Supplementary Information

Nucleophilic Dearomatisation of N-Heteroaromatics Enabled by Lewis Acids and Copper Catalysis

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1. General experimental information

All reactions using oxygen- and/or moisture-sensitive materials were carried out with anhydrous solvents under a nitrogen atmosphere using standard Schlenk techniques. Flash column chromatography was performed using Merck 60 Å 230–400 mesh silica gel. Thin layer chromatography was performed using 0.25 mm E. Merck silica plates (60F-254). The products were visualized by phosphomolybdic acid (PMA) and $KMnO_4$ staining. NMR data was collected on Varian VXR400 (^{1}H at 400 MHz; ^{13}C at 100.58 MHz) equipped with a 5 mm *z*-gradient broadband probe. Chemical shifts are reported in parts per million (ppm) relative to residual solvent peak ($CDCl_3$, ^{1}H: 7.26 ppm; ^{13}C: 77.16 ppm). Coupling constants are reported in Hertz. Multiplicity is reported with the usual abbreviations (s: singlet, bs: broad singlet, d: doublet, t: triplet, m: multiplet). Variable-temperature NMR spectra were acquired on a Bruker Advance III spectrometer paired with an Ascend 400 MHz magnet and BBFO dual-resonance probe. All temperatures were calibrated prior to acquisition with an external pure MeOH reference. ^{1}H-^{13}C HSQCED spectra were recorded with the $^1J_{CH}$ constant set to 145 Hz while the ^{1}H-^{13}C HMBC spectra were recorded with a $^nJ_{XH}$ constant set to 8 Hz. Exact mass spectra were recorded on a LTQ Orbitrap XL apparatus with ESI ionization. Enantiomeric excess (*ee*) were determined by chiral HPLC analysis using a Shimadzu LC-10AD*VP* HPLC equipped with a Shimadzu SPD-M10A*VP* diode array detector.

2. Chemicals

Unless otherwise indicated, reagents and substrates were purchased from commercial sources and used as received. The substrates for synthesis of products **5j** and **5o** were synthesized according to the literature procedures respectively,[1] the rest are commercially available. Dry solvents were freshly collected from a dry solvent purification system prior to use. Inert atmosphere experiments were performed with standard Schlenk techniques with dried (P_2O_5) nitrogen gas. PhPrMgBr (2.6 M in Et_2O) and Hept-6-en-1-ylMgBr (1.4 M in Et_2O) was prepared from the corresponding alkyl bromides and Mg activated with I_2 in Et_2O. $Me_3SiCH_2CH_2MgBr$ (0.4 M in 2-Me-THF) was prepared from the corresponding alkyl bromide and Mg in 2-Me-THF at 0 °C. Other Grignard reagents were purchased from Sigma-Aldrich: EtMgBr (3 M in Et_2O); PentMgBr, *i*BuMgBr, *i*PentMgBr (2 M in Et_2O); *i*PrMgBr (3 M in 2-Me-THF). The Grignard reagents were titrated by ^{1}H NMR before use. Chiral ligands (**L1**−**L4**) were purchased from Sigma-Aldrich and Strem Chemicals. All reported compounds were characterized by ^{1}H and ^{13}C NMR and compared with literature data. All new compounds were fully characterized by ^{1}H and ^{13}C NMR and HRMS techniques.

3. Computational details

We have used the Density Functional Theory (DFT) in the Kohn-Sham formulation[2] to optimize all the stationary points presented in this manuscript. Geometries of all the stationary points were fully optimized at the M06[3]/def2svpp[4] computational level. The effect of solvent was modeled using the polarizable continuum model (PCM)[5] with the default parameters implemented in the Gaussian 09 package.[6] All geometry optimizations have been optimized using tight convergence criteria in the SCF and requesting a pruned (99.590) grid to guarantee the accuracy of the reported results. Moreover, the calculations were performed considering 1 atm and 195 K to properly simulate the reaction conditions.

Harmonic analysis was used to establish the nature of all optimized structures as either minima or transition structures. For all stationary points, the stability of the wave function was also confirmed.[7] Moreover, for all the copper species an analysis of the spin annihilation was also performed being the value 0.00.

IRC[8] calculations were conducted for important transition states to ensure their connectivity with the expected reactants and products. The stability of the wave function was analyzed for all the presented stationary points.[9] When the substrates showed conformational freedom, conformational analysis was performed manually, it must be indicated that only the most stable conformer of each stationary point was considered and reported unless otherwise indicated.

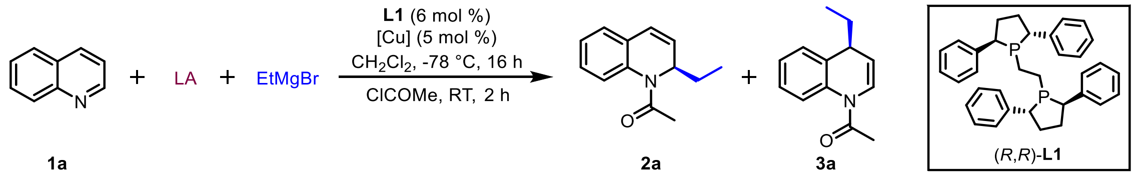
The visualization of the reported structures was performed using MOLDEN.[10] The representation of the structures here presented were generated using CYLView.[11]

The Grignard reagents used in this work are bought in ethereal solvents and then diluted. In line with this, we have confirmed the superior stability of the Grignard reagents with two solvent molecules (see Solvation studies).[12] Since solvent can be exchanged during the reaction process, we have evaluated the relative stability of each of the proposed stationary points here described with none, one and two solvent molecules directly coordinated to the magnesium center, for each step of the reaction, obtaining that the coordination two ethereal molecules (at −78 °C) lead to the more stable systems. Thus, along the mechanistic study two solvent molecules are considered in the first coordination sphere of the magnesium.

Moreover, the BF_3 was selected as the LA and **L1** as a ligand for the molecular simulations.

4. Optimization of reaction conditions

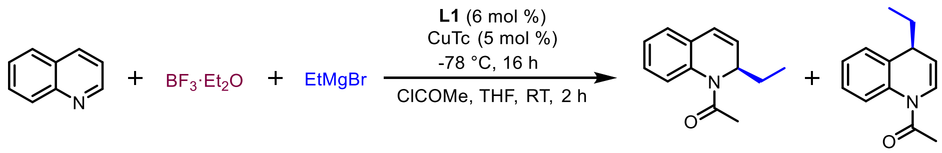
Table S1. Optimization of the copper salt and LA for the enantioselective C-4-addition of EtMgBr to quinoline followed by trapping with acetyl chloride[a]



Entry	**L**	Cu(I)	LA	**1a**:**2a**:**3a**[b]	NMR yield (**3a**) [%][c]	*ee* (**3a**) [%][d]
1[e]	–	–	–	100:0:0	–	–
2	–	–	Me_3SiOTf	1:93:6	–	–
3[f]	–	–	$BF_3{\cdot}Et_2O$	80:14:6	–	–
4	**L1**	$CuBr{\cdot}SMe_2$	–	100:0:0	–	–
5	**L1**	$CuBr{\cdot}SMe_2$	Me_3SiOTf	3:79:18	–	77
6[f]	**L1**	$CuBr{\cdot}SMe_2$	$BF_3{\cdot}Et_2O$	1:0:99	55	>99
7	**L1**	CuTc	Me_3SiOTf	0:67:33	–	83
8[f]	**L1**	CuTc	$BF_3{\cdot}Et_2O$	1:0:99	58[g]	>99
9[f]	**L1**	CuTc	BCl_3	24:0:76	35	96

[a]Reaction conditions: 0.1 M of **1a** in CH_2Cl_2, Cu(I) (5 mol%), **L1** (6 mol%), LA (2 equiv.), EtMgBr (2 equiv.) at −78 °C for 16 h, then ClCOMe (5 equiv.) at RT for 2 h. [b]The ratio was determined by ^1H NMR of reaction crude. [c]Trimethoxybenzene was added after work-up and used as the internal standard. [d]Enantiomeric excess was determined by HPLC on a chiral stationary phase. [e]In this case the reaction was quenched directly without trapping with ClCOMe. [f]In this case THF (4 mL) was added after addition of ClCOMe. [g]In this case the data reported corresponds to the isolated yield.

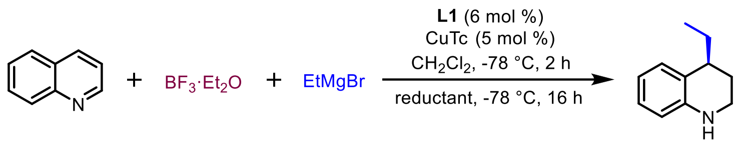
Table S2. Optimization of the of LA and EtMgBr quantities as well as the nature of solvent for the enantioselective C-4-addition of EtMgBr to quinoline followed by trapping with acetyl chloride[a]



Entry	Solvent	$BF_3 \cdot Et_2O$ [equiv.]	EtMgBr [equiv.]	**1a**:**2a**:**3a**[b]	NMR yield (**3a**) [%][c]	*ee* (**3a**) [%][d]
1	CH_2Cl_2	2	2	1:0:99	58[e]	>99
2	CH_2Cl_2	1.2	2	1:0:99	54	>99
3	CH_2Cl_2	0.4	2	35:0:65	47	98
4	CH_2Cl_2	2	1.2	34:0:66	41	>99
5	CH_2Cl_2	1.2	1.2	35:0:65	39	>99
6[f]	CH_2Cl_2	2	2	1:0:99	57	>99
7[g]	CH_2Cl_2	2	2	4:0:96	54	>99
8[h]	CH_2Cl_2	2	2	5:0:95	51	>99
9[i]	THF	2	2	12:81:7	–	42
10[i]	2-Me-THF	2	2	1:0:99	34	>99
11	MTBE	2	2	30:0:70	–	>99
12	MTBE	3	3	2:0:98	52	>99
13	Et_2O	3	3	2:0:98	41	>99
14	Toluene	3	3	1:0:99	44	>99

[a]Reaction conditions: 0.1 M of **1a**, CuTc (5 mol%), **L1** (6 mol%), $BF_3 \cdot Et_2O$, EtMgBr at −78 °C for 16 h, then ClCOMe (5 equiv.) and THF (4 mL) at RT for 2 h. [b]The ratio was determined by ^1H NMR of reaction crude. [c]Trimethoxybenzene was added after work-up and used as the internal standard. [d]Enantiomeric excess was determined by HPLC on a chiral stationary phase. [e]In this case the isolated yield is reported. [f]EtMgBr was diluted to 1 mL with MTBE and added with syringe pump in 1 h. [g]EtMgBr was first added followed by addition of $BF_3 \cdot Et_2O$. [h]The mixture of chiral catalyst **L1**/Cu(I) and EtMgBr was added to the mixture of substrate and $BF_3 \cdot Et_2O$. [i]In this case THF (4 mL) was not needed after addition of ClCOMe.

Table S3. Optimization of the reductant for the enantioselective C-4-addition of EtMgBr to quinoline followed by reduction[a]



Entry	Reductant	Conversion [%][b]	Isolated yield [%]	*ee* [%][c]
1	$NaBH_4$	99	73	>99
2	$NaBH_4$ (1 mmol)/THF (4 mL) mixture	99	49	>99
3	$NaBH_4$ (1 mmol)/MeOH (2 mL) mixture	99	33	>99
4	$BH_3 \cdot SMe_2$	99	49	>99
5[d]	Et_3SiH (1 mmol), CF_3COOH (1.2 mmol)	99	49[e]	>99
6	BH_3 (1 M in THF)	99	83	>99

[a]Reaction conditions: 0.2 mmol of **1a** in CH_2Cl_2 (2 mL), CuTc (5 mol%), **L1** (6 mol%), $BF_3 \cdot Et_2O$ (2 equiv.), EtMgBr (2 equiv.) at −78 °C for 2 h, then reductant (5 equiv.) at RT for 16 h. [b]Conversion was determined by ^1H NMR of reaction crude. [c]Enantiomeric excess was determined by HPLC on a chiral stationary phase. [d]During work-up, the solvent was evaporated before saturated $NaHCO_3$ aqueous solution was added to the residue and the mixture was extracted with CH_2Cl_2. [e]Product is not pure.

5. Solvation studies for the computational mechanistic study

Table S4. Computed relative energies for the solvation of the EtMgBr species. Calculations were performed at the PCM(CH_2Cl_2)/M06/def2svpp computational level using the Gaussian 09 program. The thermochemistry was obtained at 1 atm and 195 K.

ID	ΔG[a]
EtMgBr	0.00
EtMgBr·Et$_2$O	−7.70
EtMgBr·2Et$_2$O	−8.84

[a]Energies are calculated with respect to EtMgBr and two molecules of Et_2O and are expressed in kcal/mol.

Table S5. Summary of the energies for solvation studies of the Grignard reagent.

ID	ImFreqs	Stable	SCF[a]	SCF+ZPVE	H[b]	G[c]
EtMgBr	−	Yes	−2852.92586678	−2852.862580	−2852.858414	−2852.881361
Et_2O	−	Yes	−233.296065097	−233.161050	−233.156875	−233.179034
EtMgBr·Et_2O	−	Yes	−3086.24895436	−3086.048164	−3086.040115	−3086.072676
EtMgBr·2Et_2O	−	Yes	−3319.207607	−3319.19668	−3319.195446	−3319.252401

[a]Energies are expressed in a.u. and the imaginary frequencies in cm^{-1}. [b]H represents enthalpies. [c]G Represents Gibbs free Energies.

6. Lewis acid promoted copper-catalyzed enantioselective dearomatization of quinolines

General procedure for catalytic reactions

In a flame-dried Schlenk tube equipped with septum and magnetic stirring bar, the substrate (0.2 mmol, 1 equiv.), copper salt (0.01 mmol, 5 mol%), and ligand **L** (0.012 mmol, 6 mol%) were dissolved in the solvent (2 mL) and stirred under nitrogen atmosphere for 20 min. at RT. The mixture was cooled to −78 °C and LA (1.2–3 equiv.) was added. After 20 min., RMgBr (2–3 equiv.) was added dropwise in about 1 min.

General trapping procedure

After stirring for 16 h at −78 °C, acetyl chloride (71 μL, 1 mmol, 5 equiv.) was added and the reaction mixture was warmed up to RT. After stirring for 2 h, the resulting reaction mixture was quenched with saturated $NaHCO_3$ aqueous solution (2 mL) and stirred at RT for 1 h to hydrolyze the remaining acetyl chloride. The mixture was extracted with CH_2Cl_2 (10 mL × 3). The combined organic phase was dried over $MgSO_4$, filtered and evaporated on rotary evaporator. The crude was purified by flash chromatography on the silica gel. (Note: when $BF_3 \cdot Et_2O$ was used as LA, 4 mL of THF has to be added after addition of acetyl chloride, because when using $BF_3 \cdot Et_2O$ trapping was only successful in THF.)

General reduction procedure

After stirring for 2–16 h at −78 °C, BH_3 (1 M in THF, 1 mmol, 5 equiv.) was added. After stirring for 16 h at −78 °C, the resulting reaction mixture was quenched with saturated $NaHCO_3$ aqueous solution (2 mL) and warmed up to RT. The mixture was stirred at RT for 1 h to hydrolyze the remaining $BH_3 \cdot THF$, and extracted with CH_2Cl_2 (10 mL × 3). The combined organic phase was dried over

$MgSO_4$, filtered and evaporated on rotary evaporator. The crude was purified by flash chromatography on the silica gel.

Procedure for the reaction with the reduced catalyst loading

In a flame-dried three-neck round-bottom flask equipped with septum and mechanistic stirring bar, CuTc (0.01 mmol) and ligand (*R*,*R*)-**L1** (0.012 mmol) were dissolved in CH_2Cl_2 (10 mL) and the mixture was stirred under nitrogen atmosphere for 20 min. at RT, forming catalyst solution **1**. 2 mL of catalyst solution **1** (2 μmol, 1 mol%) was transferred to substrate **1a** (0.2 mmol, 1 equiv.) to perform the reaction with 1 mol% catalyst. 0.2 mL of catalyst solution **1** (0.2 μmol, 0.1 mol%) was transferred to substrate **1a** (0.2 mmol, 1 equiv.) dissolved in CH_2Cl_2 (2 mL) to perform the reaction with 0.1 mol% catalyst. 1 mL of catalyst solution **1** (1 μmol) was transferred to another round-bottom flask and diluted with CH_2Cl_2 to 10 mL to form catalyst solution **2**. 0.2 mL of catalyst solution **2** (0.02 μmol, 0.01 mol%) was transferred to substrate **1a** (0.2 mmol, 1 equiv.) dissolved in CH_2Cl_2 (2 mL) to perform the reaction with 0.01 mol% catalyst.

Procedure for the preparative scale (10 mmol) reaction

In a flame-dried three-neck round-bottom flask equipped with septum and mechanistic stirring bar, the substrate **1a** (10 mmol, 1 equiv.), CuTc (0.01 mmol, 0.1 mol%) and ligand (*R*,*R*)-**L1** (0.012 mmol, 0.12 mol%) were dissolved in CH_2Cl_2 (50 mL) and the mixture was stirred under nitrogen atmosphere for 20 min. at RT. The mixture was cooled to −78 °C and $BF_3{\cdot}Et_2O$ (20 mmol, 2 equiv.) was added. After 20 min., EtMgBr (3 M in Et_2O, 20 mmol, 2 equiv.) was added with syringe pump in 15 min. After stirring for 2 h at −78 °C, BH_3 (1 M in THF, 50 mmol, 5 equiv.) was added. After stirring for 16 h at −78 °C, the resulting reaction mixture was quenched with saturated $NaHCO_3$ aqueous solution (20 mL) and warmed up to RT. The mixture was stirred at RT for 1 h to hydrolyze the $BH_3{\cdot}THF$, and extracted with CH_2Cl (30 mL × 3). The combined organic phase was dried over $MgSO_4$, filtered and evaporated on rotary evaporator. The crude was purified by flash chromatography on the silica gel (SiO_2, pentane:Et_2O = 20:1) to yield the product **4a** as a colorless oil [71% yield, 96% *ee*].

Procedure for the synthesis of racemic 2a and 3a

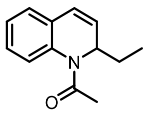
In a flame-dried Schlenk tube equipped with septum and magnetic stirring bar, **1a** (0.2 mmol, 1 equiv.) was dissolved in CH_2Cl_2 (2 mL). The temperature was cooled down to −78 °C and EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.) was added. After stirring for 16 h, acetyl chloride (1 mmol, 5 equiv.) was added and the reaction mixture was warmed up to RT. After stirring for 2 h, the resulting reaction mixture was quenched with saturated $NaHCO_3$ aqueous solution (2 mL) and stirred at RT for 1 h to hydrolyze the remaining acetyl chloride. The mixture was extracted with CH_2Cl (10 mL × 3). The combined organic phase was dried over $MgSO_4$, filtered and evaporated on rotary evaporator. Products **2a** and **3a** were obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 10:1) [**1a**:**2a**:**3a** = 37:53:10 in the crude product].

General procedure for the synthesis of racemic 4-substituted 1,2,3,4-tetrahydroquinolines

In a flame-dried Schlenk tube equipped with septum and magnetic stirring bar, the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%) and CH_2Cl_2 (2 mL) were stirred under nitrogen atmosphere for 20 min. at RT. The mixture was cooled to −78 °C and $BF_3{\cdot}Et_2O$ (0.6 mmol, 3 equiv.) was added. After 20 min., RMgBr (0.6 mmol, 3 equiv.) was added dropwise in about 1 min. After stirring for 16 h at −78 °C, $NaBH_4$ (1 mmol, 5 equiv.) was added and the reaction mixture was warmed up to RT. After stirring for 2 h, the resulting reaction mixture was quenched with saturated $NaHCO_3$ aqueous solution (2 mL) and stirred at RT for 1 h to hydrolyze the remaining $NaBH_4$. The mixture was extracted with CH_2Cl_2 (10 mL × 3). The combined organic phase was dried over $MgSO_4$, filtered and evaporated on rotary evaporator. The crude was purified by flash chromatography on the silica gel.

Specific experimental details and product characterization

1-acetyl-2-ethyl-1,2-dihydroquinoline (2a)



2a

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.21-6.98 (m, 4H, CH_{Ar}), 6.43 (d, J = 9.5 Hz, 1H, CHCH=C*H*), 6.11 (dd, J = 9.6, 5.8 Hz, 1H, CHC*H*=), 5.38-5.17 (m, 1H, CH=CHC*H*), 2.18 (s, 3H, COCH_3), 1.51-1.37 (m, 1H, CH_3C*H*H), 1.37-1.21 (m, 1H, CH_3CH*H*), 0.83 (t, J = 7.4 Hz, 3H, CH_2CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 170.2, 135.3, 132.5, 128.6, 127.0, 126.3, 125.4, 124.8, 124.3, 51.7, 25.3, 22.8, 9.9.

HRMS (ESI, m/Z): calcd. for $C_{13}H_{16}NO$ $[M+H]^+$: 202.1226, found: 202.1225.

HPLC: Chiracel-ODH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 234 nm. Retention time (min): 13.6 and 16.2.

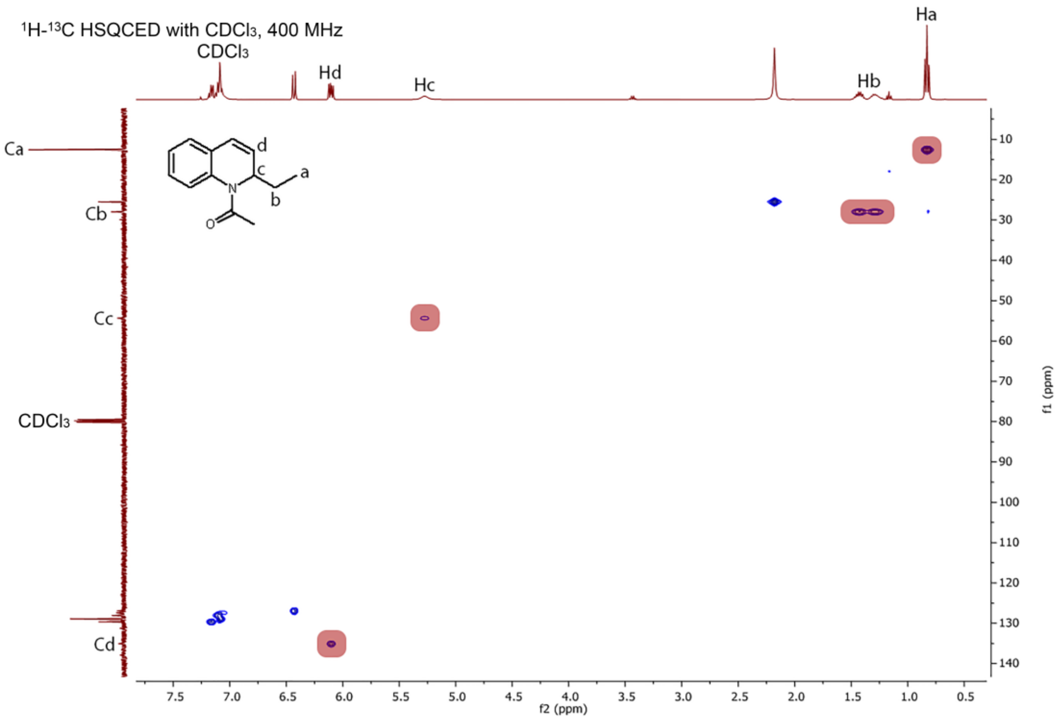


Figure S1. ^{1}H-^{13}C-HSQCED spectrum of product **2a**.

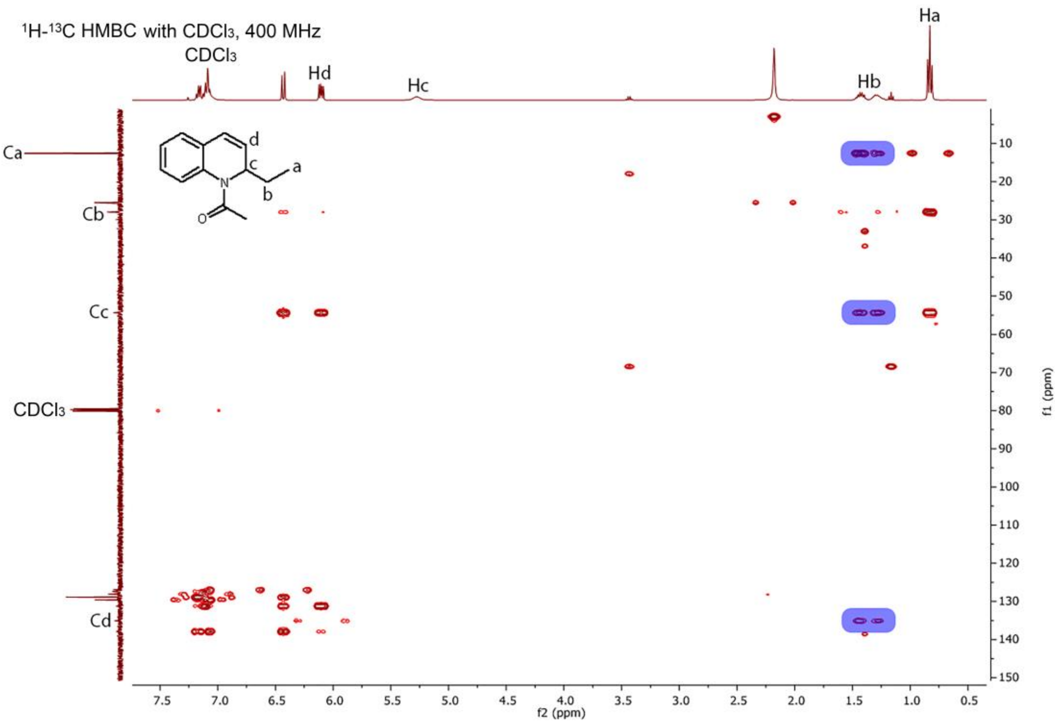
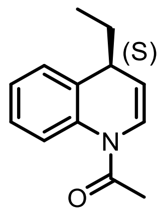


Figure S2. ^{1}H-^{13}C-HMBC spectrum of product **2a**. Correlations of Hb with Ca, Cc and Cd are highlighted. No correlation of Hb with any aromatic carbon was observed, proving that product **2a** is the C-2-addition product.

(*S*)-1-acetyl-4-ethyl-1,4-dihydroquinoline (3a)



3a

The reaction was performed with **1a** (24 μL, 0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3·Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 16 h, and following **General trapping procedure**. Product **3a** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 10:1) [99% conversion, 58% yield, >99% *ee*].

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.85 (d, *J* = 9.3 Hz, 1H, CH_{Ar}), 7.27-7.19 (m, 1H, CH_{Ar}), 7.19-7.08 (m, 2H, CH_{Ar}), 6.89 (d, *J* = 7.5 Hz, 1H, NC*H*=), 5.52 (dd, *J* = 7.5, 5.9 Hz, 1H, NCH=C*H*), 3.30-3.23 (m, 1H, CH=CHC*H*), 2.36 (s, 3H, $COCH_3$), 1.69-1.51 (m, 2H, CH_3CH_2), 0.88 (t, *J* = 7.4 Hz, 3H, CH_2CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.4, 136.8, 133.1, 128.3, 127.0, 126.0, 125.4, 123.0, 116.6, 39.9, 30.3, 24.2, 10.8.

HRMS (ESI, m/Z): calcd. for $C_{13}H_{16}NO$ $[M+H]^+$: 202.1226, found: 202.1224.

HPLC: Chiracel-ASH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 251 nm. Retention time (min): 11.1 (major) and 12.4 (minor).

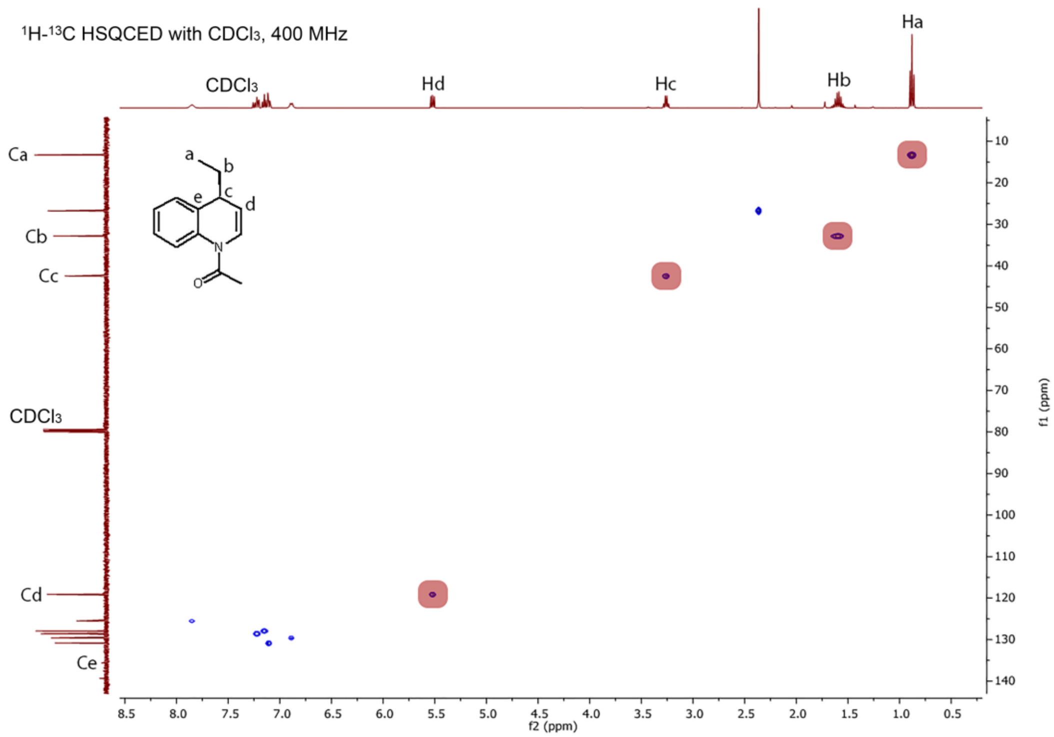


Figure S3. ^{1}H-^{13}C-HSQCED spectrum of product **3a**.

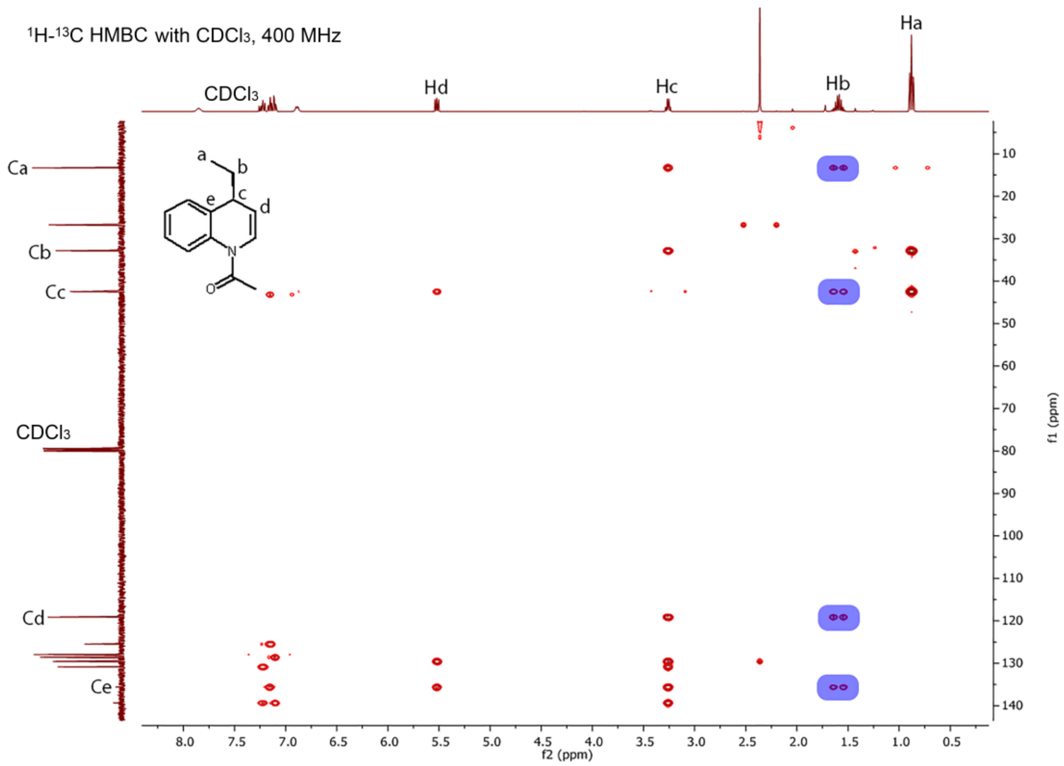
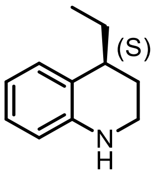


Figure S4. ^{1}H-^{13}C-HMBC spectrum of product **3a**. Correlations of Hb with Ca, Cc, Cd and Ce are highlighted. Hb correlates not only with Ca, Cc and Cd but also with the aromatic Ce, proving that product **3a** is the C-4-addition product.

(*S*)-4-Ethyl-1,2,3,4-tetrahydroquinoline (4a)[13]



4a

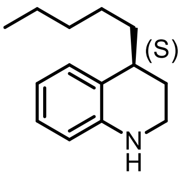
The reaction was performed with **1a** (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3{\cdot}Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **4a** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 20:1) [99% conversion, 83% yield, >99% *ee*].

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.07-7.03 (m, 1H, CH_{Ar}), 7.02-6.96 (m, 1H, CH_{Ar}), 6.68-6.61 (m, 1H, CH_{Ar}), 6.49 (dd, *J* = 8.0, 1.2 Hz, 1H, CH_{Ar}), 3.76 (bs, 1H, N*H*), 3.38-3.23 (m, 2H, $NHCH_2$), 2.72-2.63 (m, 1H, CH_3CH_2CH), 2.00-1.90 (m, 1H, CH_2), 1.89-1.71 (m, 2H, CH_2), 1.63-1.50 (m, 1H, CH_2), 1.01 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.3, 129.3, 126.9, 125.7, 116.8, 114.3, 38.6, 37.3, 29.4, 25.8, 11.8.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 247 nm. Retention time (min): 11.3 (major) and 12.8 (minor).

(*S*)-4-Pentyl-1,2,3,4-tetrahydroquinoline (4b)



4b

The reaction was performed with **1a** (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3{\cdot}Et_2O$ (0.4 mmol, 2 equiv.), PentMgBr (2 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **4b** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 30:1) [99% conversion, 96% yield, >99% *ee*].

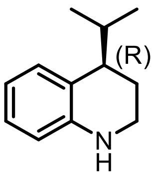
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.06-7.02 (m, 1H, CH_{Ar}), 7.01-6.95 (m, 1H, CH_{Ar}), 6.67-6.61 (m, 1H, CH_{Ar}), 6.49 (dd, *J* = 8.0, 1.2 Hz, 1H, CH_{Ar}), 3.82 (bs, 1H, N*H*), 3.34 (dt, *J* = 10.7, 3.6 Hz, 1H, NHCH*H*), 3.26 (dt, *J* = 11.1, 4.7 Hz, 1H, NHC*H*H), 2.80-2.71 (m, 1H, $NHCH_2CH_2CH$), 2.00-1.89 (m, 1H, CH_2), 1.87-1.78 (m, 1H, CH_2), 1.75-1.64 (m, 1H, CH_2), 1.60-1.27 (m, 7H, CH_2), 0.93 (t, *J* = 6.6 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.3, 129.2, 126.8, 125.9, 116.7, 114.2, 38.6, 36.8, 35.6, 32.2, 26.8, 26.2, 22.8, 14.3.

HRMS (ESI, m/Z): calcd. for $C_{14}H_{22}N$ $[M+H]^+$: 204.1747, found: 204.1746.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 247 nm. Retention time (min): 10.0 (major) and 11.1 (minor).

(*R*)-4-(1-methylethyl)-1,2,3,4-tetrahydroquinoline (4c)[14]



4c

The reaction was performed with **1a** (0.2 mmol, 1 equiv.), CuTc (0.02 mmol, 10 mol%), ligand (*R*,*R*)-**L1** (0.024 mmol, 12 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.), *i*PrMgBr (3 M in 2-Me-THF, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 16 h, and following **General reducing procedure**. Product **4c** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 30:1) [99% conversion, 82% yield, 80% *ee*].

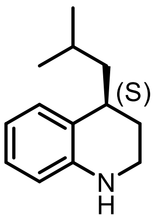
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.06-6.96 (m, 2H, CH_{Ar}), 6.66-6.60 (m, 1H, CH_{Ar}), 6.48 (d, *J* = 7.9 Hz, 1H, CH_{Ar}), 3.82 (bs, 1H, N*H*), 3.40-3.26 (m, 2H, $NHCH_2$), 2.60-2.53 (m, 1H, CH_3CHCH), 2.11-2.00 (m, 1H, CH_3CH), 2.00-1.90 (m, 1H, $NHCH_2CHH$), 1.88-1.77 (m, 1H, $NHCH_2CHH$), 1.01 (d, *J* = 6.8 Hz, 3H, CH_3), 0.90 (d, *J* = 6.8 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.7, 129.4, 126.8, 124.5, 116.3, 114.1, 42.3, 39.6, 30.5, 23.0, 21.6, 18.6.

HRMS (ESI, m/Z): calcd. for $C_{12}H_{18}N$ $[M+H]^+$: 176.1434, found: 176.1428.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 247 nm. Retention time (min): 10.2 (major) and 14.4 (minor).

(*S*)-4-(2-methylpropyl)-1,2,3,4-tetrahydroquinoline (4d)



4d

The reaction was performed with **1a** (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.), *i*BuMgBr (2 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **4d** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 30:1) [94% conversion, 72% yield, >99% *ee*].

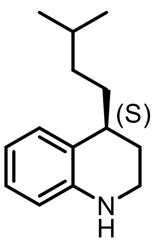
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.05-6.94 (m, 2H, CH_{Ar}), 6.66-6.60 (m, 1H, CH_{Ar}), 6.49 (dd, *J* = 8.0, 1.2 Hz, 1H, CH_{Ar}), 3.85 (bs, 1H, N*H*), 3.34 (dt, *J* = 10.9, 3.4 Hz, 1H, NHCH*H*), 3.26 (dt, *J* = 11.2, 4.6 Hz, 1H, NHC*H*H), 2.89-2.80 (m, 1H, $NHCH_2CH_2CH$), 2.00-1.88 (m, 1H, CH_2), 1.83-1.71 (m, 2H, CH_2), 1.55-1.41 (m, 2H, CH_2, CH_3CH), 1.02-0.95 (m, 6H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.3, 129.1, 126.8, 126.2, 116.8, 114.2, 46.5, 38.3, 33.1, 26.1, 24.9, 23.8, 22.1.

HRMS (ESI, m/Z): calcd. for $C_{13}H_{20}N$ $[M+H]^+$: 190.1590, found: 190.1585.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 247 nm. Retention time (min): 10.0 (major) and 11.7 (minor).

(*S*)-4-(3-methylbutyl)-1,2,3,4-tetrahydroquinoline (4e)



4e

The reaction was performed with **1a** (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.), *i*PentMgBr (2 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **4e** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 30:1) [99% conversion, 90% yield, >99% *ee*].

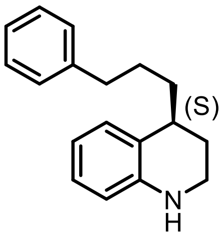
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.08-7.02 (m, 1H, CH_{Ar}), 7.02-6.96 (m, 1H, CH_{Ar}), 6.68-6.62 (m, 1H, CH_{Ar}), 6.49 (dd, *J* = 8.0, 1.2 Hz, 1H, CH_{Ar}), 3.85 (bs, 1H, N*H*), 3.34 (dt, *J* = 10.4, 5.5 Hz, 1H, NHCH*H*), 3.27 (td, *J* = 10.9, 4.7 Hz, 1H, NHC*H*H), 2.78-2.69 (m, 1H, $NHCH_2CH_2CH$), 2.00-1.89 (m, 1H, CH_2), 1.88-1.79 (m, 1H, CH_2), 1.77-1.66 (m, 1H, CH_2), 1.65-1.46 (m, 2H, CH_2, CH_3CH), 1.40-1.24 (m, 2H, CH_2), 0.96-0.90 (m, 6H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.3, 129.2, 126.8, 125.9, 116.8, 114.2, 38.5, 36.4, 35.9, 34.6, 28.4, 26.2, 23.1, 22.6.

HRMS (ESI, m/Z): calcd. for $C_{14}H_{22}N$ $[M+H]^+$: 204.1747, found: 204.1740.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 247 nm. Retention time (min): 9.8 (major) and 10.9 (minor).

(*S*)-4-(3-Phenylpropyl)-1,2,3,4-tetrahydroquinoline (4f)



4f

The reaction was performed with **1a** (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.), $Ph(CH_2)_3MgBr$ (2.6 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **4f** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 30:1) [99% conversion, 83% yield, >99% *ee*].

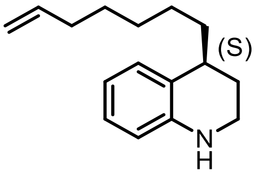
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.35-7.27 (m, 2H, CH_{Ar}), 7.25-7.18 (m, 3H, CH_{Ar}), 7.04-6.96 (m, 2H, CH_{Ar}), 6.67-6.60 (m, 1H, CH_{Ar}), 6.49 (d, *J* = 7.9 Hz, 1H, CH_{Ar}), 3.85 (bs, 1H, N*H*), 3.37-3.22 (m, 2H, NHCH_2), 2.84-2.75 (m, 1H, $NHCH_2CH_2CH$), 2.75-2.59 (m, 2H, PhCH_2), 2.01-1.90 (m, 1H, CH_2), 1.88-1.68 (m, 4H, CH_2), 1.67-1.53 (m, 1H, CH_2).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.3, 142.7, 129.2, 128.5, 128.4, 126.9, 125.8, 125.5, 116.8, 114.2, 38.5, 36.4, 36.2, 35.6, 29.1, 26.3.

HRMS (ESI, m/Z): calcd. for $C_{18}H_{22}N$ $[M+H]^+$: 252.1747, found: 252.1740.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 247 nm. Retention time (min): 18.3 (minor) and 22.4 (major).

(*S*)-4-(Hept-6-en-1-yl)-1,2,3,4-tetrahydroquinoline (4g)



4g

The reaction was performed with **1a** (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.), Hept-6-en-1-ylMgBr (1.4 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **4g** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 30:1) [99% conversion, 84% yield, >99% *ee*].

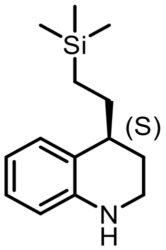
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.06-6.94 (m, 2H, CH_{Ar}), 6.67-6.59 (m, 1H, CH_{Ar}), 6.48 (d, *J* = 7.9 Hz, 1H, CH_{Ar}), 5.83 (ddt, *J* = 16.9, 10.1, 6.7 Hz, 1H, CH_2=C*H*), 5.07-4.92 (m, 2H, CH_2=), 3.85 (bs, 1H, N*H*), 3.34 (dt, *J* = 10.7, 3.6 Hz, 1H, NHCH*H*), 3.26 (dt, *J* = 10.9, 4.7 Hz, 1H, NHC*H*H), 2.80-2.69 (m, 1H, $NHCH_2CH_2$C*H*), 2.13-2.01 (m, 2H, CH_2), 2.00-1.88 (m, 1H, CH_2), 1.86-1.76 (m, 1H, CH_2), 1.75-1.64 (m, 1H, CH_2), 1.59-1.30 (m, 7H, CH_2).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.3, 139.3, 129.2, 126.8, 125.8, 116.7, 114.3, 114.2, 38.6, 36.8, 35.6, 33.9, 29.4, 29.1, 27.0, 26.3.

HRMS (ESI, m/Z): calcd. for $C_{16}H_{24}N$ $[M+H]^+$: 230.1903, found: 230.1895.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 247 nm. Retention time (min): 9.9 (major) and 11.1 (minor).

(*R*)-4-(2-Trimethylsilylethyl)-1,2,3,4-tetrahydroquinoline (4h)



4h

The reaction was performed with **1a** (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.), $Me_3Si(CH_2)_2MgBr$ (0.4 M in 2-Me-THF, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 16 h, and following **General reducing procedure**. Product **4h** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 40:1) [99% conversion, 67% yield, >99% *ee*].

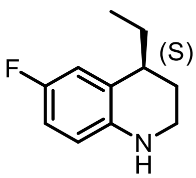
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.07-7.02 (m, 1H, CH_{Ar}), 7.02-6.95 (m, 1H, CH_{Ar}), 6.68-6.61 (m, 1H, CH_{Ar}), 6.53-6.47 (m, 1H, CH_{Ar}), 3.74 (bs, 1H, N*H*), 3.35-3.22 (m, 2H, $NHCH_2$), 2.72-2.62 (m, 1H, $NHCH_2CH_2CH$), 1.98-1.85 (m, 2H, CH_2), 1.77-1.64 (m, 1H, CH_2), 1.59-1.46 (m, 1H, CH_2), 0.67 (dt, *J* = 13.6, 4.4 Hz, 1H, SiCH*H*), 0.67 (ddd, *J* = 14.1, 12.6, 4.8 Hz, 1H, SiC*H*H), 0.01 (s, 9H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.4, 129.3, 126.9, 125.8, 116.8, 114.2, 38.5, 38.4, 30.9, 25.3, 13.9, −1.56.

HRMS (ESI, m/Z): calcd. for $C_{14}H_{24}NSi$ $[M+H]^+$: 234.1673, found: 234.1665.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 98:2, 0.5 mL/min., 40 °C, detection at 247 nm. Retention time (min): 9.7 (major) and 11.2 (minor).

(*S*)-4-Ethyl-6-fluoro-1,2,3,4-tetrahydroquinoline (5a)



5a

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (1.91 mg, 0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (6.08 mg, 0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (49 µL, 0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General**

reducing procedure. Product **5a** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 20:1) [99% conversion, 70% yield, >99% *ee*].

^1H NMR ($CDCl_3$, 400 MHz): δ 6.76 (dd, *J* = 9.8, 2.9 Hz, 1H, CH_{Ar}), 6.73-6.65 (m, 1H, CH_{Ar}), 6.40 (dd, *J* = 8.7, 4.9 Hz, 1H, CH_{Ar}), 3.74 (bs, 1H, N*H*), 3.33-3.19 (m, 2H, $NHCH_2$), 2.68-2.59 (m, 1H, CH_3CH_2CH), 1.96-1.86 (m, 1H, CH_2), 1.84-1.68 (m, 2H, CH_2), 1.61-1.47 (m, 1H, CH_2), 0.98 (t, *J* = 7.4 Hz, 3H, CH_3).

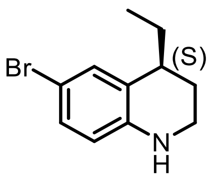
^{13}C NMR ($CDCl_3$, 400 MHz): δ 155.5 (d, *J* = 234.1 Hz), 140.6 (d, *J* = 1.9 Hz), 127.0 (d, *J* = 6.2 Hz), 115.3 (d, *J* = 21.7 Hz), 114.9 (d, *J* = 7.4 Hz), 113.4 (d, *J* = 22.4 Hz), 39.0, 37.4, 29.2, 25.8, 11.6.

^{19}F NMR ($CDCl_3$, 400 MHz): δ −128.2.

HRMS (ESI, m/Z): calcd. for $C_{11}H_{15}NF$ $[M+H]^+$: 180.1183, found: 180.1182.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 242 nm. Retention time (min): 12.7 (major) and 14.6 (minor).

(*S*)-6-Bromo-4-ethyl-1,2,3,4-tetrahydroquinoline (5b)



5b

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3·Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5b** was obtained as a white solid after column chromatography (SiO_2, pentane:Et_2O = 15:1) [99% conversion, 70% yield, >99% *ee*]. **5b** was dissolved in the mixed solvent of CH_2Cl_2 and pentane, and left for slow evaporation at RT in the air to afford the colorless single crystal.

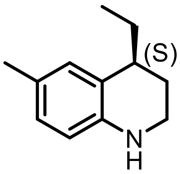
^1H NMR ($CDCl_3$, 400 MHz): δ 7.14-7.10 (m, 1H, CH_{Ar}), 7.03 (dd, *J* = 8.5, 2.3 Hz, 1H, CH_{Ar}), 6.37 (d, *J* = 8.5 Hz, 1H, CH_{Ar}), 3.87 (bs, 1H, N*H*), 3.35-3.20 (m, 2H, $NHCH_2$), 2.67-2.58 (m, 1H, CH_3CH_2CH), 1.94-1.66 (m, 3H, CH_2), 1.59-1.45 (m, 1H, CH_2), 1.61-1.47 (m, 1H, CH_2), 0.98 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.3, 131.6, 129.5, 127.5, 115.6, 108.1, 38.5, 37.3, 29.1, 25.3, 11.6.

HRMS (ESI, m/Z): calcd. for $C_{11}H_{15}NBr$ $[M+H]^+$: 240.0382, found: 240.0383.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 253 nm. Retention time (min): 13.4 (major) and 15.2 (minor).

(*S*)-4-Ethyl-6-methyl-1,2,3,4-tetrahydroquinoline (5c)



5c

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3{\cdot}Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5c** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 30:1) [98% conversion, 68% yield, 99% *ee*].

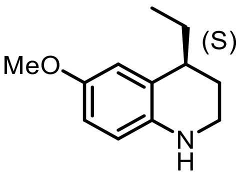
^1H NMR ($CDCl_3$, 400 MHz): δ 6.86 (d, *J* = 2.0 Hz, 1H, CH_{Ar}), 6.80 (dd, *J* = 8.1, 2.0 Hz, 1H, CH_{Ar}), 6.42 (d, *J* = 8.0 Hz, 1H, CH_{Ar}), 3.68 (bs, 1H, N*H*), 3.35-3.19 (m, 2H, $NHCH_2$), 2.68-2.58 (m, 1H, CH_3CH_2CH), 2.23 (s, 1H, $PhCH_3$), 1.98-1.88 (m, 1H, CH_2), 1.86-1.71 (m, 1H, CH_2), 1.61-1.48 (m, 1H, CH_2), 1.00 (t, *J* = 7.4 Hz, 3H, CH_2CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.0, 129.8, 127.4, 126.0, 125.9, 114.5, 38.8, 37.3, 29.5, 26.1, 20.7, 11.8.

HRMS (ESI, m/Z): calcd. for $C_{12}H_{18}N$ $[M+H]^+$: 176.1434, found: 176.1435.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 248 nm. Retention time (min): 10.4 (major) and 11.7 (minor).

(*S*)-4-Ethyl-6-methoxy-1,2,3,4-tetrahydroquinoline (5d)



5d

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5d** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 20:1) [92% conversion, 76% yield, >99% *ee*].

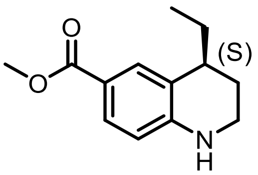
^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.66 (d, *J* = 2.9 Hz, 1H, CH_{Ar}), 6.61 (dd, *J* = 8.6, 2.9 Hz, 1H, CH_{Ar}), 6.46 (d, *J* = 8.6 Hz, 1H, CH_{Ar}), 3.74 (s, 1H, OCH_3), 3.47 (bs, 1H, N*H*), 3.34-3.16 (m, 2H, $NHCH_2$), 2.70-2.60 (m, 1H, CH_3CH_2CH), 1.98-1.88 (m, 2H, CH_2), 1.85-1.72 (m, 2H, CH_2), 1.63-1.49 (m, 1H, CH_2), 1.00 (t, *J* = 7.4 Hz, 3H, CH_2CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 152.2, 137.8, 127.7, 115.9, 114.9, 112.9, 56.0, 39.2, 37.4, 29.4, 26.0, 11.7.

HRMS (ESI, m/Z): calcd. for $C_{12}H_{18}NO$ $[M+H]^+$: 192.1383, found: 192.1383.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 245 nm. Retention time (min): 16.9 (major) and 18.5 (minor).

(*S*)-Methyl 4-ethyl-1,2,3,4-tetrahydroquinoline-6-carboxylate (5e)



5e

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.24 mmol, 1.2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5e** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 10:1) [98% conversion, 84% yield, 98% *ee*].

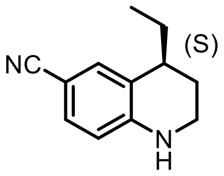
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.70 (d, *J* = 2.1 Hz, 1H, CH_{Ar}), 7.64 (dd, *J* = 8.4, 2.0 Hz, 1H, CH_{Ar}), 6.39 (d, *J* = 8.4 Hz, 1H, CH_{Ar}), 4.40 (bs, 1H, N*H*), 3.83 (s, 1H, OCH_3), 3.40-3.27 (m, 2H, $NHCH_2$), 2.70-2.62 (m, 1H, CH_3CH_2CH), 1.92-1.79 (m, 2H, CH_2), 1.77-1.68 (m, 1H, CH_2), 1.57-1.47 (m, 1H, CH_2), 0.98 (t, *J* = 7.4 Hz, 3H, CH_2CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.8, 148.4, 131.2, 129.2, 124.0, 117.2, 112.8, 51.5, 38.2, 37.2, 28.7, 25.0, 11.6.

HRMS (ESI, m/Z): calcd. for $C_{13}H_{18}NO_2$ $[M+H]^+$: 220.1332, found: 220.1331.

HPLC: Chiracel-OJH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 225 nm. Retention time (min): 24.7 (major) and 26.4 (minor).

(*S*)-6-Cyano-4-ethyl-1,2,3,4-tetrahydroquinoline (5f)



5f

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.) , EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5f** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 10:1) [99% conversion, 70% yield, 99% *ee*].

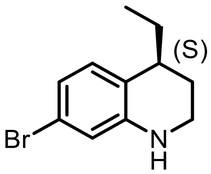
^1H NMR ($CDCl_3$, 400 MHz): δ 7.23 (d, *J* = 1.9 Hz, 1H, CH_{Ar}), 7.19 (dd, *J* = 8.3, 1.9 Hz, 1H, CH_{Ar}), 6.40 (d, *J* = 8.3 Hz, 1H, CH_{Ar}), 4.45 (bs, 1H, N*H*), 3.42-3.28 (m, 2H, $NHCH_2$), 2.67-2.57 (m, 1H, CH_3CH_2CH), 1.92-1.77 (m, 2H, CH_2), 1.72-1.59 (m, 1H, CH_2), 1.58-1.44 (m, 1H, CH_2), 0.97 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 147.8, 133.1, 131.2, 124.9, 121.1, 113.5, 97.5, 38.2, 37.1, 28.4, 24.7, 11.4.

HRMS (ESI, m/Z): calcd. for $C_{12}H_{15}N_2$ $[M+H]^+$: 187.1230, found: 187.1228.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 90:10, 0.5 mL/min., 40 °C, detection at 281 nm. Retention time (min): 18.9 (major) and 19.7 (minor).

(*S*)-7-Bromo-4-ethyl-1,2,3,4-tetrahydroquinoline (5g)



5g

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5g** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 20:1) [99% conversion, 77% yield, >99% *ee*].

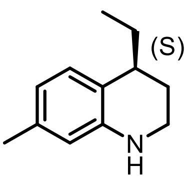
^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.85 (dd, *J* = 8.1, 0.8 Hz, 1H, CH_{Ar}), 6.70 (dd, *J* = 8.1, 2.0 Hz, 1H, CH_{Ar}), 6.60 (d, *J* = 1.9 Hz, 1H, CH_{Ar}), 3.90 (bs, 1H, N*H*), 3.35-3.21 (m, 2H, NHCH_2), 2.65-2.55 (m, 1H, CH_3CH_2CH), 1.93-1.76 (m, 2H, CH_2), 1.75-1.63 (m, 1H, CH_2), 1.58-1.45 (m, 1H, CH_2), 0.98 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.6, 130.6, 124.2, 120.1, 119.2, 116.3, 38.3, 37.0, 29.0, 25.4, 11.6.

HRMS (ESI, m/Z): calcd. for $C_{11}H_{15}NBr$ $[M+H]^+$: 240.0382, found: 240.0382.

HPLC: Chiracel-OBH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 250 nm. Retention time (min): 12.8 (major) and 15.2 (minor).

(*S*)-4-Ethyl-7-methyl-1,2,3,4-tetrahydroquinoline (5h)



5h

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5h** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 20:1) [96% conversion, 82% yield, >99% *ee*].

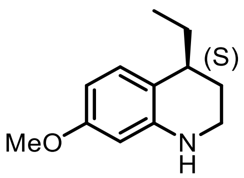
^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.94 (d, J = 7.7 Hz, 1H, CH_{Ar}), 6.50-6.44 (m, 1H, CH_{Ar}), 6.33 (s, 1H, CH_{Ar}), 3.76 (bs, 1H, N*H*), 3.37-3.19 (m, 2H, $NHCH_2$), 2.68-2.58 (m, 1H, CH_3CH_2CH), 2.23 (s, 3H, $PhCH_3$), 1.98-1.88 (m, 1H, CH_2), 1.86-1.69 (m, 2H, CH_2), 1.60-1.47 (m, 1H, CH_2), 1.00 (t, J = 7.4 Hz, 3H, CH_2CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.3, 136.5, 129.2, 122.9, 117.8, 114.8, 38.7, 37.0, 29.4, 26.1, 21.2, 11.8.

HRMS (ESI, m/Z): calcd. for $C_{12}H_{18}N$ $[M+H]^+$: 176.1434, found: 176.1433.

HPLC: Chiracel-OBH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 248 nm. Retention time (min): 10.7 (major) and 13.0 (minor).

(*S*)-4-Ethyl-7-methoxy-1,2,3,4-tetrahydroquinoline (5i)



5i

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3·Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5i** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 30:1) [98% conversion, 81% yield, >99% *ee*].

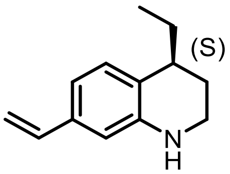
^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.94 (d, J = 8.3 Hz, 1H, CH_{Ar}), 6.23 (dd, J = 8.4, 2.5 Hz, 1H, CH_{Ar}), 6.05 (d, J = 2.5 Hz, 1H, CH_{Ar}), 3.85 (bs, 1H, N*H*), 3.74 (s, 3H, OCH_3), 3.36-3.20 (m, 2H, $NHCH_2$), 2.66-2.57 (m, 1H, CH_3CH_2CH), 1.98-1.86 (m, 1H, CH_2), 1.85-1.66 (m, 2H, CH_2), 1.59-1.45 (m, 1H, CH_2), 0.99 (t, J = 7.4 Hz, 3H, CH_2CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 158.8, 145.2, 129.9, 118.4, 102.7, 99.3, 55.2, 38.6, 36.6, 29.4, 26.1, 11.7.

HRMS (ESI, m/Z): calcd. for $C_{12}H_{18}NO$ $[M+H]^+$: 192.1383, found: 192.1381.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 245 nm. Retention time (min): 20.1 (minor) and 24.2 (major).

(*S*)-4-Ethyl-7-vinyl-1,2,3,4-tetrahydroquinoline (5j)



5j

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.24 mmol, 1.2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5j** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 50:1) [98% conversion, 60% yield, >99% *ee*].

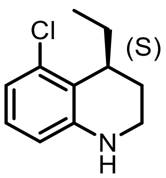
^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.99 (d, *J* = 7.8 Hz, 1H, CH_{Ar}), 6.71 (dd, *J* = 7.1, 1.6 Hz, 1H, CH_{Ar}), 6.60 (dd, *J* = 17.6, 10.9 Hz, 1H, CH_2=C*H*), 6.53 (d, *J* = 1.6 Hz, 1H, CH_{Ar}), 5.64 (dd, *J* = 17.6, 1.1 Hz, 1H, CH*H*=CH), 5.14 (dd, *J* = 10.9, 1.1 Hz, 1H, C*H*H=CH), 3.85 (bs, 1H, N*H*), 3.40-3.19 (m, 2H, NHCH_2), 2.71-2.61 (m, 1H, CH_3CH_2C*H*), 1.99-1.87 (m, 1H, CH_2), 1.87-1.68 (m, 2H, CH_2), 1.61-1.47 (m, 1H, CH_2), 0.99 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.4, 137.2, 136.4, 129.4, 125.6, 115.0, 112.7, 111.8, 38.7, 37.2, 29.3, 25.9, 11.7.

HRMS (ESI, m/Z): calcd. for $C_{13}H_{18}N$ $[M+H]^+$: 188.1434, found: 188.1432.

HPLC: Chiracel-OBH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 239 nm. Retention time (min): 15.9 (major) and 23.1 (minor).

(*S*)-5-Chloro-4-ethyl-1,2,3,4-tetrahydroquinoline (5k)



5k

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**.

Product **5k** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 20:1) [99% conversion, 77% yield, >99% *ee*].

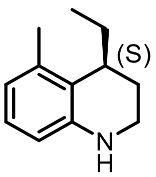
^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.92-6.84 (m, 1H, CH_{Ar}), 6.65 (dd, *J* = 7.9, 1.1 Hz, 1H, CH_{Ar}), 6.35 (dd, *J* = 8.1, 1.1 Hz, 1H, CH_{Ar}), 4.00 (bs, 1H, N*H*), 3.38-3.21 (m, 2H, NHCH_2), 3.02-2.93 (m, 1H, CH_3CH_2C*H*), 2.03-1.94 (m, 1H, CH_2), 1.85-1.68 (m, 2H, CH_2), 1.45-1.30 (m, 1H, CH_2), 1.02 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.2, 134.7, 127.3, 123.6, 117.4, 112.3, 36.8, 34.8, 27.0, 23.0, 11.8.

HRMS (ESI, m/Z): calcd. for $C_{11}H_{15}NCl$ $[M+H]^+$: 196.0888, found: 196.0887.

HPLC: Chiracel-OBH, *n*-heptane/*i*-PrOH 99:1, 0.5 mL/min., 40 °C, detection at 250 nm. Retention time (min): 11.9 (major) and 12.5 (minor).

(*S*)-4-Ethyl-5-methyl-1,2,3,4-tetrahydroquinoline (5l)



5l

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3\cdot Et_2O$ (0.6 mmol, 3 equiv.), EtMgBr (3 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 24 h, and following **General reducing procedure**. Product **5l** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 40:1) [95% conversion, 80% yield, 98% *ee*].

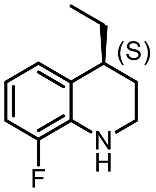
^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.92-6.86 (m, 1H, CH_{Ar}), 6.49 (d, *J* = 7.4, Hz, 1H, CH_{Ar}), 6.34 (d, *J* = 8.0 Hz, 1H, CH_{Ar}), 3.81 (bs, 1H, N*H*), 3.41-3.20 (m, 2H, NHCH_2), 2.79-2.70 (m, 1H, CH_3CH_2C*H*), 2.26 (s, 1H, PhCH_3), 2.01-1.94 (m, 1H, CH_2), 1.83-1.71 (m, 1H, CH_2), 1.68-1.55 (m, 1H, CH_2), 1.52-1.38 (m, 1H, CH_2), 1.02 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.7, 136.6, 126.5, 124.4, 118.9, 112.1, 36.8, 34.3, 27.2, 23.5, 18.9, 12.0.

HRMS (ESI, m/Z): calcd. for $C_{12}H_{18}N$ $[M+H]^+$: 176.1434, found: 176.1434.

HPLC: Chiracel-OJH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 248 nm. Retention time (min): 11.1 (major) and 12.8 (minor).

(*S*)-4-Ethyl-8-fluoro-1,2,3,4-tetrahydroquinoline (5m)



5m

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3{\cdot}Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5m** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 20:1) [92% conversion, 76% yield, >99% *ee*].

^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.85-6.77 (m, 2H, CH_{Ar}), 6.57-6.49 (m, 1H, CH_{Ar}), 6.34 (d, *J* = 8.0 Hz, 1H, CH_{Ar}), 4.05 (bs, 1H, N*H*), 3.40-3.29 (m, 2H, NHCH_2), 2.75-2.65 (m, 1H, CH_3CH_2C*H*), 2.00-1.81 (m, 2H, CH_2), 1.81-1.68 (m, 1H, CH_2), 1.63-1.48 (m, 1H, CH_2), 1.00 (t, *J* = 7.4 Hz, 3H, CH_3).

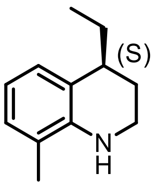
^{13}C NMR ($CDCl_3$, 100 MHz): δ 151.0 (d, *J* = 237.2 Hz), 132.8 (d, *J* = 11.9 Hz), 127.8 (d, *J* = 3.3 Hz), 124.2 (d, *J* = 2.8 Hz), 115.2 (d, *J* = 7.4 Hz), 112.1 (d, *J* = 18.2 Hz), 37.9, 37.0 (d, *J* = 2.7 Hz), 29.2, 25.5, 11.7.

^{19}F NMR ($CDCl_3$, 400 MHz): δ −138.9.

HRMS (ESI, m/Z): calcd. for $C_{11}H_{15}NF$ $[M+H]^+$: 180.1183, found: 180.1182.

HPLC: Chiracel-ODH, *n*-heptane/*i*-PrOH 98:2, 0.5 mL/min., 40 °C, detection at 243 nm. Retention time (min): 10.9 (minor) and 11.7 (major).

(*S*)-4-Ethyl-8-methyl-1,2,3,4-tetrahydroquinoline (5n)



5n

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.6 mmol, 3 equiv.), EtMgBr (3 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5n** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 80:1) [99% conversion, C-2-addition:C-4-addition = 1:5, 73% yield, >99% *ee*].

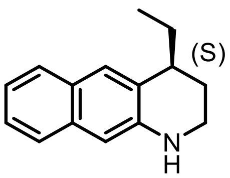
^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.94 (d, *J* = 7.6 Hz, 1H, CH_{Ar}), 6.90 (d, *J* = 7.3 Hz, 1H, CH_{Ar}), 6.90 (d, *J* = 7.3 Hz, 1H, CH_{Ar}), 3.67 (bs, 1H, N*H*), 3.44-3.31 (m, 2H, $NHCH_2$), 2.74-2.64 (m, 1H, CH_3CH_2CH), 2.09 (s, 3H, $PhCH_3$), 1.99-1.70 (m, 3H, CH_2), 1.62-1.49 (m, 1H, CH_2), 1.00 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.3, 128.0, 127.3, 125.1, 121.1, 116.1, 38.8, 37.5, 29.6, 25.6, 17.5, 11.9.

HRMS (ESI, m/Z): calcd. for $C_{12}H_{18}N$ $[M+H]^+$: 176.1434, found: 176.1433.

HPLC: Chiracel-ODH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 244 nm. Retention time (min): 9.6 (major) and 11.1 (minor).

(*S*)-4-Ethyl-1,2,3,4-tetrahydrobenzo[*g*]quinoline (5o)



5o

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3 \cdot Et_2O$ (0.6 mmol, 3 equiv.), EtMgBr (3 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5o** was obtained as a white solid after column chromatography (SiO_2, pentane:Et_2O = 40:1) [96% conversion, 66% yield, 97% *ee*].

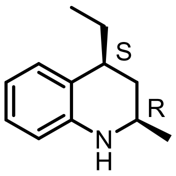
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62 (d, *J* = 8.1 Hz, 1H, CH_{Ar}), 7.54-7.46 (m, 2H, CH_{Ar}), 7.32-7.24 (m, 1H, CH_{Ar}), 7.17-7.10 (m, 1H, CH_{Ar}), 6.75 (s, 1H, CH_{Ar}), 4.17 (bs, 1H, N*H*), 3.47 – 3.32 (m, 2H, $NHCH_2$), 2.91-2.82 (m, 1H, CH_3CH_2CH), 2.08-1.96 (m, 1H, CH_2), 1.95-1.78 (m, 2H, CH_2), 1.74-1.60 (m, 1H, CH_2), 1.04 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.3, 134.0, 128.9, 127.4, 127.4, 127.2, 125.5, 124.9, 121.4, 38.8, 38.0, 28.6, 26.0, 11.7.

HRMS (ESI, m/Z): calcd. for $C_{15}H_{18}N$ $[M+H]^+$: 212.1434, found: 212.1433.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 247 nm. Retention time (min): 17.4 (major) and 20.9 (minor).

(2*R*,4*S*)-4-Ethyl-2-methyl-1,2,3,4-tetrahydroquinoline (5p)



5p

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3{\cdot}Et_2O$ (0.4 mmol, 2 equiv.), EtMgBr (3 M in Et_2O, 0.4 mmol, 2 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5p** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 30:1) [98% conversion, 79% yield, 6:1 *dr*, 99% *ee*].

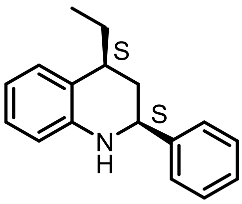
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.16 (dd, *J* = 7.7, 1.4 Hz, 1H, CH_{Ar}), 7.04-6.95 (m, 1H, CH_{Ar}), 6.72-6.60 (m, 1H, CH_{Ar}), 6.50 (d, *J* = 8.1 Hz, 1H, CH_{Ar}), 3.67 (bs, 1H, N*H*), 3.52-3.38 (m, 1H, NHC*H*), 2.93-2.82 (major) and 2.66-2.57 (minor) (m, 1H, CH_2), 2.11-1.97 (major) and 1.89-1.82 (minor) and 1.76-1.65 (minor) (m, 2H, CH_2), 1.65-1.50 (m, 1H, CH_2), 1.41-1.27 (m, 1H, CH_2), 1.23 (d, *J* = 6.2 Hz, 3H, CHCH_3), 1.05-0.94 (m, 3H, CH_2CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): Major: δ 145.6, 127.1, 126.7, 125.2, 117.5, 114.4, 47.5, 36.8, 36.7, 27.1, 23.0, 10.7. Minor: δ 144.2, 129.7, 126.9, 125.4, 116.6, 113.9, 42.6, 37.9, 33.7, 31.0, 23.0, 12.1.

HRMS (ESI, m/Z): calcd. for $C_{12}H_{18}N$ $[M+H]^+$: 176.1434, found: 176.1433.

HPLC: Chiracel-ODH, *n*-heptane/*i*-PrOH 98:2, 0.5 mL/min., 40 °C, detection at 254 nm. Retention time of major disastereomer (min): 12.1 (major) and 12.7 (minor), retention time of minor disastereomer (min): 10.3 (minor) and 11.6 (major).

(2*S*,4*S*)-4-ethyl-2-phenyl-1,2,3,4-tetrahydroquinoline (5q)



5q

The reaction was performed with the substrate (0.2 mmol, 1 equiv.), CuTc (0.01 mmol, 5 mol%), ligand (*R*,*R*)-**L1** (0.012 mmol, 6 mol%), $BF_3{\cdot}Et_2O$ (0.6 mmol, 3 equiv.), EtMgBr (3 M in Et_2O, 0.6 mmol, 3 equiv.), CH_2Cl_2 (2.0 mL) at −78 °C for 2 h, and following **General reducing procedure**. Product **5q** was obtained as a colorless oil after column chromatography (SiO_2, pentane:Et_2O = 70:1) [95% conversion, 84% yield, 6:1 *dr*, 86% *ee*]. The relative configuration of **5q** was determined by NOE experiments after transforming to **5t** (see Figure S5).

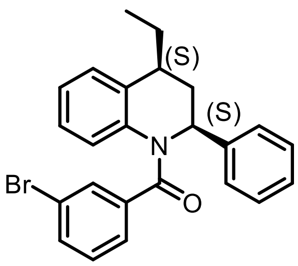
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.50-7.30 (m, 5H, CH_{Ar}), 7.28-7.20 (m, 1H, CH_{Ar}), 7.11-7.00 (m, 1H, CH_{Ar}), 6.78-6.67 (m, 1H, CH_{Ar}), 6.56 (dd, *J* = 7.9, 1.2 Hz, 1H, CH_{Ar}), 4.50-4.42 (m, 1H, NHC*H*), 4.07 (minor) and 3.97 (major) (bs, 1H, N*H*), 3.10-2.99 (major) and 2.73-2.65 (minor) (m, 1H, CH_2), 2.26-1.92 (m, 2H, CH_2), 1.88-1.69 (m, 1H, CH_2), 1.69-1.53 (m, 1H, CH_2), 1.06 and 0.98 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): Major: δ 145.6, 144.8, 128.8, 127.7, 127.2, 126.9, 126.8, 125.1, 117.8, 114.6, 57.2, 38.0, 37.4, 27.0, 10.8. Minor: δ 145.0, 144.1, 129.6, 128.7, 127.6, 127.1, 126.8, 125.2, 52.4, 37.9, 34.9, 30.7, 12.0.

HRMS (ESI, m/Z): calcd. for $C_{17}H_{20}N$ $[M+H]^+$: 238.1590, found: 238.1590.

HPLC: Chiracel-ADH, *n*-heptane/*i*-PrOH 95:5, 0.5 mL/min., 40 °C, detection at 207 nm. Retention time of major disastereomer (min): 10.5 (minor) and 11.1 (major), retention time of minor disastereomer (min): 8.9 (major) and 12.9 (minor).

(2*S*,4*S*)-1-(3-Bromophenyl)carbonyl-4-ethyl-2-phenyl-1,2,3,4-tetrahydroquinoline (5t)



5t

The reactions were performed according to the literature procedure.[14] To a solution of **5q** (75 mg, 0.316 mmol, 1 equiv.) in dry CH_2Cl_2 (2 ml) was added benzoyl chloride (54 μL, 0.411 mmol, 1.3 equiv.) dropwise, followed by DMAP (1.9 mg, 0.016 mmol, 5 mol%) and triethylamine (57 μL, 0.411 mmol, 1.3 equiv.). The reaction mixture was stirred at RT overnight. Then it is quenched with water and extracted with CH_2Cl_2 for three times. The combined organic phases were washed with brine, dried over $MgSO_4$, and concentrated in vacuo to give the crude product. The major diastereomer of **5t** was obtained as a white solid after column chromatography (SiO_2, pentane:Et_2O = 20:1) followed by recrystallization in the mixed solvent of CH_2Cl_2 and pentane. Relative configuration was determined by NOE experiments (see Figure S5).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.35-7.31 (m, 2H, CH_{Ar}), 7.26-7.22 (m, 1H, CH_{Ar}), 7.22-7.17 (m, 2H, CH_{Ar}), 7.15-7.08 (m, 4H, CH_{Ar}), 6.95-6.87 (m, 3H, CH_{Ar}), 6.55 (d, *J* = 7.1 Hz, 1H, CH_{Ar}), 5.56 (t, *J* = 9.5 Hz, 1H, NHC*H*), 2.27 (ddd, *J* = 12.6, 8.8, 3.3 Hz, 1H, NHCHCH*H*), 2.65-1.58 (m, 1H, CH_3CH_2C*H*), 2.19-2.10 (m, 1H, NHCHC*H*H), 1.59-1.48 (m, 1H, CH_3CH*H*), 1.38-1.29 (m, 1H, CH_3C*H*H), 1.10 (t, *J* = 7.4 Hz, 3H, CH_3).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.1, 144.1, 139.2, 139.0, 138.1, 133.0, 132.1, 129.3, 128.7, 127.2, 127.1, 127.1, 126.5, 126.4, 125.9, 123.7, 122.1, 58.6, 40.9, 37.3, 23.3, 11.8.

HRMS (ESI, m/Z): calcd. for $C_{24}H_{22}NOBr$ $[M+H]^+$: 420.0958, found: 420.0962.

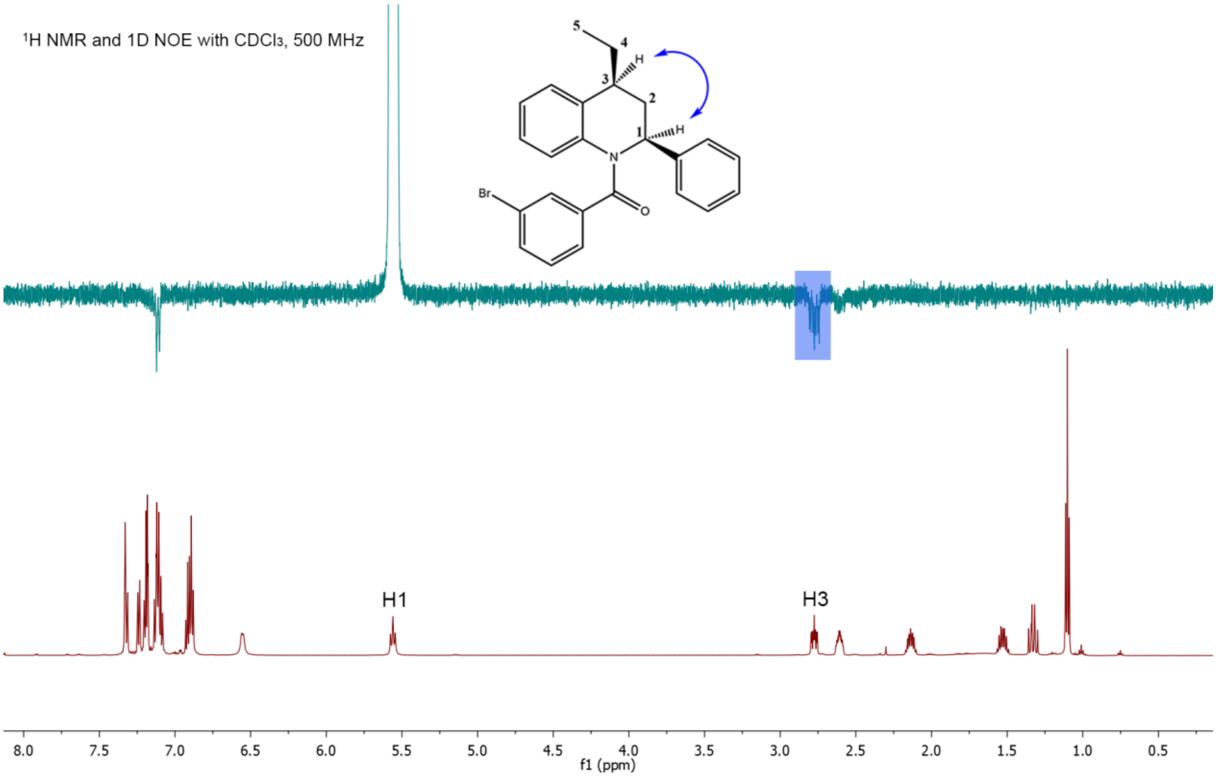


Figure S5. ^{1}H NMR and 1D NOE experiment of **5t**. Selective irradiation on H-1 showed NOE with H-3 (highlighted) which are positioned on the same side of the ring.

7. Determination of absolute configuration

The absolute configuration of **5b** was determined by X-ray single crystallography (see Figure S6), and the relative configuration of **5q** and **5t** was determined by NOE experiment (see Figure S5). The absolute configurations of other compounds were assigned by analogy.

8. X-ray crystallographic analysis

A single crystal of compound **5b** was mounted on top of a cryoloop and transferred into the cold nitrogen stream (100 K) of a Bruker-AXS D8 Venture diffractometer. Data collection and reduction was done using the Bruker software suite APEX3.[15] The final unit cell was obtained from the xyz centroids of 7072 reflections after integration. A multiscan absorption correction was applied, based on the intensities of symmetry-related reflections measured at different angular settings (SADABS). The structures were solved by direct methods using SHELXT[16] and refinement of the structure was performed using SHLELXL.[17] The hydrogen atoms were generated by geometrical considerations, constrained to idealized geometries and allowed to ride on their carrier atoms with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms. The absolute configuration of the model was chosen based on anomalous dispersion. Refinement of the Flack x parameter converged 0.040(12).

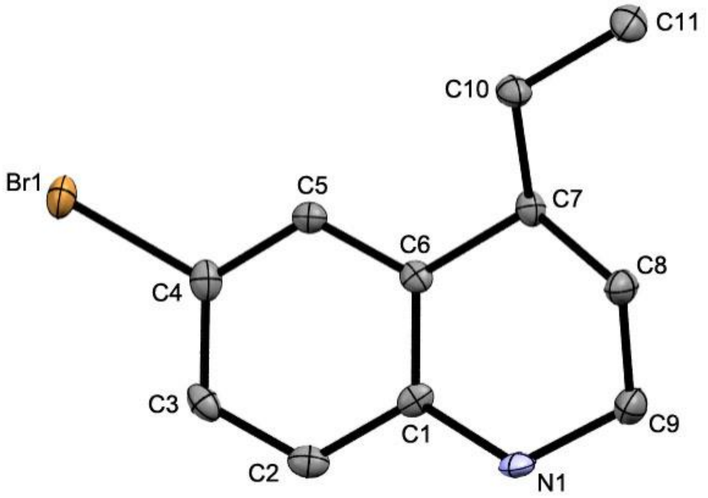


Figure S6. Molecular structure of compound **5b**, showing 50% probability ellipsoids. Hydrogen atoms are omitted for clarity.

Table S6. Crystallographic data for compound **5b**

chem. formula	$C_{11}H_{14}BrN$
M_r	240.14
cryst syst.	Monoclinic
color, habit	Orange, platelet
size (mm)	0.42 × 0.10 0.03
space group	P 21
a (Å)	8.8938(3)
b (Å)	5.9958(2)
c (Å)	9.5190(3)
α, deg	90
β, deg	94.8830(10)
γ, deg	90
V (Å^3)	505.76(3)
Z	2
ρ_{calc}, g·cm^{-3}	1.577
μ(Mo Kα), cm^{-1}	5.129
F(000)	244
temp (K)	100(2)
θ range (deg)	4.662 – 65.118
data collected (h,k,l)	-10:10, -6:7, -11:10
no. of rflns collected	6932
no. of indpndt reflns	1702
observed reflns	1689 ($F_o \geq 2(F_o)$)

R(F) (%)	1.74
$wR(F^2)$ (%)	4.21
GooF	1.076
Weighting a,b	0.0238, 0.0615
params refined	123
restraints	1
min, max resid dens	-0.552, 0.193
Flack x	0.040(12)

9. Mechanistic studies

DFT study of the copper catalyzed addition of EtMgBr·2Et$_2$O to 1a and 1a·BF$_3$

To unravel the mechanism behind the presented copper catalyzed nucleophilic addition of Grignard reagents to quinolines, we first explored the blank reaction, *i.e.* the direct addition of the Grignard reagent to the quinoline. We have found that – in line with the experimental evidence- this direct addition reaction (independently of the considered regioselectivity) is not accessible at the working temperature ($\Delta G^{\neq}_{C\text{-}2\text{-addition}}$ = 23.00 kcal/mol, $\Delta G^{\neq}_{C\text{-}4\text{-addition}}$= 41.44 kcal/mol), see Figure S7. If the LA is added to the reaction media , it will bind to the nitrogen atom decreasing the electron density of the quinoline (the charge at C-2 changes from 0.33 a.u. to 0.24 a.u. and the charge at C-4 changes from 0.44 a.u. to 0.43 a.u.) and facilitate a subsequent addition of the Grignard reagent, both at C-2 and C-4; the latter is energetically less penalized, in agreement with the experimental data presented in the manuscript.

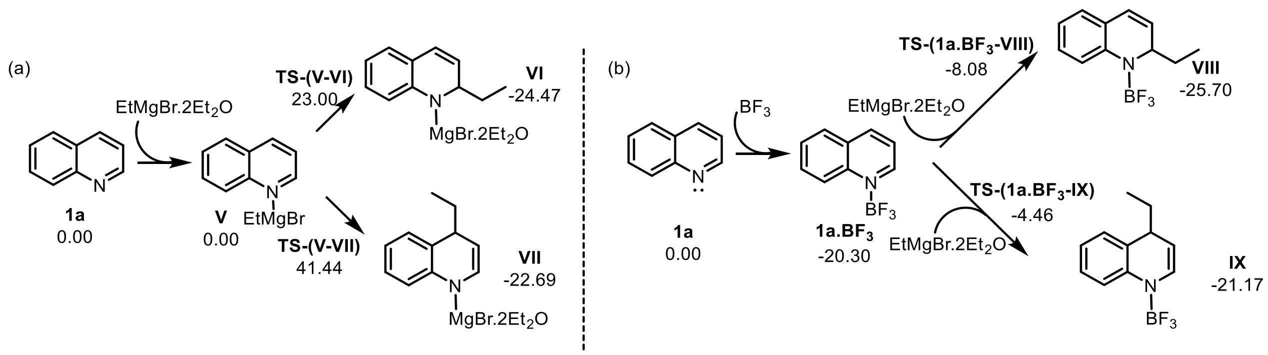


Figure S7. Computed mechanism for the (a) addition of EtMgBr·2Et$_2$O to 1a. (b) addition of EtMgBr·2Et$_2$O to the LA activated quinoline (**1a**·BF$_3$). Calculations were performed at the PCM (CH_2Cl_2)/M06/def2svpp computational level using the Gaussian 09 program. The thermochemistry was obtained at 1 atm and 195 K. Short names have been used, but all the presented systems contain two Et$_2$O molecules except for BF$_3$ and quinoline, this information is omitted for clarity.

Table S7. Summary of the energies for the study of the blank reaction and the blank reaction with BF_3 in the addition of the Grignard reagent to quinoline

ID	ImFreqs	Stable	SCF[a]	SCF+ZPVE	H[b]	G[c]
1a	−	Yes	−401.3167684	−401.181547	−401.17791	−401.200117
V	−	Yes	−3720.911052	−3720.435202	−3720.419991	−3720.468347
TS-(V-VI)	−404.649	Yes	−3720.876478	−3720.400663	−3720.386453	−3720.431694
VI	−	Yes	-3487.268379	-3487.258404	-3487.257786	-3487.296207
TS-(V-VII)	−412.972	Yes	−3720.847843	−3720.371393	−3720.357214	−3720.402308
VII	−	Yes	−3720.94771	−3720.469152	−3720.454362	−3720.502078
BF_3	−	Yes	−324.2164826	−324.203888	−324.201265	−324.219811
1a·BF_3	−	Yes	−725.5809442	−725.430379	−725.424745	−725.452271
TS-(1a·BF_3-VIII)	−381.532	Yes	−4045.14233	−4044.650201	−4044.634257	−4044.682723
VIII	−	Yes	−4045.22728	−4044.733319	−4044.71804	−4044.765589
TS-(1a·BF_3-IX)	−510.418	Yes	−4045.135857	−4044.643974	−4044.62797	−4044.676943
IX	−	Yes	−3811.900283	−3811.542546	−3811.530313	−3811.57177

[a]Energies are expressed in a.u. and the imaginary frequencies in cm^{-1}. [b]H represents enthalpies. [c]G Represents Gibbs free Energies.

At this point, we wondered whether copper could also behave as a LA and compete with the BF_3 for binding tothe nitrogen atom of **1a**, or if the BF_3 could be engaged in the coordination of any other species present in the reaction. Thus, we performed a systematic exploration of all the potential coordination of BF_3 and **L1-CuBr** with **1a** (Figure S8). This study reveals that even **L1-CuBr** can behave as a LA and coordinate the quinoline, as expected BF_3 leads to a more thermodynamically stable speciesthus displacing the copper in case complex **X** or **XI** were formed in solution. We also explored potential coordination of BF_3 with the **L1** We have found that even BF_3can coordinate **L1**, this coordination leads to a complex that is thermodynamically less stable than that resulting from its coordination to the **1a** (**1a·BF_3**) or that resulting from the coordination of **L1** with the copper source, as we detailed below (Figure S8). This is also in agreement with the NMR studies (Figures S15-16).

