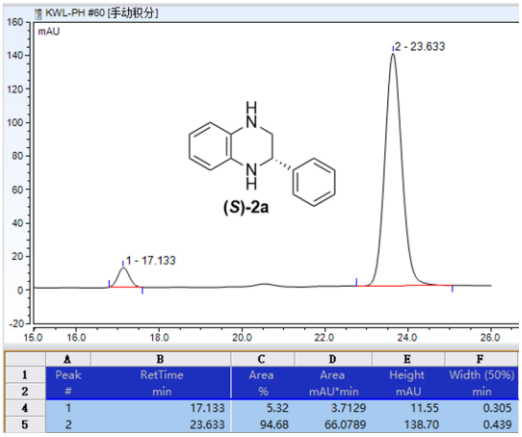
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 1 mL/min, column temp 40 °C, retention times 16.480 min (major enantiomer), 23.500 min (minor enantiomer), 97% *ee* for (*R*)-2a, retention times 17.133 min (minor enantiomer), 23.633 min (major enantiomer), 89% *ee* for (*S*)-2a.



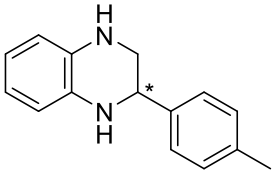
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	16.837	49.93	133.6309	392.44	0.314
5	2	23.440	50.07	134.0033	279.54	0.443



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	16.480	98.58	155.1209	473.52	0.304
5	2	23.500	1.42	2.2395	5.40	0.406



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	17.133	5.32	3.7129	11.55	0.305
5	2	23.633	94.68	66.0789	138.70	0.439



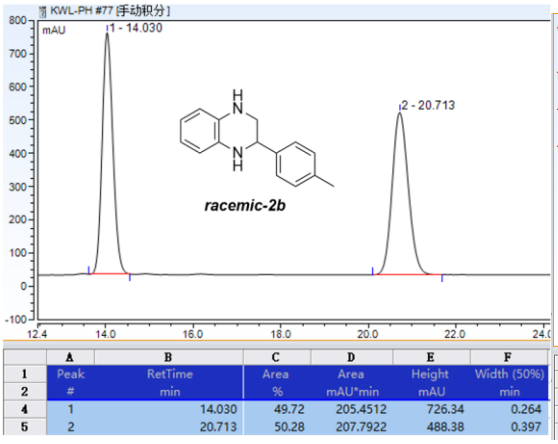
(*R*/*S*)-2-(p-tolyl)-1,2,3,4-tetrahydroquinoxaline (2b)[2]

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.31 (d, J = 8.0 Hz, 2H), 7.30 (s, 1H), 7.22 (d, J = 7.9 Hz, 2H), 6.72 – 6.57 (m, 4H), 4.49 (dd, J = 8.2, 3.1 Hz, 1H), 3.48 (dd, J = 11.0, 3.1 Hz, 1H), 3.35 (dd, J = 11.0, 8.2 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 138.88, 134.27, 132.83, 129.39, 126.95, 118.98, 118.79, 114.77, 114.46, 54.49, 49.24, 21.20.

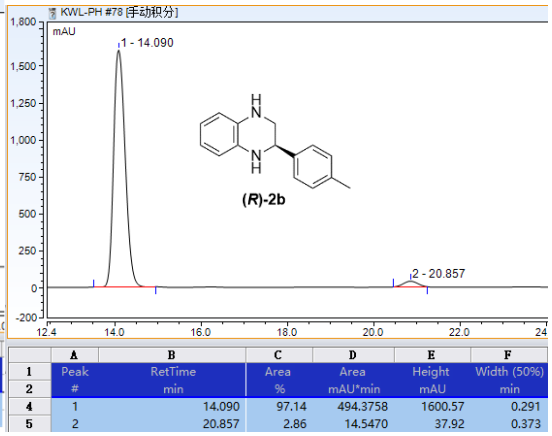
$[\alpha]_D^{25}$ = -97.074 (*c* 0.1, $CHCl_3$) for **(*R*)-2b**. $[\alpha]_D^{25}$ = 66.370 (*c* 0.1, $CHCl_3$) for **(*S*)-2b**.

HRMS (ESI) calcd for $C_{15}H_{17}N_2^+$ [$(M+H)^+$] 225.1386, found 225.1383.

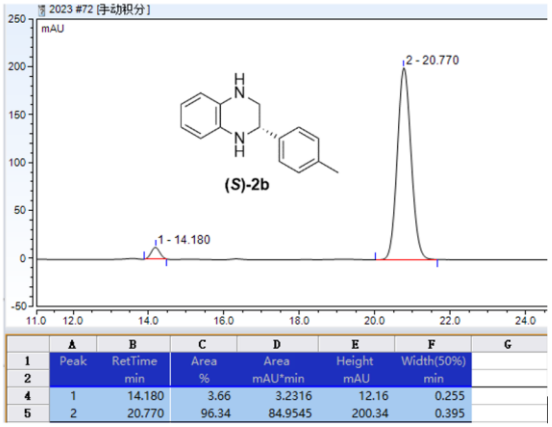
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 1 mL/min, column temp 40 °C, retention times 14.090 min (major enantiomer), 20.857 min (minor enantiomer), 94% *ee* for (*R*)-2b, retention times 14.180 min (minor enantiomer), 20.770 min (major enantiomer), 93% *ee* for (*S*)-2b.



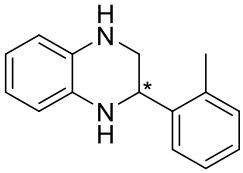
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	14.030	49.72	205.4512	726.34	0.264
5	2	20.713	50.28	207.7922	488.38	0.397



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	14.090	97.14	494.3758	1600.57	0.291
5	2	20.857	2.86	14.5470	37.92	0.373



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	14.180	3.66	3.2316	12.16	0.255	
5	2	20.770	96.34	84.9545	200.34	0.395	



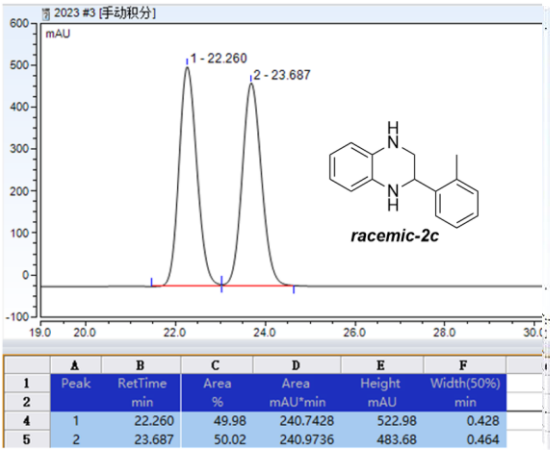
(*R*/*S*)-2-(o-tolyl)-1,2,3,4-tetrahydroquinoxaline (2c)[3]

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 7.4 Hz, 1H), 7.32 – 7.24 (m, 3H), 6.72 – 6.63 (m, 4H), 4.76 (m, 1H), 3.81 (s, 2H), 3.50 (d, *J* = 11.1 Hz, 1H), 3.32 (t, *J* = 9.7 Hz, 1H), 2.46 (s, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 139.60, 135.33, 134.53, 132.87, 130.53, 127.56, 126.72, 126.60, 118.97, 118.85, 114.78, 114.60, 50.62, 47.86, 19.31.

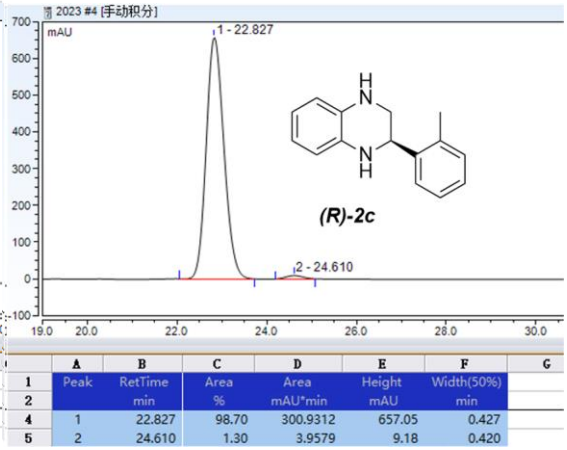
$[\alpha]_D^{25}$ = -69.149 (*c* 0.1, $CHCl_3$) for (***R*)-2c**. $[\alpha]_D^{25}$ = 68.044 (*c* 0.1, $CHCl_3$) for (***S*)-2c.**

HRMS (ESI) calcd for $C_{15}H_{16}N_2^+$ [$(M+H)^+$] 224.1313, found 224.1312.

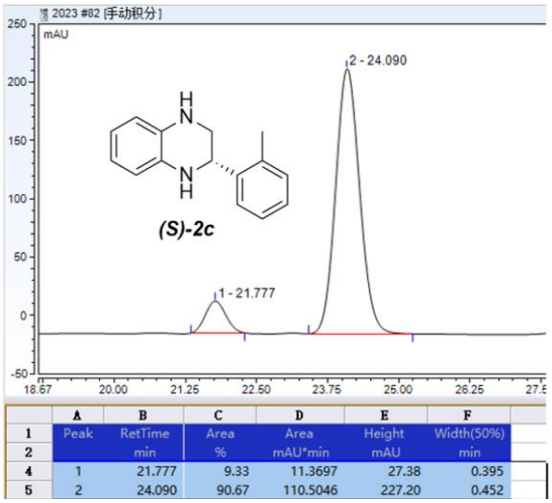
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 0.8 mL/min, column temp 40 °C, retention time 22.827 min (major enantiomer), 24.610 min (minor enantiomer), 97% *ee* for **(*R*)-2c**, retention time 21.777 min (minor enantiomer), 24.090 min (major enantiomer), 81% *ee* for **(*S*)-2c**.



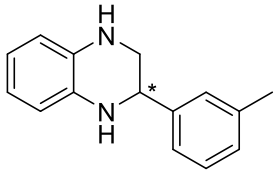
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	22.260	49.98	240.7428	522.98	0.428
5	2	23.687	50.02	240.9736	483.68	0.464



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	22.827	98.70	300.9312	657.05	0.427	
5	2	24.610	1.30	3.9579	9.18	0.420	



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	21.777	9.33	11.3697	27.38	0.395
5	2	24.090	90.67	110.5046	227.20	0.452



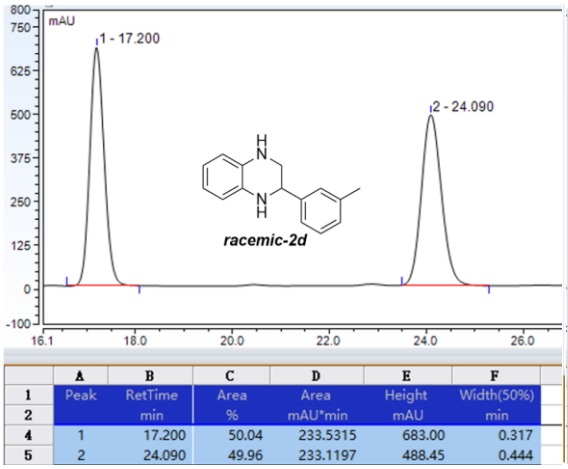
(*R*/*S*)-2-(m-tolyl)-1,2,3,4-tetrahydroquinoxaline (2d)[4]

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.29 – 7.22 (m, 1H), 7.22 – 7.16 (m, 2H), 7.13 (d, *J* = 7.5 Hz, 1H), 6.67 – 6.60 (m, 2H), 6.60 – 6.54 (m, 2H), 4.44 (dd, *J* = 8.4, 3.1 Hz, 1H), 3.84 (s, 2H), 3.44 (ddd, *J* = 11.0, 3.1, 1.1 Hz, 1H), 3.32 (ddd, *J* = 11.1, 8.3, 1.2 Hz, 1H), 2.36 (s, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 141.78, 138.43, 134.24, 132.90, 128.72, 128.62, 127.73, 124.14, 118.95, 118.83, 114.76, 114.49, 54.77, 49.27, 21.53.

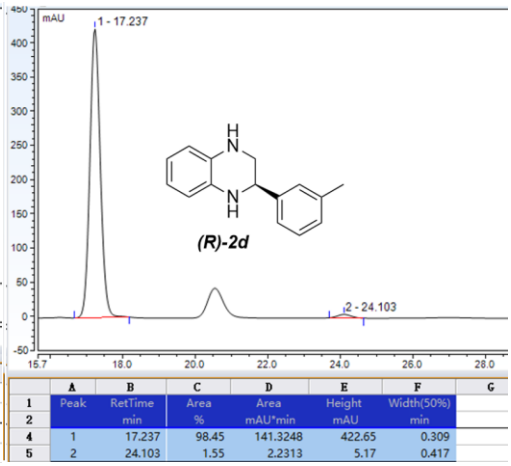
$[\alpha]_D^{25}$ = -57.041 (*c* 0.1, $CHCl_3$) for (***R*)-2d**. $[\alpha]_D^{25}$ = 66.768 (*c* 0.1, $CHCl_3$) for (***S*)-2d.**

HRMS (ESI) calcd for $C_{15}H_{16}N_2^+$ [$(M+H)^+$] 224.1313, found 224.1316.

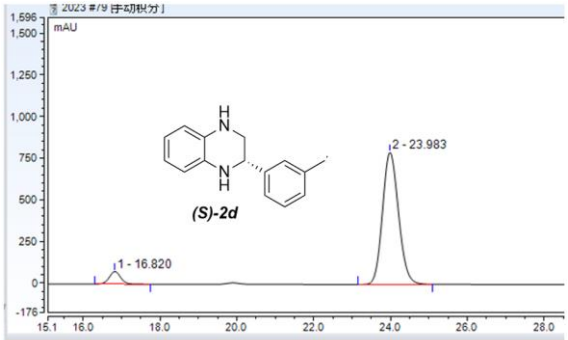
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 0.8 mL/min, column temp 40 °C, retention time 17.237 min (major enantiomer), 24.103 min (minor enantiomer), 97% *ee* for **(*R*)-2d**, retention time 16.820 min (minor enantiomer), 23.983 min (major enantiomer), 87% *ee* for **(*S*)-2d.**



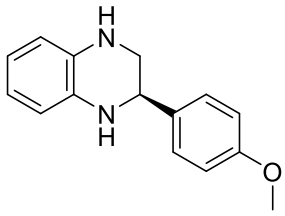
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	17.200	50.04	233.5315	683.00	0.317
5	2	24.090	49.96	233.1197	488.45	0.444



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	17.237	98.45	141.3248	422.65	0.309	
5	2	24.103	1.55	2.2313	5.17	0.417	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	16.820	6.42	26.2501	75.94	0.314	
5	2	23.983	93.58	382.7021	792.73	0.448	



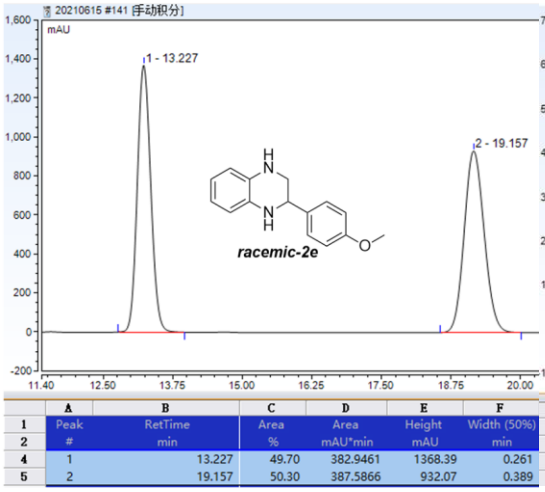
(*R*/*S*)-2-(4-methoxyphenyl)-1,2,3,4-tetrahydroquinoxaline (2e)[2]

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 (d, *J* = 8.2 Hz, 2H), 6.90 (d, *J* = 8.2 Hz, 2H), 6.63 (dd, *J* = 5.7, 3.6 Hz, 2H), 6.56 (dd, *J* = 6.2, 3.0 Hz, 2H), 4.42 (dd, *J* = 8.4, 3.1 Hz, 1H), 3.81 (s, 3H), 3.41 (dd, *J* = 11.0, 3.1 Hz, 1H), 3.29 (dd, *J* = 11.0, 8.3 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 159.36, 134.27, 133.98, 132.90, 128.18, 118.91, 118.81, 114.72, 114.47, 114.08, 55.40, 54.16, 49.34.

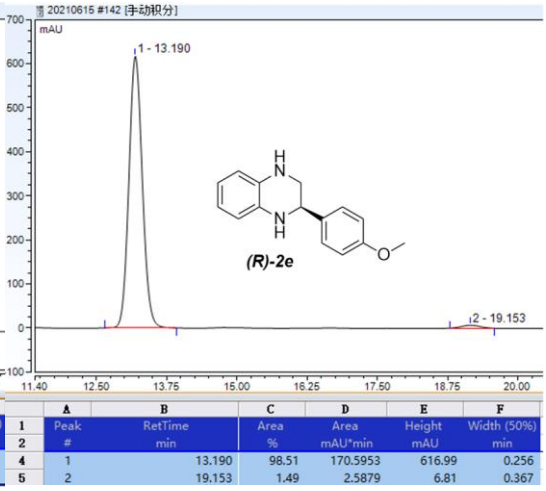
$[\alpha]_D^{25}$ = -76.372 (*c* 0.1, $CHCl_3$) for (***R***)-**2e**. $[\alpha]_D^{25}$ = 27.354 (*c* 0.1, $CHCl_3$) for (***S***)-**2e**.

HRMS (ESI) calcd for $C_{15}H_{17}N_2O^+$ [$(M+H)^+$] 241.1335 , found 241.1332.

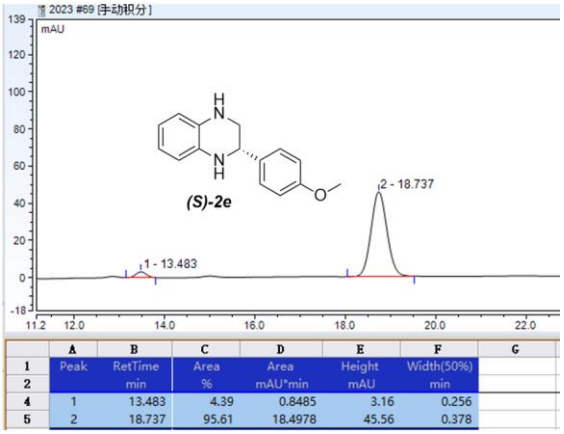
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 °C, retention times 13.190 min (major enantiomer), 19.153 min (minor enantiomer), 97% *ee* for **(*R*)-2e**, retention times 13.483 min (minor enantiomer), 18.737 min (major enantiomer), 91% *ee* for **(*S*)-2e**.



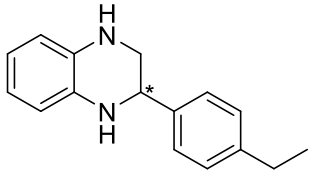
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	13.227	49.70	382.9461	1368.39	0.261
5	2	19.157	50.30	387.5866	932.07	0.389



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	13.190	98.51	170.5953	616.99	0.256
5	2	19.153	1.49	2.5879	6.81	0.367



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	13.483	4.39	0.8485	3.16	0.256	
5	2	18.737	95.61	18.4978	45.56	0.378	



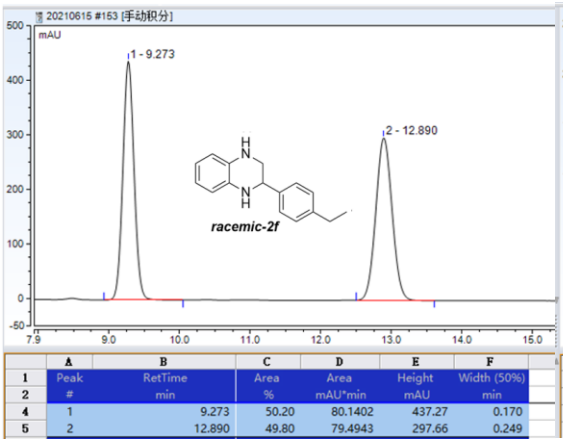
(*R/S*)-2,6,7-trimethyl-1,2,3,4-tetrahydroquinoxaline (2f)[5]

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.30 (d, *J* = 7.9 Hz, 2H), 7.20 (d, *J* = 7.8 Hz, 2H), 6.62 (m, 2H), 6.57 (m, 2H), 4.45 (dd, *J* = 8.3, 3.1 Hz, 1H), 4.05 – 3.58 (m, 2H), 3.44 (dd, *J* = 11.1, 3.1 Hz, 1H), 3.31 (dd, *J* = 11.0, 8.2 Hz, 1H), 2.65 (q, *J* = 7.6 Hz, 2H), 1.24 (t, *J* = 7.6 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 144.09, 139.14, 134.29, 132.90, 128.21, 127.05, 118.94, 118.79, 114.75, 114.46, 54.53, 49.24, 28.62, 15.70.

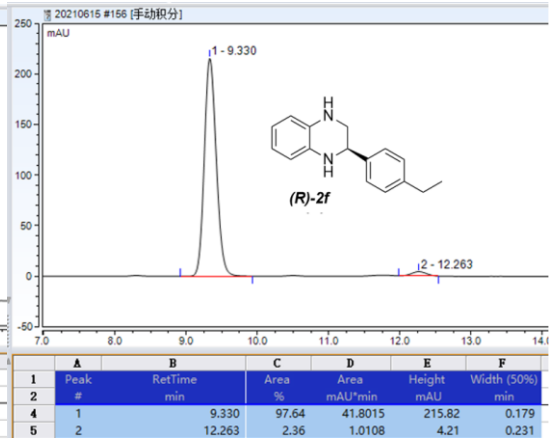
$[\alpha]_D^{25}$ = -76.725 (*c* 0.1, $CHCl_3$) for (***R*)-2f**. $[\alpha]_D^{25}$ = 62.373 (*c* 0.1, $CHCl_3$) for (***S*)-2f.**

HRMS (ESI) calcd for $C_{16}H_{19}N_2^+$ [$(M+H)^+$] 239.1543, found 239.1544.

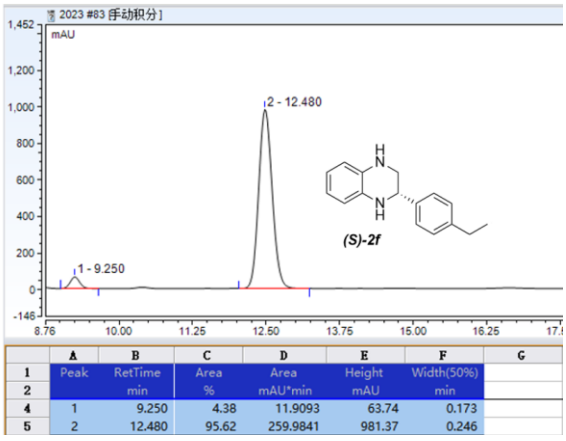
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 °C, retention times 9.330 min (major enantiomer), 12.263 min (minor enantiomer), 95% *ee* for **(*R*)-2f**, retention times 9.250 min (minor enantiomer), 12.480 min (major enantiomer), 91% *ee* for **(*S*)-2f**.



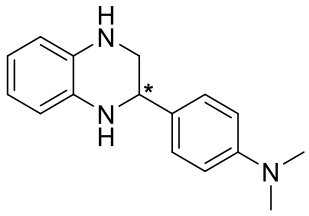
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	9.273	50.20	80.1402	437.27	0.170
5	2	12.890	49.80	79.4943	297.66	0.249



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	9.330	97.64	41.8015	215.82	0.179
5	2	12.263	2.36	1.0108	4.21	0.231



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	9.250	4.38	11.9093	63.74	0.173	
5	2	12.480	95.62	259.9841	981.37	0.246	



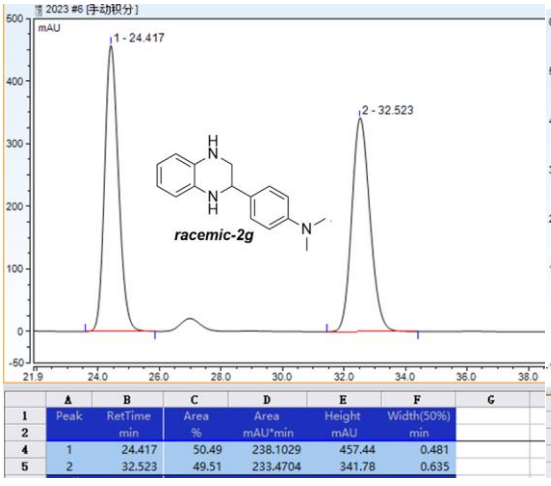
(*R*/*S*)-N,N-dimethyl-4-(1,2,3,4-tetrahydroquinoxalin-2-yl)aniline (2g)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.27 – 7.22 (m, 3H), 6.77 – 6.70 (m, 2H), 6.65 – 6.51 (m, 4H), 4.37 (dd, *J* = 8.5, 3.1 Hz, 1H), 3.40 (dd, *J* = 11.0, 3.1 Hz, 1H), 3.30 (dd, *J* = 11.0, 8.4 Hz, 1H), 2.95 (s, 6H).^{13}C NMR (101 MHz, Chloroform-d) δ 150.48, 132.93, 127.87, 118.81, 118.64, 114.64, 114.38, 54.19, 49.38, 40.74, 29.78.

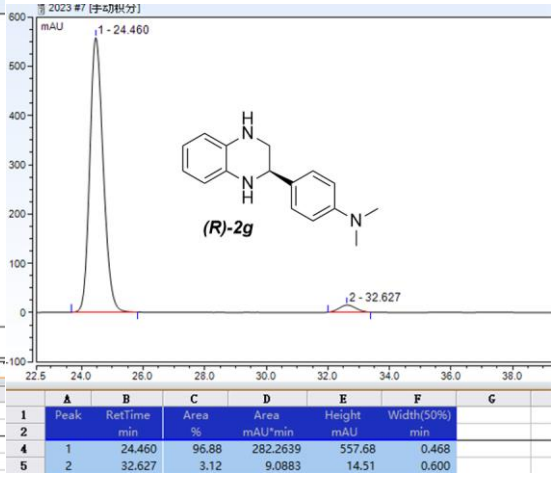
$[\alpha]_D^{25}$ = -52.359 (*c* 0.1, $CHCl_3$) for (***R***)-**2g**. $[\alpha]_D^{25}$ = 39.018 (*c* 0.1, $CHCl_3$) for (***S***)-**2g.**

HRMS (ESI) calcd for $C_{16}H_{19}N_3^+$ [$(M+H)^+$] 253.1579, found 253.1576.

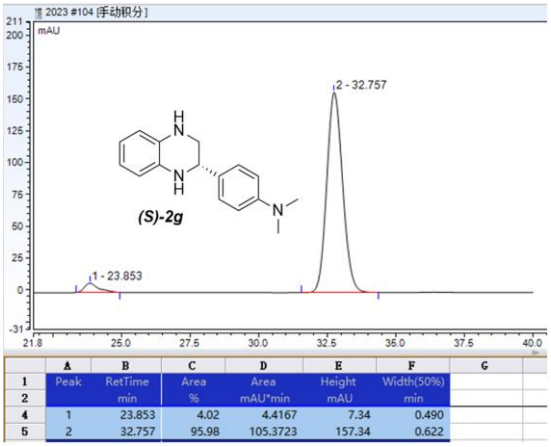
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 0.8 mL/min, column temp 40 °C, retention time 24.460 min (major enantiomer), 32.627 min (minor enantiomer), 94% *ee* for **(*R*)-2g**, retention times 23.853 min (minor enantiomer), 32.757 min (major enantiomer), 92% *ee* for **(*S*)-2g**.



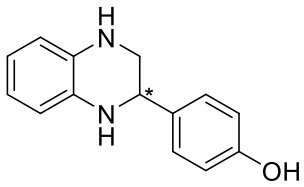
	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	24.417	50.49	238.1029	457.44	0.481	
5	2	32.523	49.51	233.4704	341.78	0.635	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	24.460	96.88	282.2639	557.68	0.468	
5	2	32.627	3.12	9.0883	14.51	0.600	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	23.853	4.02	4.4167	7.34	0.490	
5	2	32.757	95.98	105.3723	157.34	0.622	



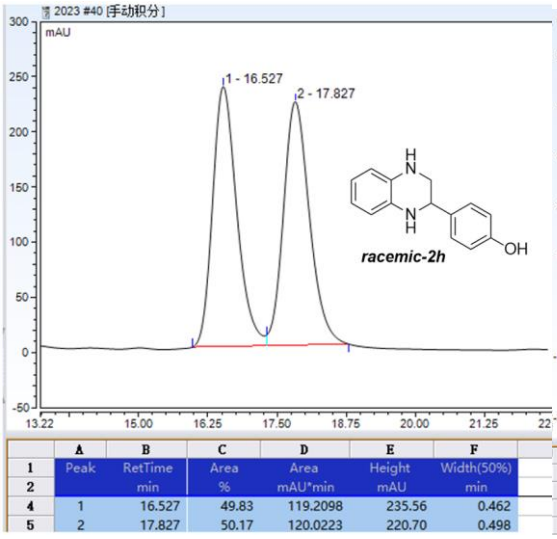
(*R*/*S*)-4-(1,2,3,4-tetrahydroquinoxalin-2-yl)phenol (2h)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.23 – 7.18 (m, 2H), 6.80 – 6.75 (m, 2H), 6.65 – 6.62 (m, 2H), 6.59 – 6.54 (m, 2H), 4.39 (dd, *J* = 8.3, 3.0 Hz, 1H), 3.39 (dd, *J* = 11.1, 3.1 Hz, 1H), 3.28 – 3.20 (m, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 150.48, 134.52, 132.93, 129.51, 127.87, 118.81, 118.64, 114.64, 114.38, 112.71, 54.19, 49.38.

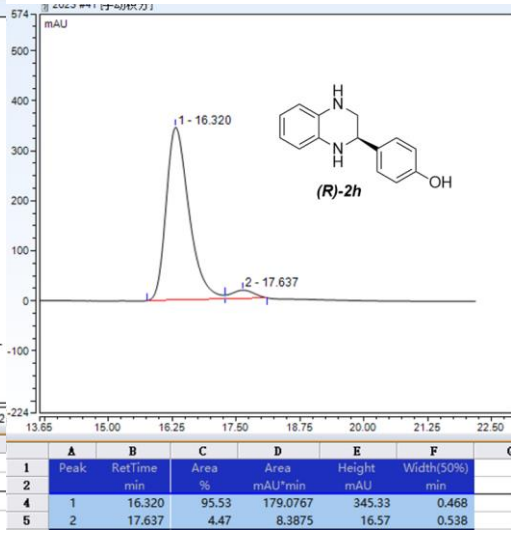
$[\alpha]_D^{25}$ = -61.045 (*c* 0.1, $CHCl_3$) for (***R***)-**2h**. $[\alpha]_D^{25}$ = 30.013 (*c* 0.1, $CHCl_3$) for (***S***)-**2h.**

HRMS (ESI) calcd for $C_{14}H_{14}N_2O^+$ [$(M+H)^+$] 226.1106, found 226.1102.

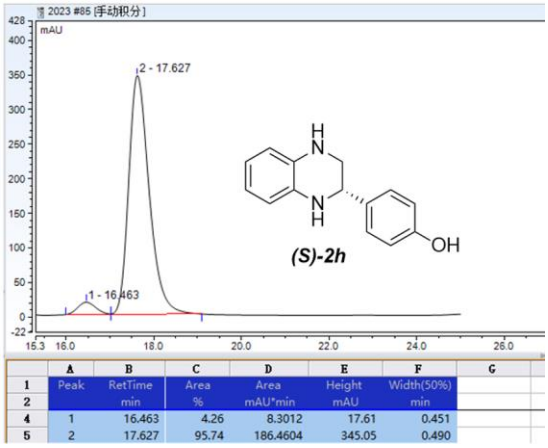
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 °C, retention time 16.320 min (major enantiomer), 17.637 min (minor enantiomer), 91% *ee* for **(*R*)-2h**, retention time 16.463 min (minor enantiomer), 17.627 min (major enantiomer), 91% *ee* for **(*S*)-2h.**



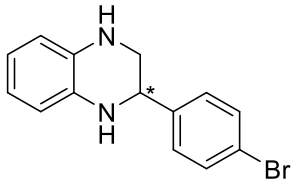
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	16.527	49.83	119.2098	235.56	0.462
5	2	17.827	50.17	120.0223	220.70	0.498



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	16.320	95.53	179.0767	345.33	0.468
5	2	17.637	4.47	8.3875	16.57	0.538



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	16.463	4.26	8.3012	17.61	0.451	
5	2	17.627	95.74	186.4604	345.05	0.490	



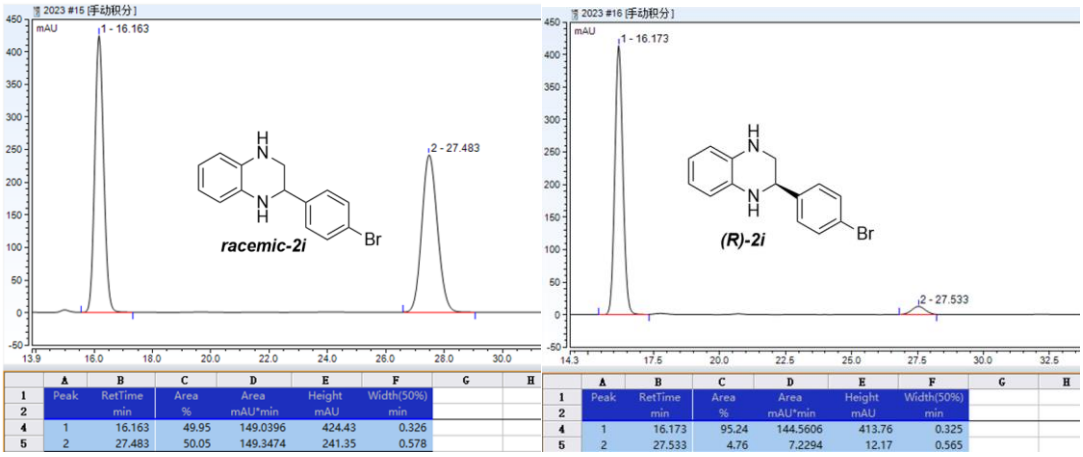
(*R*/*S*)-2-(4-bromophenyl)-1,2,3,4-tetrahydroquinoxaline (2i)[4]

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 (d, *J* = 6.0 Hz, 2H), 7.29 – 7.23 (m, 2H), 6.68 – 6.53 (m, 4H), 4.45 (dt, *J* = 8.1, 2.8 Hz, 1H), 3.87 (s, 2H), 3.43 (dt, *J* = 11.1, 2.8 Hz, 1H), 3.27 (ddd, *J* = 10.7, 7.8, 2.4 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 141.03, 133.81, 132.79, 131.82, 121.74, 119.11, 119.06, 114.84, 114.59, 54.21, 48.99.

$[\alpha]_D^{25}$ = -82.394 (*c* 0.1, $CHCl_3$) for (***R*)-2i**. $[\alpha]_D^{25}$ = 61.363 (*c* 0.1, $CHCl_3$) for (***S*)-2i.**

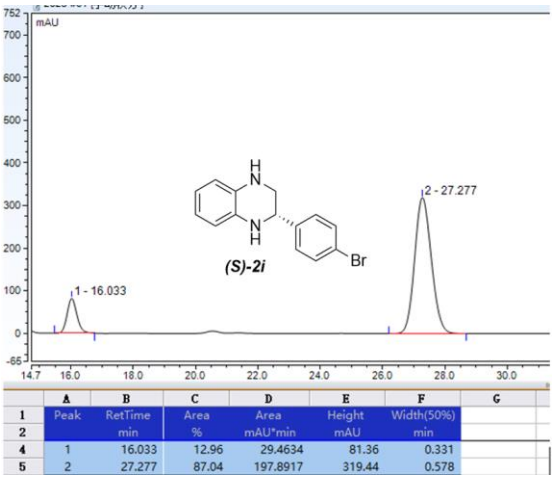
HRMS (ESI) calcd for $C_{14}H_{13}BrN_2^+$ [(M+H)$^+$] 288,0262, found 288.0265.

Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 ^{o}C, retention time 16.173 min (major enantiomer), 27.533 min (minor enantiomer), 90% *ee* for **(*R*)-2i**, retention time 16.033 min (minor enantiomer), 27.277 min (major enantiomer), 74% *ee* for **(*S*)-2i.**

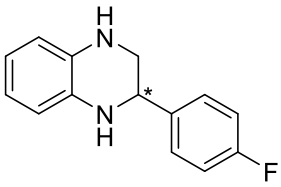


Peak	RetTime min	Area %	Area mAU*min	Height mAU	Width(50%) min
1	16.163	49.95	149.0396	424.43	0.326
2	27.483	50.05	149.3474	241.35	0.578

Peak	RetTime min	Area %	Area mAU*min	Height mAU	Width(50%) min
1	16.173	95.24	144.5606	413.76	0.325
2	27.533	4.76	7.2294	12.17	0.565



Peak	RetTime min	Area %	Area mAU*min	Height mAU	Width(50%) min
1	16.033	12.96	29.4634	81.36	0.331
2	27.277	87.04	197.8917	319.44	0.578



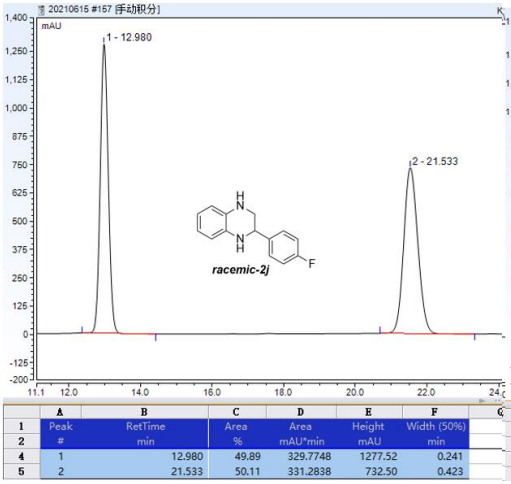
(*R*/*S*)-2-(4-fluorophenyl)-1,2,3,4-tetrahydroquinoxaline (2j)[4]

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.33 (t, J = 6.1 Hz, 2H), 7.03 (m, 2H), 6.63 (d, J = 3.2 Hz, 2H), 6.56 (d, J = 3.3 Hz, 2H), 4.45 (dt, J = 8.1, 2.6 Hz, 1H), 3.80 (s, 2H), 3.41 (dt, J = 11.2, 2.6 Hz, 1H), 3.26 (ddd, J = 10.8, 8.1, 2.1 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-d) δ 163.70, 161.25, 137.70 (d, J = 3.2 Hz), 133.99, 132.86, 119.03, 115.67, 115.46, 114.80, 114.58, 54.09, 49.25.

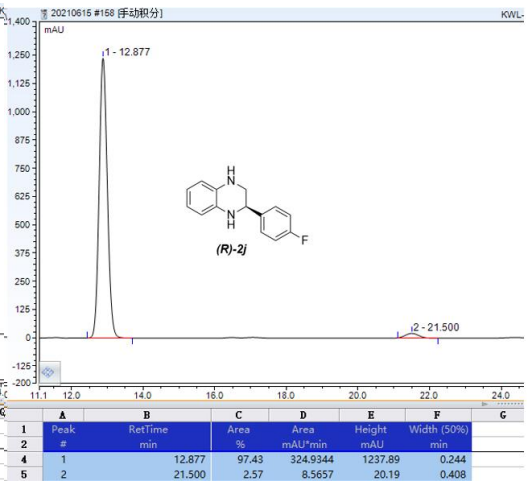
$[\alpha]_D^{25}$ = -88.047 (*c* 0.1, $CHCl_3$) for (***R*)-2j**. $[\alpha]_D^{25}$ = 79.367 (*c* 0.1, $CHCl_3$) for (***S*)-2j.**

HRMS (ESI) calcd for $C_{14}H_{14}FN_2^+$ [$(M+H)^+$] 229.1136, found 229.1134.

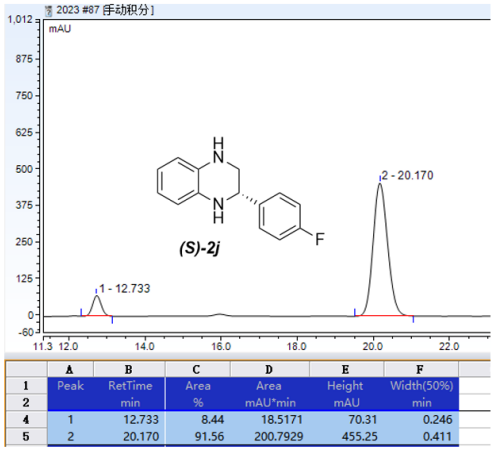
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 °C, retention times 12.877 min (major enantiomer), 21.500 min (minor enantiomer), 95% *ee* for **(*R*)-2j**, retention times 12.733 min (minor enantiomer), 20.170 min (major enantiomer), 83% *ee* for **(*S*)-2j**.



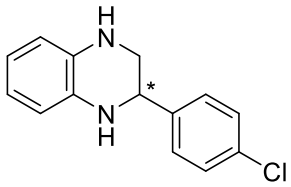
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	12.980	49.89	329.7748	1277.52	0.241
5	2	21.533	50.11	331.2838	732.50	0.423



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width (50%)	
2	#	min	%	mAU*min	mAU	min	
4	1	12.877	97.43	324.9344	1237.89	0.244	
5	2	21.500	2.57	8.5657	20.19	0.408	



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	12.733	8.44	18.5171	70.31	0.246
5	2	20.170	91.56	200.7929	455.25	0.411



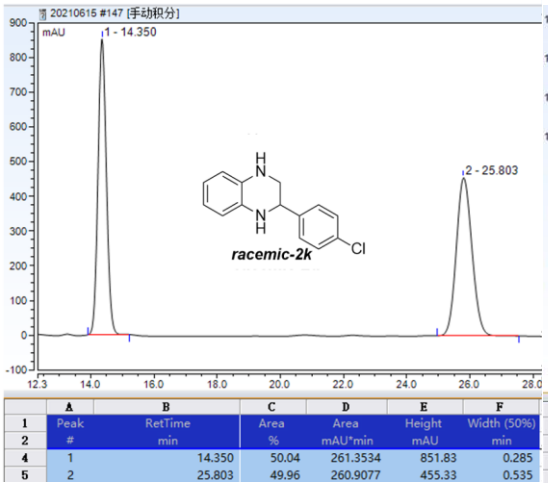
(*R*/*S*)-2-(4-chlorophenyl)-1,2,3,4-tetrahydroquinoxaline（2k）

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.27 (m, 4H), 6.64 (dd, *J* = 5.7, 3.4 Hz, 2H), 6.57 (dd, *J* = 5.8, 3.1 Hz, 2H), 4.45 (dd, *J* = 8.0, 3.1 Hz, 1H), 3.42 (dd, *J* = 11.1, 3.1 Hz, 1H), 3.26 (dd, *J* = 11.1, 8.0 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 140.50, 133.85, 133.62, 132.80, 128.86, 128.42, 119.09, 119.04, 114.84, 114.59, 54.14, 49.05.

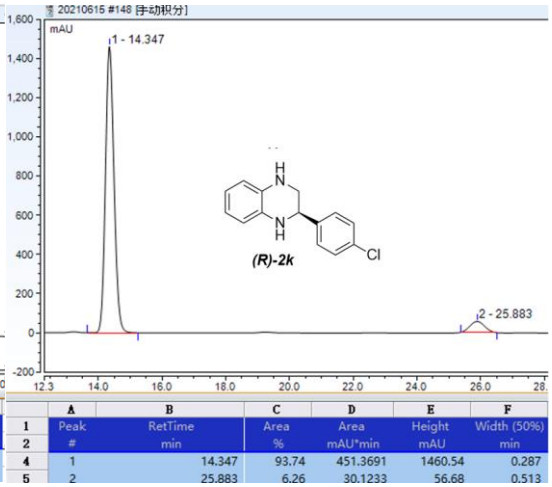
$[\alpha]_D^{25}$ = -77.044 (*c* 0.1, $CHCl_3$) for (***R***)-**2k**. $[\alpha]_D^{25}$ = 58.696 (*c* 0.1, $CHCl_3$) for (***S***)-**2k**.

HRMS (ESI) calcd for $C_{14}H_{13}ClN_2^+$ [$(M+H)^+$] 244.0767, found 244.0769.

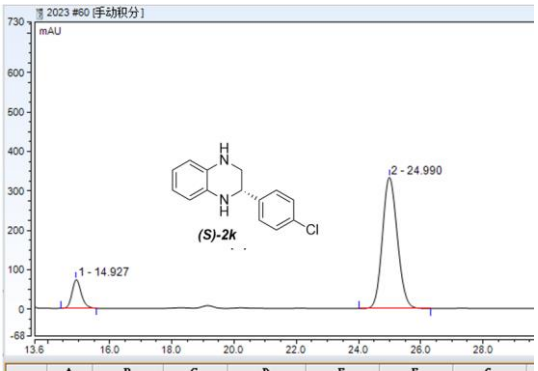
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 °C, retention times 14.347 min (major enantiomer), 25.883 min (minor enantiomer), 87% *ee* for **(*R*)-2k**, retention times 14.927 min (minor enantiomer), 24.990 min (major enantiomer), 76% *ee* for **(*S*)-2k**.



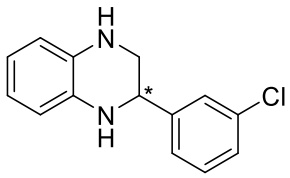
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	14.350	50.04	261.3534	851.83	0.285
5	2	25.803	49.96	260.9077	455.33	0.535



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	14.347	93.74	451.3691	1460.54	0.287
5	2	25.883	6.26	30.1233	56.68	0.513



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	14.927	11.87	24.9657	72.89	0.309	
5	2	24.990	88.13	185.4057	333.12	0.519	



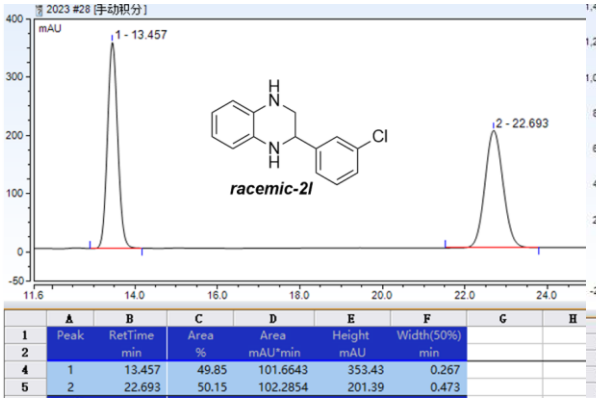
(*R*/*S*)-2-(3-chlorophenyl)-1,2,3,4-tetrahydroquinoxaline (2l)

White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.22 (m, 3H), 6.68 – 6.60 (m, 2H), 6.61 – 6.52 (m, 2H), 4.44 (dd, *J* = 8.0, 3.1 Hz, 1H), 3.86 (s, 1H), 3.43 (dd, *J* = 11.1, 3.1 Hz, 1H), 3.27 (dd, *J* = 11.1, 8.0 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 144.11, 134.62, 133.79, 132.80, 129.99, 128.10, 127.24, 125.30, 119.14, 119.09, 114.88, 114.65, 54.34, 49.00.

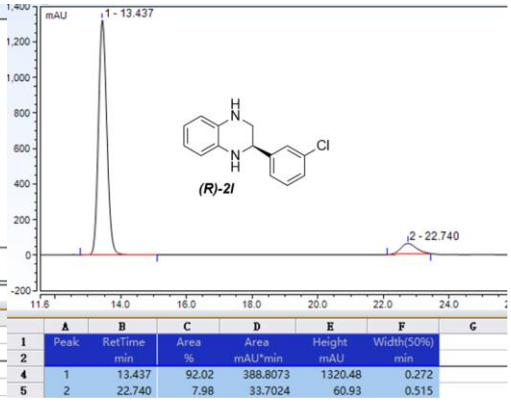
$[\alpha]_D^{25}$ = -81.135 (*c* 0.1, $CHCl_3$) for (***R***)-**2l**. $[\alpha]_D^{25}$ = 86.704 (*c* 0.1, $CHCl_3$) for (***S***)-**2l.**

HRMS (ESI) calcd for $C_{14}H_{13}ClN_2^+$ [$(M+H)^+$] 244.0767, found 244.0768.

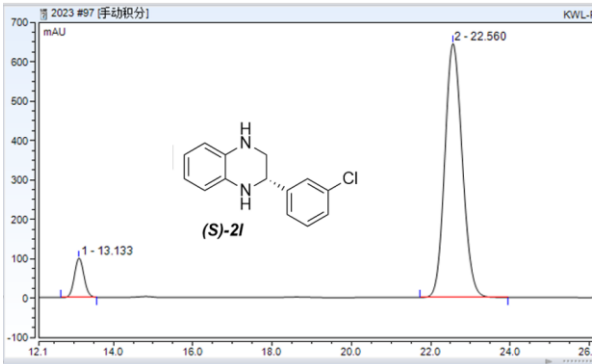
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 ^{o}C, retention times 13.437 min (major enantiomer), 22.740 min (minor enantiomer), 84% *ee* for **(*R*)-2l**, retention times 13.133 min (minor enantiomer), 22.560 min (major enantiomer), 84% *ee* for **(*S*)-2l**.



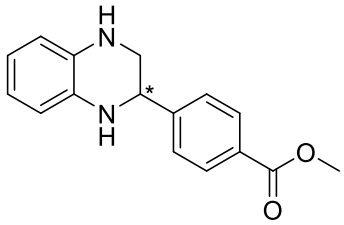
	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	13.457	49.85	101.6643	353.43	0.267		
5	2	22.693	50.15	102.2854	201.39	0.473		



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	13.437	92.02	388.8073	1320.48	0.272	
5	2	22.740	7.98	33.7024	60.93	0.515	



	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	13.133	7.79	27.7880	99.82	0.259		
5	2	22.560	92.21	328.7559	644.62	0.475		



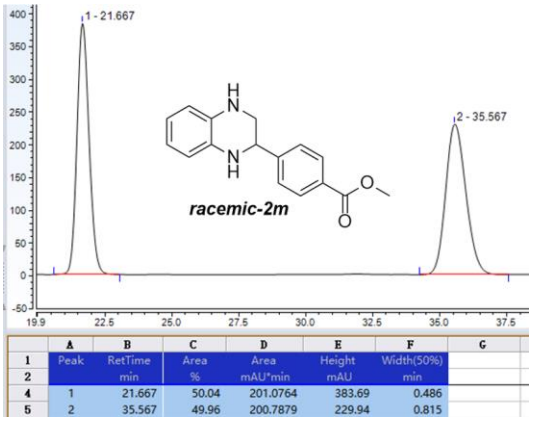
methyl (*R/S*)-4-(1,2,3,4-tetrahydroquinoxalin-2-yl)benzoate (2m)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.10 – 8.03 (m, 2H), 7.49 (d, *J* = 8.2 Hz, 2H), 6.75 – 6.57 (m, 4H), 4.57 (dd, *J* = 7.8, 3.1 Hz, 1H), 3.95 (s, 3H), 3.50 (dd, J = 11.1, 3.1 Hz, 1H), 3.33 (dd, *J* = 11.1, 7.8 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 166.97, 147.20, 133.78, 132.81, 130.01, 129.73, 127.05, 119.15, 119.06, 114.91, 114.63, 54.58, 52.24, 48.85

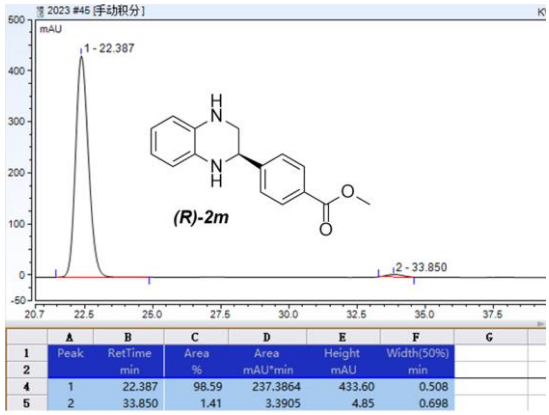
$[\alpha]_D^{25}$ = -82.359 (*c* 0.1, $CHCl_3$) for (***R***)-**2m**. $[\alpha]_D^{25}$ = 55.700 (*c* 0.1, $CHCl_3$) for (***S***)-**2m.**

HRMS (ESI) calcd for $C_{16}H_{17}N_2O_2^+$ [$(M+H)^+$] 269.1285, found 269.1287.

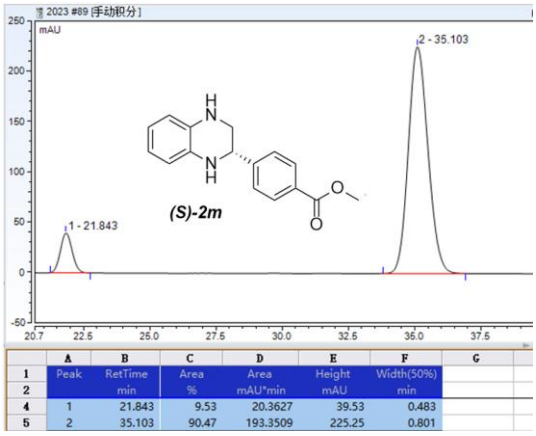
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 ºC, retention time 22.387 min (major enantiomer), 33.850 min (minor enantiomer), 97% *ee* for **(*R*)-2m**, retention time 21.843 min (minor enantiomer), 35.103 min (major enantiomer), 81% *ee* for **(*S*)-2m.**



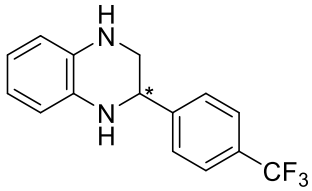
	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	21.667	50.04	201.0764	383.69	0.486	
5	2	35.567	49.96	200.7879	229.94	0.815	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	22.387	98.59	237.3864	433.60	0.508	
5	2	33.850	1.41	3.3905	4.85	0.698	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	21.843	9.53	20.3627	39.53	0.483	
5	2	35.103	90.47	193.3509	225.25	0.801	



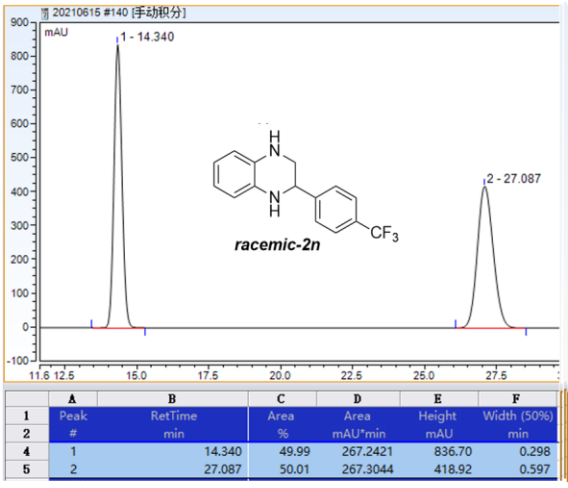
(*R*/*S*)-2-(4-(trifluoromethyl)phenyl)-1,2,3,4-tetrahydroquinoxaline (2n)[1]

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.66 (d, J = 8.0 Hz, 2H), 7.55 (d, J = 7.9 Hz, 2H), 6.78 – 6.66 (m, 2H), 6.69 – 6.56 (m, 2H), 4.61 (dd, J = 7.8, 3.1 Hz, 1H), 3.97 (s, 1H), 3.88 (s, 1H), 3.52 (dd, J = 11.1, 3.1 Hz, 1H), 3.40 – 3.30 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.12, 133.64, 132.78, 129.98, 127.41, 125.67, 119.22, 119.16, 114.93, 114.65, 54.43, 48.83.

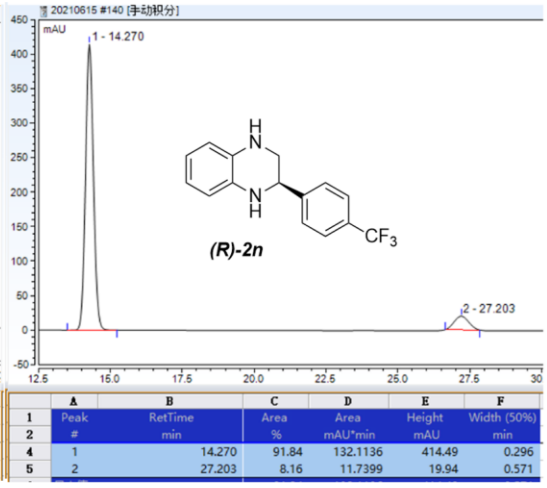
$[\alpha]_D^{25}$ = -48.696 (*c* 0.1, $CHCl_3$) for (***R***)-**2n**. $[\alpha]_D^{25}$ = 75.700 (*c* 0.1, $CHCl_3$) for (***S***)-**2n**.

HRMS (ESI) calcd for $C_{15}H_{13}F_3N_2^+$ [$(M+H)^+$] 278.1031, found 278.1034.

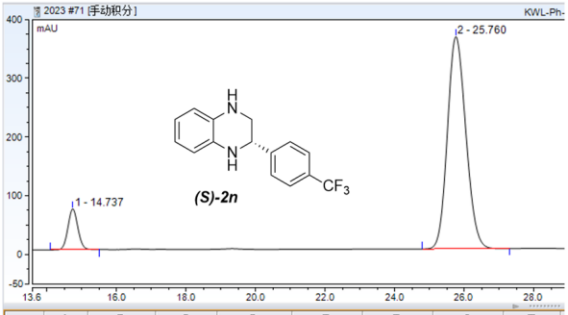
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 °C, retention times 14.270 min (major enantiomer), 27.203 min (minor enantiomer), 84% *ee* for **(*R*)-2n**, retention times 14.737 min (minor enantiomer), 25.760 min (major enantiomer), 81% *ee* for **(*S*)-2n**.



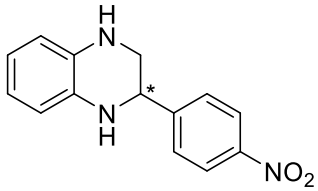
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	14.340	49.99	267.2421	836.70	0.298
5	2	27.087	50.01	267.3044	418.92	0.597



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	14.270	91.84	132.1136	414.49	0.296
5	2	27.203	8.16	11.7399	19.94	0.571



	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	14.737	9.36	22.9168	69.48	0.306		
5	2	25.760	90.64	221.8309	361.25	0.574		



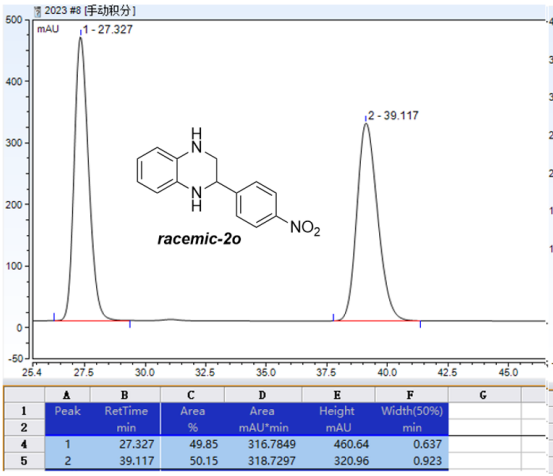
(*R*/*S*)-2-(4-nitrophenyl)-1,2,3,4-tetrahydroquinoxaline (2o)

Dark red solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.19 (dd, *J* = 8.7, 1.4 Hz, 2H), 7.58 – 7.50 (m, 2H), 6.72 – 6.54 (m, 4H), 4.62 (dd, *J* = 7.3, 3.1 Hz, 1H), 3.99 (s, 1H), 3.49 (dd, *J* = 11.1, 2.0 Hz, 1H), 3.29 (dd, *J* = 11.1, 7.2 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 149.71, 147.56, 133.26, 132.72, 127.89, 123.92, 119.39, 119.30, 115.04, 114.73, 54.32, 48.49.

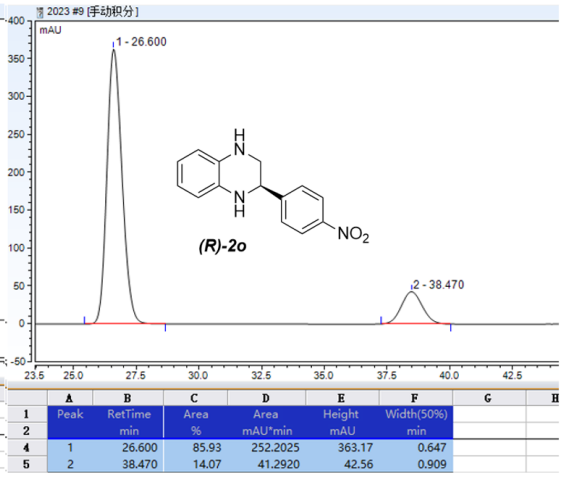
$[\alpha]_D^{25}$ = -22.009 (*c* 0.1, $CHCl_3$) for (***R***)-**2o**. $[\alpha]_D^{25}$ = 32.031 (*c* 0.1, $CHCl_3$) for (***S***)-**2o.**

HRMS (ESI) calcd for $C_{14}H_{13}N_3O_2^+$ [$(M+H)^+$] 255.1008, found 255.1003.

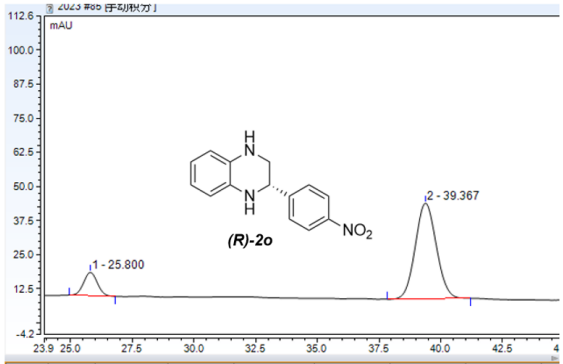
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 70:30, flow rate 1 mL/min, column temp 40 °C, retention time 26.600 min (major enantiomer), 28.470 min (minor enantiomer), 72% *ee* for **(*R*)-2o**, retention times 25.800 min (minor enantiomer), 39.367 min (major enantiomer), 73% *ee* for **(*S*)-2o**.



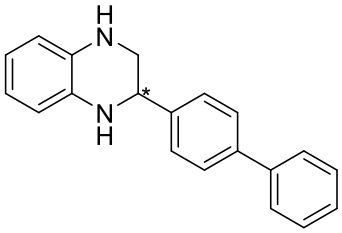
	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	27.327	49.85	316.7849	460.64	0.637	
5	2	39.117	50.15	318.7297	320.96	0.923	



	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	26.600	85.93	252.2025	363.17	0.647		
5	2	38.470	14.07	41.2920	42.56	0.909		



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	25.800	13.72	5.5068	8.56	0.604	
5	2	39.367	86.28	34.6164	35.04	0.924	



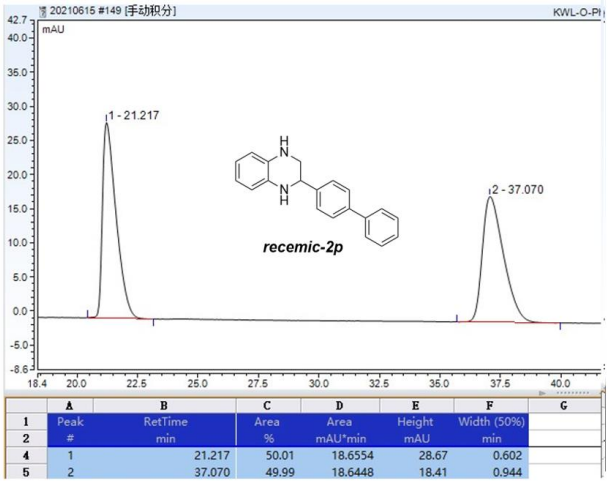
(*R*/*S*)-2-([1,1'-biphenyl]-4-yl)-1,2,3,4-tetrahydroquinoxaline（2p）

White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.29 (m, 9H), 6.66 – 6.61 (m, 2H), 6.58 (d, *J* = 5.9 Hz, 2H), 4.51 (d, *J* = 7.8 Hz, 1H), 3.88 (s, 2H), 3.51 – 3.44 (m, 1H), 3.35 (t, *J* = 9.5 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 141.01, 140.94, 140.84, 134.17, 132.92, 128.92, 127.53, 127.47, 127.20, 119.06, 118.92, 114.85, 114.57, 54.51, 49.16.

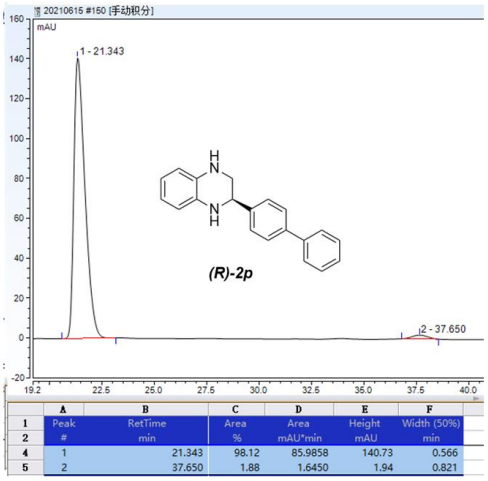
$[\alpha]_D^{25}$ = -71.373 (*c* 0.1, $CHCl_3$) for (***R***)-**2p**. $[\alpha]_D^{25}$ = 57.028 (*c* 0.1, $CHCl_3$) for (***S***)-**2p**

HRMS (ESI) calcd for $C_{20}H_{19}N_2^+$ [$(M+H)^+$] 287.1543 , found 287.1544.

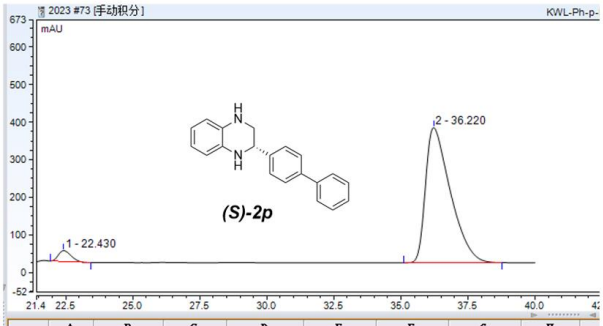
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 °C, retention times 21.343 min (major enantiomer), 37.650 min (minor enantiomer), 96% *ee* for **(*R*)-2p**, retention times 22.430 min (minor enantiomer), 36.220 min (major enantiomer), 92% *ee* for **(*S*)-2p**.



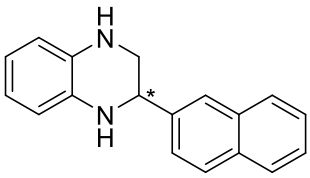
	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width (50%)	
2	#	min	%	mAU*min	mAU	min	
4	1		21.217	50.01	18.6554	28.67	0.602
5	2		37.070	49.99	18.6448	18.41	0.944



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	21.343	98.12	85.9858	140.73	0.566
5	2	37.650	1.88	1.6450	1.94	0.821



	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	22.430	3.97	15.9499	29.07	0.525		
5	2	36.220	96.03	386.0443	359.67	0.989		



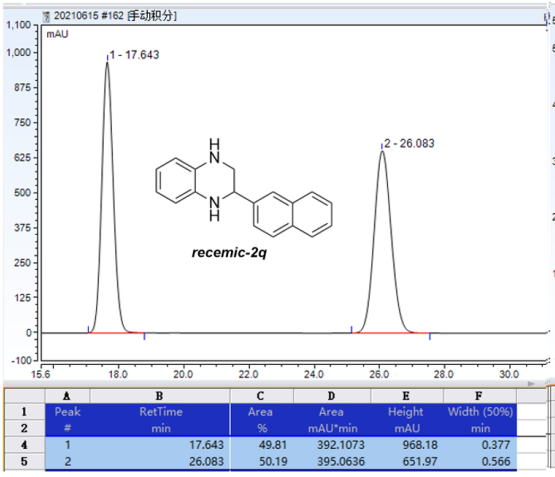
(*R*/*S*)-2-(naphthalen-2-yl)-1,2,3,4-tetrahydroquinoxaline (2q)

Gray solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 – 7.81 (m, 4H), 7.52 – 7.44 (m, 3H), 6.70 – 6.55 (m, 4H), 4.63 (dd, *J* = 8.2, 3.2 Hz, 1H), 3.98 (s, 1H), 3.50 (dd, *J* = 11.1, 3.2 Hz, 1H), 3.39 (dd, *J* = 11.1, 8.2 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 139.28, 134.21, 133.45, 133.23, 132.95, 128.50, 128.01, 127.78, 126.33, 126.07, 125.83, 125.17, 119.07, 118.95, 114.86, 114.59, 54.90, 49.22.

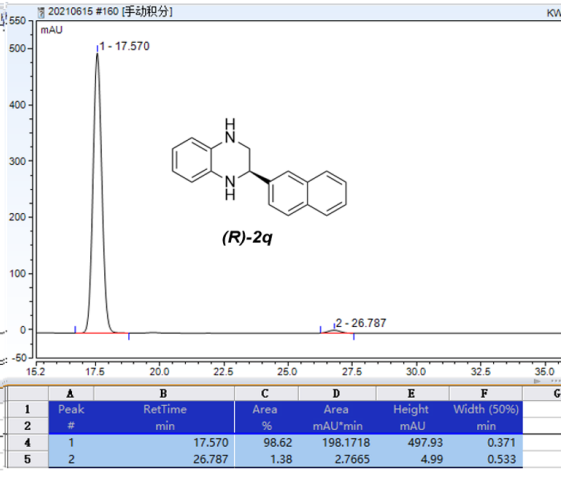
$[\alpha]_D^{25}$ = -79.049 (*c* 0.1, $CHCl_3$) for (***R***)-**2q**. $[\alpha]_D^{25}$ = 55.038 (*c* 0.1, $CHCl_3$) for (***S***)-**2q.**

HRMS (ESI) calcd for $C_{18}H_{16}N_2^+$ [$(M+H)^+$] 260.1313, found 260.1310.

