SUPPLEMENTARY INFORMATION

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1. Supplementary Methods

1.1. General Information

Unless otherwise noted, all chemicals and reagents for chemical reactions were obtained from commercial suppliers and used as received (Bide Chemical, Energy Chemical, TCI, and Titan). Kanamycin sulfate (>99%) salt, streptomycin sulfate salt (98%), and isopropyl-β-D-thiogalactopyranoside (IPTG, >99%) were purchased from Solarbio (Beijing, China). Column chromatography was performed using silica gel (300-400 mesh). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker (400 and 100 MHz, respectively) instrument, and are internally referenced to residual proton signals in $CDCl_3$ (7.26 ppm). ^{1}H NMR data are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, dt = doublet of triplet, ddd = doublet of doublet of doublet), coupling constant (Hz), and integration. Data for ^{13}C NMR are reported in terms of chemical shift relative to $CDCl_3$ (77.16 ppm). High resolution mass spectra (HRMS) were recorded on a Waters Xevo G2-XS QT of spectrometer.

1.2. Chromatography

Analytical high performance liquid chromatography (HPLC) was carried out using a Shimadzu LC-20A liquid chromatograph equipped with a UV detector. The HPLC system, utilizing isopropanol and hexanes as the mobile phases, was used to measure the yield and separate enantiomers. Chiral HPLC columns Chiral OJ-H (4.6 mmΦ×250 mmL, 5 μm particle size), Chiral OD-H (4.6 mmΦ×250 mmL, 5 μm particle size), Chiral AD-H (4.6 mmΦ×250 mmL, 5 μm particle size), Chiral OX-3 (4.6 mmΦ×250 mmL, 3 μm particle size), Chiral OZ-3 (4.6 mmΦ×250 mmL, 3 μm particle size), Chiral AS-3 (4.6 mmΦ×250 mmL, 3 μm particle size), and Chiral IH (4.6 mmΦ×250 mmL, 5 μm particle size) purchased from Daicel Chemical Industries. The HPLC conditions for analyzing synthesized chiral chemical compounds were described in the chromatogram section. The measured absolute configuration of **2a** was established by the literatures[1,2]. Absolute configurations of **2b-2n**, and **2p** were assigned by analogy, and **2o**[3] absolute configuration was judged by literature.

1.3. Cloning and expression of the $P450_{PL2}$ gene

Cloning of P450PL2 gene from ref[4], P450PL2 and co-expressed with Fdr-Fdx electron transport systems were expressed in strain *Escherichia coli* BL21 (DE3) using the pET-28b(+), pCDFDuet-1 vector. *E. coli* BL21(DE3) and pET-28b(+) were used as expression host and plasmid respectively. pCDFDuet-1 was used to express coenzyme Fdr-Fdx1. Cultivation of *E. coli* (P450PL2-1) cells was carried out using TB medium containing 50 μg/mL Kan and 50 μg/mL Str. After growing at 37 °C to an OD_{600} of 0.6-0.8, IPTG was added to the final concentration of 0.1 mM. The culture was incubated at 25 °C for another 12-14 h for enyzme expression. Recombinant *E. coli* (P450PL2-1) cells that expressed recombinant P450PL2 were harvested by centrifugation at 9000 rpm at 25°C for 3 min. The freshly prepared *E. coli* (P450PL2-1) cells were resuspended in a reaction buffer solution to a cell density (g dcw/L) for performing biotransformation.

1.4. Mutation and screening process

Preliminary screening of laboratory strains: reactions were performed 24 h in a total volume of 5 mL in 50 mM PB (Na_2HPO_4-KH_2PO_4, 50 mM, pH 7.5) buffer, at 30 ºC, 10 g dcw/L, and add **1a** to achieve a substrate concentration of 2 mM. After the reaction was completed (24 h), add ethyl acetate containing an internal standard in 1:1 for full extraction for HPLC analysis. All analytic yields of substrates were calculated using calibration curves of the corresponding racemic alcohols. The HPLC conditions for analyzing synthesized chiral alcohols **2a-2p** are described in the chromatogram section of the Supplementary Information. The analytical yields of **2** were calculated using calibration curves of the corresponding racemic alcohols.

Site saturation mutagenesis and library screening: Site-saturation mutagenesis was performed by "22c-trick" PCR using degenerate codons[5]. Target genes were amplified using PrimeSTAR HS DNA Polymerase, followed by digestion with *Dpn* I and directly transformed into competent cells of strain *E. coli* BL21(DE3) by heat shock method. Single colonies of *E. coli* cells were picked and cultured in 5-mL 24-deep-well

plates in TB-Kan-Str medium (3 mL/well, 50 μg/mL kan and str) at 37 ºC, 850 rpm for 7-8 h. Then 1 mL TB-Kan-Str medium containing IPTG (final concentration 0.1 mM) was added to each well, and the plates were shaken at 25 ºC, 800 rpm for 12 h. Induced cells were harvested (4000 rpm, 10 min, 25 ºC) and used for biotransformation. 1 mL PB solution containing 2 mM **1a** was added to resuspend *E. coli* cells. Transfer to 2 mL EP tubes shaked at 30 ºC, 250 rpm for 10-12 h. The reaction mixtures were then extracted with 1 mL ethyl acetate. The organic phases were separated, dried over anhydrous Na_2SO_4, and analyzed by chiral HPLC.

1.5. DNA and protein sequence

P450PL2 base sequence:

ATGCAGGAAATCCGGAAATCCGACCGGGCGGACGATCTCGCGGCGCTTGT
GGCGGCTTTGCCCGCAGGCGACACCATCGCCTCGCCTTATGCGCTCTATGA
CAGGCTCCGGCCCTATGGCCCCGTCTATGGCTACCGCGATTACCCGCCCGG
CACCGTGCCGGATGCGGACGAGGCGGTAACGGCCTGGGTGCTTCTGAATT
ACGACCATGTCTCCGCCGCCGCGCGCGATCACCGCATATTTTCCTCGCGCG
ATCCGCTGCAGGAGCAGTCCTCAGCGCCGACGCTGATGCTCGTGAACCAC
GACAATCCCGAGCACGACCGCCTTCGCAGCATCGTCAATCTCGCCTTTTCC
CGCCCTCGTATCGAGGCGCTCGATCCCTGGGTGCGCGAAATCGTCGGCGGC
ATGGTGGCAGGCCTTGGCGATGGCGATACCGAAGTGATGGAGGCGCTCGC
CGCCCGCATCCCGGCCCGCATCATGGTCGGCCTGCTGGGTCTCCCCGAGGA
AGTGGTAGACCGGTTTCGTCATTGGGCGACGGCCTTCATGCTGTCCGCCGA
TCTCGATCCCGCCGAACGTGAGGCGAGCAATGCCGAACTGGTCCGCTATTT
CACCGAAACCGTGGATAGCCTCTATGGCGCTCTCGAGGCGGGCGATCCCGT
TCCGGATGGCCTCATCGCCGCACTCCTGAAGGCGGAAGTCGATGGCGAGC
AACTGACCCTCGATGAAGTGATCCGCTTCTGTATCACGCTCGTTGTCGCAG
GCTCGGAAACGACAACCTTTCTCCTCGGCAACCTGCTGCACAATCTCGCTG
TCATGCCGGACATTCGTGCGCAGCTTGCGGCGAACCGCGCTCTCATCGGTC
CCTTCATCGACGAAAGCCTTCGCCATAGCGGTCCGCCGCAACGCCTCTTCC
GCATCGCGACGCAGGATGTGGAGGTCGGCGGCGCCAGAATTTCGAAGGGC

GATTGGGTGGCGCTCTTCTTCGCCGCCGCCAACCACGATCCCGCCATGTTC
CCGGATCCGGAAAAGTTCGACATCTCTAGGCCTAACCTCAACAAGCAGCTC
ACCTTCGGCGTCGGCATCCACCACTGTCTGGGTTCGGCTCTCGCCCGCATG
GAGGGCAGGGCCCTCATCGAGGCGATCCTCGACCGGATGGACGATGTCTCT
CTCGGTGCGCTGCCGCCGGTGCCGCAGCGCGCCAGTCTTCTCAATCACGGC
TTCGACAGTCTCACGCTCCGCTTCACCGCCCGGGAGGATGAAACGCAATG
A

P450PL2 amino acid sequence:

MQEIRKSDRADDLAALVAALPAGDTIASPYALYDRLRPYGPVYGYRDYPPGT
VPDADEAVTAWVLLNYDHVSAAARDHRIFSSRDPLQEQSSAPTLMLVNHDNP
EHDRLRSIVNLAFSRPRIEALDPWVREIVGGMVAGLGDGDTEVMEALAARIPA
RIMVGLLGLPEEVVDRFRHWATAFMLSADLDPAEREASNAELVRYFTETVDSL
YGALEAGDPVPDGLIAALLKAEVDGEQLTLDEVIRFCITLVVAGSETTTFLLGN
LLHNLAVMPDIRAQLAANRALIGPFIDESLRHSGPPQRLFRIATQDVEVGGARI
SKGDWVALFFAAANHDPAMFPDPEKFDISRPNLNKQLTFGVGIHHCLGSALAR
MEGRALIEAILDRMDDVSLGALPPVPQRASLLNHGFDSLTLRFTAREDETQ*

Fdr base sequence:

ATGAAGCCTTGGCAGATCGTCCTGACGATCACCGCCGTGAGTTTCGGCCTC
ACCATGATCGAAATTCCCGCAGGCACGTGGCTCAGCACCGCGGCGCTCAG
CCTCGCATGCGGCGTTGCCGCGCTCTCGCTCATGGCGGCGGCCGCCATCCT
TGCCGGCCGCTGGGGCTGGCCCGAGACCGCCCTTGGCGGGCTGGACCGCG
TTTACGCCGCTCACAAATGGCTCGCCGTCTACGCGCTGGCGCTCGCCTCGG
TGCATTTTCTCTTCAAGGCCGGCGATCCCTCATGGGCGGCCGAAAGCATCA
TGGCATTGCCGCAGGGCTGGACCCGCCTCGCGCGGCAGGCGAGCTTCGTC
GCGCTGATGAGCATCGTCATTCTCGCGCTCAACCGGAACATTCCCTACAGC
ACATGGCGCTGGTGGCATCGCCTGTCGGGGCCGCTCTTCCTGATCGTGATC
GTCCATTGGCTGAGCATCAAATCGCCCCTGGATCTCGTCAGCCCGGCCGGG
CTGTGGCTGGCCGGCCTTTCCGCACTCGGCATTGCCGCCGCCGCCTACAAG
CTGCTGCTCTATCCGTTTCTCGCCCGCCACGCCGACTACCGCGTTGTGAAG
GTTCTGCGCGGACCCTCGGCCGCCGAGATCGAGTTCGAGCCGGTAAAGCG

CGGCATCGATTTTCATGCGGGCCATTTCGGGTTCCTGCGCATGAAGGTGGA
CGGCCTGCGCGAGCCCCATCCCTTCACGATCGCCGCCGCTCCGGCACCGGA
CGGCAGGATCACCTTCGTGATCCGCGCACTCGGTGATTACACGGCGAAACT
GATCGCCGATGTCGAGCCGGGCATGGAGGCCGATGTCTATGCGCCTTACGG
GCGCTTCGAACGCAAGCCCGATTGCCGCCGCGAGATCTGGATCGGCGGCG
GCGTCGGCATATCGCCGTTCATTGCCTGGATGCGGGATGAGCAGAAAGGCG
GCTTCGCAAACGTATCGCTCTTCTACTTCTTCACGCCCGGCCGTGTATTTCC
CGACATCGATGTGTTGCGGAAGATGGCCGAAGAACGCGGCATCGAATTCGT
TCCCGTTTCCGGCGGTCCCGGGTCACGCGACTTCATCGACAGATTCGGCGA
GATCGTCCGGGATACGGCGCCGGGCACGCCCGACATCGCCCTCTGCGGTCC
TGCGGGACTGCTGGAGAGCGTGCGCGGGCTGGCCAGGGAGAATGGCCTCG
ATCCCGCCTGCATCCGCCATGAACTCTTTCAGTTCCGTTGA

Fdr amino acid sequence:

MKPWQIVLTITAVSFGLTMIEIPAGTWLSTAALSLACGVAALSLMAAAAILAGR
WGWPETALGGLDRVYAAHKWLAVYALALASVHFLFKAGDPSWAAESIMALP
QGWTRLARQASFVALMSIVILALNRNIPYSTWRWWHRLSGPLFLIVIVHWLSI
KSPLDLVSPAGLWLAGLSALGIAAAAYKLLLYPFLARHADYRVVKVLRGPSA
AEIEFEPVKRGIDFHAGHFGFLRMKVDGLREPHPFTIAAAPAPDGRITFVIRAL
GDYTAKLIADVEPGMEADVYAPYGRFERKPDCRREIWIGGGVGISPFIAWMR
DEQKGGFANVSLFYFFTPGRVFPDIDVLRKMAEERGIEFVPVSGGPGSRDFIDR
FGEIVRDTAPGTPDIALCGPAGLLESVRGLARENGLDPACIRHELFQFR*

Fdx1 base sequence:

ATGGCGAAGATTACCTATATCGAACATGACGGCACCGAGCACACGATCGAG
GTGGCGAACGGCATCACGCTGATGGAAGCGGCGGTGAAGGCGAGCATTCC
CGGCATCGACGGCGATTGCGGCGGCGCCTGCGCTTGCGCCACCTGCATGGT
CTATGTGCCCGACGAATGGAAGCCGAAGCTGCCGGAAGTCGAGACGATGG
AAGAGACGATGCTCGACTTCTGCGAACACACGGAAGCGAACTCGCGGCTT
TCCTGCCAGCTTGTGGCGAGCGACGAGCTGGACGGGATCCGGCTGCAGAT
GCCGGAAAGCCAGCACTAG

Fdx1 amino acid sequence:

MAKITYIEHDGTEHTIEVANGITLMEAAVKASIPGIDGDCGGACACATCMVYV
PDEWKPKLPEVETMEETMLDFCEHTEANSRLSCQLVASDELDGIRLQMPESQ
H*

1.6. Primer design

Primers Name	Primers Sequence (5'-3')
P50-NDT-F	GATTACCCGNDTGGCACCGTGCCGGATGCGGACG
P50-NDT-R	CACGGTGCCAHNCGGGTAATCGCGGTAGCCATAGAC
P50-VHG-F	ATTACCCGVHGGGCACCGTGCCGGATGCGGACGAG
P50-VHG-R	GCACGGTGCCCDBCGGGTAATCGCGGTAGCCATAGAC
P50-TGG-F	GATTACCCGTGGGGCACCGTGCCGGATGCGGA
P50-TGG-R	CACGGTGCCCCACGGGTAATCGCGGTAGCCATAGAC
E89-NDT-F	CGCTGCAGNDTCAGTCCTCAGCGCCGACG
E89-NDT-R	GAGGACTGAHNCTGCAGCGGATCGCGCGAG
E89-VHG-F	CGCTGCAGVHGCAGTCCTCAGCGCCGA
E89-VHG-R	GACTGCDBCTGCAGCGGATCGCGCGAG
E89-TGG-F	CGCTGCAGTGGCAGTCCTCAGCGCCGACG
E89-TGG-R	GAGGACTGCCACTGCAGCGGATCGCGCGA
L96-NDT-F	GCCGACGNDTATGCTCGTGAACCACGACAA
L96-NDT-R	ACGAGCATAHNCGTCGGCGCTGAGGACTGCT
L96-VHG-F	CGACGVHGATGCTCGTGAACCACGACAATCCC
L96-VHG-R	ACGAGCATCDBCGTCGGCGCTGAGGACT
L96-TGG-F	GCCGACGTGGATGCTCGTGAACCACGACAA
L96-TGG-R	ACGAGCATCCACGTCGGCGCTGAGGACTGCT
V99-NDT-F	ATGCTCNDTAACCACGACAATCCCGAGCACGACC
V99-NDT-R	GTGGTTAHNGAGCATCAGCGTCGGCGCTGAGGACT
V99-VHG-F	ATGCTCVHGAACCACGACAATCCCGAGCACGACC
V99-VHG-R	TGGTTCDBGAGCATCAGCGTCGGCGCTGAGGACT
V99-TGG-F	ATGCTCTGGAACCACGACAATCCCGAGCA
V99-TGG-R	TGGTTCCAGAGCATCAGCGTCGGCGCTGAGG

Primers Name	Primers Sequence (5’-3’)
L109-NDT-F	GCACGACCGCNDTCGCAGCATCGTCAATCTC
L109-NDT-R	GATGCTGCGAHNGCGGTCGTGCTCGGGATTGT
L109-VHG-F	GCACGACCGCVHGCGCAGCATCGTCAATCTC
L109-VHG-R	GATGCTGCGCDBGCGGTCGTGCTCGGGATTGT
L109-TGG-F	GCACGACCGCTGGCGCAGCATCGTCAATCTC
L109-TGG-R	GATGCTGCGCCAGCGGTCGTGCTCGGGATTGT
T179-NDT-F	TGGGCGNDTGCCTTCATGCTGTCCGC
T179-NDT-R	AGGCAHNCGCCCAATGACGAAACCGGTC
T179-VHG-F	TGGGCGVHGGCCTTCATGCTGTCCGC
T179-VHG-R	AGGCCDBCGCCCAATGACGAAACCGGTC
T179-TGG-F	TGGGCGTGGGCCTTCATGCTGTCCGC
T179-TGG-R	AGGCCCACGCCCAATGACGAAACCGGTC
M182-NDT-F	ACGGCCTTCNDTCTGTCCGCCGATCTCGATCCC
M182-NDT-R	TCGGCGGACAGAHNGAAGGCCGTCGCCCA
M182-VHG-F	ACGGCCTTCVHGCTGTCCGCCGATCTCGAT
M182-VHG-R	TCGGCGGACAGCDBGAAGGCCGTCGCCCA
M182-TGG-F	ACGGCCTTCTGGCTGTCCGCCGATCTCGATCCC
M182-TGG-R	TCGGCGGACAGCCAGAAGGCCGTCGCCCAATG
T249-NDT-F	TGTATCNDTCTCGTTGTCGCAGGCTCGGA
T249-NDT-R	CAACGAGAHNGATACAGAAGCGGATCACTTCAT
T249-VHG-F	TCTGTATCVHGCTCGTTGTCGCAGGC
T249-VHG-R	CAACGAGCDBGATACAGAAGCGGATCACT
T249-TGG-F	TCTGTATCTGGCTCGTTGTCGCAGGC
T249-TGG-R	CAACGAGCCAGATACAGAAGCGGATCACT
V252-NDT-F	CACGCTCGTTNDTGCAGGCTCGGAAACGA
V252-NDT-R	TCCGAGCCTGCAHNAACGAGCGTGATACAG
V252-VHG-F	ACGCTCGTTVHGGCAGGCTCGGAAACGACAAC
V252-VHG-R	AGCCTGCCDBAACGAGCGTGATACAGAAG
V252-TGG-F	CACGCTCGTTTGGGCAGGCTCGGAAACGA
V252-TGG-R	TCCGAGCCTGCCCAAACGAGCGTGATACAG
A253-NDT-F	TCGTTGTCNDTGGCTCGGAAACGACAACC
A253-NDT-R	TCCGAGCCAHNGACAACGAGCGTGATAC

Primers Name	Primers Sequence (5’-3’)
A253-VHG-F	TCGTTGTCVHGGGCTCGGAAACGACAACC
A253-VHG-R	TCCGAGCCCDBGACAACGAGCGTGATACAGA
A253-TGG-F	TCGTTGTCTGGGGCTCGGAAACGACAACC
A253-TGG-R	TCCGAGCCCCAGACAACGAGCGTGATAC
G254-NDT-F	GTTGTCGCANDTTCGGAAACGACAACCT
G254-NDT-R	GTCGTTTCCGAAHNTGCGACAACGAGC
G254-VHG-F	TTGTCGCAVHGTCGGAAACGACAACCT
G254-VHG-R	GTCGTTTCCGACDBTGCGACAACGAGC
G254-TGG-F	GTTGTCGCATGGTCGGAAACGACAACCTT
G254-TGG-R	GTCGTTTCCGACCATGCGACAACGAGC
T257-NDT-F	CGGAANDTACAACCTTTCTCCTCGGCAACCTGCTG
T257-NDT-R	AAGGTTGTAHNTTCCGAGCCTGCGACAACGAGCG
T257-VHG-F	CGGAAVHGACAACCTTTCTCCTCGGCAACCTGCTG
T257-VHG-R	AAGGTTGTCDBTTCCGAGCCTGCGACAACGAGCG
T257-TGG-F	CGGAATGGACAACCTTTCTCCTCGGCAACCTGCTG
T257-TGG-R	AAGGTTGTCCATTCCGAGCCTGCGACAACGAGCG
P299-NDT-F	GCCATAGCGGTNDTCCGCAACGCCTCTTCCGCATCGCGAC
P299-NDT-R	GAGGCGTTGCGGAHNACCGCTATGGCGAAGGCTTTCGTC
P299-VHG-F	GCCATAGCGGTVHGCCGCAACGCCTCTTCCGCATCGCGA
P299-VHG-R	GAGGCGTTGCGGCDBACCGCTATGGCGAAGGCTTTCGTC
P299-TGG-F	GCCATAGCGGTTGGCCGCAACGCCTCTTCC
P299-TGG-R	GCGTTGCGGCCAACCGCTATGGCGAAGGCTT
P300-NDT-F	GTCCGNDTCAACGCCTCTTCCGCATCGCGACG
P300-NDT-R	GCGTTGAHNCGGACCGCTATGGCGAAGGCT
P300-VHG-F	GTCCGVHGCAACGCCTCTTCCGCATCGCGA
P300-VHG-R	TTGCDBCGGACCGCTATGGCGAAGGCT
P300-TGG-F	GTCCGTGGCAACGCCTCTTCCGCATCGCGA
P300-TGG-R	GCGTTGCCACGGACCGCTATGGCGAAGGCT
Q301-NDT-F	TCCGCCGNDTCGCCTCTTCCGCATCGCGACGCAG
Q301-NDT-R	AGAGGCGAHNCGGCGGACCGCTATGGCGAAGGCTTTC
Q301-VHG-F	CGGTCCGCCGVHGCGCCTCTTCCGCATCGCGA
Q301-VHG-R	GAAGAGGCGCDBCGGCGGACCGCTATGGCGAA

Primers Name	Primers Sequence (5’-3’)
Q301-TGG-F	CGGTCCGCCGTGGCGCCTCTTCCGCATCGCGA
Q301-TGG-R	GAAGAGGCGCCACGGCGGACCGCTATGGCGAA
R302-NDT-F	GTCCGCCGCAANDTCTCTTCCGCATCGCGA
R302-NDT-R	GCGGAAGAGAHNTTGCGGCGGACCGCTA
R302-VHG-F	GTCCGCCGCAAVHGCTCTTCCGCATCGCGA
R302-VHG-R	GCGGAAGAGCDBTTGCGGCGGACCGCTAT
R302-TGG-F	GTCCGCCGCAATGGCTCTTCCGCATCGCGA
R302-TGG-R	GCGGAAGAGCCATTGCGGCGGACCGCTA
L303-NDT-F	AACGCNDTTTCCGCATCGCGACGCAGGATG
L303-NDT-R	TGCGGAAAHNGCGTTGCGGCGGACCGCTAT
L303-VHG-F	CGCAACGCVHGTTCCGCATCGCGACGCAGGAT
L303-VHG-R	GATGCGGAACDBGCGTTGCGGCGGACCGCT
L303-TGG-F	CGCAACGCTGGTTCCGCATCGCGACGCAGGATGT
L303-TGG-R	GATGCGGAACCAGCGTTGCGGCGGACCGCT
F304-NDT-F	CAACGCCTCNDTCGCATCGCGACGCAGGATGTG
F304-NDT-R	CGCGATGCGAHNGAGGCGTTGCGGCGGACCGCTAT
F304-VHG-F	CAACGCCTCVHGCGCATCGCGACGCAGGATGTGGA
F304-VHG-R	CGCGATGCGCDBGAGGCGTTGCGGCGGACCGCTA
F304-TGG-F	CAACGCCTCTGGCGCATCGCGACGCAGGATGTGGA
F304-TGG-R	CGCGATGCGCCAGAGGCGTTGCGGCGGACCGCTA
S401-NDT-F	GCAGCGCGCCNDTCTTCTCAATCACG
S401-NDT-R	ATTGAGAAGAHNGGCGCGCTGCGGCAC
S401-VHG-F	GCAGCGCGCCVHGCTTCTCAATCACGGC
S401-VHG-R	ATTGAGAAGCDBGGCGCGCTGCGGCACC
S401-TGG-F	GCAGCGCGCCTGGCTTCTCAATCACGG
S401-TGG-R	ATTGAGAAGCCAGGCGCGCTGCGGCACC
L403-NDT-F	AGCGCGCCAGTCTTNDTAATCACGGCTTCGACA
L403-NDT-R	AGCCGTGATTAHNAAGACTGGCGCGCTGCGGCA
L403-VHG-F	CGCCAGTCTTVHGAATCACGGCTTCGACAG
L403-VHG-R	AGCCGTGATTCDBAAGACTGGCGCGCTGC
L403-TGG-F	AGCGCGCCAGTCTTTGGAATCACGGCTTCGACA
L403-TGG-R	AGCCGTGATTCCAAAGACTGGCGCGCTGCGGCA

1.7. Quantification the concentrationof P450PL2 and its mutants

Preparation of Crude Enzyme Extract: P450PL2 (WT) and its mutant strains were cultured, then cells were resuspended in phosphate buffer (PB, 50 mM, pH 7.5) to achieve a cell density of 15 g dcw/L. The cell suspension was frozen at -20 °C for 12 h to weaken the cell wall integrity, thereby facilitating subsequent protein release. After thawing in a water bath, lysozyme and DNase I stock solutions were added to the suspension to reach final concentrations of 1 mg/mL and 5 μg/mL, respectively. The mixture was incubated in a temperature-controlled shaker at 30 °C and 150 rpm for 3 h to ensure complete cell lysis. The lysate was then centrifuged at 9,000 rpm for 20 min at 4 °C. The supernatant (crude enzyme extract) was immediately transferred to ice to prevent protein denaturation and subjected to subsequent analyses.

CO-Difference Spectral Scanning: The quantification of P450 enzyme concentration in this study was performed according to the method described by Qian et al. (2009).[6] A UV-visible spectrophotometer was utilized with two quartz cuvettes, as the instrument requires only a single blank reference for spectral calibration.

Procedure for Dataset A (Reduced Protein Spectrum): A quartz cuvette was loaded with 3 mL of the obtained cell lysate[7], wiped clean, and placed in the reference cell holder to perform baseline correction by scanning over the 400–500 nm wavelength range. After baseline calibration, the cuvette was removed, and approximately 3 mg of sodium dithionite ($Na_2S_2O_4$) was added. The mixture was homogenized by repeated pipetting, wiped clean again, and rescanned within the same wavelength range to acquire and save the reduced protein spectrum.

Procedure for Dataset B (CO-Bound P450 Spectrum): A second clean quartz cuvette was loaded with 3 mL of the obtained supernatant. CO gas was gently infused into the solution for 3 minutes in a fume hood, accompanied by continuous stirring to maximize gas-protein interaction. Subsequently, approximately 3 mg of $Na_2S_2O_4$ was added and homogenized via pipette aspiration to reduce the enzyme. The cuvette was wiped clean, inserted into the spectrophotometer, and subjected to iterative scanning across the 400–500 nm range until spectral stabilization at 450 nm (indicating complete CO-heme

complex formation). The CO-ligated reduced P450 spectrum was recorded and archived.

Calculation of P450PL2 and mutants Concentrations: The enzyme concentration was determined by subtracting Dataset A from Dataset B to generate Dataset C. A CO-difference spectral curve was plotted from Dataset C, exhibiting a characteristic absorption peak at 450 nm. The enzyme concentration was calculated using the absorbance difference between 450 nm and 490 nm in Dataset C, based on the Beer-Lambert law:

$$\mathrm{P450(\mu M)} = \frac{\mathrm{A450} - \mathrm{A490}}{\varepsilon \times l}$$

Where ε=91mM^{-1}cm^{-1} (CO difference extinction coefficient) and *l*=1cm (path length).

1.8. X-Ray Crystallography

Expression and purification of P450PL2

The P450PL2 gene coding was inserted into the pET-28b(+) expression vector. The protein was overexpressed in the *E. coli* Rossetta (DE3) strain by initially growing cells at 37 ℃ to an absorbance of 0.8 at A600, and inducing by addition of 0.5 mM IPTG and overnight growth at 16 ℃. Cells were disrupted by sonication in buffer A (20 mM Tris-HCl (pH 8.0), 350 mM NaCl, and 1 mM PMSF) and the supernatant applied to a Nickel column equilibrated with buffer A, washed with buffer A, and the P450PL2 protein eluted with 250 mM imidazole in buffer A. P450PL2-containing fractions were concentrated by microfiltration and applied to a Superdex-200 gel-filtration column in buffer B (10 mM Tris-HCl (pH 8.0), 100 mM NaCl, 1 mM DTT). Purified P450PL2 was judged to be greater than 99% pure by SDS-PAGE and concentrated by microfiltration to 10 mg/ml.

Crystallization and structure determination

Crystals of P450PL2, grown using hanging drop vapor diffusion by mixing equal volumes of protein and a buffer solution containing 1.26 M Sodium phosphate monobasic monohydrate, 0.14 M Potassium phosphate dibasic at temperature 291 K. Crystals were rapidly soaked in the reservoir solution supplemented with 20% glycerol

as cryo-protectant, mounted on loops, and flash-cooled at 100 K in a nitrogen gas cryo-stream. Crystals Diffraction data was collected from a single crystal at Shanghai Synchrotron Radiation Facility (SSRF) BL18U beamline, China, with a wavelength of 0.9793 Å at 100 K. The diffraction data were processed and scaled with HKL-3000.[8] Relevant statistics were summarized in Supplementary Table 2.

The structure was solved by the molecular replacement method and Cytochrome $P450_{terp}$ (PDB entry 1CPT) was used as the starting model.[9] Initial model was build using PHENIX.autobuild.[10] Manual adjustment of the model was carried out using the program COOT[11] and the models were refined by PHENIX.refinement[10] and Refmac.[12] Stereochemical quality of the structures was checked by using PROCHECK.[13] All of residues locate in the favored and allowed region and none in the disallowed region. Refinement resulted in a model with excellent refinement statistics and geometry (Supplementary Table 2).

Database accession number

The coordinates of the P450PL2 have been deposited with the Rutgers Collaborative Structural Bioinformatics database (Protein Data Bank) under accession number 9LW0.

1.9. QM calculations

All quantum mechanical calculations, including full geometry optimizations, transition state (TS) characterizations, and single-point energy evaluations, were performed using the Gaussian 16 software suite.[14] Geometry optimizations employed the unrestricted hybrid Becke three-parameter Lee-Yang-Parr (B3LYP) density functional theory (DFT) formalism, a benchmarked methodology for iron-containing haem systems in prior literature. To account for relativistic effects in iron (Fe), the LANL2DZ effective core potential (ECP) and its accompanying valence basis set were implemented. For non-metal atoms (S, O, N, C, H), geometry optimizations utilized the 6-31G(d) split-valence polarized basis set, while higher-accuracy single-point energy calculations were conducted with the triple-zeta 6-311+G(d,p) basis set, incorporating

diffuse and polarization functions. Thermodynamic corrections (enthalpic and entropic contributions) to Gibbs free energy were derived from vibrational frequency analyses under the harmonic oscillator approximation. Stationary point characterization was rigorously validated by inspecting the Hessian matrix eigenvalue spectrum: minima exhibited no imaginary frequencies, whereas transition states displayed a single imaginary frequency corresponding to the reaction coordinate. Frequency scaling approximations were intentionally omitted to preserve intrinsic quantum chemical accuracy. Connectivity of critical transition states was confirmed via mass-weighted intrinsic reaction coordinate (IRC) calculations, executed through a Hessian-informed predictor-corrector integration algorithm. This protocol ensured unambiguously mapped reaction pathways between designated reactants and products

1.10. Molecular dynamics simulations

The iron-oxo intermediate involved in the cytochrome catalyzed oxidative hydroxylation cycle was used to model the active form of the P450 cofactor [15]. Simulations were performed using the GPU code (pmemd) of the AMBER 22 software package [16]. The structure of P450PL2 (PDB ID: 9LW0) was used as the starting point for the preparation of the MD simulations. The L96I, L109I, A253T, P300L, and L303S mutations were manually introduced using Pymol v.1.8.2. The Amber-compatible parameters developed by Cheatham et al. [17] were used for Cpd I and its axial Cys ligand. Substrate **1a** parameters for the molecular dynamics (MD) simulations were generated within the antechamber module of AMBER 22 using the general AMBER force field (GAFF) [18], with partial charges set to fit the electrostatic potential generated at the HF/6-31G(d) level by the restrained electrostatic potential (RESP) model [19]. The charges were calculated according to the Merz-Singh-Kollman scheme [20,21] using Gaussian 16(C.01) [14]. Amino acid protonation states were predicted using the H++ server (http://biophysics.cs.vt.edu/H++)[22]. Then, the enzyme was solvated in a pre-equilibrated truncated hexagonal box with a 10-Å buffer of TIP3P [23] water molecules using the AMBER 22 leap module, resulting in the addition of ~19,000 solvent molecules. The systems were neutralized by addition of ions Na^+ and Cl^-, all

subsequent calculations were done using the Amber ff14SB force field [24]. The following MD simulation steps as reported in ref.[15], three independent 600 ns production trajectories MD simulations were performed after equilibrated. Binding free energy calculations. Based on the MD trajectories, a total of 600 snapshots were extracted to calculate the binding free energies of ligands within P450PL2 using the MM/GBSA method.[25]

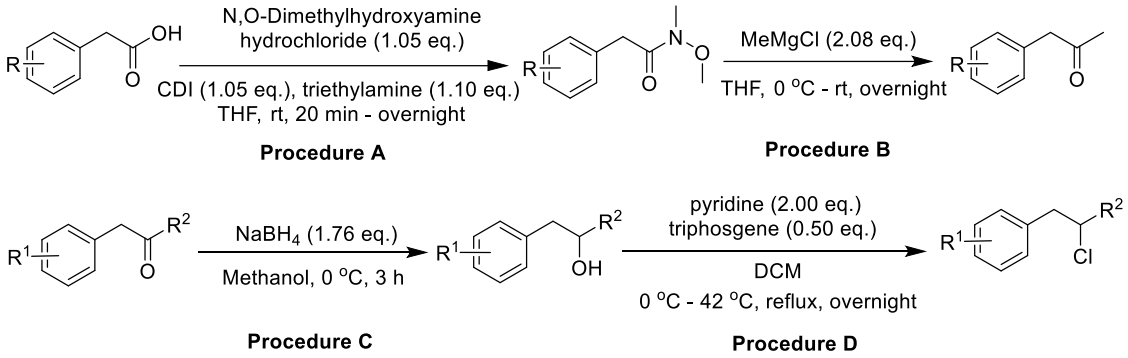
1.11. Gram-scale reactions of enantiomerization hydroxylation of halogenated compounds

General procedure: In a triangular 250 mL bottle, a resting cell suspension of *E. coli* (P450) at a concentration of 15 g cdw/L was prepared in 50 mL of PB buffer (50 mM, pH 7.5). To this suspension, 500 μL of halocompounds (*rac*)-**1** was added to a final concentration of 4 mM. The reaction mixture was then stirred at 25 °C. Upon completion of the enzymatic reaction, the mixture was subjected to extraction using ethyl acetate (3 × 50 mL). The organic phases were separated by centrifugation (9000 rpm, 3 min), combined, dried over anhydrous Na_2SO_4, and evaporated at reduced pressure. The resulting mixture was purified by flash chromatography (petroleum ether: ethyl acetate = 100:1 ~ 50:1) on silica gel to afford the desired enantiodivergent hydroxylation halocompounds (1*R*, 2*S*)-**2**.

2. Preparation of Substrates and Racemic Products

2.1 Synthesis of Substrates

Method 1



Procedure A[26]: Add tetrahydrofuran (THF, 40 mL) to a clean dry round-bottomed flask with stirrer. N, O-dimethylhydroxylamine hydrochloride (28.22 mmol, 1.05 equiv.) was added to the mixture, and then the corresponding substrate acid (26.88 mmol, 1.00 equiv.) and triethylamine (29.60 mmol, 1.10 equiv.) were added. The reaction mixture was stirred at room temperature for 20 min and then added N, N'-carbonyldiimidazole (CDI, 28.22 mmol, 1.05 equiv.). The final mixture was stirred overnight. After the reaction, the reaction was quenched with ice water, extracted with ethyl acetate for three times and dried with anhydrous Na_2SO_4. The organic solvent was evaporated under reduced pressure. The crude product was purification by silica gel column chromatography (Petroleum Ether:Ethyl Acetate=7:1) to afford the desired product.

Procedure B[26]: To the solution of product of procedure A (26.0mmol, 1.00 equiv.) in dry THF (30 mL), MeMgCl (18.0 mL, 3 M in THF) was added dropwise at 0 °C, then the final mixture was stirred overnight at room temperature. The mixture was carefully quenched by saturated NH_4Cl a.q., extracted with ethyl acetate for three times and dried with anhydrous Na_2SO_4. The organic solvent was evaporated under reduced pressure, the crude residue was used for the next step without further purification.

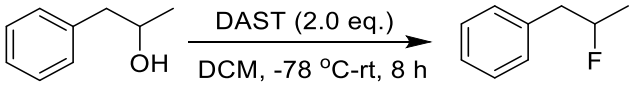
Procedure C[27]: To a stirred suspension of corresponding ketone (6.1 mmol, 1.00 equiv.) in methanol (22 mL), $NaBH_4$ (10.7 mmol, 1.76 equiv.) was added in batches under 0 °C and the resulting mixture was allowed to react at room temperature for 3 h. After that time, the reaction was quenched with water (10 ml) and extracted with CH_2Cl_2 (3 × 20

ml); after drying (anhydrous Na_2SO_4) the solvent was evaporated under vacuum, the crude residue was used for the next step without further purification.

Procedure D[28]: Add the corresponding alcohol (2.00 mmol, 1.00 equiv.) and anhydrous dichloromethane (15 mL) to a dry round-bottomed flask, the mixture was cooled to 0 ℃ and added pyridine (4.00 mmol, 2.00 equiv.) with a syringe followed by triphosgene (1.00 mmol, 0.50 equiv.) in one portion. Stir the solution for 5 min and warm to gentle reflux overnight. After that time, pour the reaction mixture into a separatory funnel containing 1 M HCl aqueous solution (30 mL) and shake the biphasic mixture vigorously, re-extract the aqueous layer with dichloromethane (3 × 15 mL) upon separation of layers. After drying the solvent with anhydrous Na_2SO_4, it was evaporated under vacuum, the crude product was purification by silica gel column chromatography (100% *n*-hexane) to afford the desired product.

Method 1 was used for the synthesis of substrates **1a**, **1d-1p**: the synthesis method of **1a** is procedure D; the synthesis methods of **1e, 1j** and **1p** are procedure A-B-C-D; except for the substrates specified above, the other substrate synthesis methods are procedure C-D.

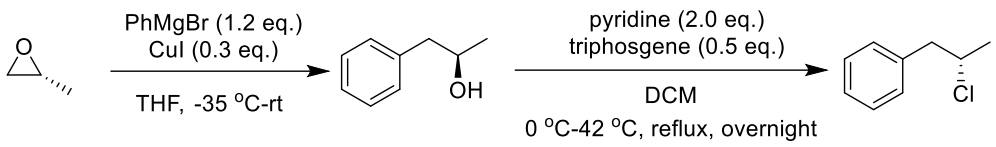
Method 2[29]



Diethylaminosulfur trifluoride (DAST, 7.6 mmol, 2.0 equiv.) was added to a solution of alcohol (3.7 mmol, 1.0 equiv.) in dichloromethane (10 mL) at -78 ℃. This solution was allowed to warm to room temperature gradually. After being stirred for 1 h at this temperature, the mixture was poured into an ice-cold aqueous dil. KOH solution (**Caution! Hydrogen fluoride was often evolved during this procedure**). Extraction with dichloromethane (3 × 10 mL), after drying the solvent with anhydrous Na_2SO_4, it was evaporated under vacuum. The crude product was purification by silica gel column chromatography (100% *n*-hexane) to afford the desired fluorides (Note: This material is easy to deteriorate, timely store to -20 ℃ refrigerator).

Method 2 was used for the synthesis of substrate **1b**.

Method 3



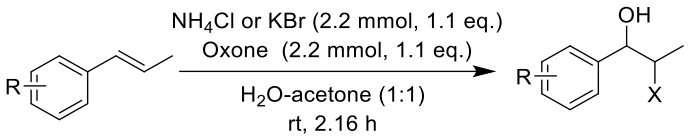
Procedure E **Procedure D**

Procedure E[30]: CuI (6.3 mmol, 0.3 equiv.) was added to the PhMgBr (90 mmol, 1.2 equiv., 3.0 M in THF) at -35 ℃. After stirring for 30 min, a solution of (*R*)-2-methyloxirane (20.8 mmol, 1.0 equiv.) was added dropwise by using a syringe, and stirring was continued for 30 min at -35 ℃ and for an additional 1 h at room temperature. The reaction mixture was poured into a cool solution of saturated NH_4Cl (aq). The aqueous layer was extracted with dichloromethane (3 × 30 mL). The combined organic layer was dried over Na_2SO_4, concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel (Petroleum Ether:Ethyl Acetate=5:1) to afford (*R*)-1-phenylpropan-2-ol. After (*R*)-alcohol underwent the reaction described in procedure D and was purified using *n*-hexane as the eluent, (*S*)-**1a** was obtained.

The preparation and purification method of (*R*)-**1a** is the same as that of (*S*)-**1a**, only by replacing (*R*)-2-methyloxirane with (*S*)-2-methyloxirane.

2.2 Synthesis of Racemic Products

Method 4



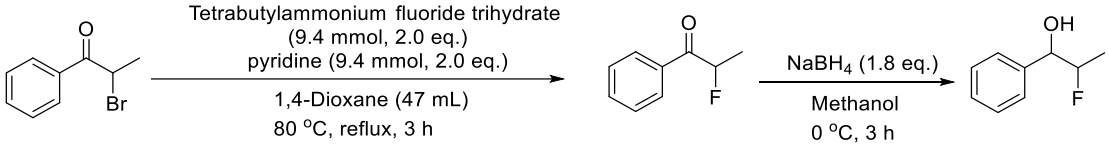
Procedure F

Procedure F[3]: Oxone (2.2 mmol, 1.1 equiv.) was slowly added to a well stirred solution of NH_4Cl or KBr (2.2 mmol, 1.1 equiv.) and the corresponding olefin (2.0 mmol, 1.0 equiv.) in acetone-H_2O (1:1; 10 mL) and the reaction mixture was allowed to stir at room temperature, until olefin was completely disappeared (monitored by TLC, eluent: Petroleum Ether-Ethyl Acetate). The organic layer was separated, and the aqueous phase was extracted with ethyl acetate (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using Petroleum

Ether-Ethyl Acetate (5:1) as eluent to give desired products.

Method 4 was used for the synthesis of racemic products **2a**, **2c** and **2m**. The synthesis of **2c** only needs to replace NH_4Cl with KBr.

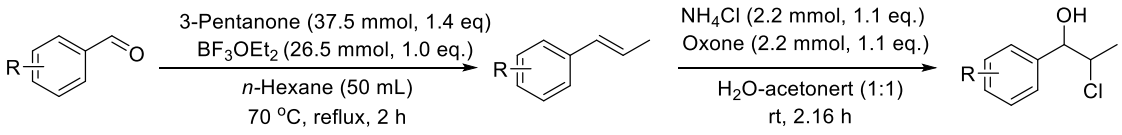
Method 5



Procedure G[31]: To a round-bottomed flask containing a stir bar, add 2-bromopropiophenone (4.7 mmol, 1.0 equiv.), tetrabutylammonium fluoride trihydrate (9.4 mmol, 2.0 equiv.), pyridine (9.4 mmol, 2.0 equiv.), and 1,4-dioxane (47 mL). Reflux the mixture at 80 °C for 24 hours. After the reaction was completed, quench the reaction by acidifying the solution with 2 M HCl aqueous solution, and the aqueous phase was extracted with ethyl acetate. The combined organic layers were dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using Petroleum Ether-Ethyl Acetate (50:1) as eluent to give desired products. The product obtained from procedure G was synthesized and purified according to the method described in procedure C, resulting in the corresponding product standard.

Method 5 was used for the synthesis of racemic product **2b**.

Method 6

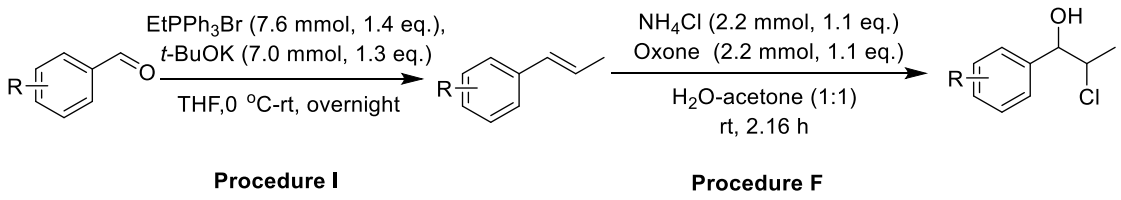


Procedure H[32]: To a round-bottomed flask containing a stir bar, add the corresponding aldehyde (41.5 mmol, 1.6 equiv.), 3-pentanone (37.5 mmol, 1.4 equiv.), *n*-hexane (50 mL), and a solution of boron trifluoride diethyl etherate (BF_3OEt_2) (26.5 mmol, 1.0 equiv.). Then, reflux the mixture at 70 °C for 2 hours. After the reaction was completed, cool the mixture to room temperature and quench it by adding water. The mixture was then extracted three times with ethyl acetate (3 × 10 mL) and dried over anhydrous

Na_2SO_4, and concentrated under reduced pressure. The crude residue was purified by column chromatography on silica gel using petroleum ether as eluent to give products. The olefin obtained from procedure H was synthesized and purified according to the method described in procedure F, resulting in the corresponding product standard.

Method 6 was used for the synthesis of racemic products **2d, 2e, and 2g**.

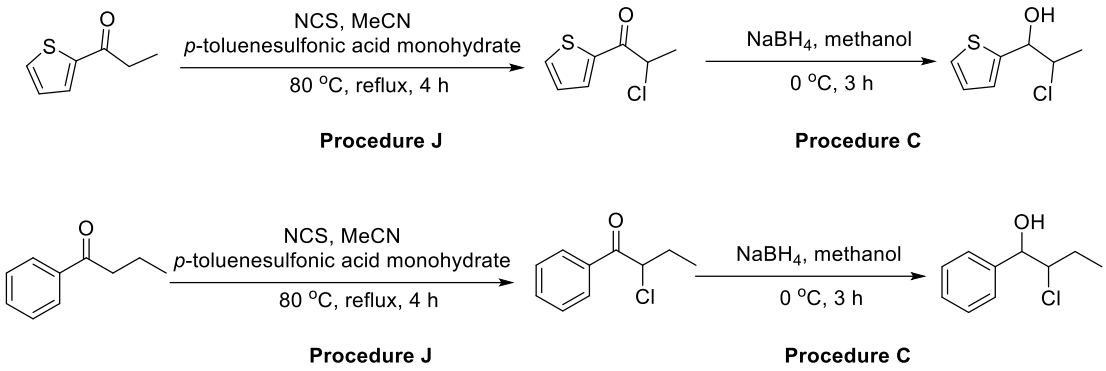
Method 7



Procedure I[33]: Add methyltriphenylphosphonium bromide ($EtPPh_3Br$, 7.6 mmol, 1.4 equiv.) and potassium tert-butoxide (*t*-BuOK, 7.0 mmol, 1.3 equiv.) to a clean dry round-bottomed flask with stirrer. Then, tetrahydrofuran (THF, 27 mL) was added at 0 °C, followed by stirring at 0 °C for 1 hour. Subsequently, the corresponding aldehyde (5.4 mmol, 1.0 equiv.) was slowly added dropwise. After the completion of the addition, the reaction mixture was allowed to warm to room temperature and stirred overnight. After the reaction was completed, the reaction was quenched by slowly adding saturated NH_4Cl solution to the reaction mixture. The mixture was then extracted three times with ethyl acetate (3 × 10 mL) and dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude residue was purified by column chromatography on silica gel using petroleum ether as eluent to give products. The olefin obtained from procedure I was synthesized and purified according to the method described in procedure F, resulting in the corresponding product standard.

Method 7 was used for the synthesis of racemic products **2f**, **2h**-**2l** and **2o**.

Method 8



Procedure J[34]: A round-bottom flask equipped with a stir bar was charged with the corresponding ketone (67.0 mmol, 1.0 equiv.), *p*-toluenesulfonic acid monohydrate (100.5 mmol, 1.5 equiv.), and acetonitrile (150 mL). The mixture was refluxed at 80 °C for 4 h. After completion, the reaction was cooled to room temperature, quenched with water, and extracted three times with dichloromethane. The combined organic layers were dried over anhydrous Na_2SO_4, and the solvent was removed under reduced pressure to yield a concentrated crude product. Purification by silica gel column chromatography using petroleum ether-ethyl acetate (80:1) as the eluent followed by concentration afforded the target product.

The products obtained from procedure J were synthesized and purified according to the method described in procedure C, resulting in the corresponding product standard.

Method 8 was used for the synthesis of racemic products **2n** and **2p**.