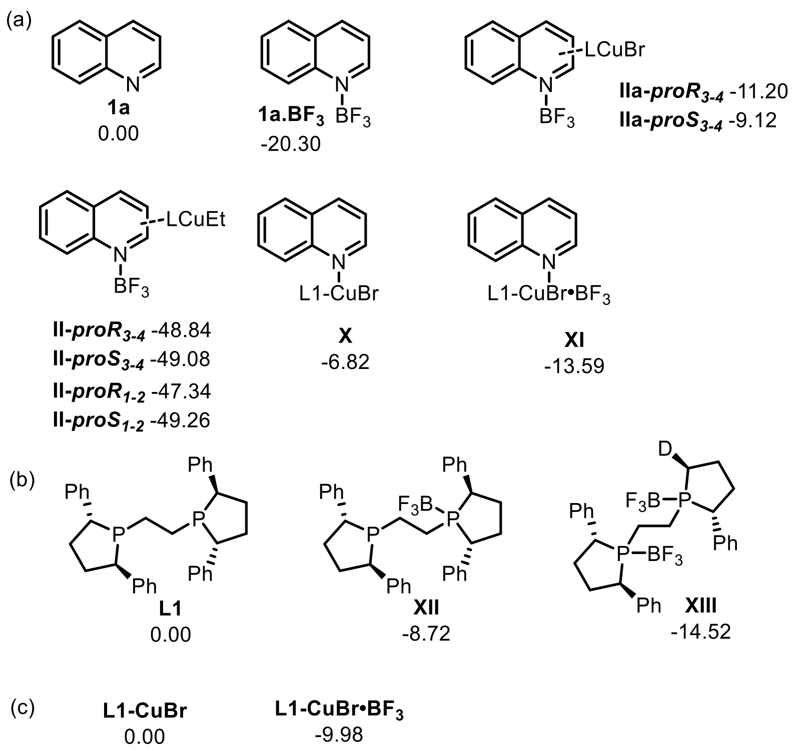


Figure S8. Computed relative stability of the coordination of BF_3 to the different species participating in the reaction. Calculations were performed at the PCM (CH_2Cl_2)/M06/def2svpp computational level using the Gaussian 09 program. The thermochemistry was obtained at 1 atm and 195 K.

Table S8. Summary of the energies for the study of the interaction of BF_3 with the different components of the catalytic system presented. All calculations were performed with the (*R*,*R*)-**L1** ligand.

ID	ImFreqs	Stable	SCF[a]	SCF+ZPVE	H[b]	G[c]
1a	–	Yes	−401.3167684	−401.181547	−401.17791	−401.200117
1a·BF$_3$	–	Yes	−725.5809442	−725.430379	−725.424745	−725.452271
IIa-*proR*$_{3-4}$	–	Yes	−6937.441863	−6936.68338	−6936.660362	−6936.72743
IIa-*proS*$_{3-4}$	–	Yes	−6937.438924	−6936.680365	−6936.657475	−6936.724125
II-*proR*$_{3-4}$	–	Yes	−4442.685582	−4441.864414	−4441.841144	−4441.907423
II-*proS*$_{3-4}$	–	Yes	−4442.684883	−4441.863422	−4441.840268	−4441.906948
II-*proR*$_{1-2}$	–	Yes	−4442.682289	−4441.86133	−4441.810951	−4441.945899
II-*proS*$_{1-2}$	–	Yes	−4442.683702	−4441.863418	−4441.812692	−4441.948965
X	–	Yes	−6613.203409	−6612.459973	−6612.439187	−6612.500643
XI	–	Yes	−6937.445992	−6936.688835	−6936.666203	−6936.731244
L1	–	Yes	−1997.721791	−1997.11694	−1997.101947	−1997.151917
XII	–	Yes	−2321.967603	−2321.348094	−2321.330934	−2321.385628
XIII	–	Yes	−2646.21189	−2645.57695	−2645.558094	−2645.61468
L1-CuBr	–	Yes	−6211.843657	−6211.236732	−6211.219631	−6211.274031
L1-CuBr·BF$_3$	–	Yes	−6536.091876	−6535.470998	−6535.451685	−6535.50974

[a]Energies are expressed in a.u. and the imaginary frequencies in cm^{-1}. [b]H represents enthalpies. [c]G Represents Gibbs free Energies.

Once we have identified the role of the LA as well as its preferred disposition in the system, we moved to the study of the speciation of the copper source in the reaction. With this goal and taking into consideration that copper(I) is known for forming dimeric species and other aggregates in solution, we performed a systematic analysis on the relative stability of some of the copper species that might be present in the reaction media (Figure S9).

We have found that once the copper source interacts with **L1** it evolves towards the formation of the complex **L1-CuBr** (ΔG=−20.91 kcal/mol). This complex can further progress towards the formation of dimeric species and even transmetalate in the presence of the Grignard reagent (Figure S9). The formation of dimeric species is energetically favourable, nonetheless we have disregarded them as potential catalyst for two reasons: a) the dilution degree in which the copper species is present in the reaction media and b) when the dimeric species are allowed to interact with the organic substrate they break towards their monomeric constituents.

The **L1-CuBr** complex can alternatively evolve through a direct transmetalation leading to **L1-CuEt**, or **I**, this species is not only thermodynamically preferred (−32.70 kcal/mol) but also key for the evolution of the catalysed reaction, as we present in the main text.

Next we explored the possibility of species **I** further interacting with the Grignard reagent via a second transmetallation resulting in the formation of a cuprate species. We have found that the formation of cuprates is highly endergonic and consequently unfeasible in the working conditions used in this protocol.

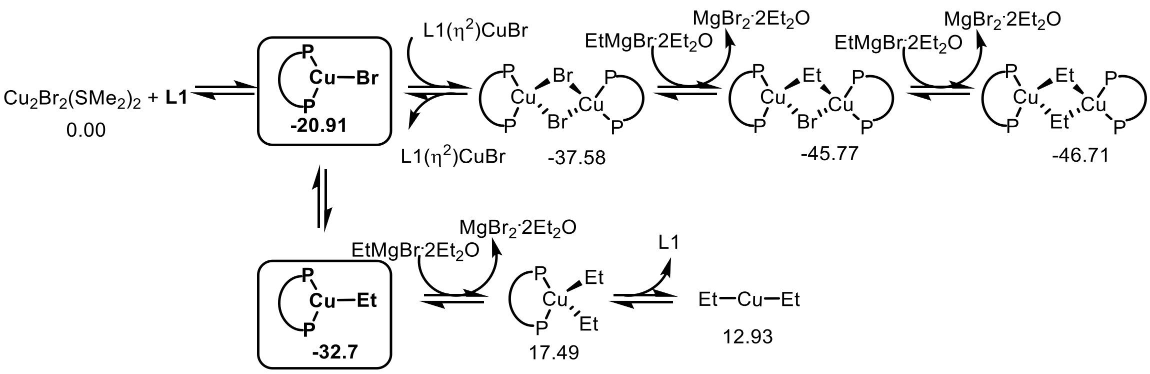


Figure S9. Computed relative energies for the potential copper species present in the reaction media. The calculations were performed at the PCM(CH_2Cl_2)/M06/def2svpp computational level using the Gaussian 09 program. The thermochemistry was obtained at 1 atm and 195 K. **L1** has been represented as a curved line to clarify that it behaves as a chelating agent.

Table S9. Summary of the energies for the study of the copper speciation in solution.

ID	Im. Freqs.	Stable	SCF[a]	SCF+ZPVE	H[b]	G[c]
Cu_2Br_2·(SMe_2)$_2$	–	Yes	−9383.671745	−9383.517717	−9383.506351	−9383.548312
L1-CuBr	–	Yes	−6211.843657	−6211.236732	−6211.219631	−6211.274031
L1$_2$Cu$_2$Br$_2$	–	Yes	−12423.732710	−12422.517483	−12422.483079	−12422.574618
L1$_2$Cu$_2$BrEt	–	Yes	−9928.977519	−9927.699335	−9927.664871	−9927.754807
L1$_2$Cu$_2$Et$_2$	–	Yes	−7434.206748	−7432.867065	−7432.831901	−7432.923431
L1-CuEt	–	Yes	−3717.080114	−3716.411863	−3716.393885	−3716.450532
L1-CuEt$_2$	–	Yes	−3796.216569	−3795.485075	−3795.465794	−3795.523754
CuEt$_2$	–	Yes	−1798.483889	−1798.359603	−1798.354567	−1798.379112

[a]Energies are expressed in a.u. and the imaginary frequencies in cm^{-1}. [b]H represents enthalpies. [c]G Represents Gibbs free Energies.

We then proceed with the exploration of the copper(I) catalysed reaction of the quinoline with the Grignard in the presence of the BF_3 as a LA, as described in the main text.

During the mechanistic exploration we also explored the potential evolution of **II$_{3-4}$** through a C-2-addition. Unfortunately, all our attempts to locate the transition state connecting **II$_{3-4}$** and **III$_{1-2}$** were unfruitful. In order to provide an estimation for the energy of **TS-(II$_{3-4}$-III)-*R*$_{1-2}$** and **TS-(II$_{3-4}$-III)-*S*$_{1-2}$,** we explored the potential energy surface via a scan of the electronic energy variation with the elongation of the bond C-2-Et at **III$_{1-2}$** (see Figure S10).

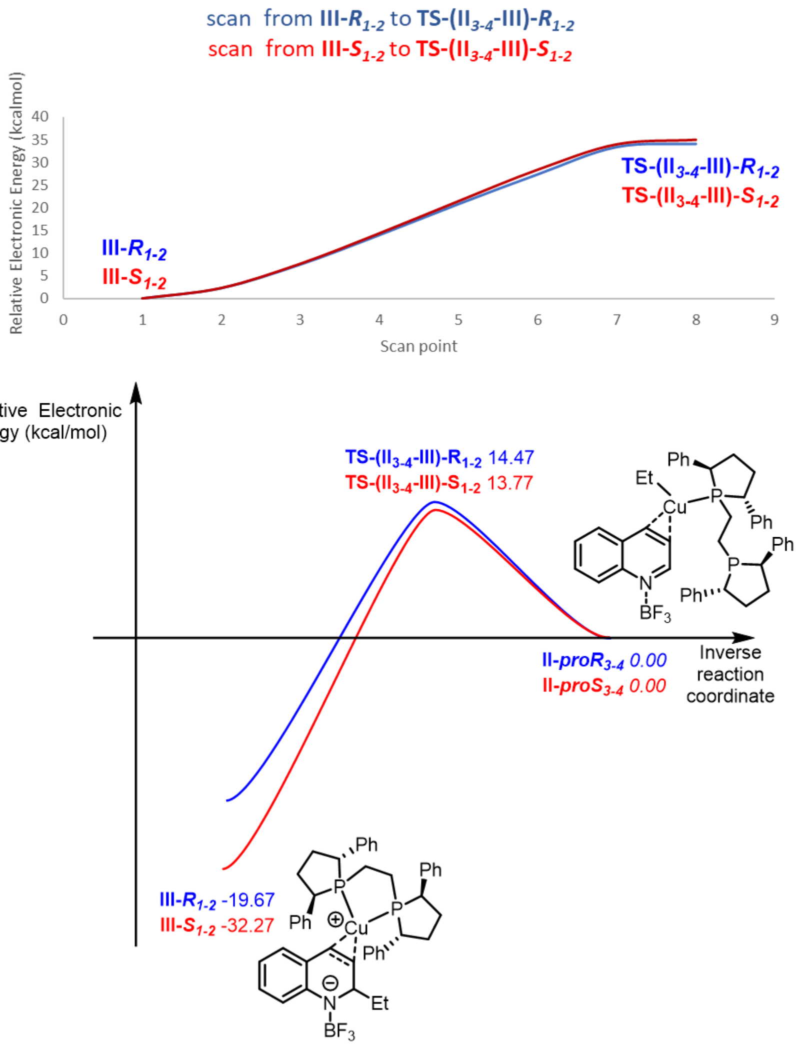


Figure S10. Representation of the energy scan (top) and reaction profile (bottom) obtained through the evaluation of the energy penalty associated with the addition of the Grignard reagent to **II$_{3-4}$** at C-2. The energies reported correspond to electronic energies. The scan point corresponds to each of the steps of the scan, the step size selected was 0.1 Å, the initial C-C bond distance is 1.54 Å and the ending one 2.34 Å.

Moreover, we explored the possibility of a direct decoordination of the copper complex in **III$_{3-4}$** yielding directly the product while creating a highly electrophilic copper species (**IIIa**), naturally we found that the formation of such an ionic pair is energetically unfeasible (see Figure S11). Alternatively, we also explored the possibility of **III$_{3-4}$** to evolve via a structural reorganization that would involve the coordination of the copper at the nitrogen with the concominant release of BF_3. We have found that the formation of **III$_b$** is too endothermic and thus it is unlikely that this species will be present in solution.

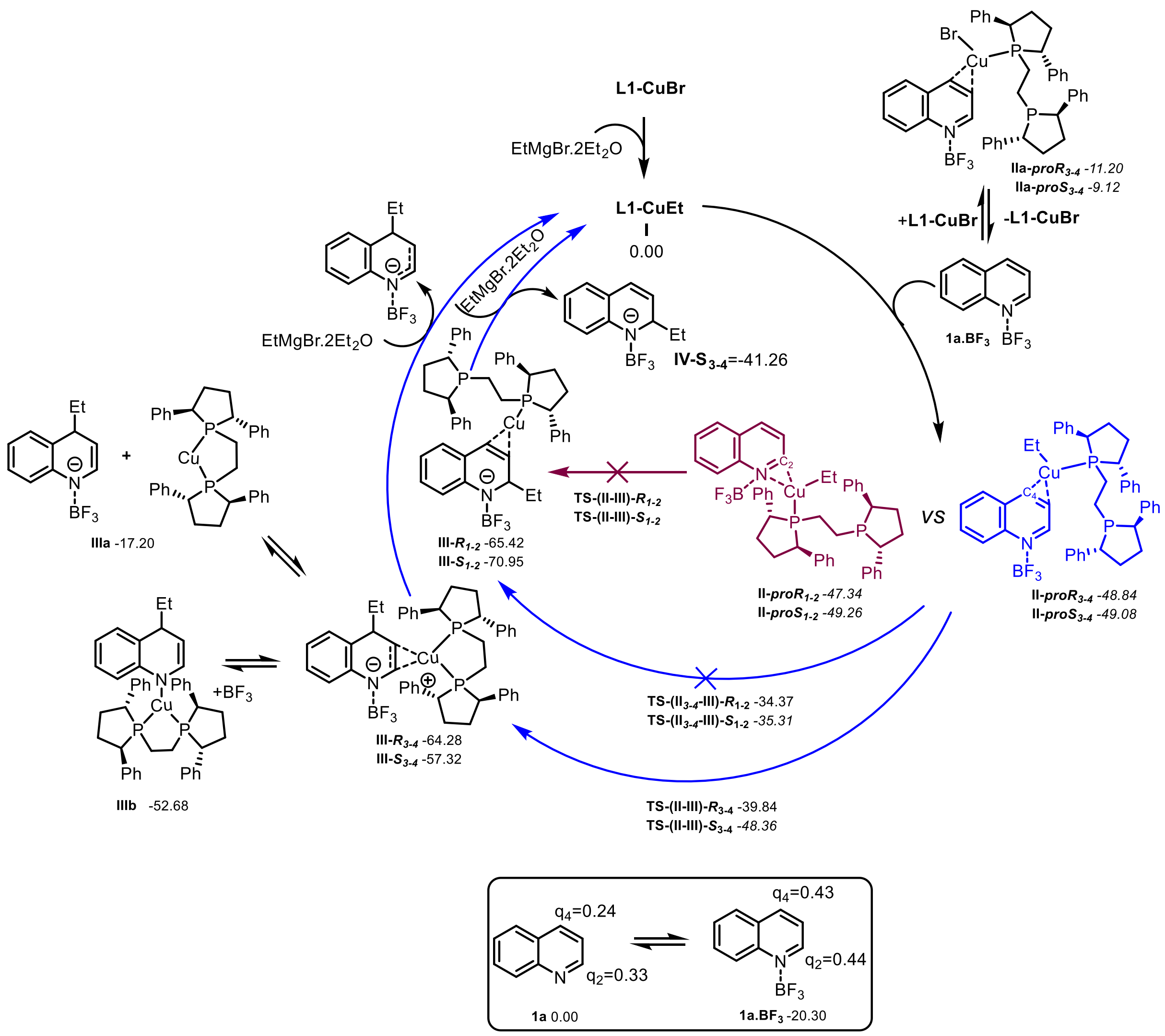


Figure S11. Computed potential reaction paths for the copper catalyzed addition of EtMgBr·2Et$_2$O to quinoline in the presence of a LA. Calculations were performed at the PCM (CH_2Cl_2)/M06/def2svpp computational level using the Gaussian 09 program. The thermochemistry was obtained at 1 atm and 195 K.

Table S10. Summary of the energies for the study of the Computed mechanism for the copper catalyzed addition of $EtMgBr\cdot 2Et_2O$ to quinoline in the presence of a LA.[a]

ID	ImFreqs	Stable	SCF	SCF+ZPVE	H	G
L1-CuBr	–	Yes	−6211.843657	−6211.236732	−6211.219631	−6211.274031
EtMgBr·2Et$_2$O	–	Yes	−3320.18153	−3319.840154	−3319.81692	−3319.893004
L1-CuEt	–	Yes	−3717.080114	−3716.411863	−3716.393885	−3716.450532
1a·BF$_3$	–	Yes	−725.5809442	−725.430379	−725.424745	−725.452271
IIa-*proR*$_{3-4}$	–	Yes	−6937.441863	−6936.68338	−6936.660362	−6936.72743
IIa-*proS*$_{3-4}$	–	Yes	−6937.438924	−6936.680365	−6936.657475	−6936.724125
II-*proR*$_{1-2}$	–	Yes	−4442.683702	−4441.863418	−4441.812692	−4441.948965
II-*proS*$_{1-2}$	–	Yes	−4442.682289	−4441.86133	−4441.810951	−4441.945899
II-*proR*$_{3-4}$	–	Yes	−4442.685582	−4441.864414	−4441.841144	−4441.907423
II-*proS*$_{3-4}$	–	Yes	−4442.684883	−4441.863422	−4441.840268	−4441.906948
TS-(II-III)-*R*$_{3-4}$	-300.38	Yes	−4442.673217	−4441.851763	−4441.802325	−4441.933955
TS-(II-III)-*S*$_{3-4}$	-318.93	Yes	−4442.683985	−4441.863683	−4441.813757	−4441.947534
III-*R*$_{3-4}$	–	Yes	−4442.744373	−4441.920167	−4441.897521	−4441.9618
III-*S*$_{3-4}$	–	Yes	−4442.755128	−4441.930912	−4441.908182	−4441.972896
III-*R*$_{1-2}$	–	Yes	−4442.71626	−4441.891792	−4441.842248	−4441.974708
III-*S*$_{1-2}$	–	Yes	−4442.736311	−4441.911465	−4441.88894	−4441.952942
III$_a$	–	Yes	−804.7923851	−804.577264	−804.57015	−804.600866
III$_b$	–	Yes	−4118.464794	−4117.656681	−4117.611087	−4117.735868
IV-*S*$_{3-4}$	–	Yes	−804.7923853	−804.577273	−804.570153	−804.600902

[a]Energies are expressed in a.u. and the imaginary frequencies in cm^{-1}. [b]H represents enthalpies. [c]G Represents Gibbs free Energies.

Scans of the variation of the energy with the reaction coordinate from II-*proR*$_{3-4}$ to TS-(II-III)-*R*$_{3-4}$

Due to the difficulties found when trying to locate **TS-(II-III)-*R*$_{1-2}$** and **TS-(II-III)-*S*$_{1-2}$**, we decided to explore the potential energy surface in the region of the reaction coordinate. To do so, we first confirmed in **TS-(II-III)-*R*$_{3-4}$** that the bending of C-4-Cu-Et is the main contributor to the energy penalization of the transition state (barrier from scan = 13.23, computed barrier = 9 kcal/mol), we chose this diastereomer and not the **II-*proS*$_{3-4}$** one because it shows a higher barrier and thus it provides a clearer scan (see Figure S12).

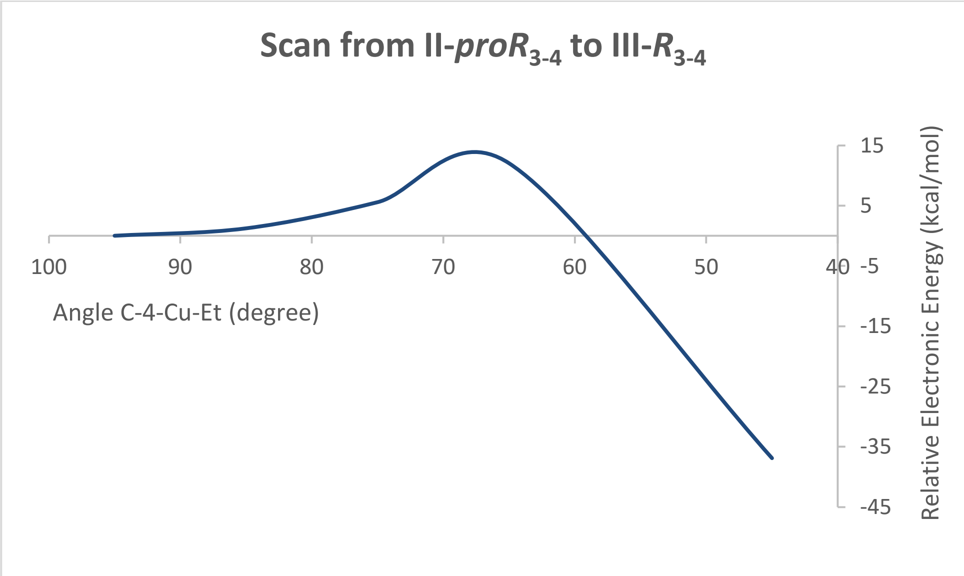


Figure S12. Computed energy profile for the formation of **III-*R*$_{3-4}$** from **II-*proR*$_{3-4}$**. The represented energies correspond to pure electronic energies. Calculations were performed at the PCM (CH_2Cl_2)/M06/def2svpp computational level using the Gaussian 09 program. The scan step chosen is 10˚.

Encouraged with these results we performed an analogous study for localizing **TS-(II-III)-*R*$_{1-2}$** obtaining, as it was described in the main text, that the variation of this internal coordinate leads to the disaggregation of the complex and the formation of an alternative one in which the **L1-**CuEt complex is establishing a weak interaction with C-3-C-4. This reveals that **II-*proR*$_{1-2}$** will not evolve via a C-2-addition but through a disaggregation of the complex and the formation of a new species **IIb-*proR*$_{1-2}$** in which the copper is already sitting at C-3-C-4 thus predisposing the system to further progress via the formation of **II-$_{3-4}$**.

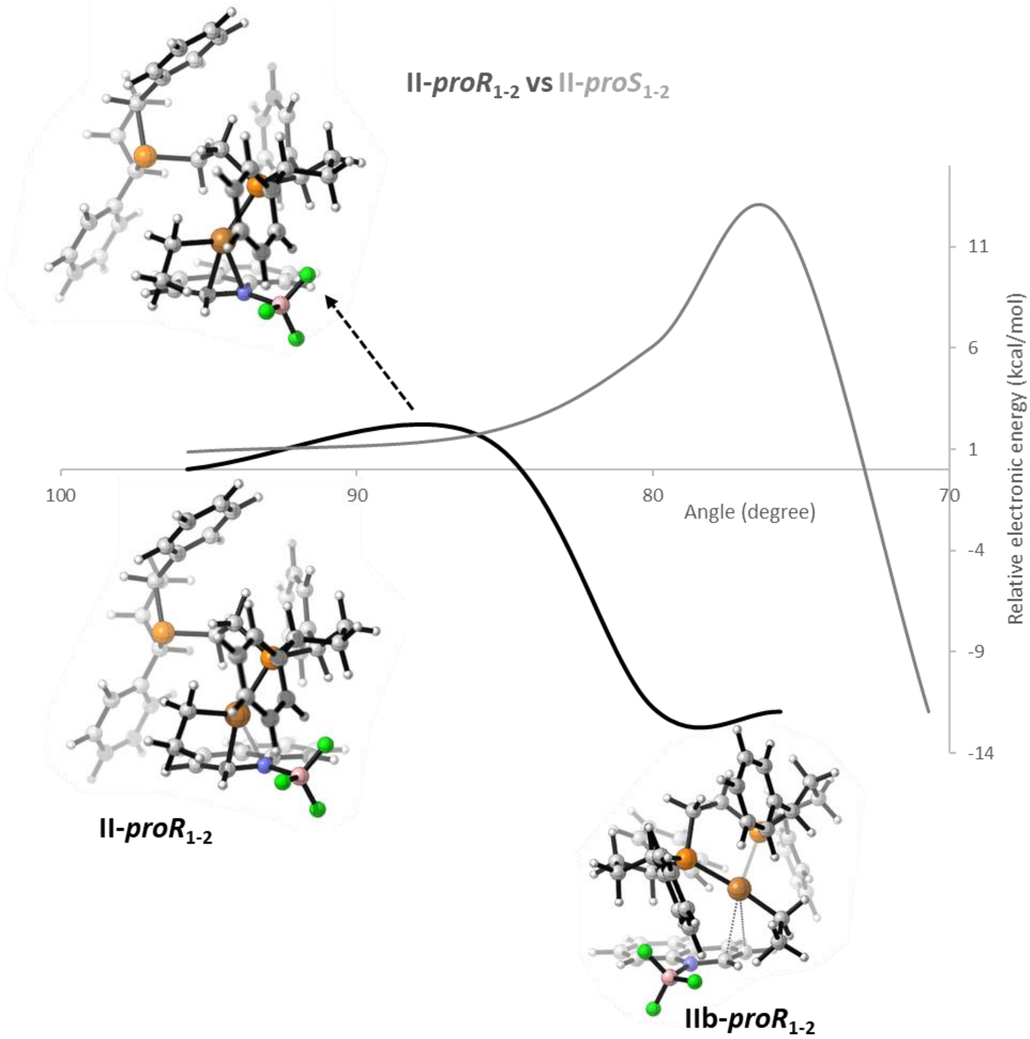


Figure S13. Scan of the internal coordinate C-2-Cu-Et at **II-**$_{1\text{-}2}$. The represented energies correspond to pure electronic energies. Calculations were performed at the PCM (CH_2Cl_2)/M06/def2svpp computational level using the Gaussian 09 program The scan step chosen is 10˚. We have used black lines to represent the energy evolution of ***II-proR***$_{1\text{-}2}$ and grey lines to represent the energy evolution of ***II-proS***$_{1\text{-}2.}$ Notice that we have used the mirror image of the compound ***IIb-proR***$_{1\text{-}2}$ for visualization purposes.

IRC obtained for TS-(II-III)-*R*$_{3\text{-}4}$

To rationalize the sensitivity of the reaction to the substituents at position C-3 but not to substituents at C-4 we have followed the intrinsic reaction coordinate (IRC) from **TS-(II-III)-*R*$_{3\text{-}4}$**. The IRC shows that once the transition state structure is met and the delivery of the *Et* group initiated, the **L1**/Cu(I) moiety starts relocating towards C-3 and it is not until the very end of the IRC that the relocation of the copper center towards C-4 is happening. As a result, the latter chemical event barely contributes to the energy of the reaction whereas the relocation to C-3 has a sound effect on the energy of this TS, as a result if the access to that position is impeded the energy penalization for this reaction is going to be increased (Figure S14).

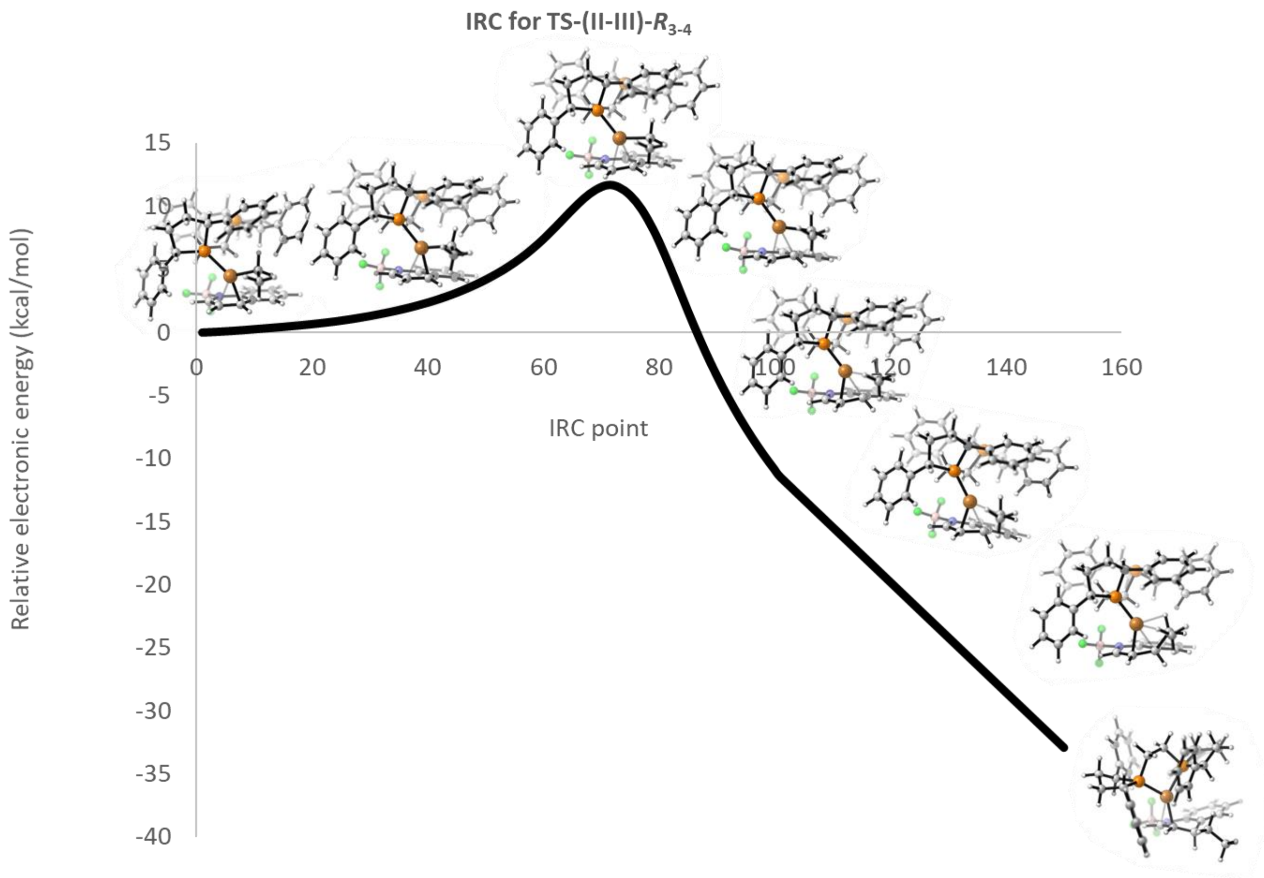


Figure S14. IRC obtained for **TS-(II-III)-*R*$_{3-4}$**. The represented energies correspond to pure electronic energies. Calculations were performed at the PCM (CH_2Cl_2)/M06/def2svpp computational level using the Gaussian 09 program. Notice that for visualization purposes we have represented the mirror images of the compounds.

NMR experiments

NMR experiments were carried out in order to detect possible species formed in the reaction. NMR studies were performed with 2-methyl-quinoline in combination with $BF_3{\cdot}Et_2O$, with CuBr·SMe_2 and with $BF_3{\cdot}Et_2O$ and **L4**-CuBr. Accordingly 3 different species were detected: 1) 2-methyl-quinoline/BF_3; 2) 2-methyl-quinoline/**L4**-CuBr; 3) 2-methyl-quinoline/BF_3/**L4**-CuBr. For the latter species we assume that Cu(I) complex binds to C-3-C-4 position of 2-methyl-quinoline**,** however we don't have a strong NMR evidence for this. All the attempts to detect species with 2-methyl-quinoline/BF_3/**L4**-CuBr/RMgBr were not successful due the immediate addition product formation upon mixing all the reagents together.

Below one can find the overlapped spectra, separate spectra with assignments and procedures for the preparation of the species.

Overlapped spectra

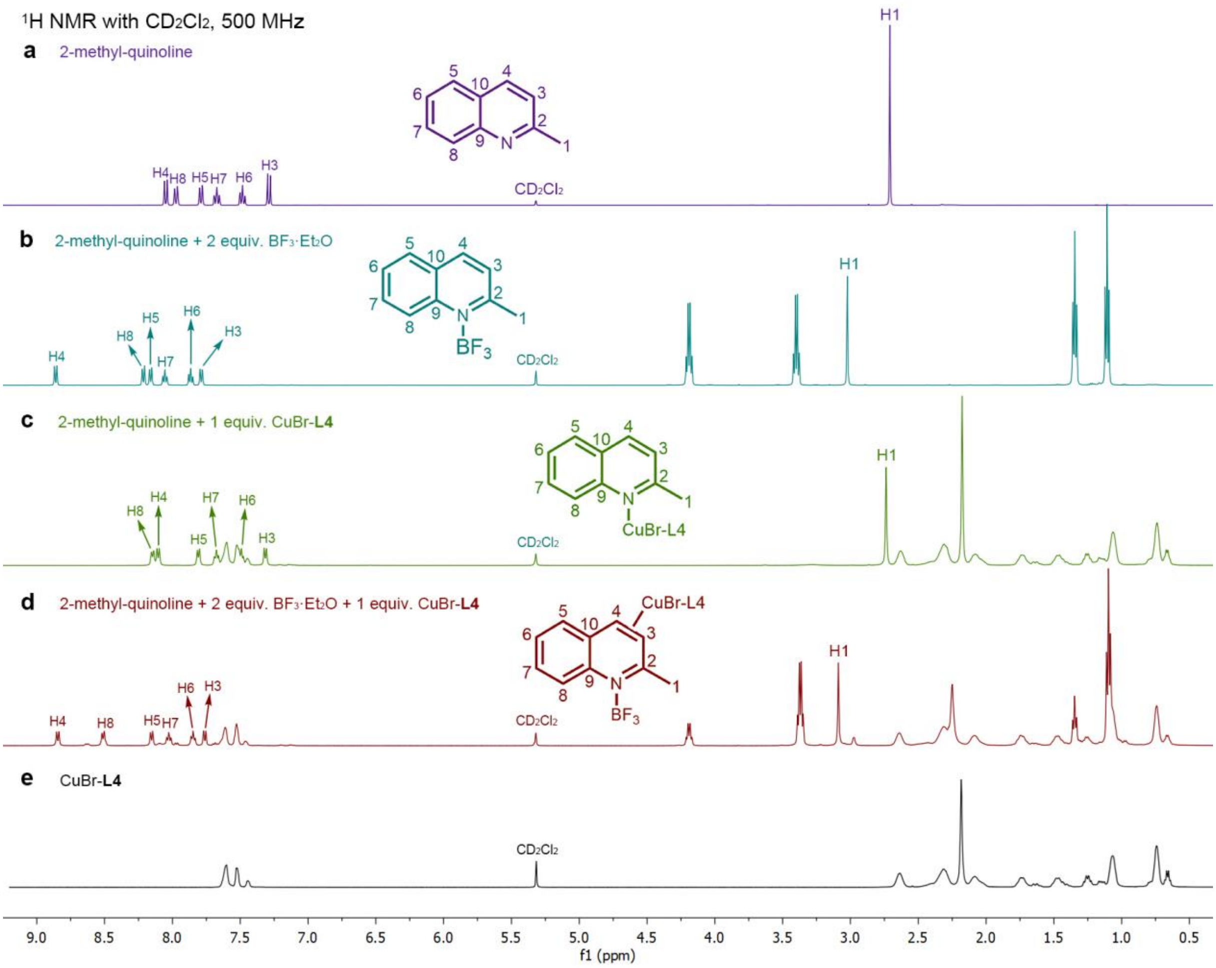


Figure S15. NMR studies performed to evaluate the interaction of 2-Me-quinoline with $BF_3{\cdot}Et_2O$, L4-CuBr and both of them. (a) ^{1}H-NMR spectra of 2-methyl-quinoline. (b) ^{1}H-NMR spectra of the 2-methyl-quinoline with 2 equiv. of $BF_3{\cdot}Et_2O$. (c) ^{1}H-NMR spectra of the 2-methyl-quinoline with 1 equiv. of **L4-**CuBr. (d) ^{1}H-NMR spectra of the 2-Me-quinoline with 1 equiv of **L4-**CuBr and 2 equiv. of $BF_3{\cdot}Et_2O$. (e) ^{1}H-NMR spectra of **L4-**CuBr.

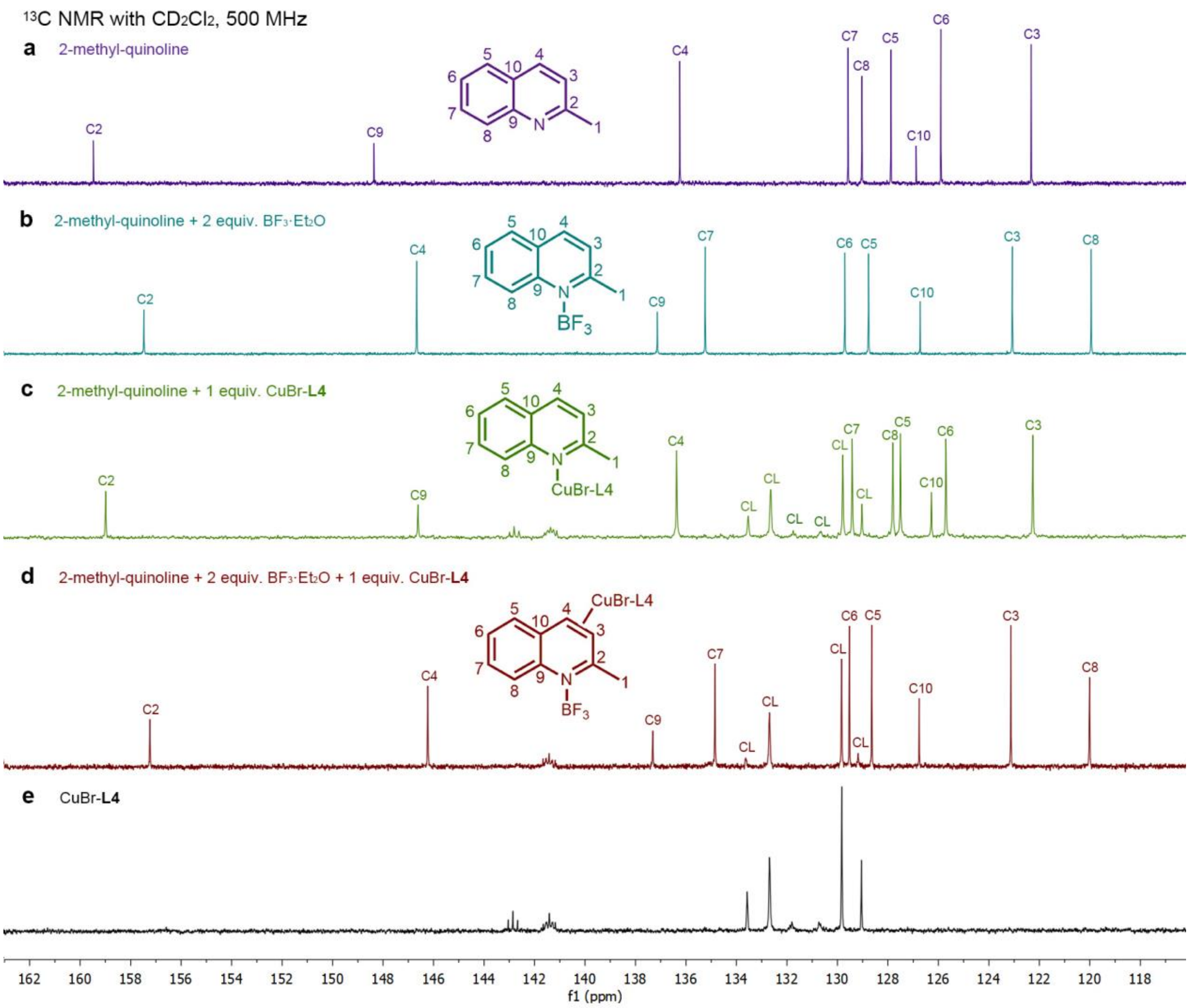
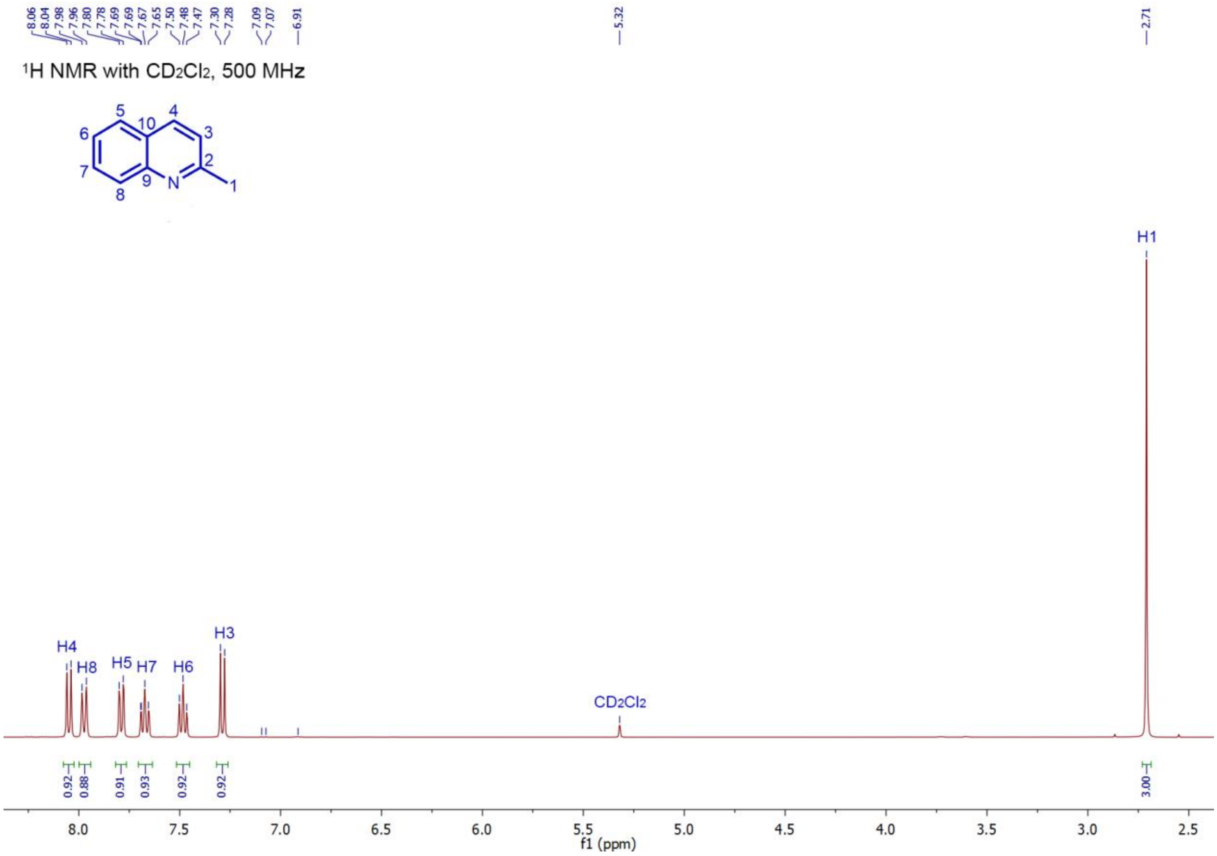


Figure S16. Amplified aromatic part of ^{13}C NMR spectra in the range of 118-162 ppm to evaluate the interaction of 2-Me-quinoline with $BF_3{\cdot}Et_2O$, **L4**-CuBr and both of them (for full spectra, see below). (a) ^{13}C-NMR spectra of 2-methyl-quinoline. (b) ^{13}C-NMR spectra of the 2-Me-quinoline with 2 equiv of $BF_3{\cdot}Et_2O$. (c) ^{13}C -NMR spectra of the 2-methyl-quinoline with 1 equiv of **L4-**CuBr. (d) ^{13}C-NMR spectra of the 2-methyl-quinoline with 1 equiv. of **L4-**CuBr and 2 equiv. of $BF_3{\cdot}Et_2O$. (e) ^{13}C-NMR spectra of **L4-**CuBr.

Full assignments of all the peaks

2-methyl-quinoline

2-methyl-quinoline was dissolved in CD_2Cl_2 in a dry NMR tube at −50 °C under N_2 atmosphere and measured by NMR spectroscopy at −50 °C. Full characterization was carried out by ^1H NMR (Figure S17), ^{13}C NMR (Figure S18), ^1H-^{13}C-HSQCED (Figure S19) and ^1H-^{13}C-HMBC (Figure S20).



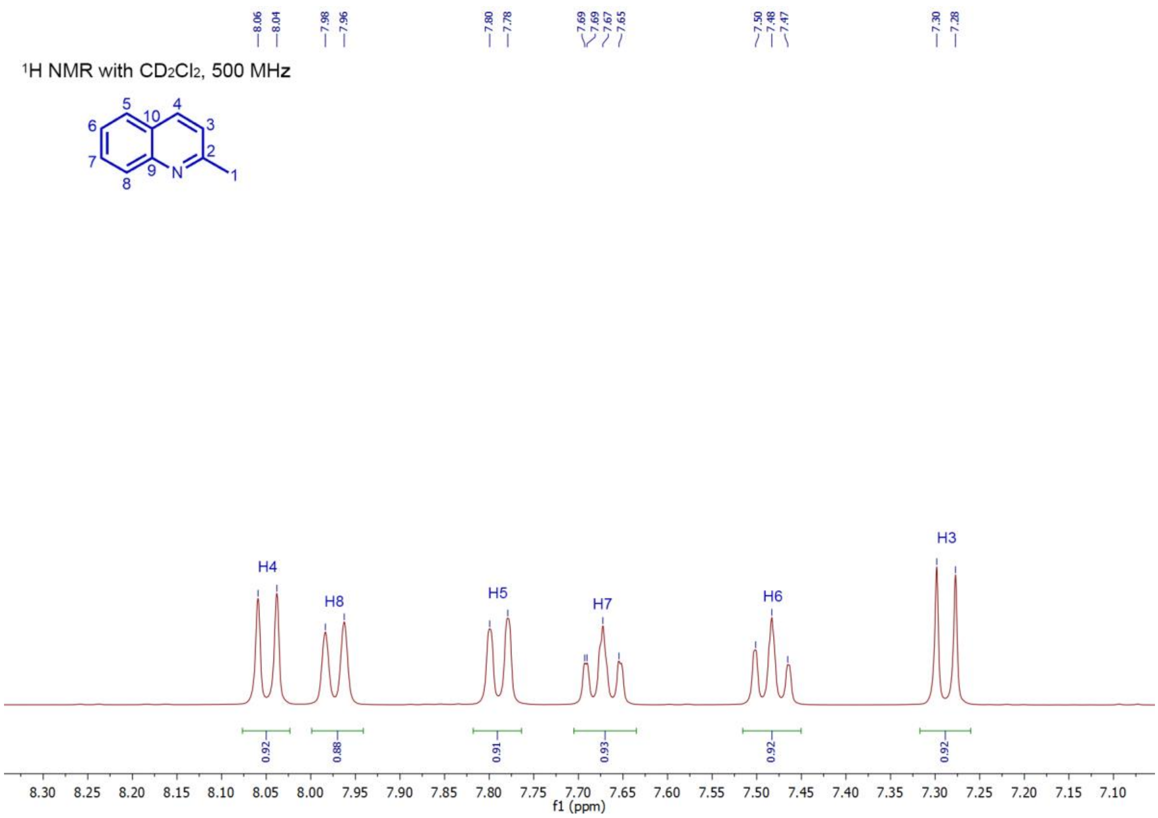
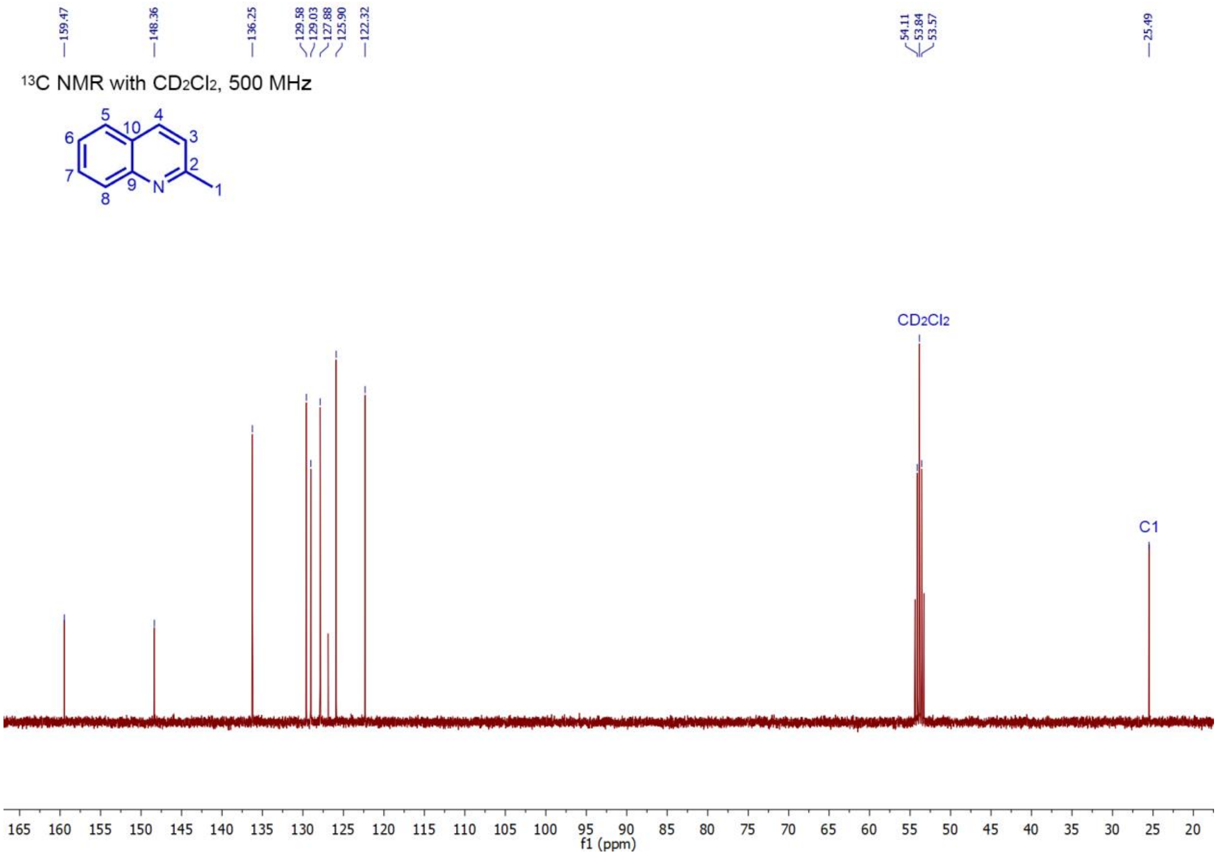


Figure S17. ^{1}H NMR spectrum of 2-methyl-quinoline (top) and amplified aromatic part of ^{1}H NMR spectra (bottom) .



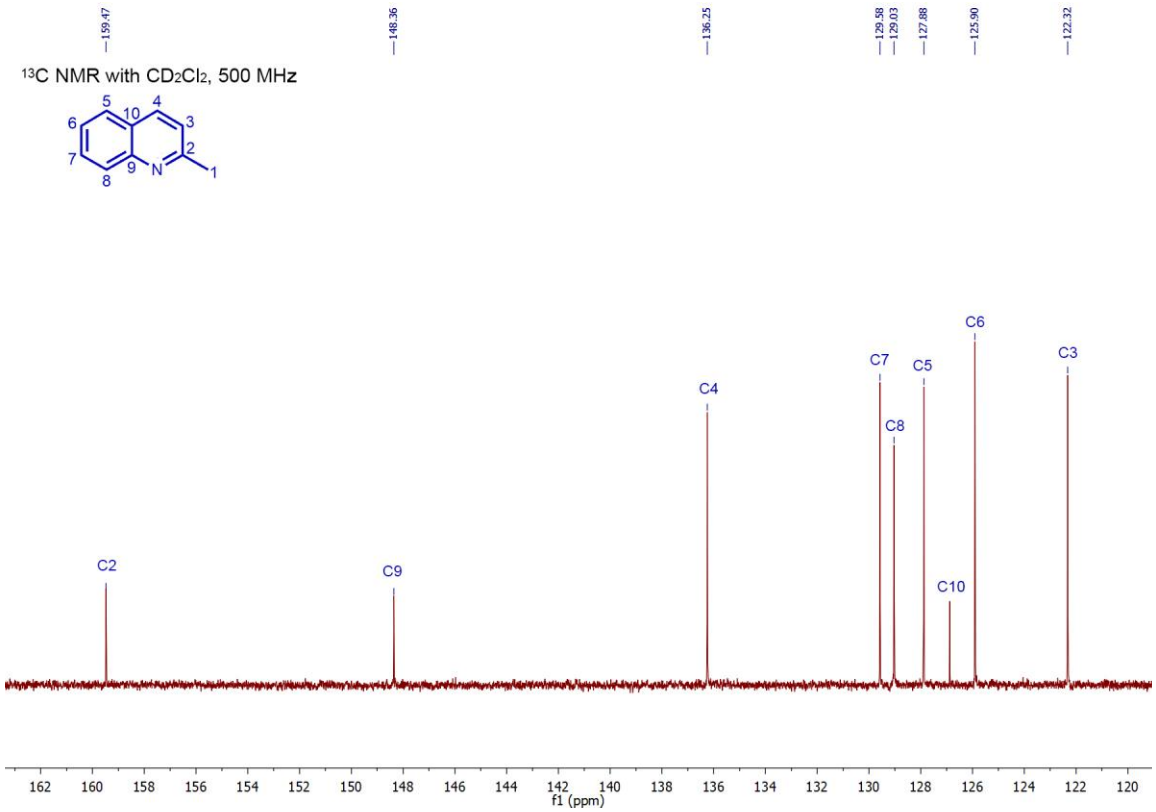
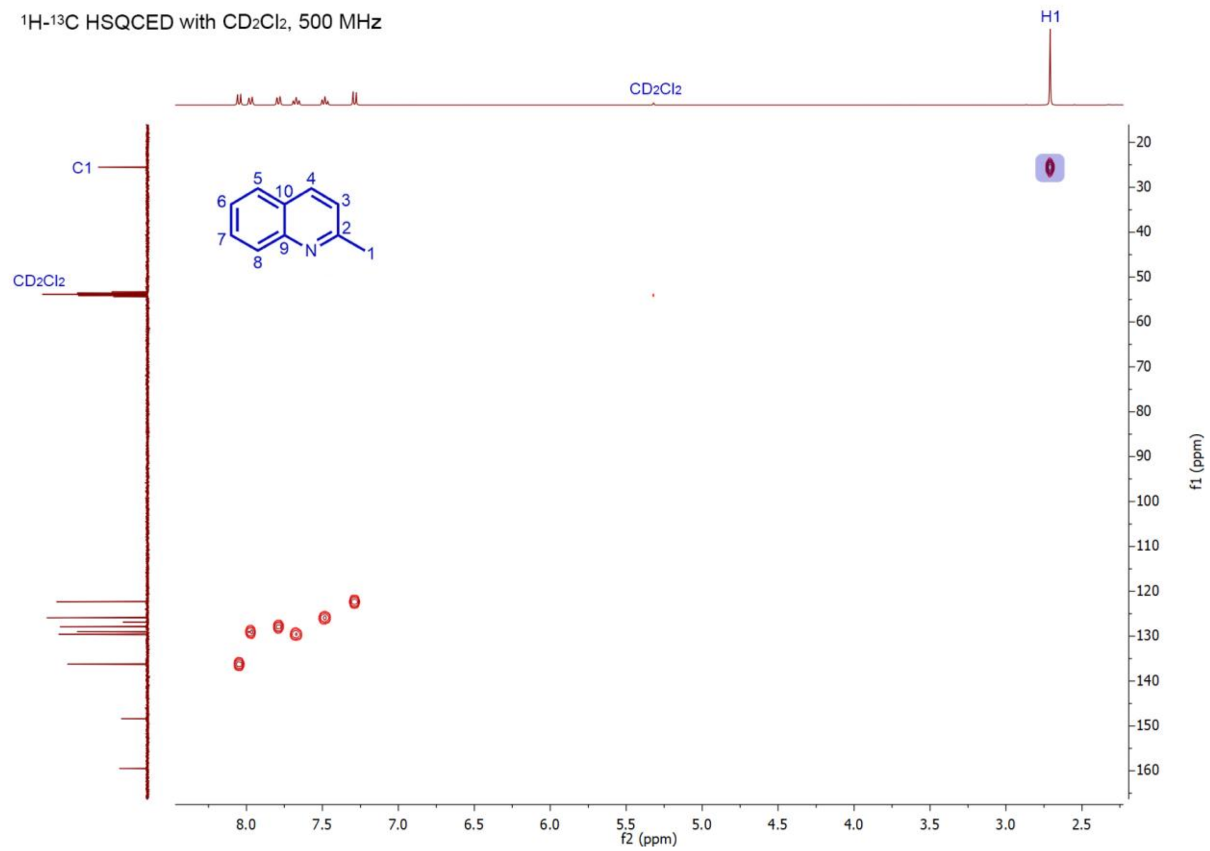


Figure S18. ^{13}C NMR spectrum of 2-methyl-quinoline (top) and amplified aromatic part of ^{1}H NMR spectra (bottom).



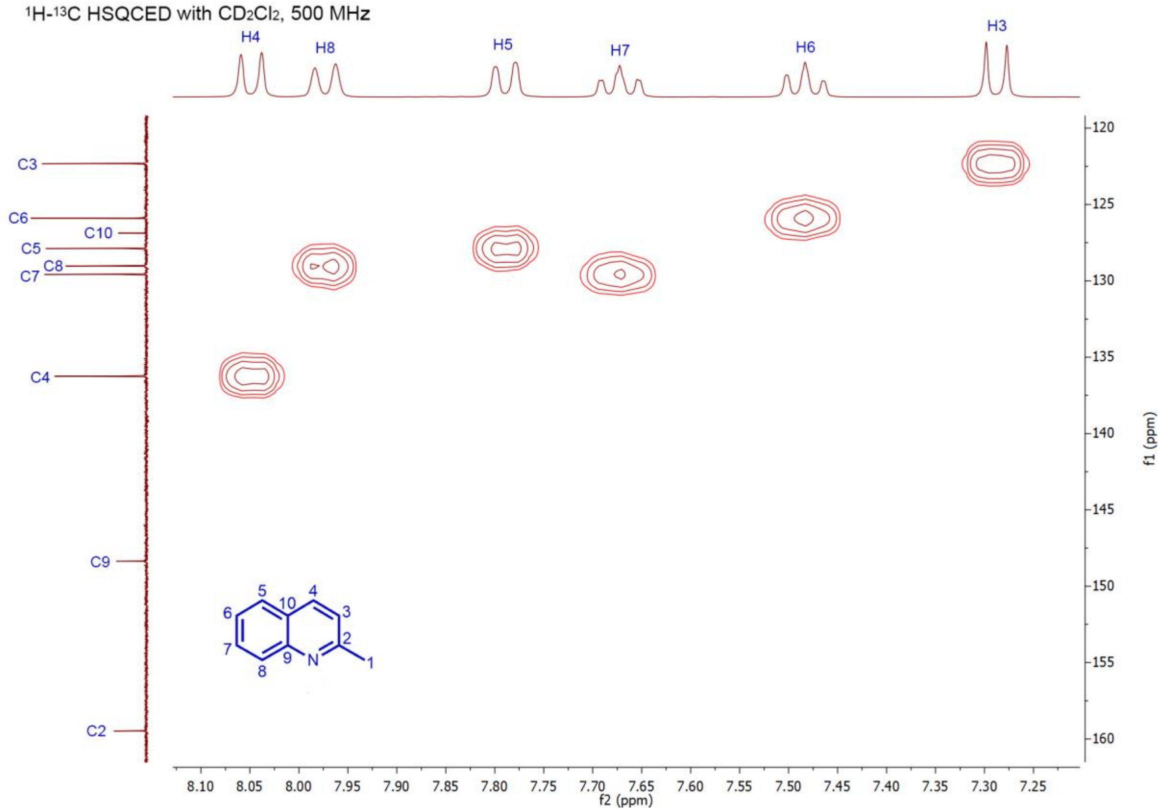


Figure S19. ^{1}H-^{13}C HSQCED spectrum of 2-methyl-quinoline (top) and amplified aromatic part of ^{1}H-^{13}C HSQCED spectra (bottom).

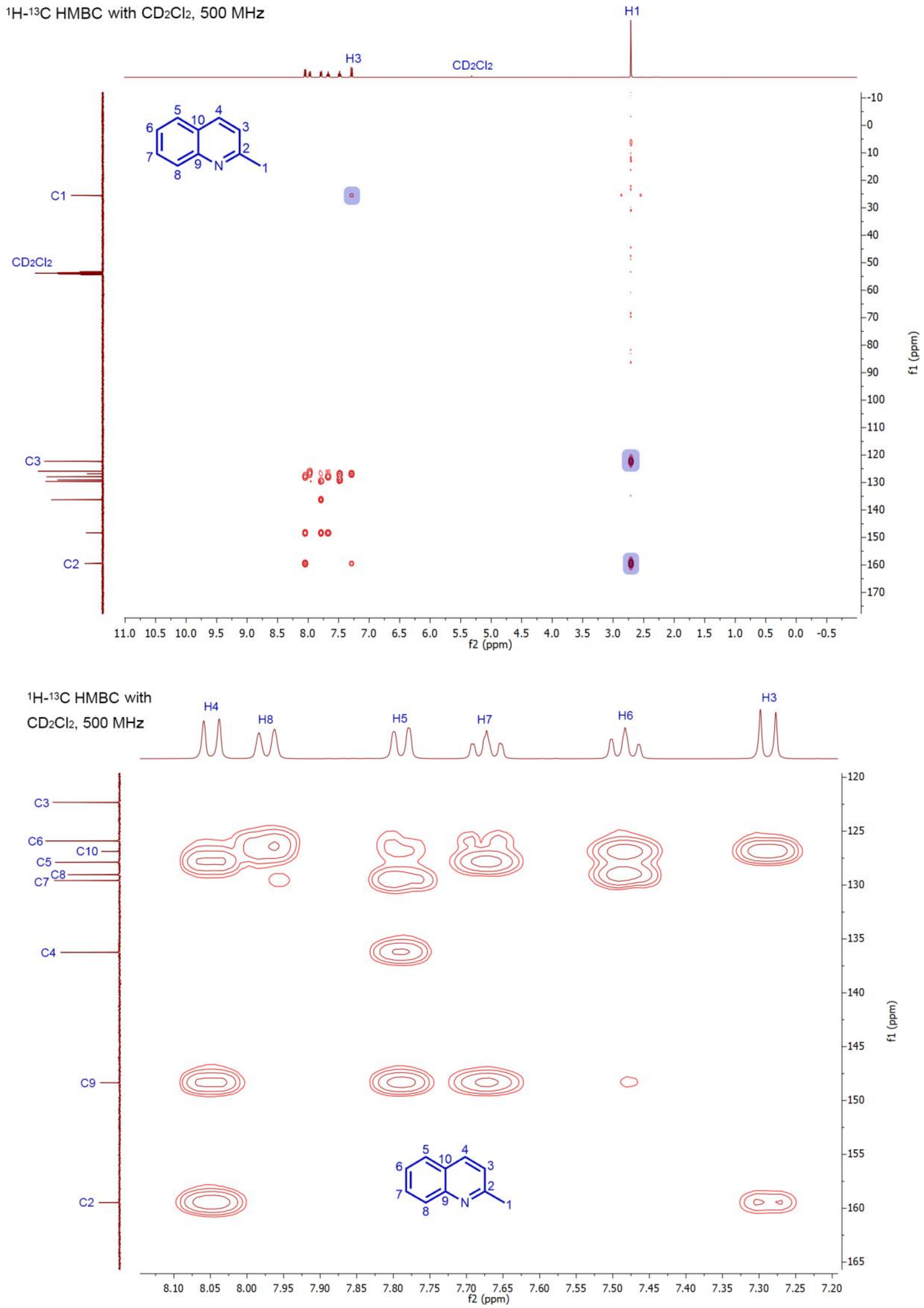
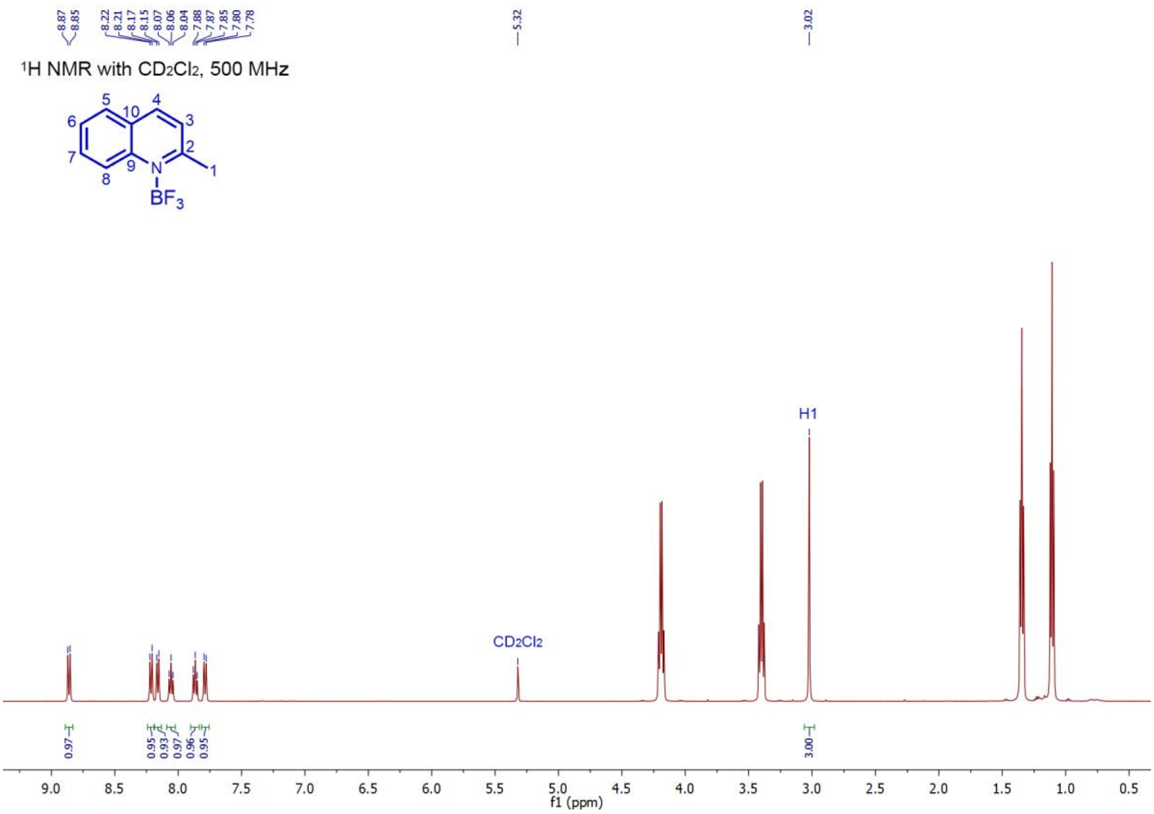


Figure S20. ^{1}H-^{13}C HMBC spectrum of 2-methyl-quinoline (top) and amplified aromatic part of ^{1}H-^{13}C HMBC spectra (bottom) .

2-methyl-quinoline-BF_3 complex

2 Equiv. of $BF_3 \cdot Et_2O$ was added to a solution of 2-methyl-quinoline in CD_2Cl_2 in a dry NMR tube at −50 °C under N_2 atmosphere, leading to instantaneous formation of a new species which was immediately measured by NMR spectroscopy at −50 °C. Full characterization was carried out by ^{1}H NMR (Figure S21), ^{13}C NMR (Figure S22), ^{1}H-^{13}C-HSQCED (Figure S23) and ^{1}H-^{13}C-HMBC (Figure S24). The peaks of 2-methyl-quinoline for both ^{1}H NMR and ^{13}C NMR have shifted after coordinating with BF_3, indicating the formation of 2-methyl-quinoline-BF_3 complex.



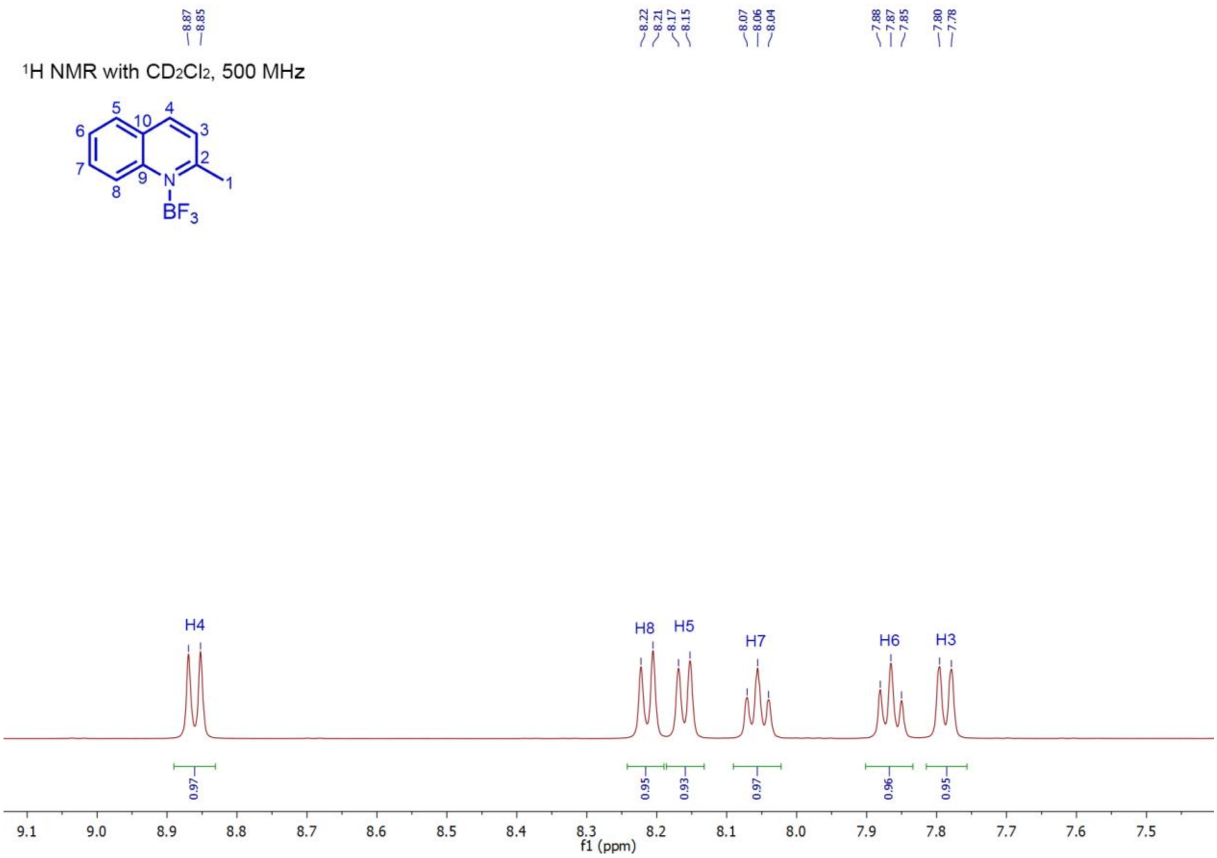
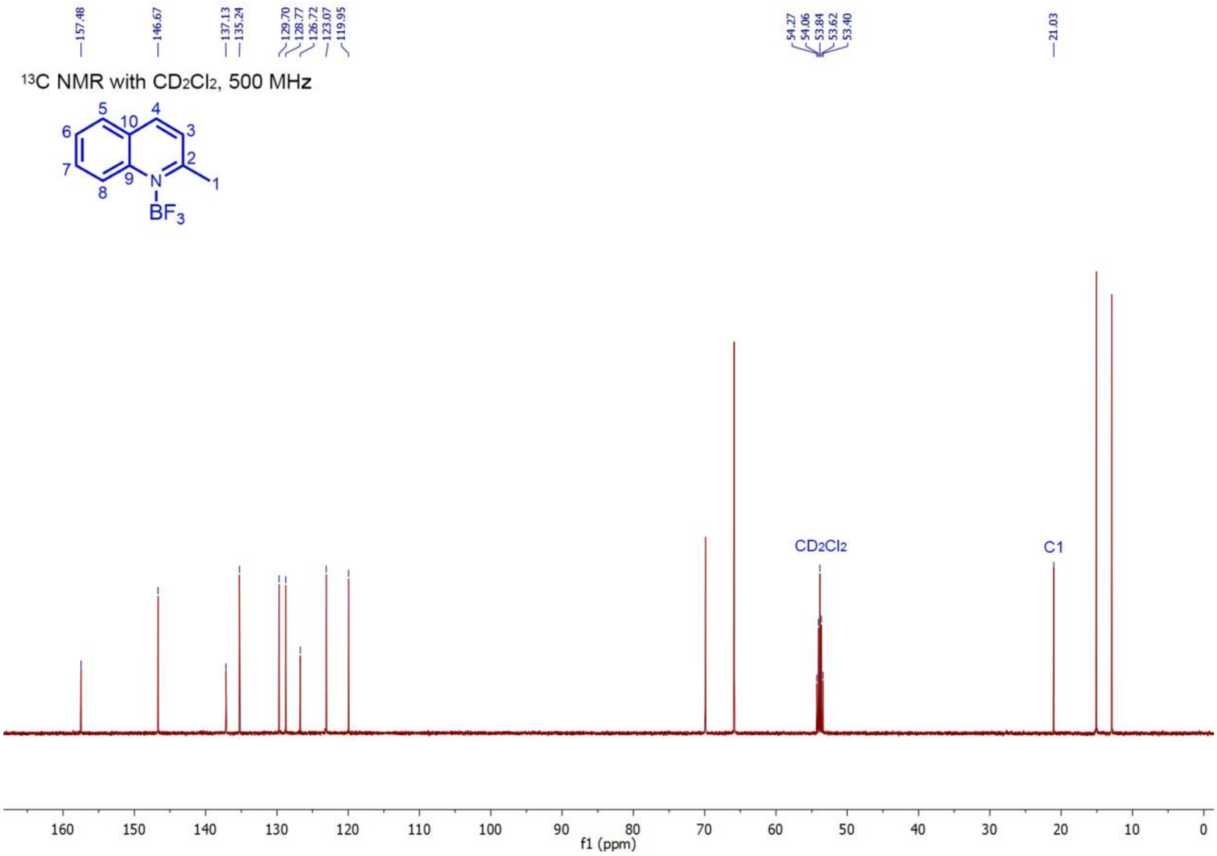


Figure S21. ^{1}H NMR spectrum of the mixture of 2-methyl-quinoline and $BF_3{\cdot}Et_2O$ (top) and amplified aromatic part of ^{1}H NMR spectra (bottom).



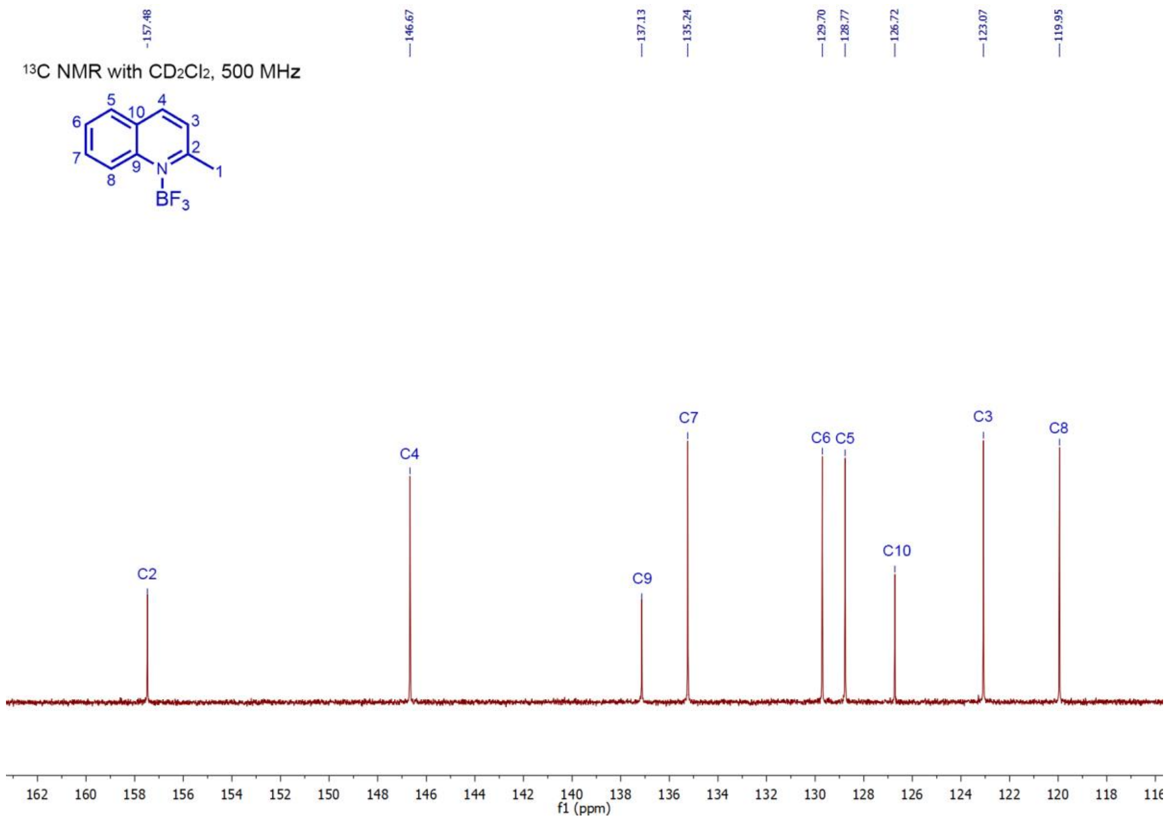
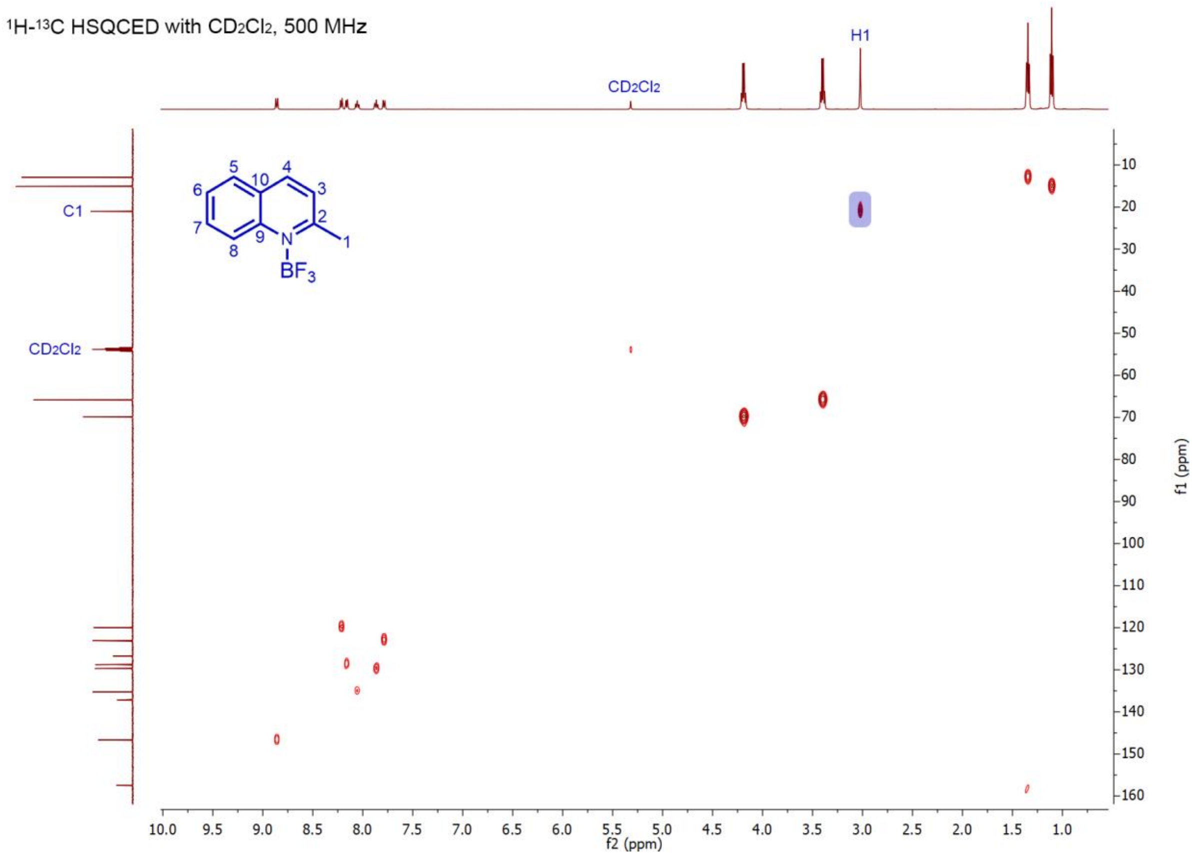


Figure S22. ^{13}C NMR spectrum of the mixture of 2-methyl-quinoline and $BF_3 \cdot Et_2O$ (top) and amplified aromatic part of ^{13}C NMR spectra (bottom).



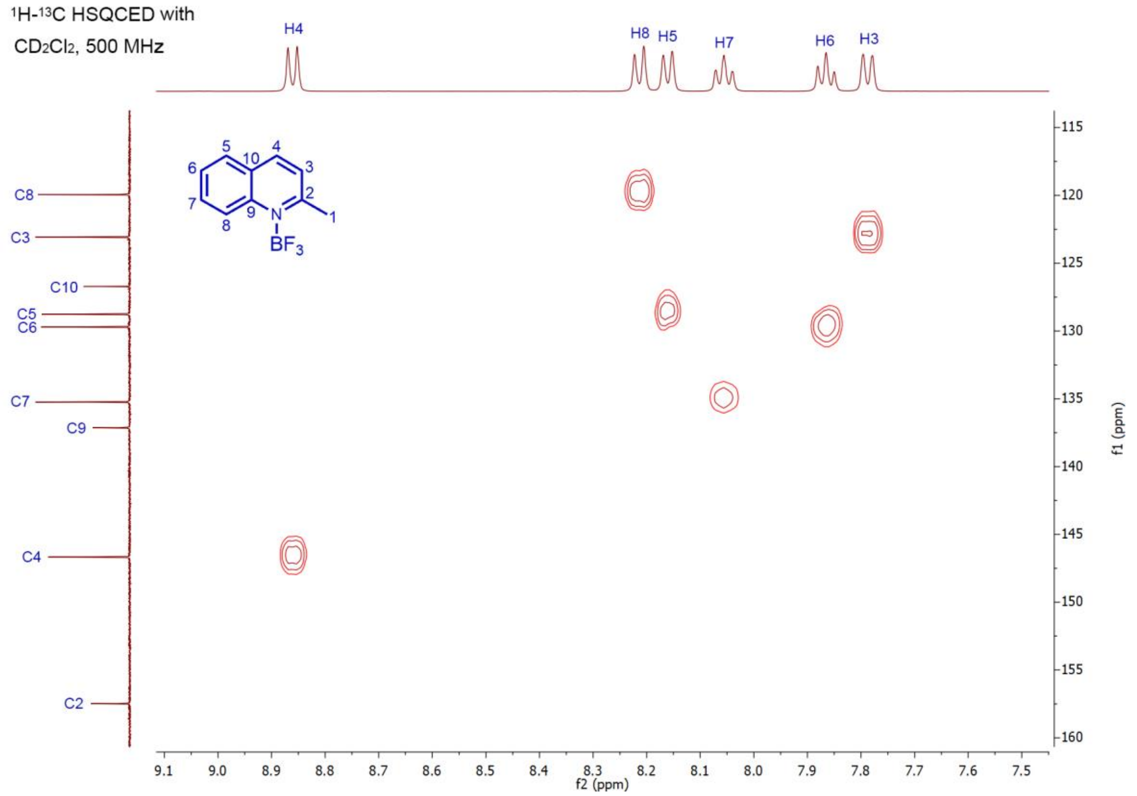
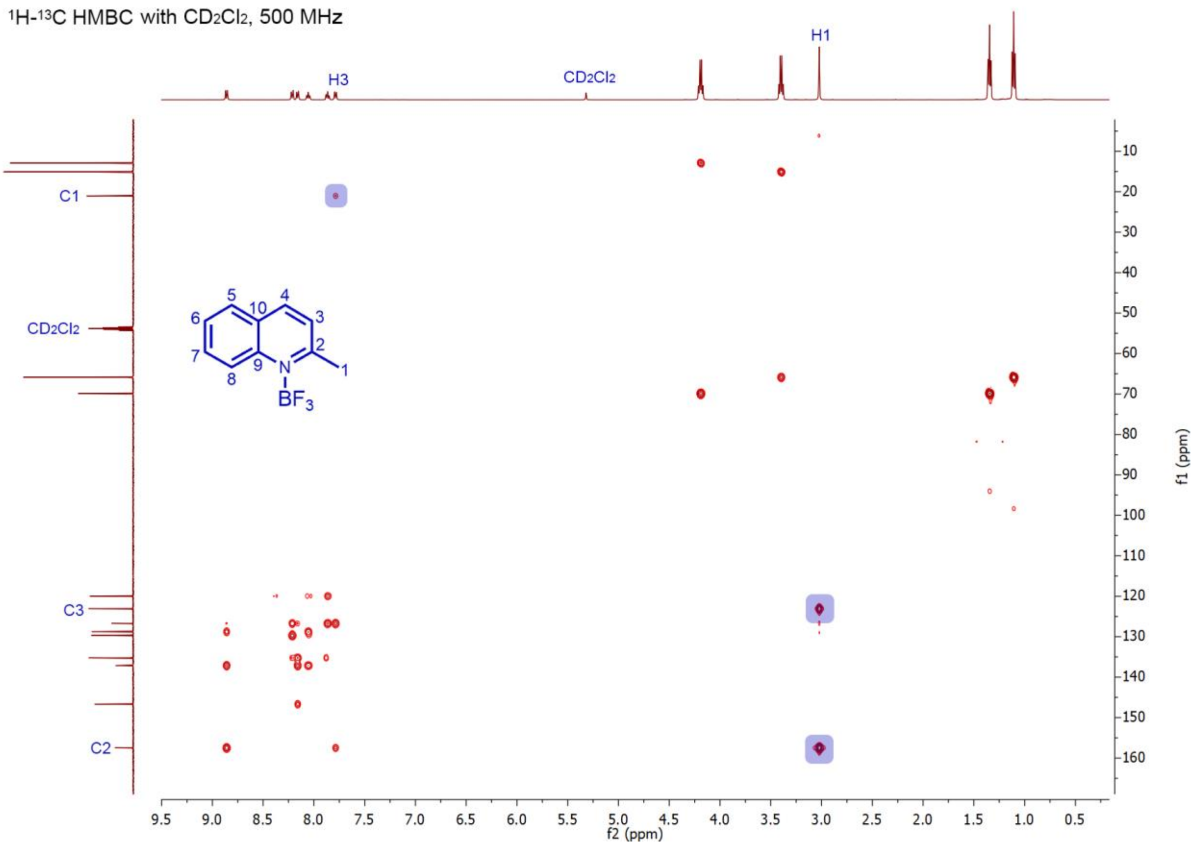


Figure S23. ^{1}H-^{13}C HSQCED spectrum of the mixture of 2-methyl-quinoline and $BF_3{\cdot}Et_2O$ (top) and amplified aromatic part of ^{1}H-^{13}C HSQCED spectra (bottom).