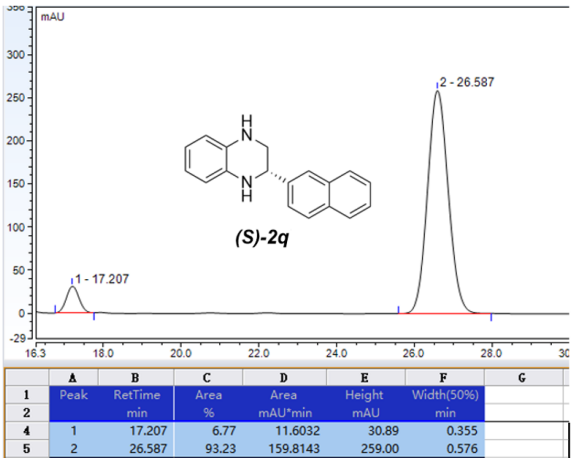
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 °C, retention times 17.570 min (major enantiomer), 26.787 min (minor enantiomer), 97% *ee* for **(*R*)-2q**, retention times 17.207 min (minor enantiomer), 26.587 min (major enantiomer), 87% *ee* for **(*S*)-2q**.



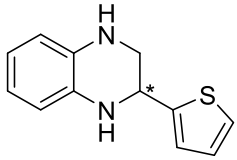
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	17.643	49.81	392.1073	968.18	0.377
5	2	26.083	50.19	395.0636	651.97	0.566



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width (50%)	
2	#	min	%	mAU*min	mAU	min	
4	1	17.570	98.62	198.1718	497.93	0.371	
5	2	26.787	1.38	2.7665	4.99	0.533	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	17.207	6.77	11.6032	30.89	0.355	
5	2	26.587	93.23	159.8143	259.00	0.576	



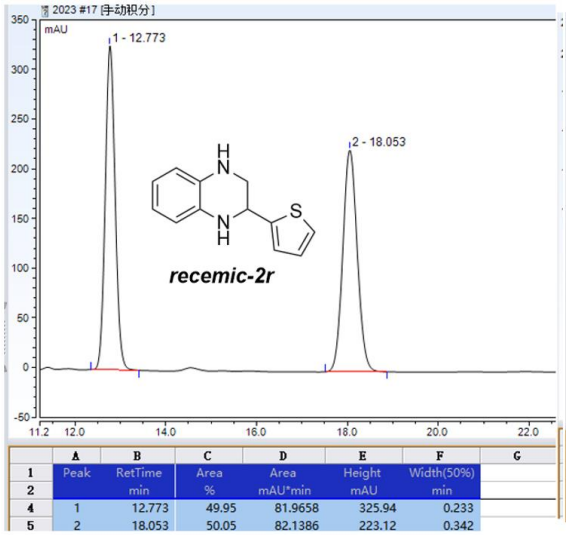
(*R*/*S*)-2-(thiophen-2-yl)-1,2,3,4-tetrahydroquinoxaline (2r)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.25 (dd, *J* = 5.4, 1.5 Hz, 1H), 7.04 (t, *J* = 2.2 Hz, 1H), 6.98 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.69 – 6.59 (m, 2H), 6.59 – 6.51 (m, 2H), 4.82 (dd, *J* = 7.6, 3.1 Hz, 1H), 3.54 (dd, *J* = 11.0, 3.1 Hz, 1H), 3.41 (dd, *J* = 11.0, 7.6 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 145.67, 133.24, 132.90, 126.68, 125.02, 124.24, 119.36, 119.10, 114.89, 114.87, 50.67, 49.49.

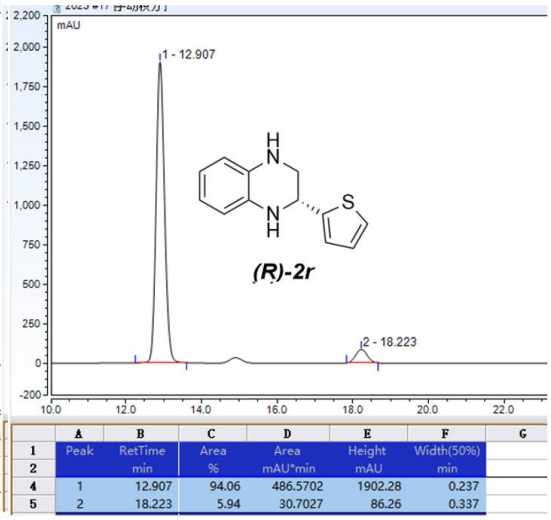
$[\alpha]_D^{25}$ = -79.062 (*c* 0.1, $CHCl_3$) for (***R*)-2r**. $[\alpha]_D^{25}$ = 17.305 (*c* 0.1, $CHCl_3$) for (***S*)-2r.**

HRMS (ESI) calcd for $C_{12}H_{12}N_2S^+$ [$(M+H)^+$] 216.0721, found 216.0724.

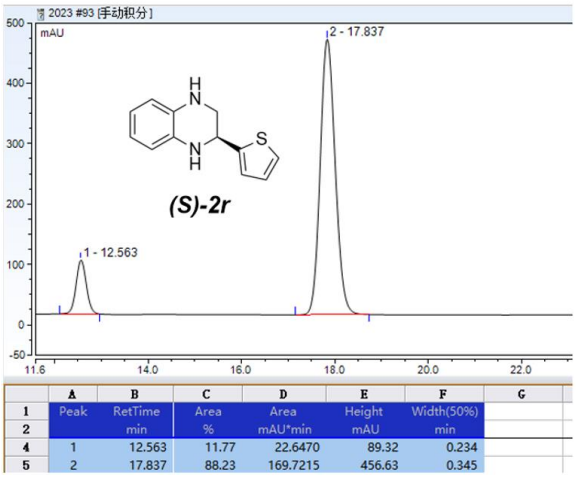
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 ^{o}C, retention time 12.907 min (major enantiomer), 18.223 min (minor enantiomer), 88% *ee* for **(*R*)-2r**, retention time 12.563 min (minor enantiomer), 17.837 min (major enantiomer), 77% *ee* for **(*S*)-2r**.



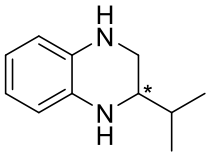
	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	12.773	49.95	81.9658	325.94	0.233	
5	2	18.053	50.05	82.1386	223.12	0.342	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	12.907	94.06	486.5702	1902.28	0.237	
5	2	18.223	5.94	30.7027	86.26	0.337	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	12.563	11.77	22.6470	89.32	0.234	
5	2	17.837	88.23	169.7215	456.63	0.345	



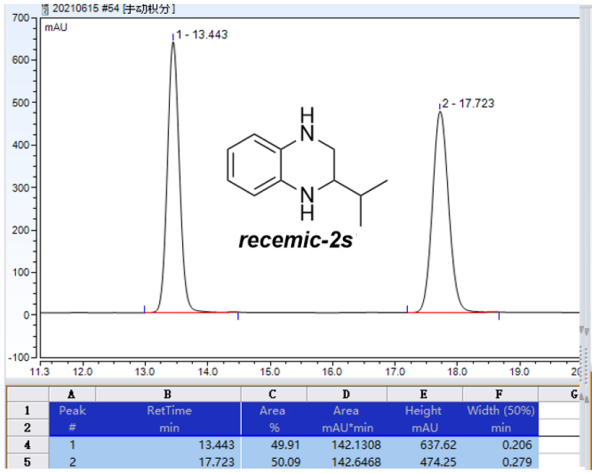
(*R*/*S*)-2-isopropyl-1,2,3,4-tetrahydroquinoxaline (2s)

Yellow oil. ^{1}H NMR (400 MHz, Chloroform-d) δ 6.59 (m, 4H), 3.41 (dd, *J* = 10.2, 2.4 Hz, 1H), 3.24 – 3.12 (m, 2H), 1.77 (m, 1H), 1.05 (dd, *J* = 18.9, 6.8 Hz, 6H).^{13}C NMR (101 MHz, Chloroform-d) δ 133.65, 133.21, 118.58, 118.17, 114.13, 114.10, 55.80, 43.85, 18.50, 18.36.

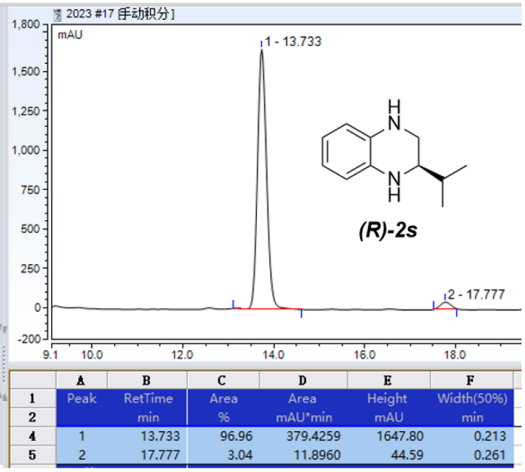
$[\alpha]_D^{25}$ = 26.683 (*c* 0.1, $CHCl_3$) for (***R*)-2s**. **$[\alpha]_D^{25}$** = 19.902 (*c* 0.1, $CHCl_3$) for (***S*)-2s.**

HRMS (ESI) calcd for $C_{11}H_{17}N_2^+$ [$(M+H)^+$] 177.1386, found 177.1382.

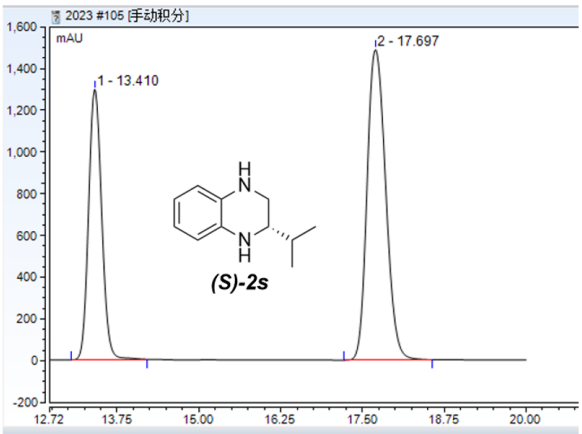
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 0.5 mL/min, column temp 40 ºC, retention time 13.733 min (major enantiomer), 17.777 min (minor enantiomer), 94% *ee* for **(*R*)-2s**, retention time 13.410 min (minor enantiomer), 17.697 min (major enantiomer), 24% *ee* for **(*S*)-2s.**



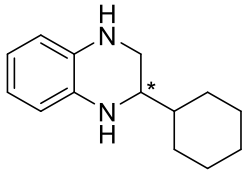
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	13.443	49.91	142.1308	637.62	0.206
5	2	17.723	50.09	142.6468	474.25	0.279



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	13.733	96.96	379.4259	1647.80	0.213
5	2	17.777	3.04	11.8960	44.59	0.261



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	13.410	38.09	300.6145	1295.41	0.215
5	2	17.697	61.91	488.5324	1487.72	0.309



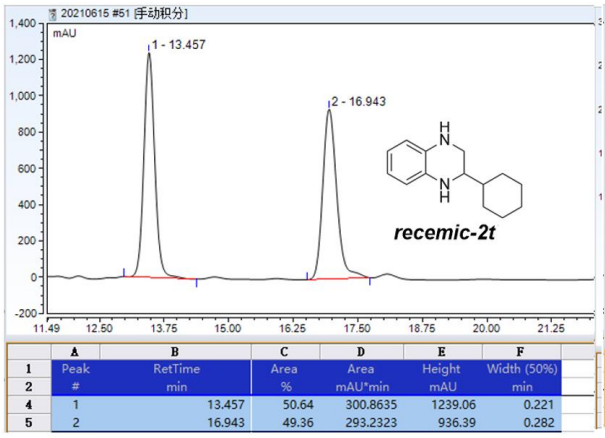
(*R*/*S*)-2-cyclohexyl-1,2,3,4-tetrahydroquinoxaline (2t)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 6.82 – 6.37 (m, 4H), 3.41 (d, *J* = 10.4 Hz, 1H), 3.18 (dt, *J* = 24.0, 8.0 Hz, 2H), 1.83 (m, 5H), 1.47 – 1.08 (m, 6H).^{13}CNMR (126 MHz, Chloroform-d) δ 133.89, 133.53, 118.81, 118.39, 114.38, 55.24, 44.03, 40.79, 29.21, 29.00, 26.49, 26.22, 26.17.

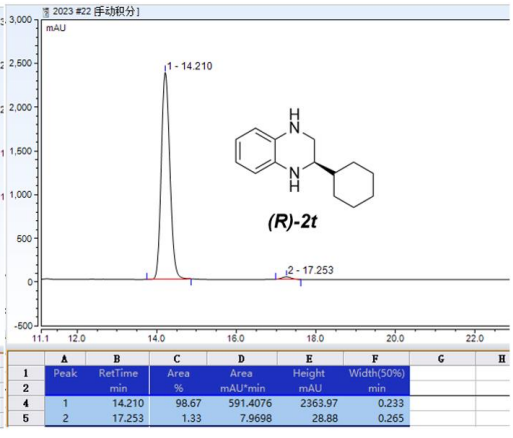
$[\alpha]_D^{25}$ = 36.697 (*c* 0.1, $CHCl_3$) for (***R***)-**2t**. $[\alpha]_D^{25}$ = -20.004 (*c* 0.1, $CHCl_3$) for (***S***)-**2t.**

HRMS (ESI) calcd for $C_{14}H_{20}N_2^+$ [$(M+H)^+$] 216.1626, found 216.1623.

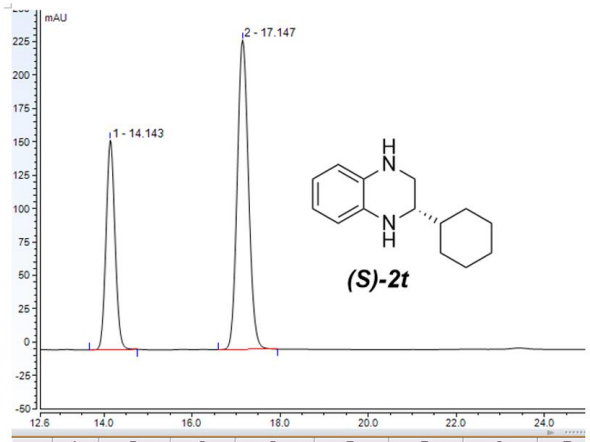
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 0.5 mL/min, column temp 40 °C, retention time 14.210 min (major enantiomer), 17.253 min (minor enantiomer), 97% *ee* for **(*R*)-2t**, retention time 14.143 min (minor enantiomer), 17.147 min (major enantiomer), 30% *ee* for **(*S*)-2t.**



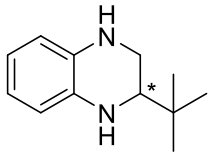
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	13.457	50.64	300.8635	1239.06	0.221
5	2	16.943	49.36	293.2323	936.39	0.282



	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	14.210	98.67	591.4076	2363.97	0.233		
5	2	17.253	1.33	7.9698	28.88	0.265		



	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	14.143	34.98	36.9499	156.89	0.218		
5	2	17.147	65.02	68.6730	231.95	0.274		



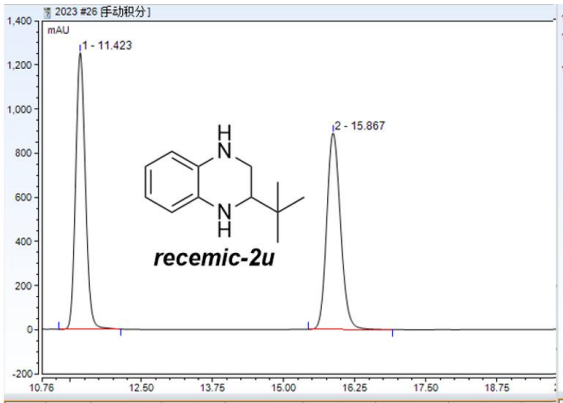
(*R/S*)-2-(tert-butyl)-1,2,3,4-tetrahydroquinoxaline (2u)

Yellow liquid. ^{1}H NMR (400 MHz, Chloroform-d) δ 6.64 – 6.47 (m, 4H), 3.40 – 3.30 (m, 1H), 3.19 – 3.09 (m, 2H), 0.98 (s, 9H).^{13}C NMR (101 MHz, Chloroform-d) δ 134.65, 133.39, 118.96, 118.31, 114.42, 114.33, 59.09, 42.59, 32.84, 26.10.

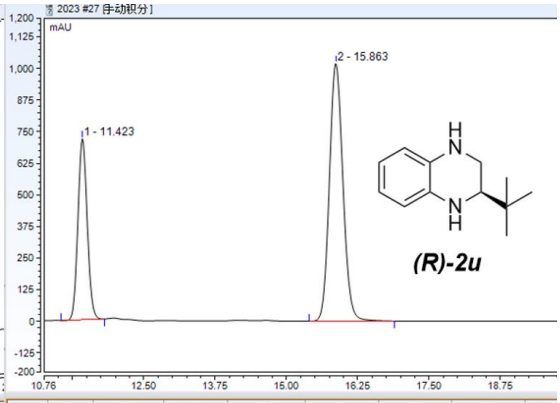
$[\alpha]_D^{25}$ = 12.009 (*c* 0.1, $CHCl_3$) for (***R***)-**2u**. $[\alpha]_D^{25}$ = -13.675 (*c* 0.1, $CHCl_3$) for (***S***)-**2u.**

HRMS (ESI) calcd for $C_{12}H_{19}N_2^+$ [$(M+H)^+$] 191.1543, found 191.1548.

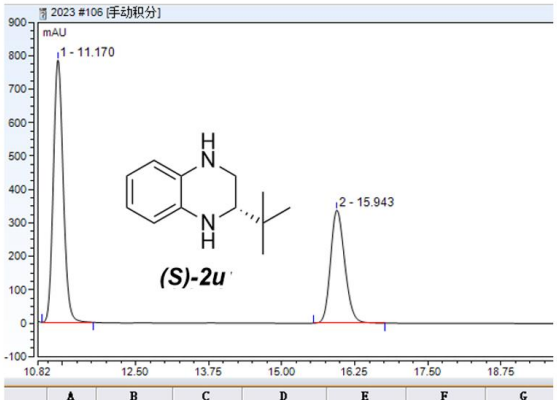
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 0.5 mL/min, column temp 40 ºC, retention time 11.423 min (minor enantiomer), 15.863 min (major enantiomer), 35% *ee* for **(*R*)-2u**, retention time 11.170 min (major enantiomer), 15.943 min (minor enantiomer), 23% *ee* for **(*S*)-2u.**



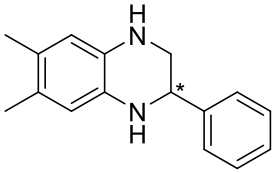
	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	11.423	49.68	245.9361	1253.24	0.181		
5	2	15.867	50.32	249.0948	890.74	0.258		



	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	11.423	32.51	135.2127	716.41	0.176		
5	2	15.863	67.49	280.6847	1019.84	0.254		



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	11.170	61.63	153.2753	784.33	0.180	
5	2	15.943	38.37	95.4106	338.88	0.260	



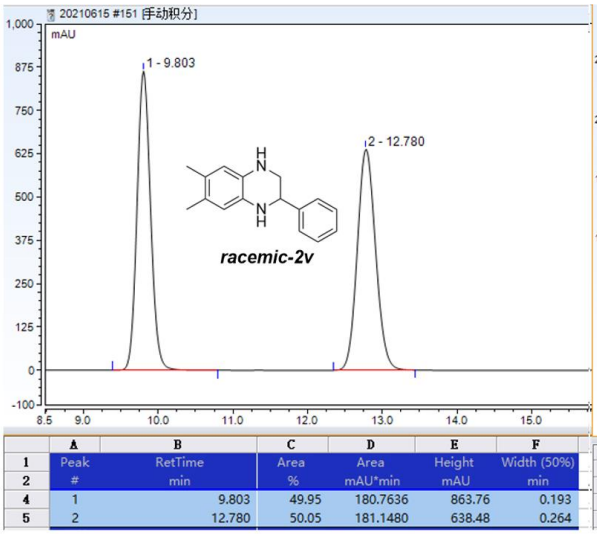
(R/S)-6,7-dimethyl-2-phenyl-1,2,3,4-tetrahydroquinoxaline（2v）

White solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.40 – 7.25 (m, 5H), 6.38 (d, *J* = 2.6 Hz, 2H), 4.42 (dd, *J* = 8.2, 3.0 Hz, 1H), 3.39 (dd, *J* = 11.1, 3.0 Hz, 1H), 3.26 (dd, *J* = 11.2, 8.3 Hz, 1H), 2.12 (s, 6H).^{13}C NMR (101 MHz, Chloroform-d) δ 142.25, 132.16, 130.60, 128.69, 127.88, 127.08, 126.96, 126.55, 116.78, 116.24, 55.16, 49.60, 19.04 (d, *J* = 2.3 Hz).

$[\alpha]_D^{25}$ = -31.990 (*c* 0.1, $CHCl_3$) for (***R***)-**2v**. $[\alpha]_D^{25}$ = 36.350 (*c* 0.1, $CHCl_3$) for (***S***)-**2v**.

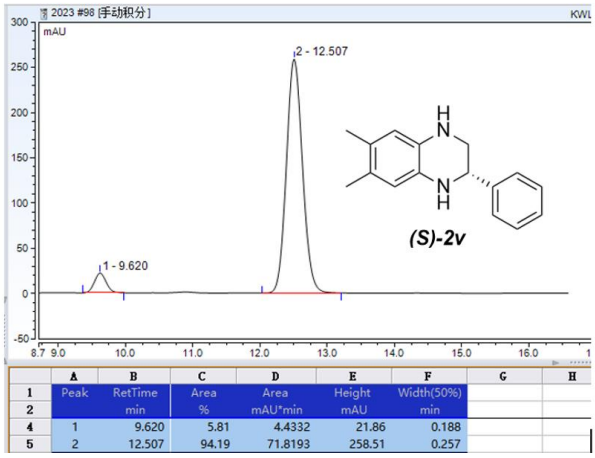
HRMS (ESI) calcd for $C_{16}H_{18}N_2^+$ [$(M+H)^+$] 238.1470, found 238.1475.

Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 ºC, retention times 9.793 min (major enantiomer), 12.807 min (minor enantiomer), 95% *ee* for **(*R*)-2v**, retention times 9.620 min (minor enantiomer), 12.507 min (major enantiomer), 88% *ee* for **(*S*)-2v**.

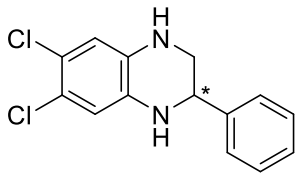


	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	9.803	49.95	180.7636	863.76	0.193
5	2	12.780	50.05	181.1480	638.48	0.264

	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%
2	#	min	%	mAU*min	mAU	min
4	1	9.793	97.32	533.6260	2523.32	0.196
5	2	12.807	2.68	14.6883	55.55	0.254



	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	9.620	5.81	4.4332	21.86	0.188		
5	2	12.507	94.19	71.8193	258.51	0.257		



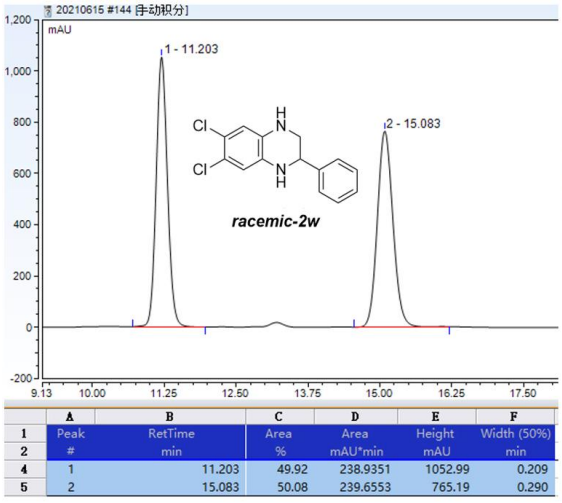
(*R*/*S*)-6,7-dichloro-2-phenyl-1,2,3,4-tetrahydroquinoxaline (2w)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.39 (m, 5H), 6.63 (d, *J* = 3.8 Hz, 2H), 4.47 (dd, *J* = 7.9, 3.2 Hz, 1H), 4.01 (s, 1H), 3.48 (dd, *J* = 11.0, 3.3 Hz, 1H), 3.31 (dd, *J* = 11.3, 7.9 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-d) δ 141.05, 133.73, 132.62, 128.85, 128.26, 126.95, 120.63, 114.96, 114.84, 54.32, 48.51.

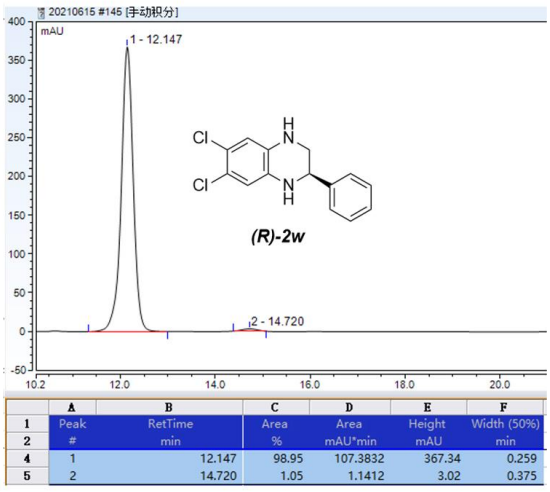
$[\alpha]_D^{25}$ = -56.024 (*c* 0.1, $CHCl_3$) for (***R***)-**2w**. $[\alpha]_D^{25}$ = 82.036 (*c* 0.1, $CHCl_3$) for (***S***)-**2w**.

HRMS (ESI) calcd for $C_{14}H_{12}Cl_2N_2^+$ [$(M+H)^+$] 278.0378 , found 278.0374.

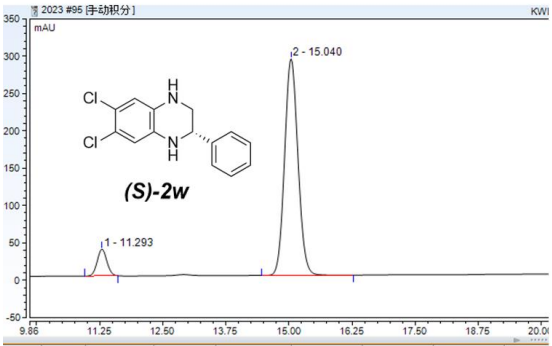
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 1 mL/min, column temp 40 °C, retention times 12.147 min (major enantiomer), 14.720 min (minor enantiomer), 98% *ee* for **(*R*)-2w**, retention times 11.293 min (minor enantiomer), 15.040 min (major enantiomer), 84% *ee* for **(*S*)-2w**.



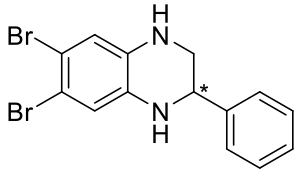
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	11.203	49.92	238.9351	1052.99	0.209
5	2	15.083	50.08	239.6553	765.19	0.290



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	12.147	98.95	107.3832	367.34	0.259
5	2	14.720	1.05	1.1412	3.02	0.375



	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	11.293	8.23	7.9683	35.77	0.208		
5	2	15.040	91.77	88.8572	289.93	0.284		



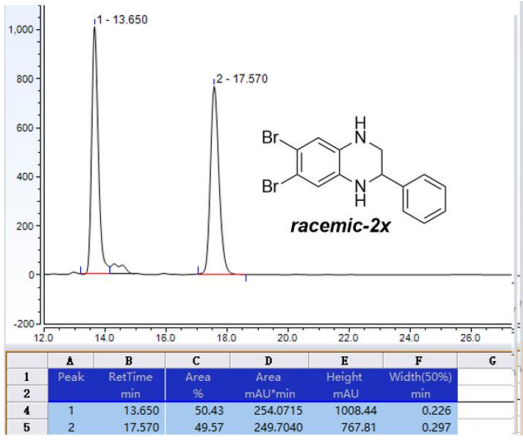
(*R/S*)-6,7-dibromo-2-phenyl-1,2,3,4-tetrahydroquinoxaline (2x)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.41 – 7.26 (m, 5H), 6.74 (d, *J* = 4.5 Hz, 2H), 4.41 (dd, *J* = 7.9, 3.2 Hz, 1H), 3.43 (dd, *J* = 11.2, 3.2 Hz, 1H), 3.24 (dd, *J* = 11.2, 7.9 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 141.11, 134.66, 133.54, 128.97, 128.38, 127.06, 118.01, 117.90, 116.80, 111.76, 54.33, 48.52.

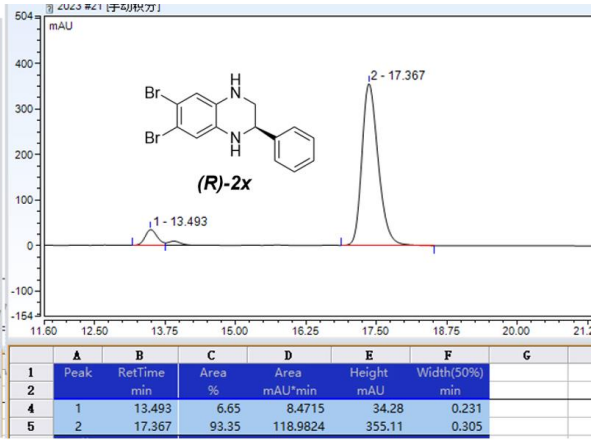
$[\alpha]_D^{25}$ = -48.359 (*c* 0.1, $CHCl_3$) for (***R***)-**2x**. $[\alpha]_D^{25}$ = 19.681 (*c* 0.1, $CHCl_3$) for (***S***)-**2x.**

HRMS (ESI) calcd for $C_{14}H_{12}Br_2N_2^+$ [$(M+H)^+$] 365.9367, found 365.9362.

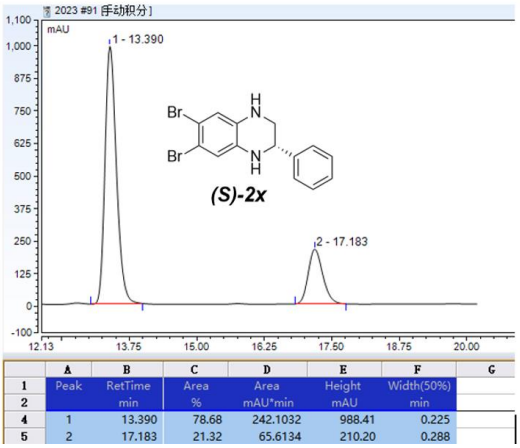
Daicel Chiralpak OZ-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 0.6 mL/min, column temp 40 °C, retention time 13.493 min (major enantiomer), 17.367 min (minor enantiomer), 87% *ee* for **(*R*)-2x**, retention time 13.390 min (minor enantiomer), 17.183 min (major enantiomer), 57% *ee* for **(*S*)-2x.**



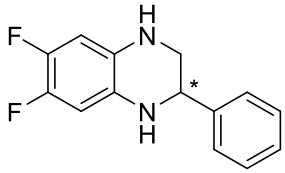
	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	13.650	50.43	254.0715	1008.44	0.226	
5	2	17.570	49.57	249.7040	767.81	0.297	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	13.493	6.65	8.4715	34.28	0.231	
5	2	17.367	93.35	118.9824	355.11	0.305	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	13.390	78.68	242.1032	988.41	0.225	
5	2	17.183	21.32	65.6134	210.20	0.288	



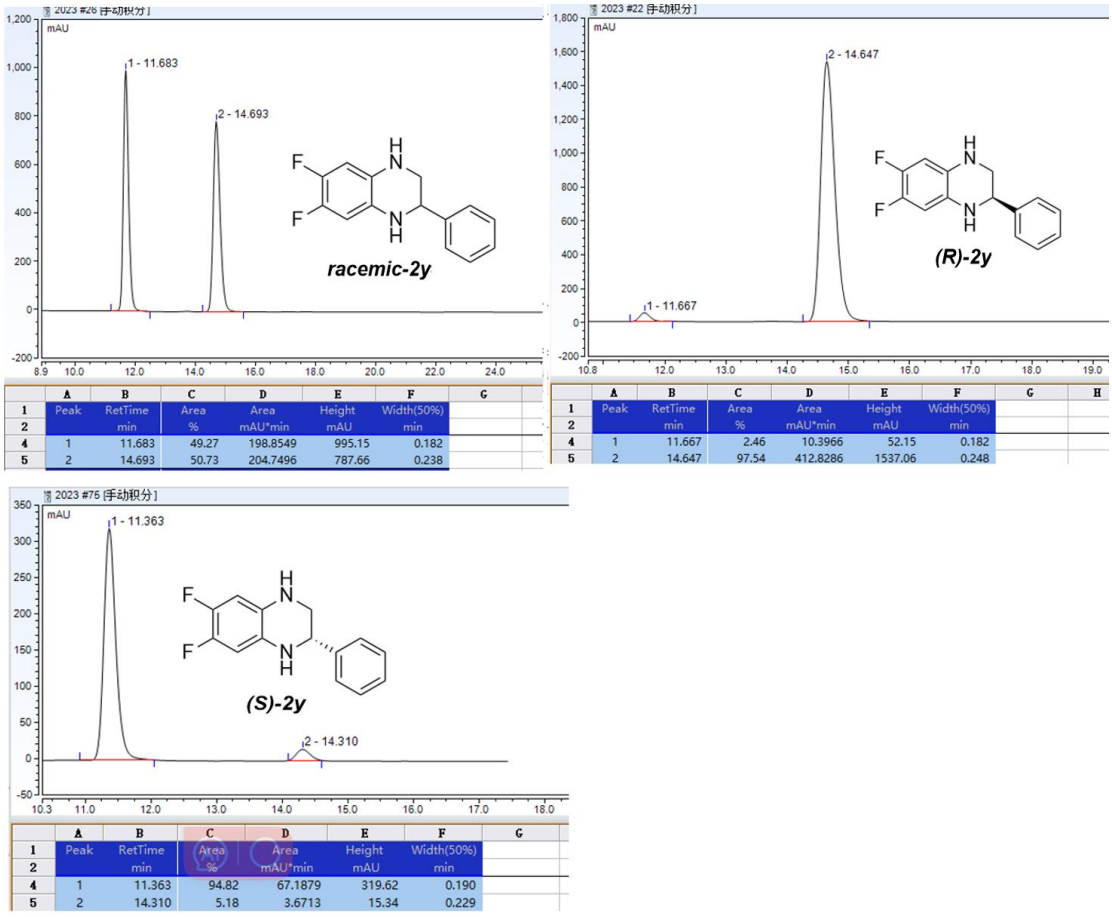
(*R*/*S*)-6,7-difluoro-2-phenyl-1,2,3,4-tetrahydroquinoxaline (2y)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.34 (m, 5H), 6.40 – 6.31 (m, 2H), 4.39 (dt, *J* = 8.2, 2.4 Hz, 1H), 3.76 (m, 2H), 3.41 (dt, *J* = 11.3, 2.5 Hz, 1H), 3.26 (ddd, *J* = 10.6, 8.1, 1.7 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 144.49 (dd, *J* = 16.2, 10.3 Hz), 142.12 (dd, *J* = 16.2, 11.0 Hz), 141.29, 130.21 – 129.80 (m), 128.81, 128.76 – 128.30 (m), 128.17, 127.97, 126.99, 103.05 (dd, *J* = 38.5, 20.5 Hz), 54.52, 48.87.

$[\alpha]_D^{25}$ = -52.704 (*c* 0.1, $CHCl_3$) for (***R***)-**2y**. $[\alpha]_D^{25}$ = 63.367 (*c* 0.1, $CHCl_3$) for (***S***)-**2y.**

HRMS (ESI) calcd for $C_{14}H_{12}F_2N_2^+$ [(M+H)$^+$] 246.0969, found 246.0965.

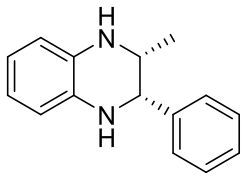
Daicel Chiralpak OZ-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 0.6 mL/min, column temp 40 °C, retention time 11.667 min (major enantiomer), 14.647 min (minor enantiomer), 95% *ee* for **(*R*)-2y**, retention time 11.363 min (minor enantiomer), 14.310 min (major enantiomer), 90% *ee* for **(*S*)-2y.**



Peak	RetTime min	Area %	Area mAU*min	Height mAU	Width(50%) min
1	11.683	49.27	198.8549	995.15	0.182
2	14.693	50.73	204.7496	787.66	0.238

Peak	RetTime min	Area %	Area mAU*min	Height mAU	Width(50%) min
1	11.667	2.46	10.3966	52.15	0.182
2	14.647	97.54	412.8286	1537.06	0.248

Peak	RetTime min	Area %	Area mAU*min	Height mAU	Width(50%) min
1	11.363	94.82	67.1879	319.62	0.190
2	14.310	5.18	3.6713	15.34	0.229



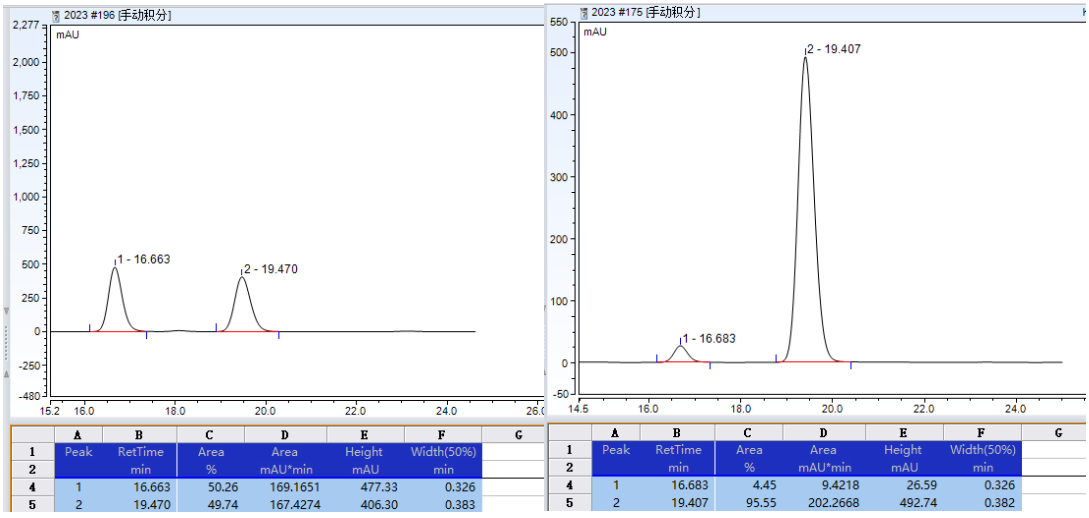
(2*R*,3*S*)-2-methyl-3-phenyl-1,2,3,4-tetrahydroquinoxaline (4a)[6]

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.26 (m, 5H), 6.74 – 6.50 (m, 4H), 4.51 (d, *J* = 3.1 Hz, 1H), 3.72 (qd, *J* = 6.5, 3.0 Hz, 1H), 0.95 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 141.82, 133.33, 132.22, 128.29, 127.65, 127.44, 119.43, 118.44, 115.00, 114.03, 58.55, 49.54, 17.61.

$[\alpha]_D^{25}$ = -30.847 (*c* 0.1, $CHCl_3$).

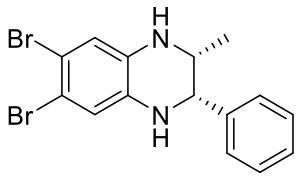
HRMS (ESI) calcd for $C_{15}H_{17}N_2^+$ [$(M+H)^+$] 225.1386, found 225.1389.

Daicel Chiralpak AD-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 1 mL/min, column temp 40 °C, retention times 16.683 min (minor enantiomer), 19.407 min (major enantiomer), 91% *ee*.



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	16.663	50.26	169.1651	477.33	0.326	
5	2	19.470	49.74	167.4274	406.30	0.383	

	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	16.683	4.45	9.4218	26.59	0.326	
5	2	19.407	95.55	202.2668	492.74	0.382	



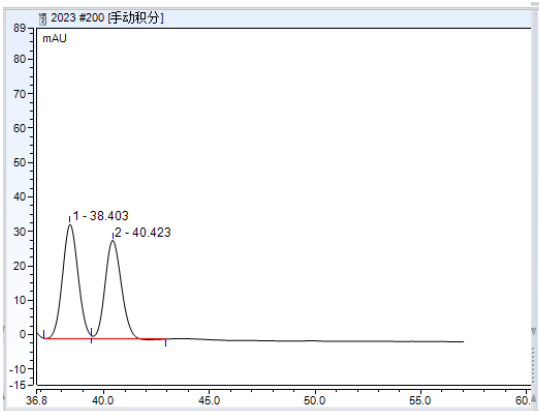
(2*R*,3*S*)-6,7-dibromo-2-methyl-3-phenyl-1,2,3,4-tetrahydroquinoxaline (4b)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 (m, 2H), 7.23 (m, 2H), 6.79 – 6.71 (m, 2H), 5.29 (d, *J* = 8.5 Hz, 1H), 4.49 – 4.42 (m, 1H), 3.67 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 140.85, 133.69, 132.91, 128.39, 127.74, 127.55, 118.05, 117.28, 112.21, 111.20, 58.12, 49.07, 17.58.

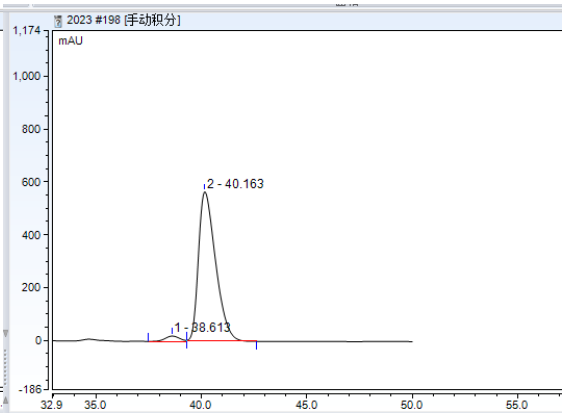
$[\alpha]_D^{25}$ = -54.506 (*c* 0.1, $CHCl_3$).

HRMS (ESI) calcd for $C_{15}H_{14}Br_2N_2^+$ [$(M+H)^+$] 379.9524, found 379.9521.

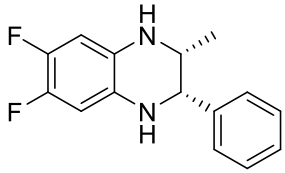
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 95:5, flow rate 0.5 mL/min, column temp 40 °C, retention times 38.613 min (minor enantiomer), 40.163 min (major enantiomer), 94% *ee*.



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	38.403	52.90	28.3452	33.18	0.802
5	2	40.423	47.10	25.2377	28.59	0.832



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	38.613	2.87	15.7722	20.27	0.743	
5	2	40.163	97.13	534.5023	566.58	0.874	



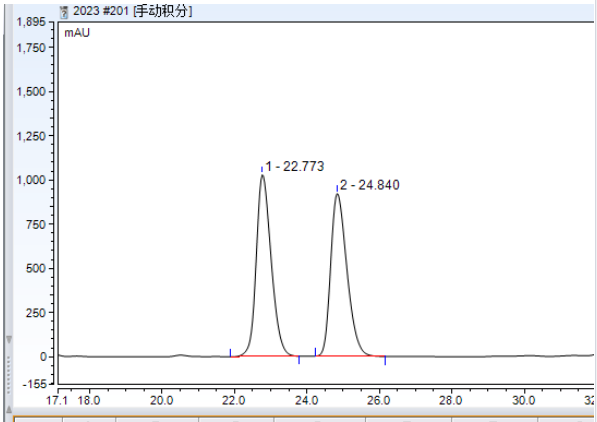
(2*R*,3*S*)-6,7-difluoro-2-methyl-3-phenyl-1,2,3,4-tetrahydroquinoxaline (4c)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.20 (m, 5H), 6.34 (m, 2H), 4.45 – 4.41 (m, 1H), 3.64 (m, 1H), 0.92 (dd, *J* = 6.6, 1.6 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.89 (d, *J* = 13.1 Hz), 144.21 (d, *J* = 13.3 Hz), 142.55 (d, *J* = 12.9 Hz), 141.87 (d, *J* = 13.2 Hz), 141.25, 129.10 (d, *J* = 8.3 Hz), 128.39, 128.02 (d, *J* = 8.0 Hz), 127.60 (d, *J* = 9.5 Hz), 103.35 (d, *J* = 20.9 Hz), 102.31 (d, *J* = 21.3 Hz), 58.24, 49.41, 17.48.

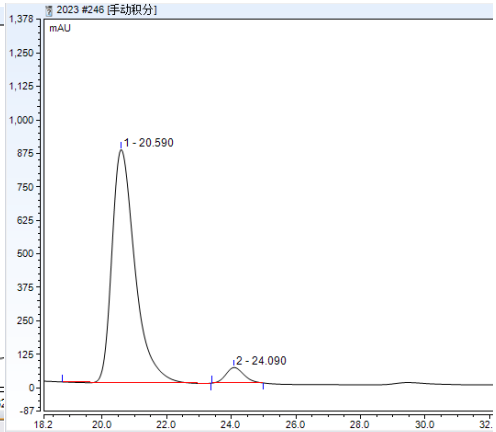
$[\alpha]_D^{25}$ = -26.672 (*c* 0.1, $CHCl_3$).

HRMS (ESI) calcd for $C_{15}H_{14}F_2N_2^+$ [$(M+H)^+$] 260.1125, found 260.1127.

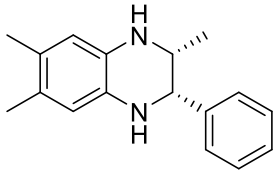
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 95:5, flow rate 0.5 mL/min, column temp 40 ºC, retention times 20.590 min (major enantiomer), 24.090 min (minor enantiomer), 90% *ee*.



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	22.773	50.64	490.6583	1029.07	0.435	
5	2	24.840	49.36	478.2122	920.74	0.481	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	20.590	95.08	714.2112	869.50	0.733	
5	2	24.090	4.92	36.9866	57.65	0.598	



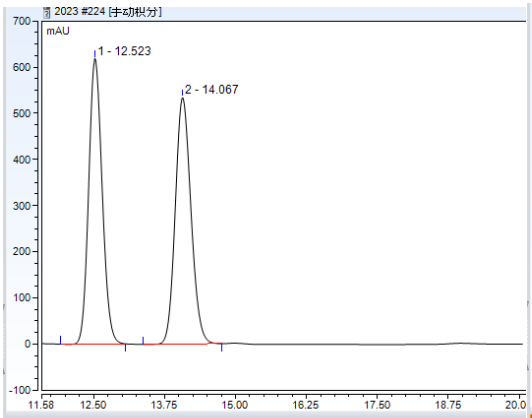
(2*R*,3*S*)-2,6,7-trimethyl-3-phenyl-1,2,3,4-tetrahydroquinoxaline(4d)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.26 (m, 5H), 6.45 (d, *J* = 9.0 Hz, 2H), 4.52 (d, *J* = 3.1 Hz, 1H), 3.71 (m, 1H), 2.18 (s, 6H), 0.98 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.03, 131.21, 129.93, 128.25, 127.62, 127.34, 126.20, 116.90, 115.76, 58.73, 49.90, 19.09, 19.01, 17.43.

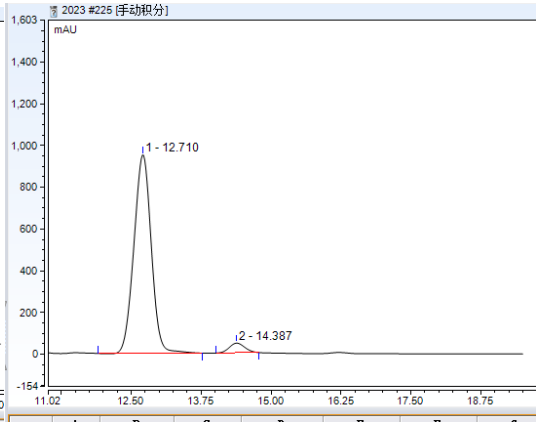
$[\alpha]_D^{25}$ = -28.670 (*c* 0.1, $CHCl_3$).

HRMS (ESI) calcd for $C_{17}H_{21}N_2^+$ [$(M+H)^+$] 253.1699, found 253.1697.

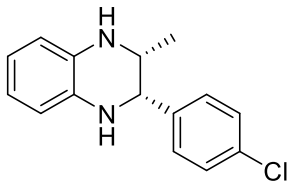
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 1 mL/min, column temp 40 °C, retention times 12.710 min (major enantiomer), 14.387 min (minor enantiomer), 92% *ee*.



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	12.523	49.85	169.8084	618.61	0.255	
5	2	14.067	50.15	170.8005	534.32	0.297	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	12.710	95.80	341.8125	952.66	0.333	
5	2	14.387	4.20	14.9749	46.68	0.303	



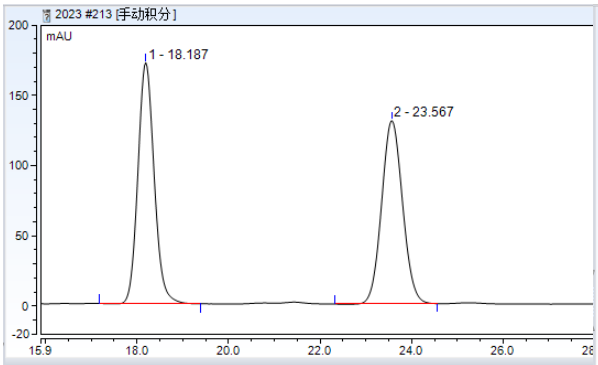
(2*S*,3*R*)-2-(4-chlorophenyl)-3-methyl-1,2,3,4-tetrahydroquinoxaline (4e)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.19 (m, 4H), 6.62 (, 4H), 4.47 (d, *J* = 3.1 Hz, 1H), 3.75 – 3.63 (m, 1H), 0.93 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 140.34, 133.17, 132.93, 132.05, 129.05, 128.37, 119.62, 118.54, 115.02, 114.03, 58.09, 49.19, 17.64.

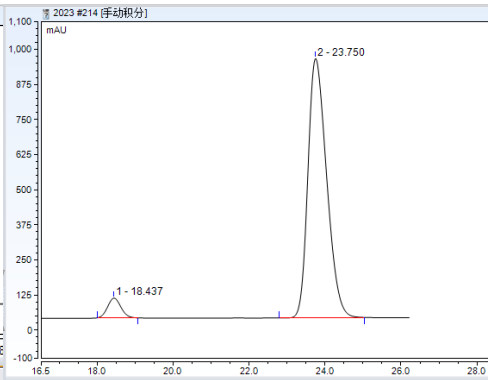
$[\alpha]_D^{25}$ = -44.350 (*c* 0.1, $CHCl_3$).

HRMS (ESI) calcd for $C_{15}H_{16}ClN_2^+$ [$(M+H)^+$] 259.0997, found 259.0994.

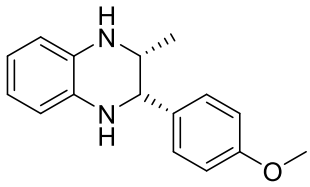
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 85:5, flow rate 1 mL/min, column temp 40 °C, retention times 18.437 min (minor enantiomer), 23.750 min (major enantiomer), 90% *ee*.



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	18.187	50.47	70.4548	171.63	0.376	
5	2	23.567	49.53	69.1390	130.57	0.494	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	18.437	5.11	28.3609	70.31	0.378	
5	2	23.750	94.89	526.9951	924.29	0.532	



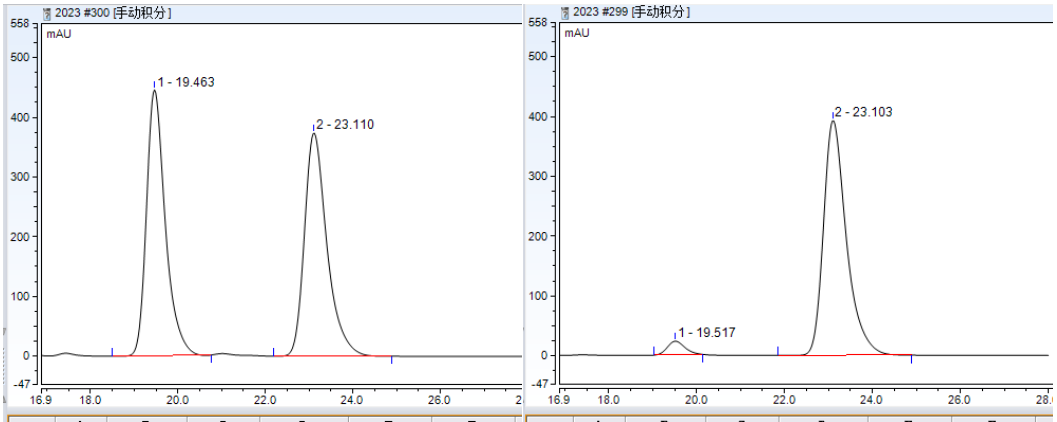
(2*S*,3*R*)-2-(4-methoxyphenyl)-3-methyl-1,2,3,4-tetrahydroquinoxaline (4f)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.26 (dd, *J* = 8.5, 1.8 Hz, 2H), 6.90 (dd, *J* = 8.6, 1.8 Hz, 2H), 6.74 – 6.56 (m, 4H), 4.50 (dd, *J* = 3.1, 1.7 Hz, 1H), 3.84 (d, *J* = 1.7 Hz, 3H), 3.78 – 3.69 (m, 1H), 0.99 (dd, *J* = 6.5, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.95, 134.08, 133.31, 132.52, 128.71, 119.25, 118.36, 114.80, 113.99, 113.63, 58.02, 55.33, 49.63, 17.75.

$[\alpha]_D^{25}$ = -48.261 (*c* 0.1, $CHCl_3$).

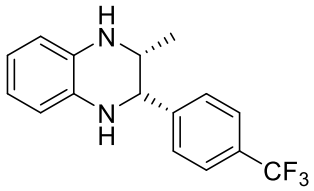
HRMS (ESI) calcd for $C_{16}H_{18}N_2O^+$ [$(M+H)^+$] 255.1492, found 255.1497.

Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 1 mL/min, column temp 40 ºC, retention times 19.517 min (minor enantiomer), 23.103 min (major enantiomer), 92% *ee*.



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	19.463	49.88	222.0269	445.67	0.443
5	2	23.110	50.12	223.0916	374.27	0.529

	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	19.517	4.24	10.4878	22.85	0.426
5	2	23.103	95.76	237.0871	392.80	0.535



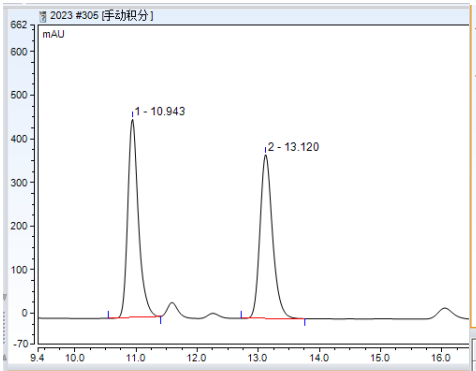
(2*R*,3*S*)-2-methyl-3-(4-(trifluoromethyl)phenyl)-1,2,3,4-tetrahydroquinoxaline (4g)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 2H), 6.66 (m, 4H), 4.60 – 4.55 (m, 1H), 3.78 (t, *J* = 5.0 Hz, 1H), 0.98 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.97, 132.65, 132.36, 128.10, 125.13 (q, *J* = 3.8 Hz), 119.56, 118.65, 114.88, 114.02, 58.53, 49.00, 17.86.

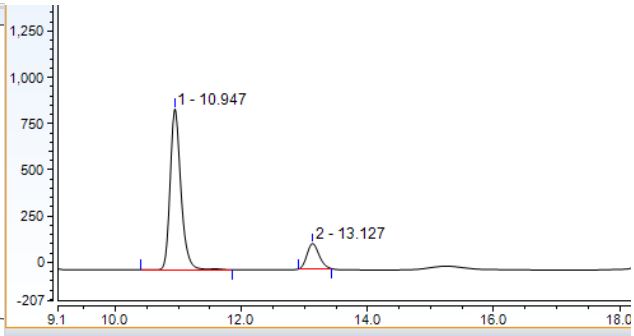
$[\alpha]_D^{25}$ = -26.093 (*c* 0.1, $CHCl_3$).

HRMS (ESI) calcd for $C_{16}H_{16}F_3N_2^+$ [$(M+H)^+$] 293.1260, found 293.1263.

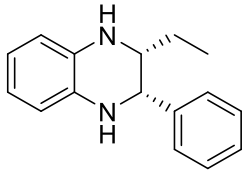
Daicel Chiralpak AD-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 0.7 mL/min, column temp 40 °C, retention times 10.947 min (major enantiomer), 13.127 min (minor enantiomer), 70% *ee*.



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	10.943	50.65	91.4738	455.37	0.178
5	2	13.120	49.35	89.1221	376.31	0.214



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	10.947	85.09	172.6946	870.40	0.176
5	2	13.127	14.91	30.2531	137.00	0.207



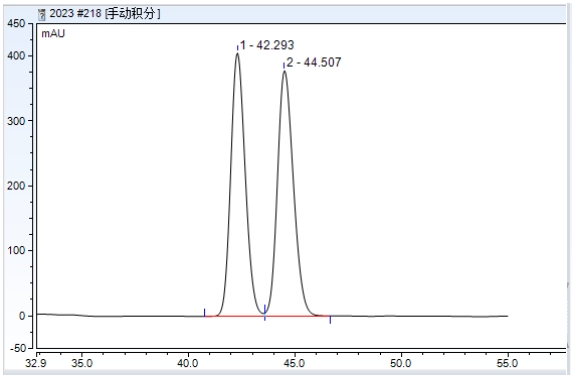
(2*R*,3*S*)-2-ethyl-3-phenyl-1,2,3,4-tetrahydroquinoxaline (4h)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.28 (m, 6H), 6.74 – 6.55 (m, 4H), 4.61 (t, *J* = 2.7 Hz, 1H), 3.48 (t, *J* = 3.0 Hz, 1H), 1.35 – 1.22 (m, 2H), 0.96 (t, *J* = 7.5 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 141.99, 133.43, 132.31, 128.30, 127.64, 127.40, 119.30, 118.40, 114.80, 114.05, 57.86, 55.72, 23.80, 10.59.

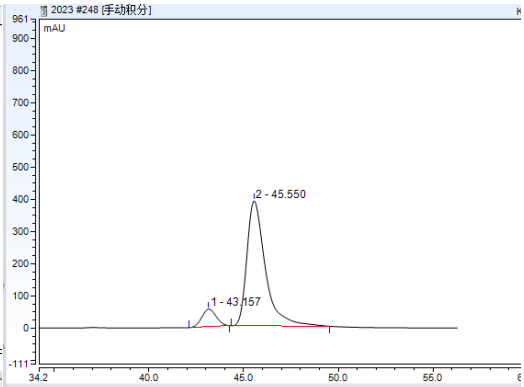
$[\alpha]_D^{25}$ = -20.582 (*c* 0.1, $CHCl_3$).

HRMS (ESI) calcd for $C_{16}H_{19}N_2^+$ [$(M+H)^+$] 239.1543, found 239.1546.

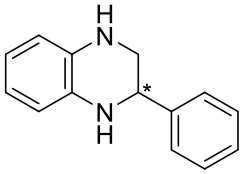
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 95:5, flow rate 0.5 mL/min, column temp 40 °C, retention times 43.157 min (minor enantiomer), 45.550 min (major enantiomer), 80% *ee*.



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	42.293	49.44	320.1658	405.43	0.735	
5	2	44.507	50.56	327.3652	377.75	0.807	



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	43.157	9.78	47.7483	54.55	0.829	
5	2	45.550	90.22	440.3609	387.99	0.972	

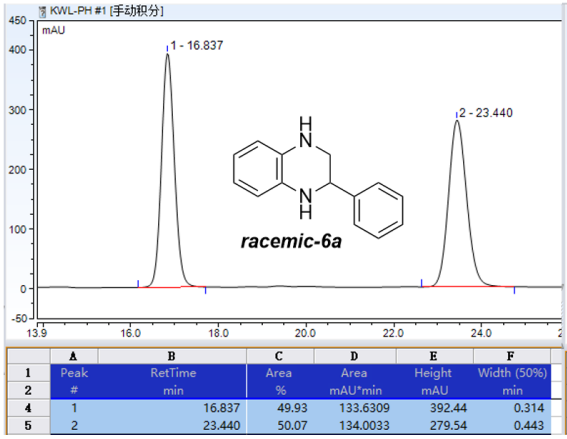


(*R*/*S*)-2-phenyl-1,2,3,4-tetrahydroquinoxaline (6a)[1]

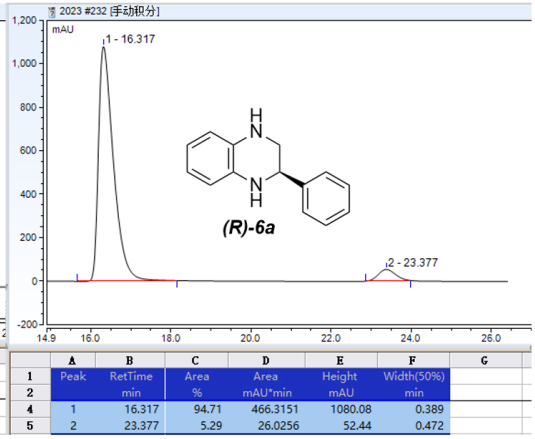
Yellow solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.48 – 7.30 (m, 5H), 6.73 – 6.66 (m, 2H), 6.66 – 6.60 (m, 2H), 4.53 (dd, *J* = 8.2, 3.1 Hz, 1H), 3.51 (dd, *J* = 11.1, 3.1 Hz, 1H), 3.37 (dd, *J* = 11.0, 8.2 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 141.92, 134.22, 132.89, 128.74, 127.99, 127.09, 119.00, 118.87, 114.81, 114.52, 54.79, 49.22.

$[\alpha]_D^{25}$ = -82.423 (*c* 0.1, $CHCl_3$) for **(*R*)-6a**. $[\alpha]_D^{25}$ = 78.134 (*c* 0.1, $CHCl_3$) for **(*S*)-6a**.

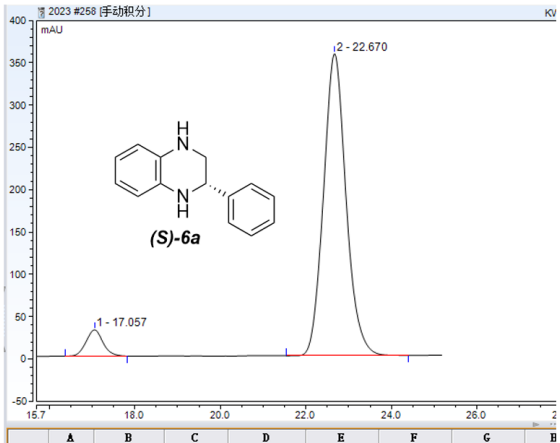
HRMS (ESI) calcd for $C_{14}H_{14}N_2^+$ [$(M+H)^+$] 211.1230, found 211.1231.
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 90:10, flow rate 1 mL/min, column temp 40 °C, retention times 16.317 min (major enantiomer), 23.377 min (minor enantiomer), 90% *ee* for (*R*)-6a, retention times 17.057 min (minor enantiomer), 22.670 min (major enantiomer), 87% *ee* for (*S*)-6a.



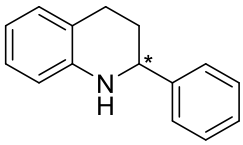
	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	16.837	49.93	133.6309	392.44	0.314
5	2	23.440	50.07	134.0033	279.54	0.443



	A	B	C	D	E	F	G
1	Peak	RetTime	Area	Area	Height	Width(50%)	
2		min	%	mAU*min	mAU	min	
4	1	16.317	94.71	466.3151	1080.08	0.389	
5	2	23.377	5.29	26.0256	52.44	0.472	



	A	B	C	D	E	F	G	H
1	Peak	RetTime	Area	Area	Height	Width(50%)		
2		min	%	mAU*min	mAU	min		
4	1	17.057	6.13	14.2308	31.12	0.417		
5	2	22.670	93.87	217.8520	356.90	0.554		



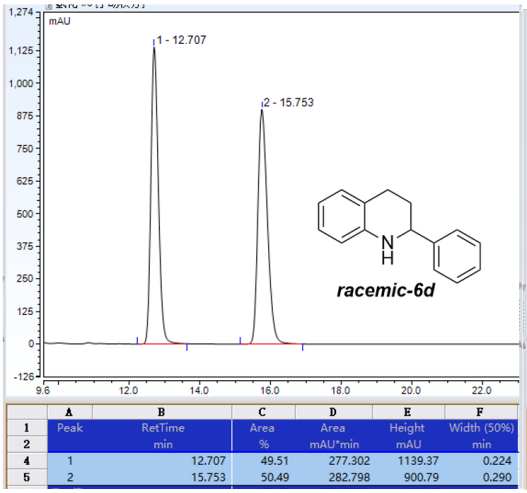
(*R/S*)-2-phenyl-1,2,3,4-tetrahydroquinoline (6b)[7]

White solid. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.42 – 7.27 (m, 5H), 7.02 (t, *J* = 7.3 Hz, 2H), 6.66 (td, *J* = 7.4, 1.1 Hz, 1H), 6.58 – 6.52 (m, 1H), 4.45 (dd, *J* = 9.3, 3.3 Hz, 1H), 4.05 (s, 1H), 2.93 (m, 1H), 2.74 (m, 1H), 2.24 – 2.08 (m, 1H), 2.08 – 1.91 (m, 1H); ^{13}C NMR (101 MHz, Chloroform-d) δ 144.92 , 144.85 , 129.43 , 128.70 , 127.57 , 127.03 , 126.67 , 121.01 , 117.28 , 114.10 , 56.38 , 31.10 , 26.51 .HRMS (ESI+) m/z [M+H]: calcd. 210.1277, found 210.1272. $[\alpha]^{25}_{589}$ = - 54.719(c = 0.100 in $CHCl_3$).

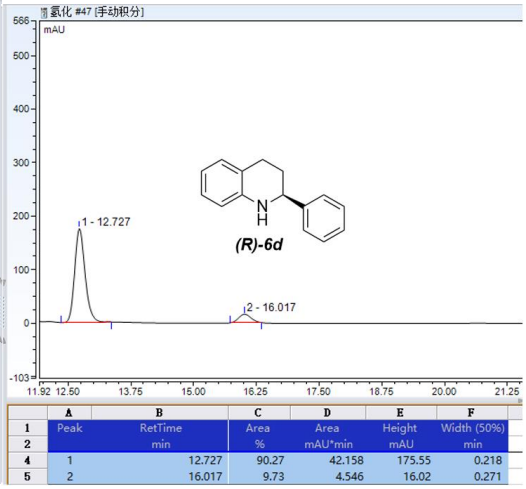
$[\alpha]^{25}_{D}$ = -52.069 (*c* 0.1, $CHCl_3$) for **(*R*)-6d**. $[\alpha]^{25}_{D}$ = 45.273 (*c* 0.1, $CHCl_3$) for **(*S*)-6d**.

HRMS (ESI) calcd for $C_{15}H_{15}N^{+}$ [$(M+H)^{+}$] 209.1204, found 209.1205.

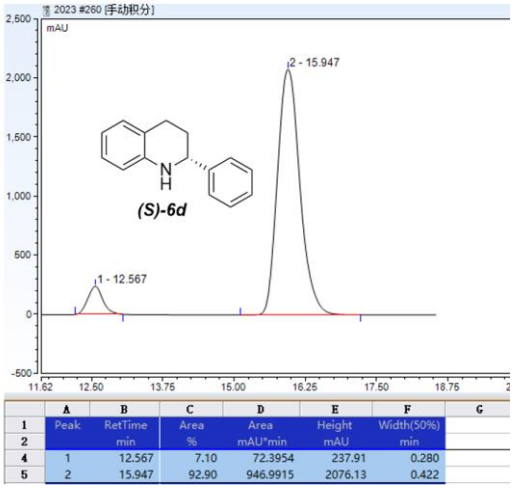
Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 0.6 mL/min, column temp 40 °C, retention times 12.727 min (major enantiomer), 16.017 min (minor enantiomer), 80% *ee* for (*R*)-6d, retention times 12.567 min (minor enantiomer), 15.947 min (major enantiomer), 87% *ee* for (*S*)-6d.



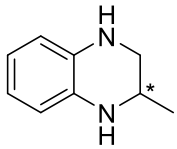
Peak	RetTime min	Area %	Area mAU*min	Height mAU	Width (50%) min
1	12.707	49.51	277.302	1139.37	0.224
2	15.753	50.49	282.798	900.79	0.290



Peak	RetTime min	Area %	Area mAU*min	Height mAU	Width (50%) min
1	12.727	90.27	42.158	175.55	0.218
2	16.017	9.73	4.546	16.02	0.271



Peak	RetTime min	Area %	Area mAU*min	Height mAU	Width(50%) min
1	12.567	7.10	72.3954	237.91	0.280
2	15.947	92.90	946.9915	2076.13	0.422



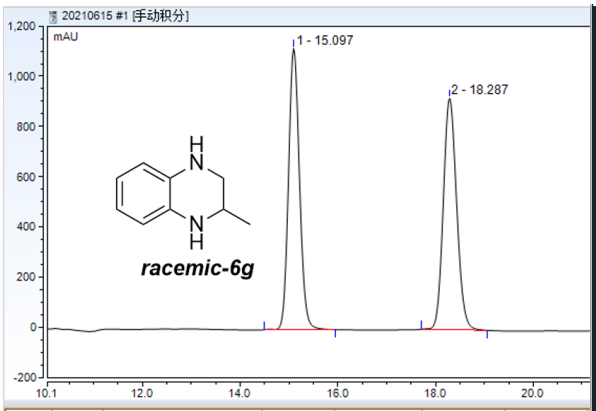
(*S*)-2-methyl-1,2,3,4-tetrahydroquinoxaline(6c)

Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.60 (dd, *J* = 5.8, 3.4 Hz, 2H), 6.52 (dd, *J* = 6.1, 3.2 Hz, 2H), 3.51 (m, 1H), 3.39 (s, 2H), 3.32 (dd, *J* = 10.8, 3.0 Hz, 1H), 3.04 (dd, *J* = 10.7, 8.2 Hz, 1H), 1.19 (d, *J* = 6.3 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 133.65, 133.26, 118.78, 114.52, 48.31, 45.78, 19.98.

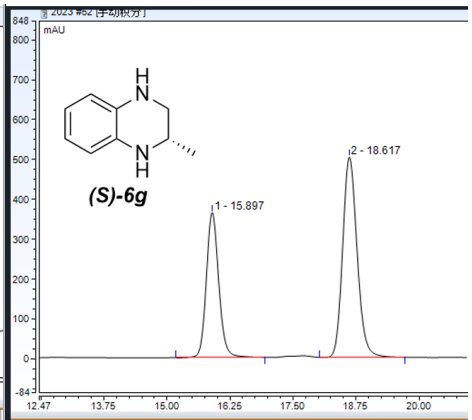
$[\alpha]_D^{25}$ = -13.3 (*c* 0.1, $CHCl_3$) for **(*R*)-6g**. $[\alpha]_D^{25}$ = 10.121 (*c* 0.1, $CHCl_3$) for **(*S*)-6g**.