3. Supplementary Tables

Supplementary Table 1. Enzymes are screened for enantioselective hydroxylation and divergent kinetics of (*rac*)-**1a**

P450s[a]	*er* of **2a**[b,c]	*dr* of **2a**[b,c]	Yield (%)[b]
P450pyr	-	-	*trace*
P450pyr-D1	-	-	*trace*
P450pyr-D2	-	-	*trace*
P450tol	-	-	*trace*
P450PL7-1	71:29	80:20	17
P450PL2-1	73.5:26.5	85:15	72
WP_161883678.1	98:2	54:46	48
P450DA-M3	98:2	53:47	70
P450DA	99:1	57:43	27
P450PD	-	-	*trace*
P450HB	-	-	*trace*
P450CL	99:1	53:47	48
A0A2T4VPV1	94:6	59:41	34
P450DG	99:1	57:43	38
A0A5C4VXA4	98:2	53:47	58

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was10 g dcw/L, substrate concentration was 2 mM, reaction was taken at 30 °C and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er* and *dr* of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20min, 214 nm). [c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 2. Summary of data collection and refinement statistics for P450PL2

P450PL2	
PDB code	9LW0
Data collection	
Temperature (K)	100
Wavelength (Å)	0.979
Space group	P41 (number 76)
a,b,c (Å)	56.7900 56.7900 112.5200
α,β,γ (°)	90.0000 90.0000 90.0000
Resolution (Å)	50.70-2.10 (2.25-2.10)
No. of observations	129054
No. of unique reflections	18344
Completeness (%)	99.8 (99.8)
<I>/δ(I)	8.7 (2.2)

Redundancy	7.0 (7.2)
R_{merge}	0.214 (1.130)
$R_{p.i.m}$	0.132 (0.681)
Structure refinement	
R_{work} /R_{free}	0.173 / 0.214
No. atoms	2626
Protein	2391
Ligand/ion	3
Water	232
B-factors	
Protein	26.105
Ligand/ion	46.880
Water	33.093
Ramachandran	
Favored (%)	97.69
Allowed (%)	2.31
Outlier (%)	0
R.m.s. deviations	
Bond lengths (Å)	0.0152
Bond angles (°)	1.6447

Supplementary Table 3. Beneficial mutant of P450PL2 single point saturation mutation

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
PL2-2(WT)	74:26	88:12	50	1*R*,2*S*
E89R	76:24	92:8	20	1*R*,2*S*
E89G	80:20	93:7	17	1*R*,2*S*
V99G	92:8	96:4	15	1*R*,2*S*
L109F	76:24	87:13	53	1*R*,2*S*
L109I	78:22	93:7	33	1*R*,2*S*
L109R	70:30	90:10	56	1*R*,2*S*
L109W	73:27	84:16	65	1*R*,2*S*
T179P	68:32	91:9	43	1*R*,2*S*
M182C	58:42	93:7	14	1*R*,2*S*
T249L	70:30	89:11	40	1*R*,2*S*
T249P	84:16	90:10	8	1*R*,2*S*
T249E	71:29	97:3	13	1*R*,2*S*
T249V	77:23	88:12	46	1*R*,2*S*
T249M	75:25	90:10	50	1*R*,2*S*

V252N	78:22	95:5	13	1*R*,2*S*
A253G	74:26	94:6	49	1*R*,2*S*
A253P	79:21	89:11	20	1*R*,2*S*
G254L	84:16	94:6	15	1*R*,2*S*
G254Q	85:15	93:7	16	1*R*,2*S*
T257D	94:6	95:5	8	1*R*,2*S*
A281T	68:32	88:12	71	1*R*,2*S*
A281C	70:30	88:12	69	1*R*,2*S*
P300H	97:3	84:16	25	1*R*,2*S*
P300L	96:4	79:21	25	1*R*,2*S*
P300D	72:28	93:7	53	1*R*,2*S*
L303G	60:40	93:7	50	1*S*,2*R*
L303K	55:45	94:6	3	1*R*,2*S*
L303S	62:38	89:11	34	1*S*,2*R*
L303P	75:25	93:7	20	1*S*,2*R*
L303A	64:36	92:8	29	1*S*,2*R*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)] or *er* = [(1*S*,2*R*)]/[(1*R*,2*S*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 4. Beneficial mutant of iteration saturation mutation using P300H as template

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
P300H	97:3	84:16	25	1*R*,2*S*
P300H/E89D	97:3	89:11	12	1*R*,2*S*
P300H/L96V	98:2	94:6	4	1*R*,2*S*
P300H/V99I	98:2	92:8	10	1*R*,2*S*
P300H/L109C	98:2	90:10	14	1*R*,2*S*
P300H/L109K	97:3	94:6	9	1*R*,2*S*
P300H/L109N	97:3	93:7	7	1*R*,2*S*
P300H/L109A	97:3	93:7	12	1*R*,2*S*
P300H/T179E	97:3	90:10	10	1*R*,2*S*
P300H/T179K	97:3	89:11	16	1*R*,2*S*
P300H/T179Q	95:5	91:9	5	1*R*,2*S*
P300H/T179W	93:7	91:9	5	1*R*,2*S*
P300H/T179A	97:3	89:11	18	1*R*,2*S*

P300H/T249V	95:5	92:8	4	1*R*,2*S*
P300H/V252L	96:4	90:10	16	1*R*,2*S*
P300H/A253G	91:9	93:7	8	1*R*,2*S*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 5. Beneficial mutant of iteration saturation mutation using P300H as template

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
P300L	96:4	79:21	25	1*R*,2*S*
P300L/L96I	98:2	94:6	13	1*R*,2*S*
P300L/L96P	98:2	97:3	9	1*R*,2*S*
P300L/L96V	98:2	95:5	11	1*R*,2*S*
P300L/L96A	98:2	97:3	6	1*R*,2*S*
P300L/V99C	97:3	94:6	12	1*R*,2*S*
P300L/V99G	96:4	96:4	12	1*R*,2*S*
P300L/L109C	98:2	88:12	16	1*R*,2*S*
P300L/T179M	97:3	81:19	41	1*R*,2*S*
P300L/T179G	96:4	78:22	48	1*R*,2*S*
P300L/T249V	95:5	85:15	24	1*R*,2*S*
P300L/T249L	95:5	93:7	13	1*R*,2*S*
P300L/V252A	98:2	85:15	19	1*R*,2*S*
P300L/V252G	96:4	92:8	10	1*R*,2*S*
P300L/V252N	98:2	88:12	9	1*R*,2*S*
P300L/T257F	85:15	83:17	trace	1*S*,2*R*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)] or *er* = [(1*S*,2*R*)]/[(1*R*,2*S*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 6. The screening results of CCM and site-saturation mutagenesis at dual sites using P450PL2 as a template

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
PL2-2(WT)	73:27	88:12	50	1*R*,2*S*
T249V/P300N	96:4	86:14	16	1*R*,2*S*

T249L/P300S	80:20	96:4	10	1*R*,2*S*
T249M/P300H	92:8	91:9	4	1*R*,2*S*
T249L/P300S	79:21	95:5	18	1*R*,2*S*
T249L/P300N	93:7	95:5	3	1*R*,2*S*
P300S/L303P	66:34	92:8	3	1*S*,2*R*
P300G/L303A	59:41	92:8	33	1*S*,2*R*
P300G/L303P	62:38	92:8	7	1*S*,2*R*
E89D/T179C/P300H	98:2	89:11	8	1*R*,2*S*
E89Y/P300H	97:3	91:9	7	1*R*,2*S*
E89S/A281D/P300H	97:3	90:10	3	1*R*,2*S*
A281G/P300L	97:3	85:15	12	1*R*,2*S*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)] or *er* = [(1*S*,2*R*)]/[(1*R*,2*S*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 7. The screening results of site-saturation mutagenesis at the L303 position using P450PL2 as a template

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
PL2-2(WT)	73:27	88:12	50	1*R*,2*S*
L303S	62:38	89:11	34	1*S*,2*R*
L303G	60:40	93:7	50	1*S*,2*R*
L303P	75:25	93:7	20	1*S*,2*R*
L303A	64:36	92:8	29	1*S*,2*R*
L303K	54:46	94:6	3	1*R*,2*S*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er, dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)] or *er* = [(1*S*,2*R*)]/[(1*R*,2*S*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 8. The screening results of iterative saturation mutagenesis using P450PL2-L303G as a template

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
L303G	60:40	93:7	50	1*S*,2*R*
L303G/L96F	62:38	91:9	50	1*S*,2*R*
L303G/L96W	73:27	91:9	19	1*S*,2*R*
L303G/V99P	68:32	91:9	15	1*S*,2*R*

L303G/V99P	72:28	91:9	10	1*S*,2*R*
L303G/A253S	62:38	96:4	36	1*S*,2*R*
L303G/L109V	65:35	93:7	28	1*S*,2*R*
L303G/T179Y	73:27	94:6	10	1*S*,2*R*
L303G/T179G	58:42	93:7	41	1*S*,2*R*
L303G/M182L	66:34	91:9	46	1*S*,2*R*
L303G/M182K	68:32	90:10	18	1*S*,2*R*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 °C and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er, dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*S*,2*R*)]/[(1*R*,2*S*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 9. The screening results of iterative saturation mutagenesis using P450PL2-L303G/L96W as a template

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
L303G/L96W	73:27	91:9	19	1*S*,2*R*
L303G/L96W/T249A	87:13	> 99:1	*trace*	1*S*,2*R*
L303G/L96W/L109D	79:21	93:7	3	1*S*,2*R*
L303G/L96W/L109V	78:22	93:7	2	1*S*,2*R*
L303G/L96W/L109A	80:20	94:6	4	1*S*,2*R*
L303G/L96W/E89D	77:23	93:7	3	1*S*,2*R*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 °C and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er, dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*S*,2*R*)]/[(1*R*,2*S*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 10. The screening results of iterative saturation mutagenesis using P450PL2-L303P as a template

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
L303P	75:25	93:7	20	1*S*,2*R*
L303P/G254E	76:24	96:4	3	1*S*,2*R*
L303P/G254Q	75:25	94:6	6	1*S*,2*R*
L303P/G254P	74:26	92:8	13	1*S*,2*R*
L303P/E89N	77:23	92:8	9	1*S*,2*R*
L303P/E89R	79:21	89:11	2	1*S*,2*R*
L303P/E89V	76:24	93:7	9	1*S*,2*R*
L303P/E89S	76:24	93:7	17	1*S*,2*R*

L303P/E89F	76:24	92:8	9	1*S*,2*R*
L303P/E89A	76:24	94:6	9	1*S*,2*R*
L303P/L109I	78:22	94:6	20	1*S*,2*R*
L303P/L109C	79:21	94:6	16	1*S*,2*R*
L303P/L109V	82:18	95:5	12	1*S*,2*R*
L303P/T179Y	82:18	> 99:1	2	1*S*,2*R*
L303P/A253T	90:10	92:8	3	1*S*,2*R*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*S*,2*R*)]/[(1*R*,2*S*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 11. The screening results of iterative saturation mutagenesis at the L303 position using P450PL2 mutants as templates

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
L109W/L303S	59:41	93:7	49	1*S*,2*R*
L109W/L303P	66:34	95:5	35	1*S*,2*R*
L109I/L303S	71:29	90:10	38	1*S*,2*R*
L109I/L303A	70:30	93:7	38	1*S*,2*R*
E89D/T179C/L303P	73:27	93:7	32	1*S*,2*R*
T179A/L303P	70:30	92:8	46	1*S*,2*R*
T179P/L303P	70:30	92:8	46	1*S*,2*R*
T249L/L303S	75:25	88:12	32	1*S*,2*R*
T249L/L303P	85:15	94:6	9	1*S*,2*R*
T249M/L303P	82:18	93:3	12	1*S*,2*R*
L109I/A253S/L303P	86:14	96:4	13	1*S*,2*R*
L109I/A253A/L303P	78:22	92:8	37	1*S*,2*R*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*S*,2*R*)]/[(1*R*,2*S*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 12. The screening results of iterative saturation mutagenesis using P450PL2-L109I/L303S as a template

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
L109I/L303S	71:29	90:10	38	1*S*,2*R*
L109I/L303S/A253S	75:25	93:7	31	1*S*,2*R*

L109I/L303S/A253V	92:8	82:18	6	1*S*,2*R*
L109I/L303S/A253T	94:6	86:14	15	1*S*,2*R*
L109I/L303S/V99P	81:19	88:12	11	1*S*,2*R*
L109I/L303S/T249L	78:22	88:12	21	1*S*,2*R*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*S*,2*R*)]/[(1*R*,2*S*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 13. The screening results of iterative saturation mutagenesis using P450PL2-L109I/L303S/A253S as a template

Mutants [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
L109I/L303S/A253S	75:25	93:7	31	1*S*,2*R*
L109I/L303S/A253S/L96L	73:27	92:8	31	1*S*,2*R*
L109I/L303S/A253S/L96V	75:25	94:6	11	1*S*,2*R*
L109I/L303S/A253S/T249L	76:24	86:4	16	1*S*,2*R*
L109I/L303S/A253S/T249I	75:25	94:6	4	1*S*,2*R*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*S*,2*R*)]/[(1*R*,2*S*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 14. Investigation of the optimal pH for reaction

pH [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
6.0	＞99:1	94:6	10	1*R*,2*S*
6.5	99:1	93:7	17	1*R*,2*S*
7.0	98.5:1.5	93:7	19	1*R*,2*S*
7.5	98:2	93:7	19	1*R*,2*S*
8.0	98:2	94:6	13	1*R*,2*S*
8.5	98:2	94:6	11	1*R*,2*S*

[a] All experiments were performed with resting cells in 5 mL system, cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 30 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 15. Investigation of the optimal reaction temperature

T (℃) [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
10	＞99:1	96:4	10	1*R*,2*S*
15	99:1	95:5	14	1*R*,2*S*
20	98.5:1.5	95:5	17	1*R*,2*S*
25	98:2	94:6	17	1*R*,2*S*
30	97.5:2.5	94:6	13	1*R*,2*S*
35	94.1±0.8	94:6	8	1*R*,2*S*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm). [c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 16. Investigation of the optimal reaction time

t (h) [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
0	-	-	-	-
2	＞99:1	94:6	19	1*R*,2*S*
6	＞99:1	94:6	23	1*R*,2*S*
10	＞99:1	93:7	23	1*R*,2*S*
12	＞99:1	93:7	24	1*R*,2*S*
24	99:1	93:7	24	1*R*,2*S*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm).[c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 17. Investigation of the optimal substrate concentration for the reaction

Concentration (mM) [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
1	99:1	92:8	23	1*R*,2*S*
2	＞99:1	92:8	27	1*R*,2*S*
4	＞99:1	93:7	20	1*R*,2*S*
6	＞99:1	94:6	10	1*R*,2*S*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), cell density was 10 g dcw/L, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation

reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm).[c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 18. Investigation of the optimal cell concentration for reaction

Cell dry weight (g dcw/L) [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
5	98.5:1.5	94:6	8	1*R*,2*S*
10	98.5:1.5	92:8	20	1*R*,2*S*
15	98.5:1.5	92:8	24	1*R*,2*S*
20	98.5:1.5	92:8	26	1*R*,2*S*
25	99:1	93:7	23	1*R*,2*S*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm).[c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 19. The influence of co-solvents on the yield

P450s	Organic solvents [a]	*er* [b,c]	*dr* [b,c]	Yield (%) [b]	Config. [b]
P300L/L96I	PB buffer	99:1	94:6	20	1*R*,2*S*
	pentane	98:2	96:4	3	1*R*,2*S*
	n-hexane	98:2	95:5	5	1*R*,2*S*
	dibutyl phthalate	98.5:1.5	84:16	7	1*R*,2*S*
	n-octane	98.5:1.5	93:7	5	1*R*,2*S*
	n-decane	99:1	94:6	6	1*R*,2*S*
	n-dodecane	98.5:1.5	93:7	6	1*R*,2*S*
	oleic acid	98.5:1.5	93:7	7	1*R*,2*S*
	n-tetradecane	98:2	94:6	5	1*R*,2*S*
	n-cetane	98:2	95:5	5	1*R*,2*S*
PL2-2	PB buffer	72.5:27.5	88:12	58	1*R*,2*S*
	pentane	81.5:18.5	90:10	19	1*R*,2*S*
	n-hexane	80:20	89:11	16	1*R*,2*S*
	dibutyl phthalate	77:23	89:11	14	1*R*,2*S*
	n-octane	84:16	89:11	26	1*R*,2*S*
	n-decane	84:16	89:11	30	1*R*,2*S*
	n-dodecane	83.5:16.5	88:12	30	1*R*,2*S*
	oleic acid	72.5:27.5	88:12	37	1*R*,2*S*
	n-tetradecane	83:17	88:12	30	1*R*,2*S*

	n-cetane	83:17	89:11	18	1*R*,2*S*

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), organic solvents (10%), substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (5 mL) were taken from biotransformation reactions. [b] The yield, *er*, *dr* and absolute configuration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane : *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm).[c] *er* = [(1*R*,2*S*)]/[(1*S*,2*R*)]; *dr* = [(1*R*,2*S*)+(1*S*,2*R*)]/[(1*R*,2*R*)+(1*S*,2*S*)].

Supplementary Table 20. Enzymatic reactions of enantiomerically pure substrates (*R*)-**1a** and (*S*)-**1a** with P450PL2 and mutants.

P450s[a]	**1a** config.	**(1*R*, 2*S*)-2a** (mM) [b]	**(1*R*, 2*R*)-2a** (mM) (mM) [b]	**(1*S*, 2*R*)-2a** (mM) [b]	**(1*S*, 2*S*)-2a** (mM) [b]
PL2-WT	*rac*	1.26±0.03	0.23±0.01	0.52±0.02	0.02±0.00
	R	0.01±0.00	0.25±0.00	0.59±0.00	-
	S	1.39±0.02	-	-	0.03±0.00
DS	*rac*	0.50±0.02	0.03±0.00	0.01±0.00	-
	R	-	0.13±0.01	0.03±0.00	-
	S	0.79±0.02	-	-	-
DR	*rac*	0.04±0.00	0.004±0.002	0.46±0.06	0.08±0.01
	R	-	0.01±0.00	0.37±0.10	-
	S	0.08±0.01	-	0.01±0.00	0.19±0.02

[a] All experiments were performed with resting cells in 5 mL system, PB (50 mM, pH 7.5), substrate concentration was 4 mM, reaction was taken at 25 ℃ and 250 rpm for 24 h. Samples (1 mL) were taken from biotransformation reactions. [b] The concentration of products were determined by chiral HPLC analysis (used a CHIRALCEL OD-H column, *n*-hexane: *i*-PrOH = 95 : 5, 0.8 mL/min, 20 min, 214 nm).

Supplementary Table 21. Energies, enthalpies, free energies, and entropies of the QM structures calculated for the heme iron catalyzed H-abstraction.

Structure [a]	E0 [b] (Hartree) [d]	ZPE [c] (Hartree /particle) [d,e]	H correction [c] (Hartree /particle) [d,f]	S [c] (cal mol-^{1}K^{-1}) [f]	G correction [c] (Hartree /particle) [d,f]
1*R*-2*R*-S	-3575.633498	0.495328	0.530982	231.360	0.421056
1*R*-2*R*-TS	-3575.594035	0.488817	0.523374	212.897	0.422219
1*R*-2*R*-P	-3575.641219	0.492959	0.528761	225.667	0.421539
1*R*-2*S*-S	-3575.633330	0.495115	0.530807	231.651	0.420742
1*R*-2*S*-TS	-3575.599578	0.488616	0.523286	213.187	0.421994
1*R*-2*S*-P	-3575.636098	0.492946	0.528832	226.355	0.421284
1*S*-2*R*-S	-3575.633396	0.495115	0.530802	230.529	0.421270
1*S*-2*R*-TS	-3575.598924	0.488906	0.523521	214.568	0.421573
1*S*-2*R*-P	-3575.638331	0.492572	0.528535	228.502	0.419967
1*S*-2*S*-S	-3575.633343	0.495133	0.530802	230.469	0.421299

1*S*-2*S*-TS	-3575.592589	0.488441	0.523156	214.224	0.421372
1*S*-2*S*-P	-3575.634682	0.492193	0.528227	229.358	0.419252

[a] All species correspond to duet spin states; all species are neutral.

[b] Energy obtained from single-point calculations with UB3LYP/6-311+G(d,p)+LANL2DZ(Fe).

[c] Vibrational, thermal and entropic corrections obtained from frequency calculations on geometries optimized at the UB3LYP/6-31G(d) level.

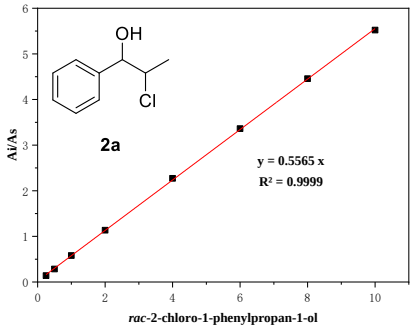
[d] 1 Hartree = 627.51 kcal mol^{-1}.

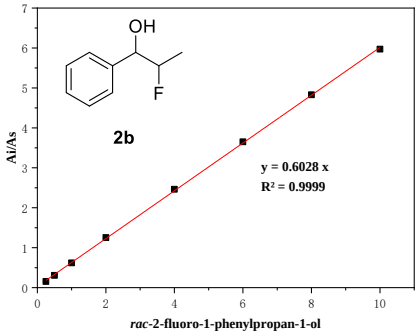
[e] Zero-point energy obtained from vibrational frequencies.

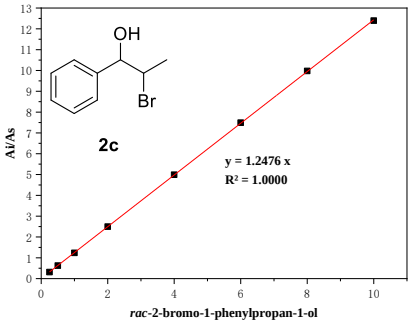
[f] Thermal corrections at 298.15 K.

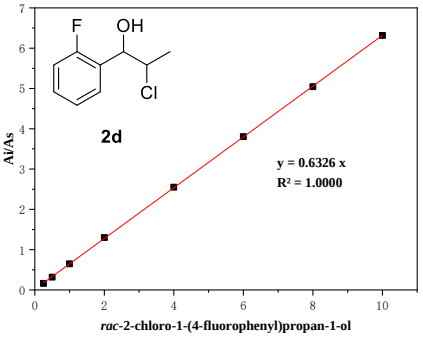
4. Supplementary Figures

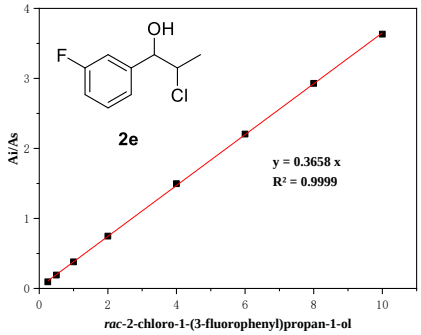
Supplementary Figure 1. Fig. HPLC standard curves of the products

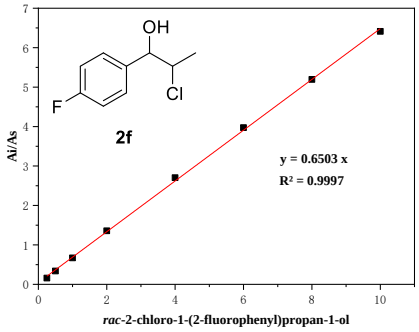


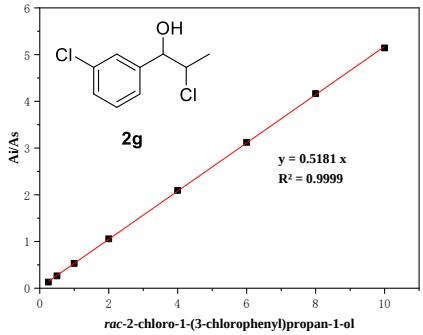


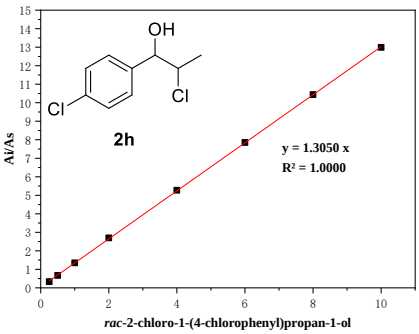


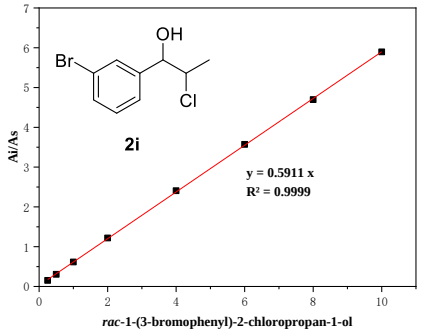


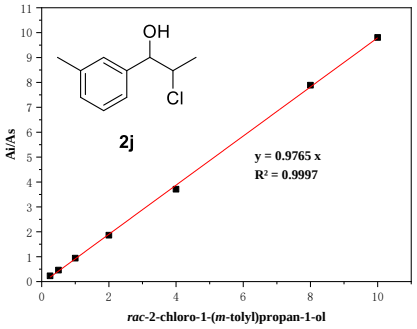


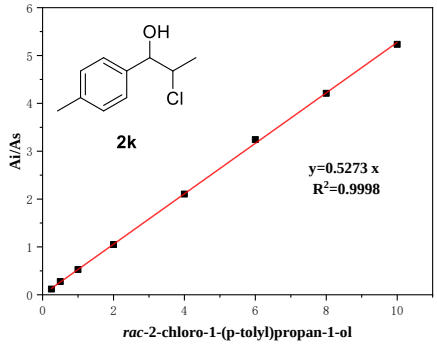


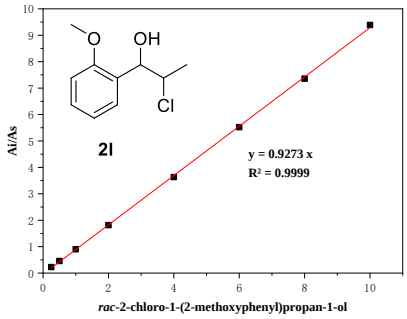


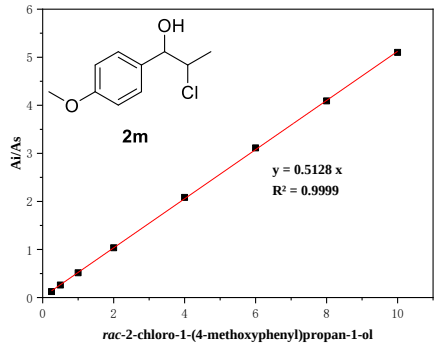


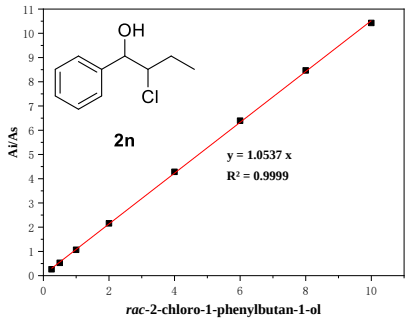

Br
OH
Cl
2i
y = 0.5911 x
R² = 0.9999
Ai/As
rac-1-(3-bromophenyl)-2-chloropropan-1-ol

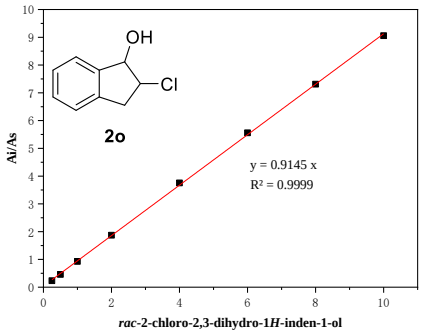

OH
Cl
2j
y = 0.9765 x
R² = 0.9997
Ai/As
rac-2-chloro-1-(m-tolyl)propan-1-ol

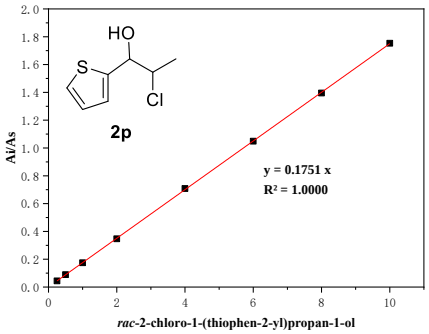

OH
Cl
2k
y=0.5273 x
R²=0.9998
Ai/As
rac-2-chloro-1-(p-tolyl)propan-1-ol


O
OH
Cl
2l
y = 0.9273 x
R² = 0.9999
Ai/As
rac-2-chloro-1-(2-methoxyphenyl)propan-1-ol

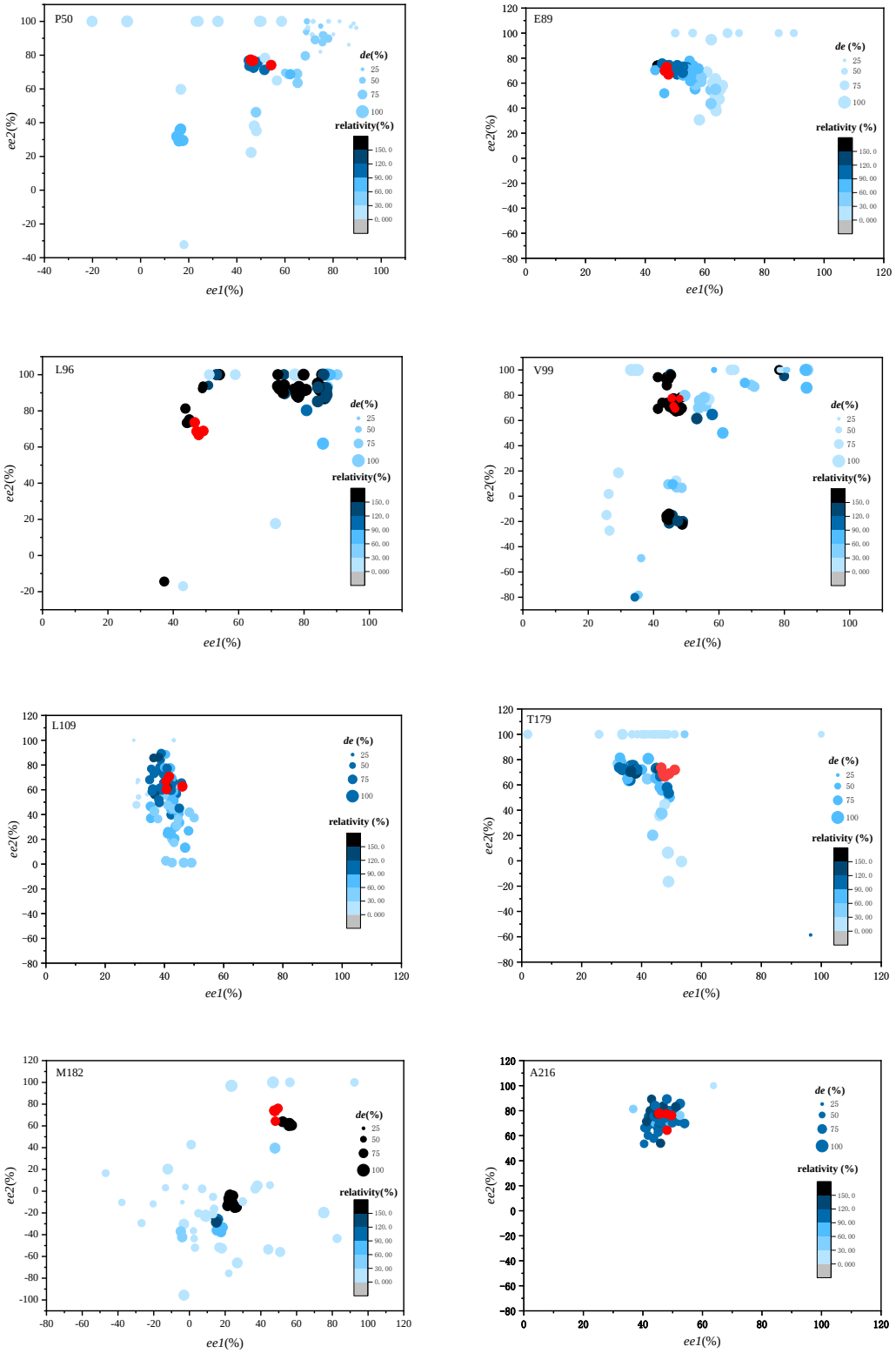

OH
O
Cl
2m
y = 0.5128 x
R² = 0.9999
Ai/As
rac-2-chloro-1-(4-methoxyphenyl)propan-1-ol

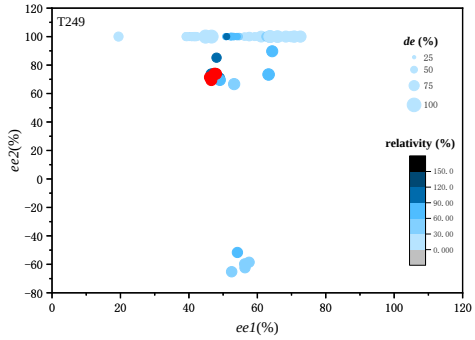

OH
Cl
2n
y = 1.0537 x
R² = 0.9999
Ai/As
rac-2-chloro-1-phenylbutan-1-ol

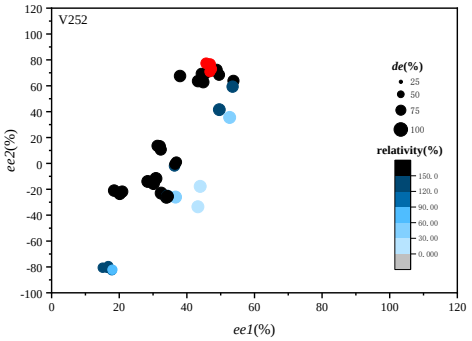

OH
Cl
2o
y = 0.9145 x
R² = 0.9999
Ai/As
rac-2-chloro-2,3-dihydro-1H-inden-1-ol

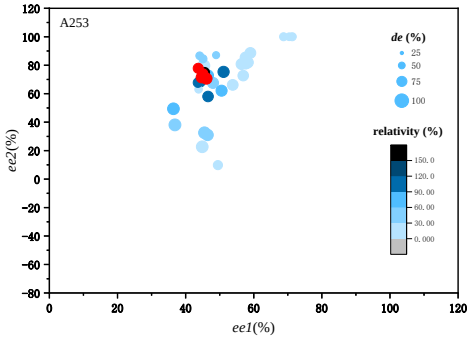

HO
S
Cl
2p
y = 0.1751 x
R² = 1.0000
Ai/As
rac-2-chloro-1-(thiophen-2-yl)propan-1-ol

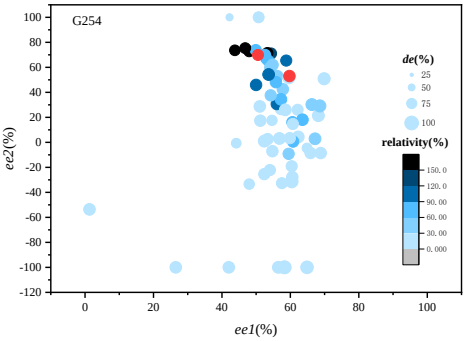
Supplementary Figure 2. The first-round single-site saturation mutagenesis scatter plot.

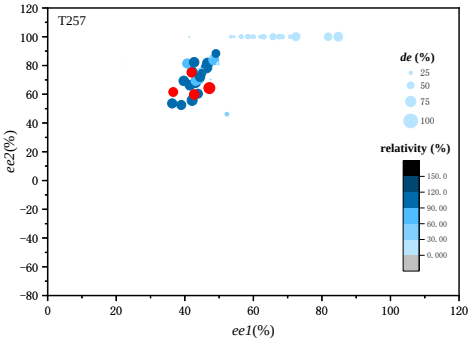


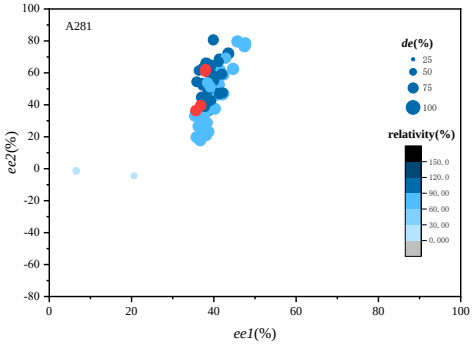

T249
de (%)
25
50
75
100
relativity (%)
150. 0
120. 0
90. 00
60. 00
30. 00
0. 000
ee2(%)
ee1(%)

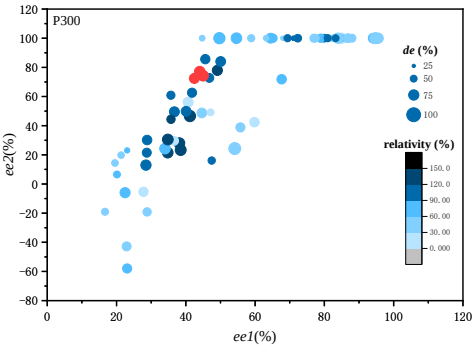

V252
de(%)
25
50
75
100
relativity(%)
150. 0
120. 0
90. 00
60. 00
30. 00
0. 000
ee2(%)
ee1(%)

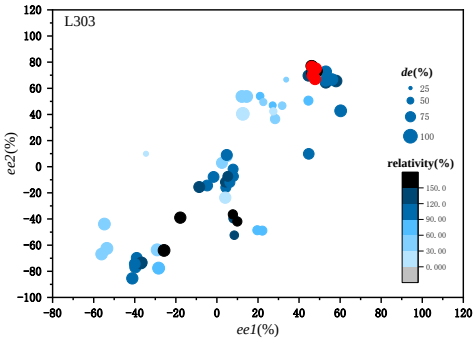

A253
de (%)
25
50
75
100
relativity (%)
150. 0
120. 0
90. 00
60. 00
30. 00
0. 000
ee2(%)
ee1(%)

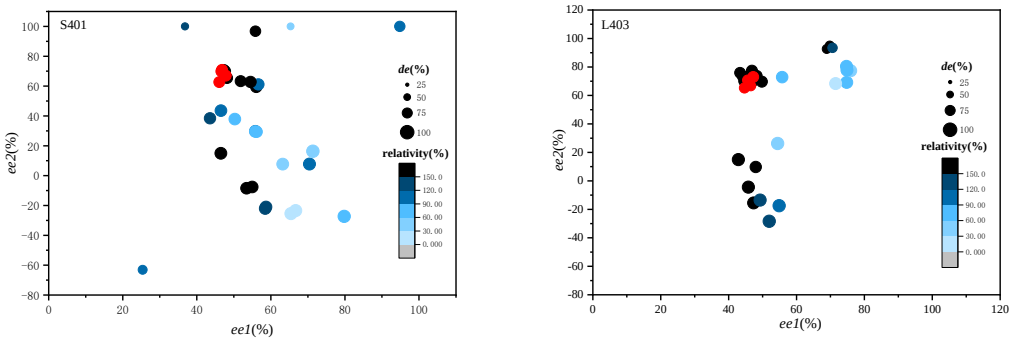

G254
de(%)
25
50
75
100
relativity(%)
150. 0
120. 0
90. 00
60. 00
30. 00
0. 000
ee2(%)
ee1(%)


T257
de (%)
25
50
75
100
relativity (%)
150. 0
120. 0
90. 00
60. 00
30. 00
0. 000
ee2(%)
ee1(%)

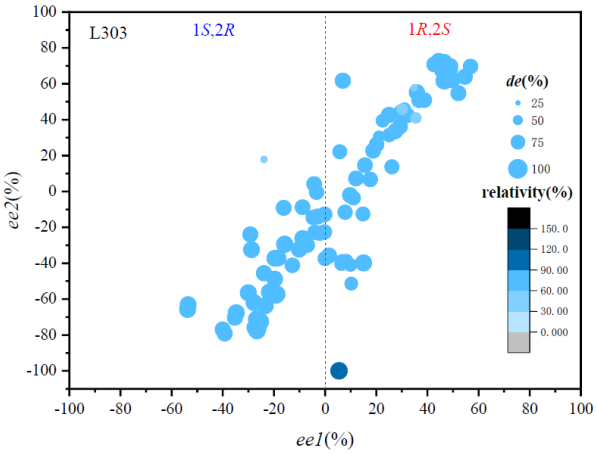

A281
de(%)
25
50
75
100
relativity(%)
150. 0
120. 0
90. 00
60. 00
30. 00
0. 000
ee2(%)
ee1(%)


P300
de (%)
25
50
75
100
relativity (%)
150. 0
120. 0
90. 00
60. 00
30. 00
0. 000
ee2(%)
ee1(%)

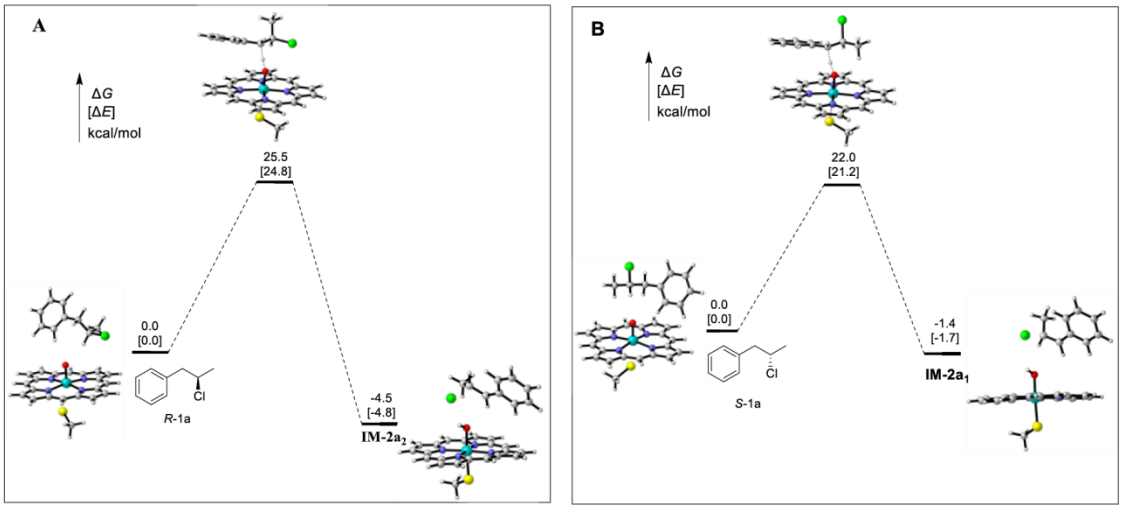

L303
de(%)
25
50
75
100
relativity(%)
150. 0
120. 0
90. 00
60. 00
30. 00
0. 000
ee2(%)
ee1(%)

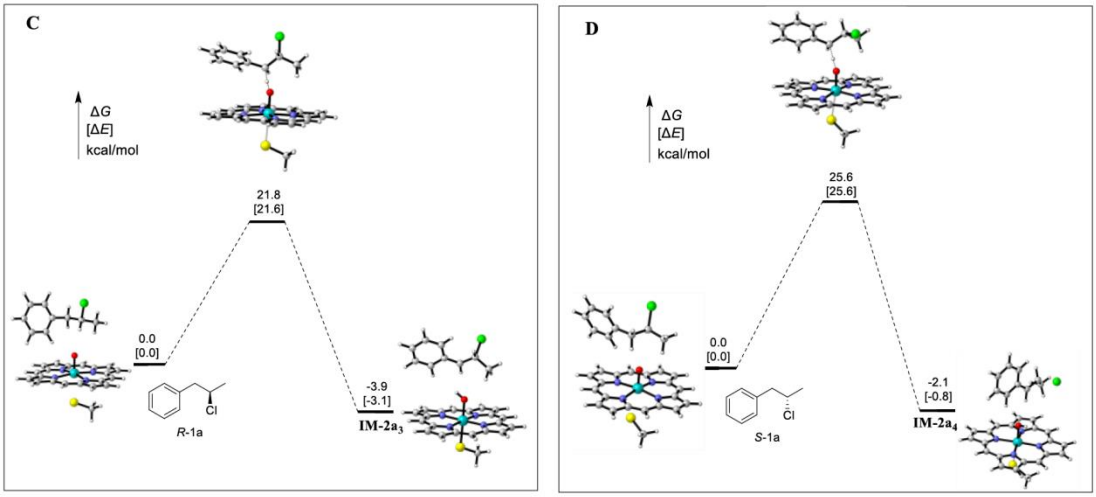


Supplementary Figure 3. Preliminary screening results of L303 saturated mutation

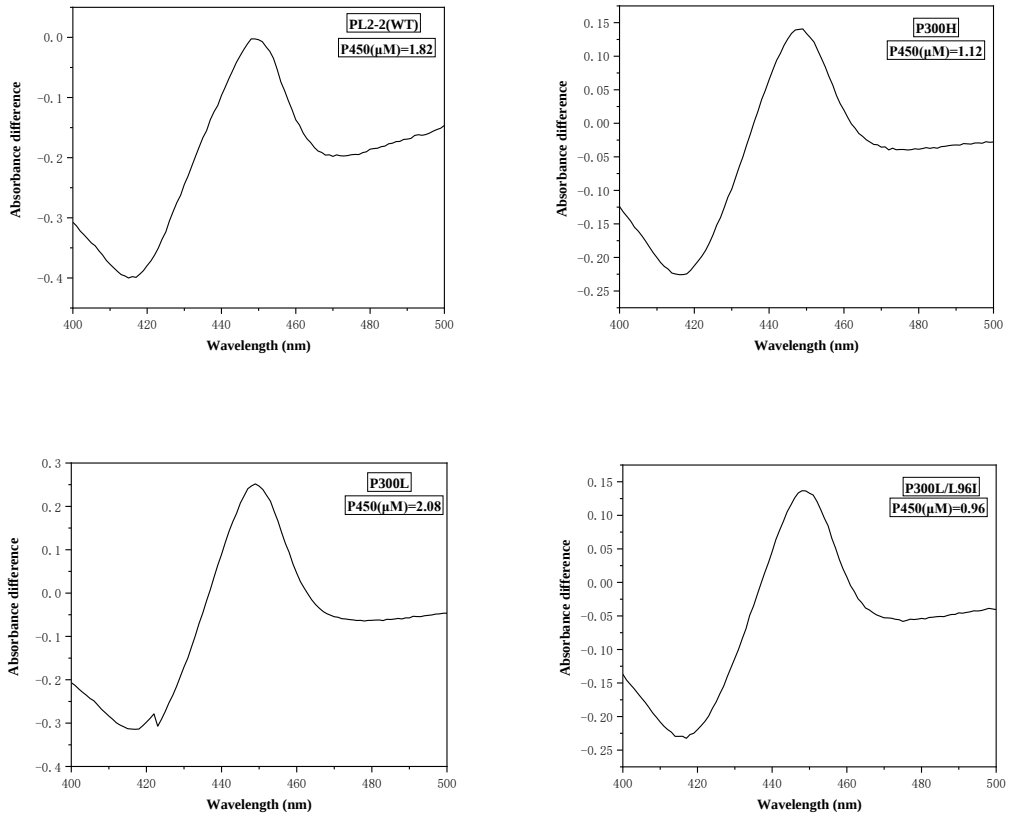


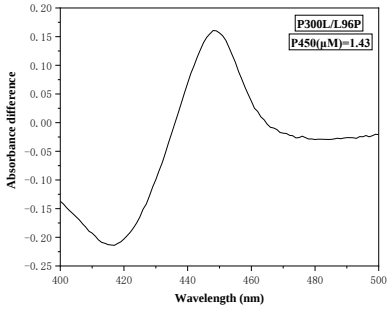
Supplementary Figure 4. Energy barriers of transition states for heme hydrogen abstraction reactions of four configuration products

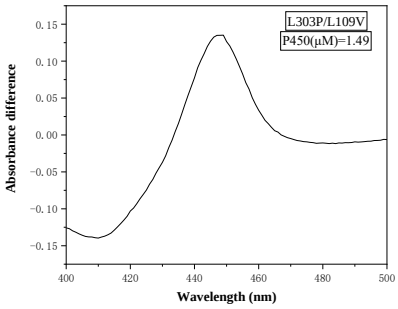


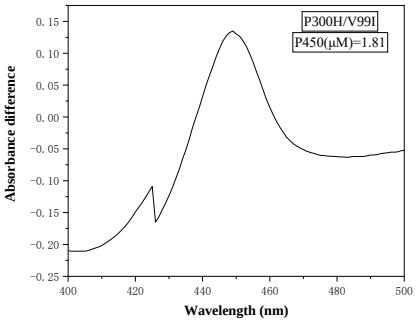


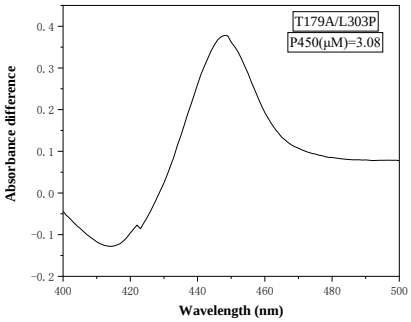
Supplementary Figure 5. CO difference spectroscopy of P450PL2 and its mutants

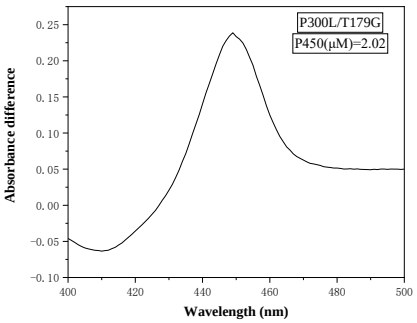


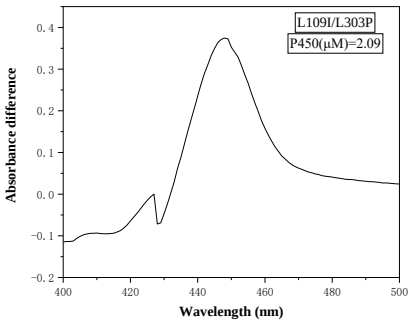

P300L/L96P
P450(μM)=1.43
Absorbance difference
Wavelength (nm)

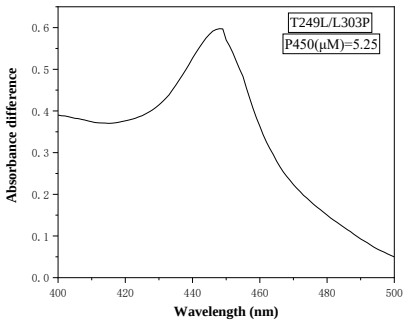

L303P/L109V
P450(μM)=1.49
Absorbance difference
Wavelength (nm)

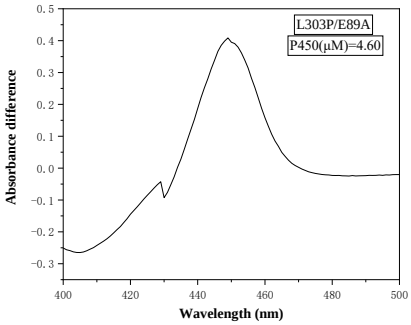

P300H/V99I
P450(μM)=1.81
Absorbance difference
Wavelength (nm)

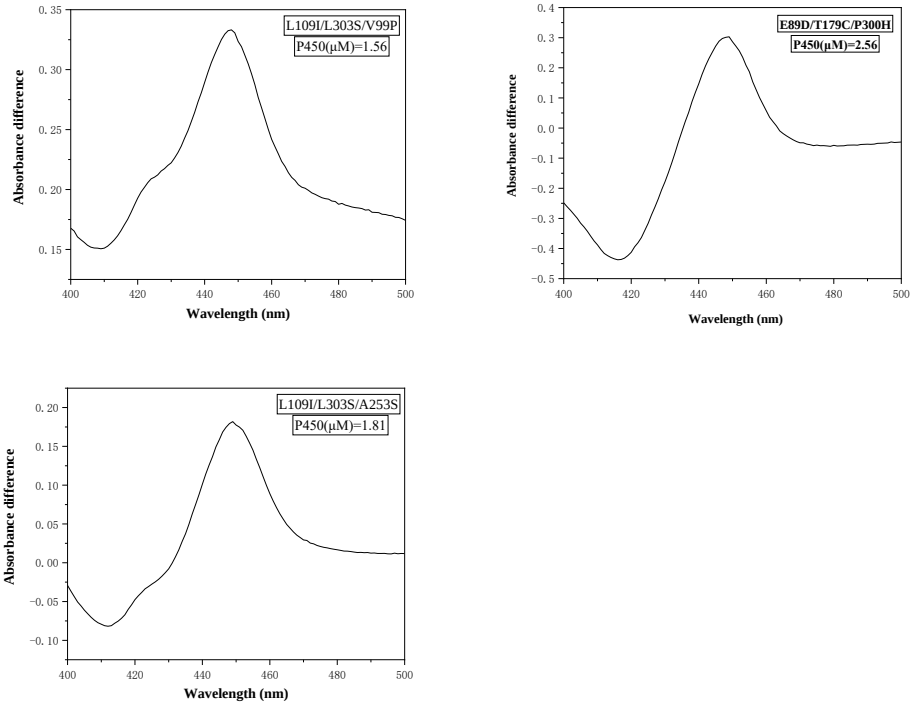

T179A/L303P
P450(μM)=3.08
Absorbance difference
Wavelength (nm)


P300L/T179G
P450(μM)=2.02
Absorbance difference
Wavelength (nm)

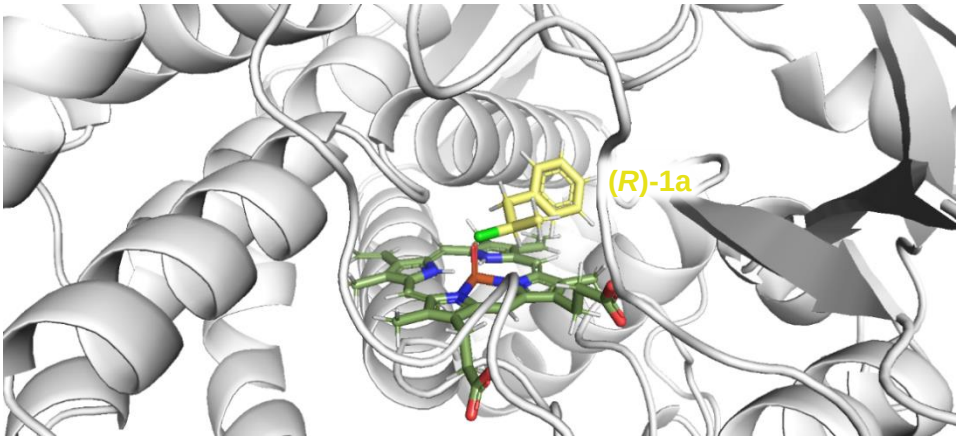

L109I/L303P
P450(μM)=2.09
Absorbance difference
Wavelength (nm)


T249L/L303P
P450(μM)=5.25
Absorbance difference
Wavelength (nm)

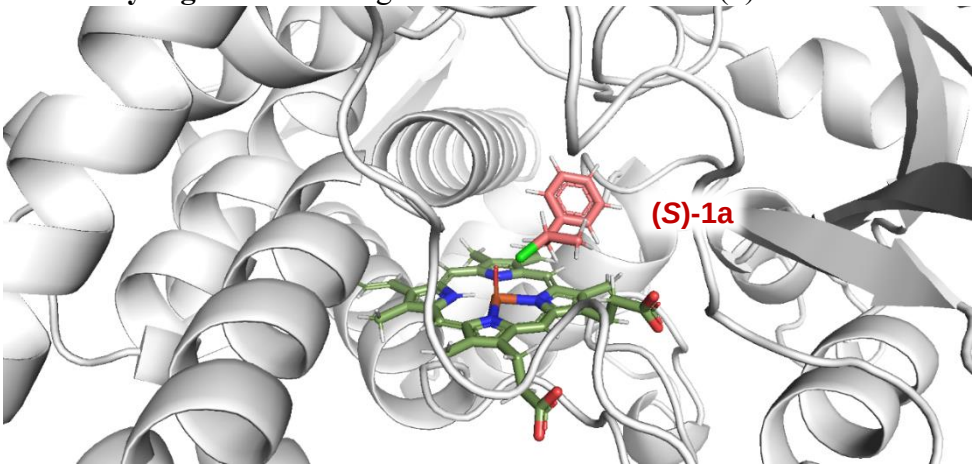

L303P/E89A
P450(μM)=4.60
Absorbance difference
Wavelength (nm)