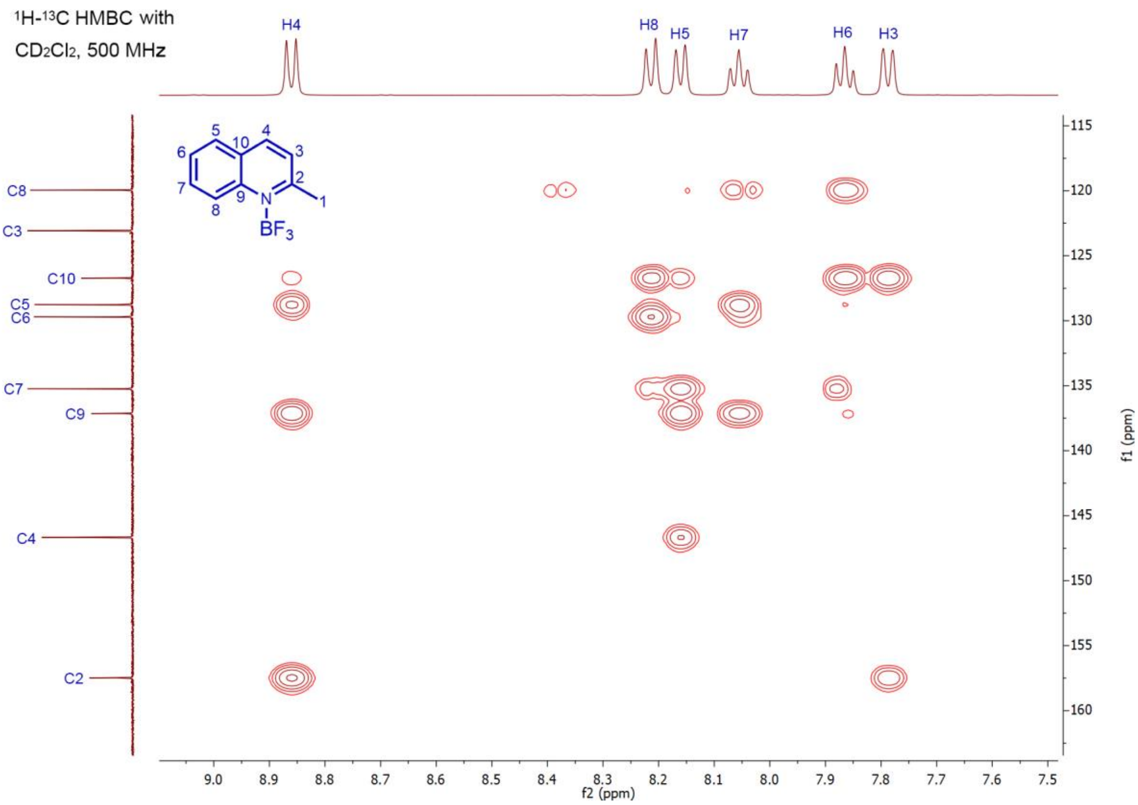
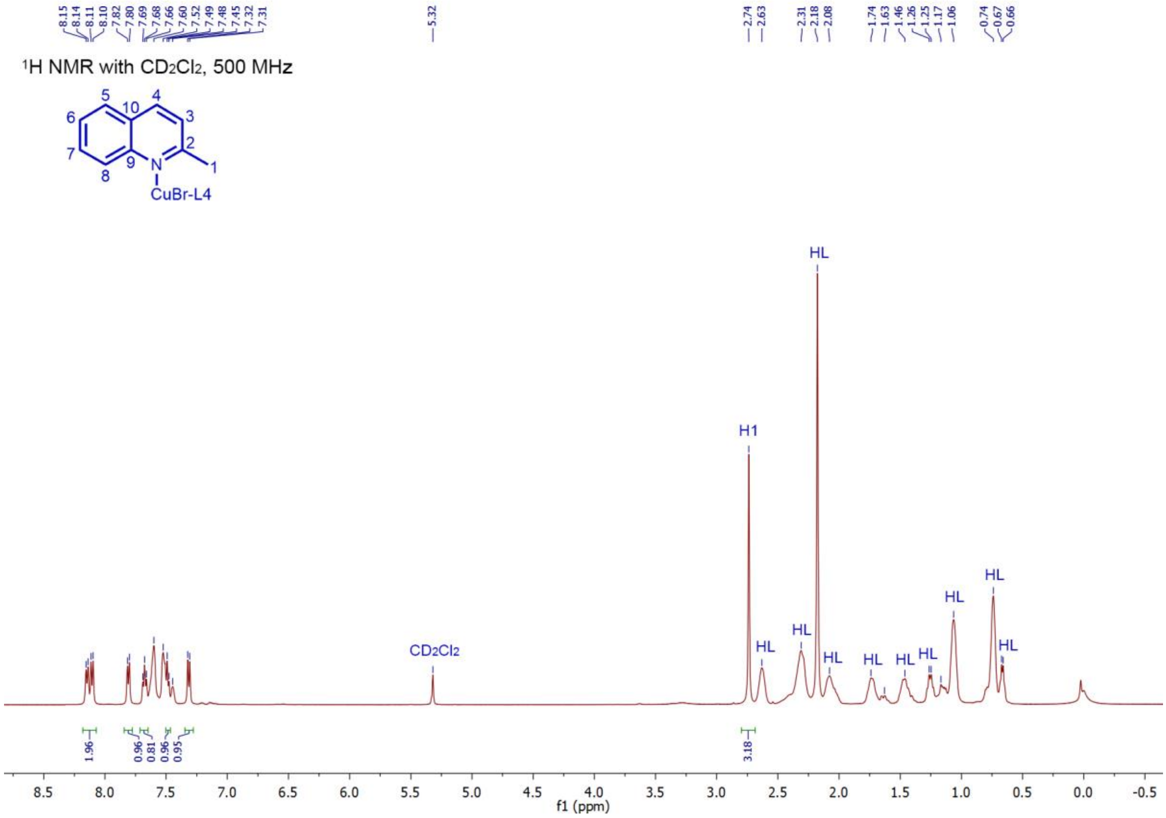


Figure S24. ^{1}H-^{13}C HMBC spectrum of the mixture of 2-methyl-quinoline and $BF_3{\cdot}Et_2O$ (top) and amplified aromatic part of ^{1}H-^{13}C HMBC spectra (bottom).

2-methyl-quinoline-L4-CuBr complex

1 Equiv. of **L4-**CuBr catalyst was added to a solution of 2-methyl-quinoline in CD_2Cl_2 in a dry NMR tube at −50 °C under N_2 atmosphere, leading to instantaneous formation of a new species which was immediately measured by NMR spectroscopy at −50 °C. Full characterization was carried out by ^{1}H NMR (Figure S25), ^{13}C NMR (Figure S26), ^{1}H-^{13}C-HSQCED (Figure S27) and ^{1}H-^{13}C-HMBC (Figure S28). The peaks of 2-methyl-quinoline for both ^{1}H NMR and ^{13}C NMR have shifted after coordinating with CuBr, indicating the formation of 2-methyl-quinoline- **L4-**CuBr complex.



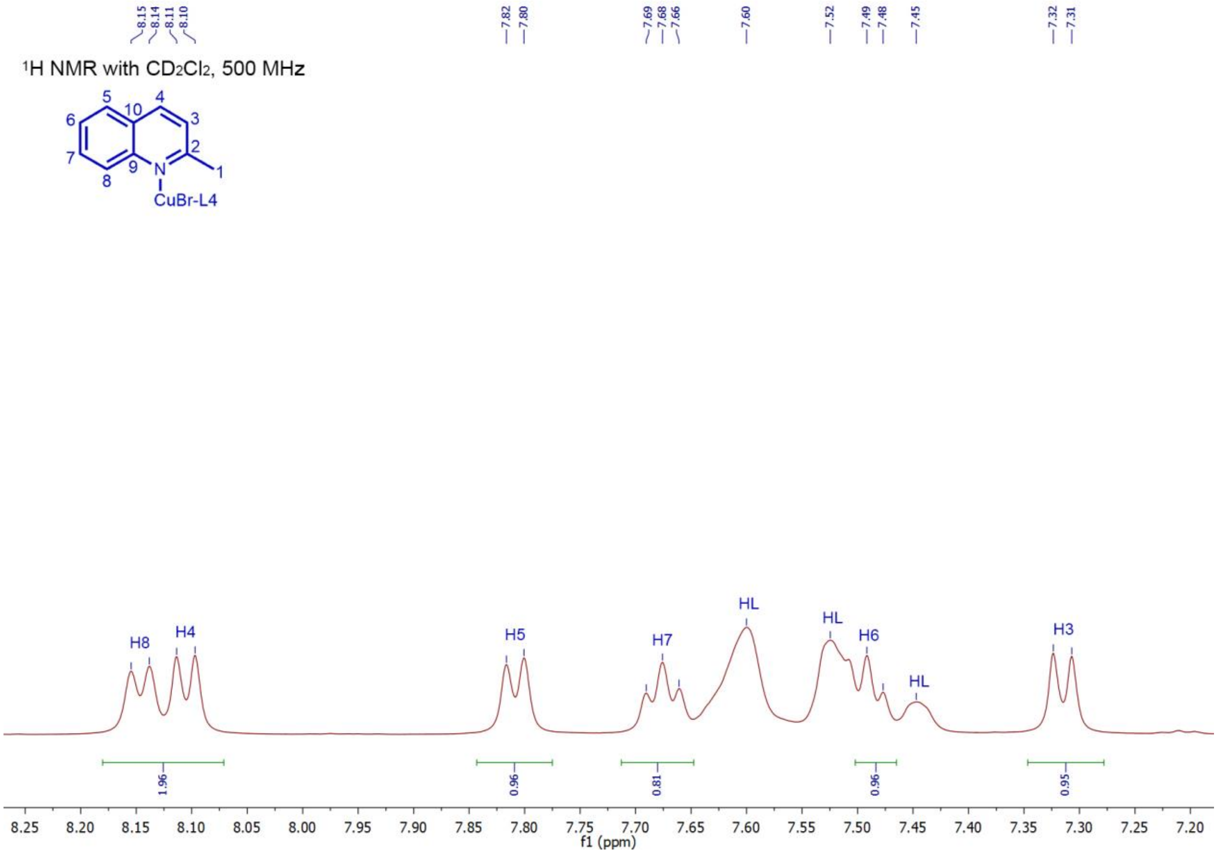
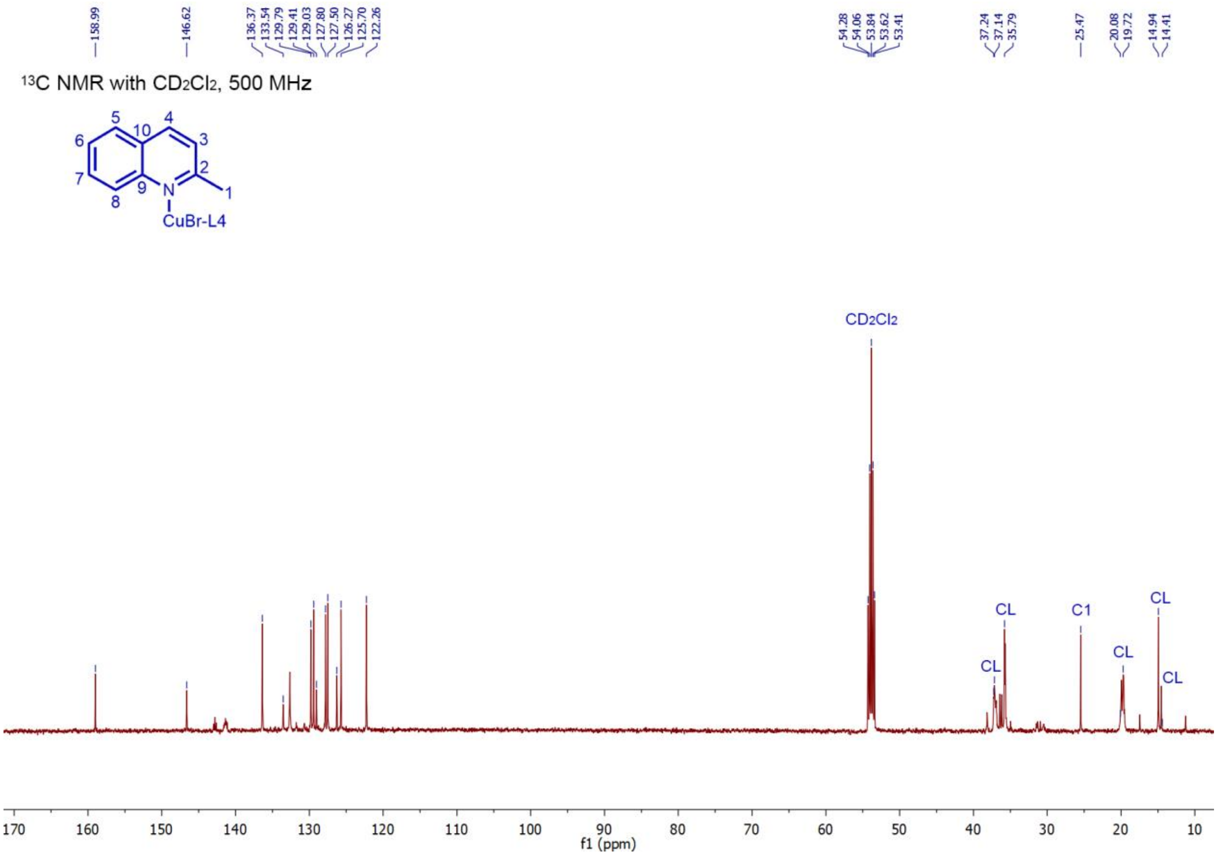


Figure S25. ^{1}H NMR spectrum of the mixture of 2-methyl-quinoline and **L4**-CuBr catalyst (top) and amplified aromatic part of ^{1}H NMR spectra (bottom).



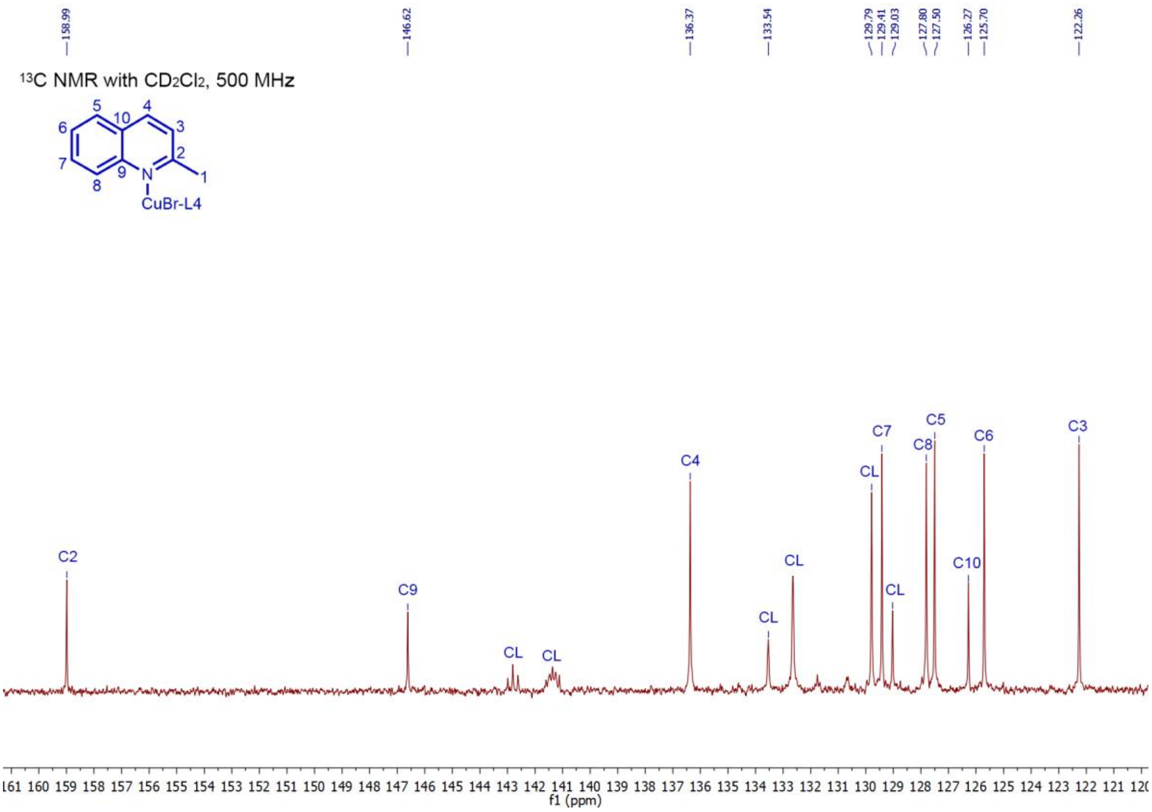
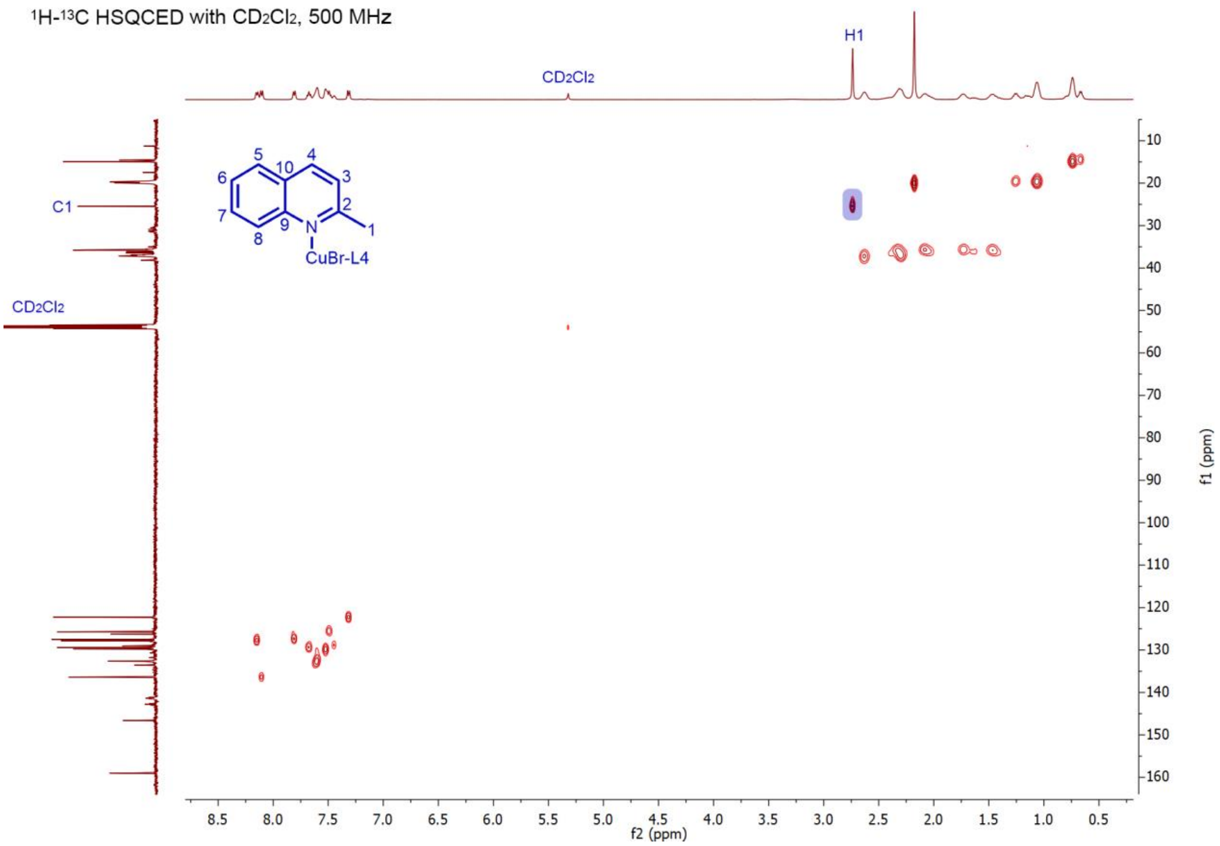


Figure S26. ^{13}C NMR spectrum of the mixture of 2-methyl-quinoline and **L4**-CuBr catalyst (top) and amplified aromatic part of ^{13}C NMR spectra (bottom).



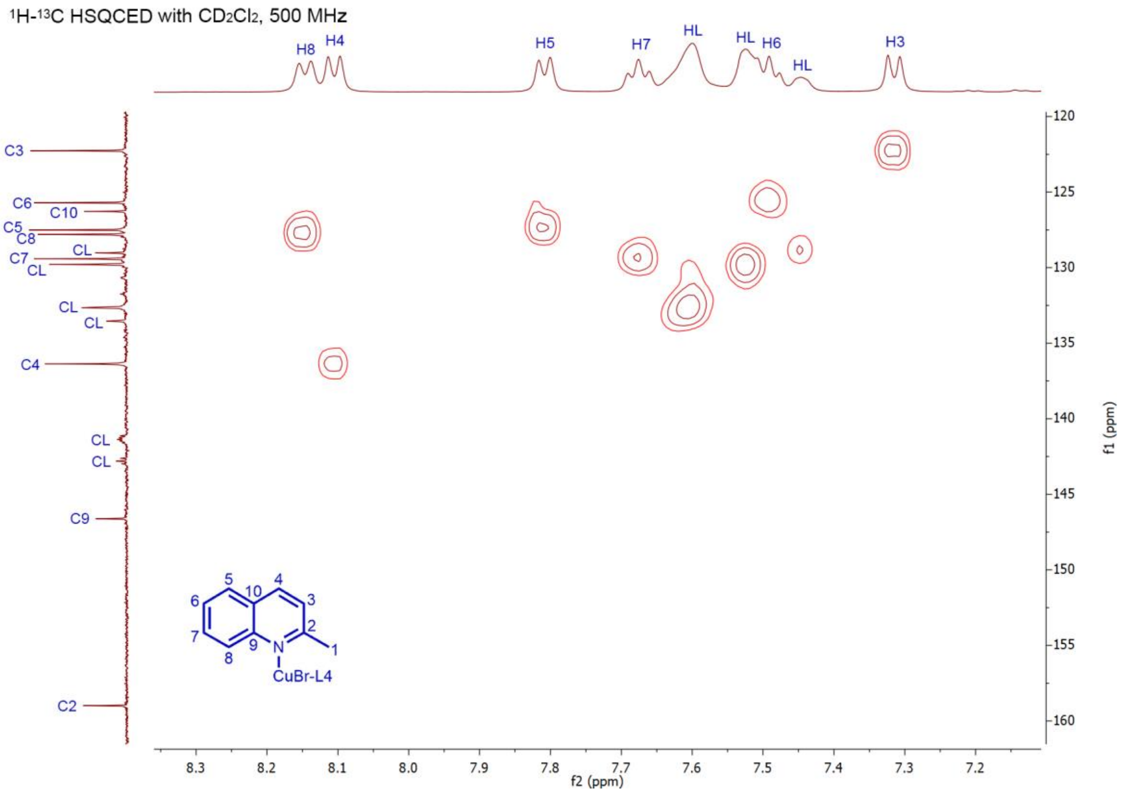
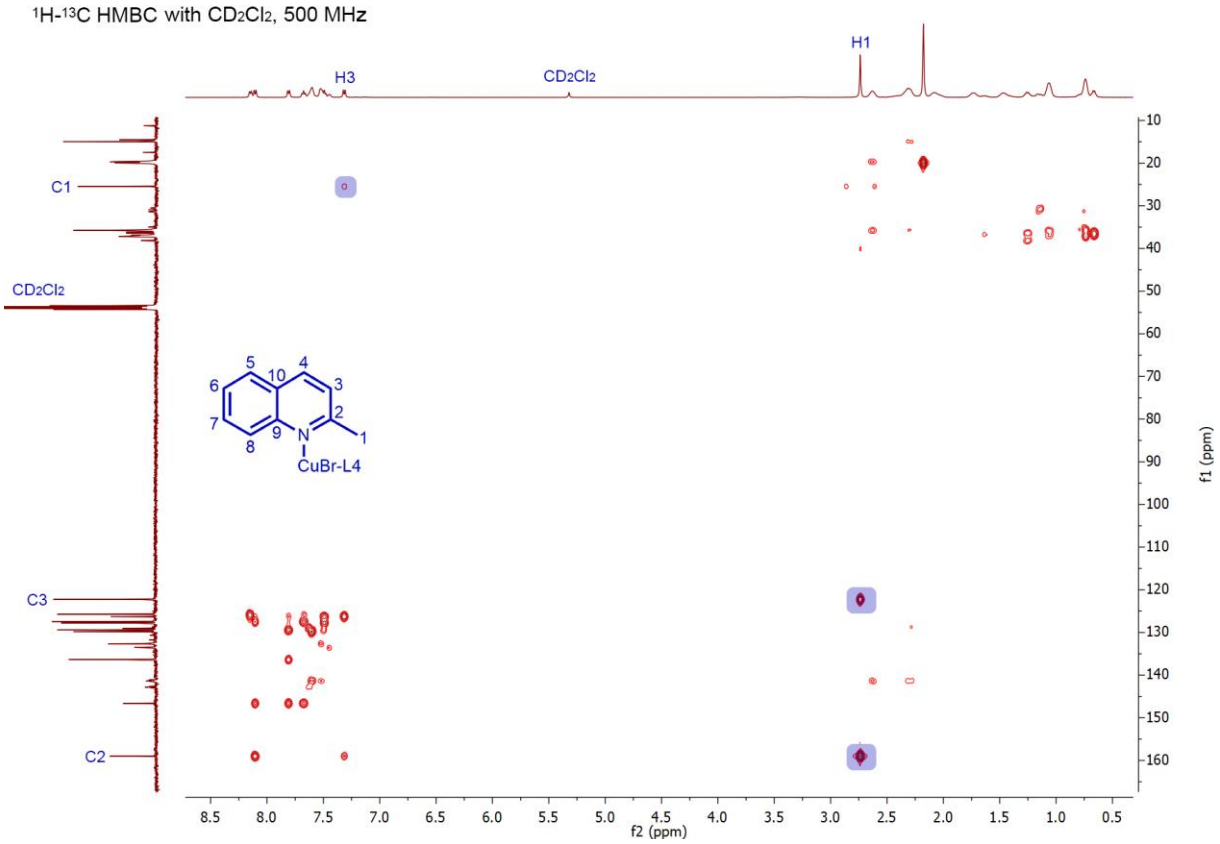


Figure S27. ^{1}H-^{13}C HSQCED spectrum of the mixture of 2-methyl-quinoline and **L4**-CuBr catalyst (top) and amplified aromatic part of ^{1}H-^{13}C HSQCED spectra (bottom).



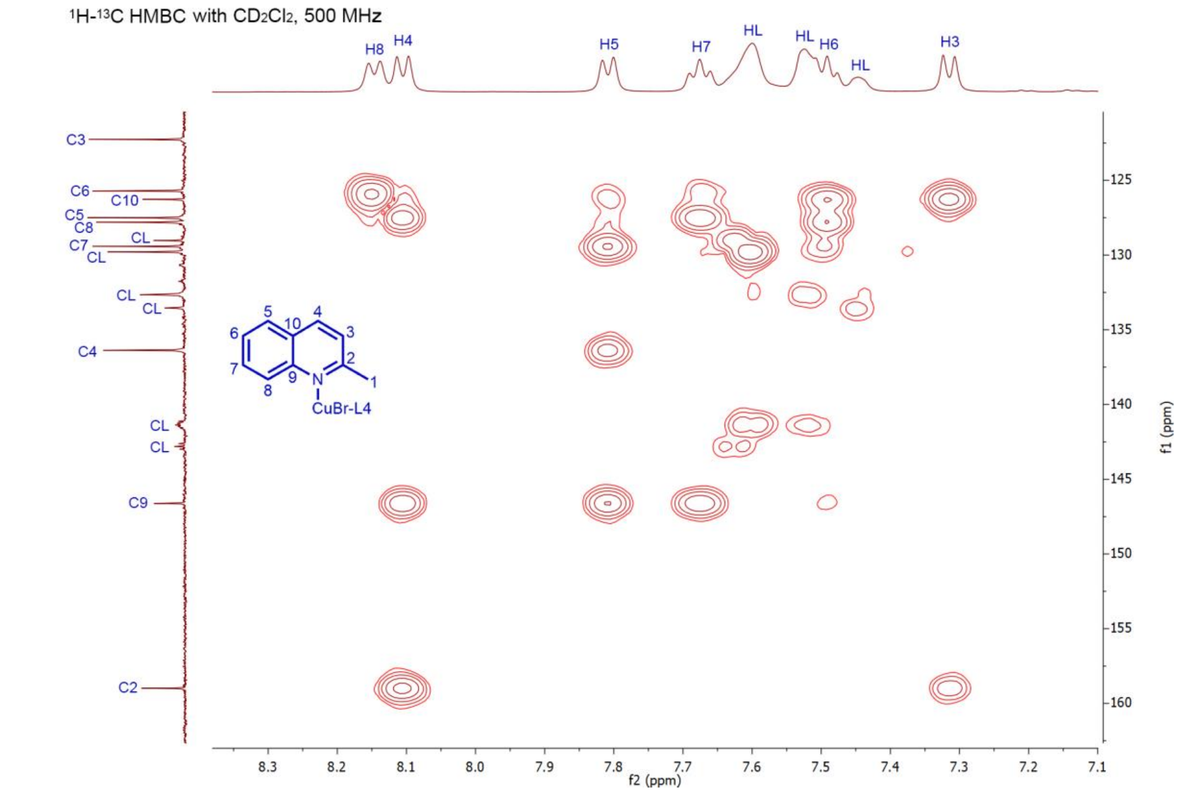
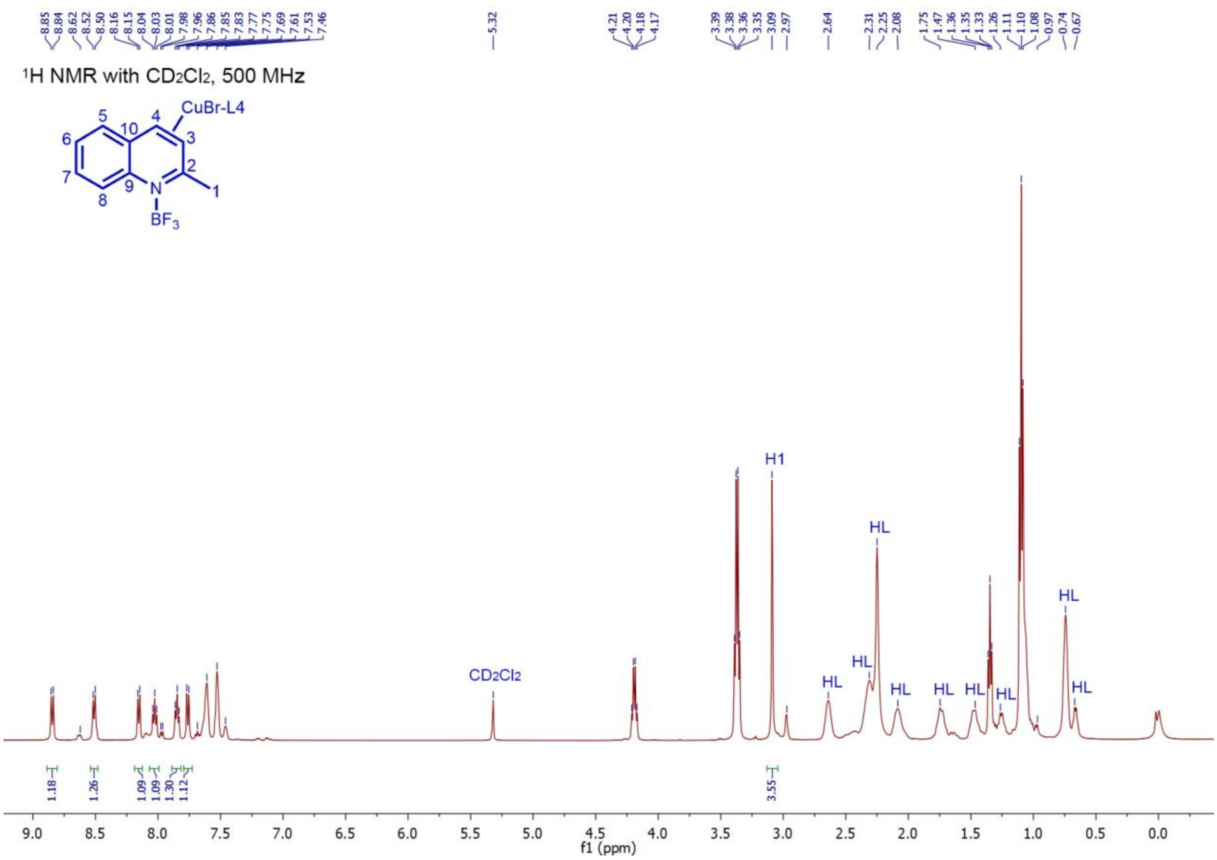


Figure S28. ^{1}H-^{13}C HMBC spectrum of the mixture of 2-methyl-quinoline and **L4**-CuBr catalyst (top) and amplified aromatic part of ^{1}H-^{13}C HMBC spectra (bottom).

Formation of 2-methyl-quinoline/BF_3/L4-CuBr complex

1 Equiv. of **L4-**CuBr catalyst and 2 equiv. of $BF_3{\cdot}Et_2O$ was added to a solution of 2-methyl-quinoline in CD_2Cl_2 in a dry NMR tube at −50 °C under N_2 atmosphere, leading to instantaneous formation of a new species which was immediately measured by NMR spectroscopy at −50 °C. Full characterization was carried out by ^{1}H NMR (Figure S29), ^{13}C NMR (Figure S30), ^{1}H-^{13}C-HSQCED (Figure S31) and ^{1}H-^{13}C-HMBC (Figure S32). The peaks of 2-methyl-quinoline for both ^{1}H NMR and ^{13}C NMR have shifted after adding $BF_3{\cdot}Et_2O$ and **L4-**CuBr, and the spectra are different from 2-methyl-quinoline-BF_3 complex and 2-methyl-quinoline- **L4-**CuBr complex.



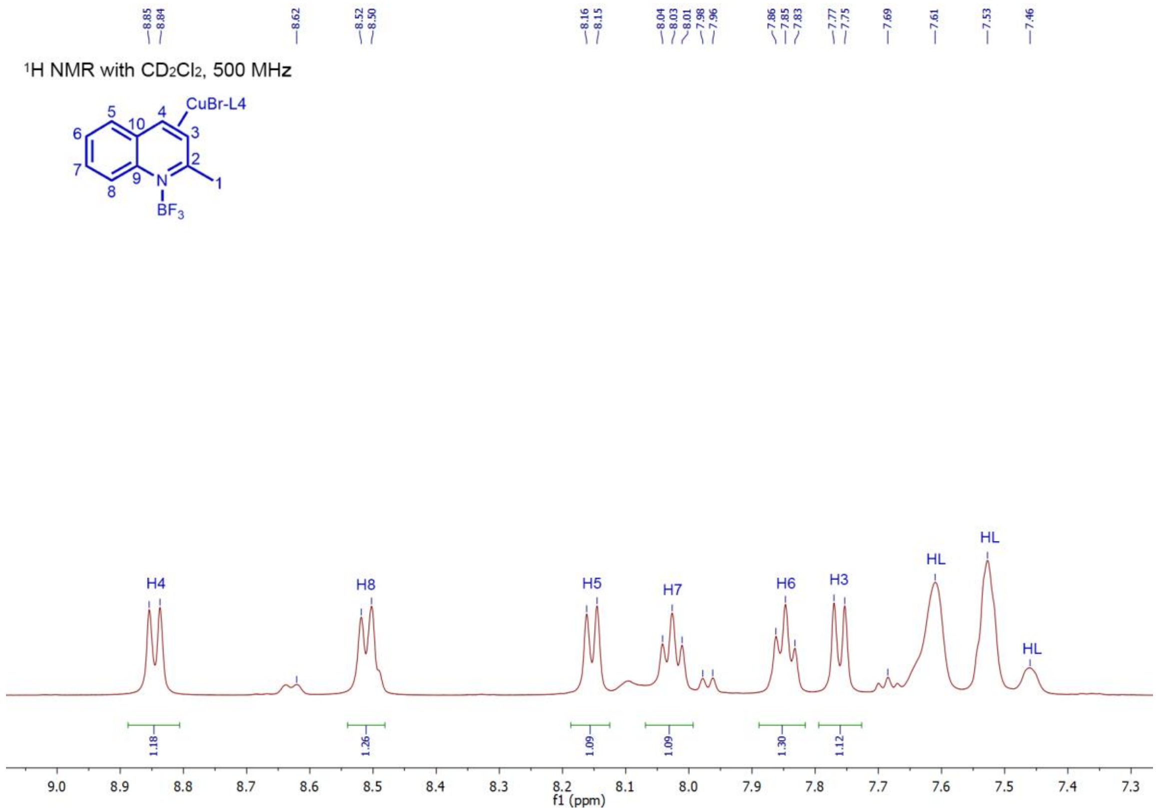
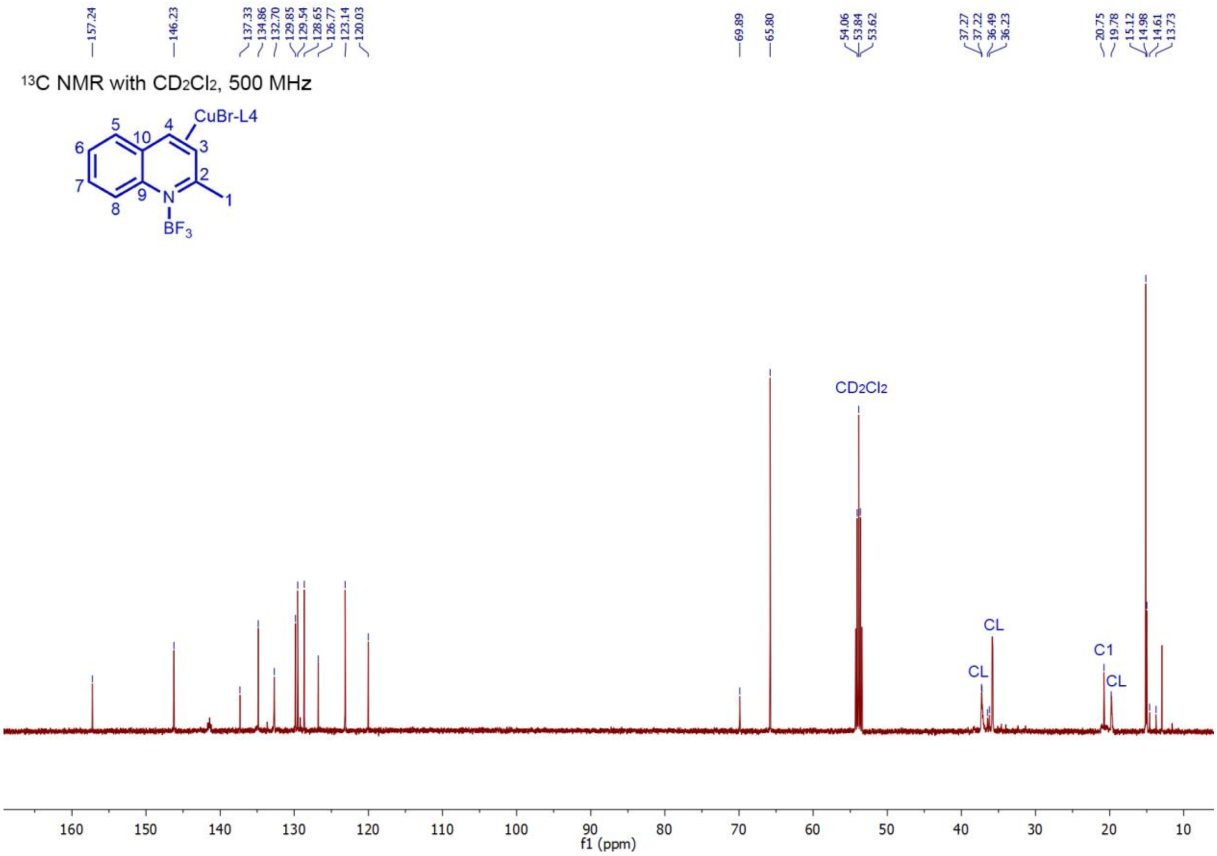


Figure S29. ^{1}H NMR spectrum of the mixture of 2-methyl-quinoline, $BF_3{\cdot}Et_2O$ and **L4**-CuBr catalyst (top) and amplified aromatic part of ^{1}H NMR spectra (bottom).



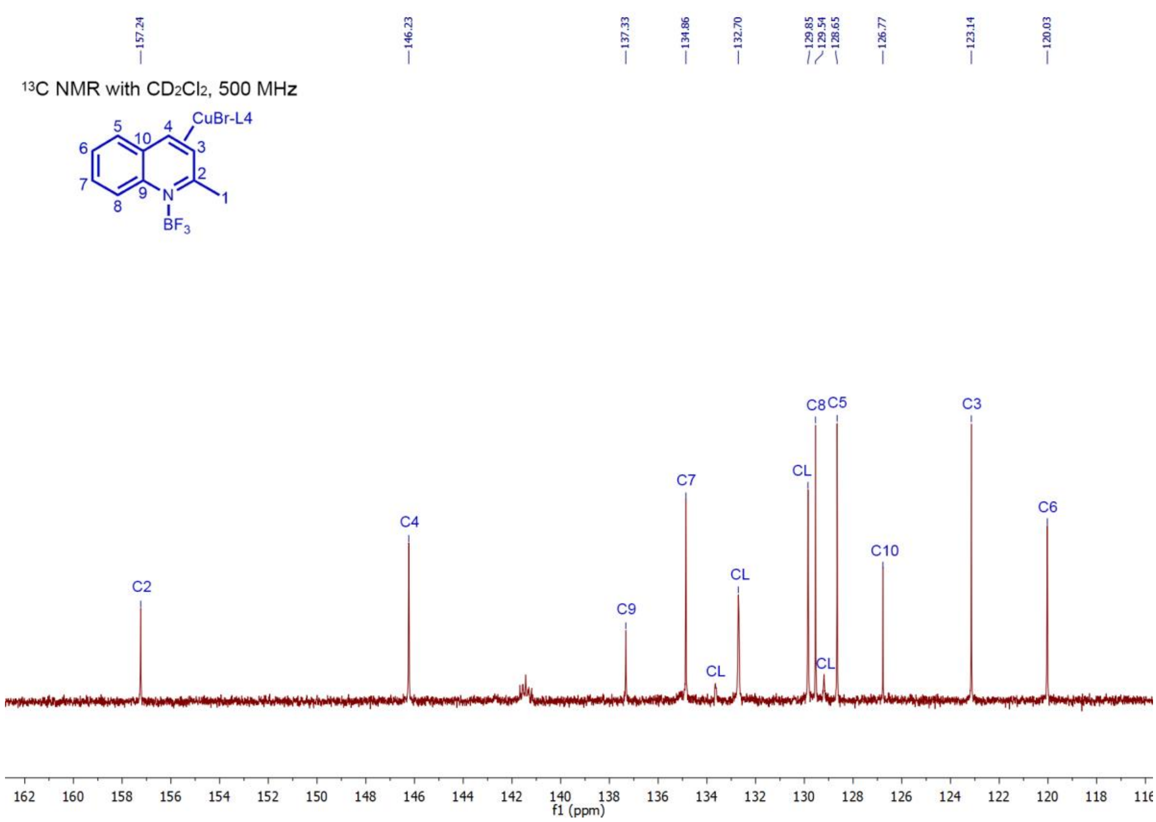
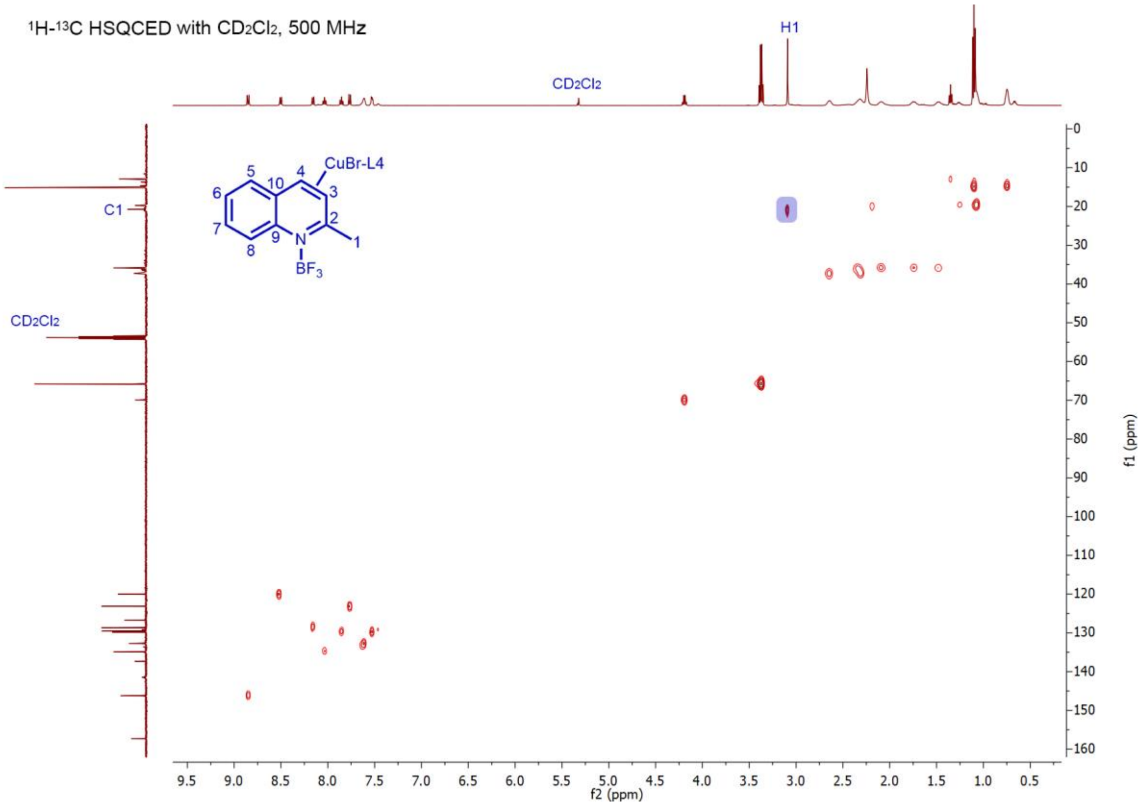


Figure S30. ^{13}C NMR spectrum of the mixture of 2-methyl-quinoline, $BF_3{\cdot}Et_2O$ and **L4**-CuBr catalyst (top) and amplified aromatic part of ^{13}C NMR spectra (bottom).



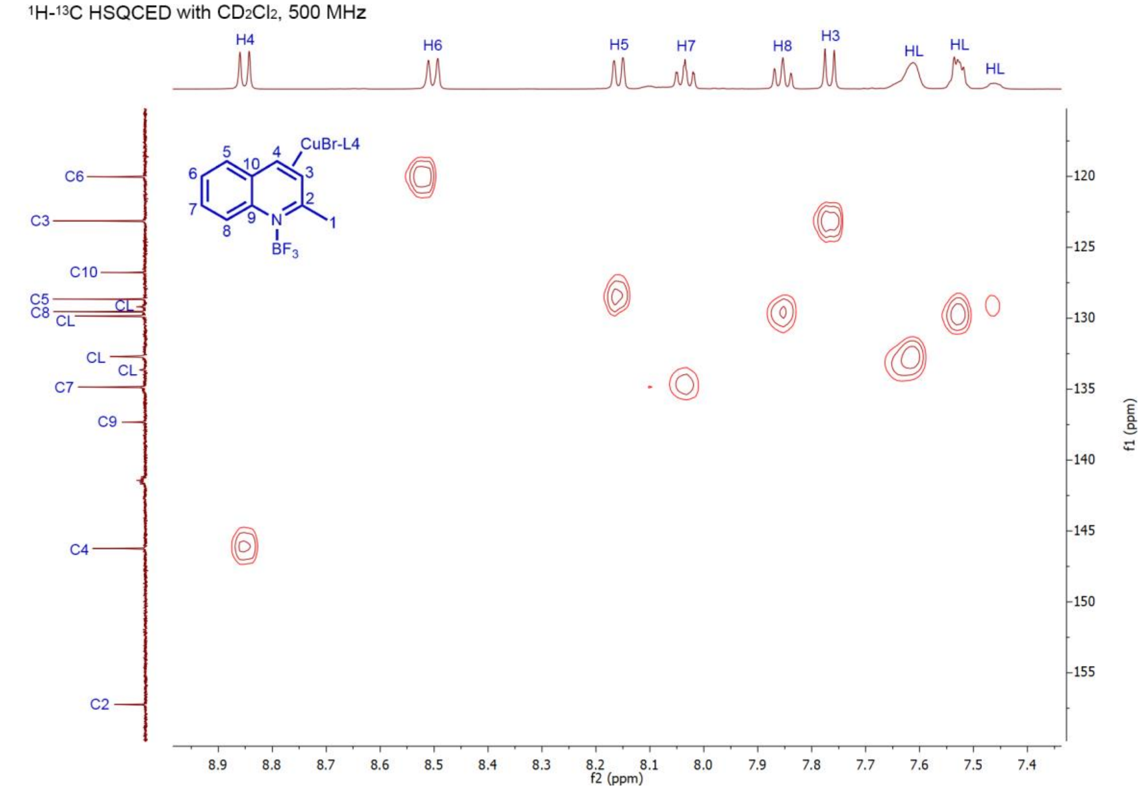
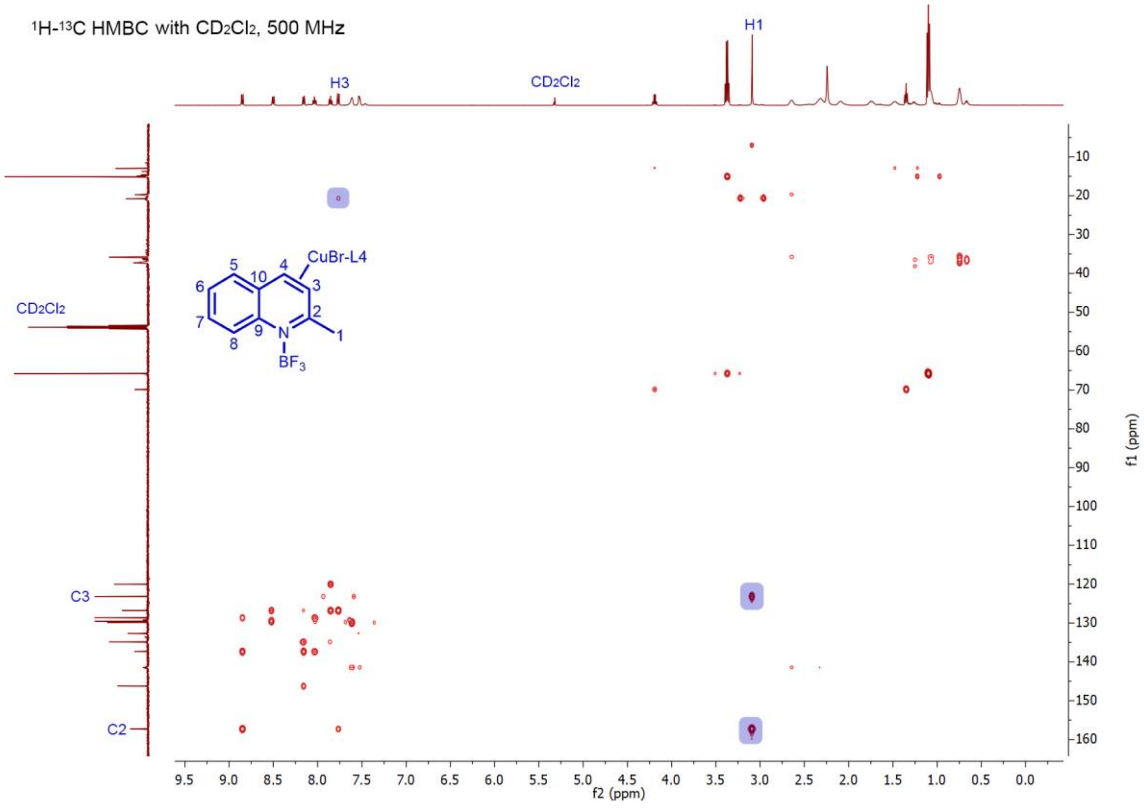


Figure S31. ^{1}H-^{13}C HSQCED spectrum of the mixture of 2-methyl-quinoline, $BF_3 \cdot Et_2O$ and **L4**-CuBr catalyst (top) and amplified aromatic part of ^{1}H-^{13}C HSQCED spectra (bottom).



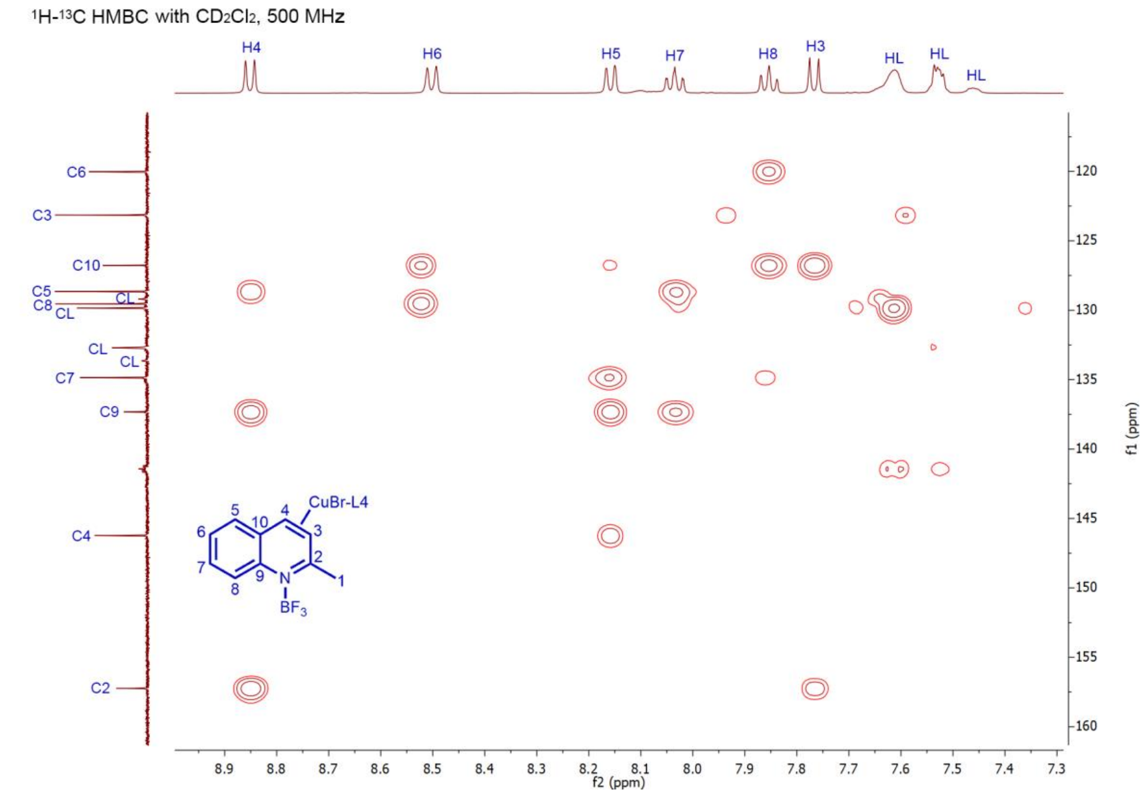


Figure S32. ^{1}H-^{13}C HMBC spectrum of the mixture of 2-methyl-quinoline, $BF_3 \cdot Et_2O$ and **L4**-CuBr catalyst (top) and amplified aromatic part of ^{1}H-^{13}C HMBC spectra (bottom).

Comparison of the ^{1}H NMR spectra of L4-CuBr with the mixture of L4-CuBr catalyst and $BF_3·Et_2O$

L4-CuBr catalyst was added to CD_2Cl_2 in a dry NMR tube at −50 °C under N_2 atmosphere, and immediately measured by NMR spectroscopy at −50 °C. 2 Equiv. of $BF_3·Et_2O$ was added to a solution of **L4**-CuBr in CD_2Cl_2 in a dry NMR tube at −50 °C under N_2 atmosphere, and immediately measured by NMR spectroscopy at −50 °C. Comparison were made for ^{1}H NMR (Figure S33), ^{13}C NMR (Figure S34) and ^{31}P NMR (Figure S35). The peaks of **L4**-CuBr catalyst for ^{1}H NMR, ^{13}C NMR and ^{31}P NMR have no shifted after addition of $BF_3·Et_2O$, indicating that BF_3 cannot displace CuBr to coordinate with **L4**.

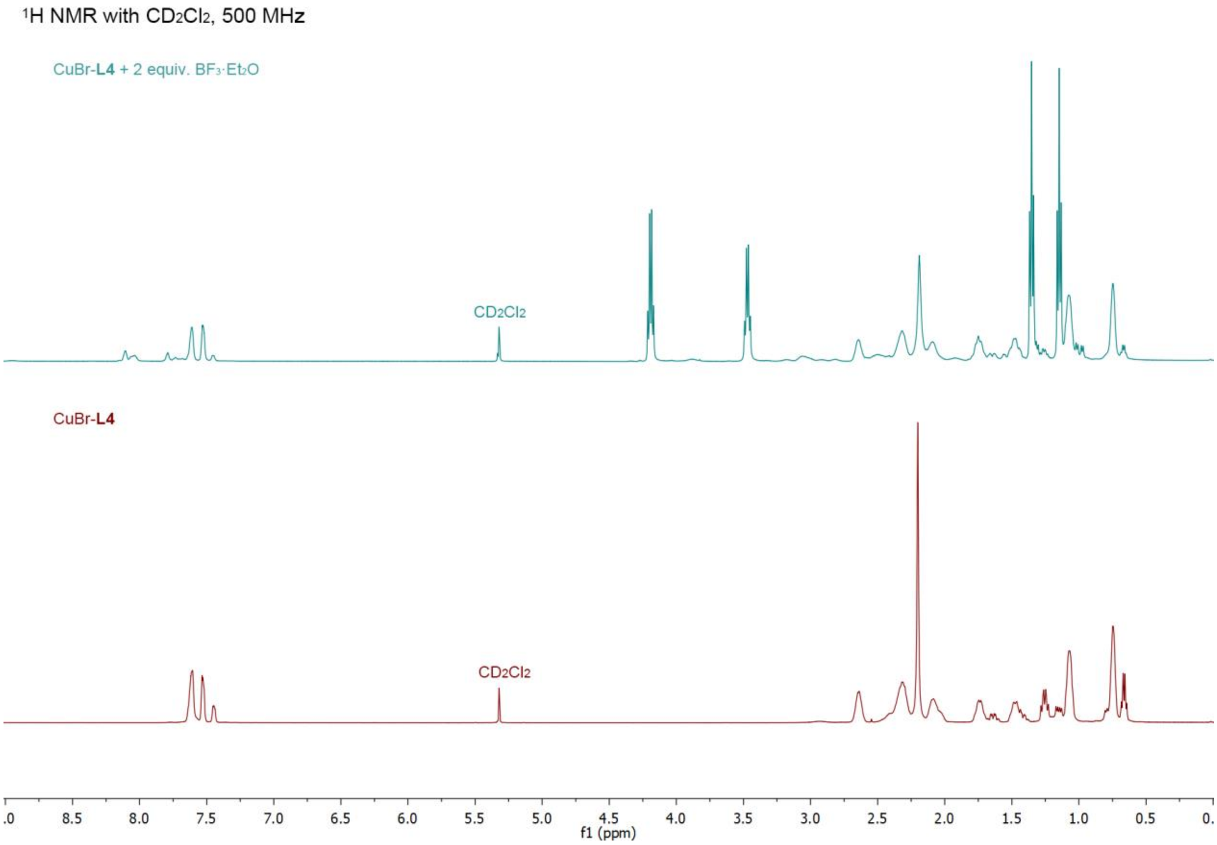


Figure S33. Comparison of the ^{1}H NMR spectra of **L4**-CuBr with the mixture of **L4**-CuBr catalyst and $BF_3·Et_2O$.

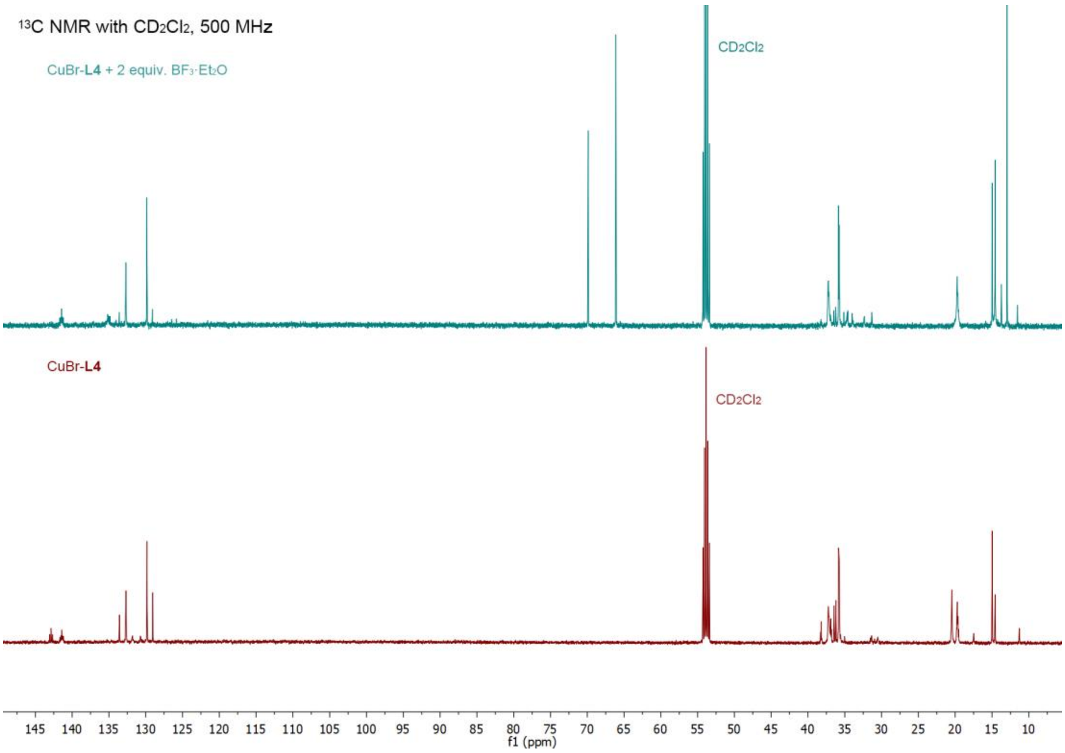


Figure S34. Comparison of the ^{13}C NMR spectra of **L4**-CuBr with the mixture of **L4**-CuBr catalyst and $BF_3 \cdot Et_2O$.

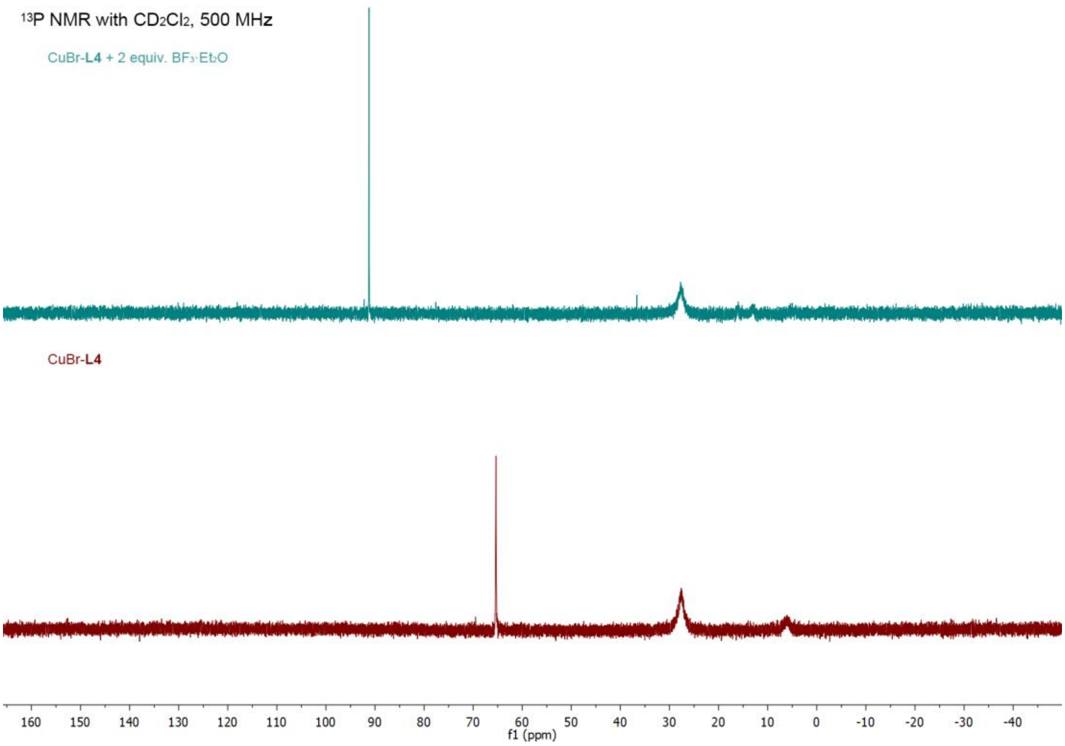
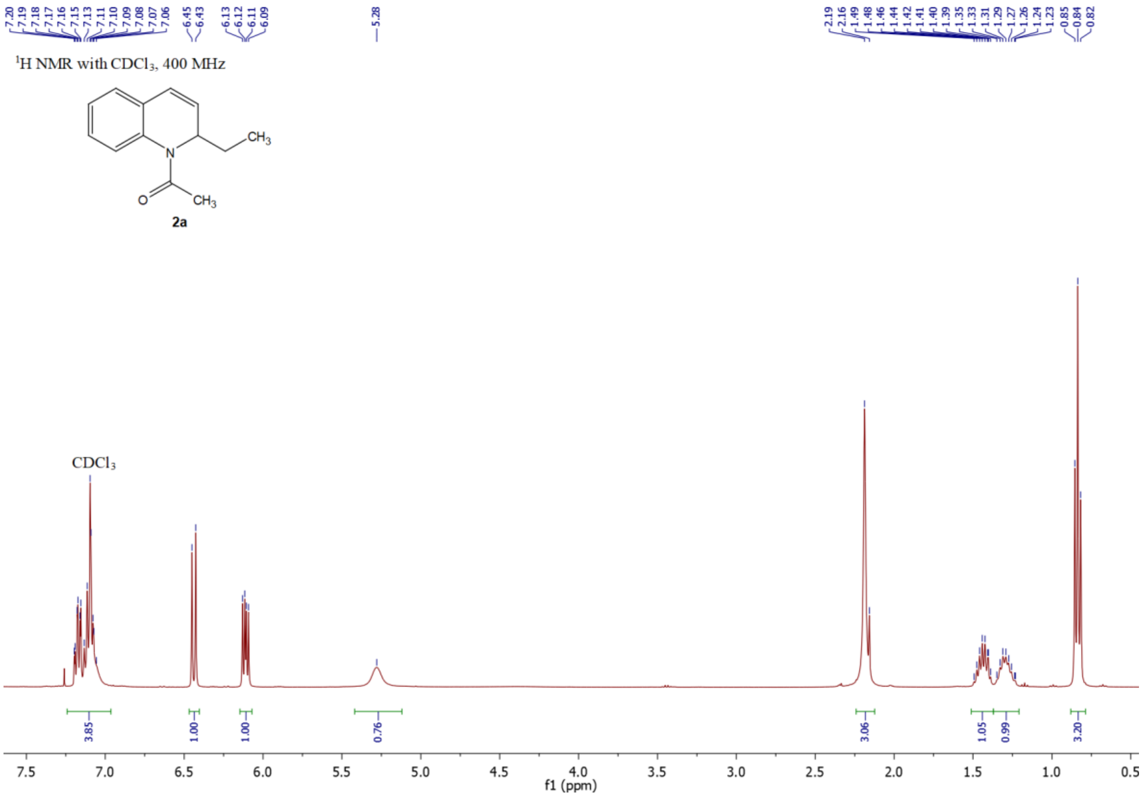


Figure S35. Comparison of the ^{31}P NMR spectra of **L4**-CuBr with the mixture of **L4**-CuBr catalyst and $BF_3 \cdot Et_2O$.

10. NMR spectra



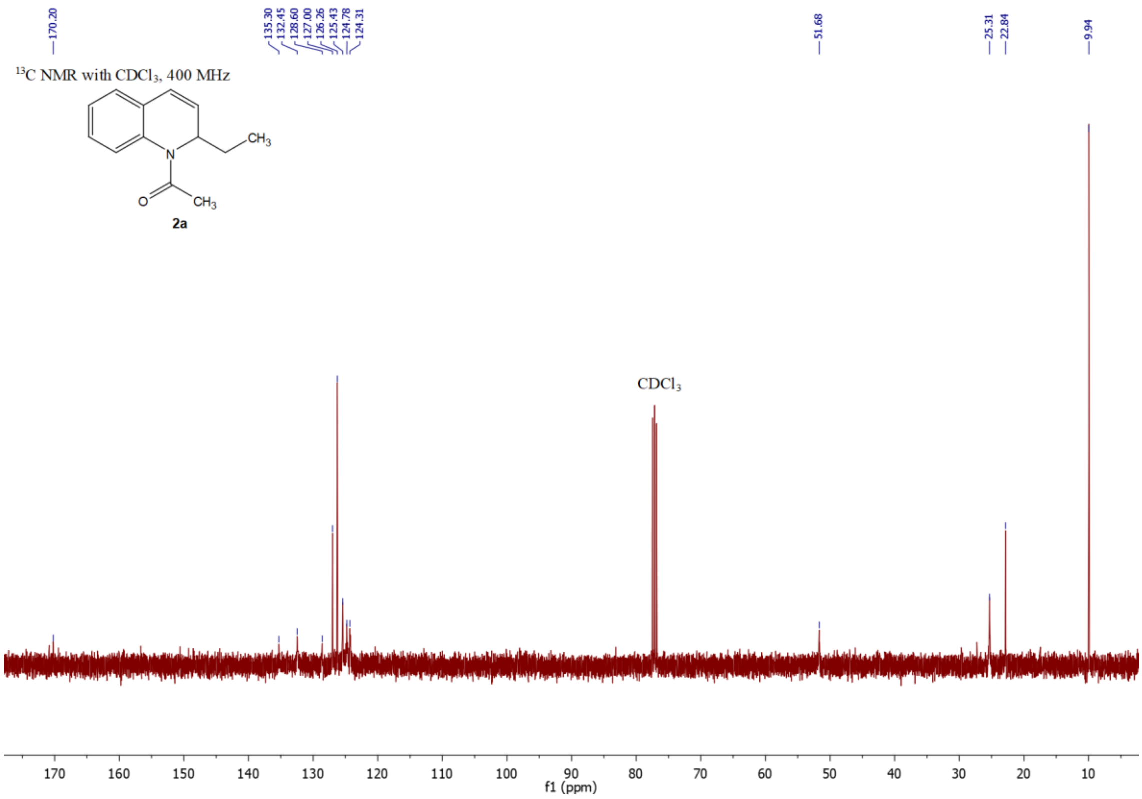
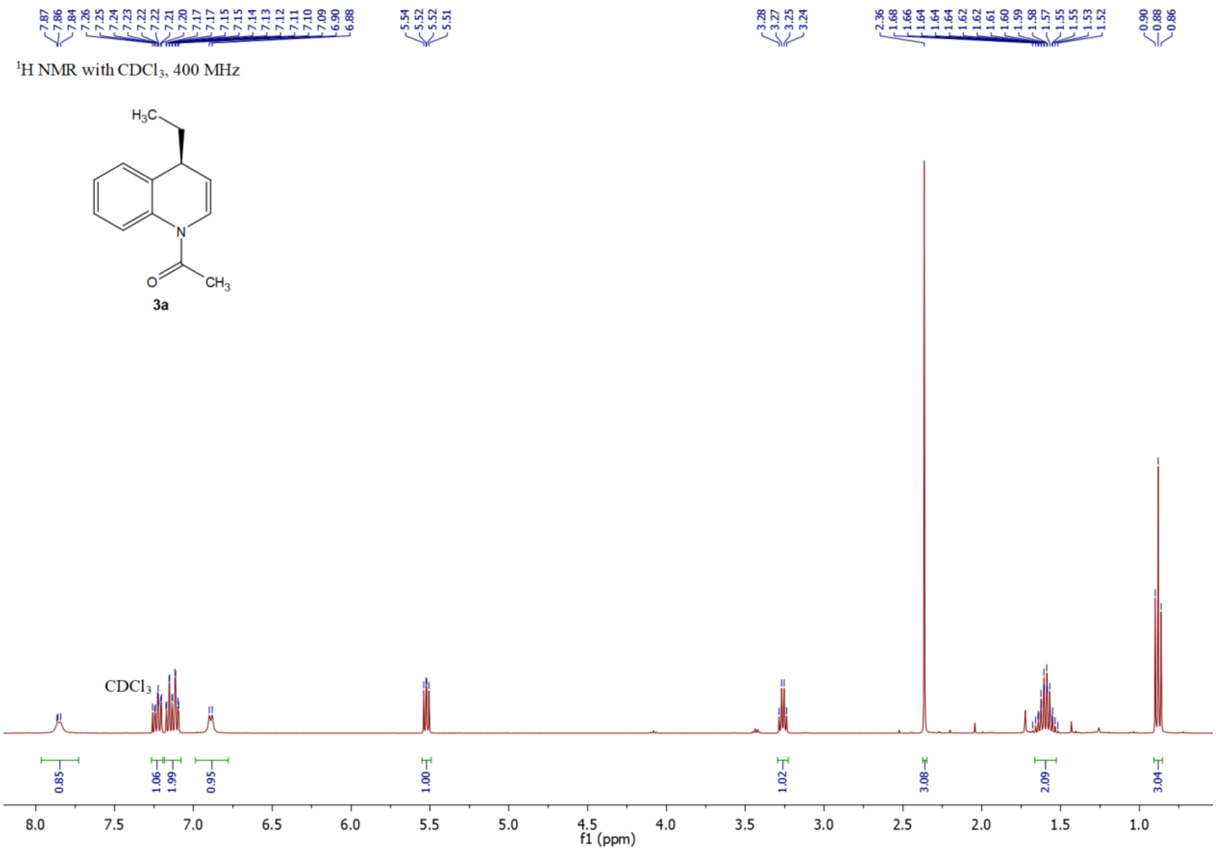


Figure S36. NMR spectra of 1-acetyl-2-ethyl-C2-dihydroquinoline (**2a**)



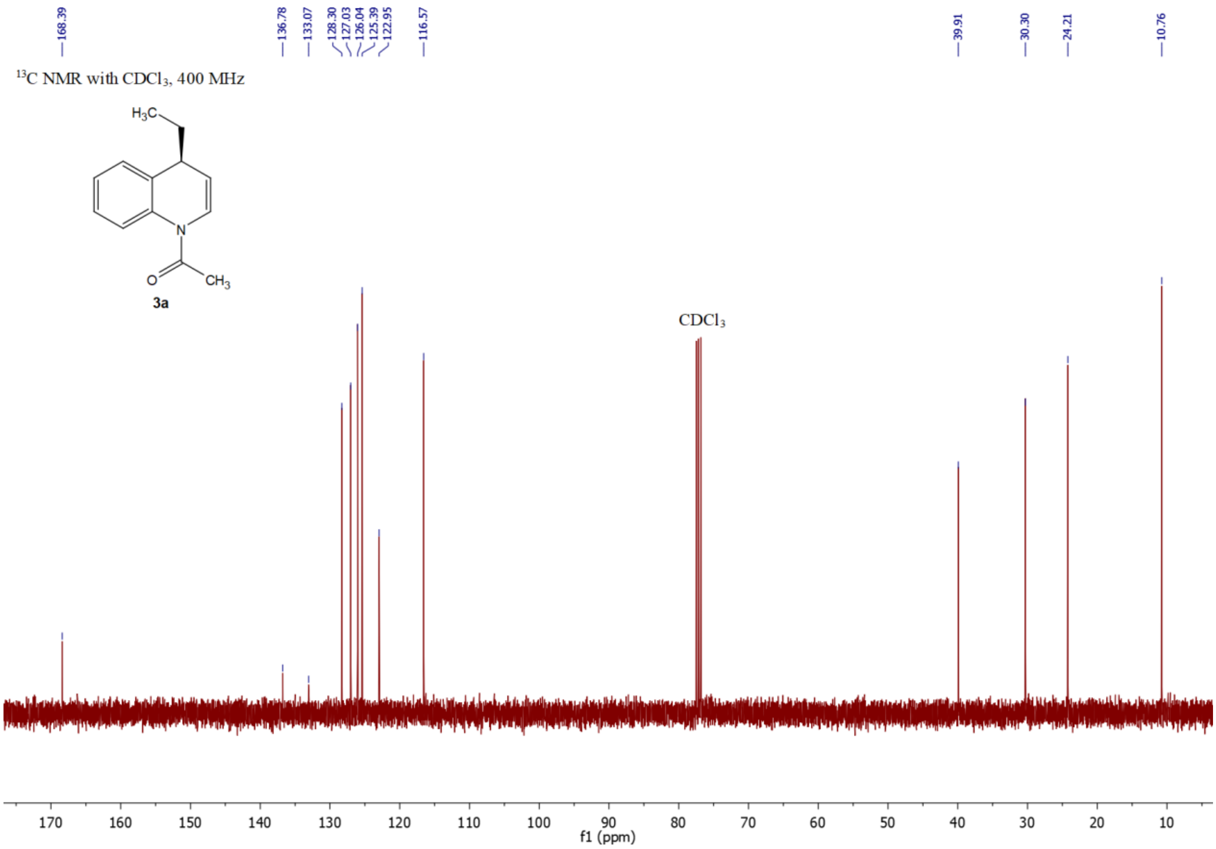
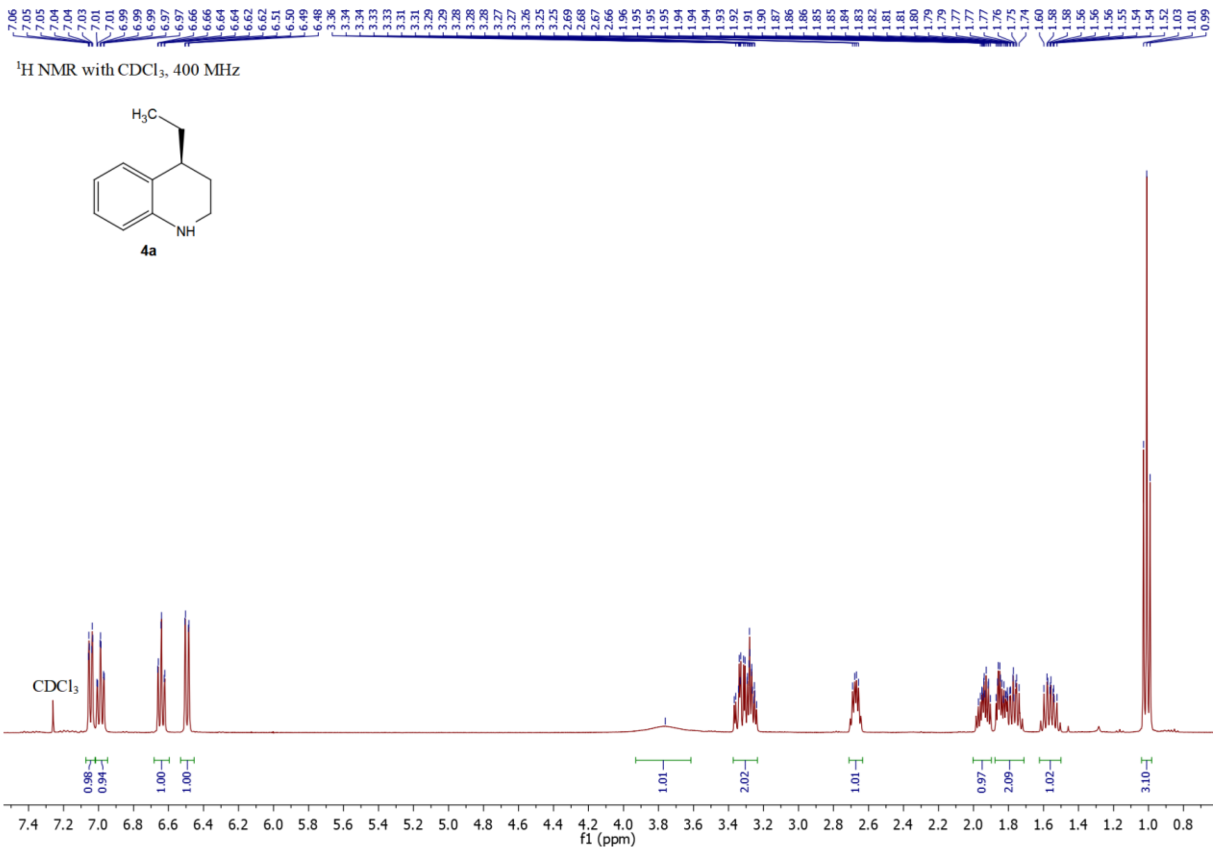


Figure S37. NMR spectra of (*S*)-1-acetyl-4-ethyl-C4-dihydroquinoline (**3a**)



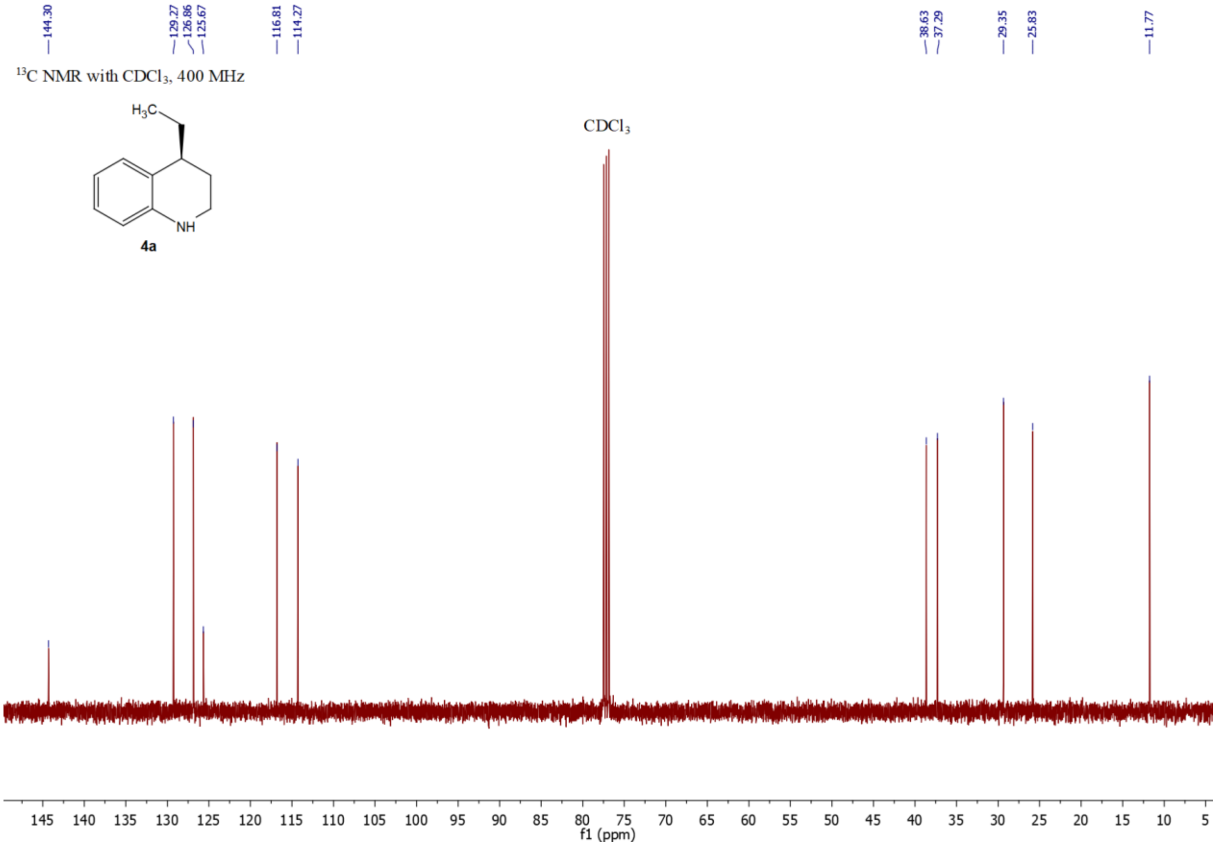
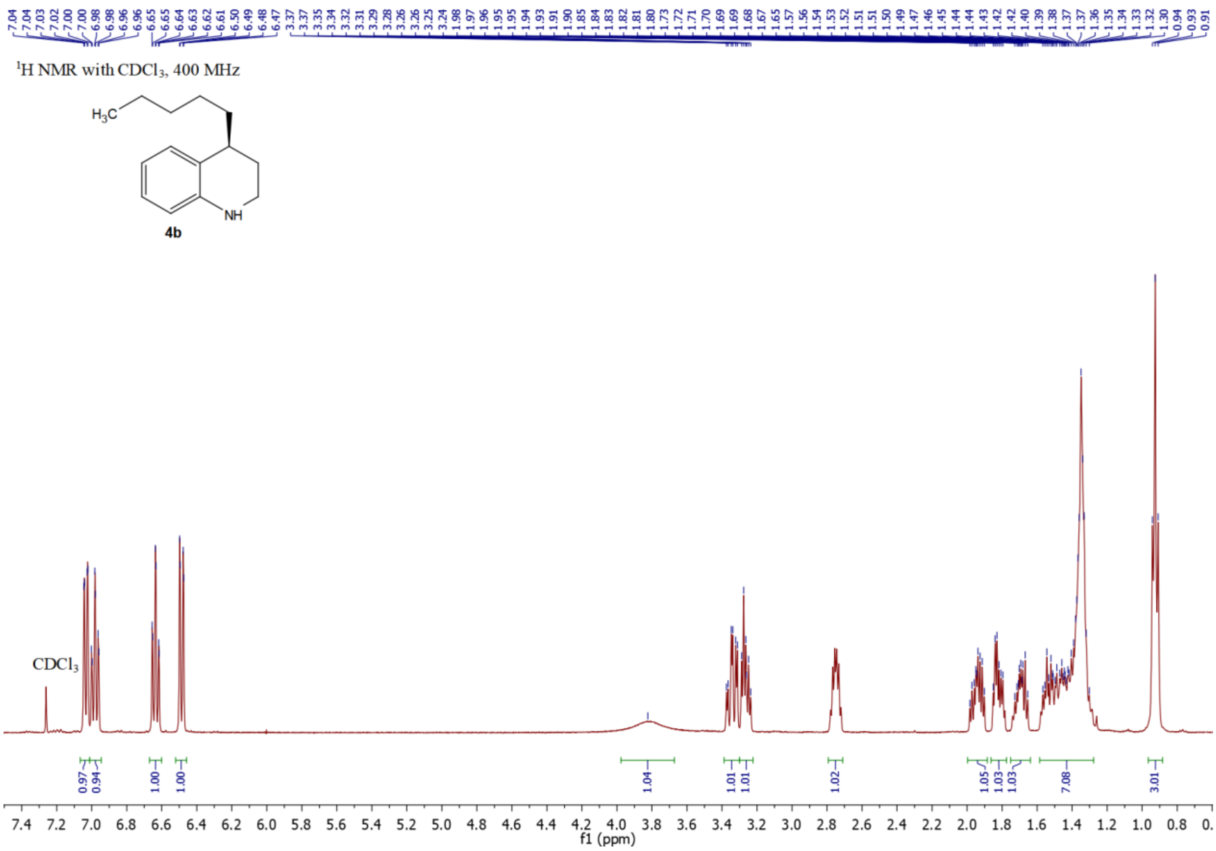


Figure S38. NMR spectra of (*S*)-4-Ethyl-1,2,3,4-tetrahydroquinoline (**4a**)