HRMS (ESI) calcd for $C_9H_{13}N_2^+$ [$(M+H)^+$] 149.1073, found 149.1070.

Daicel Chiralpak OD-H column, isocratic elution: n-hexane/2-propanol 80:20, flow rate 0.5 mL/min, column temp 40 °C, retention times 15.897 min (minor enantiomer), 18.617 min (major enantiomer), 23% *ee* for (*S*)-6d, retention times 19. min (minor enantiomer), 15.947 min (major enantiomer), 87% *ee* for (*S*)-6d.



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width (50%)
2	#	min	%	mAU*min	mAU	min
4	1	15.097	49.98	292.0190	1121.30	0.239
5	2	18.287	50.02	292.1980	921.94	0.294



	A	B	C	D	E	F
1	Peak	RetTime	Area	Area	Height	Width(50%)
2		min	%	mAU*min	mAU	min
4	1	15.897	38.36	103.6764	363.99	0.258
5	2	18.617	61.64	166.5820	502.33	0.304

10. Supporting references

1 Q.-A. Chen; D.-S. Wang; Y.-G. Zhou; Y. Duan; H.-J. Fan; Y. Yang; Z. Zhang, Convergent Asymmetric Disproportionation Reactions: Metal/Brønsted Acid Relay Catalysis for Enantioselective Reduction of Quinoxalines**,** *J. Am. Chem. Soc*, **2011**, *133* (16), 6126-6129.

2 F. Shi; W. Tan; H. H. Zhang; M. Li; Q. Ye; G. H. Ma; S. J. Tu; G. Li, Asymmetric Organocatalytic Tandem Cyclization/Transfer Hydrogenation: A Synthetic Strategy for Enantioenriched Nitrogen Heterocycles**,** *Advanced Synthesis & Catalysis*, **2013**, *355* (18), 3715-3726.

3 D. Cartigny; T. Nagano; T. Ayad; J. P. Gen ê t; T. Ohshima; K. Mashima; V. Ratovelomanana‐Vidal, Iridium‐Difluorphos‐Catalyzed Asymmetric Hydrogenation of 2‐Alkyl‐and 2‐Aryl‐Substituted Quinoxalines: A General and Efficient Route into Tetrahydroquinoxalines**,** *Advanced Synthesis & Catalysis*, **2010**, *352* (11-12), 1886-1891.

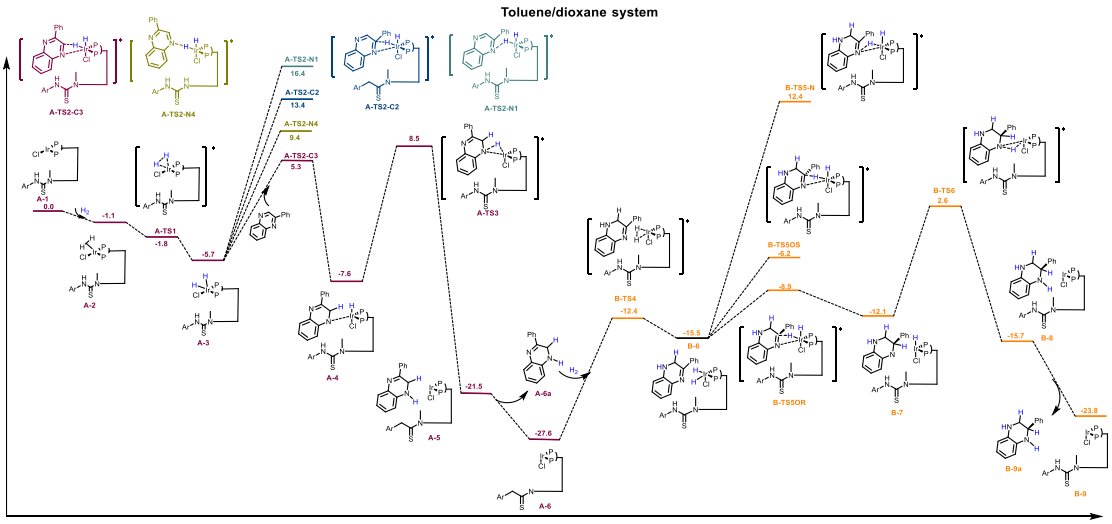
4 Z. Han; X. Feng; H. Du, Asymmetric Transfer Hydrogenation of 2-Substituted Quinoxalines with Regenerable Dihydrophenanthridine**,** *The Journal of Organic Chemistry*, **2024**, *89* (5), 3666-3671.

5 H.-X. Lei; K. Zhang; Y.-X. Qin; R.-J. Dong; D.-Z. Chen; H. Zhou; X.-H. Sheng, A Quantum-Chemical Approach to Develop Tetrahydroquinoxaline as Potent Ferroptosis Inhibitors**,** *Journal of Molecular Structure*, **2021**, *1228*.

6 C. Liu; X. Liu; Q. Liu, Stereodivergent Asymmetric Hydrogenation of Quinoxalines**,** *Chem*, **2023**, *9* (9), 2585-2600.

7 Z. Han; G. Liu; X. Yang; X.-Q. Dong; X. Zhang, Enantiodivergent Synthesis of Chiral Tetrahydroquinoline Derivatives Via Ir-Catalyzed Asymmetric Hydrogenation: Solvent-Dependent Enantioselective Control and Mechanistic Investigations**,** *ACS Catal*, **2021**, *11* (12), 7281-7291.

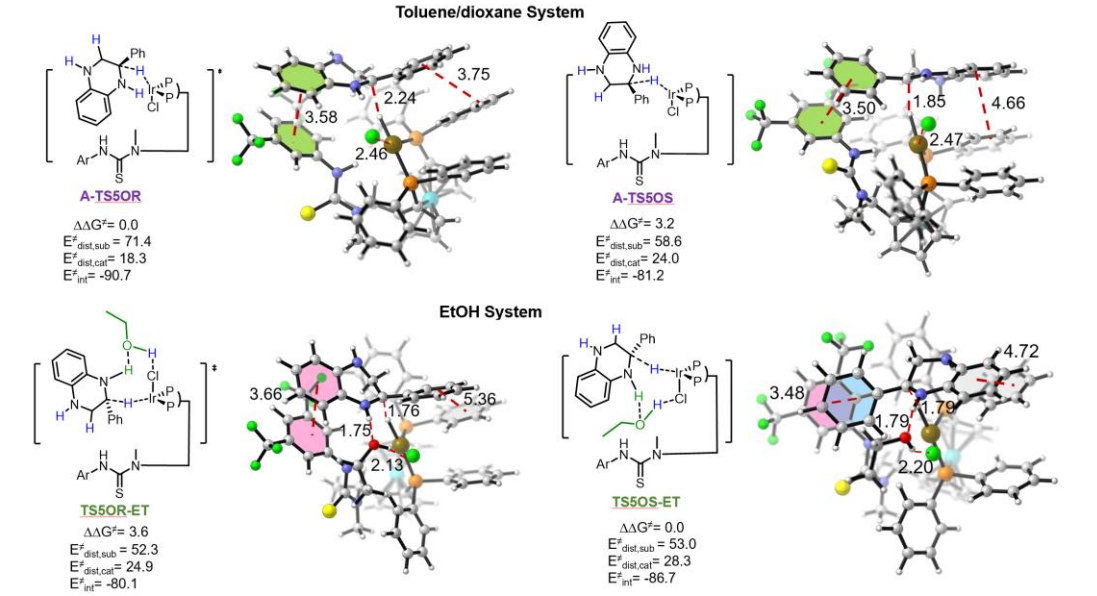
11. DFT computational studies



Scheme S2. DFT calculated energy potential surface for the proposed inner-sphere pathway in toluene/dioxane system (Ar=3,5-di-CF_3Ph; the phenyl groups on the phosphorus atoms are omitted for clarity; the relative Gibbs energies are labeled in kcal·mol^{-1}).

11.1 Distortion calculation

Absolute distortion energies (Hartree) of the catalyst complex (E_{cat}), and of the substrate (E_{sub}), as well as electronic energy (EE) for **A-TS5OR** and **A-TS5OS**, **TS5OR-ET** and **TS5OS-ET** were calculated at B3LYP-D3(BJ)/def2-tzvp//B3LYP-D3(BJ)/6-31g* level of theory and in kcal/mol.



Distortion-interaction analysis method in enantio-determining step for the single-point energy calculations, the relative Gibbs energies are labeled in kcal·mol^{-1}.

	A-TS5OR	A-TS5OS	TS5OR-ET	TS5OS-ET
sub	-651.6153034	-651.6353907	-651.6456249	-651.6442523
cat	-5395.104874	-5395.096697	-5550.224905	-5550.219508
EE	-6046.864721	-6046.861502	-6201.998148	-6202.001996

11.2 Method for DFT calculation

All quantum chemistry calculations were conducted using Gaussian 16 packages[8] at China National Supercomputing Center in Shenzhen with Density functional theory (DFT) method. B3LYP-D3(BJ) functional was used for optimization of all geometries.[8-9] SDD basis set was used for Ir and Fe,[10] and 6-31g* basis set was used for other elements.[8, 11] Then frequency calculations (at 298.15 K) were performed on the optimized geometries to confirm the local minimums (without imaginary frequency) and the transition states (with one imaginary frequency).[12] Solvent effect was included employing SMD solvation model as the solvent（solvent=generic，eps=2.34，epsinf=2.05，to the model the slovent mixture Toluene/dioxane=4:1）in mixture system. To gain more accurate energetics, the single-point solvation energies were calculated at B3LYP-D3(BJ)/def2-tzvp level of theory with SMD solvation model as the solvent (solvent=generic， eps=2.34， epsinf=2.05， to the model the slovent mixture Toluene/dioxane=4:1) in mixture system and employing SMD solvation model with etnanol as the solvent in EtOH system.

Table S4. Energetics of Computed Intermediates and TSs.

Geometries	E(correction)	E (SCF Done)	G(correction)
A-1	0.652008	-5395.151361	-5394.499353
H_2	-0.001353	-1.179184754	-1.180537754
A-2	0.668999	-5396.350628	-5395.681629
A-TS1	0.667064	-5396.349755	-5395.682691
A-3	0.670421	-5396.359427	-5395.689006
Substrate	0.167065	-649.3266804	-649.1596154
A-TS2-C3	0.863012	-6045.694007	-6044.830995
A-TS2-N4	0.859572	-6045.685811	-6044.826239
A-TS2-N1	0.855927	-6045.669307	-6044.81338
A-TS2-C2	0.860593	-6045.67881	-6044.818217
A-4	0.864809	-6045.696927	-6044.832118
A-TS3	0.861012	-6045.667531	-6044.806519
A-5	0.868631	-6045.722926	-6044.854295
A-6	0.647341	-5395.172008	-5394.524667
A-6a	0.188301	-650.5276533	-650.3393523
B-TS4	0.879589	-6046.899927	-6046.020338
B-6	0.884915	-6046.910298	-6046.025383
A-TS4-2	0.883072	-6046.819385	-6045.936313
A-TS4-1	0.882945	-6046.885132	-6046.002187
A-7	0.882532	-6046.915234	-6046.032702
A-TS4	0.882728	-6046.902872	-6046.020144
A-8	0.885564	-6046.907301	-6046.021737
A-9	0.886157	-6046.912429	-6046.026272
A-TS5OS	0.887792	-6046.897309	-6046.009517
A-TS5OR	0.886999	-6046.901644	-6046.014645
A-10	0.889114	-6046.930427	-6046.041313
A-11	0.648983	-5395.169779	-5394.520796
A-11a	0.212968	-651.741423	-651.528455
B-TS5OR	0.882431	-6046.877735	-6045.995304
B-7	0.882431	-6046.896247	-6046.013816
B-TS5OS	0.88079	-6046.891332	-6046.010542
B-TS6	0.886816	-6046.882359	-6045.995543
B-8	0.894122	-6046.91877	-6046.024648
B-9	0.650539	-5395.161115	-5394.510576
B-9a	0.213094	-651.7401446	-651.5270506
TS5OR-ET	0.968197	-6202.060126	-6201.091929
TS5OS-ET	0.963544	-6202.061206	-6201.097662

11.3 Cartesian coordinates

H_2

H	0.00000000	0.00000000	0.37142100
H	0.00000000	0.00000000	-0.37142100

Substrate

C	-0.44322400	0.30272400	-0.02965300
C	1.69824200	-0.52374400	0.05682300
C	2.22620300	0.79648400	-0.07927400
C	0.10276900	1.61781600	-0.19343300
H	2.16725700	-2.61222100	0.27859700
C	2.59134800	-1.61843400	0.17689900
C	3.62796800	0.99269600	-0.08680900
H	-0.55810400	2.46973900	-0.33268600
C	4.47272700	-0.08838000	0.03476300
C	3.95064800	-1.40018900	0.16588100
H	3.99965600	2.00692600	-0.19179100
H	5.54867100	0.05930800	0.02964200
H	4.63485000	-2.23860600	0.25915600
N	1.39087000	1.86777200	-0.21490900
N	0.35719200	-0.74618200	0.08049500
C	-1.90484600	0.06821600	-0.00444900
C	-2.40158900	-1.21723300	-0.27453200
C	-2.81535100	1.09479500	0.29138200
C	-3.77029600	-1.46431500	-0.26266600
H	-1.69332200	-2.00872500	-0.49188800
C	-4.18619200	0.84432100	0.30579800
H	-2.45835700	2.08935200	0.53825000
C	-4.66898100	-0.43392800	0.02496200
H	-4.13915500	-2.46277800	-0.48006900
H	-4.87664200	1.64847000	0.54352400
H	-5.73784100	-0.62756600	0.03400700

Toluene/dioxane system

A-1

C	-0.96126200	3.87425200	1.73708600
C	-0.69298100	3.96664000	0.34698100
H	-0.69419500	4.87770000	-0.23093000
C	-0.46032800	2.66212800	-0.18108300
C	-0.59018100	1.73409300	0.92824900
C	-0.88366700	2.50863800	2.10478900
H	-1.03002100	2.10895400	3.09611500
C	1.42246400	-0.30085400	1.26187000
C	2.15393500	0.75172100	1.82973400
H	1.71911000	1.73898000	1.91552800
C	3.46175200	0.53894900	2.26589400
H	4.03496200	1.36852900	2.66695200
C	4.04586900	-0.72175700	2.15565100
H	5.07106700	-0.87066400	2.47838600
C	3.32872100	-1.76945400	1.57641600
H	3.79642400	-2.73828400	1.43749000
C	2.02633000	-1.56102300	1.12354600
H	1.48724800	-2.36858900	0.64430100
C	-1.09320500	-0.70091900	2.48564600
C	-2.22980600	-0.12969300	3.07147400
H	-2.67835900	0.74193800	2.62461600
C	-2.79317500	-0.66982900	4.22561400
H	-3.67740000	-0.20796100	4.65487400
C	-2.24259000	-1.81094400	4.80570600
H	-2.68594500	-2.24041200	5.69926400
C	-1.11974900	-2.40048400	4.22359900
H	-0.67823200	-3.28969200	4.66445500
C	-0.54724100	-1.85039400	3.07799900
H	0.33466200	-2.31659800	2.65834800
P	-0.36415200	-0.06942000	0.90553300
Fe	-2.34138100	2.74467600	0.63085400
C	-3.73260100	1.38704500	-0.05020000
C	-4.21640200	1.99492700	1.15943100
H	-4.47794200	1.47242500	2.06636700
C	-4.29562900	3.40272700	0.96205000
C	-3.88679500	3.68516800	-0.37380100
C	-3.53364600	2.45177100	-0.99442600
H	-3.15696400	2.33026500	-1.99997500
C	-4.22257100	-1.32775600	0.89159900
C	-5.50945500	-1.00189100	1.34200000
H	-6.02500100	-0.13756900	0.93478800
C	-6.13917700	-1.79588700	2.29944900
H	-7.13343400	-1.53320300	2.65032500
C	-5.49963000	-2.93553600	2.79405000
H	-5.99232700	-3.55365600	3.53944900
C	-4.23354600	-3.28328800	2.32185600
H	-3.73205200	-4.16819900	2.70168000
C	-3.59673500	-2.48300300	1.37437800
H	-2.60313000	-2.72732500	1.01010600
C	-4.52084800	-0.74614900	-1.83464600
C	-4.49590600	-2.06531100	-2.31791400
H	-3.82773400	-2.79271000	-1.86242000
C	-5.32780900	-2.45252200	-3.36544400
H	-5.29628900	-3.47587900	-3.72812400

C	-6.20064200	-1.52709800	-3.94384900
H	-6.84956800	-1.82750300	-4.76137800
C	-6.23631900	-0.21799400	-3.46476700
H	-6.91751500	0.50547300	-3.90416700
C	-5.40081400	0.17424000	-2.41578800
H	-5.45067400	1.19216300	-2.04879500
P	-3.37851300	-0.36818700	-0.43299900
H	-1.21041400	4.69640300	2.39454400
H	-3.80350000	4.66611800	-0.82226000
H	-4.58570900	4.13035500	1.70837600
S	2.59084700	3.18504300	-0.65515100
N	0.90303800	1.59828700	-2.02039200
N	2.86083500	0.60669700	-1.49996200
H	2.28339200	-0.21138300	-1.70791400
F	5.68557500	-3.72248000	0.01373100
F	5.43822300	-3.56426100	-2.14013100
F	7.39331800	-3.23075600	-1.23469400
F	6.77600000	1.42341800	2.10720300
F	7.11140700	2.77531700	0.43833300
F	8.46271100	1.09863100	0.77256300
C	-0.29310700	2.37443700	-1.66130500
H	-1.09591100	1.67249900	-1.91759300
C	-0.44542600	3.64483100	-2.51264700
H	0.36131700	4.34912600	-2.29632800
H	-1.40844500	4.12590000	-2.31675500
H	-0.41237400	3.39856300	-3.57672800
C	2.12854000	1.76293600	-1.41637800
C	4.15723000	0.26321000	-1.11205100
C	4.52047700	-1.07457200	-1.34838200
H	3.81800500	-1.74099200	-1.83750400
C	5.75222800	-1.55539500	-0.92464800
C	6.65367400	-0.72460700	-0.25799000
H	7.60800600	-1.10356700	0.08547400
C	6.29331100	0.60317000	-0.04577800
C	5.06818000	1.11251100	-0.47364100
H	4.79638800	2.13717200	-0.27047000
C	6.06907700	-3.01487400	-1.08283600
C	7.16761100	1.47971800	0.80429200
Cl	0.62303700	-2.12511800	-1.87279300
Ir	-1.28796200	-1.01277500	-0.90625100
C	0.79001600	0.96350600	-3.33813200
H	-0.11444900	0.35165600	-3.36977300
H	0.74900600	1.72803300	-4.12488100
H	1.64049500	0.31846500	-3.53695000

A-2

C	-0.91974200	3.80654500	1.87019900
C	-0.66478900	3.94881500	0.48189800
H	-0.67131800	4.88033000	-0.06242700
C	-0.43659200	2.66362600	-0.09374000
C	-0.55853300	1.69689000	0.98289800
C	-0.83776700	2.42874100	2.18798200
H	-0.97443800	1.99375300	3.16572800
C	1.44984700	-0.33517000	1.26366100
C	2.17821300	0.69212700	1.88062900
H	1.74111700	1.67421700	2.00630900
C	3.48474700	0.46497400	2.31309300
H	4.05460200	1.27736800	2.75268400
C	4.07134000	-0.78960300	2.15394200
H	5.09476900	-0.95114300	2.47645500
C	3.35823600	-1.81295300	1.52900700
H	3.82767500	-2.77505900	1.35352800
C	2.05732600	-1.58763400	1.07819600
H	1.52207800	-2.37632900	0.56456200
C	-1.06559600	-0.79289600	2.45108300
C	-2.19844700	-0.24225000	3.06275000
H	-2.64457300	0.64864600	2.65320000
C	-2.76202400	-0.82639000	4.19570600
H	-3.64355200	-0.37852400	4.64509800
C	-2.21428000	-1.99081300	4.72969900
H	-2.65677100	-2.45362200	5.60693700
C	-1.09423700	-2.55910800	4.12227900
H	-0.65384200	-3.46598700	4.52688900
C	-0.52205400	-1.96527800	2.99799700
H	0.35837600	-2.41653600	2.55901200
P	-0.33587900	-0.10464400	0.89122700
Fe	-2.31027500	2.71676900	0.73837000
C	-3.71219500	1.38459700	0.02118900
C	-4.17600100	1.94793400	1.26001400
H	-4.42788700	1.39294600	2.15019300
C	-4.25962900	3.36170600	1.11344300
C	-3.86553800	3.69292700	-0.21568300
C	-3.52194200	2.48314800	-0.88534600
H	-3.15939100	2.39817300	-1.89983800
C	-4.16808700	-1.35905300	0.88512100
C	-5.42338900	-1.03651400	1.41854700
H	-5.94851500	-0.15036700	1.07578300
C	-6.00940000	-1.86181900	2.37700400
H	-6.97881600	-1.60211200	2.79325500

C	-5.35888600	-3.02778500	2.78924800
H	-5.81772300	-3.66980600	3.53593800
C	-4.12609700	-3.37120000	2.23347000
H	-3.61665800	-4.27658300	2.54869600
C	-3.53235100	-2.54065800	1.28444300
H	-2.56530400	-2.78497000	0.85527800
C	-4.64184300	-0.64916900	-1.77596200
C	-4.75732900	-1.95802200	-2.27313200
H	-4.11719600	-2.74311100	-1.88022400
C	-5.69689800	-2.26606500	-3.25306600
H	-5.77073100	-3.28335400	-3.62662800
C	-6.54216400	-1.27060600	-3.75115700
H	-7.27318100	-1.50888800	-4.51830400
C	-6.44702900	0.02622600	-3.25105600
H	-7.10759500	0.80454000	-3.62290200
C	-5.50636600	0.33625600	-2.26455700
H	-5.45872000	1.34646800	-1.87653300
P	-3.38839000	-0.35641700	-0.44419000
H	-1.16279600	4.60436500	2.55918300
H	-3.78703400	4.68945000	-0.62921800
H	-4.54148400	4.06157400	1.88881100
S	2.60757000	3.20444500	-0.55956700
N	0.91798400	1.66364200	-1.97278000
N	2.87241900	0.65054800	-1.47763300
H	2.29238200	-0.16188800	-1.70255100
F	5.69484400	-3.72220100	-0.08619700
F	5.43902800	-3.50719100	-2.23405700
F	7.39813000	-3.20044700	-1.32826900
F	6.80558500	1.37176500	2.13235500
F	7.13731900	2.76146900	0.49416900
F	8.48508700	1.07367900	0.78263700
C	-0.27709300	2.42860800	-1.58496200
H	-1.08278500	1.74006600	-1.86685400
C	-0.42900800	3.72916500	-2.38924700
H	0.38044300	4.42224500	-2.14864500
H	-1.39017200	4.20554200	-2.17363700
H	-0.39864000	3.52191600	-3.46168500
C	2.14315300	1.80548000	-1.36117100
C	4.16902900	0.29460100	-1.10196000
C	4.52830500	-1.03751100	-1.37340400
H	3.82197000	-1.68989600	-1.87560900
C	5.76116400	-1.53102200	-0.96794900
C	6.66736800	-0.71888000	-0.28493300
H	7.62268600	-1.10802400	0.04407100
C	6.31060300	0.60369900	-0.03740200
C	5.08429900	1.12575600	-0.44620300
H	4.81548500	2.14545200	-0.21603500
C	6.07483000	-2.98640400	-1.16519100
C	7.19112100	1.45736600	0.82935900
Cl	0.78661100	-1.92065600	-1.89122200
H	-1.97801800	-2.01644100	-2.25733500
H	-1.85070900	-1.23884400	-2.65332300
Ir	-1.30151100	-0.99679500	-1.02754500
C	0.80994000	1.08222900	-3.31597100
H	-0.09118400	0.46966700	-3.37675100
H	0.76987000	1.87819600	-4.07109100
H	1.66360800	0.44903100	-3.53775500

A-TS1

C	-0.92654100	3.81665200	1.86021100
C	-0.67276200	3.94856600	0.47042800
H	-0.68585900	4.87524000	-0.08203300
C	-0.43740000	2.65987100	-0.09416700
C	-0.55091400	1.70248300	0.99156900
C	-0.83558500	2.44220900	2.19018800
H	-0.97035600	2.01396000	3.17132700
C	1.47482800	-0.31542500	1.28596000
C	2.20058000	0.71359500	1.90294200
H	1.75840700	1.69306200	2.03316800
C	3.50957700	0.49028900	2.32945900
H	4.07816800	1.30317300	2.76981200
C	4.10041700	-0.76179600	2.16422300
H	5.12563100	-0.92003900	2.48255800
C	3.38973000	-1.78622100	1.53846200
H	3.86282300	-2.74559200	1.35792800
C	2.08635600	-1.56460700	1.09239100
H	1.55280200	-2.35264500	0.57552400
C	-1.04460000	-0.78796200	2.46705800
C	-2.18469900	-0.24349800	3.07073600
H	-2.63295500	0.64470600	2.65759100
C	-2.75116900	-0.83047500	4.20069900
H	-3.63816400	-0.38796500	4.64455900
C	-2.19908500	-1.99095000	4.73904600
H	-2.64398200	-2.45581500	5.61395600
C	-1.07185000	-2.55276100	4.13906200
H	-0.62817400	-3.45640000	4.54728100
C	-0.49657800	-1.95653300	3.01752800
H	0.38980400	-2.40202800	2.58428200
P	-0.31038000	-0.09586300	0.91274300

Fe	-2.31085300	2.70998700	0.73825800
C	-3.71093700	1.37388700	0.02234400
C	-4.17244900	1.93326000	1.26369800
H	-4.42071000	1.37546700	2.15312600
C	-4.26101000	3.34698500	1.11984500
C	-3.87263200	3.68159100	-0.21020800
C	-3.52798500	2.47414300	-0.88316800
H	-3.17302500	2.39098500	-1.90055900
C	-4.16448100	-1.37131900	0.88046700
C	-5.41708500	-1.05312200	1.42307900
H	-5.95029300	-0.17195400	1.07990900
C	-5.99016600	-1.87649900	2.39085100
H	-6.95762800	-1.62024600	2.81371100
C	-5.32939900	-3.03648800	2.80377900
H	-5.77834600	-3.67731200	3.55746400
C	-4.09932000	-3.37564300	2.23967200
H	-3.58216200	-4.27652500	2.55509300
C	-3.51833900	-2.54680600	1.28123400
H	-2.55444600	-2.79021100	0.84465600
C	-4.67263800	-0.63626000	-1.77315500
C	-4.76635200	-1.92144700	-2.33152300
H	-4.08800600	-2.70372400	-2.00370400
C	-5.73158600	-2.21013200	-3.29246600
H	-5.78757600	-3.20930400	-3.71478300
C	-6.62333700	-1.21877000	-3.71054200
H	-7.37356800	-1.44179600	-4.46362200
C	-6.54871700	0.05454100	-3.14984700
H	-7.24410300	0.82947300	-3.46018700
C	-5.58345300	0.34459800	-2.18163000
H	-5.55057000	1.33614300	-1.74652900
P	-3.40096400	-0.36596600	-0.45563200
H	-1.17492800	4.61894500	2.54206400
H	-3.79843300	4.67906900	-0.62225600
H	-4.54194200	4.04474700	1.89744800
S	2.60309700	3.19675600	-0.57690000
N	0.90886600	1.63483300	-1.96506800
N	2.87138100	0.63694500	-1.47483300
H	2.29326300	-0.17845900	-1.69458100
F	5.71036800	-3.71889400	-0.09063800
F	5.46177500	-3.50699500	-2.23957600
F	7.41681400	-3.19374600	-1.32724000
F	6.82191000	1.38558800	2.11315300
F	7.13349300	2.77494700	0.47074700
F	8.49376900	1.09600300	0.75220200
C	-0.28151200	2.41065200	-1.58362800
H	-1.09110900	1.72431200	-1.85921700
C	-0.43165300	3.70361800	-2.40030500
H	0.38024000	4.39713300	-2.16950700
H	-1.39092700	4.18448500	-2.18629000
H	-0.40585500	3.48464400	-3.47050300
C	2.13880000	1.78957200	-1.36295600
C	4.17168900	0.28855500	-1.10549400
C	4.53627000	-1.04235800	-1.37539000
H	3.83086500	-1.69944800	-1.87290000
C	5.77356600	-1.52869500	-0.97454600
C	6.67894700	-0.71019300	-0.29817300
H	7.63781900	-1.09367800	0.02707200
C	6.31682100	0.61133300	-0.05236200
C	5.08587900	1.12604400	-0.45624100
H	4.81298100	2.14493400	-0.22739300
C	6.09244200	-2.98333700	-1.16912700
C	7.19785100	1.47172100	0.80730000
Cl	0.78123700	-1.93565000	-1.88428400
H	-1.98124300	-2.07313200	-2.11536500
H	-1.83038300	-1.14738400	-2.60574500
Ir	-1.31543600	-1.01018600	-1.04386000
C	0.80755700	1.06522000	-3.31516300
H	-0.12560500	0.50641800	-3.40149300
H	0.83542700	1.86371400	-4.06839200
H	1.62510900	0.37998000	-3.51576500

A-3

C	-1.01921500	3.96603100	1.60458100
C	-0.85426800	3.92318100	0.19550800
H	-0.94388200	4.76775900	-0.47034600
C	-0.60366600	2.57788600	-0.20963300
C	-0.60046000	1.76640300	0.99800500
C	-0.84768200	2.65053200	2.10167800
H	-0.89957500	2.35394800	3.13811800
C	1.53709300	-0.07686600	1.51957800
C	2.22362200	1.05285900	1.98722600
H	1.72787700	2.01508800	2.02589900
C	3.55712000	0.95045300	2.38285400
H	4.09111500	1.83664900	2.71170400
C	4.21549700	-0.27844500	2.33168700
H	5.25839900	-0.34378700	2.62373000
C	3.54535100	-1.40324500	1.85139800
H	4.06746200	-2.34940900	1.75465600
C	2.21743400	-1.30224500	1.43487200

H	1.72185400	-2.16652800	1.00926000
C	-0.98212100	-0.62237100	2.69459900
C	-2.05285400	-0.00895500	3.35491000
H	-2.45757800	0.91578000	2.97603900
C	-2.61714000	-0.58133600	4.49605400
H	-3.44790000	-0.08267200	4.98791000
C	-2.12744900	-1.78573500	4.99516400
H	-2.56822900	-2.23391800	5.88084700
C	-1.06413000	-2.41264900	4.34192000
H	-0.66850400	-3.35186400	4.71827900
C	-0.49788400	-1.83844700	3.20580600
H	0.32847200	-2.34289300	2.71994000
P	-0.25532600	-0.02102000	1.10145400
Fe	-2.41553400	2.67764200	0.70915600
C	-3.71817000	1.27513900	-0.03265600
C	-4.16043600	1.68620600	1.27182000
H	-4.30553000	1.02672300	2.11234800
C	-4.39683800	3.08836100	1.25152100
C	-4.12242300	3.56324000	-0.06412200
C	-3.70436200	2.45304200	-0.85412100
H	-3.41264500	2.49138900	-1.89404300
C	-4.17115900	-1.40957600	0.72959200
C	-5.54715600	-1.19703400	0.91709600
H	-6.07202100	-0.47141300	0.30438400
C	-6.24933600	-1.91546400	1.88088000
H	-7.31299100	-1.73968000	2.01465400
C	-5.58911600	-2.86546300	2.66591400
H	-6.13781000	-3.42726700	3.41658400
C	-4.22751100	-3.09073300	2.47757700
H	-3.70052500	-3.81934400	3.08502100
C	-3.52210300	-2.36631700	1.51495300
H	-2.46164200	-2.53605200	1.39283600
C	-4.40687100	-0.67868500	-2.00137400
C	-4.26889900	-1.84860400	-2.76406600
H	-3.45810800	-2.53523300	-2.54959000
C	-5.15835700	-2.12895800	-3.79930200
H	-5.03410000	-3.03868700	-4.37964400
C	-6.19739100	-1.24386000	-4.09439500
H	-6.88473900	-1.45916100	-4.90750800
C	-6.34827800	-0.08346200	-3.33697500
H	-7.15607600	0.61004700	-3.55355300
C	-5.46478900	0.19457500	-2.29181200
H	-5.60846900	1.09406300	-1.70530500
P	-3.27757600	-0.42715500	-0.55667400
H	-1.26263100	4.84167400	2.19150500
H	-4.17197500	4.59152700	-0.39679000
H	-4.70168900	3.69157000	2.09632700
S	2.34616200	3.03665500	-1.02233100
N	0.56939300	1.19054000	-1.93871700
N	2.64845000	0.38985800	-1.49279400
H	2.11508200	-0.48211100	-1.60060600
F	5.74389200	-3.61175200	0.27939100
F	5.44576500	-3.68121700	-1.87229200
F	7.40106000	-3.17051200	-1.05454700
F	6.76540000	1.79996400	1.74383400
F	6.87537000	2.96809100	-0.08517700
F	8.35080000	1.41274000	0.30701100
C	-0.53328300	2.14536200	-1.66495800
H	-1.41425300	1.52577700	-1.85636600
C	-0.61464700	3.33116700	-2.64028300
H	0.21908200	4.01966100	-2.50382000
H	-1.55545100	3.86955500	-2.48934400
H	-0.60712300	2.97239400	-3.67251800
C	1.87492100	1.50360700	-1.48621800
C	3.98511200	0.15565100	-1.14494400
C	4.40792100	-1.17996000	-1.26192000
H	3.71710000	-1.92930300	-1.63134100
C	5.68763700	-1.54951800	-0.86962500
C	6.57906400	-0.60702600	-0.35617800
H	7.57318500	-0.89834000	-0.04121400
C	6.15826700	0.71588200	-0.26054700
C	4.88088900	1.11232600	-0.65457500
H	4.56980400	2.13927000	-0.54718900
C	6.07144200	-3.00172200	-0.89069500
C	7.04187800	1.72701700	0.41331000
Cl	0.92772200	-2.27107700	-1.51601900
H	-1.60273600	-2.43218500	-0.37197800
H	-1.60882000	-1.65689500	-2.31006300
Ir	-1.11320900	-1.06982000	-0.90073700
C	0.52200600	0.64246300	-3.31721900
H	-0.52238500	0.46775400	-3.58157200
H	0.97449600	1.33944700	-4.03403700
H	1.02906300	-0.31826900	-3.36729400

A-TS2-C3

C	-3.44942900	-3.65602700	2.43118600
C	-2.04365900	-3.84476100	2.36745300
H	-1.46943100	-4.50901800	2.99699200

C	-1.49856700	-2.97501900	1.37018300
C	-2.60696800	-2.22857200	0.80829900
C	-3.80066000	-2.67303100	1.46778900
H	-4.79192000	-2.28565300	1.28718300
C	-2.05627700	-2.04699800	-1.93621600
C	-2.65121100	-3.31412900	-2.06882100
H	-3.37831200	-3.65083100	-1.33589400
C	-2.31681700	-4.14163000	-3.13642600
H	-2.78049200	-5.12001500	-3.22620300
C	-1.37107400	-3.72145300	-4.07681500
H	-1.09500200	-4.37511800	-4.89912700
C	-0.78318200	-2.46480100	-3.95266000
H	-0.05152100	-2.12573500	-4.67929500
C	-1.13130800	-1.62345400	-2.89399200
H	-0.66507000	-0.65415600	-2.80468400
C	-4.36731200	-0.71521600	-0.87247700
C	-5.15386100	-0.02810300	0.06518900
H	-4.70581500	0.31872800	0.98690100
C	-6.50324000	0.21792700	-0.17488400
H	-7.09443200	0.74398400	0.56947300
C	-7.08886700	-0.19589300	-1.37407500
H	-8.13801500	0.00659100	-1.56866400
C	-6.31392700	-0.86286600	-2.32039400
H	-6.75447200	-1.18231000	-3.26050800
C	-4.96495900	-1.12703200	-2.07038600
H	-4.38146900	-1.65145000	-2.81667300
P	-2.56838200	-0.97973700	-0.53073500
Fe	-2.46498400	-1.86110400	2.81536900
C	-1.56811200	-0.04950500	3.15615700
C	-2.99811300	0.06877500	3.25510900
H	-3.60710000	0.69899300	2.62564700
C	-3.45669000	-0.78448800	4.29403500
C	-2.32264400	-1.43787300	4.85527200
C	-1.16117200	-0.97806400	4.17251300
H	-0.15499400	-1.29220300	4.39497900
C	-0.84193200	2.62891000	2.80355100
C	0.05741500	2.98532000	3.81780200
H	0.86303200	2.31125700	4.08796300
C	-0.05990600	4.21419600	4.46663200
H	0.65236400	4.48162300	5.24195400
C	-1.08292200	5.09834100	4.11886500
H	-1.17000300	6.05744800	4.62135900
C	-1.99572600	4.74125100	3.12497400
H	-2.79798200	5.42054800	2.85023700
C	-1.87594500	3.51401500	2.47200700
H	-2.57899600	3.24519600	1.69130500
C	1.12359600	0.72196100	2.05346800
C	1.73712500	-0.40313200	2.60926800
H	1.14160600	-1.19885100	3.02197200
C	3.12854900	-0.52512500	2.61968100
H	3.59435300	-1.40974700	3.04302200
C	3.92020400	0.48172500	2.07458500
H	4.99907900	0.37573600	2.07417100
C	3.31611000	1.60252500	1.50035800
H	3.92038600	2.37135400	1.03442700
C	1.93056800	1.72232000	1.48251600
H	1.47896900	2.58994600	1.01759400
P	-0.68423800	0.99164800	1.95147900
H	-4.12801500	-4.13972200	3.12121800
H	-2.33656400	-2.18464400	5.63816100
H	-4.48977600	-0.94710200	4.57076900
S	2.42740900	-4.69130400	-1.49011700
N	0.26891000	-3.61964200	-0.27763800
N	1.99198800	-2.15322600	-0.73494600
H	1.31435100	-1.38994400	-0.82376600
F	6.44220100	1.25214700	-2.59330800
F	4.32764600	1.76416200	-2.71047200
F	5.48228300	2.26580900	-0.93392800
F	6.40097900	-3.81309300	1.19260200
F	6.31531100	-1.98775500	2.36958300
F	7.82369700	-2.20507100	0.81660600
C	-0.03192500	-2.91579500	1.00885200
H	0.23947000	-1.86981900	0.87323800
C	0.85402600	-3.53468700	2.10502500
H	0.75689300	-4.62381900	2.11035300
H	0.58730500	-3.16959100	3.09928500
H	1.90050000	-3.29130400	1.90968800
C	1.53311700	-3.44839500	-0.80870800
C	3.32972900	-1.73189900	-0.73485300
C	3.67243200	-0.54562000	-1.39705300
H	2.93172300	-0.02570800	-1.98662000
C	4.95213600	-0.01534000	-1.26258200
C	5.92246600	-0.66287200	-0.49910500
H	6.91678200	-0.24580000	-0.39183000
C	5.57900200	-1.85467800	0.13852200
C	4.30013000	-2.39287000	0.02514600
H	4.04854800	-3.30918700	0.54276500
C	5.29223700	1.30820300	-1.88699800

C	6.53574000	-2.47472300	1.11302900
Cl	0.63055500	0.64510000	-1.27425500
H	-2.92950500	1.52684000	0.50559600
H	-0.97003200	2.68699400	-0.12180400
Ir	-1.55677900	1.09252700	-0.15721000
C	-0.34459100	-4.93552600	-0.43229400
H	-1.39567400	-4.86270600	-0.15595100
H	-0.26859600	-5.23983600	-1.47370200
H	0.14991800	-5.69883300	0.18182600
C	-0.21413800	3.63798500	-1.95897700
C	-0.72345000	2.44033900	-3.86557900
C	-1.86604300	1.86131800	-3.25706600
C	-1.49667100	3.18937500	-1.34097700
H	0.49350800	2.55584400	-5.62285100
C	-0.39264500	2.10155900	-5.19091400
C	-2.65413500	0.95926200	-3.99279600
H	-2.07541200	3.92998500	-0.78471400
C	-2.30854600	0.63221400	-5.29370700
C	-1.17232400	1.20153100	-5.89927800
H	-3.53429700	0.54133800	-3.51768500
H	-2.92196800	-0.07020700	-5.85089100
H	-0.91039600	0.93740100	-6.91937900
N	-2.26828800	2.23541600	-1.98467600
N	0.10830800	3.28943400	-3.16402200
C	0.77918900	4.30681800	-1.09604000
C	2.14497200	4.16055600	-1.39272800
C	0.40870300	4.96186700	0.08977500
C	3.11183800	4.66243200	-0.52755800
H	2.42627200	3.61042300	-2.28241400
C	1.37899100	5.46279200	0.95720100
H	-0.63652100	5.07846700	0.35454700
C	2.73253700	5.31255200	0.65187500
H	4.16172700	4.51000300	-0.75724800
H	1.07169800	5.94909200	1.87793800
H	3.48955300	5.68650300	1.33547600

A-TS2-N4

C	-3.45658800	-2.95380500	3.15183900
C	-2.27932500	-2.42901300	3.75192900
H	-2.09367100	-2.34347100	4.81349900
C	-1.39932300	-1.97495600	2.72096000
C	-2.05297500	-2.22542300	1.45546400
C	-3.31934000	-2.83687700	1.74150500
H	-4.05153000	-3.14352300	1.01162100
C	0.10571800	-2.96485100	-0.17285100
C	1.35308900	-2.47804000	-0.56276300
H	1.45895700	-1.43262700	-0.82175500
C	2.45639400	-3.33232200	-0.60494600
H	3.41450000	-2.95543300	-0.93989600
C	2.31915800	-4.66712100	-0.23511000
H	3.18268100	-5.32479500	-0.25402200
C	1.07541500	-5.15697800	0.17672700
H	0.96985300	-6.19603700	0.47607400
C	-0.02837500	-4.31063600	0.20685100
H	-0.99711000	-4.69058100	0.51864500
C	-2.49799200	-2.75874300	-1.33184500
C	-3.85790100	-2.41417700	-1.35861300
H	-4.23765300	-1.66377100	-0.67523600
C	-4.72523600	-3.00321100	-2.27573900
H	-5.77403000	-2.72020000	-2.27762600
C	-4.24155200	-3.93200800	-3.20045600
H	-4.91478700	-4.38801300	-3.92070400
C	-2.88667500	-4.26332700	-3.19743300
H	-2.49881100	-4.97803700	-3.91802600
C	-2.01911300	-3.68428600	-2.26821700
H	-0.96875200	-3.95300200	-2.27551400
P	-1.35320200	-1.86049700	-0.20048900
Fe	-3.19014500	-0.96517200	2.62443300
C	-3.55836000	0.83430900	1.63523500
C	-4.78712600	0.23106800	2.07258100
H	-5.60081800	-0.07446400	1.43216600
C	-4.73993500	0.09584200	3.48931200
C	-3.48129000	0.59454900	3.93901300
C	-2.74341700	1.02917700	2.79997200
H	-1.72623600	1.39095200	2.78819600
C	-4.71141600	1.17973700	-0.95803900
C	-5.86086400	1.78794700	-0.42211000
H	-5.79849900	2.32462300	0.51916600
C	-7.07712000	1.72080600	-1.09626600
H	-7.95701900	2.19270600	-0.66858000
C	-7.16206200	1.05599400	-2.32358400
H	-8.11086900	1.00524000	-2.85013800
C	-6.02292100	0.47062000	-2.87294000
H	-6.07519100	-0.03903400	-3.83065000
C	-4.80267100	0.53665300	-2.19548500
H	-3.91810100	0.08317000	-2.62421900
C	-2.96468900	3.18178000	0.03586000
C	-3.48404800	3.96146600	-1.01108000
H	-4.03731400	3.49082300	-1.81649800

C	-3.29651400	5.34331200	-1.02792500
H	-3.70981000	5.92994800	-1.84353000
C	-2.58334000	5.96812000	-0.00258300
H	-2.43904300	7.04469600	-0.01414000
C	-2.05169300	5.19795600	1.03186400
H	-1.48160700	5.66945900	1.82696500
C	-2.23565100	3.81551900	1.05091200
H	-1.78568500	3.23700600	1.84380700
P	-3.11324300	1.34179500	-0.05757700
H	-4.32389800	-3.33500900	3.67456500
H	-3.12327600	0.58681600	4.95986400
H	-5.50625000	-0.35178100	4.10821800
S	3.69761800	-2.84564300	2.89770800
N	1.06331600	-2.33479700	2.78872200
N	2.44661200	-0.69728200	1.89744700
H	1.61568700	-0.14692400	1.68411500
F	5.59368200	4.14850200	0.59165400
F	3.96587300	4.02609800	2.03587700
F	6.00090400	3.55934700	2.64002800
F	6.70757300	-0.14903700	-1.92195400
F	6.43703200	-2.01640300	-0.83840300
F	7.95026000	-0.58356700	-0.19877600
C	-0.04320600	-1.34974700	2.93012300
H	0.04707000	-0.61238300	2.13726200
C	0.09772800	-0.62851600	4.27831900
H	0.03705200	-1.33359500	5.11347300
H	-0.67922100	0.12762300	4.40567000
H	1.07297200	-0.13609800	4.32545400
C	2.34051000	-1.92233800	2.50338100
C	3.62674300	-0.06239600	1.45705200
C	3.77936900	1.29704400	1.73573900
H	3.02346700	1.81322500	2.31454200
C	4.89715800	1.98578900	1.26248500
C	5.86059300	1.33573500	0.49544800
H	6.72386500	1.87439700	0.12090200
C	5.68808600	-0.01964400	0.20634900
C	4.58907700	-0.72282800	0.68655900
H	4.46985100	-1.77139200	0.46980600
C	5.10660300	3.42599400	1.63520800
C	6.69321000	-0.70007800	-0.67758900
Ir	-1.27724500	0.38284200	-0.89789600
H	-2.11312400	-0.14084400	-2.13296700
Cl	0.23534200	1.40627300	0.83514300
H	-1.25273000	1.81660900	-1.88456400
C	1.79657300	0.50636900	-2.67223200
C	2.10297500	2.58185000	-1.72304100
C	0.74378600	2.93368300	-1.94428400
C	0.41484500	0.81203000	-2.89016000
H	3.99747100	3.26570900	-0.99414300
C	2.95967700	3.53643600	-1.13281200
C	0.25475500	4.18965100	-1.54662300
H	-0.20719300	0.20430400	-3.53348200
C	1.10850000	5.09006400	-0.93970300
C	2.46799900	4.76349100	-0.73755200
H	-0.79317400	4.41986400	-1.70295900
H	0.72782400	6.05314300	-0.61406700
H	3.13207300	5.47463800	-0.25702800
N	-0.09961000	2.03292200	-2.57158600
N	2.61043800	1.37015800	-2.09337800
C	2.37541200	-0.77363800	-3.14731200
C	3.76129000	-0.96879100	-3.03662200
C	1.58967500	-1.80061300	-3.69471600
C	4.34708500	-2.15769100	-3.46146700
H	4.36221700	-0.17581900	-2.61196800
C	2.17879300	-2.98680300	-4.12632500
H	0.51149700	-1.69815100	-3.75852600
C	3.55761000	-3.17121900	-4.01117600
H	5.41843200	-2.29013600	-3.35009100
H	1.55570100	-3.77465200	-4.53997900
H	4.01253100	-4.10095400	-4.34076600
C	0.88841200	-3.61796300	3.46248700
H	1.15972700	-3.56576100	4.52471100
H	-0.15380900	-3.91984400	3.36340000
H	1.52499900	-4.36001500	2.98622300

A-TS2-N1

C	-0.53578800	-4.44956700	-0.04523100
C	-0.98984400	-3.80475700	-1.22400900
H	-1.38364400	-4.29217600	-2.10282500
C	-0.84466000	-2.39831400	-1.07245200
C	-0.25007300	-2.16598000	0.22411600
C	-0.09001300	-3.45001200	0.85731600
H	0.31355700	-3.62521500	1.84093000
C	-1.38922100	0.19731600	1.35479000
C	-1.51189700	1.58297600	1.50256500
H	-0.66962700	2.21910300	1.25165400
C	-2.69339700	2.14264600	1.99721200
H	-2.77013100	3.21975800	2.11941600
C	-3.76433100	1.31787600	2.34778500

H	-4.68514400	1.74749900	2.72951400
C	-3.65646600	-0.06516900	2.17648400
H	-4.49759200	-0.71047600	2.40935300
C	-2.47710600	-0.62422000	1.68929800
H	-2.40682600	-1.69826300	1.55941900
C	0.77752200	-1.06577500	2.65402800
C	1.82009400	-1.98864200	2.81361100
H	2.27398400	-2.44457500	1.94446700
C	2.28899100	-2.32608500	4.08114200
H	3.10250900	-3.03883100	4.17660800
C	1.73535500	-1.72786900	5.21399500
H	2.10410800	-1.98371900	6.20320700
C	0.70743200	-0.79650400	5.06619400
H	0.26960800	-0.32325000	5.94061800
C	0.22680800	-0.47009600	3.79664800
H	-0.57673000	0.25062100	3.70349800
P	0.23638400	-0.57032700	0.95559700
Fe	1.00780300	-3.34171900	-0.88941500
C	2.90784600	-2.47033700	-1.07708800
C	2.99503900	-3.79148400	-0.51756600
H	3.40154200	-4.04241700	0.45077000
C	2.44310000	-4.71383300	-1.45320400
C	1.99313500	-3.97471400	-2.58701900
C	2.25657500	-2.59470000	-2.35109000
H	1.97501800	-1.76884600	-2.98637900
C	4.56179000	-1.40227700	1.05588600
C	5.46498100	-2.47377600	0.94450200
H	5.51680300	-3.04386700	0.02296300
C	6.31519100	-2.79444500	2.00044600
H	7.00226000	-3.63041800	1.90454300
C	6.29614100	-2.03004300	3.17153600
H	6.96497000	-2.27591300	3.99172800
C	5.42756700	-0.94515200	3.27553400
H	5.41308800	-0.33254100	4.17144800
C	4.56237000	-0.63513900	2.22530400
H	3.88527900	0.20418800	2.31698800
C	4.83573900	-0.32417100	-1.54159800
C	6.10075000	0.04845200	-1.05604800
H	6.35317600	-0.10826000	-0.01486000
C	7.04271800	0.63311500	-1.90370600
H	8.01520100	0.91459100	-1.50878100
C	6.74028400	0.85140300	-3.24835400
H	7.47202200	1.31102700	-3.90644700
C	5.48809500	0.47961200	-3.73907200
H	5.23421400	0.65623300	-4.77987600
C	4.54118600	-0.09803000	-2.89505300
H	3.55922800	-0.32589300	-3.28281900
P	3.52466300	-0.89869000	-0.37523800
H	-0.49907300	-5.51733200	0.12527400
H	1.48672000	-4.38203100	-3.45190700
H	2.34084200	-5.78060300	-1.30400800
S	-3.99801400	-2.47514700	-1.16219200
N	-2.31349600	-0.44194300	-1.71408500
N	-4.38607500	0.19249000	-1.00051700
H	-3.90975200	1.06422200	-0.81470100
F	-9.03237500	2.87387300	1.66888000
F	-7.12871800	2.63822500	2.69687300
F	-7.24042200	3.84831200	0.89878300
F	-8.89169400	-2.64629600	0.49950900
F	-8.74054500	-2.39697600	-1.65335200
F	-10.22499300	-1.26988800	-0.52375300
C	-1.20916600	-1.36417100	-2.10681400
H	-0.34806700	-0.70547300	-2.18195200
C	-1.45478200	-1.94286000	-3.50271100
H	-2.34036300	-2.58159000	-3.52443500
H	-0.58268700	-2.52281700	-3.82078700
H	-1.59334900	-1.12377800	-4.21541700
C	-3.54224600	-0.86336200	-1.31074300
C	-5.71135000	0.21778500	-0.55021200
C	-6.10177100	1.37190700	0.14293200
H	-5.38255200	2.16611900	0.31034800
C	-7.39302000	1.50280500	0.64359300
C	-8.33945500	0.50181300	0.44091000
H	-9.34579700	0.60273800	0.82593500
C	-7.96074500	-0.62434200	-0.29018800
C	-6.66823000	-0.77983800	-0.78895500
H	-6.40099000	-1.66223100	-1.34883000
C	-7.71073800	2.71594800	1.46907200
C	-8.95571900	-1.73538200	-0.49779200
Ir	1.84716000	0.68042800	-0.01527300
H	2.27863500	0.83155500	1.48664700
Cl	1.33413600	0.75153500	-2.48528600
H	1.02556200	2.18938500	0.33120300
C	3.06214300	2.88717500	-0.18592600
C	1.14123400	3.72576900	-1.29728200
C	1.89326800	3.81994100	-2.49364100
C	3.73368300	2.94706600	-1.46377000
H	-0.76583900	4.02822600	-0.34856200

C	-0.20753900	4.12191400	-1.27536300
C	1.27601300	4.34994800	-3.64490100
C	-0.05137900	4.73525700	-3.61362200
C	-0.79993200	4.61446200	-2.42446400
H	1.87017200	4.41355000	-4.55045800
H	-0.52429500	5.12781300	-4.50888700
H	-1.84214600	4.91992500	-2.40866800
N	3.20506300	3.40364200	-2.56244000
N	1.72755000	3.25708500	-0.12608900
C	3.82288100	2.88772200	1.09082100
C	3.16510100	3.17723200	2.30029100
C	5.19632000	2.59647900	1.13355700
C	3.84920700	3.13604800	3.51117000
H	2.10950200	3.42080500	2.27585600
C	5.87954700	2.56385500	2.34752400
H	5.73787300	2.37012400	0.22425100
C	5.21151500	2.82452800	3.54411600
H	3.31714400	3.35296500	4.43326500
H	6.93918900	2.32480700	2.35515100
H	5.74597400	2.79636900	4.48933400
C	-2.08251600	0.97459300	-2.03034100
H	-2.03552500	1.58750500	-1.12110500
H	-1.11614200	1.08052600	-2.51800600
H	-2.86665800	1.35925000	-2.69160700
H	4.76071200	2.60311700	-1.52822200

A-TS2-C2

C	1.38383500	-3.86540400	-3.46603700
C	0.03609100	-3.47161500	-3.27144600
H	-0.77975300	-3.67144600	-3.95003300
C	-0.06292400	-2.71941400	-2.05823000
C	1.26682600	-2.65668300	-1.47809200
C	2.14369800	-3.36401000	-2.37540100
H	3.21501700	-3.42998500	-2.28448000
C	0.91177400	-2.86180400	1.37798300
C	1.36096900	-4.13445800	1.76777500
H	2.26064800	-4.56050400	1.34806400
C	0.66848200	-4.86655900	2.73091600
H	1.03401300	-5.84861200	3.01817000
C	-0.48387900	-4.34365300	3.32214900
H	-1.02409200	-4.91755600	4.06951500
C	-0.92959600	-3.07754500	2.95074000
H	-1.81737600	-2.64949400	3.40326300
C	-0.23289400	-2.34311000	1.99211900
H	-0.56428000	-1.34492600	1.75356000
C	3.54666100	-2.40557100	0.29089100
C	4.47313800	-1.51564300	0.85537100
H	4.15089600	-0.52401100	1.13872000
C	5.79197700	-1.90687600	1.09230700
H	6.48570200	-1.19467500	1.53041700
C	6.21500600	-3.19600300	0.77483100
H	7.24237700	-3.49884900	0.95559600
C	5.30128100	-4.09973600	0.23066800
H	5.61047400	-5.11251900	-0.01167400
C	3.98282900	-3.71120700	-0.00254900
H	3.29779700	-4.43922600	-0.41780000
P	1.78497600	-1.85060700	0.09158800
Fe	1.28233000	-1.80044100	-3.33633400
C	1.33273900	0.23412200	-3.18094400
C	2.65899700	-0.29914600	-3.34213500
H	3.45022600	-0.22408300	-2.60910600
C	2.71901400	-0.98187600	-4.58703700
C	1.44023300	-0.88097900	-5.20776200
C	0.59142900	-0.11843000	-4.35731300
H	-0.43242500	0.14024700	-4.57388300
C	1.91047900	2.76600200	-2.26648300
C	1.36704700	3.62746300	-3.23304600
H	0.35848900	3.46368900	-3.59813200
C	2.11397700	4.69649500	-3.72291600
H	1.68003300	5.36034100	-4.46526200
C	3.41613400	4.91221300	-3.26308200
H	3.99732300	5.74612300	-3.64653600
C	3.96411700	4.05534400	-2.31011400
H	4.96903100	4.21926400	-1.93420700
C	3.21506300	2.98719100	-1.81255800
H	3.64365000	2.33138100	-1.06434500
C	-0.76123300	1.85746600	-1.83053200
C	-1.78786000	1.15065000	-2.46028400
H	-1.57199100	0.23153100	-2.97861400
C	-3.10567300	1.60822000	-2.40833800
H	-3.89178700	1.03895200	-2.89536500
C	-3.41120900	2.77635100	-1.71523900
H	-4.43601200	3.12225300	-1.64705400
C	-2.39377800	3.48447700	-1.06959400
H	-2.63663500	4.37237600	-0.49540100
C	-1.08063600	3.02884000	-1.12375000
H	-0.30094800	3.57207800	-0.59943800
P	0.96725900	1.27018800	-1.73586200
H	1.77815300	-4.39689900	-4.32189700

H	1.14831900	-1.33418200	-6.14597300
H	3.56832400	-1.53584800	-4.96429600
S	-4.13753100	-3.40728400	1.02202600
N	-1.90663700	-2.90071900	-0.38207800
N	-3.11010000	-1.03675700	0.24659600
H	-2.23922300	-0.51244900	0.35961800
F	-6.05657300	3.60089900	2.41313400
F	-3.89553400	3.46705200	2.16024000
F	-5.14747800	4.17431400	0.52852700
F	-8.73400500	0.74655500	-0.87435800
F	-8.62052000	-0.95155700	0.47549100
F	-7.83086400	-1.12184100	-1.54062300
C	-1.35966000	-2.13948900	-1.54309100
H	-1.15143200	-1.12527400	-1.20217100
C	-2.43938700	-2.10858400	-2.64068900
H	-2.79090800	-3.12319400	-2.85080600
H	-2.06081100	-1.67955000	-3.57194700
H	-3.29196800	-1.51782000	-2.30168600
C	-3.01800600	-2.41852800	0.26058200
C	-4.26509800	-0.26123200	0.40521100
C	-4.13598900	1.01554500	0.97042800
H	-3.17171000	1.34710700	1.33276900
C	-5.23596000	1.86466300	1.03207500
C	-6.48504100	1.46440200	0.55758000
H	-7.33918400	2.12839200	0.61144100
C	-6.60544600	0.19260600	-0.00034000
C	-5.51150400	-0.66670300	-0.08866100
H	-5.62549300	-1.64211400	-0.54042600
C	-5.07639500	3.26690200	1.54608700
C	-7.94675700	-0.28307200	-0.48569500
Cl	-0.67296300	0.85576000	1.29582800
H	3.08852500	0.47328000	-0.28745900
H	1.75400500	2.13573800	0.89899700
Ir	1.62550900	0.48266200	0.31083900
C	-1.63748100	-4.33330300	-0.32401000
H	-0.60104900	-4.50828700	-0.60730200
H	-1.79203900	-4.67925000	0.69591600
H	-2.30576400	-4.90027700	-0.98475900
C	2.37749400	2.00442900	2.10424500
C	1.88476700	0.09264100	3.44685200
C	1.05863000	0.88417600	4.28156200
C	1.44064000	2.74800000	2.99775800
H	2.79529300	-1.83560400	3.18130500
C	2.13803600	-1.24271400	3.80612200
C	0.47241100	0.32030100	5.42618300
H	1.26539500	3.80012900	2.77946700
C	0.70735300	-1.00746100	5.75052100
C	1.55380900	-1.78379400	4.94036800
H	-0.16004300	0.95672000	6.03687600
H	0.24810500	-1.44355400	6.63237600
H	1.74583900	-2.82166600	5.19407000
N	0.83791200	2.22696300	4.00469100
N	2.52078600	0.63177100	2.33807100
C	3.65077800	2.75090600	1.77071500
C	4.88983100	2.17162700	2.05970400
C	3.60462600	4.03865000	1.22531800
C	6.06900400	2.86645900	1.78988600
H	4.90981600	1.18144800	2.50063800
C	4.78217200	4.73912000	0.97230600
H	2.64792200	4.48550100	0.96917000
C	6.01925800	4.15259500	1.24852400
H	7.02773100	2.40730800	2.01457900
H	4.73256700	5.73566700	0.54357700
H	6.93772000	4.69661200	1.04751200

A-4

C	3.43115500	-3.81383800	-2.20240300
C	2.02511900	-3.99383000	-2.12159800
H	1.44757400	-4.70102400	-2.69924600
C	1.48423800	-3.05314800	-1.18898100
C	2.59518700	-2.26880500	-0.68695000
C	3.78714800	-2.76342000	-1.31539800
H	4.77985200	-2.36692800	-1.16578800
C	2.05339800	-1.87668200	2.04715200
C	2.60876800	-3.15178600	2.25345200
H	3.29694000	-3.56830600	1.52423700
C	2.28488600	-3.88533500	3.39062800
H	2.71596600	-4.87177800	3.53652900
C	1.39249100	-3.36034700	4.33031100
H	1.12520500	-3.94048300	5.20872600
C	0.84786700	-2.09333500	4.13482400
H	0.16057300	-1.67151900	4.86137700
C	1.18391300	-1.34656700	3.00391300
H	0.75137000	-0.36867300	2.86093200
C	4.37638500	-0.65994100	0.87482000
C	5.16607500	-0.03707900	-0.10418100
H	4.71749100	0.26864800	-1.04021600
C	6.52105700	0.19883300	0.11297300
H	7.11453400	0.67528300	-0.66225600

C	7.10963700	-0.16109800	1.32803200
H	8.16340800	0.03416700	1.50400100
C	6.33191800	-0.76422200	2.31398000
H	6.77455600	-1.04020800	3.26671500
C	4.97679200	-1.01823100	2.08853800
H	4.39057100	-1.49015100	2.86684600
P	2.57320200	-0.93121900	0.56205500
Fe	2.45026900	-2.04841600	-2.71370300
C	1.54579900	-0.26985100	-3.18251000
C	2.97593000	-0.15218000	-3.28380900
H	3.57991600	0.51836600	-2.69268900
C	3.44271300	-1.07186400	-4.26030500
C	2.31407500	-1.76803000	-4.77919200
C	1.14764900	-1.26839600	-4.13383500
H	0.14474000	-1.60461300	-4.33775700
C	0.80241400	2.42859600	-2.95728400
C	-0.13226800	2.76368200	-3.94674300
H	-0.95685500	2.09306600	-4.16156100
C	-0.02462300	3.96781700	-4.64200700
H	-0.76324500	4.21810000	-5.39816800
C	1.02179500	4.84952800	-4.36496000
H	1.10031900	5.79008200	-4.90261400
C	1.96908800	4.51368700	-3.39629800
H	2.78989200	5.19071500	-3.17644700
C	1.86080300	3.31041000	-2.69837500
H	2.59296300	3.05974200	-1.93850000
C	-1.14659300	0.54815900	-2.10443900
C	-1.76369500	-0.59493800	-2.61873000
H	-1.17107000	-1.40256400	-3.01189700
C	-3.15485900	-0.72005200	-2.61210100
H	-3.62190300	-1.61969500	-3.00125100
C	-3.94427300	0.30266900	-2.09385500
H	-5.02274100	0.19439400	-2.07949300
C	-3.33781700	1.44324100	-1.56319600
H	-3.93952100	2.22700200	-1.11889700
C	-1.95212100	1.56554400	-1.56080100
H	-1.50083800	2.45126600	-1.13147800
P	0.66185200	0.82947900	-2.03091400
H	4.10690800	-4.34836900	-2.85674200
H	2.33456400	-2.56621800	-5.50941600
H	4.47761700	-1.24769200	-4.52170100
S	-2.41870000	-4.56446400	1.81222500
N	-0.27038900	-3.58432400	0.50903400
N	-1.98762600	-2.08539800	0.87846700
H	-1.31023200	-1.31786400	0.91582300
F	-6.44405900	1.38162100	2.57613100
F	-4.33987700	1.94521000	2.60039800
F	-5.55268400	2.30263900	0.82696400
F	-6.39341100	-3.89972200	-0.90231500
F	-6.33810100	-2.15431100	-2.19624100
F	-7.82916600	-2.28458700	-0.61706500
C	0.01998600	-2.96939100	-0.82452800
H	-0.25172800	-1.91684200	-0.75844000
C	-0.87188100	-3.66193400	-1.87038300
H	-0.77881500	-4.74900300	-1.79814700
H	-0.60653400	-3.36997100	-2.88870100
H	-1.91653800	-3.40028100	-1.69020700
C	-1.52928000	-3.37325000	1.03869300
C	-3.32690600	-1.66950400	0.85852800
C	-3.67368900	-0.44482500	1.44401900
H	-2.93166100	0.12013400	1.98942000
C	-4.96115200	0.06138700	1.28978200
C	-5.93195200	-0.64331600	0.57938400
H	-6.93174100	-0.24387200	0.45691700
C	-5.58215200	-1.86930400	0.01450200
C	-4.29698200	-2.38617200	0.15028200
H	-4.04053700	-3.33123600	-0.31004200
C	-5.31483500	1.41531900	1.83597600
C	-6.54142900	-2.56038700	-0.90844900
Cl	-0.60840000	0.74355000	1.22669800
H	2.95206100	1.44795400	-0.62697600
H	1.02302100	2.79117700	0.00303600
Ir	1.58082300	1.07871000	0.07346800
C	0.33623800	-4.89192200	0.74278300
H	1.38324900	-4.84717800	0.44577200
H	0.27413000	-5.12525600	1.80325700
H	-0.17358400	-5.69052800	0.18920200
C	0.20255400	3.76546800	1.70576600
C	0.84701200	2.76400900	3.68480800
C	1.94979300	2.11837500	3.06766700
C	1.46990900	3.28624900	1.04635400
H	-0.25507000	3.07478900	5.49030400
C	0.60246500	2.57081300	5.05530700
C	2.77826000	1.29217300	3.84777300
H	2.06777100	4.06007900	0.54733200
C	2.51494800	1.10483600	5.19586400
C	1.42337700	1.74490300	5.80906800
H	3.62747600	0.81943000	3.36777400

H	3.16304100	0.45995400	5.78304600
H	1.22564300	1.59455900	6.86605200
N	2.26729500	2.34174400	1.73888200
N	-0.04284700	3.53184800	2.95076200
C	-0.84064200	4.34208800	0.83593000
C	-2.19006500	4.21477600	1.20590600
C	-0.52956800	4.89812300	-0.41622200
C	-3.19932300	4.63524900	0.34593600
H	-2.42454900	3.74350300	2.15258400
C	-1.54246600	5.32124000	-1.27663500
H	0.50200100	4.99940800	-0.73607200
C	-2.87927100	5.18746800	-0.89941300
H	-4.23657400	4.49552100	0.63262300
H	-1.28123900	5.73440000	-2.24601500
H	-3.66991300	5.49917600	-1.57619300

A-TS3

C	5.15774800	2.14126400	-1.51029000
C	3.99910000	2.96670900	-1.52788000
H	3.98939300	4.04347400	-1.62398800
C	2.84684600	2.14176100	-1.34840100
C	3.30445800	0.78137800	-1.20056700
C	4.73675800	0.79589900	-1.31943200
H	5.38346700	-0.06176000	-1.21284800
C	1.58791700	-0.89242600	-2.63652500
C	2.36214100	-0.58873700	-3.76658100
H	3.38116300	-0.23412700	-3.65046900
C	1.81500600	-0.69364300	-5.04454700
H	2.42377000	-0.45272600	-5.91155100
C	0.48297400	-1.07854900	-5.20752500
H	0.05221700	-1.14080900	-6.20218600
C	-0.30017100	-1.35829500	-4.08805400
H	-1.34112500	-1.64190300	-4.20067300
C	0.24985100	-1.26580600	-2.81205500
H	-0.36503900	-1.47768000	-1.94725100
C	3.62538400	-1.95616800	-0.76208500
C	3.94008700	-2.41665700	0.52323200
H	3.34810200	-2.07367800	1.36535800
C	4.96528800	-3.34246900	0.72037800
H	5.18990500	-3.69235600	1.72401300
C	5.68314200	-3.83127600	-0.37184900
H	6.47332700	-4.56146900	-0.22409800
C	5.36661100	-3.39035000	-1.65880900
H	5.90812300	-3.77964000	-2.51625500
C	4.34776700	-2.45771700	-1.85317400
H	4.09669100	-2.14609100	-2.85975200
P	2.27149700	-0.70496900	-0.93715000
Fe	4.10027100	1.92403300	0.26422700
C	3.06923700	1.54414600	1.97970500
C	4.30325400	0.80533600	1.95052600
H	4.40550700	-0.26691400	1.91129500
C	5.38343000	1.73028900	1.88092800
C	4.83866000	3.04630100	1.85787400
C	3.42198800	2.93804200	1.92040200
H	2.72367900	3.75966100	1.89779800
C	1.31349000	0.06892800	3.71135300
C	0.18326300	0.22548300	4.52595000
H	-0.63042100	0.86275700	4.20345600
C	0.09015500	-0.45535100	5.73910700
H	-0.79269400	-0.32459700	6.35825600
C	1.11796100	-1.30406100	6.15340500
H	1.04183000	-1.83412300	7.09845900
C	2.24423600	-1.46837100	5.34588800
H	3.05160800	-2.12422900	5.65959100
C	2.33878800	-0.78894400	4.13178900
H	3.21910000	-0.93098100	3.51782100
C	0.39340500	2.39956300	2.31250100
C	0.70056300	3.23318600	3.40161700
H	1.51015100	2.96801100	4.07464400
C	-0.03449500	4.39365600	3.63160300
H	0.21268400	5.02942900	4.47704300
C	-1.09501900	4.72897900	2.78453300
H	-1.67525400	5.62845800	2.96946000
C	-1.41859800	3.89854500	1.71261900
H	-2.26257500	4.13686300	1.07396000
C	-0.67671900	2.73859500	1.47957100
H	-0.95346200	2.08514200	0.66668700
P	1.37380700	0.86489800	2.04520200
H	6.18318100	2.48016500	-1.57581400
H	5.39806500	3.96747200	1.76297900
H	6.43053800	1.47028300	1.79994400
S	-1.41544800	2.50164500	-4.19736000
N	0.81642100	2.25954300	-2.72214700
N	-1.12455100	1.49186200	-1.72950400
H	-0.59778000	0.77968000	-1.22373800
F	-6.68764900	-0.47911000	-0.63381300
F	-4.94862600	-1.72323100	-1.05591400
F	-5.26209400	-0.91578300	0.94383500
F	-4.68244700	5.14083900	-1.87663400