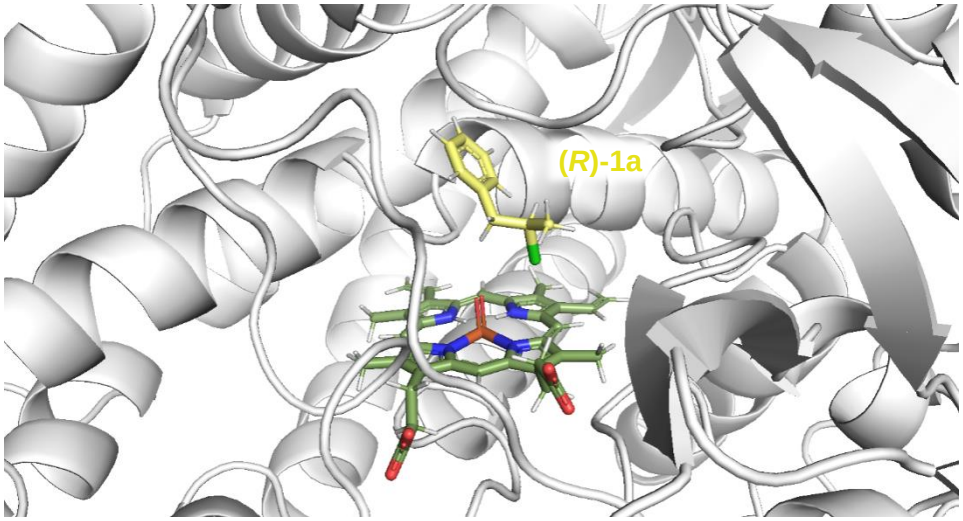
Supplementary Figure 6. Docking results of P450PL2 with (*R*)-**1a**



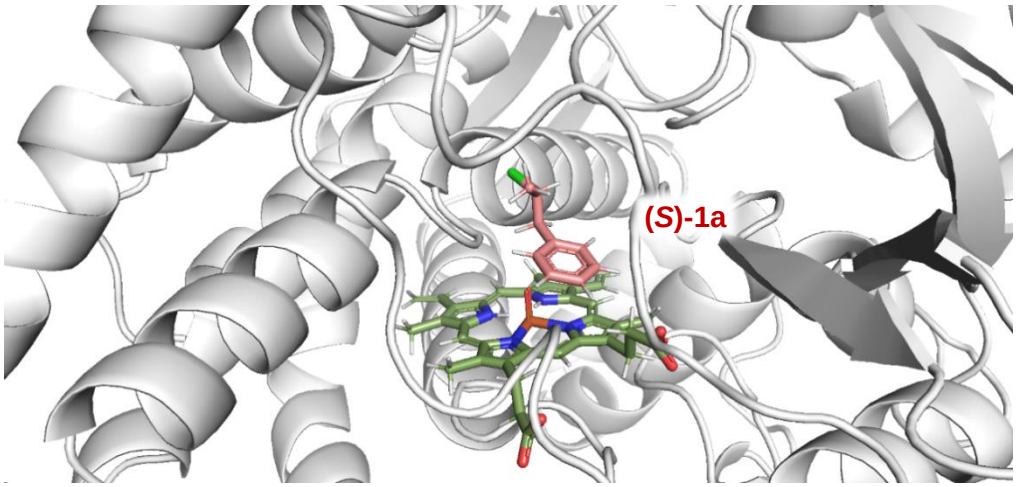
Supplementary Figure 7. Docking results of P450PL2 with (*S*)-**1a**



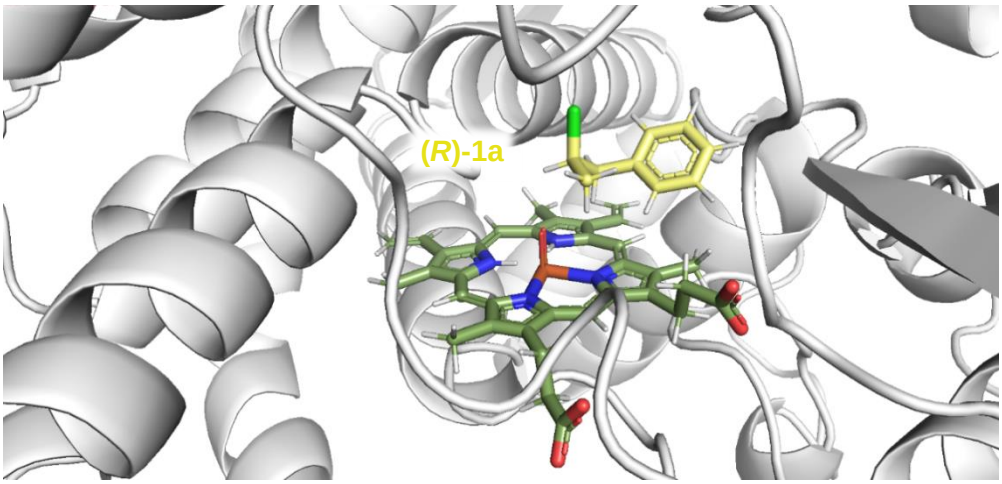
Supplementary Figure 8. Docking results of P450PL2-P300L/L96I with (*R*)-**1a**



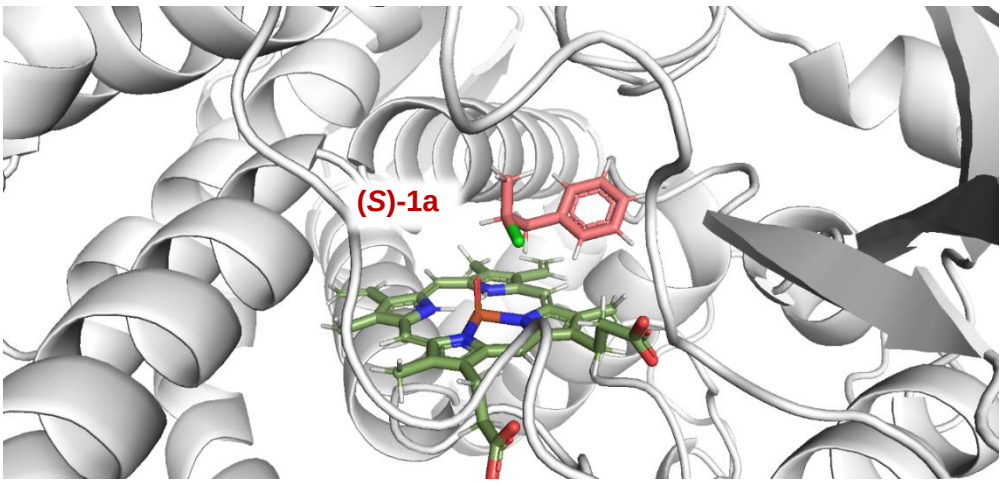
Supplementary Figure 9. Docking results of P450PL2-P300L/L96I with (*S*)-**1a**



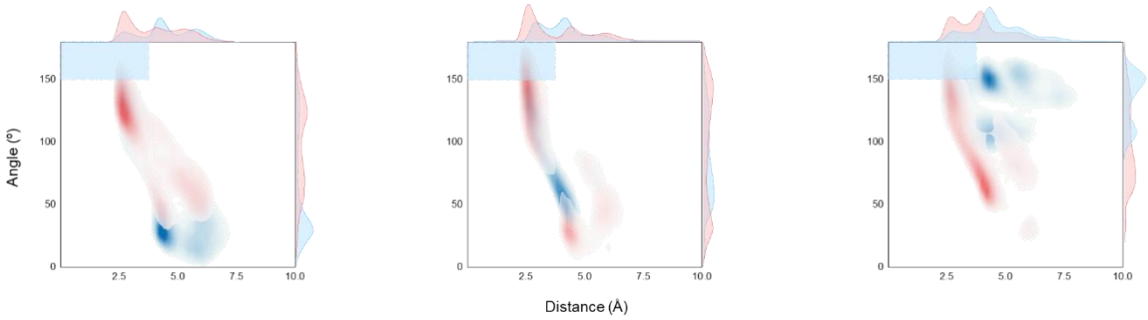
Supplementary Figure 10. Docking results of P450PL2-L109I/L303S/A253T with (*R*)-**1a**



Supplementary Figure 11. Docking results of P450PL2-L109I/L303S/A253T with (*S*)-**1a**

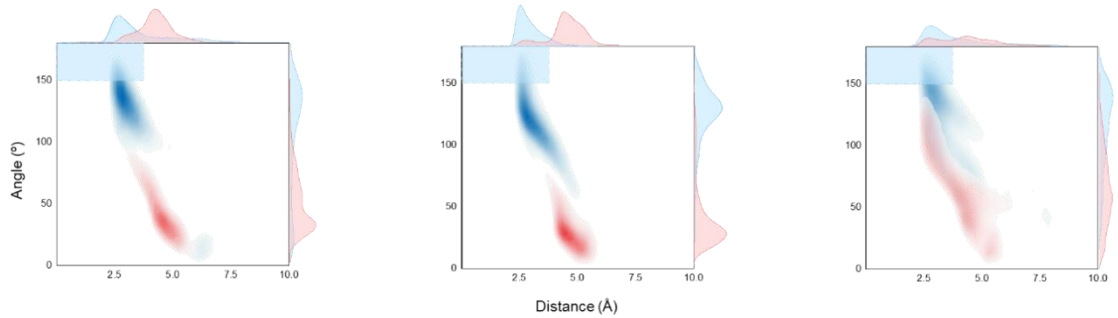


Supplementary Figure 12. Conformational population analysis of key geometric parameters for hydroxylation of P450PL2-WT with (*R*)-**1a**.



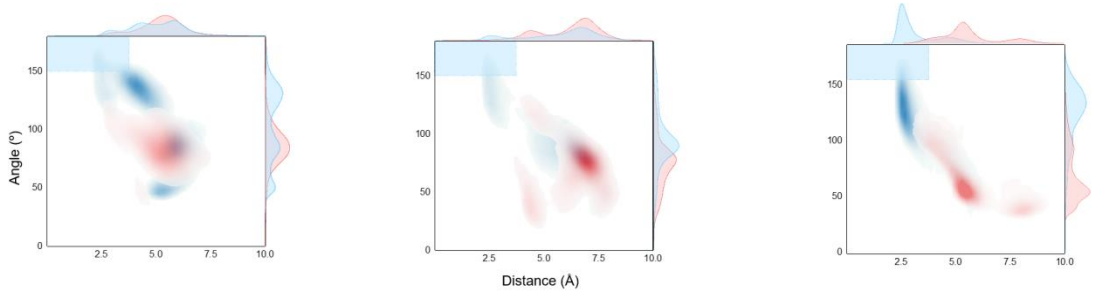
Distances determined between the oxygen atom of heme-Fe=O and the C-atom that have been hydroxylated of **1a** (x-axis) and angles formed by O(Fe=O) – H-atom that have been hydroxylated of **1a** – C-atom that have been hydroxylated of **1a** (y-axis) from the first replica of the MD dataset. The pro-*R* hydrogen at the benzyl position of 1a is shown in blue and the pro-*S* hydrogen is shown in red. The gray field indicates satisfactory conditions of active poses showing both the distance ≤ 3.8 Å and the angle ≥ 150º.

Supplementary Figure 13. Conformational population analysis of key geometric parameters for hydroxylation of P450PL2-WT with (*S*)-**1a**.



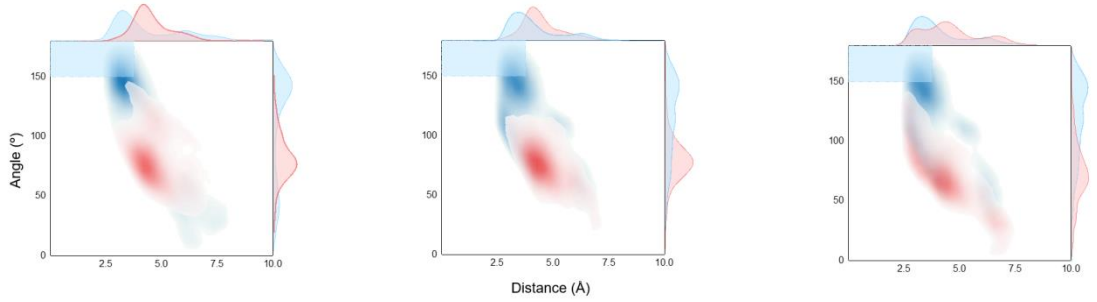
Distances determined between the oxygen atom of heme-Fe=O and the C-atom that have been hydroxylated of **1a** (x-axis) and angles formed by O(Fe=O) – H-atom that have been hydroxylated of **1a** – C-atom that have been hydroxylated of **1a** (y-axis) from the first replica of the MD dataset. The pro-*R* hydrogen at the benzyl position of 1a is shown in blue and the pro-*S* hydrogen is shown in red. The gray field indicates satisfactory conditions of active poses showing both the distance ≤ 3.8 Å and the angle ≥ 150º.

Supplementary Figure 14. Conformational population analysis of key geometric parameters for hydroxylation of DS with (*R*)-**1a**.



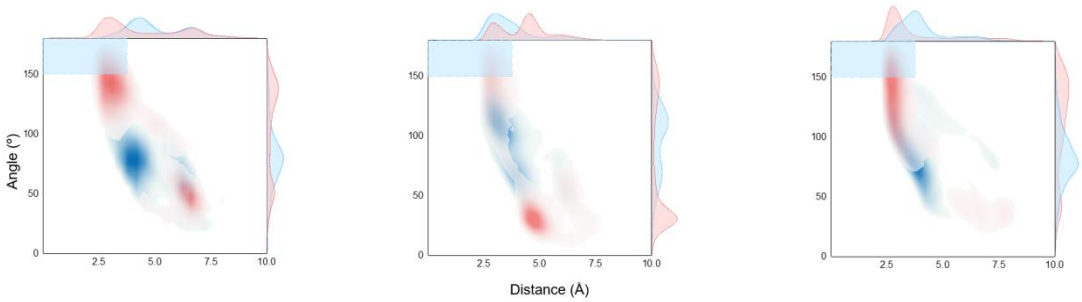
Distances determined between the oxygen atom of heme-Fe=O and the C-atom that have been hydroxylated of **1a** (x-axis) and angles formed by O(Fe=O) – H-atom that have been hydroxylated of **1a** – C-atom that have been hydroxylated of **1a** (y-axis) from the first replica of the MD dataset. The pro-*R* hydrogen at the benzyl position of 1a is shown in blue and the pro-*S* hydrogen is shown in red. The gray field indicates satisfactory conditions of active poses showing both the distance ≤ 3.8 Å and the angle ≥ 150º.

Supplementary Figure 15. Conformational population analysis of key geometric parameters for hydroxylation of DS with (*S*)-**1a**.



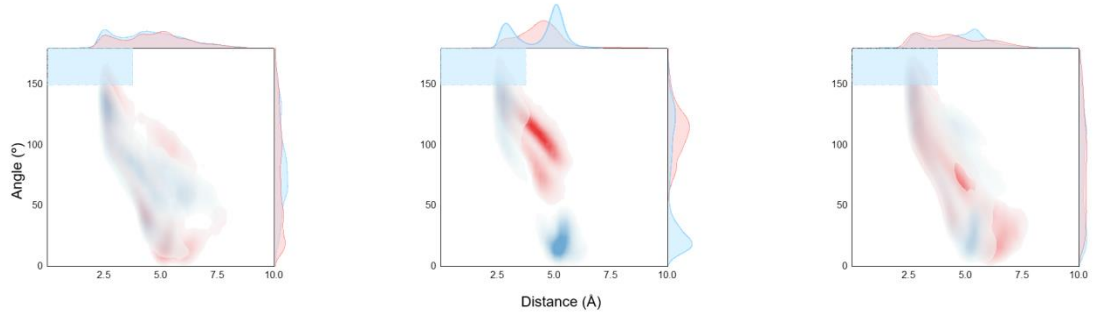
Distances determined between the oxygen atom of heme-Fe=O and the C-atom that have been hydroxylated of **1a** (x-axis) and angles formed by O(Fe=O) – H-atom that have been hydroxylated of **1a** – C-atom that have been hydroxylated of **1a** (y-axis) from the first replica of the MD dataset. The pro-*R* hydrogen at the benzyl position of 1a is shown in blue and the pro-*S* hydrogen is shown in red. The gray field indicates satisfactory conditions of active poses showing both the distance ≤ 3.8 Å and the angle ≥ 150º.

Supplementary Figure 16. Conformational population analysis of key geometric parameters for hydroxylation of DR with (*R*)-**1a**.



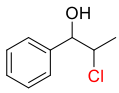
Distances determined between the oxygen atom of heme-Fe=O and the C-atom that have been hydroxylated of **1a** (x-axis) and angles formed by O(Fe=O) – H-atom that have been hydroxylated of **1a** – C-atom that have been hydroxylated of **1a** (y-axis) from the first replica of the MD dataset. The pro-*R* hydrogen at the benzyl position of 1a is shown in blue and the pro-*S* hydrogen is shown in red. The gray field indicates satisfactory conditions of active poses showing both the distance ≤ 3.8 Å and the angle ≥ 150º.

Supplementary Figure 17. Conformational population analysis of key geometric parameters for hydroxylation of DR with (*S*)-**1a**.

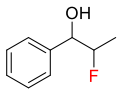


Distances determined between the oxygen atom of heme-Fe=O and the C-atom that have been hydroxylated of **1a** (x-axis) and angles formed by O(Fe=O) – H-atom that have been hydroxylated of **1a** – C-atom that have been hydroxylated of **1a** (y-axis) from the first replica of the MD dataset. The pro-*R* hydrogen at the benzyl position of 1a is shown in blue and the pro-*S* hydrogen is shown in red. The gray field indicates satisfactory conditions of active poses showing both the distance ≤ 3.8 Å and the angle ≥ 150º.

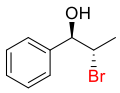
Supplementary Figure 18. Scope of the biocatalytic enantioselective synthesis of (1*R*,2S)-**2** and (1*S*,2*R*)-**2**.



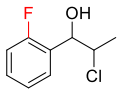
(1*R*, 2*S*)-2a: P300L/L96I
98:2 *er*, 93:7 *dr*, 1200 TTN, 29% yield
(1*S*, 2*R*)-2a: L109I/L303S/A253T
94:6 *er*, 86:14 *dr*, 140 TTN, 15% yield



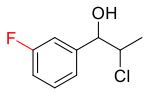
(1*R*, 2*S*)-2b: P300H/V99I
>99:1 *er*, 88:12 *dr*, 266 TTN, 14% yield
(1*S*, 2*R*)-2b: L109I/L303S/A253S
>99:1 *er*, >99:1 *dr*, 80 TTN, 4% yield



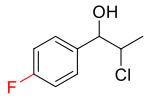
(1*R*, 2*S*)-2c: P300H
92:8 *er*, 83:17 *dr*, 180 TTN,19% yield



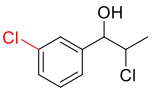
(1*R*, 2*S*)-2d: P300H
99:1 *er*, >99:1 *dr*, 430 TTN, 12% yield
(1*S*, 2*R*)-2d: L109I/L303S/A253S
95:5 *er*, 94:6 *dr*, 290 TTN, 14% yield



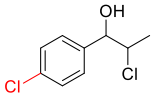
(1*R*, 2*S*)-2e: P300L/T179G
97:3 *er*, 86:14 *dr*, 849 TTN, 43% yield
(1*S*, 2*R*)-2e: L109I/L303S/A253T
94:6 *er*, 87:13 *dr*, 90 TTN, 10% yield



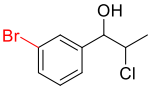
(1*R*, 2*S*)-2f: P300L/L96P
>99:1 *er*, 99:1 *dr*, 500 TTN, 18% yield
(1*S*, 2*R*)-2f: L109I/L303S/A253T
84:16 *er*, 81:19 *dr*, 110 TTN, 12% yield



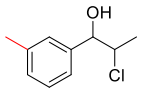
(1*R*, 2*S*)-2g: P300H
97:3 *er*, 87:13 *dr*, 286 TTN, 8% yield
(1*S*, 2*R*)-2g: L303P/L109V
90:10 *er*, 70:30 *dr*, 480 TTN, 18% yield



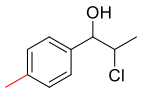
(1*R*, 2*S*)-2h: P300L/L96P
>99:1 *er*, >99:1 *dr*, 60 TTN, 2% yield
(1*S*, 2*R*)-2h: L109I/L303S/V99P
90:10 *er*, >99:1 *dr*, 310 TTN, 12% yield



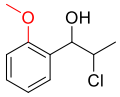
(1*R*, 2*S*)-2i: P300L
96:4 *er*, 92:8 *dr*, 80 TTN, 4% yield
(1*S*, 2*R*)-2i: L109I/L303P
91:9 *er*, 67:33 *dr*, 170 TTN, 15% yield



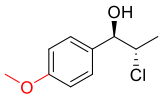
(1*R*, 2*S*)-2j: P300L/L96I
98:2 *er*, 90:10 *dr*, 830 TTN, 20% yield
(1*S*, 2*R*)-2j: T279L/L303P
94:6 *er*, 79:21 *dr*, 40 TTN, 5% yield



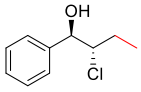
(1*R*, 2*S*)-2k: P300L/L96P
95:5 *er*, >99:1 *dr*, 140 TTN, 5% yield
(1*S*, 2*R*)-2k: L109I/L303S/A253T
99:1 *er*, >99:1 *dr*, 20 TTN, 2% yield



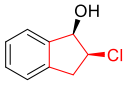
(1*S*, 2*R*)-2l: L303P/E89A
>99:1 *er*, >99:1 *dr*, 50 TTN, 6% yield



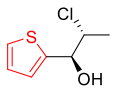
(1*R*, 2*S*)-2m: P300L/L96I
99:1 *er*, 93:7 *dr*, 460 TTN, 11% yield



(1*R*, 2*S*)-2n: P300H
98:2 *er*, 70:30 *dr*, 680 TTN, 19% yield



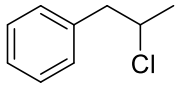
(1*R*, 2*S*)-2o: P300L/L96I
>99:1 *er*, 89:11 *dr*, 2130 TTN, 51% yield



(1*R*, 2*S*)-2p: P300H/V99I
96:4 *er*, 86:14 *dr*, 421 TTN, 22% yield

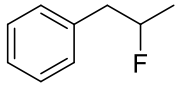
5. Characterizations of substrates and products

(*rac*)-(2-chloropropyl) benzene (1a)



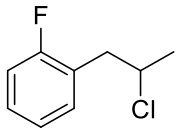
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 – 7.11 (m, 5H), 4.23 (q, J = 6.7 Hz, 1H), 3.10 (dd, J = 13.8, 7.0 Hz, 1H), 2.97 (dd, J = 13.9, 6.9 Hz, 1H), 1.52 (d, J = 6.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.1, 129.5, 128.6, 126.9, 58.7, 46.8, 24.8.

(*rac*)-(2-fluoropropyl) benzene (1b)



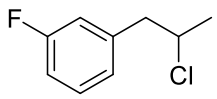
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 – 7.20 (m, 5H), 4.97 – 4.77 (m, 1H), 3.08 – 2.77 (m, 2H), 1.35 (dd, J = 23.8, 6.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.4 (d, J = 5.1 Hz, 1C), 129.5, 128.6, 126.7, 91.3 (q, J = 166.7 Hz, 1C), 43.4 (d, J = 21.2 Hz, 1C), 20.7 (d, J = 22.2 Hz, 1C).

(*rac*)-1-(2-chloropropyl)-2-fluorobenzene (1d)



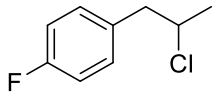
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 – 7.15 (m, 2H), 7.04 – 6.97 (m, 2H), 4.23 – 4.14 (m, 1H), 3.07 – 2.92 (m, 2H), 1.51 (d, J = 6.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.4 (d, J = 246.4 Hz, 1C), 132.0 (d, J = 5.1 Hz, 1C), 128.8 (d, J = 8.1 Hz, 1C), 125.1 (d, J = 15.2 Hz, 1C), 124.1 (d, J = 4.0 Hz, 1C), 115.5 (d, J = 22.2 Hz, 1C), 57.5, 40.0 (d, J = 2.0 Hz, 1C), 24.9.

(*rac*)-1-(2-chloropropyl)-3-fluorobenzene (1e)



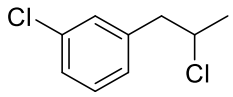
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.23 (m, 1H), 7.01 – 6.89 (m, 3H), 4.24 – 4.16 (m, 1H), 3.09 – 2.93 (m, 2H), 1.51 (d, J = 6.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.9 (d, J = 247.4 Hz, 1C), 140.5 (d, J = 7.1 Hz, 1C), 130.0 (d, J = 9.1 Hz, 1C), 125.2 (d, J = 3.0 Hz, 1C), 116.4 (d, J = 21.2 Hz, 1C), 113.9 (d, J = 21.2 Hz, 1C), 58.2, 46.4 (d, J = 2.0 Hz, 1C), 24.9.

(*rac*)-1-(2-chloropropyl)-4-fluorobenzene (1f)



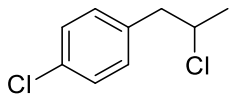
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 – 7.14 (m, 2H), 7.04 – 6.97 (m, 2H), 4.23 – 4.14 (m, 1H), 3.07 – 2.92 (m, 2H), 1.51 (d, J = 6.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.0 (d, J = 246.4 Hz, 1C), 133.8 (d, J = 4.0 Hz, 1C), 131.0 (d, J = 8.1 Hz, 1C), 115.4 (d, J = 21.2 Hz, 1C), 58.6, 45.8, 24.8.

(*rac*)-1-chloro-3-(2-chloropropyl) benzene (1g)



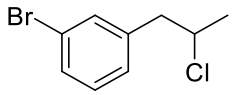
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.20 (m, 3H), 7.15 – 7.07 (m, 1H), 4.26 – 4.16 (m, 1H), 3.09 – 2.92 (m, 2H), 1.53 (d, J = 6.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.0, 134.3, 129.8, 129.6, 127.7, 127.2, 58.1, 46.3, 24.9.

(*rac*)-1-chloro-4-(2-chloropropyl) benzene (1h)



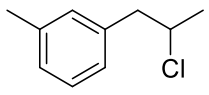
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 – 7.25 (m, 2H), 7.20 – 7.11 (m, 2H), 4.23 – 4.14 (m, 1H), 3.05 – 2.92 (m, 2H), 1.51 (d, J = 6.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.5, 132.8, 130.8, 128.6, 58.4, 46.0, 24.8.

(*rac*)-1-bromo-3-(2-chloropropyl) benzene (1i)



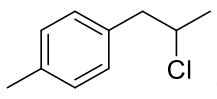
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42 – 7.35 (m, 2H), 7.23 – 7.11 (m, 2H), 4.24 – 4.15 (m, 1H), 3.05 – 2.92 (m, 2H), 1.52 (d, J = 6.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.3, 132.5, 130.1, 128.2, 122.5, 58.2, 46.2, 24.9.

(*rac*)-1-(2-chloropropyl)-3-methylbenzene (1j)



Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 (t, J = 7.5 Hz, 1H), 7.10 – 6.98 (m, 3H), 4.27 – 4.18 (m, 1H), 3.07 (dd, J = 13.8, 7.0 Hz, 1H), 2.93 (dd, J = 13.8, 7.0 Hz, 1H), 2.35 (s, 3H), 1.51 (d, J = 6.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.1, 138.1, 130.2, 128.4, 127.7 126.5, 58.7, 46.8, 24.8, 21.5.

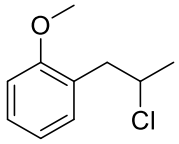
(*rac*)-1-(2-chloropropyl)-4-methylbenzene (1k)



Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.17 – 7.07 (m, 4H), 4.25

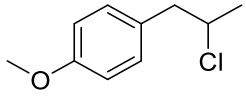
– 4.16 (m, 1H), 3.05 (dd, *J* = 13.9, 7.0 Hz, 1H), 2.93 (dd, *J* = 13.9, 6.9 Hz, 1H), 2.34 (s, 3H), 1.51 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ* 136.5, 135.1, 129.4, 129.2, 77.5, 77.2, 76.8, 58.9, 46.4, 24.8, 21.2.

(*rac*)-1-(2-chloropropyl)-2-methoxybenzene (1l)



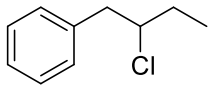
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.12 (m, 2H), 6.95 – 6.83 (m, 2H), 4.40 – 4.32 (m, 1H), 3.83 (s, 3H), 3.13 – 2.97 (m, 2H), 1.50 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 131.5, 128.3, 126.6, 120.4, 110.4, 57.7, 55.3, 55.3, 41.8, 25.0.

(*rac*)-1-(2-chloropropyl)-4-methoxybenzene (1m)



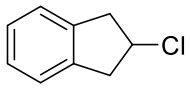
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.16 – 7.10 (m, 2H), 6.88 – 6.83 (m, 2H), 4.22 – 4.14 (m, 1H), 3.05 (dd, *J* = 13.9, 7.0 Hz, 1H), 2.93 (dd, *J* = 13.9, 6.9 Hz, 1H), 2.34 (s, 3H), 1.51 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ* 136.5, 135.1, 129.4, 129.2, 58.9, 46.4, 24.8, 21.2.

(*rac*)-(2-chlorobutyl) benzene (1n)



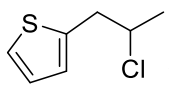
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.39 – 7.07 (m, 5H), 4.08 – 4.01 (m, 1H), 3.04 (d, *J* = 7.0 Hz, 2H), 1.89 – 1.79 (m, 1H), 1.76 – 1.62 (m, 1H), 1.06 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ* 138.2, 129.5, 128.5, 126.8, 65.8, 44.8, 30.8, 11.1.

2-chloro-2,3-dihydro-1*H*-indene (1o)



Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.35 – 7.07 (m, 4H), 4.74 (m, 1H), 3.45 (dd, *J* = 16.7, 6.3 Hz, 2H), 3.23 (dd, *J* = 16.7, 3.9 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ* 140.3, 127.1, 124.8, 59.4, 44.0.

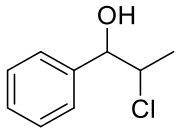
(*rac*)-2-(2-chloropropyl) thiophene (1p)



Yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.19 (dd, *J* = 5.1, 1.2 Hz, 1H),

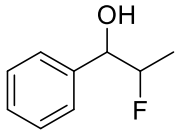
6.96 (dd, *J* = 5.2, 3.5 Hz, 1H), 6.89 (d, *J* = 3.4 Hz, 1H), 4.28 – 4.15 (m, 1H), 3.29 (dd, *J* = 14.9, 6.7 Hz, 1H), 3.19 (dd, *J* = 15.0, 6.7 Hz, 1H), 1.54 (dd, *J* = 6.4, 1.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ* 139.9, 127.0, 126.5, 124.5, 58.2, 40.7, 24.6.

(*rac*)-2-chloro-1-phenylpropan-1-ol (2a)[3]



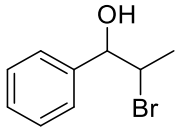
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.40 – 7.24 (m, 5H), 5.01 – 4.51 (m, 1H), 4.42 – 4.15 (m, 1H), 2.48 (s, 1H), 1.38 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ* 139.7, 128.7, 128.5, 126.5, 77.5, 62.9, 18.1. **HRMS** (**ESI**) *m/z*: calculated for $C_9H_{10}OCl$ ($[M-H]^-$): 169.0420, found: 169.0412.

(*rac*)-2-fluoro-1-phenylpropan-1-ol (2b)[35]



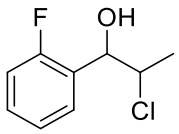
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.64 – 7.09 (m, 5H), 4.98 – 4.72 (m, 1H), 4.71 – 4.55 (m, 1H), 2.54 (s, 1H), 1.31 – 1.14 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ* 139.1 (d, *J* = 7.1 Hz, 1C), 128.7, 128.6, 127.2, 94.1 (d, *J* = 171.7 Hz, 1C), 77.8 (d, *J* = 20.2 Hz, 1C), 17.1 (d, *J* = 22.2 Hz, 1C). **HRMS** (**ESI**) *m/z*: calculated for $C_9H_{10}OF$ ($[M-H]^-$): 153.0716, found: 153.0725.

(*rac*)-2-bromo-1-phenylpropan-1-ol (2c)[36]



Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.40 – 7.27 (m, 5H), 5.02 (d, *J* = 3.5 Hz, 1H), 4.46 – 4.40 (m, 1H), 2.41 (s, 1H), 1.55 (d, *J* = 6.8, 0.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ* 139.7, 128.5, 128.2, 126.5, 76.8, 56.3, 18.9. **HRMS** (**ESI**) *m/z*: calculated for $C_9H_{10}OBr$ ($[M-H]^-$): 212.9915, found: 212.9914.

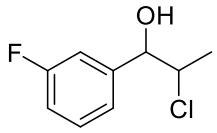
(*rac*)-2-chloro-1-(2-fluorophenyl) propan-1-ol (2d)



Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ* 7.60 – 7.43 (m, 1H), 7.37 – 7.25 (m, 1H), 7.18 (td, *J* = 7.5, 1.2 Hz, 1H), 7.12 – 6.99 (m, 1H), 5.49 – 4.78 (m, 1H), 4.47 – 4.20 (m, 1H), 2.53 (s, 1H), 1.42 (ddd, *J* = 35.9, 6.7, 1.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ* 159.8 (d, *J* = 246.4 Hz, 1C), 129.7 (d, *J* = 8.1 Hz, 1C), 128.2 (d, *J* = 4.0 Hz, 1C), 126.7 (d, *J* = 13.1 Hz, 1C), 124.4 (d, *J* = 3.0 Hz, 1C), 115.3 (d, *J* = 21.2 Hz,

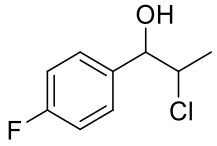
1C), 71.5, 61.4 (d, *J* = 1.0 Hz, 1C), 18.3. **HRMS** (**ESI**) *m/z*: calculated for C_9H_9OFCl ($[M-H]^-$): 187.0326, found: 187.0330.

(*rac*)-2-chloro-1-(3-fluorophenyl) propan-1-ol (2e)



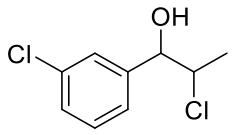
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 (dt, *J* = 7.9, 5.8 Hz, 1H), 7.18 – 6.86 (m, 3H), 4.59 (d, *J* = 7.2 Hz, 1H), 4.18 (p, *J* = 6.8 Hz, 1H), 2.72 (s, 1H), 1.40 (dd, *J* = 6.7, 0.9 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.0 (d, *J* = 247.5 Hz, 1C), 142.3 (d, *J* = 7.1 Hz, 1C), 130.2 (d, *J* = 8.1 Hz, 1C), 122.7 (d, *J* = 3.0 Hz, 1C), 115.5 (d, *J* = 20.2 Hz, 1C), 113.9 (d, *J* = 22.2 Hz, 1C), 78.5 (d, *J* = 2.0 Hz, 1C), 64.2, 21.6. **HRMS** (**ESI**) *m/z*: calculated for C_9H_9OFCl ($[M-H]^-$): 187.0326, found: 187.0334.

(*rac*)-2-chloro-1-(4-fluorophenyl) propan-1-ol (2f)



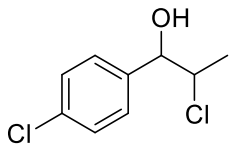
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 – 7.30 (m, 1H), 7.11 – 7.02 (m, 2H), 4.58 (d, *J* = 7.6 Hz, 1H), 4.17 (m, *J* = 7.6, 6.7 Hz, 1H), 2.61 (s, 1H), 1.36 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.68 (dd, *J* = 246.6, 30.0 Hz, 1C), 135.40, 128.46 (dd, *J* = 48.9, 8.2 Hz, 2C), 115.53 (dd, *J* = 23.6, 21.5 Hz, 2C), 78.57, 63.66 (d, *J* = 178.7 Hz, 1C), 19.83 (d, *J* = 339.6 Hz, 1C). **HRMS** (**ESI**) *m/z*: calculated for C_9H_9OFCl ($[M-H]^-$): 187.0326, found: 187.0319.

(*rac*)-2-chloro-1-(3-chlorophenyl) propan-1-ol (2g)



Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.35 (m, 1H), 7.33 – 7.20 (m, 3H), 4.57 (d, *J* = 7.3 Hz, 1H), 4.18 (p, *J* = 6.8 Hz, 1H), 2.64 (s, 1H), 1.40 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.8, 134.7, 129.9, 128.8, 127.1, 125.2, 78.4, 64.2, 21.6. **HRMS** (**ESI**) *m/z*: calculated for $C_9H_9OCl_2$ ($[M-H]^-$): 203.0030, found: 203.0036.

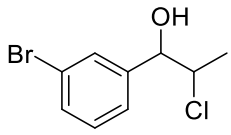
(*rac*)-2-chloro-1-(4-chlorophenyl) propan-1-ol (2h)



Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 – 7.24 (m, 4H), 5.13 – 4.51 (m, 1H), 4.37 – 4.05 (m, 1H), 2.82 (s, 1H), 1.37 (dd, *J* = 8.6, 6.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.2, 134.4, 128.9, 128.4, 78.4, 64.3, 21.5. **HRMS**

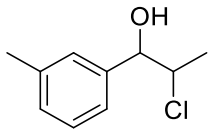
(**ESI**) *m/z*: calculated for $C_9H_9OCl_2$ ([M-H]$^-$): 203.0030, found: 203.0021.

(*rac*)-1-(3-bromophenyl)-2-chloropropan-1-ol (2i)



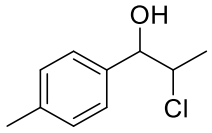
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 (d, J = 6.7 Hz, 1H), 7.45 (dd, J = 7.7, 1.8 Hz, 1H), 7.33 – 7.20 (m, 2H), 5.09 – 4.44 (m, 1H), 4.38 – 4.09 (m, 1H), 2.54 (s, 1H), 1.39 (dd, J = 14.2, 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.9, 131.3, 130.1, 129.6, 125.2, 122.7, 76.5, 62.5, 18.1. **HRMS** (**ESI**) *m/z*: calculated for C_9H_9OClBr ([M-H]$^-$): 246.9525, found: 246.9530.

(*rac*)-2-chloro-1-(*m*-tolyl) propan-1-ol (2j)



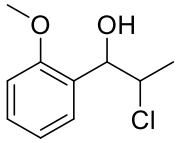
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 – 7.06 (m, 4H), 5.08 – 4.48 (m, 1H), 4.36 – 4.16 (m, 1H), 2.37 (s, 3H), 1.38 (dd, J = 6.7, 5.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 139.6, 138.4, 129.4, 128.6, 127.5, 124.2, 79.3, 64.8, 21.7, 18.2. **HRMS** (**ESI**) *m/z*: calculated for $C_{10}H_{12}OCl$ ([M-H]$^-$): 183.0577, found: 183.0575.

(*rac*)-2-chloro-1-(*p*-tolyl) propan-1-ol (2k)[37]



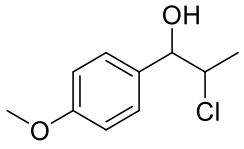
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 – 7.03 (m, 4H), 4.55 (d, J = 7.7 Hz, 1H), 4.24 – 4.17 (m, 1H), 2.59 (s, 1H), 2.35 (s, 3H), 1.37 (d, J = 6.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.4, 136.7, 129.4, 126.9, 79.1, 64.7, 21.7, 21.3. **HRMS** (**ESI**) *m/z*: calculated for $C_{10}H_{12}OCl$ ([M-H]$^-$): 183.0577, found: 183.0582.

(*rac*)-2-chloro-1-(2-methoxyphenyl) propan-1-ol (2l)



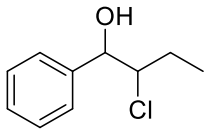
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 – 7.20 (m, 2H), 7.09 – 6.78 (m, 2H), 5.04 (dd, J = 67.3, 5.3 Hz, 1H), 4.53 – 4.30 (m, 1H), 3.85 (d, J = 2.0 Hz, 3H), 2.61 (s, 1H), 1.42 (dd, J = 19.1, 6.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.2, 129.0, 128.5, 128.0, 120.7, 110.4, 73.9, 61.1, 55.4, 18.5. **HRMS** (**ESI**) *m/z*: calculated for $C_{10}H_{12}O_2Cl$ ([M-H]$^-$): 199.0526, found: 199.0532.

(*rac*)-2-chloro-1-(4-methoxyphenyl) propan-1-ol (2m)[38]



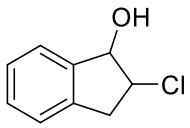
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.26 (m, J = 8.6, 7.3, 1.5 Hz, 2H), 6.92 – 6.84 (m, 2H), 5.08 – 4.40 (m, 1H), 4.30 – 4.12 (m, 1H), 3.79 (s, 3H), 2.33 (s, 1H), 1.34 (dd, J = 15.9, 6.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.4, 131.9, 127.7, 113.8, 78.9, 63.0, 55.4, 18.4. **HRMS** (**ESI**) *m/z*: calculated for $C_{10}H_{12}O_2Cl$ ([M-H]$^-$): 199.0526, found: 199.0528.

(*rac*)-2-chloro-1-phenylbutan-1-ol (2n)[39]



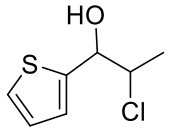
Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42 – 7.29 (m, 5H), 4.67 (d, J = 7.2 Hz, 1H), 4.08 – 4.03 (m, 1H), 2.66 (s, 1H), 1.76 – 1.54 (m, 2H), 1.02 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ140.1, 128.7, 128.5, 126.9, 77.6, 72.1, 27.6, 11.2. **HRMS** (**ESI**) *m/z*: calculated for $C_{10}H_{12}OCl$ ([M-H]$^-$): 183.0577, found: 183.0570.

(*rac*)-2-chloro-2,3-dihydro-1H-inden-1-ol (2o)[40]



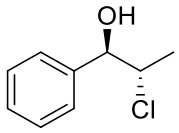
White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 – 7.09 (m, 4H), 5.19 (d, J = 17.5, 5.3 Hz, 1H), 4.94 – 4.07 (m, 1H), 3.58 – 3.31 (m, 1H), 3.30 – 3.01 (m, 1H), 1.93 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.5, 139.1, 129.2, 127.8, 124.8, 124.3, 83.2, 64.8, 39.9. **HRMS** (**ESI**) *m/z*: calculated for C_9H_8OCl ([M-H]$^-$): 167.0264, found: 167.0259.

(*rac*)-2-chloro-1-(thiophen-2-yl) propan-1-ol (2p)



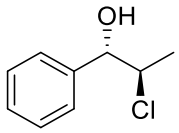
Yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 (dd, J = 5.0, 1.3 Hz, 1H), 7.08 – 6.96 (m, 2H), 4.88 (d, J = 7.0 Hz, 1H), 4.25 (p, J = 6.8 Hz, 1H), 2.80 (s, 1H), 1.45 (d, J = 6.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.9, 126.9, 125.7, 75.1, 64.0, 21.6. **HRMS** (**ESI**) *m/z*: calculated for C_7H_8OClS ([M-H]$^-$): 174.9984, found: 174.9977.

(1*R*,2*S*)-2-chloro-1-phenylpropan-1-ol (2a)[3]



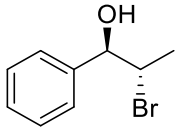
Prepared according to the general procedure: 50 mL PB buffer (50 mM, pH 7.5) containing 4 mM **1a** (2 mmol) and 15 g cdw/L *E. coli* (P450PL2-P300L/L96I) cells, 25 °C, reaction for 24 h. The crude product was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100:1 ~ 50:1) to provide (1*R*, 2*S*)-**2a** as a colorless oil in 21.8% yield (25.3 mg). $[\alpha]D^{25}$ = - 14.2 (*c* = 0.50, $CHCl_3$).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.27 (m, 5H), 4.94 (d, *J* = 3.8 Hz, 1H), 4.34 – 4.28 (m, 1H), 2.31 (s, 1H), 1.38 (d, *J* = 6.7 Hz, 3H).
^{13}C NMR (100 MHz, $CHCl_3$) δ 139.7, 128.5, 128.2, 126.5, 77.3, 62.9, 18.2.

(1*S*,2*R*)-2-chloro-1-phenylpropan-1-ol (2a)[3]



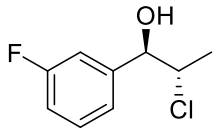
Prepared according to the general procedure: 50 mL PB buffer (50 mM, pH 7.5) containing 4 mM **1a** (2 mmol) and 15 g cdw/L *E. coli* (P450PL2-L109I/L303S/A253T) cells, 25 °C, reaction for 24 h. The crude product was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100:1 ~ 50:1) to provide (1*S*, 2*R*)-**2a** as a colorless oil in 14.6% yield (29.9 mg). $[\alpha]D^{25}$ = + 6.1 (*c* = 0.50, $CHCl_3$).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.28 (m, 5H), 4.95 (d, *J* = 3.8 Hz, 1H), 4.34 – 4.28 (m, 1H), 2.30 (s, 1H), 1.38 (dd, *J* = 6.7, 2.0 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 128.5, 128.2, 126.5, 77.3, 62.9, 18.2.

(1*R*,2*S*)-2-bromo-1-phenylpropan-1-ol (2c)[36]



Prepared according to the general procedure: 50 mL PB buffer (50 mM, pH 7.5) containing 4 mM **1c** (2 mmol) and 15 g cdw/L *E. coli* (P450PL2-P300H) cells, 25 °C, reaction for 1 h. The crude product was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100:1 ~ 50:1) to provide (1*R*, 2*S*)-**2c** as a light yellow oil in 19.1% yield (278.2 mg). $[\alpha]D^{25}$ = - 7.4 (*c* = 0.50, CH_2Cl_2).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.28 (m, 5H), 5.02 (d, *J* = 3.5 Hz, 1H), 4.60 – 4.46 (m, 1H), 2.47 (s, 1H), 1.56 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 128.7, 128.5, 126.5, 77.4, 56.3, 18.9.

(1*R*,2*S*)-2-chloro-1-(3-fluorophenyl) propan-1-ol (2e)

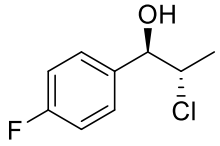


Prepared according to the general procedure: 50 mL PB buffer (50 mM, pH 7.5) containing 4 mM **1e** (2 mmol) and 15 g cdw/L *E. coli* (P450PL2-P300H) cells, 25 °C, reaction for 24 h. The crude product was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100:1 ~ 50:1) to provide (1*R*, 2*S*)-**2e** as a light yellow oil in 27.3% yield (56.6 mg). $[\alpha]D^{25}$ = - 18.0 (*c* = 0.50, CH_2Cl_2).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.30 (m, 1H), 7.17 – 7.08 (m, 2H), 7.05 – 6.95 (m, 1H), 4.94 (d, *J* = 3.6 Hz, 1H), 4.32 – 4.26 (m, 1H), 2.51 (s, 1H), 1.36 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0 (d, *J* = 246.2 Hz, 1C), 142.3 (d, *J* = 7.0 Hz, 1C), 130.0 (d, *J* = 8.1 Hz, 1C), 122.1 (d, *J* = 3.0 Hz, 1C), 115.1 (d, *J* = 21.3 Hz, 1C), 113.6 (d, *J* = 22.4 Hz, 1C), 76.7 – 76.5 (m, 1C), 62.6, 18.0.

(1*R*,2*S*)-2-chloro-1-(4-fluorophenyl) propan-1-ol (2f)

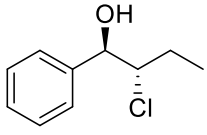


Prepared according to the general procedure: 50 mL PB buffer (50 mM, pH 7.5) containing 4 mM **1f** (2 mmol) and 15 g cdw/L *E. coli* (P450PL2-P300L/L96P) cells, 25 °C, reaction for 24 h. The crude product was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100:1 ~ 50:1) to provide (1*R*, 2*S*)-**2f** as a light yellow oil in 16.7% yield (34.7 mg). $[\alpha]D^{25}$ = - 16.8 (*c* = 0.50, CH_2Cl_2).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.31 (m, 2H), 7.09 – 7.02 (m, 2H), 4.91 (d, *J* = 3.8 Hz, 1H), 4.29 – 4.23 (m, 1H), 2.52 (s, 1H), 1.36 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5 (d, *J* = 246.4 Hz, 1C), 135.4 (d, *J* = 3.1 Hz, 1C), 128.2 (d, *J* = 8.1 Hz, 2C), 115.4 (d, *J* = 21.6 Hz, 2C), 76.8 (d, *J* = 17.8 Hz, 1C), 62.7, 18.2.

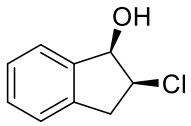
(1*R*,2*S*)-2-chloro-1-phenylbutan-1-ol (2n)[39]



Prepared according to the general procedure: 50 mL PB buffer (50 mM, pH 7.5) containing 4 mM **1n** (2 mmol) and 15 g cdw/L *E. coli* (P450PL2-P300H) cells, 25 °C, reaction for 24 h. The crude product was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100:1 ~ 50:1) to provide (1*R*, 2*S*)-**2n** as a light yellow oil in 17.5% yield (38.8 mg). $[\alpha]D^{25}$ = - 22.9 (*c* = 0.50, CH_2Cl_2).

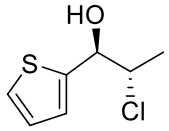
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.28 (m, 5H), 4.95 (d, J = 4.4 Hz, 1H), 4.13 – 4.08 (m, 1H), 2.34 (s, 1H), 1.83 – 1.54 (m, 2H), 1.04 – 1.0 (m, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 128.7, 128.5, 126.7, 77.0, 70.4, 24.8, 11.4.

(1*R*,2*S*)-2-chloro-2,3-dihydro-1H-inden-1-ol (2o)[40]



Prepared according to the general procedure: 50 mL PB buffer (50 mM, pH 7.5) containing 4 mM **1o** (2 mmol) and 15 g cdw/L *E. coli* (P450PL2-P300L/L96I) cells, 25 °C, reaction for 24 h. The crude product was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100:1 ~ 30:1) to provide (1*R*, 2*S*)-**2o** as white solid in 49.6% yield (50.2 mg). M.p. = 110.5 - 111.4 °C. [α]D^{25} = + 57.2 (c = 0.50, CH_2Cl_2).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.41 (m, 1H), 7.35 – 7.21 (m, 3H), 5.15 (d, J = 4.7 Hz, 1H), 4.79 (q, J = 5.1Hz, 1H), 3.37 – 3.21 (m, 2H), 2.57 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ (100 MHz, $CDCl_3$) δ 141.5, 139.0, 128.9, 127.6, 125.1, 124.2, 76.5, 66.1, 39.8.

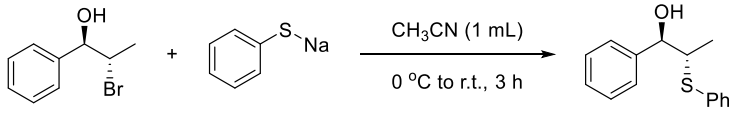
(1*R*,2*S*)-2-chloro-1-(thiophen-2-yl) propan-1-ol (2p)



Prepared according to the general procedure: 50 mL PB buffer (50 mM, pH 7.5) containing 4 mM **1p** (2 mmol) and 15 g cdw/L *E. coli* (P450PL2-P300H/V99I) cells, 25 °C, reaction for 24 h. The crude product was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100:1 ~ 50:1) to provide **(1*R*, 2*S*)-2p** as red brown oil in 19.8% yield (42.0 mg). [α]D^{25} = - 4.1 (c = 0.50, CH_2Cl_2).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.29 (m, 1H), 7.06 – 7.0 (m, 2H), 5.15 (dd, J = 3.9, 0.9 Hz, 1H), 4.37 – 4.31 (m, 1H), 2.45 (s, 1H), 1.46 (d, J = 6.7 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 126.8, 125.3, 125.2, 74.2, 62.4, 19.0.

6. Transformations of chiral halohydrins

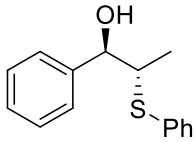
Synthesis of chiral compound **3**



(1*R*,2*S*)-**2c** **3**

To a 4 mL tube with oven-dried stir bar was added **2c** (0.1 mmol, 21.5 mg) and Sodium thiophenolate (0.3 mmol) in dry CH_3CN (1 mL). The mixture was allowed to stir at 25 °C for 3 hours and then subjected to column chromatography on silica gel (20:1 petroleum ether / EtOAc) directly to give the desired pure product **3**.

(1*R*,2*S*)-1-phenyl-2-(phenylthio)propan-1-ol (3)

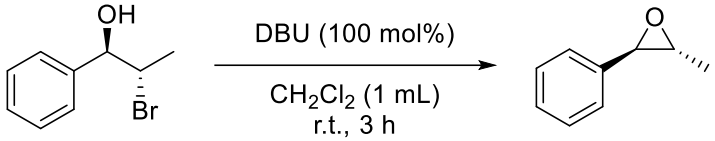


Colorless oil (24.4 mg, 83% yield, 91:9 *er*, 84:16 *dr*). $[\alpha]D^{25}$ = + 1.1 (c = 0.17, CH_2Cl_2).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.48 (m, 2H), 7.37 – 7.29 (m, 8H), 4.38 (dd, *J* = 8.7, 1.4 Hz, 1H), 3.36 (d, *J* = 1.8 Hz, 1H), 3.29 (dq, *J* = 8.9, 6.9 Hz, 1H), 1.08 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 140.8, 133.9, 132.2, 129.0, 128.4, 128.1, 128.0, 127.1, 76.8, 52.8, 18.3.