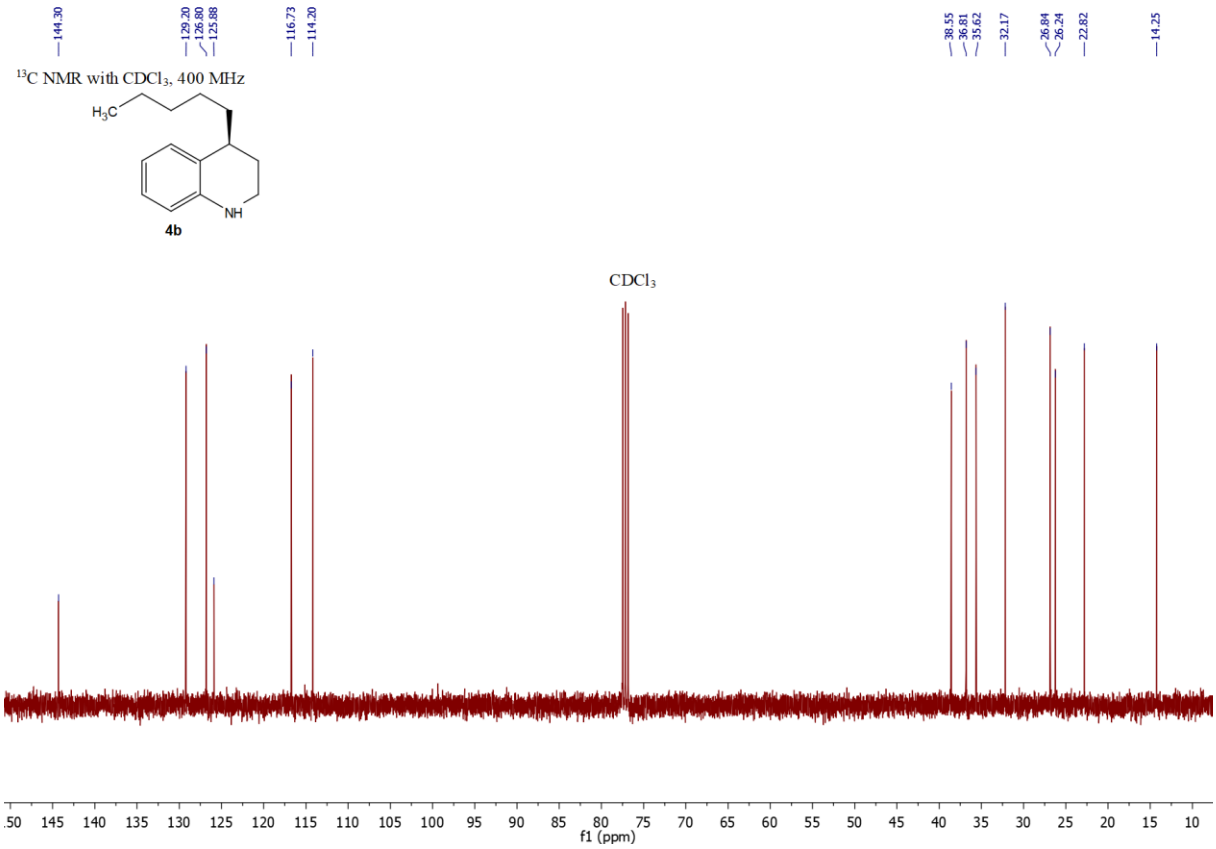
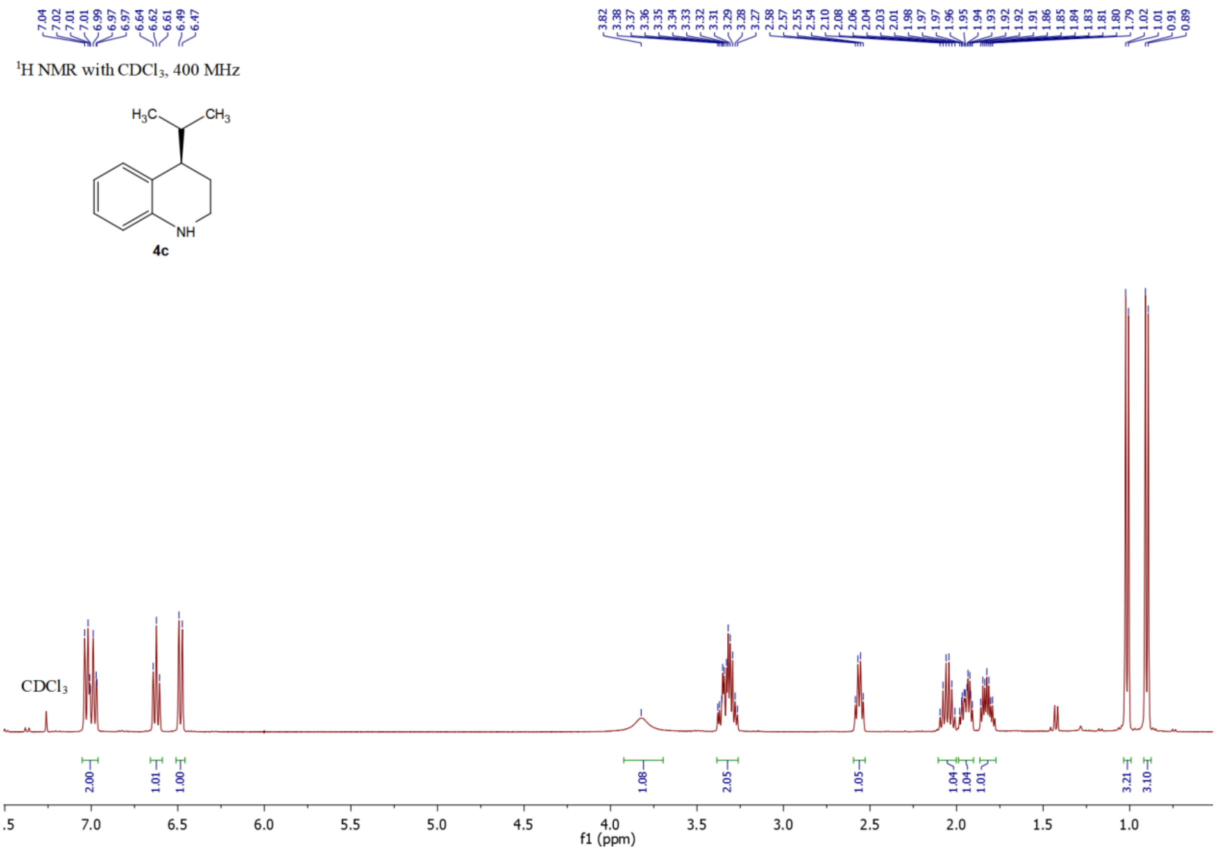


Figure S39. NMR spectra of (*S*)-4-Pentyl-1,2,3,4-tetrahydroquinoline (**4b**)



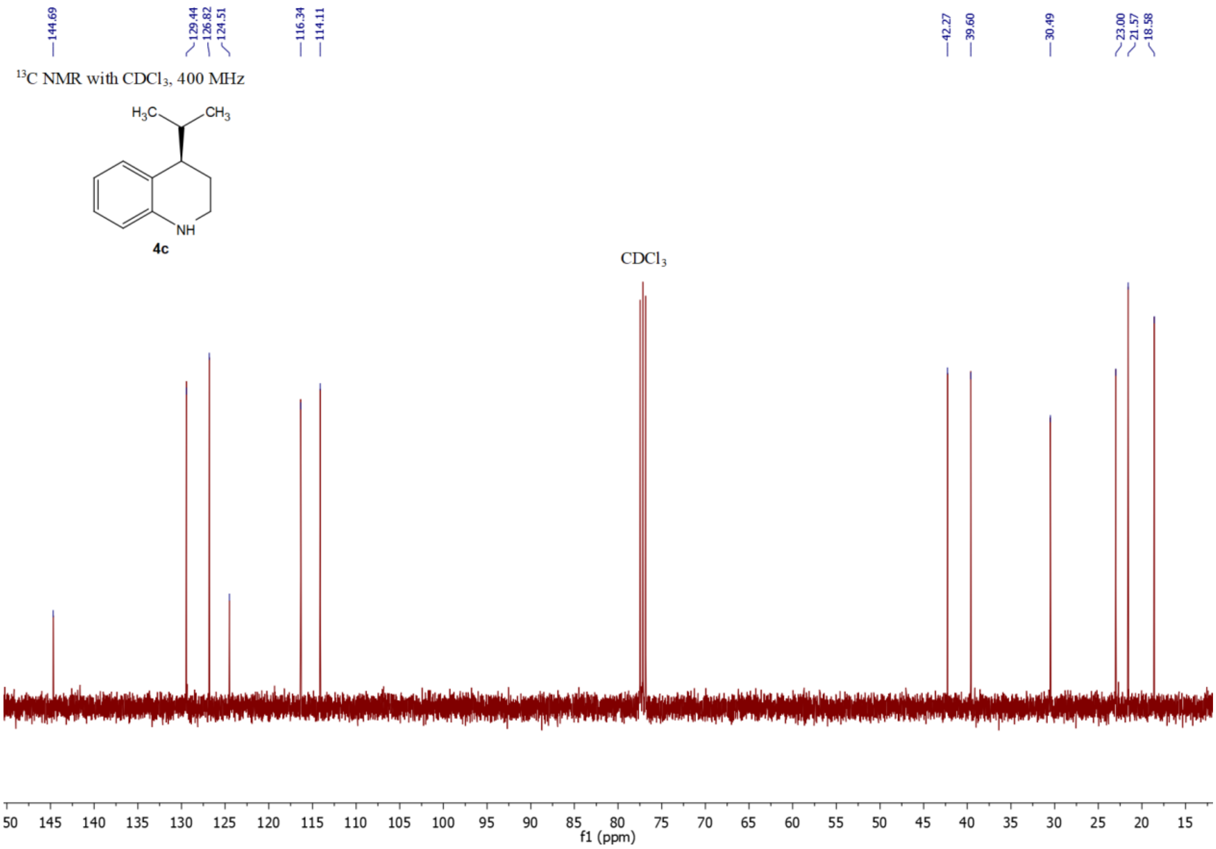
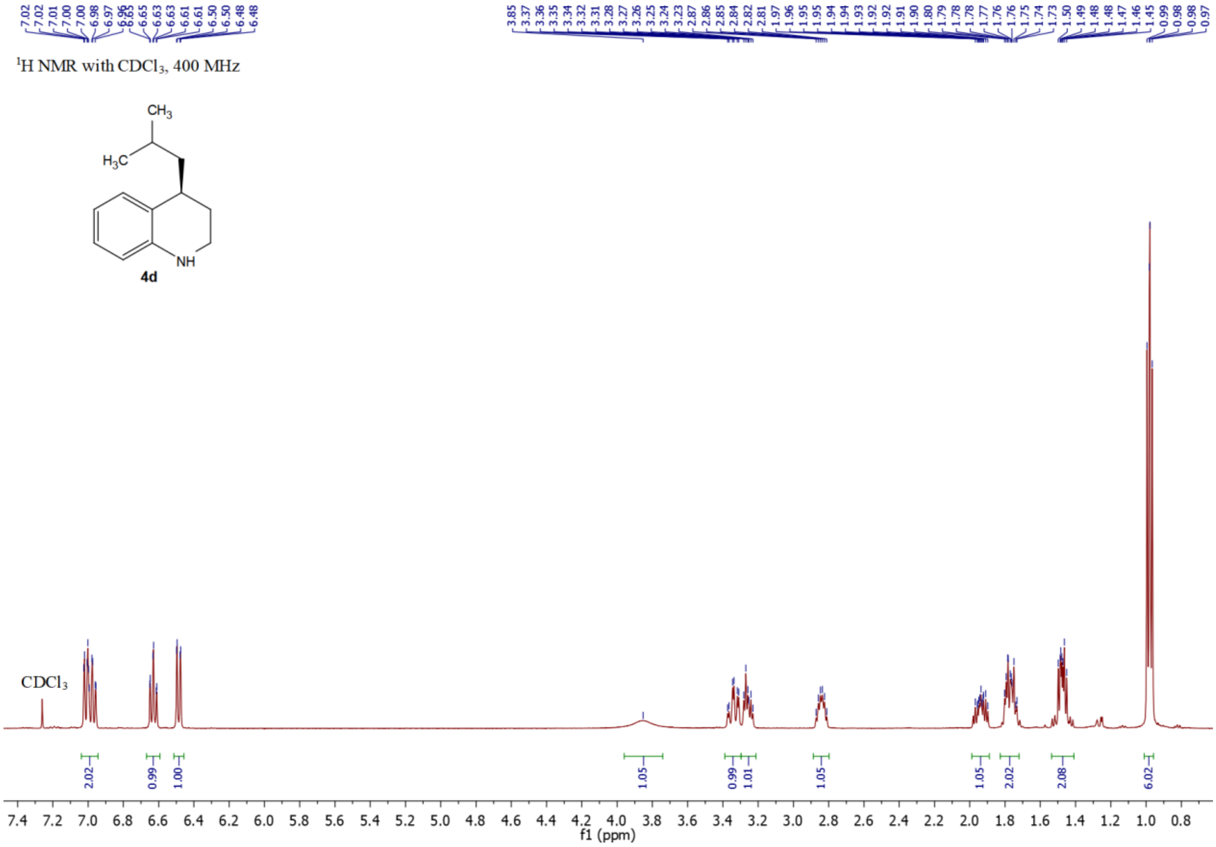


Figure S40. NMR spectra of (*R*)-4-(1-methylethyl)-1,2,3,4-tetrahydroquinoline (**4c**)



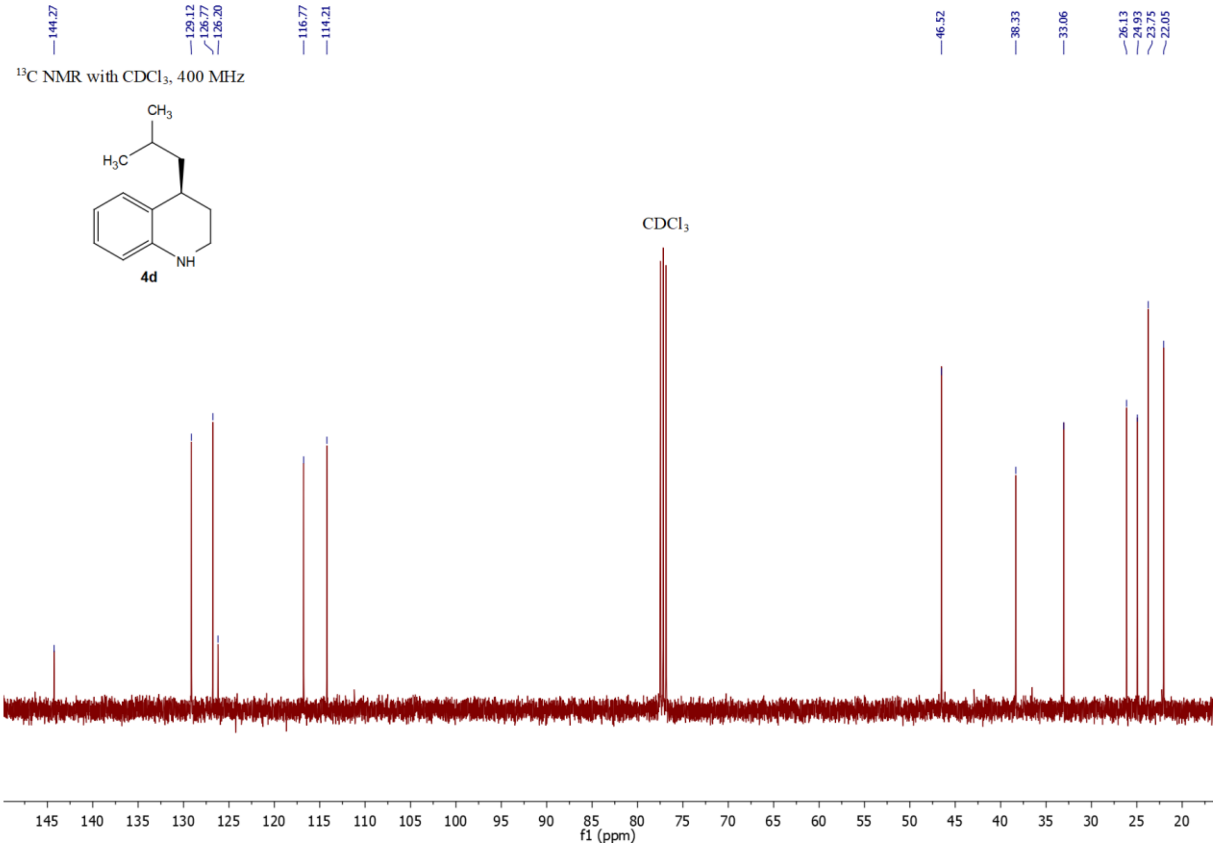
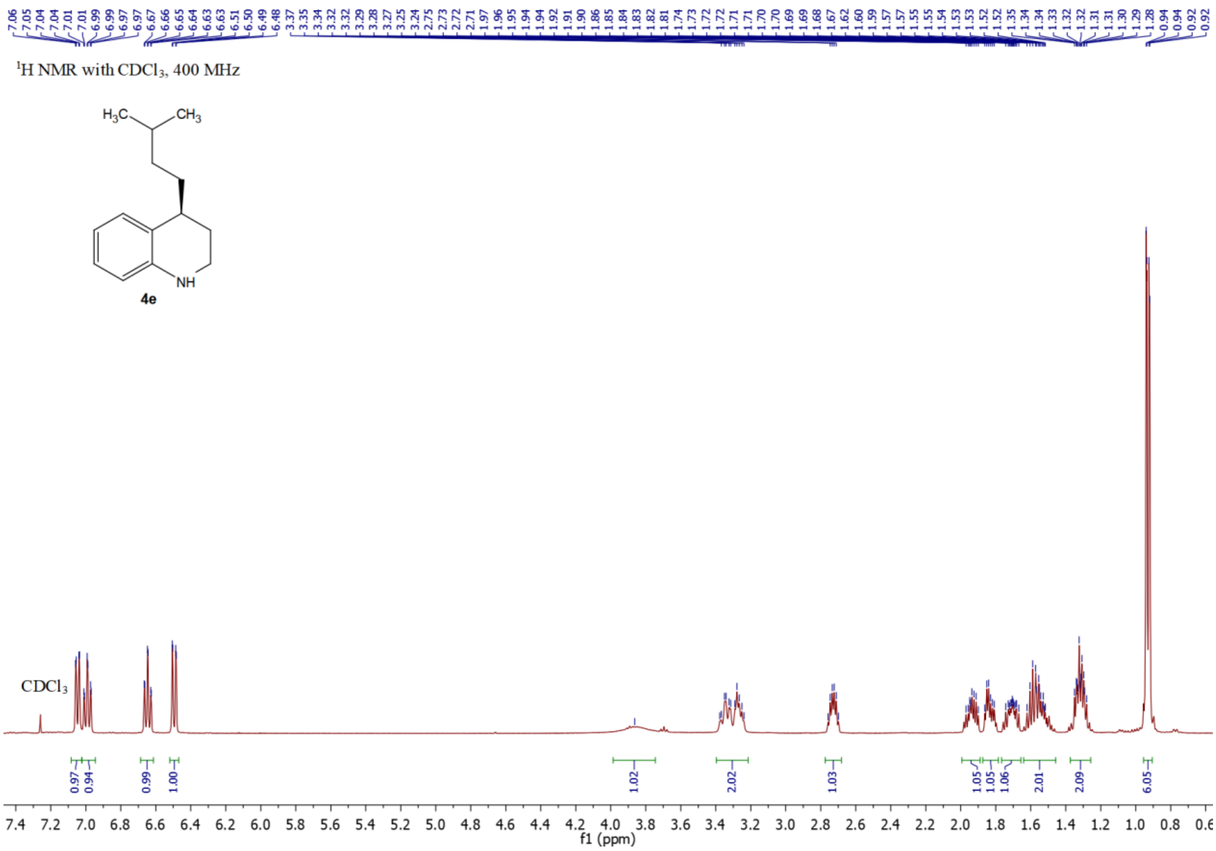


Figure S41. NMR spectra of (*S*)-4-(2-methylpropyl)-1,2,3,4-tetrahydroquinoline (**4d**)



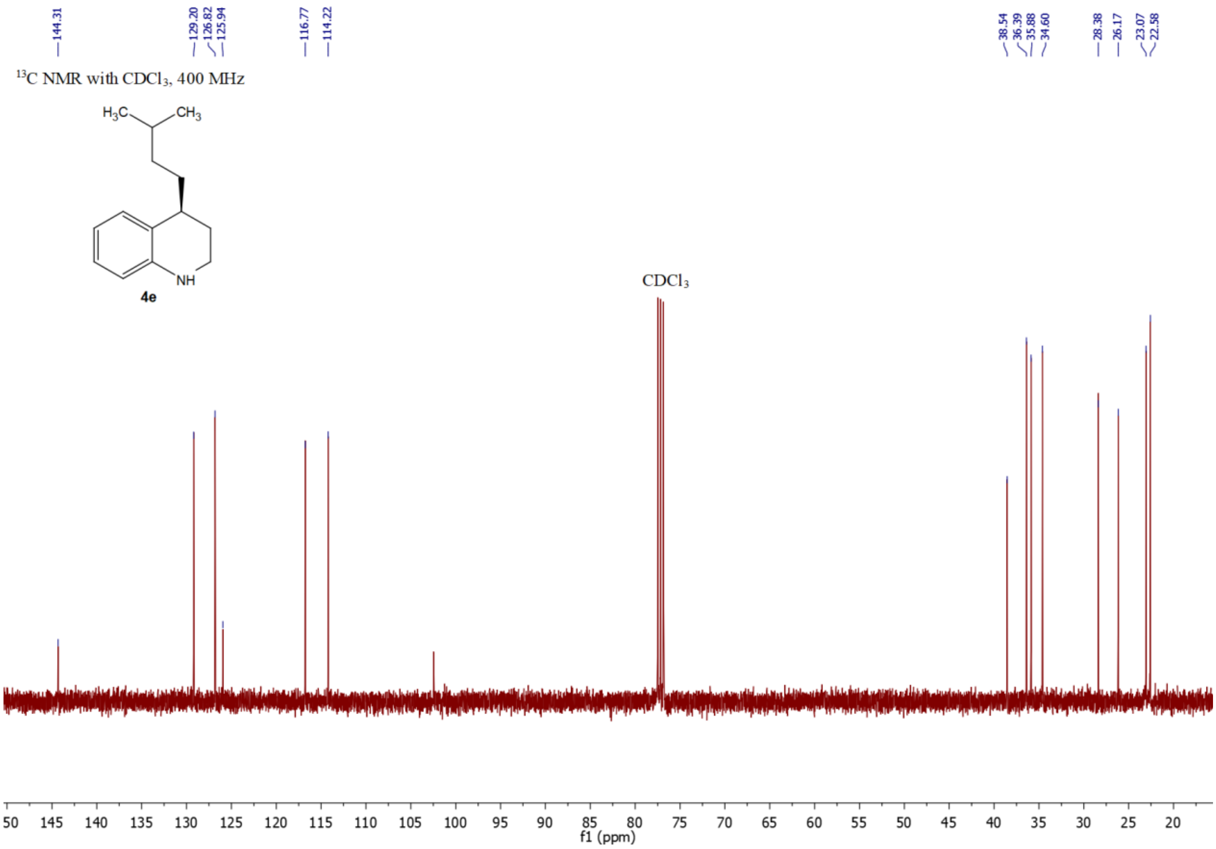
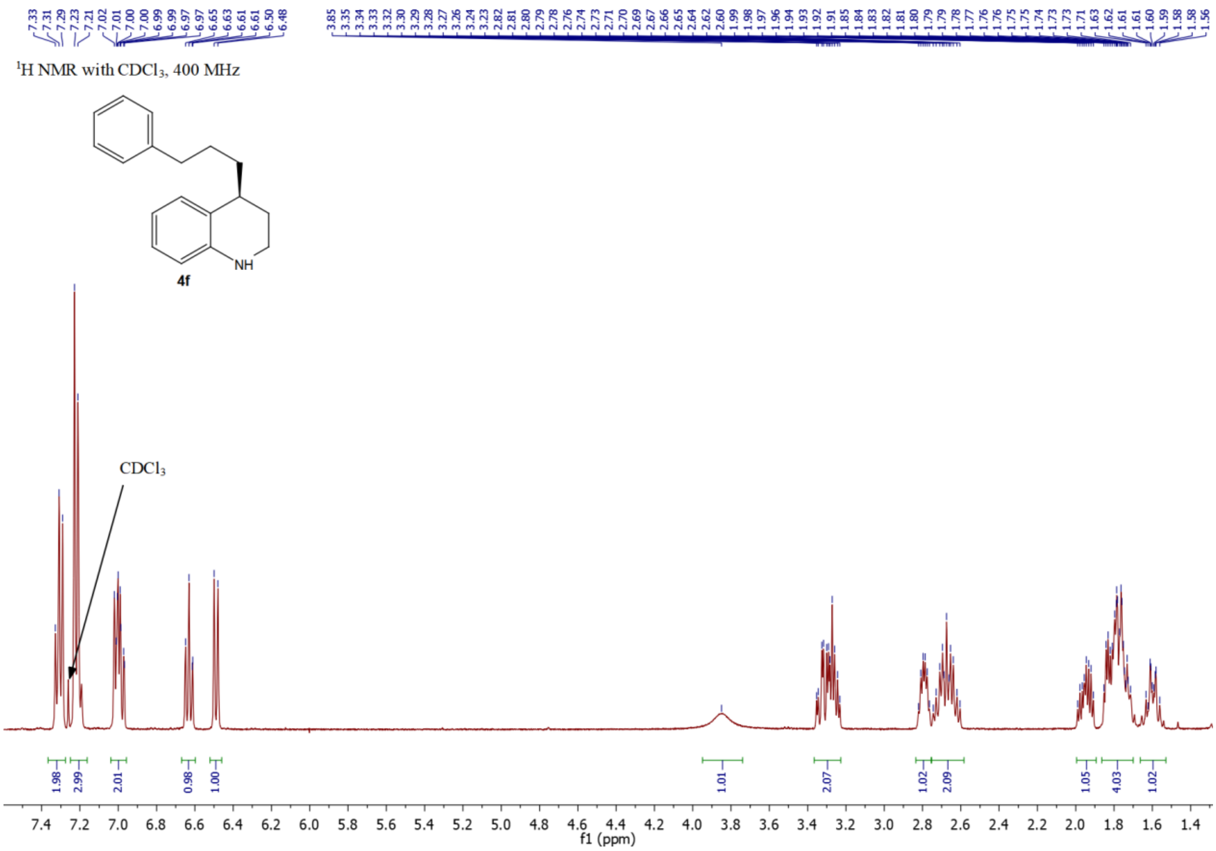


Figure S42. NMR spectra of (*S*)-4-(3-methylbutyl)-1,2,3,4-tetrahydroquinoline (**4e**)



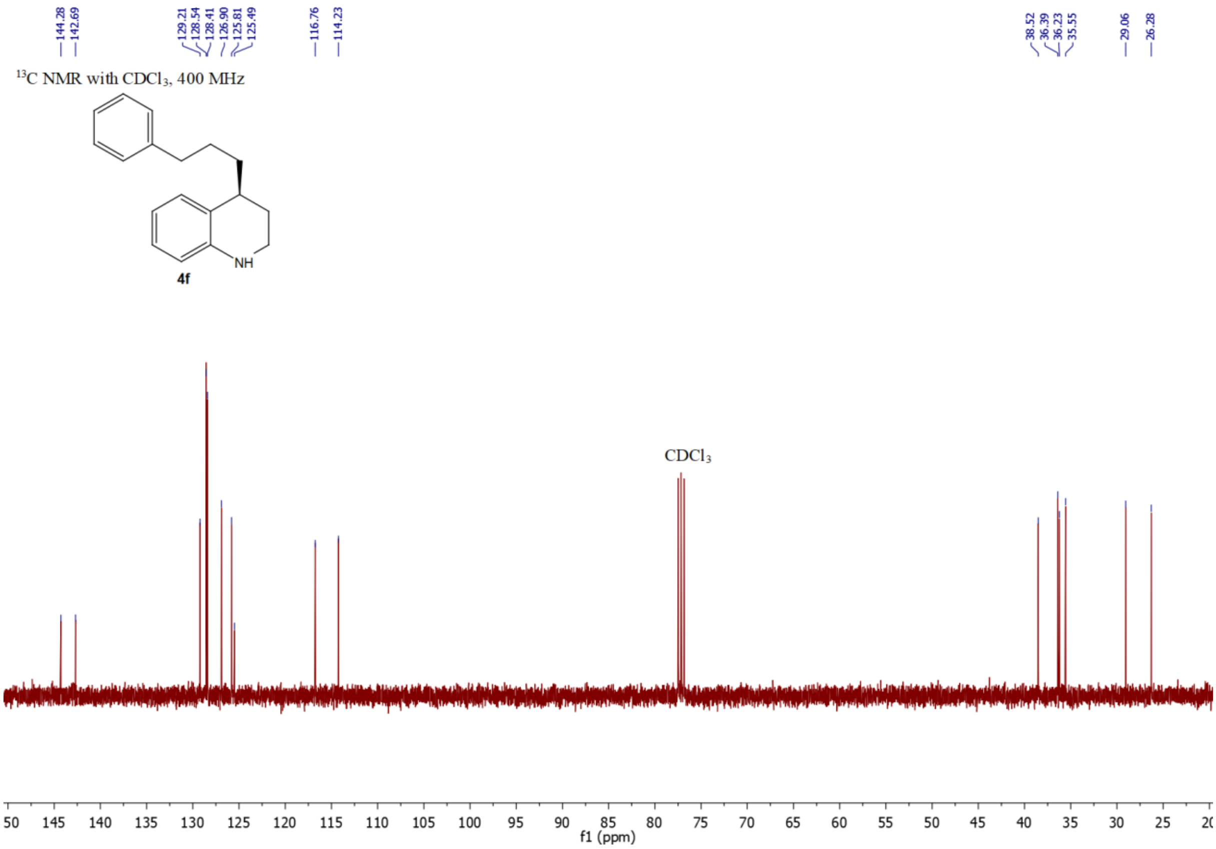
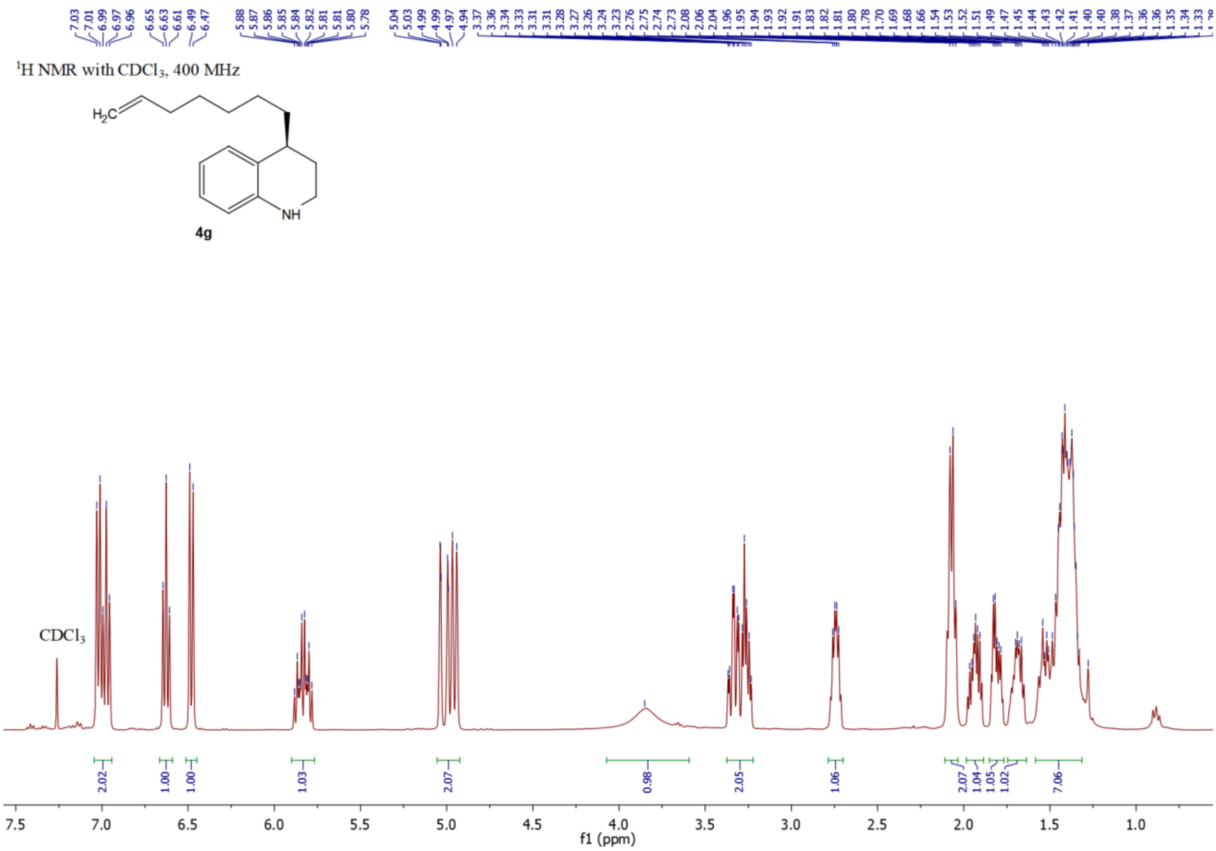


Figure S43. NMR spectra of (*S*)-4-(3-Phenylpropyl)-1,2,3,4-tetrahydroquinoline (**4f**)



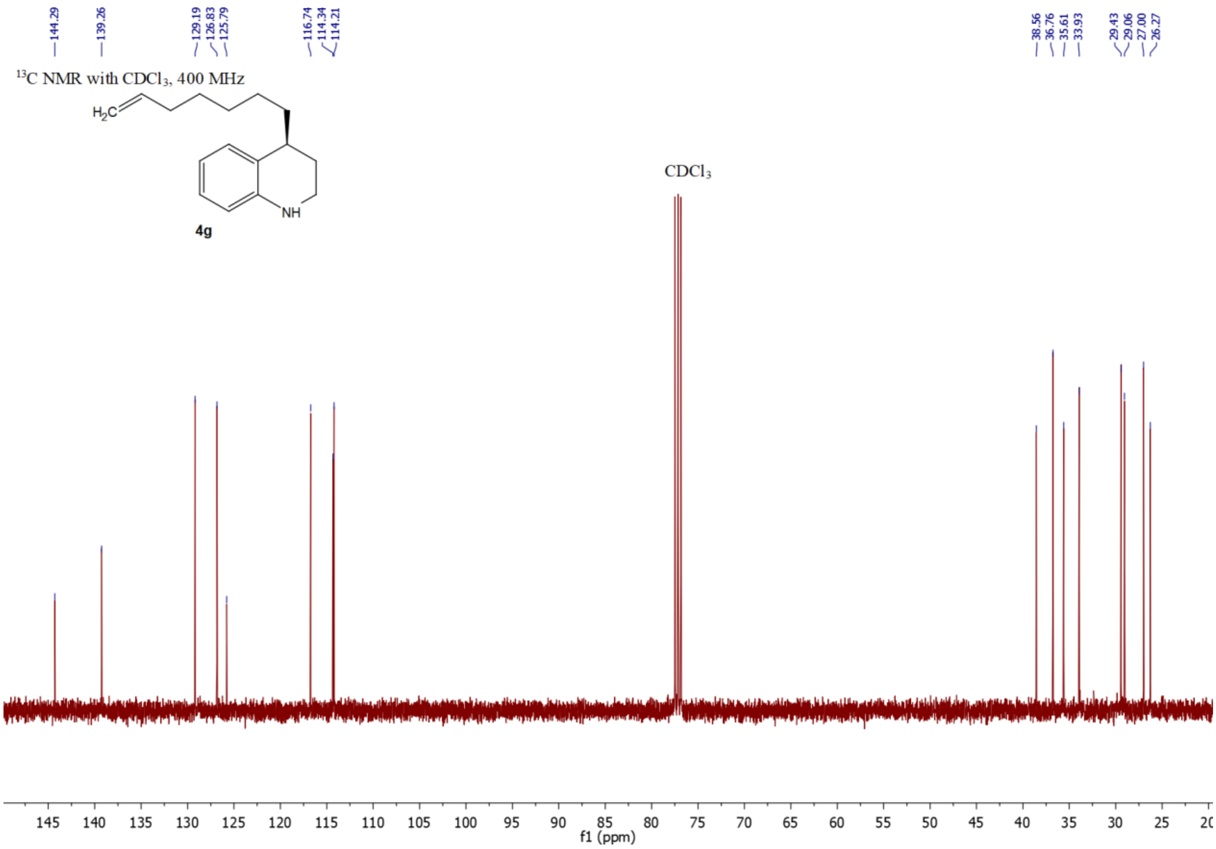
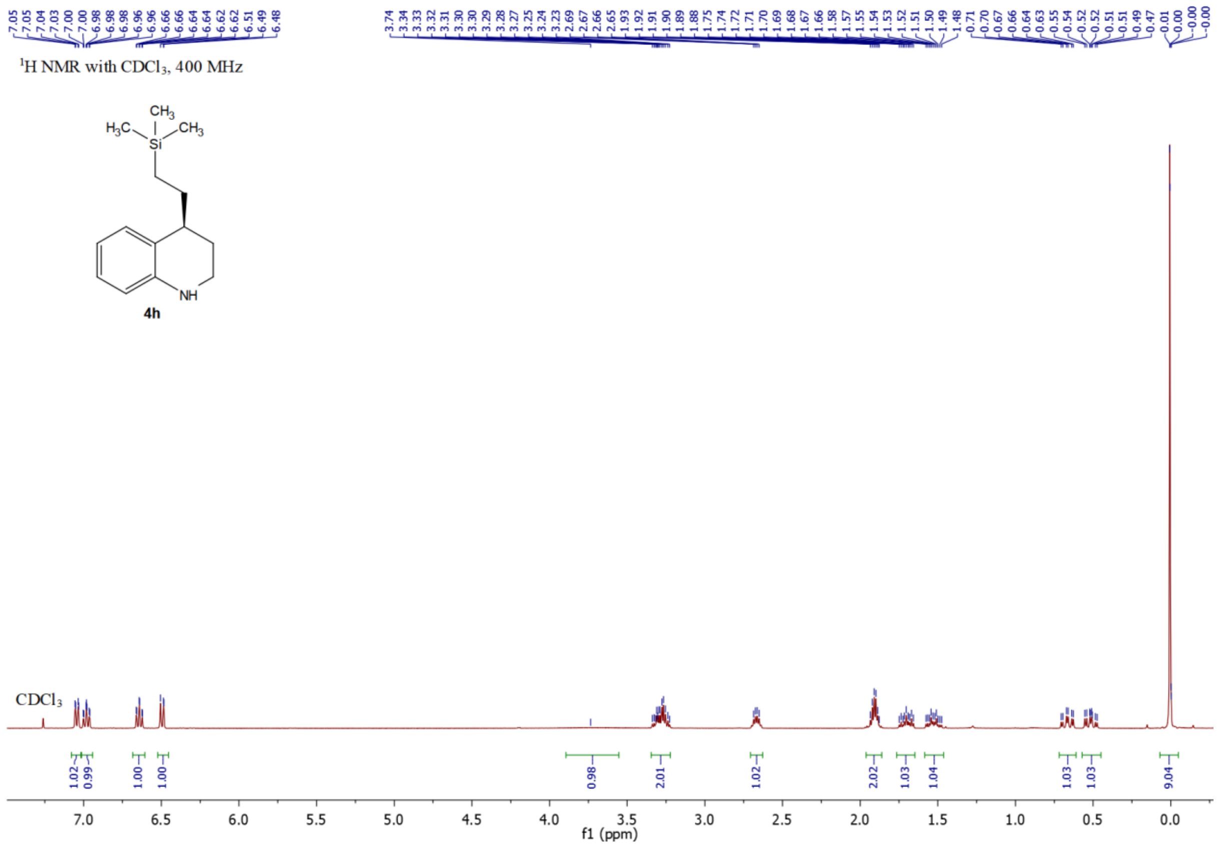


Figure S44. NMR spectra of (*S*)-4-(Hept-6-en-1-yl)-1,2,3,4-tetrahydroquinoline (**4g**)



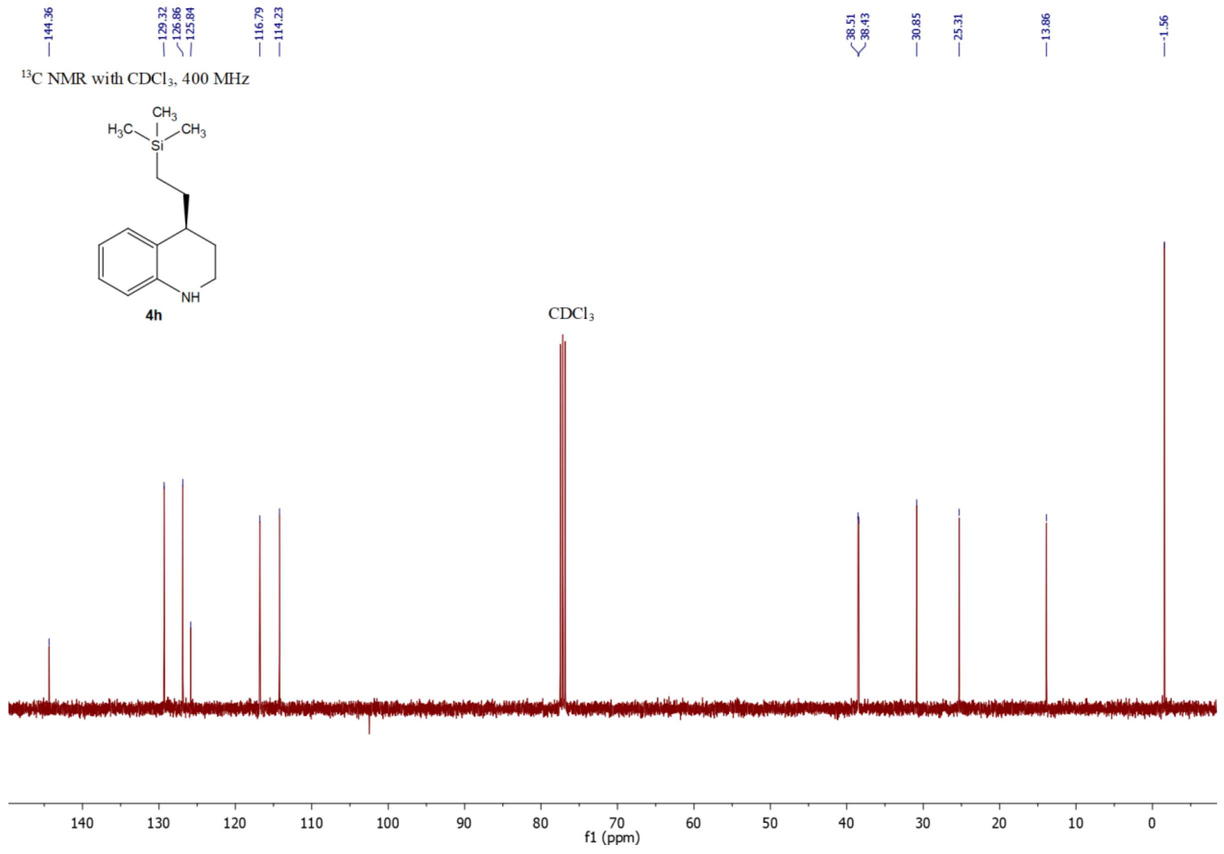
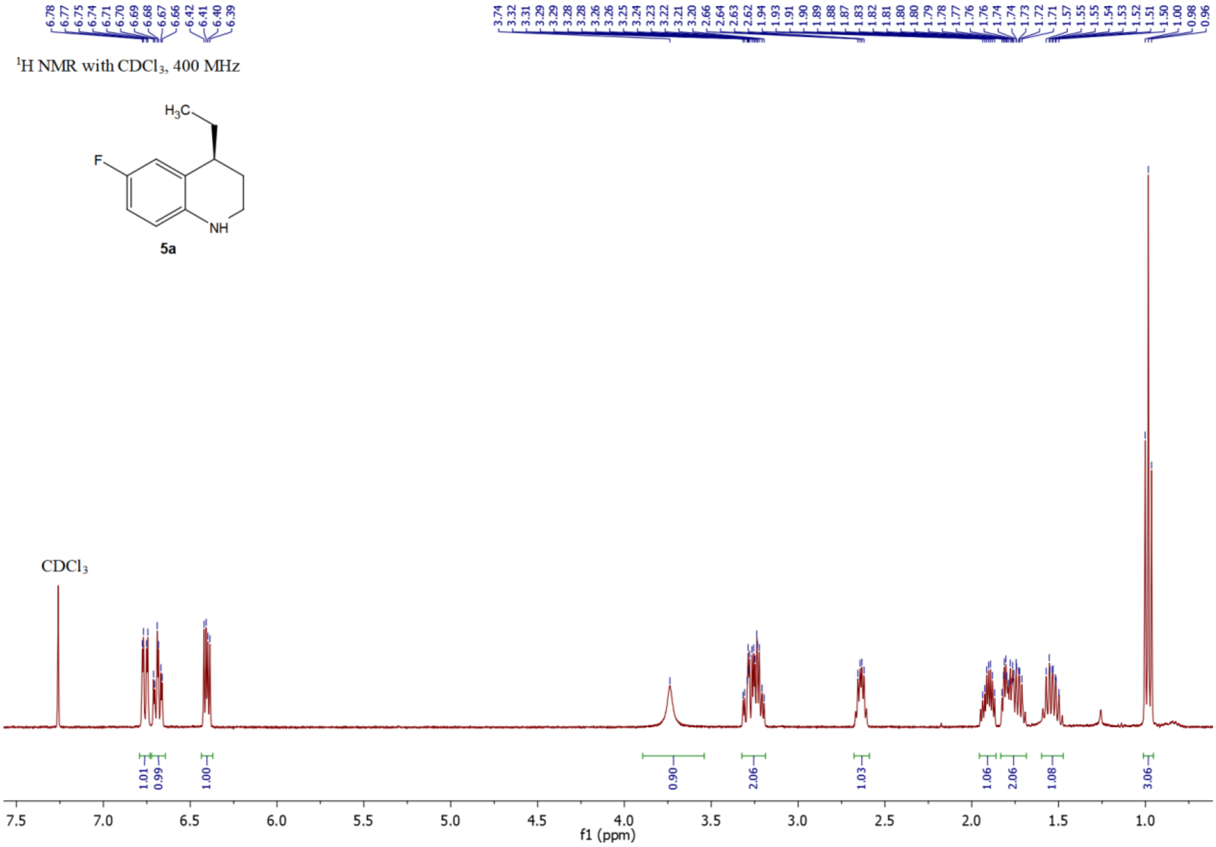
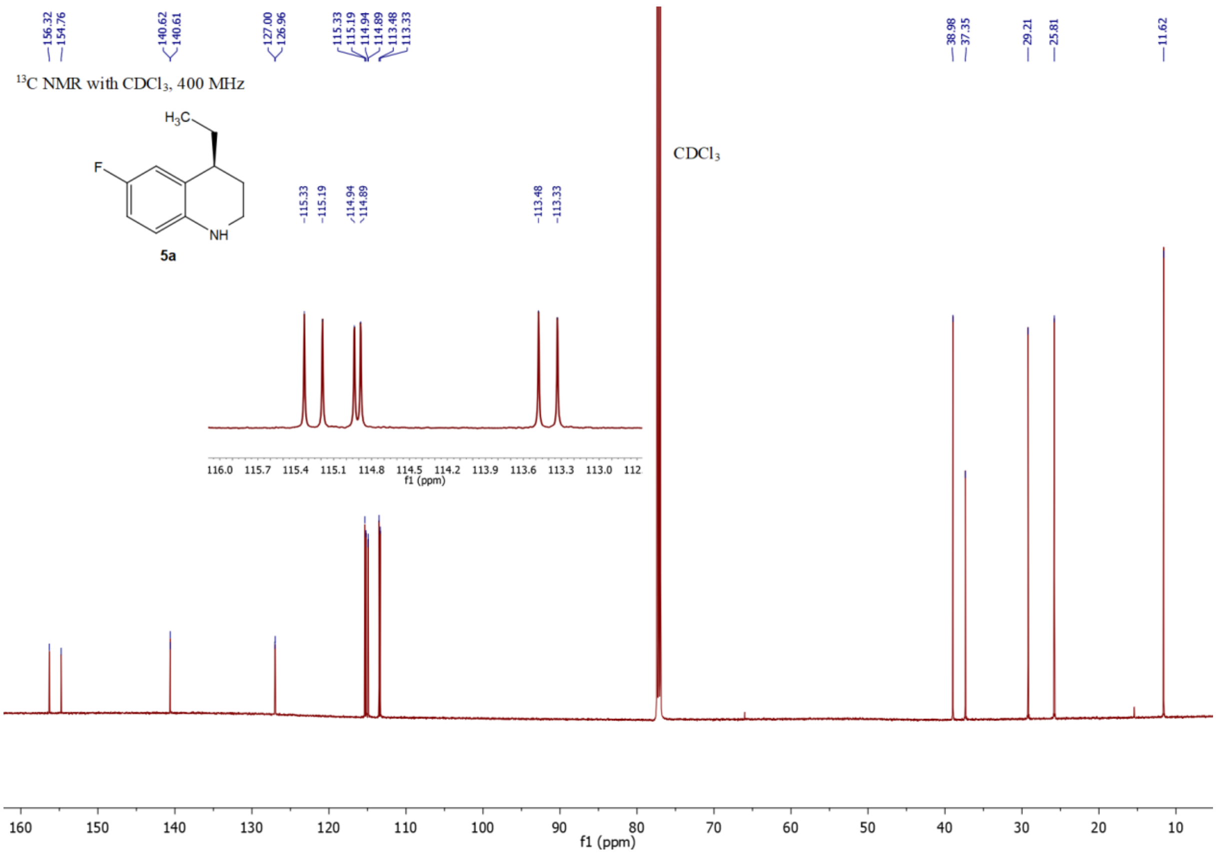


Figure S45. NMR spectra of (*R*)-4-(2-Trimethylsilylethyl)-1,2,3,4-tetrahydroquinoline (**4h**)



^{1}H NMR with $CDCl_3$, 400 MHz
5a
CDCl3
f1 (ppm)



^{13}C NMR with $CDCl_3$, 400 MHz
5a
CDCl3
f1 (ppm)

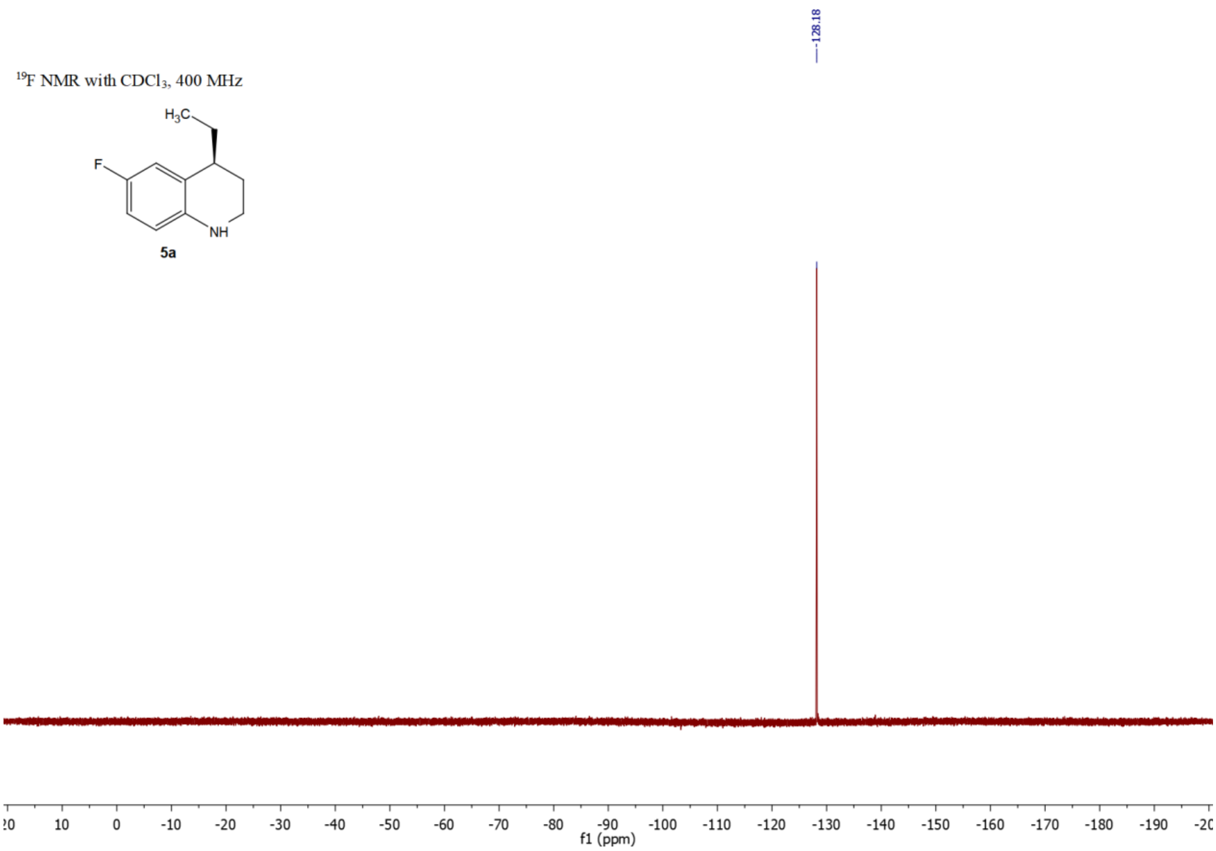
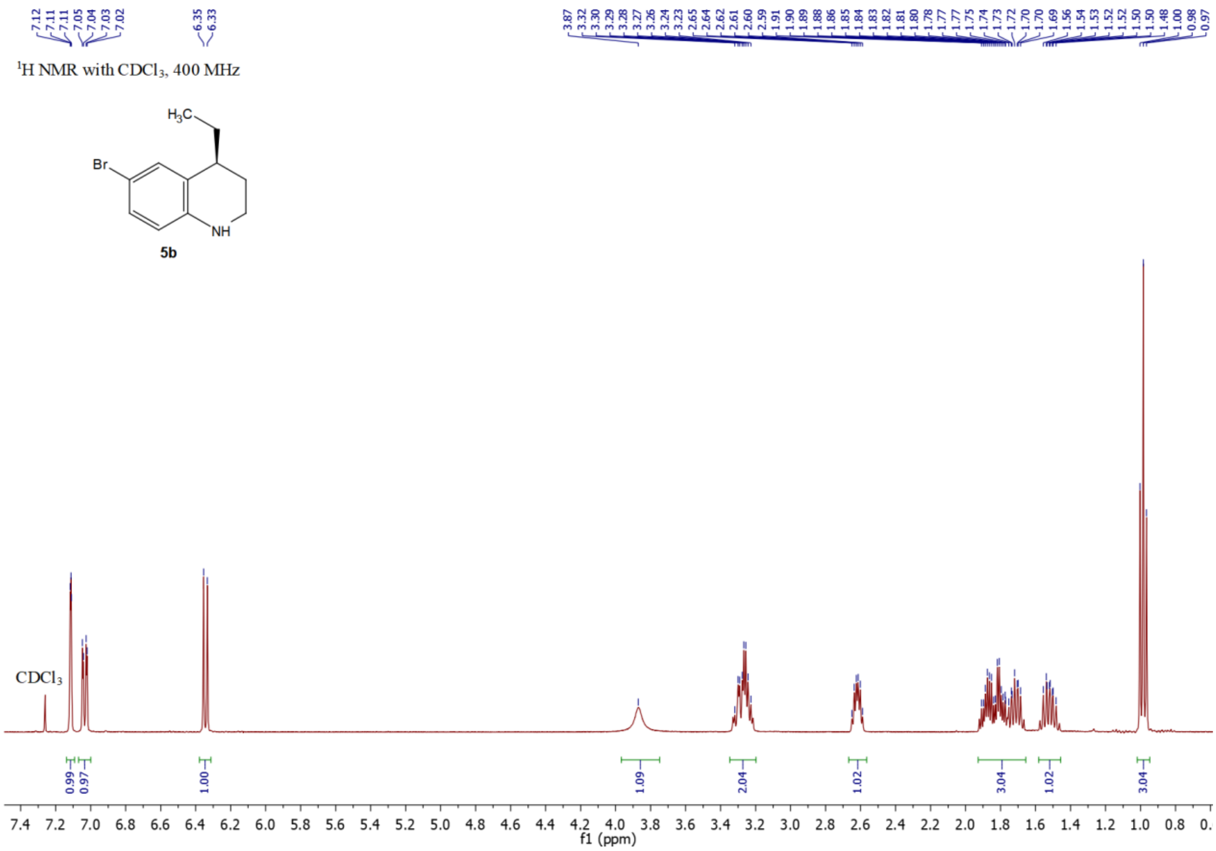


Figure S46. NMR spectra of (*S*)-4-Ethyl-6-fluoro-1,2,3,4-tetrahydroquinoline (**5a**)



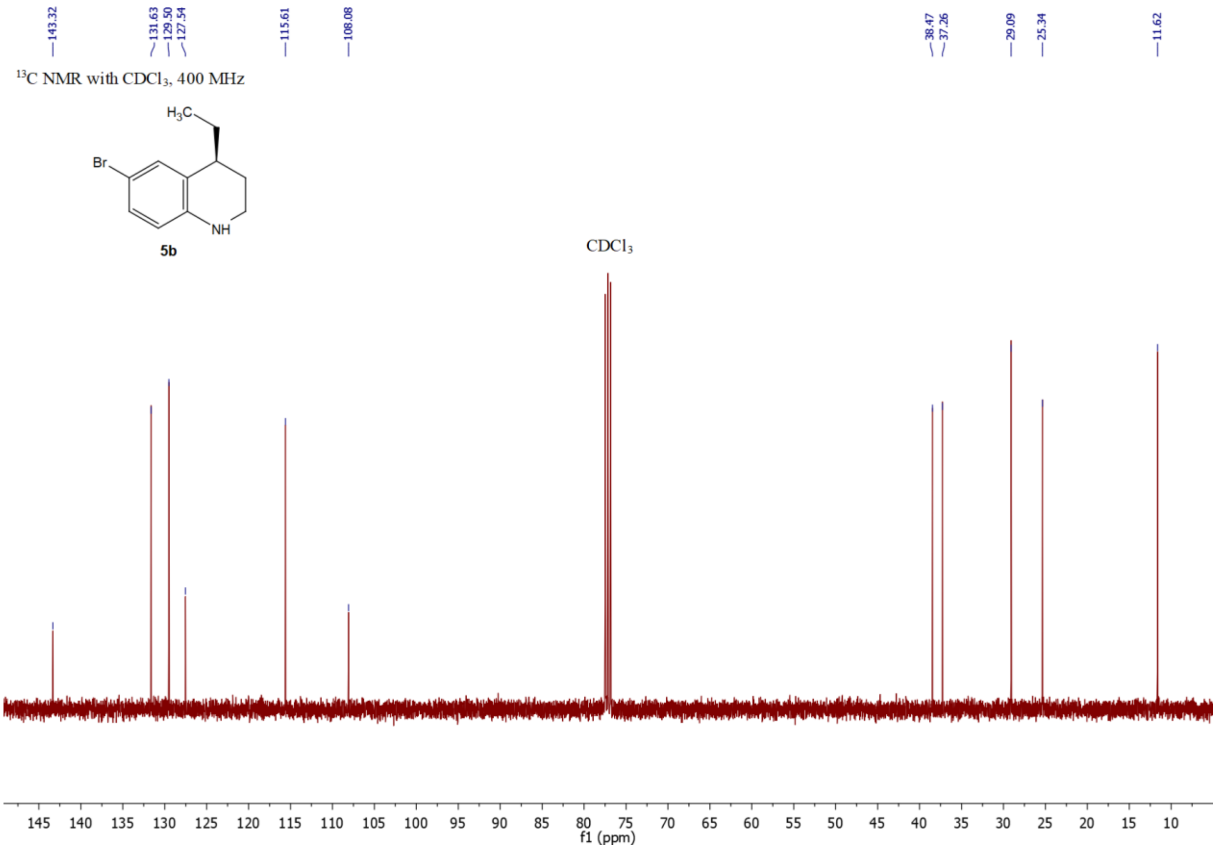
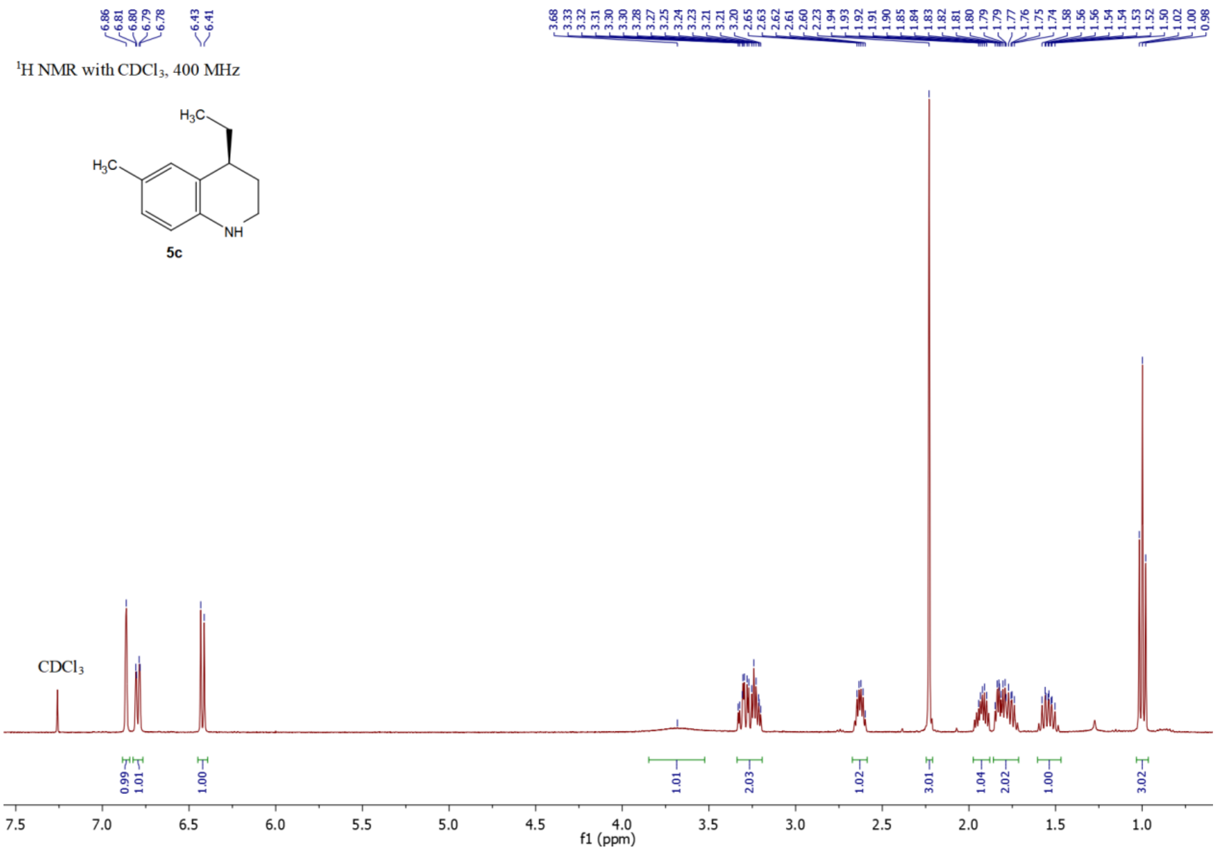


Figure S47. NMR spectra of (*S*)-6-Bromo-4-ethyl-1,2,3,4-tetrahydroquinoline (**5b**)



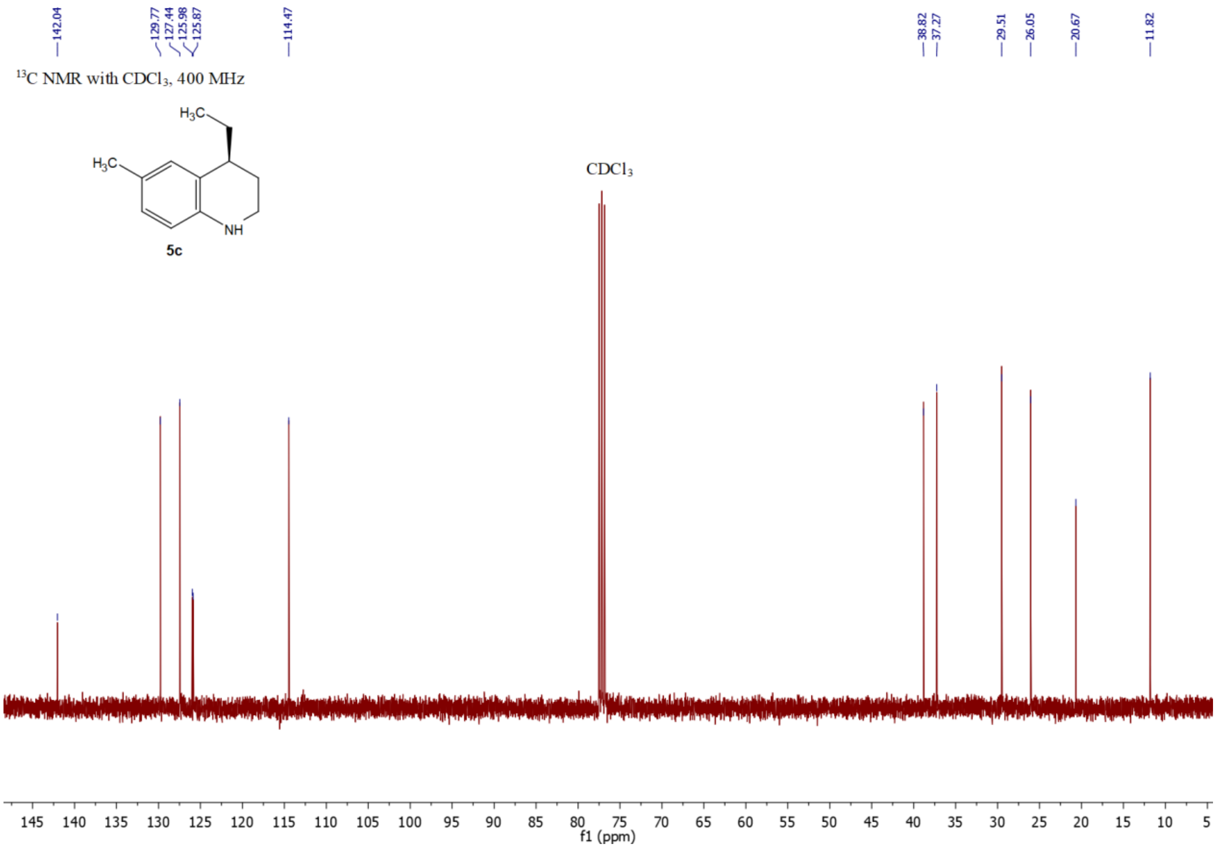
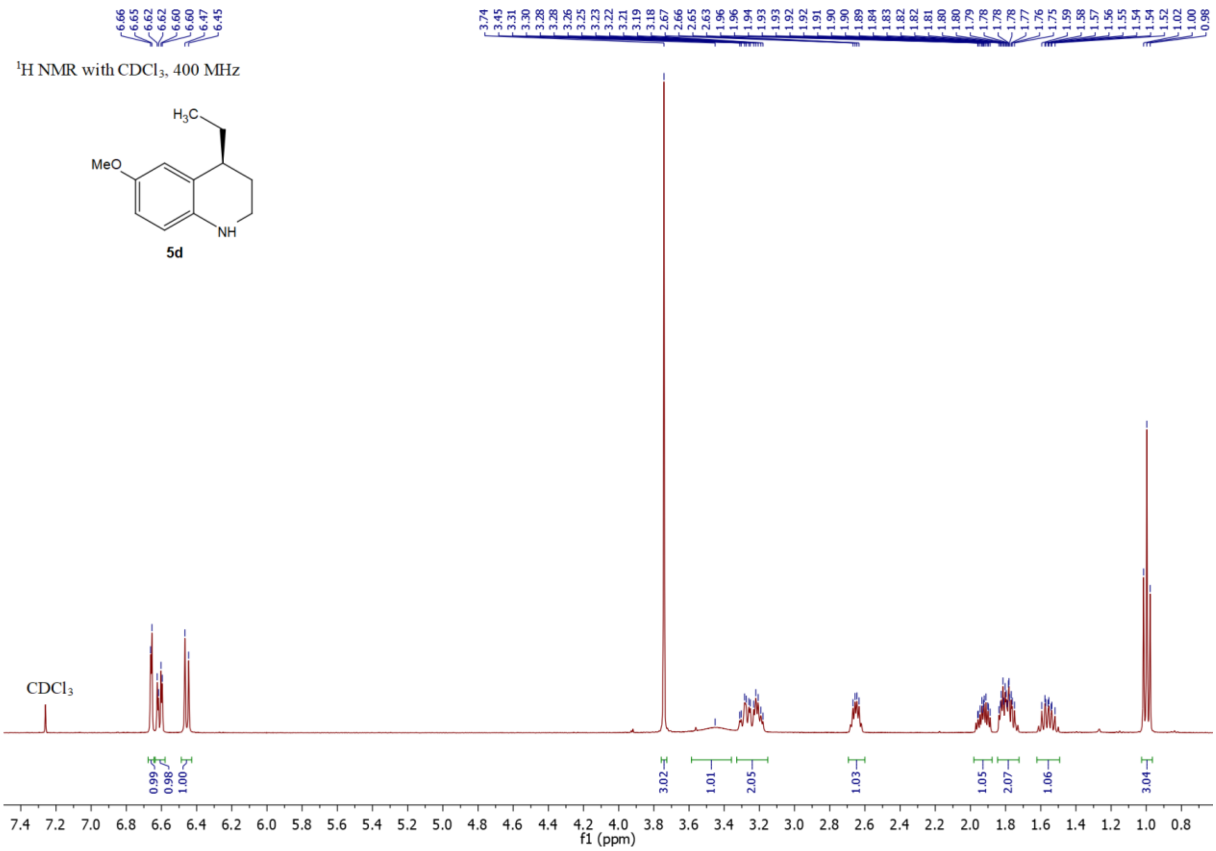


Figure S48. NMR spectra of (*S*)-4-Ethyl-6-methyl-1,2,3,4-tetrahydroquinoline (**5c**)



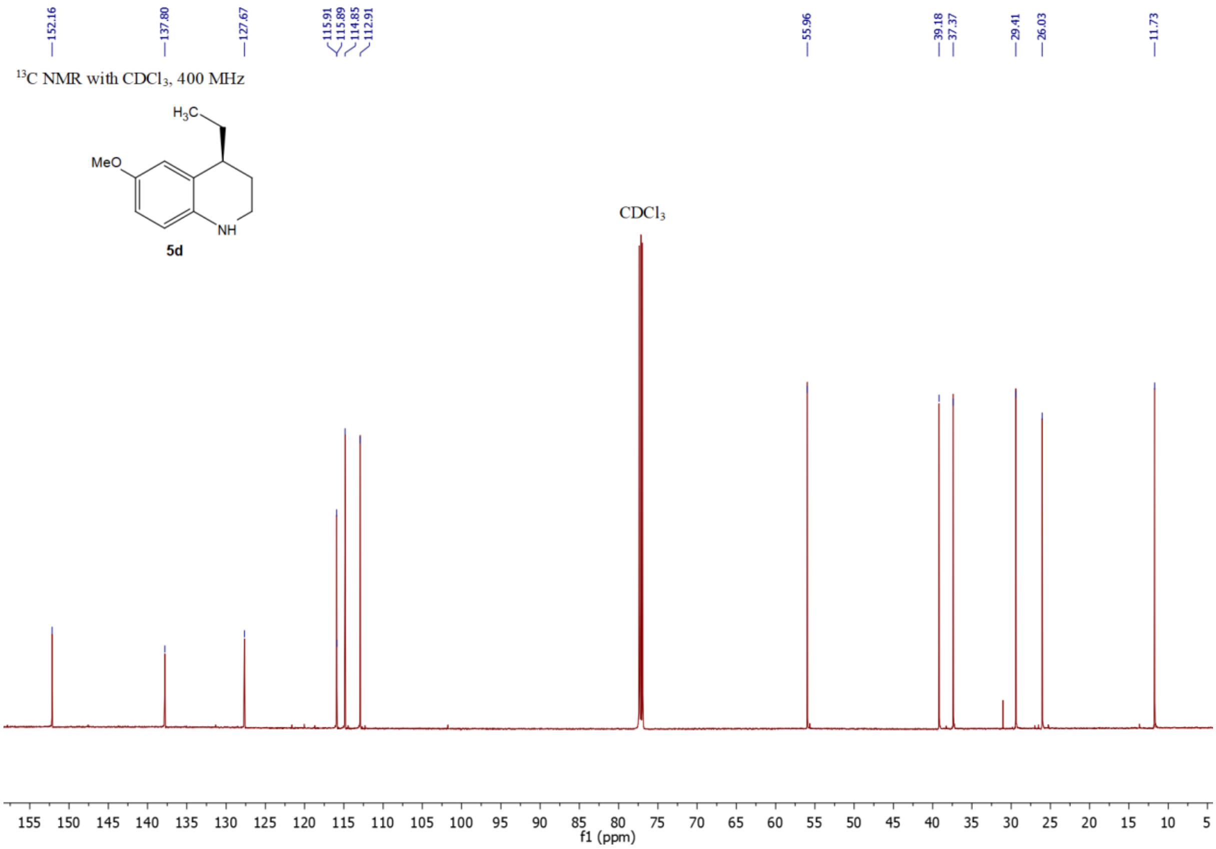
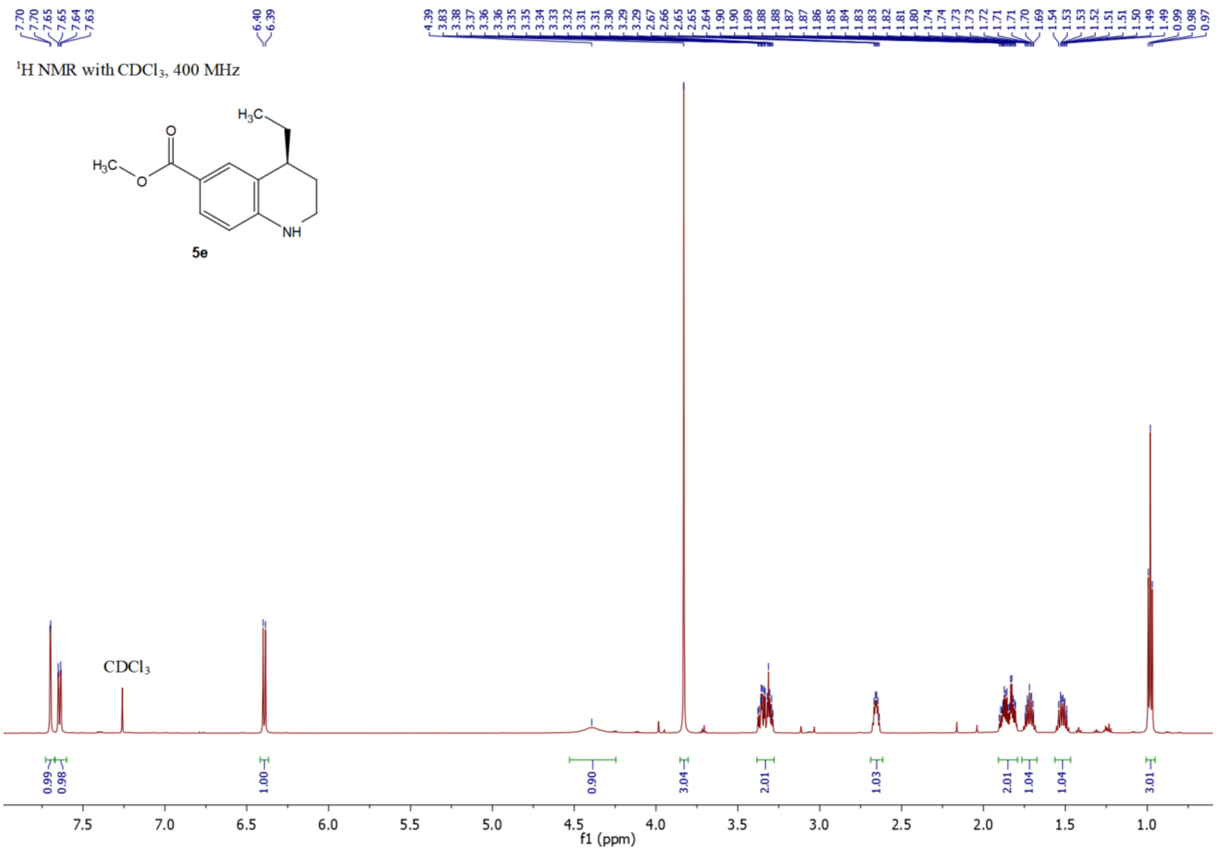


Figure S49. NMR spectra of (*S*)-4-Ethyl-6-methoxy-1,2,3,4-tetrahydroquinoline (**5d**)



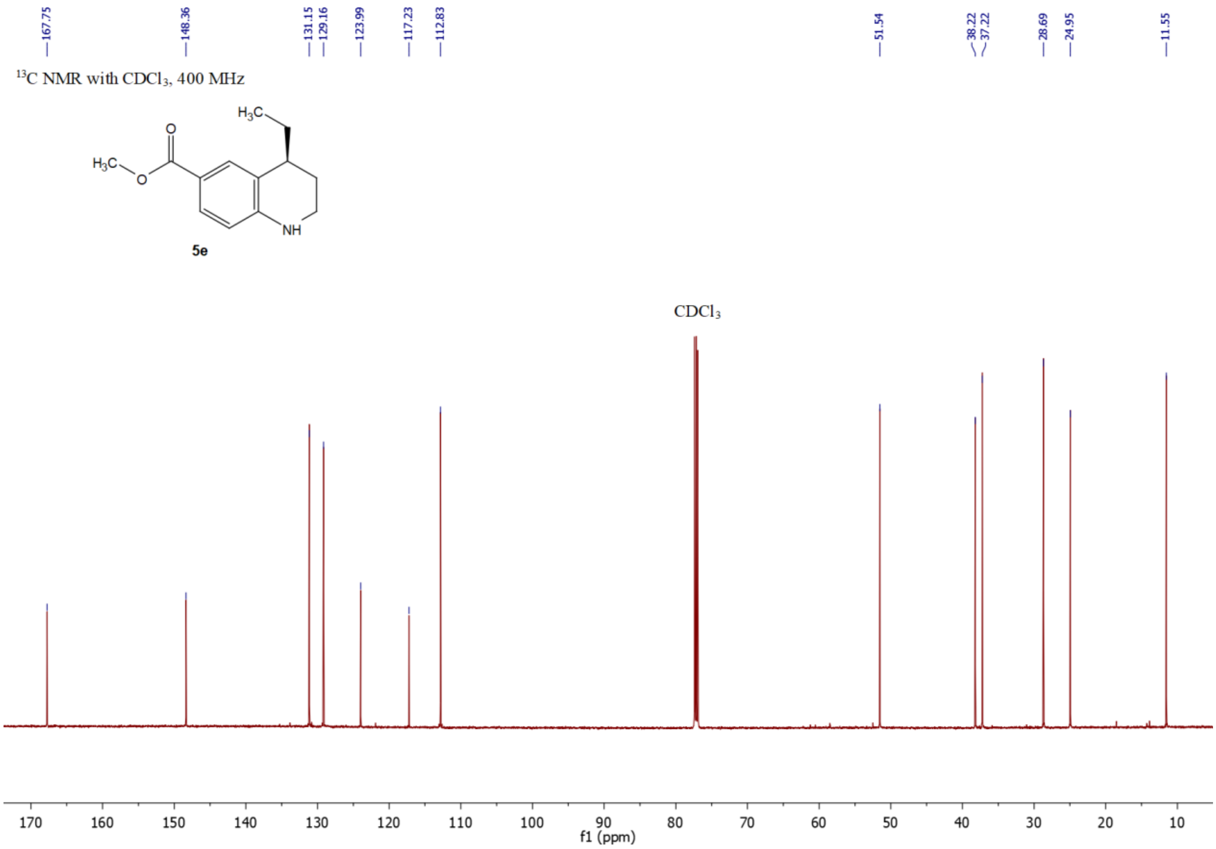
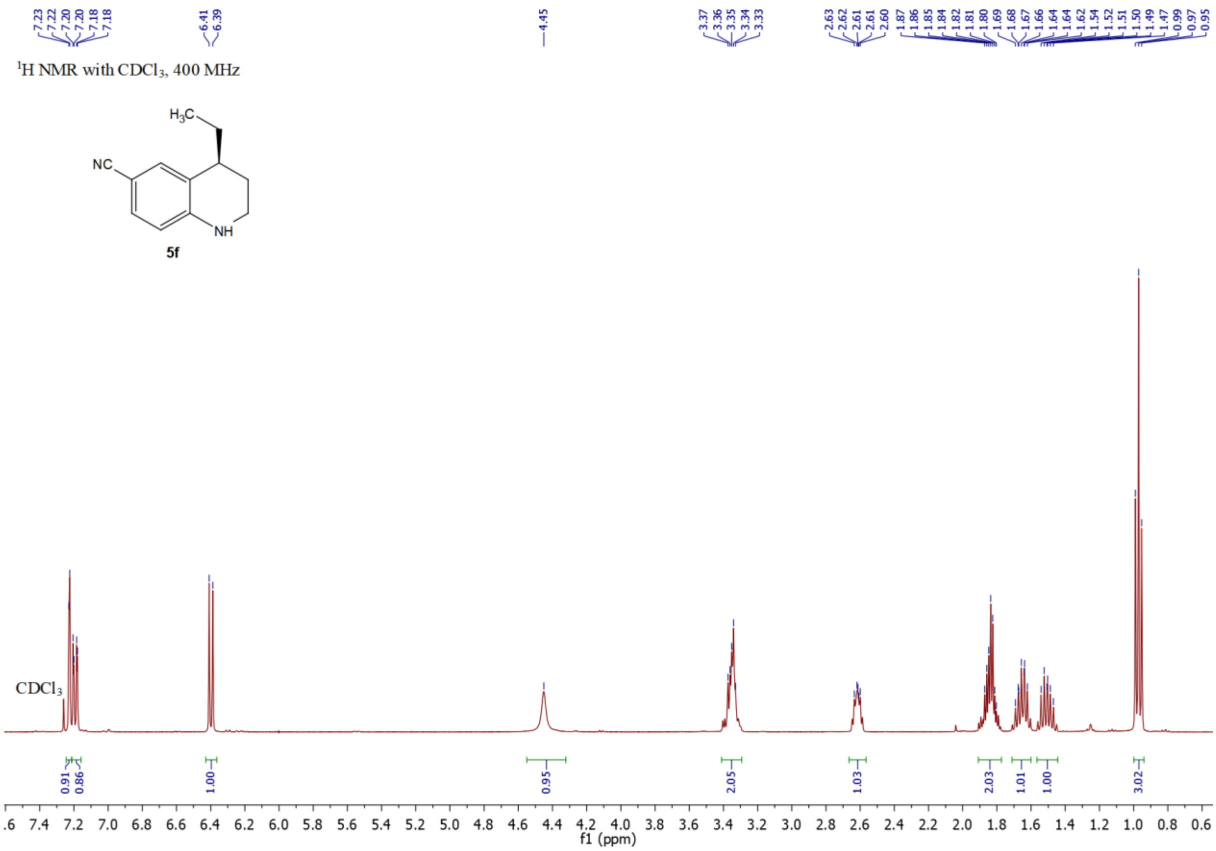


Figure S50. NMR spectra of (*S*)-Methyl 4-ethyl-1,2,3,4-tetrahydroquinoline-6-carboxylate (**5e**)



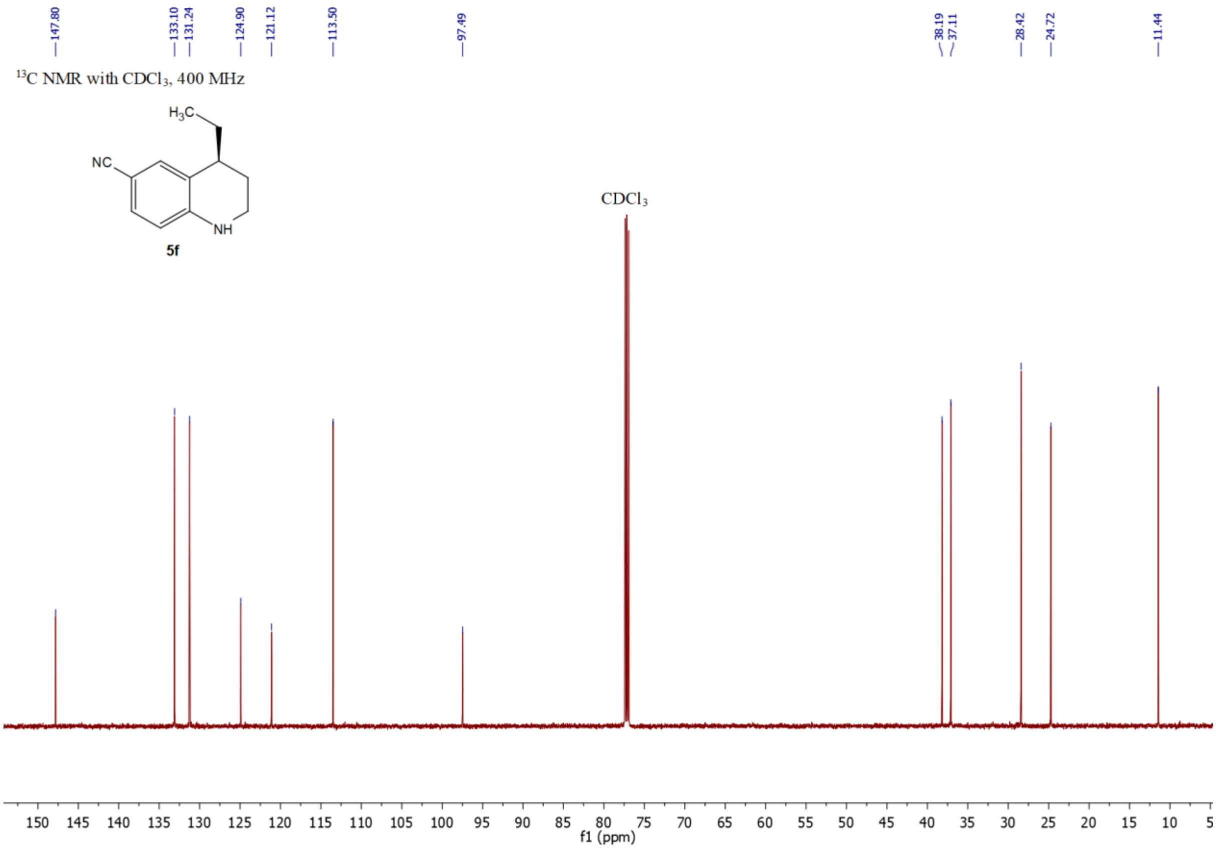
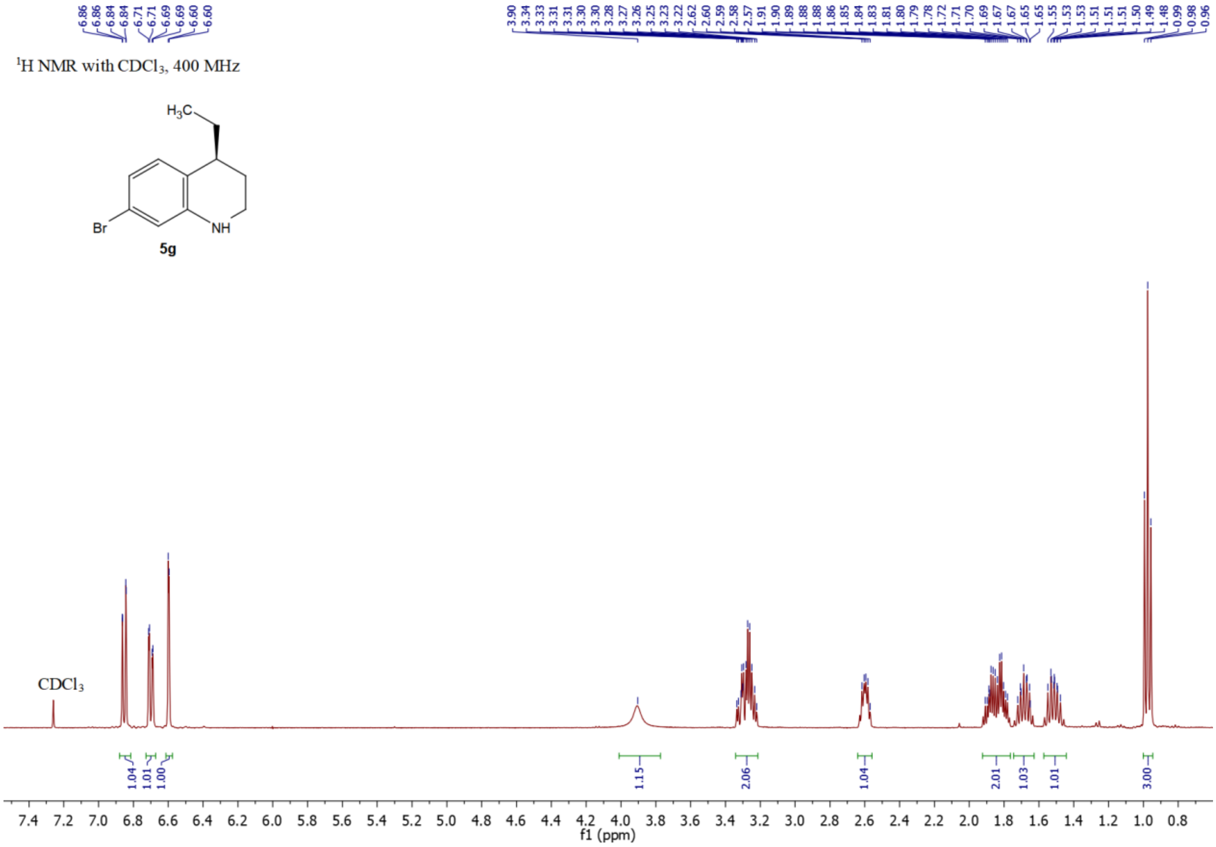