F	-4.53366500	4.96083500	0.28056400
F	-6.35260900	4.33033200	-0.73483300
C	1.41132800	2.58411100	-1.39517300
H	0.87238100	2.00130200	-0.65325000
C	1.21146200	4.06848000	-1.07346300
H	1.69429700	4.71082600	-1.81615100
H	1.61861000	4.30419800	-0.08723700
H	0.14341700	4.30013500	-1.06410400
C	-0.53512300	2.07640400	-2.83678300
C	-2.49503000	1.58817400	-1.42247500
C	-3.23714400	0.44911400	-1.10857700
H	-2.77870700	-0.53165100	-1.14941200
C	-4.57665400	0.58401800	-0.74082900
C	-5.18275300	1.83605100	-0.67058800
H	-6.22388700	1.92780400	-0.38948800
C	-4.42815900	2.96720500	-0.98020500
C	-3.09478800	2.84900400	-1.35701700
H	-2.51578400	3.72967400	-1.60666200
C	-5.36844000	-0.63955400	-0.37238100
C	-5.00892200	4.34382800	-0.83790200
Cl	-1.51100600	-0.43502800	1.70614600
H	1.21805400	-2.42750900	0.99785700
Ir	0.62443900	-0.75772700	0.63500000
C	1.54661200	2.72272100	-3.89771900
H	2.61257200	2.57084400	-3.72733900
H	1.23291600	2.13894500	-4.76104800
H	1.35040900	3.78036000	-4.11109500
C	-2.35657900	-3.62486400	0.45186500
C	-1.15683900	-4.10106900	-1.45848800
C	0.07552300	-3.68111300	-0.88896100
C	-1.02821200	-3.48793300	1.17763300
H	-2.10782400	-5.02959800	-3.12588000
C	-1.14974900	-4.74793500	-2.69970300
C	1.27005300	-4.03040800	-1.51552400
H	-0.70240300	-4.49796500	1.48742700
C	1.26010400	-4.69319900	-2.74242400
C	0.04971100	-5.03297700	-3.35029200
H	2.20516400	-3.78874400	-1.03494100
H	2.20432100	-4.94307700	-3.21811600
H	0.04037200	-5.53716500	-4.31196800
N	-0.03493100	-2.90348500	0.27730300
N	-2.38097600	-3.88756100	-0.81585000
C	-3.62075000	-3.60540100	1.21096600
C	-4.77739000	-4.14715000	0.62055400
C	-3.70376500	-3.10963200	2.52200100
C	-5.97921400	-4.18223800	1.31549400
H	-4.70234400	-4.53054800	-0.39012700
C	-4.91118400	-3.14732600	3.21737700
H	-2.84201700	-2.65229600	2.99168000
C	-6.05162000	-3.68140700	2.61902700
H	-6.86343500	-4.60167100	0.84349700
H	-4.96121600	-2.74583600	4.22561100
H	-6.99235900	-3.70698500	3.16223300
H	-1.11072100	-2.87337600	2.06676600

A-5

C	5.50365200	1.98056100	0.00459500
C	4.46387600	2.86262100	0.41600000
H	4.59881700	3.79384100	0.94861000
C	3.20463500	2.28481000	0.06575200
C	3.47839200	1.01603400	-0.56808300
C	4.90144300	0.84776000	-0.61294700
H	5.41564900	-0.02261100	-0.99517900
C	1.74614400	0.76134200	-2.72640000
C	2.69246300	1.49369800	-3.46168100
H	3.72509900	1.53441900	-3.12940200
C	2.30729100	2.20965600	-4.59356800
H	3.04849800	2.77560000	-5.15108600
C	0.96757600	2.22605300	-4.99021600
H	0.66302100	2.80780700	-5.85492600
C	0.01819300	1.51867600	-4.25520400
H	-1.02851800	1.54362800	-4.53870400
C	0.40924800	0.78463400	-3.13698500
H	-0.33205400	0.24112000	-2.56667800
C	3.27235600	-1.54885200	-1.80127500
C	3.31565700	-2.70543400	-1.00578800
H	2.73361800	-2.71935700	-0.08739000
C	4.05933100	-3.81975800	-1.39693700
H	4.07971800	-4.70521600	-0.76752800
C	4.76453500	-3.79654500	-2.60153500
H	5.33777100	-4.66382500	-2.91574000
C	4.71744000	-2.65755300	-3.40830700
H	5.25354800	-2.63866600	-4.35296500
C	3.97662900	-1.54210800	-3.01313500
H	3.93447000	-0.67266600	-3.65912800
P	2.22271500	-0.14430500	-1.19076100
Fe	4.21371100	1.00958400	1.31358300
C	2.89487700	0.00592800	2.50239900
C	3.98138600	-0.85093100	2.10907100

H	3.90534000	-1.73353100	1.49463300
C	5.19963000	-0.29394000	2.59156900
C	4.88994300	0.91397100	3.28010500
C	3.47980500	1.10084600	3.22893300
H	2.94135800	1.94183600	3.63607800
C	0.76126000	-1.81675900	3.06855000
C	-0.32133300	-1.88192000	3.95407200
H	-0.92395400	-1.00121200	4.13659100
C	-0.65472500	-3.08487000	4.57732100
H	-1.50416900	-3.11760300	5.25314700
C	0.08326100	-4.24081900	4.32279800
H	-0.17848300	-5.17653200	4.80881600
C	1.15723200	-4.18926700	3.43113900
H	1.73731300	-5.08384900	3.22088400
C	1.48838800	-2.98729500	2.80683700
H	2.31367600	-2.96819000	2.10599100
C	0.29505500	1.01887600	3.13181700
C	0.64234800	1.21695600	4.47907300
H	1.42115000	0.61294000	4.93372900
C	-0.02410100	2.17071600	5.24567400
H	0.25527200	2.31777900	6.28525300
C	-1.05991900	2.92255800	4.68299600
H	-1.58416400	3.65998800	5.28422300
C	-1.43546700	2.70743800	3.35737400
H	-2.26870700	3.25457400	2.92816800
C	-0.76055900	1.75769400	2.58785900
H	-1.07573700	1.56322300	1.57470500
P	1.12694700	-0.26797400	2.11372500
H	6.56275800	2.12214500	0.17482000
H	5.60177000	1.59704700	3.72433700
H	6.18964500	-0.69258300	2.41383500
S	-0.78362900	4.59772000	-2.21563500
N	1.30668800	3.42945000	-1.00486900
N	-0.73640400	2.37268200	-0.72357200
H	-0.25303200	1.47883500	-0.53667600
F	-6.27615800	0.14370400	-1.51804100
F	-4.46887700	-0.56196600	-2.50902100
F	-4.87405600	-1.11773100	-0.44422600
F	-4.53714300	5.55535700	0.60670000
F	-4.53462400	4.26783300	2.35265300
F	-6.22653400	4.23163400	0.98363300
C	1.83923000	2.89207200	0.27326900
H	1.17654000	2.08774500	0.57893800
C	1.79956100	3.97145900	1.36018200
H	2.41711700	4.83604600	1.09800100
H	2.14983400	3.56814600	2.31318000
H	0.76944100	4.31226200	1.49368200
C	-0.03868800	3.42566800	-1.26749300
C	-2.14100900	2.32077000	-0.61340100
C	-2.84145100	1.20385300	-1.07096200
H	-2.31872600	0.39919100	-1.57069400
C	-4.21965900	1.11732500	-0.86633100
C	-4.90892200	2.12931700	-0.20363800
H	-5.97754600	2.05766700	-0.04937900
C	-4.19947400	3.24183400	0.25117400
C	-2.82740500	3.34369700	0.04684300
H	-2.28171900	4.21079100	0.39759400
C	-4.95768500	-0.10773300	-1.33230600
C	-4.88230100	4.32338800	1.03614500
Cl	-1.72464800	-1.09748300	1.00603400
H	1.00109700	-2.77765200	-1.58434000
Ir	0.46497100	-0.79596900	0.03916500
C	2.13757800	4.41949100	-1.68246300
H	3.18383800	4.14753700	-1.53450300
H	1.91060800	4.40891900	-2.74722500
H	1.95920000	5.43303800	-1.30514500
C	-2.14274100	-3.50000800	-0.77124900
C	-1.94898300	-2.59665600	-2.89043600
C	-0.55933900	-2.40673900	-2.78399400
C	-0.63042500	-3.62399500	-0.70968400
H	-3.63550300	-2.50902700	-4.19179600
C	-2.55964900	-2.38743300	-4.13306700
C	0.21068600	-2.11259200	-3.90353000
H	-0.34664900	-4.59353000	-1.15284400
C	-0.41042700	-1.93461000	-5.14155900
C	-1.79725700	-2.05254400	-5.25128200
H	1.28591000	-2.00056000	-3.80713000
H	0.19149000	-1.68637800	-6.01012500
H	-2.28324300	-1.89729900	-6.20979500
N	0.02204400	-2.52426500	-1.47115900
N	-2.73218500	-3.02169600	-1.81341100
C	-2.95747900	-4.05832600	0.32531000
C	-4.34730100	-4.17155000	0.14785700
C	-2.39516800	-4.47833400	1.54125200
C	-5.14877500	-4.69295400	1.15645100
H	-4.77367500	-3.82566400	-0.78565900
C	-3.20079500	-5.00403900	2.54852900
H	-1.33595200	-4.36430500	1.73637100

C	-4.57859400	-5.11584300	2.36106700
H	-6.22211200	-4.76837400	1.00630300
H	-2.74736900	-5.31027900	3.48664000
H	-5.20628800	-5.52219100	3.14952000
H	-0.25439300	-3.58117100	0.30872700

A-6

C	-3.95771000	-2.41454900	2.52624800
C	-2.95800100	-1.74970800	3.28960600
H	-3.03754500	-1.47601200	4.33252400
C	-1.85576000	-1.43747000	2.43652100
C	-2.18314200	-1.93065800	1.11224100
C	-3.48525000	-2.53355500	1.19178400
H	-4.03762300	-2.94070900	0.35857600
C	0.02746100	-2.89129100	-0.55994200
C	0.36690200	-3.74829100	0.49233000
H	-0.23157600	-3.75627900	1.39529500
C	1.49337100	-4.56561700	0.39068900
H	1.77064300	-5.20408100	1.22311900
C	2.27922600	-4.53880700	-0.76341200
H	3.17185000	-5.15315000	-0.82703100
C	1.93230800	-3.70343400	-1.82852400
H	2.55528500	-3.66033200	-2.71512900
C	0.81175000	-2.88068300	-1.72909500
H	0.55070800	-2.22011700	-2.55294700
C	-2.47749100	-2.12311700	-1.73421600
C	-2.96656400	-1.16440700	-2.63079700
H	-2.61601800	-0.13983000	-2.55528400
C	-3.87010400	-1.53144500	-3.62961500
H	-4.24256900	-0.78025800	-4.32022500
C	-4.27803100	-2.86113500	-3.74888200
H	-4.97635600	-3.14848700	-4.52969900
C	-3.77012900	-3.82794700	-2.87644300
H	-4.06889100	-4.86708900	-2.98094300
C	-2.86897000	-3.46216300	-1.87707600
H	-2.45958000	-4.21795100	-1.21245200
P	-1.27822100	-1.61742700	-0.43736700
Fe	-3.54474800	-0.54412200	1.70742400
C	-3.17308900	1.19331700	0.68327400
C	-4.31634000	0.51463400	0.13338100
H	-4.39854700	0.13668900	-0.87482700
C	-5.30345100	0.40425800	1.15309200
C	-4.78489200	1.00118600	2.34049400
C	-3.47864500	1.48963200	2.05336700
H	-2.81674000	1.99063400	2.74344500
C	-2.39057300	2.58972200	-1.64933800
C	-1.63309800	2.75382500	-2.81901800
H	-0.64347000	2.31503200	-2.88493500
C	-2.14875700	3.48166900	-3.89159500
H	-1.55199100	3.60036100	-4.79133500
C	-3.41999700	4.05191200	-3.81073200
H	-3.82041900	4.61477700	-4.64921200
C	-4.17591700	3.89727600	-2.64745100
H	-5.16550100	4.33994100	-2.57558700
C	-3.66602400	3.17056700	-1.57189100
H	-4.26808300	3.05181900	-0.67796300
C	-0.93598700	2.97907900	0.82921200
C	-1.72103700	4.05704200	1.26834000
H	-2.77346600	4.10753700	1.00804500
C	-1.15155300	5.07489300	2.03032300
H	-1.76735700	5.90400900	2.36721000
C	0.21043600	5.03893700	2.34497800
H	0.65412500	5.84174100	2.92682800
C	0.99971100	3.98081900	1.89621100
H	2.06653300	3.96328600	2.09845700
C	0.42759600	2.95154700	1.14667100
H	1.04393000	2.14131900	0.77993000
P	-1.66169700	1.66088800	-0.23119900
H	-4.92910200	-2.72862900	2.88444300
H	-5.27706000	1.03935600	3.30325200
H	-6.25848900	-0.09475600	1.05554500
S	3.12693000	-2.34866500	3.06659500
N	0.51696200	-1.73684400	2.97843600
N	1.89617800	-0.46576600	1.62006500
H	1.07418400	-0.23360800	1.02914900
F	6.24806200	-1.21912500	-2.51136200
F	5.13485900	-2.84895900	-1.58400000
F	4.15088000	-1.53359000	-2.99974200
F	6.21333000	2.79386700	1.61021100
F	4.45236700	3.74155800	0.76724600
F	6.12787200	3.20645600	-0.52294800
C	-0.58034000	-0.74883700	2.85375100
H	-0.32714400	-0.06099800	2.05125500
C	-0.70221800	0.06937300	4.14433100
H	-0.92354200	-0.56283500	5.00965900
H	-1.49322000	0.81767500	4.05428800
H	0.24459300	0.58356400	4.33227400
C	1.78609600	-1.48413800	2.52892700
C	3.10841600	-0.17639500	0.93063700

C	3.58265600	-1.04395100	-0.05022900
H	3.10467100	-2.00453600	-0.18598600
C	4.64157900	-0.65026400	-0.86209500
C	5.24105000	0.59989900	-0.69521600
H	6.04964700	0.91135700	-1.34393800
C	4.77214300	1.44823100	0.30447900
C	3.70888700	1.06032600	1.12200100
H	3.32424600	1.72210300	1.88903900
C	5.05332000	-1.55790900	-1.98474500
C	5.39589000	2.79451000	0.53154600
Cl	1.61995100	1.41699500	-1.86820700
Ir	-0.14287200	0.23069300	-0.89114400
C	0.32903400	-2.78776800	3.97418300
H	-0.74207800	-2.95231700	4.10395500
H	0.79807600	-3.70993500	3.62910700
H	0.78428400	-2.52600200	4.93562500

A-6a

H	1.76901700	2.69844400	-0.42491200
H	-0.60514500	2.39838000	-0.28551700
C	-0.46968900	0.26506800	0.05663000
C	1.70516300	-0.54081700	0.05824600
C	2.25604300	0.74045900	-0.16995800
C	0.05476000	1.68684900	0.21120000
H	2.10088100	-2.60101400	0.41607500
C	2.55584700	-1.63021100	0.25393600
C	3.64378400	0.89423400	-0.21624700
H	0.07041000	1.94693800	1.28665800
C	4.47397300	-0.20397100	-0.01251200
C	3.93638200	-1.46856900	0.23194700
H	4.06984600	1.87531800	-0.40801000
H	5.55012800	-0.06846800	-0.04295100
H	4.58903100	-2.31939700	0.39105700
N	1.36575900	1.77344800	-0.41226500
N	0.32421200	-0.74441500	0.02044900
C	-1.92720200	0.03280600	0.01257600
C	-2.41538300	-1.25456000	-0.26606400
C	-2.85096900	1.05661800	0.26512400
C	-3.77869400	-1.50316600	-0.29901900
H	-1.69731800	-2.04270500	-0.45288000
C	-4.21995100	0.80285400	0.23968700
H	-2.51343000	2.05940400	0.49914600
C	-4.68911300	-0.47487800	-0.04627000
H	-4.13798200	-2.50224700	-0.52274300
H	-4.91914300	1.60706300	0.44327600
H	-5.75580100	-0.67123300	-0.07216000

A-7

C	5.93930600	0.45320500	-1.22669800
C	5.16660800	-0.27585100	-2.17266700
H	5.44296900	-0.46823200	-3.19971200
C	3.92802200	-0.64958400	-1.56640000
C	3.94181800	-0.13856000	-0.21099800
C	5.19896700	0.52427500	-0.01623100
H	5.51562100	1.02064500	0.88838900
C	3.18470000	-2.11249900	1.60715400
C	4.46042100	-2.23339200	2.18135100
H	5.06885700	-1.34888900	2.34571700
C	4.95075700	-3.48457300	2.54735800
H	5.93743500	-3.56767300	2.99419700
C	4.17436400	-4.62762900	2.33642700
H	4.55838800	-5.60438300	2.61672000
C	2.90785100	-4.51197900	1.76396500
H	2.30025100	-5.39252500	1.58213500
C	2.41176500	-3.25846700	1.40287700
H	1.42567100	-3.17780400	0.97203400
C	3.00968400	0.61518700	2.48680000
C	3.52568200	1.91231300	2.38713500
H	3.84112900	2.29540900	1.42717000
C	3.61713500	2.72624500	3.51695500
H	4.02055600	3.73048800	3.42298500
C	3.17605200	2.25938900	4.75445300
H	3.24202100	2.89477800	5.63301400
C	2.64302600	0.97136500	4.85799800
H	2.28871500	0.60264600	5.81625200
C	2.55966700	0.15158900	3.73442000
H	2.12370900	-0.83873700	3.81576800
P	2.65293000	-0.44979100	1.03599800
Fe	4.09952600	1.38284200	-1.55342400
C	2.31353900	2.39283800	-1.53526800
C	3.35786900	3.22587100	-1.00267600
H	3.36743500	3.66085500	-0.01527300
C	4.35588100	3.39670500	-2.00365500
C	3.94074200	2.68227300	-3.16468500
C	2.68716800	2.06880200	-2.88019200
H	2.11894000	1.45481300	-3.56088000
C	0.60702300	3.29137400	0.49800900
C	0.67379400	4.61699700	0.04123400
H	0.80369600	4.81861000	-1.01766600

C	0.57939900	5.67657000	0.94085700
H	0.63046700	6.69875500	0.57691600
C	0.42180300	5.42498900	2.30773600
H	0.35313100	6.25305500	3.00760100
C	0.35734000	4.11039700	2.76971200
H	0.25070300	3.90449900	3.83035200
C	0.44967500	3.04793800	1.86826000
H	0.42182100	2.02040600	2.21964300
C	-0.49730600	2.09139000	-1.94059400
C	-0.51751500	1.18098000	-3.01162300
H	0.23102700	0.39591400	-3.06970000
C	-1.51669900	1.24651500	-3.97829300
H	-1.52739000	0.52958200	-4.79387500
C	-2.52622000	2.20720400	-3.87409700
H	-3.32211200	2.23862800	-4.61176500
C	-2.52354500	3.10075800	-2.80637100
H	-3.31517100	3.83393900	-2.69761400
C	-1.51241700	3.04782100	-1.84271200
H	-1.54186900	3.73966900	-1.01069500
P	0.79325800	1.86413600	-0.65123200
H	6.90324800	0.90999100	-1.40728700
H	4.49532900	2.58571200	-4.08860200
H	5.28157700	3.94462300	-1.88817100
S	1.31772000	-5.09089600	-1.77876400
N	2.67330600	-2.77675400	-1.66137400
N	0.38459300	-2.57653100	-1.52257000
H	0.57703600	-1.64427900	-1.10180300
F	-5.43029300	-1.15682600	-1.90099600
F	-3.80335300	0.25344200	-1.56134400
F	-3.97809200	-0.75503000	-3.47472800
F	-2.72292700	-6.27539700	0.35704700
F	-4.67785800	-5.31494700	0.44312300
F	-3.13387200	-4.78622900	1.88006100
C	2.80838200	-1.41296000	-2.23195700
H	1.89677900	-0.86713700	-2.00070800
C	2.94695500	-1.50132100	-3.75748300
H	3.82928700	-2.08052800	-4.04580000
H	3.02895400	-0.50750100	-4.20655700
H	2.06636400	-2.00285400	-4.16963800
C	1.45281900	-3.42072300	-1.64968000
C	-0.98858000	-2.88651400	-1.36329800
C	-1.87810700	-1.95377400	-1.89829000
H	-1.49509400	-1.14212900	-2.50379600
C	-3.24252900	-2.03386500	-1.62529300
C	-3.74564500	-3.07339700	-0.85101700
H	-4.80138600	-3.13043000	-0.62594200
C	-2.85314300	-4.01922900	-0.34187400
C	-1.48150200	-3.93040200	-0.57605100
H	-0.80054900	-4.65114600	-0.14692000
C	-4.12527600	-0.93244800	-2.13607200
C	-3.34936600	-5.10070000	0.57665100
Cl	-0.30862900	-1.66000300	2.13669500
H	-2.08328400	2.25451400	1.94458300
Ir	0.46569000	-0.05659100	0.48663800
C	3.88457700	-3.59335000	-1.68032700
H	4.73927500	-2.93463400	-1.51859800
H	3.84102500	-4.32108400	-0.87125500
H	4.00416400	-4.13591000	-2.62484900
C	-4.10888800	2.31286800	1.16222200
C	-5.21282000	0.27517200	1.27511700
C	-4.08806600	-0.37671600	1.83542900
C	-3.05513000	1.79598000	2.13433700
H	-7.24353000	0.08664600	0.64830500
C	-6.40504000	-0.43584200	1.09817900
C	-4.16903300	-1.73037300	2.18193800
H	-3.35128700	2.06893000	3.16773500
C	-5.37360200	-2.41240100	2.01925100
C	-6.49736700	-1.77051000	1.48370900
H	-3.28964100	-2.24038100	2.56099300
H	-5.42454500	-3.46114800	2.29263600
H	-7.42872900	-2.31355300	1.35579100
N	-2.92096700	0.36339800	1.94238200
N	-5.12146100	1.59079600	0.81978200
C	-4.01115100	3.68967200	0.63683000
C	-4.93536000	4.12395000	-0.33240700
C	-3.02442700	4.58948300	1.07158800
C	-4.86514900	5.40894600	-0.85621900
H	-5.69416200	3.42199700	-0.65870800
C	-2.95746500	5.88046900	0.54475100
H	-2.29610800	4.29643100	1.81884800
C	-3.87070000	6.29457600	-0.42350500
H	-5.58513700	5.72515500	-1.60638800
H	-2.18355600	6.55674500	0.89352000
H	-3.81452700	7.29811700	-0.83590700
H	-2.15648400	-0.09315100	2.43147500
H	-1.11461400	-0.13817600	-0.27083200
H	-1.30707900	0.28978100	0.43659500

A-TS4

C	5.85733300	-0.17889000	-1.49073100
C	4.95252600	-0.84548600	-2.36296700
H	5.14058700	-1.09440500	-3.39785100
C	3.72301100	-1.06604600	-1.66852500
C	3.87819200	-0.52677700	-0.33380100
C	5.20726600	0.00278700	-0.24000100
H	5.63124200	0.48748800	0.62627300
C	3.02871100	-2.36036200	1.57495400
C	4.32333000	-2.61382900	2.05553200
H	5.03913400	-1.80140300	2.13996900
C	4.69721900	-3.90257400	2.42938800
H	5.70108400	-4.08661600	2.80201400
C	3.78261500	-4.95399900	2.32089900
H	4.07498200	-5.96058900	2.60666200
C	2.49614700	-4.70814300	1.84165700
H	1.78079700	-5.51763700	1.73734700
C	2.11889100	-3.41591200	1.47261200
H	1.11846400	-3.23461600	1.10993200
C	3.22143900	0.37520300	2.38763400
C	3.85419800	1.61254100	2.21981800
H	4.12605800	1.94756900	1.22887600
C	4.12028300	2.43005800	3.31928700
H	4.61331500	3.38658600	3.16924800
C	3.74031500	2.02884400	4.59939700
H	3.94356900	2.66619000	5.45540000
C	3.09252300	0.80236000	4.77402000
H	2.78634900	0.48377100	5.76651400
C	2.83469600	-0.02028400	3.67938300
H	2.31324700	-0.96150300	3.81936900
P	2.62859000	-0.65994500	0.98907400
Fe	4.11055200	0.93381300	-1.73797000
C	2.43229100	2.11118800	-1.66269100
C	3.57603300	2.84908100	-1.19823900
H	3.67487200	3.29826100	-0.22220900
C	4.53873400	2.90370800	-2.24598400
C	4.00297000	2.21114800	-3.37033300
C	2.71060100	1.72792100	-3.01541200
H	2.05628700	1.15784600	-3.65575400
C	0.94577100	3.23760000	0.40597100
C	1.09994900	4.53437000	-0.10860100
H	1.14772700	4.68739700	-1.18233100
C	1.20644800	5.62635500	0.75028500
H	1.32504300	6.62517000	0.33977000
C	1.16705000	5.43703200	2.13564300
H	1.25941900	6.28922100	2.80338200
C	1.02013600	4.15106800	2.65621700
H	1.01382900	3.98953600	3.73002300
C	0.91167400	3.05680600	1.79462800
H	0.82898000	2.04625200	2.18576800
C	-0.39604900	2.09564900	-1.94349500
C	-0.55061900	1.17055700	-2.98990700
H	0.10229900	0.30414000	-3.04405300
C	-1.56069500	1.32665700	-3.93477900
H	-1.67522100	0.59517400	-4.72918100
C	-2.45040200	2.39943200	-3.83432700
H	-3.25521800	2.50619900	-4.55522500
C	-2.31617800	3.31114900	-2.79050200
H	-3.01366500	4.13571900	-2.68602800
C	-1.29283800	3.16419500	-1.84970300
H	-1.21734400	3.87657600	-1.03805600
P	0.90975900	1.74956800	-0.69070500
H	6.85056100	0.16670800	-1.74513100
H	4.50225500	2.04297800	-4.31539800
H	5.51757100	3.36054000	-2.18419800
S	0.65540700	-5.20334900	-1.60157300
N	2.24280100	-3.04171700	-1.60760600
N	-0.00006000	-2.59890300	-1.33957500
H	0.29983900	-1.67287500	-0.94994600
F	-5.65915400	-0.65536300	-1.82753000
F	-3.90057800	0.60494600	-1.56366000
F	-4.19630600	-0.46079300	-3.42910600
F	-3.55200300	-6.06339600	0.27787100
F	-5.35494500	-4.85564500	0.48139500
F	-3.71206700	-4.61784600	1.88774100
C	2.48624300	-1.71882000	-2.23578400
H	1.65504100	-1.07051500	-1.96745400
C	2.51641200	-1.87031100	-3.76228400
H	3.31077500	-2.55174800	-4.08152400
H	2.67683600	-0.90586800	-4.25229100
H	1.56221400	-2.28413300	-4.10199300
C	0.96565400	-3.55122900	-1.51152600
C	-1.39541500	-2.76292500	-1.19601400
C	-2.18295100	-1.73762100	-1.72404800
H	-1.70794100	-0.93070600	-2.26567100
C	-3.56254900	-1.72916400	-1.53372800
C	-4.18440500	-2.75558500	-0.83023400
H	-5.25366700	-2.74808800	-0.67427200
C	-3.39148800	-3.77193900	-0.29579200

C	-2.00645100	-3.78334000	-0.46152500
H	-1.40426600	-4.56681300	-0.02467700
C	-4.33816900	-0.56906600	-2.08410100
C	-4.00536300	-4.82974800	0.57519300
Cl	-0.36274400	-1.51081700	2.33540600
H	-1.60053900	2.40788200	1.88027000
Ir	0.47334700	-0.06945800	0.53015200
C	3.36138900	-3.97965200	-1.65633500
H	4.28458200	-3.41098300	-1.53482800
H	3.27248400	-4.68908200	-0.83515800
H	3.39038600	-4.54294500	-2.59606700
C	-3.65327600	2.69013000	1.21599700
C	-4.93218600	0.75664500	1.31848900
C	-3.88020200	-0.02306500	1.83029100
C	-2.60350400	2.04397400	2.10787000
H	-7.00313600	0.79717700	0.80306100
C	-6.20572100	0.18765900	1.21481900
C	-4.08049600	-1.34505600	2.21236200
H	-2.81949400	2.27340600	3.16269100
C	-5.36575700	-1.88632500	2.12950800
C	-6.42602100	-1.12233800	1.63479700
H	-3.24178000	-1.94556200	2.54900400
H	-5.52464100	-2.91687500	2.42470800
H	-7.41915300	-1.55479700	1.56079800
N	-2.58957600	0.58946800	1.88220900
N	-4.73313900	2.07061900	0.88452400
C	-3.45999500	4.08031800	0.76030600
C	-4.37293300	4.63059200	-0.15878600
C	-2.39611100	4.87572800	1.21406200
C	-4.21695900	5.93241400	-0.61765700
H	-5.18969300	4.00621600	-0.50177300
C	-2.24779300	6.18570400	0.75713900
H	-1.66872400	4.48864200	1.91832600
C	-3.15064500	6.71675600	-0.16245200
H	-4.92594900	6.34063100	-1.33258200
H	-1.41686900	6.78221800	1.11813000
H	-3.02857600	7.73424600	-0.52281800
H	-1.96909600	0.09472700	2.53516500
H	-1.16324600	0.22416100	0.03444200
H	-1.75277300	0.38113200	0.81796700

A-TS4-1

C	0.20761800	-5.02812400	-0.74311100
C	0.01300000	-4.25786100	-1.91816100
H	-0.04265000	-4.65173900	-2.92113700
C	-0.05565000	-2.87451300	-1.57304900
C	0.10006200	-2.79295100	-0.12944500
C	0.24271600	-4.13676500	0.35762200
H	0.36980500	-4.41405900	1.39253100
C	-1.73094600	-1.20514800	1.39011900
C	-2.22470700	-0.06094100	2.03707900
H	-1.59538000	0.81541500	2.12881600
C	-3.52651100	-0.03535000	2.53808700
H	-3.90281600	0.86570400	3.01129500
C	-4.35887000	-1.14392600	2.38224100
H	-5.38340900	-1.11721300	2.73905400
C	-3.88713300	-2.27177000	1.71213900
H	-4.54682900	-3.11755500	1.54496900
C	-2.57965400	-2.30890800	1.22663500
H	-2.23372500	-3.19047600	0.70267100
C	0.75946800	-1.80301200	2.55939000
C	1.79840700	-2.73250900	2.68812000
H	2.16225300	-3.24480700	1.81331500
C	2.37402800	-3.00881500	3.92767300
H	3.18129000	-3.73305600	3.99210600
C	1.93217600	-2.34482100	5.06982200
H	2.38290700	-2.55248200	6.03610300
C	0.90744700	-1.40432500	4.95614900
H	0.54960800	-0.87712700	5.83641100
C	0.32651800	-1.13776100	3.71729300
H	-0.47571600	-0.41311100	3.66170500
P	0.05089100	-1.29583600	0.91589000
Fe	1.75621100	-3.63555300	-0.99087600
C	3.30224500	-2.27914700	-0.80760400
C	3.63551500	-3.49750600	-0.11837200
H	3.87317500	-3.58424700	0.92962800
C	3.61758700	-4.57235800	-1.05243700
C	3.28586900	-4.03799600	-2.33070400
C	3.09113400	-2.63482300	-2.18127100
H	2.80108400	-1.95590800	-2.96861800
C	3.96583500	-0.65797700	1.47327200
C	5.15356700	-1.37918000	1.67330900
H	5.60652000	-1.91883300	0.84766600
C	5.76201800	-1.39965300	2.92773200
H	6.67908700	-1.96374200	3.07424300
C	5.19405600	-0.69357600	3.99193400
H	5.66466100	-0.71721900	4.97109900
C	4.02469000	0.03994200	3.79420300
H	3.57502700	0.58921700	4.61502000

C	3.41460500	0.05974400	2.54096800
H	2.49987000	0.61839900	2.37155600
C	4.33509700	0.34257500	-1.20964700
C	3.99252700	0.61159400	-2.54493300
H	3.02383100	0.30000700	-2.92153500
C	4.85826400	1.31753100	-3.37617000
H	4.57892300	1.50646800	-4.40950500
C	6.07528900	1.79492100	-2.88047800
H	6.74602300	2.35580200	-3.52496900
C	6.41615100	1.55198200	-1.55169500
H	7.35485700	1.92574800	-1.15210900
C	5.55531100	0.82529400	-0.72292800
H	5.83854200	0.64210600	0.30706800
P	3.10922200	-0.56432800	-0.15066700
H	0.33658000	-6.10138400	-0.69743700
H	3.15423300	-4.60097400	-3.24518900
H	3.79412200	-5.61446000	-0.82096400
S	-3.12144800	-2.66985200	-2.24297600
N	-1.20641500	-0.79717800	-2.43722000
N	-3.06540300	-0.08475500	-1.37440400
H	-2.39390800	0.61553500	-1.05171600
F	-7.15592100	3.35977200	1.21974600
F	-5.46763600	2.80909100	2.46953000
F	-5.13260300	3.92323700	0.63466500
F	-7.28247100	-2.40665100	1.06010600
F	-7.65026100	-2.41883200	-1.08189000
F	-8.82541400	-1.12487300	0.21914200
C	-0.10923200	-1.76340800	-2.60684000
H	0.76976100	-1.13674300	-2.41442800
C	-0.04021600	-2.30680200	-4.04242700
H	-0.92116500	-2.91424100	-4.26242300
H	0.86129100	-2.91036100	-4.18462100
H	-0.00298100	-1.48313100	-4.76048900
C	-2.46564000	-1.14123500	-2.01563400
C	-4.33597400	0.11085200	-0.83378100
C	-4.53658900	1.35583600	-0.21166400
H	-3.73260500	2.08338600	-0.20830800
C	-5.73404000	1.64042200	0.43025800
C	-6.76362900	0.69946500	0.47351800
H	-7.69280400	0.91502900	0.98570700
C	-6.56309300	-0.52426800	-0.15977500
C	-5.37421300	-0.82810000	-0.82158700
H	-5.22768100	-1.79539000	-1.27800700
C	-5.87541000	2.93354000	1.17865900
C	-7.58526700	-1.61338700	-0.00321700
Ir	1.13191900	0.45603300	-0.12140800
H	1.81677600	1.50492300	-1.24745900
Cl	-0.81720500	1.98358400	-0.06886100
H	2.04939900	2.35505100	-0.66901100
C	-0.93739800	0.49432200	-3.07859000
H	-1.76949500	1.17768400	-2.93631300
H	-0.04079100	0.94692100	-2.65337700
H	-0.80008200	0.35365200	-4.15842000
H	-0.51304900	4.20351400	1.38767100
H	1.04381700	6.23518200	-0.04882700
C	1.13865500	4.27591300	-0.88473900
C	2.40278400	3.78601800	1.04102200
C	1.43390500	4.34881700	1.89357400
C	0.43215800	5.32061200	-0.04935600
H	4.32567500	2.85262800	0.86663600
C	3.60614000	3.29241900	1.55012800
C	1.66224100	4.35150200	3.27055400
H	-0.53726700	5.58487300	-0.47157200
C	2.86009300	3.84822100	3.77957400
C	3.84102600	3.34020500	2.92081900
H	0.90607700	4.77428900	3.92494500
H	3.03695400	3.86957300	4.85112500
H	4.77123000	2.95268900	3.32211000
N	0.24602300	4.88325800	1.33131200
N	2.09996000	3.59644600	-0.32270600
C	0.81371900	3.98682000	-2.28178700
C	1.79312700	3.40813600	-3.11079400
C	-0.46540500	4.23210200	-2.81042900
C	1.49352800	3.07050700	-4.42705500
H	2.78984300	3.24214900	-2.71895600
C	-0.76006400	3.89314300	-4.12685600
H	-1.24716000	4.63656700	-2.17790300
C	0.21681500	3.30947100	-4.93910700
H	2.26038500	2.62551700	-5.05451100
H	-1.75701600	4.07236000	-4.51794200
H	-0.01733000	3.04684400	-5.96668000

A-TS4-2

C	-0.42988500	-4.43088600	-0.77069600
C	-0.80463000	-3.58363300	-1.84359200
H	-1.14374800	-3.90321000	-2.81708100
C	-0.65993400	-2.22715100	-1.44143200
C	-0.14134000	-2.23116700	-0.09028800
C	-0.03845500	-3.61038300	0.31805200

H	0.29699800	-3.96478400	1.27810000
C	-1.37646000	-0.10013400	1.33878500
C	-1.52229400	1.23011100	1.74491300
H	-0.67564300	1.90088500	1.69830500
C	-2.74688000	1.68351500	2.24377300
H	-2.84032800	2.71551600	2.57067600
C	-3.83377500	0.81264000	2.33934600
H	-4.78593500	1.16259200	2.72603400
C	-3.69923400	-0.50971800	1.90565500
H	-4.54947000	-1.18381100	1.93542300
C	-2.47882300	-0.96700900	1.41444900
H	-2.38791700	-1.99511700	1.08376500
C	0.62049700	-1.64774700	2.57346800
C	1.65525800	-2.58646000	2.66815900
H	2.23757200	-2.83601500	1.79144000
C	1.94958100	-3.21240300	3.87867300
H	2.76238500	-3.93108200	3.92446100
C	1.21382000	-2.90073100	5.02295600
H	1.44276900	-3.38349400	5.96877300
C	0.17950400	-1.96761400	4.94133300
H	-0.40093100	-1.71741200	5.82486000
C	-0.11721600	-1.34707100	3.72749900
H	-0.91801800	-0.62083500	3.68714700
P	0.28606800	-0.79677400	0.96425100
Fe	1.16821700	-3.21009000	-1.30348100
C	3.01783800	-2.26405300	-1.21970400
C	3.14358800	-3.65015500	-0.85807600
H	3.51264700	-4.02266800	0.08626800
C	2.69775500	-4.44421800	-1.95311200
C	2.28846500	-3.56380500	-2.99817300
C	2.46643600	-2.22352100	-2.54757100
H	2.19986300	-1.32069900	-3.07526200
C	4.60241100	-1.64212400	1.06277800
C	5.69896600	-2.40429400	0.62236000
H	5.86418800	-2.54326200	-0.44139000
C	6.57851800	-2.97423300	1.53800100
H	7.41742200	-3.56611200	1.18306200
C	6.38872100	-2.77679700	2.91014400
H	7.07969100	-3.21644300	3.62386900
C	5.31358100	-2.01126700	3.35517600
H	5.15266400	-1.85334900	4.41773000
C	4.42697000	-1.44756700	2.43371700
H	3.57883200	-0.88221700	2.78550800
C	4.84302000	0.00392000	-1.13870900
C	5.03804800	-0.13567000	-2.51502000
H	4.37664800	-0.76176200	-3.09857500
C	6.09361900	0.52647600	-3.14588100
H	6.23592600	0.40491100	-4.21600800
C	6.95610100	1.34044700	-2.41274400
H	7.77570100	1.85425100	-2.90692600
C	6.75746700	1.49585200	-1.03791800
H	7.41684500	2.13546800	-0.45843300
C	5.70913100	0.83258100	-0.40683000
H	5.56305600	0.95888100	0.66159700
P	3.50445900	-0.83431800	-0.19042500
H	-0.41075300	-5.51250200	-0.78614800
H	1.86251000	-3.85834700	-3.94812200
H	2.63994700	-5.52453800	-1.96843400
S	-3.80835600	-2.23952900	-1.80084600
N	-2.07612400	-0.17247300	-1.85192000
N	-4.19411200	0.36488000	-1.19690800
H	-3.72933700	1.17363500	-0.80718800
F	-9.04003100	2.55549400	1.56739000
F	-7.22950600	2.08245300	2.67838500
F	-7.18771000	3.62964400	1.15726300
F	-8.82630200	-2.61442800	-0.69013100
F	-8.48982100	-1.93350700	-2.72545300
F	-10.05962700	-1.02776300	-1.51495000
C	-0.94705200	-1.02952400	-2.31019400
H	-0.08221300	-0.37975200	-2.20838900
C	-1.08580800	-1.35990200	-3.79894200
H	-1.96996600	-1.96971000	-3.99641500
H	-0.19447000	-1.89277100	-4.14458500
H	-1.16515100	-0.42932000	-4.36974300
C	-3.33375400	-0.63531100	-1.62517500
C	-5.55217300	0.33031000	-0.85981600
C	-5.99465700	1.32935600	0.01786800
H	-5.28791500	2.05597800	0.40305700
C	-7.32417000	1.38595000	0.42394500
C	-8.25471300	0.46847000	-0.05663800
H	-9.29017300	0.51249800	0.25480700
C	-7.82018700	-0.49511300	-0.96723600
C	-6.49012300	-0.57578700	-1.37668600
H	-6.18045600	-1.33177500	-2.08101400
C	-7.70636800	2.41505700	1.44792100
C	-8.79940700	-1.51727500	-1.48017100
Ir	1.86041800	0.74281300	0.37153800
H	0.48297200	2.26091700	-0.00379500

Cl	1.66209000	1.00280500	-2.13532900
H	0.71268000	3.07602500	-0.34745000
C	-1.81354800	1.27321300	-1.89357300
H	-1.82851200	1.71359500	-0.88851700
H	-0.81324600	1.44244000	-2.28710400
H	-2.54561400	1.78111100	-2.53069300
H	0.49183800	5.38845700	2.23512600
H	2.66617500	5.59150000	0.99034100
C	2.22363600	3.87162500	-0.21617600
C	2.19410800	2.62103300	1.74100300
C	1.22593500	3.49673300	2.36314600
C	1.77095600	5.07183800	0.59722900
H	3.64723400	1.12344500	2.28903300
C	2.59795100	1.38496900	2.38419300
C	0.67065800	3.12320700	3.56624000
H	1.23789200	5.78088700	-0.03681200
C	1.03196200	1.88978800	4.18661800
C	1.96849000	1.05787000	3.64452000
H	-0.06463100	3.76868700	4.04060400
H	0.56234700	1.63162900	5.13181500
H	2.26944400	0.15934200	4.17145800
N	0.88066400	4.64377200	1.66971700
N	2.73397900	2.82867200	0.50181300
C	2.69657900	4.11312400	-1.58545000
C	3.84347500	3.46622000	-2.07411700
C	2.01424000	5.00009900	-2.43841100
C	4.29015200	3.69995700	-3.37103400
H	4.37325800	2.78256100	-1.42648100
C	2.45877600	5.22623800	-3.73667100
H	1.10252600	5.48372300	-2.09946900
C	3.60217900	4.57740400	-4.21040600
H	5.17872100	3.18680700	-3.72369100
H	1.90819200	5.90439100	-4.38308900
H	3.95099400	4.75506900	-5.22396800

A-8

C	5.95860900	-0.43141000	-1.34426800
C	5.03720300	-1.04088900	-2.24229200
H	5.23228800	-1.28691700	-3.27677100
C	3.78403600	-1.20047300	-1.57220300
C	3.94411600	-0.69291000	-0.22743800
C	5.29292500	-0.22878800	-0.10339200
H	5.71744400	0.23189600	0.77651900
C	2.93449800	-2.52462000	1.60588800
C	4.21678500	-2.91037800	2.02750500
H	5.01453200	-2.17476600	2.07280400
C	4.47462100	-4.23078400	2.38880400
H	5.47149100	-4.51775100	2.71243900
C	3.45330400	-5.18369100	2.32885300
H	3.65522400	-6.21543400	2.60323500
C	2.17753600	-4.80743300	1.90963600
H	1.38098900	-5.54144100	1.84009000
C	1.91840100	-3.48269800	1.55222300
H	0.92801100	-3.19939100	1.22591100
C	3.28437600	0.16706800	2.48755200
C	3.89001000	1.42145600	2.34027900
H	4.11480200	1.79211400	1.34989500
C	4.19272200	2.20310500	3.45528000
H	4.66378600	3.17293200	3.31922200
C	3.87879800	1.74781500	4.73625100
H	4.11041600	2.35676500	5.60571100
C	3.26226000	0.50382900	4.89279600
H	3.00931600	0.14206000	5.88567300
C	2.96718500	-0.28184400	3.77948900
H	2.47669000	-1.24089400	3.90985400
P	2.64308900	-0.78849400	1.05125000
Fe	4.28742000	0.77608300	-1.61919800
C	2.68102400	2.06419600	-1.59837100
C	3.85174700	2.72201700	-1.08544100
H	3.94186300	3.16167500	-0.10407000
C	4.85739800	2.71755900	-2.09378200
C	4.32246100	2.06552400	-3.24252600
C	2.98795200	1.66718300	-2.94058900
H	2.32420500	1.14288300	-3.60973200
C	1.16349400	3.27251100	0.41116400
C	1.41860000	4.55819900	-0.08965700
H	1.55688900	4.70353800	-1.15687100
C	1.50464000	5.64931800	0.77387000
H	1.70286200	6.64014800	0.37403400
C	1.34485900	5.46802700	2.15176000
H	1.42178600	6.31804000	2.82440100
C	1.10158100	4.19108700	2.65981000
H	1.00178900	4.03658200	3.73040900
C	1.01201500	3.09911300	1.79311900
H	0.84987700	2.09284900	2.17243000
C	-0.13666400	2.21549400	-1.98091200
C	-0.31477500	1.32181300	-3.04979000
H	0.30208100	0.43000600	-3.11526300
C	-1.30649400	1.53893100	-4.00342800

H	-1.43541700	0.83193200	-4.81799500
C	-2.15627300	2.64255000	-3.89097800
H	-2.94612600	2.79696200	-4.61996000
C	-1.99931600	3.52514000	-2.82475100
H	-2.66608800	4.37441700	-2.70962200
C	-0.99260200	3.31694700	-1.87824300
H	-0.90009700	4.00680600	-1.04944600
P	1.10494200	1.78045700	-0.68363500
H	6.97279300	-0.13444900	-1.57708000
H	4.84709000	1.86715000	-4.16788400
H	5.86099200	3.10858900	-1.99051700
S	0.47396400	-5.14264100	-1.59152600
N	2.16837400	-3.07246200	-1.54867700
N	-0.05571800	-2.50001800	-1.34074500
H	0.28635900	-1.57848700	-0.95033800
F	-5.53185300	-0.08167200	-1.69388100
F	-3.65610800	0.98809400	-1.39794600
F	-4.11437800	0.11290300	-3.33266800
F	-3.90344500	-5.87028300	-0.28559100
F	-5.64120900	-4.57472400	-0.05570900
F	-4.08631600	-4.60036200	1.46463200
C	2.51509000	-1.76517000	-2.16414300
H	1.72619400	-1.06241500	-1.90142900
C	2.56364200	-1.91492500	-3.68998700
H	3.31556400	-2.64864600	-3.99653800
H	2.80080200	-0.96224300	-4.17170900
H	1.59012900	-2.25997200	-4.05140500
C	0.86396900	-3.50543300	-1.48632100
C	-1.45706600	-2.57714400	-1.25657400
C	-2.15223300	-1.43822400	-1.68728800
H	-1.59818900	-0.60543300	-2.10033200
C	-3.53856700	-1.36140600	-1.56380100
C	-4.26774400	-2.42005400	-1.02615600
H	-5.34192000	-2.35620000	-0.92170100
C	-3.57072400	-3.54479800	-0.58819800
C	-2.18065500	-3.63208100	-0.68570700
H	-1.65698200	-4.50453700	-0.32343200
C	-4.22031600	-0.10039100	-2.00437800
C	-4.30201500	-4.65042400	0.11827700
Cl	-0.57123100	-1.38020700	2.25324800
H	-1.74356500	2.01811600	1.57491700
Ir	0.54098200	0.00646800	0.50316600
C	3.23181100	-4.07416600	-1.55501800
H	4.18089200	-3.55835400	-1.40412700
H	3.07433800	-4.77320200	-0.73524900
H	3.25981600	-4.64221100	-2.49194000
C	-3.85191600	2.54732000	1.26265100
C	-5.28600400	0.73470700	1.47417400
C	-4.25369200	-0.18785400	1.69727200
C	-2.74157200	1.72797100	1.90250500
H	-7.40869200	0.98346200	1.41222900
C	-6.60442000	0.27875600	1.59441000
C	-4.48353500	-1.51435600	2.02080100
H	-2.79244500	1.76782700	2.99641300
C	-5.80645500	-1.94665400	2.14542400
C	-6.85784000	-1.04995000	1.93301400
H	-3.65288900	-2.19969200	2.14860500
H	-6.00409600	-2.98655100	2.37866300
H	-7.88411200	-1.39323900	2.02090800
N	-2.90205400	0.30910800	1.48912400
N	-5.03542100	2.05830200	1.09752600
C	-3.55920400	3.91697900	0.81035800
C	-4.46631600	4.56183800	-0.04973100
C	-2.39073700	4.59203000	1.19912500
C	-4.20236900	5.84327500	-0.51767700
H	-5.36201900	4.02821600	-0.34591700
C	-2.13611000	5.88313000	0.73851000
H	-1.66553700	4.12598200	1.85676700
C	-3.03453000	6.50806100	-0.12653000
H	-4.90409100	6.32666300	-1.19135600
H	-1.22605500	6.38528400	1.04712400
H	-2.82789600	7.50838700	-0.49619900
H	-2.16344100	-0.29860400	1.95628200
H	-0.95761800	0.55863800	0.08888700
H	-2.60715400	0.24687700	0.49633100

A-9

C	4.85730000	3.24667300	1.44221400
C	3.55478400	3.65148400	1.84625800
H	3.32844200	4.33110600	2.65560900
C	2.59255100	2.94611100	1.05927600
C	3.32050800	2.09440400	0.14098300
C	4.71645400	2.30851100	0.38388500
H	5.52838000	1.81903400	-0.13186600
C	2.47371300	2.23279400	-2.51270700
C	3.67707600	2.69632900	-3.06764700
H	4.62443100	2.31661200	-2.69575600
C	3.66670500	3.63350700	-4.09809200
H	4.60497000	3.98492800	-4.51902500

C	2.45044400	4.11864700	-4.58870400
H	2.44133300	4.84920500	-5.39313600
C	1.25164100	3.66166600	-4.04287600
H	0.29939200	4.03441900	-4.40848200
C	1.26253900	2.72270500	-3.00884100
H	0.32700500	2.37777500	-2.59336000
C	3.78088000	-0.15782300	-1.72483500
C	4.86947000	-0.64491900	-0.99396000
H	5.10396100	-0.22182800	-0.02821400
C	5.64556100	-1.69972500	-1.48251500
H	6.48334200	-2.06414600	-0.89402200
C	5.34087100	-2.28927900	-2.70722300
H	5.94248800	-3.11129900	-3.08537900
C	4.25384900	-1.81100300	-3.44723000
H	4.00657900	-2.25935800	-4.40606500
C	3.48281600	-0.75704500	-2.96373400
H	2.62627200	-0.40983600	-3.53304900
P	2.51337500	1.03650500	-1.10593700
Fe	3.73467100	1.60339900	2.07940700
C	2.71478200	-0.14164400	2.51139200
C	4.12780100	-0.39360100	2.44221300
H	4.59717700	-1.09492200	1.77028400
C	4.78863400	0.40851300	3.41516800
C	3.79582300	1.16373100	4.10397500
C	2.52519800	0.82471500	3.55277700
H	1.57977400	1.23776400	3.86651000
C	2.32666100	-2.63194000	1.40277900
C	2.71361800	-3.32167000	2.56348000
H	2.42347300	-2.94262300	3.53894000
C	3.48234600	-4.47985700	2.47294300
H	3.77068400	-5.00968000	3.37680400
C	3.89980000	-4.94752300	1.22179600
H	4.51546100	-5.84063800	1.15397200
C	3.53607000	-4.25628600	0.06758000
H	3.87814600	-4.59466600	-0.90633800
C	2.74395300	-3.10904100	0.15684000
H	2.45582200	-2.55643100	-0.73118100
C	0.09775000	-1.24020000	2.70017700
C	-0.57609100	-0.10576000	3.17864500
H	-0.30121600	0.87982800	2.81917600
C	-1.63851000	-0.22716000	4.07116000
H	-2.15109100	0.66432600	4.42109000
C	-2.06366400	-1.49072800	4.48372500
H	-2.90228700	-1.58890000	5.16592500
C	-1.42813300	-2.62635100	3.98282100
H	-1.77204200	-3.61493900	4.27461600
C	-0.35584800	-2.50381600	3.09755900
H	0.11993900	-3.39589400	2.70596000
P	1.44867700	-1.00609000	1.46438700
H	5.79050300	3.56791300	1.88588000
H	3.97217000	1.89603000	4.88101300
H	5.85738500	0.45968500	3.57671800
S	-1.82836200	4.06801200	-1.33914200
N	0.41975800	3.55697100	0.02089200
N	-1.24391000	1.99218100	0.31555500
H	-0.54680700	1.18976300	0.18082700
F	-5.31189600	-2.17135300	0.79269400
F	-3.18866400	-2.46303400	1.19003900
F	-4.55025100	-1.92145600	2.80172000
F	-5.68419100	4.16543600	1.64006200
F	-7.06412700	2.49717600	1.88842200
F	-6.50374200	3.16292700	-0.10392000
C	1.09534800	3.01139600	1.22656200
H	0.75992900	1.98447400	1.32369500
C	0.65116500	3.80547400	2.46067400
H	0.91920100	4.86330300	2.37384600
H	1.11322700	3.40871500	3.36897700
H	-0.43593000	3.73621400	2.56232900
C	-0.85847000	3.18479200	-0.27939600
C	-2.53727300	1.59300000	0.63556500
C	-2.75751500	0.22173000	0.86280000
H	-1.93254000	-0.46819000	0.72764700
C	-4.01843900	-0.23358800	1.22488100
C	-5.09989800	0.64019700	1.34824100
H	-6.08875400	0.27487600	1.59542400
C	-4.87057500	1.99679400	1.14088700
C	-3.60522300	2.48418100	0.81660400
H	-3.46143000	3.54349900	0.66415500
C	-4.25215000	-1.68491900	1.50546800
C	-6.02599800	2.95443700	1.15187200
Cl	-0.16881500	-0.18721700	-2.82386200
H	-4.08610300	-4.76125300	-2.02073700
Ir	0.74910200	-0.35428800	-0.52656700
C	0.94243900	4.81500600	-0.50613100
H	2.00915800	4.86144100	-0.28419100
H	0.80016900	4.85366700	-1.58389600
H	0.42794100	5.67431300	-0.05984500
C	-2.69891800	-3.14891100	-1.88096900

C	-3.74399900	-0.99828700	-2.16762800
C	-5.02483200	-1.57629100	-2.16444400
C	-4.06051500	-3.75106000	-1.60384700
H	-2.56172200	0.80237500	-2.19183800
C	-3.56269600	0.38735200	-2.18655000
C	-6.13697900	-0.73135900	-2.15733400
H	-4.17531000	-3.83606200	-0.51202500
C	-5.95870800	0.65193700	-2.14435000
C	-4.67875300	1.21538200	-2.16692100
H	-7.13472300	-1.16175300	-2.14027100
H	-6.82824300	1.29921500	-2.09424400
H	-4.54012000	2.28945300	-2.13329700
N	-5.10866100	-2.96320200	-2.23571400
N	-2.63431400	-1.86652500	-2.12374300
C	-1.50615300	-3.97680800	-1.79465700
C	-0.28404700	-3.58358600	-2.37570200
C	-1.56542600	-5.19254700	-1.08283000
C	0.84025800	-4.38874900	-2.24688700
H	-0.20671600	-2.65343800	-2.92464000
C	-0.42854400	-5.97907900	-0.93868400
H	-2.48874100	-5.50826000	-0.60948400
C	0.77583900	-5.58088800	-1.52391100
H	1.77423500	-4.06703400	-2.69651800
H	-0.48052700	-6.90155100	-0.36880900
H	1.66398900	-6.19297800	-1.40476000
H	-1.70867100	-1.39813300	-2.26442200
H	-0.40202800	-1.50760100	-0.26002600
H	-6.03739300	-3.33184500	-2.07395100

A-TS5OR

C	4.52909000	3.18725000	2.06168100
C	3.23182300	3.31796700	2.63187900
H	3.00506200	3.73743600	3.60206300
C	2.28353000	2.73205900	1.73790300
C	3.00742200	2.24312500	0.58646600
C	4.39268500	2.54182900	0.80136600
H	5.20213700	2.29070100	0.13307700
C	1.75344600	3.07037400	-1.75872900
C	2.76657600	3.99271100	-2.06378100
H	3.80030100	3.75780900	-1.82751400
C	2.45641400	5.20859200	-2.66907500
H	3.24913000	5.91521000	-2.89958400
C	1.12768400	5.51828900	-2.97362500
H	0.88375000	6.46933100	-3.43902400
C	0.11655600	4.60583000	-2.67309400
H	-0.92070800	4.84229400	-2.88873700
C	0.42813500	3.38562000	-2.07011100
H	-0.35999000	2.68355100	-1.83824600
C	3.55596500	0.87979300	-1.93821800
C	4.70317900	0.25572100	-1.43385600
H	4.86236400	0.20402900	-0.36548300
C	5.63516000	-0.32563900	-2.29494000
H	6.51932500	-0.80415300	-1.88284200
C	5.42042600	-0.31449900	-3.67225000
H	6.14336500	-0.77062500	-4.34296300
C	4.26364600	0.28122100	-4.18397300
H	4.08152400	0.28715300	-5.25521400
C	3.33993000	0.87503500	-3.32660100
H	2.43940200	1.32700000	-3.73037000
P	2.18863900	1.50731200	-0.87572900
Fe	3.63260400	1.32348200	2.30630500
C	2.94108600	-0.61098700	2.25003000
C	4.37642800	-0.59062000	2.16529200
H	4.96048100	-0.99342600	1.35211100
C	4.89218500	0.03618600	3.33621100
C	3.78780300	0.40648400	4.15844600
C	2.59178100	0.00834000	3.49321800
H	1.58637900	0.15939000	3.85644000
C	2.90457100	-2.53961600	0.24496100
C	3.68808800	-3.42149500	1.00994200
H	3.59539600	-3.43001100	2.09163500
C	4.61433400	-4.26080400	0.39418400
H	5.21235200	-4.93967800	0.99621000
C	4.79351500	-4.20679200	-0.99233800
H	5.53224300	-4.84544100	-1.46947600
C	4.02980000	-3.32584000	-1.75477500
H	4.17036300	-3.26378000	-2.82895200
C	3.08040700	-2.50717400	-1.14183800
H	2.47508000	-1.82146800	-1.72672700
C	0.66573400	-2.26634300	2.14821800
C	-0.33729000	-1.54132600	2.81193400
H	-0.41014800	-0.47228100	2.63612700
C	-1.25463100	-2.17598600	3.64552800
H	-2.03341700	-1.60061800	4.13542100
C	-1.19615000	-3.56238300	3.81641300
H	-1.92051500	-4.06356300	4.45185500
C	-0.20481300	-4.29451500	3.16446500
H	-0.14832100	-5.37219200	3.29529500
C	0.72520700	-3.65018800	2.34104700

H	1.48552500	-4.23547900	1.83826200
P	1.76337600	-1.30155000	1.00809600
H	5.46126800	3.48661100	2.52255500
H	3.84178000	0.93619900	5.10048600
H	5.93611100	0.23028200	3.54457400
S	-2.31320500	4.59481200	0.47166200
N	0.08805300	3.54467100	1.00132000
N	-1.58014500	1.99534600	0.61657300
H	-0.83226600	1.28498000	0.44353600
F	-6.10991600	-1.48022700	2.57539500
F	-4.11491900	-2.28642600	2.27379000
F	-4.45096100	-0.80688800	3.81826900
F	-5.88235600	2.45152000	-2.15483800
F	-6.69215500	3.36103900	-0.35859900
F	-7.39985500	1.40636200	-0.98796500
C	0.79668700	2.63411500	1.93897400
H	0.52590300	1.61253500	1.67041300
C	0.34593100	2.92023700	3.37632700
H	0.55104000	3.95694900	3.66084700
H	0.85652100	2.26348500	4.08617700
H	-0.73290000	2.75738500	3.45937200
C	-1.23186600	3.32201800	0.70006500
C	-2.89853600	1.49566100	0.61848800
C	-3.20089000	0.44404000	1.48688600
H	-2.41571600	0.02596900	2.10323400
C	-4.50702000	-0.04328300	1.57905800
C	-5.52797900	0.52039600	0.81977300
H	-6.54257600	0.15803100	0.90501500
C	-5.21244200	1.54055700	-0.07555200
C	-3.90896400	2.01543400	-0.20078200
H	-3.67281500	2.78985700	-0.91415100
C	-4.80580600	-1.14210900	2.55289900
C	-6.29520700	2.18697600	-0.89248800
Cl	-0.55443800	0.26592500	-2.64512800
H	-1.76350800	-4.06013000	0.61248500
Ir	0.65242200	-0.19204500	-0.55158200
C	0.59356800	4.91401000	0.93677300
H	1.68291300	4.87617700	0.93509100
H	0.25437200	5.37657500	0.01228300
H	0.24228300	5.52463000	1.77700300
C	-1.53660400	-2.88527000	-1.20409000
C	-3.60308800	-1.79919500	-1.79441600
C	-4.33082700	-2.64667500	-0.93355300
C	-2.24243100	-3.23552400	0.09296600
H	-3.64870700	-0.16517800	-3.18637700
C	-4.24385800	-0.81876100	-2.55629100
C	-5.72260700	-2.51489200	-0.87803600
H	-2.20242100	-2.35571500	0.74634800
C	-6.36048100	-1.55434500	-1.65842700
C	-5.62701600	-0.70212900	-2.49243900
H	-6.29267600	-3.15960200	-0.21475500
H	-7.43872800	-1.44729300	-1.59624800
H	-6.13005300	0.06557800	-3.06677200
N	-3.60919100	-3.61723200	-0.25061200
N	-2.25245600	-2.10701800	-2.00408100
C	-0.36838600	-3.59827000	-1.72316500
C	0.07796400	-3.39439400	-3.04473500
C	0.26104000	-4.59015200	-0.95043600
C	1.09887900	-4.17322800	-3.57223900
H	-0.37073000	-2.62835700	-3.66514900
C	1.27533600	-5.37533200	-1.48718700
H	-0.03669600	-4.75030000	0.07629000
C	1.69278200	-5.17708700	-2.80162700
H	1.42744100	-4.00151900	-4.59275900
H	1.75213100	-6.13054500	-0.87054700
H	2.48578400	-5.78903500	-3.21994600
H	-1.74059900	-1.50826000	-2.67259300
H	-0.46537000	-1.40109500	-0.29342900
H	-4.11032200	-4.04553200	0.51737700

A-TS5OS

C	3.14218500	4.15212000	2.35509200
C	1.72146400	4.19123400	2.43323400
H	1.14469800	4.74745100	3.15879700
C	1.18521100	3.30537000	1.44703600
C	2.30161300	2.71997600	0.73729200
C	3.50025200	3.26257800	1.30533800
H	4.50527600	3.00509100	1.00610500
C	1.86660800	2.87102200	-2.00352300
C	2.78122500	3.93100100	-2.11531700
H	3.64009500	3.97662600	-1.45271800
C	2.60140900	4.92262100	-3.07664000
H	3.31771600	5.73603000	-3.15357800
C	1.50240300	4.86832600	-3.93926700
H	1.35999700	5.64185300	-4.68884400
C	0.58603400	3.82372400	-3.82689300
H	-0.28554500	3.78228700	-4.47228300
C	0.76600900	2.83036300	-2.86203100
H	0.04418500	2.03216600	-2.77633900

C	3.86429300	1.06600600	-1.07323900
C	4.73731600	0.61710200	-0.07436200
H	4.44140600	0.68366200	0.96257700
C	5.97943000	0.07431600	-0.40190200
H	6.64091900	-0.26767400	0.38935600
C	6.35940800	-0.04577200	-1.73885700
H	7.32417200	-0.47350800	-1.99728200
C	5.48877800	0.38378500	-2.74300500
H	5.77165500	0.28747600	-3.78758600
C	4.25134200	0.93666800	-2.41616500
H	3.57609800	1.25094800	-3.20318800
P	2.14228400	1.59884900	-0.69314900
Fe	2.36876400	2.25038100	2.71956500
C	1.83871700	0.27134600	2.87405000
C	3.22282600	0.44424300	3.22654700
H	4.05576800	-0.04251800	2.74442300
C	3.31019700	1.33699700	4.33209800
C	1.98587600	1.72341000	4.68681100
C	1.08490900	1.07094000	3.79622400
H	0.01251500	1.17921300	3.81060200
C	2.58644600	-2.04828200	1.53548900
C	3.05156300	-2.63459400	2.72708800
H	2.54292700	-2.43011800	3.66402300
C	4.17569500	-3.45598000	2.71988400
H	4.52214700	-3.90512400	3.64662200
C	4.86809400	-3.68590600	1.52505100
H	5.75505200	-4.31381300	1.52421200
C	4.42033200	-3.10296500	0.34225700
H	4.94972900	-3.26771500	-0.59014900
C	3.27917900	-2.29627200	0.34456400
H	2.92510000	-1.83522100	-0.57317300
C	-0.14330100	-1.66725800	2.49372400
C	-1.25771200	-0.89977400	2.86891300
H	-1.34565700	0.12462500	2.52176300
C	-2.26973700	-1.44031600	3.65556500
H	-3.12605300	-0.83061400	3.92560200
C	-2.20861600	-2.77783400	4.05225100
H	-3.01118200	-3.20636800	4.64402300
C	-1.13393700	-3.56537500	3.64670700
H	-1.08677100	-4.61338100	3.92916700
C	-0.10453500	-3.01347600	2.87926400
H	0.73568200	-3.63943600	2.60188700
P	1.18977900	-0.82619400	1.52256300
H	3.82989400	4.67537500	3.00625400
H	1.70885200	2.42269700	5.46474900
H	4.22418600	1.68527400	4.79472700
S	-2.65318600	3.45759600	-1.97311600
N	-0.75048300	3.41346900	-0.09731800
N	-2.03084500	1.49054900	-0.21005200
H	-1.18878800	0.86162300	-0.15974700
F	-5.53735500	-3.14636100	0.66363700
F	-3.43952900	-3.08635300	1.23207100
F	-4.97841400	-2.45151600	2.63484600
F	-6.83904000	3.08621600	0.21149000
F	-7.96262100	1.33345400	0.85413900
F	-7.40226600	1.56248900	-1.23341700
C	-0.27182100	2.97655300	1.24069700
H	-0.34391800	1.89283800	1.25313300
C	-1.19027600	3.55631300	2.32294700
H	-1.19262300	4.65070800	2.30023800
H	-0.87162700	3.23575000	3.31884100
H	-2.21399800	3.20928000	2.15492600
C	-1.78710100	2.77307500	-0.70427700
C	-3.27362400	0.92225000	0.04795500
C	-3.31762700	-0.41842500	0.47878900
H	-2.39767100	-0.98419000	0.52983200
C	-4.53093000	-1.00584800	0.82031700
C	-5.73284100	-0.30402000	0.72067700
H	-6.67600600	-0.77675700	0.96497900
C	-5.68518400	1.01531900	0.28465800
C	-4.48010300	1.63794000	-0.02985400
H	-4.48173800	2.66448200	-0.36302500
C	-4.60931200	-2.41487500	1.33003900
C	-6.96923800	1.75450700	0.03831500
Cl	1.02640500	-0.36144800	-3.03749300
H	-1.52934100	-3.58117600	0.19781800
Ir	0.78449500	-0.25654200	-0.58480700
C	-0.42780600	4.78403400	-0.49033000
H	0.52524300	5.05725100	-0.03817800
H	-0.34400000	4.84824400	-1.57229500
H	-1.21219400	5.47729600	-0.16413200
C	-1.08460600	-2.89637200	-1.78713100
C	0.98451200	-3.80108200	-2.62504800
C	1.25693900	-4.42498800	-1.39822400
C	-1.00732500	-3.93743500	-0.68605600
H	1.65508500	-3.36589300	-4.61930900
C	1.88231100	-3.87983000	-3.69031200
C	2.45368300	-5.12986500	-1.25769900

H	-1.54069800	-4.82981700	-1.05022700
C	3.35831700	-5.20463000	-2.31508200
C	3.07330300	-4.58278200	-3.53452600
H	2.66428200	-5.60475800	-0.30530900
H	4.28633700	-5.75419600	-2.18842900
H	3.77614800	-4.64124200	-4.35926600
N	0.34664500	-4.31837400	-0.32143600
N	-0.20215000	-3.05106600	-2.76474200
C	-2.34721700	-2.18617600	-2.09082900
C	-2.36004700	-0.89842200	-2.64903000
C	-3.56505700	-2.84278400	-1.85158700
C	-3.56883400	-0.26696100	-2.92673500
H	-1.42652100	-0.37227700	-2.80059500
C	-4.77055200	-2.21701400	-2.16404200
H	-3.58098100	-3.83421700	-1.41358100
C	-4.77723500	-0.92329400	-2.68532900
H	-3.55882700	0.75863400	-3.28176500
H	-5.70436200	-2.72834200	-1.95737400
H	-5.71858900	-0.41218600	-2.86355800
H	-0.18504000	-2.33504700	-3.49165900
H	-0.27395600	-1.59801900	-0.69078200
H	0.71910000	-3.71686200	0.40763800