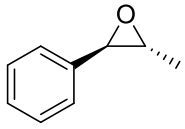
Synthesis of chiral compound **4**



(1*R*,2*S*)-**2c** **4**

To a 4.0 mL vial equipped with a magnetic stir bar was added **2c** (0.1 mmol), dried DCM (1.0 mL) and DBU (0.10 mmol) was added *via* syringe. Then the reaction mixture was stirred for 3 hours at 25 ℃ and then subjected to column chromatography on silica gel (20:1 petroleum ether / EtOAc) directly to give the desired pure product **4**.

(2*R*,3*R*)-2-methyl-3-phenyloxirane (4)

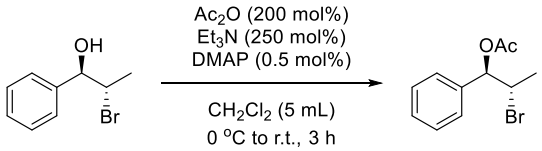


Colorless oil (12.8 mg, 95% yield, 92:8 *er*, 83:17 *dr*). $[\alpha]D^{25}$ = + 2.3 (*c* = 0.20, CH_2Cl_2).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.23 (m, 5H), 3.57 (d, *J* = 2.1 Hz, 1H), 3.04 (dd, *J* = 5.1, 2.1 Hz, 1H), 1.45 (d, *J* = 5.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 128.5, 128.1, 125.6, 59.6, 59.1, 17.9.

Synthesis of chiral compound **5**

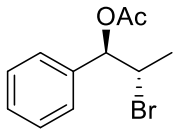


(1*R*,2*S*)-**2c** **5**

To a 4 mL tube with oven-dried stir bar was added **2c** (0.5 mmol, 107.6 mg), DMAP and Et_3N (1.25 mmol) in dry CH_2Cl_2 (5 mL) at 0 °C was added Ac_2O (1.0 mmol). The solution was warmed to room temperature and stirred for 3 hours, then the solvent

was removed in vacuo and the residue was chromatographed on silica gel (20:1 petroleum ether / EtOAc) to give the product **5**.

(1*R*,2*S*)-2-bromo-1-phenylpropyl acetate (5)

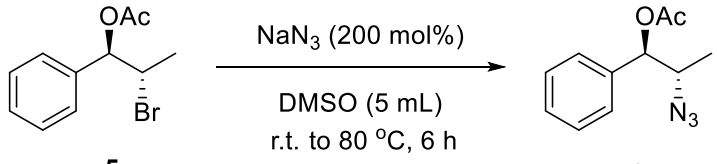


Colorless oil (128.6 mg, 95% yield, 92:8 *er*, 82:18 *dr*). $[\alpha]D^{25}$ = - 9.4 (*c* = 0.50, CH_2Cl_2).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.28 (m, 5H), 5.96 (d, *J* = 5.2 Hz, 1H), 4.36 (qd, *J* = 6.8, 5.3 Hz, 1H), 2.16 (s, 3H), 2.13 (s, 1H), 1.65 (d, *J* = 6.8 Hz, 3H), 1.53 (d, *J* = 6.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 137.1, 128.5, 128.4, 127.1, 78.3, 50.2, 21.0, 20.8.

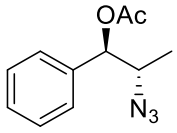
Synthesis of chiral compound **6**



5 **6**

To a 4 mL tube with oven-dried stir bar was added **5** (0.4 mmol, 102.9 mg) and NaN_3 (0.8 mmol, 52.0 mg) in dry DMSO (2 mL). The mixture was allowed to stir at 80 °C for 6 h and cooled to room temperature. The residue was purified by silica gel chromatography with hexanes:EtOAc (20:1) as the eluent to yield product **6**.

(1*R*,2*S*)-2-azido-1-phenylpropyl acetate (6)

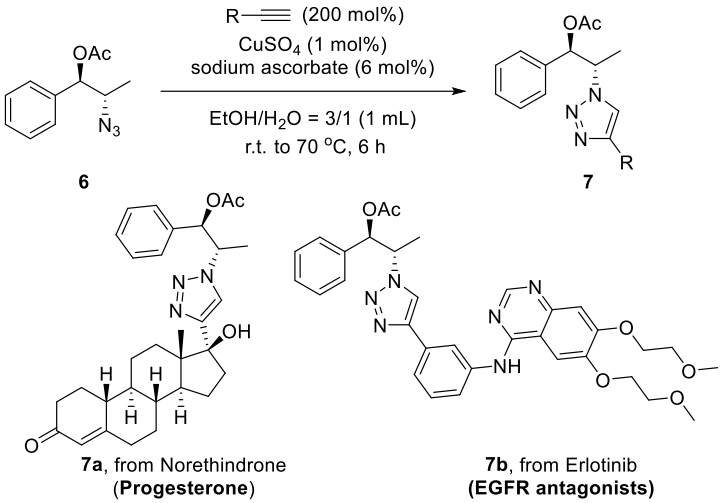


Colorless oil (76.8 mg, 87% yield, 90:10 *er*, 77:23 *dr*). $[\alpha]D^{25}$ = - 10.9 (*c* = 0.27, CH_2Cl_2).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.28 (m, 7H), 5.64 (d, *J* = 7.5 Hz, 1H), 3.85 – 3.75 (m, 1H), 2.13 (s, 3H), 1.21 (d, *J* = 6.7 Hz, 1H), 1.08 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 137.2, 128.7, 128.7, 127.2, 78.9, 60.7, 21.1, 16.2.

Synthesis of chiral compound **7a** and **7b**



To a 4 mL tube with oven-dried stir bar was added $CuSO_4$ (0.01 mmol, 0.2 mg), sodium ascorbate (0.06 mmol, 1.2 mg) and MonoPhos (0.01 mmol, 0.4 mg) were dissolved in 1 mL EtOH/H_2O (v/v = 3/1) and the solution was stirred at room temperature for 15 min. To this solution was added **6** (0.1 mmol, 21.9 mg) and Norethindrone (or Erlotinib) (0.2 mmol). The reaction mixture was stirred at 70 °C for 6 hours. Then the mixture was concentrated under reduced pressure to yield the crude product. The residue was purified by silica gel chromatography with CH_2Cl_2: MeOH (30:1) as the eluent to yield products **7** (**7a**, 42.5 mg, 82% yield; **7b**, 49.0 mg, 80% yield, $[\alpha]D^{25}$ = - 7.0 (*c* = 0.50, CH_2Cl_2); **7b**, 49.0 mg, 80% yield, $[\alpha]D^{25}$ = - 2.0 (*c* = 0.27, CH_2Cl_2)).

7a:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 – 7.04 (m, 6H), 5.90 – 5.83 (m, 1H), 5.68 – 5.62 (m, 1H), 4.95 – 4.78 (m, 1H), 2.36 – 2.00 (m, 7H), 1.98 – 1.84 (m, 2H), 1.77 (s, 4H), 1.52 (t, *J* = 7.5 Hz, 1H), 1.40 – 1.21 (m, 7H), 1.17 – 1.01 (m, 3H), 0.88 (d, *J* = 20.6 Hz, 4H), 0.52 – 0.37 (m, 1H), 0.26 (td, *J* = 13.1, 4.3 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.9, 169.2, 166.6, 153.3, 136.2, 129.1, 128.8, 127.1, 124.6, 120.0, 82.3, 77.3, 60.4, 49.2, 48.2, 47.1, 42.5, 41.1, 37.9, 36.5, 35.5, 32.7, 30.8, 26.6, 26.1, 23.6, 20.8, 17.5, 14.2.

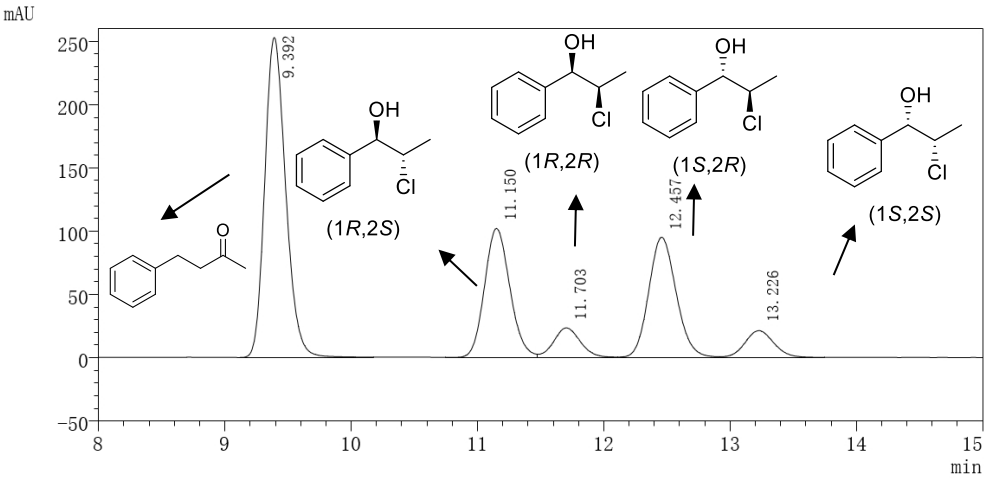
7b:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (d, *J* = 6.3 Hz, 1H), 7.98 (dt, *J* = 14.2, 1.9 Hz, 1H), 7.86 – 7.70 (m, 3H), 7.49 – 7.43 (m, 1H), 7.38 – 7.18 (m, 8H), 7.16 (d, *J* = 2.1 Hz, 1H), 6.00 (d, *J* = 8.4 Hz, 1H), 5.01 (dt, *J* = 8.7, 7.0 Hz, 1H), 4.25 (q, *J* = 4.8 Hz, 2H), 4.19 (dd, *J* = 5.6, 3.8 Hz, 2H), 3.81 – 3.74 (m, 4H), 3.40 (dd, *J* = 4.9, 1.0 Hz, 6H), 1.87 (s, 3H), 1.42 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.5, 156.5, 154.6, 153.1, 149.0, 147.3, 139.2, 136.3, 131.3, 129.6, 129.2, 128.9, 128.6, 127.2, 126.6, 121.8, 121.4, 118.9, 109.1, 108.2, 102.4, 70.9, 70.4, 69.2, 68.4, 60.5, 59.3, 59.3, 29.7, 20.8, 17.5.

7. Chiral HPLC and NMR Spectra

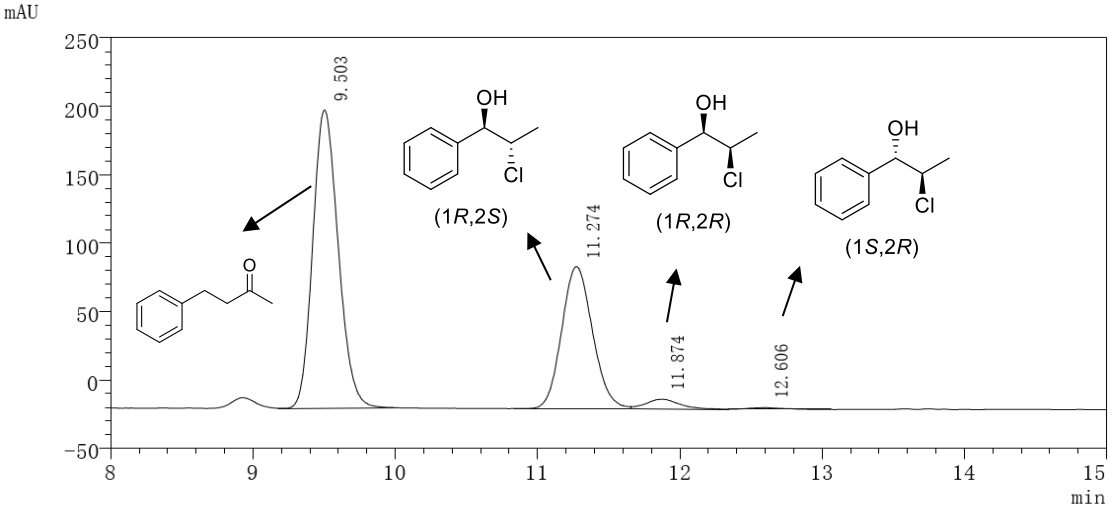
HPLC trace for the chemical synthesized (*rac*)-**2a**



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.392	2907017	252584	45.058
2	11.150	1420555	101745	22.018
3	11.703	344543	23335	5.340
4	12.457	1438274	94953	22.293
5	13.226	341283	21227	5.290

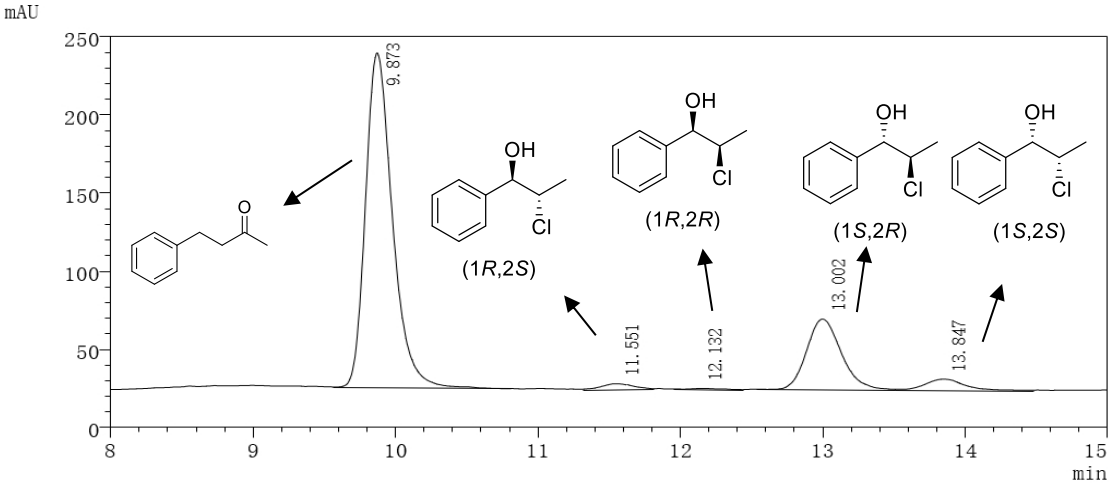
HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2a**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.503	2716478	218005	61.287
2	11.274	1568807	103660	35.394
3	11.874	124219	7246	2.803
4	12.606	22888	1307	0.516

HPLC trace for the enzymatic synthesized (1*S*,2*R*)-**2a**.

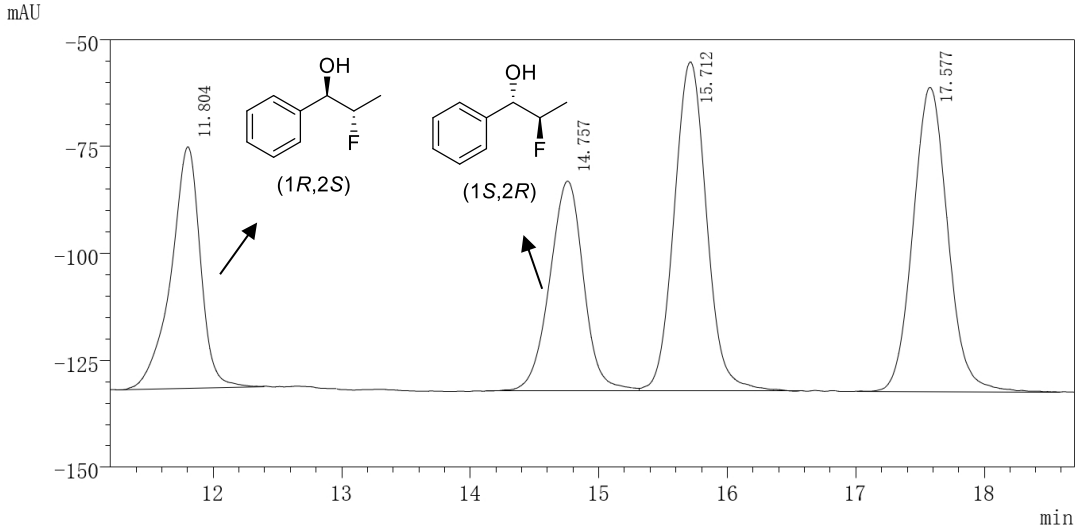


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.873	2811687	214227	75.096
2	11.551	47299	3395	1.263
3	12.132	6446	491	0.172
4	13.002	756436	45010	20.203
5	13.847	122271	6819	3.266

Chiral HPLC analysis: Diacel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 95/5, 0.8 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 11.6 min, $t_{(1R,2R)}$ = 12.1 min, $t_{(1S,2R)}$ = 13.0 min, $t_{(1S,2S)}$ = 13.8 min, interior label: 4-phenyl-2-butanone.

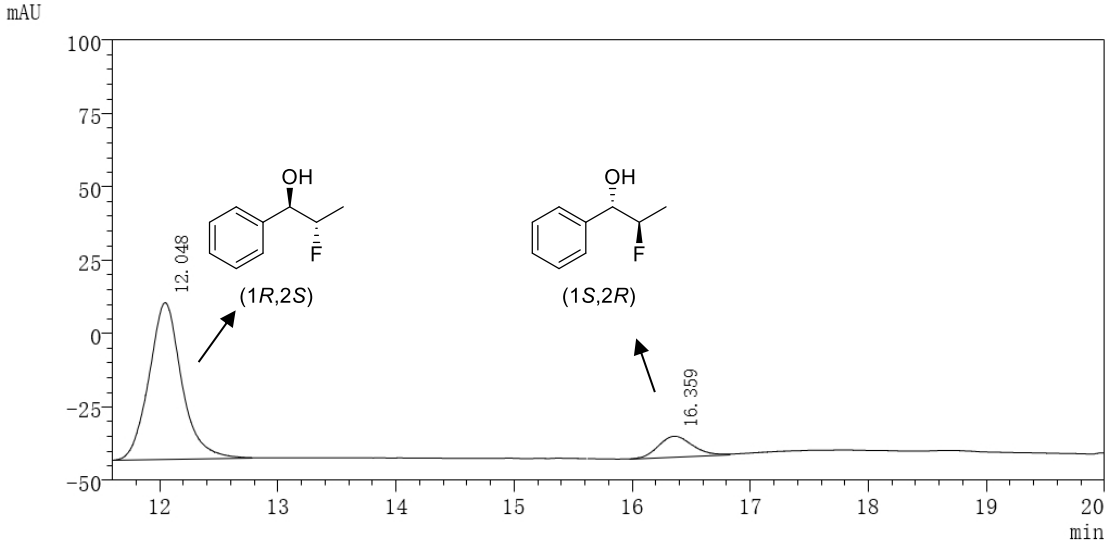
HPLC trace for the chemical synthesized (*rac*)-**2b**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.804	896352	56457	19.990
2	14.757	904979	49115	20.183
3	15.712	1343143	77033	29.955
4	17.577	1339441	71130	29.872

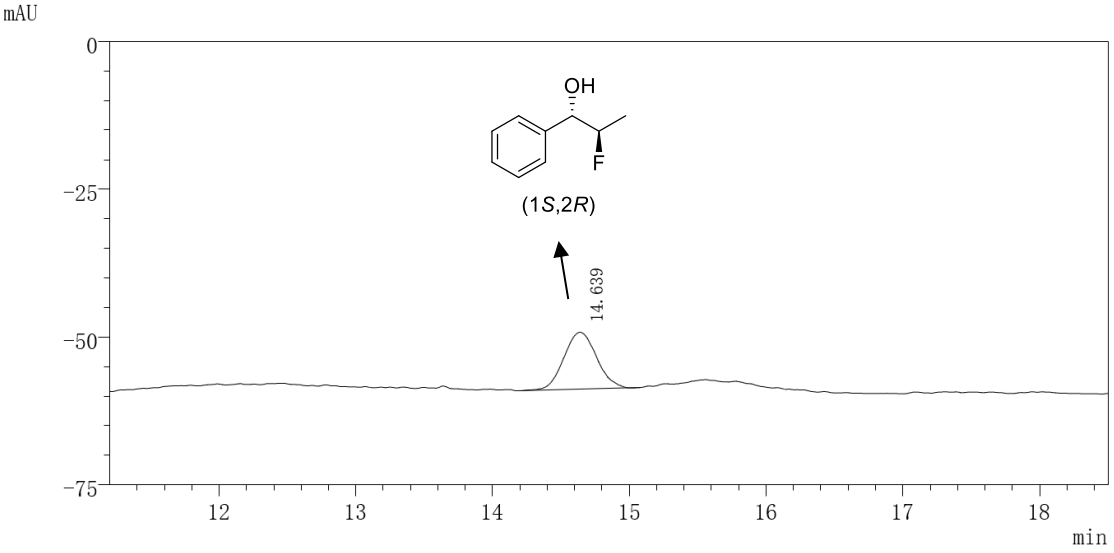
HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2b**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	12.048	1022905	53355	88.098
2	16.359	138195	7028	11.902

HPLC trace for the enzymatic synthesized (1*S*,2*R*)-**2b**.

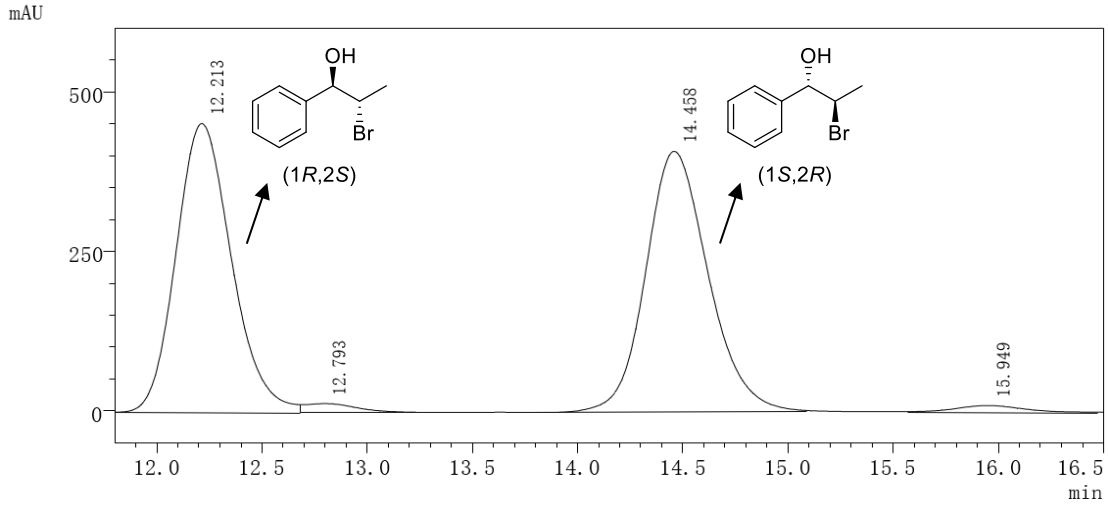


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	14.639	160338	9696	100.000

Chiral HPLC analysis: Diacel Chiralpak OX-3, *n*-Hexane /*i*-PrOH = 97/3, 0.7 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 12.0 min, $t_{(1S,2R)}$ = 14.6 min.

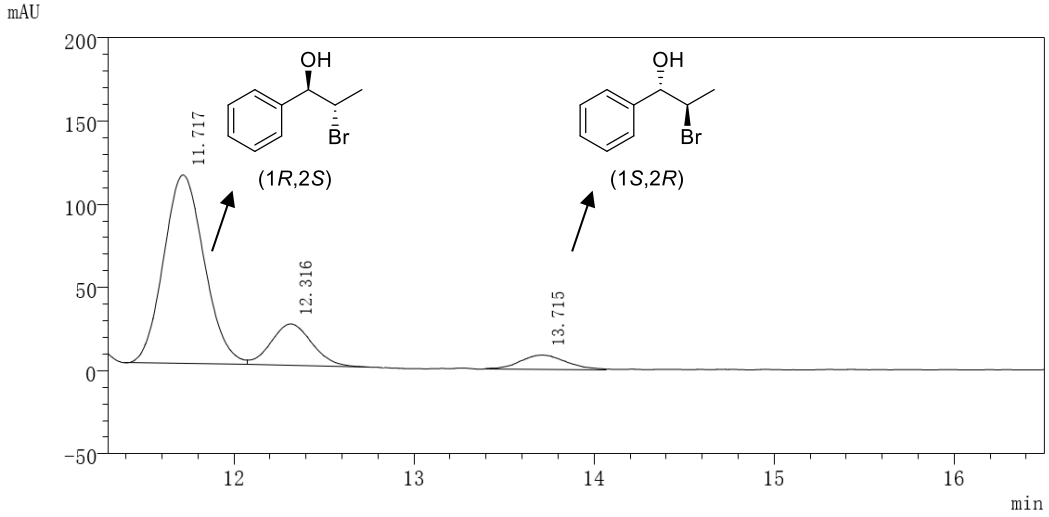
HPLC trace for the chemical synthesized (*rac*)-**2c**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	12.213	8270069	452070	48.367
2	12.793	227378	13567	1.330
3	14.458	8396939	408372	49.109
4	15.949	204323	9860	1.195

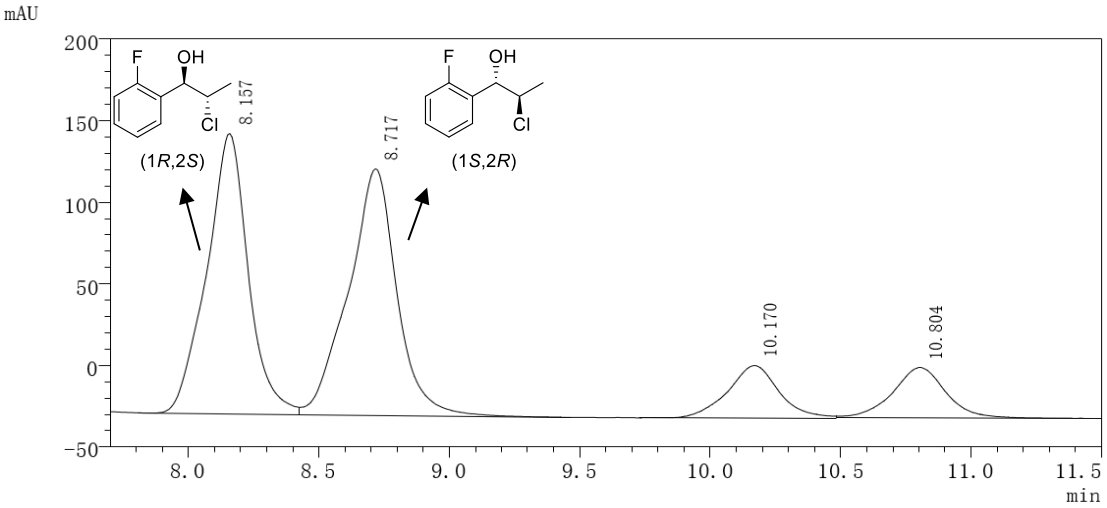
HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2c**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.717	1790257	113705	76.594
2	12.316	399851	25173	17.107
3	13.715	147219	8601	6.299

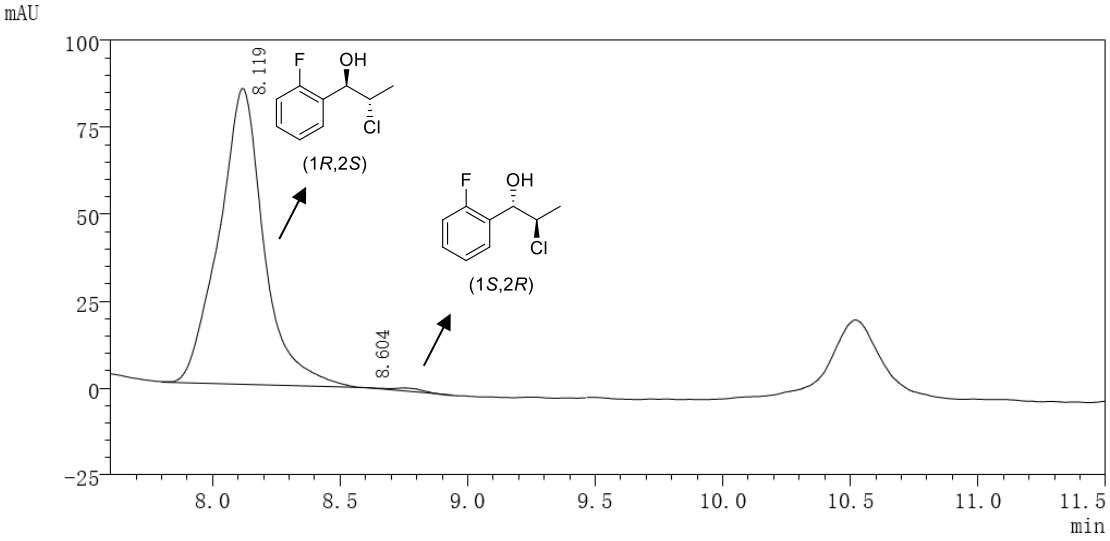
HPLC trace for the chemical synthesized (*rac*)-**2d**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	8.157	1896789	171645	40.097
2	8.717	1952338	150974	41.271
3	10.170	437607	31900	9.251
4	10.804	443749	30898	9.381

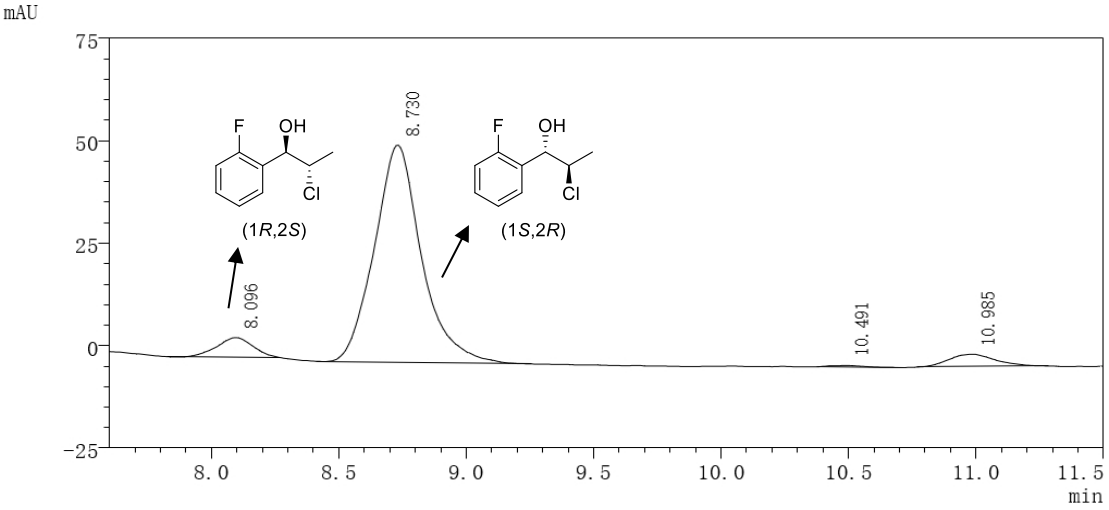
HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2d**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	8.119	1039592	85080	23.402
2	8.604	7874	27	0.177
3	21.024	3394797	158214	76.420

HPLC trace for the enzymatic synthesized (1*S*,2*R*)-**2d**.

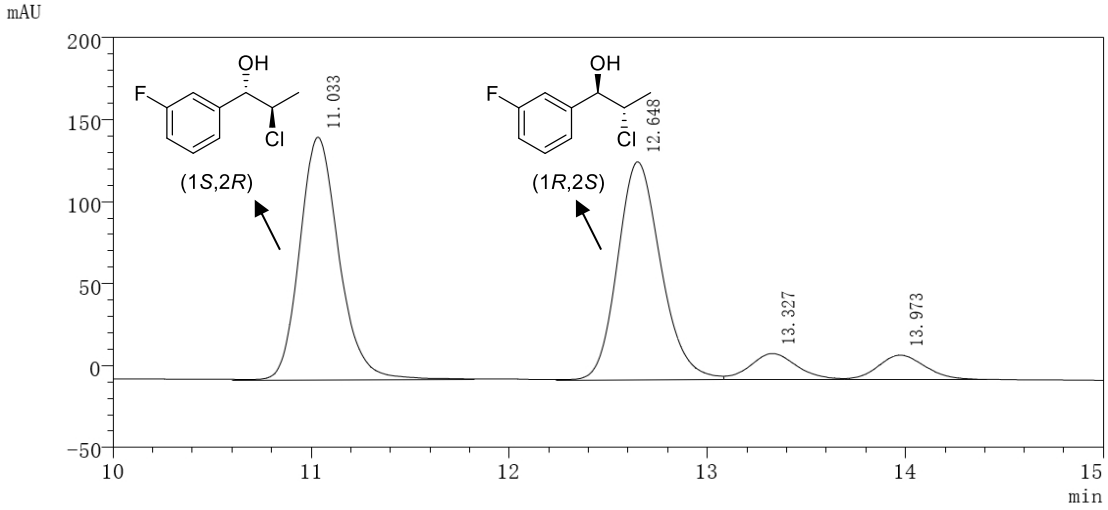


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	8.096	46226	4732	6.020
2	8.730	680780	52955	88.652
3	10.491	3457	394	0.450
4	10.985	37459	2920	4.878

Chiral HPLC analysis: Diacel Chiralpak OX-3, *n*-Hexane /*i*-PrOH = 97/3, 0.7 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 8.1 min, $t_{(1S,2R)}$ = 8.7 min.

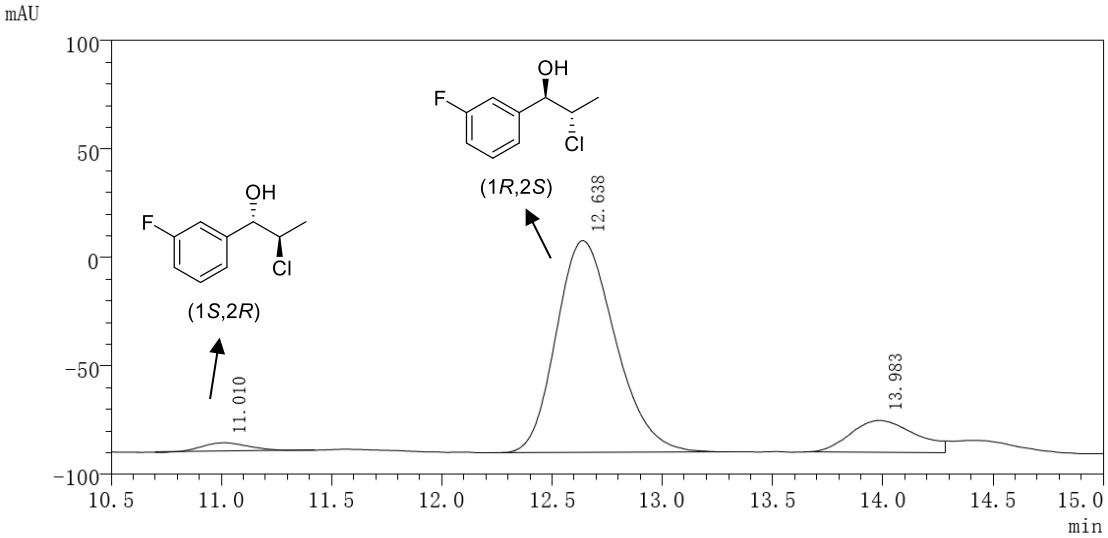
HPLC trace for the chemical synthesized (*rac*)-**2e**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.033	2014189	147836	44.555
2	12.648	2011972	132834	44.506
3	13.327	255466	15747	5.651
4	13.973	239024	14724	5.287

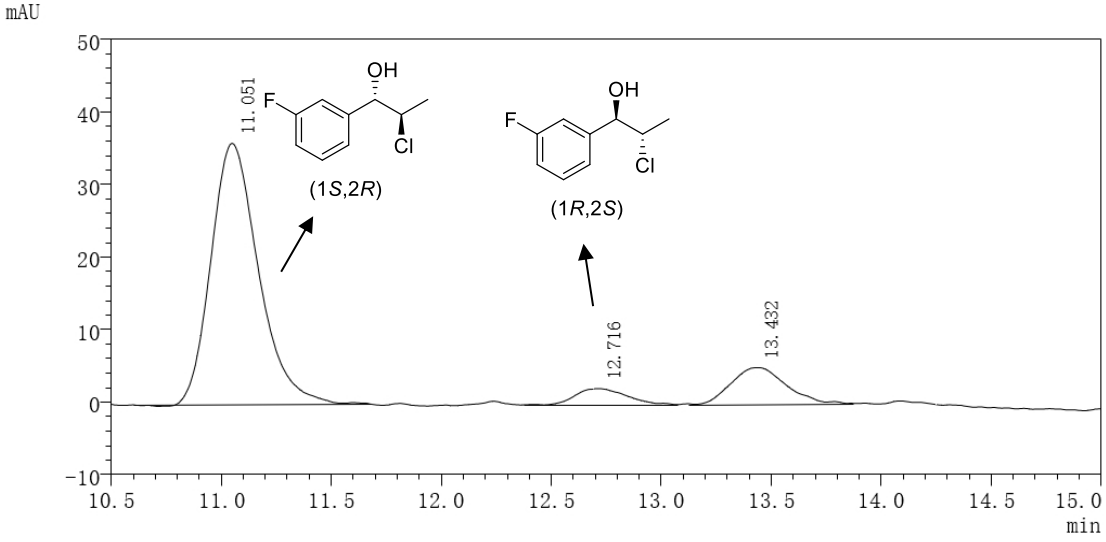
HPLC trace for the enzymatic synthesized (1*R,2S*)-**2e**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.010	60740	3994	2.776
2	12.638	1818583	97447	83.124
3	13.983	308461	14802	14.099

HPLC trace for the enzymatic synthesized (1*S*,2*R*)-**2e**.

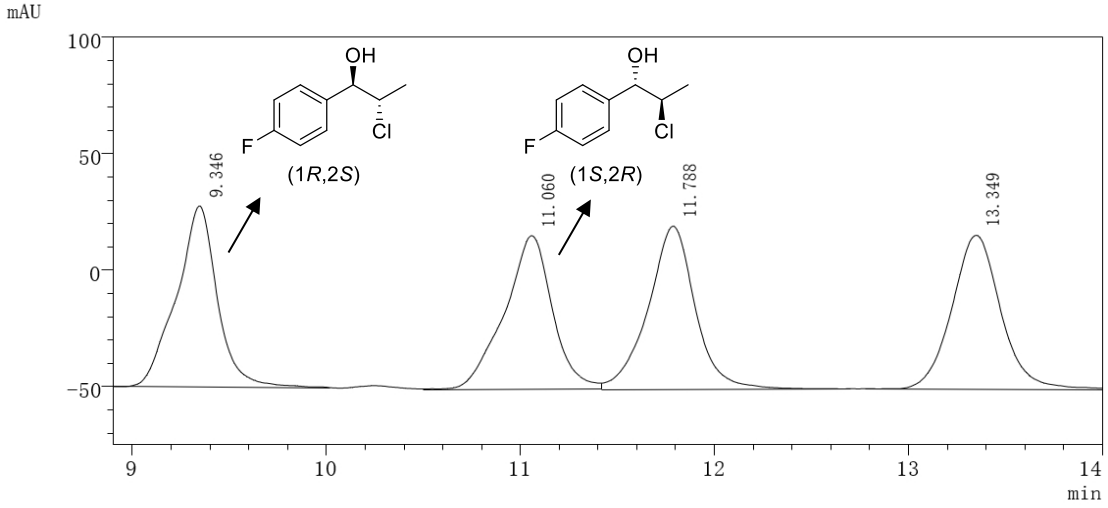


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.051	541019	36097	81.714
2	12.716	35983	2236	5.435
3	13.432	85087	5025	12.851

Chiral HPLC analysis: Diacel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 95/5, 0.8 mL/min, λ = 214 nm, $t_{(1S,2R)}$ = 11.1 min, $t_{(1R,2S)}$ = 12.7 min.

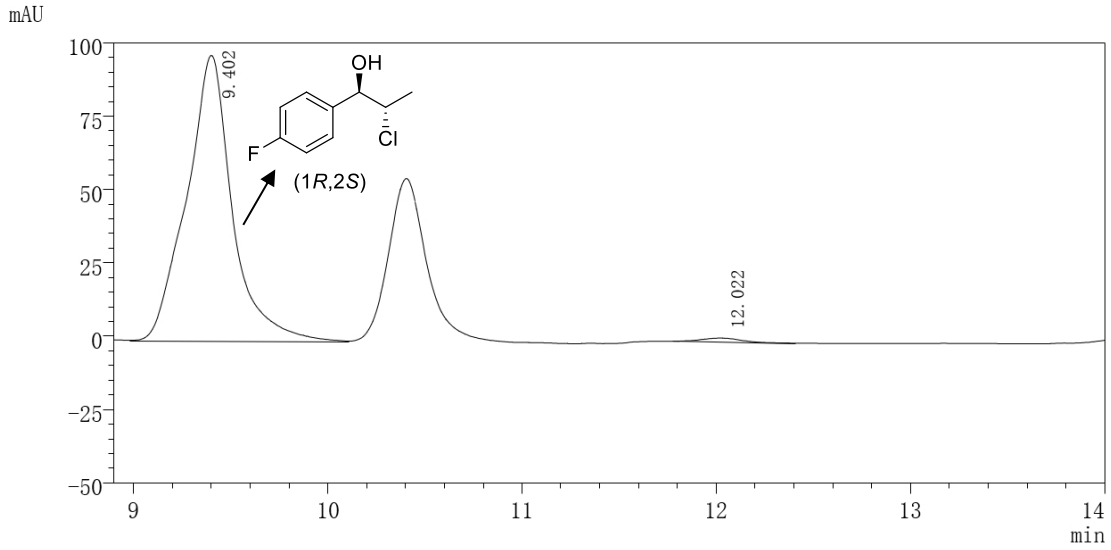
HPLC trace for the chemical synthesized (*rac*)-**2f**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.346	1138378	77785	24.782
2	11.060	1127827	65898	24.552
3	11.788	1176244	70138	25.606
4	13.349	1151167	66151	25.060

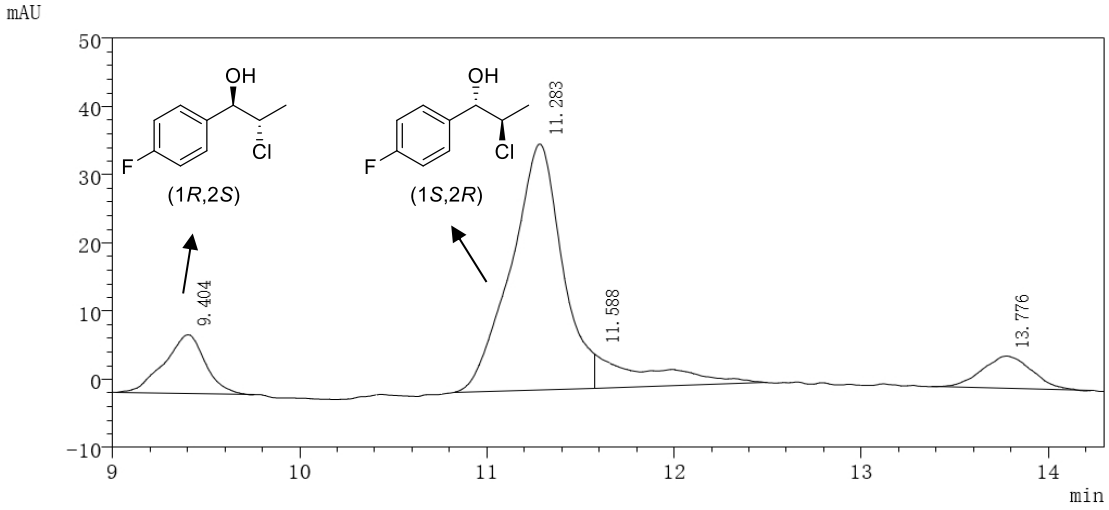
HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2f**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.402	1579637	97327	98.827
2	12.022	18744	1360	1.173

HPLC trace for the enzymatic synthesized (1*S*,2*R*)-**2f**.

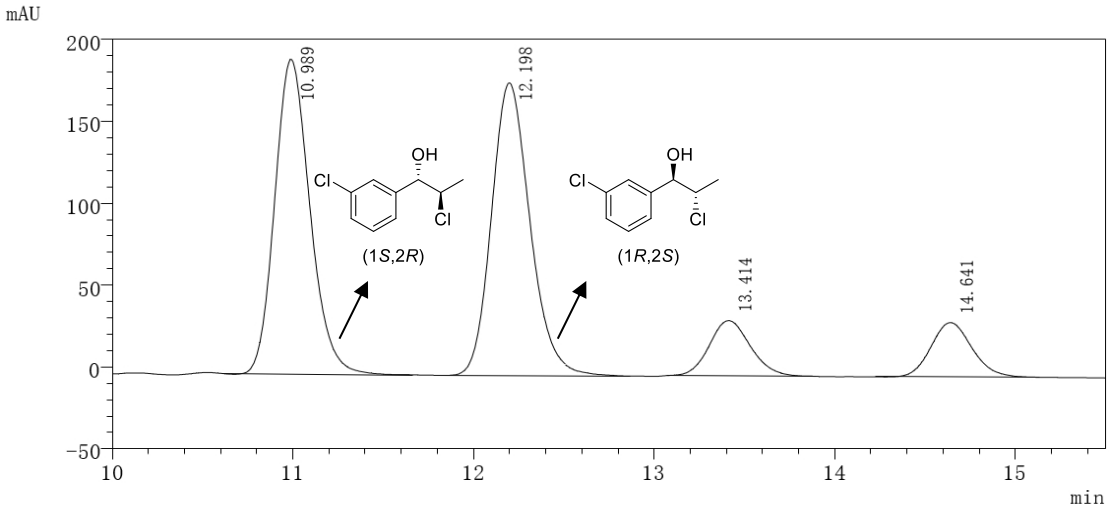


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.404	131126	8602	13.049
2	11.283	685540	36014	68.222
3	11.588	102327	4825	10.183
4	13.776	85873	4631	8.546

Chiral HPLC analysis: Diacel Chiralpak OX-3, Hexane/*i*-PrOH = 97/3, 0.7 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 9.4 min, $t_{(1R,2S)}$ = 11.3 min.

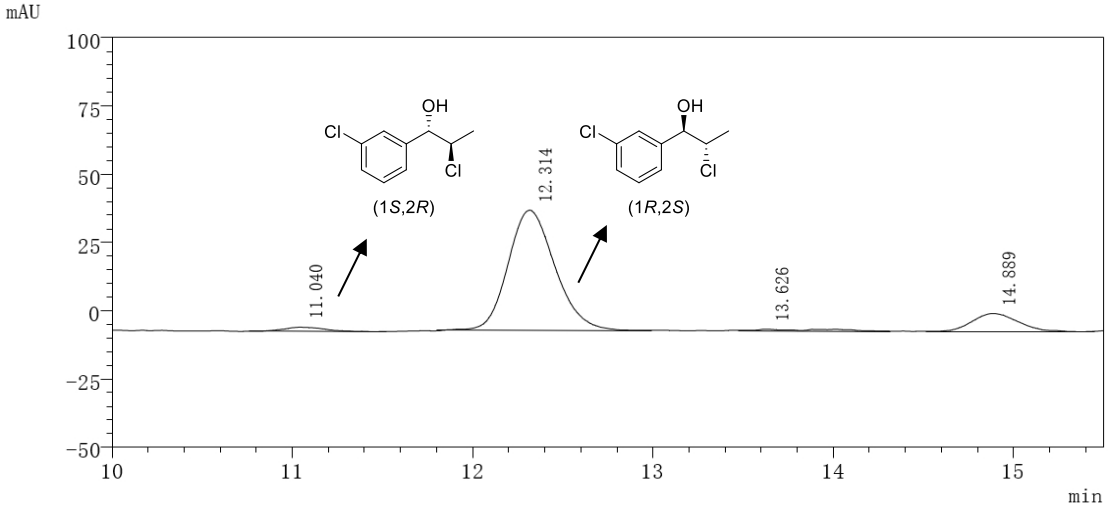
HPLC trace for the chemical synthesized (*rac*)-**2g**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	10.989	2605132	192386	41.193
2	12.198	2651417	178870	41.924
3	13.414	538651	33923	8.517
4	14.641	529080	33461	8.366

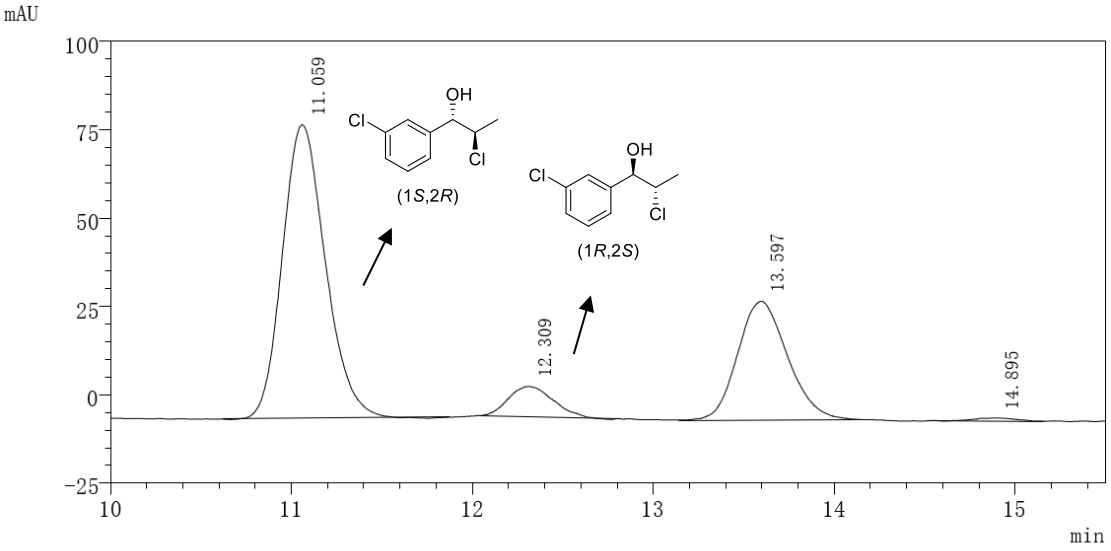
HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2g**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.040	23162	1515	2.436
2	12.314	801534	44099	84.294
3	13.626	13229	495	1.391
4	14.889	112956	6596	11.879

HPLC trace for the enzymatic synthesized (1*S,2R*)-**2g**.

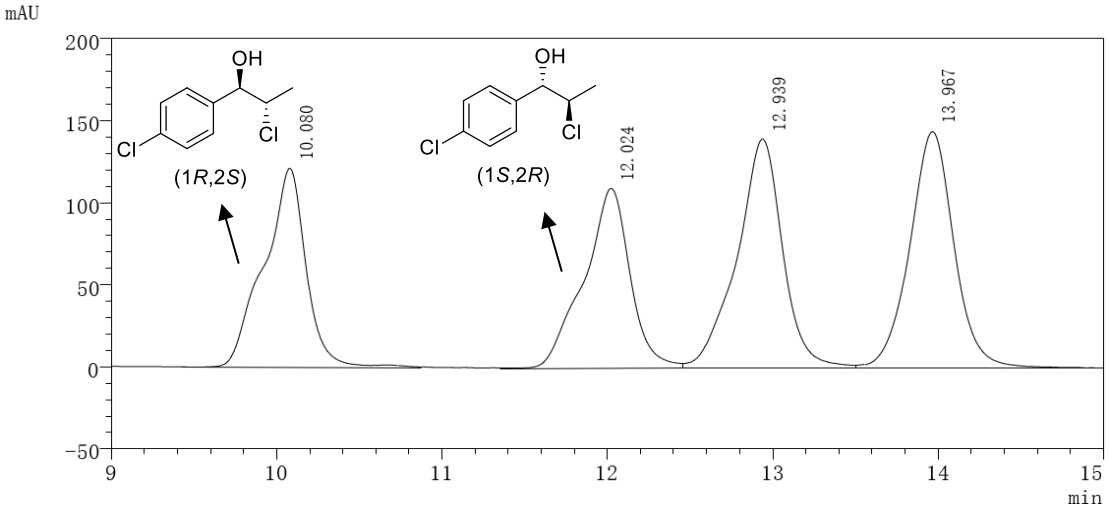


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.059	1375707	83263	63.175
2	12.309	146270	8554	6.717
3	13.597	641837	33596	29.474
4	14.895	13809	863	0.634

Chiral HPLC analysis: Diacel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 95/5, 0.8 mL/min, λ = 214 nm, $t_{(1S,2R)}$ = 11.0 min, $t_{(1R,2S)}$ = 12.3 min.