Figure S51. NMR spectra of (*S*)-6-Cyano-4-ethyl-1,2,3,4-tetrahydroquinoline (**5f**)



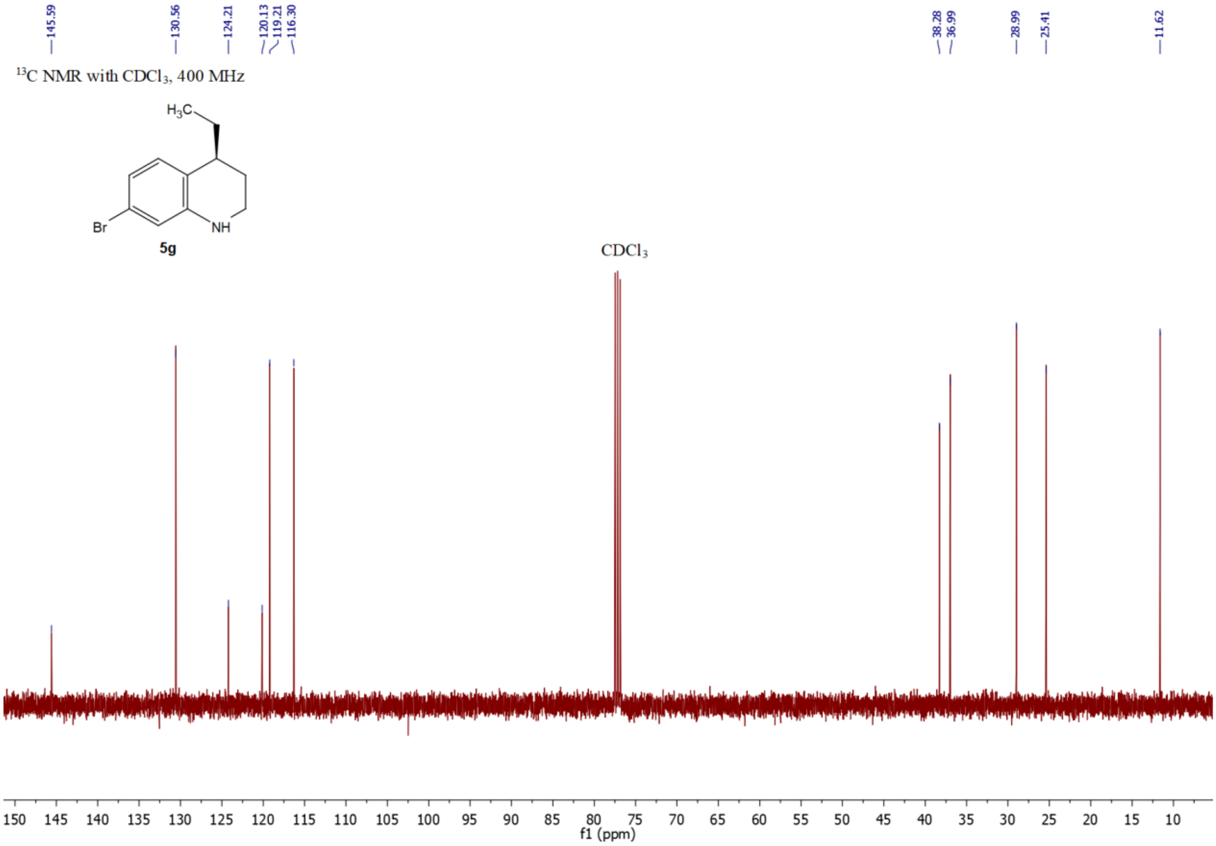
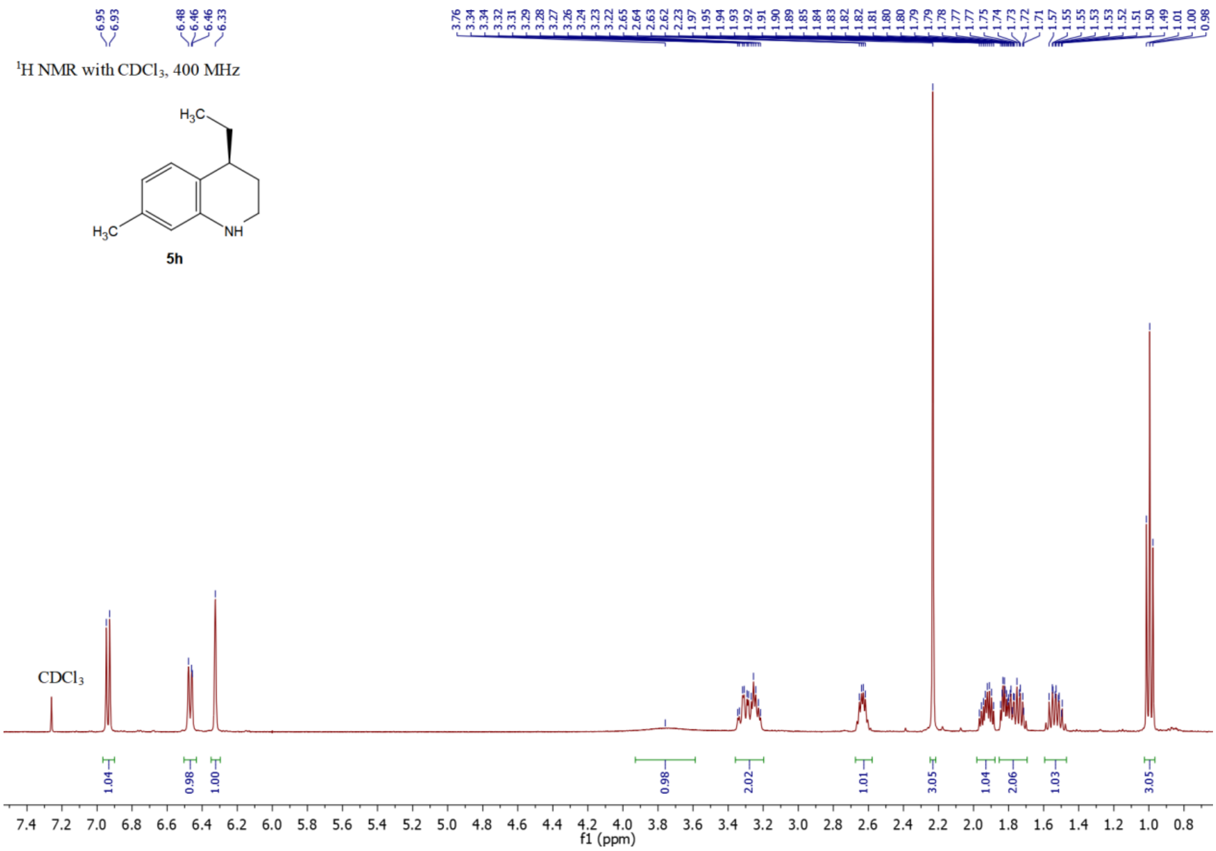


Figure S52. NMR spectra of (*S*)-7-Bromo-4-ethyl-1,2,3,4-tetrahydroquinoline (**5g**)



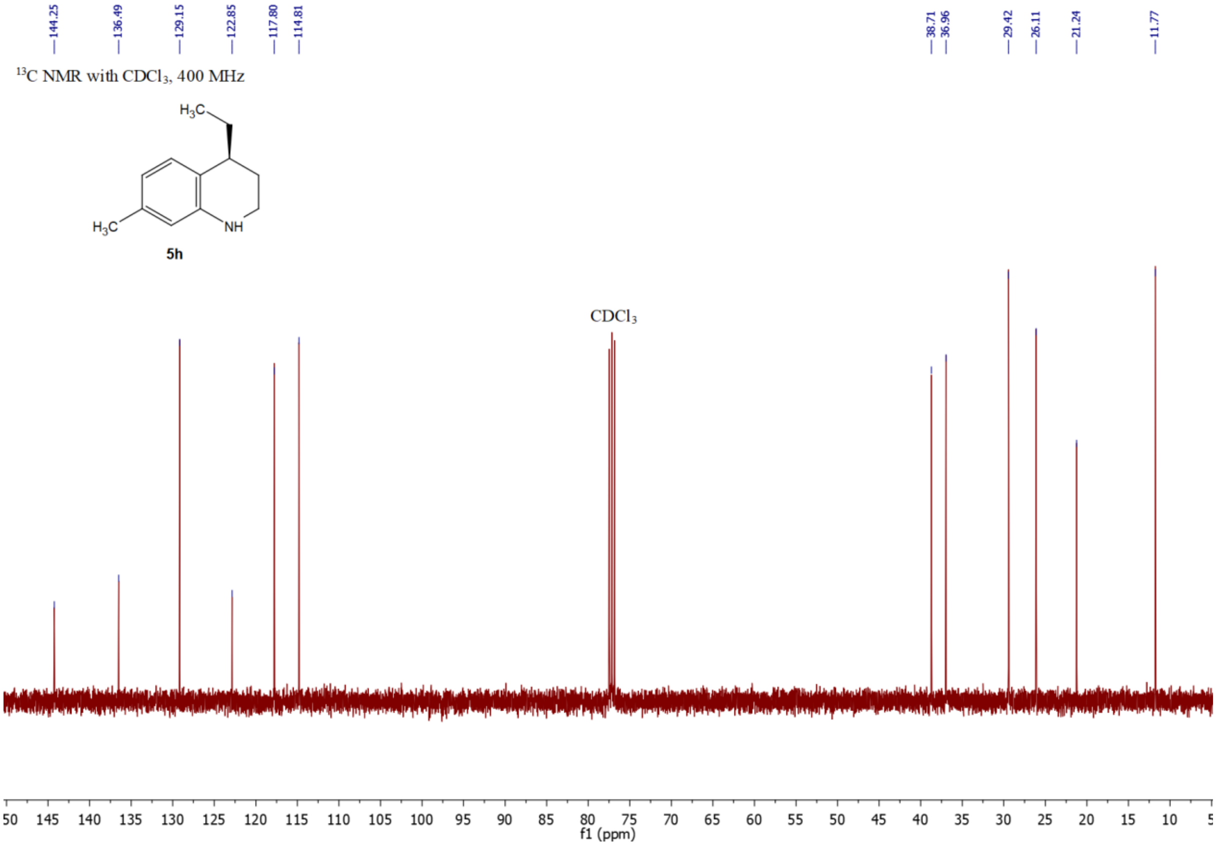
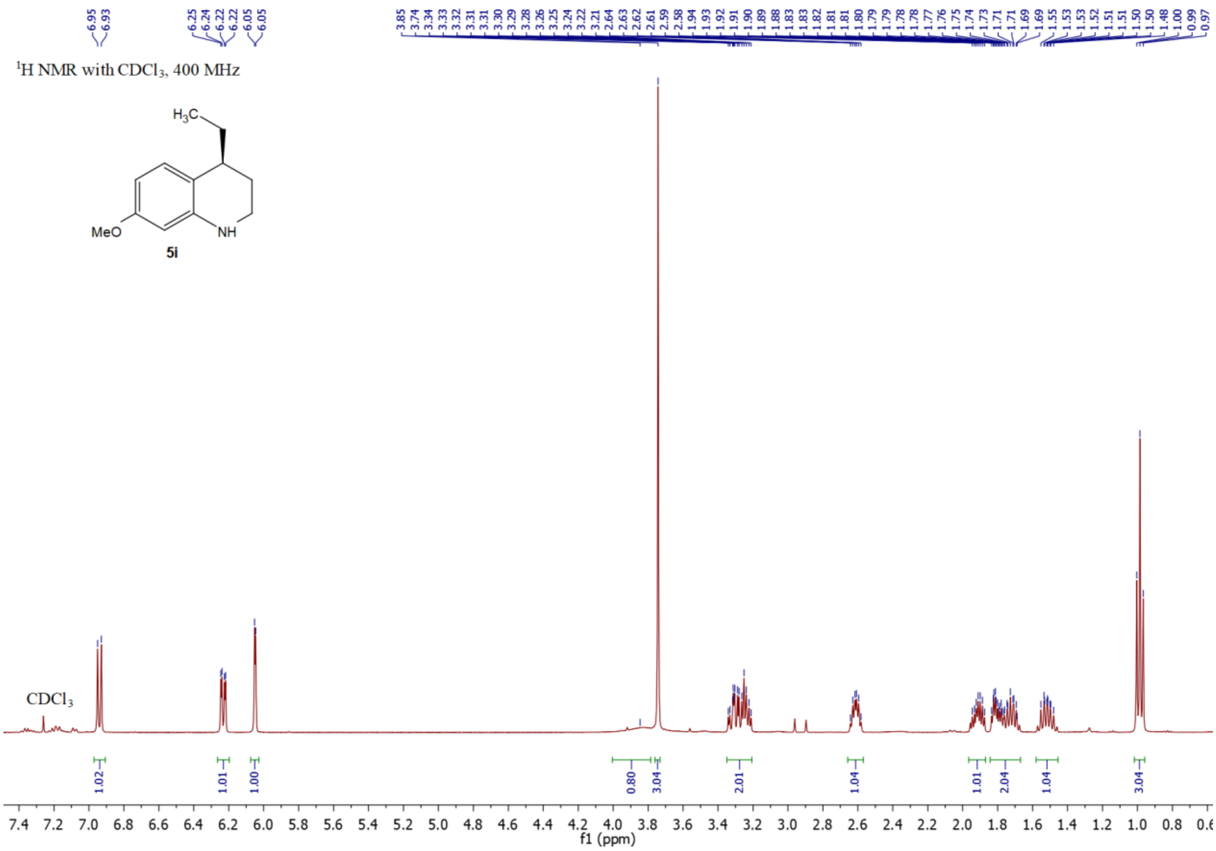


Figure S53. NMR spectra of (*S*)-4-Ethyl-7-methyl-1,2,3,4-tetrahydroquinoline (**5h**)



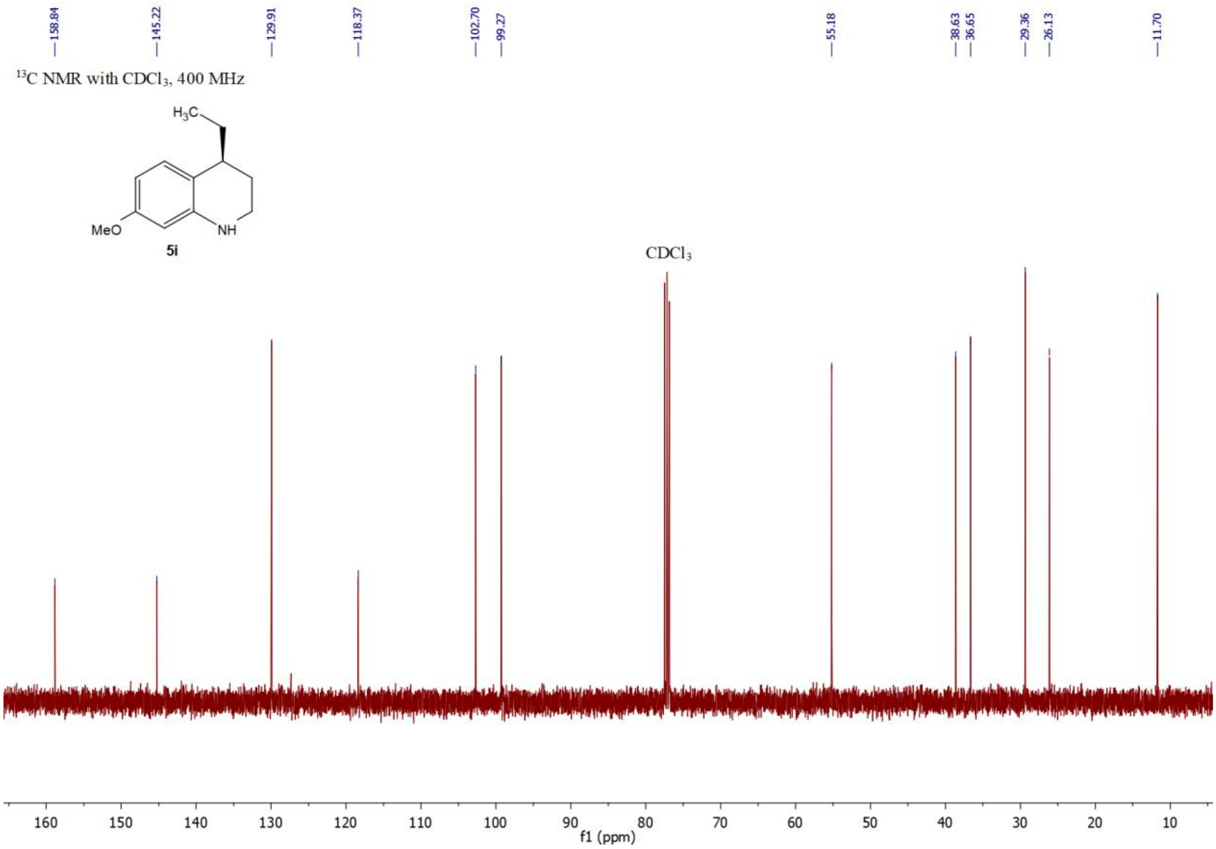
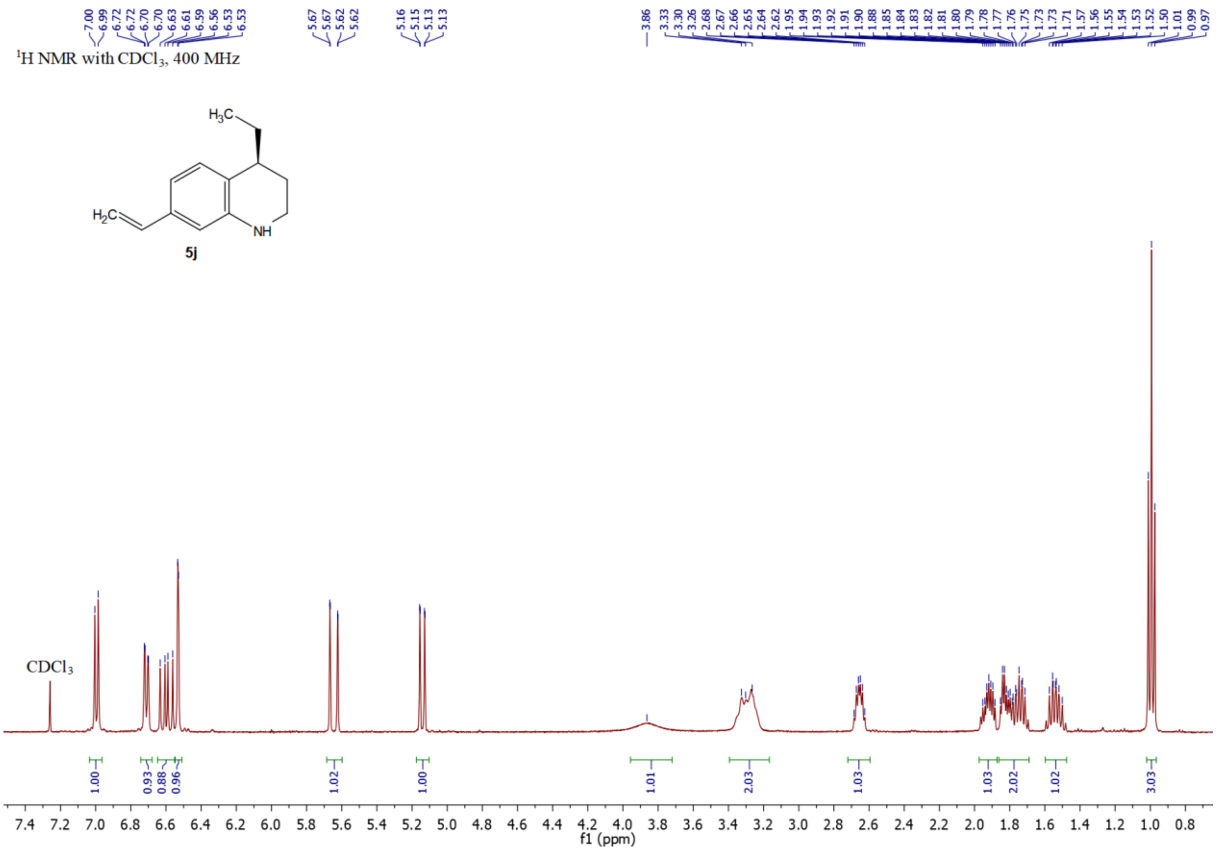


Figure S54. NMR spectra of (*S*)-4-Ethyl-7-methoxy-1,2,3,4-tetrahydroquinoline (**5i**)



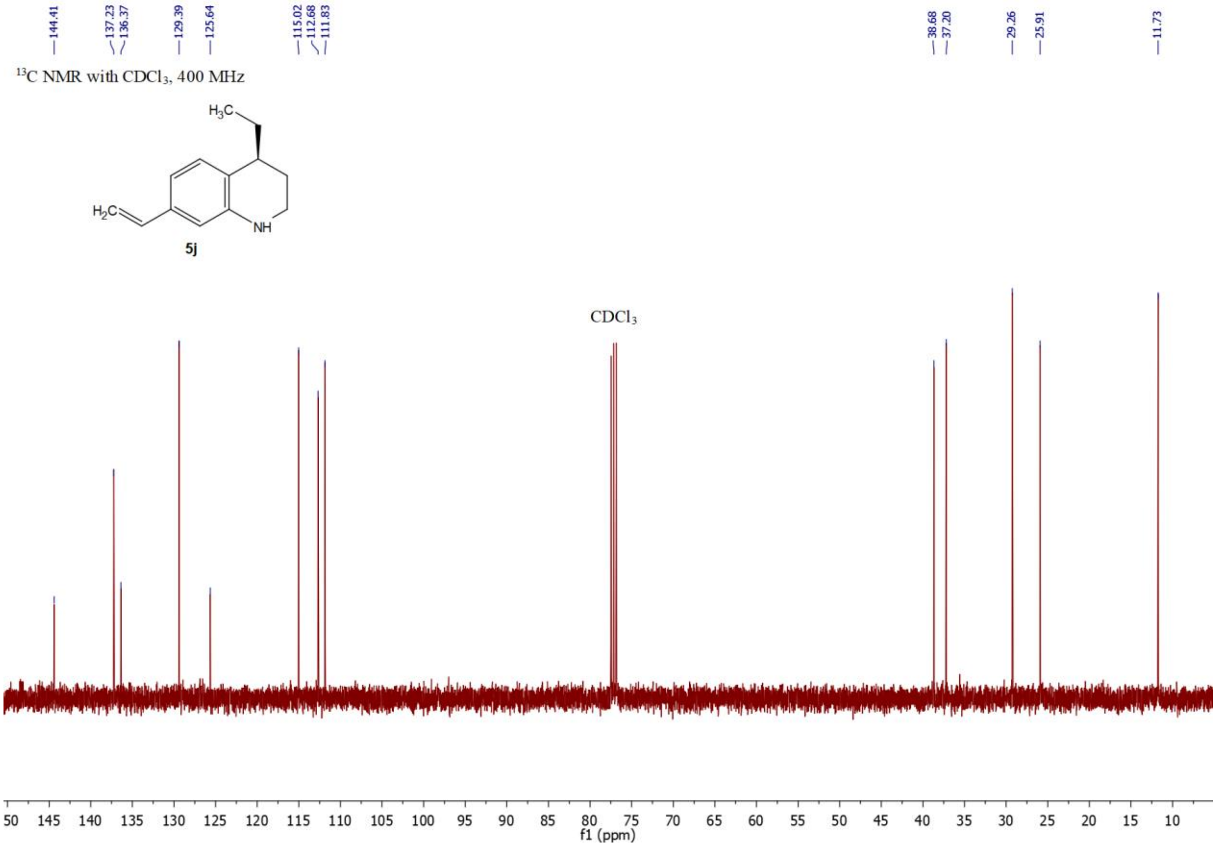
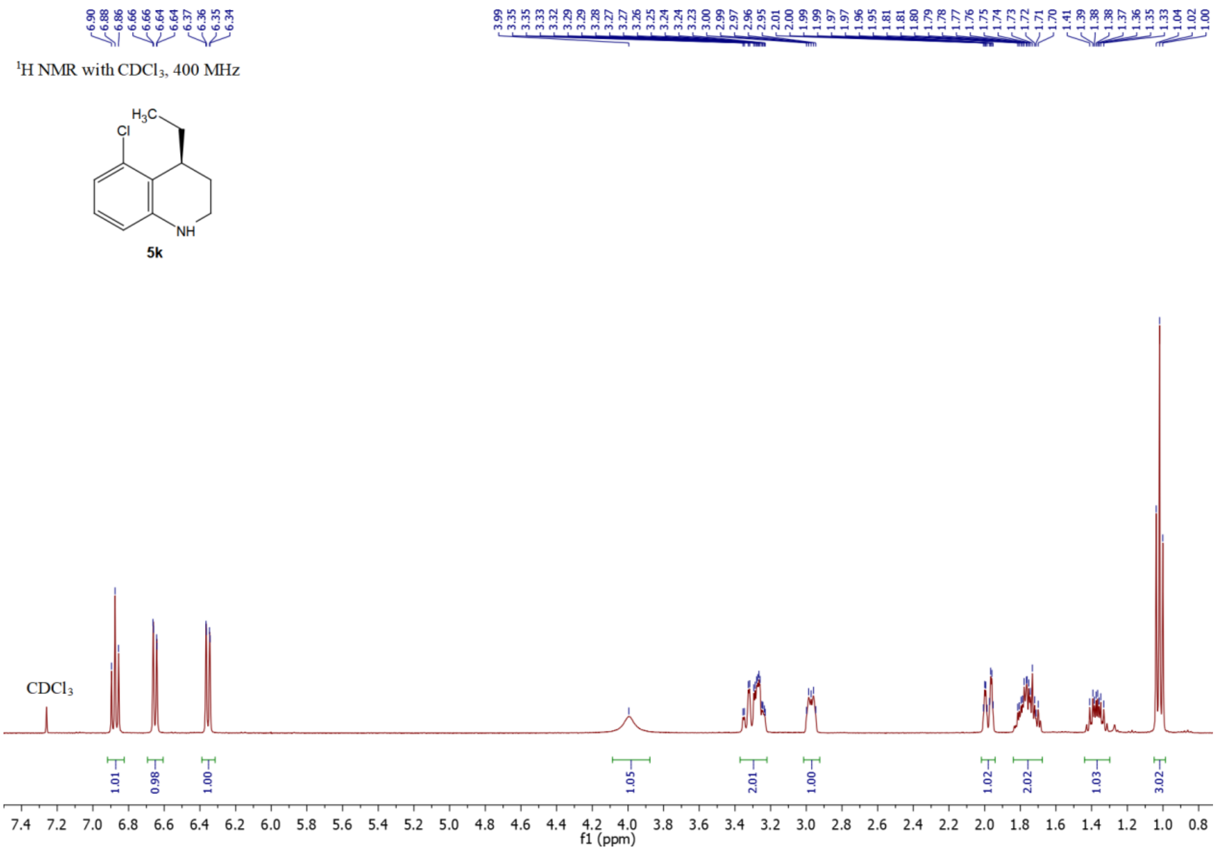


Figure S55. NMR spectra of (*S*)-4-Ethyl-7-vinyl-1,2,3,4-tetrahydroquinoline (**5j**)



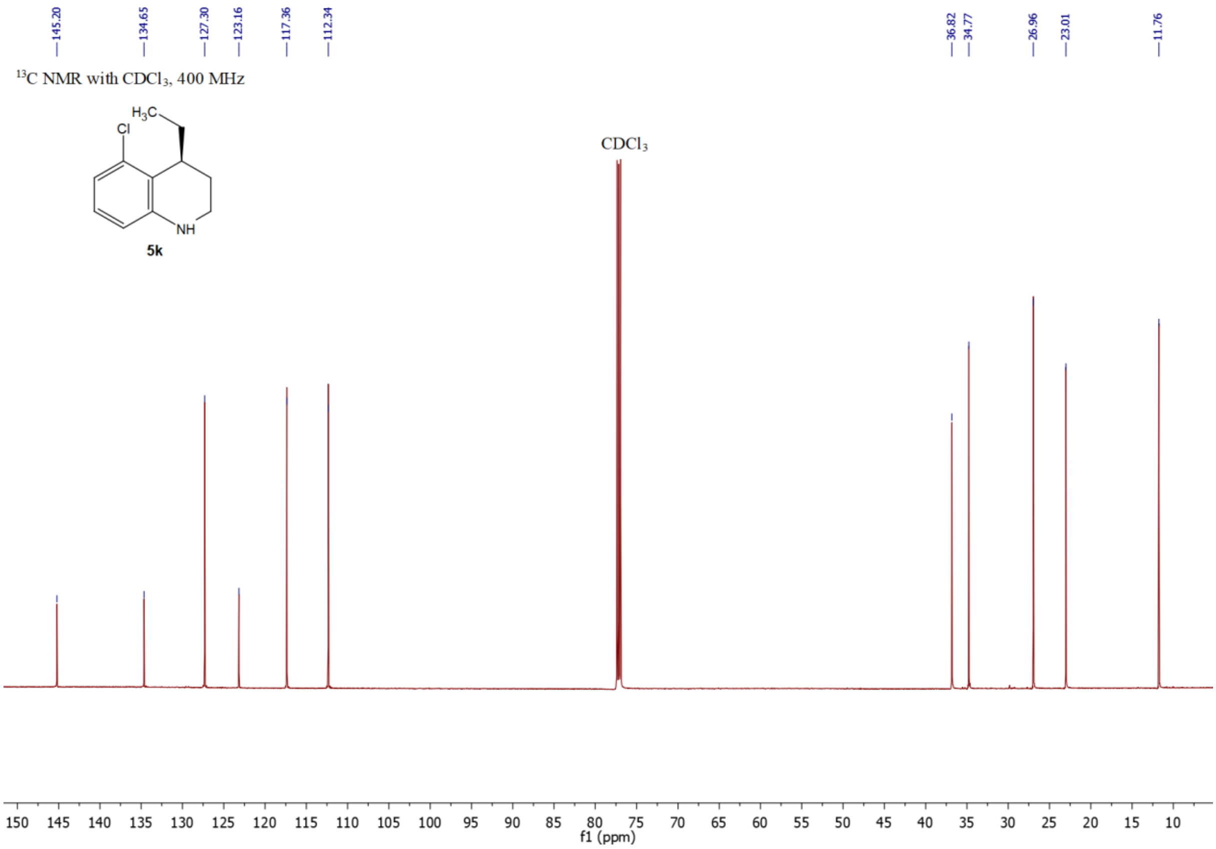
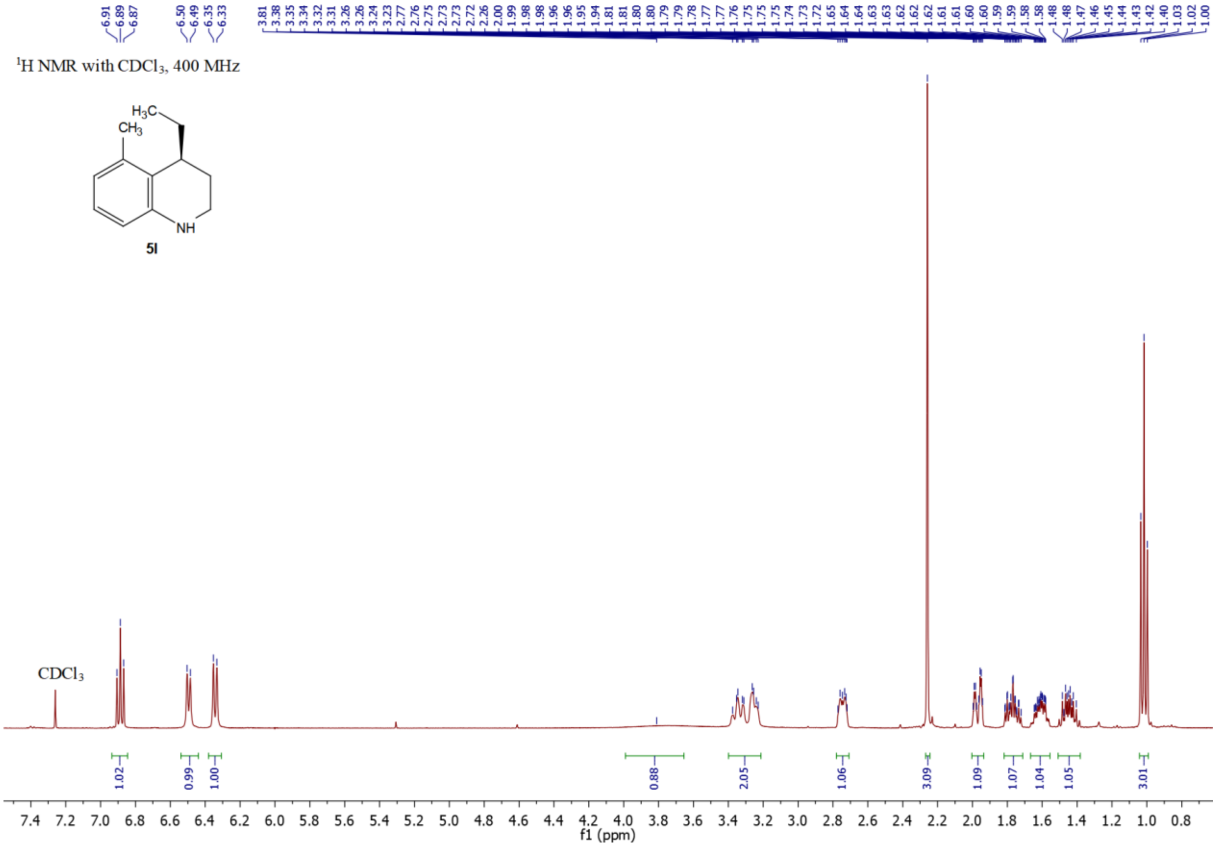


Figure S56. NMR spectra of (*S*)-5-Chloro-4-ethyl-1,2,3,4-tetrahydroquinoline (**5k**)



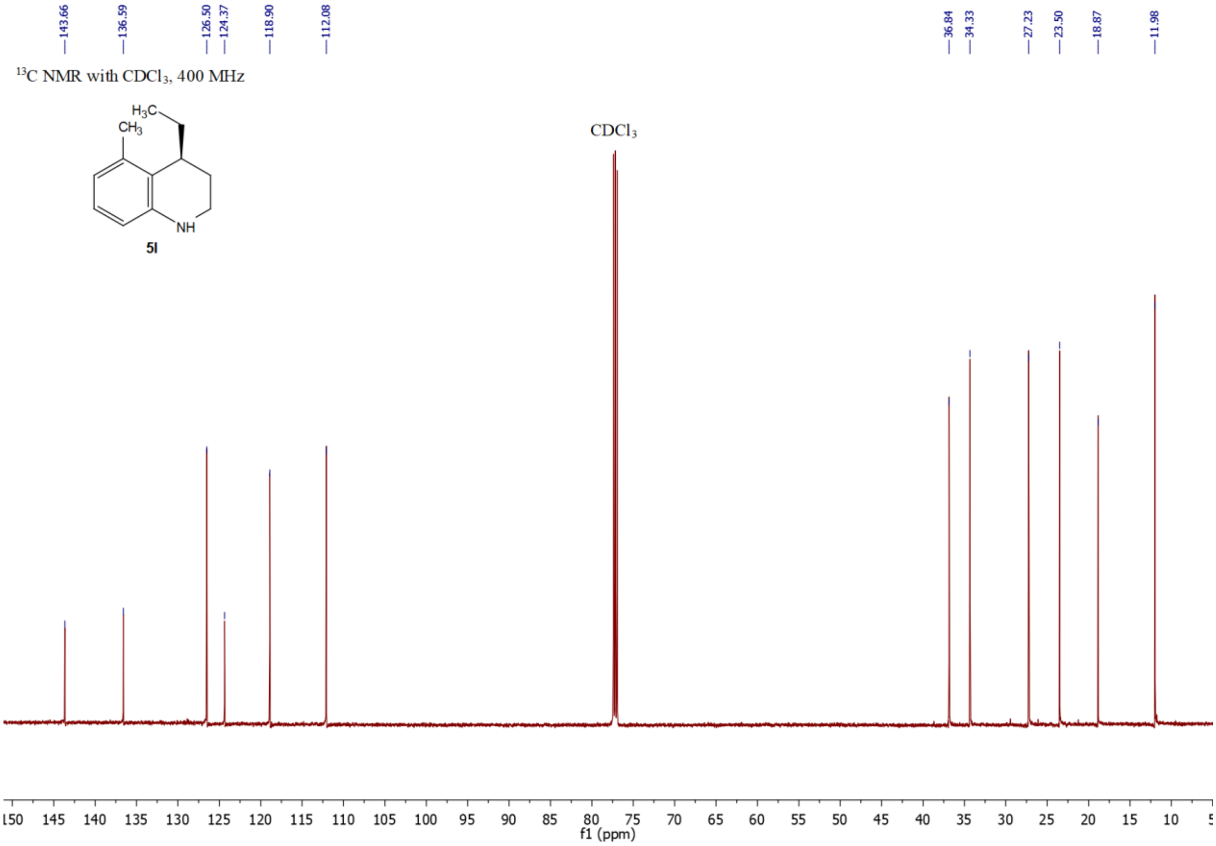
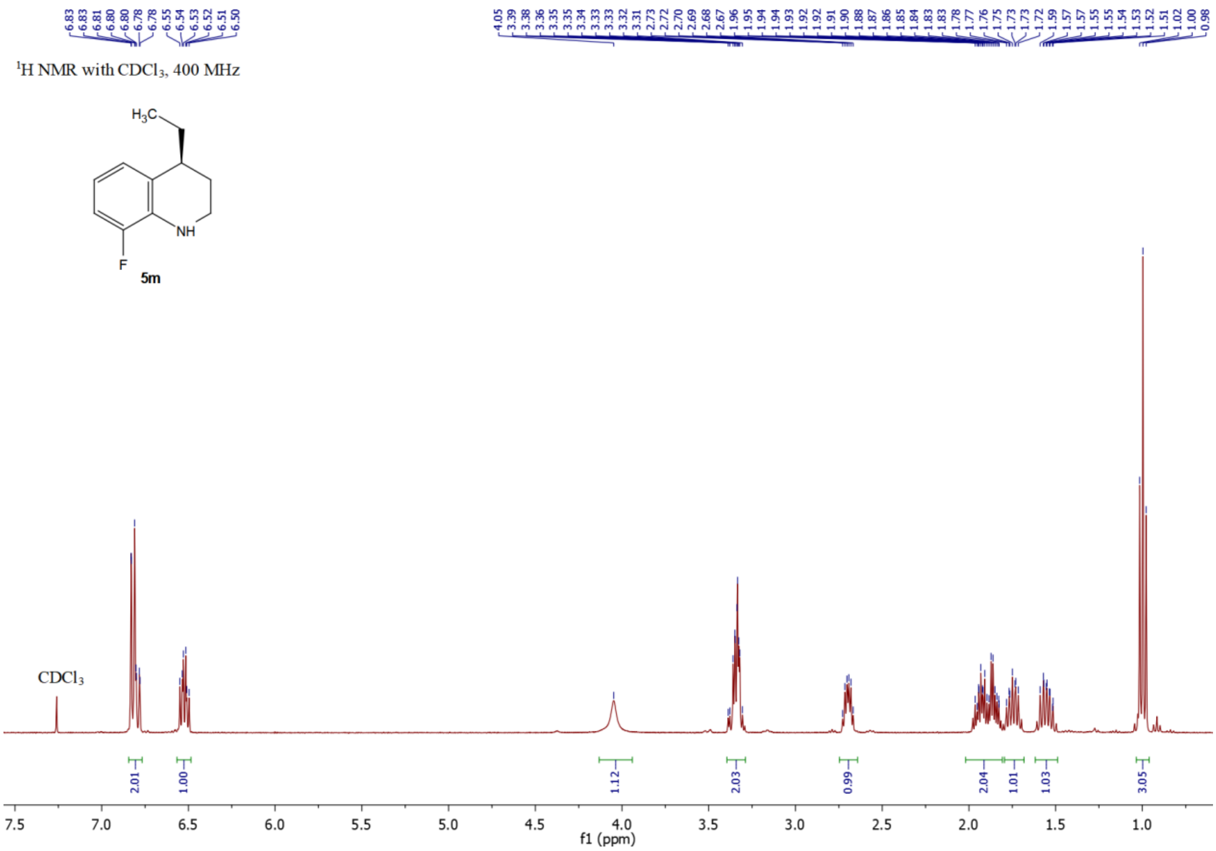
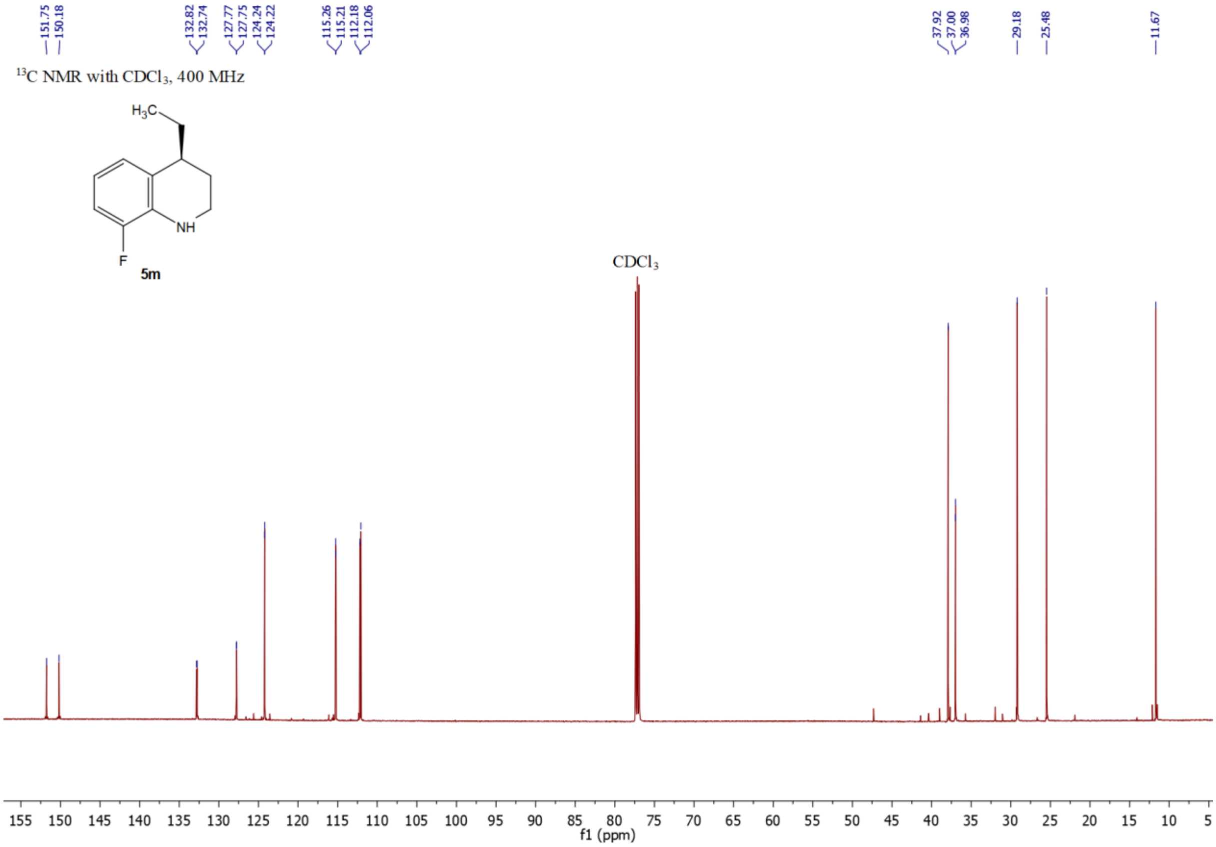


Figure S57. NMR spectra of (*S*)-4-Ethyl-5-methyl-1,2,3,4-tetrahydroquinoline (**5l**)


6.83 6.83 6.81 6.80 6.80 6.78 6.55 6.54 6.53 6.52 6.51 6.50
4.05 3.39 3.38 3.36 3.35 3.35 3.34 3.33 3.33 3.32 3.31 2.73 2.72 2.70 2.69 2.68 2.67 1.96 1.95 1.94 1.94 1.93 1.92 1.92 1.91 1.90 1.88 1.87 1.86 1.85 1.84 1.83 1.83 1.78 1.77 1.76 1.75 1.73 1.73 1.72 1.59 1.57 1.57 1.55 1.55 1.54 1.53 1.52 1.51 1.02 1.00 0.98
1H NMR with CDCl3, 400 MHz
H3C
NH
F
5m
CDCl3
2.01
1.00
1.12
2.03
0.99
2.04
1.01
1.03
3.05
f1 (ppm)


151.75 150.18
132.82 132.74 127.77 127.75 124.24 124.22
115.26 115.21 112.18 112.06
37.92 37.00 36.98
29.18
25.48
11.67
13C NMR with CDCl3, 400 MHz
H3C
NH
F
5m
CDCl3
f1 (ppm)

^{19}F NMR with $CDCl_3$, 400 MHz

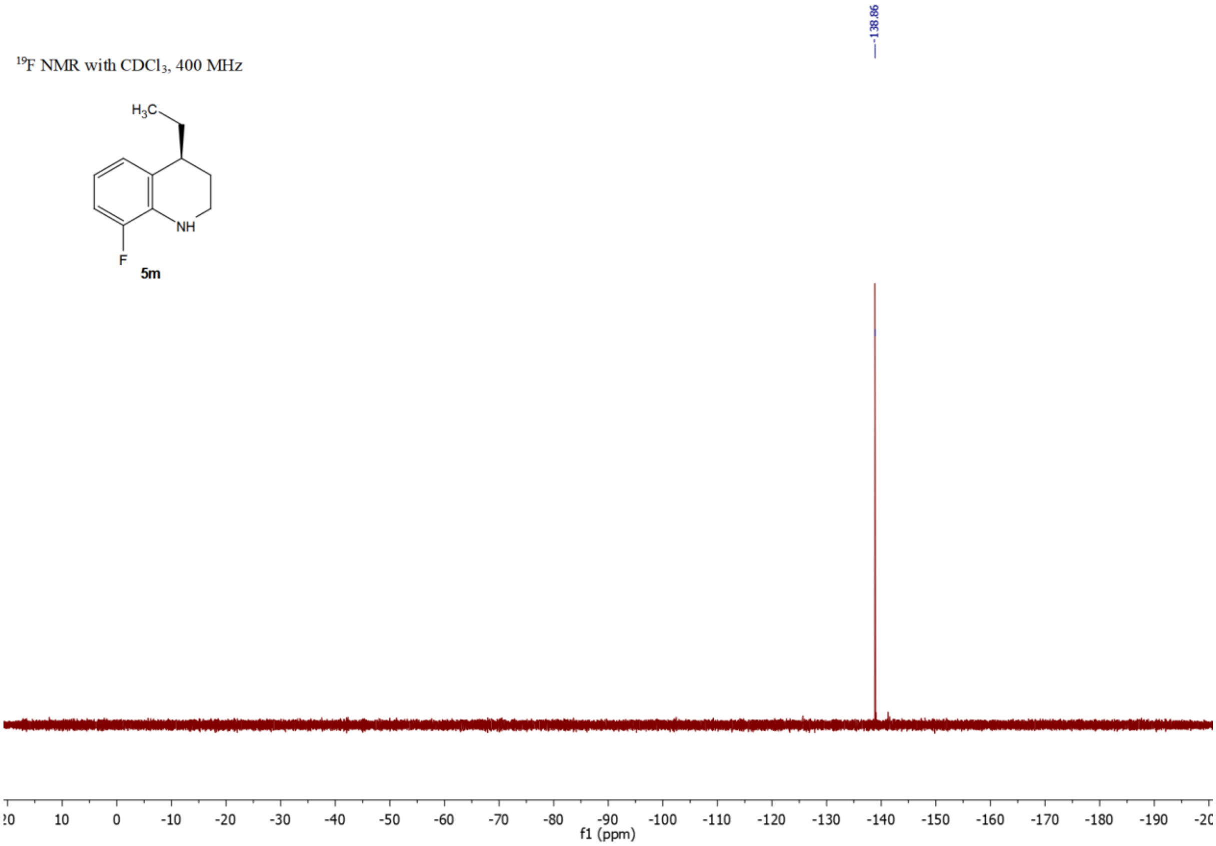
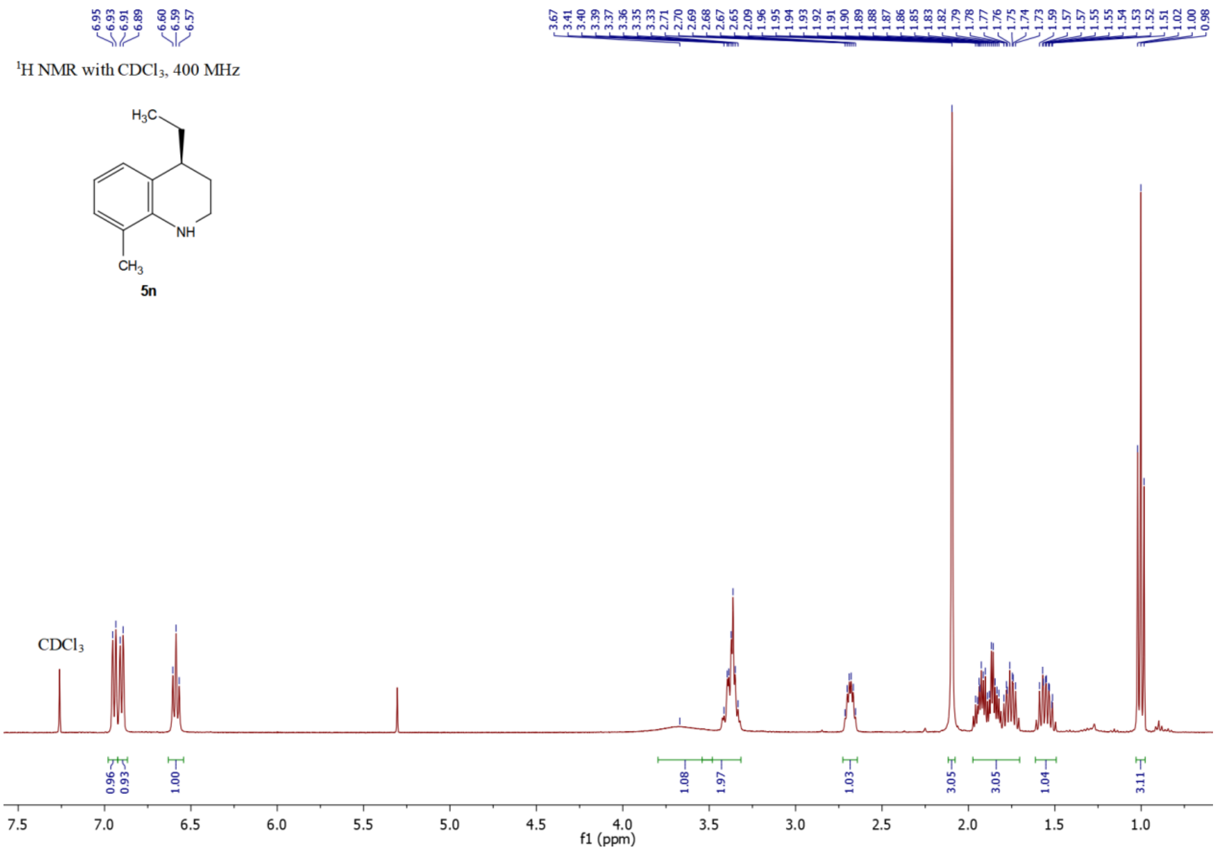


Figure S58. NMR spectra of (*S*)-4-Ethyl-8-fluoro-1,2,3,4-tetrahydroquinoline (**5m**)



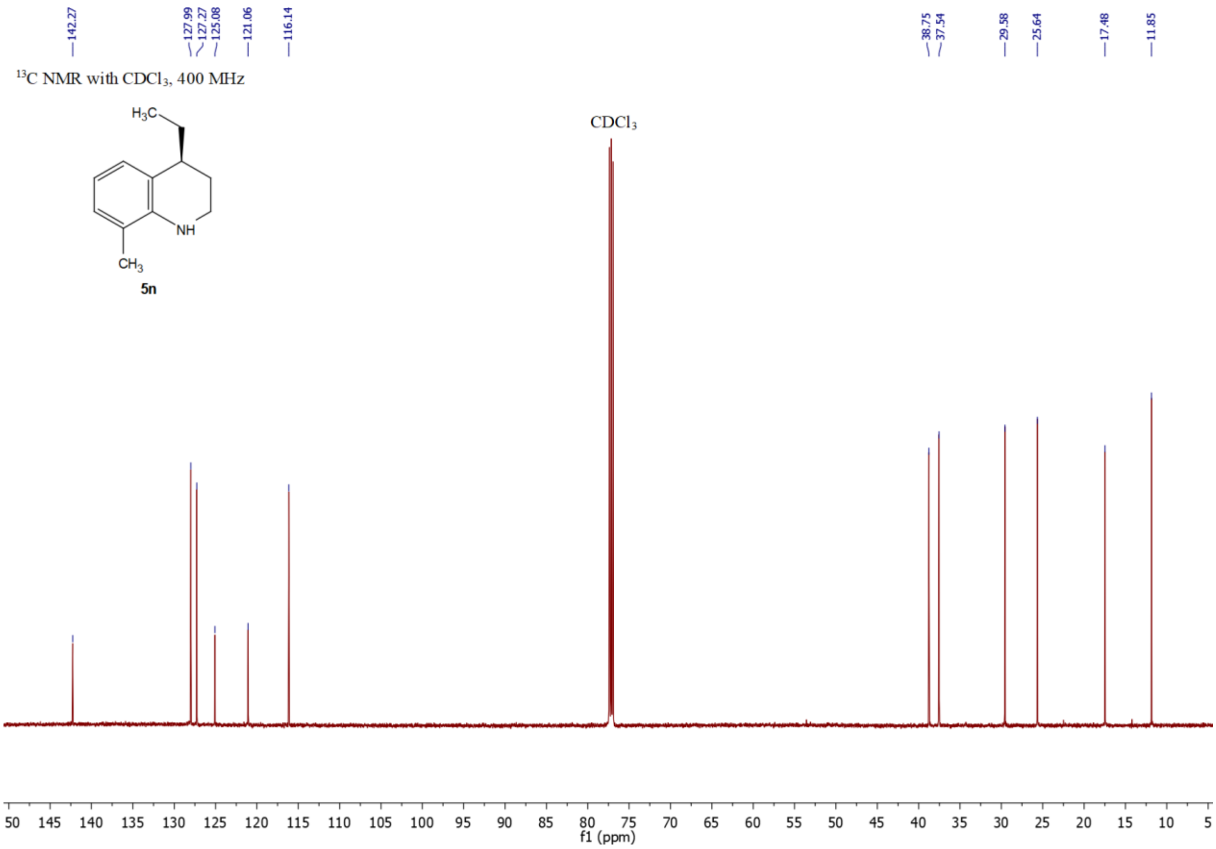
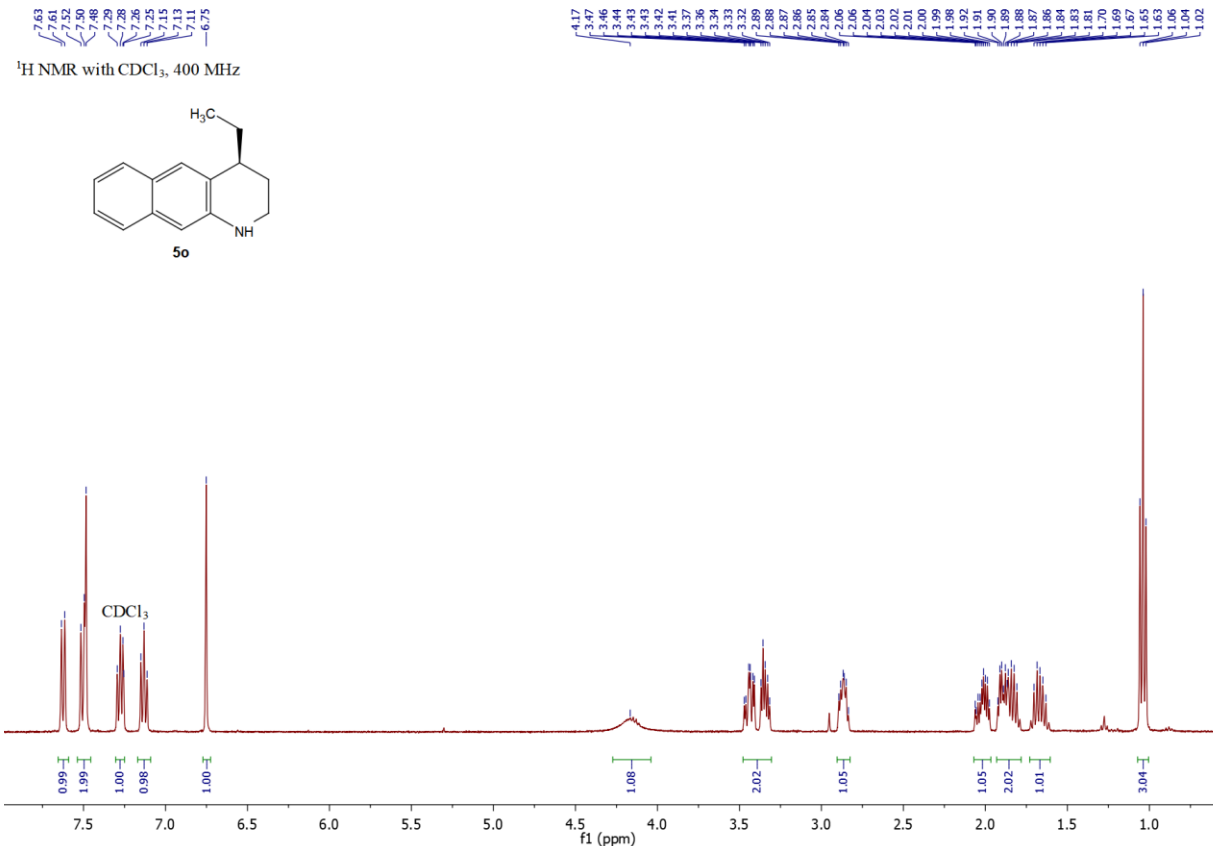


Figure S59. NMR spectra of (*S*)-4-Ethyl-8-methyl-1,2,3,4-tetrahydroquinoline (**5n**)



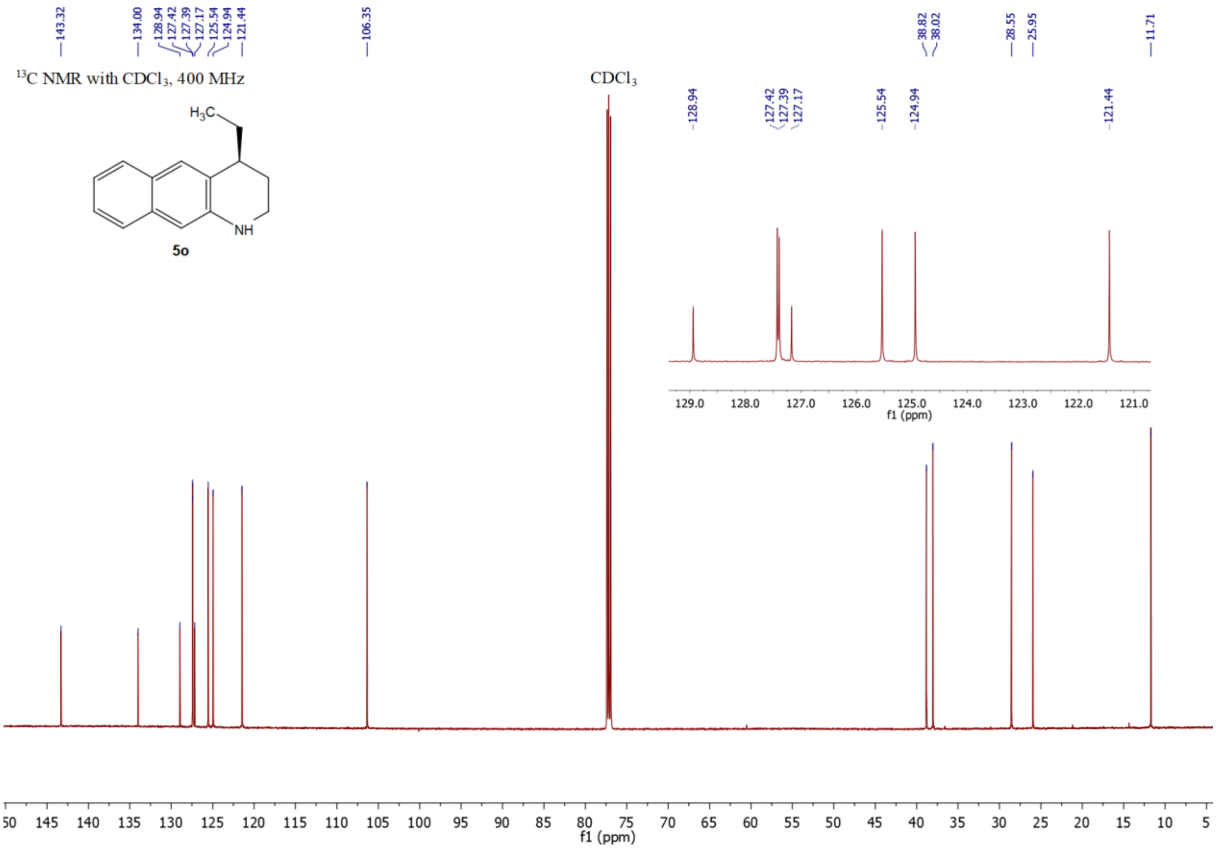
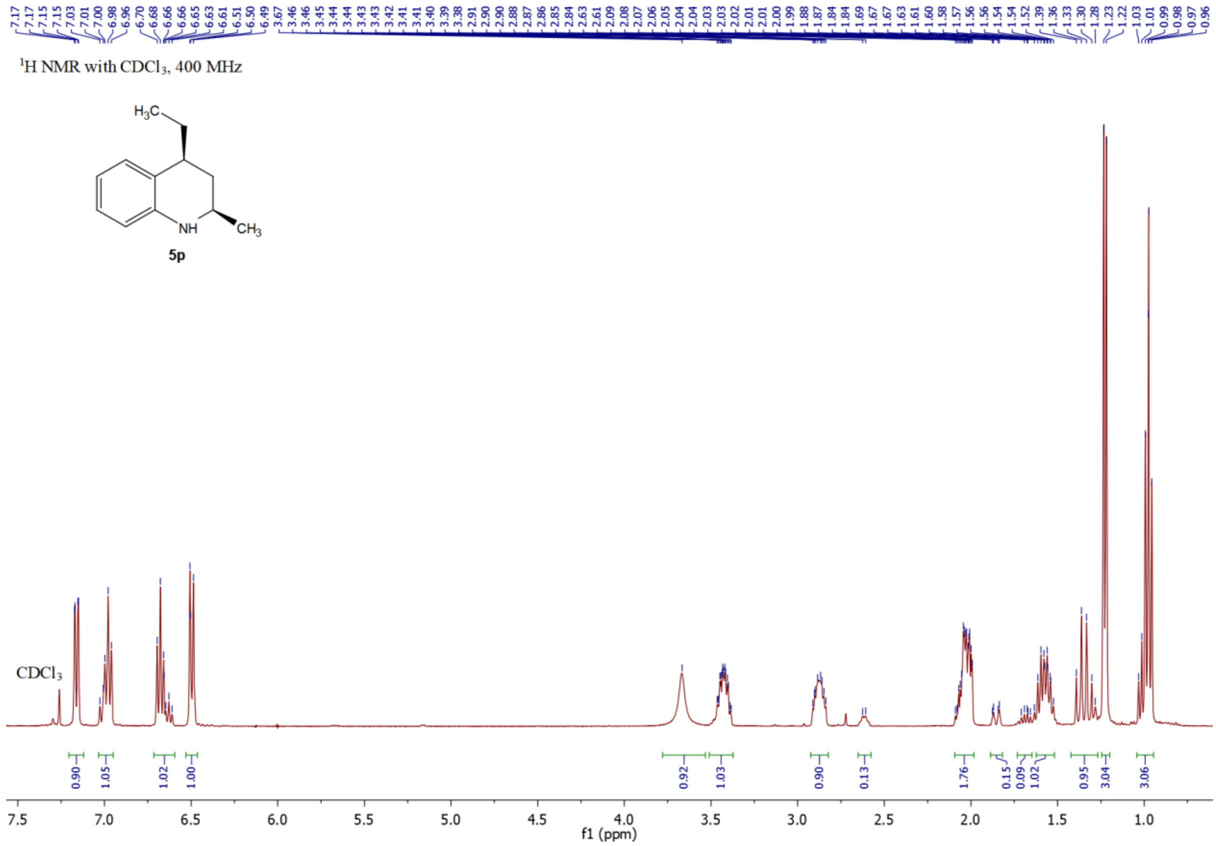
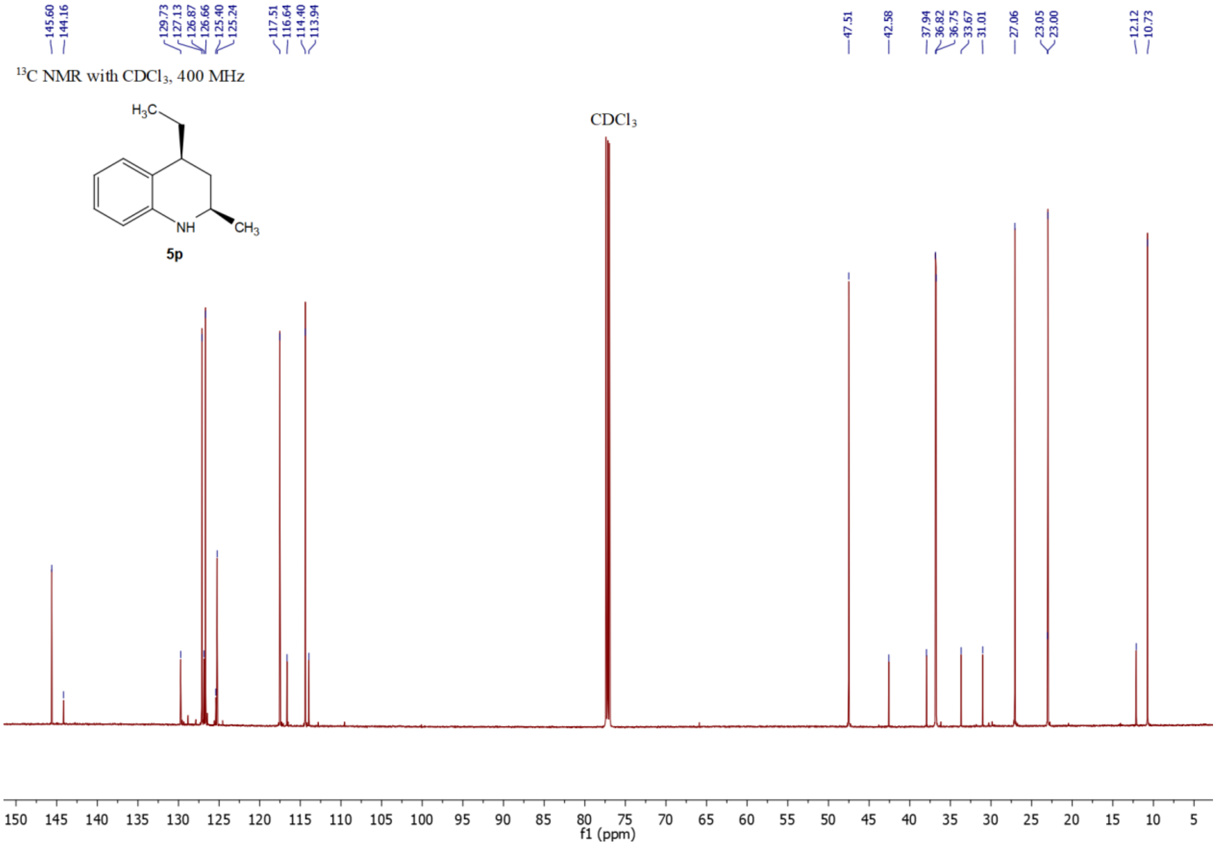
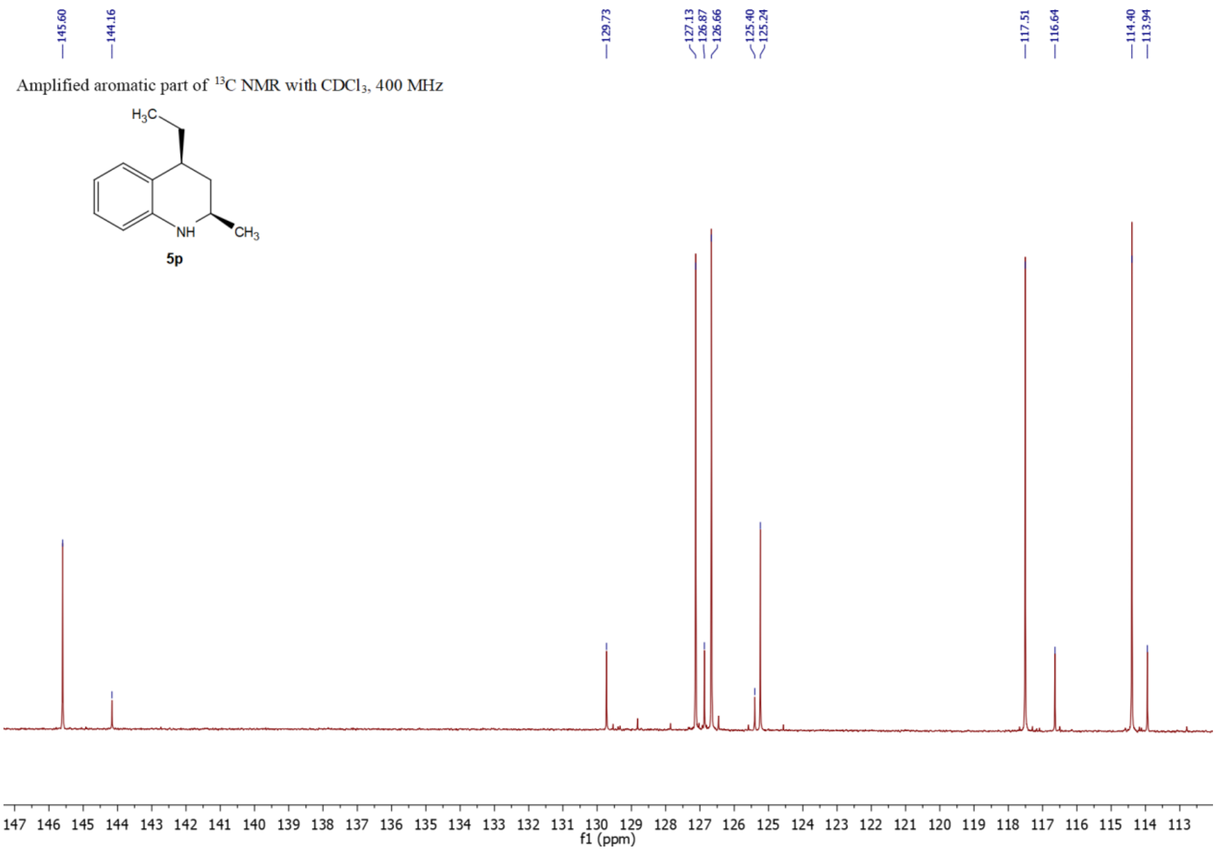


Figure S60. NMR spectra of (*S*)-4-Ethyl-1,2,3,4-tetrahydrobenzo[*g*]quinoline (**5o**)


7.17 7.17 7.15 7.15 7.03 7.01 7.00 6.98 6.96 6.70 6.68 6.66 6.66 6.65 6.63 6.61 6.51 6.50 6.49 3.67 3.46 3.46 3.45 3.44 3.44 3.43 3.43 3.42 3.41 3.41 3.40 3.39 3.38 2.91 2.90 2.90 2.88 2.87 2.86 2.85 2.84 2.63 2.61 2.09 2.08 2.07 2.06 2.05 2.04 2.04 2.03 2.03 2.02 2.01 2.01 2.00 1.99 1.88 1.87 1.84 1.84 1.69 1.67 1.67 1.63 1.61 1.60 1.58 1.57 1.56 1.56 1.54 1.54 1.52 1.39 1.36 1.33 1.30 1.28 1.23 1.22 1.03 1.01 0.99 0.98 0.97 0.96
^{1}H NMR with $CDCl_3$, 400 MHz
H_3C
NH
CH_3
5p
$CDCl_3$
0.90 1.05 1.02 1.00 0.92 1.03 0.90 0.13 1.76 0.15 0.09 1.02 0.95 3.04 3.06
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)


145.60 144.16 129.73 127.13 126.87 126.66 125.40 125.24 117.51 116.64 114.40 113.94 47.51 42.58 37.94 36.82 36.75 33.67 31.01 27.06 23.05 23.00 12.12 10.73
^{13}C NMR with $CDCl_3$, 400 MHz
H_3C
NH
CH_3
5p
$CDCl_3$
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
f1 (ppm)



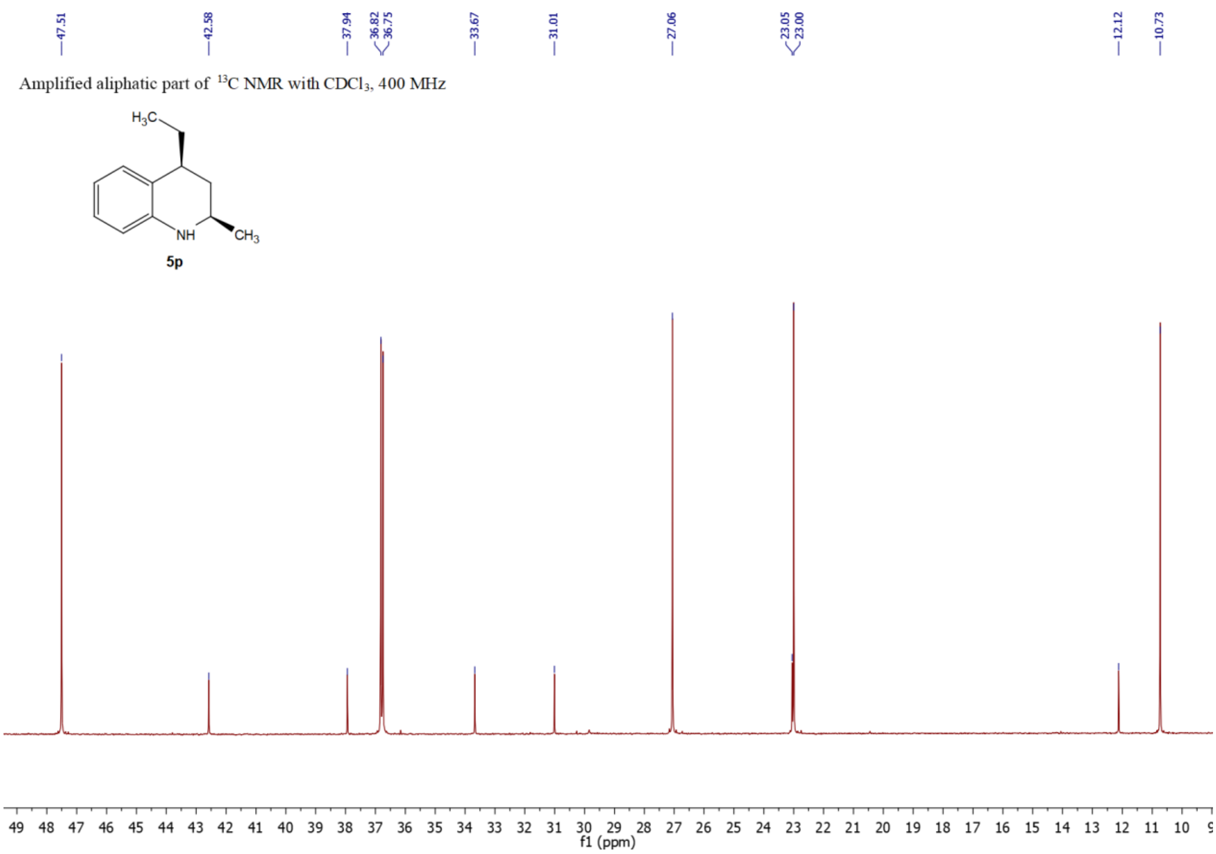
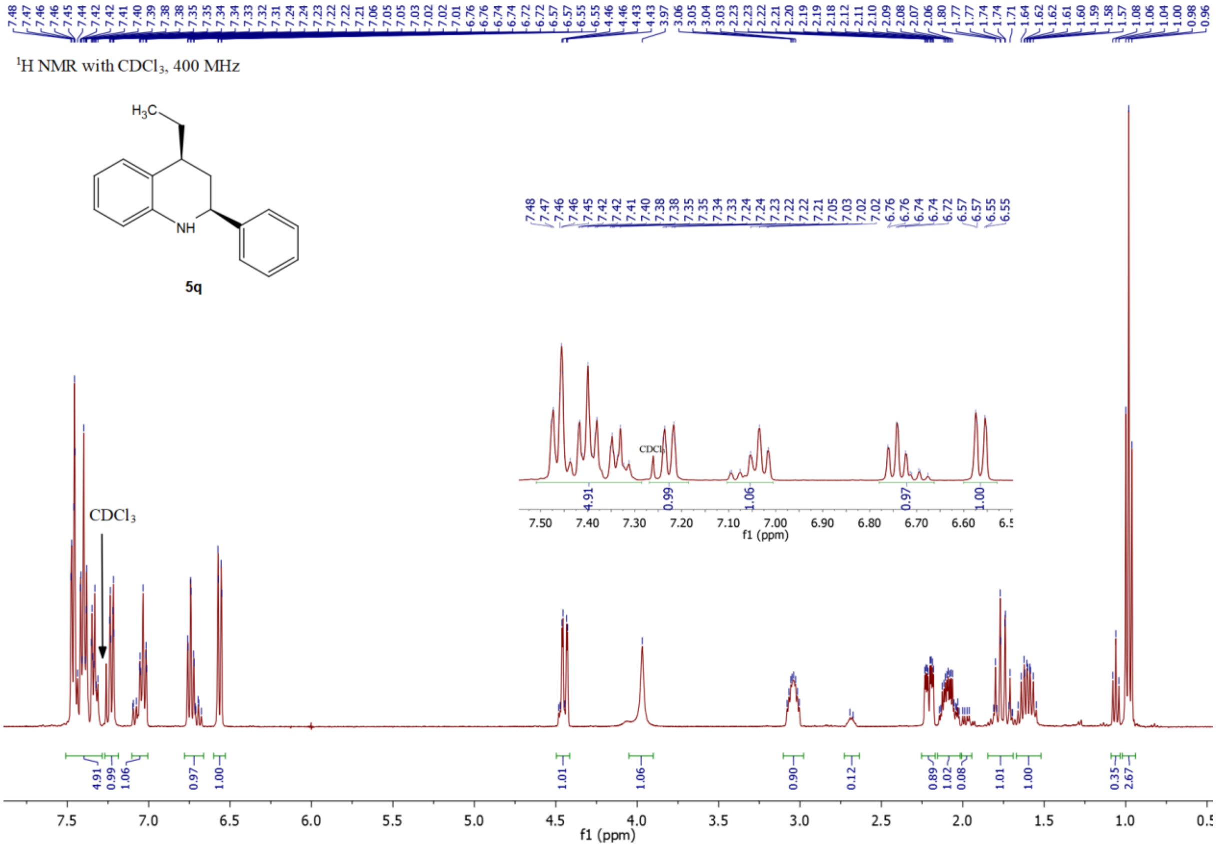
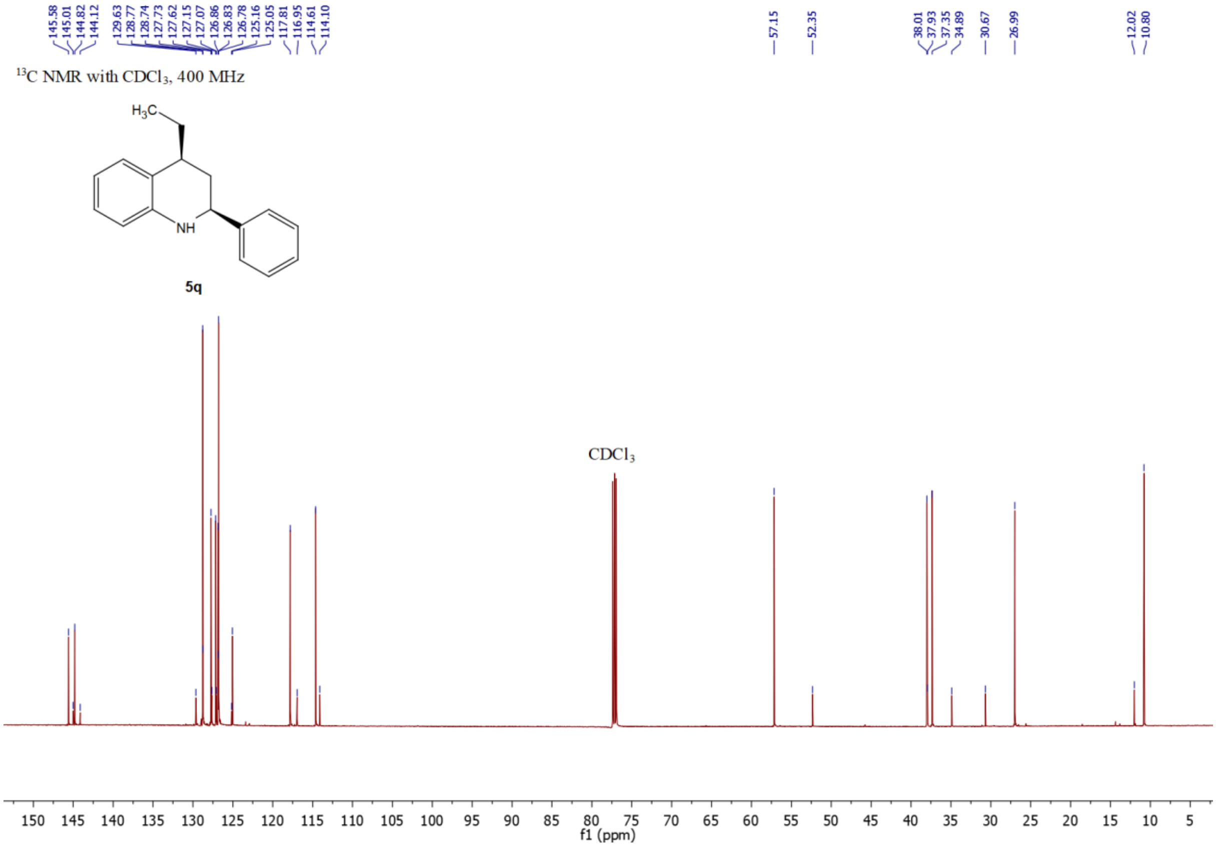
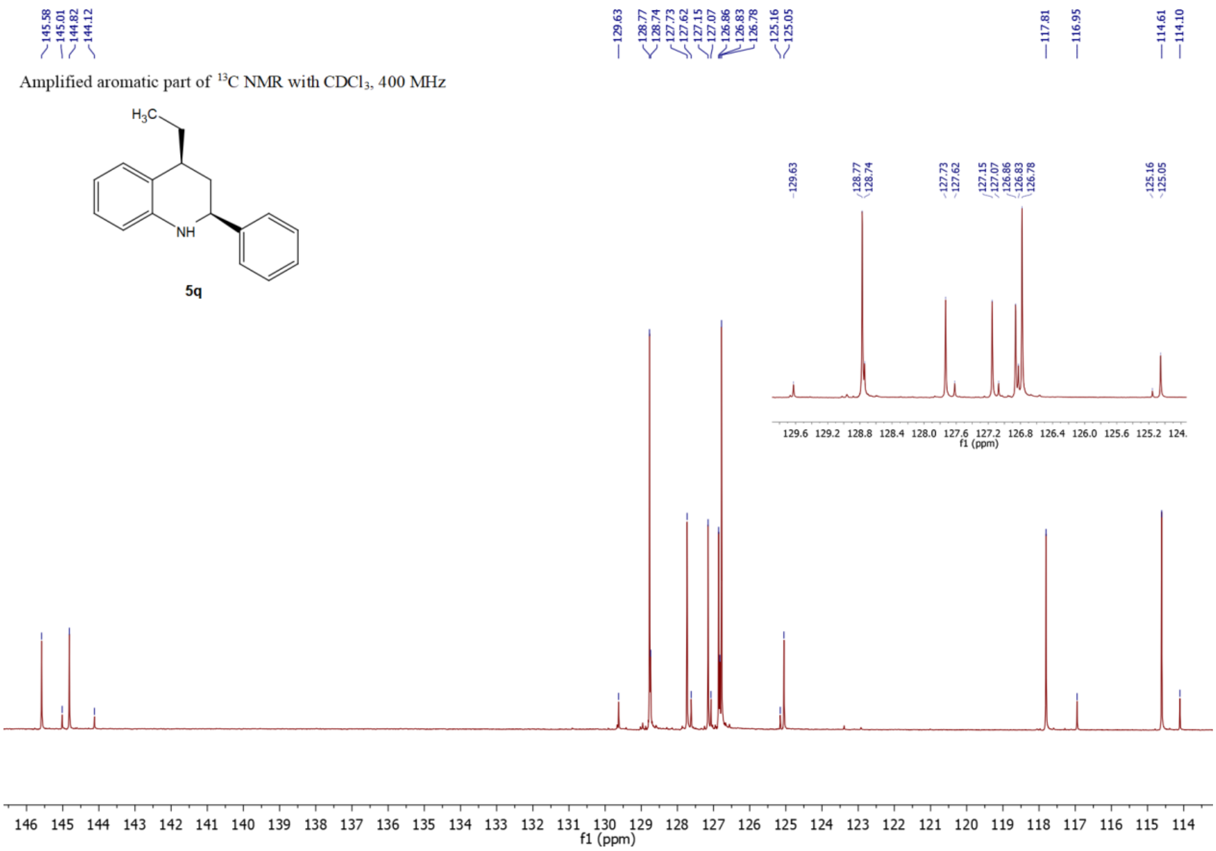


Figure S61. NMR spectra of (2*R*,4*S*)-4-Ethyl-2-methyl-1,2,3,4-tetrahydroquinoline (**5p**)


7.48 7.47 7.46 7.45 7.44 7.42 7.42 7.41 7.40 7.39 7.38 7.38 7.35 7.35 7.34 7.34 7.33 7.32 7.31 7.24 7.24 7.23 7.22 7.22 7.21 7.06 7.05 7.05 7.03 7.02 7.02 7.01 6.76 6.76 6.74 6.74 6.72 6.72 6.57 6.57 6.55 6.55 4.46 4.46 4.43 4.43 3.97 3.06 3.05 3.04 3.03 2.23 2.23 2.22 2.21 2.20 2.19 2.19 2.18 2.12 2.11 2.10 2.09 2.08 2.07 2.06 1.80 1.77 1.77 1.74 1.74 1.71 1.64 1.62 1.61 1.60 1.59 1.58 1.57 1.08 1.06 1.04 1.00 0.98 0.96
^{1}H NMR with $CDCl_3$, 400 MHz
H_3C
NH
5q
CDCl3
4.91 0.99 1.06 0.97 1.00 1.01 1.06 0.90 0.12 0.89 1.02 0.08 1.01 1.00 0.35 2.67
f1 (ppm)