A-10

C	5.43660300	2.19674900	1.38885300
C	4.33633100	2.64177700	2.17389300
H	4.40284500	3.10827300	3.14662800
C	3.12204500	2.29981000	1.50200500
C	3.48647600	1.63353400	0.26982500
C	4.92050000	1.58991800	0.21209400
H	5.50356500	1.14188400	-0.57831300
C	2.10204500	2.75217900	-1.86491700
C	3.24410800	3.37589200	-2.39429500
H	4.20259100	2.86624600	-2.37242100
C	3.15384600	4.64739900	-2.95569500
H	4.04201800	5.11857400	-3.36703500
C	1.92497200	5.31266700	-2.98686200
H	1.85565700	6.30636100	-3.42010600
C	0.79003900	4.69948900	-2.45710900
H	-0.16711900	5.21087100	-2.45873700
C	0.87815400	3.42301800	-1.90004200
H	-0.00488200	2.95339200	-1.49653600
C	3.29379700	0.16655300	-2.27078900
C	4.25866100	-0.77924500	-1.90420700
H	4.54487600	-0.88110300	-0.86712400
C	4.83917000	-1.60675100	-2.86480300
H	5.58343700	-2.33841900	-2.56389900
C	4.44890500	-1.50907700	-4.20026300
H	4.89494400	-2.15858800	-4.94791300
C	3.47449300	-0.57842000	-4.57125400
H	3.15756600	-0.50386900	-5.60742900
C	2.89759100	0.25461000	-3.61509400
H	2.12384600	0.95814800	-3.90451900
P	2.32915200	1.12333500	-1.03940900
Fe	4.17882800	0.60476600	1.87474200
C	3.06568200	-1.10327400	1.95286000
C	4.44238500	-1.42437900	1.68758300
H	4.80891900	-1.95436400	0.82199800
C	5.23308000	-0.94522100	2.77129100
C	4.35979800	-0.33364500	3.71819400
C	3.02941600	-0.43643600	3.22040800
H	2.13711000	-0.06344700	3.70134100
C	2.17697400	-2.99510600	0.06746500
C	2.89907700	-4.00139100	0.72975600
H	3.12910300	-3.90250000	1.78582600
C	3.35235700	-5.11912700	0.03080300
H	3.90815100	-5.89277000	0.55328300
C	3.10297900	-5.23634800	-1.33886000
H	3.46015600	-6.10640600	-1.88268800
C	2.39700200	-4.23616000	-2.00559500
H	2.19621700	-4.31946800	-3.06805200
C	1.93360800	-3.12345200	-1.30667000
H	1.39586100	-2.33421600	-1.82357800
C	0.43829200	-1.98635700	2.25369600
C	-0.36918500	-0.98970400	2.82392300
H	-0.33374000	0.01833000	2.42391600
C	-1.24281700	-1.29398800	3.86777400
H	-1.87791700	-0.52100600	4.28905300
C	-1.32906300	-2.60161600	4.34693900
H	-2.02158000	-2.84327700	5.14772500
C	-0.52943400	-3.59946400	3.78540200
H	-0.59734000	-4.62085800	4.14898900
C	0.35370700	-3.29382900	2.74882500
H	0.95568700	-4.08079100	2.31108500
P	1.59707500	-1.46769200	0.91228800
H	6.48193100	2.26807000	1.65837400
H	4.65610600	0.15810400	4.63523000
H	6.31086300	-1.00592900	2.84365800
S	-1.22923800	4.98635600	0.90003400

N	1.04238400	3.59283000	1.20189400
N	-0.88513900	2.32270700	1.07979300
H	-0.29954500	1.55192200	0.67871000
F	-6.32200200	0.03452700	2.41369200
F	-4.43438000	-0.92095100	2.93848900
F	-5.00047100	0.93767700	3.89130200
F	-4.31849400	2.18321800	-2.86274300
F	-4.84109000	4.01504900	-1.83270200
F	-6.22840600	2.34014700	-1.81990100
C	1.72290600	2.54979400	2.00659800
H	1.17339400	1.62345700	1.86257200
C	1.66529700	2.92574000	3.49308900
H	2.15705600	3.88458000	3.68268100
H	2.14845300	2.16533900	4.11267100
H	0.61921100	3.01725700	3.79959300
C	-0.32477600	3.58090000	1.06688100
C	-2.27790100	2.09597700	0.87466700
C	-2.98680200	1.39867900	1.84586900
H	-2.48921200	1.12688100	2.76870900
C	-4.32650100	1.05751800	1.63249700
C	-4.97467700	1.43761000	0.46101400
H	-6.00392500	1.15664200	0.28276700
C	-4.26361300	2.16706500	-0.49426200
C	-2.92150400	2.48313900	-0.30255000
H	-2.37529200	3.03161200	-1.05678700
C	-5.03453200	0.28464400	2.70499500
C	-4.92211400	2.66675000	-1.75071800
Cl	-0.79473400	0.67485000	-2.36150500
H	-2.04026700	-2.82409000	1.47683500
Ir	0.56643700	-0.11371000	-0.57645900
C	1.74115300	4.87068700	1.09137400
H	2.81283600	4.66871300	1.05400200
H	1.44156600	5.36595700	0.16893300
H	1.51479100	5.53942600	1.92941300
C	-1.95977000	-2.24939200	-0.62605300
C	-4.20986000	-1.50529900	-1.34624700
C	-4.79643700	-2.13542200	-0.22599300
C	-2.61991000	-2.25222100	0.75729600
H	-4.57201700	-0.30737400	-3.08807900
C	-5.02848800	-0.80251600	-2.23727600
C	-6.17504700	-2.04665600	-0.02727700
H	-2.65147600	-1.21140500	1.10433600
C	-6.98426700	-1.34947600	-0.92618300
C	-6.40514300	-0.72394300	-2.03141700
H	-6.60906000	-2.51941700	0.85072700
H	-8.05513500	-1.29133400	-0.75593300
H	-7.01731700	-0.16307100	-2.73003200
N	-3.94660900	-2.83826200	0.64506400
N	-2.84228600	-1.62885500	-1.57972800
C	-1.43394300	-3.59891700	-1.11099400
C	-1.39001200	-3.86720900	-2.48407400
C	-0.95830800	-4.57343700	-0.22643100
C	-0.88238800	-5.07527300	-2.96074900
H	-1.78245200	-3.12805700	-3.17318900
C	-0.45606700	-5.78498300	-0.69933500
H	-0.98475300	-4.39940400	0.84114600
C	-0.41406600	-6.04140100	-2.06924300
H	-0.86326800	-5.26490800	-4.03072200
H	-0.09402900	-6.52769700	0.00623100
H	-0.02208400	-6.98522600	-2.43811100
H	-2.41846500	-0.91158300	-2.16042600
H	-1.05180300	-1.57420700	-0.51883500
H	-4.37016300	-2.98598600	1.55386700

A-11

C	-3.61541600	-2.09143400	3.00316600
C	-2.24241600	-2.43216900	3.16302400
H	-1.79651200	-2.84716100	4.05582300
C	-1.53349100	-2.05638300	1.98004800
C	-2.49788000	-1.48335700	1.06730500
C	-3.77934400	-1.51996100	1.71189300
H	-4.70001200	-1.14219900	1.29238800
C	-2.01216800	-2.59862300	-1.46204700
C	-3.00712300	-3.55920700	-1.21647600
H	-3.85136200	-3.31724800	-0.57775200
C	-2.91854400	-4.82424000	-1.79319500
H	-3.69483600	-5.55952200	-1.60124900
C	-1.82954000	-5.14654800	-2.60786200
H	-1.75477700	-6.13651200	-3.04853900
C	-0.83505000	-4.19781300	-2.84628500
H	0.02363800	-4.44367400	-3.46258400
C	-0.92723600	-2.92459700	-2.28111900
H	-0.15273900	-2.19385200	-2.47470200
C	-3.76830600	-0.31308900	-1.26081700
C	-4.42005100	0.72593900	-0.58080700
H	-4.02142900	1.08269100	0.35904500
C	-5.56846800	1.30954300	-1.11021100
H	-6.06154800	2.11294100	-0.57031400
C	-6.07187200	0.87246300	-2.33791200

H	-6.96348500	1.33085400	-2.75576800
C	-5.41994600	-0.14991400	-3.02876700
H	-5.79996900	-0.48815000	-3.98834300
C	-4.27376600	-0.74125600	-2.49611800
H	-3.76785800	-1.52769100	-3.04491700
P	-2.16465400	-0.95925300	-0.64501900
Fe	-2.40821100	-0.40406700	2.79224900
C	-1.48299400	1.36374600	2.32562400
C	-2.85345700	1.60480700	2.69399300
H	-3.59794600	2.07549700	2.06998300
C	-3.05291500	1.14324900	4.02524000
C	-1.81470600	0.62158000	4.49929100
C	-0.84956100	0.75984700	3.46033600
H	0.18057000	0.44689600	3.51834700
C	-1.70697900	3.27993400	0.30208100
C	-1.79099100	4.32188600	1.23910800
H	-1.29302000	4.22683600	2.19977800
C	-2.51034800	5.47657200	0.94009300
H	-2.56922600	6.28060300	1.66816000
C	-3.15674800	5.59880400	-0.29454300
H	-3.71952300	6.49921100	-0.52426800
C	-3.07708000	4.56682300	-1.22919800
H	-3.57697600	4.65643300	-2.18913400
C	-2.35169300	3.41021000	-0.93420000
H	-2.28370500	2.59778800	-1.65259600
C	0.94397200	2.30455800	1.00339200
C	1.86935300	1.43610000	1.60986200
H	1.56332300	0.44601800	1.92662300
C	3.20058500	1.81025400	1.76318600
H	3.90896100	1.12515800	2.21718500
C	3.63837400	3.04200400	1.27060700
H	4.68451900	3.31833400	1.35525300
C	2.73863200	3.89668300	0.63605300
H	3.08140200	4.84166800	0.22596700
C	1.39616600	3.53643800	0.50826100
H	0.70420100	4.20825100	0.01253300
P	-0.77428200	1.73918200	0.67483000
H	-4.39117400	-2.20852600	3.74811800
H	-1.64086100	0.16419700	5.46420600
H	-3.98937000	1.15724300	4.56661300
S	2.47886200	-4.20079300	-0.46852500
N	0.30597800	-3.10602500	0.68246300
N	1.78415000	-1.61020900	-0.23329700
H	0.97309800	-0.99059800	-0.45083400
F	7.63008700	-0.50696100	0.77433800
F	6.22537600	-0.28660100	2.42014300
F	6.53376400	-2.23878900	1.51524800
F	3.12873000	2.60356700	-2.39756300
F	4.86956600	1.78456600	-3.40844700
F	5.12964800	3.03322700	-1.64927400
C	-0.04388200	-2.15299100	1.76423400
H	0.28397000	-1.17553100	1.42091900
C	0.73092200	-2.50689500	3.04131800
H	0.48329400	-3.51198500	3.39542300
H	0.51265600	-1.79828500	3.84526700
H	1.80461000	-2.47975000	2.83296000
C	1.50191100	-2.93343000	0.02092900
C	3.03465200	-1.01262700	-0.41204400
C	4.14866000	-1.38280800	0.35077700
H	4.09377300	-2.23871700	1.01096100
C	5.31566600	-0.62620200	0.27548700
C	5.40218800	0.49881200	-0.54525700
H	6.30455900	1.09669300	-0.56847500
C	4.29083500	0.85090300	-1.30862000
C	3.12366000	0.09608300	-1.26322600
H	2.26967400	0.37341200	-1.86719200
C	6.43215400	-0.92512400	1.23277300
C	4.35105000	2.06454300	-2.19373400
Cl	0.12550300	0.24610400	-3.35842800
Ir	-0.60247500	0.47294600	-1.15393200
C	-0.22754400	-4.45630900	0.81872000
H	-1.25474000	-4.38184100	1.17992100
H	-0.22756400	-4.93913700	-0.15722900
H	0.36818200	-5.06973000	1.50485400

A-11a

H	-0.87546600	2.37969900	-1.25319500
C	-0.63073900	1.34030300	0.62778500
C	1.56595900	0.19293000	0.72253800
C	1.73081200	0.37823200	-0.67058900
C	-0.05353400	2.02661100	-0.62465500
H	2.37636900	-0.70703300	2.49195700
C	2.50726200	-0.56980800	1.42068500
C	2.83434400	-0.19007400	-1.31121500
H	0.53647000	2.89826500	-0.29672800
C	3.76685300	-0.94855500	-0.60260100
C	3.60085400	-1.13952700	0.76832900
H	2.94770600	-0.04422300	-2.38361300
H	4.61492900	-1.38343500	-1.12280500

H	4.31699000	-1.72782000	1.33423300
N	0.73407700	1.06550500	-1.37571200
N	0.49384500	0.80494600	1.38771500
C	-1.71882900	0.33325400	0.29088700
C	-1.41760500	-0.96097800	-0.15236500
C	-3.06140700	0.70989100	0.40757300
C	-2.44112900	-1.85080500	-0.47628800
H	-0.38356600	-1.27422900	-0.24048400
C	-4.08678200	-0.17728600	0.07997800
H	-3.30580900	1.70976400	0.76122500
C	-3.77767200	-1.46302100	-0.36416300
H	-2.19281200	-2.85168600	-0.81886800
H	-5.12354800	0.13269600	0.17924700
H	-4.57210900	-2.15992500	-0.61637500
H	0.21999400	0.33365800	2.24111400
H	-1.08622200	2.13125500	1.23778300
H	1.02129500	1.38285700	-2.29291400

B-TS4

C	-0.47183200	-5.07899600	-0.15034000
C	-0.59941800	-4.45174800	-1.41714200
H	-0.69434300	-4.96502900	-2.36148100
C	-0.53728900	-3.03567300	-1.25541700
C	-0.36795100	-2.78727900	0.16570900
C	-0.34782900	-4.06197200	0.82791000
H	-0.24243800	-4.21162500	1.89139900
C	-2.03006000	-0.82866500	1.44042300
C	-2.98489000	-1.85546900	1.42899000
H	-2.73285200	-2.83212600	1.03634200
C	-4.27719500	-1.61871100	1.89754500
H	-5.02033400	-2.40818300	1.84772600
C	-4.62667000	-0.36572700	2.39913600
H	-5.63991500	-0.18619200	2.74327100
C	-3.68704300	0.66536600	2.40140700
H	-3.96765700	1.65724200	2.73946400
C	-2.39877300	0.43993500	1.91629000
H	-1.68707700	1.25517500	1.88497800
C	0.43158200	-1.48215200	2.67971300
C	1.38222900	-2.47873500	2.93041800
H	1.67618900	-3.14588500	2.13688800
C	1.95850000	-2.62169100	4.19159800
H	2.69819700	-3.39985700	4.35557300
C	1.60829800	-1.75555900	5.22498800
H	2.06370100	-1.85859400	6.20551100
C	0.67153000	-0.74969700	4.98535800
H	0.38731900	-0.06644700	5.78066900
C	0.08609700	-0.61499300	3.72747900
H	-0.65007300	0.16347400	3.57312100
P	-0.27934600	-1.17745100	0.99754500
Fe	1.19770000	-3.87859900	-0.56369100
C	2.87782900	-2.67121900	-0.55988800
C	3.11308200	-3.82988100	0.25953800
H	3.37453400	-3.81717200	1.30573200
C	2.96097800	-4.99640500	-0.54182400
C	2.63832300	-4.58324000	-1.86629400
C	2.57521200	-3.15958900	-1.87734700
H	2.29802300	-2.55130500	-2.72519300
C	3.74589600	-0.85825600	1.54574700
C	4.85729000	-1.66068400	1.84240900
H	5.23550300	-2.36077500	1.10430800
C	5.49219700	-1.54754200	3.07761900
H	6.34738600	-2.17807300	3.30489700
C	5.03989600	-0.61350200	4.01390700
H	5.53759900	-0.52533500	4.97572100
C	3.96220100	0.21552800	3.70552000
H	3.61740600	0.95819600	4.41586800
C	3.31706200	0.09619700	2.47567700
H	2.48162300	0.74172000	2.22406100
C	4.31688400	-0.22718200	-1.13408000
C	5.00723800	0.88634500	-0.63255500
H	4.74512800	1.30162700	0.33333100
C	6.02948000	1.47695500	-1.37171700
H	6.54388600	2.34479600	-0.97102200
C	6.37634800	0.97100300	-2.62537500
H	7.17200100	1.43427300	-3.20175100
C	5.69266500	-0.13395800	-3.13274200
H	5.95794400	-0.54289900	-4.10381700
C	4.67078700	-0.73053200	-2.39171200
H	4.16930200	-1.59738600	-2.79937600
P	2.93319400	-0.89546300	-0.09981700
H	-0.44440500	-6.14476800	0.03328200
H	2.42082300	-5.23210400	-2.70408500
H	3.04338900	-6.01727300	-0.19334500
S	-3.55078600	-2.60351800	-1.98125500
N	-1.45715600	-0.95874900	-2.36077900
N	-3.25997800	0.05394400	-1.45428800
H	-2.52846300	0.72934500	-1.22218700
F	-5.39600200	3.61181900	1.96917000
F	-4.95885300	4.45459900	0.01417700

F	-7.02556700	4.14987800	0.63812000
F	-7.64513600	-1.54840800	1.24346800
F	-8.02348100	-1.82213000	-0.87941400
F	-9.07977300	-0.26908800	0.22545900
C	-0.48063600	-2.05787700	-2.41708400
H	0.46602800	-1.51570100	-2.30817000
C	-0.48527500	-2.77780600	-3.77492000
H	-1.43103000	-3.30369300	-3.92313100
H	0.33994600	-3.49364600	-3.83636000
H	-0.35785800	-2.05868900	-4.58782400
C	-2.75617000	-1.12634800	-1.93726400
C	-4.50845500	0.43076000	-0.95642900
C	-4.59660400	1.75935200	-0.50460700
H	-3.73514600	2.41212400	-0.59475500
C	-5.76109100	2.22694000	0.08933600
C	-6.86690600	1.39127900	0.25042200
H	-7.77036000	1.75126900	0.72628800
C	-6.77719500	0.08278700	-0.21646300
C	-5.62328400	-0.40561400	-0.82767600
H	-5.56506800	-1.43280700	-1.15398700
C	-5.78745300	3.61284400	0.66674900
C	-7.88698300	-0.88517800	0.07927100
Cl	-0.76622700	1.99238500	-0.45426900
H	2.07203600	1.61526600	-0.53745100
H	1.77667700	1.17326600	-1.46747000
Ir	1.06359200	0.35965300	-0.22817000
C	-1.07272900	0.18434700	-3.20201500
H	-0.07589600	0.52882900	-2.92477800
H	-1.08141700	-0.10571200	-4.26078800
H	-1.76150800	1.01378800	-3.07433300
H	0.40978000	3.57030400	0.99492500
C	2.30266000	4.05077500	-1.19583900
C	3.49362300	3.92815700	0.79280300
C	2.31525500	4.04069600	1.57417700
C	1.24091800	4.82566200	-0.43214200
H	5.62616900	3.71357000	0.82227900
C	4.73319600	3.77823700	1.43694800
C	2.39010900	3.87604000	2.96401700
C	3.62578100	3.70253700	3.58080200
C	4.80459400	3.68042300	2.82100900
H	1.47676900	3.93752500	3.54975100
H	3.67615300	3.60882500	4.66225700
H	5.76670600	3.56334900	3.31027300
N	1.10898900	4.30657800	0.92526000
N	3.40209800	3.73928700	-0.58641900
C	2.09147500	3.55551900	-2.57174100
C	3.10815000	2.80580300	-3.19633000
C	0.87422600	3.72412400	-3.25102800
C	2.90573800	2.23308700	-4.44582000
H	4.04325700	2.66535800	-2.67002300
C	0.67434000	3.15136200	-4.50744100
H	0.06242200	4.27860900	-2.79666600
C	1.68416200	2.39935000	-5.10790200
H	3.70170900	1.64890000	-4.89856700
H	-0.27776300	3.28849500	-5.01239100
H	1.52328700	1.94895300	-6.08355800
H	1.54368300	5.88233100	-0.38065700
H	0.25999800	4.77975400	-0.89886200

B-6

C	-0.41378200	-4.91526600	-1.40325700
C	-0.30071400	-3.90795400	-2.39654800
H	-0.21664700	-4.08438000	-3.45796400
C	-0.27295700	-2.62813200	-1.76951000
C	-0.36784500	-2.85557200	-0.33338600
C	-0.47719100	-4.27561000	-0.14049000
H	-0.59293800	-4.77461500	0.80912500
C	-2.18501900	-1.47992800	1.38713800
C	-3.11710800	-2.39530500	0.87770300
H	-2.80756100	-3.15107500	0.16706100
C	-4.45800900	-2.32173200	1.25629000
H	-5.17590500	-3.01638100	0.83143900
C	-4.88534300	-1.34010300	2.14934300
H	-5.93448500	-1.27461400	2.41864200
C	-3.96809000	-0.41526300	2.64917000
H	-4.30150600	0.38548200	3.30119800
C	-2.62840900	-0.48007100	2.26754600
H	-1.93783200	0.27009000	2.63039600
C	0.35016300	-2.15820700	2.51080100
C	0.85954600	-3.43435300	2.77471700
H	0.83492300	-4.20151800	2.01507500
C	1.44631000	-3.72746500	4.00896500
H	1.84655400	-4.72206800	4.18558400
C	1.51742800	-2.75748400	5.00651600
H	1.97190300	-2.98940000	5.96526300
C	1.00296500	-1.48266200	4.75981100
H	1.05689600	-0.71247800	5.52422100
C	0.43798400	-1.18456200	3.52276500
H	0.08636900	-0.17651100	3.32872700

P	-0.39739800	-1.55325900	0.93322200
Fe	1.29674600	-3.73717300	-1.08662400
C	2.87100500	-2.45972300	-0.82818700
C	2.91228300	-3.49312900	0.17071800
H	2.86884500	-3.32376300	1.23506900
C	3.01618400	-4.75275200	-0.47909800
C	3.04847300	-4.52039700	-1.88455500
C	2.96681200	-3.11317600	-2.10269400
H	2.95849000	-2.63524700	-3.06955600
C	3.97165700	-0.76491800	1.01824700
C	5.26816100	-1.24174400	0.75205000
H	5.56768000	-1.45243900	-0.26966800
C	6.16913300	-1.45392400	1.78990400
H	7.17012900	-1.81318900	1.56864700
C	5.78160300	-1.22111400	3.11398700
H	6.48193500	-1.39938600	3.92516200
C	4.49576400	-0.76410400	3.38487300
H	4.17732900	-0.58503700	4.40684500
C	3.59843800	-0.52787300	2.34096200
H	2.60323200	-0.17612000	2.56726300
C	3.71338800	0.16111500	-1.71346900
C	4.76995200	1.02014100	-1.38648000
H	5.03096600	1.18828100	-0.34987600
C	5.48339300	1.68007900	-2.38675000
H	6.29317200	2.34827800	-2.10937800
C	5.14896300	1.50184600	-3.72877000
H	5.70753400	2.01496200	-4.50611900
C	4.07574000	0.67431800	-4.06368900
H	3.79110800	0.53886600	-5.10333200
C	3.35967200	0.01795600	-3.06409700
H	2.52050200	-0.60025100	-3.35463800
P	2.76190500	-0.67423500	-0.37099600
H	-0.41951700	-5.98318400	-1.57640000
H	3.09063000	-5.27553900	-2.65831200
H	3.03033100	-5.71838100	0.00881000
S	-3.07248500	-1.68291900	-2.69204200
N	-0.87463800	-0.20290700	-2.02585800
N	-2.85461600	0.48586800	-1.10540100
H	-2.18404500	1.06629400	-0.58883300
F	-5.51264200	2.66263000	3.02461000
F	-4.87650000	4.13538200	1.55856400
F	-6.99125400	3.65269400	1.77847600
F	-7.59483000	-1.83186400	0.22519200
F	-7.59164600	-1.35879300	-1.89592600
F	-8.85212300	-0.22522300	-0.52603600
C	-0.04283300	-1.33556900	-2.53393000
H	0.95577700	-0.99204000	-2.27700200
C	-0.03762400	-1.53399000	-4.05770100
H	-0.97899500	-1.93893700	-4.42578100
H	0.77655500	-2.21668000	-4.32369100
H	0.15725200	-0.58468400	-4.56277800
C	-2.28525200	-0.44050900	-1.90806600
C	-4.17506600	0.68944600	-0.67319500
C	-4.35913800	1.77531300	0.20000500
H	-3.51305100	2.39626000	0.46715800
C	-5.60744900	2.03291300	0.75025800
C	-6.70360400	1.22470200	0.44831400
H	-7.67474200	1.42129100	0.88509300
C	-6.51690800	0.16126500	-0.42896000
C	-5.27408900	-0.11338300	-0.99886800
H	-5.15218000	-0.95607500	-1.66000500
C	-5.74739500	3.12731100	1.76977300
C	-7.64143000	-0.80604700	-0.66771600
Cl	-0.89390400	2.03428700	0.77350000
H	1.54147800	0.80395600	1.38226600
H	1.55247500	1.63562600	-0.51207300
Ir	0.79325000	0.36587800	0.10526700
C	-0.58663500	1.07949300	-2.73031000
H	0.48988600	1.17278900	-2.86756200
H	-1.09163700	1.11748800	-3.70306700
H	-0.90465300	1.92328400	-2.12281400
H	0.95773700	3.05296900	2.10347000
C	2.18575600	4.16296000	-0.36860400
C	3.87339400	3.51896300	1.08105800
C	2.97574100	3.38914900	2.17109200
C	1.39275000	4.63485200	0.83980000
H	5.90686900	3.35592700	0.43208900
C	5.23361100	3.22776600	1.27505900
C	3.43830600	2.86826000	3.38656400
C	4.78464600	2.55436400	3.54768600
C	5.69267800	2.75720100	2.49987100
H	2.73623000	2.75352600	4.20870500
H	5.13441500	2.16440600	4.49913100
H	6.74485300	2.52729800	2.63738500
N	1.65015100	3.78949100	1.99942100
N	3.39642300	3.73931400	-0.21109900
C	1.59301400	4.14890600	-1.72163100
C	2.31731700	3.57839300	-2.78441900

C	0.31046900	4.65627000	-1.98358600
C	1.77443400	3.51366500	-4.06144800
H	3.30148900	3.18073300	-2.57712900
C	-0.23359900	4.59134300	-3.26733400
H	-0.27840000	5.10006800	-1.18919800
C	0.49291800	4.01796300	-4.31106900
H	2.35030100	3.06088000	-4.86372900
H	-1.22857800	4.98826900	-3.44853300
H	0.06704400	3.96567600	-5.30936100
H	1.68728300	5.66984300	1.07434000
H	0.31973700	4.62223600	0.66274100

B-TS5OR

C	-0.61340900	-4.49567000	0.67060500
C	-1.03426100	-4.02588300	-0.60081400
H	-1.42827000	-4.63092000	-1.40319200
C	-0.84867000	-2.61709200	-0.66230800
C	-0.26454000	-2.20787100	0.59401800
C	-0.15180500	-3.38202500	1.42050500
H	0.24463100	-3.41292300	2.42278500
C	-1.37521600	0.27271800	1.41181600
C	-1.51113000	1.66509100	1.46208500
H	-0.67091000	2.29163100	1.18807100
C	-2.70445500	2.25173500	1.89054100
H	-2.78745600	3.33452100	1.93293700
C	-3.78061600	1.44949200	2.27531600
H	-4.71223600	1.90112400	2.60088500
C	-3.66013600	0.05964600	2.20800800
H	-4.50175800	-0.57475200	2.46728200
C	-2.46708800	-0.52540700	1.78769600
H	-2.39402700	-1.60519400	1.73816800
C	0.84006900	-0.80081600	2.81066200
C	1.91371700	-1.66778200	3.05315000
H	2.35544100	-2.21798700	2.23526000
C	2.42360800	-1.83436500	4.33855100
H	3.26356800	-2.50408200	4.49674500
C	1.87430100	-1.12264200	5.40613100
H	2.27426800	-1.24476500	6.40860200
C	0.80914400	-0.25201000	5.17554700
H	0.37199400	0.30559600	5.99908500
C	0.29116900	-0.09369700	3.88847500
H	-0.54057000	0.58261000	3.73185800
P	0.25222100	-0.53268500	1.07683200
Fe	0.96666100	-3.55399400	-0.29887800
C	2.81532600	-2.67941500	-0.60151100
C	2.94752400	-3.86863100	0.19348500
H	3.35132700	-3.91987300	1.19417300
C	2.44987500	-4.96924600	-0.56355200
C	2.00942300	-4.47277500	-1.82762700
C	2.22415400	-3.06599600	-1.85225500
H	1.98232100	-2.37817500	-2.64959100
C	4.61060300	-1.21132500	1.12788000
C	5.55163500	-2.25401900	1.14082100
H	5.58010500	-2.97357600	0.33169700
C	6.45915300	-2.37788400	2.19066400
H	7.17571900	-3.19440600	2.18807600
C	6.45332100	-1.45054000	3.23644900
H	7.16608100	-1.54418600	4.05105800
C	5.53331600	-0.40382200	3.22470300
H	5.52121900	0.32763400	4.02712900
C	4.61567200	-0.28893000	2.18038600
H	3.89514200	0.51833400	2.18188000
C	4.56667300	-0.80101100	-1.72180200
C	5.28035000	-1.90677800	-2.20918700
H	5.12319400	-2.89137400	-1.78291800
C	6.17395600	-1.76027700	-3.26842500
H	6.71835100	-2.62571600	-3.63593100
C	6.35855000	-0.50906800	-3.85994800
H	7.05344100	-0.39506600	-4.68739000
C	5.63371400	0.58768200	-3.39500400
H	5.75393500	1.56036200	-3.86382500
C	4.73553200	0.44539500	-2.33685600
H	4.14371900	1.28959800	-2.00717200
P	3.43249400	-0.99025000	-0.27687800
H	-0.60725200	-5.52622900	0.99991900
H	1.54251500	-5.05507700	-2.61087100
H	2.37860600	-5.99240500	-0.21885200
S	-4.00680700	-2.64236000	-0.85501200
N	-2.24613300	-0.73822300	-1.60072900
N	-4.31279600	0.03509000	-1.01713200
H	-3.81513600	0.90968000	-0.92408600
F	-8.93146300	3.10908200	1.24235800
F	-7.09603600	2.87658900	2.38744600
F	-7.05805000	3.93590900	0.49351800
F	-8.94894000	-2.50854400	0.61400100
F	-8.73170400	-2.46510800	-1.54721700
F	-10.20568200	-1.19082600	-0.57064200
C	-1.15822300	-1.73006000	-1.84077700
H	-0.27685700	-1.10816200	-1.98414600

C	-1.38590300	-2.48956400	-3.14986700
H	-2.28859700	-3.10273900	-3.10935100
H	-0.52268300	-3.12936700	-3.35838000
H	-1.48124100	-1.77333800	-3.97186900
C	-3.49520200	-1.07353000	-1.18151300
C	-5.64552100	0.14485000	-0.60298400
C	-6.01295300	1.36895700	-0.02785000
H	-5.27079200	2.15106000	0.08841100
C	-7.31166100	1.58596800	0.42152200
C	-8.28584700	0.60052800	0.28433000
H	-9.29776200	0.76805500	0.62960300
C	-7.92750200	-0.59961700	-0.33005200
C	-6.62909900	-0.84003600	-0.77688100
H	-6.37832700	-1.77726300	-1.24827400
C	-7.61068600	2.87673400	1.12729100
C	-8.95452100	-1.69261800	-0.46422500
Ir	1.82704000	0.71550200	-0.04527900
H	2.21929700	1.10353200	1.43283800
Cl	1.45293600	0.26587400	-2.52696800
H	0.76164700	2.01938700	-0.00679400
C	-1.95805000	0.62787400	-2.05822000
H	-1.91838100	1.33166400	-1.21725100
H	-0.97503200	0.65304600	-2.52393300
H	-2.70825400	0.96499000	-2.78159800
H	2.52646700	5.80446200	1.20515200
H	0.59173800	4.62111900	0.53257000
C	1.75386900	3.09811200	-0.51210300
C	4.00065500	3.01943400	0.27426500
C	3.86796700	4.30881500	0.84694900
C	1.51652100	4.05957300	0.66859100
H	5.32949500	1.35587800	0.00906600
C	5.21320600	2.33817200	0.44510300
C	4.93615200	4.88513500	1.54167700
H	1.45734700	3.47680500	1.60180700
C	6.13294300	4.18976800	1.69667400
C	6.26601000	2.90850400	1.15382200
H	4.81533000	5.87913000	1.96735000
H	6.95193900	4.64288300	2.24747500
H	7.18911800	2.35079800	1.27871200
N	2.64760300	4.96389100	0.65394500
N	2.99875200	2.52694800	-0.58527400
C	1.05412700	3.42420900	-1.79461400
C	1.77098100	3.46701200	-2.99229800
C	-0.31673800	3.71277100	-1.80571100
C	1.12730200	3.79832200	-4.18376900
H	2.82634900	3.22633100	-2.97294700
C	-0.96294900	4.03323300	-2.99601500
H	-0.88940300	3.65774900	-0.88325500
C	-0.23883700	4.07873900	-4.19091900
H	1.69352700	3.82553000	-5.11009800
H	-2.02801500	4.24840700	-2.99381800
H	-0.73993400	4.33149600	-5.12103000

B-TS5OS

C	-0.63740700	-4.27983000	1.24513300
C	-1.06628200	-4.03993300	-0.08481000
H	-1.45568600	-4.77868600	-0.76836200
C	-0.89560200	-2.65990100	-0.39024200
C	-0.31805900	-2.03322600	0.77746100
C	-0.18621900	-3.04903300	1.78903000
H	0.20740500	-2.90455300	2.78203300
C	-1.45395200	0.56441800	0.95315900
C	-1.61730100	1.84506800	0.41488700
H	-0.80895100	2.28876500	-0.15586300
C	-2.80950000	2.55042600	0.60973400
H	-2.91528800	3.55100900	0.19839100
C	-3.85223000	1.97826800	1.34040500
H	-4.77509800	2.52668800	1.49999500
C	-3.71681100	0.67578700	1.82969000
H	-4.54089600	0.20269000	2.35430600
C	-2.52953900	-0.02638700	1.63805500
H	-2.43367500	-1.03412700	2.02736500
C	0.57819900	-0.19970700	2.78481400
C	1.63552700	-0.97026300	3.29195100
H	2.15504100	-1.66682600	2.64609500
C	2.04489200	-0.83654200	4.61584600
H	2.87044300	-1.43906100	4.98269000
C	1.41490800	0.08667700	5.45357300
H	1.73868600	0.19933200	6.48430900
C	0.37340600	0.86720500	4.95503700
H	-0.11792300	1.59467500	5.59503600
C	-0.04566500	0.72486100	3.63055400
H	-0.85175800	1.34614200	3.25996200
P	0.17890900	-0.29134900	0.98154800
Fe	0.92373900	-3.50743500	0.10931000
C	2.80601300	-2.72281600	-0.30099800
C	2.89825300	-3.83108500	0.61034700
H	3.29149300	-3.79225400	1.61491400
C	2.35825600	-4.98477100	-0.02817600

C	1.91423600	-4.60175400	-1.32858300
C	2.16953100	-3.20942500	-1.49312600
H	1.89124000	-2.60070000	-2.34030700
C	4.50375600	-1.13108000	1.41282300
C	5.36558800	-2.22660600	1.59947700
H	5.38704800	-3.02779400	0.86907800
C	6.21679200	-2.28249200	2.70101600
H	6.86996000	-3.14045500	2.83265300
C	6.24067500	-1.23235100	3.62325600
H	6.90658600	-1.27533900	4.48061700
C	5.41812500	-0.12450300	3.42620100
H	5.43398000	0.70678100	4.12508900
C	4.55811900	-0.07372200	2.32796700
H	3.92662500	0.79381100	2.18677900
C	4.75913200	-0.93101000	-1.40220800
C	6.08073900	-0.59132400	-1.07321000
H	6.35506600	-0.39150100	-0.04499000
C	7.05835300	-0.50476800	-2.06504500
H	8.07644200	-0.24300000	-1.79054500
C	6.73153500	-0.75551200	-3.39801100
H	7.49452900	-0.69438400	-4.16906100
C	5.41422400	-1.06641400	-3.73499800
H	5.13853100	-1.22812500	-4.77277800
C	4.43204200	-1.14187300	-2.74942900
H	3.40548800	-1.31595500	-3.03719200
P	3.45350700	-1.02427700	-0.10032100
H	-0.61858000	-5.23818800	1.74685600
H	1.41501300	-5.24209000	-2.04349400
H	2.25733100	-5.96538000	0.41772600
S	-4.01540600	-2.76309300	-0.48227700
N	-2.33511400	-1.04913000	-1.71702100
N	-4.40446400	-0.20897200	-1.27145400
H	-3.92330200	0.67080700	-1.40042600
F	-9.09436300	3.28831800	0.01509400
F	-7.18239700	3.52113400	1.02943100
F	-7.31846500	3.86872600	-1.10840700
F	-8.89947200	-2.21469500	1.24602600
F	-8.73992300	-2.88637100	-0.81380300
F	-10.24126600	-1.40702500	-0.25960800
C	-1.20065600	-2.01725900	-1.71999700
H	-0.33922200	-1.39161800	-1.95542000
C	-1.37814300	-3.02509100	-2.86025900
H	-2.26977200	-3.63854000	-2.71022500
H	-0.50123400	-3.67543900	-2.92938300
H	-1.47787300	-2.48956000	-3.80963600
C	-3.56123300	-1.30648800	-1.18621600
C	-5.73765200	-0.01948900	-0.89313600
C	-6.14653600	1.31503800	-0.75323700
H	-5.43837100	2.11532900	-0.93800400
C	-7.44184700	1.62975600	-0.35729400
C	-8.37945300	0.62663600	-0.12570000
H	-9.38938900	0.86890300	0.17824900
C	-7.98459600	-0.69745700	-0.31598300
C	-6.68570200	-1.03466900	-0.69422500
H	-6.40534200	-2.06788000	-0.82513600
C	-7.77187500	3.07361500	-0.11298400
C	-8.96747100	-1.80470400	-0.04109700
Ir	1.91372700	0.71766700	-0.12555500
H	2.36245900	1.03477000	1.33660900
Cl	1.29791800	0.17734600	-2.54341000
H	1.03613800	2.18082500	-0.15552600
C	-2.14192400	0.11165100	-2.59705500
H	-2.08067700	1.04667000	-2.02616000
H	-1.18737600	0.01467300	-3.10859200
H	-2.95284900	0.17892000	-3.32981600
H	0.73044500	4.37628700	-2.90593900
H	0.56967400	4.44904300	-0.51184000
C	2.23065400	3.09144400	-0.20863200
C	3.39859100	2.60754500	-2.21362900
C	2.41355500	3.25213300	-2.99682200
C	1.50989000	4.18209100	-0.99968100
H	5.31807300	1.67920500	-2.21672800
C	4.56584500	2.15637800	-2.83232900
C	2.60363400	3.39818900	-4.37056200
H	2.17218200	5.06988000	-0.95758100
C	3.76448700	2.91649900	-4.97649600
C	4.75327900	2.30525100	-4.20542000
H	1.83331900	3.88557700	-4.96481200
H	3.89729400	3.03439600	-6.04834800
H	5.66448700	1.93741500	-4.66579500
N	1.25812100	3.71546000	-2.34721400
N	3.24942400	2.41177100	-0.82026700
C	2.43987000	3.45120900	1.24262900
C	1.35657500	3.72388600	2.08537100
C	3.74090800	3.52699500	1.74981000
C	1.56893600	4.03864500	3.42521800
H	0.34169700	3.63486000	1.70740500
C	3.95221200	3.84221400	3.09243100

H	4.56726800	3.30697100	1.08297900
C	2.86811900	4.09380900	3.93538600
H	0.71945400	4.22534100	4.07578400
H	4.96653100	3.89108700	3.47953300
H	3.03276300	4.33263700	4.98219300

B-TS5-N

C	-1.16107800	-3.74431800	2.16886800
C	-1.58979000	-3.78415100	0.81606700
H	-2.02860100	-4.63147200	0.31141100
C	-1.33066400	-2.52196200	0.21196500
C	-0.70362200	-1.68536800	1.21014900
C	-0.63051700	-2.45157000	2.42495300
H	-0.21147200	-2.11290600	3.35922300
C	-1.68107800	0.95753800	1.12042200
C	-1.68132400	2.33613700	0.87357500
H	-0.77194700	2.80984900	0.52872000
C	-2.82738500	3.10145300	1.09784800
H	-2.80700000	4.17122300	0.90645600
C	-3.99036900	2.49482400	1.57889900
H	-4.88944600	3.08022400	1.74622000
C	-3.99639400	1.12009400	1.82684800
H	-4.90039300	0.63281700	2.17873700
C	-2.85047700	0.35591500	1.60645000
H	-2.87949900	-0.70925900	1.80073700
C	0.62175000	0.38875000	2.63733300
C	1.63005800	-0.43494400	3.15456600
H	1.94290400	-1.30599900	2.60043600
C	2.23444900	-0.15779100	4.37868000
H	3.01945700	-0.81236200	4.74600000
C	1.85329200	0.96849800	5.10812000
H	2.32694400	1.19290000	6.05963800
C	0.85531000	1.80170900	4.60278100
H	0.54131000	2.67870000	5.16234800
C	0.23946800	1.51225900	3.38331600
H	-0.54519100	2.16654300	3.02512200
P	-0.09846500	0.01838800	0.96286100
Fe	0.43580700	-3.34087000	0.89778000
C	2.29515600	-2.74280200	0.23383100
C	2.42516100	-3.53253600	1.42786200
H	2.87550400	-3.21004700	2.35536700
C	1.85963100	-4.81688200	1.17896500
C	1.38305700	-4.83656400	-0.16678500
C	1.64158900	-3.56363500	-0.74807400
H	1.39423900	-3.23502500	-1.74707000
C	4.24960400	-0.84436800	1.18999600
C	5.17441700	-1.83850900	1.54711100
H	5.14510300	-2.80891100	1.06770900
C	6.15220700	-1.58763700	2.50731300
H	6.86320800	-2.36719800	2.76626100
C	6.22367100	-0.33719700	3.12657000
H	6.99365800	-0.13875500	3.86667700
C	5.30322400	0.65162600	2.78720200
H	5.34438100	1.62616400	3.26463000
C	4.32421100	0.39831200	1.82772500
H	3.60909700	1.16727100	1.56603700
C	4.08933100	-1.66045700	-1.58436800
C	4.69362600	-2.92682700	-1.57309700
H	4.47749600	-3.62855600	-0.77581500
C	5.55183700	-3.31432700	-2.60161400
H	6.01073900	-4.29872600	-2.57514700
C	5.80652900	-2.44764500	-3.66528100
H	6.47244600	-2.75024900	-4.46851300
C	5.18838400	-1.19774900	-3.69849200
H	5.36374000	-0.52168800	-4.53011000
C	4.33301200	-0.81019000	-2.66891600
H	3.84718800	0.15335700	-2.70797800
P	3.02318200	-1.10992100	-0.16881400
H	-1.19690000	-4.56478000	2.87340100
H	0.86341800	-5.65657100	-0.64447600
H	1.76985700	-5.61804600	1.90071300
S	-4.52658900	-2.57015000	-0.09243400
N	-2.66500600	-1.10582600	-1.38726200
N	-4.69095700	-0.08499000	-1.13456200
H	-4.14789000	0.76013900	-1.24918600
F	-9.21828200	3.62995100	0.16829900
F	-7.38762300	3.63910600	1.34480700
F	-7.32168700	4.18075400	-0.75524700
F	-9.53300700	-1.94555500	0.82200600
F	-9.20137700	-2.44341300	-1.26670300
F	-10.64580400	-0.90367000	-0.72515600
C	-1.60437400	-2.14255700	-1.22001500
H	-0.70424600	-1.64237300	-1.57250400
C	-1.84602000	-3.33176900	-2.15253000
H	-2.76827900	-3.85908200	-1.90176400
H	-1.00305500	-4.02596300	-2.08758700
H	-1.91072700	-2.97471200	-3.18497200
C	-3.93003800	-1.22582300	-0.90678800
C	-6.02627500	0.18846400	-0.81069500

C	-6.34565500	1.52640100	-0.55049300
H	-5.56541300	2.27888500	-0.57536600
C	-7.64885900	1.89901900	-0.23205500
C	-8.66804300	0.95226300	-0.18760900
H	-9.68235300	1.23980600	0.05676400
C	-8.35258200	-0.37392700	-0.48844500
C	-7.05331100	-0.76687700	-0.80297700
H	-6.83639000	-1.79765100	-1.03619100
C	-7.90543000	3.33482300	0.12411000
C	-9.43349400	-1.41955400	-0.41933500
Ir	1.61569500	0.61695800	-0.65544000
H	2.02182000	1.55675600	0.54614000
Cl	1.11095700	-0.78580000	-2.77325300
H	3.49989200	1.25597100	-0.96157600
C	-2.30584600	0.01469100	-2.26328600
H	-2.16092900	0.94084900	-1.68957900
H	-1.35996100	-0.21341700	-2.75214100
H	-3.07589100	0.17059600	-3.02541800
H	6.69307800	5.11785300	-0.17676300
H	4.34747600	5.44029600	-0.52308600
C	3.98186600	3.35641400	-0.93115700
C	5.87574600	1.96912800	-0.65580500
C	6.69169500	3.09856800	-0.39739100
C	4.71344400	4.46228300	-0.20482000
H	5.83877000	-0.16540500	-0.82255100
C	6.44740100	0.69414400	-0.59914100
C	8.04126600	2.92013000	-0.07413600
H	4.51900500	4.36549200	0.88298200
C	8.58384100	1.64014100	0.00099000
C	7.78451700	0.52415300	-0.25902500
H	8.65854100	3.79421600	0.12061500
H	9.63034000	1.51704400	0.26448500
H	8.19695600	-0.47765300	-0.20298000
N	6.12401400	4.36173500	-0.53667600
N	4.53645700	2.16435300	-1.04669300
C	2.62007800	3.46411700	-1.34285100
C	2.04669400	2.31967800	-2.05402500
C	1.80526900	4.50930400	-0.91713000
C	0.61387100	2.27030600	-2.14171300
H	2.63399500	1.89009400	-2.86071800
C	0.41599800	4.47835100	-1.11059900
H	2.24014700	5.35237200	-0.38867800
C	-0.16370800	3.35842000	-1.68689500
H	0.16340700	1.55849600	-2.81929800
H	-0.19706200	5.31225200	-0.78299600
H	-1.24005100	3.32618900	-1.83175800

B-7

C	-0.72293200	-4.48669500	0.51712000
C	-1.14289500	-3.94938900	-0.72754600
H	-1.55326400	-4.50865100	-1.55450700
C	-0.93035200	-2.54247700	-0.72555100
C	-0.33428700	-2.20518000	0.54728500
C	-0.23627800	-3.41834300	1.31573500
H	0.17363400	-3.50231200	2.30986500
C	-1.28674700	0.32480400	1.45406400
C	-1.28275300	1.71015300	1.66411900
H	-0.36069500	2.26839300	1.55372400
C	-2.44677100	2.37645300	2.05189600
H	-2.42354200	3.45034100	2.21559000
C	-3.63230500	1.66191200	2.24013300
H	-4.54275000	2.17270900	2.53845000
C	-3.64340000	0.28060100	2.03311600
H	-4.56269700	-0.28293000	2.15616400
C	-2.48026200	-0.38510000	1.64822300
H	-2.51171400	-1.45593300	1.48439900
C	0.82886800	-0.97618100	2.82561600
C	1.94781200	-1.79916900	3.01250900
H	2.44634000	-2.22977100	2.15740600
C	2.43067100	-2.07552900	4.28864200
H	3.30782000	-2.70552400	4.40274100
C	1.80183800	-1.52399900	5.40705200
H	2.17955100	-1.73048400	6.40429400
C	0.68612200	-0.70579100	5.23392300
H	0.18648700	-0.27473800	6.09688500
C	0.19831500	-0.43501000	3.95294400
H	-0.67286700	0.19889000	3.84157300
P	0.27749800	-0.58624200	1.10352000
Fe	0.86800600	-3.52961100	-0.41726400
C	2.73841300	-2.68804700	-0.67779000
C	2.83571500	-3.91903900	0.05857600
H	3.22970700	-4.03143200	1.05797500
C	2.31414800	-4.96629000	-0.75524300
C	1.88840000	-4.39542600	-1.99295700
C	2.13882100	-2.99567200	-1.94676400
H	1.91753100	-2.26234500	-2.70889600
C	4.62738600	-1.34644000	1.07102200
C	5.48512700	-2.45859900	1.04508500
H	5.42754400	-3.17603800	0.23609700

C	6.41877500	-2.65813600	2.06010400
H	7.06831500	-3.52822800	2.02787600
C	6.52337000	-1.74028700	3.10810500
H	7.25523400	-1.89416700	3.89604800
C	5.68875200	-0.62407000	3.13230000
H	5.76552900	0.10307400	3.93501600
C	4.74554200	-0.43067300	2.12348600
H	4.09563000	0.43340600	2.15383800
C	4.51385700	-0.80498300	-1.76351100
C	5.21596000	-1.90343800	-2.28447200
H	5.07402600	-2.89411100	-1.86753100
C	6.08015600	-1.74034000	-3.36489200
H	6.61615300	-2.59934200	-3.75863400
C	6.24519900	-0.48027700	-3.94370500
H	6.91696900	-0.35311700	-4.78811200
C	5.53181200	0.60823800	-3.44383900
H	5.63775000	1.58783900	-3.90103900
C	4.66353800	0.45125300	-2.36295100
H	4.08238000	1.29163600	-2.00436100
P	3.42366000	-1.04057900	-0.29336000
H	-0.73339200	-5.53191700	0.79630300
H	1.40787800	-4.92542300	-2.80452600
H	2.21492500	-6.00317800	-0.46255200
S	-4.09884600	-2.54609300	-0.98054600
N	-2.31653700	-0.61470300	-1.59702400
N	-4.42929800	0.12537700	-1.12568900
H	-3.95627500	1.01401500	-1.04680700
F	-9.00361000	2.96784000	1.51993400
F	-7.05580700	2.78521700	2.47473900
F	-7.25104800	3.91133500	0.63045300
F	-9.02791400	-2.54174400	0.43987900
F	-8.83970500	-2.36712400	-1.71763500
F	-10.30320100	-1.15867600	-0.64604400
C	-1.22646800	-1.59921800	-1.86510900
H	-0.34183500	-0.97495200	-1.97053800
C	-1.43920800	-2.29708300	-3.21078900
H	-2.34548900	-2.90619900	-3.21159800
H	-0.57718500	-2.93236800	-3.43631300
H	-1.51899900	-1.54306300	-3.99985500
C	-3.58498900	-0.96752600	-1.25749800
C	-5.75404500	0.20174900	-0.67137800
C	-6.11159800	1.37886000	-0.00262800
H	-5.36784300	2.15214100	0.15739100
C	-7.40234600	1.55746200	0.48729900
C	-8.37331000	0.57741600	0.30279900
H	-9.37812400	0.71410700	0.68082900
C	-8.02369000	-0.57639400	-0.40052400
C	-6.73517400	-0.77552400	-0.89332900
H	-6.49025100	-1.67379900	-1.43805900
C	-7.69128100	2.80502300	1.27125400
C	-9.04985400	-1.66261900	-0.58685400
Ir	1.93184200	0.65884500	0.03161200
H	2.37694900	0.93183600	1.52175000
Cl	1.41758400	0.41046700	-2.44052300
H	0.95335800	2.22545900	0.07537100
C	-1.99634900	0.78120000	-1.92456700
H	-2.05416500	1.42041100	-1.03420700
H	-0.97183400	0.84326300	-2.28601500
H	-2.66517300	1.17019800	-2.70105900
H	2.78075000	5.76651800	1.31868700
H	0.76246200	4.62110800	0.86866400
C	1.75222500	3.06164300	-0.29033200
C	4.10306500	2.94568900	0.27233000
C	4.04920200	4.25074500	0.82812600
C	1.69071500	4.04703500	0.89809200
H	5.37856400	1.24723300	-0.03933600
C	5.31708800	2.24699200	0.36694000
C	5.18353800	4.81986600	1.41265700
H	1.72995300	3.46540700	1.83594700
C	6.38229300	4.11217000	1.47737800
C	6.44003000	2.81544200	0.96125000
H	5.11339500	5.82440700	1.82574900
H	7.25437400	4.56455800	1.94000900
H	7.35932900	2.23996400	1.01949000
N	2.82509100	4.93148300	0.74718800
N	3.02229900	2.43660800	-0.46156300
C	1.10367000	3.58376900	-1.55415100
C	1.85956700	3.81455000	-2.70177500
C	-0.26990800	3.84956700	-1.56757800
C	1.24809600	4.31146500	-3.85283700
H	2.91720600	3.58127400	-2.68101300
C	-0.88468800	4.33632300	-2.71910100
H	-0.86603500	3.65597700	-0.67773500
C	-0.12305100	4.56992800	-3.86700700
H	1.84293400	4.48645500	-4.74480600
H	-1.95347800	4.53335100	-2.72270500
H	-0.59802100	4.94957800	-4.76729700

B-TS6

C	-1.09201500	-4.95897000	-0.04821400
C	-1.02489600	-4.39208400	-1.34628400
H	-1.09435200	-4.93885900	-2.27400100
C	-0.82109700	-2.98534100	-1.23661400
C	-0.75033400	-2.67510700	0.18049400
C	-0.93408000	-3.91167800	0.89368000
H	-0.88855600	-4.02881500	1.96451300
C	-2.09603400	-0.50390700	1.47556500
C	-2.21367800	0.65321200	2.26297800
H	-1.33573700	1.25636200	2.46707600
C	-3.45106500	1.03100000	2.77380200
H	-3.53992000	1.94180300	3.35740100
C	-4.58631100	0.25682200	2.51181800
H	-5.55258600	0.56959000	2.89357700
C	-4.47736600	-0.89105600	1.73167600
H	-5.35987800	-1.47631000	1.49264600
C	-3.23409200	-1.27486800	1.21815400
H	-3.16921700	-2.16288600	0.60221400
C	0.13326200	-1.61119100	2.70603400
C	1.44374500	-1.38990300	3.13742300
H	2.13828600	-0.88954800	2.48235000
C	1.86259200	-1.78670900	4.40830500
H	2.89031400	-1.60451900	4.71016400
C	0.96176900	-2.40117900	5.27746900
H	1.27960300	-2.70994600	6.26927900
C	-0.36167300	-2.59612800	4.87238500
H	-1.07803100	-3.05059200	5.55094800
C	-0.77635800	-2.19609500	3.60272700
H	-1.81421900	-2.32517900	3.31507000
P	-0.41282100	-1.08686200	1.00984600
Fe	0.72392500	-3.95984300	-0.30385300
C	2.45295100	-2.88466200	-0.23765100
C	2.37554400	-3.77639800	0.88945700
H	2.35832400	-3.47772700	1.92673800
C	2.30184000	-5.11021800	0.39786900
C	2.32851000	-5.06316400	-1.02794100
C	2.42910500	-3.69850100	-1.42187800
H	2.46145700	-3.32672800	-2.43543400
C	4.21143000	-1.07527400	0.92684800
C	5.13735900	-2.13320800	0.88601900
H	4.98456600	-2.96392400	0.20618300
C	6.24259200	-2.14187000	1.73399600
H	6.94918900	-2.96552300	1.68634500
C	6.43281000	-1.10377800	2.64940500
H	7.29320100	-1.11288100	3.31252500
C	5.50625900	-0.06521200	2.71446900
H	5.63315000	0.74776200	3.42275700
C	4.40270000	-0.05379300	1.86164600
H	3.68752100	0.75144200	1.95063100
C	3.40849500	-0.86553700	-1.90423700
C	4.69992200	-1.25655900	-2.27456700
H	5.38918400	-1.63979900	-1.53287700
C	5.12415400	-1.12085200	-3.59616900
H	6.13372800	-1.41631400	-3.86709900
C	4.26393800	-0.60021300	-4.56558200
H	4.59984500	-0.49440500	-5.59296000
C	2.97680500	-0.20143900	-4.20263200
H	2.30574300	0.22772400	-4.94129200
C	2.55855900	-0.32778500	-2.87869100
H	1.58591900	0.04324200	-2.58225600
P	2.74370900	-1.07302600	-0.19350600
H	-1.19664200	-6.01053900	0.18343500
H	2.24450300	-5.90971800	-1.69642600
H	2.18961200	-5.99969200	1.00370700
S	-3.74803400	-2.41070200	-2.15694600
N	-1.53504800	-0.92379500	-2.47965600
N	-3.29298400	0.23289700	-1.65573600
H	-2.52719200	0.84105100	-1.35941900
F	-6.62087300	4.43133100	0.73964000
F	-5.69454500	3.29370700	2.33770300
F	-4.44915500	4.28502700	0.85372600
F	-8.03075000	-1.35868600	0.31222900
F	-8.29971300	-1.01188800	-1.81577000
F	-9.22680600	0.32664300	-0.36763400
C	-0.61078300	-2.07086900	-2.42605400
H	0.36308800	-1.59830000	-2.27964400
C	-0.56613000	-2.83866100	-3.75425300
H	-1.52777300	-3.31792600	-3.94905500
H	0.22399800	-3.59545900	-3.73029800
H	-0.34660000	-2.15681400	-4.58063300
C	-2.85250900	-0.99205200	-2.09679400
C	-4.52533800	0.65772100	-1.14422900
C	-4.49935800	1.87329500	-0.43719300
H	-3.56457700	2.40958800	-0.32547500
C	-5.64841300	2.35457200	0.17099100
C	-6.85252000	1.65105300	0.09096400
H	-7.74522300	2.02036000	0.58073700
C	-6.87410000	0.46262300	-0.62987500

C	-5.73331100	-0.03668100	-1.26121700
H	-5.77186300	-0.97322300	-1.79555800
C	-5.59483200	3.59549300	1.01553900
C	-8.11233400	-0.38833900	-0.63440400
Ir	1.04299800	0.43708100	0.10926200
H	1.95679600	1.21003300	1.20765700
Cl	-0.81422700	1.96704400	-0.29194100
H	0.73658800	3.41143900	0.76296900
C	-1.02932500	0.23775800	-3.21809600
H	-0.39876500	0.88172000	-2.60113700
H	-0.45514200	-0.11261200	-4.08180400
H	-1.86855900	0.82792100	-3.58877800
H	4.34136500	3.81509500	2.82438000
H	2.24994800	4.72966100	2.41168200
C	1.81541900	3.51045800	0.66842700
C	3.73546000	2.33888100	-0.05226000
C	4.47233000	2.92311600	1.00825700
C	2.37441300	3.68842400	2.08668800
H	3.82843600	1.64089000	-2.06213700
C	4.41077400	1.98179200	-1.21948700
C	5.86150900	3.04482300	0.90580400
H	1.78342100	3.06102800	2.76485500
C	6.52489100	2.60222700	-0.23805100
C	5.79957300	2.08128600	-1.31024900
H	6.42087700	3.47649300	1.73378400
H	7.60598100	2.69220000	-0.29777300
H	6.30250200	1.77490000	-2.22217900
N	3.78637100	3.28494900	2.16549900
N	2.33097700	2.24436900	0.08037200
C	2.09043700	4.65204400	-0.29906300
C	1.37401600	4.67393000	-1.50431300
C	3.04435600	5.64722400	-0.06886800
C	1.60073100	5.67131400	-2.44923700
H	0.63862500	3.89665300	-1.68720800
C	3.27574800	6.64754500	-1.01614300
H	3.62600500	5.64281900	0.84701700
C	2.55538700	6.66360600	-2.20902600
H	1.03060200	5.67755200	-3.37468700
H	4.02458300	7.41034500	-0.82022400
H	2.73486700	7.44130400	-2.94635200

B-8

C	-1.04098500	-4.57862100	-1.68399200
C	-0.81652100	-3.57026100	-2.65606500
H	-0.77494700	-3.72333500	-3.72369800
C	-0.62515800	-2.32004800	-1.99943300
C	-0.72049700	-2.56595300	-0.57196400
C	-0.99353300	-3.96905300	-0.40454800
H	-1.07354000	-4.48437200	0.53856900
C	-2.23922500	-1.05335700	1.30757100
C	-2.47734200	-0.35683800	2.50433100
H	-1.64653300	0.07863700	3.04784200
C	-3.77297200	-0.22104300	2.99236300
H	-3.95031800	0.34257600	3.90304900
C	-4.84946600	-0.78428900	2.29910000
H	-5.86018800	-0.65473600	2.67244200
C	-4.62117200	-1.48001400	1.11527900
H	-5.45281300	-1.89118700	0.55113200
C	-3.31913400	-1.62049500	0.62368100
H	-3.16383900	-2.15565900	-0.30410500
C	-0.08485200	-2.49819700	2.24966400
C	1.13758200	-2.35844900	2.90967800
H	1.81758100	-1.58873900	2.58329600
C	1.47420000	-3.17836000	3.98825500
H	2.43785700	-3.05026600	4.47364000
C	0.57114600	-4.14158000	4.43617600
H	0.82408400	-4.78343000	5.27546000
C	-0.67802800	-4.25608300	3.81791000
H	-1.40206200	-4.97910000	4.18322200
C	-1.01017400	-3.43327400	2.74290400
H	-1.99936500	-3.50212500	2.30307600
P	-0.49263900	-1.39651800	0.81282600
Fe	0.79465400	-3.64921000	-1.33713000
C	2.50220600	-2.72974100	-0.71561200
C	2.28208700	-3.93640400	0.03659800
H	2.12816800	-3.99094700	1.10404900
C	2.26968300	-5.03237900	-0.87303000
C	2.47644600	-4.52285700	-2.18978700
C	2.62564600	-3.10972000	-2.09594300
H	2.78302000	-2.42812200	-2.91890000
C	3.94652100	-1.35021300	1.25903400
C	4.87300600	-2.40012300	1.17580200
H	4.85760900	-3.07214300	0.32489700
C	5.79777400	-2.61456600	2.19847900
H	6.50678600	-3.43390400	2.11869600
C	5.80190100	-1.79054900	3.32526100
H	6.51845200	-1.96237200	4.12360300
C	4.87251700	-0.75401800	3.42701900
H	4.86040400	-0.11125800	4.30241900

C	3.95304700	-0.53880300	2.40203900
H	3.21331400	0.24965400	2.48886600
C	3.67331000	-0.32757300	-1.46689900
C	4.95867700	-0.79142500	-1.78483100
H	5.42975100	-1.55292800	-1.17466600
C	5.64636800	-0.26992600	-2.87890700
H	6.64400800	-0.63315800	-3.10982500
C	5.05521900	0.71382400	-3.67666200
H	5.59320000	1.12056700	-4.52833700
C	3.77815800	1.17907100	-3.36859600
H	3.31848000	1.95948400	-3.96355600
C	3.09606400	0.66500200	-2.26533600
H	2.12029100	1.04911100	-1.99883900
P	2.68457100	-1.02402800	-0.06262400
H	-1.17596600	-5.63416200	-1.87931700
H	2.47825100	-5.10032200	-3.10479100
H	2.08125100	-6.06555100	-0.61226600
S	-3.44733900	-1.31387300	-2.94579000
N	-1.21910800	0.07687300	-2.43455800
N	-3.04771800	0.87798800	-1.36395900
H	-2.32811700	1.27344500	-0.75768500
F	-6.59432600	3.87839500	2.17679000
F	-6.04110700	2.07386200	3.24550300
F	-4.49356200	3.43911700	2.55386800
F	-8.02225500	-1.11228200	-0.86676600
F	-7.99005600	0.14019600	-2.64174600
F	-9.09909100	0.77771500	-0.87769700
C	-0.28445000	-1.03011600	-2.71238700
H	0.64705000	-0.67249600	-2.26389500
C	-0.06354800	-1.21959800	-4.21736100
H	-0.98436200	-1.55570900	-4.69926300
H	0.73265200	-1.94855000	-4.39789300
H	0.24056900	-0.27357000	-4.67545100
C	-2.56164000	-0.07949500	-2.22853500
C	-4.33473700	1.10944400	-0.86083400
C	-4.39872000	1.89345800	0.30475900
H	-3.48442400	2.26563700	0.75083200
C	-5.61670400	2.13091200	0.92247100
C	-6.80202100	1.60744400	0.40098500
H	-7.75045100	1.77933800	0.89521600
C	-6.73186600	0.85530100	-0.76597800
C	-5.51876300	0.61112400	-1.41286500
H	-5.48980300	0.00542700	-2.30516900
C	-5.67536400	2.88595300	2.21922900
C	-7.96318800	0.17469600	-1.29298000
Ir	0.96378300	0.30505400	0.52858600
H	1.62293700	2.40542000	1.57767400
Cl	-0.82042800	1.91823900	1.06463900
H	0.62622000	3.36752300	-0.25704600
C	-0.59695100	1.39497400	-2.47500300
H	0.00198700	1.57017300	-1.57606700
H	0.05753600	1.45405200	-3.35137800
H	-1.36267200	2.16633500	-2.56757900
H	2.57914000	5.28515600	2.79101800
H	1.99837800	5.68931600	0.49128500
C	1.66075000	3.59487400	-0.01882900
C	3.52963900	2.63095900	1.14403900
C	3.64947600	3.77708300	1.95647300
C	1.64569200	4.77948100	0.99539900
H	4.57125400	1.10027900	0.07865000
C	4.65922400	1.92618300	0.76382300
C	4.90111400	4.13777600	2.46520300
H	0.61857200	4.94469700	1.33169400
C	6.02540200	3.38126800	2.12854900
C	5.91173800	2.29302000	1.26324100
H	4.99323600	5.01577200	3.09993600
H	6.99675200	3.66404100	2.52442800
H	6.78894400	1.72227900	0.97634900
N	2.46370200	4.47781800	2.18913100
N	2.16821300	2.35686400	0.70740600
C	2.36818600	3.93047600	-1.31749200
C	1.58726300	3.98658100	-2.48030300
C	3.71883800	4.30264100	-1.41324700
C	2.12921200	4.37710500	-3.70551800
H	0.53084800	3.74789000	-2.41744700
C	4.26792800	4.67642300	-2.63941400
H	4.34986200	4.31458900	-0.53459300
C	3.47920300	4.71744600	-3.79026600
H	1.49499000	4.42031500	-4.58664900
H	5.31780900	4.95074700	-2.68987700
H	3.91028100	5.02164700	-4.73990000

B-9

C	0.96060300	-3.53580500	2.38758800
C	0.87086800	-3.80360400	0.99760000
H	0.99454400	-4.77273600	0.53961600
C	0.62272000	-2.58819100	0.29364300
C	0.56604200	-1.53142500	1.28956400
C	0.76815300	-2.14464100	2.57630300

H	0.82857800	-1.62039300	3.51672900
C	-1.41043200	0.58817100	1.35200500
C	-1.86907800	1.91100900	1.23992600
H	-1.20324700	2.68268100	0.86824300
C	-3.17789300	2.22767400	1.58959400
H	-3.53625000	3.24533600	1.47614700
C	-4.04297200	1.22965300	2.04905500
H	-5.07113100	1.47697000	2.29307400
C	-3.59518200	-0.08537000	2.15384800
H	-4.27688900	-0.86995100	2.46668700
C	-2.27710800	-0.40767900	1.81646900
H	-1.94322100	-1.43503400	1.88932600
C	1.05307400	1.00111600	2.61675200
C	2.18685300	1.81840800	2.57519100
H	2.64800600	2.03628800	1.62313900
C	2.70833600	2.37495800	3.74448400
H	3.59271300	3.00325800	3.68746300
C	2.08682000	2.13394600	4.96970800
H	2.48758600	2.56725100	5.88165500
C	0.92650900	1.35581800	5.01551400
H	0.41818500	1.18999400	5.96113300
C	0.40486200	0.80319900	3.84684000
H	-0.51842500	0.23441300	3.88864400
P	0.37139400	0.26287100	1.06490300
Fe	2.38334500	-2.41549800	1.34536300
C	3.69399700	-1.10336800	0.48624800
C	3.87288800	-1.12944300	1.91435700
H	3.73269600	-0.29116400	2.58062600
C	4.23100600	-2.45513600	2.29281100
C	4.26971900	-3.26073300	1.11610200
C	3.94356300	-2.43256000	0.00392900
H	3.86946100	-2.74653300	-1.02734900
C	4.43593800	1.60523000	-0.02876700
C	5.64106500	1.29674800	0.61514400
H	5.87586300	0.26789100	0.86589200
C	6.53689000	2.31149100	0.95652700
H	7.46541400	2.06121000	1.46212100
C	6.23981300	3.64143800	0.65561400
H	6.93643000	4.42972600	0.92640600
C	5.04181800	3.95644500	0.00990200
H	4.80130900	4.98978300	-0.22289200
C	4.14458900	2.94484400	-0.32851200
H	3.19579300	3.18797300	-0.80113900
C	3.86145800	-0.16739600	-2.18968600
C	5.20379200	-0.53674600	-2.35991000
H	5.87599500	-0.54317200	-1.50800000
C	5.68038600	-0.89730600	-3.61833400
H	6.72028200	-1.18772600	-3.73803500
C	4.82592900	-0.88119600	-4.72521200
H	5.20151300	-1.15979800	-5.70558200
C	3.49379900	-0.50054300	-4.56804800
H	2.82577000	-0.47515800	-5.42430700
C	3.01500800	-0.14778400	-3.30442300
H	1.97533900	0.13784900	-3.17595900
P	3.20088500	0.32832300	-0.53673100
H	1.18425400	-4.25691900	3.16243200
H	4.47004900	-4.32317800	1.07646400
H	4.39415800	-2.79919700	3.30557500
S	-2.36119000	-3.22405900	-0.26211100
N	-0.62622200	-1.84314100	-1.76563700
N	-2.60485600	-0.79210900	-1.48475600
H	-2.03680700	0.00478700	-1.76670500
F	-6.96762800	3.14366000	-1.61655800
F	-5.78012400	3.47168700	0.16933400
F	-4.83811000	3.57462200	-1.79040300
F	-6.82043200	-1.77919300	1.71645500
F	-7.09344300	-2.91696200	-0.11451000
F	-8.38473600	-1.21485600	0.31436800
C	0.57633400	-2.49834000	-1.22154000
H	1.37696800	-1.81326700	-1.51524800
C	0.82112300	-3.85717900	-1.89154200
H	0.03219800	-4.56265100	-1.62091500
H	1.79378700	-4.26366900	-1.59677500
H	0.82344200	-3.74550600	-2.97962100
C	-1.86433800	-1.91545700	-1.19130700
C	-3.91102200	-0.41457200	-1.15042100
C	-4.21495400	0.94632500	-1.32961300
H	-3.45446200	1.62223900	-1.70510900
C	-5.46526700	1.43485500	-0.97968300
C	-6.44359700	0.59230800	-0.44778900
H	-7.41334400	0.98017200	-0.16085400
C	-6.13955900	-0.75549900	-0.29258300
C	-4.89415600	-1.27373500	-0.64901700
H	-4.67458300	-2.31942700	-0.49937700
C	-5.75575700	2.90564900	-1.06730600
C	-7.11508900	-1.66829400	0.39442200
Ir	1.11963200	1.10821100	-0.80319500
Cl	-0.63557400	2.19648300	-