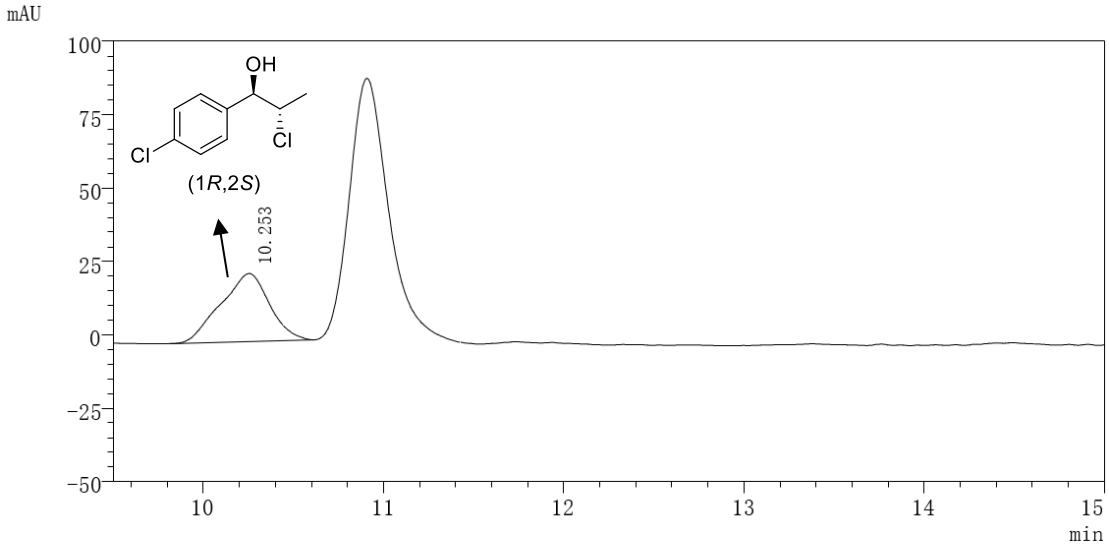
HPLC trace for the chemical synthesized (*rac*)-**2h**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	10.080	2138395	121298	22.275
2	12.024	2115051	109433	22.032
3	12.939	2671670	139206	27.830
4	13.967	2674767	143776	27.862

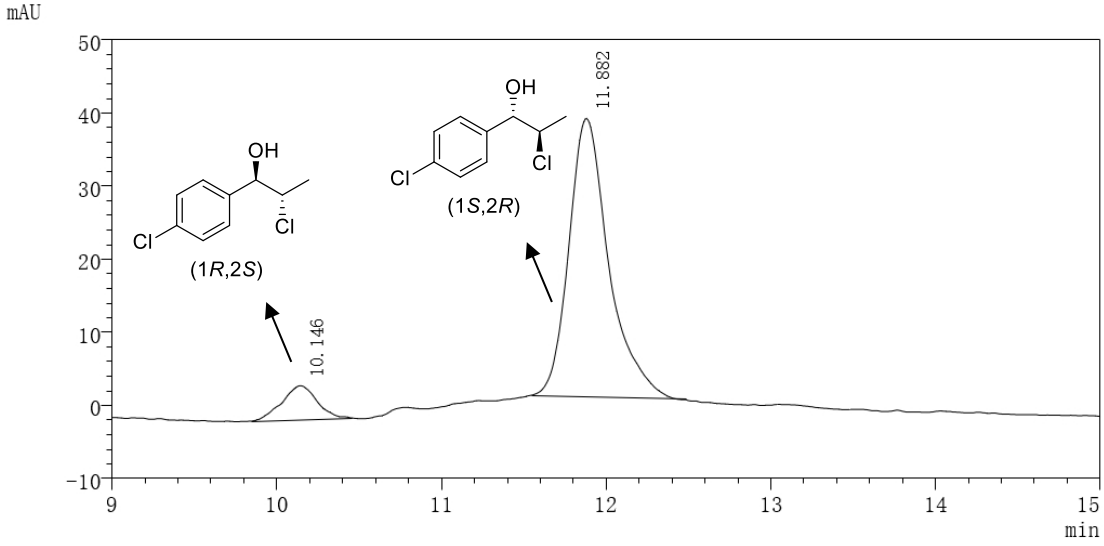
HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2h**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	10.253	434907	23122	100.000

HPLC trace for the enzymatic synthesized (1*S,2R*)-**2h**.

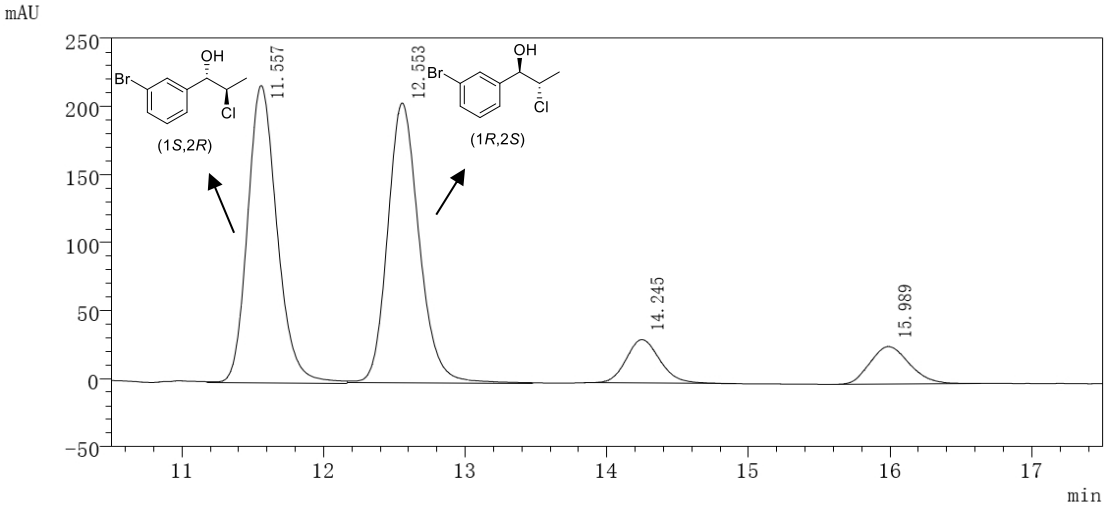


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	10.146	67925	4616	9.528
2	11.882	644953	38057	90.472

Chiral HPLC analysis: Diacel Chiralpak OX-3, *n*-Hexane/*i*-PrOH = 97/3, 0.7 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 10.1 min, $t_{(1S,2R)}$ = 11.9 min.

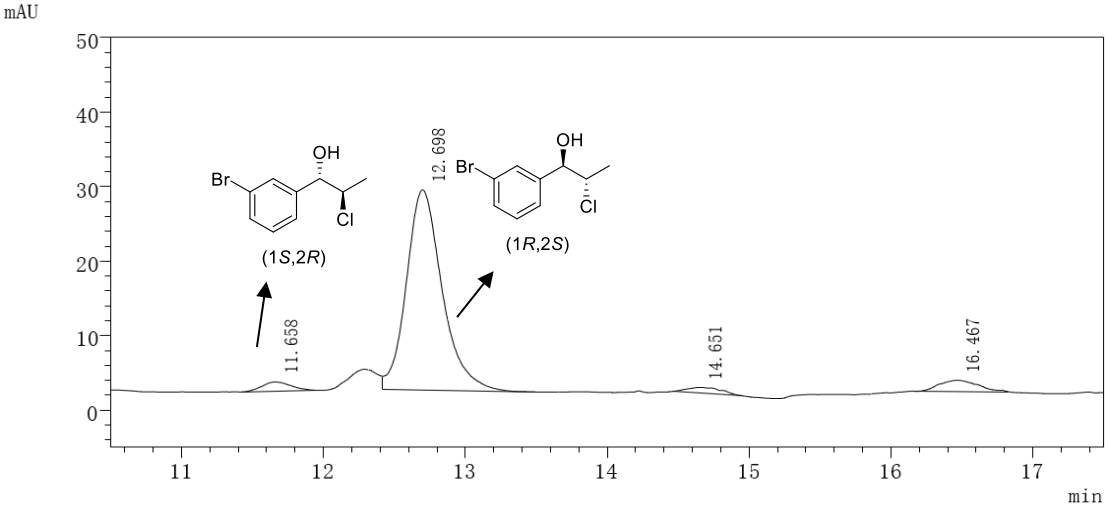
HPLC trace for the chemical synthesized (*rac*)-**2i**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.557	3118785	218076	42.582
2	12.553	3143220	205313	42.916
3	14.245	531775	31944	7.261
4	15.989	530364	27438	7.241

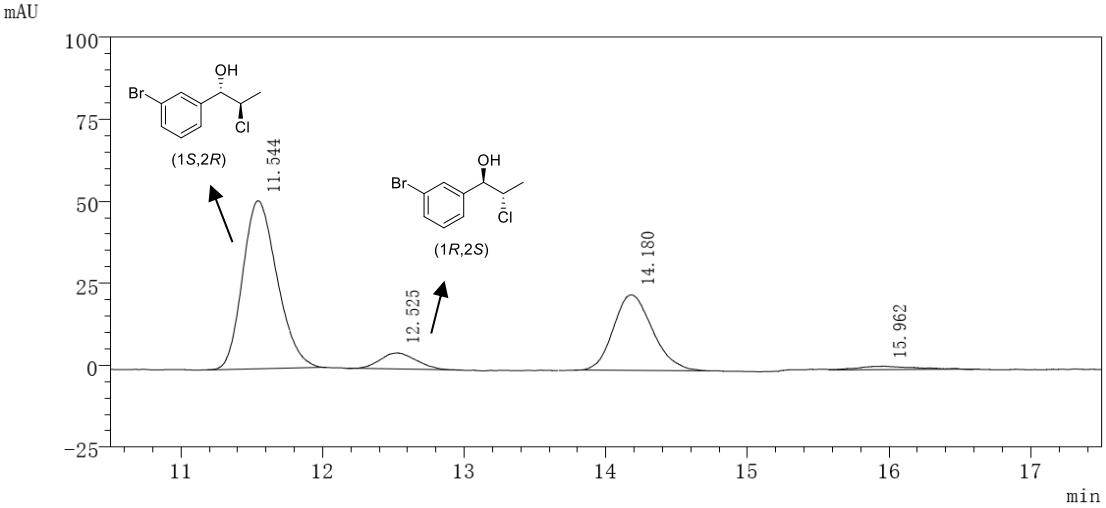
HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2i**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.658	17862	1255	3.364
2	12.698	472233	26901	88.947
3	14.651	12982	743	2.445
4	16.467	27838	1483	5.243

HPLC trace for the enzymatic synthesized (1*S*,2*R*)-**2i**.

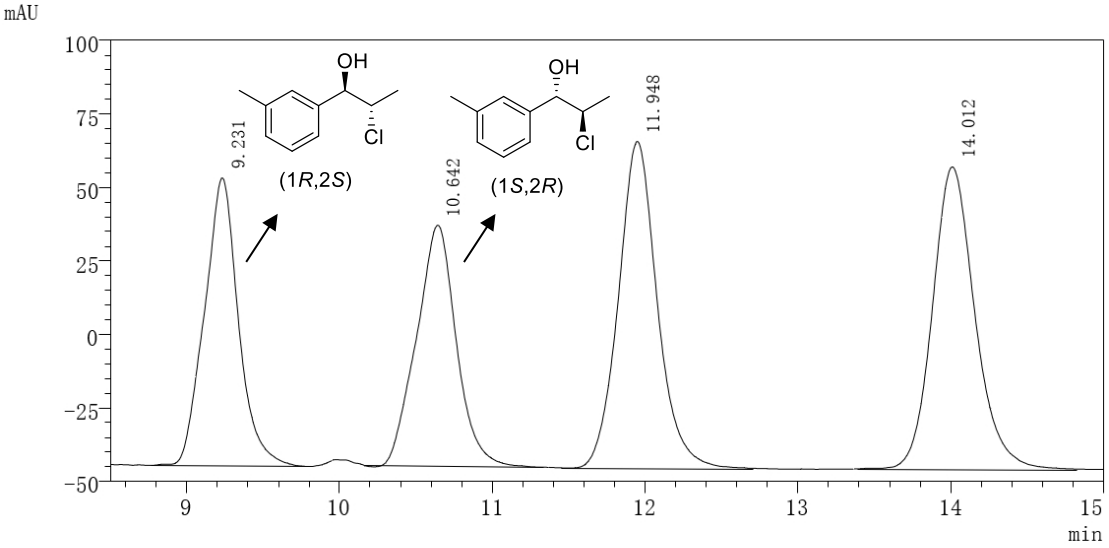


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.544	866891	51133	60.622
2	12.525	88793	4927	6.209
3	14.180	447542	23229	31.297
4	15.962	26775	983	1.872

Chiral HPLC analysis: Diacel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 95/5, 0.8 mL/min, λ = 214 nm, $t_{(1S,2R)}$ = 11.5 min, $t_{(1R,2S)}$ = 12.5 min.

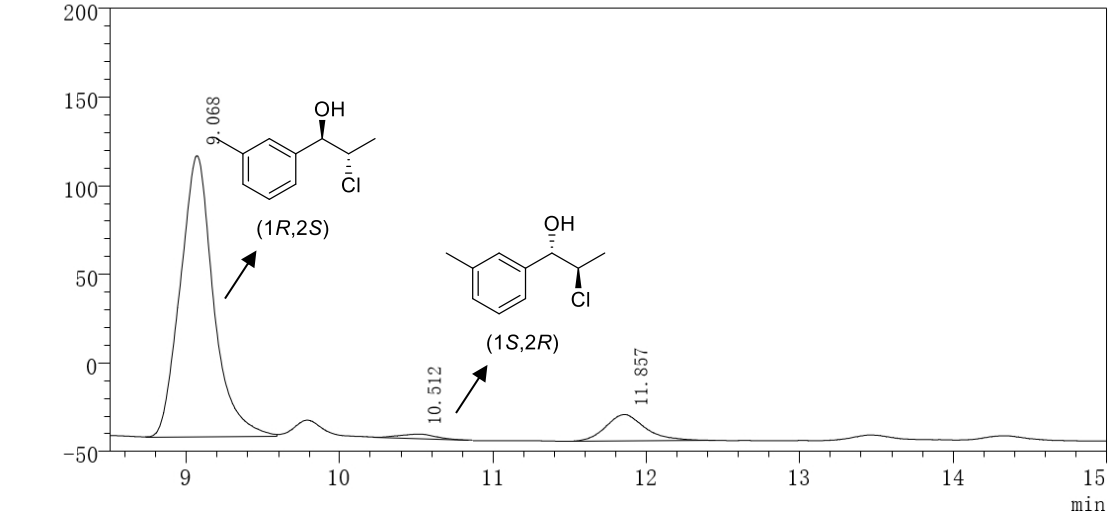
HPLC trace for the chemical synthesized (*rac*)-**2j**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.231	1513740	97724	21.845
2	10.642	1479891	81970	21.356
3	11.948	1961458	111125	28.306
4	14.012	1974419	102783	28.493

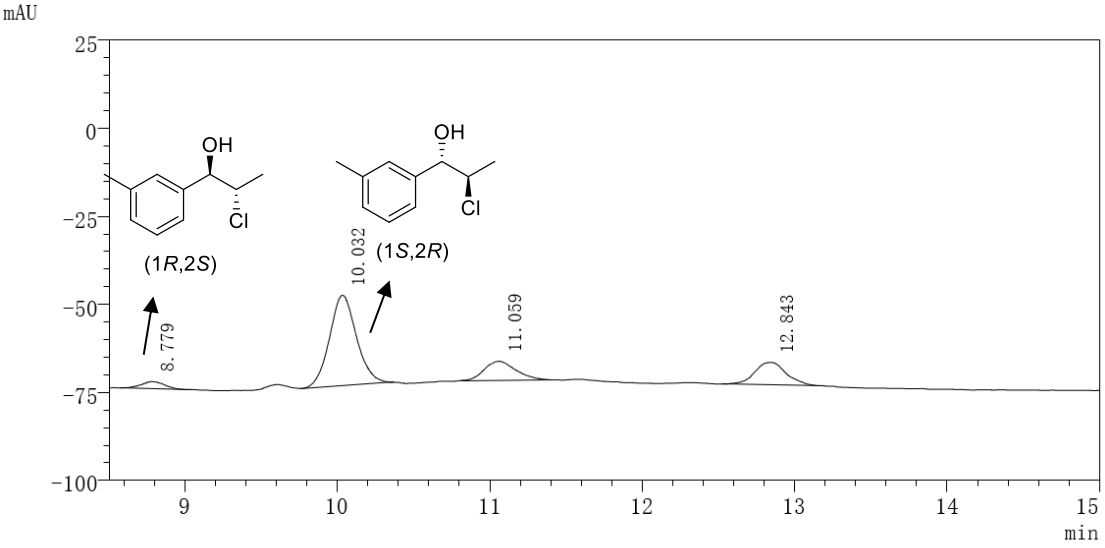
HPLC trace for the enzymatic synthesized (1*R,2S*)-**2j**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.068	2401983	159245	88.893
2	10.512	38938	2496	1.441
3	11.857	261188	14580	9.666

HPLC trace for the enzymatic synthesized (1*S*,2*R*)-**2j**.

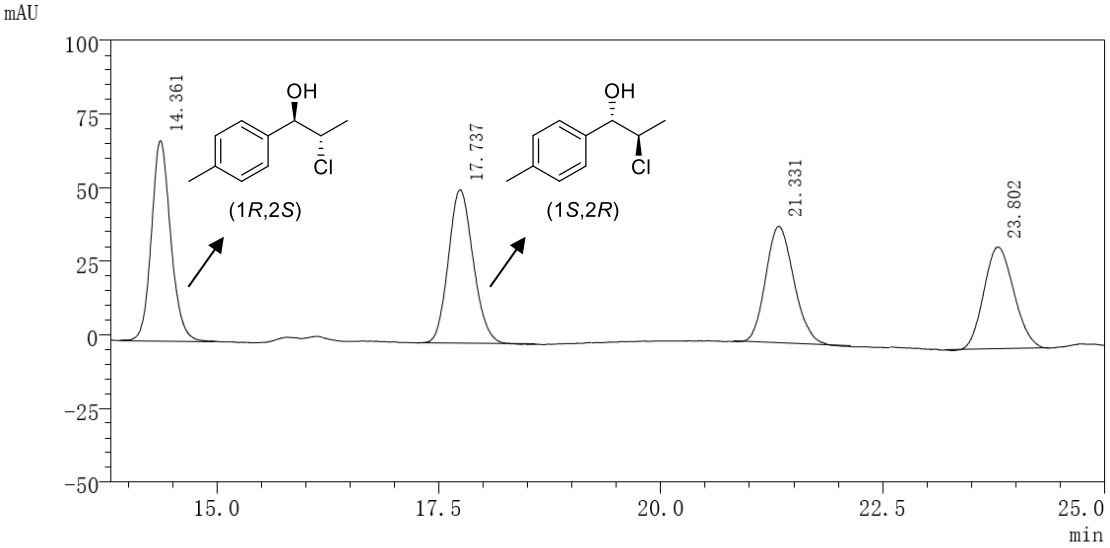


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	8.779	21174	1995	4.150
2	10.032	317576	25683	62.245
3	11.059	77651	5425	15.220
4	12.843	93798	6425	18.385

Chiral HPLC analysis: Diacel Chiralpak OX-3, *n*-Hexane/*i*-PrOH = 97/3, 0.7 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 8.8 min, $t_{(1S,2R)}$ = 10.0 min.

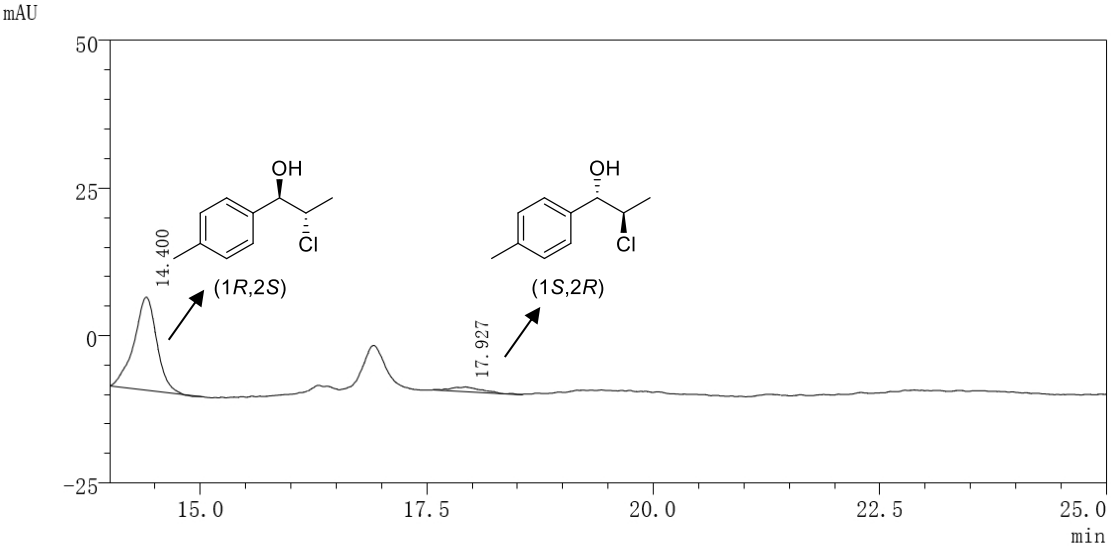
HPLC trace for the chemical synthesized (*rac*)-**2k**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	14.361	1026689	68035	27.434
2	17.737	1012240	51869	27.048
3	21.331	887852	39766	23.724
4	23.802	815594	34574	21.793

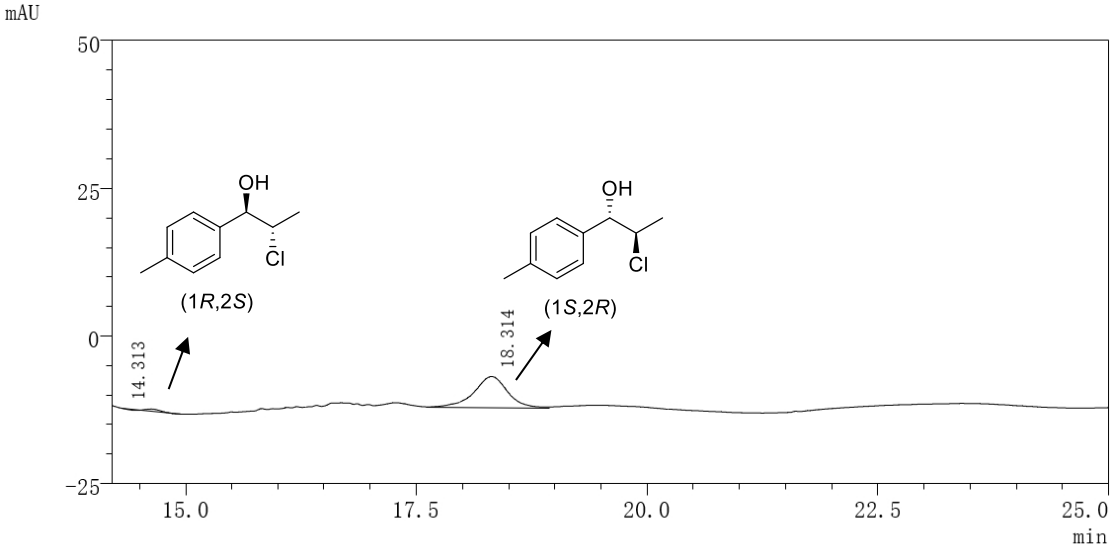
HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2k**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	14.400	276178	15810	94.731
2	17.927	15361	756	5.269

HPLC trace for the enzymatic synthesized (1*S*,2*R*)-**2k**.

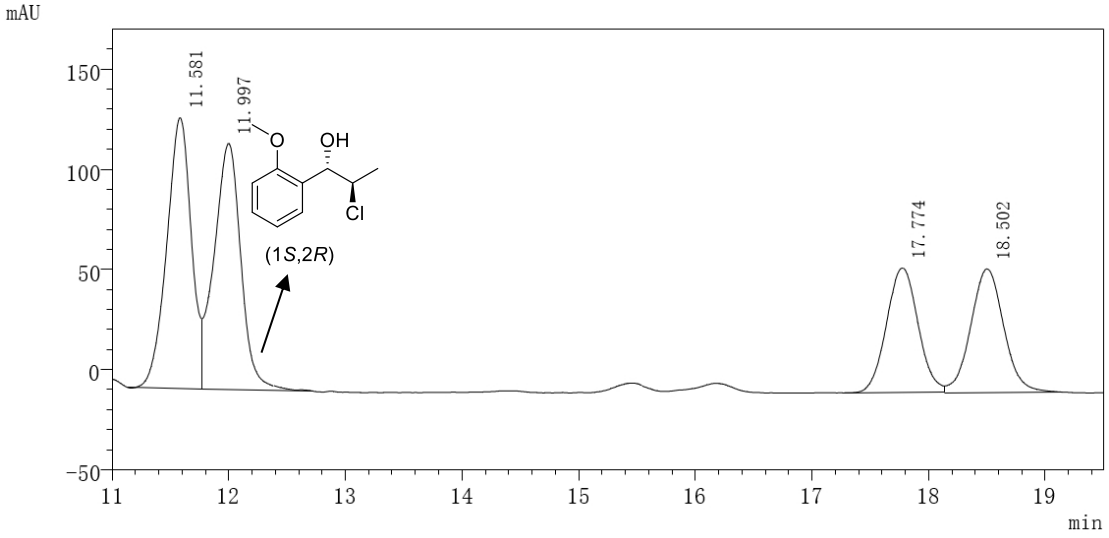


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	14.313	1578	-10	1.253
2	18.314	124313	5099	98.747

Chiral HPLC analysis: Diacel Chiralpak OX-3, *n*-Hexane/*i*-PrOH = 99/1, 0.8 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 14.3 min, $t_{(1S,2R)}$ = 18.3 min.

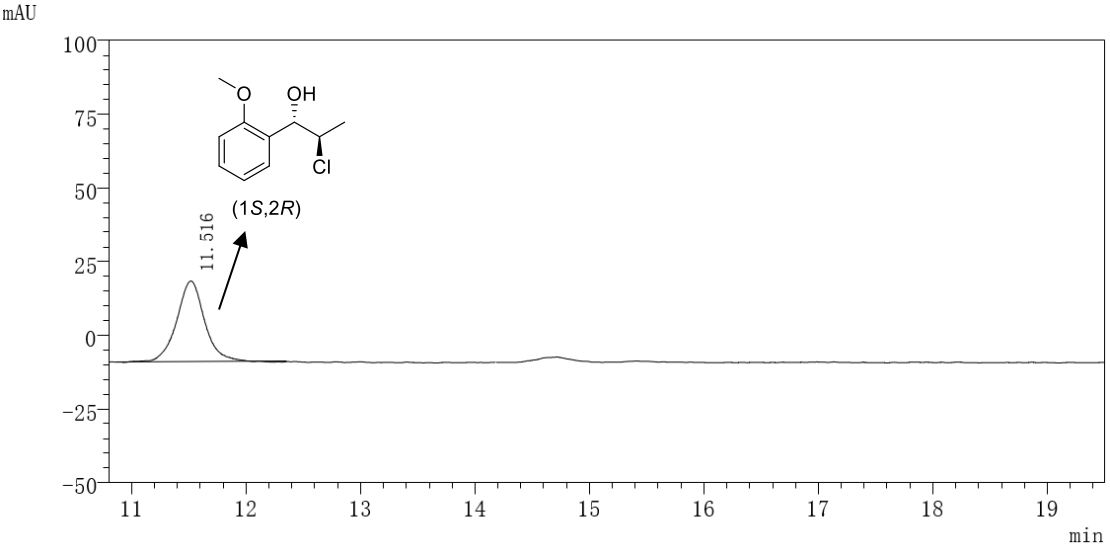
HPLC trace for the chemical synthesized (*rac*)-**2l**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.581	1991156	135330	31.441
2	11.997	1961852	122912	30.979
3	17.774	1172671	62177	18.517
4	18.502	1207269	61447	19.063

HPLC trace for the enzymatic synthesized (1*S*,2*R*)-**2l**.

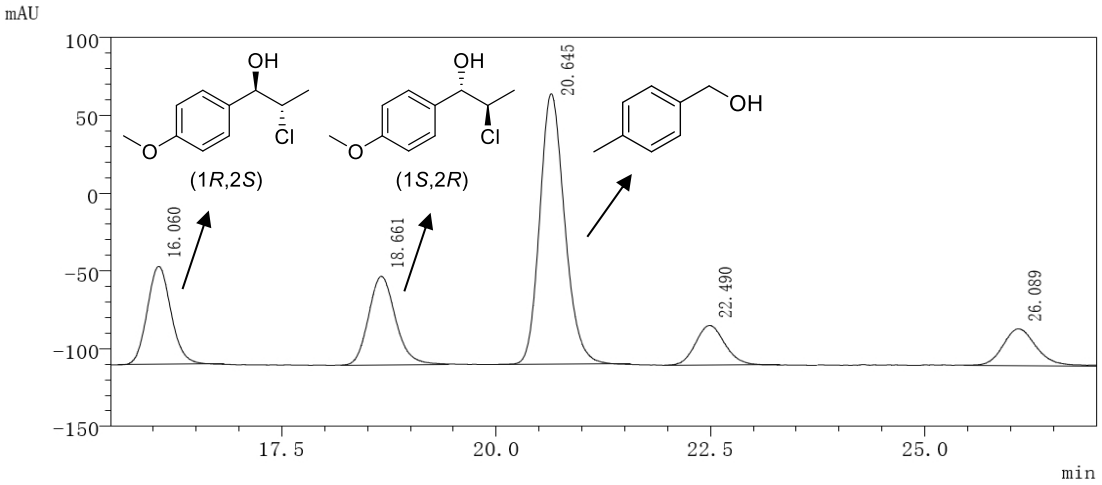


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.516	468212	27344	100.000

Chiral HPLC analysis: Diacel Chiralpak OX-3, *n*-Hexane/*i*-PrOH = 97/3, 0.7 mL/min, λ = 214 nm, $t_{(1S,2R)}$ = 11.5 min.

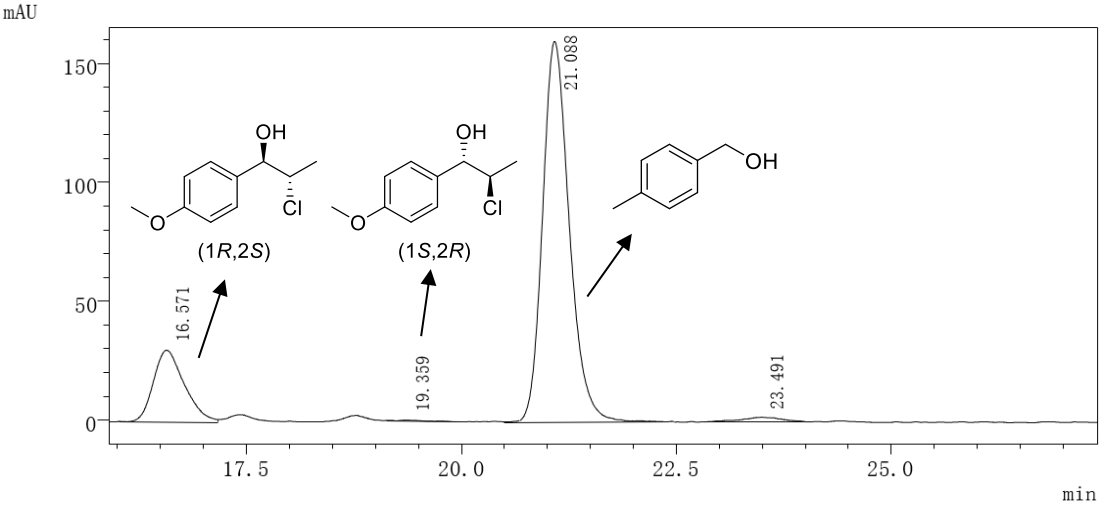
HPLC trace for the chemical synthesized (*rac*)-**2m**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	16.060	1228028	62976	17.030
2	18.661	1231243	56594	17.075
3	20.645	3541602	173989	49.115
4	22.490	601614	25228	8.343
5	26.089	608362	23069	8.437

HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2m**.

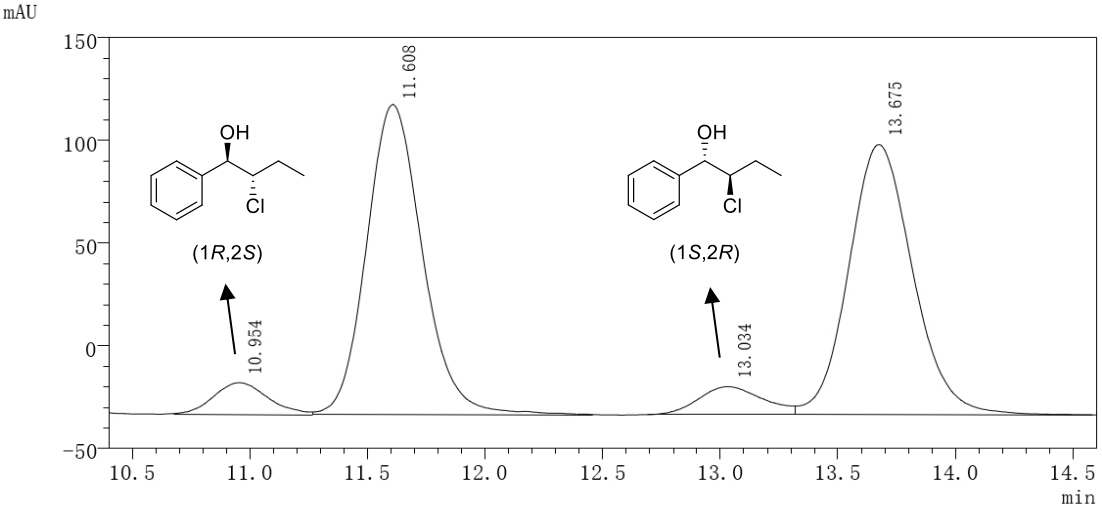


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	16.571	746940	30098	17.547
2	19.359	5357	335	0.126
3	21.088	3447243	159967	80.983
4	23.491	57226	1727	1.344

Chiral HPLC analysis: Diacel Chiralpak OX-3, *n*-Hexane/*i*-PrOH = 97/3, 0.7 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 16.6 min, interior label: 4-methylbenzyl alcohol.

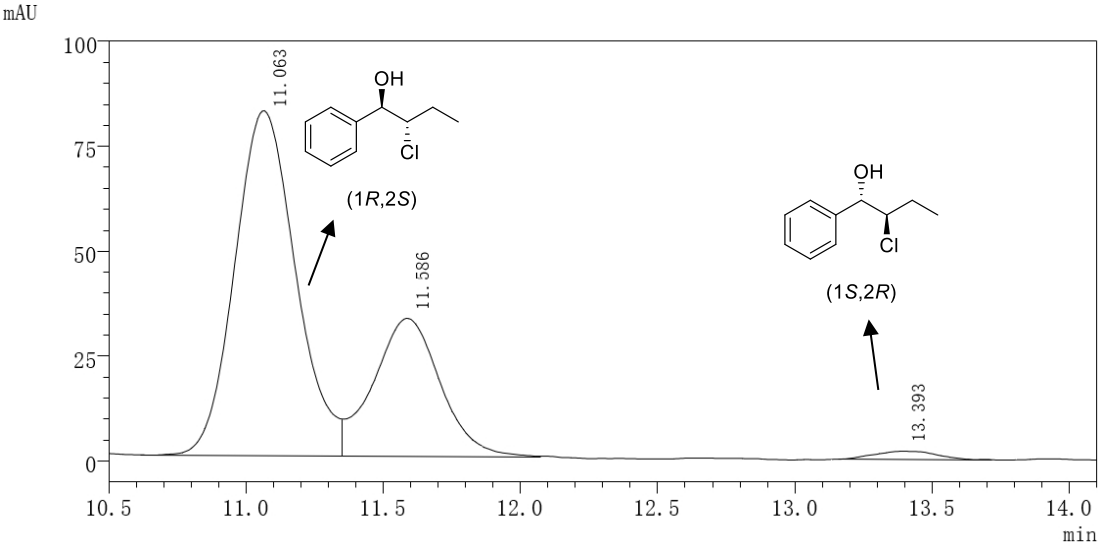
HPLC trace for the chemical synthesized (*rac*)-**2n**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	10.954	236289	15113	4.311
2	11.608	2487834	151020	45.391
3	13.034	262032	13658	4.781
4	13.675	2494762	131798	45.517

HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2n**.

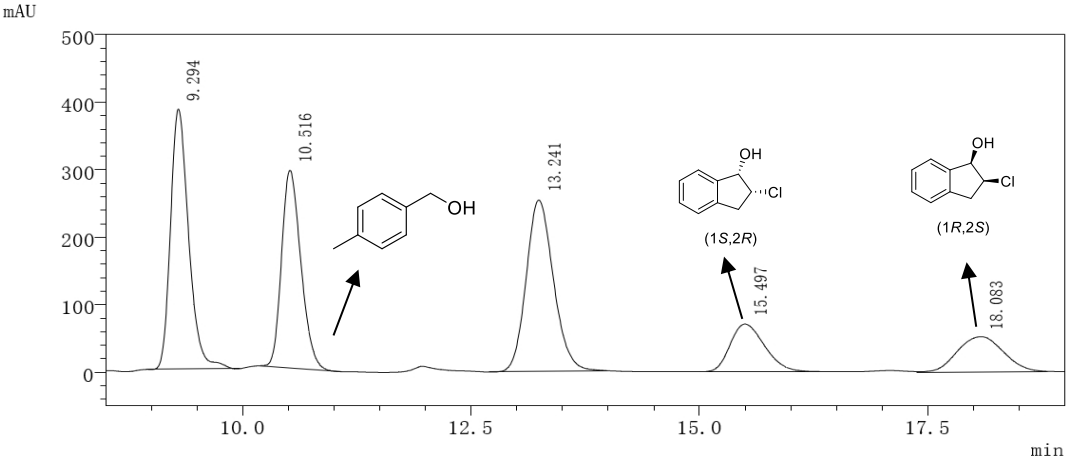


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	11.063	1266352	82145	68.630
2	11.586	548161	32727	29.708
3	13.393	30661	1956	1.662

Chiral HPLC analysis: Diacel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 95/5, 0.8 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 11.1 min.

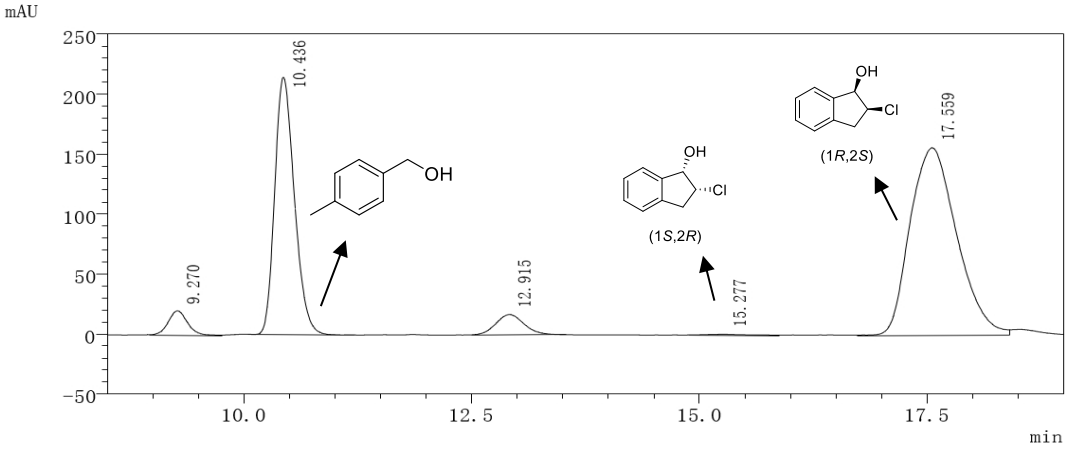
HPLC trace for the chemical synthesized (*rac*)-**2o**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.294	5336777	385203	28.758
2	10.516	4308358	292766	23.216
3	13.241	5282611	254510	28.466
4	15.497	1848089	70773	9.959
5	18.083	1781820	51522	9.602

HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2o**.

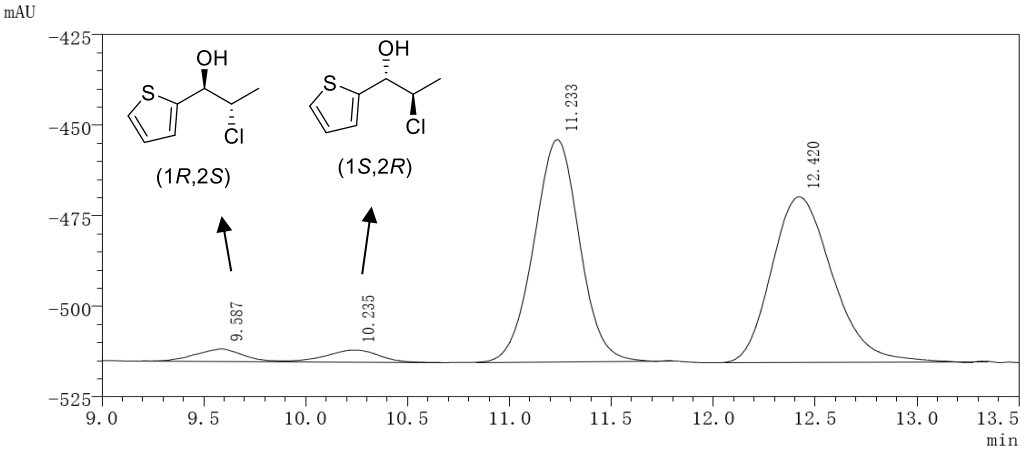


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.270	288806	20041	3.056
2	10.436	3228474	214322	34.165
3	12.915	363568	16936	3.847
4	15.277	14620	599	0.155
5	17.559	5554088	156095	58.776

Chiral HPLC analysis: Diacel Chiralpak AY-H, *n*-Hexane/*i*-PrOH = 95/5, 0.8 mL/min, λ = 214 nm, $t_{(1S,2R)}$ = 15.3 min, $t_{(1R,2S)}$ = 17.6 min, interior label: 4-methylbenzyl alcohol.

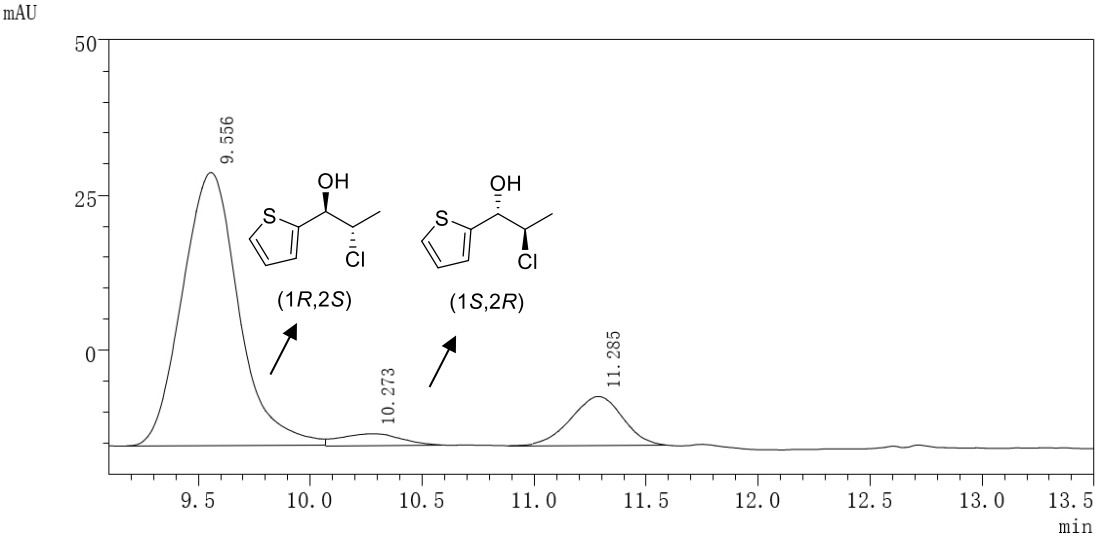
HPLC trace for the chemical synthesized (*rac*)-**2p**:



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.587	55841	3465	2.769
2	10.235	59716	3319	2.961
3	11.233	954534	61457	47.338
4	12.420	946344	45700	46.932

HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**2p**.

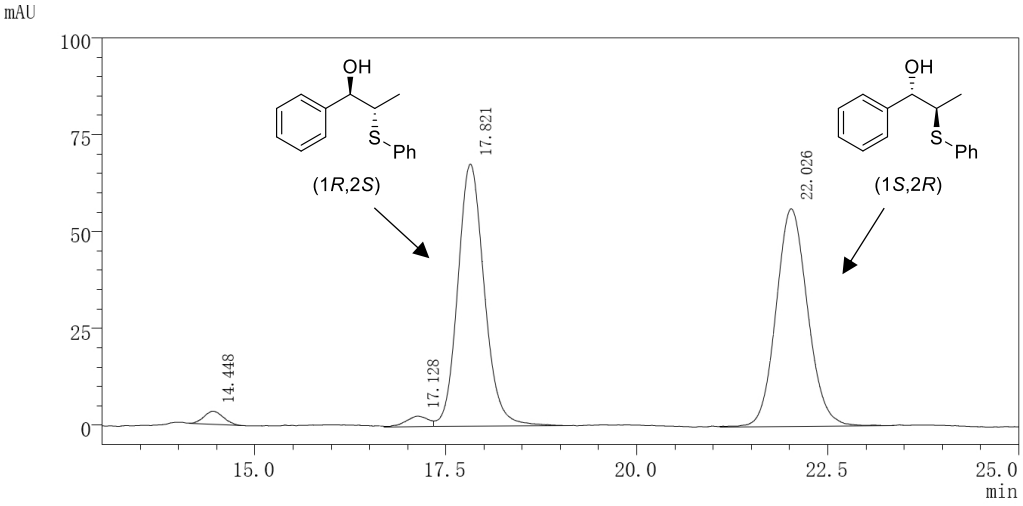


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	9.556	772059	43977	82.734
2	10.273	34598	1853	3.708
3	11.285	126528	7844	13.559

Chiral HPLC analysis: Diacel Chiralpak AY-H, *n*-Hexane/*i*-PrOH = 95/5, 0.8 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 9.6 min, $t_{(1S,2R)}$ = 10.3 min.

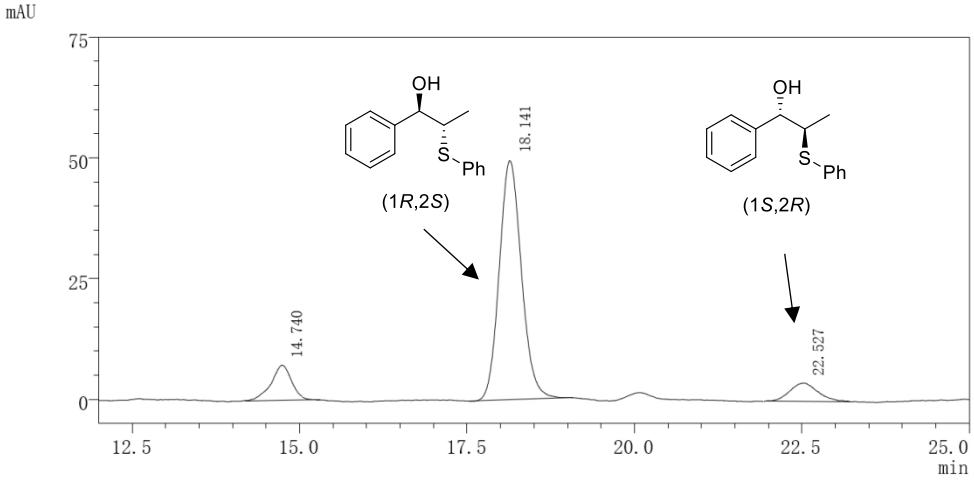
HPLC trace for the chemical synthesized (*rac*)-**3**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	14.448	59334	3406	1.770
2	17.128	50513	2558	1.507
3	17.821	1631124	67573	48.655
4	22.026	1611443	56235	48.068

HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**3**.

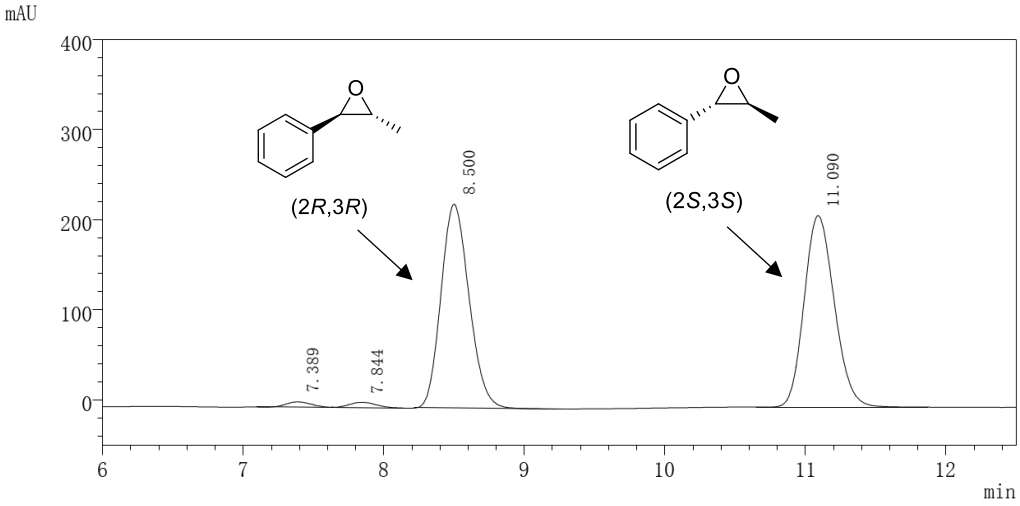


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	14.740	155463	7256	11.060
2	18.141	1142091	49444	81.254
3	22.527	108022	3707	7.685

Chiral HPLC analysis: Diacel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 97/3, 0.8 mL/min, λ = 214 nm, $t_{(1R,2S)}$ = 18.1 min, $t_{(1S,2R)}$ = 22.5 min.

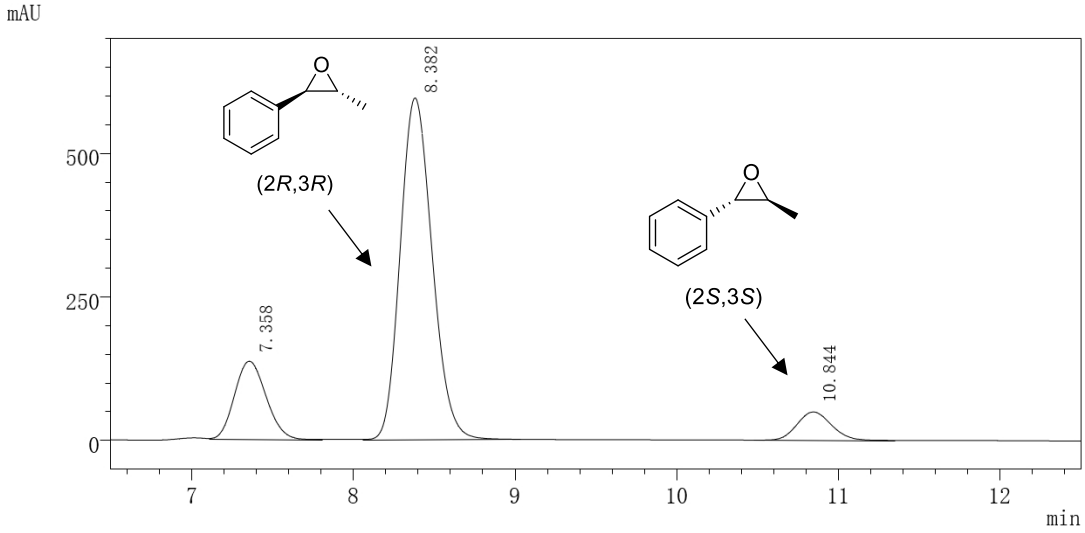
HPLC trace for the chemical synthesized (*rac*)-**4**.



PDA 210nm

ID#	Rt. Time	Area	Height	Area %
1	7.389	77258	6066	1.190
2	7.844	83084	6145	1.280
3	8.500	3149405	226595	48.515
4	11.090	3181819	212867	49.015

HPLC trace for the enzymatic synthesized (2*R*,3*R*)-**4**.

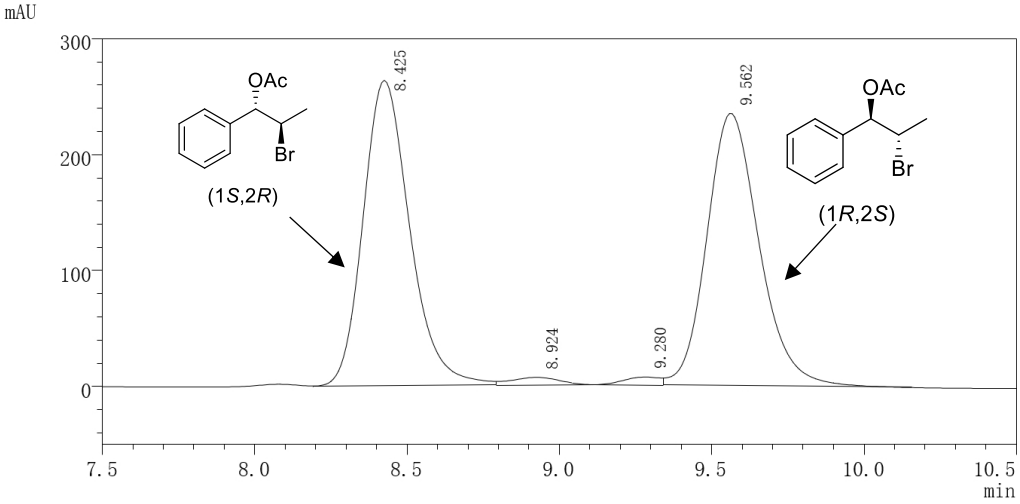


PDA 210nm

ID#	Rt. Time	Area	Height	Area %
1	7.358	1812062	135312	16.936
2	8.382	8158880	594933	76.255
3	10.844	728475	49365	6.809

Chiral HPLC analysis: Diacel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 99/1, 0.8 mL/min, λ = 210 nm, $t_{(2R,2R)}$ = 8.4 min, $t_{(2S,2S)}$ = 10.8 min.