145.58 145.01 144.82 144.12 129.63 128.77 128.74 127.73 127.62 127.15 127.07 126.86 126.83 126.78 125.16 125.05 117.81 116.95 114.61 114.10 57.15 52.35 38.01 37.93 37.35 34.89 30.67 26.99 12.02 10.80
^{13}C NMR with $CDCl_3$, 400 MHz
H_3C
NH
5q
CDCl3
f1 (ppm)



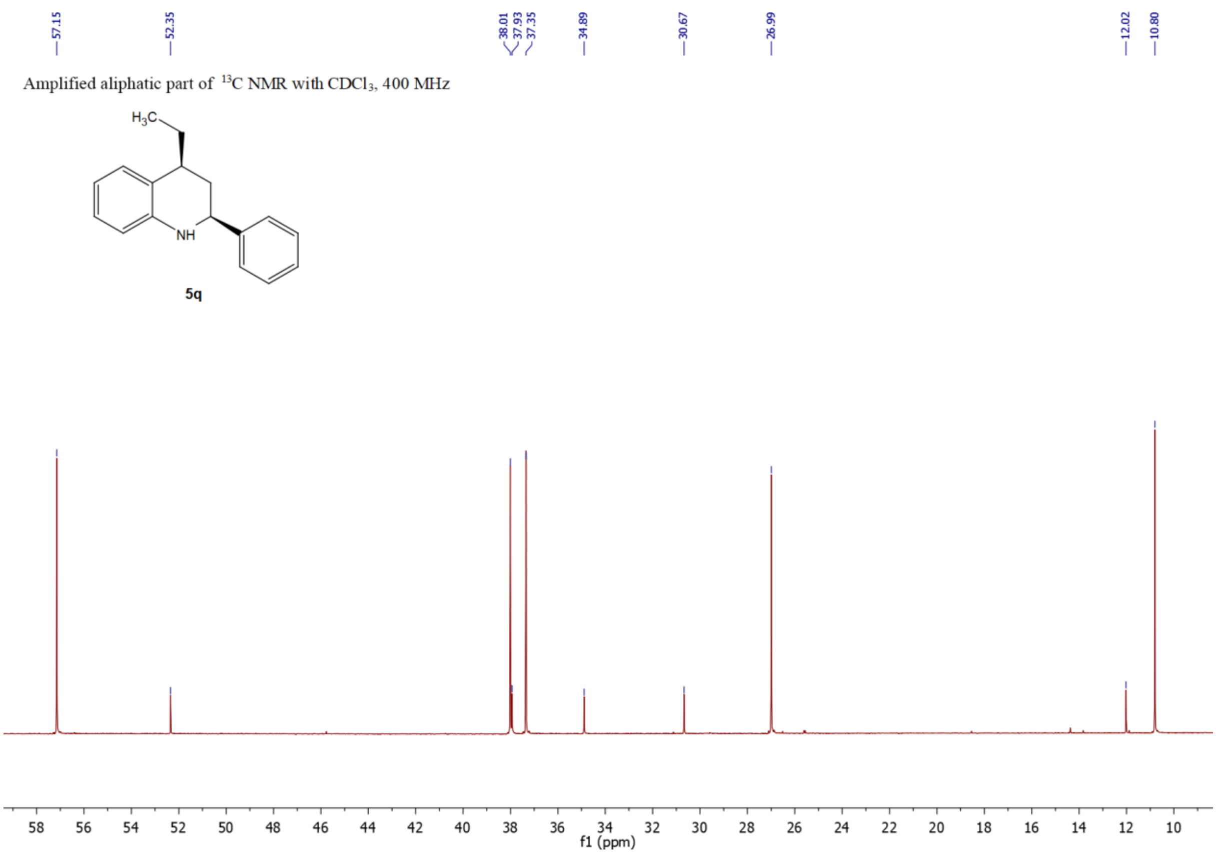
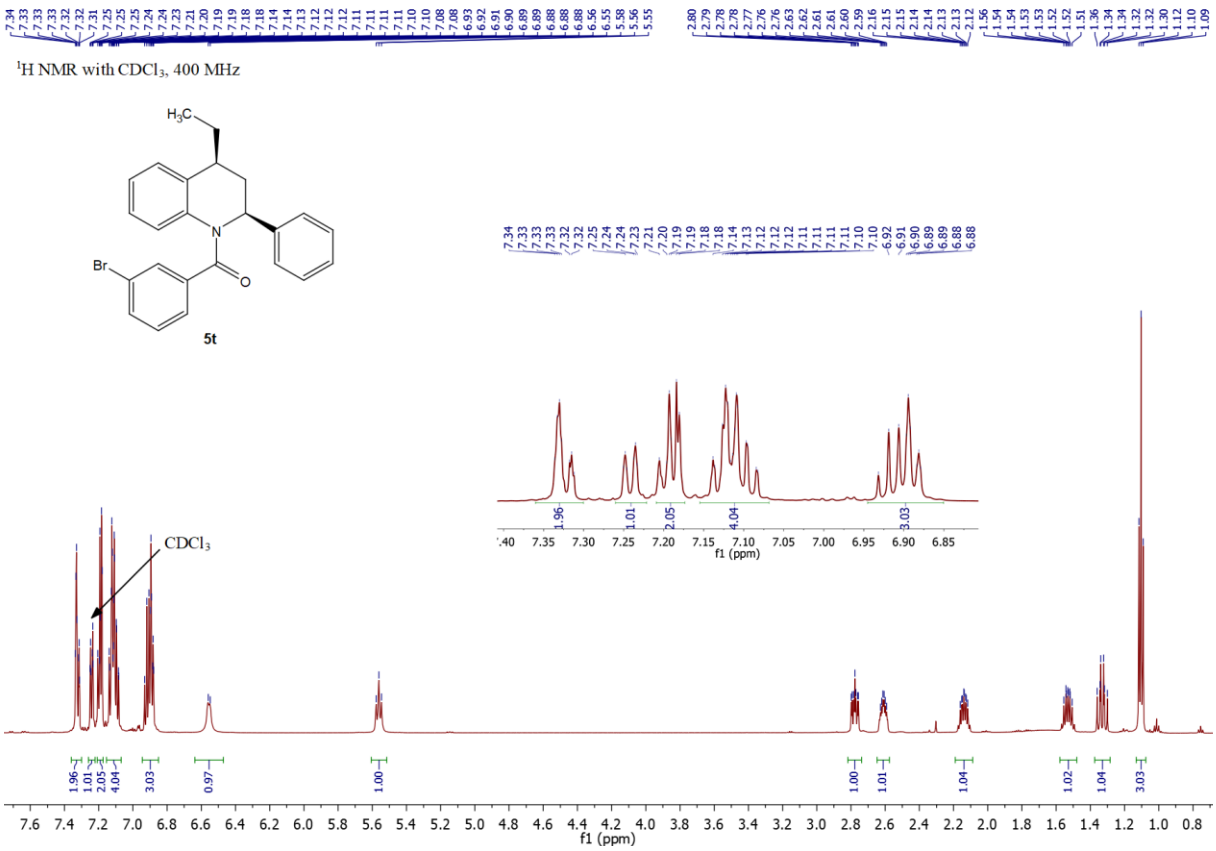
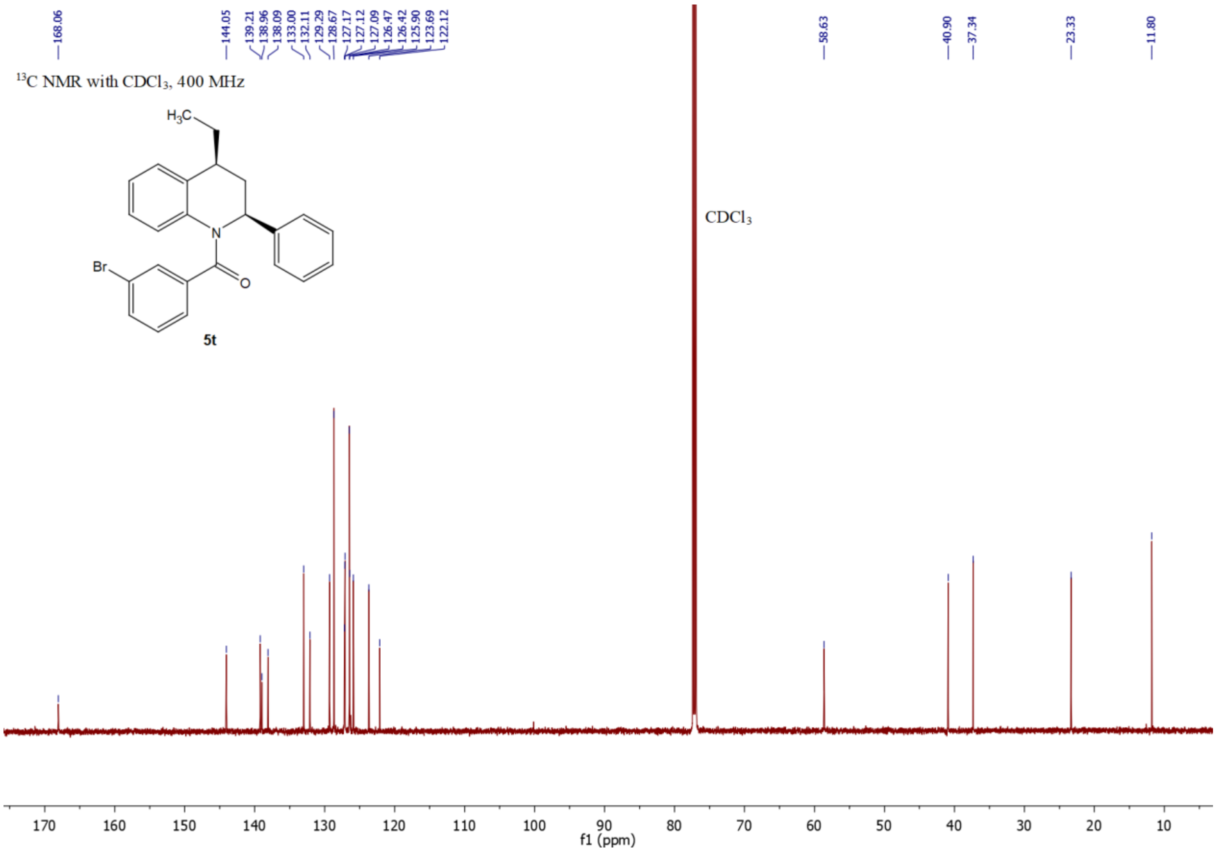


Figure S62. NMR spectra of (2*S*,4*S*)-4-ethyl-2-phenyl-1,2,3,4-tetrahydroquinoline (**5q**)


^{1}H NMR with CDCl$_3$, 400 MHz
5t
CDCl$_3$
f1 (ppm)


168.06
144.05
139.21
138.96
138.09
133.00
132.11
129.29
128.67
127.17
127.12
127.09
126.42
125.90
123.69
122.12
58.63
40.90
37.34
23.33
11.80
^{13}C NMR with CDCl$_3$, 400 MHz
5t
CDCl$_3$
f1 (ppm)

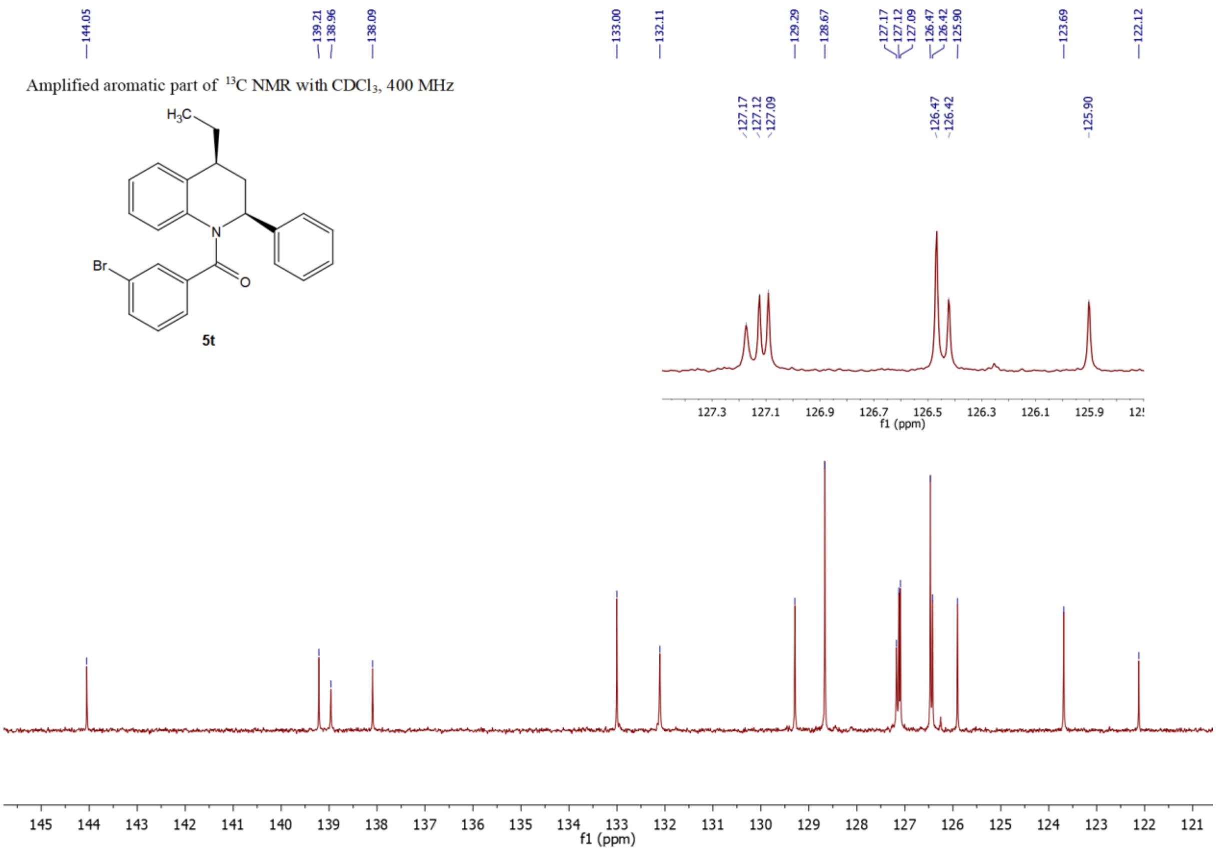
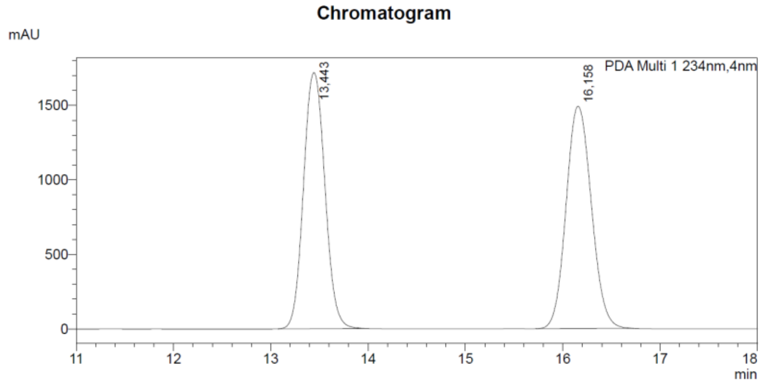


Figure S63. NMR spectra of (2*S*,4*S*)-1-(3-Bromophenyl)carbonyl-4-ethyl-2-phenyl-1,2,3,4-tetrahydroquinoline (**5t**)

11. HPLC and UV spectra

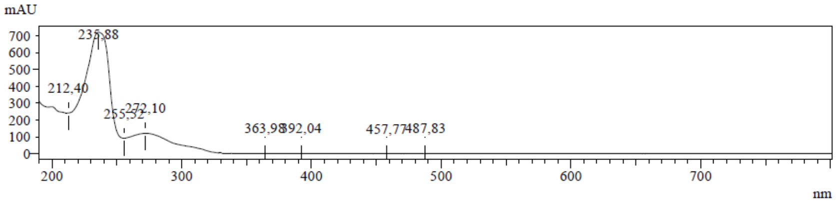


Peak Table

PDA Ch1 234nm

Peak#	Ret. Time	Area	Height	Conc.
1	13,443	26259763	1718345	49,311
2	16,158	26993870	1492601	50,689
Total		53253633	3210946	

Peak# : 14
Retention Time : 13,483 min
Compound Name :
Spectrum Operation : None



Peak# : 17
Retention Time : 16,217 min
Compound Name :
Spectrum Operation : None

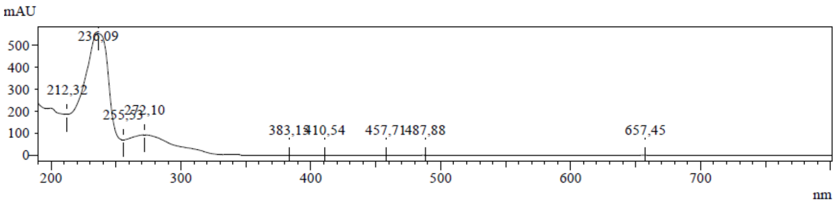
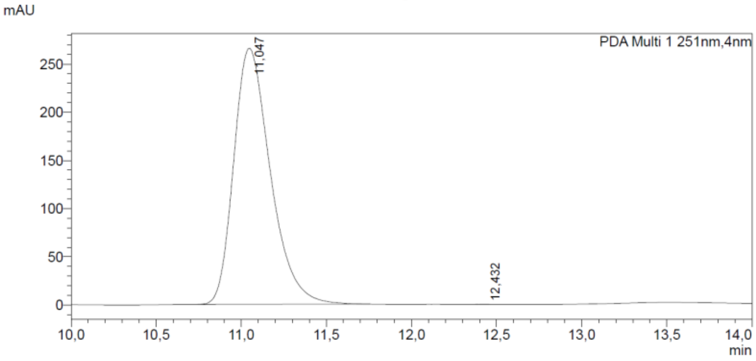


Figure S64. HPLC and UV spectra of 1-acetyl-2-ethyl-C2-dihydroquinoline (**2a**)

Chromatogram

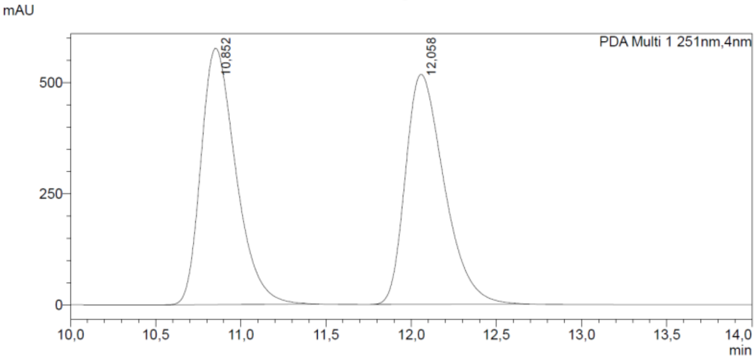


Peak Table

PDA Ch1 251nm

Peak#	Ret. Time	Area	Height	Conc.
1	11,047	3984112	265756	99,986
2	12,432	557	60	0,014
Total		3984669	265816	

Chromatogram

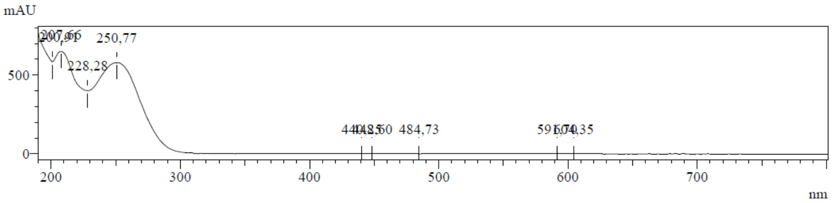


Peak Table

PDA Ch1 251nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,852	8227019	576334	50,053
2	12,058	8209518	516897	49,947
Total		16436537	1093230	

Peak# : 9
Retention Time : 10,852 min
Compound Name :
Spectrum Operation : None



Peak# : 10
Retention Time : 12,058 min
Compound Name :
Spectrum Operation : None

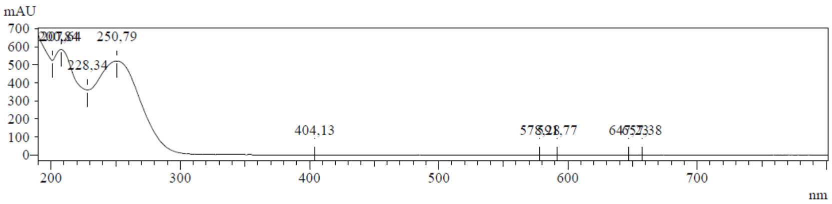
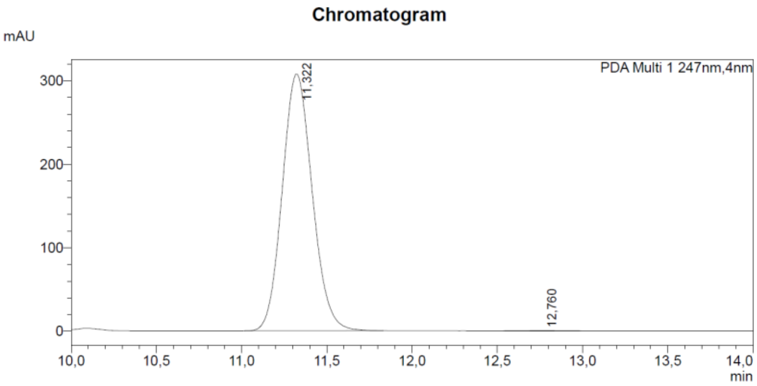


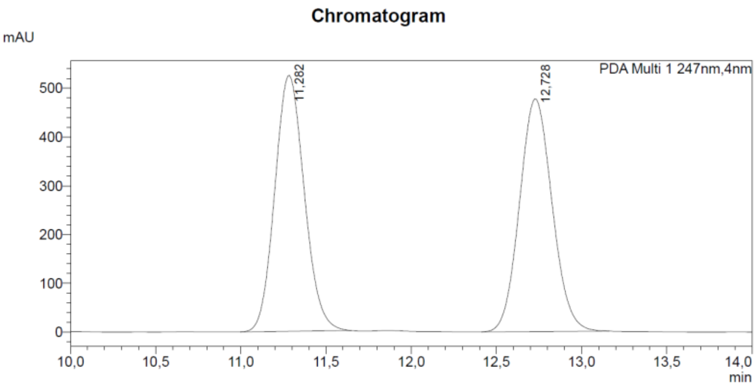
Figure S65. HPLC and UV spectra of (*S*)-1-acetyl-4-ethyl-C4-dihydroquinoline (**3a**)



Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	11,322	3768046	307485	99,887
2	12,760	4249	309	0,113
Total		3772295	307794	

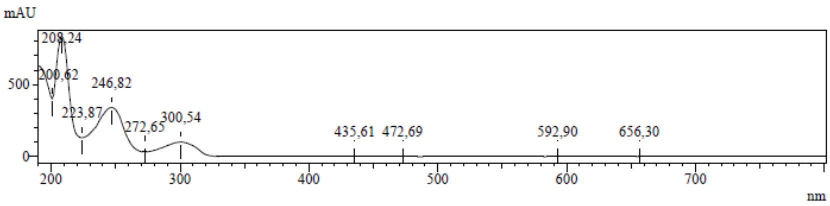


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	11,282	6331790	525036	49,883
2	12,728	6361409	477410	50,117
Total		12693199	1002446	

Peak# : 1
Retention Time : 11,397 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 12,890 min
Compound Name :
Spectrum Operation : None

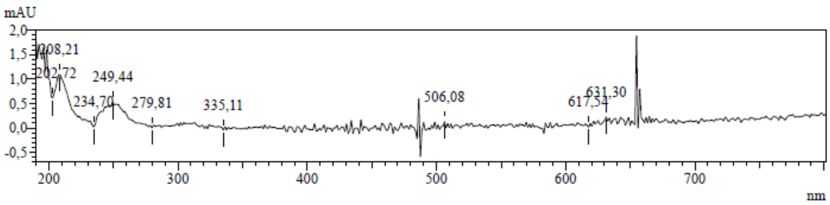
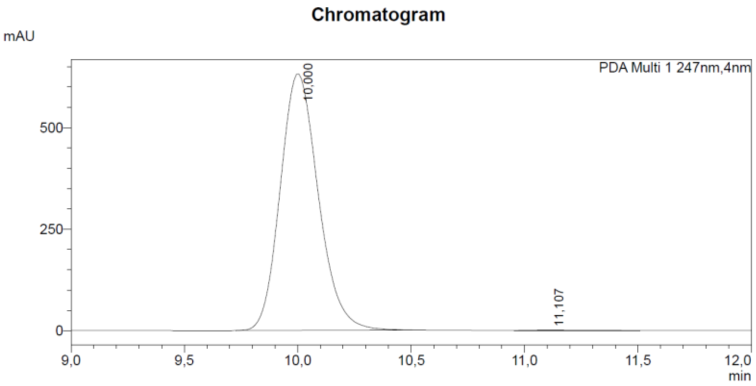


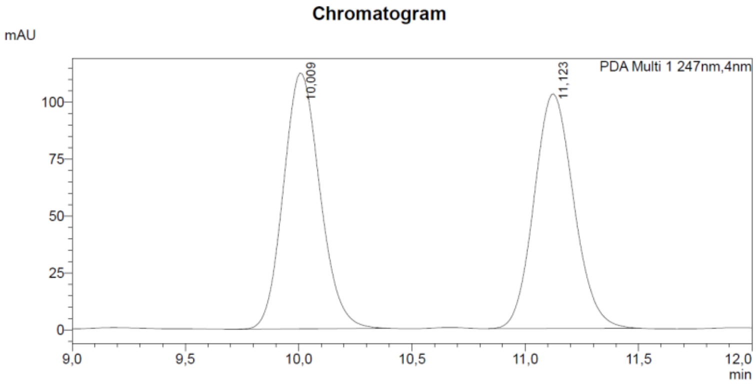
Figure S66. HPLC and UV spectra of (*S*)-4-Ethyl-1,2,3,4-tetrahydroquinoline (**4a**)



Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,000	7384579	630868	99,802
2	11,107	14623	716	0,198
Total		7399202	631584	

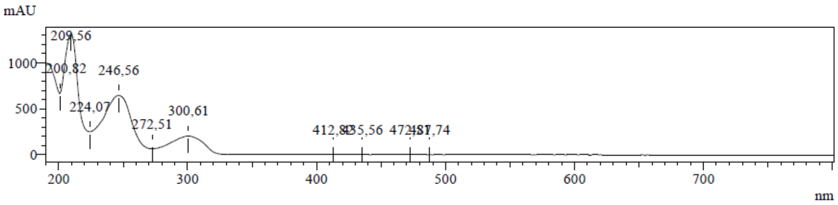


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,009	1263546	112336	50,144
2	11,123	1256313	103048	49,856
Total		2519858	215384	

Peak# : 9
Retention Time : 10,000 min
Compound Name :
Spectrum Operation : None



Peak# : 10
Retention Time : 11,109 min
Compound Name :
Spectrum Operation : None

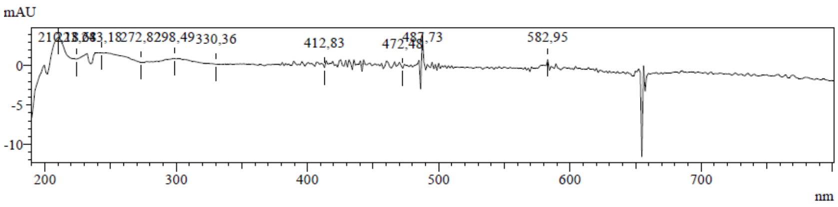
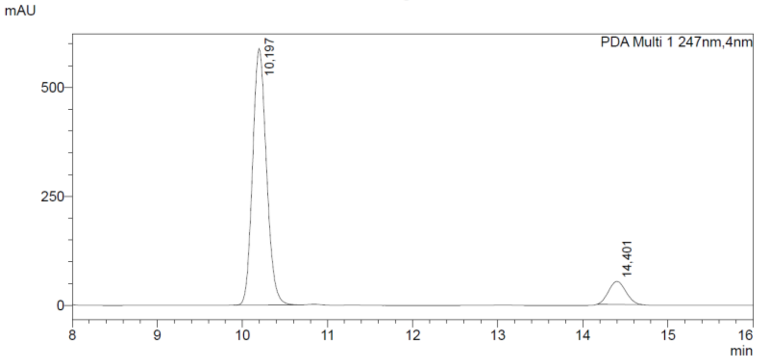


Figure S67. HPLC and UV spectra of (*S*)-4-Pentyl-1,2,3,4-tetrahydroquinoline (**4b**)

Chromatogram

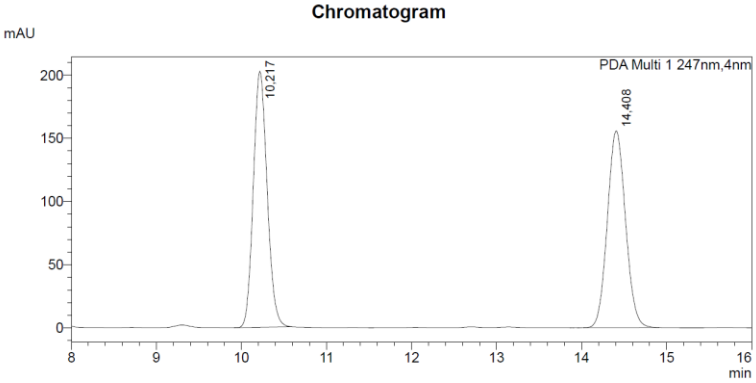


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,197	6685332	588080	89,922
2	14,401	749245	52988	10,078
Total		7434577	641068	

Chromatogram

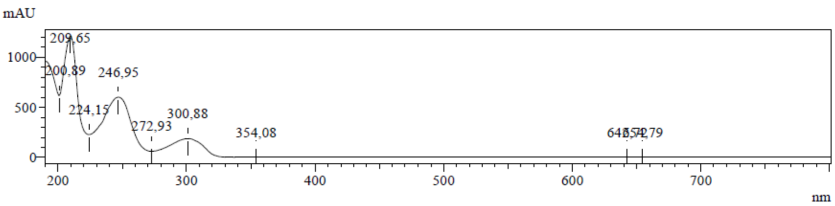


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,217	2293884	202647	49,821
2	14,408	2310375	155734	50,179
Total		4604259	358381	

Peak# : 5
Retention Time : 10,197 min
Compound Name :
Spectrum Operation : None



Peak# : 10
Retention Time : 14,401 min
Compound Name :
Spectrum Operation : None

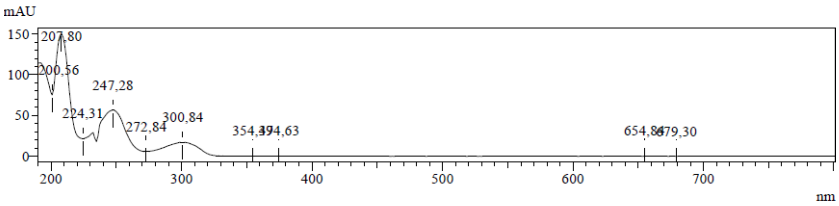
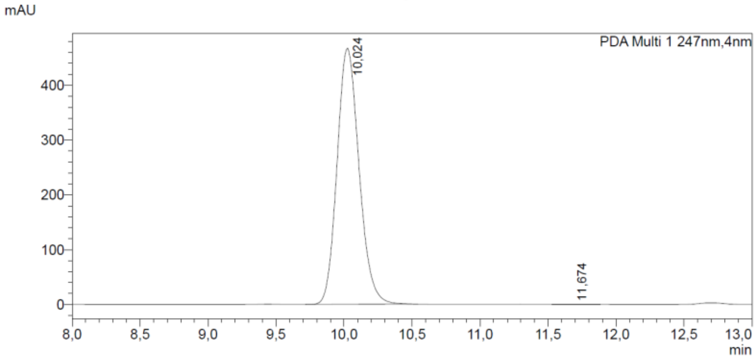


Figure S68. HPLC and UV spectra of (*R*)-4-(1-methylethyl)-1,2,3,4-tetrahydroquinoline (**4c**)

Chromatogram

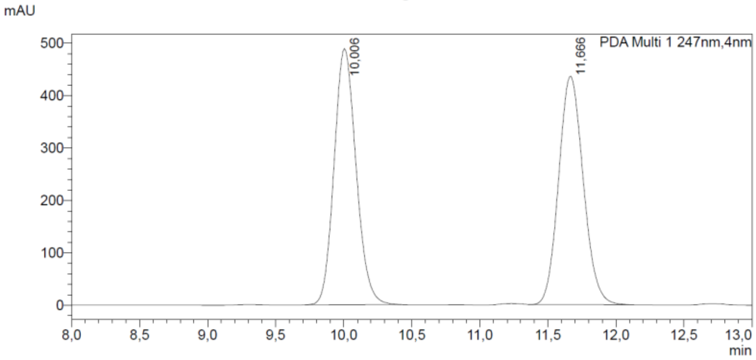


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,024	5264042	467234	99,952
2	11,674	2550	247	0,048
Total		5266592	467481	

Chromatogram

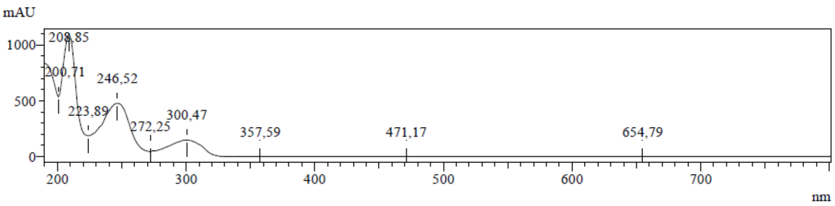


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,006	5500897	488819	50,038
2	11,666	5492561	435884	49,962
Total		10993458	924703	

Peak# : 7
Retention Time : 10,024 min
Compound Name :
Spectrum Operation : None



Peak# : 9
Retention Time : 11,681 min
Compound Name :
Spectrum Operation : None

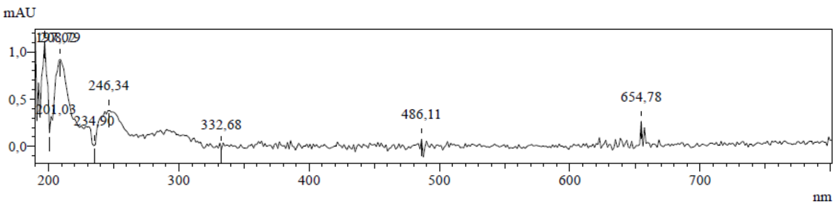
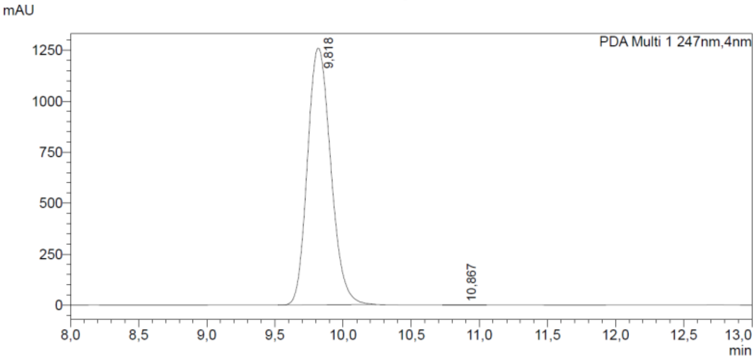


Figure S69. HPLC and UV spectra of (*S*)-4-(2-methylpropyl)-1,2,3,4-tetrahydroquinoline (**4d**)

Chromatogram

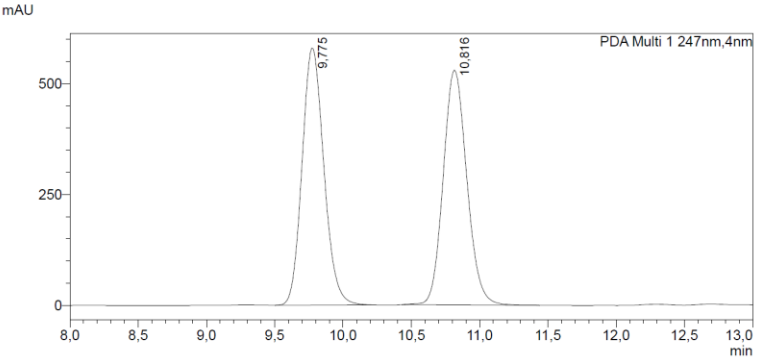


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	9,818	15010420	1258592	99,971
2	10,867	4423	450	0,029
Total		15014843	1259041	

Chromatogram

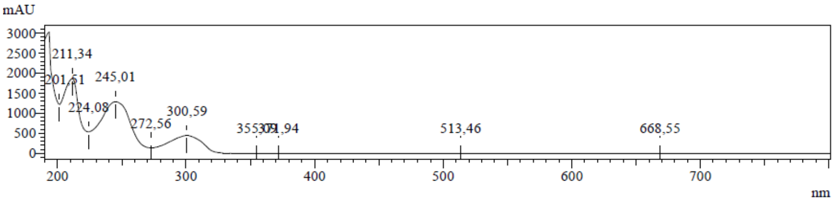


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	9,775	6437798	579345	50,238
2	10,816	6376736	529746	49,762
Total		12814534	1109091	

Peak# : 10
Retention Time : 9,818 min
Compound Name :
Spectrum Operation : None



Peak# : 11
Retention Time : 10,868 min
Compound Name :
Spectrum Operation : None

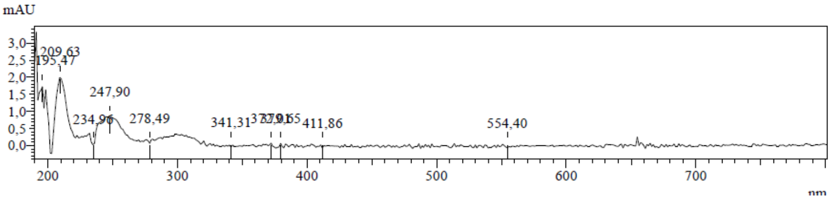
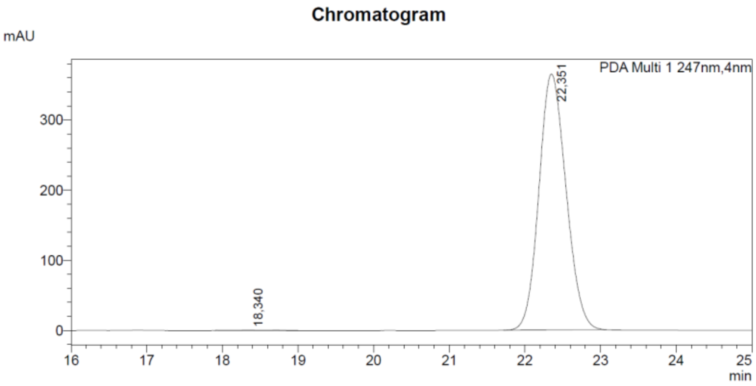


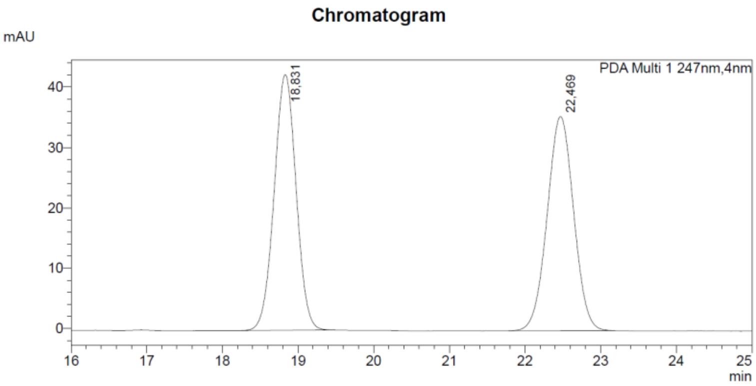
Figure S70. HPLC and UV spectra of (*S*)-4-(3-methylbutyl)-1,2,3,4-tetrahydroquinoline (**4e**)



Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	18,340	12520	338	0,137
2	22,351	9095544	364729	99,863
Total		9108064	365066	

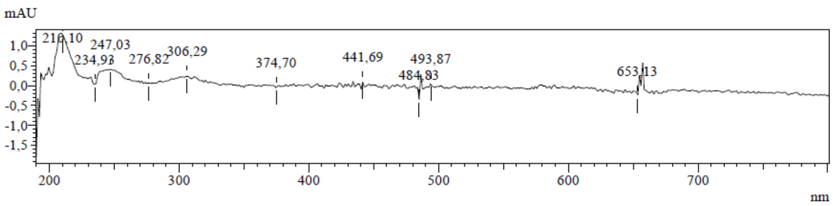


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	18,831	853385	42328	49,700
2	22,469	863700	35476	50,300
Total		1717085	77804	

Peak# : 1
Retention Time : 18,340 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 22,351 min
Compound Name :
Spectrum Operation : None

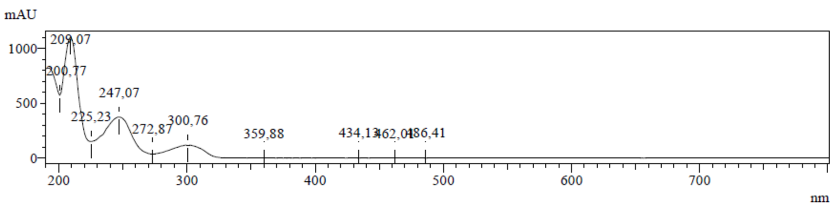
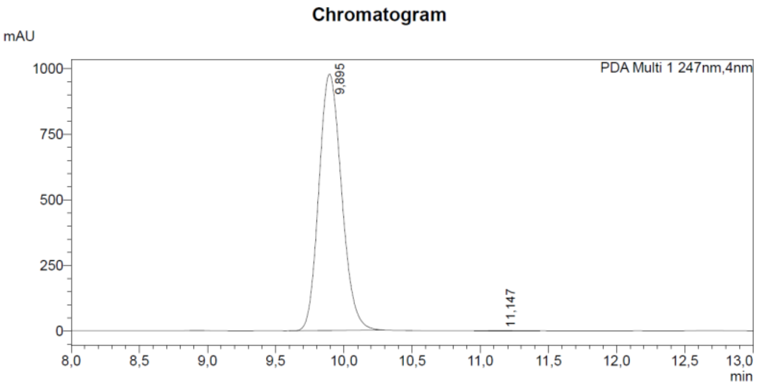


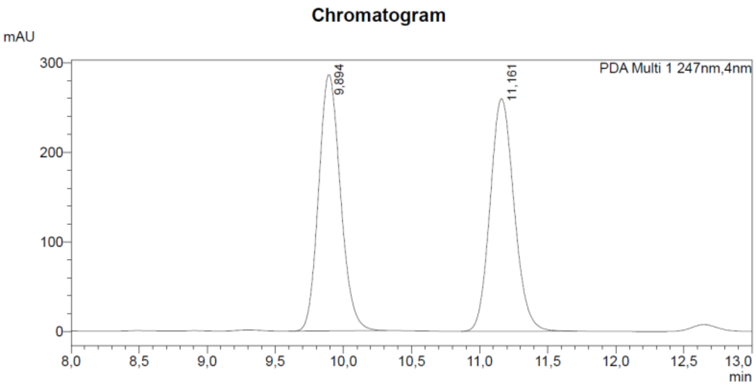
Figure S71. HPLC and UV spectra of (*S*)-4-(3-Phenylpropyl)-1,2,3,4-tetrahydroquinoline (**4f**)



Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	9,895	11349938	976578	99,879
2	11,147	13775	1135	0,121
Total		11363713	977713	

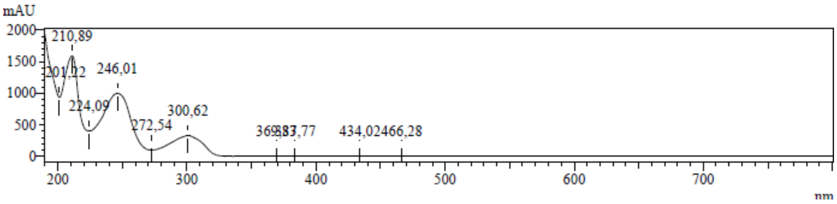


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	9,894	3198899	285786	50,032
2	11,161	3194796	259732	49,968
Total		6393695	545518	

Peak# : 13
Retention Time : 9,895 min
Compound Name :
Spectrum Operation : None



Peak# : 15
Retention Time : 11,148 min
Compound Name :
Spectrum Operation : None

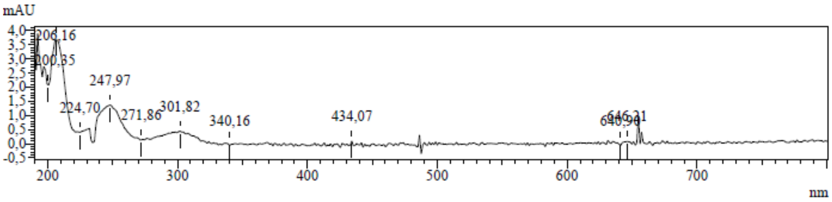
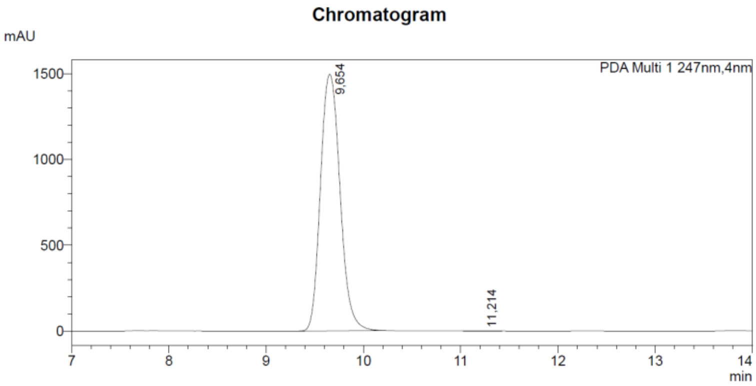


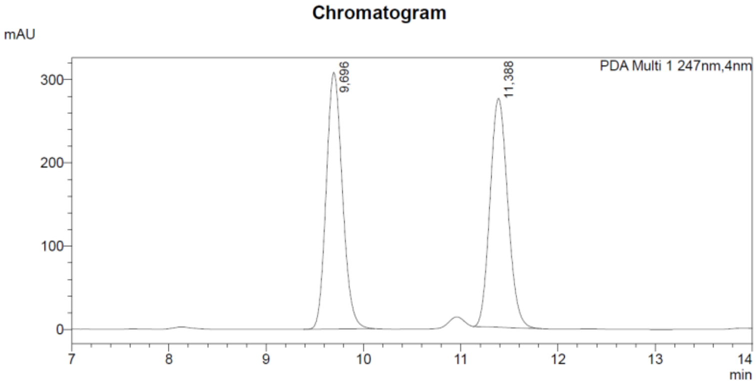
Figure S72. HPLC and UV spectra of (*S*)-4-(Hept-6-en-1-yl)-1,2,3,4-tetrahydroquinoline (**4g**)



Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	9,654	20936113	1496918	99,968
2	11,214	6667	576	0,032
Total		20942781	1497494	

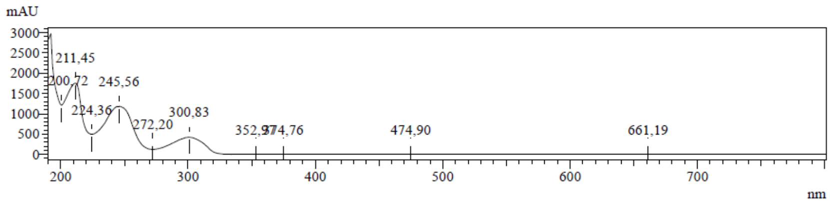


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	9,696	3559109	308222	50,489
2	11,388	3490126	274976	49,511
Total		7049235	583199	

Peak# : 7
Retention Time : 9,643 min
Compound Name :
Spectrum Operation : None



Peak# : 9
Retention Time : 11,305 min
Compound Name :
Spectrum Operation : None

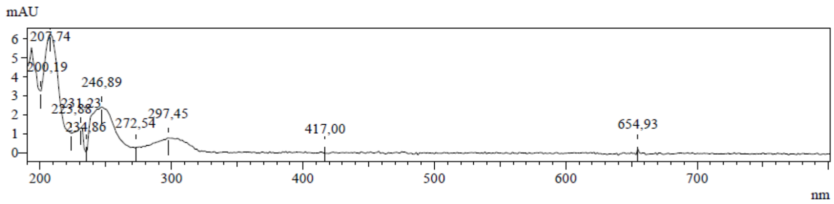
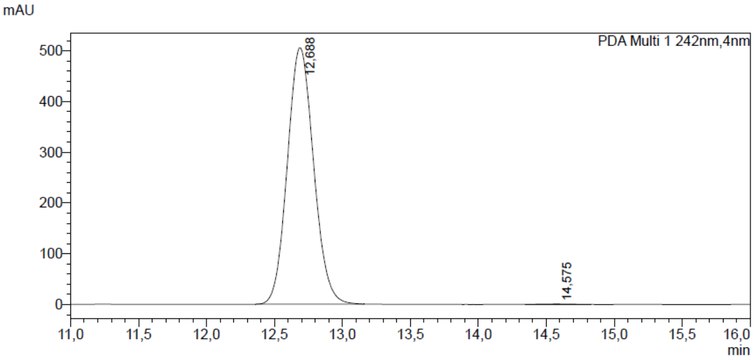


Figure S73. HPLC and UV spectra of (*R*)-4-(2-Trimethylsilylethyl)-1,2,3,4-tetrahydroquinoline (**4h**)

Chromatogram

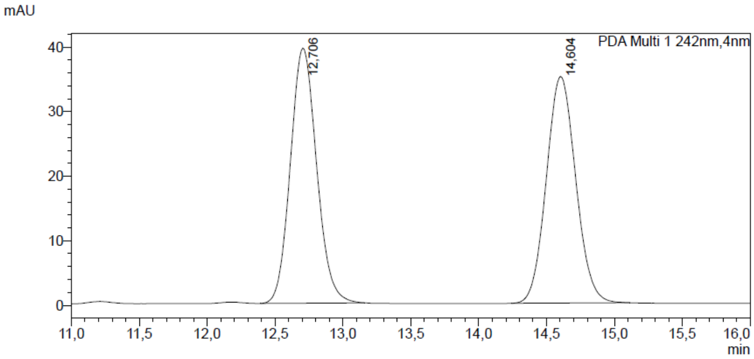


Peak Table

PDA Ch1 242nm

Peak#	Ret. Time	Area	Height	Conc.
1	12,688	6803348	505018	99,793
2	14,575	14085	1033	0,207
Total		6817433	506051	

Chromatogram

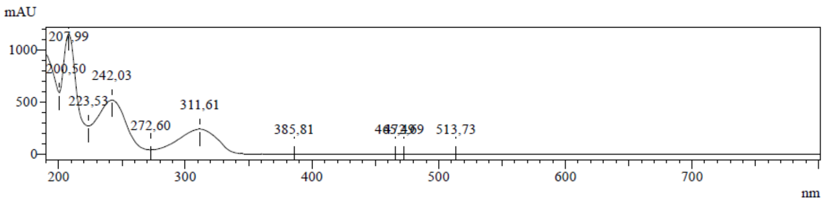


Peak Table

PDA Ch1 242nm

Peak#	Ret. Time	Area	Height	Conc.
1	12,706	532195	39526	50,108
2	14,604	529903	35125	49,892
Total		1062098	74651	

Peak# : 10
Retention Time : 12,688 min
Compound Name :
Spectrum Operation : None



Peak# : 11
Retention Time : 14,579 min
Compound Name :
Spectrum Operation : None

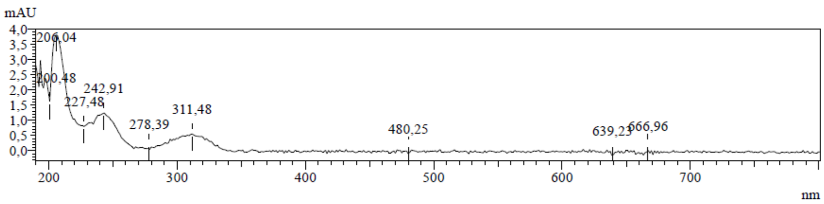
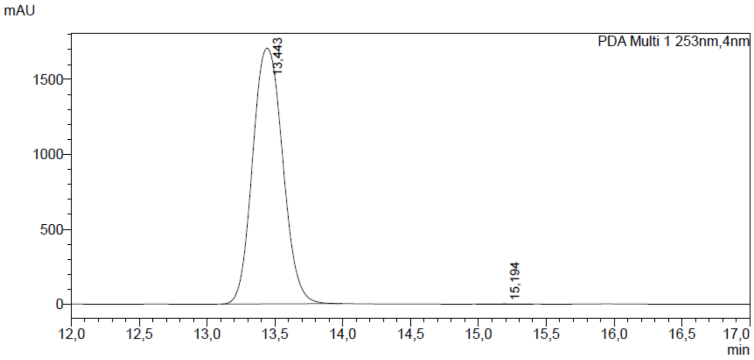


Figure S74. HPLC and UV spectra of (*S*)-4-Ethyl-6-fluoro-1,2,3,4-tetrahydroquinoline (**5a**)

Chromatogram

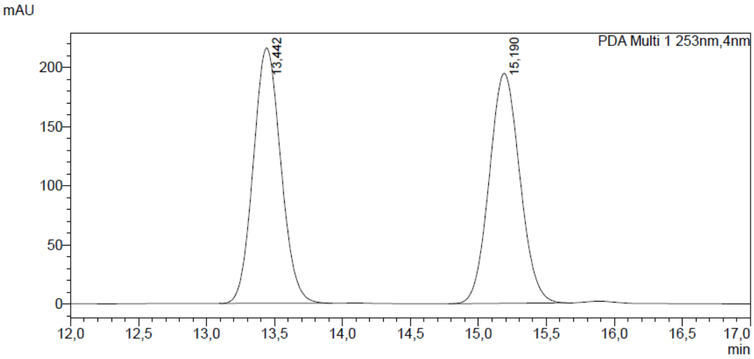


Peak Table

PDA Ch1 253nm

Peak#	Ret. Time	Area	Height	Conc.
1	13,443	26305351	1706658	99,941
2	15,194	15399	1164	0,059
Total		26320750	1707823	

Chromatogram

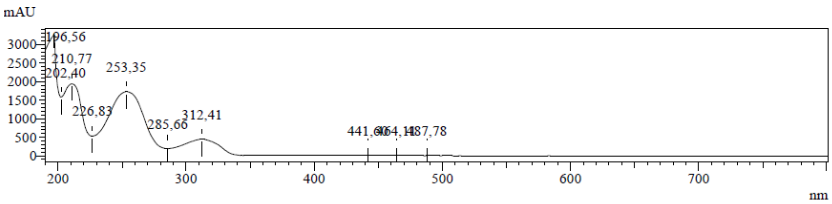


Peak Table

PDA Ch1 253nm

Peak#	Ret. Time	Area	Height	Conc.
1	13,442	3045739	215923	49,991
2	15,190	3046884	194456	50,009
Total		6092623	410378	

Peak# : 1
Retention Time : 13,443 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 15,195 min
Compound Name :
Spectrum Operation : None

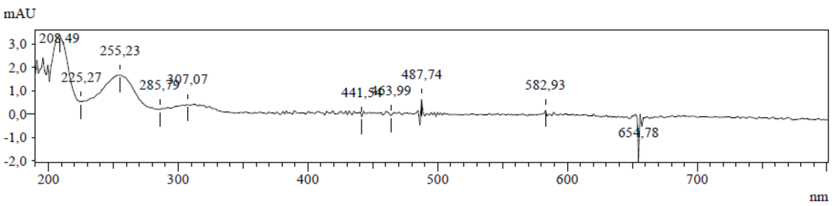
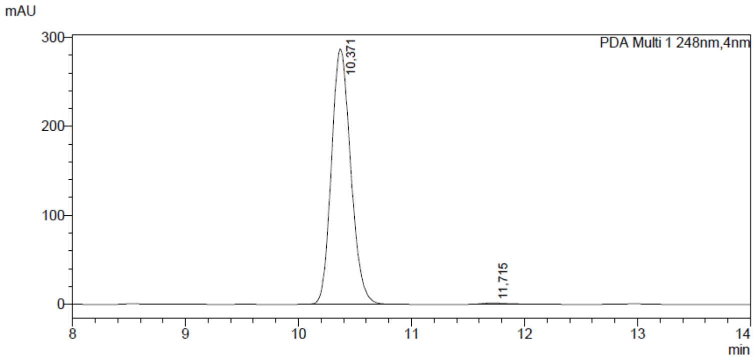


Figure S75. HPLC and UV spectra of (S)-6-Bromo-4-ethyl-1,2,3,4-tetrahydroquinoline (**5b**)

Chromatogram

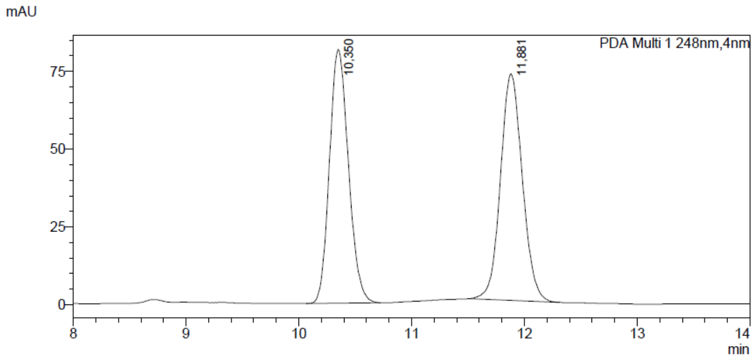


Peak Table

PDA Ch1 248nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,371	3402911	286634	99,549
2	11,715	15425	1218	0,451
Total		3418337	287852	

Chromatogram

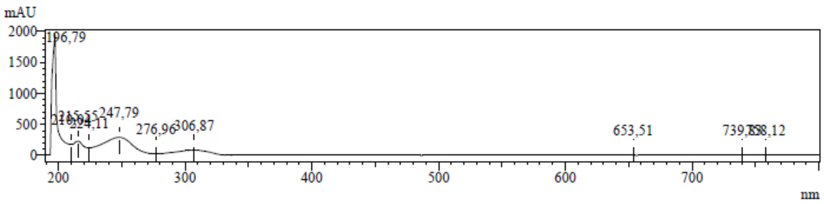


Peak Table

PDA Ch1 248nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,350	956839	81551	49,310
2	11,881	983624	72828	50,690
Total		1940463	154379	

Peak# : 1
Retention Time : 10,371 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 11,715 min
Compound Name :
Spectrum Operation : None

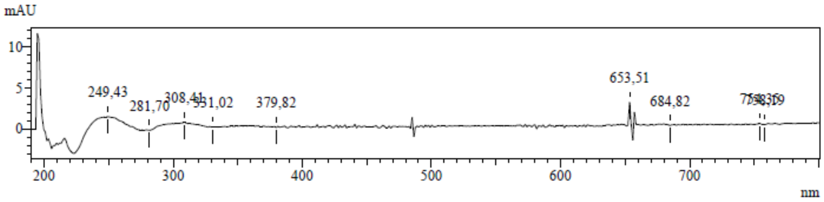
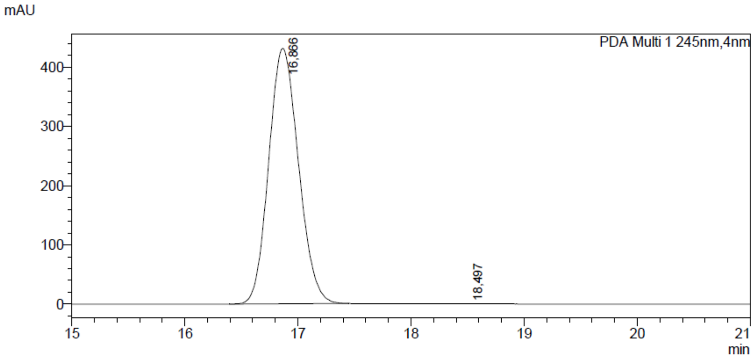


Figure S76. HPLC and UV spectra of (*S*)-4-Ethyl-6-methyl-1,2,3,4-tetrahydroquinoline (**5c**)

Chromatogram

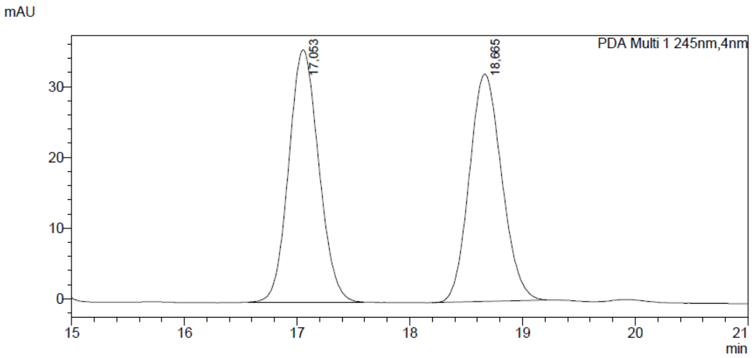


Peak Table

PDA Ch1 245nm

Peak#	Ret. Time	Area	Height	Conc.
1	16,866	7894517	431093	99,944
2	18,497	4418	231	0,056
Total		7898935	431324	

Chromatogram

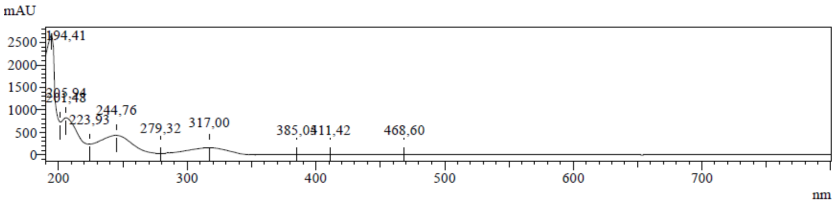


Peak Table

PDA Ch1 245nm

Peak#	Ret. Time	Area	Height	Conc.
1	17,053	660523	35666	50,683
2	18,665	642728	32142	49,317
Total		1303251	67808	

Peak# : 1
Retention Time : 16,866 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 18,497 min
Compound Name :
Spectrum Operation : None

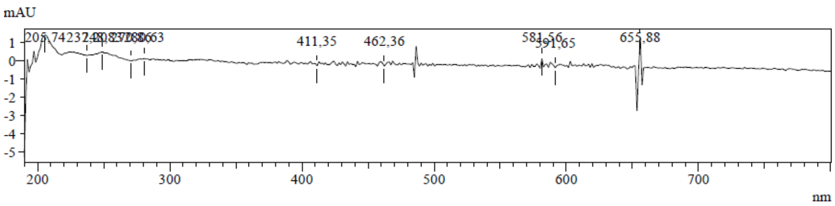
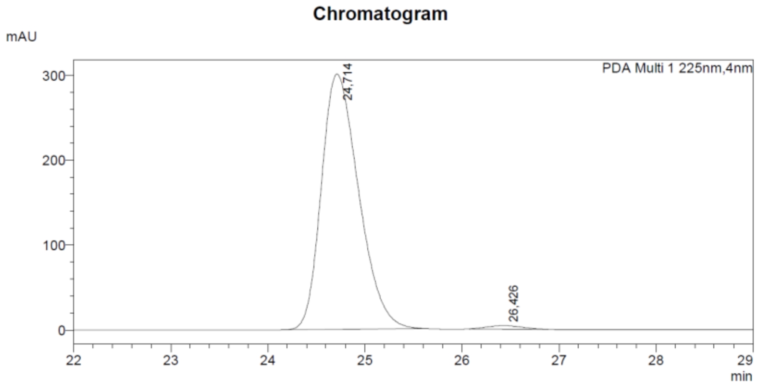


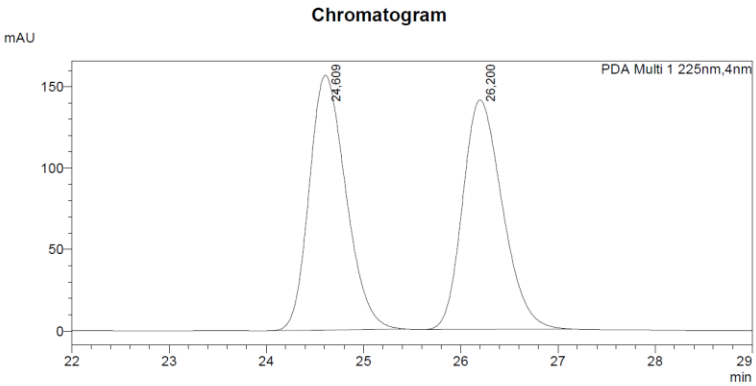
Figure S77. HPLC and UV spectra of (*S*)-4-Ethyl-6-methoxy-1,2,3,4-tetrahydroquinoline (**5d**)



Peak Table

PDA Ch1 225nm

Peak#	Ret. Time	Area	Height	Conc.
1	24,714	8050347	300692	98,764
2	26,426	100733	4079	1,236
Total		8151079	304771	

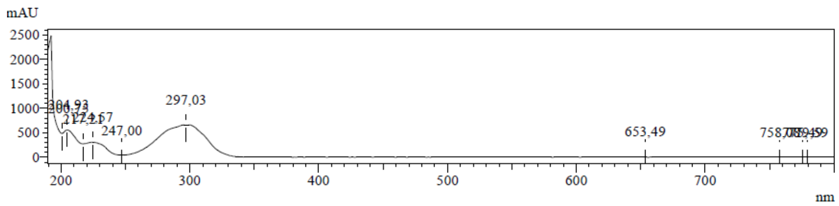


Peak Table

PDA Ch1 225nm

Peak#	Ret. Time	Area	Height	Conc.
1	24,609	4110255	156552	50,631
2	26,200	4007820	140949	49,369
Total		8118075	297501	

Peak# : 1
Retention Time : 24,714 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 26,426 min
Compound Name :
Spectrum Operation : None

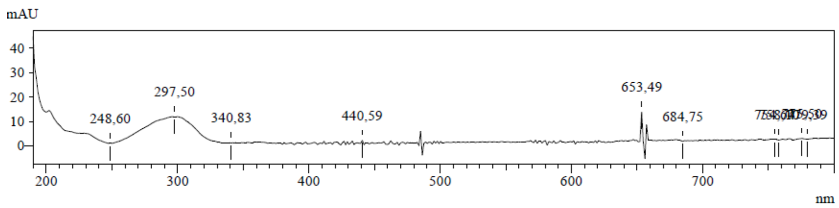
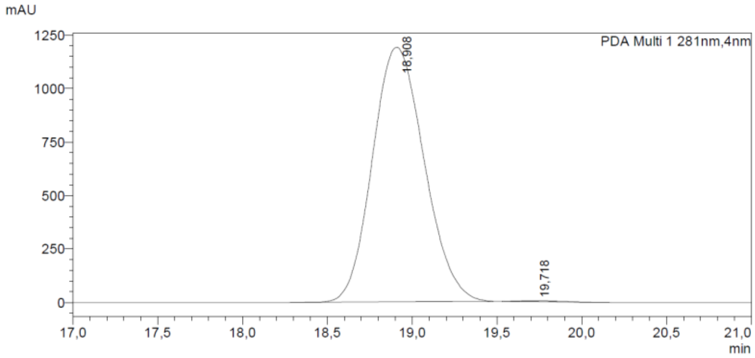


Figure S78. HPLC and UV spectra of (*S*)-Methyl 4-ethyl-1,2,3,4-tetrahydroquinoline-6-carboxylate (**5e**)

Chromatogram

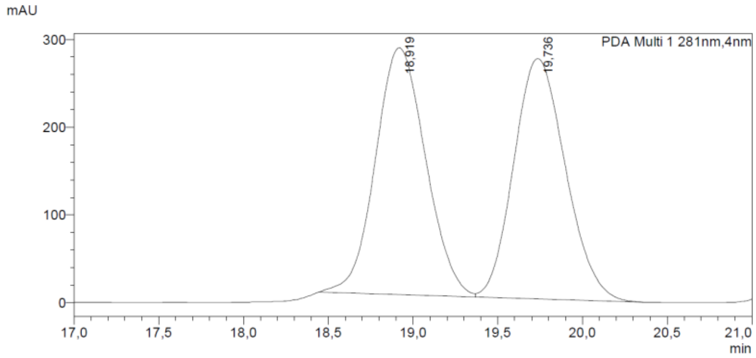


Peak Table

PDA Ch1 281nm

Peak#	Ret. Time	Area	Height	Conc.
1	18,908	25316226	1190497	99,666
2	19,718	84800	5209	0,334
Total		25401026	1195706	

Chromatogram

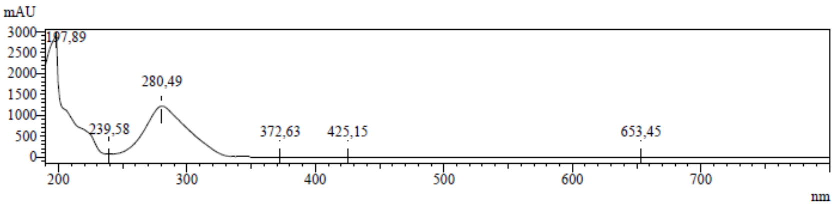


Peak Table

PDA Ch1 281nm

Peak#	Ret. Time	Area	Height	Conc.
1	18,919	5805412	281541	49,917
2	19,736	5824703	274092	50,083
Total		11630115	555633	

Peak# : 1
Retention Time : 18,915 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 19,726 min
Compound Name :
Spectrum Operation : None

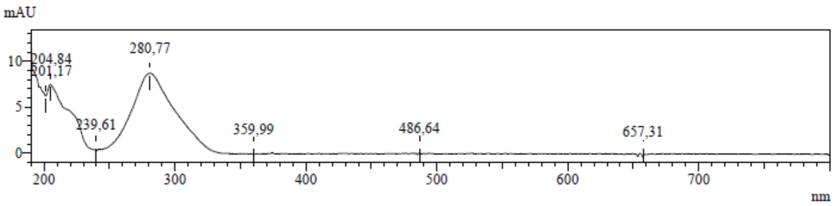
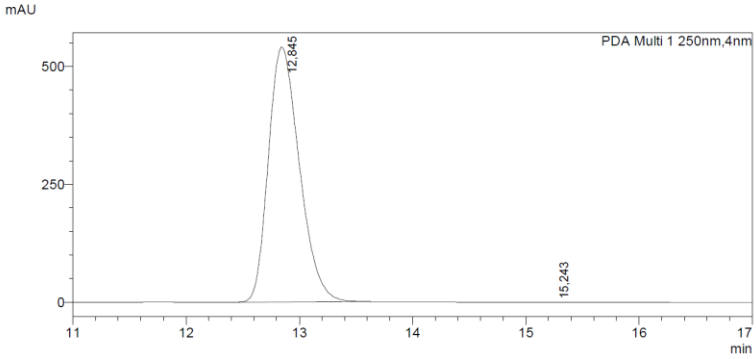


Figure S79. HPLC and UV spectra of (*S*)-6-Cyano-4-ethyl-1,2,3,4-tetrahydroquinoline (**5f**)

Chromatogram

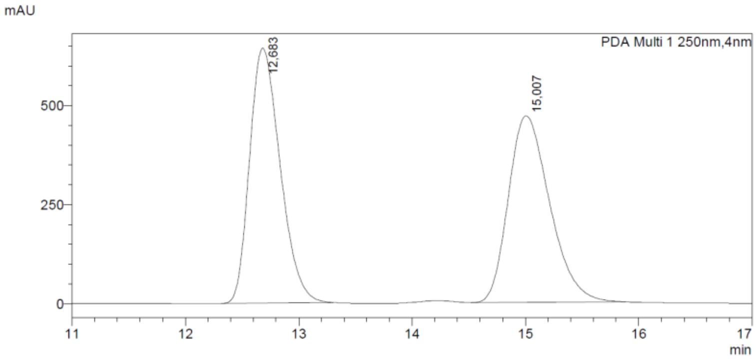


Peak Table

PDA Ch1 250nm

Peak#	Ret. Time	Area	Height	Conc.
1	12,845	10307813	540507	99,966
2	15,243	3485	152	0,034
Total		10311298	540659	

Chromatogram

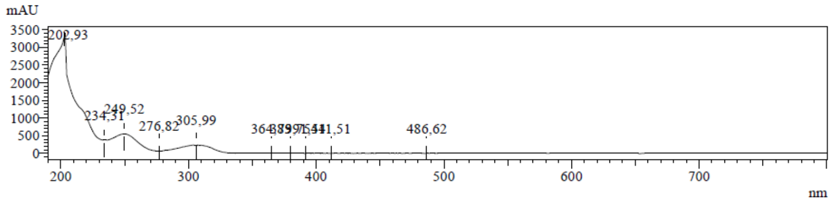


Peak Table

PDA Ch1 250nm

Peak#	Ret. Time	Area	Height	Conc.
1	12,683	12064487	643122	50,290
2	15,007	11925215	470107	49,710
Total		23989703	1113230	

Peak# : 1
Retention Time : 12,845 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 15,235 min
Compound Name :
Spectrum Operation : None

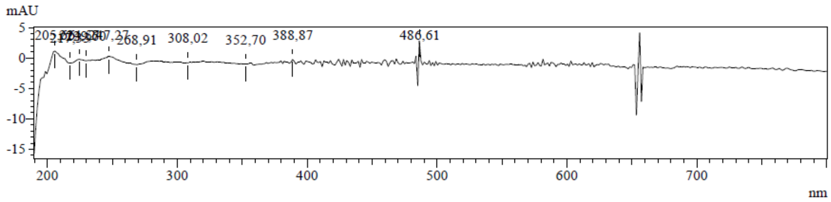
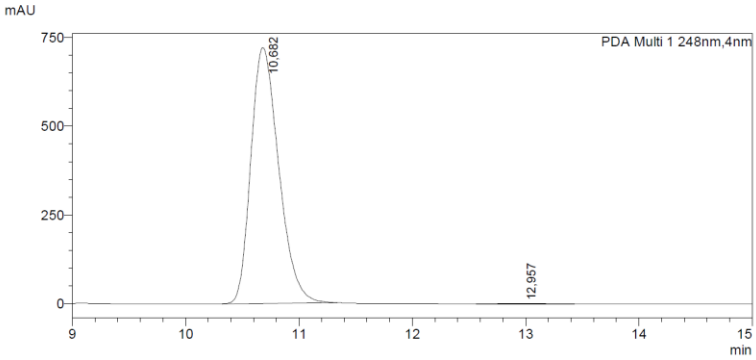


Figure S80. HPLC and UV spectra of (*S*)-7-Bromo-4-ethyl-1,2,3,4-tetrahydroquinoline (**5g**)

Chromatogram

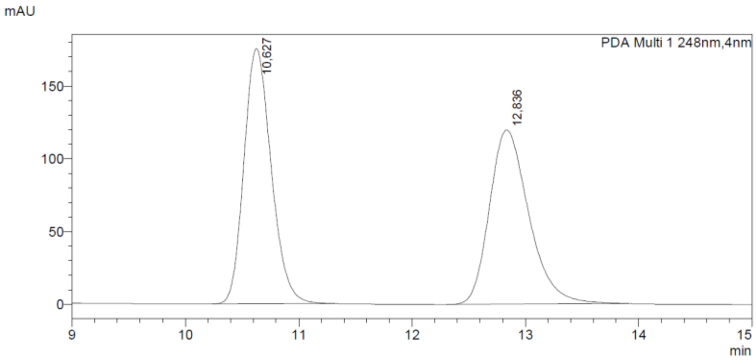


Peak Table

PDA Ch1 248nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,682	12328349	720178	99,948
2	12,957	6408	284	0,052
Total		12334757	720462	

Chromatogram

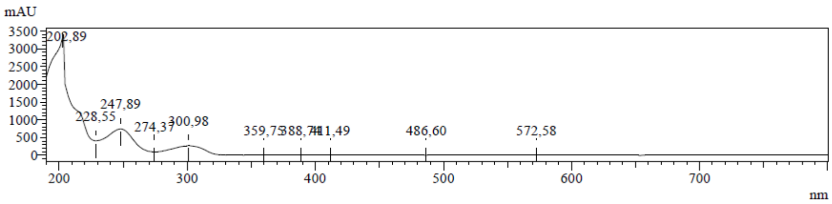


Peak Table

PDA Ch1 248nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,627	2934148	175261	50,334
2	12,836	2895161	119567	49,666
Total		5829309	294828	

Peak# : 1
Retention Time : 10,682 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 12,981 min
Compound Name :
Spectrum Operation : None

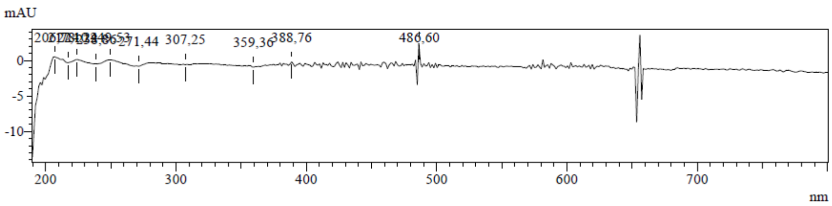
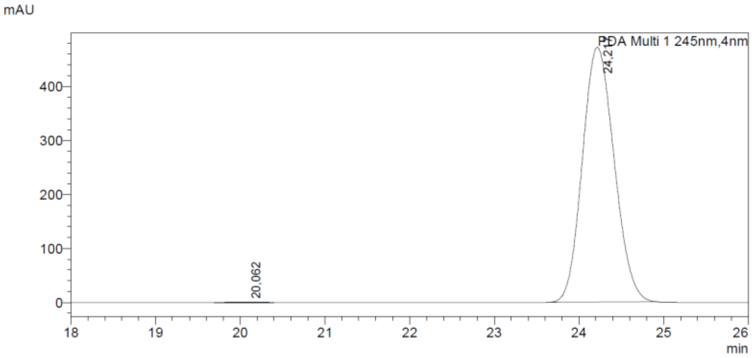


Figure S81. HPLC and UV spectra of (*S*)-4-Ethyl-7-methyl-1,2,3,4-tetrahydroquinoline (**5h**)

Chromatogram

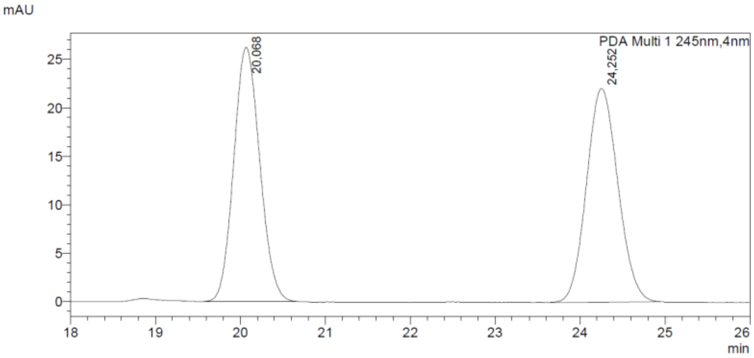


Peak Table

PDA Ch1 245nm

Peak#	Ret. Time	Area	Height	Conc.
1	20,062	14321	738	0,116
2	24,217	12335148	472239	99,884
Total		12349468	472977	

Chromatogram

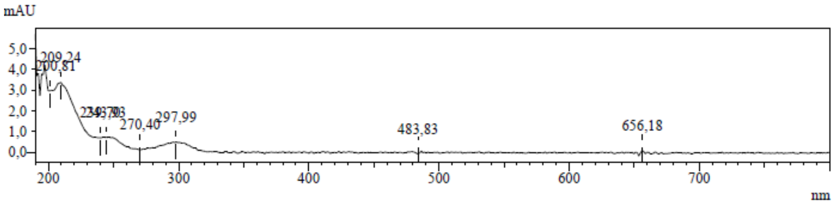


Peak Table

PDA Ch1 245nm

Peak#	Ret. Time	Area	Height	Conc.
1	20,068	559152	26223	49,670
2	24,252	566571	22034	50,330
Total		1125722	48257	

Peak# : 1
Retention Time : 20,062 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 24,215 min
Compound Name :
Spectrum Operation : None

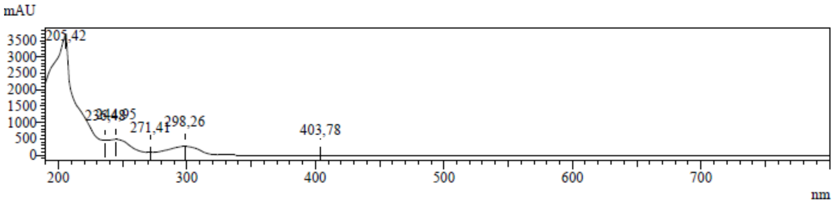
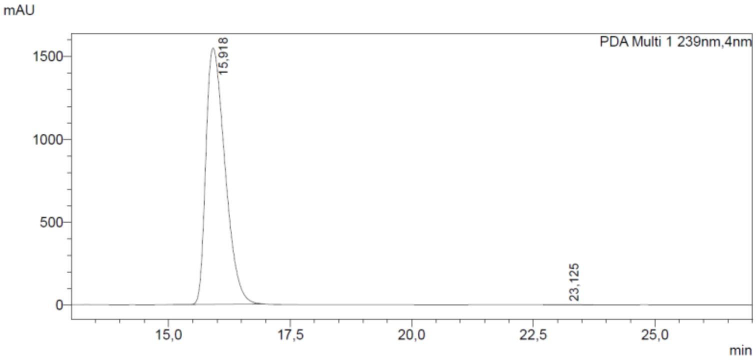


Figure S82. HPLC and UV spectra of (*S*)-4-Ethyl-7-methoxy-1,2,3,4-tetrahydroquinoline (**5i**)

Chromatogram

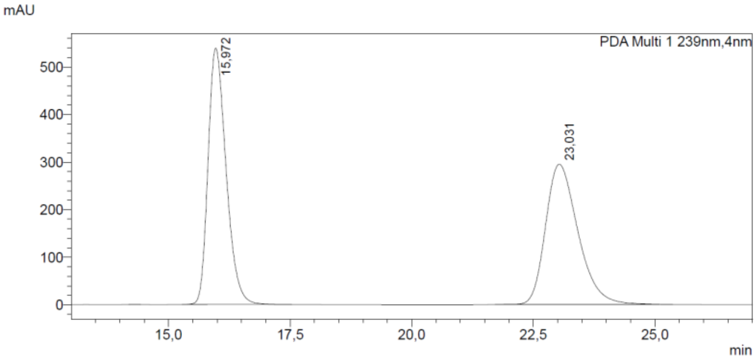


Peak Table

PDA Ch1 239nm

Peak#	Ret. Time	Area	Height	Conc.
1	15,918	42283955	1546021	99,987
2	23,125	5572	136	0,013
Total		42289527	1546156	

Chromatogram

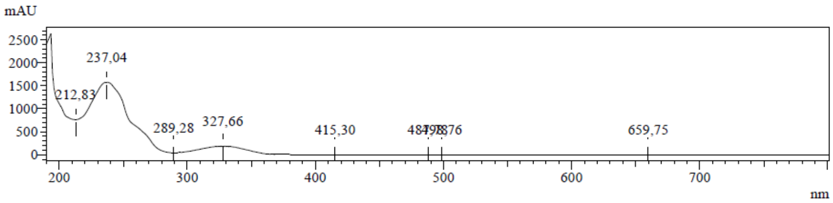


Peak Table

PDA Ch1 239nm

Peak#	Ret. Time	Area	Height	Conc.
1	15,972	13842551	538365	50,472
2	23,031	13583622	294318	49,528
Total		27426173	832683	

Peak# : 1
Retention Time : 15,918 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 23,125 min
Compound Name :
Spectrum Operation : None

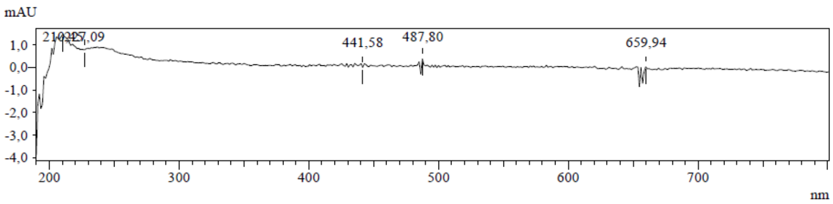
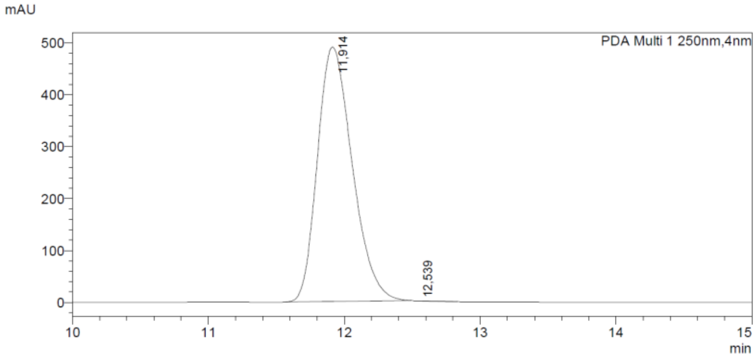


Figure S83. HPLC and UV spectra of(*S*)-4-Ethyl-7-vinyl-1,2,3,4-tetrahydroquinoline (**5j**)

Chromatogram

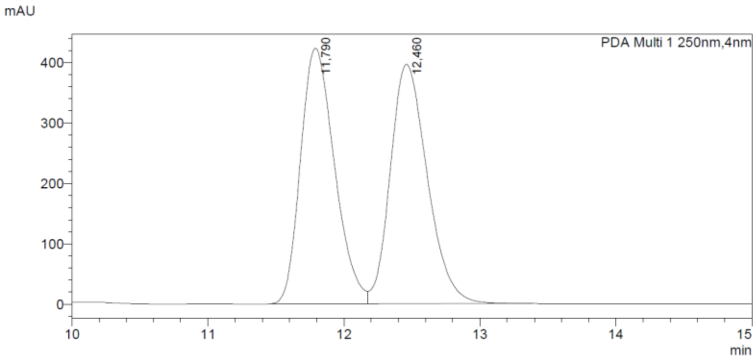


Peak Table

PDA Ch1 250nm

Peak#	Ret. Time	Area	Height	Conc.
1	11,914	8755398	490739	99,999
2	12,539	90	32	0,001
Total		8755488	490772	

Chromatogram

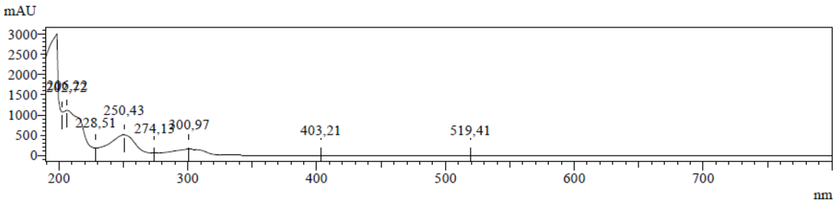


Peak Table

PDA Ch1 250nm

Peak#	Ret. Time	Area	Height	Conc.
1	11,790	7357462	422825	49,538
2	12,460	7494707	396461	50,462
Total		14852168	819286	

Peak# : 1
Retention Time : 11,914 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 12,613 min
Compound Name :
Spectrum Operation : None