1.94673000

C	-0.46399300	-1.23249500	-3.08845900
H	-0.23698900	-0.16499400	-3.03167500
H	0.35808300	-1.73423200	-3.60355100
H	-1.37563000	-1.37818300	-3.67340700

B-9a

H	0.32584100	0.52730000	2.28402400
H	-1.10172900	2.18928500	1.23301700
H	0.15458500	0.52988600	-2.05054300
H	-0.92293800	2.39274400	-1.27460800
C	-0.62835700	1.39504900	0.64095500
C	1.57584400	0.28799400	0.69890100
C	1.67227600	0.37613100	-0.70819000
C	-0.09186000	2.03617300	-0.66151400
H	2.46928400	-0.50876300	2.48463700
C	2.54186800	-0.44763600	1.40069200
C	2.70917000	-0.28701300	-1.36806100
H	0.52403000	2.89924900	-0.38334800
C	3.64735000	-1.04019900	-0.66491400
C	3.56472000	-1.10984800	0.72749800
H	2.76450200	-0.19789900	-2.44984700
H	4.44235900	-1.55351500	-1.19712400
H	4.29579200	-1.68029700	1.29327300
N	0.71857900	1.12365800	-1.44987300
N	0.53815200	0.93459500	1.38168700
C	-1.68113200	0.33900000	0.34465900
C	-1.34775800	-0.99826200	0.09478900
C	-3.02657200	0.72109500	0.26625200
C	-2.33888600	-1.92588500	-0.23113000
H	-0.31401700	-1.31967700	0.16473600
C	-4.01728800	-0.20309200	-0.06055000
H	-3.29846500	1.75557600	0.46698400
C	-3.67483400	-1.53295600	-0.31234000
H	-2.06352000	-2.95993300	-0.42011600
H	-5.05586800	0.11229200	-0.11189000
H	-4.44422100	-2.25732300	-0.56417600

TS5OS-ET

C	-3.34411100	4.61620600	-1.41342400
C	-1.92885100	4.70474000	-1.53821600
H	-1.39274000	5.42332400	-2.14208400
C	-1.33738800	3.63099800	-0.80183200
C	-2.41316200	2.87554200	-0.19815400
C	-3.64331400	3.50451700	-0.57911500
H	-4.63005500	3.16155500	-0.30584700
C	-1.82796500	2.38817100	2.48100300
C	-2.71459900	3.40091700	2.88093500
H	-3.59658800	3.61395500	2.28462500
C	-2.47765500	4.12997200	4.04400100
H	-3.17287100	4.90941900	4.34346800
C	-1.34874000	3.85695600	4.82233700
H	-1.16213200	4.42571000	5.72901900
C	-0.45841600	2.86057300	4.42403200
H	0.43664100	2.65713000	5.00329700
C	-0.69604800	2.13111100	3.25761800
H	0.00563300	1.37063900	2.94922600
C	-3.88767500	0.84242900	1.25632800
C	-4.78817400	0.58921400	0.21362000
H	-4.52439700	0.86381700	-0.79735200
C	-6.01691200	-0.02078600	0.46241200
H	-6.69986700	-0.20774100	-0.36171700
C	-6.35624600	-0.40508400	1.76016900
H	-7.31009500	-0.88681100	1.95640300
C	-5.45902900	-0.17081300	2.80411500
H	-5.70972200	-0.47425200	3.81670800
C	-4.23426000	0.44858600	2.55766600
H	-3.53877500	0.60930200	3.37249900
P	-2.18292600	1.45815000	0.92609300
Fe	-2.56238600	2.86389400	-2.23058800
C	-2.01807200	0.98095300	-2.84997700
C	-3.41691100	1.20297200	-3.10304300
H	-4.22519500	0.60370800	-2.71481400
C	-3.55745900	2.32119600	-3.97288500
C	-2.25235100	2.80305900	-4.27862200
C	-1.30997400	1.98294600	-3.59312500
H	-0.24002900	2.11131700	-3.62194900
C	-2.68865800	-1.59881000	-2.04811200
C	-3.19877100	-1.90826000	-3.32225600
H	-2.73868300	-1.47951800	-4.20703700
C	-4.30432500	-2.74386100	-3.45773000
H	-4.68596700	-2.97765400	-4.44779100
C	-4.93072600	-3.26815400	-2.32100000
H	-5.80090600	-3.91005700	-2.42856200
C	-4.43835500	-2.96067300	-1.05477900
H	-4.91457600	-3.35788100	-0.16454800
C	-3.31891700	-2.13560700	-0.91833700
H	-2.93195100	-1.88732500	0.06603600
C	-0.00589200	-0.95899800	-3.00253300
C	1.08928800	-0.10991100	-3.22911400

H	1.18102600	0.81145100	-2.66319200
C	2.08104100	-0.44581700	-4.14519900
H	2.92459300	0.22051900	-4.29451100
C	2.01714000	-1.66051500	-4.83076500
H	2.80516800	-1.93481100	-5.52470700
C	0.95939600	-2.53265600	-4.58471300
H	0.91108000	-3.49091100	-5.09422400
C	-0.04899500	-2.18301400	-3.68292400
H	-0.87030200	-2.87142500	-3.52329600
P	-1.30352700	-0.38525000	-1.81350300
H	-4.06693700	5.25741000	-1.90035500
H	-2.01369800	3.66539800	-4.88716100
H	-4.49275500	2.74772400	-4.31044100
S	2.64906100	3.01915000	2.38943600
N	0.66956600	3.40584600	0.63709400
N	1.96238200	1.53323100	0.22367100
F	5.51539500	-2.71984900	-1.74234100
F	3.38972500	-2.60891200	-2.18921100
F	4.84093700	-1.65190600	-3.49962400
F	6.69740600	3.34092600	-0.11124200
F	7.82954400	1.78295200	-1.13059800
F	7.37661200	1.59175500	0.98634200
C	0.13046500	3.29176100	-0.74335700
H	0.21219500	2.24414300	-1.01672400
C	0.99140200	4.12930300	-1.69621100
H	0.98422500	5.18723900	-1.41523900
H	0.62889400	4.04604000	-2.72471800
H	2.02500900	3.77300100	-1.66014400
C	1.73280900	2.65272200	1.02694400
C	3.20078900	1.06883400	-0.20798900
C	3.25165200	-0.15246800	-0.90708500
H	2.34264500	-0.72180800	-1.03770400
C	4.45942600	-0.62576800	-1.40662600
C	5.65000700	0.07684700	-1.21472300
H	6.59057000	-0.30946300	-1.58725100
C	5.59454000	1.28316000	-0.52561200
C	4.39206400	1.79343000	-0.04221800
H	4.38737700	2.73412700	0.48714900
C	4.53896800	-1.89766100	-2.19924700
C	6.87129400	2.00543500	-0.20217300
Cl	-1.06717100	-1.01429200	2.69720900
H	1.29480100	-3.12650400	-1.36732500
Ir	-0.83281600	-0.31193400	0.35614700
C	0.35858800	4.63644100	1.36223200
H	-0.61036900	5.00136100	1.02265400
H	0.31406800	4.43582200	2.42986200
H	1.12976900	5.39579200	1.18683200
C	1.09214000	-3.09944000	0.77819800
C	-0.80046000	-4.37073000	1.53926000
C	-1.22200400	-4.60546500	0.22097700
C	0.91826800	-3.76822000	-0.57547300
H	-1.19076800	-4.60675000	3.63491100
C	-1.54321000	-4.82429000	2.63136100
C	-2.42075600	-5.29172200	0.01640100
H	1.53927900	-4.67801300	-0.56086700
C	-3.17723900	-5.73159700	1.10189500
C	-2.73629200	-5.50628400	2.40982500
H	-2.74797200	-5.46953700	-1.00260900
H	-4.10814900	-6.26262600	0.92532500
H	-3.32186300	-5.85542400	3.25435900
N	-0.45493300	-4.14190300	-0.87291700
N	0.37023200	-3.62219700	1.75747800
C	2.37509800	-2.46358700	1.18384300
C	2.39560000	-1.30183800	1.96579900
C	3.58617200	-3.07517200	0.83017700
C	3.60740900	-0.73993500	2.36094000
H	1.46024600	-0.81720500	2.21329500
C	4.79634900	-2.52130600	1.24689000
H	3.59171500	-3.97299400	0.22202600
C	4.81109700	-1.34772600	2.00150800
H	3.60186000	0.19955700	2.90463200
H	5.72752600	-2.99150700	0.94915700
H	5.75547100	-0.88785400	2.27704800
H	0.58478400	-3.37319300	2.73743000
H	-0.94735600	-3.40928300	-1.37453600
H	0.22418000	-1.65574700	0.18770300
H	1.12874600	0.90836100	0.08055400
O	0.62308400	-2.92389900	4.46985400
H	0.12113500	-2.13415900	4.17895600
C	1.84333100	-2.49756700	5.09530200
H	2.04130400	-3.20767400	5.90575300
H	2.66752800	-2.56809100	4.37510800
C	1.74460900	-1.07746400	5.63399600
H	2.67862100	-0.78851600	6.12844900
H	1.56036100	-0.36624100	4.82064200
H	0.92670800	-0.99116800	6.35784200

TS5OR-ET

C	-4.18212600	2.72832400	-3.08388000

C	-2.79748200	2.92127800	-3.34623600
H	-2.37330800	3.29663200	-4.26687400
C	-2.05405500	2.46339600	-2.21581400
C	-2.99872200	1.98494400	-1.23115100
C	-4.31023100	2.17348400	-1.78161300
H	-5.23978500	1.91245900	-1.30102600
C	-2.36146600	2.99156500	1.28442200
C	-3.46850600	3.85547000	1.28640700
H	-4.40158600	3.53974800	0.82972000
C	-3.38384500	5.11459800	1.87640200
H	-4.24908200	5.77181600	1.87174400
C	-2.18868900	5.52795500	2.47133800
H	-2.11975800	6.51057100	2.92977100
C	-1.08371200	4.67734700	2.46746600
H	-0.14387000	4.99265800	2.90837800
C	-1.16923700	3.41522000	1.87654300
H	-0.30741800	2.76525400	1.87628200
C	-4.09242900	0.74769500	1.16242800
C	-5.07387700	0.06065800	0.43636600
H	-4.95793700	-0.08172900	-0.62887900
C	-6.19241500	-0.47111900	1.07742700
H	-6.94087800	-1.00176500	0.49593600
C	-6.33043400	-0.35180600	2.45952500
H	-7.19745400	-0.77270300	2.96097600
C	-5.33762100	0.29724800	3.19782900
H	-5.42724900	0.38144000	4.27733700
C	-4.22805300	0.84526400	2.55663100
H	-3.45589600	1.33835300	3.13802700
P	-2.52109100	1.36276000	0.42246800
Fe	-3.14305200	0.92178000	-2.96313700
C	-2.47280000	-0.98320800	-2.54133200
C	-3.85491300	-1.01049900	-2.94100600
H	-4.67597300	-1.36689400	-2.33893800
C	-3.96232800	-0.47471500	-4.25762500
C	-2.65547200	-0.10567100	-4.68973600
C	-1.74491900	-0.40631800	-3.63482300
H	-0.68660400	-0.19258700	-3.64251300
C	-3.10055200	-2.49979900	-0.18926400
C	-3.91246600	-3.37703000	-0.92674400
H	-3.74177100	-3.50733500	-1.99049500
C	-4.92077200	-4.10787900	-0.30000800
H	-5.54381300	-4.77870300	-0.88533900
C	-5.11860100	-3.98882700	1.07875200
H	-5.90498500	-4.55855500	1.56637800
C	-4.29981300	-3.14133500	1.82348200
H	-4.44739000	-3.03277800	2.89341400
C	-3.29989600	-2.39995700	1.19328200
H	-2.67029400	-1.72684600	1.76602500
C	-0.69521600	-2.98354900	-1.60811000
C	0.32023200	-2.76906800	-2.55074100
H	0.51689400	-1.77195600	-2.92543600
C	1.10418900	-3.82347200	-3.01715800
H	1.87691000	-3.62706600	-3.75047400
C	0.90960200	-5.11493700	-2.52458300
H	1.52286700	-5.93588400	-2.88553700
C	-0.08150200	-5.34133000	-1.57002400
H	-0.24412700	-6.34060800	-1.17519600
C	-0.87971400	-4.28704600	-1.12158200
H	-1.65302900	-4.48919900	-0.39097300
P	-1.70211200	-1.55598100	-0.96398700
H	-4.99508200	2.93157300	-3.76840300
H	-2.40262300	0.37014400	-5.62804000
H	-4.88109800	-0.33534200	-4.81190100
S	2.00176000	4.53236200	0.15897100
N	-0.11086500	3.40930900	-1.03529100
N	1.49661100	1.91613100	-0.31184000
F	5.14408200	-1.64622500	-3.47036100
F	3.73425800	-2.62538900	-2.14418700
F	3.00178600	-1.38631900	-3.76837700
F	6.54495000	3.41670600	-0.98939900
F	7.53251600	1.48825100	-0.78818100
F	6.49003900	2.36911200	0.91073700
C	-0.55789300	2.44496000	-2.07808600
H	-0.30764300	1.44531600	-1.72605100
C	0.18758100	2.71953700	-3.38919300
H	0.00580900	3.73727500	-3.74857700
H	-0.12632300	2.01932300	-4.16901600
H	1.26378900	2.60383100	-3.23027100
C	1.10028900	3.24115200	-0.42782900
C	2.75020700	1.40789200	-0.68239800
C	2.77359400	0.23341300	-1.45058100
H	1.83473500	-0.25827500	-1.68299700
C	3.98334100	-0.26547800	-1.93326000
C	5.18929600	0.36767700	-1.63882400
H	6.12578800	-0.02713600	-2.00599000
C	5.16008600	1.50366400	-0.83600800
C	3.96329800	2.02813700	-0.35563100
H	3.95446200	2.91416000	0.26291400

C	3.97689500	-1.47342800	-2.82220300
C	6.43412100	2.19192500	-0.43464500
Cl	-0.48082100	0.43227900	2.92160300
H	1.22684800	-3.84305100	0.40608600
Ir	-0.84577800	-0.22130700	0.59604000
C	-0.68659800	4.75044200	-1.10527000
H	-1.73829200	4.66166200	-1.37639700
H	-0.60786100	5.22747600	-0.13091800
H	-0.16153000	5.37454100	-1.83794000
C	1.71585200	-2.17947600	1.69865000
C	4.02545800	-1.51528300	1.42425500
C	4.32622500	-2.73023100	0.77028300
C	1.97064200	-3.05547500	0.47910200
H	4.78413600	0.34404300	2.18556600
C	5.02981700	-0.57585000	1.66941200
C	5.63929500	-2.96974400	0.35292300
H	1.90811400	-2.43730900	-0.42071100
C	6.63479200	-2.02757100	0.59997700
C	6.33520600	-0.83311900	1.26183500
H	5.87009200	-3.89834000	-0.16220600
H	7.64999100	-2.22455000	0.26849900
H	7.10755800	-0.09527100	1.44183000
N	3.29149100	-3.64656300	0.63976200
N	2.74652600	-1.37413800	1.98931500
C	0.82461900	-2.61025800	2.79480000
C	1.15828700	-2.34911000	4.13171200
C	-0.34701200	-3.32941600	2.51613200
C	0.32771600	-2.78364400	5.16322300
H	2.07204900	-1.81848900	4.37369800
C	-1.16568200	-3.77452000	3.54445400
H	-0.63703100	-3.49979200	1.48735300
C	-0.83419300	-3.49699700	4.87466400
H	0.59566100	-2.56643400	6.19275800
H	-2.07450300	-4.31796400	3.30621100
H	-1.47919900	-3.83816800	5.67944500
H	2.64775200	-0.63442400	2.71310500
H	0.50661600	-1.25749500	0.80537800
H	3.47585500	-4.41537100	0.00763300
H	0.73739400	1.20064000	-0.25930500
O	2.45960900	0.74740000	3.76219500
H	1.48130800	0.63637300	3.73618500
C	2.70845900	2.01292100	3.12263800
H	3.79531700	2.09585800	3.02139400
H	2.27125700	2.01617700	2.11802200
C	2.15788200	3.17192900	3.93945700
H	2.36413000	4.11790600	3.42695700
H	1.07253300	3.07355300	4.05283300
H	2.60935900	3.19623500	4.93697400

12. Supporting references for DFT calculation

8. Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Al-Laham, M. A.; Shirley, W. A.; Mantzaris, J., A complete basis set model chemistry. I. The total energies of closed-shell atoms and hydrides of the first-row elements, *J. Chem. Phys.***, 1988**, *89* (4), 2193-2218.

9. Becke, A. D., Density-functional thermochemistry. III. The role of exact exchange, *J. Chem. Phys.***, 1993**, *98* (7), 5648-5652.

10. Yang, T.; Sun, Y.; Wang, H.; Lin, Z.; Wen, J.; Zhang, X., Iridium-Catalyzed Enantioselective Hydrogenation of Oxocarbenium Ions: A Case of Ionic Hydrogenation, *Angew. Chem. Int. Ed.***, 2020**, *59* (15), 6108-6114.

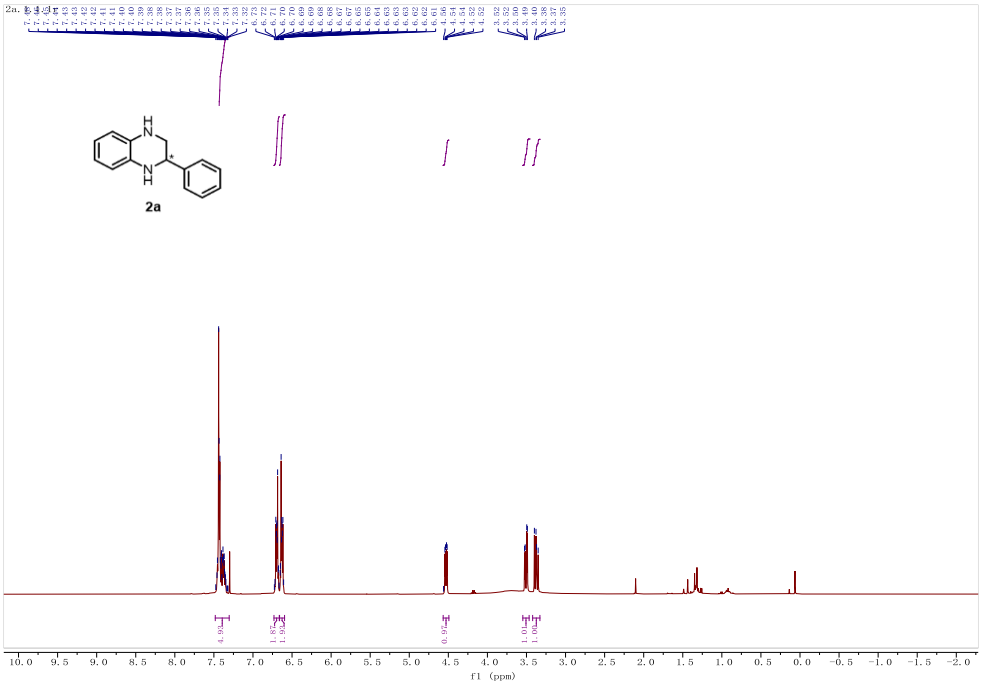
11. Wen, J. L.; Fan, X. R.; Tan, R. C.; Chien, H. C.; Zhou, Q. H.; Chung, L. W.; Zhang, X. M., Brønsted-Acid-Promoted Rh-Catalyzed Asymmetric Hydrogenation of N-Unprotected Indoles: A Cocatalysis of Transition Metal and Anion Binding, *Org. Lett.***, 2018**, *20*, 2143−2147.

12. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions, *J. Phys. Chem B.***, 2009**, *113* (18), 6378- 96.

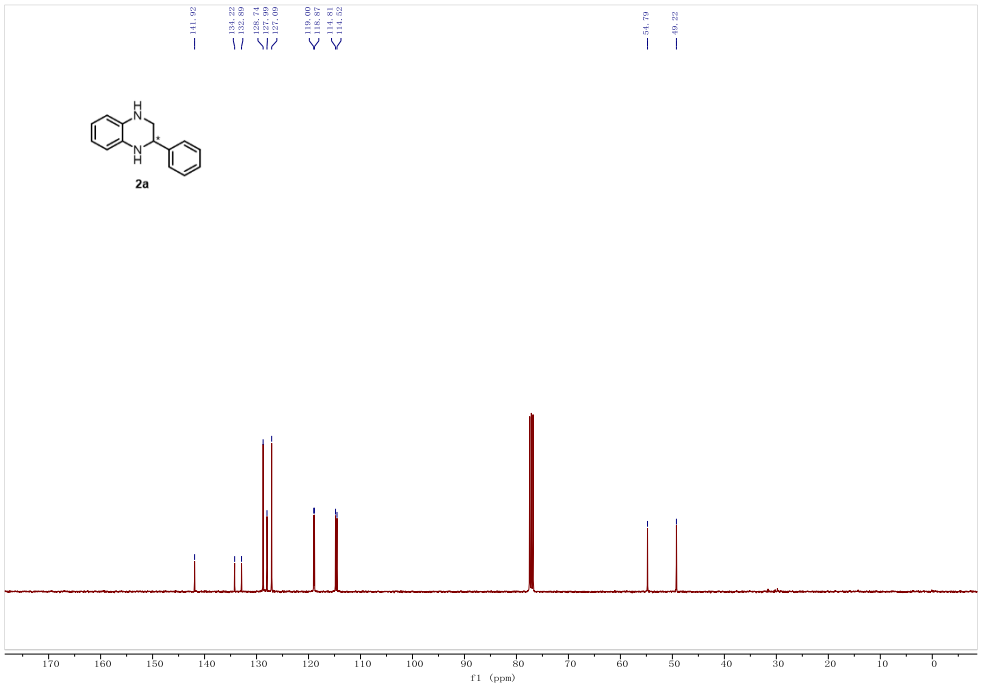
13. NMR spectra

Note: All the target compounds are correctly identified and of high purity. However, it is unavoidable that the sample will be contaminated during the post-processing stage due to the presence of vacuum grease, plastic or high-boiling impurities in solvents. Accordingly, a few of the compounds show an impurity peak at approximately 1.25 ppm in the ^{1}H NMR spectra. However, this does not affect the structural identification.