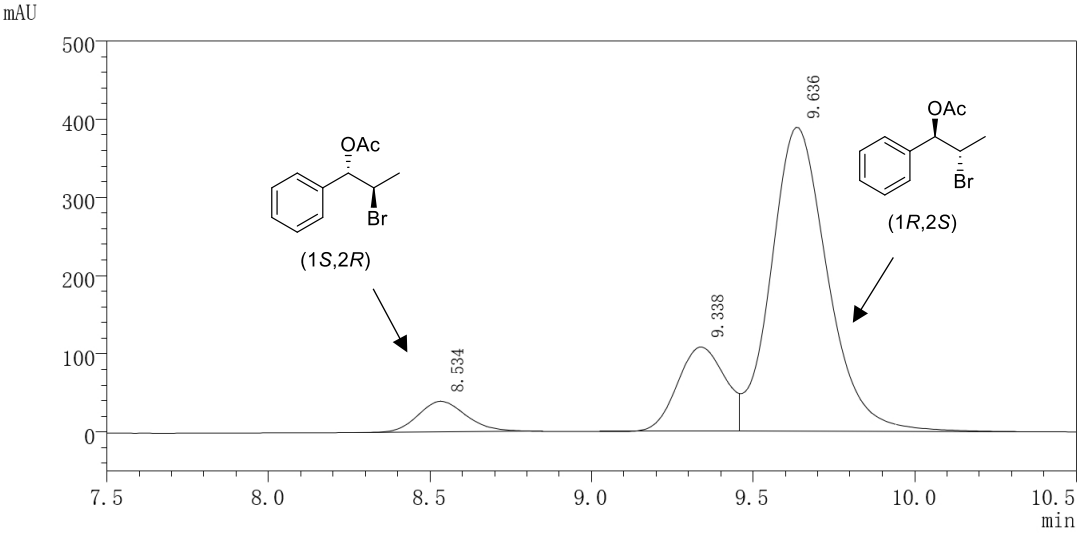
HPLC trace for the chemical synthesized (*rac*)-**5**.



PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	8.425	2809875	263838	48.826
2	8.924	69291	6489	1.204
3	9.280	58181	6945	1.011
4	9.562	2817544	234878	48.959

HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**5**.

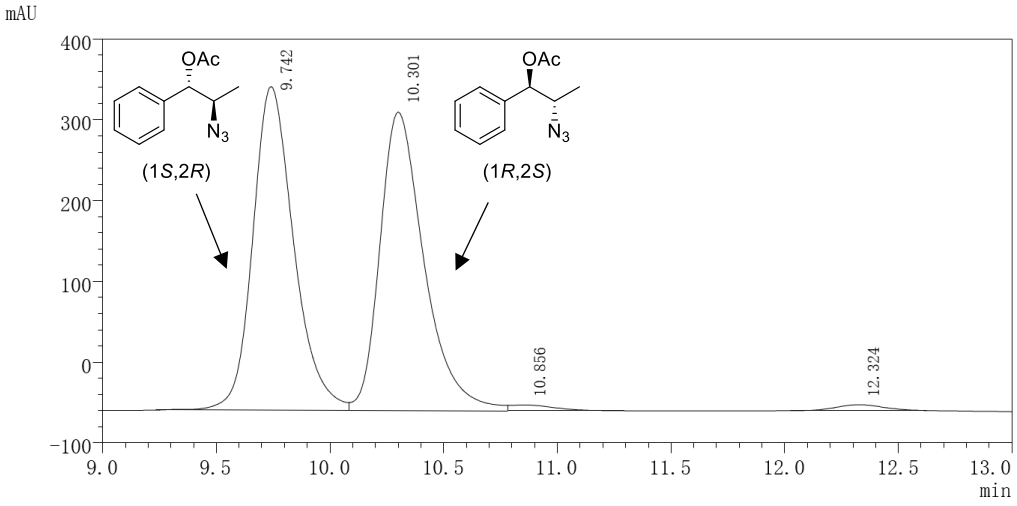


PDA 214nm

ID#	Rt. Time	Area	Height	Area %
1	8.534	410870	39139	6.581
2	9.338	1118407	107741	17.913
3	9.636	4714430	388239	75.507

Chiral HPLC analysis: Diacel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 99/1, 0.8 mL/min, λ = 214 nm, $t_{(1S,2R)}$ = 8.5 min, $t_{(1R,2S)}$ = 9.6 min.

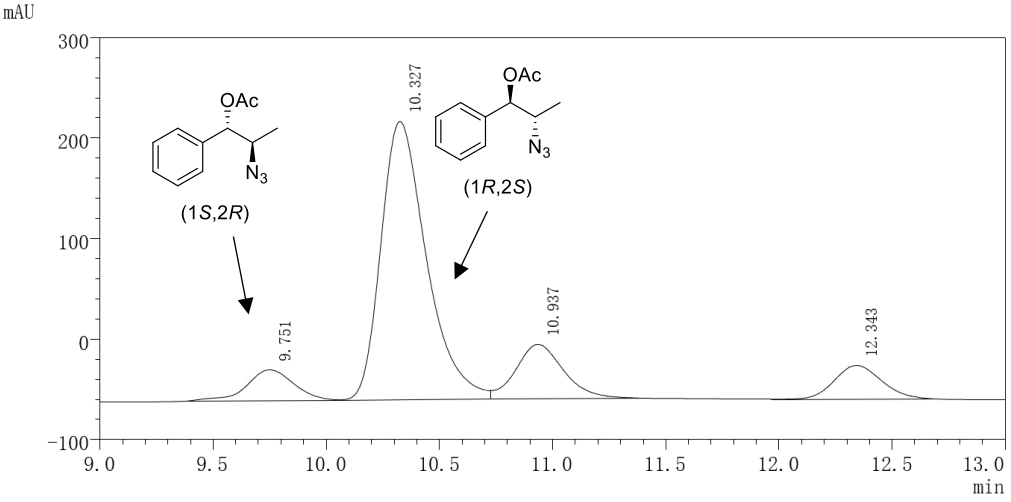
HPLC trace for the chemical synthesized (*rac*)-**6**.



PDA 210nm

ID#	Rt. Time	Area	Height	Area %
1	9.742	5030034	401124	49.211
2	10.301	4995256	369574	48.871
3	10.856	90441	6904	0.885
4	12.324	105604	7292	1.033

HPLC trace for the enzymatic synthesized (1*R*,2*S*)-**6**.

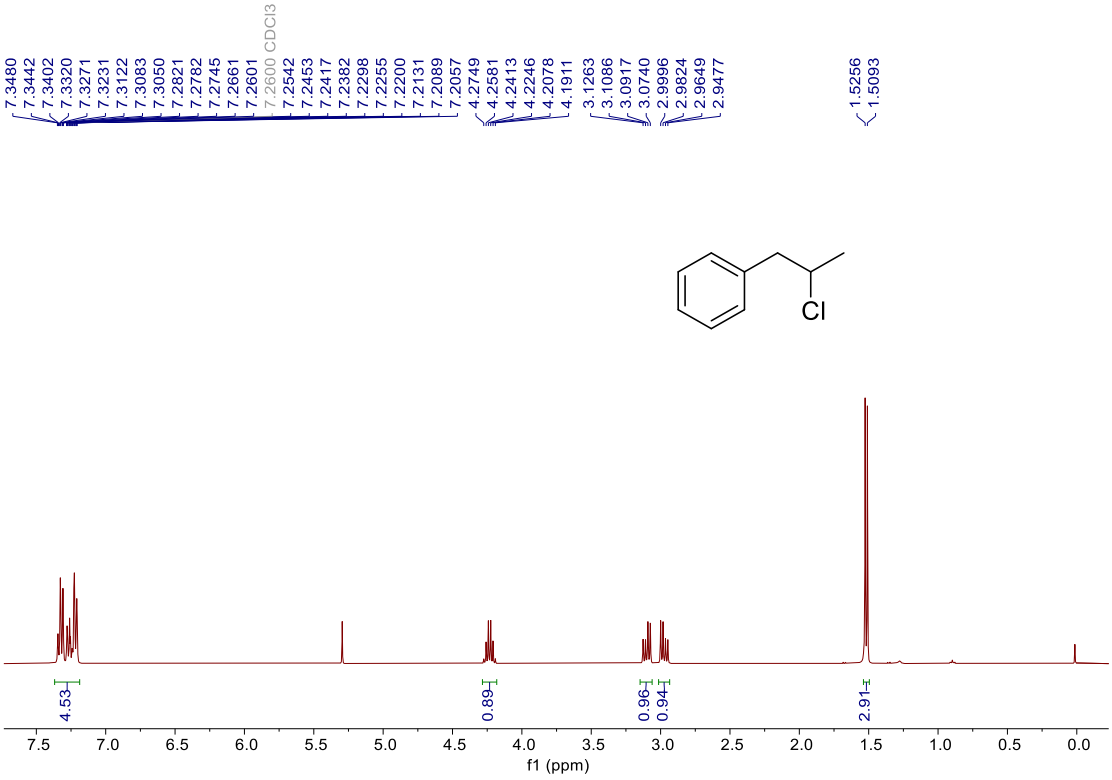


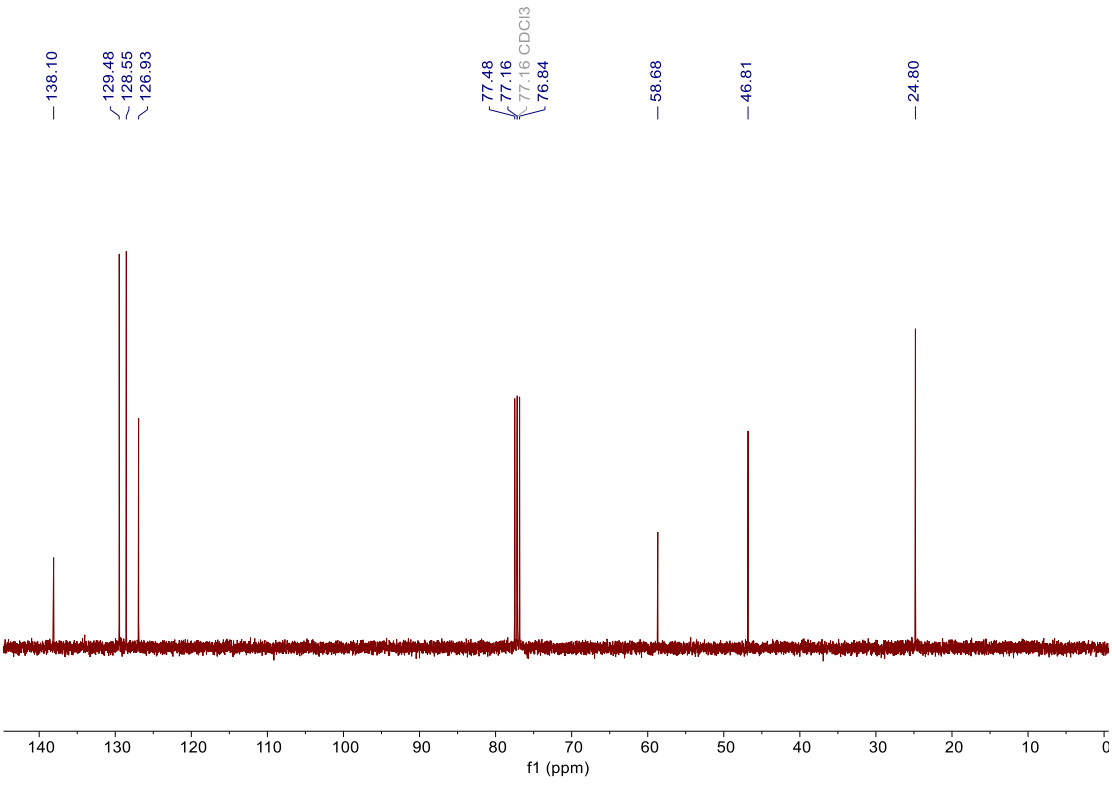
PDA 210nm

ID#	Rt. Time	Area	Height	Area %
1	9.751	441428	30579	7.871
2	10.327	3881351	277392	69.211
3	10.937	800505	54197	14.274
4	12.343	484712	33401	8.643

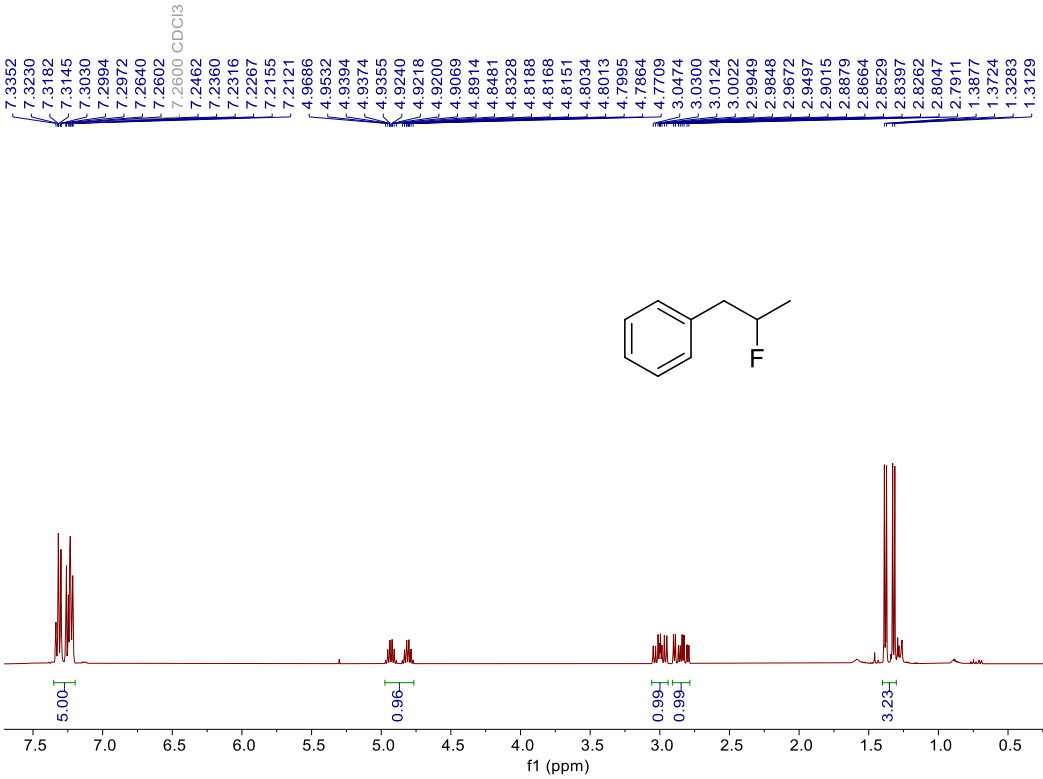
Chiral HPLC analysis: Diacel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 99/1, 0.8 mL/min, λ = 210 nm, $t_{(1S,2R)}$ = 9.8 min, $t_{(1R,2S)}$ = 10.3 min.