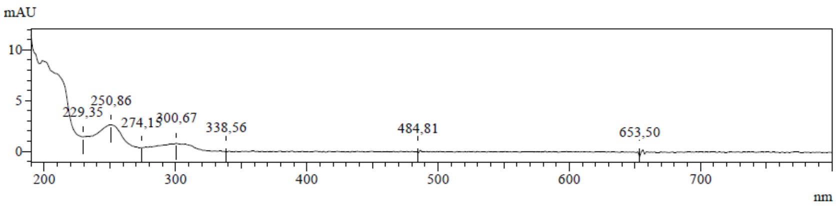
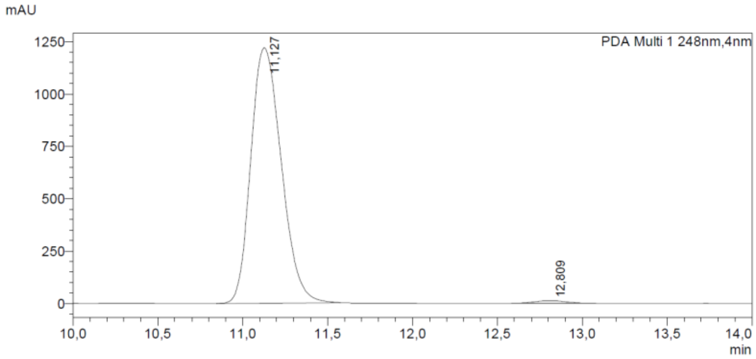


Figure S84. HPLC and UV spectra of (*S*)-5-Chloro-4-ethyl-1,2,3,4-tetrahydroquinoline (**5k**)

Chromatogram

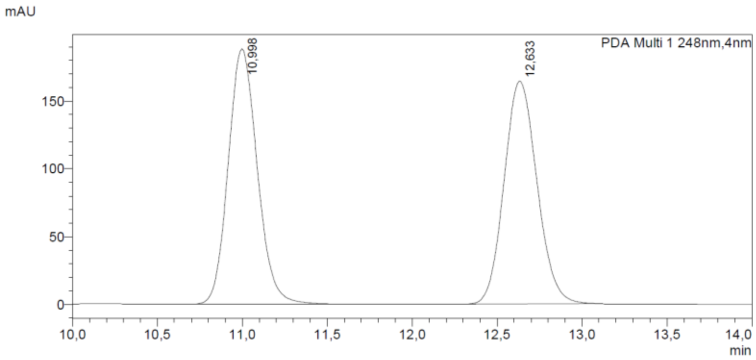


Peak Table

PDA Ch1 248nm

Peak#	Ret. Time	Area	Height	Conc.
1	11,127	15238899	1220681	99,040
2	12,809	147678	11860	0,960
Total		15386577	1232542	

Chromatogram

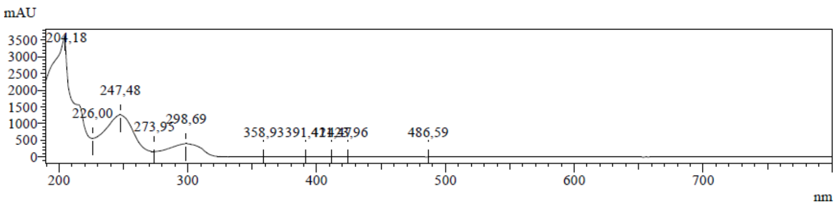


Peak Table

PDA Ch1 248nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,998	2235054	188254	50,207
2	12,633	2216662	164480	49,793
Total		4451716	352734	

Peak# : 1
Retention Time : 11,127 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 12,809 min
Compound Name :
Spectrum Operation : None

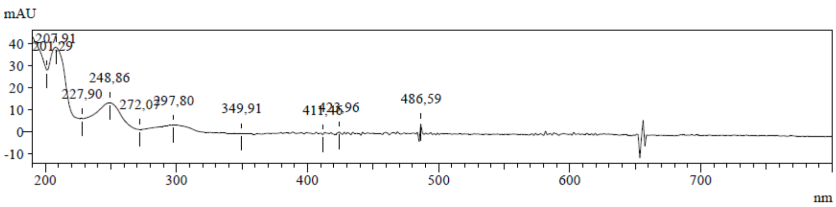
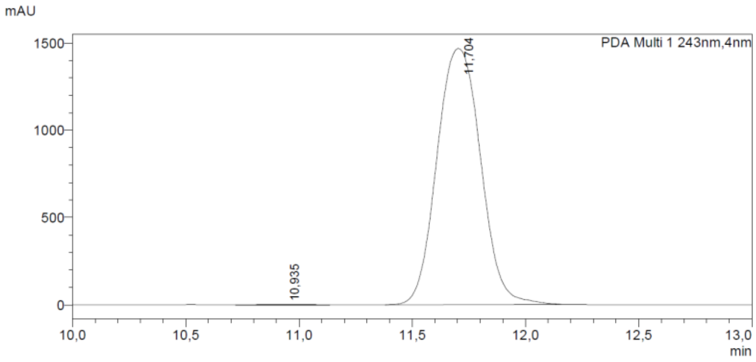


Figure S85. HPLC and UV spectra of (*S*)-4-Ethyl-5-methyl-1,2,3,4-tetrahydroquinoline (**5l**)

Chromatogram

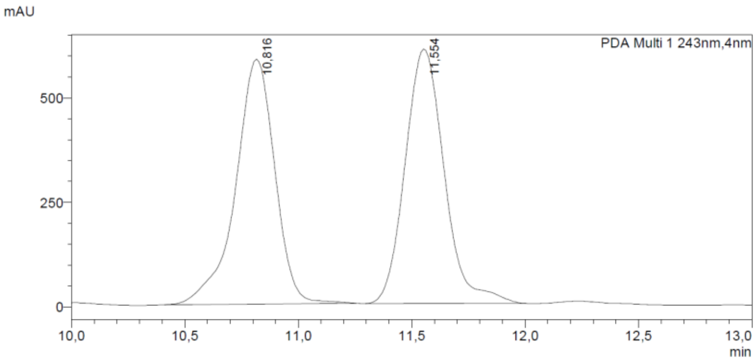


Peak Table

PDA Ch1 243nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,935	22323	2117	0,113
2	11,704	19763030	1467830	99,887
Total		19785353	1469946	

Chromatogram

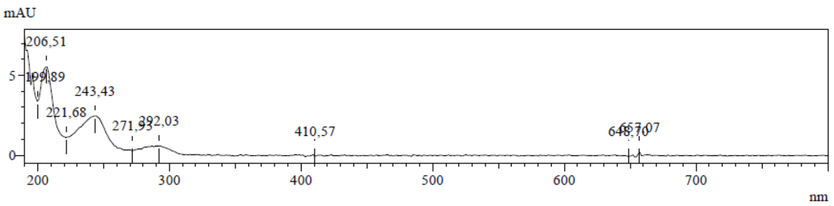


Peak Table

PDA Ch1 243nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,816	7077740	586689	49,113
2	11,554	7333525	609431	50,887
Total		14411265	1196121	

Peak# : 15
Retention Time : 10,932 min
Compound Name :
Spectrum Operation : None



Peak# : 17
Retention Time : 11,704 min
Compound Name :
Spectrum Operation : None

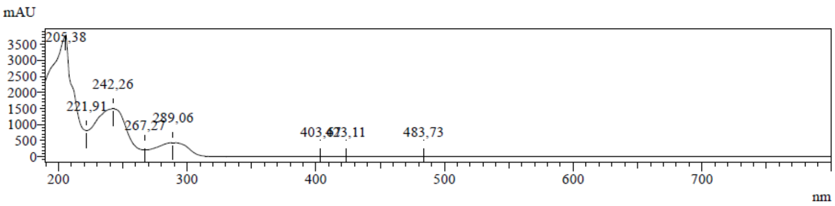
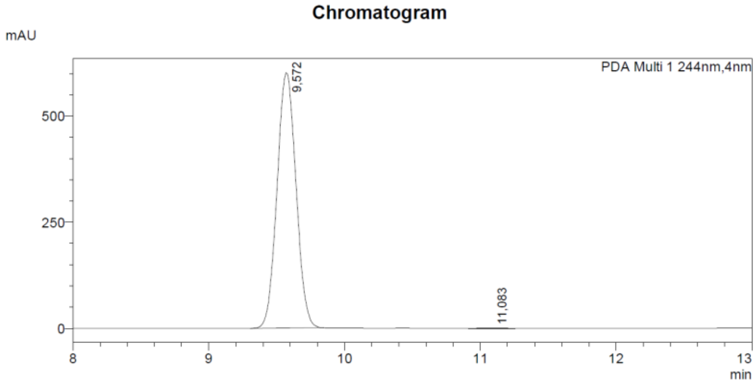


Figure S86. HPLC and UV spectra of (*S*)-4-Ethyl-8-fluoro-1,2,3,4-tetrahydroquinoline (**5m**)

Chromatogram

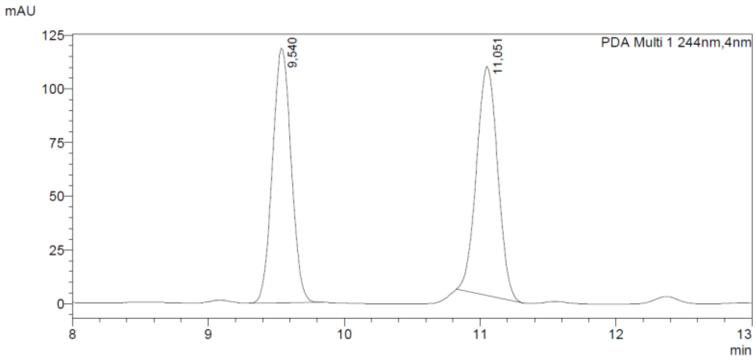


Peak Table

PDA Ch1 244nm

Peak#	Ret. Time	Area	Height	Conc.
1	9,572	5844967	601893	99,903
2	11,083	5669	574	0,097
Total		5850636	602467	

Chromatogram

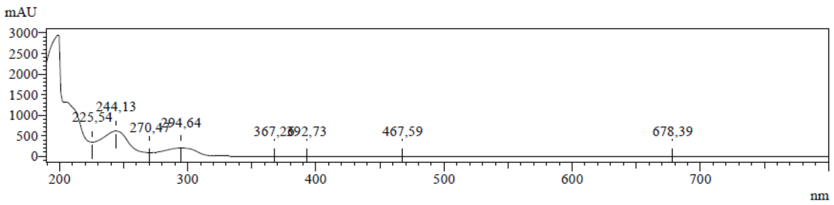


Peak Table

PDA Ch1 244nm

Peak#	Ret. Time	Area	Height	Conc.
1	9,540	1132750	118320	49,558
2	11,051	1152938	106443	50,442
Total		2285688	224762	

Peak# : 1
Retention Time : 9,572 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 11,082 min
Compound Name :
Spectrum Operation : None

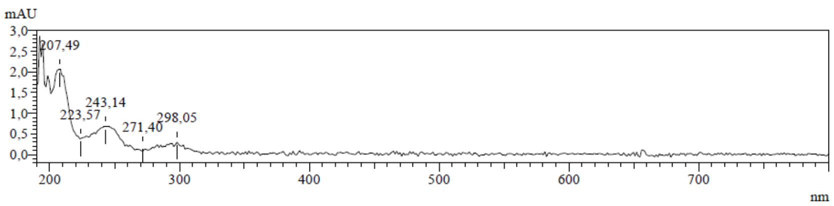
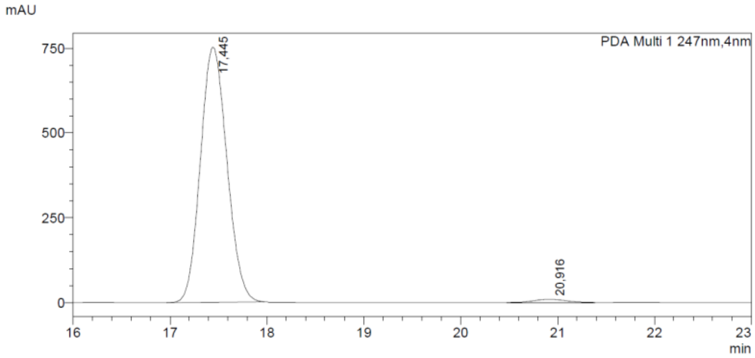


Figure S87. HPLC and UV spectra of (*S*)-4-Ethyl-8-methyl-1,2,3,4-tetrahydroquinoline (**5n**)

Chromatogram

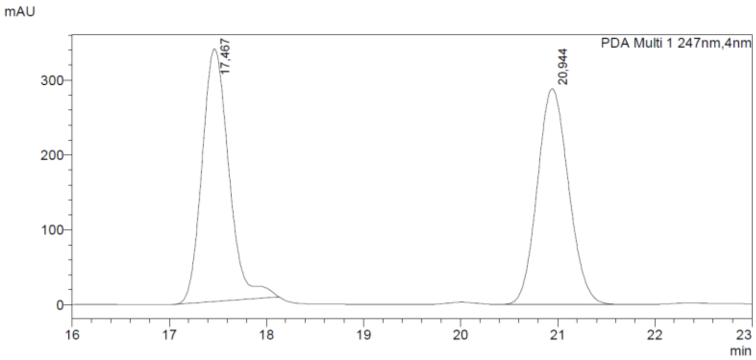


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	17,445	14294269	751503	98,539
2	20,916	211995	9605	1,461
Total		14506264	761108	

Chromatogram

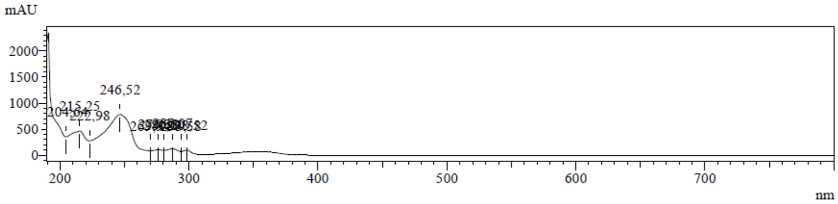


Peak Table

PDA Ch1 247nm

Peak#	Ret. Time	Area	Height	Conc.
1	17,467	6492333	337203	50,233
2	20,944	6432143	287761	49,767
Total		12924476	624964	

Peak# : 1
Retention Time : 17,445 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 20,917 min
Compound Name :
Spectrum Operation : None

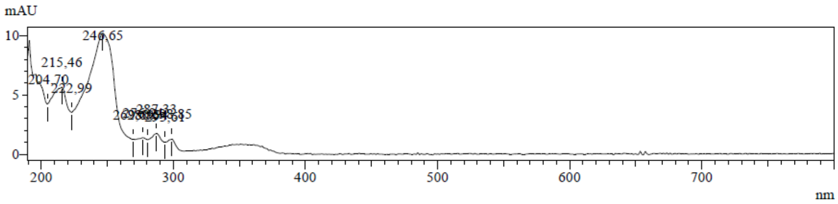
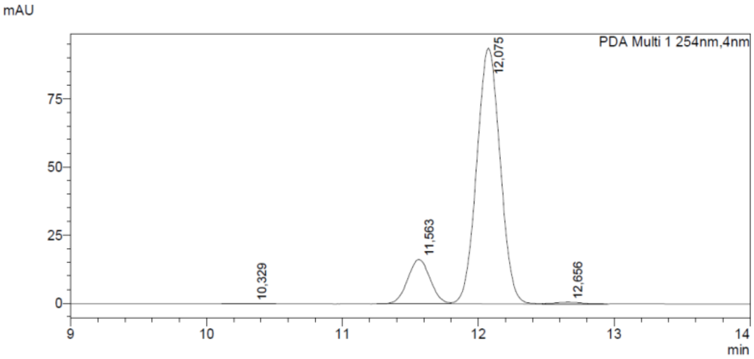


Figure S88. HPLC and UV spectra of (*S*)-4-Ethyl-1,2,3,4-tetrahydrobenzo[*g*]quinoline (**5o**)

Chromatogram

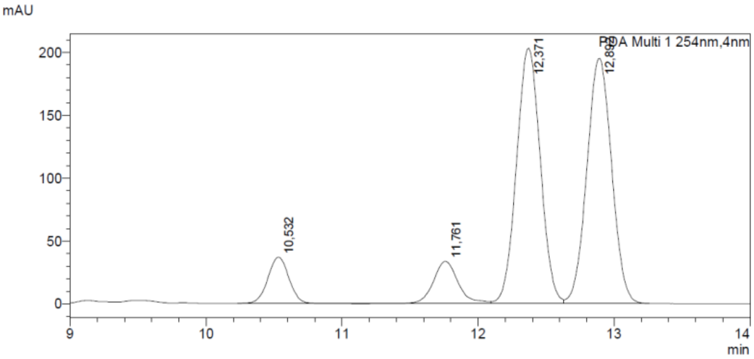


Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,329	1372	113	0,104
2	11,563	187350	16278	14,162
3	12,075	1126806	93819	85,175
4	12,656	7410	567	0,560
Total		1322938	110777	

Chromatogram

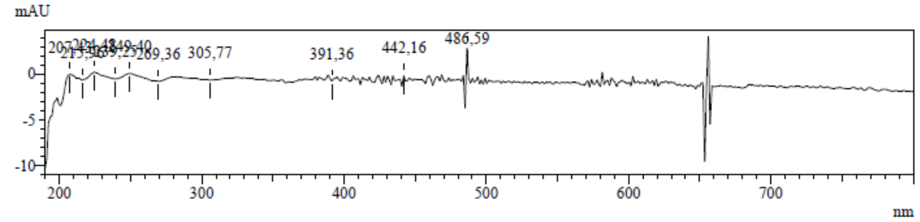


Peak Table

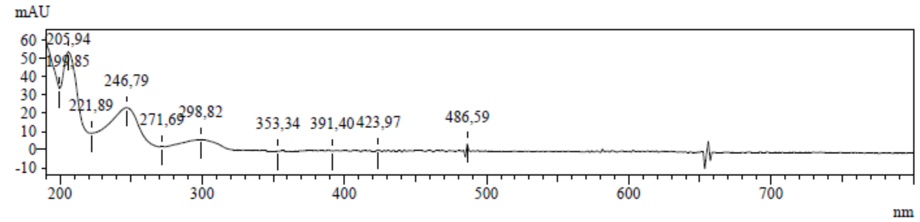
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	10,532	390604	36904	6,779
2	11,761	422686	33562	7,336
3	12,371	2473178	203149	42,925
4	12,892	2475117	195140	42,959
Total		5761585	468754	

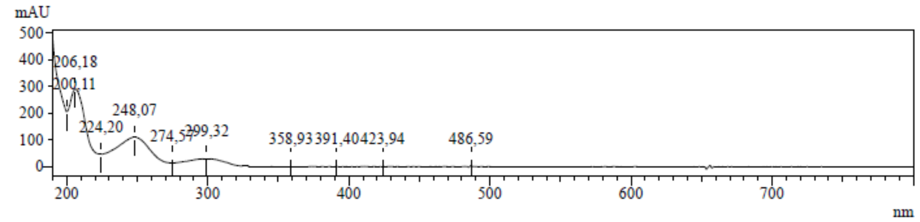
Peak# : 1
Retention Time : 10,329 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 11,563 min
Compound Name :
Spectrum Operation : None



Peak# : 3
Retention Time : 12,075 min
Compound Name :
Spectrum Operation : None



Peak# : 4
Retention Time : 12,656 min
Compound Name :
Spectrum Operation : None

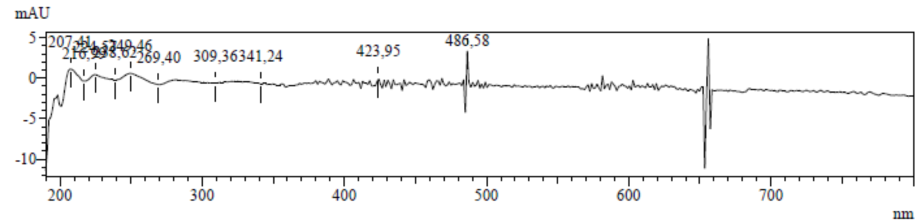
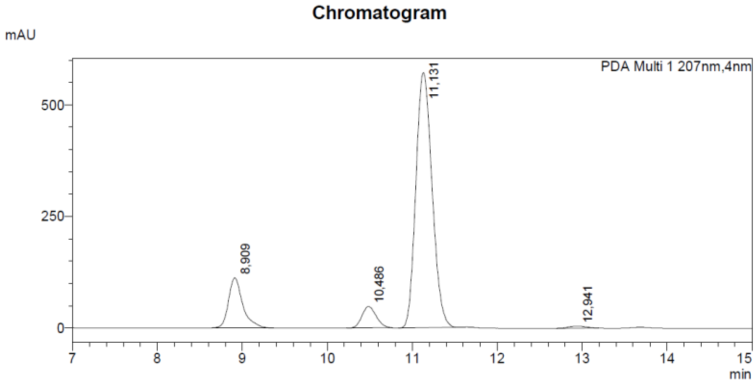


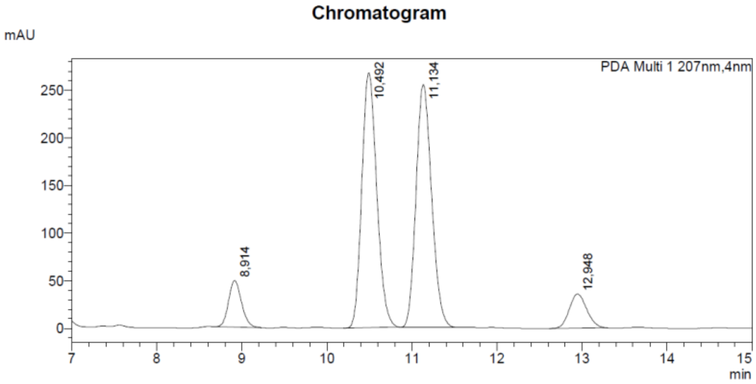
Figure S89. HPLC and UV spectra of (2*R*,4*S*)-4-Ethyl-2-methyl-1,2,3,4-tetrahydroquinoline (**5p**)



Peak Table

PDA Ch1 207nm

Peak#	Ret. Time	Area	Height	Conc.
1	8,909	1310056	112350	13,734
2	10,486	564663	48023	5,920
3	11,131	7598115	571325	79,657
4	12,941	65740	4893	0,689
Total		9538574	736592	

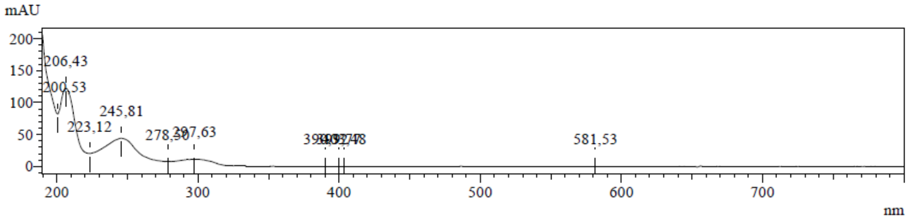


Peak Table

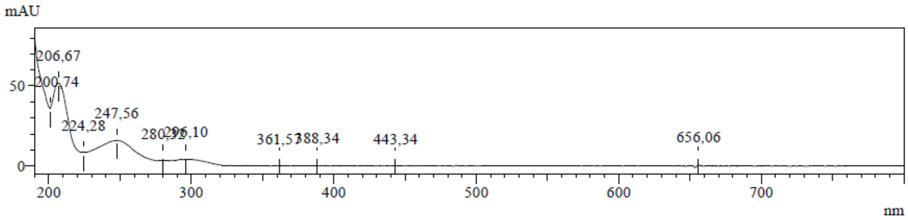
PDA Ch1 207nm

Peak#	Ret. Time	Area	Height	Conc.
1	8,914	514587	48804	6,811
2	10,492	3271041	267440	43,294
3	11,134	3255741	254849	43,091
4	12,948	514121	35937	6,805
Total		7555490	607031	

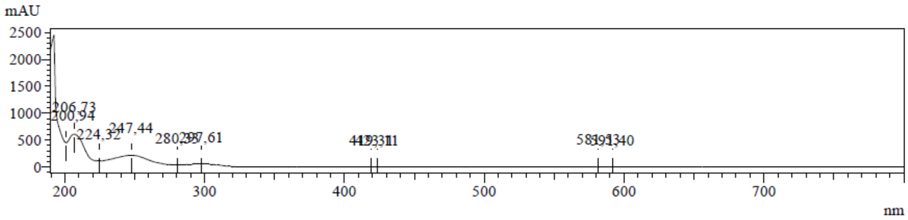
Peak# : 1
Retention Time : 8,909 min
Compound Name :
Spectrum Operation : None



Peak# : 2
Retention Time : 10,486 min
Compound Name :
Spectrum Operation : None



Peak# : 3
Retention Time : 11,131 min
Compound Name :
Spectrum Operation : None



Peak# : 4
Retention Time : 12,945 min
Compound Name :
Spectrum Operation : None

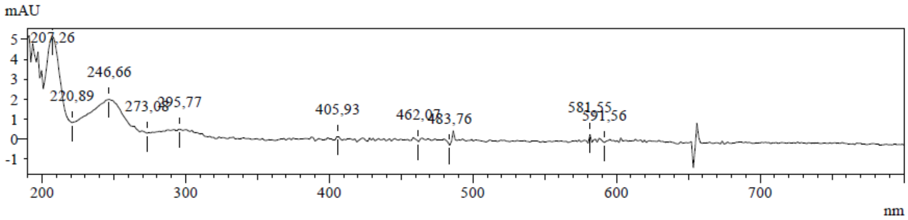


Figure S90. HPLC and UV spectra of (2*S*,4*S*)-4-ethyl-2-phenyl-1,2,3,4-tetrahydroquinoline (**5q**)

12. Cartesian coordinates

1a

C	2.397159	-0.714056	-0.000000
C	1.206261	-1.402185	-0.000000
C	-0.029944	-0.706194	-0.000000
C	-0.014619	0.721539	0.000000
C	1.227478	1.404892	0.000000
C	2.409716	0.701711	-0.000000
H	3.346520	-1.261799	-0.000001
H	1.171169	-2.497390	-0.000001
C	-1.263859	1.389338	0.000000
H	1.225213	2.502122	0.000000
H	3.366985	1.235015	-0.000000
C	-2.421719	0.651247	0.000000
C	-2.320994	-0.762076	0.000000
H	-1.285869	2.486493	0.000001
H	-3.406324	1.130259	0.000001
H	-3.243645	-1.363141	0.000000
N	-1.187275	-1.419551	-0.000000

BF_3

B	0.000257	0.000487	-0.001301
F	1.253539	0.370729	0.000241
F	-0.948350	0.898888	0.000241
F	-0.305332	-1.269887	0.000241

1a·BF_3

C	-1.968237	-2.040057	-0.000526
C	-0.696620	-1.511858	-0.001214
C	-0.519610	-0.108328	-0.000901
C	-1.668866	0.735216	0.000120
C	-2.961901	0.155312	0.000749
C	-3.110928	-1.209980	0.000438
H	-2.093294	-3.128338	-0.000960
H	0.172212	-2.171522	-0.002866
C	-1.481808	2.136403	0.000393
H	-3.832626	0.821077	0.001430
H	-4.110040	-1.657995	0.000818
C	-0.211488	2.659655	-0.000460
C	0.875886	1.775481	-0.001493
H	-2.362121	2.789929	0.001286
H	-0.028464	3.737211	-0.000291
N	0.735606	0.458699	-0.001601
B	2.092769	-0.479098	0.000476
F	2.045389	-1.233838	1.146460
F	2.039541	-1.249093	-1.135088
F	3.159143	0.383047	-0.008162
H	1.906023	2.142137	-0.002128

L1-CuBr

C	-3.067425	-1.264577	-0.795234
C	-0.759306	-2.702564	-1.133429

C	-3.185221	-2.781709	-1.024005
H	-3.345186	-0.749519	-1.737825
C	-1.995577	-3.215932	-1.864499
H	-0.676796	-3.250198	-0.171153
H	-3.160395	-3.299623	-0.042973
H	-4.157364	-3.026928	-1.492073
H	-1.953970	-4.313069	-2.007476
H	-2.077363	-2.760984	-2.872414
C	2.880539	1.902988	-0.613361
C	0.457337	3.110975	-0.202430
C	2.836763	3.440495	-0.574669
H	3.068762	1.584617	-1.661347
C	1.460769	3.904067	-1.030292
H	0.593220	3.392952	0.862483
H	3.002499	3.780640	0.467363
H	3.643808	3.880576	-1.189110
H	1.324800	4.994691	-0.897196
H	1.333379	3.695757	-2.111555
P	1.105248	1.351141	-0.272609
P	-1.221018	-0.960483	-0.574999
Cu	0.240005	-0.260775	1.095818
Br	0.705847	-1.576424	2.959409
C	-1.004720	3.183463	-0.528872
C	-1.928274	2.679010	0.400216
C	-1.486044	3.682607	-1.743301
C	-3.289521	2.651154	0.115868
H	-1.565654	2.293681	1.364439
C	-2.852621	3.654739	-2.031784
H	-0.791353	4.099033	-2.482565

C	-3.756874	3.132487	-1.109393
H	-3.994114	2.248034	0.853438
H	-3.210800	4.048922	-2.990087
H	-4.829317	3.106619	-1.337271
C	3.927376	1.261702	0.267877
C	3.793068	-0.061799	0.706760
C	5.084885	1.958830	0.639607
C	4.768117	-0.668024	1.495117
H	2.893878	-0.633658	0.443051
C	6.068098	1.354250	1.422830
H	5.234243	2.993641	0.310552
C	5.913832	0.039071	1.857516
H	4.619309	-1.700241	1.835488
H	6.963673	1.923198	1.699211
H	6.682443	-0.432229	2.480828
C	-3.949223	-0.755584	0.311457
C	-5.195898	-0.199851	0.003015
C	-3.584523	-0.874016	1.658928
C	-6.055744	0.237274	1.009722
H	-5.492693	-0.101406	-1.050230
C	-4.439034	-0.433050	2.667915
H	-2.606448	-1.300614	1.925382
C	-5.677241	0.125462	2.347232
H	-7.026934	0.672900	0.746595
H	-4.132647	-0.526011	3.716337
H	-6.347725	0.472926	3.141787
C	0.575070	-2.748462	-1.816008
C	0.710557	-2.761308	-3.209192
C	1.740519	-2.724331	-1.033911

C	1.972972	-2.732063	-3.803932
H	-0.178386	-2.799750	-3.850112
C	3.000919	-2.694232	-1.625978
H	1.647659	-2.728550	0.063149
C	3.122189	-2.692454	-3.016742
H	2.055968	-2.744461	-4.897043
H	3.898254	-2.677536	-0.995484
H	4.112933	-2.671567	-3.484885
C	0.582340	0.739222	-1.959124
H	0.689618	1.547944	-2.709619
H	1.335797	-0.032589	-2.220822
C	-0.822560	0.141794	-2.019357
H	-0.970918	-0.394460	-2.977990
H	-1.583695	0.946896	-1.986090

IIa-*proR*$_{3\text{-}4}$

C	-3.749576	1.480906	-0.386426
C	-4.241072	-0.192039	1.709189
C	-5.197256	1.019228	-0.204584
H	-3.278605	0.756394	-1.078028
C	-5.101208	-0.349665	0.454455
H	-4.876484	0.271147	2.493340
H	-5.755788	1.722587	0.447941
H	-5.729881	0.984607	-1.174201
H	-6.094057	-0.779048	0.692575
H	-4.614474	-1.042736	-0.262097
C	0.697834	-2.199081	1.421722
C	0.025830	-3.154808	-1.071093

C	0.907973	-3.694595	1.140774
H	-0.246160	-2.096531	1.996519
C	-0.135637	-4.106710	0.112343
H	0.992790	-3.374454	-1.568634
H	1.924323	-3.867596	0.731932
H	0.831099	-4.274936	2.079820
H	-0.024051	-5.160725	-0.206060
H	-1.141736	-4.006437	0.568380
P	0.321555	-1.476069	-0.272308
P	-2.997324	1.224874	1.331217
Cu	1.983879	-0.394065	-1.373658
C	2.819187	2.388853	0.184252
C	0.872965	2.310353	-1.122378
C	3.472707	2.727000	1.387835
C	3.568901	1.772715	-0.860171
C	1.533225	1.644227	-2.178701
H	-0.187172	2.580467	-1.213392
C	4.819909	2.469208	1.532682
H	2.912255	3.187755	2.202340
C	4.946516	1.519402	-0.677968
C	2.904108	1.411318	-2.072653
H	0.985585	1.451218	-3.107295
C	5.566072	1.867085	0.500593
H	5.314728	2.735456	2.473250
H	5.498398	1.032363	-1.489926
H	3.494637	1.067891	-2.929093
H	6.634364	1.671773	0.640944
N	1.477516	2.679821	-0.010376
B	0.603586	3.485849	1.142612

F	0.603838	2.687809	2.260637
F	-0.654774	3.644347	0.620485
F	1.240808	4.681580	1.347066
Br	3.595442	-1.920635	-2.199005
C	-3.633913	-1.431958	2.305407
C	-3.835382	-2.708988	1.765386
C	-2.827125	-1.326942	3.450597
C	-3.227619	-3.833649	2.327746
H	-4.481179	-2.839469	0.888652
C	-2.213561	-2.444888	4.010009
H	-2.673699	-0.339448	3.909066
C	-2.404498	-3.707548	3.444658
H	-3.403922	-4.821083	1.883165
H	-1.582839	-2.330291	4.899975
H	-1.923229	-4.589725	3.882451
C	-3.514169	2.857080	-0.931073
C	-2.736722	3.030792	-2.082528
C	-4.030350	3.997513	-0.301442
C	-2.470767	4.303898	-2.588326
H	-2.335014	2.144732	-2.596266
C	-3.773657	5.269346	-0.806299
H	-4.630494	3.887283	0.611611
C	-2.988763	5.428894	-1.950133
H	-1.857579	4.415817	-3.490646
H	-4.184425	6.149119	-0.296972
H	-2.782800	6.431372	-2.342729
C	1.798608	-1.492354	2.160400
C	1.518778	-0.765736	3.322947
C	3.124357	-1.537148	1.703404

C	2.532814	-0.110902	4.022470
H	0.485830	-0.719944	3.694388
C	4.139012	-0.888893	2.403519
H	3.371136	-2.081485	0.780990
C	3.847773	-0.175638	3.567528
H	2.290094	0.450393	4.932201
H	5.169753	-0.940362	2.032191
H	4.648275	0.333910	4.117174
C	-1.052764	-3.061426	-2.109395
C	-2.376440	-3.443462	-1.864201
C	-0.747517	-2.470388	-3.345176
C	-3.372107	-3.215895	-2.815629
H	-2.645452	-3.922058	-0.914391
C	-1.739602	-2.240170	-4.294424
H	0.292846	-2.183703	-3.556337
C	-3.060638	-2.605928	-4.029273
H	-4.403564	-3.521278	-2.602573
H	-1.479570	-1.774845	-5.252398
H	-3.844177	-2.424372	-4.773735
C	-1.366512	-0.758004	-0.086535
H	-2.061287	-1.573609	0.195322
H	-1.664494	-0.408050	-1.095604
C	-1.389562	0.366545	0.930494
H	-0.993702	0.028043	1.908507
H	-0.717040	1.190996	0.631148

IIa-*proS*$_{3-4}$

C	-4.347354	1.412405	0.595102

C	-3.312983	3.603808	-0.657721
C	-4.896885	2.782514	1.005620
H	-3.573301	1.144908	1.343925
C	-3.761314	3.768725	0.791023
H	-4.109683	4.031232	-1.303512
H	-5.765139	3.052181	0.368403
H	-5.258641	2.764029	2.051452
H	-4.053079	4.813990	1.012588
H	-2.931073	3.511151	1.481889
C	-0.451375	-0.655259	2.105647
C	-1.024376	-2.974761	0.743732
C	-0.528642	-1.959782	2.912492
H	-1.429359	-0.140591	2.209184
C	-1.511403	-2.867181	2.188637
H	-0.096510	-3.582109	0.735816
H	0.471229	-2.438576	2.950418
H	-0.827369	-1.749594	3.956413
H	-1.585263	-3.868354	2.653706
H	-2.522417	-2.414593	2.236994
P	-0.398257	-1.243620	0.322494
P	-3.429860	1.740958	-1.040257
Cu	1.648956	-1.403173	-0.659219
C	4.080329	-0.923981	-1.816843
C	4.018421	1.100470	-0.629817
C	2.780402	-0.726181	-2.343978
C	2.687806	1.345224	-1.069472
C	2.059398	0.392239	-1.932585
H	1.088781	0.637233	-2.381671
N	4.662849	-0.072891	-1.001515

B	6.082770	-0.517659	-0.290881
F	6.404621	-1.744972	-0.805634
F	5.817623	-0.563594	1.056952
F	7.020161	0.436605	-0.606471
C	2.036419	2.534731	-0.679345
C	2.690353	3.460442	0.104357
H	2.179978	4.383535	0.398925
C	4.674061	2.065073	0.159413
C	4.014400	3.223668	0.514426
H	4.533489	3.968626	1.127617
H	1.011410	2.722873	-1.026402
H	5.703999	1.896940	0.477754
H	2.408032	-1.410584	-3.113908
H	4.649660	-1.823647	-2.066742
C	-1.955800	-3.497682	-0.310473
C	-1.410839	-4.022291	-1.491800
C	-3.348621	-3.405373	-0.204933
C	-2.231589	-4.424000	-2.542763
H	-0.318649	-4.111510	-1.580032
C	-4.172877	-3.804672	-1.257031
H	-3.813642	-3.006699	0.705220
C	-3.618489	-4.311280	-2.431241
H	-1.784705	-4.831793	-3.457047
H	-5.261266	-3.715242	-1.151714
H	-4.265989	-4.623900	-3.258494
C	0.639884	0.294627	2.507277
C	0.320894	1.554842	3.025127
C	1.992240	-0.065465	2.405596
C	1.322936	2.429316	3.447943

H	-0.734297	1.852232	3.107073
C	2.994358	0.807151	2.822549
H	2.275186	-1.048025	1.997310
C	2.661379	2.055571	3.351416
H	1.051841	3.409486	3.857813
H	4.044319	0.505635	2.724657
H	3.451025	2.741433	3.680948
C	-5.356220	0.301056	0.543936
C	-5.351315	-0.703974	1.519252
C	-6.335198	0.247568	-0.457442
C	-6.292254	-1.734125	1.497401
H	-4.591794	-0.675517	2.314378
C	-7.277242	-0.777924	-0.483358
H	-6.352638	1.021228	-1.237210
C	-7.258906	-1.774846	0.493982
H	-6.268196	-2.510540	2.271538
H	-8.033074	-0.801574	-1.277120
H	-7.999679	-2.582547	0.472713
C	-2.015537	4.238708	-1.070241
C	-1.213500	4.957975	-0.176569
C	-1.595650	4.147444	-2.407604
C	-0.040036	5.579292	-0.609712
H	-1.515439	5.066107	0.871428
C	-0.416059	4.748071	-2.836639
H	-2.217735	3.596102	-3.126745
C	0.368343	5.472673	-1.936629
H	0.555283	6.162801	0.103559
H	-0.110751	4.660633	-3.885972
H	1.293455	5.955678	-2.272284

C	-1.863763	-0.419746	-0.430501
H	-2.028277	-0.863804	-1.432884
H	-2.741192	-0.718889	0.179555
C	-1.751716	1.095869	-0.528995
H	-1.011655	1.384049	-1.301925
H	-1.420819	1.558520	0.425399
Br	2.721727	-3.376286	0.089336

EtMgBr·2Et_2O

C	1.612756	0.643570	2.261893
H	1.400422	0.002463	3.145844
H	2.589630	0.272646	1.878413
C	1.778851	2.101148	2.732178
H	2.567851	2.251243	3.503045
H	2.034729	2.777135	1.890987
H	0.838143	2.496894	3.163560
Mg	0.116652	0.321632	0.755580
Br	-2.240637	1.191963	0.472938
O	1.015676	0.640204	-1.103090
O	-0.182589	-1.694263	0.262796
C	2.290313	1.309435	-1.196660
H	2.276434	1.980121	-2.072533
H	2.364889	1.933881	-0.293470
C	0.390126	0.269401	-2.348606
H	1.165117	-0.122300	-3.030812
H	-0.285187	-0.560899	-2.092789
C	3.443552	0.321446	-1.265778
H	3.356872	-0.342922	-2.143264

H	4.399588	0.868680	-1.346216
H	3.474462	-0.298698	-0.353969
C	-0.379572	1.423492	-2.969563
H	-0.860682	1.086603	-3.905282
H	-1.160751	1.771166	-2.272873
H	0.284568	2.270440	-3.215468
C	0.943485	-2.517194	-0.101960
H	0.590184	-3.334271	-0.754334
H	1.600414	-1.869277	-0.701609
C	-1.439753	-2.381403	0.444341
H	-1.239201	-3.374146	0.883324
H	-2.002101	-1.786851	1.179651
C	1.670156	-3.044193	1.124680
H	1.012344	-3.686762	1.735644
H	2.545218	-3.643183	0.815529
H	2.018779	-2.203617	1.749107
C	-2.207723	-2.479562	-0.862620
H	-2.446946	-1.467671	-1.230615
H	-1.626638	-3.015695	-1.633618
H	-3.153509	-3.027635	-0.703109

L1-CuEt

Cu	0.021730	-0.184070	1.529246
C	0.273710	-0.054244	-1.847178
H	0.868132	0.072295	-2.773002
H	-0.468459	-0.850058	-2.060575
C	-0.433135	1.249928	-1.481254
H	0.301136	2.069686	-1.342136

H	-1.108320	1.568677	-2.299296
C	2.957813	0.164587	-0.865011
C	1.921454	-2.381838	-0.882734
C	3.537777	-0.778716	-1.933278
H	2.734053	1.152978	-1.314513
C	3.343990	-2.208929	-1.443257
H	1.965413	-2.914387	0.086565
H	3.005884	-0.621959	-2.892639
H	4.605054	-0.552780	-2.125399
H	3.562745	-2.950355	-2.234404
H	4.067613	-2.404796	-0.628725
C	-2.927212	0.206392	-0.487532
C	-2.213469	2.729246	0.416056
C	-3.798945	1.365292	-0.969339
H	-2.618438	-0.427926	-1.344131
C	-3.687324	2.505627	0.039030
H	-2.129152	2.895645	1.505596
H	-3.430432	1.697773	-1.959182
H	-4.849249	1.056370	-1.130348
H	-4.151816	3.436384	-0.337402
H	-4.243365	2.234609	0.956282
P	1.321690	-0.636956	-0.416911
P	-1.357014	1.055489	0.130482
C	-3.510439	-0.707482	0.565755
C	-2.723839	-1.769481	1.038352
C	-4.804335	-0.574517	1.077907
C	-3.210462	-2.672108	1.977244
H	-1.699051	-1.887757	0.654733
C	-5.295698	-1.472785	2.029211

H	-5.457845	0.235307	0.733616
C	-4.504702	-2.525059	2.480937
H	-2.572651	-3.495223	2.322228
H	-6.313358	-1.344225	2.416282
H	-4.892290	-3.229789	3.225535
C	-1.473371	3.841918	-0.271542
C	-0.317246	4.357025	0.333148
C	-1.847126	4.346916	-1.522160
C	0.449922	5.333812	-0.296000
H	-0.013400	3.973620	1.317317
C	-1.083197	5.329296	-2.153005
H	-2.747567	3.969921	-2.023106
C	0.070064	5.823722	-1.546387
H	1.350066	5.719862	0.196508
H	-1.395323	5.711135	-3.132233
H	0.669926	6.594117	-2.044348
C	0.891952	-3.068224	-1.731401
C	-0.232299	-3.625601	-1.104529
C	0.948825	-3.086698	-3.129507
C	-1.284094	-4.154244	-1.848802
H	-0.279122	-3.637313	-0.005612
C	-0.096416	-3.628445	-3.877938
H	1.815474	-2.659900	-3.650516
C	-1.221190	-4.154161	-3.243068
H	-2.157145	-4.573900	-1.334422
H	-0.032553	-3.632871	-4.972443
H	-2.044863	-4.571109	-3.833735
C	3.898630	0.368761	0.301398
C	5.022254	1.187665	0.116580

C	3.723645	-0.238465	1.549467
C	5.941128	1.391849	1.142285
H	5.172079	1.678467	-0.854987
C	4.642370	-0.037177	2.580891
H	2.836464	-0.857947	1.739947
C	5.754712	0.776757	2.381649
H	6.808632	2.041218	0.975221
H	4.477504	-0.520959	3.551200
H	6.475034	0.937797	3.192064
C	0.314200	-0.949651	3.332049
H	-0.600054	-0.880090	3.961987
H	1.090935	-0.370656	3.882359
C	0.751039	-2.411350	3.251595
H	0.906357	-2.907884	4.238928
H	0.010270	-3.038988	2.709516
H	1.707449	-2.532665	2.697754

II-*proR*$_{1-2}$

C	-3.717465	-0.604320	-0.810611
C	-3.757500	2.085387	-1.279554
C	-5.084677	0.094063	-0.845520
H	-3.447777	-0.740691	0.258334
C	-4.853618	1.521919	-0.381614
H	-4.182743	2.210799	-2.296979
H	-5.475989	0.087783	-1.884731
H	-5.820465	-0.449471	-0.221053
H	-5.771494	2.141231	-0.419884
H	-4.522665	1.499698	0.676950

C	2.544338	2.438103	0.570629
C	1.133749	1.103624	2.526290
C	3.186571	2.357653	1.959236
H	1.983874	3.393363	0.501619
C	2.039812	2.265060	2.954120
H	1.619287	0.152358	2.822084
H	3.823526	1.453026	2.030861
H	3.836696	3.232994	2.144780
H	2.390769	2.121508	3.993320
H	1.479402	3.219908	2.932842
P	1.253060	1.083797	0.633969
P	-2.492709	0.673645	-1.503607
Cu	1.690175	-0.624261	-0.834835
C	1.118905	-2.973746	1.214988
C	1.788010	-2.652109	-1.067904
C	1.425916	-3.018140	2.587442
C	-0.181888	-3.350451	0.787843
C	0.491937	-3.054733	-1.517606
H	2.647008	-2.703720	-1.744998
C	0.471853	-3.438898	3.501872
H	2.421948	-2.734709	2.932668
C	-1.137699	-3.745800	1.741970
C	-0.475761	-3.367621	-0.617058
H	0.309659	-3.089725	-2.597091
C	-0.817872	-3.800008	3.087525
H	0.735274	-3.479982	4.564743
H	-2.135789	-4.032775	1.387414
H	-1.477532	-3.674008	-0.942844
H	-1.562924	-4.124838	3.821943

N	2.081898	-2.609869	0.270063
B	3.620153	-2.333331	0.708437
F	4.121012	-3.479448	1.274513
F	3.622291	-1.279261	1.612992
F	4.299872	-1.986027	-0.442107
C	1.565110	-0.212173	-2.767894
H	0.496082	-0.336056	-3.047008
H	1.794601	0.874945	-2.783887
C	2.480039	-0.966056	-3.708210
H	3.536127	-0.930306	-3.368366
H	2.207285	-2.038209	-3.797090
H	2.466966	-0.564163	-4.745343
C	-3.718248	-1.962161	-1.459021
C	-4.099958	-3.076643	-0.698510
C	-3.401136	-2.160587	-2.807959
C	-4.148611	-4.351655	-1.259671
H	-4.361081	-2.935121	0.360006
C	-3.445355	-3.435077	-3.374035
H	-3.100153	-1.303079	-3.423932
C	-3.814679	-4.536184	-2.601896
H	-4.444547	-5.208735	-0.642919
H	-3.185542	-3.568332	-4.430845
H	-3.844680	-5.537745	-3.046144
C	-3.093698	3.373501	-0.891446
C	-2.360494	4.080482	-1.857801
C	-3.125400	3.882708	0.412089
C	-1.664297	5.240003	-1.530529
H	-2.332041	3.699117	-2.887943
C	-2.431820	5.048281	0.743394

H	-3.695549	3.364615	1.192528
C	-1.692859	5.728513	-0.222354
H	-1.096389	5.770906	-2.303761
H	-2.473632	5.427972	1.771977
H	-1.148501	6.643376	0.038870
C	3.456732	2.313165	-0.614147
C	4.341048	1.231128	-0.731688
C	3.407701	3.253290	-1.648425
C	5.161001	1.104312	-1.849911
H	4.385391	0.464584	0.053098
C	4.228861	3.127352	-2.769967
H	2.711599	4.099704	-1.572436
C	5.110661	2.053151	-2.872740
H	5.842213	0.248098	-1.923494
H	4.178045	3.876762	-3.568658
H	5.756956	1.951806	-3.752412
C	-0.280536	1.098441	3.035633
C	-1.023104	2.270686	3.225623
C	-0.915199	-0.128633	3.270847
C	-2.358445	2.213799	3.626626
H	-0.566840	3.253243	3.052324
C	-2.249064	-0.191002	3.663652
H	-0.344877	-1.055736	3.130443
C	-2.980805	0.984519	3.841073
H	-2.917607	3.145742	3.776028
H	-2.718391	-1.167115	3.838327
H	-4.029723	0.943182	4.156756
C	-0.288260	1.827052	-0.045621
H	-0.024784	2.075641	-1.096645

H	-0.535490	2.783922	0.454542
C	-1.453195	0.839355	0.033747
H	-1.085973	-0.201304	0.187350
H	-2.086107	1.062521	0.914766

II-*proS*$_{1\text{-}2}$

C	-3.905993	1.824165	-0.545570
C	-4.718801	-0.449877	0.727714
C	-5.314239	1.294784	-0.852682
H	-3.255385	1.576959	-1.408189
C	-5.279007	-0.213807	-0.669611
H	-5.461350	-0.065029	1.458295
H	-6.045327	1.736837	-0.144683
H	-5.633624	1.595965	-1.868757
H	-6.275804	-0.681370	-0.795098
H	-4.617782	-0.658290	-1.442031
C	1.472030	-2.205714	1.626311
C	0.771182	-2.640866	-0.999902
C	2.199369	-3.328117	0.883298
H	0.638854	-2.663434	2.197629
C	1.213640	-3.838381	-0.157355
H	1.616630	-2.331262	-1.646811
H	3.110540	-2.941723	0.381409
H	2.524919	-4.120546	1.582623
H	1.637967	-4.638904	-0.793192
H	0.340154	-4.272483	0.371794
P	0.654569	-1.223938	0.249206
P	-3.264910	0.768891	0.910169

Cu	1.476940	0.931701	0.184945
C	4.200333	0.603271	-1.151606
C	2.653797	2.369467	-0.624425
C	4.533587	-0.584203	-1.827093
C	5.136894	1.160069	-0.241679
C	3.600015	2.955193	0.273666
H	1.861341	2.999477	-1.045930
C	5.753706	-1.203223	-1.596320
H	3.828120	-1.022483	-2.534174
C	6.369257	0.513249	-0.034435
C	4.808398	2.370022	0.458970
H	3.315216	3.877953	0.789354
C	6.680306	-0.660887	-0.696474
H	5.989915	-2.129260	-2.132367
H	7.078612	0.961634	0.672550
H	5.552485	2.804818	1.137137
H	7.640391	-1.158148	-0.522579
N	2.965247	1.241993	-1.359788
B	2.064459	1.015173	-2.689830
F	2.683668	1.669073	-3.724537
F	0.818689	1.560325	-2.401373
F	1.936467	-0.335746	-2.945169
C	0.602758	2.085468	1.538098
H	-0.072745	1.404753	2.098539
H	1.383110	2.430954	2.248312
C	-0.177429	3.243485	0.947990
H	-0.791338	3.792224	1.697973
H	0.479823	4.000850	0.472797
H	-0.888599	2.911350	0.161941

C	-4.343417	-1.841279	1.140526
C	-4.108429	-2.870991	0.222378
C	-4.164751	-2.119251	2.505759
C	-3.696486	-4.133313	0.655198
H	-4.234612	-2.695823	-0.853778
C	-3.746633	-3.373404	2.938827
H	-4.350930	-1.322376	3.239080
C	-3.506907	-4.390003	2.011195
H	-3.519940	-4.923623	-0.084647
H	-3.610758	-3.562678	4.010284
H	-3.183176	-5.381764	2.347803
C	-3.818782	3.302256	-0.296091
C	-4.459364	3.889742	0.803854
C	-3.078491	4.128310	-1.149077
C	-4.360904	5.257698	1.044398
H	-5.034795	3.258252	1.495445
C	-2.973611	5.498993	-0.911098
H	-2.563517	3.683151	-2.011294
C	-3.614472	6.068882	0.187412
H	-4.866849	5.695444	1.913121
H	-2.384168	6.125629	-1.590899
H	-3.532578	7.145250	0.378384
C	-0.447819	-2.815434	-1.868648
C	-0.846014	-1.774973	-2.723722
C	-1.203659	-3.993363	-1.870187
C	-1.970454	-1.900578	-3.533749
H	-0.259739	-0.848618	-2.746195
C	-2.325984	-4.125475	-2.690801
H	-0.917185	-4.836790	-1.231623

C	-2.719905	-3.079019	-3.520126
H	-2.261631	-1.070411	-4.188323
H	-2.895839	-5.062796	-2.679438
H	-3.601694	-3.182917	-4.163023
C	2.261703	-1.321943	2.546241
C	1.752410	-0.992097	3.807703
C	3.480414	-0.751904	2.150791
C	2.434779	-0.117420	4.652686
H	0.798859	-1.429690	4.132222
C	4.168171	0.115140	2.997268
H	3.906924	-0.985899	1.163952
C	3.647225	0.439652	4.250222
H	2.015066	0.127768	5.635191
H	5.124648	0.542433	2.671441
H	4.188722	1.124312	4.912876
C	-1.912077	-0.120665	-0.019990
H	-1.254252	0.702003	-0.379184
H	-2.312186	-0.609925	-0.928984
C	-1.100136	-1.109096	0.808173
H	-1.029000	-0.777739	1.866650
H	-1.559335	-2.117710	0.819533

II-*proR*$_{3-4}$

C	3.256710	2.111440	0.009200
C	3.972726	0.398742	-1.980197
C	4.752642	2.022392	-0.295454
H	3.057508	1.340111	0.776996
C	4.956666	0.608616	-0.826805

H	4.403762	0.880365	-2.882738
H	5.049167	2.771150	-1.059644
H	5.359241	2.222719	0.608483
H	6.000645	0.416140	-1.142330
H	4.734753	-0.097828	-0.001262
C	-0.378127	-2.589261	-0.982992
C	0.661333	-3.003227	1.536467
C	-0.213667	-4.039066	-0.503957
H	0.476934	-2.360563	-1.652878
C	0.956236	-4.057721	0.470941
H	-0.176887	-3.361752	2.168705
H	-1.135275	-4.385511	0.006428
H	-0.051032	-4.711959	-1.367325
H	1.114972	-5.054759	0.924439
H	1.880033	-3.801351	-0.086545
P	-0.078529	-1.566364	0.566674
P	2.468392	1.543030	-1.611956
Cu	-1.924330	-0.764023	1.642709
C	-3.442020	1.610337	-0.169548
C	-1.414347	2.045959	0.935521
C	-4.256066	1.706671	-1.314377
C	-3.960477	0.978909	0.994108
C	-1.824151	1.386811	2.101531
H	-0.433420	2.535270	0.893840
C	-5.547825	1.211880	-1.295272
H	-3.866861	2.180853	-2.217103
C	-5.283312	0.497078	0.986646
C	-3.116841	0.813269	2.155952
H	-1.174615	1.428156	2.984166

C	-6.073968	0.612837	-0.140480
H	-6.165953	1.296826	-2.196234
H	-5.669541	0.023874	1.897850
H	-3.585921	0.553610	3.112647
H	-7.102740	0.236762	-0.134441
N	-2.162647	2.165569	-0.152305
B	-1.557900	2.965012	-1.433832
F	-1.452015	2.064206	-2.473371
F	-0.320843	3.441268	-1.052870
F	-2.426708	3.990289	-1.732293
C	-3.107161	-2.165313	2.436440
H	-4.131643	-2.010612	2.034890
H	-2.753707	-3.143966	2.044901
C	-3.106389	-2.187599	3.953771
H	-3.449957	-1.228916	4.394662
H	-3.764355	-2.975635	4.383423
H	-2.092925	-2.374873	4.364328
C	3.619489	-1.013263	-2.358180
C	4.122734	-2.133295	-1.683572
C	2.739716	-1.238533	-3.430427
C	3.736607	-3.426251	-2.044497
H	4.835144	-2.005763	-0.859695
C	2.345221	-2.525142	-3.787574
H	2.350487	-0.377574	-3.992731
C	2.836713	-3.629824	-3.088316
H	4.149367	-4.284218	-1.499123
H	1.651041	-2.668178	-4.624590
H	2.529611	-4.644449	-3.367394
C	2.690501	3.405587	0.506940

C	1.932478	3.424164	1.684646
C	2.859518	4.607781	-0.192495
C	1.347862	4.603395	2.147375
H	1.799152	2.490177	2.251701
C	2.285253	5.788631	0.270274
H	3.437758	4.614495	-1.126022
C	1.521893	5.790961	1.439706
H	0.753815	4.592731	3.069440
H	2.426941	6.718773	-0.292656
H	1.064343	6.720317	1.798123
C	-1.658343	-2.237866	-1.688067
C	-1.631968	-1.582271	-2.923800
C	-2.905679	-2.524274	-1.113920
C	-2.813959	-1.223739	-3.572480
H	-0.665131	-1.348632	-3.390312
C	-4.087359	-2.168217	-1.758938
H	-2.958662	-3.032770	-0.143142
C	-4.046045	-1.515357	-2.991795
H	-2.767443	-0.709228	-4.539272
H	-5.051536	-2.399481	-1.289821
H	-4.976743	-1.230966	-3.497006
C	1.766531	-2.507523	2.423128
C	3.120325	-2.668749	2.110113
C	1.431292	-1.746746	3.554148
C	4.109410	-2.063968	2.887802
H	3.418077	-3.265608	1.239342
C	2.415121	-1.139718	4.329451
H	0.370709	-1.619717	3.817216
C	3.762085	-1.290051	3.993175

H	5.164563	-2.200943	2.622505
H	2.129528	-0.545450	5.205196
H	4.539458	-0.811298	4.599356
C	1.391478	-0.536264	0.139111
H	2.242937	-1.208672	-0.086732
H	1.646568	0.012730	1.067481
C	1.113006	0.409950	-1.011344
H	0.776756	-0.141332	-1.911569
H	0.277791	1.094674	-0.774521

II-*proS*$_{3-4}$

C	-4.289677	0.720279	-0.444702
C	-2.956512	2.407178	-2.147402
C	-5.012228	1.994574	-0.900033
H	-3.892574	0.904610	0.574723
C	-3.941070	3.039733	-1.168092
H	-3.458818	2.325695	-3.133145
H	-5.581376	1.797444	-1.831709
H	-5.748069	2.322457	-0.140871
H	-4.360011	3.984555	-1.566440
H	-3.441320	3.290629	-0.210563
C	-0.428218	1.148780	2.799539
C	0.181394	-1.529118	2.923213
C	-0.133630	0.555657	4.183566
H	-1.530052	1.134773	2.666731
C	-0.553072	-0.906528	4.111275
H	1.246680	-1.661381	3.204815
H	0.949556	0.636849	4.411964

H	-0.673389	1.114287	4.970779
H	-0.345099	-1.458709	5.047281
H	-1.649124	-0.948460	3.946766
P	0.235614	-0.163438	1.630088
P	-2.767923	0.590000	-1.589160
Cu	2.356351	0.286727	0.848553
C	1.647375	-0.174544	-1.758551
C	3.643090	-1.429998	-1.733444
C	2.253767	0.947730	-1.167033
C	4.334358	-0.351400	-1.124769
C	3.589456	0.816582	-0.707635
H	4.152356	1.700413	-0.379242
N	2.268260	-1.322850	-1.977347
B	1.407603	-2.577505	-2.548483
F	0.079015	-2.214710	-2.470850
F	1.682558	-3.660102	-1.737577
F	1.800773	-2.805898	-3.847014
C	3.714412	-0.131995	2.238116
C	4.847062	0.851803	2.458594
H	3.161331	-0.294162	3.189217
C	5.723710	-0.446991	-0.935161
C	6.416575	-1.582433	-1.317856
H	7.499506	-1.643814	-1.165586
C	4.357778	-2.577588	-2.117674
C	5.725402	-2.649683	-1.906349
H	6.268048	-3.550089	-2.214700
H	6.251506	0.401978	-0.484506
H	3.835169	-3.409119	-2.592943
H	1.711689	1.902662	-1.140504

H	0.595426	-0.141471	-2.066949
C	-0.325260	-2.827183	2.356974
C	0.378183	-3.425966	1.300152
C	-1.492156	-3.447743	2.814197
C	-0.075573	-4.601663	0.710817
H	1.295385	-2.950852	0.917322
C	-1.945144	-4.632541	2.229772
H	-2.060718	-3.013884	3.644963
C	-1.242121	-5.211227	1.176661
H	0.485318	-5.032145	-0.125112
H	-2.860933	-5.104201	2.605389
H	-1.603207	-6.137004	0.714176
C	0.070767	2.541163	2.533509
C	-0.830407	3.592752	2.332811
C	1.443015	2.824301	2.480897
C	-0.377663	4.888795	2.082404
H	-1.910384	3.392560	2.374209
C	1.899899	4.114130	2.219878
H	2.169921	2.017413	2.652231
C	0.989331	5.153356	2.020437
H	-1.102339	5.697743	1.930808
H	2.978532	4.309317	2.180637
H	1.346726	6.169929	1.819129
C	-5.122345	-0.528269	-0.407516
C	-5.246311	-1.267893	0.774687
C	-5.780153	-0.997382	-1.553276
C	-6.007017	-2.436561	0.816951
H	-4.734516	-0.920727	1.683345
C	-6.544450	-2.160635	-1.514791

H	-5.681530	-0.447501	-2.499296
C	-6.662099	-2.885743	-0.327717
H	-6.086087	-3.000077	1.754281
H	-7.049113	-2.509469	-2.423463
H	-7.260599	-3.803585	-0.298462
C	-1.615932	3.049281	-2.356682
C	-1.040151	3.933717	-1.436043
C	-0.860081	2.689550	-3.484311
C	0.248007	4.435274	-1.631073
H	-1.593549	4.242592	-0.540579
C	0.425114	3.187422	-3.682415
H	-1.294968	1.996414	-4.217671
C	0.987242	4.065092	-2.753287
H	0.672779	5.126789	-0.892458
H	0.992796	2.889197	-4.571773
H	1.998275	4.460148	-2.906507
C	-1.182058	-0.451385	0.486515
H	-0.921017	-1.288088	-0.193610
H	-2.070565	-0.771310	1.070311
C	-1.444635	0.823432	-0.297995
H	-0.523744	1.146731	-0.821401
H	-1.714415	1.662525	0.374061
H	4.107963	-1.123836	1.921750
H	5.539150	0.543758	3.273070
H	5.474471	0.978750	1.554625
H	4.480607	1.863344	2.732825

TS-(II-III)- $R_{3\text{-}4}$

C	-2.160424	2.713496	-0.138907
C	-0.076407	3.628997	-1.659930
C	-2.022336	4.225671	-0.317810
H	-1.726817	2.455981	0.848893
C	-0.533332	4.499981	-0.493386
H	-0.529194	4.035712	-2.587425
H	-2.562894	4.569075	-1.223258
H	-2.456464	4.770683	0.542615
H	-0.317239	5.570930	-0.675371
H	-0.005297	4.219740	0.440993
C	-0.233514	-1.456399	-2.679541
C	2.225828	-2.321724	-1.807441
C	0.661364	-2.212869	-3.677039
H	-0.271608	-0.388824	-2.972259
C	2.113348	-1.970257	-3.290700
H	2.012775	-3.405149	-1.697127
H	0.447408	-3.298881	-3.629975
H	0.441477	-1.891368	-4.711584
H	2.816404	-2.572176	-3.897364
H	2.368112	-0.904391	-3.462911
P	0.728438	-1.480571	-1.055425
P	-0.972698	1.961783	-1.424394
Cu	-0.231753	-2.099149	0.865978
C	-0.048791	0.376900	3.152152
C	1.534674	-1.299140	2.669314
C	-0.357694	1.714259	3.468372
C	-1.071465	-0.599558	3.269961
C	0.612597	-2.317578	2.789226
H	2.594346	-1.536225	2.519332

C	-1.621253	2.068507	3.918625
H	0.414262	2.479422	3.364730
C	-2.328498	-0.216732	3.761714
C	-0.816339	-2.010038	2.896313
H	0.965907	-3.355855	2.820663
C	-2.615634	1.100800	4.086299
H	-1.827807	3.117760	4.159892
H	-3.099038	-0.988393	3.889838
H	-1.393512	-2.744053	3.473871
H	-3.606504	1.375812	4.463633
N	1.249416	0.017620	2.775308
B	2.468953	1.044938	2.752642
F	3.529393	0.407438	2.129171
F	2.785881	1.385054	4.056380
F	2.118481	2.186773	2.035405
C	-2.199372	-2.565840	1.380678
H	-2.961754	-2.129761	2.043223
H	-2.389973	-2.133345	0.371703
C	-2.221995	-4.075507	1.358415
H	-1.978930	-4.509828	2.349041
H	-3.218084	-4.468661	1.069202
H	-1.495952	-4.494459	0.632317
C	1.385478	3.406492	-1.906771
C	2.348309	3.495556	-0.895117
C	1.799952	2.975371	-3.177963
C	3.674430	3.133171	-1.135157
H	2.066268	3.824599	0.110395
C	3.124205	2.621980	-3.423670
H	1.057064	2.904288	-3.984935

C	4.068889	2.692762	-2.397076
H	4.403079	3.189574	-0.317443
H	3.422568	2.288593	-4.425124
H	5.111743	2.409114	-2.583977
C	-3.521059	2.086767	-0.222179
C	-3.794652	0.946633	0.548208
C	-4.516741	2.549236	-1.091808
C	-5.025444	0.299204	0.467806
H	-3.022902	0.564097	1.233095
C	-5.751945	1.905811	-1.171807
H	-4.330912	3.429274	-1.720422
C	-6.014568	0.780903	-0.389770
H	-5.214464	-0.588484	1.084868
H	-6.519940	2.291872	-1.852821
H	-6.987668	0.279559	-0.450931
C	-1.637872	-1.970258	-2.525205
C	-2.733210	-1.110152	-2.667621
C	-1.882813	-3.310869	-2.196583
C	-4.036458	-1.574237	-2.487074
H	-2.558346	-0.054764	-2.914167
C	-3.182977	-3.778504	-2.021299
H	-1.040483	-4.005477	-2.065450
C	-4.266550	-2.909858	-2.162479
H	-4.877969	-0.879632	-2.598198
H	-3.351333	-4.831313	-1.764459
H	-5.289823	-3.276883	-2.021126
C	3.494757	-2.008217	-1.069747
C	4.352087	-0.970561	-1.454136
C	3.811594	-2.741421	0.082609

C	5.490186	-0.673359	-0.705000
H	4.132740	-0.371959	-2.347133
C	4.946810	-2.445015	0.832480
H	3.148016	-3.561171	0.393376
C	5.791547	-1.406887	0.440363
H	6.146240	0.146038	-1.022436
H	5.175352	-3.031264	1.730421
H	6.683717	-1.168466	1.030336
C	1.272904	0.252792	-0.759589
H	1.717260	0.680652	-1.680271
H	2.093478	0.189196	-0.014118
C	0.153560	1.121763	-0.194291
H	-0.526843	0.509980	0.439606
H	0.586764	1.872105	0.492583

TS-(II-III)-*S*$_{3-4}$

C	-2.235278	3.227324	-0.349997
C	-4.178203	1.312261	-0.492977
C	-3.684960	3.689934	-0.558888
H	-1.704963	3.319738	-1.319034
C	-4.408232	2.582980	-1.304831
H	-4.704776	1.437427	0.475803
H	-4.169063	3.854855	0.425961
H	-3.711666	4.658388	-1.093773
H	-5.489147	2.789933	-1.431820
H	-3.977474	2.488814	-2.321876
C	-1.712464	-2.208274	0.936605
C	0.368402	-3.082624	-0.544175

C	-2.066540	-3.434644	0.090392
H	-2.551301	-1.483949	0.921960
C	-0.815498	-4.070865	-0.542856
H	1.039390	-3.342796	0.297085
H	-2.645178	-4.166455	0.685725
H	-2.756858	-3.106049	-0.708625
H	-0.511871	-4.981540	0.006909
H	-1.055135	-4.414604	-1.564053
P	-0.295341	-1.410526	0.003815
P	-2.341771	1.360255	0.020485
Cu	1.366021	-0.492778	1.341190
C	1.462336	2.075425	0.043427
C	3.530440	1.146099	-0.577619
C	1.595414	1.686876	1.379431
C	3.766343	0.745002	0.764580
C	2.740535	0.949977	1.767270
H	3.012288	0.848964	2.824170
N	2.352549	1.822544	-0.907570
B	1.976701	2.208136	-2.433557
F	3.021456	2.914102	-2.985746
F	0.832821	2.990076	-2.380089
F	1.740925	1.024889	-3.102723
C	2.308804	-1.952633	2.333327
C	2.813709	-1.674948	3.735053
H	2.028069	-1.222217	4.374224
H	3.149367	-2.595598	4.262428
H	3.681165	-0.984114	3.750684
C	-4.606455	0.000279	-1.077724
C	-4.603653	-0.252553	-2.455908

C	-5.002366	-1.037229	-0.219050
C	-4.966544	-1.504170	-2.955177
H	-4.322799	0.538350	-3.161537
C	-5.368846	-2.285986	-0.714091
H	-5.028044	-0.851130	0.863856
C	-5.347785	-2.527111	-2.088596
H	-4.958119	-1.676508	-4.037857
H	-5.674738	-3.078249	-0.020142
H	-5.637288	-3.507783	-2.483330
C	-1.483949	4.016169	0.686835
C	-0.474402	4.910267	0.310044
C	-1.785358	3.893269	2.050997
C	0.222966	5.650977	1.265235
H	-0.219934	5.013238	-0.753331
C	-1.095810	4.634800	3.007503
H	-2.572770	3.195618	2.369710
C	-0.084822	5.515331	2.617529
H	1.014468	6.339491	0.946973
H	-1.347099	4.521929	4.068764
H	0.462318	6.095105	3.369878
C	-1.319161	-2.444273	2.372264
C	-1.213669	-1.338910	3.232735
C	-1.041699	-3.712979	2.887550
C	-0.846566	-1.499359	4.564500
H	-1.438223	-0.334893	2.842782
C	-0.669160	-3.876393	4.224385
H	-1.114615	-4.598624	2.245059
C	-0.571129	-2.773362	5.067163
H	-0.777929	-0.622784	5.219828

H	-0.456905	-4.881571	4.607077
H	-0.281344	-2.902848	6.116330
C	1.224403	-2.954005	-1.775752
C	0.742967	-3.192857	-3.068734
C	2.543577	-2.495880	-1.637072
C	1.554488	-2.989919	-4.184877
H	-0.288768	-3.533974	-3.219425
C	3.356053	-2.293482	-2.750099
H	2.939194	-2.294568	-0.630361
C	2.864749	-2.541475	-4.031443
H	1.153506	-3.184577	-5.186484
H	4.384368	-1.939331	-2.610997
H	3.501983	-2.383806	-4.909042
C	-1.106005	-0.747523	-1.531677
H	-1.993341	-1.374296	-1.753272
H	-0.383288	-0.918155	-2.354153
C	-1.466658	0.731801	-1.507676
H	-0.539349	1.328708	-1.577243
H	-2.039120	0.985950	-2.422229
H	0.848478	2.032899	2.105010
H	0.586199	2.654115	-0.263812
C	4.980134	0.113311	1.090481
C	5.933894	-0.139889	0.121883
H	6.874361	-0.633563	0.389016
C	5.687556	0.241457	-1.204895
H	6.436616	0.041610	-1.979597
C	4.507714	0.876966	-1.553424
H	4.336003	1.180130	-2.587699
H	5.149977	-0.183368	2.132628

H	3.136807	-2.291141	1.671920
H	1.554817	-2.767189	2.364775

III-$R_{1\text{-}2}$

C	-4.150875	-1.853425	0.721740
C	-3.570263	0.343472	2.240354
C	-4.253194	-1.995712	2.243781
H	-3.179208	-2.288338	0.412221
C	-3.247060	-1.022799	2.835745
H	-4.535681	0.680933	2.670764
H	-5.274469	-1.733681	2.588530
H	-4.069039	-3.041816	2.554126
H	-3.273838	-0.998656	3.942749
H	-2.227094	-1.349551	2.547688
C	0.088543	0.184569	-2.725178
C	0.585788	2.791432	-2.013476
C	0.831674	1.077368	-3.729907
H	-0.966462	0.111460	-3.057543
C	0.367864	2.508613	-3.500359
H	1.680078	2.761141	-1.830243
H	1.926011	1.010048	-3.563342
H	0.641370	0.728682	-4.761574
H	0.919889	3.237060	-4.123272
H	-0.704447	2.599464	-3.767263
P	-0.010169	1.232553	-1.161717
P	-4.010806	0.021047	0.406203
Cu	1.101793	0.678554	0.703910
C	4.278266	-0.691608	0.290129

C	2.724894	-1.437558	2.034725
C	5.176663	-0.976304	-0.771152
C	3.815738	0.656123	0.381486
C	2.469136	0.024358	2.324655
H	2.915491	-1.935863	3.003176
C	5.524530	-0.008584	-1.698674
H	5.582120	-1.986912	-0.864757
C	4.192884	1.622806	-0.565268
C	3.007172	1.004566	1.533116
H	1.985983	0.280186	3.278353
C	5.028674	1.303539	-1.622621
H	6.205071	-0.282830	-2.514290
H	3.820584	2.649622	-0.436575
H	2.919391	2.067084	1.812513
H	5.317266	2.057946	-2.362121
N	3.914757	-1.632541	1.208765
B	4.787657	-2.914742	1.410690
F	4.673384	-3.777796	0.306237
F	4.354694	-3.572015	2.557871
F	6.124863	-2.547912	1.552203
C	1.457411	-2.082743	1.449733
H	0.599658	-1.765724	2.084739
H	1.285857	-1.657211	0.431563
C	1.485982	-3.596080	1.355963
H	1.673583	-4.045625	2.348934
H	0.524067	-3.984198	0.972321
H	2.287470	-3.935692	0.677088
C	-2.579655	1.456815	2.407767
C	-1.234950	1.245236	2.740833

C	-3.002372	2.778055	2.185607
C	-0.345560	2.320995	2.839687
H	-0.875352	0.232740	2.966499
C	-2.114759	3.846655	2.262069
H	-4.055809	2.961772	1.933512
C	-0.776444	3.621671	2.589575
H	0.690321	2.146067	3.155717
H	-2.468337	4.867097	2.071872
H	-0.077632	4.461804	2.669405
C	-5.237642	-2.504777	-0.082317
C	-4.922335	-3.425285	-1.088566
C	-6.587925	-2.195958	0.134886
C	-5.923177	-4.027835	-1.851462
H	-3.868882	-3.676614	-1.273957
C	-7.590169	-2.797664	-0.621276
H	-6.859518	-1.461509	0.905503
C	-7.261535	-3.718160	-1.618334
H	-5.652707	-4.747770	-2.632882
H	-8.639961	-2.542797	-0.433931
H	-8.050430	-4.191287	-2.214427
C	0.626980	-1.203768	-2.531782
C	-0.217492	-2.312014	-2.670014
C	1.967156	-1.424420	-2.189303
C	0.261694	-3.607514	-2.475060
H	-1.269753	-2.158475	-2.946132
C	2.447438	-2.716315	-1.986397
H	2.653585	-0.575230	-2.054596
C	1.596729	-3.812191	-2.132747
H	-0.415986	-4.461342	-2.592997

H	3.487939	-2.866681	-1.675204
H	1.976602	-4.826897	-1.965034
C	0.049635	4.059767	-1.417798
C	-1.177617	4.612771	-1.806132
C	0.785587	4.709078	-0.418089
C	-1.650402	5.782321	-1.212497
H	-1.775983	4.133819	-2.590843
C	0.317615	5.880037	0.173512
H	1.752534	4.288945	-0.106028
C	-0.904912	6.421168	-0.221872
H	-2.610265	6.202295	-1.534564
H	0.916269	6.376682	0.946272
H	-1.274883	7.344974	0.237521
C	-1.816813	1.362039	-0.853558
H	-2.354436	1.678617	-1.768909
H	-1.962210	2.153755	-0.092907
C	-2.308510	0.003066	-0.363416
H	-2.375528	-0.708381	-1.212145
H	-1.585000	-0.445005	0.353535

III-*S*$_{1-2}$

C	-3.959835	0.163008	-1.309831
C	-2.145107	1.942317	-2.325633
C	-4.328057	0.905069	-2.604449
H	-4.594709	0.544430	-0.485547
C	-3.610582	2.249237	-2.613026
H	-1.757396	1.315439	-3.157059
H	-3.996379	0.326220	-3.487257

H	-5.424817	1.012731	-2.691518
H	-3.732139	2.779737	-3.577031
H	-4.037418	2.907881	-1.829949
C	1.599911	2.222717	1.916408
C	-0.092822	0.453602	3.159522
C	1.953504	1.755653	3.337236
H	1.155556	3.236101	1.994248
C	0.648308	1.447338	4.050541
H	0.484760	-0.490455	3.171330
H	2.579952	0.841077	3.276307
H	2.556916	2.525514	3.853728
H	0.802950	1.029282	5.063679
H	0.071467	2.385915	4.173084
P	0.161275	1.116299	1.407747
P	-2.215075	0.747545	-0.877726
Cu	-0.178493	-0.306892	-0.398062
C	1.720640	-3.362696	0.671893
C	2.013467	-1.993377	-1.332374
C	0.321976	-3.635247	0.197482
C	0.590377	-1.960288	-1.544351
C	-0.225572	-2.921282	-0.798606
H	-1.261638	-3.087811	-1.127823
N	2.563013	-2.786984	-0.380701
B	4.091492	-3.129651	-0.415596
F	4.858137	-1.982196	-0.145683
F	4.433594	-3.610451	-1.678125
F	4.356196	-4.099860	0.543021
C	0.057411	-1.265259	-2.663390
C	0.864587	-0.534273	-3.522163

H	0.436898	-0.000610	-4.378050
C	2.807753	-1.218407	-2.221567
C	2.245654	-0.514206	-3.271098
H	2.906976	0.063921	-3.928736
H	-1.018444	-1.373889	-2.862029
H	3.890452	-1.204586	-2.083552
H	-0.259697	-4.401143	0.727127
H	2.188099	-4.315297	0.979769
C	-1.522322	0.119280	3.469229
C	-2.046769	-1.105394	3.027520
C	-2.365888	0.990040	4.169053
C	-3.372952	-1.447382	3.278033
H	-1.395599	-1.806245	2.484194
C	-3.699118	0.654462	4.407907
H	-1.983013	1.945908	4.545616
C	-4.208761	-0.563959	3.963329
H	-3.755284	-2.419335	2.944147
H	-4.342072	1.351108	4.958210
H	-5.252662	-0.832257	4.161852
C	2.782274	2.293300	0.992889
C	3.390859	3.532564	0.758537
C	3.353078	1.149465	0.422055
C	4.535091	3.632810	-0.030492
H	2.953926	4.436744	1.204063
C	4.501320	1.244649	-0.363614
H	2.902956	0.158227	0.583855
C	5.093021	2.486347	-0.595964
H	4.994450	4.613340	-0.203249
H	4.935149	0.328435	-0.778212

H	5.995560	2.558906	-1.213891
C	-4.031220	-1.340692	-1.311359
C	-4.335571	-2.006999	-0.116849
C	-3.717975	-2.113614	-2.436505
C	-4.322506	-3.398163	-0.042908
H	-4.584876	-1.415112	0.775377
C	-3.710614	-3.507241	-2.368252
H	-3.472285	-1.632587	-3.391632
C	-4.009734	-4.156348	-1.171562
H	-4.568424	-3.896188	0.902774
H	-3.464493	-4.090438	-3.263167
H	-4.002973	-5.250889	-1.119165
C	-1.171427	3.057888	-2.083407
C	-1.571334	4.362324	-1.778181
C	0.201944	2.765320	-2.101986
C	-0.622690	5.341953	-1.472985
H	-2.635572	4.626831	-1.773217
C	1.147653	3.738329	-1.798064
H	0.533443	1.748417	-2.360598
C	0.736151	5.033173	-1.472319
H	-0.954593	6.359175	-1.234262
H	2.214439	3.482653	-1.812146
H	1.479010	5.801883	-1.227665
C	-1.201115	2.370872	1.210570
H	-1.403353	2.848634	2.189803
H	-0.777846	3.159286	0.557357
C	-2.493195	1.823860	0.611072
H	-3.188816	2.653542	0.374385
H	-3.013758	1.171895	1.343998

C	1.652328	-2.456756	1.907643
H	1.218677	-1.496162	1.555780
H	0.908544	-2.890798	2.610573
C	2.963729	-2.208036	2.626685
H	3.692288	-1.689328	1.977537
H	2.805509	-1.586280	3.529681
H	3.428468	-3.157670	2.950703

EtMgBr

C	3.665331	-0.579973	0.000017
H	3.519564	-1.231160	0.885705
H	3.519604	-1.231090	-0.885728
H	4.741290	-0.296031	0.000053
C	2.712398	0.614969	0.000042
H	2.932050	1.259539	-0.879254
H	2.932029	1.259483	0.879386
Mg	0.639519	0.186040	0.000021
Br	-1.816718	-0.062949	-0.000022

Et_2O

O	0.074236	-0.590758	-0.295823
C	-1.238248	-0.626216	0.200003
C	0.913893	0.349567	0.318735
C	2.329842	0.105674	-0.138276
H	0.605332	1.388573	0.065481
H	0.837191	0.257885	1.427558
H	3.023002	0.835334	0.316312

H	2.659764	-0.911734	0.140545
H	2.401651	0.197739	-1.237525
H	-1.699881	-1.533260	-0.232872
H	-1.220991	-0.767730	1.305642
C	-2.063347	0.593358	-0.157041
H	-3.116891	0.448261	0.143324
H	-1.699099	1.507907	0.346398
H	-2.036806	0.768790	-1.248799

V·2Et$_2$O

C	-3.622484	-0.704994	1.755425
C	-2.355823	-0.531554	1.246125
C	-2.047203	-0.987087	-0.060723
C	-3.061656	-1.630678	-0.828429
C	-4.355882	-1.794366	-0.273713
C	-4.632313	-1.337819	0.993067
H	-3.852564	-0.350431	2.766342
H	-1.568446	-0.046380	1.837490
C	-2.725284	-2.082193	-2.126761
H	-5.126208	-2.291060	-0.875687
H	-5.633763	-1.464620	1.418405
C	-1.451286	-1.893219	-2.605544
C	-0.514676	-1.235841	-1.781569
H	-3.492040	-2.578611	-2.734120
H	-1.155806	-2.229002	-3.603647
H	0.504226	-1.042292	-2.148990
N	-0.792001	-0.796024	-0.568938
Mg	0.774770	0.380319	0.455606

Br	2.250179	1.377171	-1.403123
C	0.884139	0.434971	2.606945
H	0.633230	-0.582500	2.991761
C	2.299481	0.789565	3.066651
H	0.155213	1.110165	3.113442
H	2.479295	0.731948	4.166054
H	3.056945	0.123339	2.597777
H	2.584051	1.821435	2.764444
O	-0.587005	2.120262	0.186447
C	-0.306855	3.224866	1.038256
H	0.138298	4.049565	0.446079
H	0.477101	2.860690	1.725528
C	-1.518649	3.683532	1.814019
H	-1.225921	4.442795	2.561159
H	-2.288897	4.139267	1.164179
H	-1.977584	2.830275	2.349667
C	-1.487922	2.361924	-0.888253
H	-1.498846	1.424279	-1.471217
H	-2.512769	2.499583	-0.483173
C	-1.092801	3.513879	-1.783078
H	-0.043938	3.397699	-2.114447
H	-1.742163	3.521186	-2.676919
H	-1.203101	4.497372	-1.290639
O	1.926076	-1.539224	0.420009
C	3.284788	-1.700369	0.024537
H	3.892661	-2.002385	0.900816
H	3.612340	-0.690094	-0.274166
C	3.452359	-2.665673	-1.124744
H	4.503183	-2.664256	-1.465773

H	3.196378	-3.706096	-0.850144
H	2.817006	-2.363065	-1.978938
C	1.283896	-2.687853	0.959405
H	0.276916	-2.344147	1.256016
H	1.139438	-3.443364	0.158008
C	1.991931	-3.284193	2.153451
H	2.945877	-3.774209	1.885908
H	2.197379	-2.503045	2.909780
H	1.347880	-4.052386	2.617561

TS-(V-VI)·2Et_2O

C	-3.388601	2.041363	0.762698
C	-2.264879	1.578500	0.103255
C	-2.280927	0.334838	-0.576765
C	-3.496852	-0.411453	-0.575643
C	-4.626283	0.084866	0.102793
C	-4.581323	1.294243	0.773989
H	-3.348803	3.006663	1.282145
H	-1.338568	2.165572	0.087471
C	-3.509635	-1.650632	-1.294276
H	-5.548366	-0.511056	0.087510
H	-5.464788	1.671680	1.300532
C	-2.382229	-2.105903	-1.901742
C	-1.169814	-1.343127	-1.781571
H	-4.450243	-2.213766	-1.356726
H	-2.370249	-3.046541	-2.463097
H	-0.386683	-1.540882	-2.527002
N	-1.166145	-0.104726	-1.230689

C	0.011048	-2.758048	-0.372797
H	-0.050317	-3.463839	-1.225190
H	1.076205	-2.843112	-0.044276
C	-0.914861	-3.179002	0.749095
H	-0.729296	-2.603295	1.677332
H	-1.982813	-3.015109	0.487641
H	-0.833852	-4.253769	1.027399
Mg	0.740250	-0.483250	-0.345984
Br	3.130113	-0.930116	-1.116915
O	0.774585	-0.403500	1.742173
O	1.170506	1.649680	-0.504995
C	-0.049620	0.455683	2.544304
H	0.543657	0.788139	3.418407
H	-0.251937	1.351547	1.929758
C	-1.339861	-0.203161	2.962405
H	-1.166597	-1.089078	3.600641
H	-1.950051	0.514538	3.540648
H	-1.928356	-0.513826	2.077787
C	1.632605	-1.279055	2.494261
H	1.082674	-1.610696	3.395669
H	1.792017	-2.172074	1.864546
C	2.943560	-0.622506	2.844889
H	2.797924	0.292412	3.449144
H	3.561626	-1.319077	3.439376
H	3.503453	-0.362257	1.927669
C	2.105002	2.264581	0.381177
H	3.124040	2.150378	-0.042322
H	2.074597	1.663136	1.305884
C	1.779354	3.708327	0.675714

H	2.473871	4.098996	1.440943
H	1.879771	4.349332	-0.219054
H	0.747539	3.810829	1.062787
C	1.224569	2.125221	-1.858540
H	2.199771	2.628985	-2.008210
H	1.231776	1.237234	-2.518639
C	0.069073	3.027157	-2.214192
H	0.005966	3.901958	-1.542056
H	0.194543	3.398302	-3.247846
H	-0.885132	2.474031	-2.161940

VI·2Et_2O

C	-2.316472	2.473229	1.331594
C	-1.485462	1.415228	0.981898
C	-1.936616	0.333519	0.179739
C	-3.300832	0.391175	-0.248000
C	-4.117313	1.463990	0.117423
C	-3.647819	2.514146	0.906704
H	-1.915099	3.281968	1.956013
H	-0.451336	1.413154	1.357828
C	-3.749895	-0.645470	-1.160544
H	-5.154137	1.471507	-0.248598
H	-4.303657	3.346663	1.185242
C	-2.949279	-1.672109	-1.486942
C	-1.603974	-1.863263	-0.844342
H	-4.748689	-0.543026	-1.608882
H	-3.280598	-2.439118	-2.201121
H	-0.890301	-2.164587	-1.647174

N	-1.080997	-0.648112	-0.216869
C	-1.621209	-3.056633	0.129388
H	-1.954215	-3.956901	-0.429955
H	-0.571481	-3.259420	0.432720
C	-2.490307	-2.855874	1.355794
H	-2.464176	-3.740061	2.019796
H	-2.153776	-1.982431	1.946014
H	-3.546771	-2.678102	1.076450
Mg	0.889652	-0.296464	-0.270709
Br	2.406854	-1.770056	-1.549810
O	1.624587	-0.268618	1.665542
O	1.088294	1.582636	-1.109136
C	1.113372	-1.252069	2.592701
H	1.969312	-1.638682	3.178355
H	0.730100	-2.100925	1.993133
C	0.029623	-0.690344	3.476406
H	-0.814037	-0.312440	2.870970
H	-0.355424	-1.486499	4.139005
H	0.400633	0.135597	4.109002
C	2.918447	0.255871	1.990784
H	3.226980	0.854567	1.114646
H	3.629325	-0.590376	2.072561
C	2.913877	1.108672	3.235031
H	2.710306	0.515779	4.144456
H	3.903305	1.582128	3.363520
H	2.153230	1.909012	3.163662
C	1.629182	2.754617	-0.492403
H	1.536677	2.597141	0.598255
H	0.978857	3.616135	-0.739798