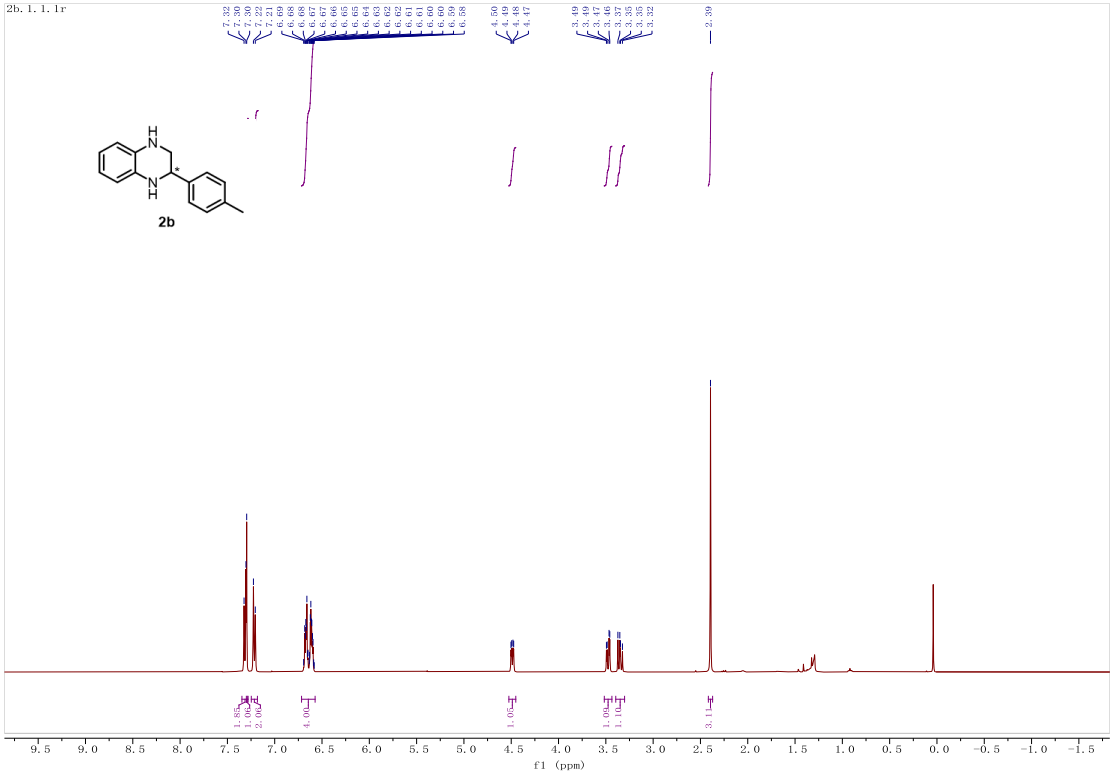
^{1}H NMR spectra for 2a



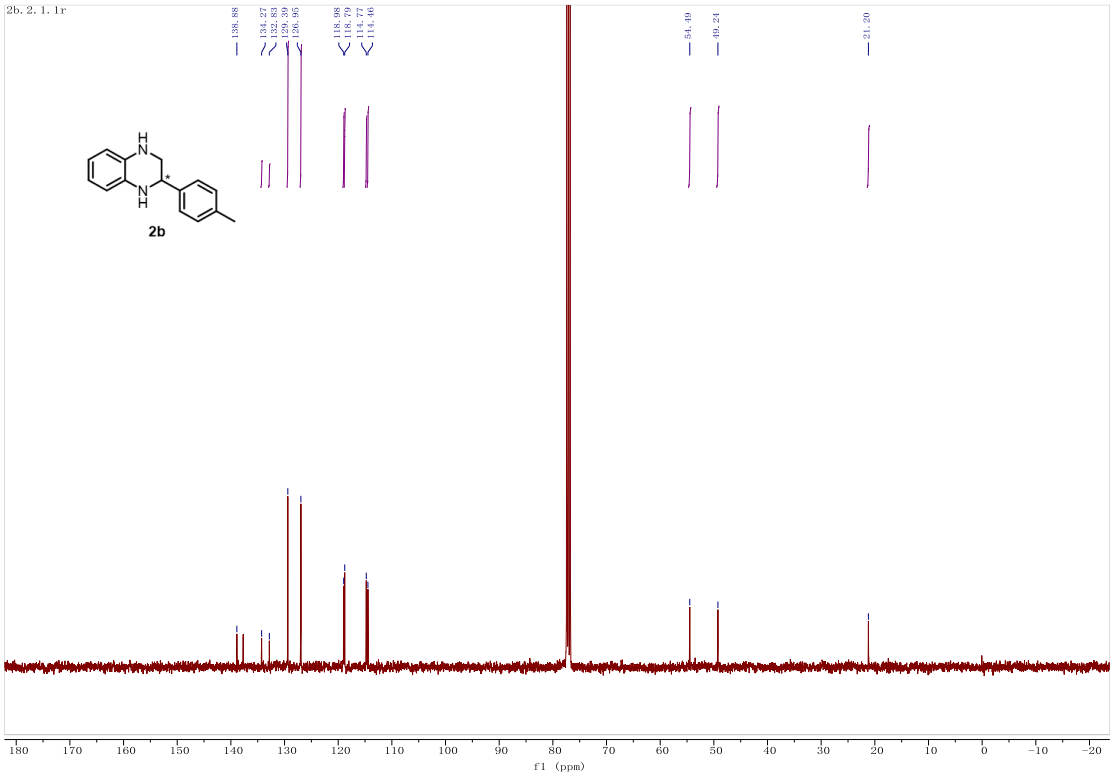
^{13}C NMR spectra for 2a



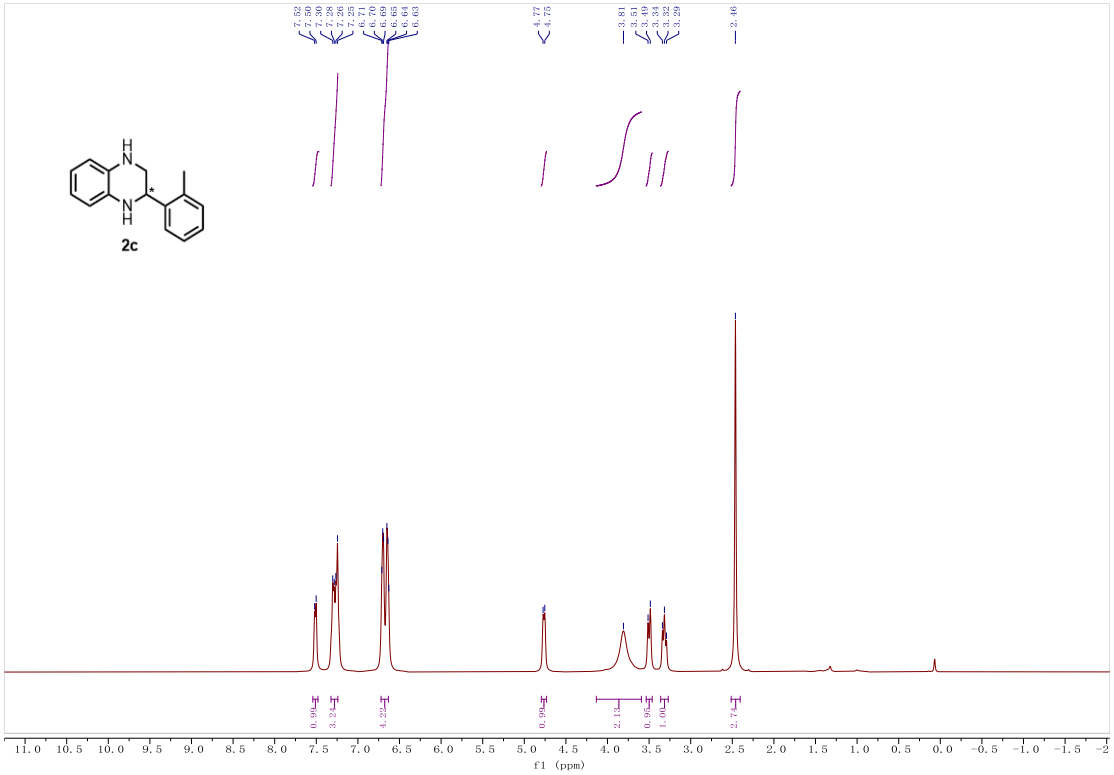
^{1}H NMR spectra for 2b



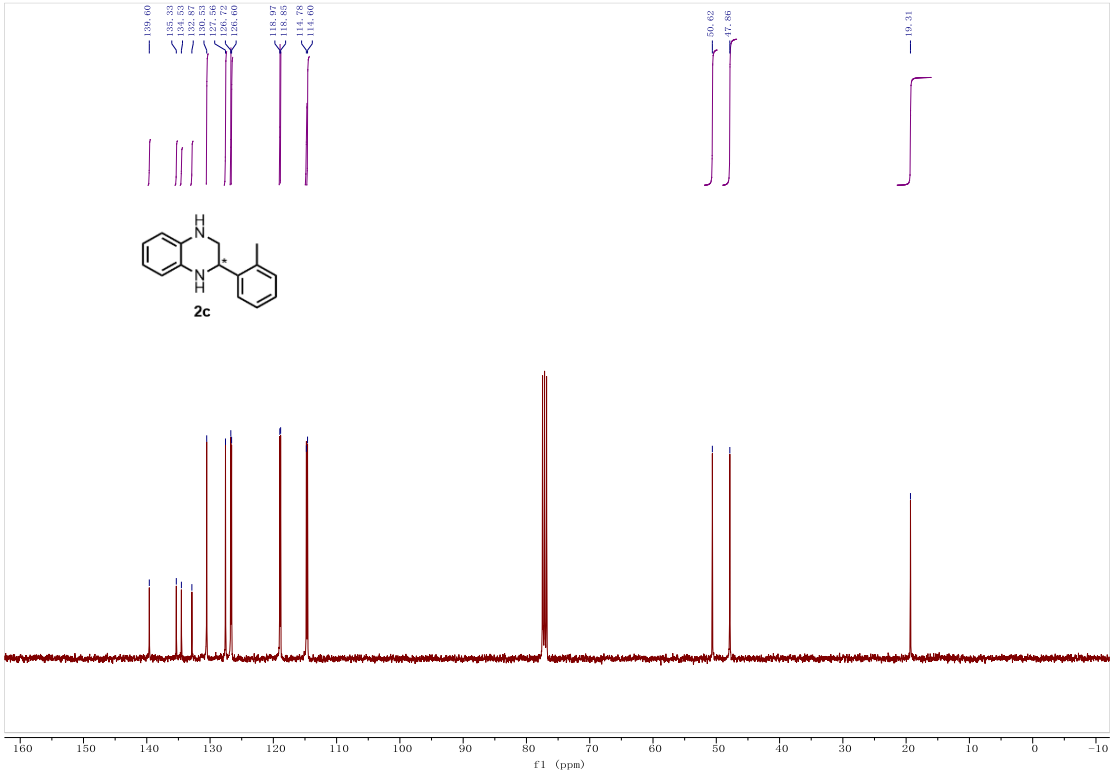
^{13}C NMR spectra for 2b



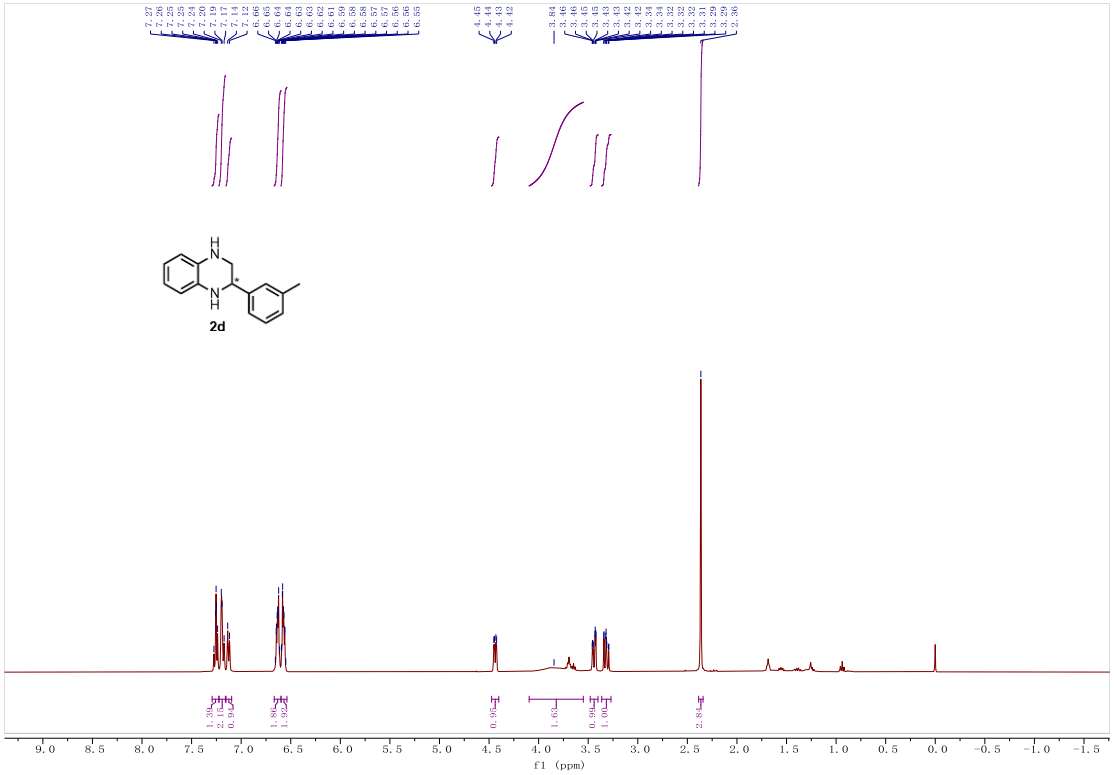
^{1}H NMR spectra for 2c



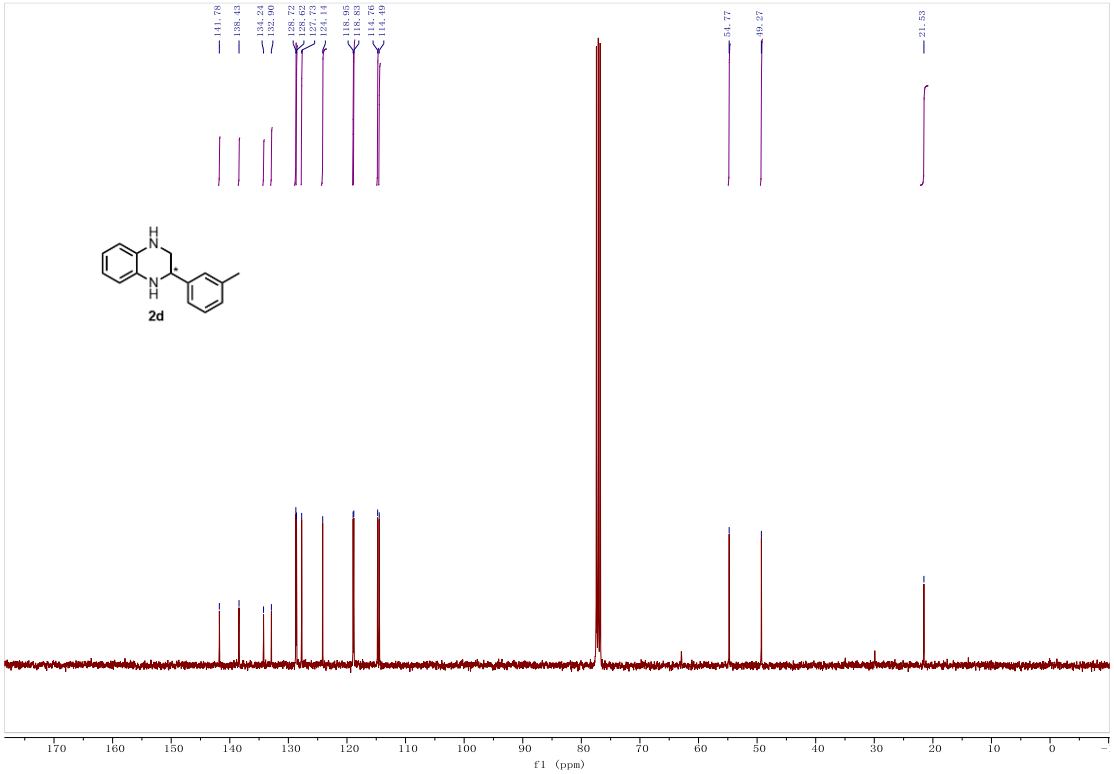
^{13}C NMR spectra for 2c



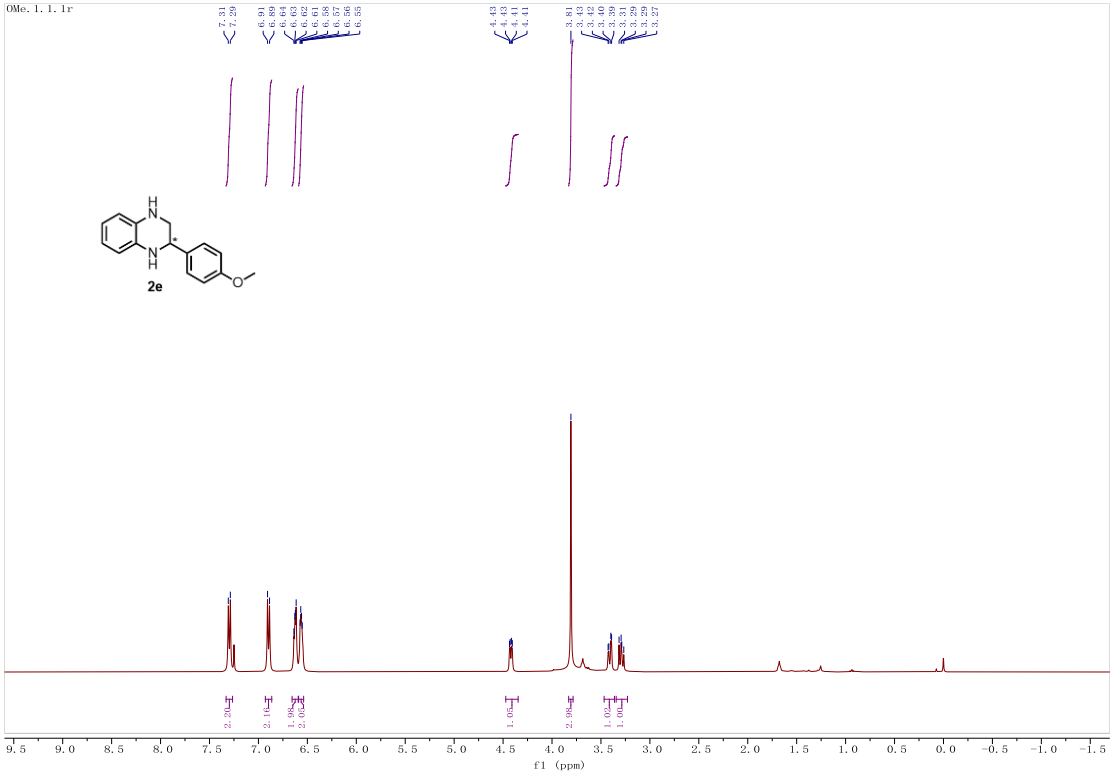
^{1}H NMR spectra for 2d



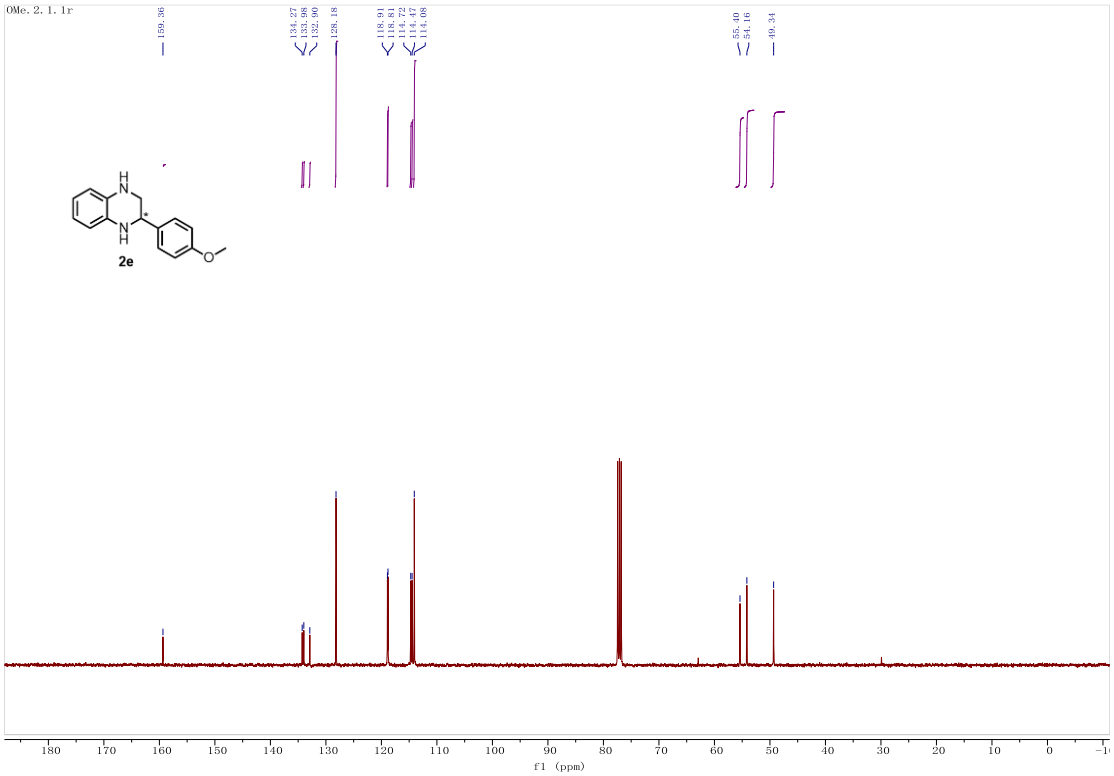
^{13}C NMR spectra for 2d



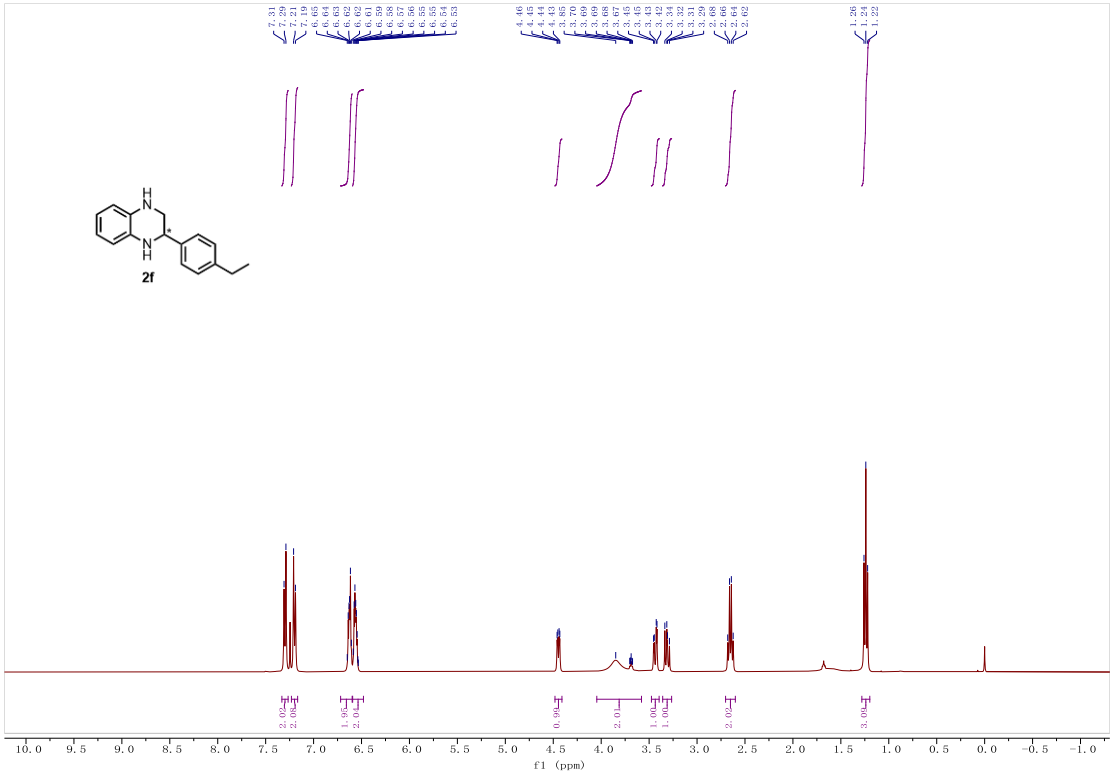
^{1}H NMR spectra for 2e



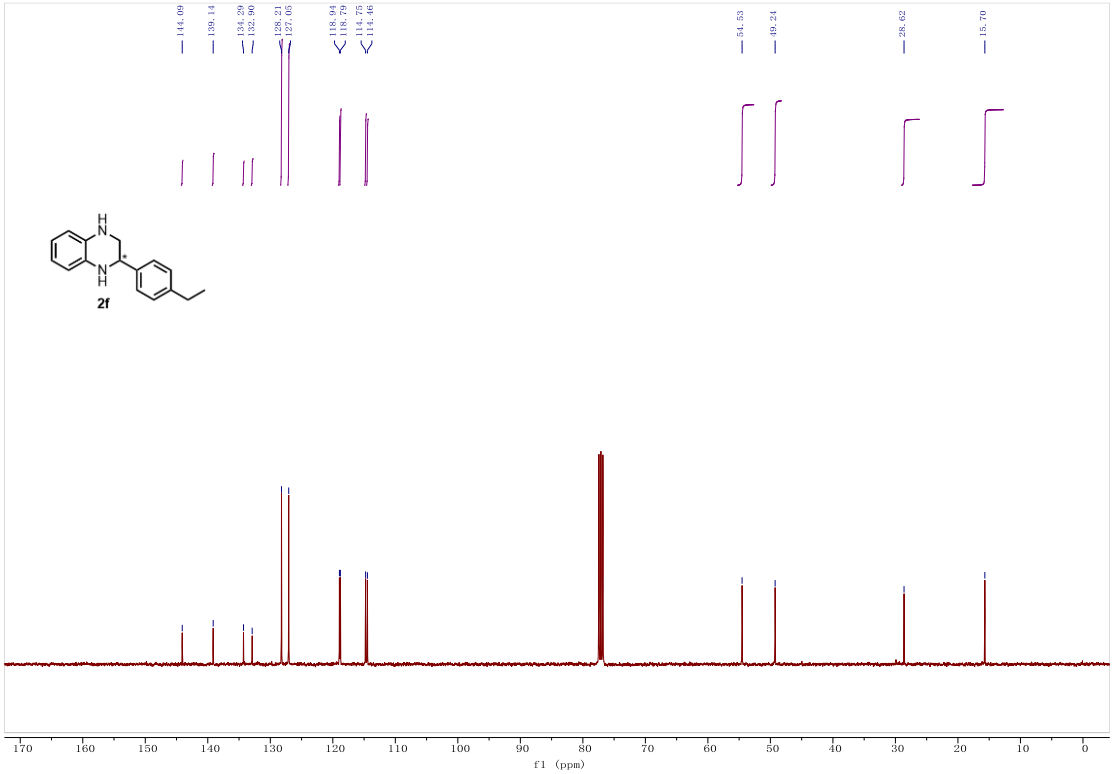
^{13}C NMR spectra for 2e



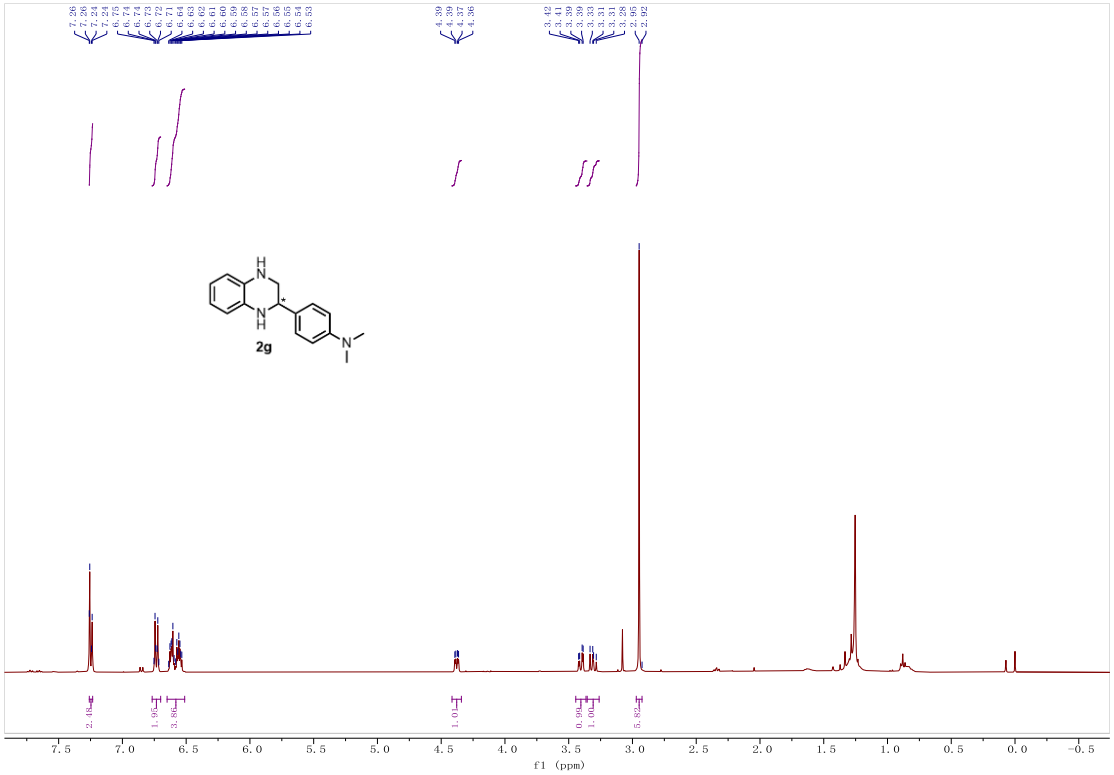
^{1}H NMR spectra for 2f



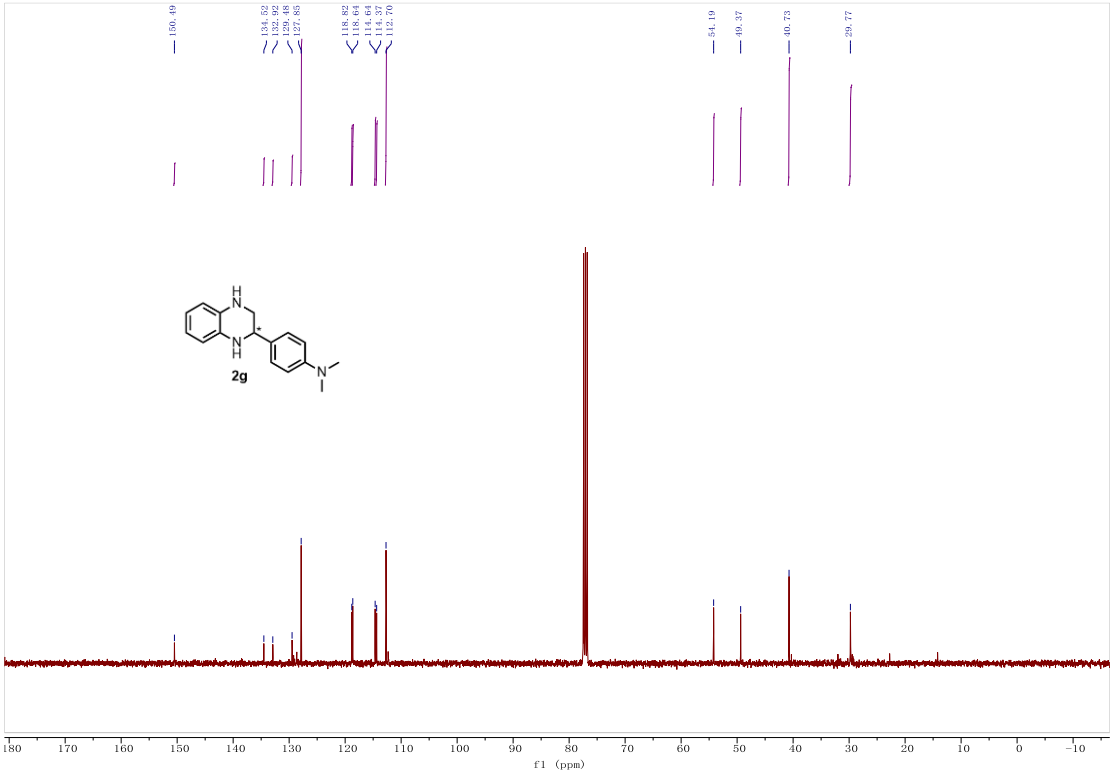
^{13}C NMR spectra for 2f



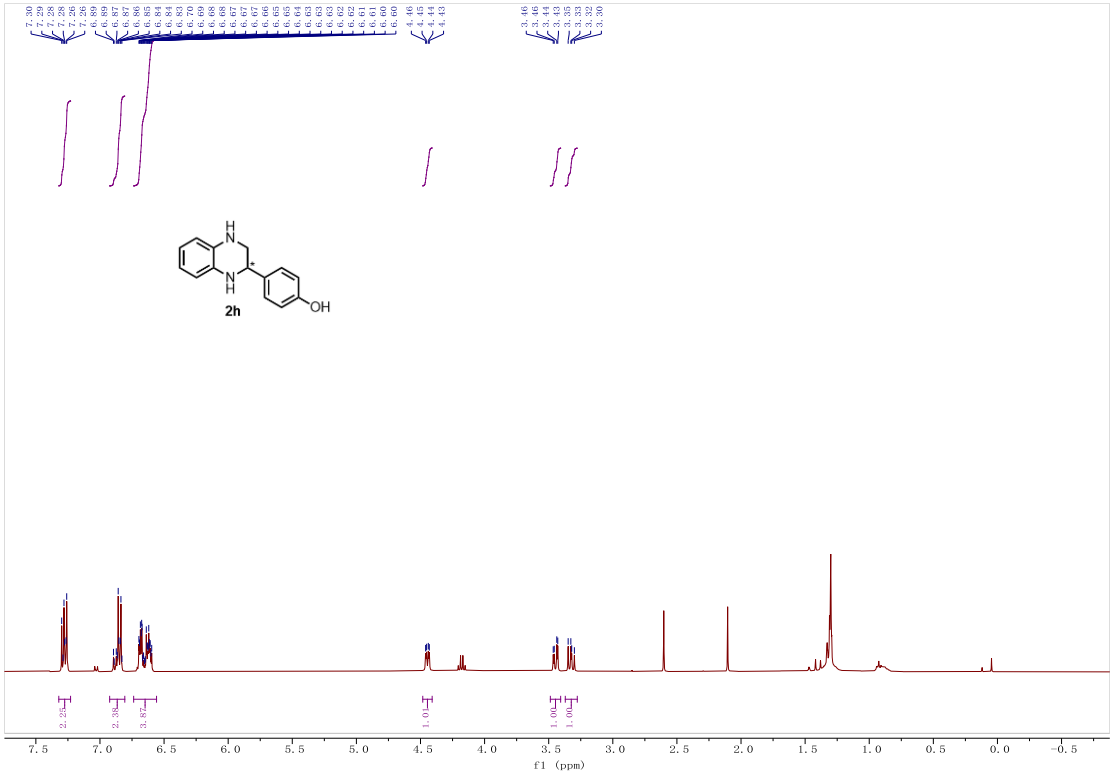
^{1}H NMR spectra for 2g



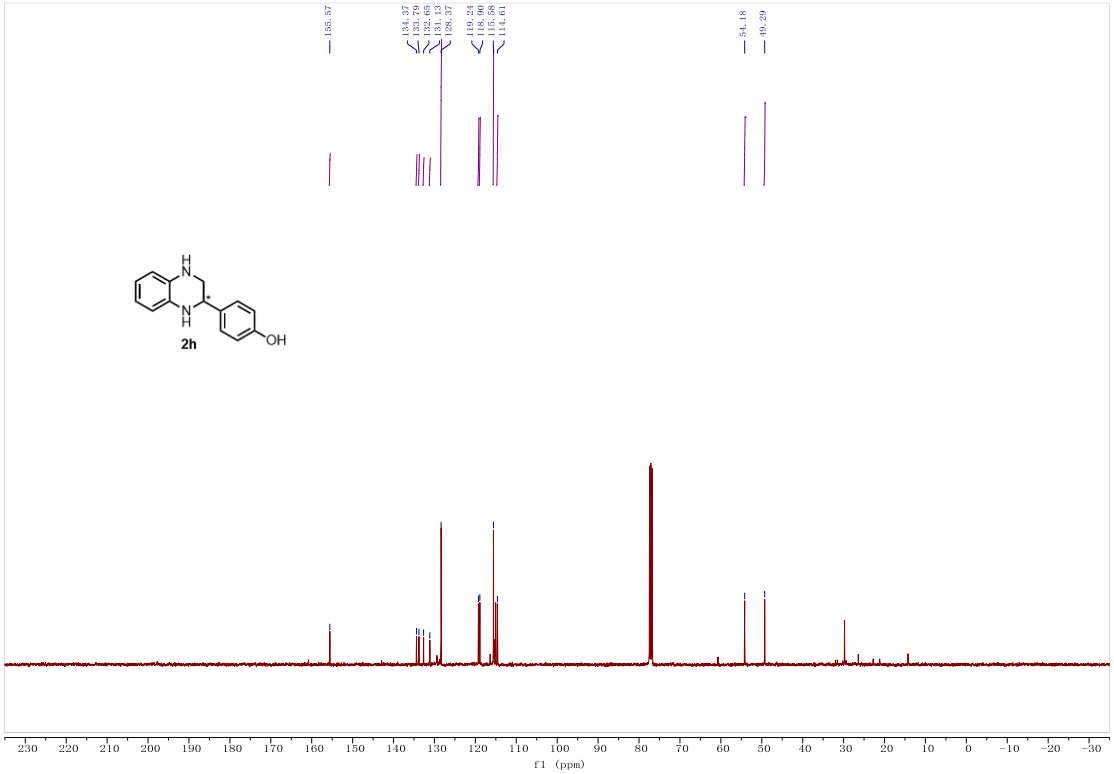
^{13}C NMR spectra for 2g



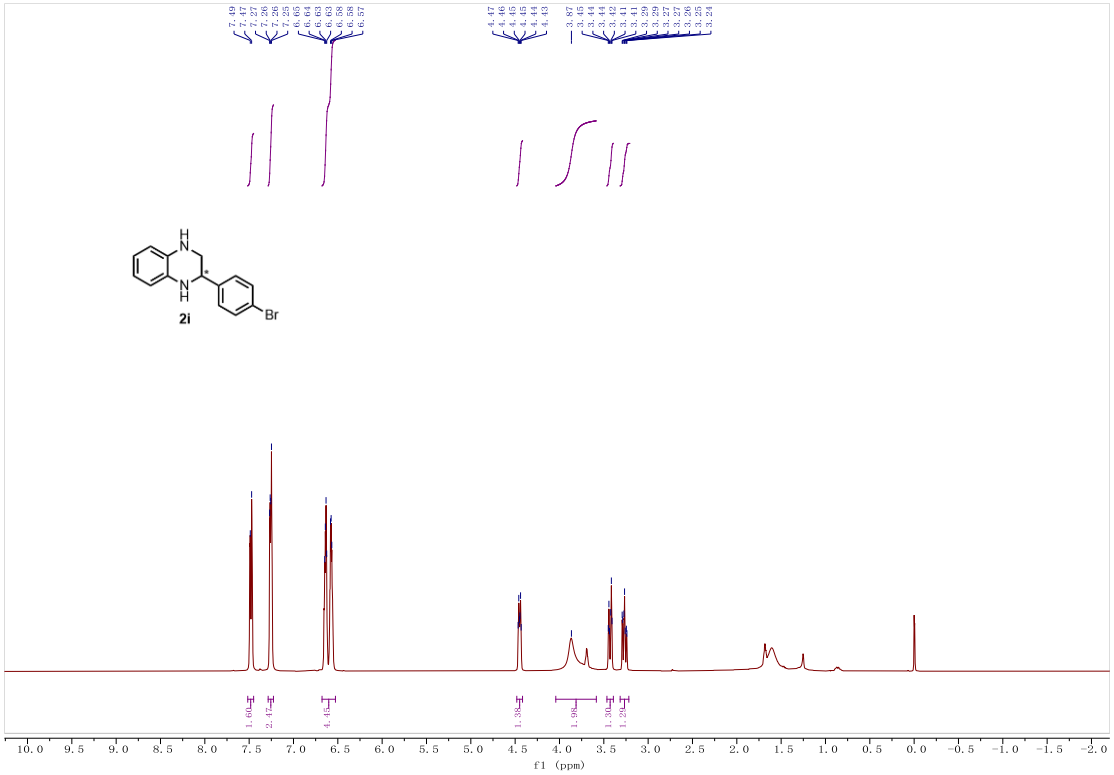
^{1}H NMR spectra for 2h



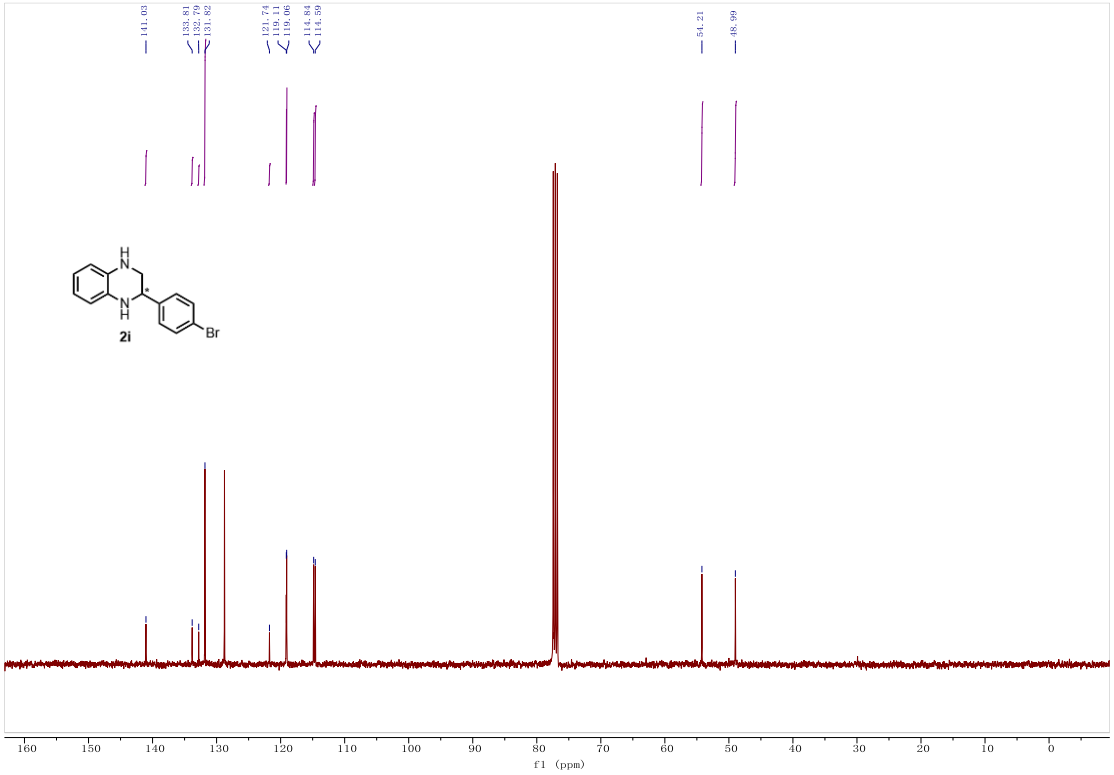
^{13}C NMR spectra for 2h



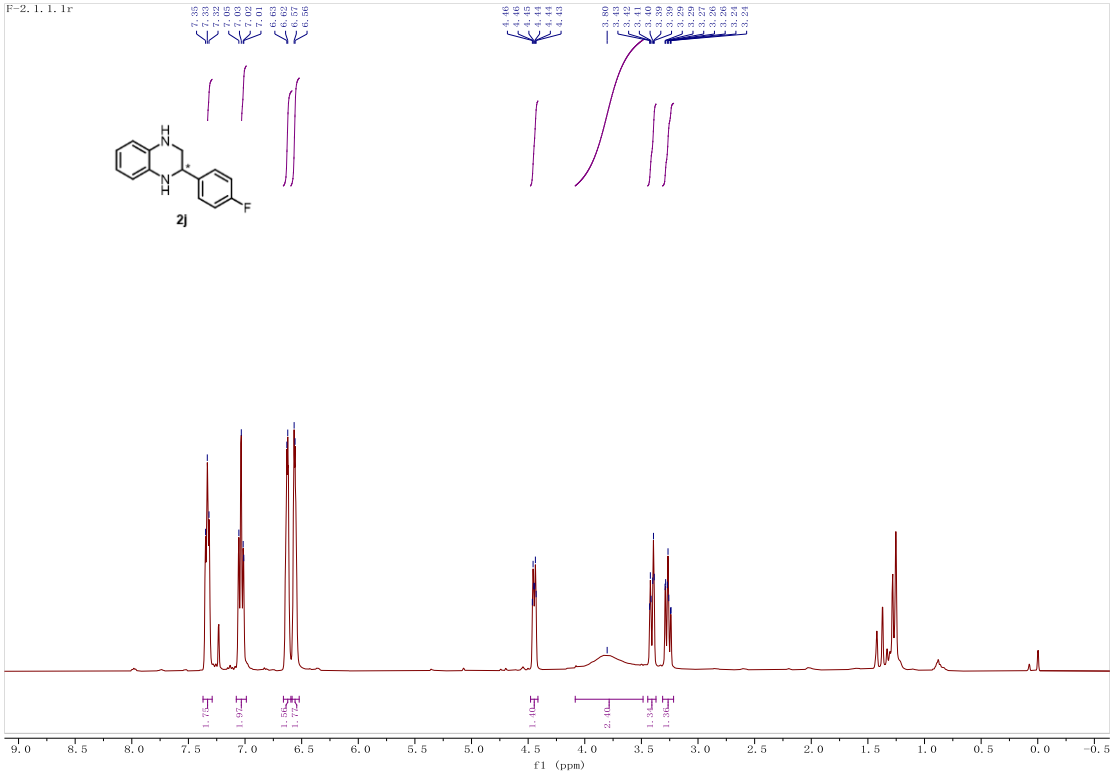
^{1}H NMR spectra for 2i



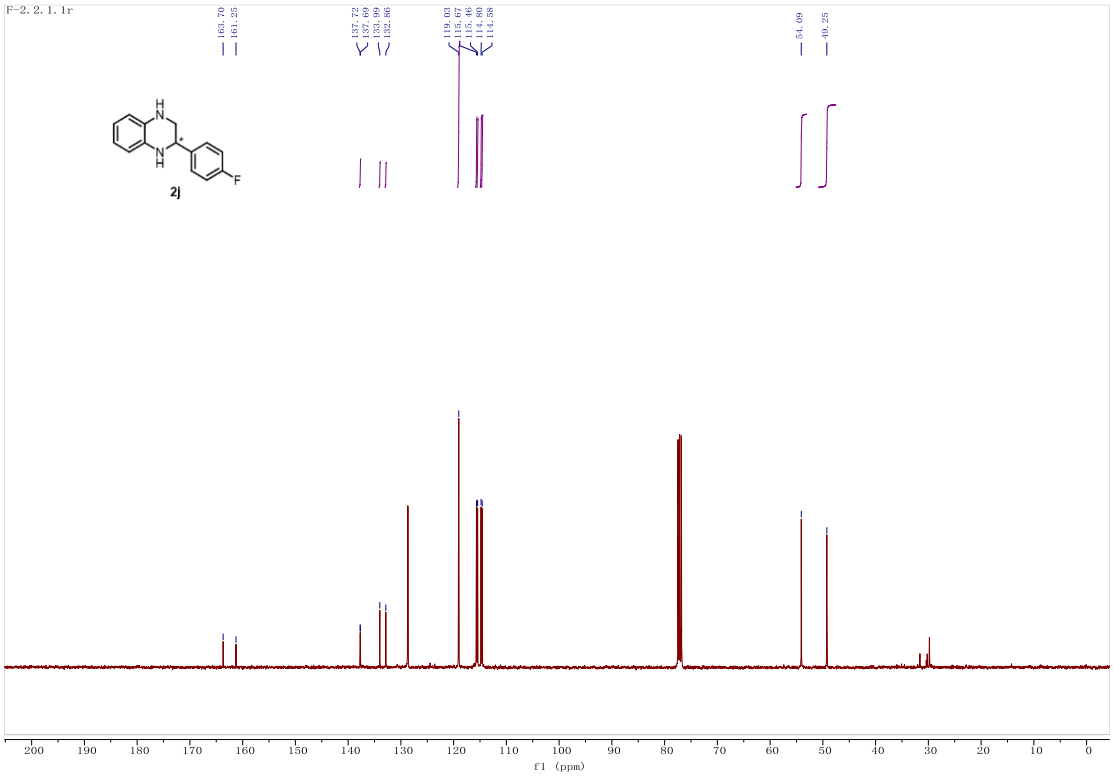
^{13}C NMR spectra for 2i



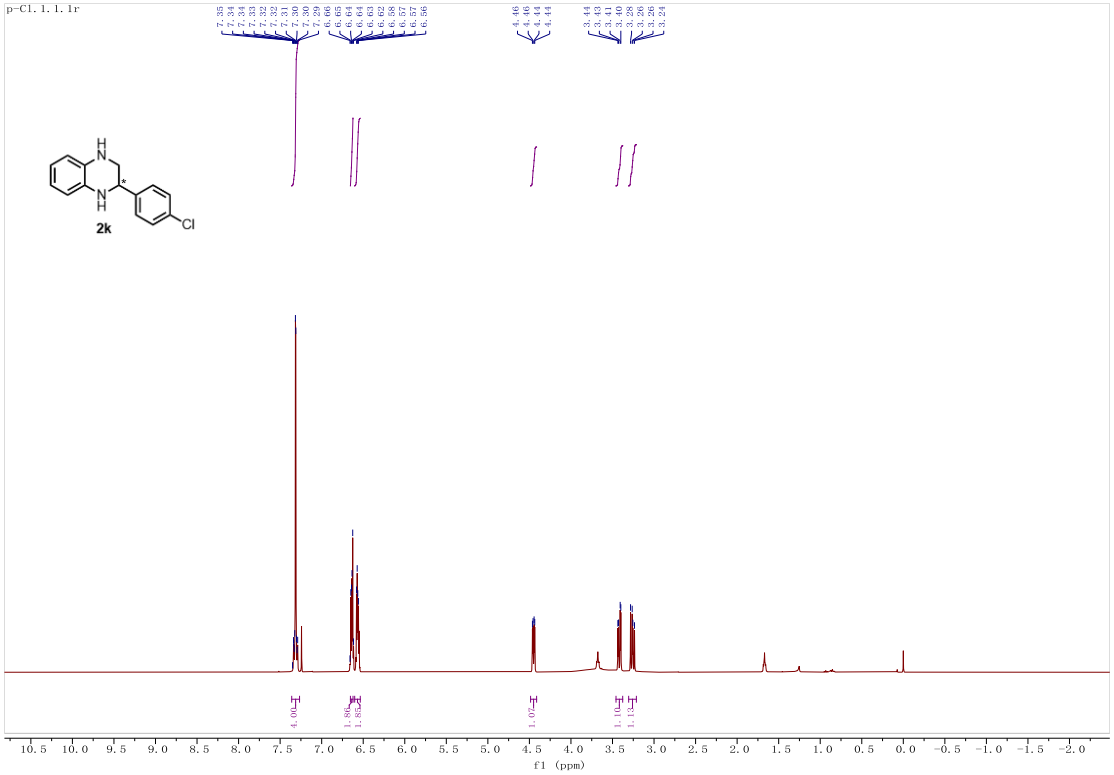
^{1}H NMR spectra for 2j



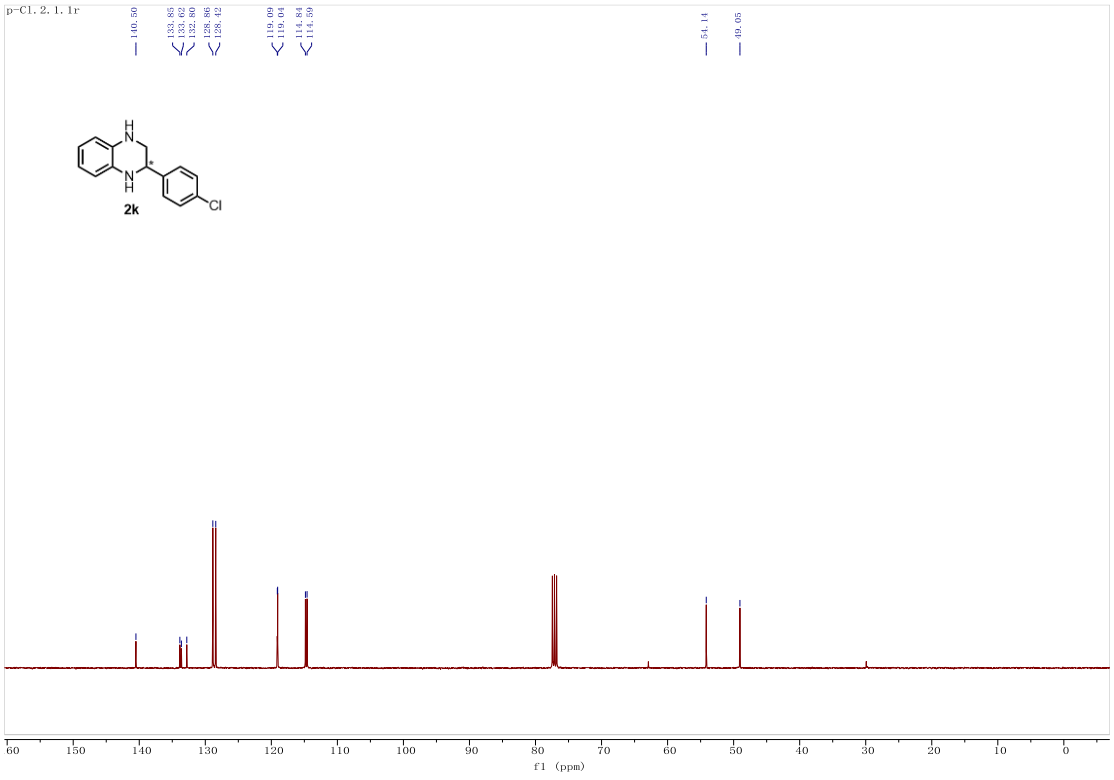
^{13}C NMR spectra for 2j



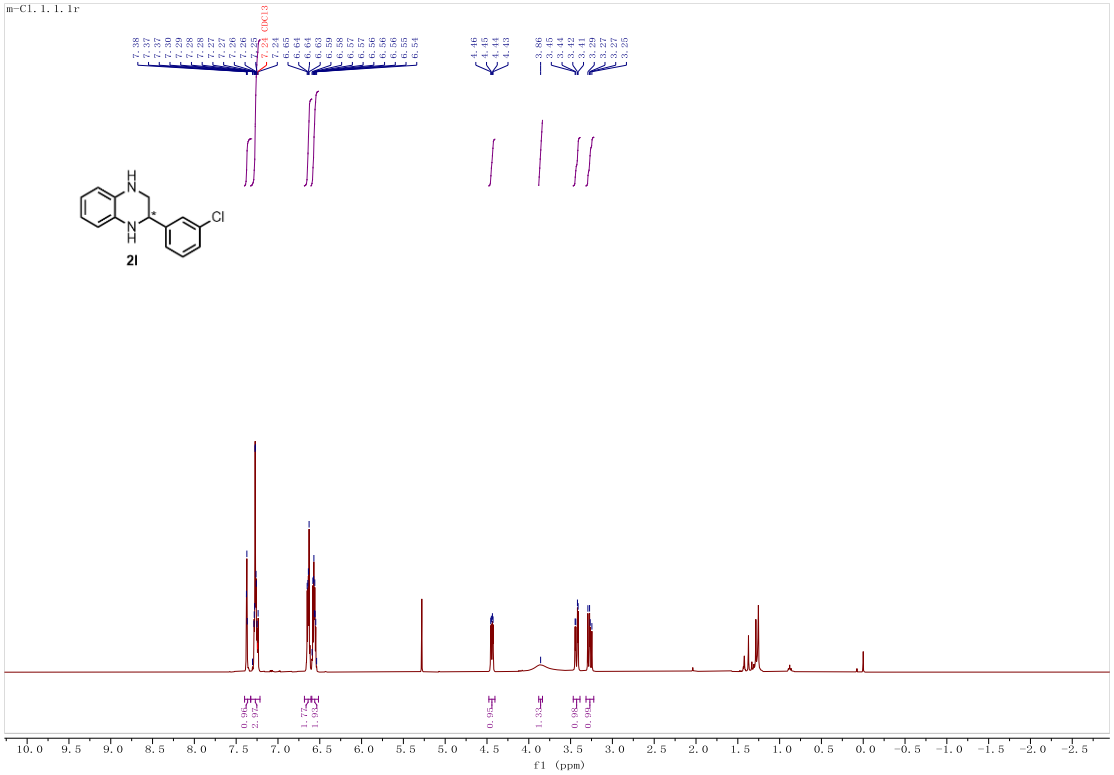
^{1}H NMR spectra for 2k



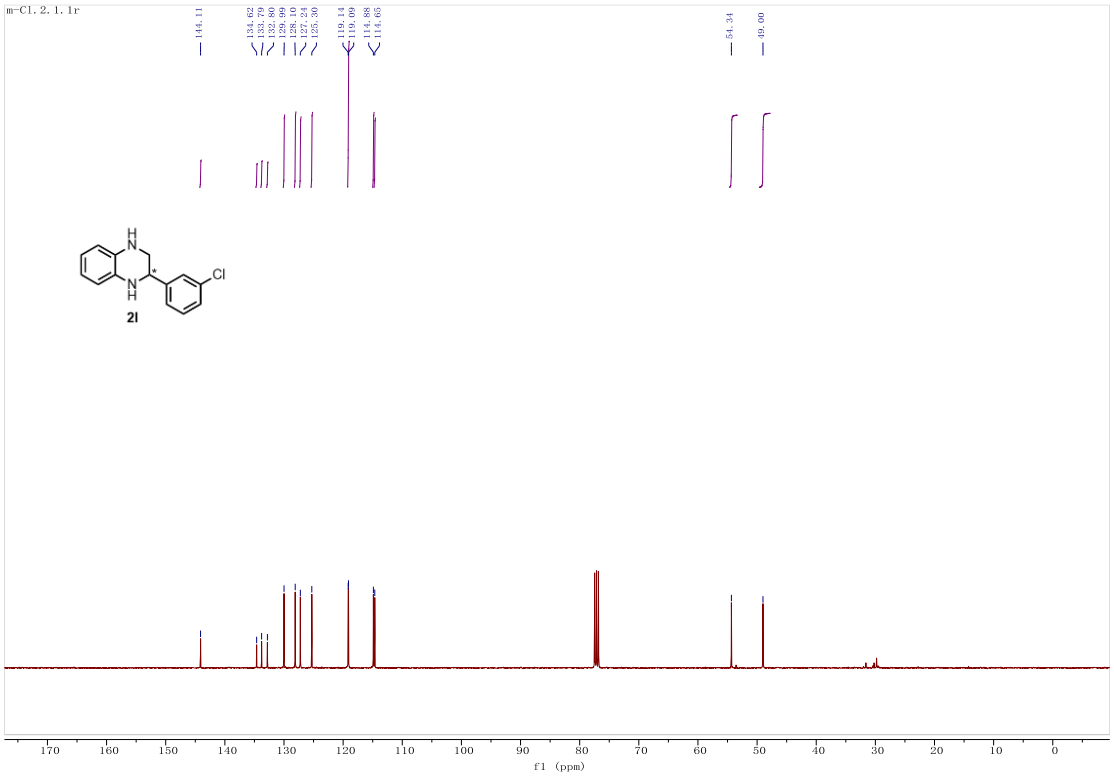
^{13}C NMR spectra for 2k



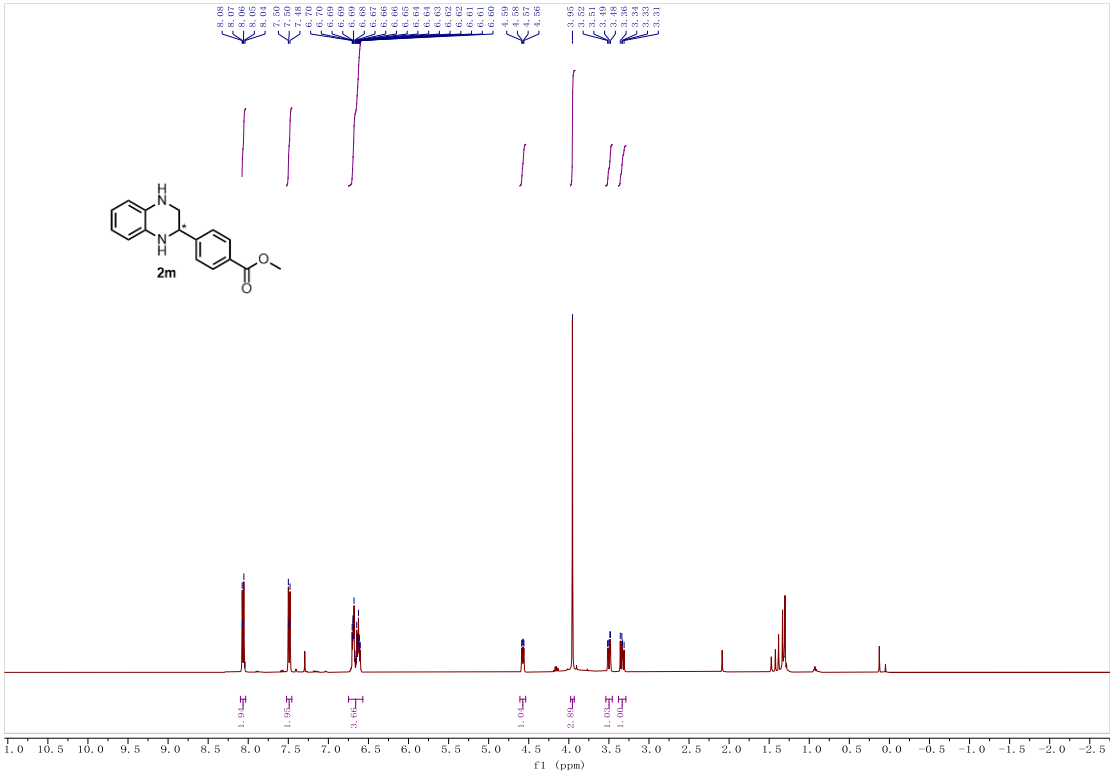
^{1}H NMR spectra for 2l



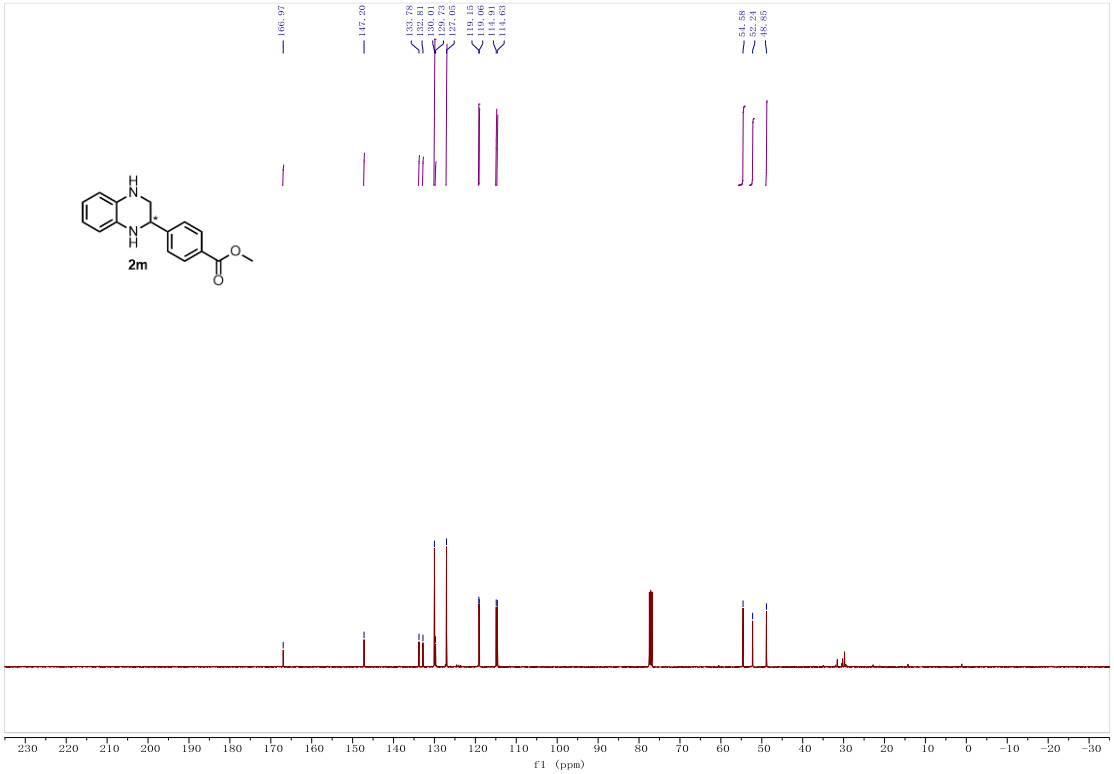
^{13}C NMR spectra for 2l



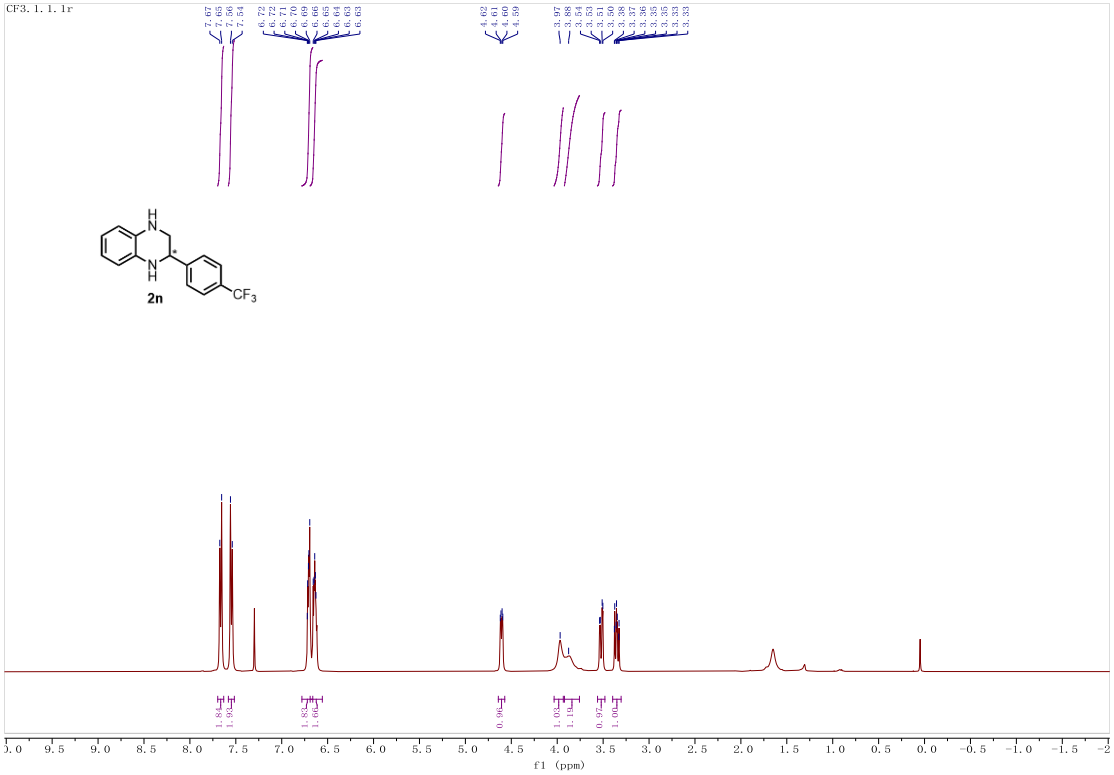
^{1}H NMR spectra for 2m



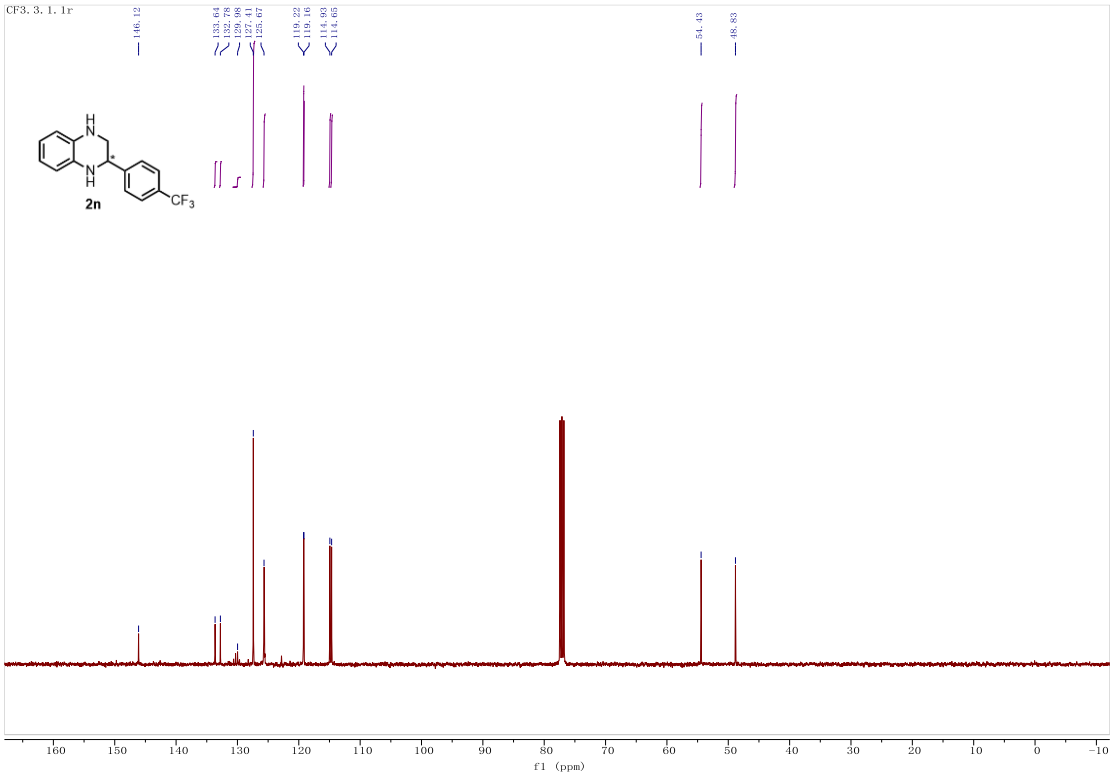
^{13}C NMR spectra for 2m



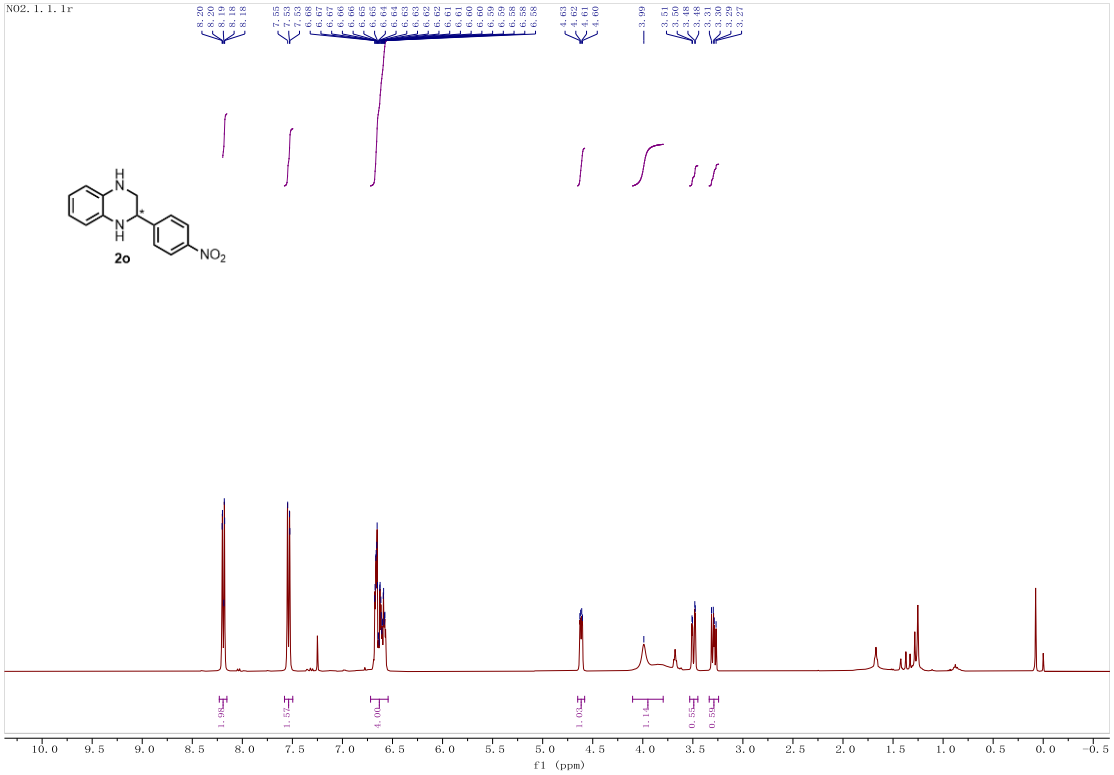
^{1}H NMR spectra for 2n



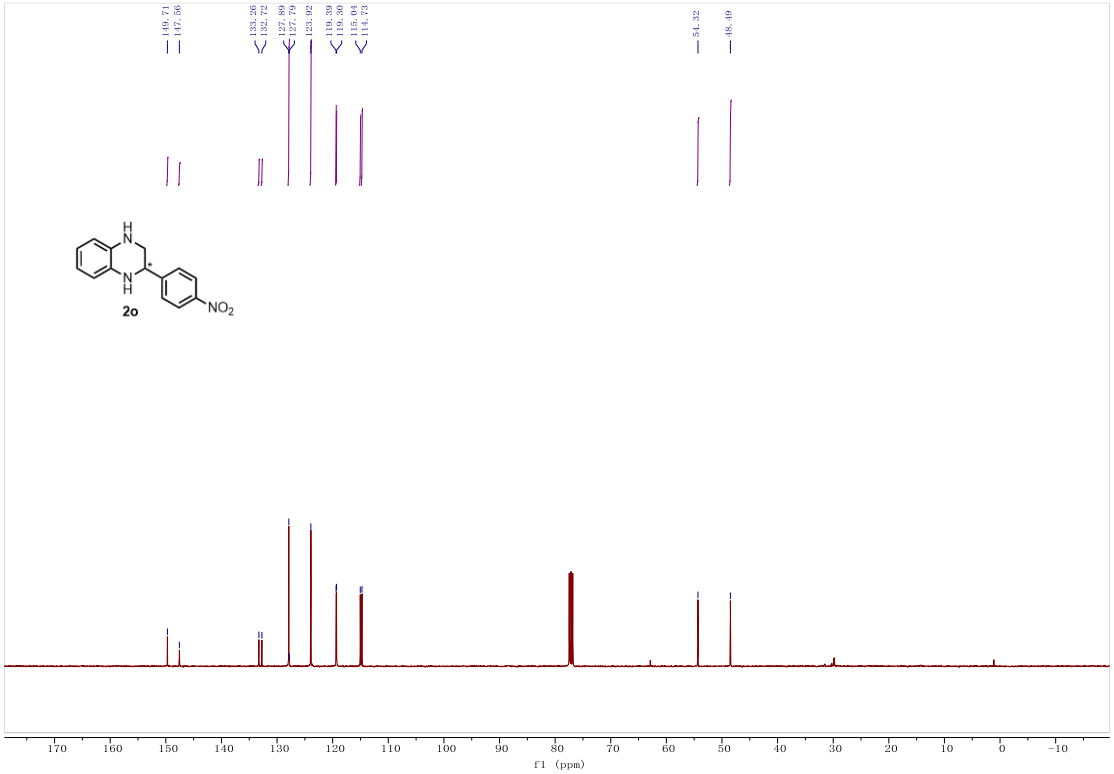
^{13}C NMR spectra for 2n



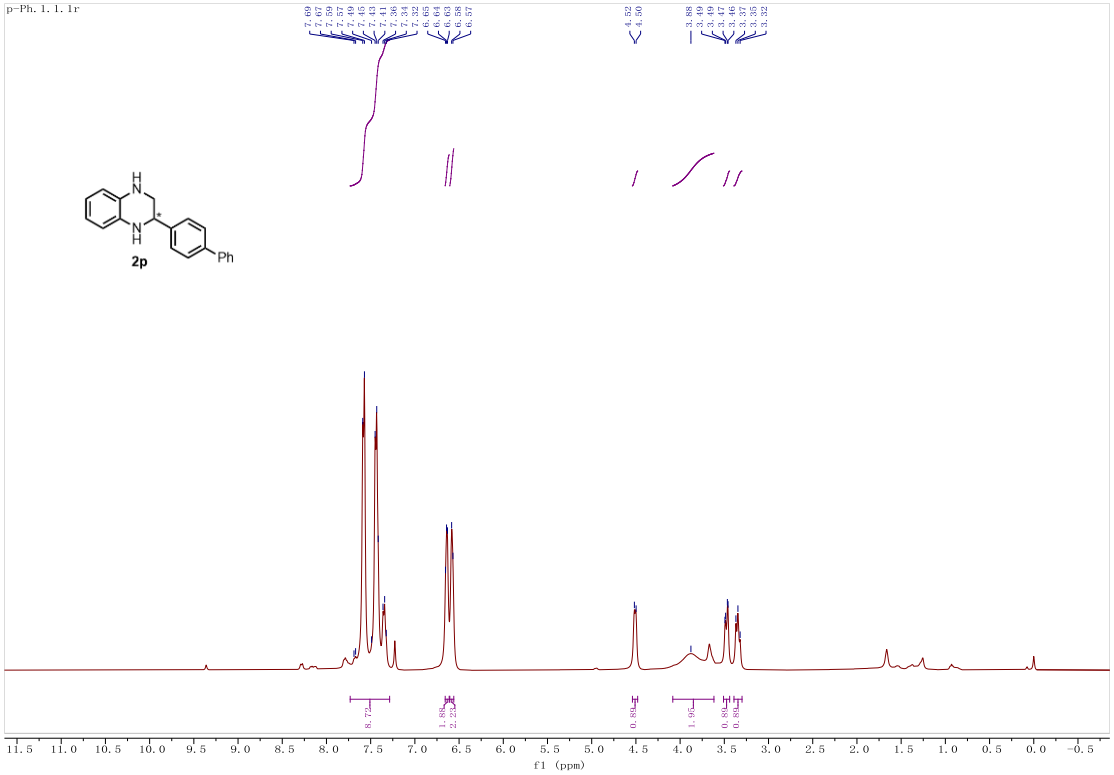
^{1}H NMR spectra for 2o



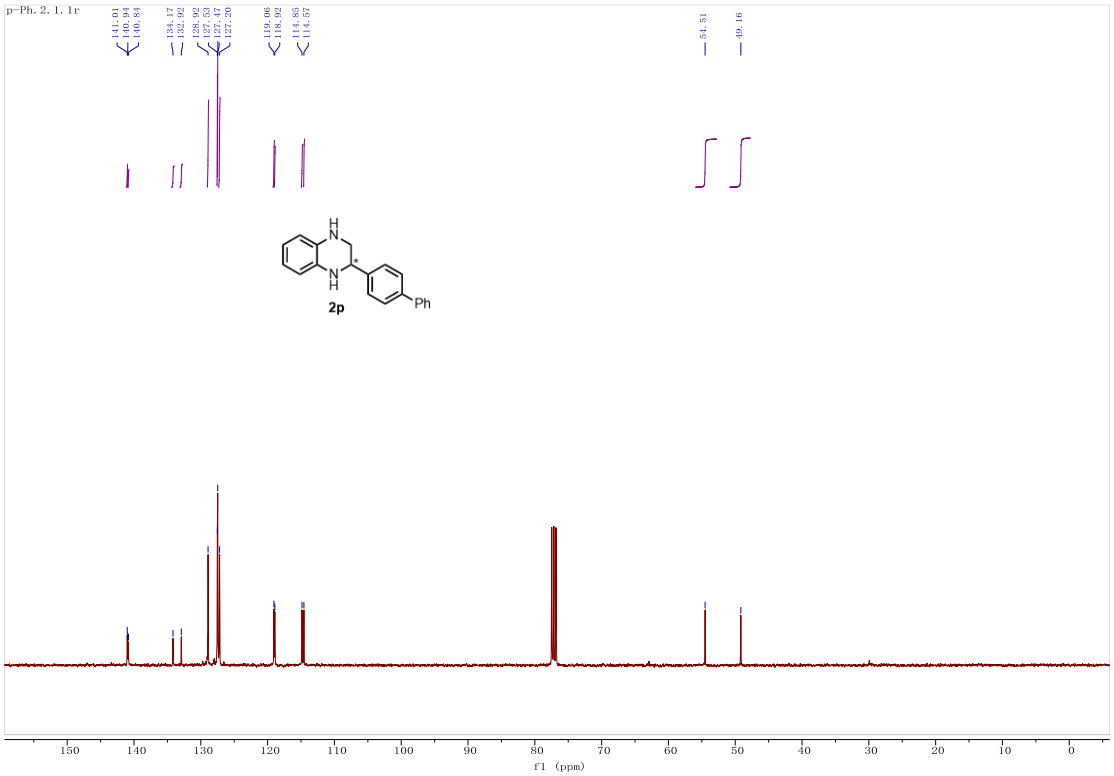
^{13}C NMR spectra for 2o



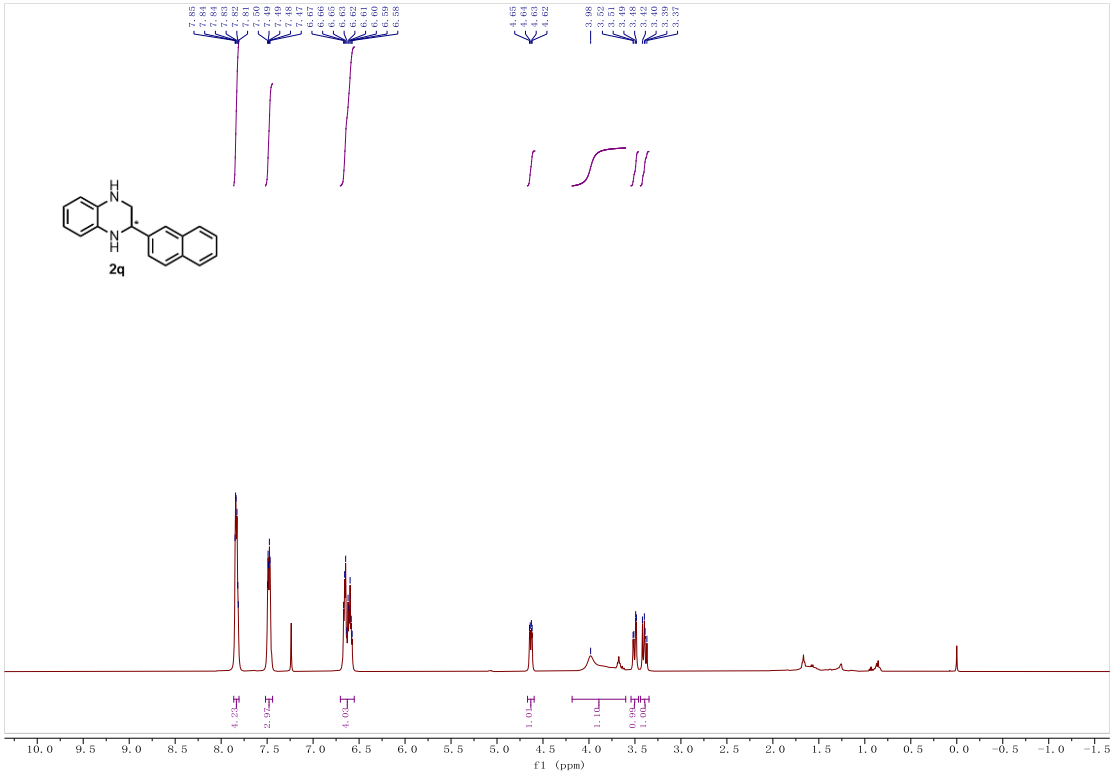
^{1}H NMR spectra for 2p



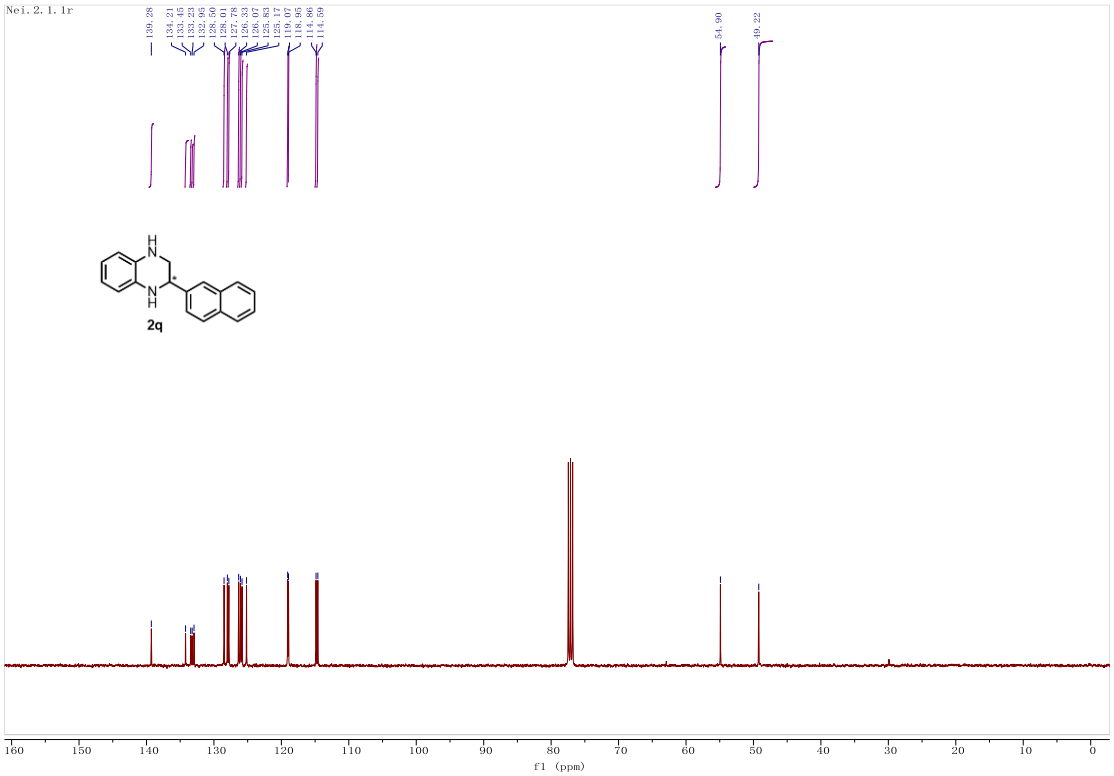
^{13}C NMR spectra for 2p



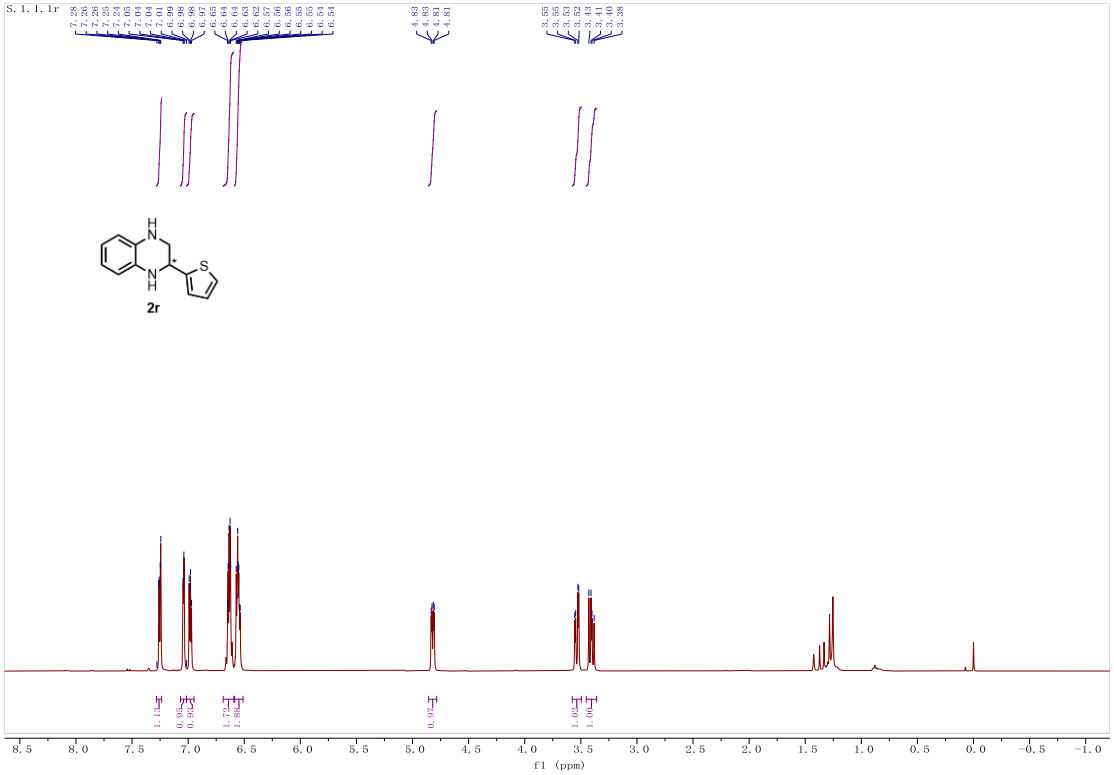
^{1}H NMR spectra for 2q



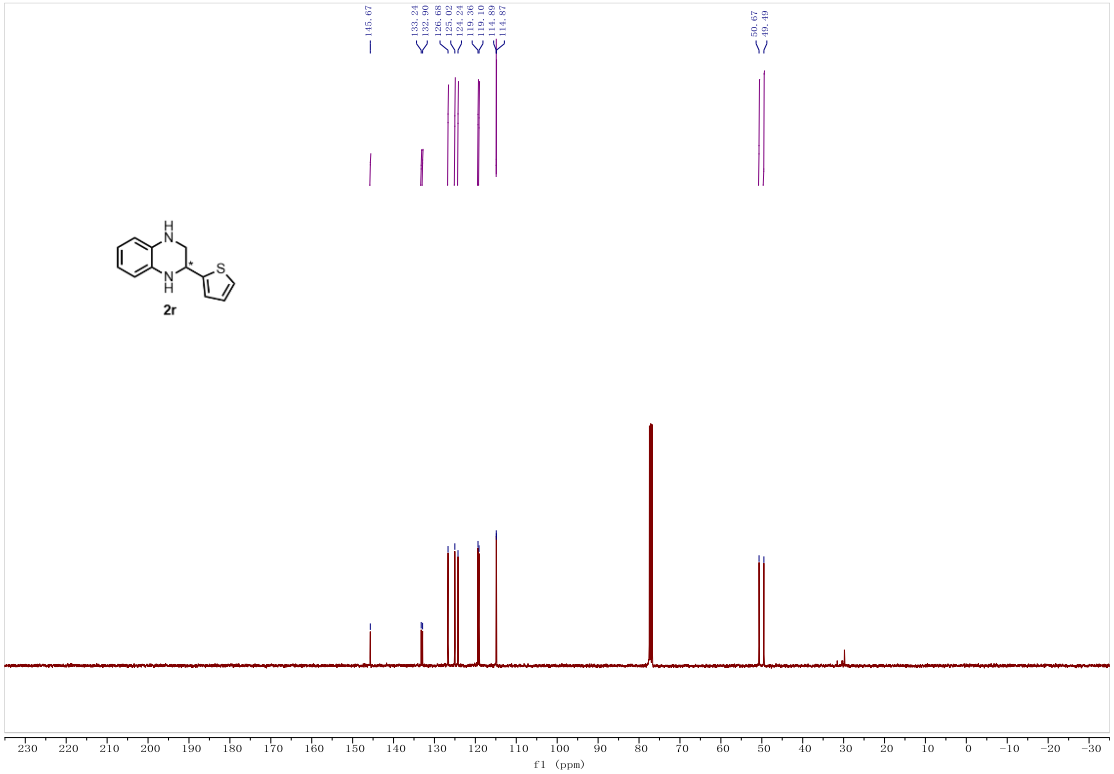
^{13}C NMR spectra for 2q



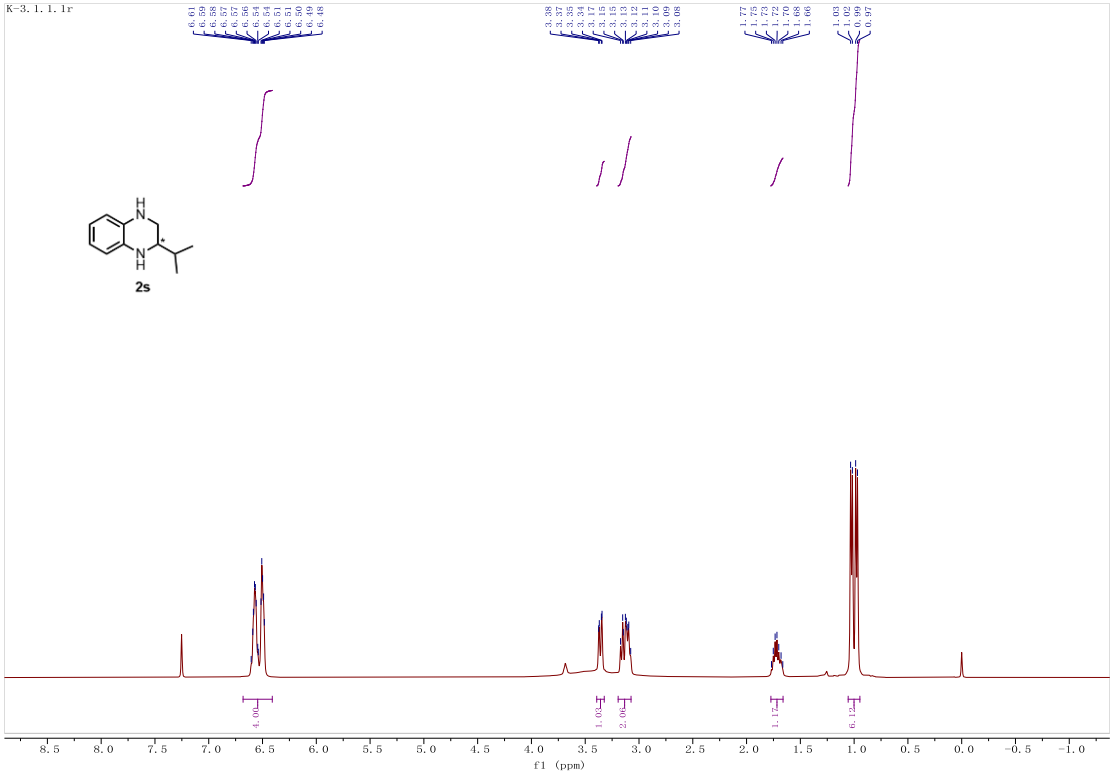
^{1}H NMR spectra for 2r