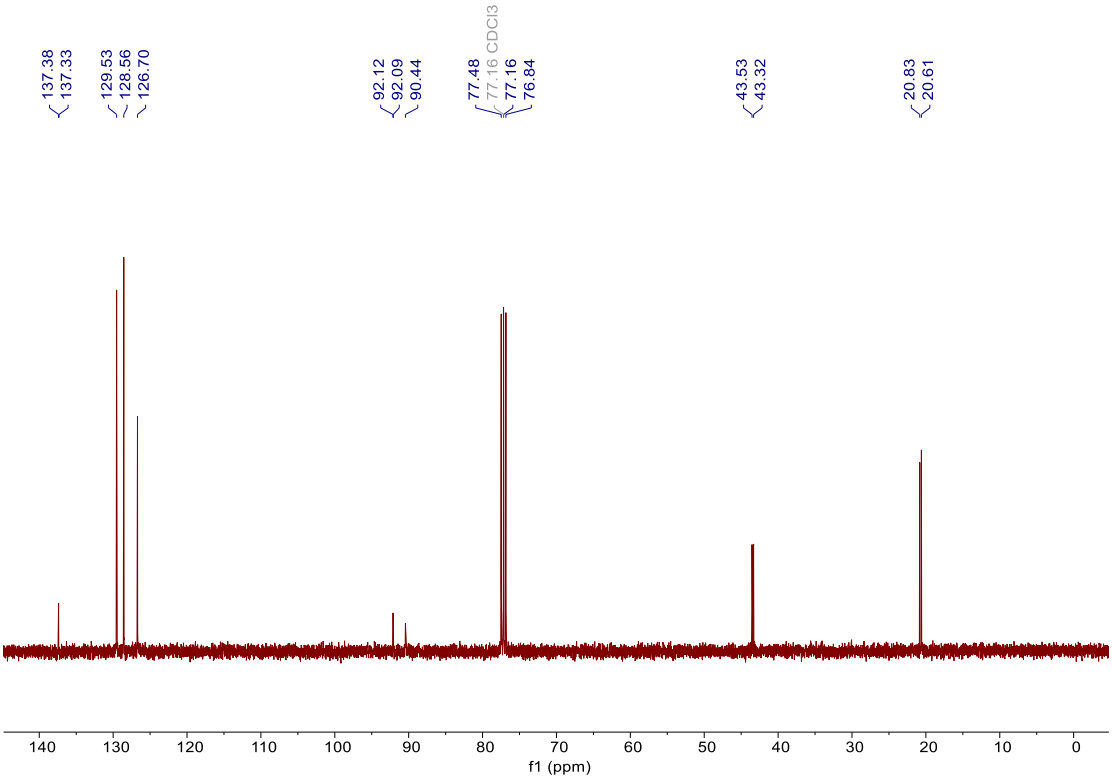
^{1}H and ^{13}C NMR of compound **1a**



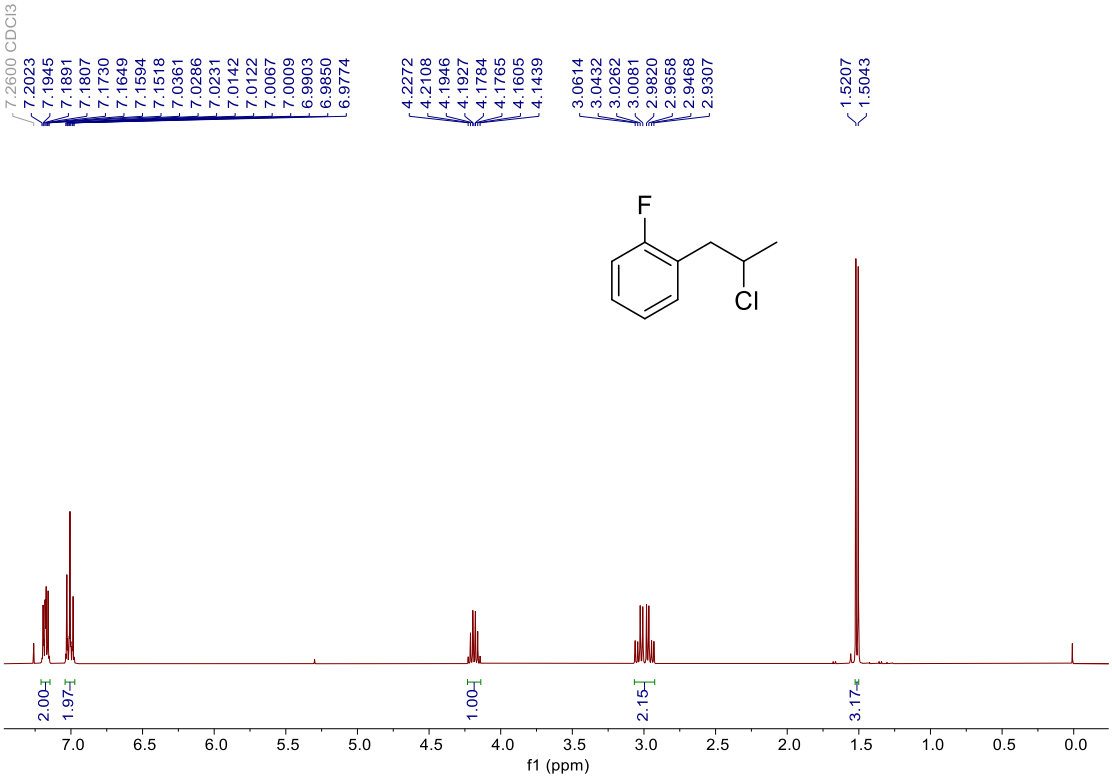


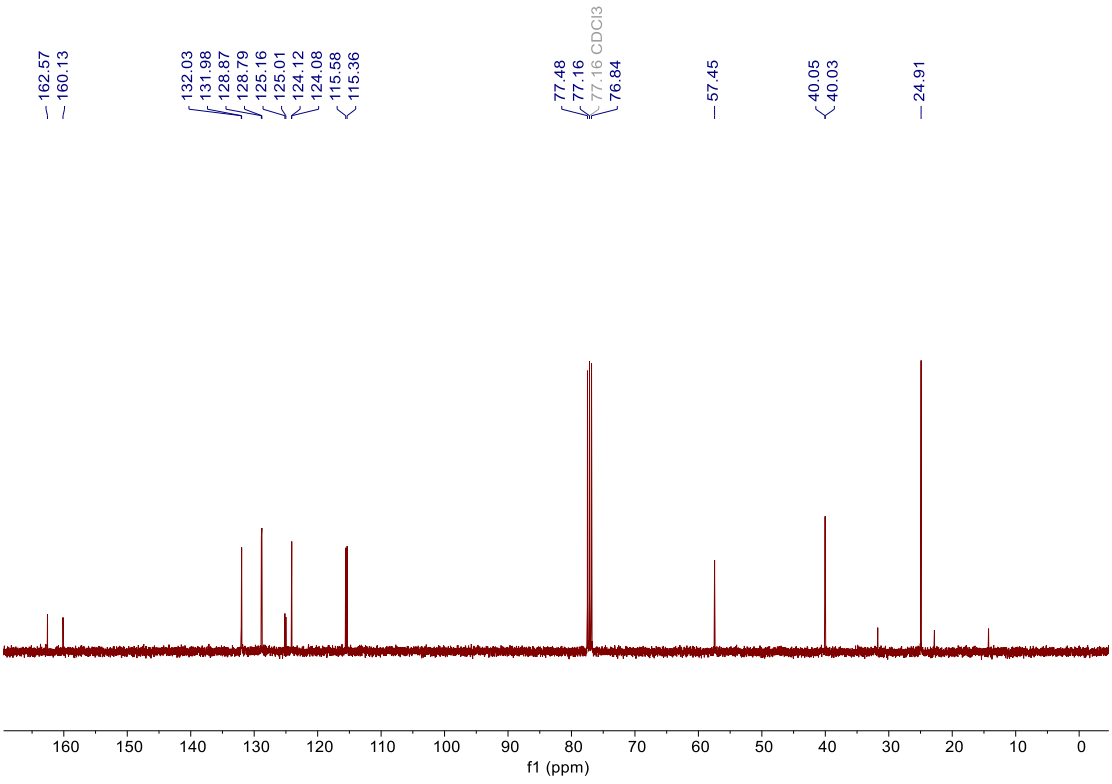
^{1}H and ^{13}C NMR of compound **1b**



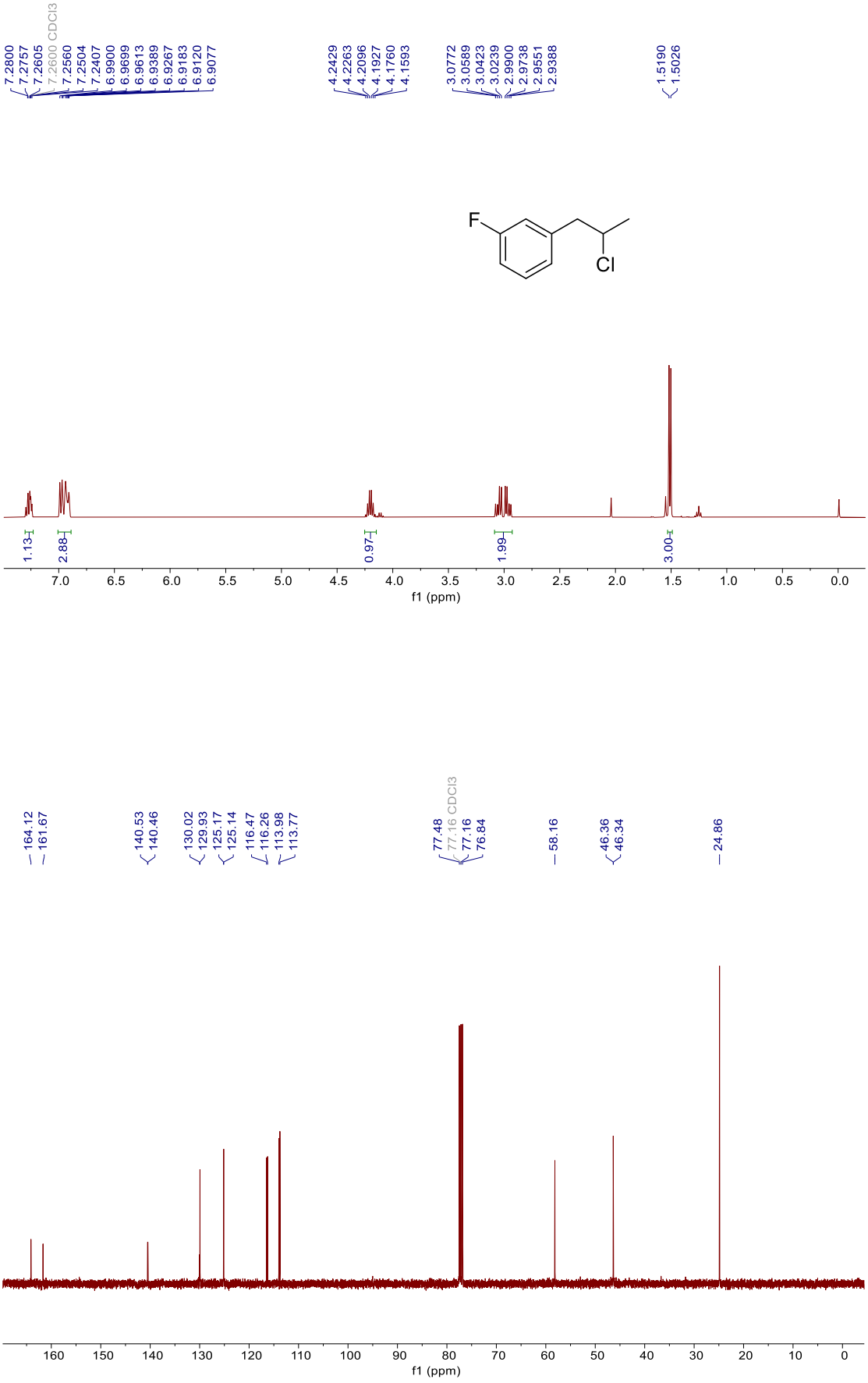


^{1}H and ^{13}C NMR of compound **1d**

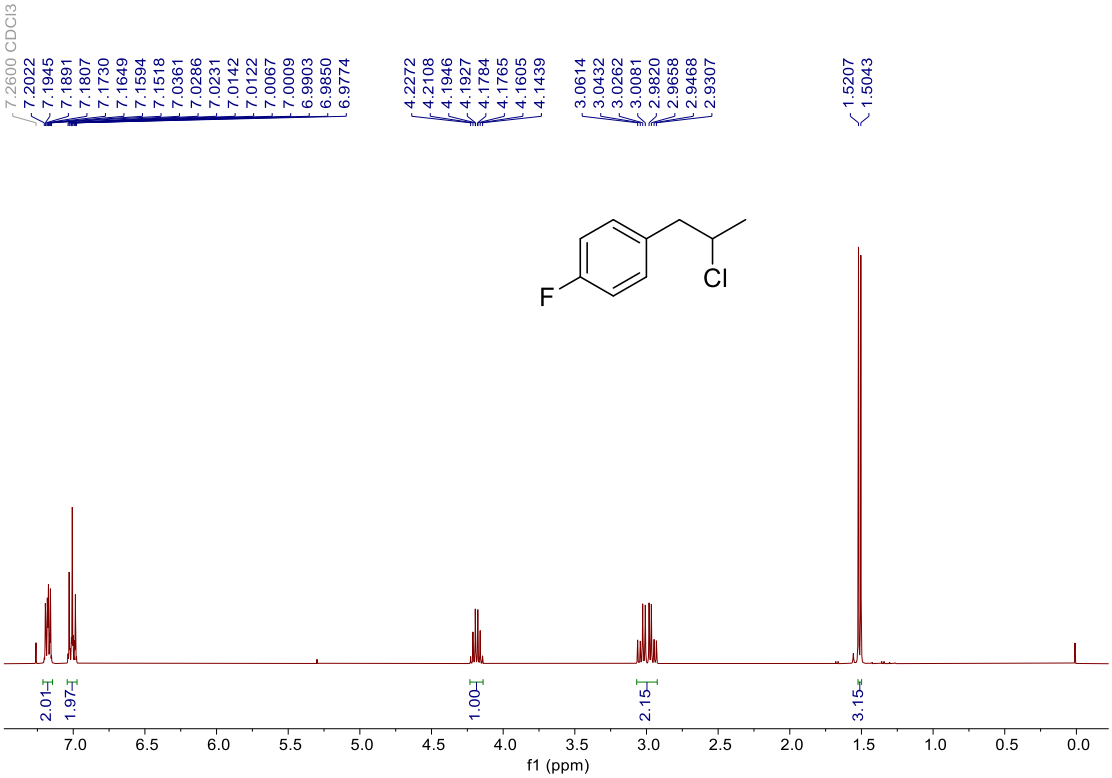


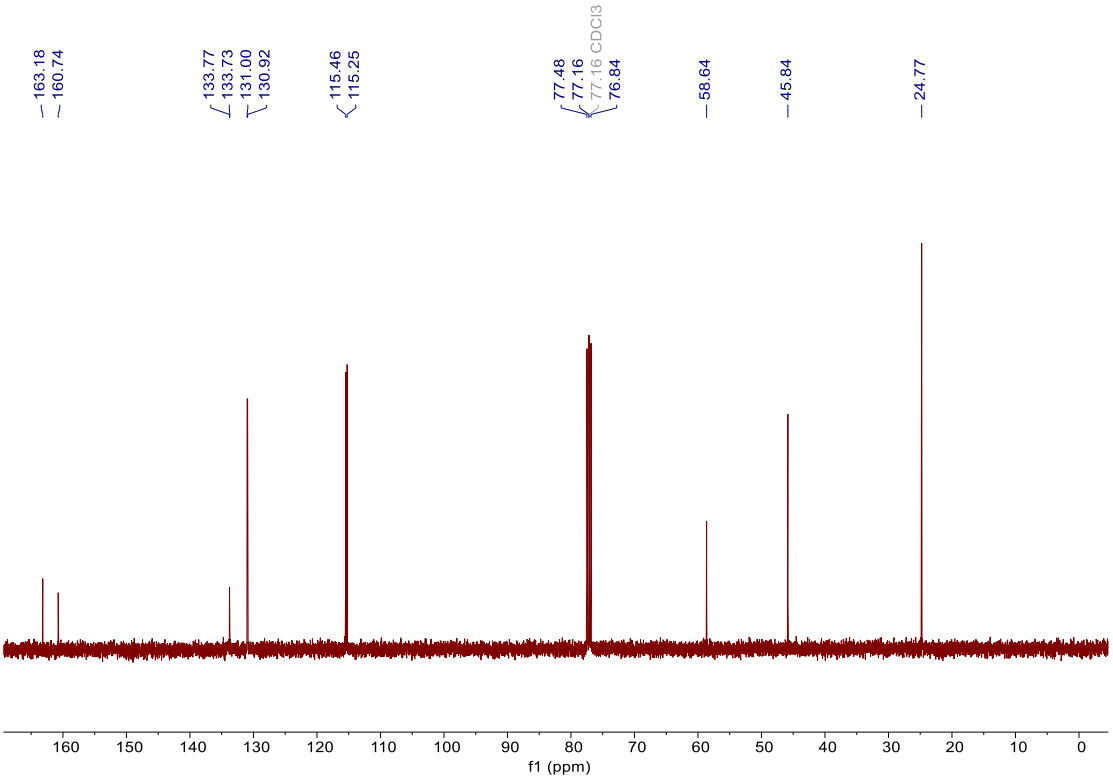


^{1}H and ^{13}C NMR of compound **1e**

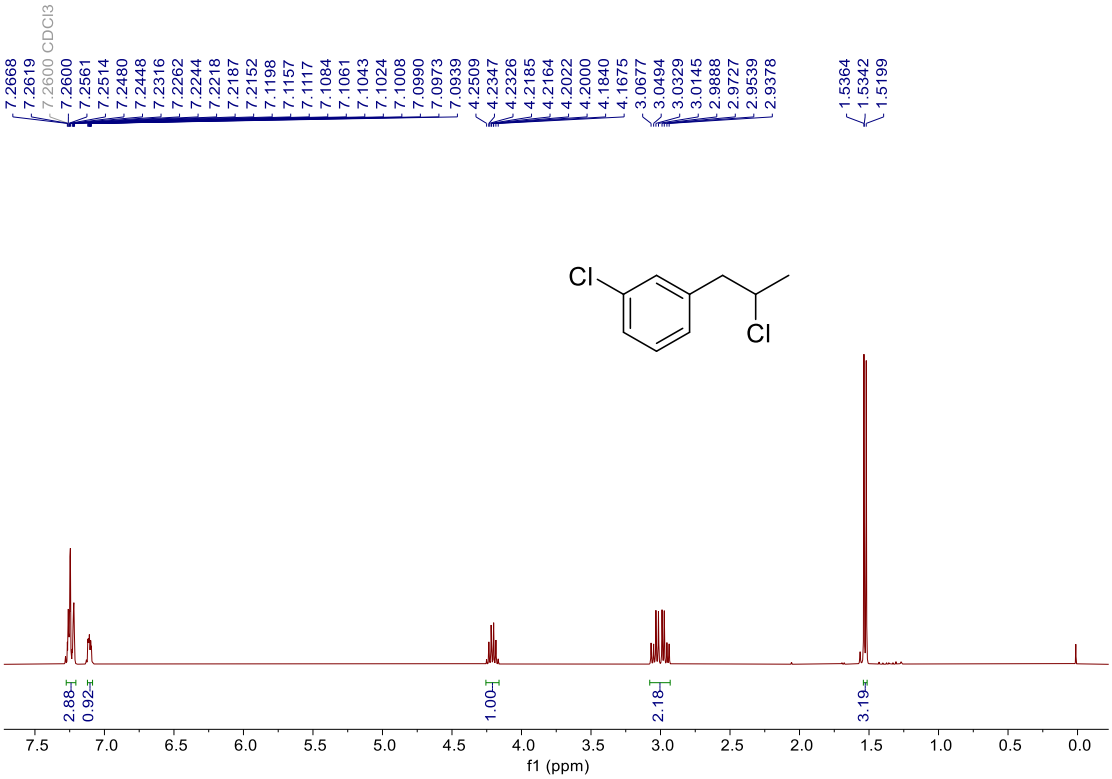


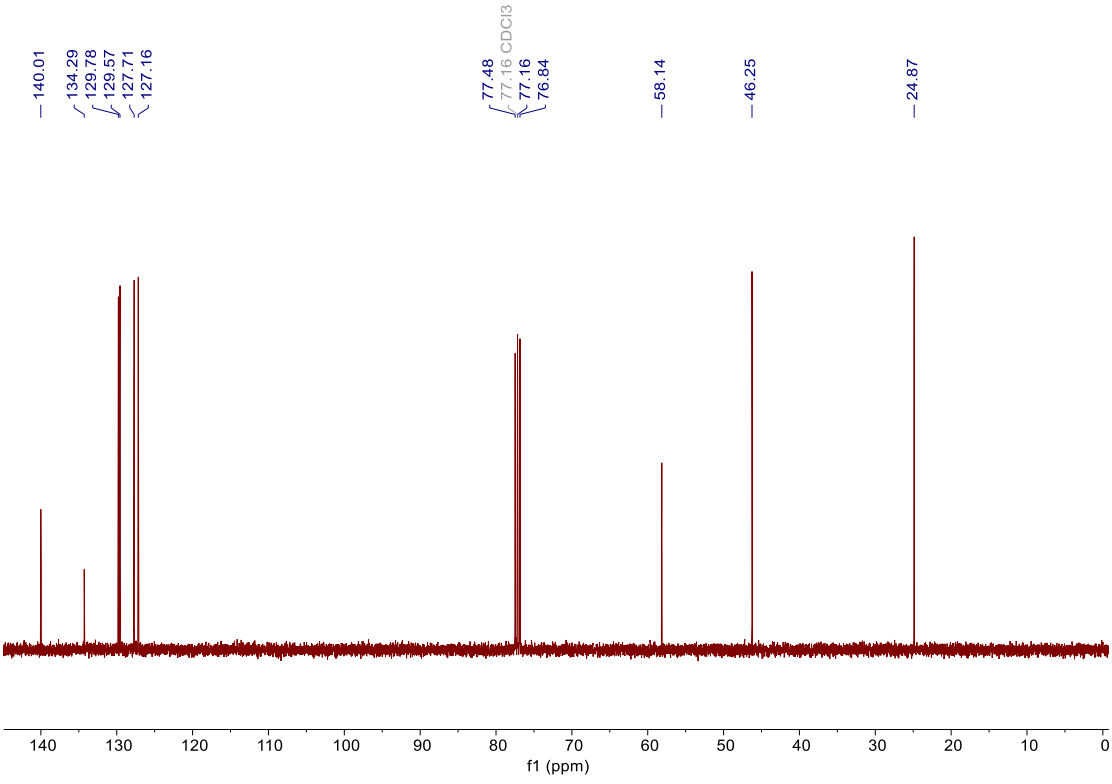
^{1}H and ^{13}C NMR of compound **1f**



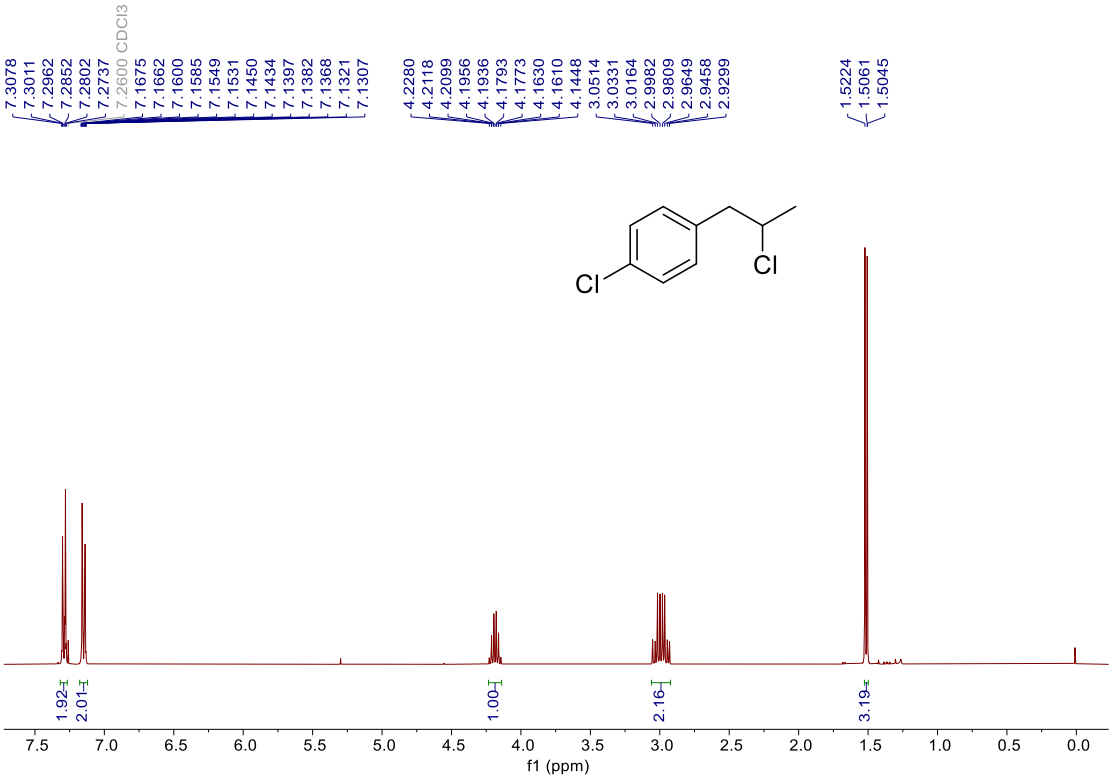


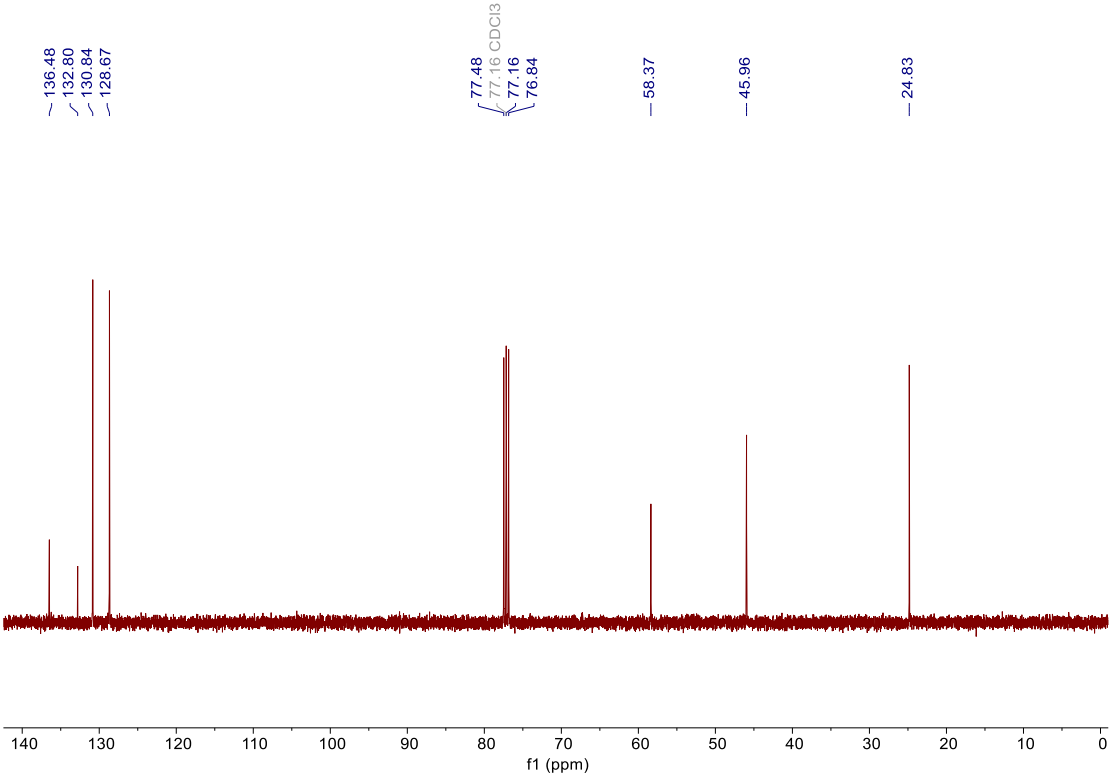
^{1}H and ^{13}C NMR of compound **1g**



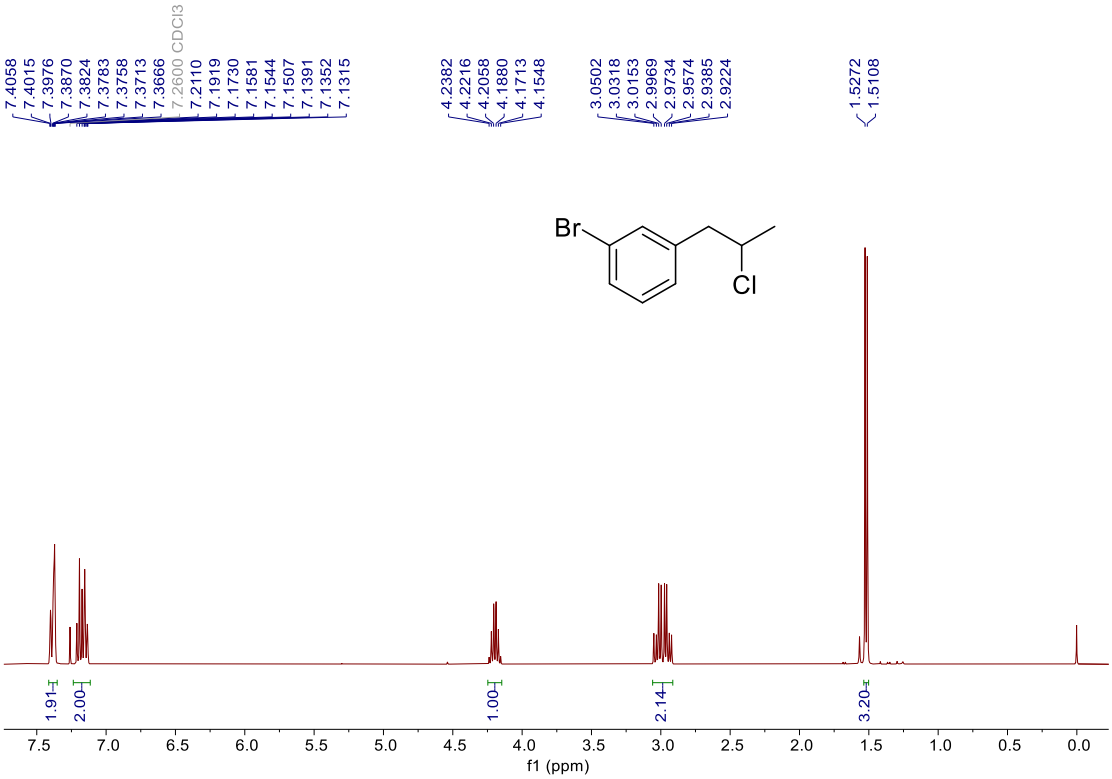


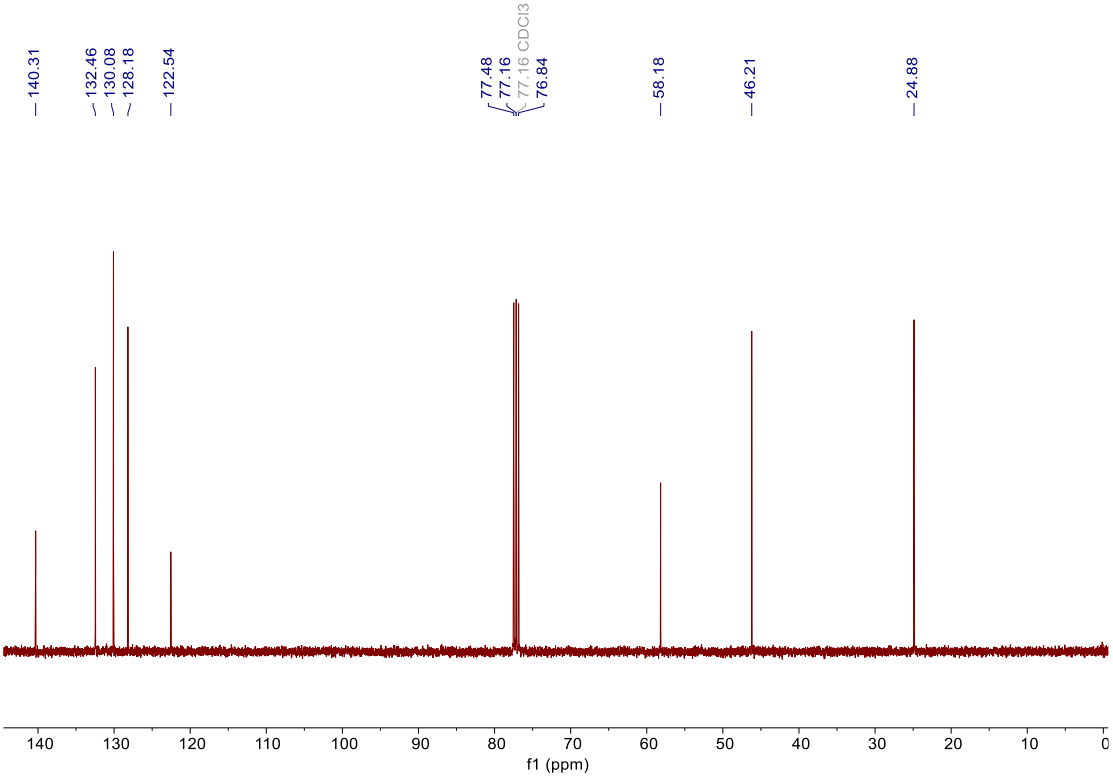
^{1}H and ^{13}C NMR of compound **1h**



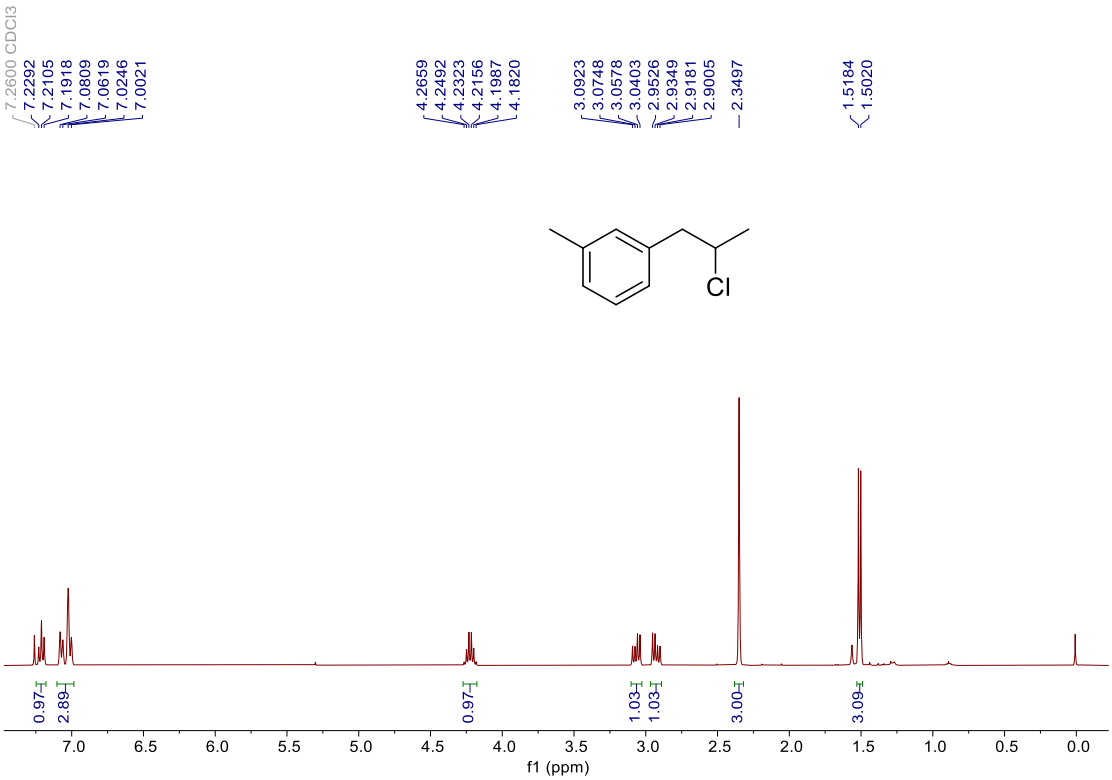


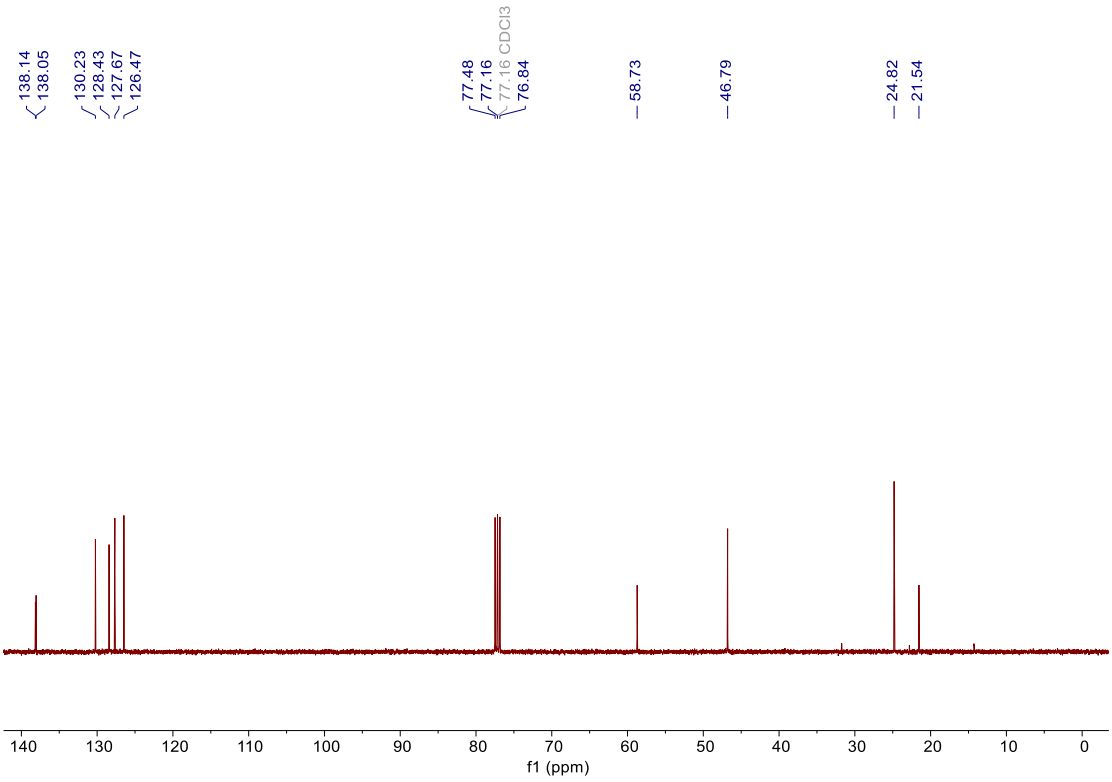
^{1}H and ^{13}C NMR of compound **1i**



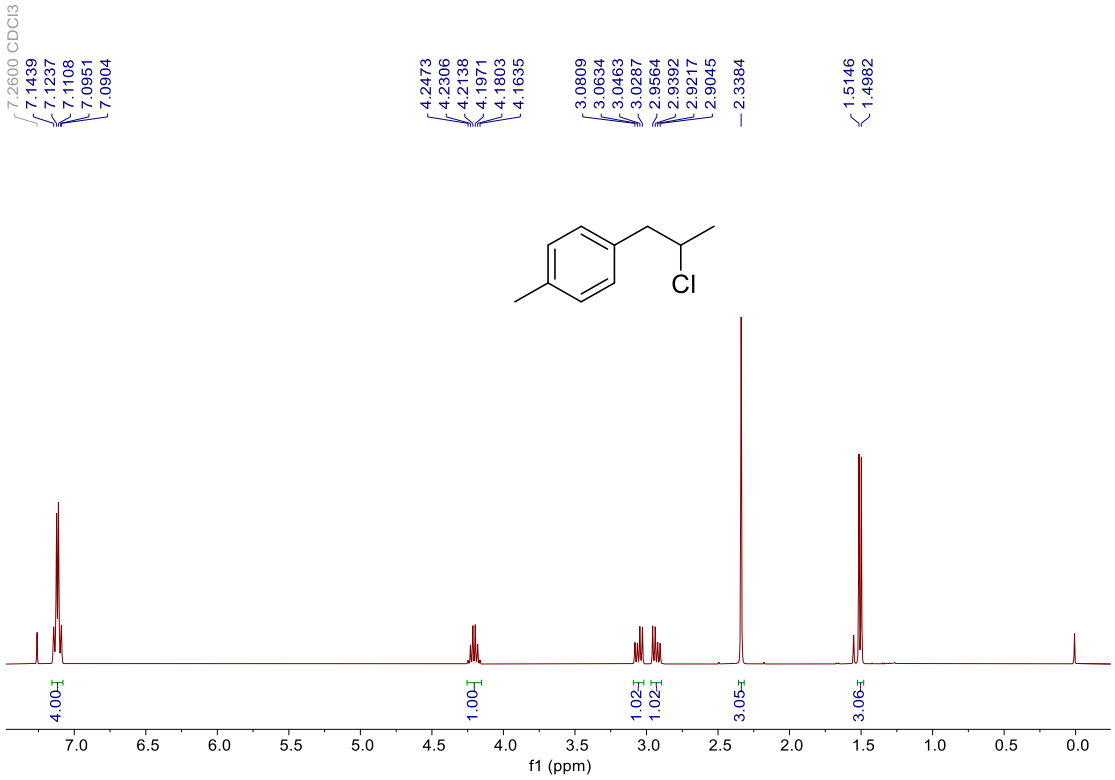


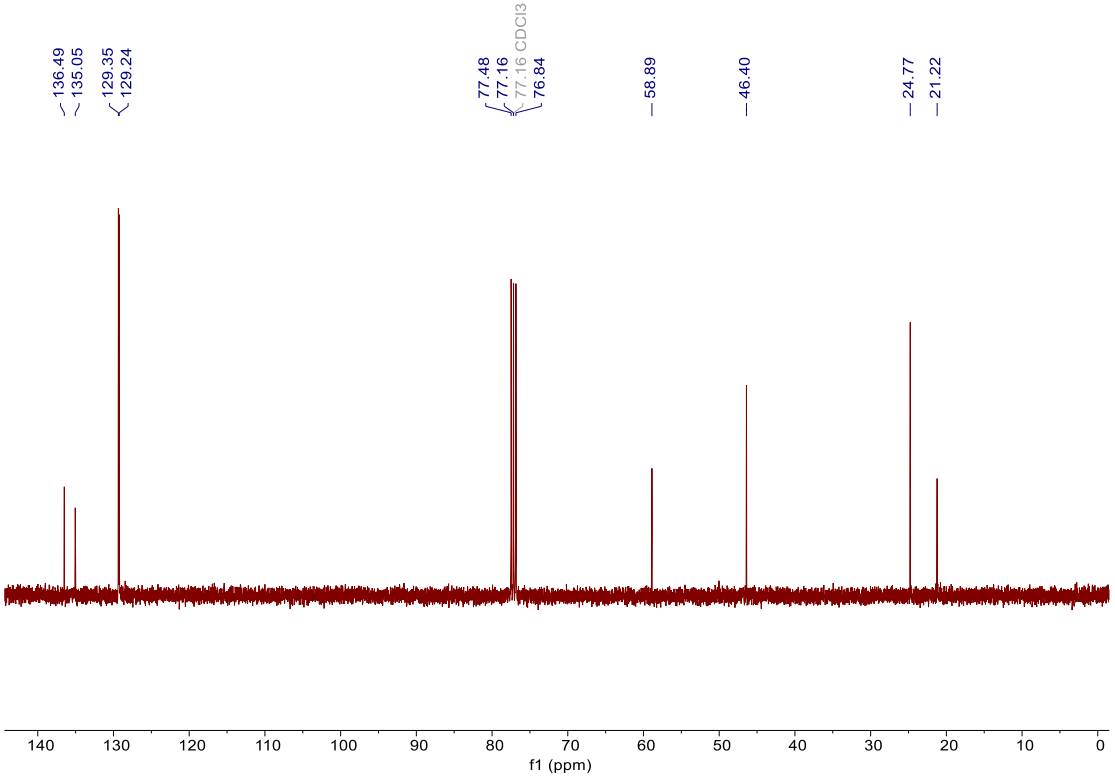
^{1}H and ^{13}C NMR of compound **1j**



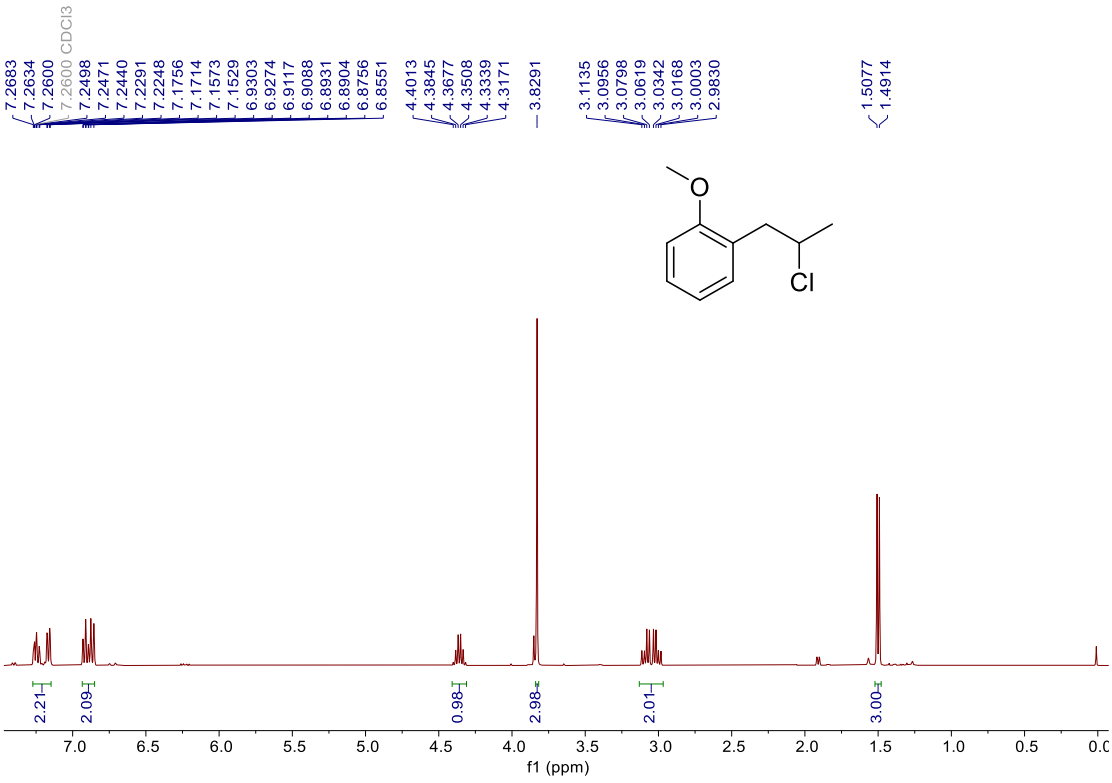


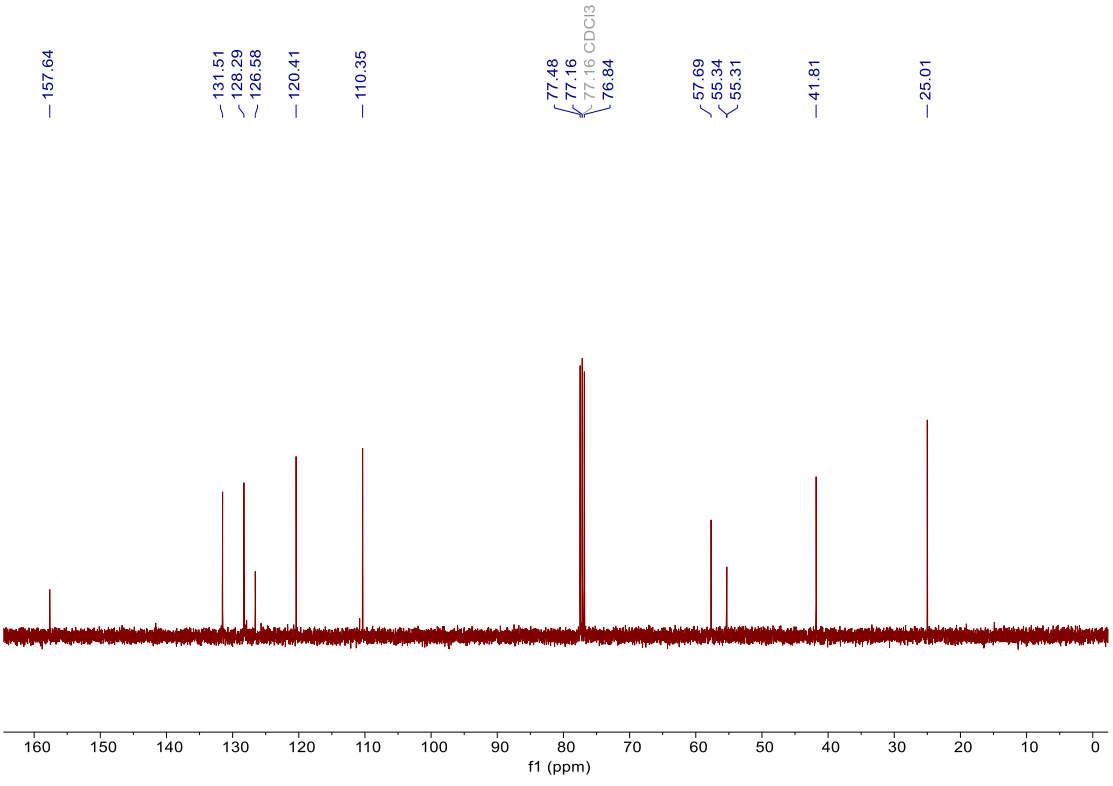
^{1}H and ^{13}C NMR of compound **1k**



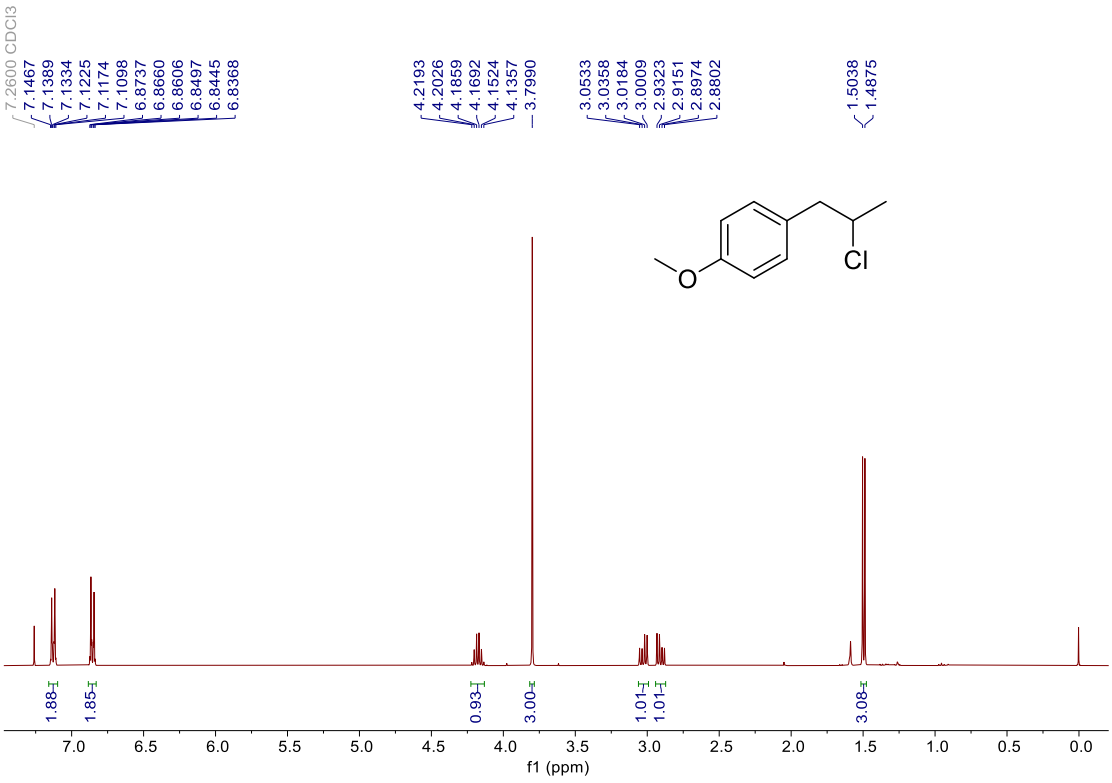


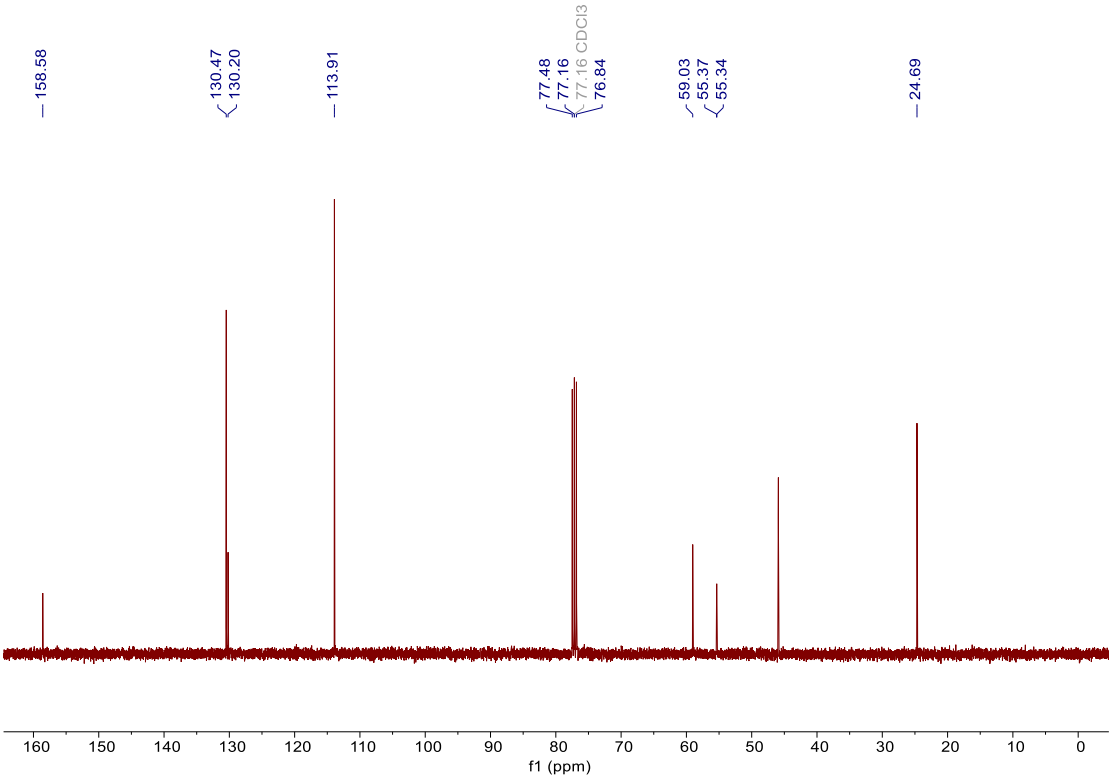
^{1}H and ^{13}C NMR of compound **1l**



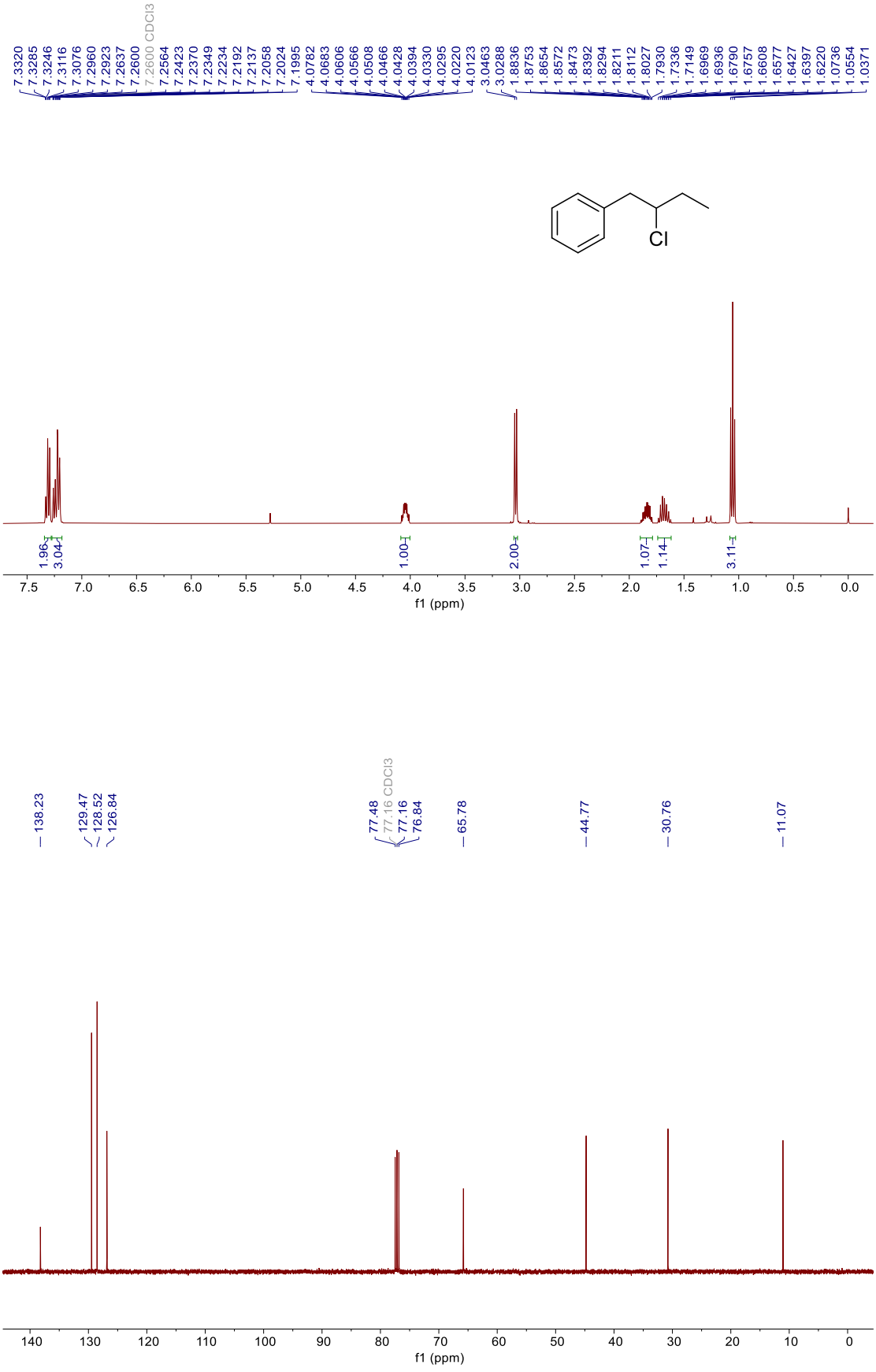


^{1}H and ^{13}C NMR of compound **1m**

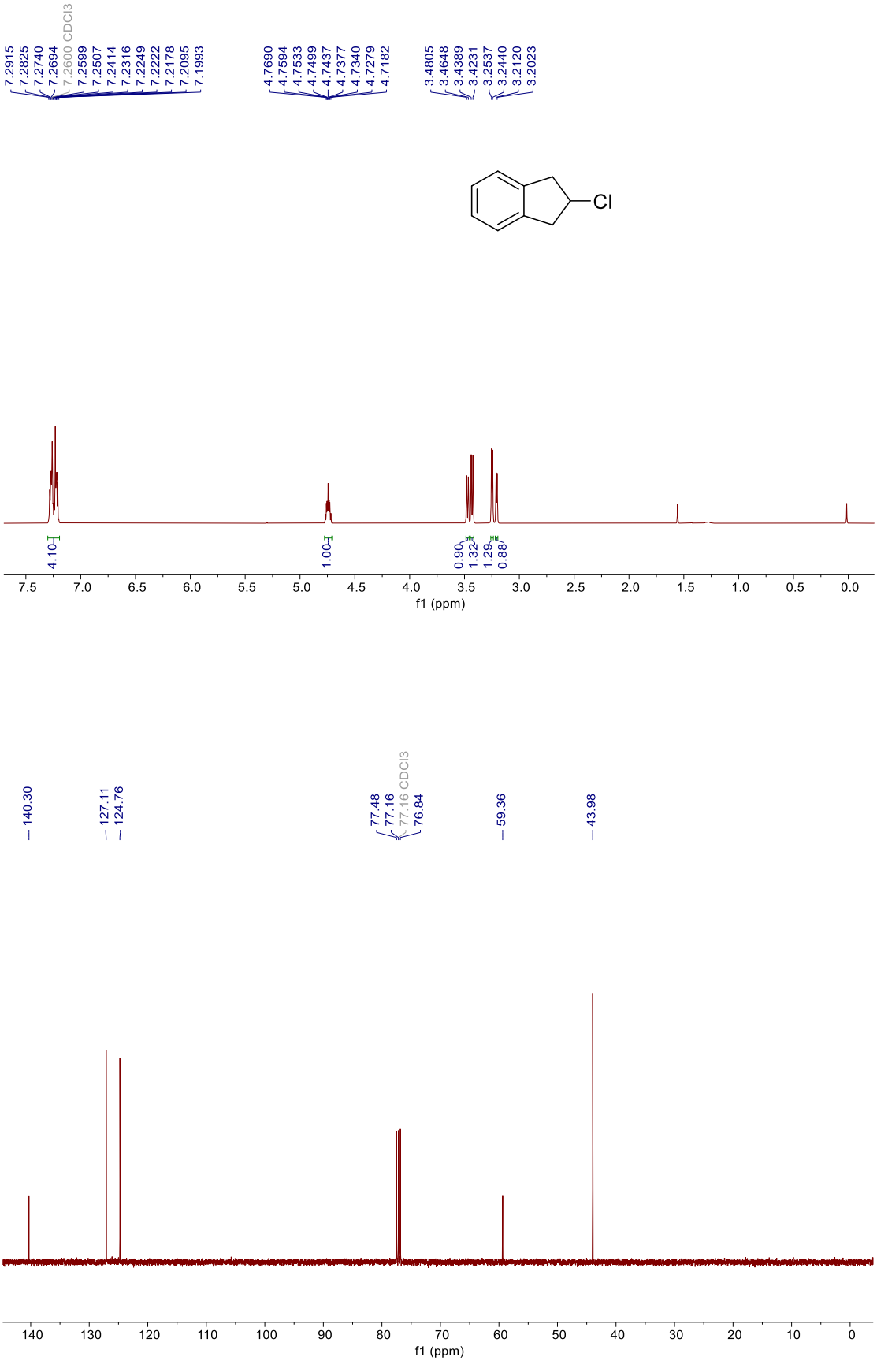




^{1}H and ^{13}C NMR of compound **1n**



^{1}H and ^{13}C NMR of compound **1o**



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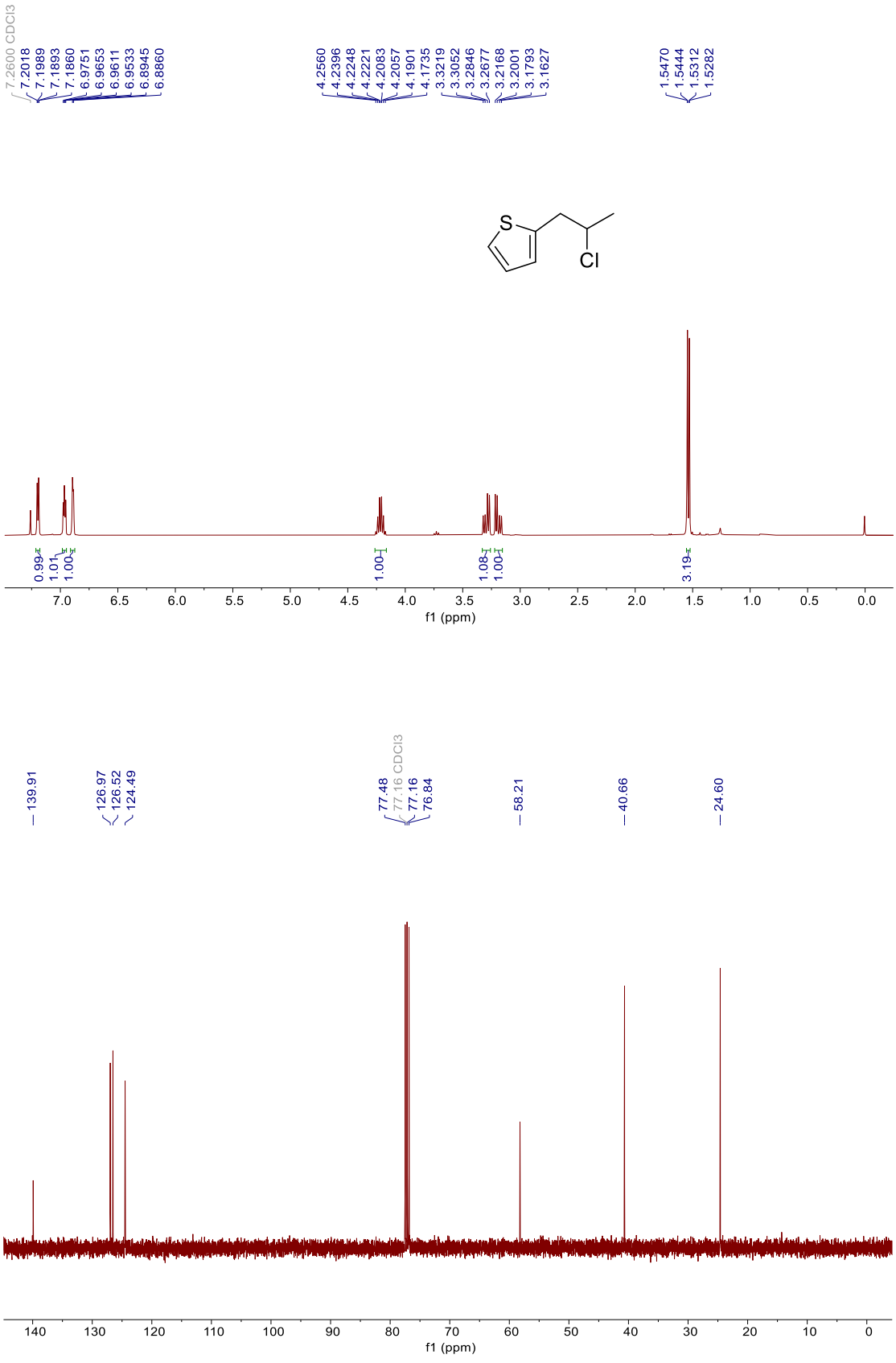
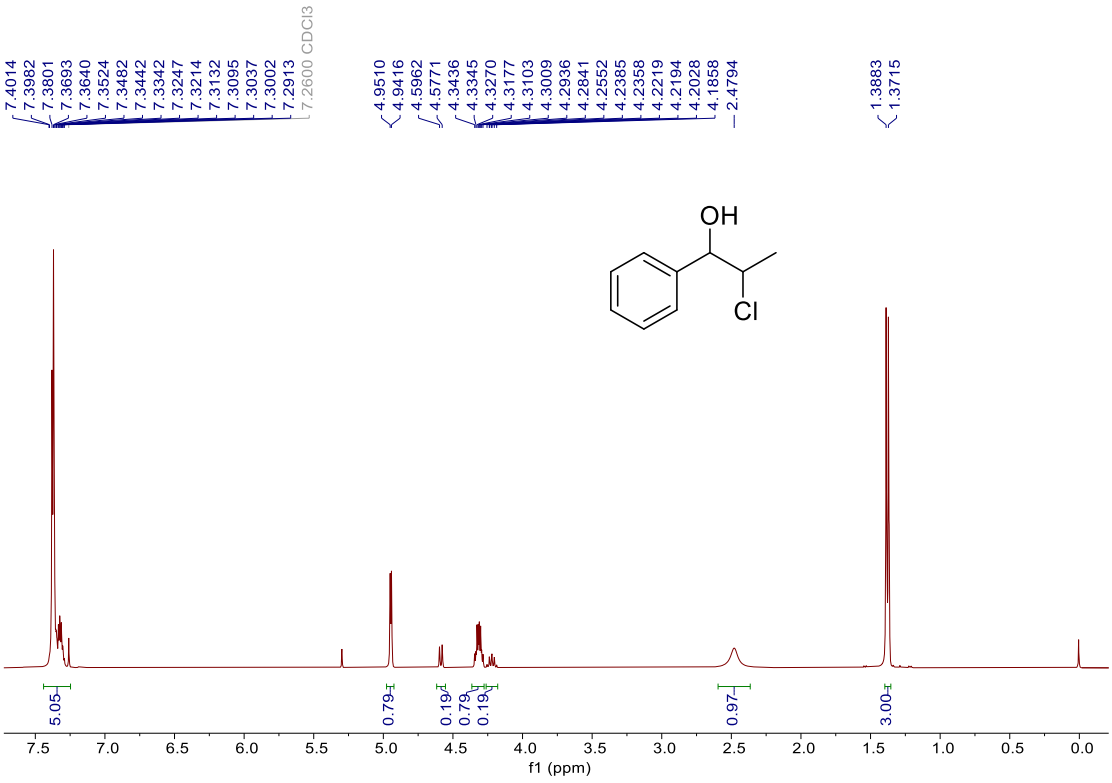
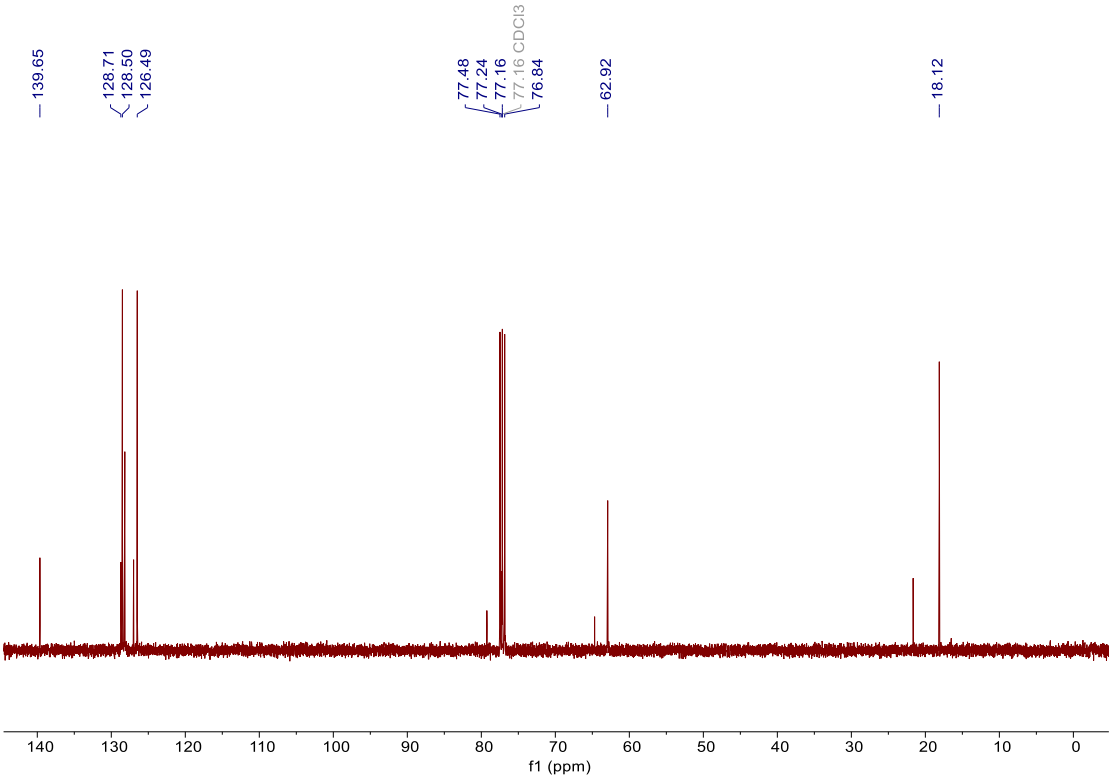
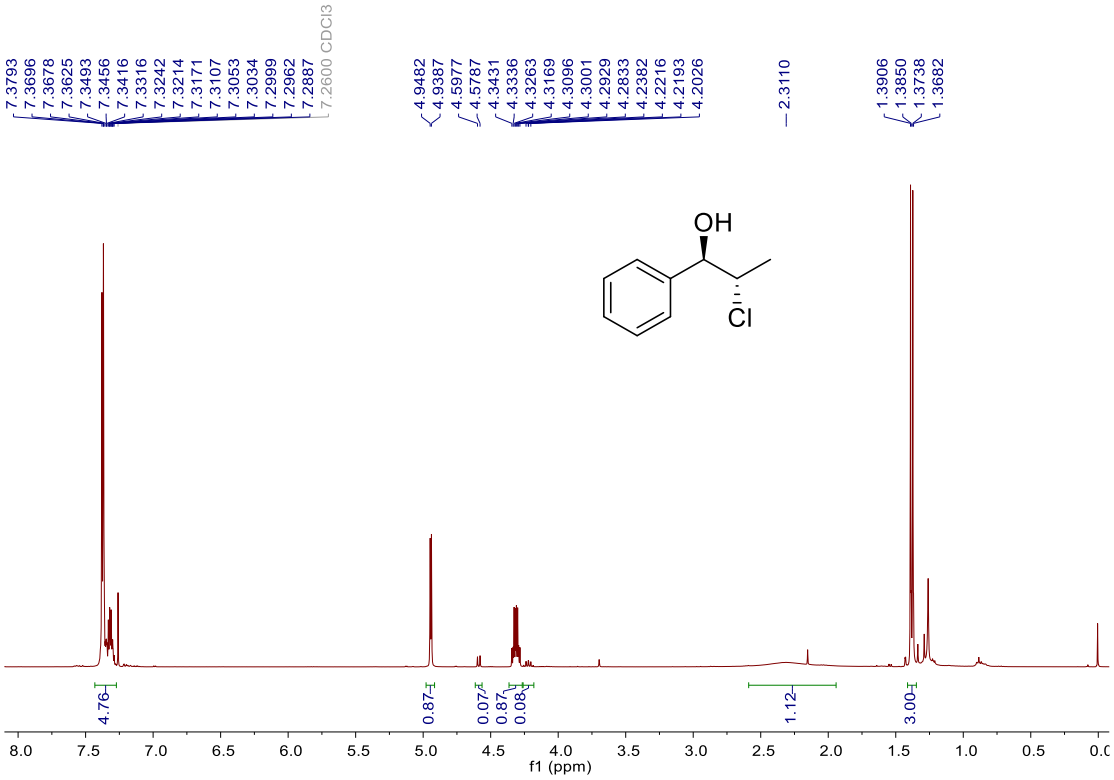