C	3.060970	3.002640	-0.895386
H	3.154965	3.206073	-1.977103
H	3.459740	3.878696	-0.353831
H	3.698086	2.130097	-0.660576
C	0.617722	1.767945	-2.457387
H	1.301995	2.474101	-2.964248
H	0.742444	0.790100	-2.957661
C	-0.812817	2.241857	-2.509444
H	-0.946178	3.193883	-1.962655
H	-1.107191	2.411706	-3.560265
H	-1.497849	1.495688	-2.069151

TS-(V-VII)·2Et_2O

C	5.120567	-0.228570	0.032548
C	4.223783	-0.840427	-0.821478
C	2.976888	-0.246790	-1.130627
C	2.647374	0.992831	-0.512342
C	3.592105	1.611041	0.329458
C	4.811799	1.017688	0.606265
H	6.082119	-0.708358	0.251834
H	4.452266	-1.799545	-1.301346
C	1.334101	1.579501	-0.763666
H	3.345678	2.581514	0.778400
H	5.530669	1.515672	1.266754
C	0.591538	0.948457	-1.812504
C	1.065708	-0.249761	-2.380136
H	1.250936	2.668098	-0.666283
H	-0.273208	1.456823	-2.262409

H	0.454777	-0.717390	-3.170155
N	2.173205	-0.877701	-2.046903
C	0.466089	1.642333	1.289677
H	-0.474133	1.300636	1.785971
H	1.275621	1.099136	1.816941
C	0.558145	3.135764	1.526679
H	-0.159316	3.706172	0.900576
H	0.355295	3.420487	2.579993
H	1.560586	3.540970	1.289447
Mg	-0.614965	-0.018418	0.000347
Br	-1.396521	-2.219851	-1.041066
O	-2.454657	1.014732	-0.189126
O	-0.670746	-1.069843	1.864426
C	-3.512922	0.526489	-1.045134
H	-4.441676	1.051503	-0.753768
H	-3.634689	-0.544602	-0.807034
C	-3.212869	0.708829	-2.511412
H	-4.077382	0.360996	-3.105874
H	-3.024725	1.766396	-2.769753
H	-2.338629	0.104117	-2.814367
C	-2.743958	2.266556	0.449136
H	-2.036569	2.355156	1.289567
H	-3.758046	2.201899	0.889762
C	-2.617304	3.442399	-0.486317
H	-3.398168	3.438582	-1.268397
H	-2.717200	4.385460	0.080812
H	-1.627001	3.442281	-0.981698
C	-1.955061	-1.112805	2.491756
H	-2.640839	-0.536256	1.841575

H	-2.315393	-2.161158	2.482642
C	-1.926882	-0.532225	3.885062
H	-1.586142	0.519527	3.863987
H	-2.939381	-0.558136	4.325760
H	-1.256761	-1.098317	4.556679
C	0.171725	-2.172349	2.205511
H	0.232934	-2.233874	3.309625
H	-0.308438	-3.101424	1.834701
C	1.541201	-1.998132	1.606100
H	1.521533	-2.057579	0.501097
H	1.997916	-1.034988	1.903764
H	2.203808	-2.808166	1.958811

VII·2Et$_2$O

C	-2.135000	2.989758	-0.002348
C	-1.307094	1.873793	0.003760
C	-1.795813	0.570808	-0.231935
C	-3.192097	0.424263	-0.444456
C	-4.003185	1.560126	-0.470479
C	-3.499991	2.843710	-0.257053
H	-1.705008	3.982793	0.181670
H	-0.230952	2.008101	0.184366
C	-3.805665	-0.955243	-0.535608
H	-5.079446	1.421624	-0.651066
H	-4.164194	3.715230	-0.278870
C	-2.753581	-1.935949	-0.970087
C	-1.445933	-1.682840	-0.750396
H	-4.639072	-0.928376	-1.274740

H	-3.050248	-2.903476	-1.393566
H	-0.697706	-2.458899	-0.983013
N	-0.915871	-0.494146	-0.279828
C	-4.437512	-1.347986	0.814641
H	-3.638826	-1.326275	1.587248
H	-5.167869	-0.562479	1.102240
C	-5.116817	-2.704586	0.800570
H	-5.618377	-2.920098	1.762091
H	-5.885556	-2.755669	0.003788
H	-4.392595	-3.519976	0.614812
Mg	1.073489	-0.420600	0.052925
Br	2.354083	-2.530940	-0.074878
O	1.515417	0.482072	1.865976
O	2.009787	0.898217	-1.234292
C	0.418564	0.661464	2.784570
H	0.547988	-0.058028	3.616350
H	-0.493231	0.368588	2.232175
C	0.322522	2.084124	3.273266
H	-0.546537	2.187591	3.947033
H	1.220127	2.395294	3.837778
H	0.180992	2.781749	2.427282
C	2.780326	0.277085	2.521261
H	2.810016	-0.768940	2.887198
H	2.821081	0.945916	3.400663
C	3.922121	0.567881	1.586255
H	4.876033	0.392356	2.113857
H	3.908492	-0.095908	0.700717
H	3.907028	1.620808	1.252924
C	2.225395	2.296798	-1.008981

H	1.915567	2.475989	0.037742
H	3.315943	2.489969	-1.062172
C	1.463093	3.182094	-1.962710
H	0.378719	2.966663	-1.926124
H	1.615786	4.239834	-1.682543
H	1.810602	3.065246	-3.005186
C	2.516502	0.375234	-2.477985
H	3.224549	1.112783	-2.898855
H	3.095529	-0.532219	-2.223122
C	1.394643	0.054972	-3.433268
H	0.703900	-0.692287	-2.999226
H	0.805836	0.954737	-3.686508
H	1.803257	-0.368860	-4.368073

TS-(1a·BF_3-VIII)·2Et_2O

C	3.981840	-1.825269	1.274446
C	2.920960	-0.960702	1.494490
C	2.780581	0.203843	0.718465
C	3.746518	0.472607	-0.281122
C	4.817961	-0.415230	-0.478071
C	4.940100	-1.561739	0.286703
H	4.063205	-2.731915	1.885044
H	2.186765	-1.200571	2.265462
C	3.594913	1.660530	-1.071332
H	5.551365	-0.180652	-1.259587
H	5.772937	-2.254070	0.122972
C	2.499108	2.442602	-0.936591
C	1.461851	2.076886	-0.006762

H	4.385731	1.919918	-1.786004
H	2.366525	3.347204	-1.537592
N	1.725399	1.099273	0.908764
B	0.693142	0.904343	2.053908
F	-0.143274	-0.226009	1.586208
F	1.249784	0.564917	3.246224
F	-0.134601	1.992139	2.149088
H	0.791634	2.860108	0.356059
C	-0.066150	1.779421	-1.670169
H	0.678873	1.317872	-2.341055
H	-1.029596	1.272549	-1.959489
C	-0.275899	3.260380	-1.976367
H	0.039518	3.940736	-1.153417
H	0.286604	3.591098	-2.871279
H	-1.334861	3.510727	-2.175787
Mg	-0.771904	-0.054262	-0.327621
Br	0.777189	-1.595607	-1.619783
O	-2.412499	1.037222	0.502199
O	-2.152481	-1.700115	-0.226553
C	-2.677242	2.427288	0.271698
H	-3.082797	2.861423	1.205158
H	-1.703055	2.914503	0.091894
C	-3.616547	2.647598	-0.888644
H	-4.600216	2.174029	-0.718685
H	-3.778823	3.730624	-1.039307
H	-3.199064	2.238555	-1.827900
C	-3.076004	0.487675	1.647580
H	-2.878740	1.153670	2.510755
H	-2.577463	-0.469302	1.863473

C	-4.552148	0.273535	1.428838
H	-4.987080	-0.237129	2.307278
H	-5.100308	1.223869	1.294999
H	-4.727300	-0.363308	0.541037
C	-1.788794	-2.792304	0.628278
H	-1.114524	-2.362630	1.389131
H	-1.193120	-3.513796	0.033591
C	-2.978936	-3.449816	1.284709
H	-2.625584	-4.177721	2.036243
H	-3.608763	-2.702876	1.803690
H	-3.611291	-4.001583	0.566777
C	-2.876468	-2.104034	-1.388853
H	-3.866503	-2.490416	-1.078151
H	-2.321083	-2.931955	-1.876488
C	-3.040086	-0.939839	-2.327304
H	-3.646880	-1.242050	-3.198114
H	-3.556547	-0.095598	-1.833927
H	-2.062534	-0.597408	-2.722592

VIII·2Et_2O

C	1.810446	3.298571	0.447981
C	1.755039	1.997109	0.941657
C	2.310674	0.920876	0.223871
C	2.948145	1.213238	-1.013385
C	2.990798	2.529067	-1.488570
C	2.425009	3.579598	-0.773079
H	1.371567	4.109401	1.042424
H	1.292799	1.816030	1.914681

C	3.476962	0.108008	-1.797851
H	3.480433	2.716248	-2.453904
H	2.470485	4.605266	-1.155945
C	3.589792	-1.116369	-1.263980
C	3.276072	-1.334489	0.189322
H	3.758384	0.304151	-2.841725
H	3.966225	-1.962048	-1.853302
N	2.244950	-0.399829	0.662519
B	1.138645	-1.032112	1.425540
F	0.252888	-0.101422	2.059767
F	0.125122	-1.652483	0.487728
F	1.516750	-2.013645	2.286439
H	2.868649	-2.358391	0.306882
Mg	-1.363513	-0.248958	0.691505
Br	-2.760070	1.410669	1.910288
O	-0.833459	0.679117	-1.077048
C	-1.150086	2.063796	-1.318566
H	-0.957279	2.597848	-0.369981
H	-0.423857	2.448552	-2.060195
C	-2.578100	2.253911	-1.765422
H	-2.776572	3.328720	-1.929655
H	-2.794328	1.718272	-2.707096
H	-3.277420	1.900835	-0.984621
C	-0.087140	0.027552	-2.116939
H	0.797162	0.656202	-2.339761
H	0.295811	-0.903448	-1.666276
C	-0.901269	-0.250950	-3.354483
H	-0.303965	-0.861280	-4.055916
H	-1.819529	-0.817191	-3.108355

H	-1.189643	0.674524	-3.884996
C	4.537199	-1.245015	1.058142
H	4.927091	-0.207456	0.995822
H	4.227247	-1.403823	2.109970
C	5.617746	-2.238490	0.672100
H	6.465100	-2.206393	1.380509
H	5.225847	-3.274965	0.669640
H	6.025152	-2.034185	-0.336101
O	-2.731718	-1.636385	-0.016496
C	-4.110477	-1.270365	-0.190982
H	-4.179848	-0.220965	0.146725
H	-4.716502	-1.877973	0.509946
C	-4.590796	-1.421936	-1.611187
H	-5.626187	-1.044769	-1.689311
H	-3.961926	-0.836744	-2.308318
H	-4.598754	-2.476327	-1.942542
C	-2.443114	-3.042111	-0.131785
H	-1.779415	-3.301584	0.710978
H	-3.390382	-3.594432	0.014953
C	-1.793255	-3.387491	-1.447387
H	-0.841934	-2.838791	-1.569328
H	-1.562848	-4.467797	-1.476196
H	-2.448125	-3.155016	-2.306285

TS-(1a·BF_3-IX)·$2Et_2O$

C	4.422906	1.139177	-0.714511
C	3.591722	0.106321	-1.119890
C	2.946060	-0.693221	-0.159776

C	3.155024	-0.429603	1.214869
C	3.985765	0.637489	1.601163
C	4.621867	1.413211	0.647637
H	4.933422	1.744753	-1.472078
H	3.442046	-0.103295	-2.181419
C	2.431082	-1.239871	2.156530
H	4.123615	0.836367	2.671114
H	5.278928	2.234754	0.953364
C	2.069072	-2.542312	1.729195
C	1.832177	-2.707407	0.386502
H	2.528561	-1.014092	3.224830
H	1.821326	-3.338144	2.437327
N	2.087594	-1.731647	-0.524819
B	1.073208	-1.531015	-1.715917
F	0.267753	-0.383414	-1.329765
F	1.693047	-1.238129	-2.900873
F	0.265817	-2.633768	-1.810500
H	1.343094	-3.604808	-0.007861
C	0.335668	-0.088999	1.969937
H	0.885971	0.849064	2.132942
H	0.657260	-0.688336	1.114443
C	-0.388188	-0.732308	3.121324
H	-1.491106	-0.585061	3.123090
H	-0.224395	-1.831767	3.144915
H	-0.029494	-0.339647	4.093614
Mg	-1.058521	0.479339	0.242890
Br	-3.118432	1.651102	1.166593
O	-2.138006	-1.248571	-0.225242
O	-0.311019	2.220855	-0.628541

C	1.071619	2.563656	-0.518374
H	1.592027	1.655769	-0.165029
H	1.470138	2.780783	-1.530255
C	-1.060639	2.974702	-1.588417
H	-2.068832	3.106906	-1.155562
H	-0.603641	3.978123	-1.679609
C	-1.108913	2.259201	-2.915724
H	-1.622577	1.282879	-2.819654
H	-1.658690	2.861937	-3.660623
H	-0.092029	2.066953	-3.305863
C	1.279915	3.709961	0.438945
H	2.356438	3.942817	0.528889
H	0.761218	4.626435	0.102206
H	0.894178	3.445936	1.441792
C	-1.946001	-2.501175	0.431260
H	-1.713160	-3.275479	-0.324015
H	-1.030316	-2.368462	1.036235
C	-3.114676	-2.885653	1.305435
H	-2.845335	-3.757632	1.927788
H	-3.389306	-2.050319	1.977160
H	-4.006982	-3.165324	0.715718
C	-3.224401	-1.163190	-1.150495
H	-4.180907	-1.267253	-0.600827
H	-3.196901	-0.125083	-1.527685
C	-3.109684	-2.146088	-2.288369
H	-3.871365	-1.914975	-3.053837
H	-2.108839	-2.082095	-2.752372
H	-3.275770	-3.189558	-1.963808

IX·Et_2O

C	3.127318	2.088594	1.183433
C	1.816014	2.036869	0.724927
C	1.447203	1.168593	-0.316440
C	2.425363	0.334172	-0.888386
C	3.741892	0.423858	-0.426367
C	4.106099	1.286340	0.601065
H	3.382861	2.775830	1.997915
H	1.071855	2.692284	1.185504
C	2.087804	-0.699080	-1.936836
H	4.499573	-0.220346	-0.892747
H	5.144731	1.330518	0.946837
C	0.773941	-0.369906	-2.573477
C	-0.120168	0.437782	-1.995513
H	2.883611	-0.681312	-2.714078
H	0.514503	-0.823536	-3.537305
N	0.081016	1.102874	-0.757607
B	-0.871519	2.313933	-0.473692
F	-1.306136	2.044133	0.940706
F	-0.284494	3.535685	-0.512381
F	-2.002728	2.239229	-1.235264
H	-1.094606	0.633759	-2.454119
C	2.103491	-2.115239	-1.329624
H	3.093587	-2.277239	-0.857834
H	1.367513	-2.152781	-0.498344
C	1.833624	-3.217152	-2.337338
H	1.943914	-4.215947	-1.877115
H	0.810587	-3.159821	-2.755359

H	2.541554	-3.161031	-3.187659
Mg	-0.895800	0.078182	1.011830
Br	0.407864	-1.441120	2.412734
O	-2.651440	-0.604200	0.165864
C	-2.899748	-1.842950	-0.522287
H	-3.733170	-2.352694	0.001833
H	-3.237029	-1.604596	-1.548506
C	-1.672136	-2.708796	-0.562173
H	-1.910709	-3.648456	-1.090753
H	-0.851299	-2.217053	-1.119952
H	-1.312425	-2.967173	0.451273
C	-3.857818	0.130683	0.464596
H	-4.435068	-0.461778	1.202495
H	-3.524030	1.058598	0.958549
C	-4.683469	0.455837	-0.754053
H	-5.479518	1.165239	-0.466913
H	-4.060078	0.936399	-1.528046
H	-5.176216	-0.433106	-1.185253

IIa-*proR*$_{3-4}$

C	-3.749576	1.480906	-0.386426
C	-4.241072	-0.192039	1.709189
C	-5.197256	1.019228	-0.204584
H	-3.278605	0.756394	-1.078028
C	-5.101208	-0.349665	0.454455
H	-4.876484	0.271147	2.493340
H	-5.755788	1.722587	0.447941
H	-5.729881	0.984607	-1.174201

H	-6.094057	-0.779048	0.692575
H	-4.614474	-1.042736	-0.262097
C	0.697834	-2.199081	1.421722
C	0.025830	-3.154808	-1.071093
C	0.907973	-3.694595	1.140774
H	-0.246160	-2.096531	1.996519
C	-0.135637	-4.106710	0.112343
H	0.992790	-3.374454	-1.568634
H	1.924323	-3.867596	0.731932
H	0.831099	-4.274936	2.079820
H	-0.024051	-5.160725	-0.206060
H	-1.141736	-4.006437	0.568380
P	0.321555	-1.476069	-0.272308
P	-2.997324	1.224874	1.331217
Cu	1.983879	-0.394065	-1.373658
C	2.819187	2.388853	0.184252
C	0.872965	2.310353	-1.122378
C	3.472707	2.727000	1.387835
C	3.568901	1.772715	-0.860171
C	1.533225	1.644227	-2.178701
H	-0.187172	2.580467	-1.213392
C	4.819909	2.469208	1.532682
H	2.912255	3.187755	2.202340
C	4.946516	1.519402	-0.677968
C	2.904108	1.411318	-2.072653
H	0.985585	1.451218	-3.107295
C	5.566072	1.867085	0.500593
H	5.314728	2.735456	2.473250
H	5.498398	1.032363	-1.489926

H	3.494637	1.067891	-2.929093
H	6.634364	1.671773	0.640944
N	1.477516	2.679821	-0.010376
B	0.603586	3.485849	1.142612
F	0.603838	2.687809	2.260637
F	-0.654774	3.644347	0.620485
F	1.240808	4.681580	1.347066
Br	3.595442	-1.920635	-2.199005
C	-3.633913	-1.431958	2.305407
C	-3.835382	-2.708988	1.765386
C	-2.827125	-1.326942	3.450597
C	-3.227619	-3.833649	2.327746
H	-4.481179	-2.839469	0.888652
C	-2.213561	-2.444888	4.010009
H	-2.673699	-0.339448	3.909066
C	-2.404498	-3.707548	3.444658
H	-3.403922	-4.821083	1.883165
H	-1.582839	-2.330291	4.899975
H	-1.923229	-4.589725	3.882451
C	-3.514169	2.857080	-0.931073
C	-2.736722	3.030792	-2.082528
C	-4.030350	3.997513	-0.301442
C	-2.470767	4.303898	-2.588326
H	-2.335014	2.144732	-2.596266
C	-3.773657	5.269346	-0.806299
H	-4.630494	3.887283	0.611611
C	-2.988763	5.428894	-1.950133
H	-1.857579	4.415817	-3.490646
H	-4.184425	6.149119	-0.296972

H	-2.782800	6.431372	-2.342729
C	1.798608	-1.492354	2.160400
C	1.518778	-0.765736	3.322947
C	3.124357	-1.537148	1.703404
C	2.532814	-0.110902	4.022470
H	0.485830	-0.719944	3.694388
C	4.139012	-0.888893	2.403519
H	3.371136	-2.081485	0.780990
C	3.847773	-0.175638	3.567528
H	2.290094	0.450393	4.932201
H	5.169753	-0.940362	2.032191
H	4.648275	0.333910	4.117174
C	-1.052764	-3.061426	-2.109395
C	-2.376440	-3.443462	-1.864201
C	-0.747517	-2.470388	-3.345176
C	-3.372107	-3.215895	-2.815629
H	-2.645452	-3.922058	-0.914391
C	-1.739602	-2.240170	-4.294424
H	0.292846	-2.183703	-3.556337
C	-3.060638	-2.605928	-4.029273
H	-4.403564	-3.521278	-2.602573
H	-1.479570	-1.774845	-5.252398
H	-3.844177	-2.424372	-4.773735
C	-1.366512	-0.758004	-0.086535
H	-2.061287	-1.573609	0.195322
H	-1.664494	-0.408050	-1.095604
C	-1.389562	0.366545	0.930494
H	-0.993702	0.028043	1.908507
H	-0.717040	1.190996	0.631148

II-*proR*$_{3\text{-}4}$

C	3.256710	2.111440	0.009200
C	3.972726	0.398742	-1.980197
C	4.752642	2.022392	-0.295454
H	3.057508	1.340111	0.776996
C	4.956666	0.608616	-0.826805
H	4.403762	0.880365	-2.882738
H	5.049167	2.771150	-1.059644
H	5.359241	2.222719	0.608483
H	6.000645	0.416140	-1.142330
H	4.734753	-0.097828	-0.001262
C	-0.378127	-2.589261	-0.982992
C	0.661333	-3.003227	1.536467
C	-0.213667	-4.039066	-0.503957
H	0.476934	-2.360563	-1.652878
C	0.956236	-4.057721	0.470941
H	-0.176887	-3.361752	2.168705
H	-1.135275	-4.385511	0.006428
H	-0.051032	-4.711959	-1.367325
H	1.114972	-5.054759	0.924439
H	1.880033	-3.801351	-0.086545
P	-0.078529	-1.566364	0.566674
P	2.468392	1.543030	-1.611956
Cu	-1.924330	-0.764023	1.642709
C	-3.442020	1.610337	-0.169548
C	-1.414347	2.045959	0.935521
C	-4.256066	1.706671	-1.314377

C	-3.960477	0.978909	0.994108
C	-1.824151	1.386811	2.101531
H	-0.433420	2.535270	0.893840
C	-5.547825	1.211880	-1.295272
H	-3.866861	2.180853	-2.217103
C	-5.283312	0.497078	0.986646
C	-3.116841	0.813269	2.155952
H	-1.174615	1.428156	2.984166
C	-6.073968	0.612837	-0.140480
H	-6.165953	1.296826	-2.196234
H	-5.669541	0.023874	1.897850
H	-3.585921	0.553610	3.112647
H	-7.102740	0.236762	-0.134441
N	-2.162647	2.165569	-0.152305
B	-1.557900	2.965012	-1.433832
F	-1.452015	2.064206	-2.473371
F	-0.320843	3.441268	-1.052870
F	-2.426708	3.990289	-1.732293
C	-3.107161	-2.165313	2.436440
H	-4.131643	-2.010612	2.034890
H	-2.753707	-3.143966	2.044901
C	-3.106389	-2.187599	3.953771
H	-3.449957	-1.228916	4.394662
H	-3.764355	-2.975635	4.383423
H	-2.092925	-2.374873	4.364328
C	3.619489	-1.013263	-2.358180
C	4.122734	-2.133295	-1.683572
C	2.739716	-1.238533	-3.430427
C	3.736607	-3.426251	-2.044497

H	4.835144	-2.005763	-0.859695
C	2.345221	-2.525142	-3.787574
H	2.350487	-0.377574	-3.992731
C	2.836713	-3.629824	-3.088316
H	4.149367	-4.284218	-1.499123
H	1.651041	-2.668178	-4.624590
H	2.529611	-4.644449	-3.367394
C	2.690501	3.405587	0.506940
C	1.932478	3.424164	1.684646
C	2.859518	4.607781	-0.192495
C	1.347862	4.603395	2.147375
H	1.799152	2.490177	2.251701
C	2.285253	5.788631	0.270274
H	3.437758	4.614495	-1.126022
C	1.521893	5.790961	1.439706
H	0.753815	4.592731	3.069440
H	2.426941	6.718773	-0.292656
H	1.064343	6.720317	1.798123
C	-1.658343	-2.237866	-1.688067
C	-1.631968	-1.582271	-2.923800
C	-2.905679	-2.524274	-1.113920
C	-2.813959	-1.223739	-3.572480
H	-0.665131	-1.348632	-3.390312
C	-4.087359	-2.168217	-1.758938
H	-2.958662	-3.032770	-0.143142
C	-4.046045	-1.515357	-2.991795
H	-2.767443	-0.709228	-4.539272
H	-5.051536	-2.399481	-1.289821
H	-4.976743	-1.230966	-3.497006

C	1.766531	-2.507523	2.423128
C	3.120325	-2.668749	2.110113
C	1.431292	-1.746746	3.554148
C	4.109410	-2.063968	2.887802
H	3.418077	-3.265608	1.239342
C	2.415121	-1.139718	4.329451
H	0.370709	-1.619717	3.817216
C	3.762085	-1.290051	3.993175
H	5.164563	-2.200943	2.622505
H	2.129528	-0.545450	5.205196
H	4.539458	-0.811298	4.599356
C	1.391478	-0.536264	0.139111
H	2.242937	-1.208672	-0.086732
H	1.646568	0.012730	1.067481
C	1.113006	0.409950	-1.011344
H	0.776756	-0.141332	-1.911569
H	0.277791	1.094674	-0.774521

X

C	1.700844	1.723807	2.314339
C	-0.715338	0.699387	3.136508
C	1.559178	1.342460	3.788659
H	1.537470	2.820439	2.229154
C	0.092444	1.507839	4.149471
H	-0.558182	-0.380349	3.338040
H	1.867858	0.284165	3.928662
H	2.211821	1.959044	4.435107
H	-0.128441	1.187305	5.185855

H	-0.163070	2.584230	4.083784
C	-3.171796	0.166474	-1.957749
C	-1.012507	1.525908	-2.966324
C	-3.172370	0.505861	-3.453728
H	-3.846728	0.880510	-1.444185
C	-2.365030	1.780300	-3.626125
H	-0.482682	0.763360	-3.574380
H	-2.698726	-0.315347	-4.029089
H	-4.208074	0.602502	-3.830390
H	-2.244554	2.070013	-4.688204
H	-2.897660	2.612929	-3.124634
P	-1.430528	0.604549	-1.353171
P	0.190043	0.937242	1.491023
Cu	-0.002401	-0.756756	-0.090817
Br	-0.888203	-2.761882	1.019975
C	2.783203	-1.996392	-0.467674
C	1.725734	-1.400850	-2.433111
C	2.781636	-2.080924	0.946614
C	3.915832	-2.480733	-1.187334
C	2.804327	-1.843581	-3.227002
H	0.830923	-0.983463	-2.917885
C	3.858836	-2.619773	1.609298
H	1.894778	-1.722057	1.482478
C	5.010004	-3.033782	-0.474953
C	3.900199	-2.383454	-2.598100
H	2.748489	-1.757504	-4.316370
C	4.982963	-3.101664	0.897238
H	3.847086	-2.679364	2.703850
H	5.872427	-3.403944	-1.042790

H	4.763301	-2.746617	-3.169761
H	5.829550	-3.530686	1.444878
N	1.705895	-1.460839	-1.117198
C	-3.602047	-1.229817	-1.615752
C	-2.944555	-2.345165	-2.150214
C	-4.680027	-1.445602	-0.751562
C	-3.359958	-3.636035	-1.837937
H	-2.075349	-2.201637	-2.808155
C	-5.093463	-2.737699	-0.426960
H	-5.206528	-0.579664	-0.327995
C	-4.437854	-3.838233	-0.974906
H	-2.827920	-4.495571	-2.262231
H	-5.939593	-2.883206	0.255799
H	-4.760648	-4.855358	-0.724111
C	-0.086008	2.689183	-2.769750
C	-0.543796	4.008043	-2.648596
C	1.294831	2.460563	-2.669500
C	0.345382	5.056661	-2.412459
H	-1.612209	4.233011	-2.745726
C	2.185465	3.505552	-2.436149
H	1.676976	1.434479	-2.777264
C	1.712498	4.810628	-2.298795
H	-0.038223	6.079620	-2.321519
H	3.259819	3.299694	-2.359648
H	2.410348	5.635255	-2.114312
C	3.013176	1.381911	1.656557
C	3.109506	1.313868	0.260629
C	4.171479	1.142564	2.405810
C	4.312908	1.007609	-0.368595

H	2.213150	1.478119	-0.352595
C	5.382083	0.842253	1.780184
H	4.137732	1.188688	3.500455
C	5.458692	0.770400	0.390843
H	4.352452	0.940871	-1.464374
H	6.274590	0.657386	2.389933
H	6.407636	0.523431	-0.099789
C	-2.196337	0.945620	3.059519
C	-2.773407	2.175583	3.403032
C	-3.041088	-0.075162	2.594686
C	-4.147174	2.385132	3.275475
H	-2.150149	2.994343	3.781741
C	-4.413831	0.130670	2.478085
H	-2.603946	-1.042003	2.303044
C	-4.974928	1.364196	2.812567
H	-4.573420	3.357254	3.550609
H	-5.053002	-0.688611	2.126535
H	-6.055460	1.525789	2.721756
C	-0.635745	2.405748	0.698566
H	0.146292	2.898730	0.082937
H	-0.948711	3.143074	1.465404
C	-1.819927	1.993283	-0.168094
H	-2.638938	1.602956	0.469659
H	-2.231945	2.863131	-0.717351

XI

C	1.447519	0.565313	2.995279
C	-0.858090	-0.933801	2.981192

C	1.299724	-0.528328	4.053655
H	1.203024	1.540598	3.468756
C	-0.188600	-0.679138	4.330603
H	-0.537892	-1.929583	2.622851
H	1.694381	-1.484556	3.655056
H	1.873682	-0.286736	4.968377
H	-0.404518	-1.500112	5.041134
H	-0.566395	0.255626	4.792348
C	-3.230325	1.150769	-1.695968
C	-1.365044	3.163338	-1.609780
C	-3.382656	2.319008	-2.683209
H	-3.997543	1.259379	-0.903087
C	-2.777960	3.552999	-2.035361
H	-0.777419	2.979462	-2.533347
H	-2.838972	2.088393	-3.621841
H	-4.444768	2.458973	-2.958023
H	-2.766053	4.427745	-2.714263
H	-3.390063	3.837703	-1.156272
P	-1.571907	1.442050	-0.837095
P	0.026180	0.241749	1.793163
Cu	0.145671	-0.112337	-0.491989
Br	-0.478083	-2.591115	-0.815730
C	2.922718	-0.659651	-1.613963
C	1.689005	0.869851	-2.828006
C	3.034549	-1.531157	-0.507847
C	4.011735	-0.557398	-2.528748
C	2.721073	1.051987	-3.771046
H	0.743416	1.416920	-2.949803
C	4.168575	-2.286304	-0.328911

H	2.198295	-1.589473	0.194134
C	5.172671	-1.343527	-2.315263
C	3.882949	0.334063	-3.618613
H	2.577191	1.746520	-4.604002
C	5.247955	-2.196629	-1.239483
H	4.231650	-2.961898	0.532478
H	6.002072	-1.258010	-3.027897
H	4.711096	0.434628	-4.330955
H	6.144264	-2.807223	-1.083216
N	1.773509	0.062678	-1.788719
C	-3.355383	-0.214844	-2.308180
C	-2.449858	-0.655825	-3.282743
C	-4.386043	-1.076292	-1.920890
C	-2.575458	-1.917859	-3.855959
H	-1.618629	-0.004133	-3.588710
C	-4.512645	-2.344912	-2.487767
H	-5.103507	-0.743462	-1.158972
C	-3.608815	-2.768387	-3.459622
H	-1.853097	-2.246122	-4.612405
H	-5.326541	-3.005921	-2.166643
H	-3.704187	-3.764902	-3.905988
C	-0.585880	4.105739	-0.740174
C	-1.199953	5.071295	0.067192
C	0.813020	4.000934	-0.695819
C	-0.442592	5.887986	0.907859
H	-2.288350	5.200094	0.043003
C	1.571577	4.816050	0.140069
H	1.315684	3.257220	-1.331649
C	0.944157	5.760562	0.953518

H	-0.946271	6.635871	1.531288
H	2.663389	4.713931	0.157786
H	1.537673	6.402875	1.613893
C	2.782281	0.689045	2.309688
C	2.908585	1.531080	1.195668
C	3.918086	-0.002279	2.743425
C	4.119196	1.668106	0.524281
H	2.028803	2.081086	0.832670
C	5.138170	0.139867	2.078965
H	3.860363	-0.665249	3.614411
C	5.244318	0.970179	0.965982
H	4.180824	2.319184	-0.358696
H	6.014940	-0.413730	2.435970
H	6.200178	1.068965	0.438003
C	-2.354881	-0.867155	2.894344
C	-3.132021	-0.083754	3.756685
C	-3.008195	-1.589208	1.882791
C	-4.516269	-0.002572	3.597128
H	-2.658962	0.475918	4.572567
C	-4.389400	-1.511204	1.724590
H	-2.413449	-2.221700	1.209281
C	-5.150888	-0.709853	2.577478
H	-5.104381	0.617610	4.283981
H	-4.875718	-2.092315	0.931573
H	-6.238759	-0.649012	2.456686
C	-0.960849	1.818119	1.902123
H	-0.248718	2.644790	1.695036
H	-1.336846	1.975371	2.932948
C	-2.111815	1.839251	0.901603

H	-2.858533	1.062979	1.163070
H	-2.641869	2.811687	0.929994
B	0.442980	-3.805705	0.785590
F	1.185189	-2.943343	1.548680
F	1.193822	-4.720547	0.127835
F	-0.616797	-4.323061	1.458835

L1

C	0.113218	0.752128	0.817374
H	0.668116	1.077342	-0.086644
H	0.732942	1.049085	1.687866
C	-0.113219	-0.752125	0.817377
H	-0.732941	-1.049078	1.687871
H	-0.668119	-1.077343	-0.086639
C	-2.142644	1.380796	-0.830573
C	-0.990614	3.488527	0.581000
C	-1.688243	2.593405	-1.643497
H	-1.623322	0.472943	-1.193474
C	-1.683613	3.824761	-0.743731
H	-1.449304	4.078642	1.396608
H	-0.664401	2.397447	-2.015343
H	-2.313727	2.743539	-2.544867
H	-1.213506	4.699211	-1.234892
H	-2.728715	4.119464	-0.524233
C	2.142644	-1.380797	-0.830569
C	0.990615	-3.488525	0.581009
C	1.688241	-2.593408	-1.643489
H	1.623322	-0.472944	-1.193473

C	1.683616	-3.824761	-0.743721
H	1.449304	-4.078638	1.396618
H	0.664398	-2.397451	-2.015332
H	2.313722	-2.743542	-2.544862
H	1.213514	-4.699215	-1.234879
H	2.728720	-4.119458	-0.524221
P	-1.507714	1.671371	0.946419
P	1.507713	-1.671368	0.946423
C	3.616759	-1.066086	-0.814272
C	4.024323	0.190646	-0.337867
C	4.605931	-1.959602	-1.237210
C	5.368422	0.544522	-0.291197
H	3.262750	0.909082	0.002746
C	5.957698	-1.610009	-1.186878
H	4.330361	-2.948687	-1.622384
C	6.345864	-0.358709	-0.715704
H	5.656585	1.535840	0.079520
H	6.713913	-2.328558	-1.524875
H	7.406642	-0.084874	-0.679259
C	-0.495491	-3.703889	0.654846
C	-1.102957	-3.796034	1.917066
C	-1.322484	-3.771373	-0.473635
C	-2.482185	-3.927327	2.050702
H	-0.471055	-3.751880	2.815404
C	-2.705889	-3.906992	-0.344980
H	-0.889897	-3.720342	-1.479623
C	-3.293890	-3.980137	0.916223
H	-2.928099	-3.994262	3.050060
H	-3.329935	-3.955157	-1.245692

H	-4.380299	-4.087447	1.016679
C	0.495491	3.703891	0.654841
C	1.102953	3.796052	1.917061
C	1.322489	3.771358	-0.473639
C	2.482181	3.927343	2.050701
H	0.471048	3.751912	2.815398
C	2.705894	3.906975	-0.344981
H	0.889904	3.720312	-1.479627
C	3.293890	3.980136	0.916223
H	2.928092	3.994292	3.050058
H	3.329943	3.955125	-1.245691
H	4.380300	4.087444	1.016682
C	-3.616759	1.066084	-0.814275
C	-4.024322	-0.190652	-0.337880
C	-4.605933	1.959605	-1.237199
C	-5.368421	-0.544528	-0.291207
H	-3.262748	-0.909092	0.002723
C	-5.957700	1.610011	-1.186864
H	-4.330365	2.948693	-1.622365
C	-6.345864	0.358708	-0.715702
H	-5.656582	-1.535850	0.079501
H	-6.713916	2.328565	-1.524852
H	-7.406642	0.084872	-0.679254

XII

C	-0.289933	0.855721	0.352409
H	0.008485	1.274939	-0.630284
H	0.446699	1.217238	1.096094

C	-0.300879	-0.666829	0.326532
H	-0.751846	-1.073153	1.255338
H	-0.889706	-1.073579	-0.520517
C	-2.900890	1.232156	-0.767137
C	-1.779108	3.394607	0.588601
C	-2.834231	2.566684	-1.512398
H	-2.329237	0.464358	-1.323602
C	-2.813368	3.705070	-0.497022
H	-2.097611	3.852192	1.544397
H	-1.902749	2.584532	-2.109925
H	-3.663176	2.674572	-2.238354
H	-2.621053	4.686794	-0.971733
H	-3.808589	3.785659	-0.016906
C	2.148126	-0.893858	-1.382116
C	1.325206	-3.192336	-0.002881
C	2.031175	-2.192831	-2.190672
H	1.505162	-0.108931	-1.824564
C	2.191834	-3.391796	-1.254949
H	1.825588	-3.632756	0.880265
H	1.031326	-2.217120	-2.664911
H	2.763035	-2.214550	-3.019125
H	1.950399	-4.346339	-1.758129
H	3.247401	-3.468445	-0.930459
P	-1.962786	1.504734	0.873523
P	1.397415	-1.340980	0.265952
C	3.527641	-0.310386	-1.177831
C	3.629270	0.984688	-0.650387
C	4.704381	-1.009547	-1.458809
C	4.870103	1.557001	-0.392965

H	2.716039	1.556163	-0.426111
C	5.951142	-0.435714	-1.203909
H	4.665213	-2.019599	-1.882839
C	6.039546	0.845596	-0.666256
H	4.924219	2.568603	0.026464
H	6.862202	-1.002380	-1.428372
H	7.018958	1.292471	-0.460842
C	-0.095995	-3.694686	-0.036043
C	-0.782147	-3.830185	1.179889
C	-0.782138	-3.977605	-1.221664
C	-2.118707	-4.217109	1.210906
H	-0.252130	-3.609438	2.117234
C	-2.122254	-4.368233	-1.193219
H	-0.274981	-3.899183	-2.190477
C	-2.796966	-4.484300	0.020216
H	-2.634563	-4.314131	2.173104
H	-2.641383	-4.585273	-2.133870
H	-3.849739	-4.789355	0.040040
C	-0.360490	3.828190	0.336270
C	0.541840	3.839408	1.412259
C	0.124781	4.191036	-0.926065
C	1.879512	4.179101	1.235088
H	0.180102	3.561557	2.412489
C	1.464042	4.541972	-1.107637
H	-0.546394	4.214008	-1.792481
C	2.348160	4.534817	-0.031345
H	2.561016	4.172085	2.093903
H	1.816148	4.828194	-2.105778
H	3.398070	4.815445	-0.175867

C	-4.265752	0.653574	-0.493305
C	-4.355169	-0.695563	-0.114628
C	-5.450815	1.391484	-0.576266
C	-5.581251	-1.287768	0.168698
H	-3.435175	-1.295489	-0.041403
C	-6.684228	0.801570	-0.289683
H	-5.426501	2.446522	-0.874441
C	-6.756492	-0.537998	0.083454
H	-5.619431	-2.345262	0.457227
H	-7.599130	1.401502	-0.362584
H	-7.725391	-0.999360	0.306701
B	2.408293	-0.975369	2.025379
F	1.595115	-1.627064	2.933637
F	3.631147	-1.577144	1.883415
F	2.479530	0.373369	2.256114

XIII

C	0.066029	-0.760918	-0.313254
H	-0.246465	-1.216632	-1.273661
H	-0.562965	-1.211896	0.479687
C	-0.066100	0.760968	-0.313025
H	0.562866	1.211727	0.480059
H	0.246471	1.216952	-1.273285
C	2.842481	-0.928854	-1.397540
C	1.897478	-3.118840	0.082149
C	2.999157	-2.321084	-2.025617
H	2.257394	-0.269640	-2.068259

C	3.030862	-3.379185	-0.921135
H	2.222085	-3.395412	1.103436
H	2.133830	-2.500341	-2.692208
H	3.896901	-2.369184	-2.669158
H	2.974671	-4.405288	-1.328639
H	3.990945	-3.313874	-0.374314
C	-2.842472	0.928993	-1.397368
C	-1.897399	3.118897	0.082400
C	-2.999151	2.321265	-2.025357
H	-2.257317	0.269835	-2.068090
C	-3.030862	3.379276	-0.920783
H	-2.221875	3.395508	1.103721
H	-2.133845	2.500579	-2.691953
H	-3.896902	2.369401	-2.668882
H	-2.974770	4.405422	-1.328193
H	-3.990904	3.313835	-0.373902
P	1.778141	-1.252459	0.097207
P	-1.778198	1.252515	0.097440
C	-4.095173	0.189126	-0.987189
C	-3.980596	-1.163821	-0.638191
C	-5.351910	0.794150	-0.906083
C	-5.085985	-1.889204	-0.207476
H	-2.998345	-1.656740	-0.692794
C	-6.463860	0.067775	-0.476185
H	-5.482879	1.847471	-1.179775
C	-6.335591	-1.272785	-0.122493
H	-4.970340	-2.945128	0.064163
H	-7.440800	0.561181	-0.417101
H	-7.208869	-1.839755	0.219469

C	-0.554066	3.755173	-0.172909
C	0.384528	3.766482	0.869933
C	-0.175120	4.273961	-1.415010
C	1.670779	4.259455	0.673275
H	0.102344	3.355009	1.849402
C	1.113002	4.774973	-1.613139
H	-0.885522	4.295533	-2.249974
C	2.041699	4.764085	-0.574480
H	2.389313	4.244129	1.501087
H	1.390233	5.178291	-2.593928
H	3.053365	5.154707	-0.734707
C	0.554155	-3.755203	-0.172992
C	-0.384270	-3.766689	0.869998
C	0.175041	-4.273891	-1.415086
C	-1.670516	-4.259741	0.673503
H	-0.101965	-3.355308	1.849468
C	-1.113076	-4.774980	-1.613054
H	0.885310	-4.295315	-2.250170
C	-2.041604	-4.764272	-0.574238
H	-2.388915	-4.244564	1.501434
H	-1.390438	-5.178219	-2.593838
H	-3.053267	-5.154959	-0.734320
C	4.095153	-0.189017	-0.987222
C	3.980549	1.163920	-0.638202
C	5.351876	-0.794052	-0.905998
C	5.085882	1.889280	-0.207307
H	2.998316	1.656856	-0.692966
C	6.463776	-0.067701	-0.475926
H	5.482864	-1.847365	-1.179711

C	6.335470	1.272842	-0.122181
H	4.970205	2.945197	0.064348
H	7.440707	-0.561114	-0.416737
H	7.208708	1.839786	0.219924
B	-2.307853	0.554851	1.974283
F	-1.336735	1.146695	2.753446
F	-3.561352	1.054969	2.202456
F	-2.245739	-0.814576	1.998461
B	2.307844	-0.554905	1.974260
F	1.336686	-1.146840	2.753288
F	3.561320	-1.055141	2.202304
F	2.245795	0.814494	1.998606

L1-CuBr BF_3

C	-3.095730	-1.587256	0.754479
C	-0.772424	-2.764736	1.623802
C	-3.180174	-2.554277	1.945284
H	-3.424165	-2.137310	-0.151569
C	-2.061824	-3.568886	1.777199
H	-0.557435	-2.282105	2.598591
H	-3.042596	-1.987849	2.889761
H	-4.181993	-3.021228	1.992417
H	-1.991993	-4.273647	2.627733
H	-2.260412	-4.174351	0.870204
C	2.705698	0.162736	-2.220907
C	0.267634	1.224205	-2.857648
C	2.620327	1.097276	-3.433766
H	2.817018	-0.877850	-2.594129

C	1.220987	0.986009	-4.022167
H	0.422478	2.263169	-2.498176
H	2.787666	2.142956	-3.106484
H	3.407271	0.860903	-4.174266
H	1.051816	1.712123	-4.840379
H	1.076328	-0.025015	-4.453655
P	0.975477	0.191523	-1.457481
P	-1.248928	-1.306367	0.521163
Cu	-0.014247	0.612076	0.583039
Br	-0.196785	2.711922	1.750669
C	-1.204599	1.003491	-3.029536
C	-2.080682	1.544909	-2.075352
C	-1.740263	0.233079	-4.066524
C	-3.448978	1.304655	-2.141569
H	-1.675842	2.165689	-1.261663
C	-3.114214	-0.009634	-4.134639
H	-1.082500	-0.188987	-4.835872
C	-3.971048	0.516860	-3.170223
H	-4.115599	1.733024	-1.383208
H	-3.516060	-0.616666	-4.954442
H	-5.049357	0.323182	-3.221154
C	3.813564	0.430327	-1.234561
C	3.804745	-0.219158	0.005865
C	4.877338	1.292875	-1.519288
C	4.816555	-0.014597	0.937159
H	2.967975	-0.884450	0.257819
C	5.897207	1.500274	-0.588559
H	4.924372	1.814228	-2.482207
C	5.871879	0.849347	0.642619

H	4.770626	-0.522253	1.908953
H	6.719836	2.182914	-0.832299
H	6.669578	1.019363	1.374924
C	-3.945905	-0.356475	0.902263
C	-5.202127	-0.305648	0.287799
C	-3.541639	0.730405	1.686844
C	-6.030767	0.805043	0.440637
H	-5.531213	-1.151739	-0.330770
C	-4.361033	1.848286	1.832346
H	-2.557559	0.715371	2.175252
C	-5.609052	1.889914	1.209065
H	-7.010359	0.826458	-0.051475
H	-4.018182	2.695113	2.438862
H	-6.253755	2.768999	1.323705
C	0.470951	-3.468939	1.165819
C	0.435925	-4.619110	0.367544
C	1.722893	-2.940227	1.513996
C	1.615749	-5.214692	-0.079509
H	-0.523863	-5.069848	0.088531
C	2.901874	-3.535308	1.070892
H	1.767502	-2.038022	2.141494
C	2.852865	-4.674254	0.266400
H	1.564152	-6.115505	-0.702065
H	3.869573	-3.105131	1.355889
H	3.779206	-5.144469	-0.082521
C	0.388816	-1.549129	-1.797760
H	0.415230	-1.760109	-2.885770
H	1.160059	-2.200548	-1.334080
C	-0.988796	-1.881626	-1.228807

H	-1.188193	-2.969072	-1.306994
H	-1.780063	-1.371798	-1.815026
B	1.943801	2.080347	2.318719
F	2.121718	2.614156	3.537245
F	1.824604	0.720142	2.305766
F	2.682493	2.600532	1.329044

Cu_2Br_2·$(SMe_2)_2$

Cu	-1.186680	-0.074589	-0.272952
Br	0.396508	-1.889383	-0.118612
Br	-0.441304	2.229344	-0.032088
Cu	1.199109	0.477401	0.033810
S	-3.428659	-0.500968	-0.423254
S	3.492204	0.497582	0.193635
C	-4.073822	0.768413	0.700223
H	-5.145608	0.593623	0.898316
H	-3.502313	0.773412	1.644832
H	-3.941985	1.739061	0.193751
C	-3.542418	-1.963018	0.644505
H	-3.012562	-1.786514	1.596920
H	-4.599988	-2.217280	0.832843
H	-3.050151	-2.789846	0.105903
C	3.905610	-0.548550	-1.230363
H	3.751167	0.056302	-2.139242
H	4.964539	-0.855035	-1.169768
H	3.243817	-1.432627	-1.255880
C	3.734396	-0.717601	1.518986
H	4.795262	-1.021725	1.552747

H	3.464243	-0.227428	2.468966
H	3.081697	-1.593412	1.354043

$L1_2Cu_2Br_2$

Cu	1.616502	-0.331108	-0.047830
C	3.826743	1.885101	0.938480
H	4.808780	2.022463	1.432269
H	3.675057	2.771856	0.291154
C	2.708330	1.793608	1.972366
H	2.832593	0.899739	2.615354
H	2.707713	2.682934	2.634576
C	5.225072	-0.612414	0.603415
C	4.844847	0.847027	-1.697427
C	6.486056	0.041215	0.012293
H	5.180415	-0.453471	1.699151
C	6.240288	0.237622	-1.479538
H	4.328441	0.327638	-2.528446
H	6.663701	1.017713	0.506278
H	7.382257	-0.581051	0.204229
H	7.030487	0.848867	-1.954037
H	6.277255	-0.750314	-1.976708
C	0.772096	3.426097	0.603430
C	-0.251378	1.628373	2.489320
C	-0.220222	3.958002	1.654510
H	1.746149	3.941740	0.731178
C	-1.128708	2.808272	2.071947
H	-0.785050	0.671921	2.321616

H	0.347330	4.333341	2.526959
H	-0.810878	4.806833	1.262019
H	-1.839248	3.094848	2.871482
H	-1.746925	2.508203	1.199358
P	3.828399	0.372571	-0.157293
P	1.060542	1.624844	1.123148
C	0.336717	3.682702	-0.826400
C	0.136498	2.684162	-1.780757
C	0.170382	5.016291	-1.231914
C	-0.225839	3.000268	-3.092505
H	0.283576	1.631999	-1.512840
C	-0.203046	5.338426	-2.533006
H	0.344497	5.824818	-0.508640
C	-0.406713	4.326929	-3.474813
H	-0.350999	2.189261	-3.822429
H	-0.326505	6.389986	-2.819317
H	-0.692350	4.576030	-4.503693
C	0.238092	1.628945	3.917851
C	0.789054	0.450077	4.444280
C	0.128943	2.736117	4.769957
C	1.225048	0.382903	5.764077
H	0.889874	-0.430713	3.791986
C	0.566030	2.670762	6.094186
H	-0.318325	3.671325	4.416279
C	1.118318	1.496240	6.598137
H	1.650328	-0.552977	6.145533
H	0.465446	3.552426	6.738308
H	1.459443	1.446085	7.638702
C	4.751753	2.321869	-1.956331

C	3.578260	2.825210	-2.534903
C	5.738192	3.229613	-1.554697
C	3.385338	4.195100	-2.692063
H	2.790107	2.124180	-2.847932
C	5.550002	4.602261	-1.715779
H	6.665972	2.867923	-1.093635
C	4.371500	5.091417	-2.277889
H	2.451760	4.562622	-3.136481
H	6.333920	5.297503	-1.392538
H	4.223603	6.170903	-2.398307
C	5.169324	-2.094895	0.330500
C	4.569471	-2.645761	-0.807521
C	5.792214	-2.963411	1.235523
C	4.600506	-4.020884	-1.035931
H	4.038309	-2.001854	-1.522517
C	5.817045	-4.338492	1.017026
H	6.262735	-2.546282	2.136375
C	5.222695	-4.873161	-0.125848
H	4.127658	-4.427486	-1.937152
H	6.303785	-4.997489	1.745741
H	5.241193	-5.954770	-0.305352
Br	0.680908	-1.001235	-2.270413
Br	1.618640	-1.991756	1.767302
Cu	-0.887546	-0.551406	-0.474930
P	-2.112034	-1.929539	0.896386
P	-2.960646	0.339206	-1.423651
C	-3.866702	-1.465958	0.485112
C	-2.176419	-3.797351	0.575135
C	-2.028815	-2.064039	2.784268

C	-3.958966	-1.184128	-1.010215
C	-4.352174	1.624827	-1.196966
C	-2.969237	0.414471	-3.324716
H	-4.567226	-2.267444	0.792329
H	-4.138512	-0.565264	1.073708
C	-2.357085	-4.419112	1.967549
H	-3.099800	-3.941122	-0.018511
C	-1.033976	-4.309876	-0.263311
C	-1.684790	-3.541141	3.021148
H	-1.158681	-1.442456	3.074733
C	-3.256576	-1.520259	3.466560
H	-3.557454	-2.033522	-1.598925
H	-5.010244	-1.051427	-1.333739
C	-4.867360	1.892209	-2.624121
H	-5.127733	1.081012	-0.626846
C	-4.031098	2.858092	-0.396671
C	-3.745322	1.698534	-3.641127
H	-1.902366	0.539981	-3.589485
C	-3.449471	-0.851635	-3.985899
H	-3.441003	-4.501102	2.176735
H	-1.960900	-5.452205	1.992158
C	0.162031	-4.790675	0.281236
C	-1.168844	-4.302091	-1.658292
H	-1.954719	-3.851263	4.048716
H	-0.585621	-3.638650	2.936192
C	-3.374099	-0.136854	3.670774
C	-4.319555	-2.333009	3.878342
H	-5.690064	1.183507	-2.835764
H	-5.307612	2.905235	-2.695339

C	-4.530348	2.974207	0.909097
C	-3.318514	3.941042	-0.928235
H	-4.133263	1.682810	-4.677665
H	-3.041143	2.552943	-3.590208
C	-2.549365	-1.913365	-4.167594
C	-4.770732	-1.031232	-4.416014
C	1.190853	-5.245974	-0.547483
H	0.307695	-4.807478	1.367568
C	-0.143791	-4.746771	-2.486143
H	-2.103436	-3.935351	-2.108558
C	-4.516211	0.416971	4.243121
H	-2.550143	0.522501	3.368000
C	-5.465122	-1.782686	4.454076
H	-4.262651	-3.420192	3.752997
C	-4.351450	4.140895	1.650278
H	-5.090407	2.135359	1.346607
C	-3.144667	5.110825	-0.191394
H	-2.894285	3.887702	-1.939834
C	-2.960300	-3.113018	-4.745232
H	-1.506084	-1.794856	-3.838330
C	-5.183445	-2.231867	-4.993785
H	-5.502667	-0.222683	-4.310152
C	1.043264	-5.223305	-1.932192
H	2.129226	-5.601605	-0.100700
H	-0.269565	-4.722409	-3.575322
C	-5.572923	-0.405532	4.633993
H	-4.575723	1.501709	4.391406
H	-6.282645	-2.443153	4.766197
C	-3.665170	5.220348	1.097374

H	-4.765646	4.213850	2.663084
H	-2.593141	5.947909	-0.636457
C	-4.282192	-3.281116	-5.157150
H	-2.237932	-3.927038	-4.883015
H	-6.223511	-2.343237	-5.322313
H	1.854000	-5.576297	-2.580244
H	-6.474018	0.025735	5.084827
H	-3.533215	6.145386	1.670798
H	-4.605539	-4.224375	-5.612094

$L1_2Cu_2BrEt$

Cu	-1.423738	0.448208	-0.002935
C	-3.992458	-1.523900	0.825392
H	-4.953108	-1.518543	1.376918
H	-4.081269	-2.321725	0.061260
C	-2.835543	-1.845231	1.767667
H	-2.786842	-1.117497	2.599983
H	-2.957569	-2.857426	2.204100
C	-4.892757	1.239871	0.826681
C	-4.969676	-0.067770	-1.583480
C	-6.296633	0.845969	0.341245
H	-4.766763	1.023780	1.904598
C	-6.238609	0.704730	-1.175805
H	-4.458029	0.467595	-2.407042
H	-6.593562	-0.114768	0.807936
H	-7.049798	1.595615	0.654794
H	-7.151708	0.229327	-1.579559
H	-6.199331	1.714610	-1.625827

C	-1.210517	-3.343756	-0.091863
C	0.136695	-2.221904	2.083905
C	-0.249623	-4.239560	0.712763
H	-2.237677	-3.757337	-0.016564
C	0.828358	-3.346496	1.314990
H	0.782511	-1.324386	2.117002
H	-0.819619	-4.744329	1.515783
H	0.192143	-5.033163	0.080872
H	1.540992	-3.905674	1.952555
H	1.429807	-2.904506	0.491163
P	-3.752721	0.084949	-0.107225
P	-1.219383	-1.708123	0.865417
C	-0.875736	-3.296981	-1.571504
C	-0.526563	-2.145041	-2.281717
C	-0.950689	-4.505895	-2.282592
C	-0.255491	-2.203897	-3.652371
H	-0.466948	-1.176338	-1.763177
C	-0.671264	-4.571475	-3.643626
H	-1.246398	-5.421341	-1.751380
C	-0.318708	-3.412963	-4.339886
H	0.001373	-1.281857	-4.191491
H	-0.739902	-5.531713	-4.169151
H	-0.104603	-3.453326	-5.414356
C	-0.272728	-2.536575	3.502340
C	-0.627081	-1.480525	4.357007
C	-0.271950	-3.833334	4.034002
C	-0.981134	-1.711991	5.683438
H	-0.644015	-0.455006	3.958155
C	-0.627396	-4.067719	5.363572

H	0.024365	-4.689494	3.418418
C	-0.986833	-3.010152	6.195075
H	-1.253981	-0.865670	6.325124
H	-0.615641	-5.093511	5.751091
H	-1.264616	-3.195142	7.239332
C	-5.134233	-1.493307	-2.020397
C	-4.140854	-2.073462	-2.821489
C	-6.197442	-2.299789	-1.595581
C	-4.197888	-3.418655	-3.178457
H	-3.297472	-1.456605	-3.164354
C	-6.258841	-3.646525	-1.952460
H	-6.987390	-1.879018	-0.960319
C	-5.257520	-4.213816	-2.740522
H	-3.403519	-3.845372	-3.802910
H	-7.099164	-4.260251	-1.606692
H	-5.306880	-5.272962	-3.018725
C	-4.610530	2.702880	0.589098
C	-4.117641	3.197343	-0.625051
C	-4.928820	3.627796	1.592145
C	-3.972064	4.567859	-0.839370
H	-3.826718	2.506988	-1.427755
C	-4.779477	4.997595	1.386715
H	-5.302337	3.258695	2.556842
C	-4.307259	5.475163	0.163329
H	-3.586814	4.925006	-1.802254
H	-5.034923	5.698963	2.189940
H	-4.190040	6.552914	-0.003150
C	-0.585509	1.768014	-1.441046
Br	-1.580999	1.524922	2.407116

Cu	0.915352	0.661781	-0.466508
P	2.365176	1.492565	1.154511
P	2.823790	-0.111464	-1.708585
C	4.044581	1.038092	0.495291
C	2.604681	3.363202	1.361641
C	2.365325	1.097926	3.006190
C	3.999744	1.173692	-1.025694
C	4.094421	-1.526355	-1.829895
C	2.770481	0.217935	-3.583290
H	4.833704	1.676295	0.940005
H	4.276326	-0.005093	0.794256
C	2.827678	3.564120	2.871414
H	3.540002	3.594286	0.817504
C	1.509940	4.172496	0.720474
C	2.127031	2.462233	3.664189
H	1.464639	0.471636	3.157286
C	3.569894	0.305016	3.433353
H	3.638746	2.179211	-1.325260
H	5.005685	1.053219	-1.473639
C	4.596689	-1.474258	-3.285221
H	4.913531	-1.206789	-1.159959
C	3.659217	-2.881127	-1.344588
C	3.488885	-0.982415	-4.211205
H	1.695041	0.180372	-3.839157
C	3.266587	1.591973	-3.939013
H	3.916987	3.532987	3.068592
H	2.482915	4.567377	3.187821
C	0.262277	4.352073	1.327797
C	1.719837	4.744808	-0.541491

H	2.445152	2.453927	4.724395
H	1.033543	2.639005	3.665568
C	3.603954	-1.074181	3.172021
C	4.686818	0.881813	4.049202
H	5.459620	-0.782569	-3.332839
H	4.976814	-2.464739	-3.601140
C	4.199318	-3.377843	-0.150038
C	2.784956	-3.704431	-2.066712
H	3.877804	-0.732193	-5.216843
H	2.748135	-1.791957	-4.363059
C	2.382524	2.677264	-3.845181
C	4.590197	1.850822	-4.316543
C	-0.750209	5.063386	0.688183
H	0.046864	3.889757	2.297411
C	0.716687	5.476319	-1.176183
H	2.694093	4.618975	-1.037218
C	4.714972	-1.846432	3.498553
H	2.740217	-1.551507	2.688346
C	5.802171	0.110526	4.380153
H	4.695655	1.952550	4.284380
C	3.899987	-4.662661	0.299615
H	4.885095	-2.746261	0.433232
C	2.489506	-4.992549	-1.623246
H	2.320013	-3.342747	-2.993358
C	2.810726	3.978548	-4.096887
H	1.335015	2.494465	-3.567045
C	5.021072	3.152792	-4.570535
H	5.308236	1.028053	-4.415947
C	-0.525868	5.635480	-0.563494

H	-1.734982	5.145207	1.167695
H	0.909109	5.926703	-2.158037
C	5.824869	-1.254845	4.103635
H	4.709240	-2.922159	3.283365
H	6.663282	0.587130	4.863241
C	3.049742	-5.480206	-0.442631
H	4.344621	-5.030816	1.232298
H	1.807521	-5.618878	-2.211363
C	4.136532	4.223922	-4.454833
H	2.097800	4.808333	-4.020103
H	6.062630	3.329512	-4.863550
H	-1.321361	6.202591	-1.062578
H	6.701633	-1.858496	4.364472
H	2.818349	-6.495465	-0.099270
H	4.476675	5.246580	-4.653879
H	0.372546	2.347370	-1.549285
C	-1.103298	1.444694	-2.838180
H	-1.231141	2.535728	-0.957912
H	-1.271776	2.347077	-3.468641
H	-0.398978	0.796114	-3.398738
H	-2.063399	0.887846	-2.813165

$L1_2Cu_2Et_2$

Cu	-1.173250	0.176221	0.276355
C	-4.431310	1.075991	0.086349
H	-5.207352	1.764263	0.475976
H	-4.707964	0.858856	-0.963700
C	-4.395100	-0.218067	0.889781

H	-4.173039	-0.012778	1.958062
H	-5.379619	-0.725136	0.862164
C	-3.022824	3.192494	1.410899
C	-2.883264	3.180036	-1.346761
C	-3.747822	4.341098	0.690364
H	-3.685491	2.737907	2.174449
C	-3.066044	4.540557	-0.658171
H	-1.891693	3.137558	-1.836254
H	-4.813607	4.071873	0.547525
H	-3.732459	5.265231	1.301224
H	-3.616776	5.252906	-1.301012
H	-2.067302	4.989893	-0.490807
C	-3.847940	-2.122740	-1.226969
C	-3.160970	-2.881822	1.325509
C	-4.692335	-3.259812	-0.632334
H	-4.502667	-1.372401	-1.712904
C	-3.877084	-3.937921	0.464609
H	-2.106995	-3.184136	1.475281
H	-5.623153	-2.831401	-0.209209
H	-5.003490	-3.979724	-1.415226
H	-4.503661	-4.607874	1.083711
H	-3.111940	-4.589572	-0.000233
P	-2.751425	1.899939	0.071226
P	-3.026373	-1.312403	0.255872
C	-2.823551	-2.583199	-2.232602
C	-1.627783	-3.211816	-1.854204
C	-3.061462	-2.392926	-3.599707
C	-0.719044	-3.653465	-2.812563
H	-1.369955	-3.346086	-0.793509

C	-2.142203	-2.812783	-4.560714
H	-3.990742	-1.898802	-3.914416
C	-0.966712	-3.452954	-4.170173
H	0.198424	-4.157499	-2.483043
H	-2.349994	-2.642681	-5.623833
H	-0.242974	-3.790986	-4.921122
C	-3.734501	-2.581121	2.679596
C	-2.897146	-2.034600	3.663501
C	-5.089050	-2.756102	2.987802
C	-3.397392	-1.659354	4.908044
H	-1.832889	-1.884528	3.431917
C	-5.591937	-2.387592	4.235663
H	-5.773408	-3.178151	2.240570
C	-4.750838	-1.833642	5.200073
H	-2.721618	-1.227334	5.656289
H	-6.656566	-2.532909	4.454524
H	-5.148734	-1.540910	6.178624
C	-3.912690	2.768490	-2.361003
C	-3.609844	1.724037	-3.248908
C	-5.195999	3.324807	-2.411447
C	-4.559125	1.246373	-4.148645
H	-2.610587	1.268046	-3.218051
C	-6.149293	2.847227	-3.312084
H	-5.471137	4.141459	-1.732847
C	-5.838372	1.804226	-4.182232
H	-4.293837	0.433662	-4.835922
H	-7.148623	3.298145	-3.330485
H	-6.588185	1.430221	-4.888826
C	-1.755719	3.646348	2.086767

C	-0.523648	3.690605	1.426668
C	-1.808895	4.078278	3.419051
C	0.617413	4.156459	2.077465
H	-0.426222	3.321896	0.394862
C	-0.668637	4.535412	4.076313
H	-2.768975	4.045914	3.952247
C	0.553480	4.578002	3.403936
H	1.565124	4.185240	1.526920
H	-0.734671	4.858941	5.121952
H	1.455917	4.936575	3.914299
Cu	1.110323	0.322553	-0.448956
P	3.109136	1.258093	0.226655
P	2.543906	-2.051188	-0.417272
C	4.472462	0.082383	-0.255498
C	3.895168	2.846597	-0.446813
C	3.496420	1.720527	2.047248
C	4.220980	-1.378928	0.076879
C	2.821720	-3.807579	0.269585
C	2.815420	-2.625745	-2.227360
H	4.567367	0.215731	-1.350339
H	5.436120	0.398432	0.186861
C	4.945032	3.191429	0.608315
H	4.378923	2.548543	-1.400451
C	2.893053	3.937537	-0.761883
C	4.294333	3.037908	1.980714
H	2.500265	1.901668	2.497679
C	4.149414	0.595241	2.804114
H	5.039999	-1.994793	-0.343929
H	4.251413	-1.521726	1.175289

C	3.655654	-4.523596	-0.793097
H	3.420758	-3.663713	1.190581
C	1.528251	-4.461215	0.683597
C	3.164523	-4.123942	-2.182396
H	1.819715	-2.491332	-2.692075
C	3.766432	-1.726584	-2.962211
H	5.800872	2.497479	0.508896
H	5.372580	4.201137	0.466130
C	3.043331	5.260950	-0.328422
C	1.786862	3.637610	-1.570085
H	5.039891	3.093804	2.795807
H	3.600480	3.884479	2.148884
C	3.357864	-0.351745	3.471074
C	5.541116	0.431812	2.846777
H	4.713603	-4.220348	-0.671701
H	3.640069	-5.623033	-0.655314
C	0.909382	-4.026988	1.867606
C	0.919893	-5.501482	-0.028062
H	3.906130	-4.386207	-2.960625
H	2.257484	-4.705105	-2.437546
C	3.269752	-0.556047	-3.553842
C	5.142892	-1.972920	-3.043601
C	2.115432	6.243913	-0.676386
H	3.894455	5.548392	0.298767
C	0.863900	4.616886	-1.926954
H	1.643346	2.604646	-1.911387
C	3.930872	-1.441483	4.123661
H	2.267754	-0.228163	3.475455
C	6.118556	-0.656770	3.500029

H	6.197202	1.165743	2.361902
C	-0.256374	-4.624697	2.334284
H	1.364465	-3.202070	2.435041
C	-0.264476	-6.088956	0.424984
H	1.376839	-5.884957	-0.947666
C	4.117411	0.356272	-4.176621
H	2.190574	-0.365116	-3.510751
C	5.995930	-1.064350	-3.671793
H	5.565739	-2.887563	-2.607650
C	1.019708	5.928334	-1.475971
H	2.256524	7.269761	-0.316147
H	0.015883	4.351880	-2.572561
C	5.316461	-1.604978	4.133631
H	3.286967	-2.165521	4.637382
H	7.209821	-0.762068	3.514159
C	-0.854109	-5.660051	1.610697
H	-0.708604	-4.277468	3.272200
H	-0.720082	-6.901013	-0.154419
C	5.490375	0.108150	-4.232983
H	3.699821	1.265598	-4.627283
H	7.070415	-1.277254	-3.722190
H	0.291660	6.700472	-1.751026
H	5.770713	-2.460956	4.645861
H	-1.778472	-6.126356	1.973164
H	6.163265	0.820710	-4.723976
C	-0.110396	0.098707	-2.072875
H	0.240593	-0.884887	-2.460233
H	-1.200074	-0.093428	-1.911150
C	-0.012574	1.136665	-3.186800

H	-0.424553	2.119147	-2.876459
H	1.032418	1.343868	-3.498824
H	-0.556567	0.852927	-4.118849
C	0.031010	-0.328475	1.848386
H	-0.289335	-1.383890	2.008590
H	1.135510	-0.412954	1.756666
C	-0.289162	0.509850	3.082540
H	0.123666	1.536331	2.992240
H	-1.383159	0.643410	3.230459
H	0.101356	0.090458	4.043508

L1-CuEt$_2$

Cu	-1.643595	0.812514	-2.210233
C	0.192403	-0.343847	1.721937
H	-0.202872	-0.263555	2.754727
H	0.974197	-1.127537	1.765997
C	0.812466	0.987736	1.310996
H	0.041601	1.784367	1.275835
H	1.550860	1.301170	2.076587
C	-2.616422	-0.205982	1.420700
C	-1.516794	-2.708810	1.250322
C	-2.865194	-1.119103	2.630909
H	-2.319481	0.807626	1.758984
C	-2.757600	-2.557800	2.143325
H	-1.778158	-3.302557	0.352651
H	-2.107873	-0.918316	3.414459
H	-3.853227	-0.914185	3.090680
H	-2.756248	-3.282652	2.980499

H	-3.656126	-2.790357	1.538745
C	3.103120	-0.163331	0.029125
C	2.667585	2.544277	-0.382257
C	4.181122	0.790188	0.535661
H	2.779619	-0.840427	0.845434
C	4.120045	2.059543	-0.306120
H	2.480245	2.994417	-1.375503
H	3.964988	1.031260	1.594754
H	5.190633	0.334278	0.530397
H	4.795461	2.850961	0.074032
H	4.465903	1.826135	-1.332394
P	-1.124746	-0.952935	0.531317
P	1.599175	0.938804	-0.390379
C	3.449078	-1.038673	-1.152449
C	2.462218	-1.905891	-1.651105
C	4.702965	-1.054950	-1.771737
C	2.719896	-2.764790	-2.713890
H	1.462353	-1.895438	-1.191376
C	4.964975	-1.910636	-2.845395
H	5.503634	-0.394875	-1.417402
C	3.978765	-2.770748	-3.319924
H	1.926818	-3.429421	-3.078847
H	5.956798	-1.900313	-3.313476
H	4.185472	-3.440731	-4.162716
C	2.221372	3.544589	0.646114
C	1.043355	4.270680	0.409603
C	2.895565	3.768138	1.852872
C	0.547504	5.172360	1.345897
H	0.495596	4.107000	-0.528760

C	2.404587	4.676612	2.792876
H	3.823909	3.227764	2.075327
C	1.227303	5.380181	2.547785
H	-0.378895	5.720185	1.133196
H	2.952999	4.833337	3.729714
H	0.841581	6.090724	3.288226
C	-0.288228	-3.320603	1.848091
C	0.690789	-3.847653	0.990634
C	-0.017408	-3.307185	3.222287
C	1.908970	-4.311199	1.480428
H	0.489998	-3.878804	-0.090291
C	1.196853	-3.781885	3.718510
H	-0.758996	-2.903344	3.923301
C	2.170449	-4.276731	2.851444
H	2.659938	-4.704723	0.784210
H	1.386341	-3.757470	4.798501
H	3.127452	-4.641115	3.242666
C	-3.848050	-0.068666	0.559300
C	-4.863023	0.805576	0.970660
C	-4.039628	-0.790068	-0.622904
C	-6.027197	0.965888	0.223077
H	-4.724621	1.383912	1.895154
C	-5.204546	-0.636291	-1.375578
H	-3.257620	-1.470753	-0.984807
C	-6.200957	0.244124	-0.959328
H	-6.802200	1.664449	0.561302
H	-5.325997	-1.205564	-2.305529
H	-7.112284	0.370820	-1.555877
C	-1.120958	-0.655239	-3.429256

H	-0.003390	-0.676375	-3.420643
H	-1.381480	-0.422846	-4.489771
C	-1.623184	-2.060857	-3.113957
H	-1.229001	-2.868249	-3.779775
H	-1.361419	-2.363678	-2.075158
H	-2.731145	-2.132119	-3.180442
C	-2.082893	2.441466	-1.184568
C	-1.766837	3.730669	-1.940354
H	-3.159842	2.443459	-0.891832
H	-1.529852	2.452566	-0.212677
H	-1.930671	4.679181	-1.367740
H	-0.709132	3.759768	-2.283773
H	-2.372838	3.824571	-2.866304

$CuEt_2$

Cu	0.000002	0.000008	-0.075759
C	-1.842341	-0.677331	-0.070996
H	-1.957512	-1.479895	0.695599
H	-2.074399	-1.185931	-1.036607
C	-2.904618	0.392549	0.182891
H	-3.958189	0.020250	0.188647
H	-2.755369	0.900347	1.159110
H	-2.870591	1.199000	-0.579629
C	1.842350	0.677336	-0.070986
C	2.904600	-0.392573	0.182889
H	2.074412	1.185902	-1.036614
H	1.957560	1.479914	0.695588
H	3.958183	-0.020307	0.188603

H	2.755366	-0.900344	1.159126
H	2.870523	-1.199041	-0.579610

V-R$_{3-4}$

C	1.934007	-0.372031	2.794257
C	-0.410780	-1.762060	2.583423
C	1.815779	-1.702387	3.550786
H	1.756794	0.437052	3.535871
C	0.349448	-1.906062	3.893558
H	-0.115138	-2.611323	1.931211
H	2.178570	-2.527745	2.902802
H	2.444983	-1.701333	4.459373
H	0.156406	-2.888099	4.366265
H	0.035587	-1.130248	4.620847
C	-3.696289	1.746622	-0.351808
C	-1.375047	3.154846	-0.691635
C	-3.760234	3.071439	-1.133377
H	-4.148217	1.907247	0.648215
C	-2.657456	3.976942	-0.614216
H	-1.170102	2.948440	-1.763324
H	-3.595189	2.865051	-2.210760
H	-4.767168	3.520622	-1.044445
H	-2.567490	4.913369	-1.197539
H	-2.880520	4.268259	0.431854
P	-1.856875	1.461990	-0.022990
P	0.381950	-0.290118	1.713241
Cu	-0.388556	-0.295731	-0.481338
C	2.493824	-1.469210	-1.987716

C	0.477240	-0.468294	-2.687165
C	3.859733	-1.341370	-1.699703
C	1.786105	-2.593150	-1.492860
C	-0.289082	-1.504242	-2.175981
H	-0.000880	0.419226	-3.124046
C	4.507112	-2.260168	-0.881636
H	4.417136	-0.493497	-2.103109
C	2.447377	-3.471156	-0.630598
C	0.377639	-2.843778	-1.997668
H	-1.360460	-1.501831	-2.432178
C	3.795882	-3.311878	-0.311882
H	5.573677	-2.127124	-0.664664
H	1.904720	-4.324938	-0.209831
H	0.480240	-3.298959	-3.016120
H	4.289862	-4.023221	0.360148
N	1.823628	-0.455583	-2.704158
B	2.574025	0.809219	-3.285010
F	1.626818	1.617448	-3.900650
F	3.532001	0.392063	-4.192276
F	3.178448	1.521261	-2.243793
C	-0.468464	-3.822402	-1.180560
H	-0.280721	-3.663343	-0.097675
H	-1.536078	-3.563080	-1.336375
C	-0.278528	-5.284333	-1.553336
H	0.774356	-5.611023	-1.468665
H	-0.887527	-5.948198	-0.913000
H	-0.585679	-5.459953	-2.601969
C	-1.908175	-1.687334	2.599267
C	-2.639892	-1.336139	3.738258

C	-2.607882	-1.938157	1.409003
C	-4.030918	-1.219280	3.681739
H	-2.126443	-1.149146	4.688835
C	-3.992849	-1.828927	1.350698
H	-2.048414	-2.234459	0.508878
C	-4.711406	-1.459045	2.489701
H	-4.586585	-0.941866	4.585133
H	-4.516874	-2.035842	0.410131
H	-5.803468	-1.368808	2.445941
C	3.270425	-0.099346	2.149814
C	4.445307	-0.494676	2.810277
C	3.398150	0.614129	0.955015
C	5.700591	-0.167542	2.304761
H	4.383723	-1.056649	3.749574
C	4.654977	0.947641	0.448295
H	2.505956	0.915378	0.387724
C	5.810688	0.564895	1.122320
H	6.601132	-0.484806	2.844120
H	4.714310	1.488701	-0.502640
H	6.797572	0.826636	0.722748
C	-4.423608	0.623619	-1.034594
C	-3.866441	-0.045396	-2.131195
C	-5.708067	0.262102	-0.615990
C	-4.558034	-1.073044	-2.769130
H	-2.866532	0.242729	-2.487680
C	-6.411192	-0.756106	-1.258896
H	-6.159743	0.783688	0.238605
C	-5.833621	-1.434707	-2.331381
H	-4.098891	-1.592570	-3.618805

H	-7.415923	-1.026799	-0.913555
H	-6.379500	-2.242227	-2.832580
C	-0.120768	3.692396	-0.073031
C	-0.131849	4.553552	1.031141
C	1.115651	3.285642	-0.592736
C	1.063399	4.981008	1.610750
H	-1.082585	4.905395	1.449762
C	2.308259	3.716501	-0.018941
H	1.152482	2.625430	-1.471420
C	2.287434	4.560649	1.091907
H	1.034803	5.655618	2.474601
H	3.257102	3.383046	-0.453764
H	3.225580	4.899545	1.546430
C	-1.776387	1.614137	1.828895
H	-2.570343	0.935376	2.201493
H	-2.061332	2.637035	2.146050
C	-0.431378	1.226792	2.437222
H	0.314067	2.034474	2.271057
H	-0.530253	1.114757	3.535835

V-S_{3-4}

C	3.788853	0.543886	1.489032
C	2.042113	2.649776	1.747971
C	3.953979	1.459860	2.709295
H	4.509777	0.884137	0.717318
C	3.459489	2.835678	2.290251
H	1.376024	2.432184	2.607829
H	3.345912	1.071501	3.553148

H	5.007061	1.468676	3.047851
H	3.473703	3.566975	3.120634
H	4.132544	3.228244	1.502313
C	-1.422479	1.047733	-2.684702
C	0.381713	-1.013935	-2.866846
C	-1.621117	0.011197	-3.799897
H	-0.970115	1.953180	-3.136856
C	-0.241605	-0.521466	-4.169851
H	-0.205862	-1.884151	-2.514651
H	-2.247249	-0.824648	-3.433858
H	-2.144421	0.468206	-4.660626
H	-0.293342	-1.335825	-4.917796
H	0.360063	0.293791	-4.621352
P	-0.049440	0.322532	-1.616159
P	2.096307	1.005074	0.813501
Cu	0.116201	-0.218210	0.643501
C	-0.926283	-2.136179	1.251587
C	-3.277681	-2.066990	1.047070
C	-0.889586	-1.220967	2.281433
C	-3.362922	-1.189435	2.152588
C	-2.140725	-0.479216	2.694056
H	-2.207729	-0.475855	3.803692
N	-2.035872	-2.477607	0.543978
B	-1.885818	-3.342544	-0.752224
F	-0.527604	-3.587093	-0.952408
F	-2.390869	-2.622121	-1.843808
F	-2.566706	-4.545143	-0.635406
C	-2.049516	0.997067	2.261596
H	-1.059779	1.363167	2.614233

H	-2.029435	1.034965	1.147155
C	-3.133367	1.924252	2.778378
H	-3.206417	1.879562	3.883067
H	-2.919260	2.973670	2.498473
H	-4.123953	1.671530	2.357699
C	-4.613585	-0.955156	2.733045
C	-5.785032	-1.489210	2.204637
H	-6.752534	-1.280589	2.675101
C	-4.467379	-2.583015	0.499433
C	-5.702260	-2.289168	1.064399
H	-6.609994	-2.712807	0.618093
H	-4.661998	-0.322005	3.628730
H	-4.414107	-3.249272	-0.364897
H	-0.042699	-1.255259	2.979996
H	-0.027665	-2.726567	1.018004
C	1.839497	-1.357429	-2.799290
C	2.283966	-2.159121	-1.735282
C	2.788690	-0.851394	-3.693798
C	3.638446	-2.415417	-1.548022
H	1.539854	-2.589140	-1.051358
C	4.148693	-1.112657	-3.510518
H	2.472219	-0.239438	-4.547359
C	4.580036	-1.883213	-2.432088
H	3.963358	-3.036128	-0.703757
H	4.877829	-0.705878	-4.221290
H	5.648682	-2.081007	-2.284673
C	-2.633522	1.461125	-1.901237
C	-2.922146	2.818419	-1.718677
C	-3.472587	0.510989	-1.303099

C	-4.027521	3.221889	-0.968409
H	-2.269879	3.572796	-2.180259
C	-4.579560	0.911613	-0.558230
H	-3.248998	-0.559990	-1.406592
C	-4.863201	2.268056	-0.390220
H	-4.239734	4.290887	-0.842573
H	-5.219127	0.149484	-0.093754
H	-5.734367	2.580669	0.197900
C	4.025767	-0.917096	1.746878
C	5.247243	-1.497983	1.388364
C	3.067244	-1.719234	2.377841
C	5.503670	-2.844168	1.646107
H	6.008811	-0.882675	0.890453
C	3.312495	-3.068096	2.626190
H	2.104104	-1.277532	2.667025
C	4.533949	-3.635712	2.260278
H	6.466855	-3.280228	1.356148
H	2.542974	-3.680621	3.110699
H	4.728834	-4.696548	2.454817
C	1.420086	3.755451	0.943627
C	2.175690	4.676181	0.207814
C	0.021634	3.848223	0.881636
C	1.551412	5.650450	-0.572691
H	3.271269	4.645418	0.239430
C	-0.604131	4.822472	0.109166
H	-0.586873	3.135246	1.453731
C	0.161027	5.727677	-0.627746
H	2.163650	6.361570	-1.139362
H	-1.699449	4.873576	0.085444

H	-0.326149	6.497831	-1.236571
C	1.260708	1.634683	-1.815723
H	1.543899	1.726376	-2.883343
H	0.751498	2.582809	-1.539370
C	2.496162	1.425160	-0.949564
H	3.160667	2.311423	-0.989282
H	3.087380	0.563994	-1.323878

IIIa

C	0.669612	-1.647452	-0.793722
C	0.065235	0.547364	-0.158102
C	-0.591653	-1.996605	-1.109670
C	-1.289465	0.263597	-0.469622
C	-1.745227	-1.170095	-0.620573
H	-2.586980	-1.199265	-1.348310
N	1.025429	-0.457096	-0.187959
B	2.501684	-0.211970	0.244571
F	3.190755	-1.421322	0.180498
F	2.534956	0.278390	1.552518
F	3.123965	0.714508	-0.601512
C	-2.283357	-1.749906	0.704035
H	-2.449836	-2.836747	0.549350
H	-1.476846	-1.672249	1.463478
C	-3.556570	-1.106464	1.221247
H	-4.364438	-1.153456	0.463608
H	-3.924357	-1.614495	2.132257
H	-3.403975	-0.040439	1.474962
C	-2.204210	1.315679	-0.565084

C	-1.842699	2.636556	-0.309131
H	-2.582153	3.442587	-0.383915
C	0.418444	1.885191	0.118052
C	-0.521269	2.906499	0.051699
H	-0.207896	3.935729	0.268387
H	-3.241588	1.077216	-0.839934
H	1.456266	2.121634	0.364269
H	-0.780867	-2.950117	-1.618647
H	1.516118	-2.301235	-1.030948

IIIb

C	-3.396185	-0.327323	-1.745024
C	-1.542901	1.422050	-2.752925
C	-3.408846	-0.055712	-3.257506
H	-4.205423	0.280888	-1.289702
C	-2.893864	1.360007	-3.461246
H	-0.835679	0.781308	-3.318304
H	-2.739115	-0.781678	-3.765081
H	-4.424034	-0.209745	-3.670383
H	-2.799206	1.631223	-4.530278
H	-3.611705	2.072694	-3.007231
C	1.175081	1.898274	2.543845
C	-0.939215	0.298057	3.231095
C	1.017163	1.496958	4.013086
H	0.871921	2.960877	2.434496
C	-0.469160	1.297514	4.282524
H	-0.409068	-0.659326	3.417497
H	1.537034	0.534760	4.196536

H	1.477761	2.245269	4.685233
H	-0.665212	0.930809	5.308497
H	-1.000445	2.265256	4.176245
P	-0.158514	0.915892	1.633279
P	-1.791129	0.452512	-1.149695
Cu	0.096249	-0.441700	-0.185958
C	1.585700	-1.860562	-2.195385
C	2.527304	-2.038564	-0.060986
C	2.682191	-2.342755	-2.823032
C	3.731432	-2.552553	-0.614144
C	3.996667	-2.394572	-2.095568
H	4.606371	-3.259947	-2.442110
N	1.492032	-1.577293	-0.850872
C	4.817363	-1.124465	-2.402914
H	4.839688	-0.998350	-3.506103
H	4.250800	-0.254261	-2.006927
C	6.233535	-1.118569	-1.858344
H	6.805937	-1.997363	-2.217929
H	6.784061	-0.211604	-2.173909
H	6.246114	-1.145598	-0.751653
C	4.680489	-3.129930	0.233366
C	4.514094	-3.173246	1.617886
H	5.279422	-3.628206	2.257793
C	2.378456	-2.079479	1.343742
C	3.352684	-2.623517	2.168816
H	3.195279	-2.636931	3.255471
H	5.590425	-3.552224	-0.217386
H	1.444482	-1.686064	1.771049
H	2.645749	-2.571581	-3.896253

H	0.654058	-1.695117	-2.763410
C	-2.395855	-0.005243	3.058928
C	-2.756429	-1.178472	2.378254
C	-3.410819	0.859787	3.481300
C	-4.088679	-1.467899	2.101426
H	-1.968342	-1.873357	2.052600
C	-4.749115	0.571243	3.205633
H	-3.160880	1.775579	4.030848
C	-5.092507	-0.585685	2.507825
H	-4.345224	-2.387309	1.560832
H	-5.531438	1.261447	3.542719
H	-6.143737	-0.808165	2.289778
C	2.525913	1.714348	1.902419
C	2.682225	2.089065	0.559464
C	3.625449	1.162050	2.563840
C	3.887461	1.903611	-0.107529
H	1.832028	2.537651	0.025807
C	4.840934	0.977816	1.899417
H	3.547174	0.863792	3.615726
C	4.976479	1.339705	0.562247
H	3.980055	2.201116	-1.160059
H	5.688161	0.536248	2.437521
H	5.928293	1.187625	0.039815
C	-3.629679	-1.770518	-1.386312
C	-4.945845	-2.217083	-1.211412
C	-2.590938	-2.703009	-1.280287
C	-5.220525	-3.554102	-0.931576
H	-5.770522	-1.495111	-1.290786
C	-2.860969	-4.040613	-0.991668

H	-1.547737	-2.376248	-1.397931
C	-4.175715	-4.471474	-0.816387
H	-6.258212	-3.881101	-0.796066
H	-2.031817	-4.752063	-0.902258
H	-4.386268	-5.522990	-0.589352
C	-0.887988	2.751833	-2.530058
C	-1.617745	3.939173	-2.391221
C	0.508669	2.813140	-2.409985
C	-0.973074	5.147698	-2.125920
H	-2.709251	3.931268	-2.497079
C	1.154356	4.019648	-2.149561
H	1.097986	1.890509	-2.522941
C	0.414132	5.193142	-1.999932
H	-1.564562	6.064841	-2.022328
H	2.247750	4.045485	-2.064274
H	0.920424	6.143360	-1.795557
C	-1.315306	2.239210	1.006721
H	-1.751419	2.816164	1.846677
H	-0.672616	2.944511	0.437380
C	-2.414426	1.683623	0.103316
H	-2.964462	2.504938	-0.397584
H	-3.157343	1.125378	0.708109

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