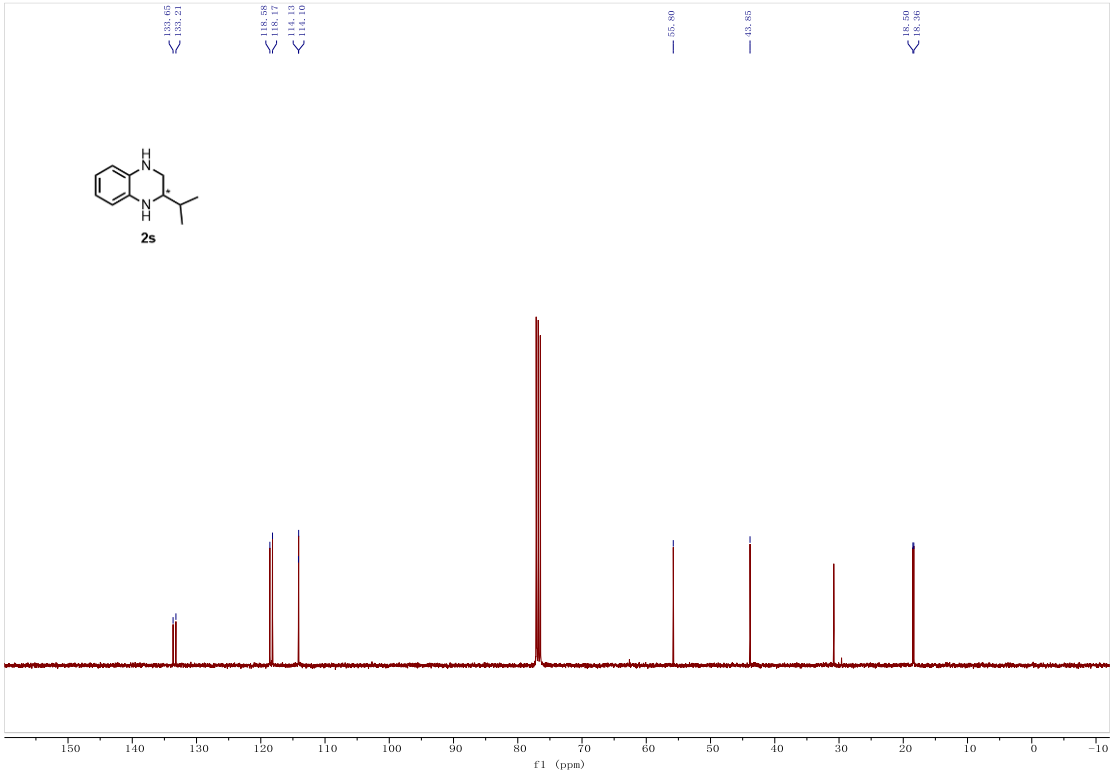
^{13}C NMR spectra for 2r



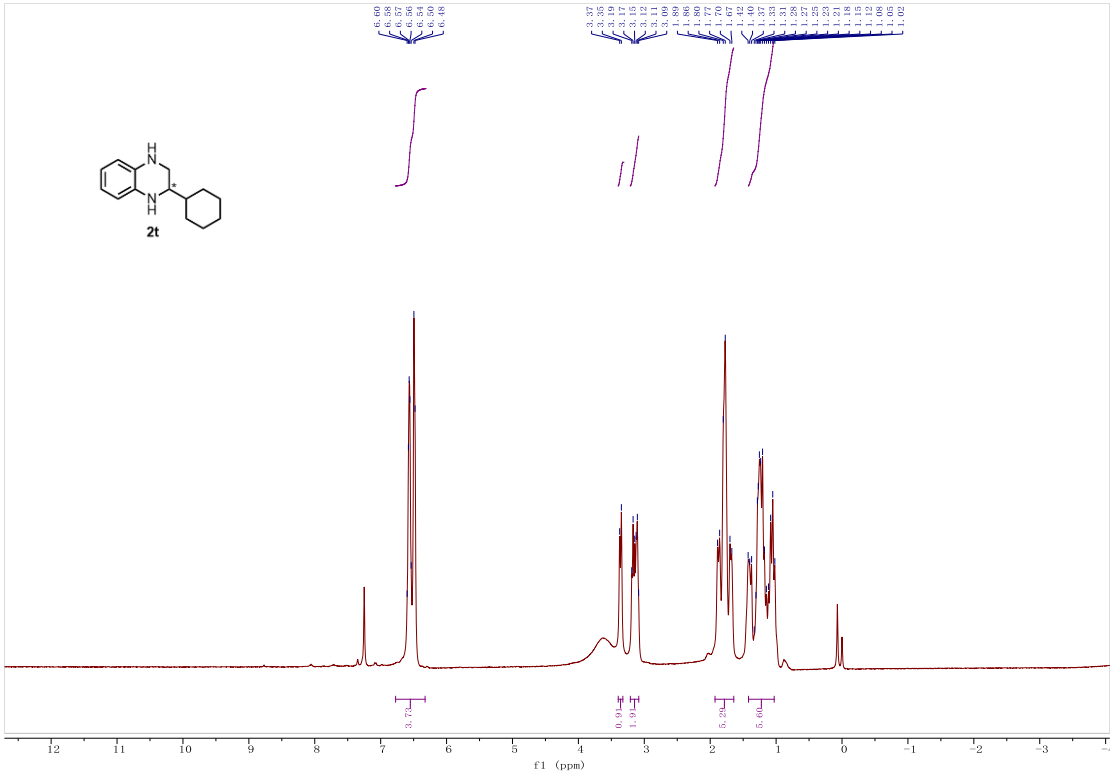
^{1}H NMR spectra for 2s



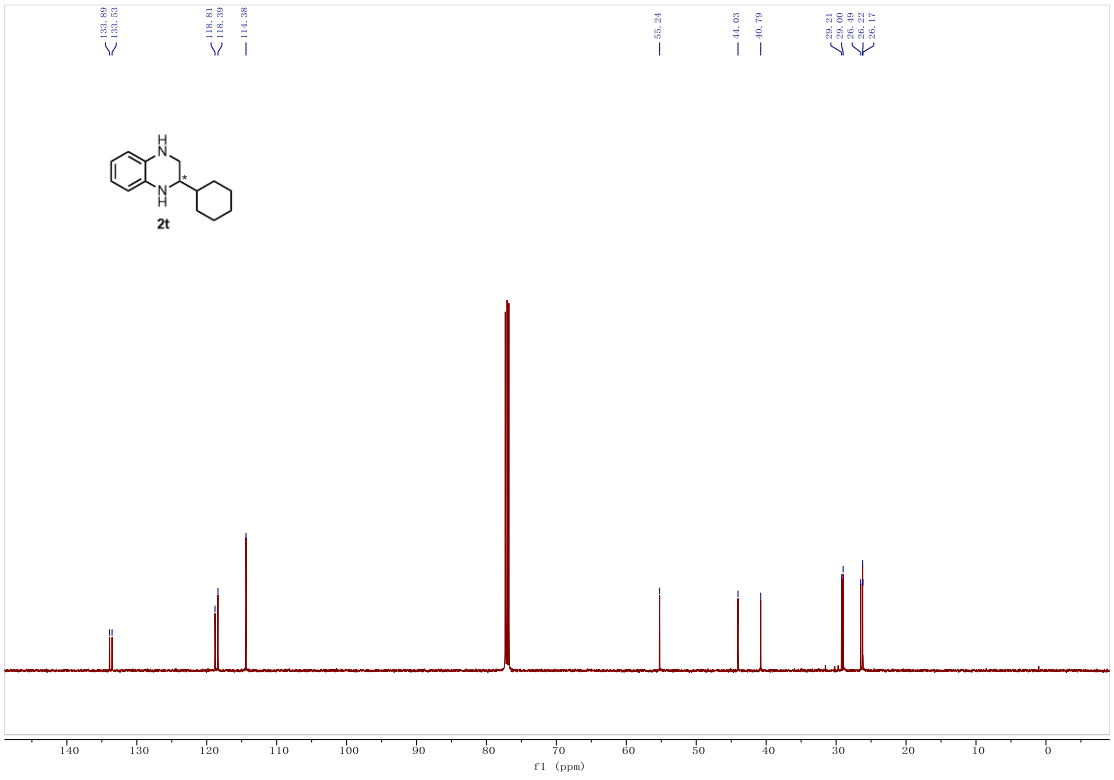
^{13}C NMR spectra for 2s



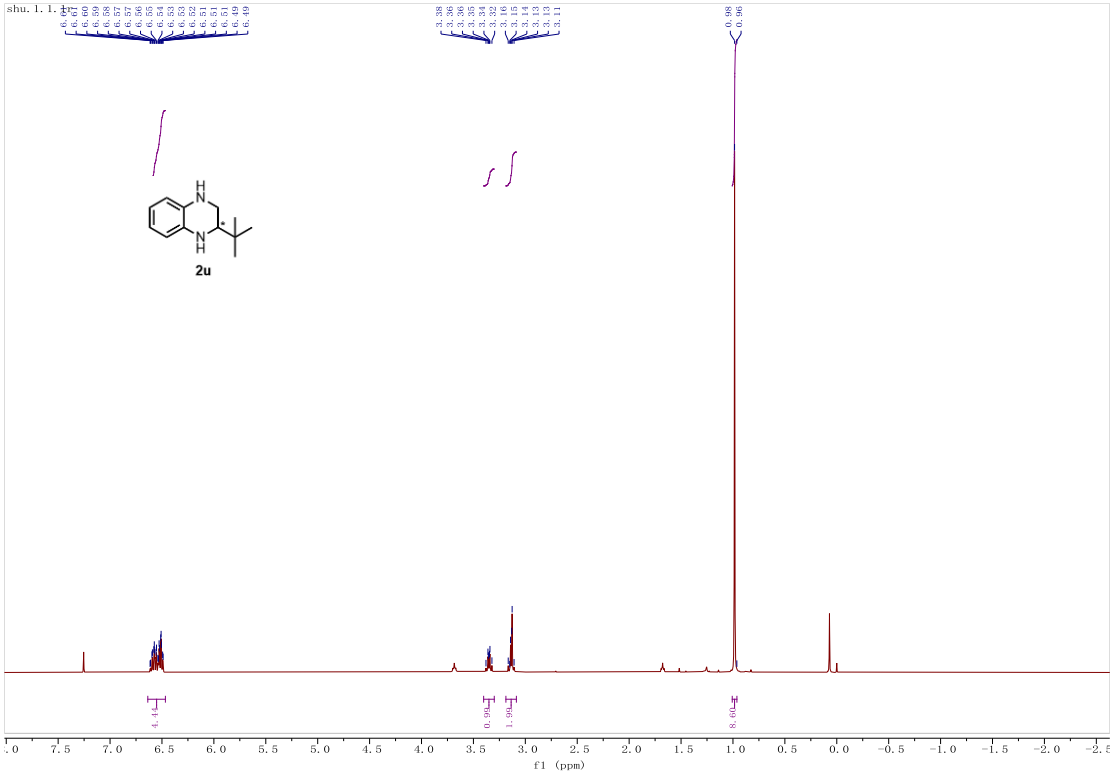
^{1}H NMR spectra for 2t



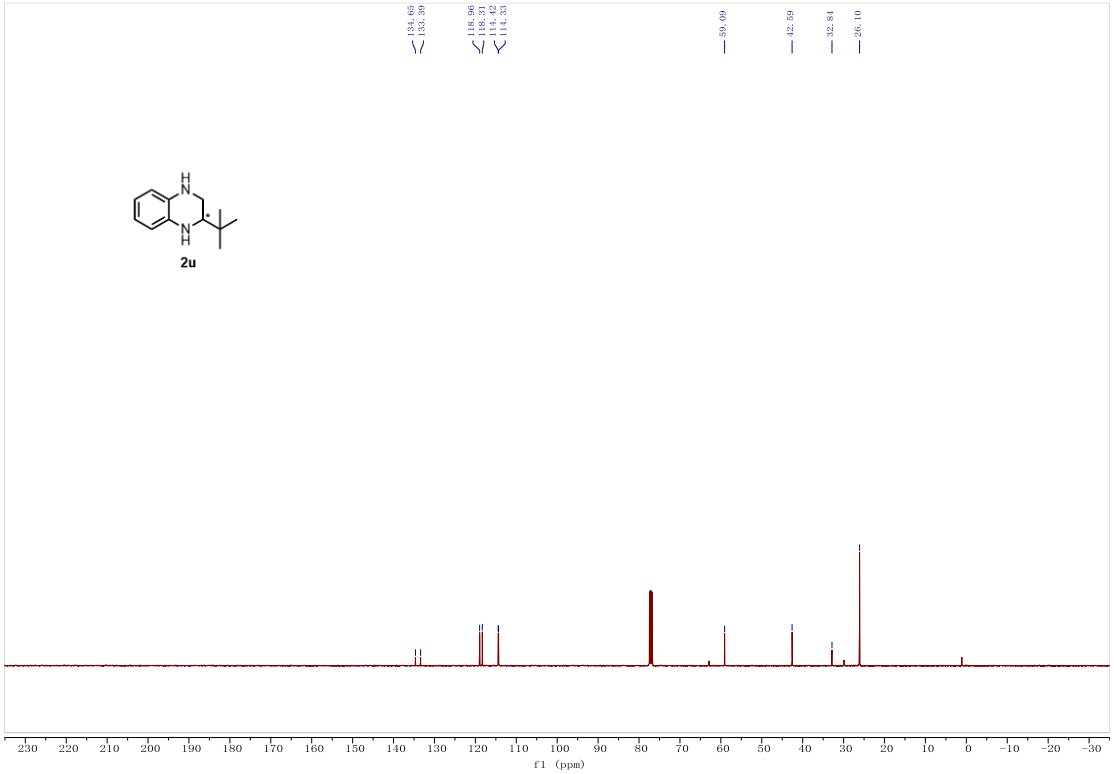
^{13}C NMR spectra for 2t



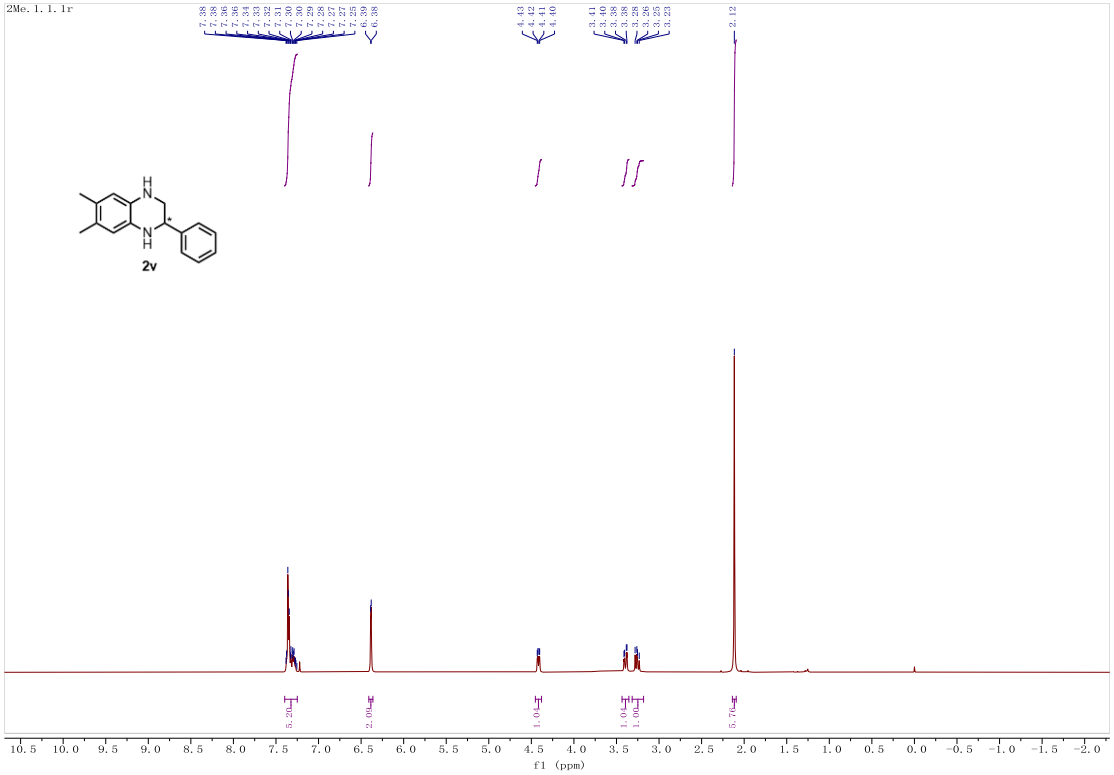
^{1}H NMR spectra for 2u



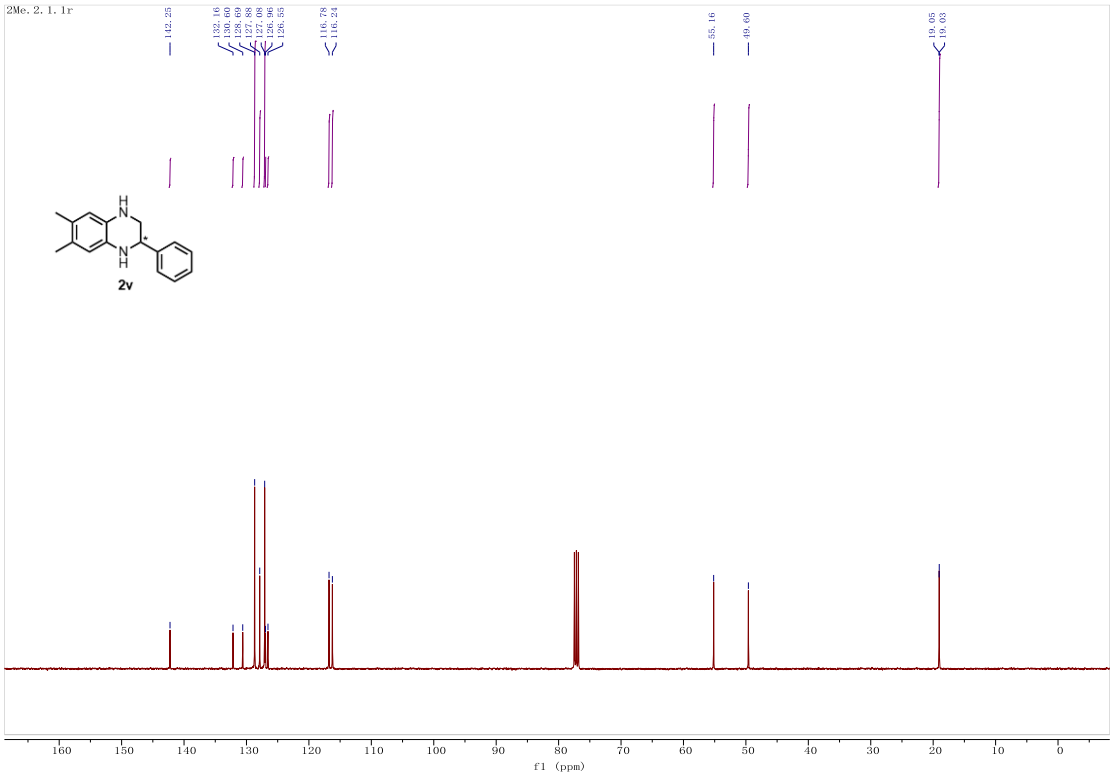
^{13}C NMR spectra for 2u



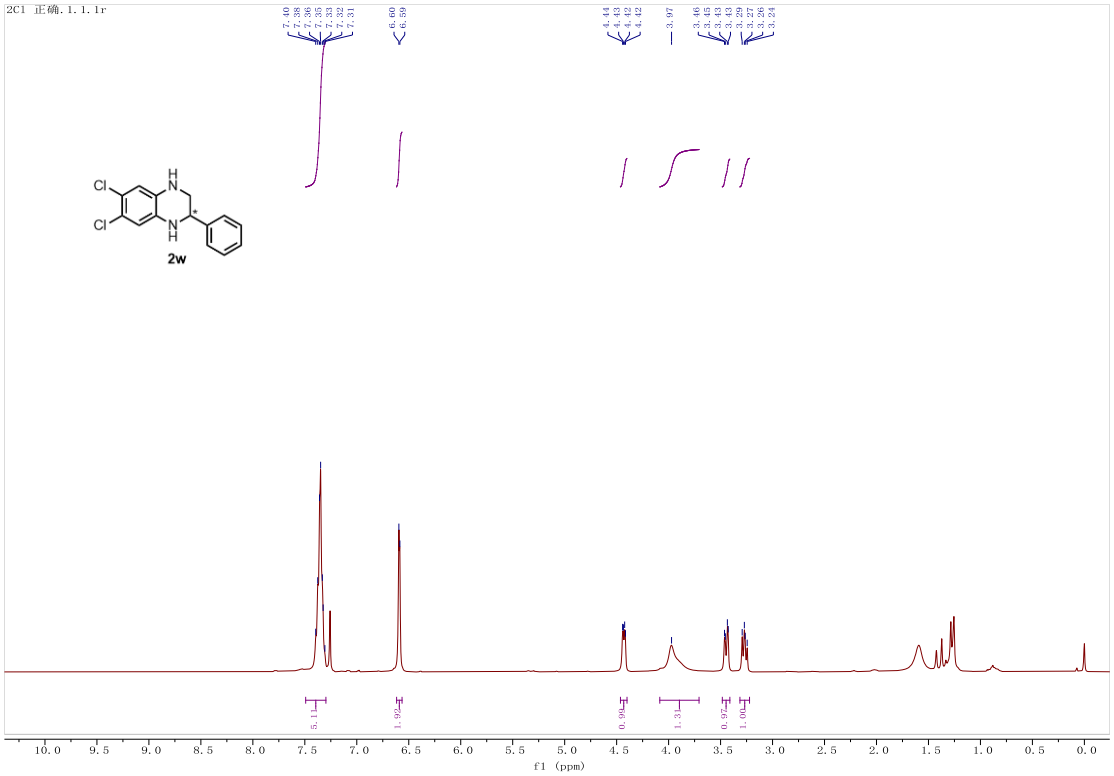
^{1}H NMR spectra for 2v



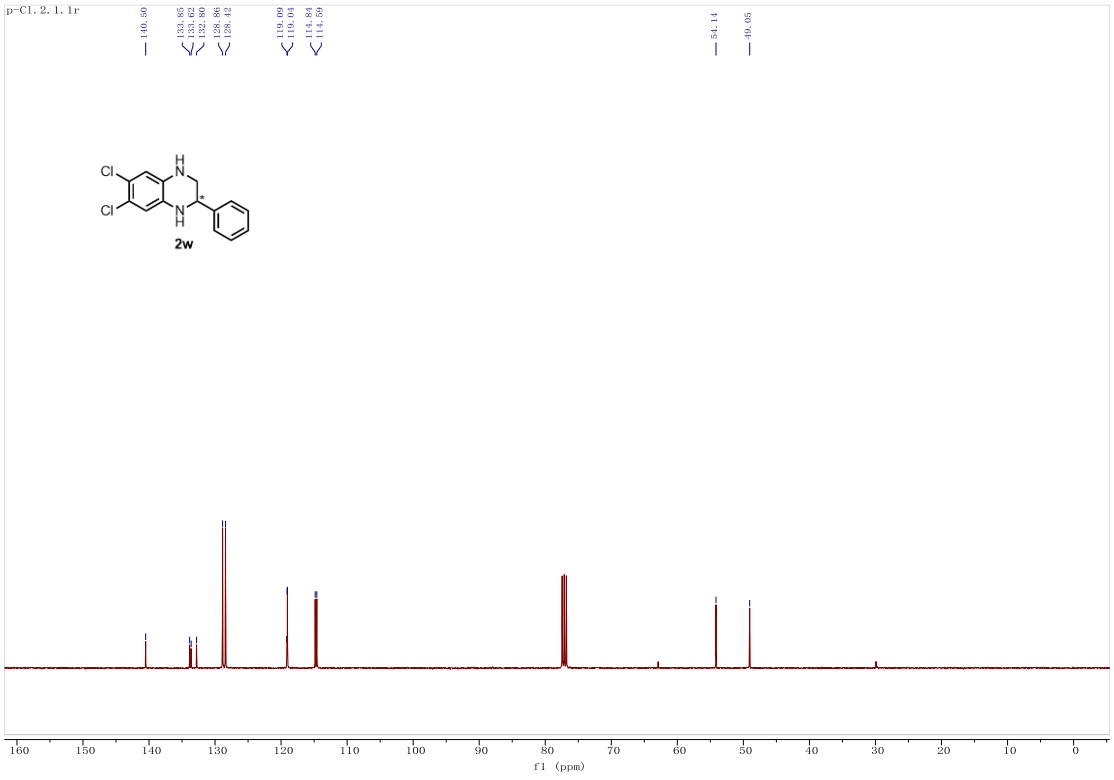
^{13}C NMR spectra for 2v



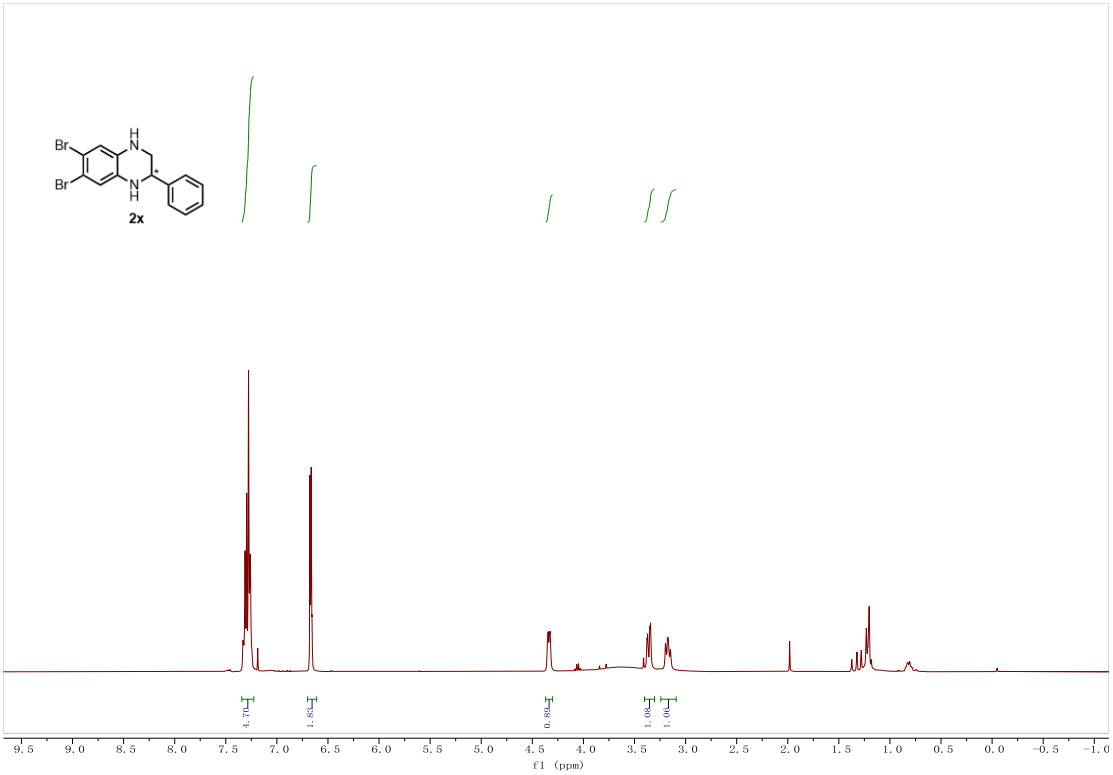
^{1}H NMR spectra for 2w



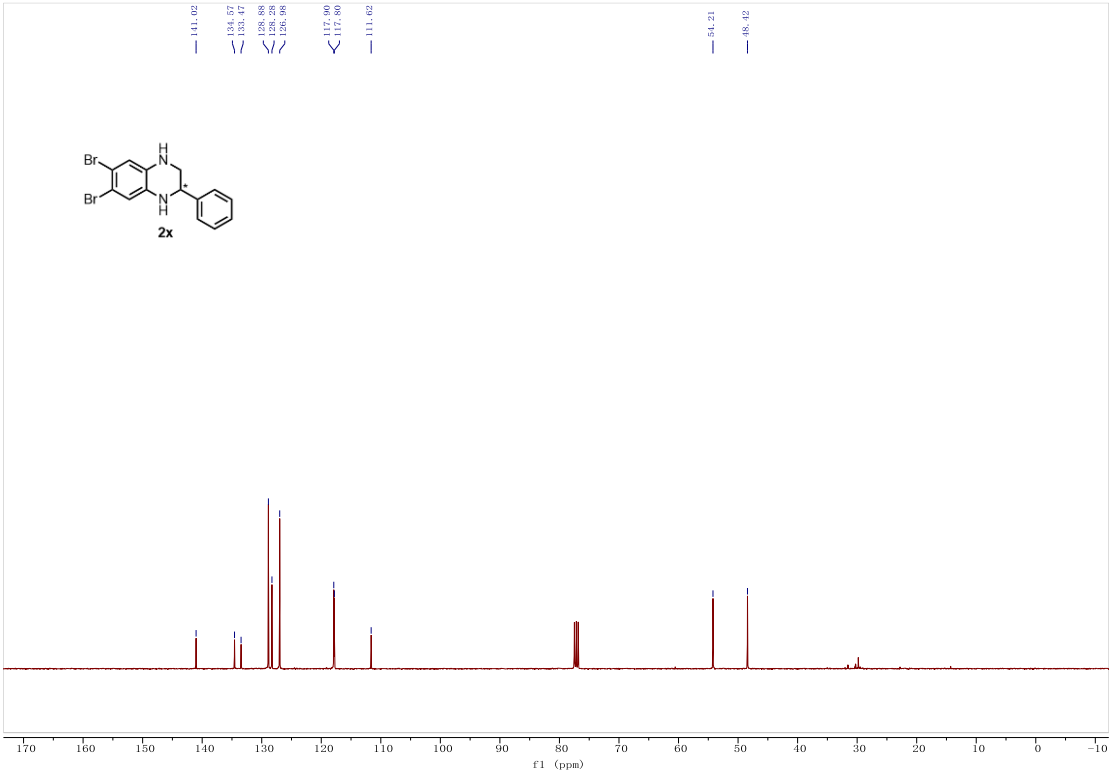
^{13}C NMR spectra for 2w



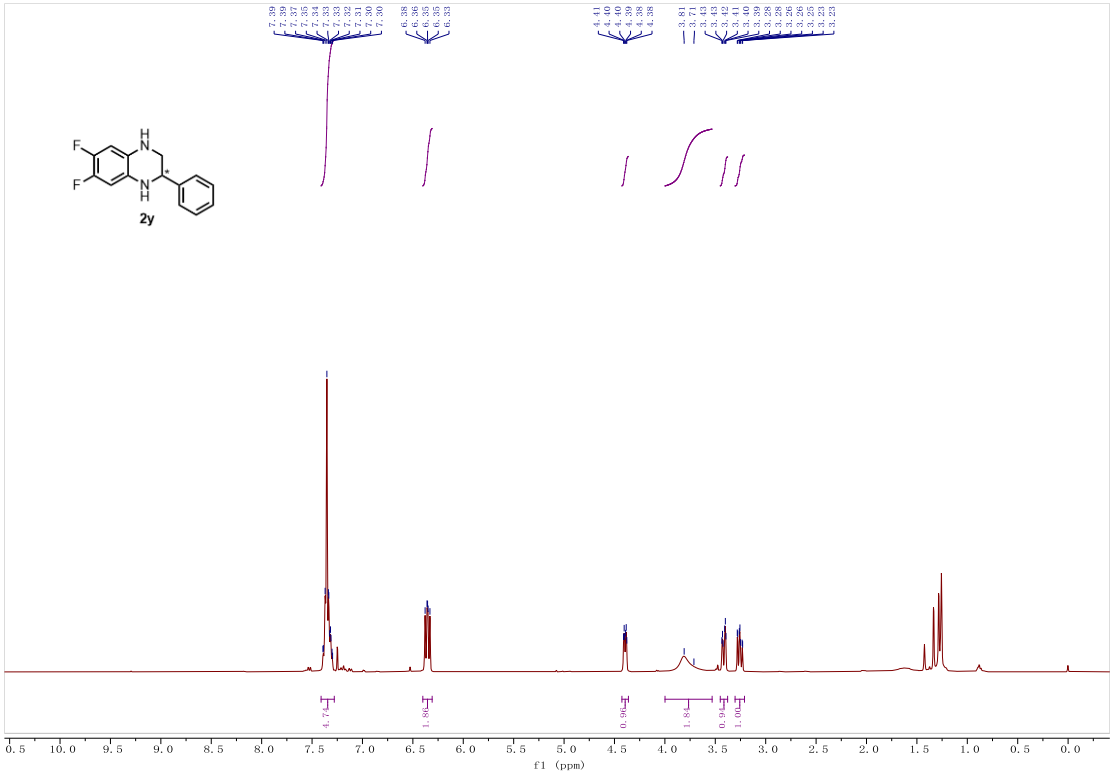
^{1}H NMR spectra for 2x



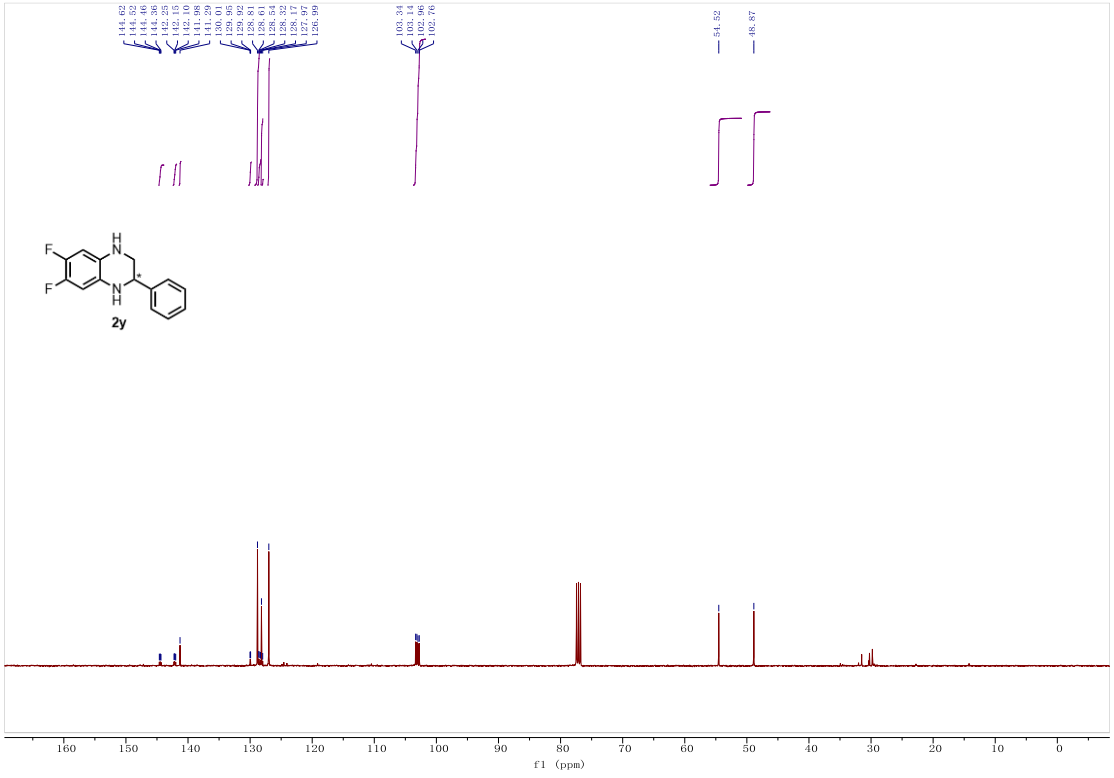
^{13}C NMR spectra for 2x



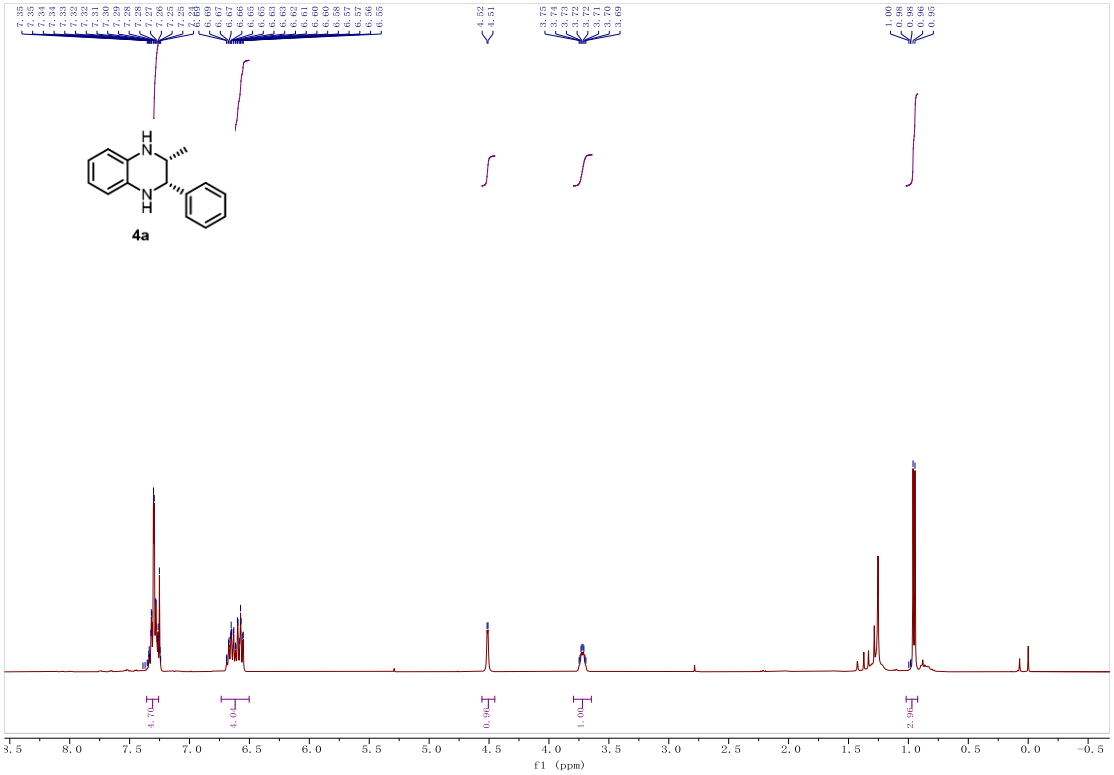
^{1}H NMR spectra for 2y



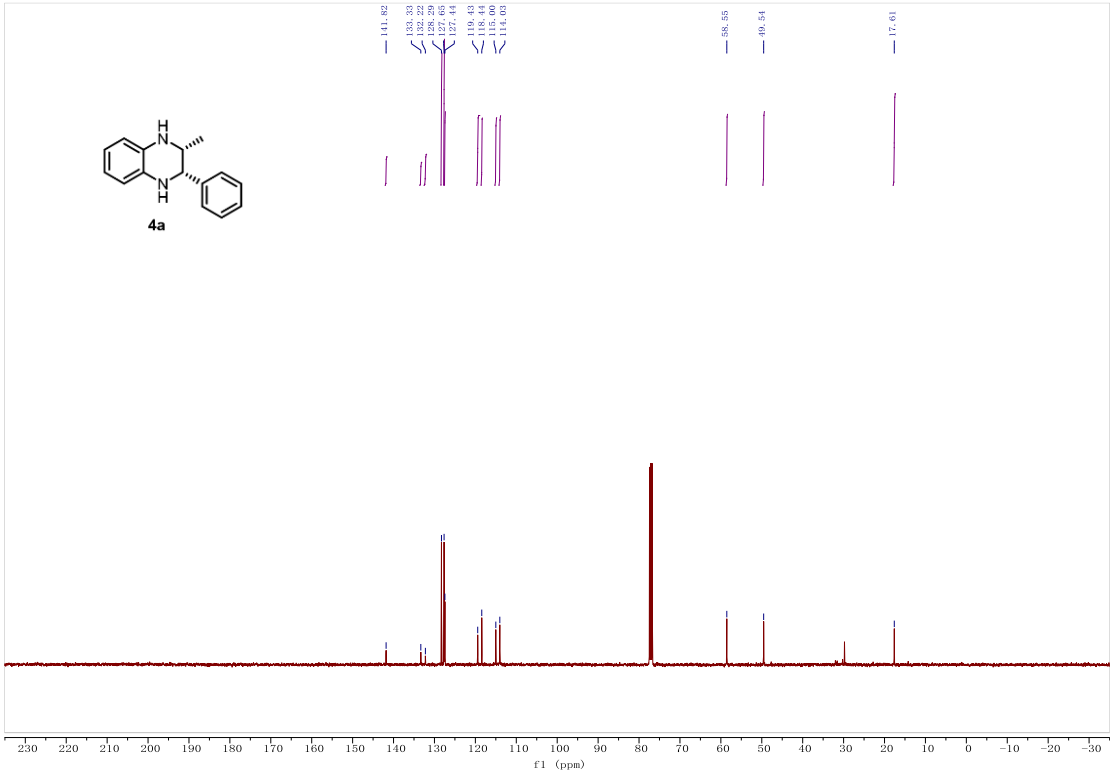
^{13}C NMR spectra for 2y



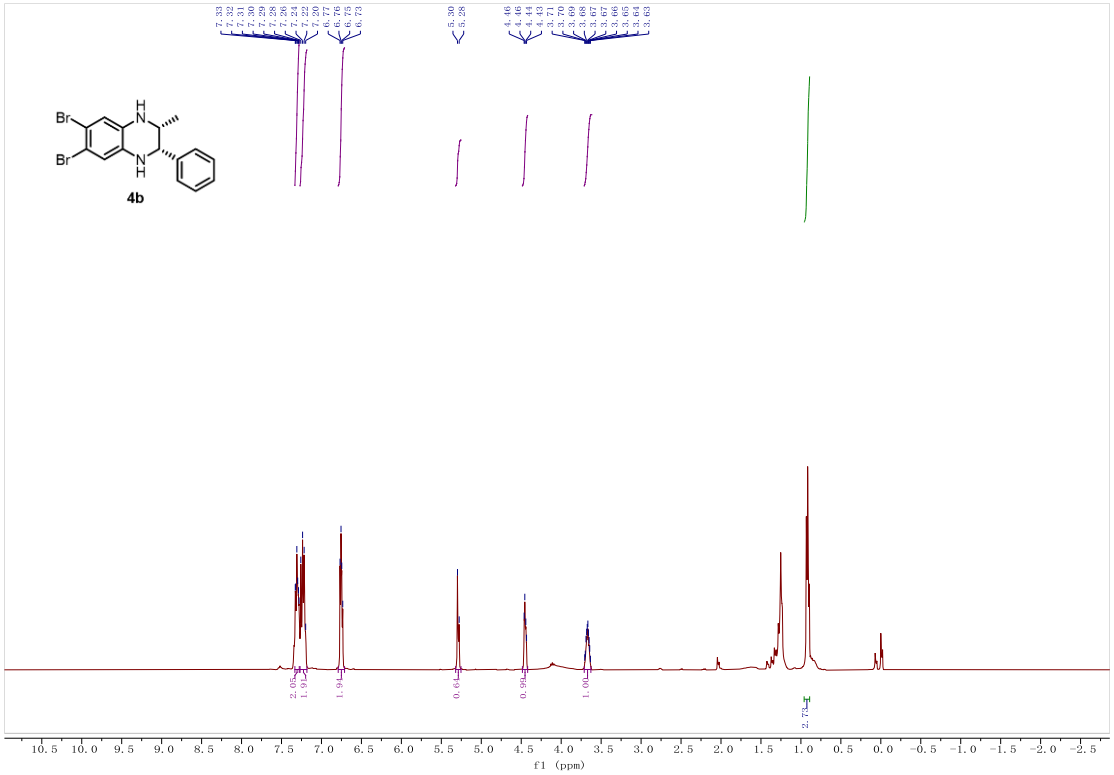
^{1}H NMR spectra for 4a



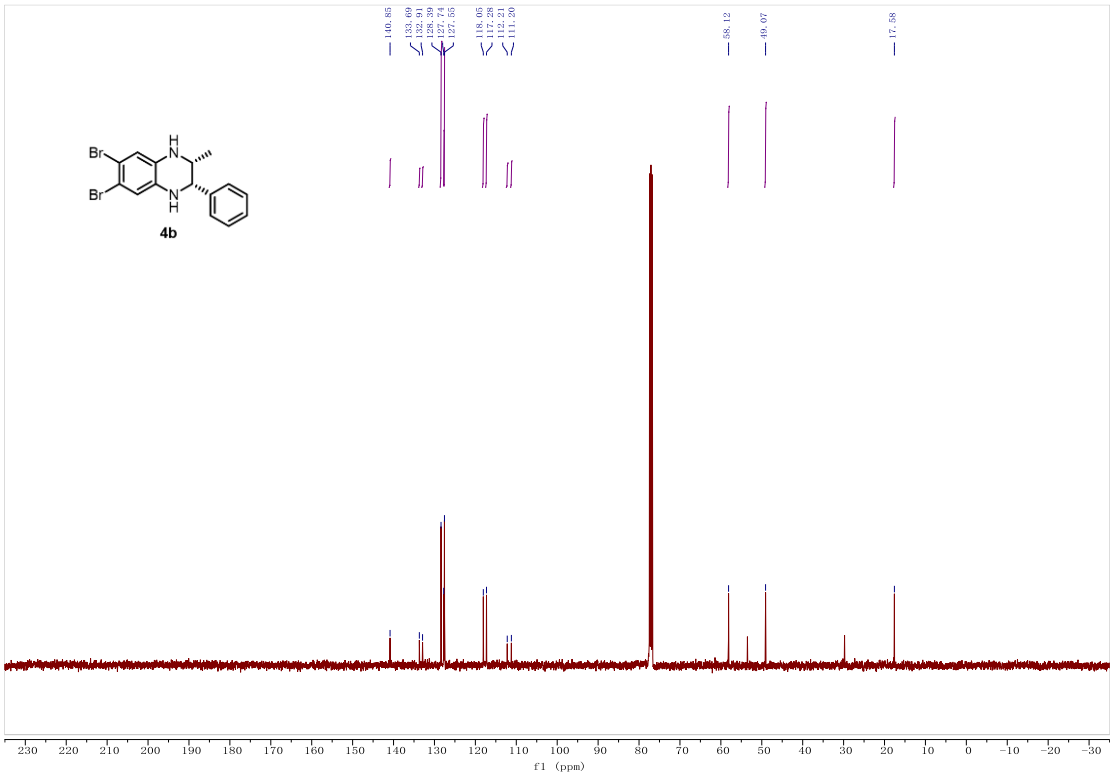
^{13}C NMR spectra for 4a



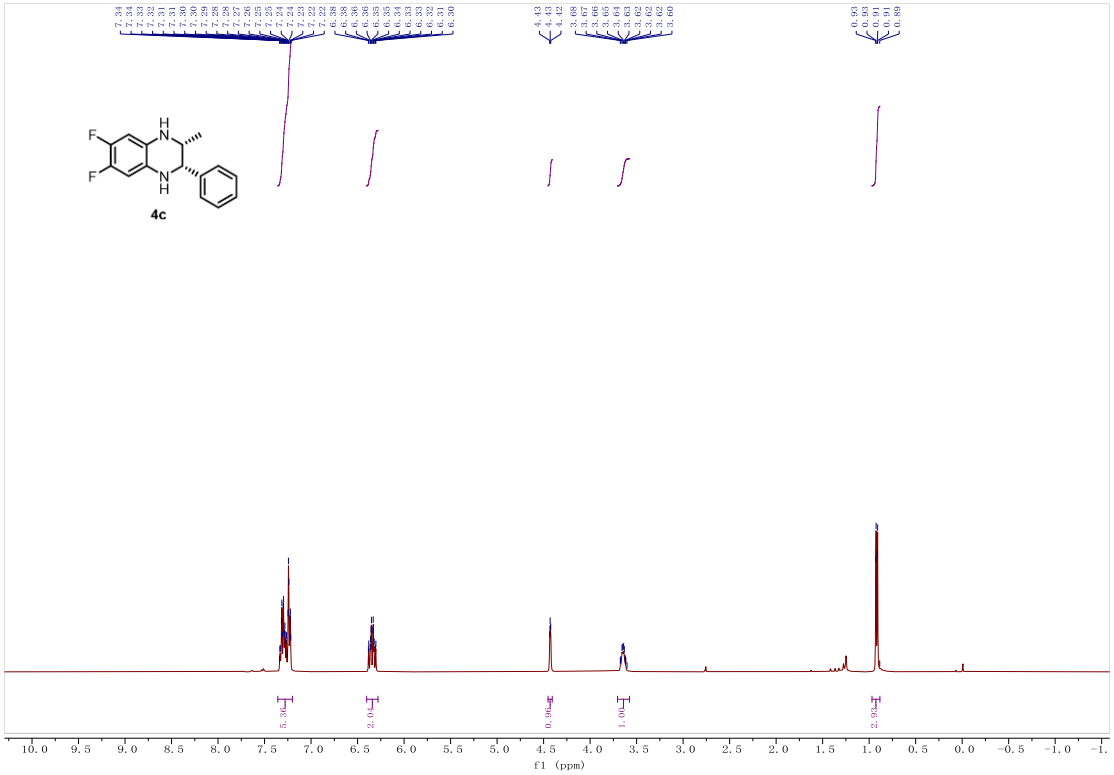
^{1}H NMR spectra for 4b



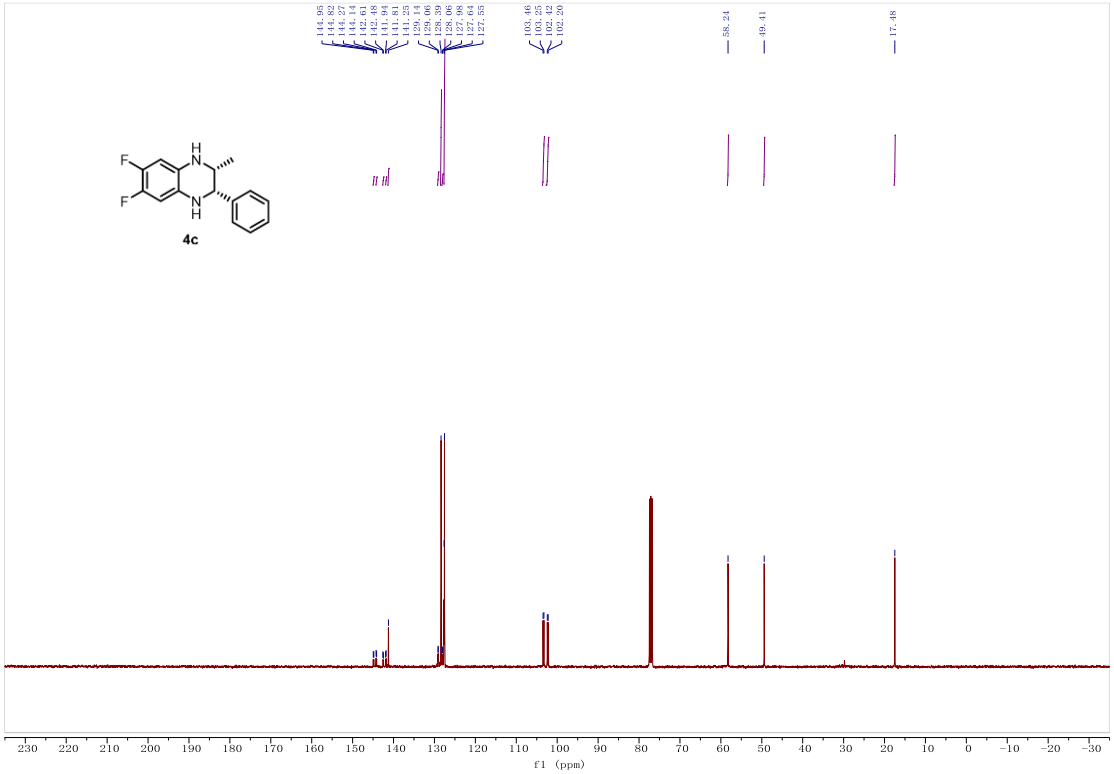
^{13}C NMR spectra for 4b



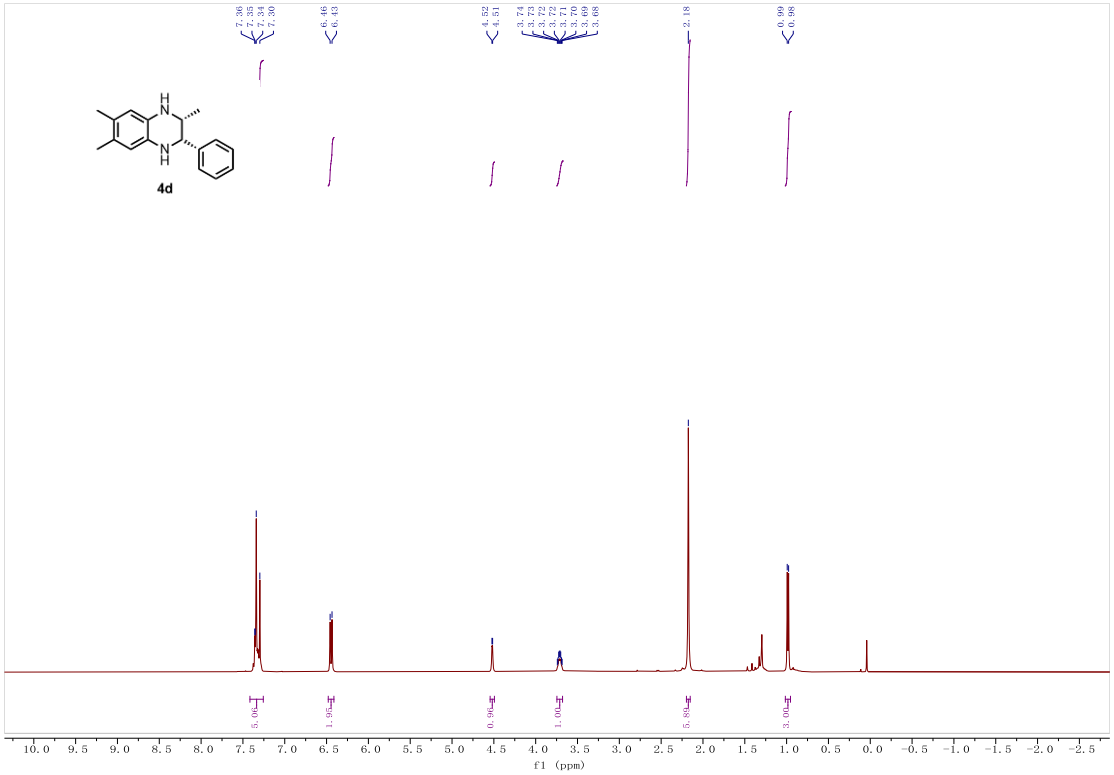
^{1}H NMR spectra for 4c



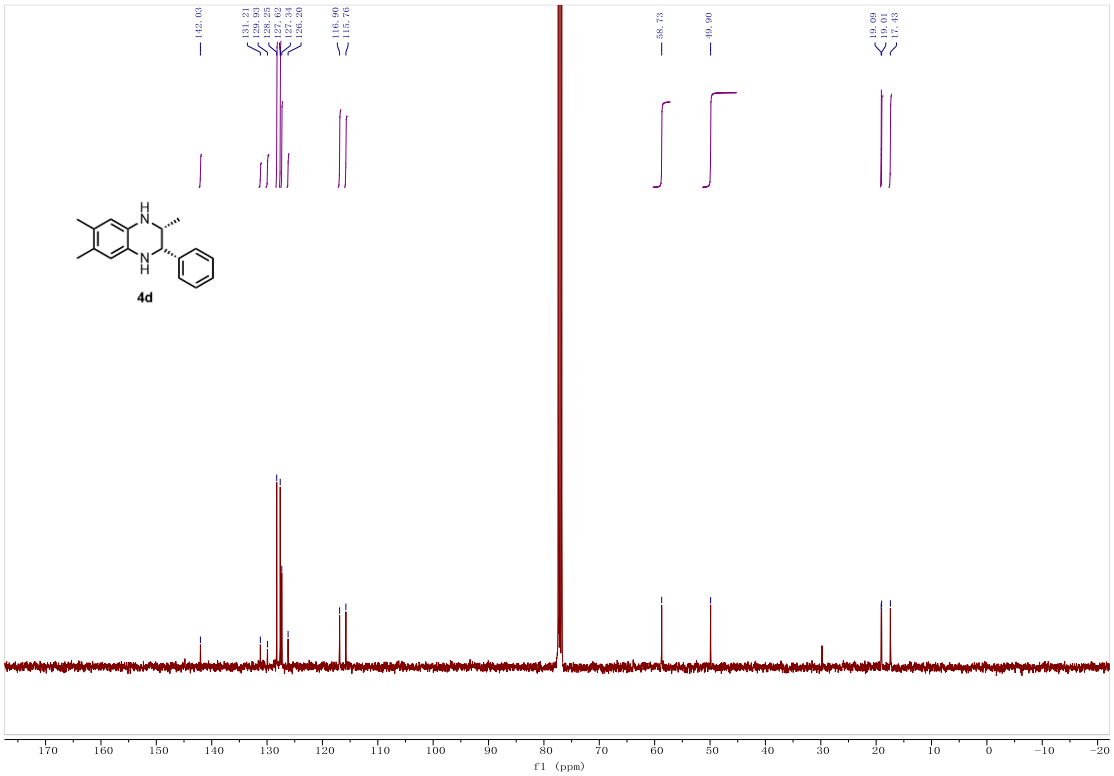
^{13}C NMR spectra for 4c



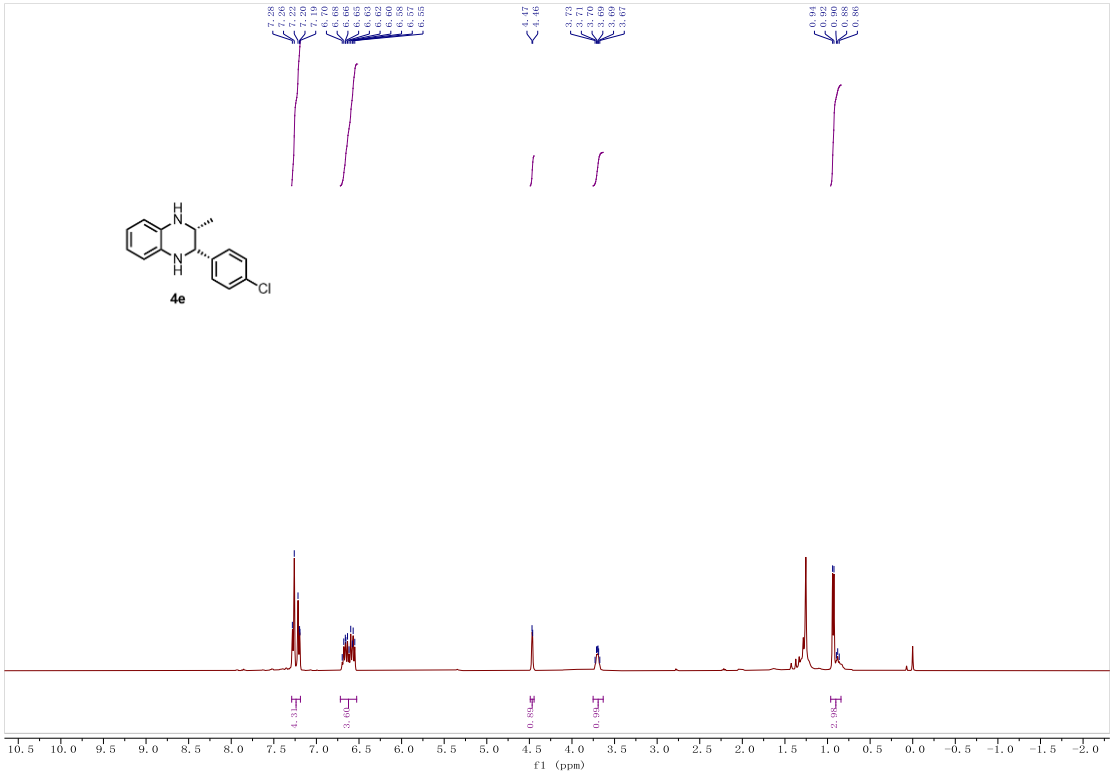
^{1}H NMR spectra for 4d



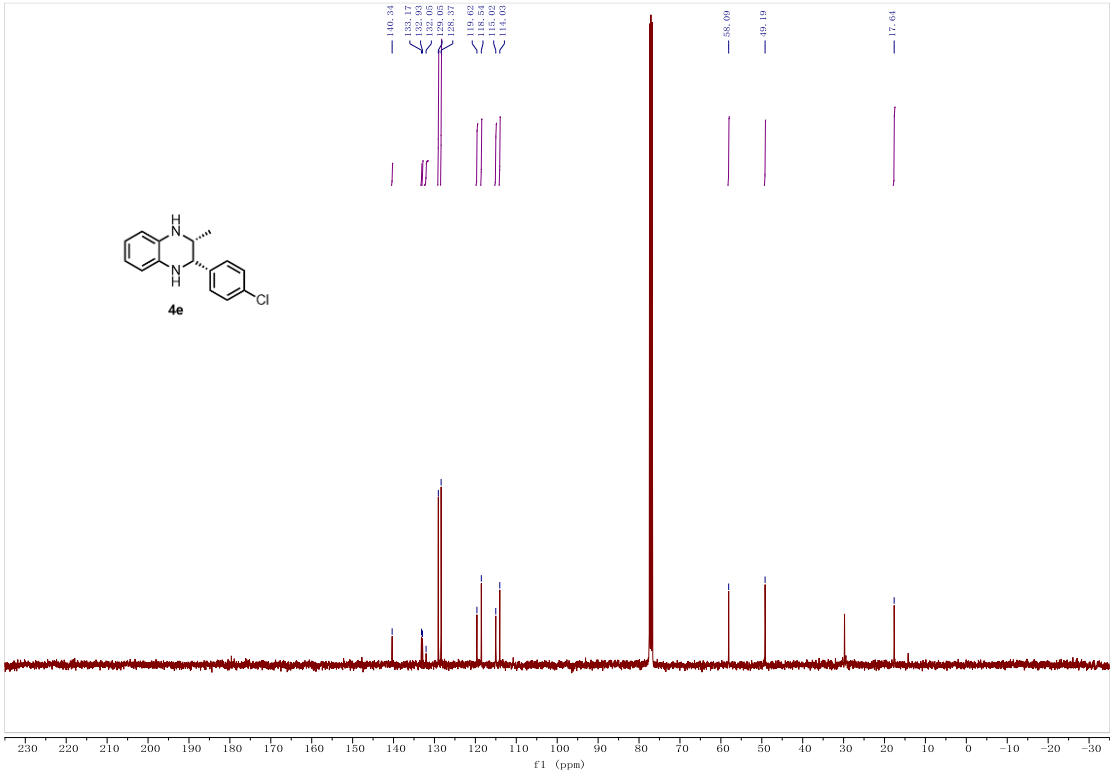
^{13}C NMR spectra for 4d



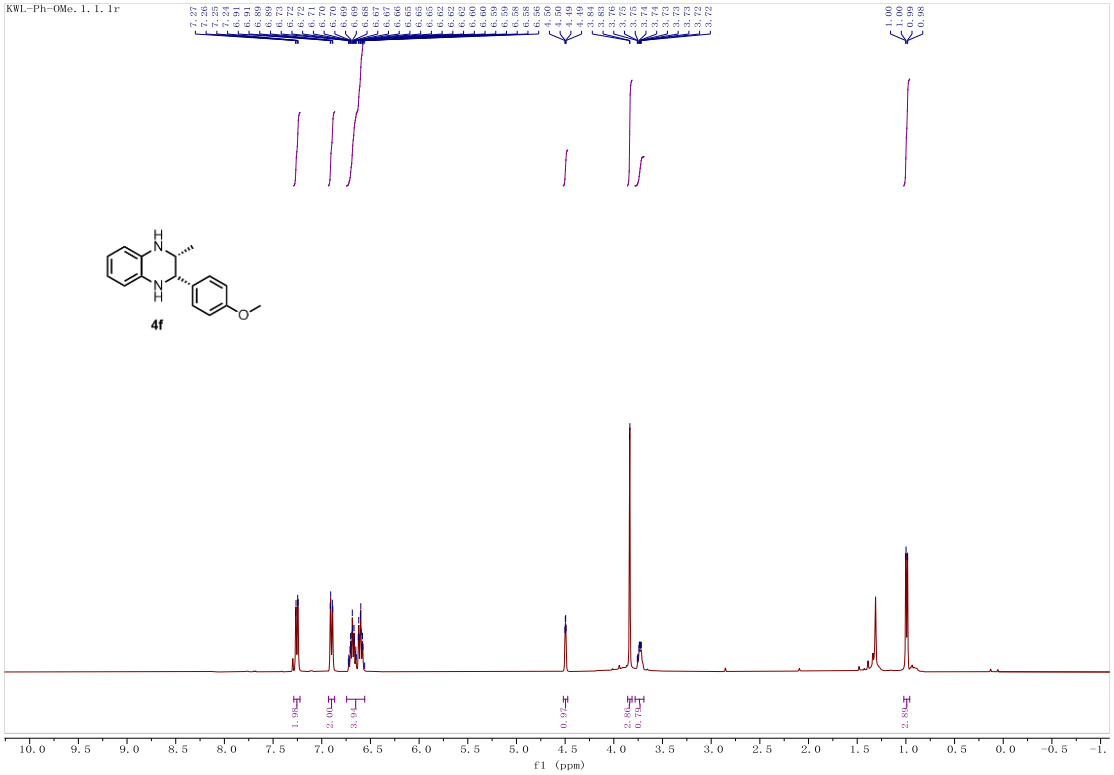
^{1}H NMR spectra for 4e



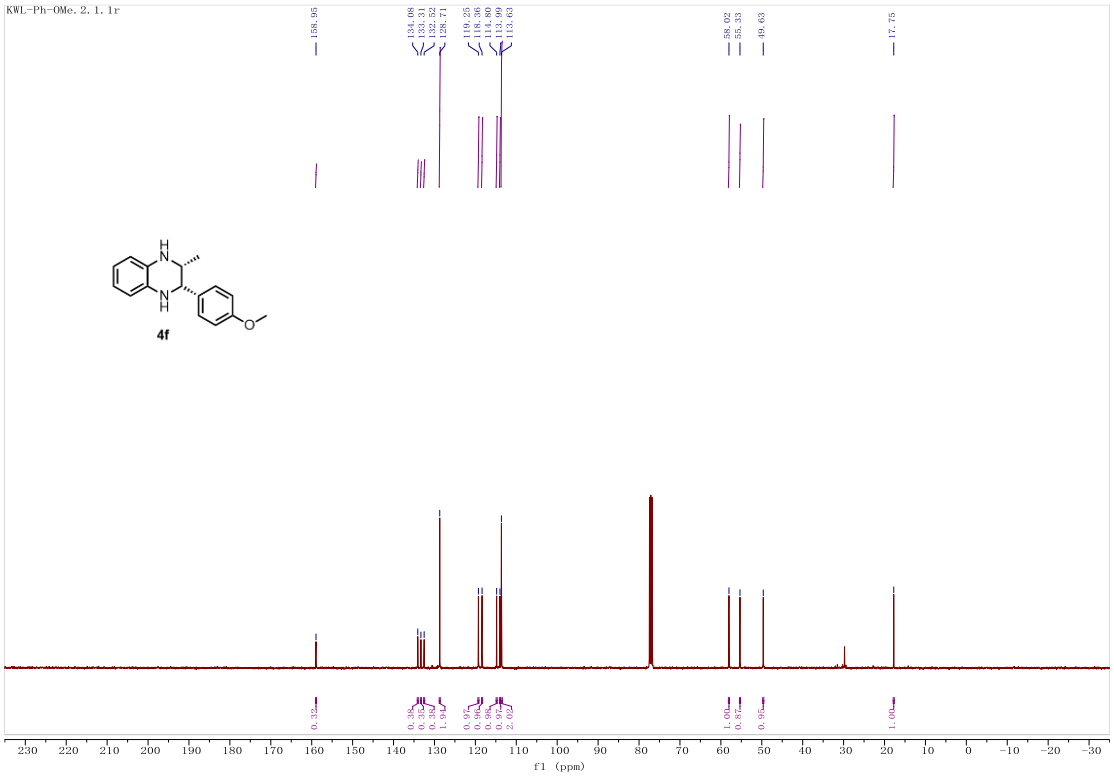
^{13}C NMR spectra for 4e



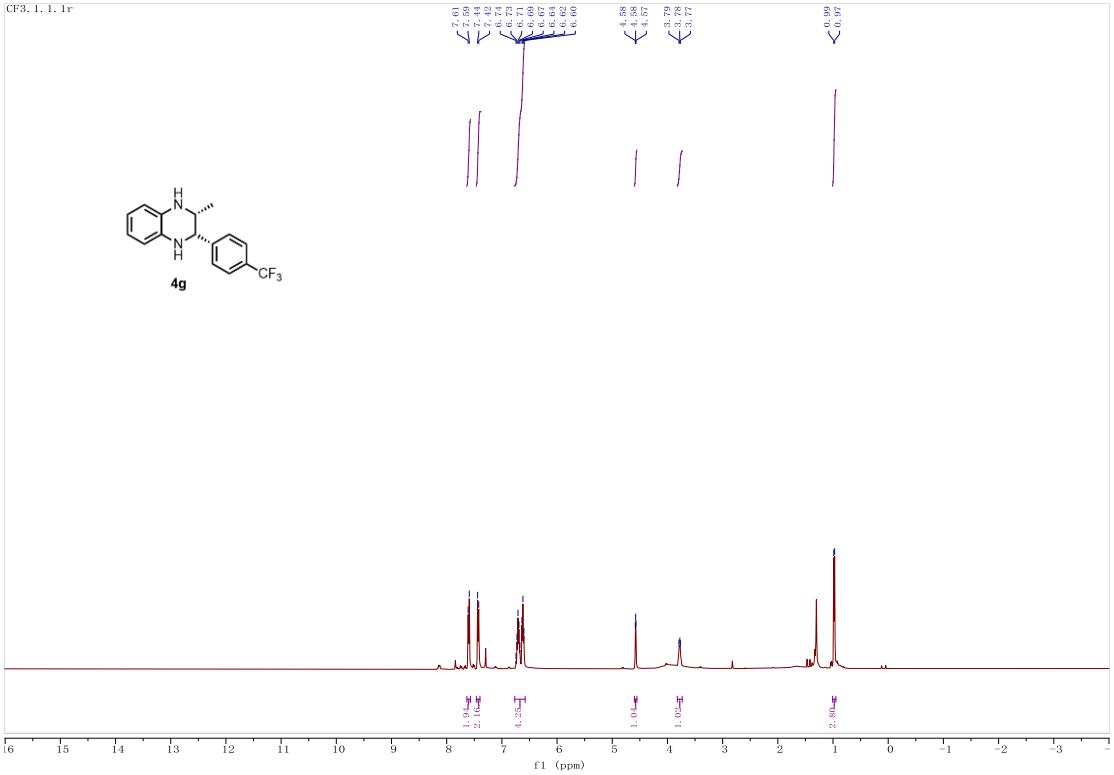
^{1}H NMR spectra for 4f



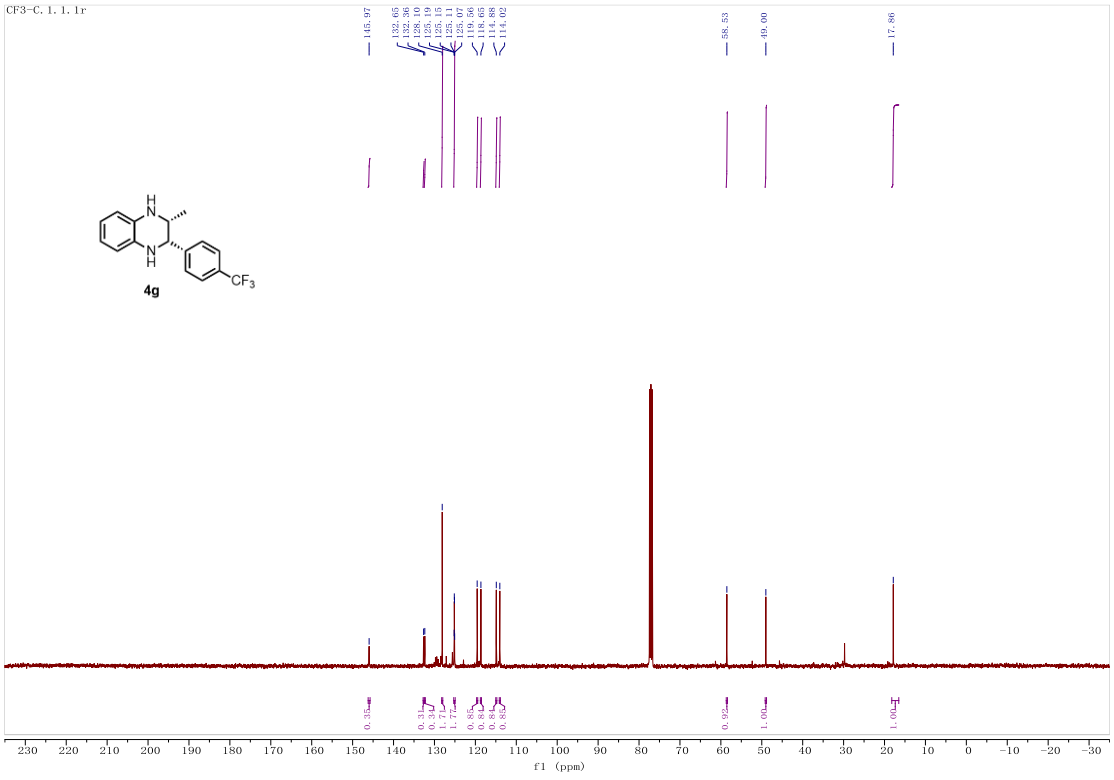
^{13}C NMR spectra for 4f



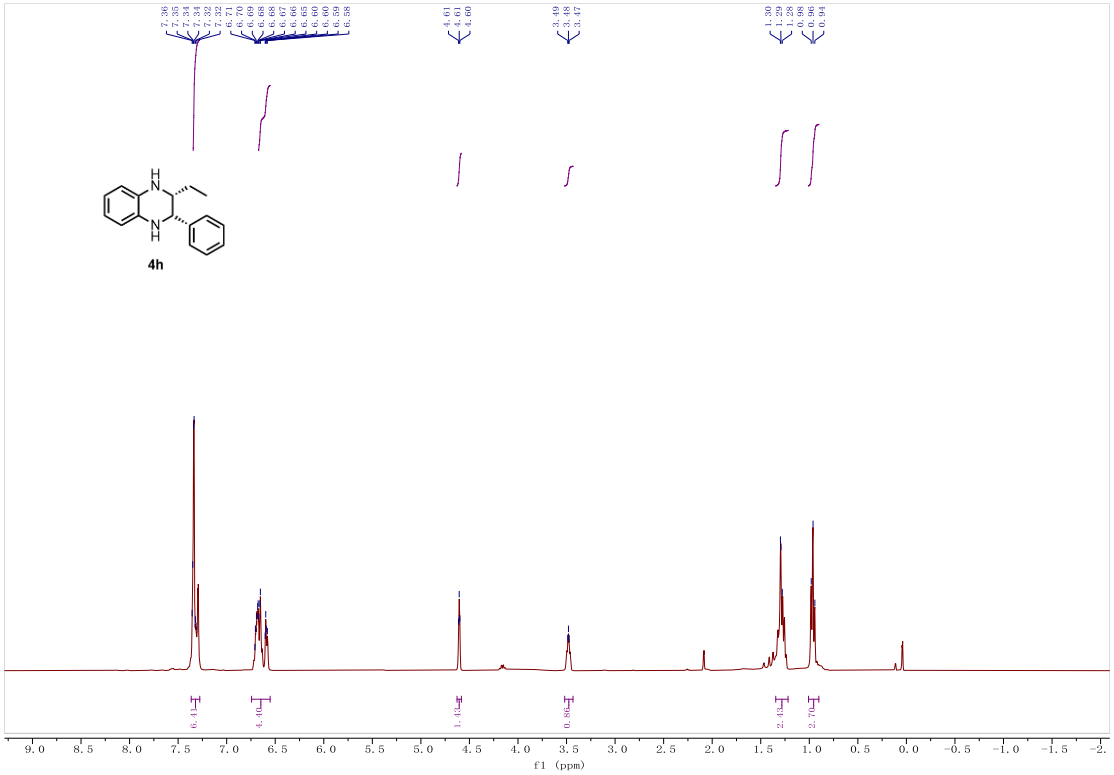
^{1}H NMR spectra for 4g



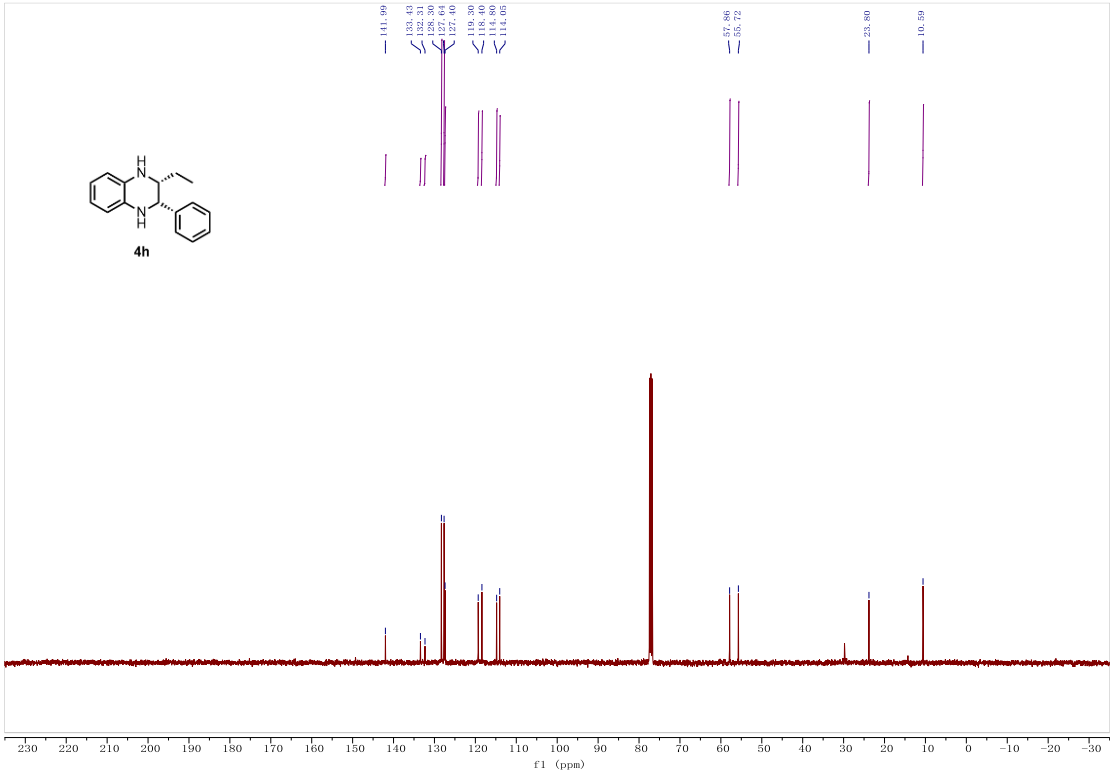
^{13}C NMR spectra for 4g



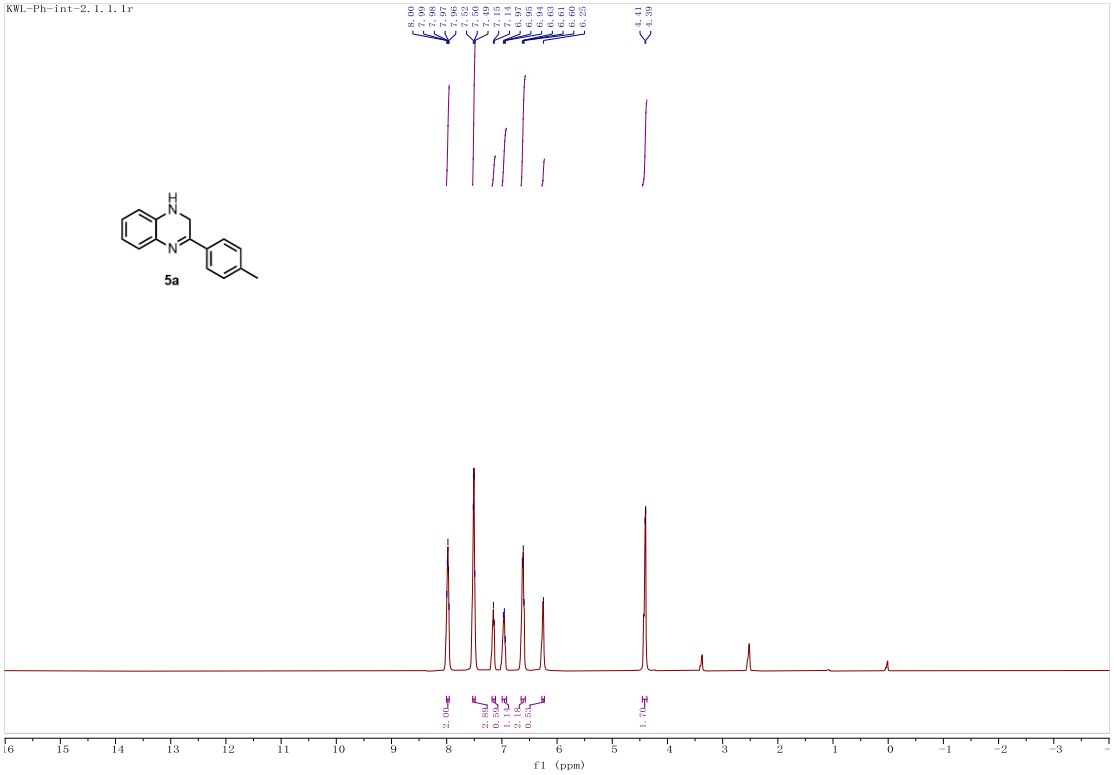
^{1}H NMR spectra for 4h



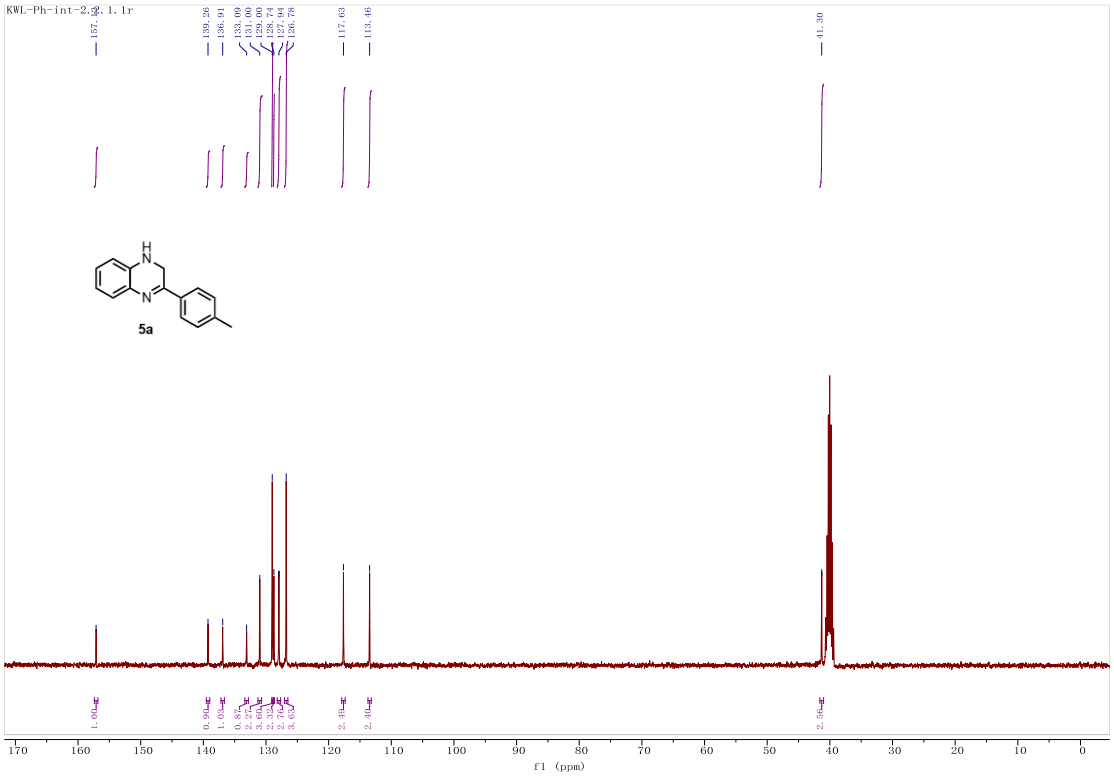
^{13}C NMR spectra for 4h



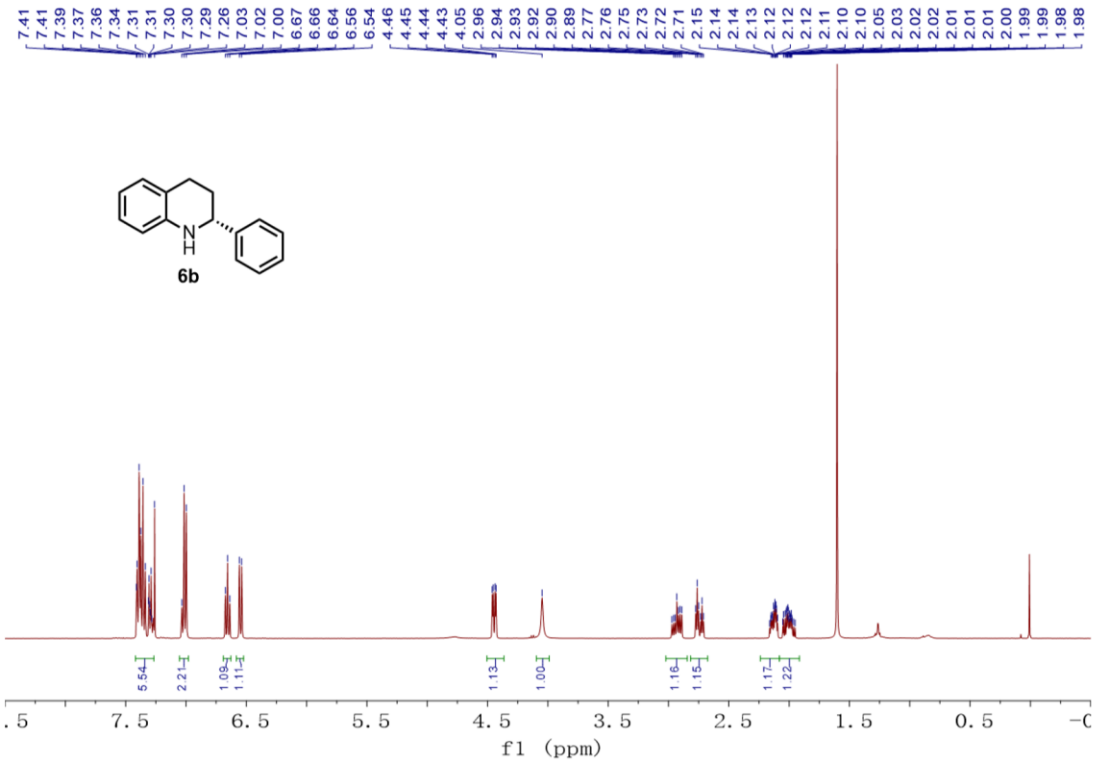
^{1}H NMR spectra for 5a



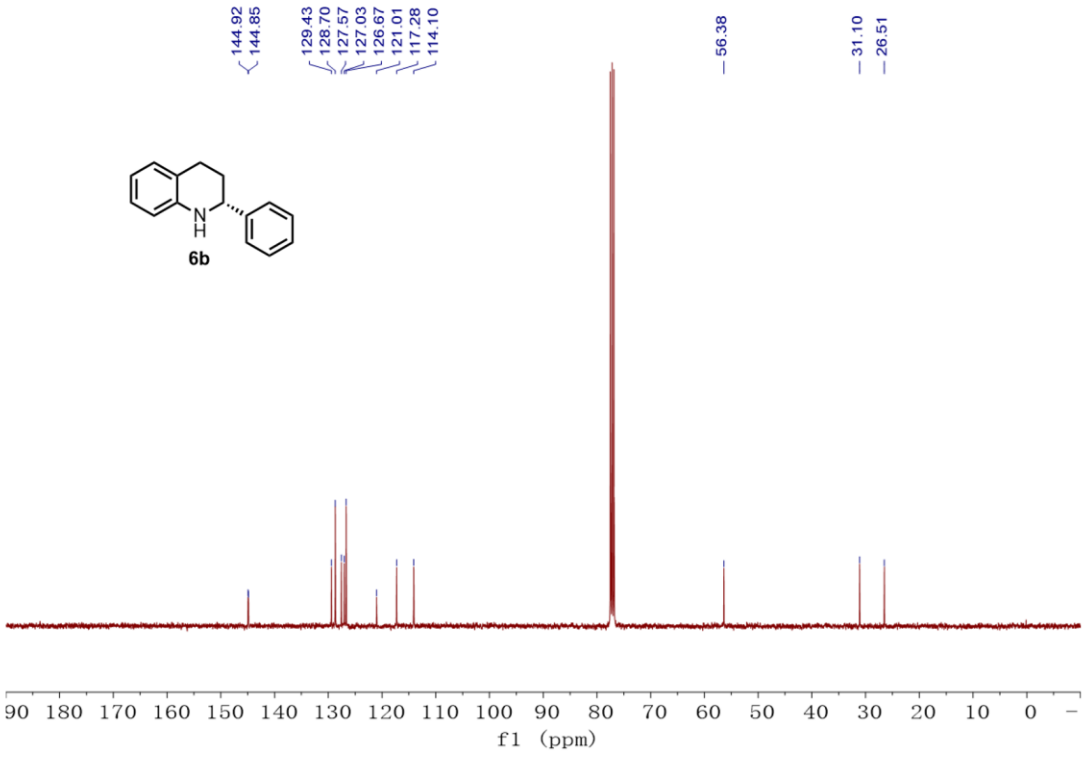
^{13}C NMR spectra for 5a



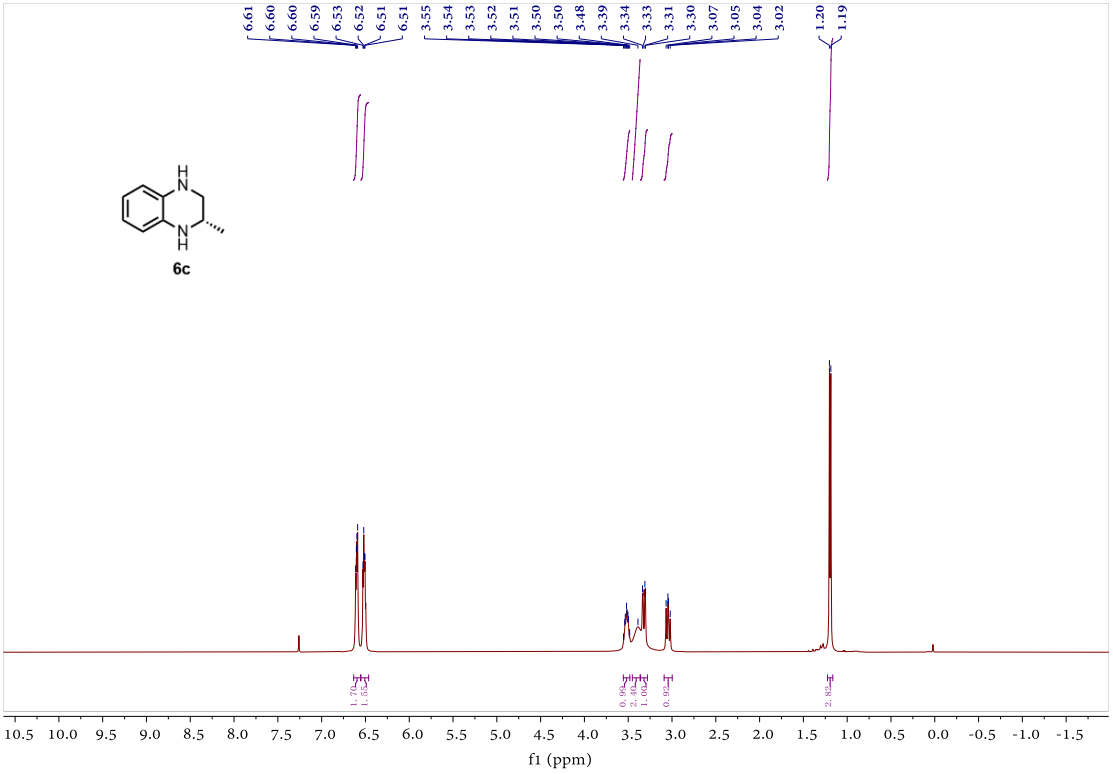
^{1}H NMR spectra for 6b



^{13}C NMR spectra for 6b



^{1}H NMR spectra for 6c



^{13}C NMR spectra for 6c