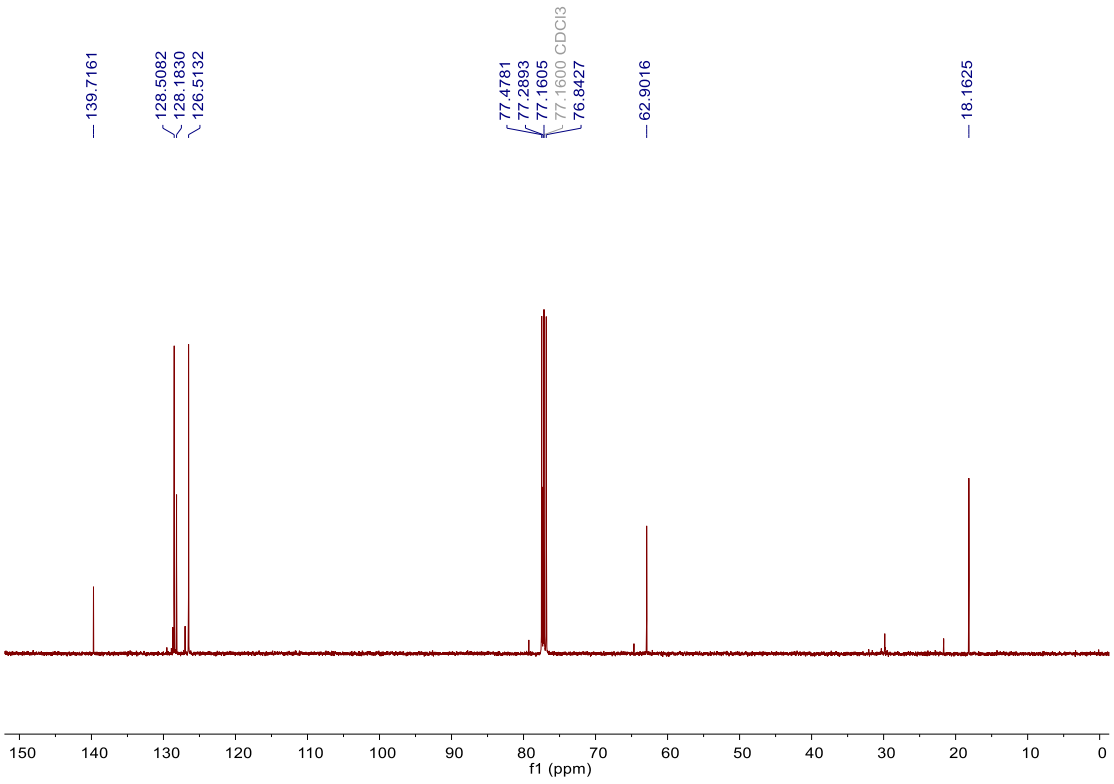
^{1}H and ^{13}C NMR of compound **2a**



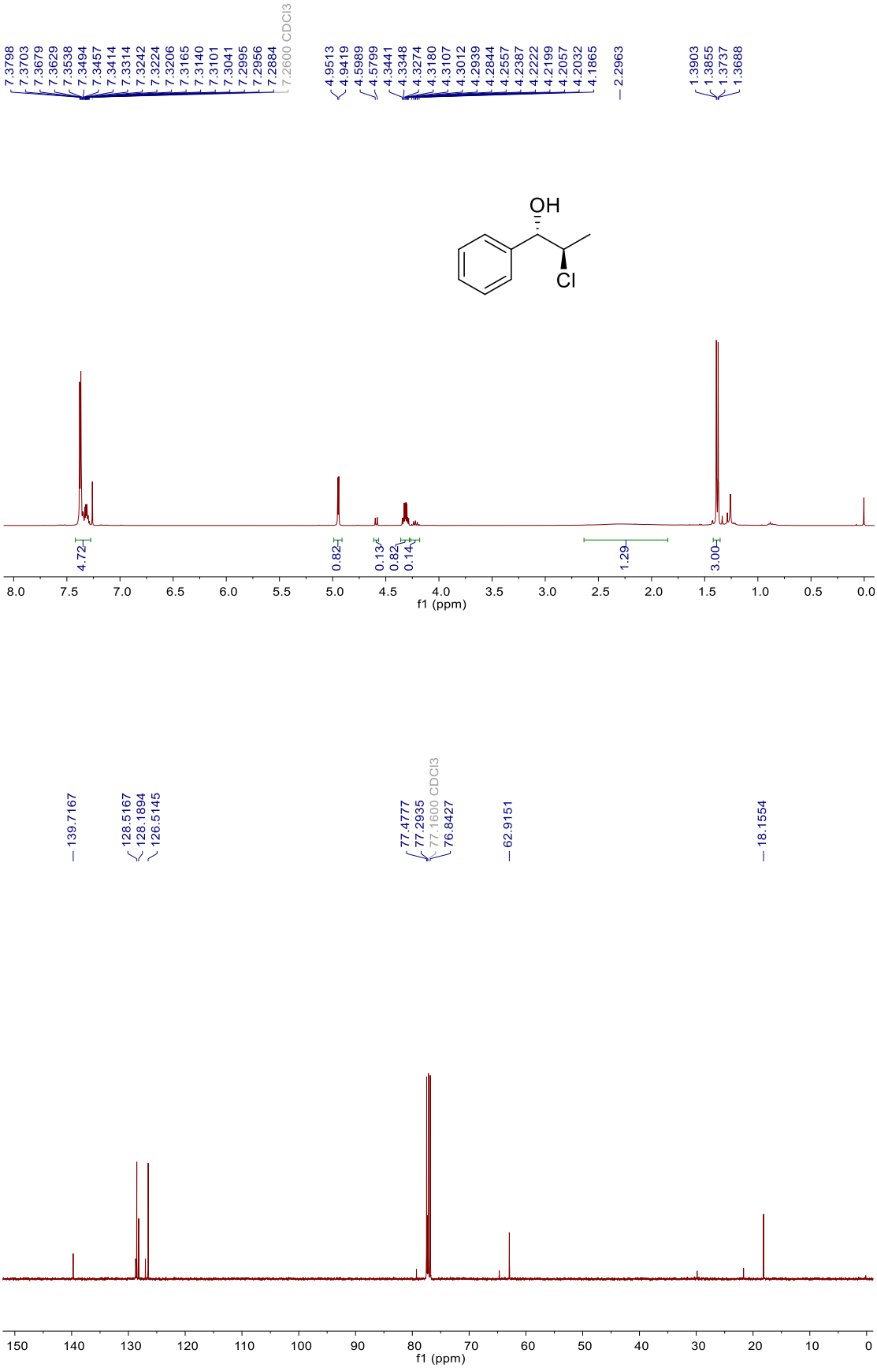


^{1}H and ^{13}C NMR of compound (1*R*,2*S*)-**2a**

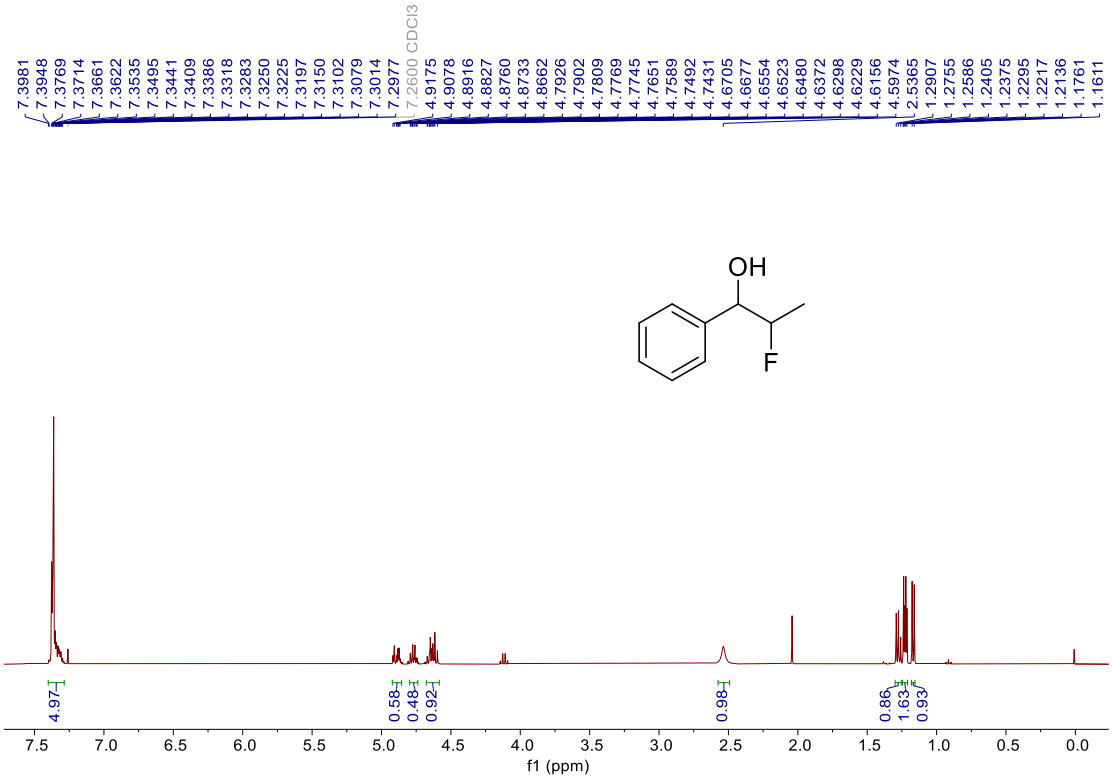


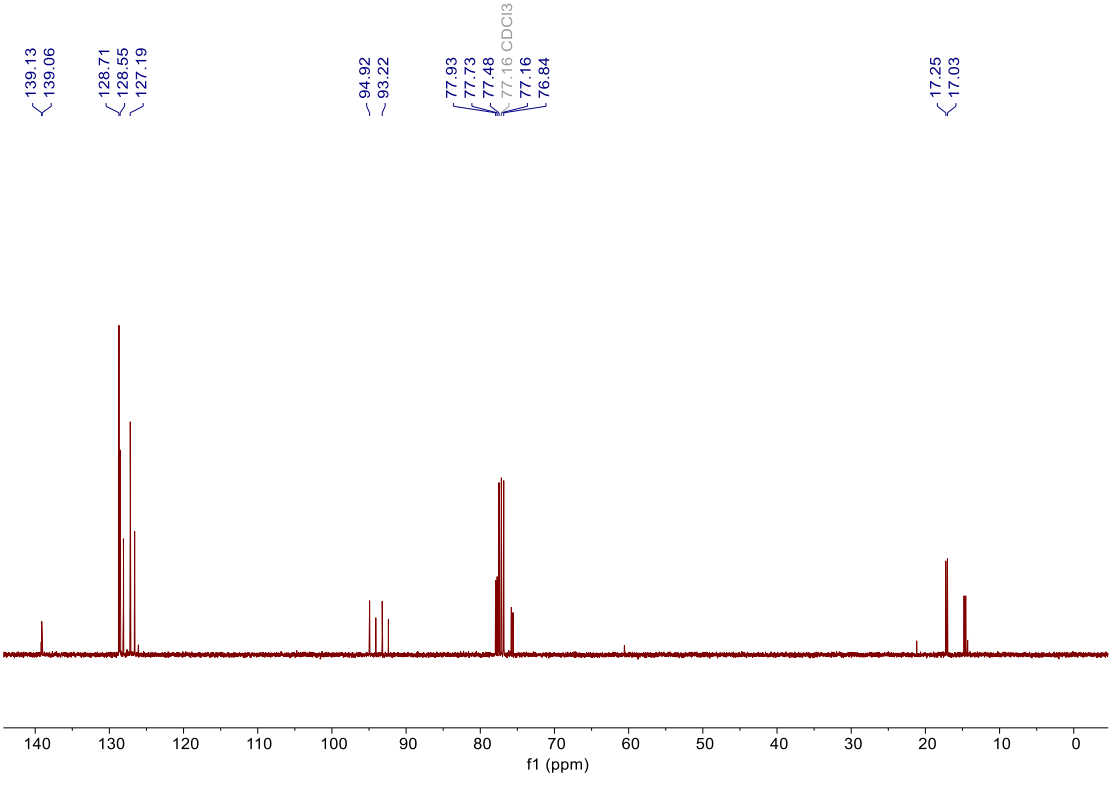


^{1}H and ^{13}C NMR of compound (1*S*,2*R*)-**2a**

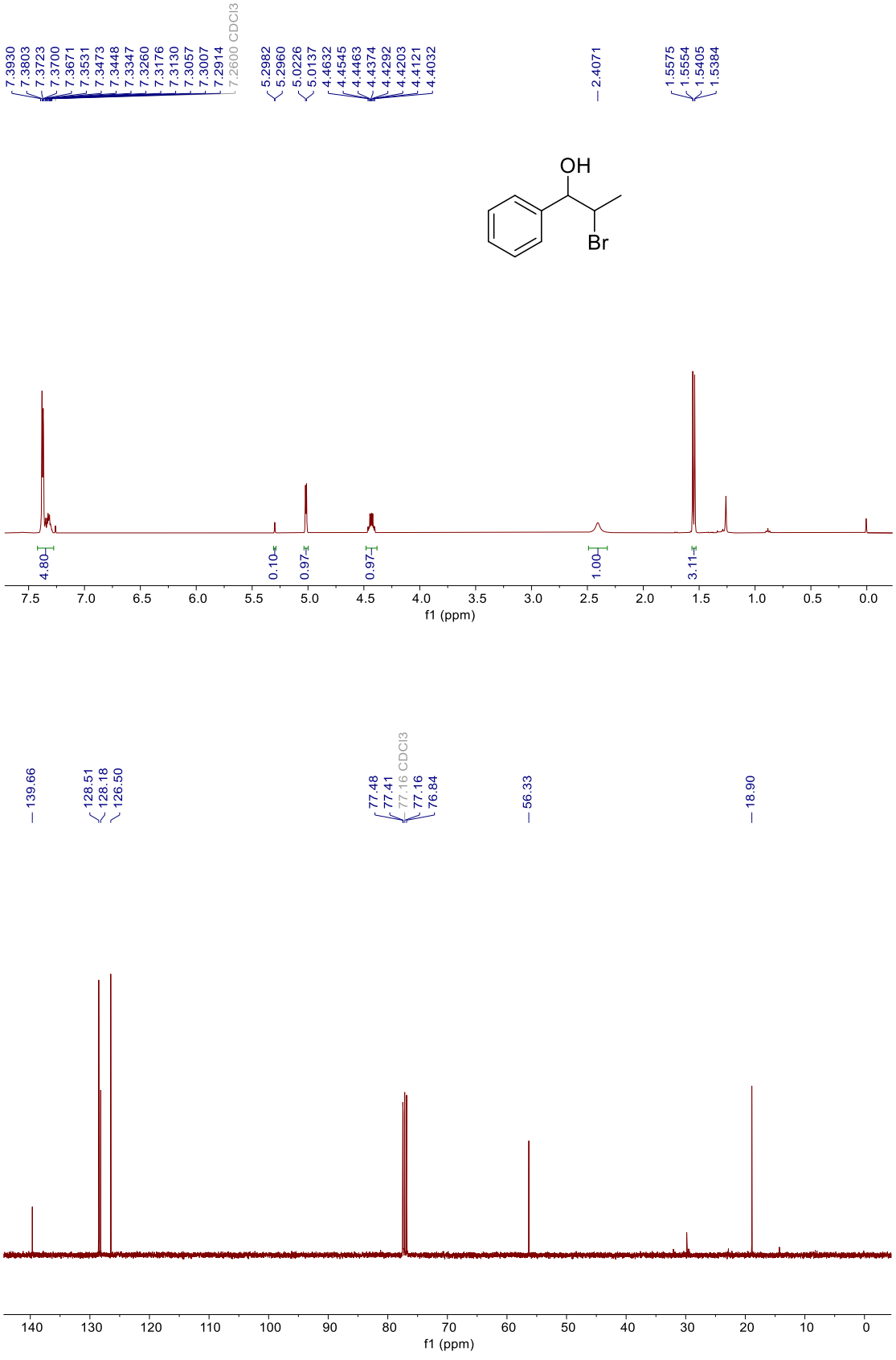


^{1}H and ^{13}C NMR of compound **2b**

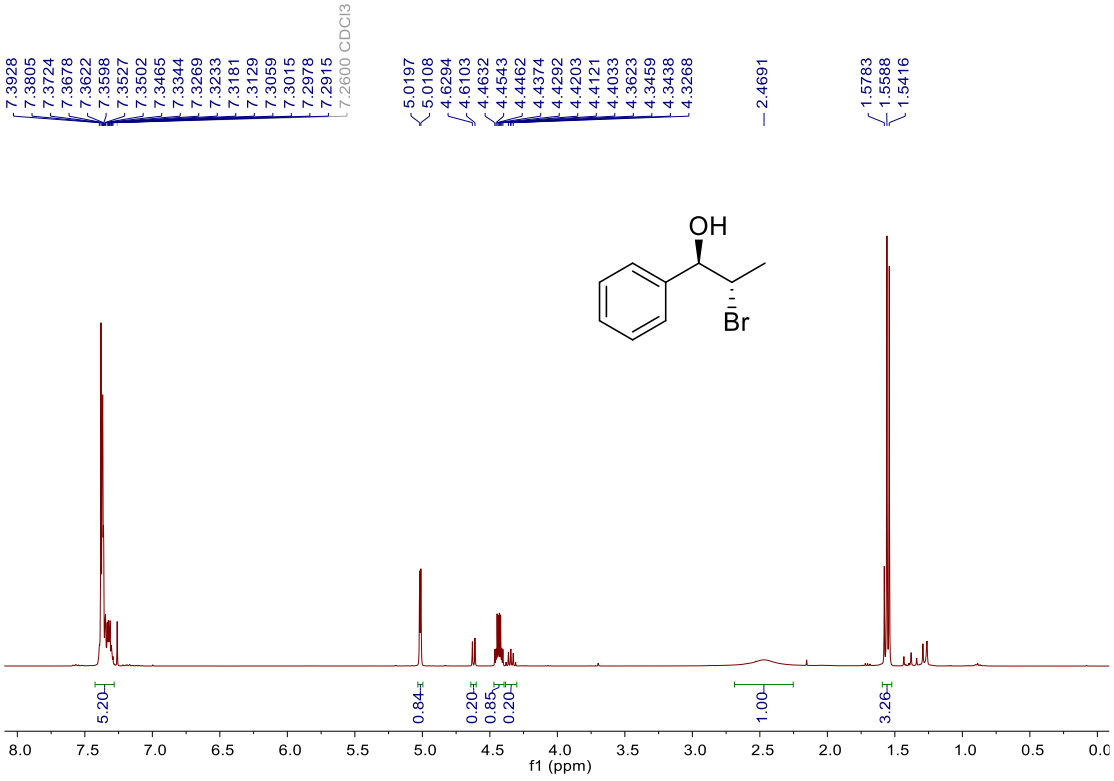


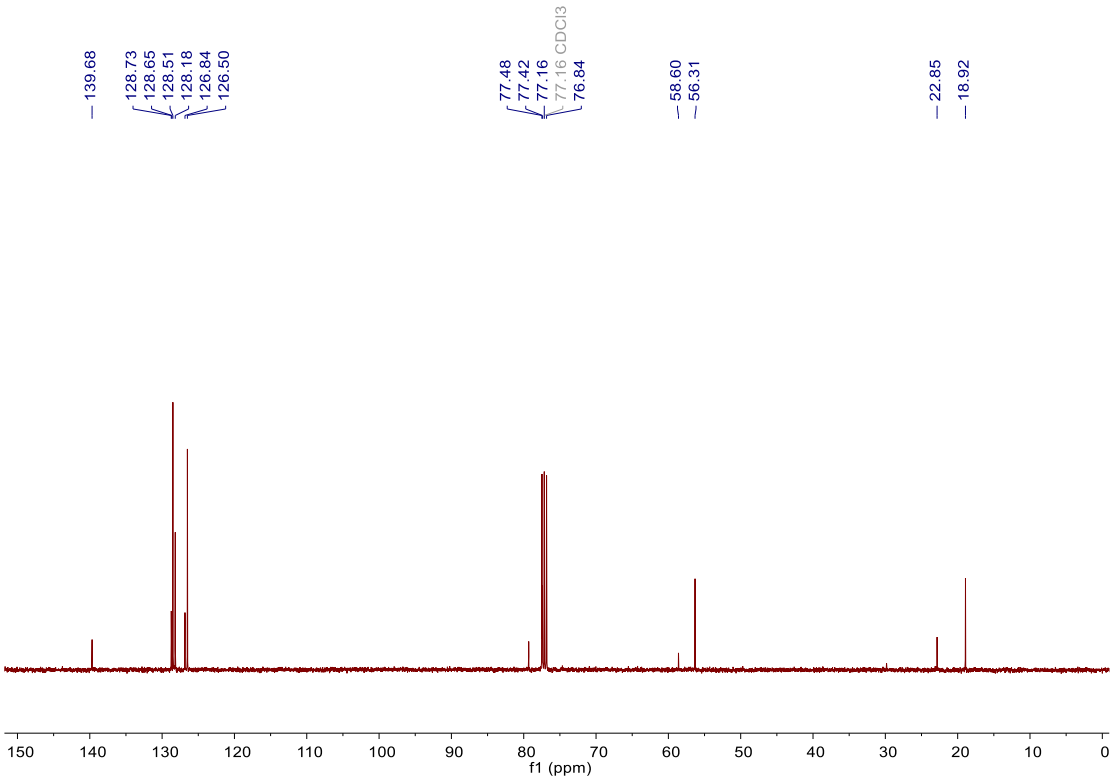


^{1}H and ^{13}C NMR of compound **2c**

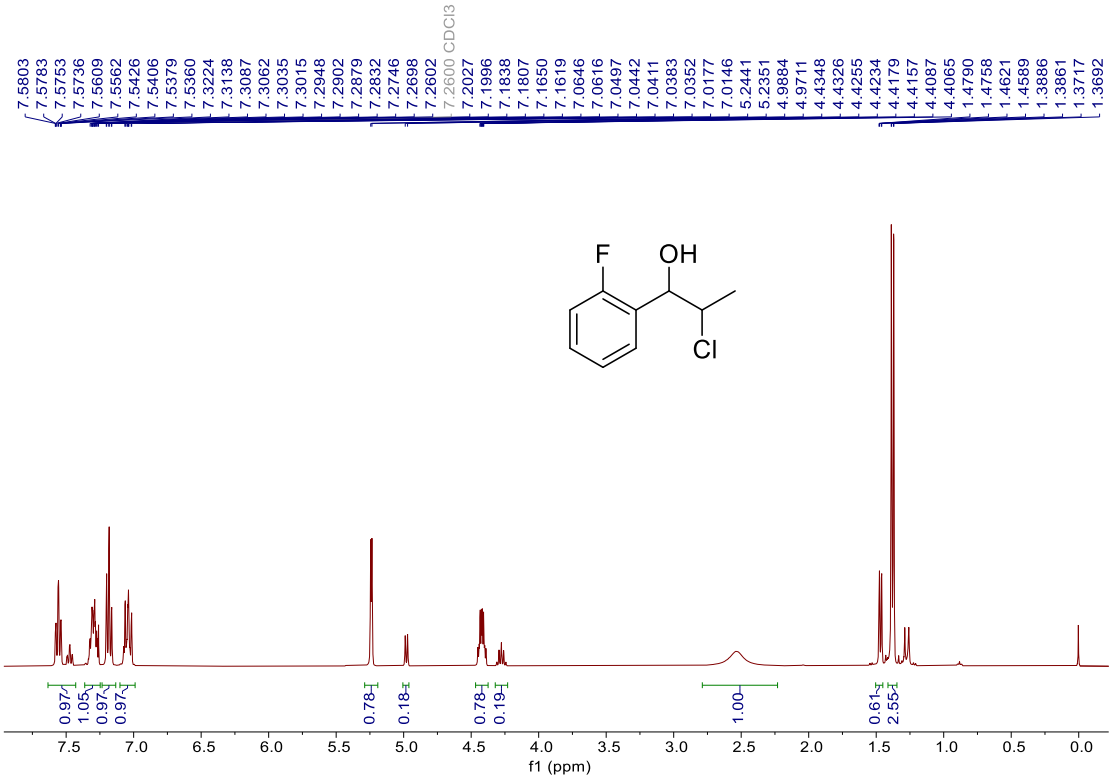


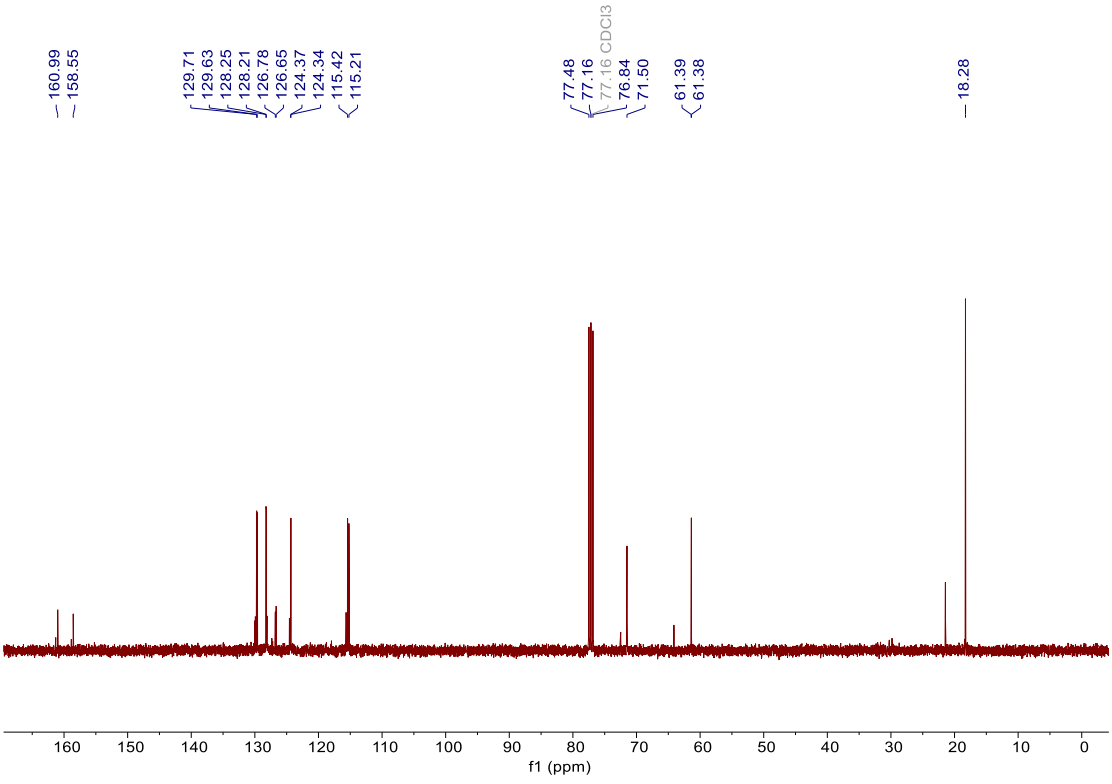
^{1}H and ^{13}C NMR of compound (1*R*,2*S*)-**2c**



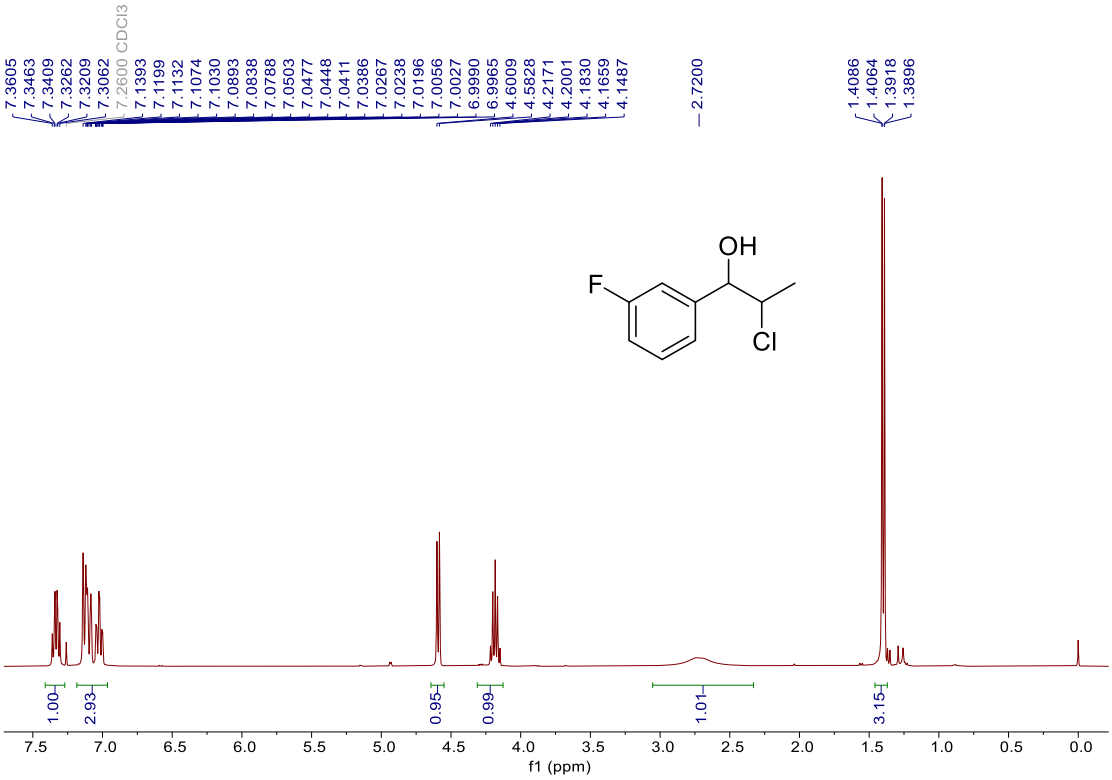


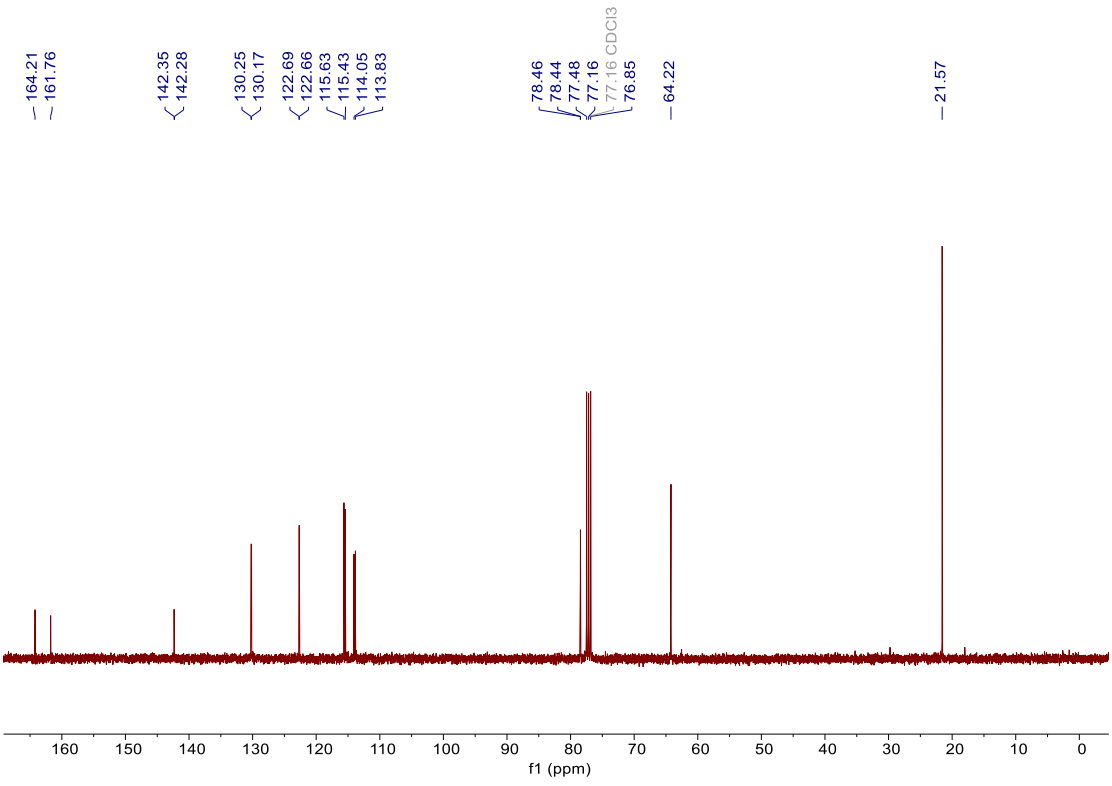
^{1}H and ^{13}C NMR of compound **2d**



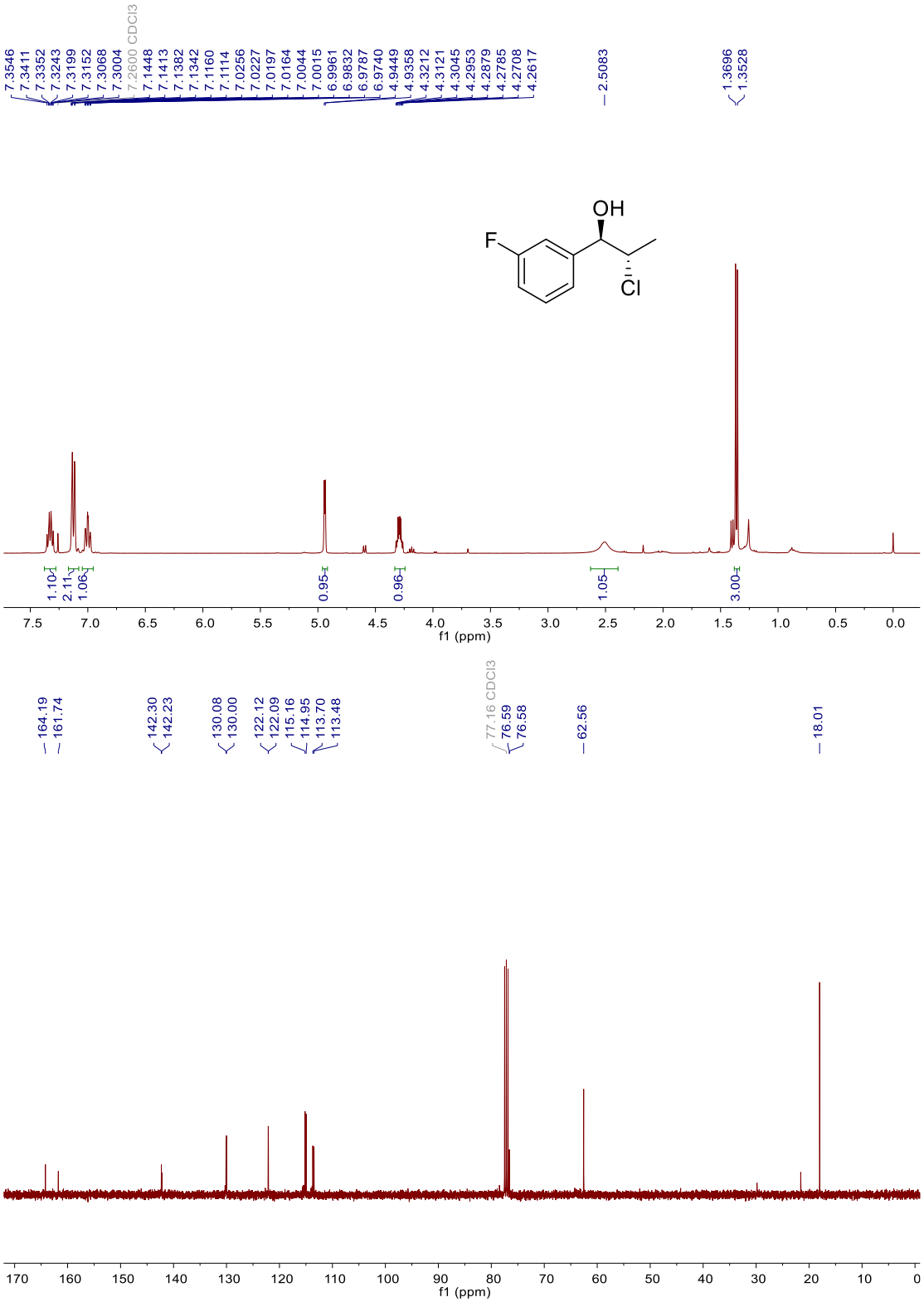


^{1}H and ^{13}C NMR of compound **2e**

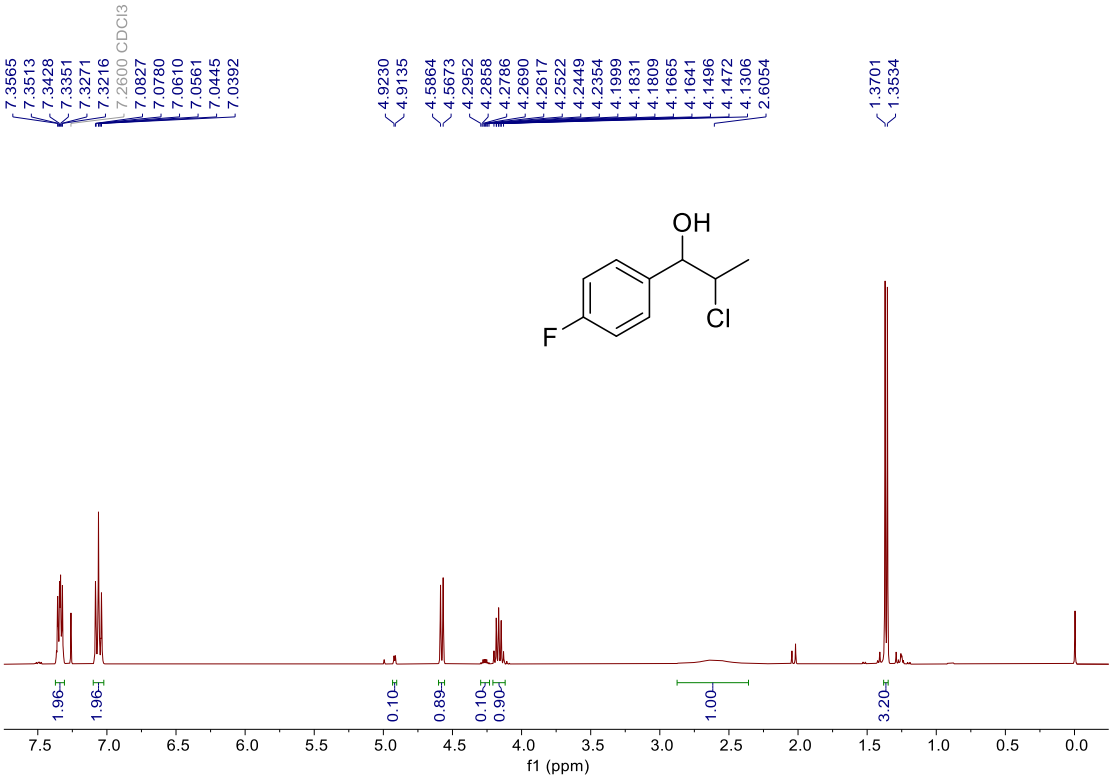


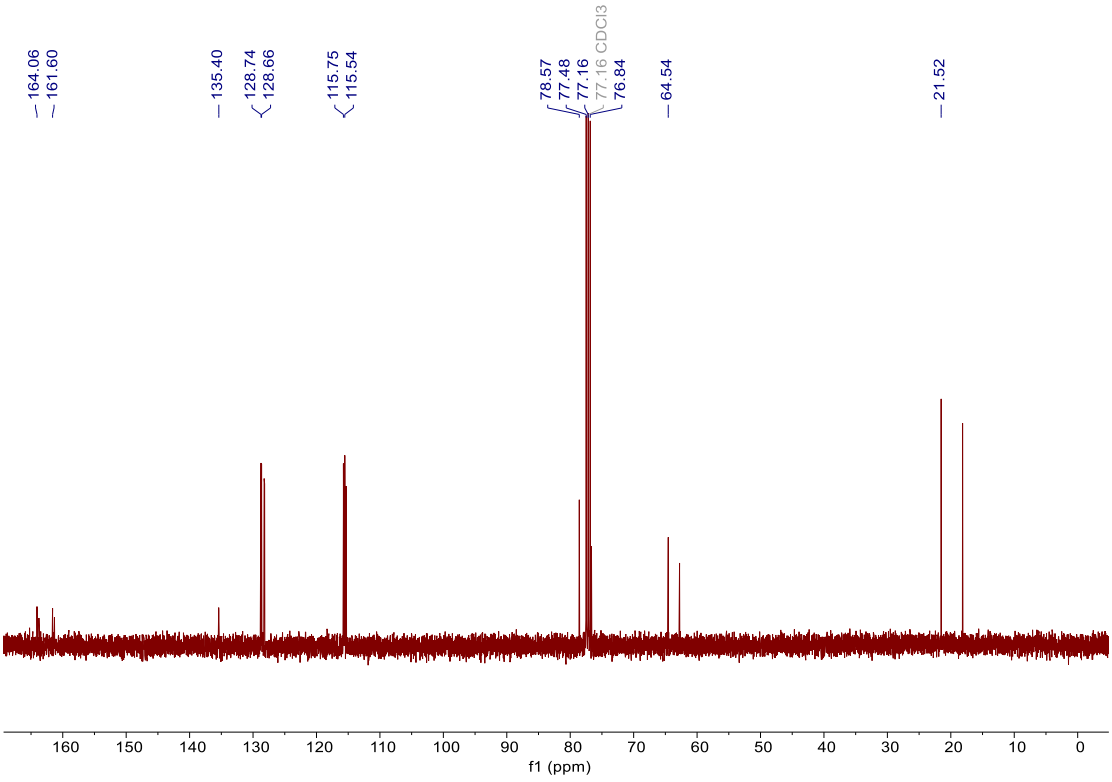


^{1}H and ^{13}C NMR of compound (1*R*,2*S*)-**2e**

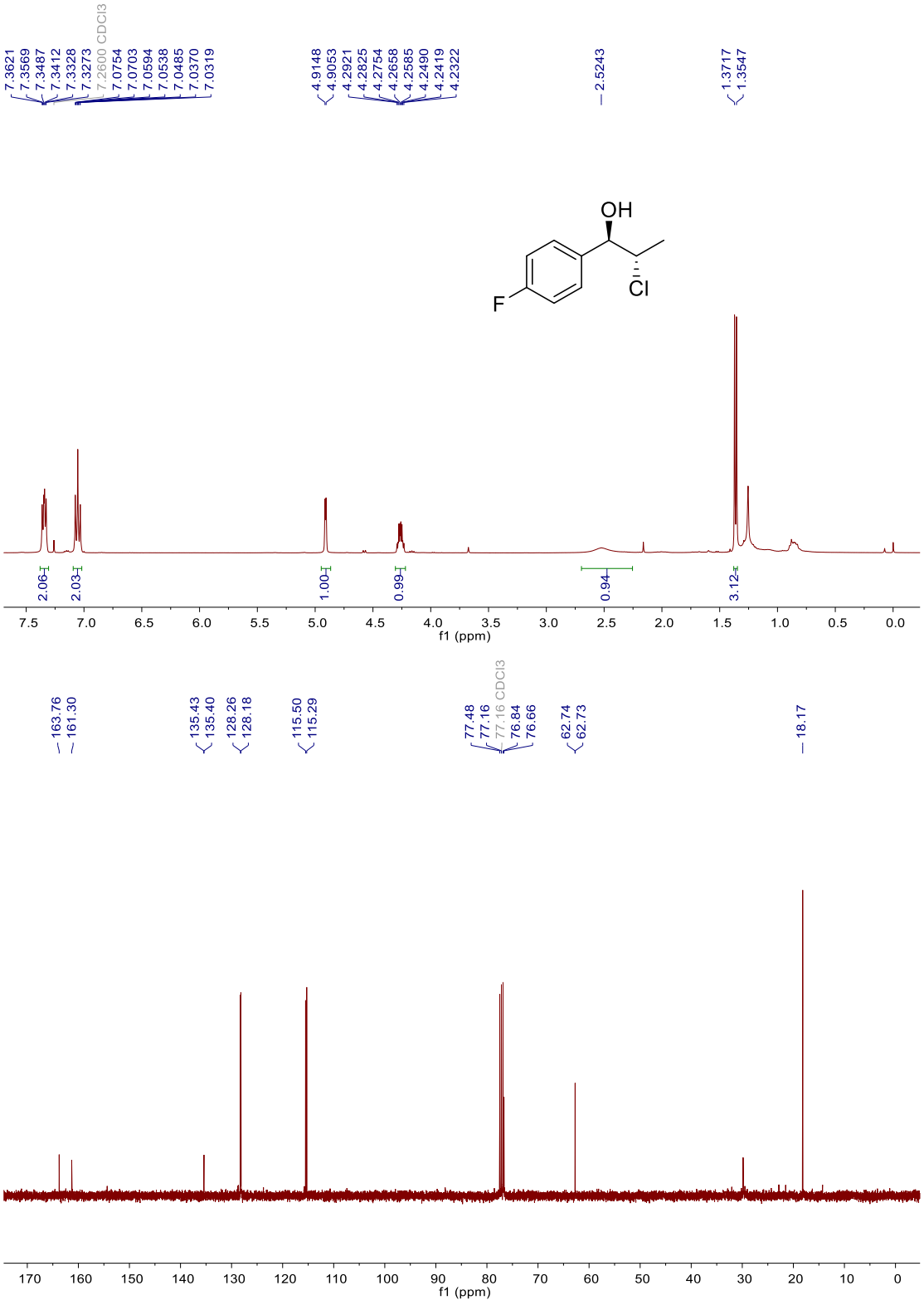


^{1}H and ^{13}C NMR of compound **2f**

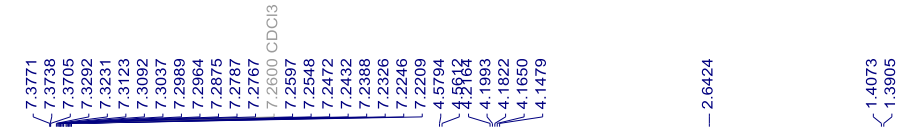


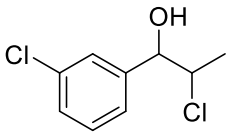


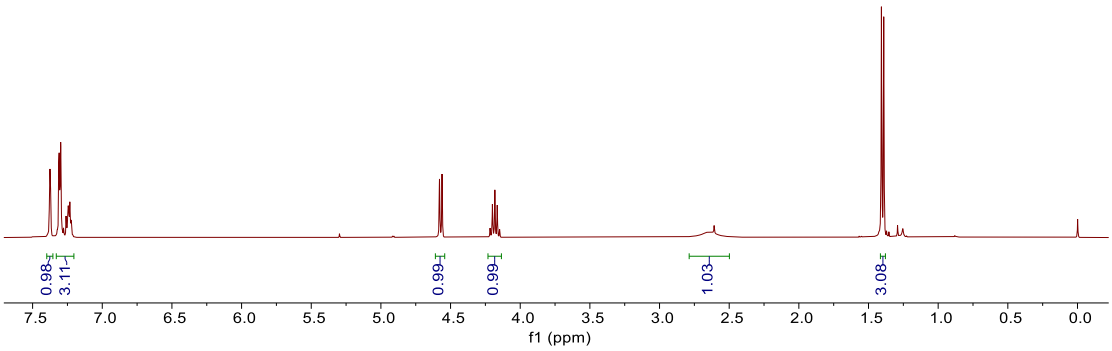
^{1}H and ^{13}C NMR of compound (1*R*,2*S*)-**2f**

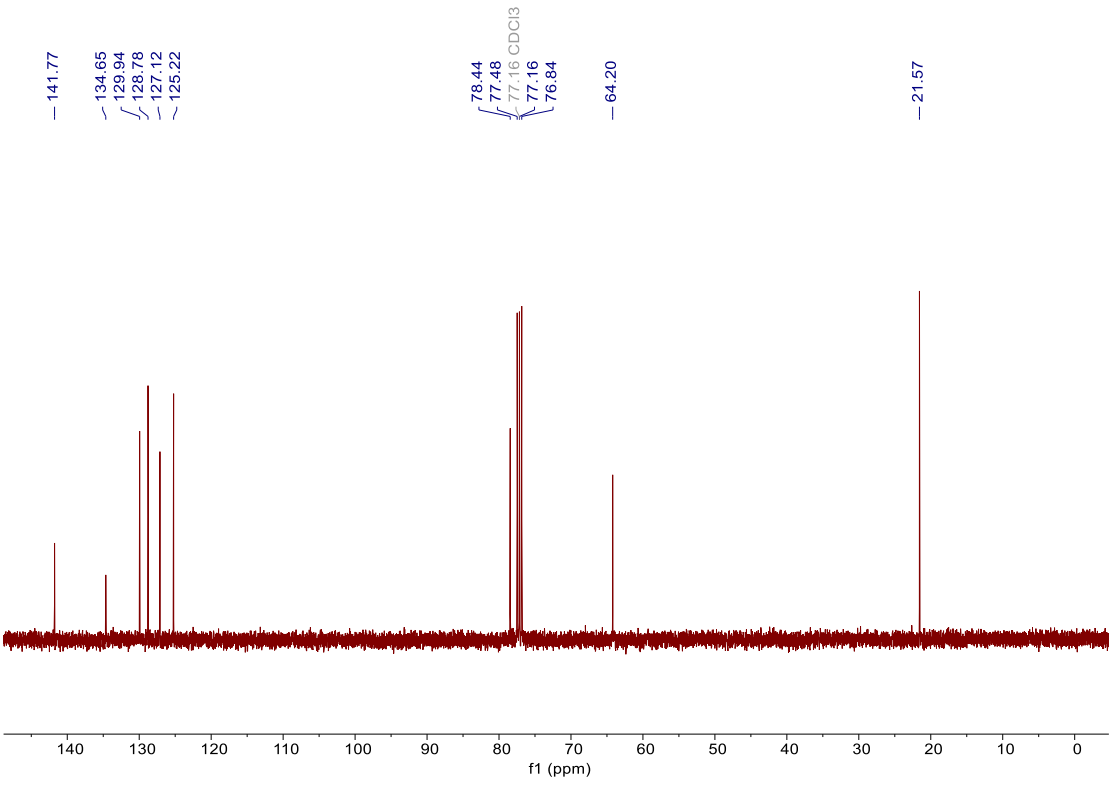


^{1}H and ^{13}C NMR of compound **2g**

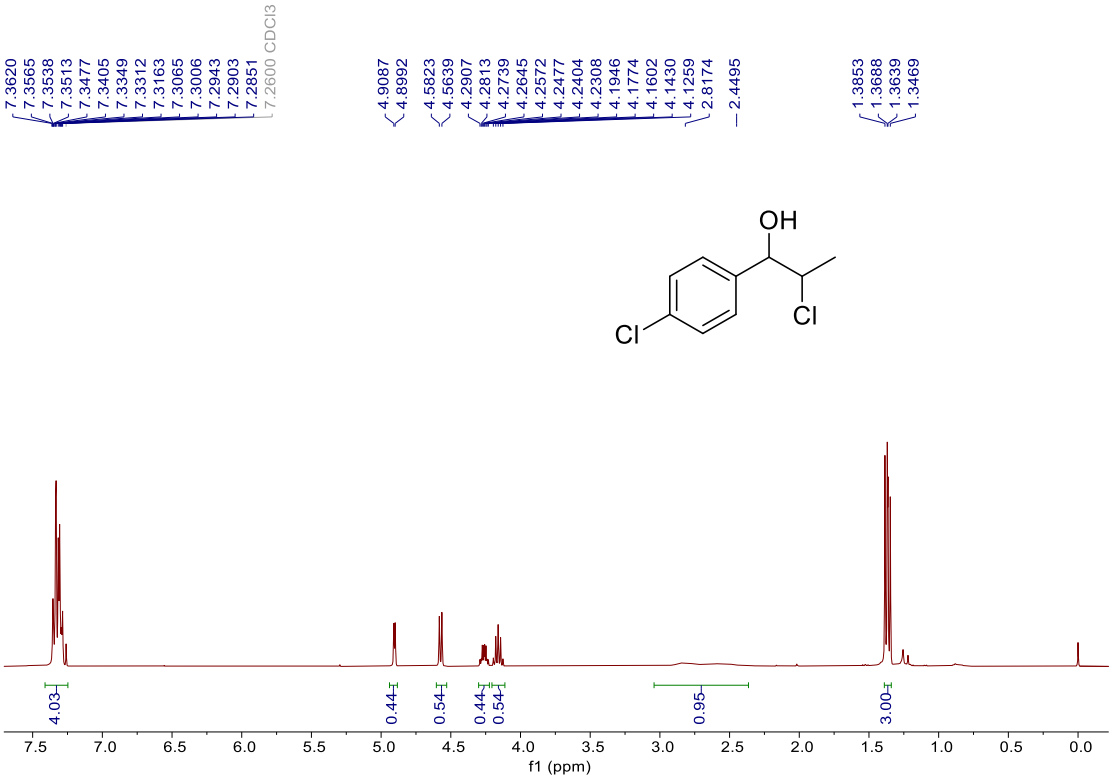


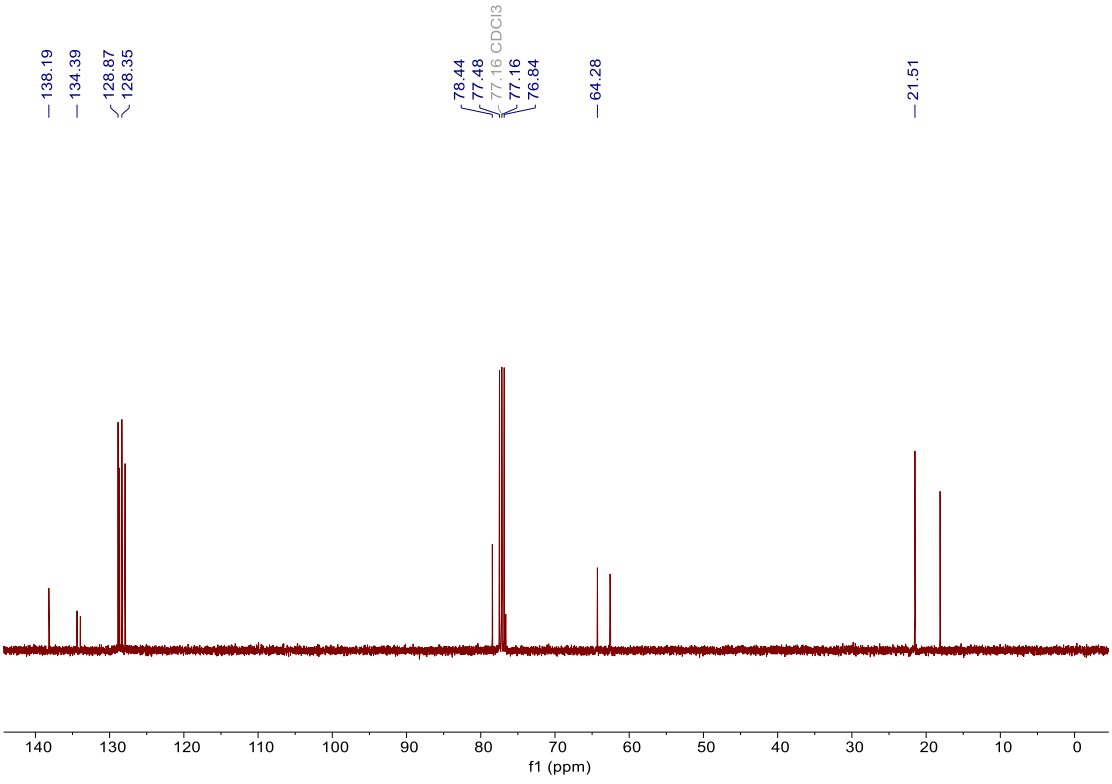




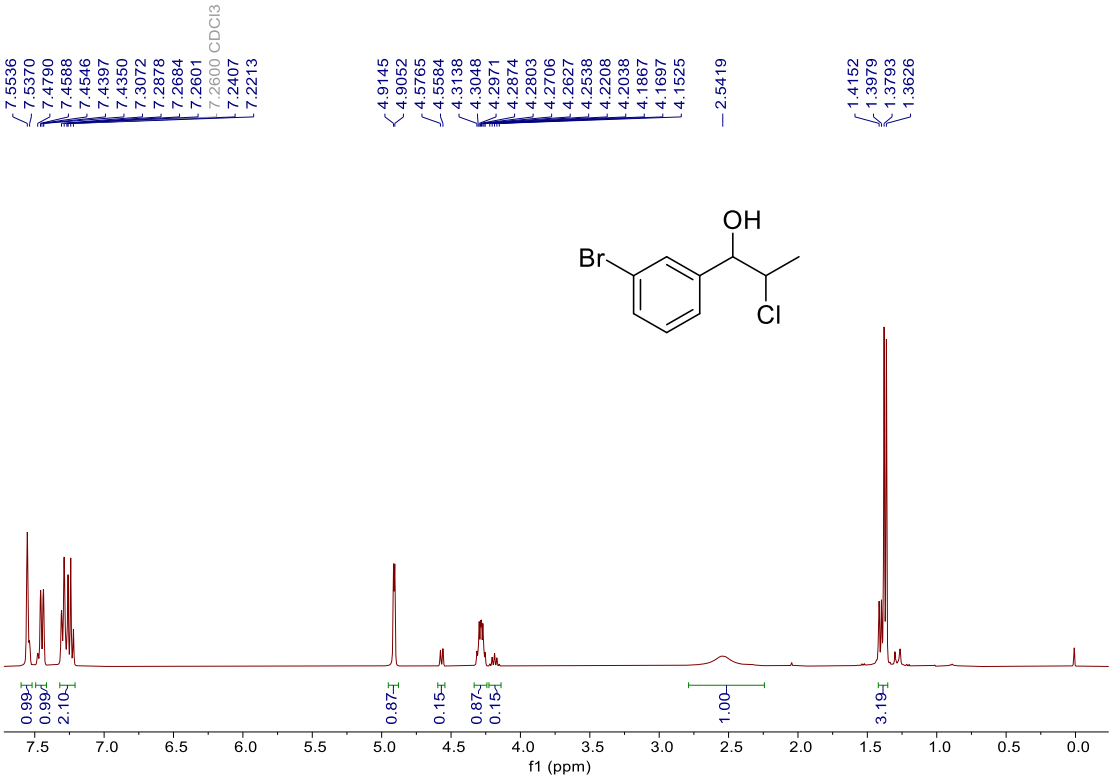


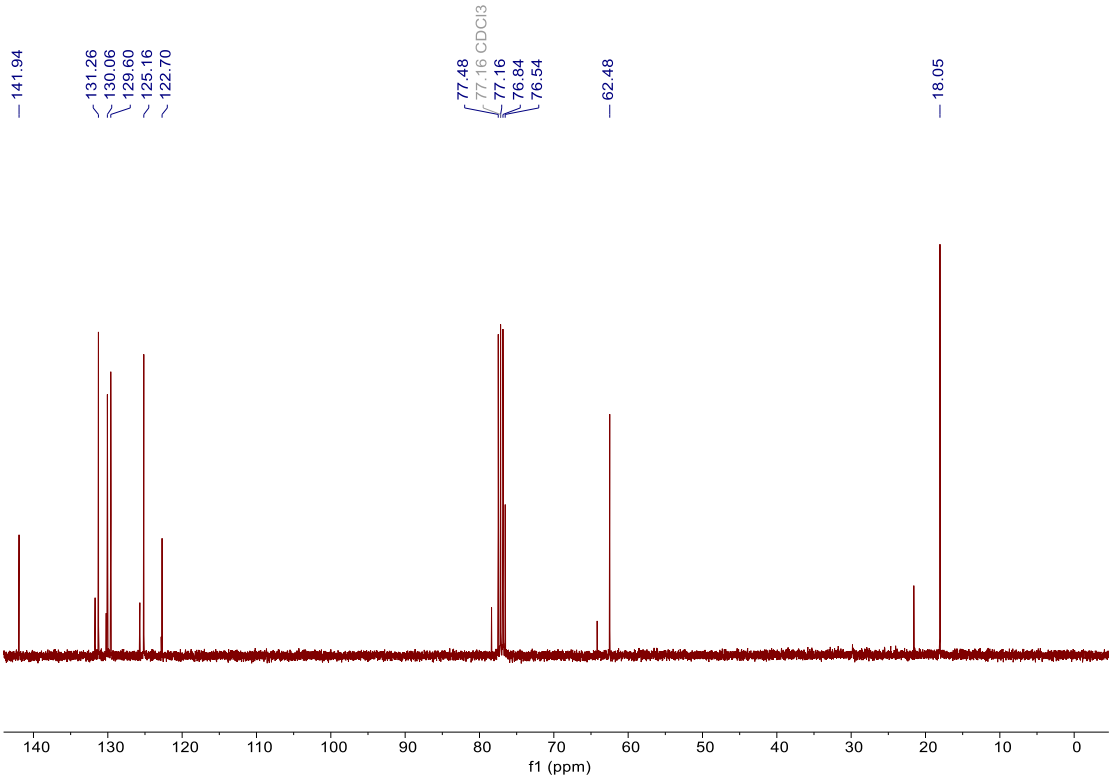
^{1}H and ^{13}C NMR of compound **2h**



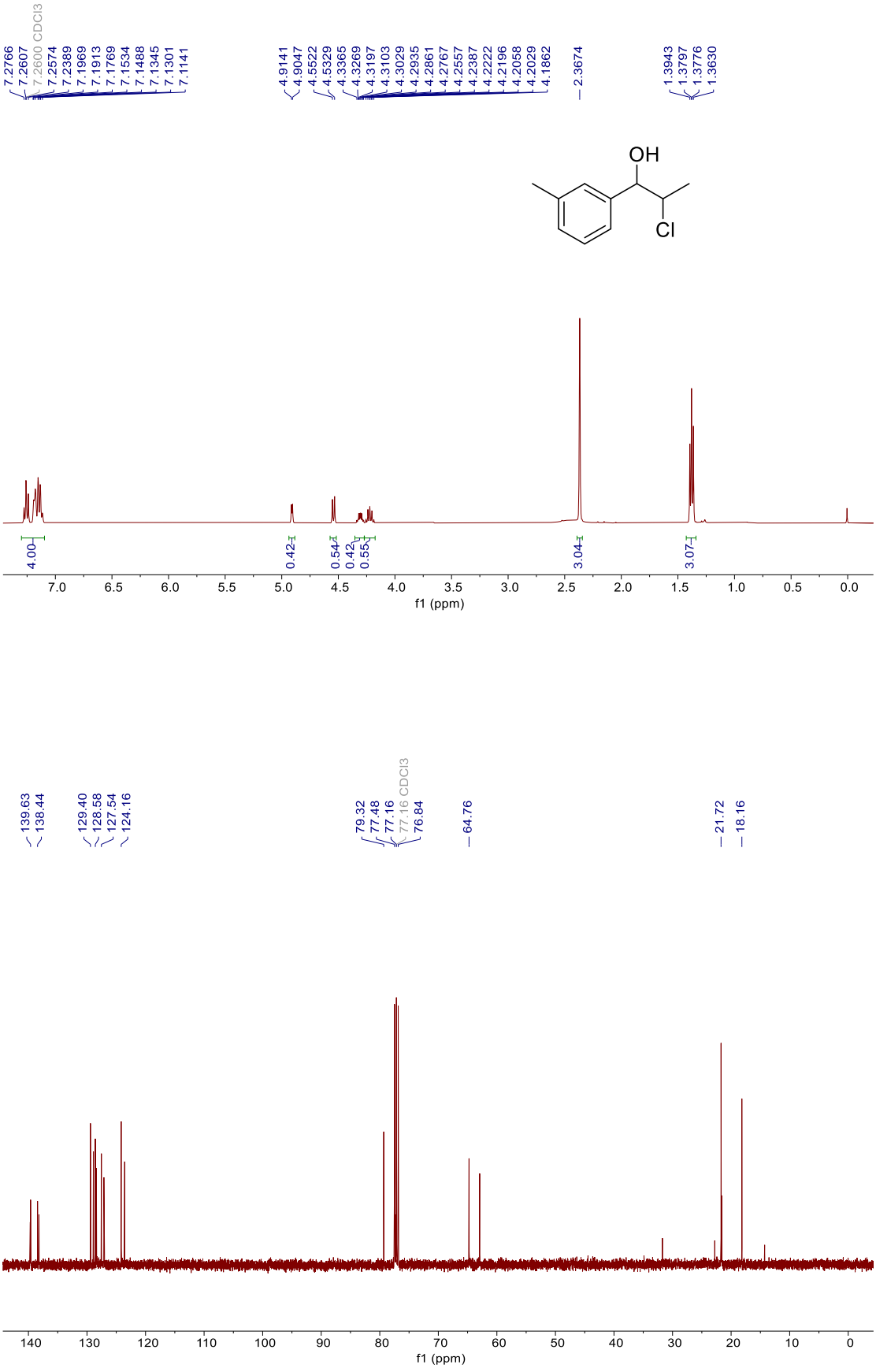


^{1}H and ^{13}C NMR of compound **2i**

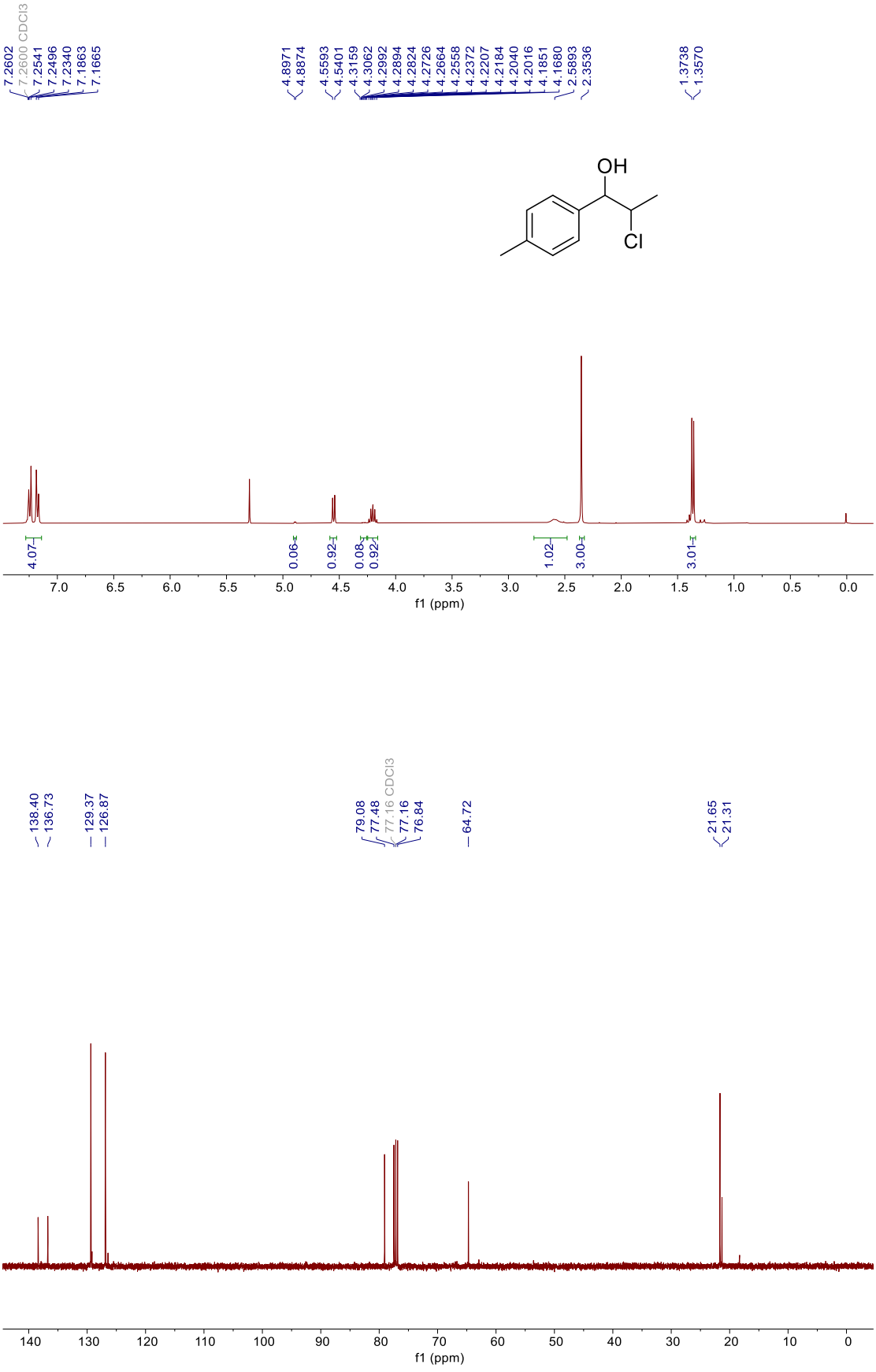




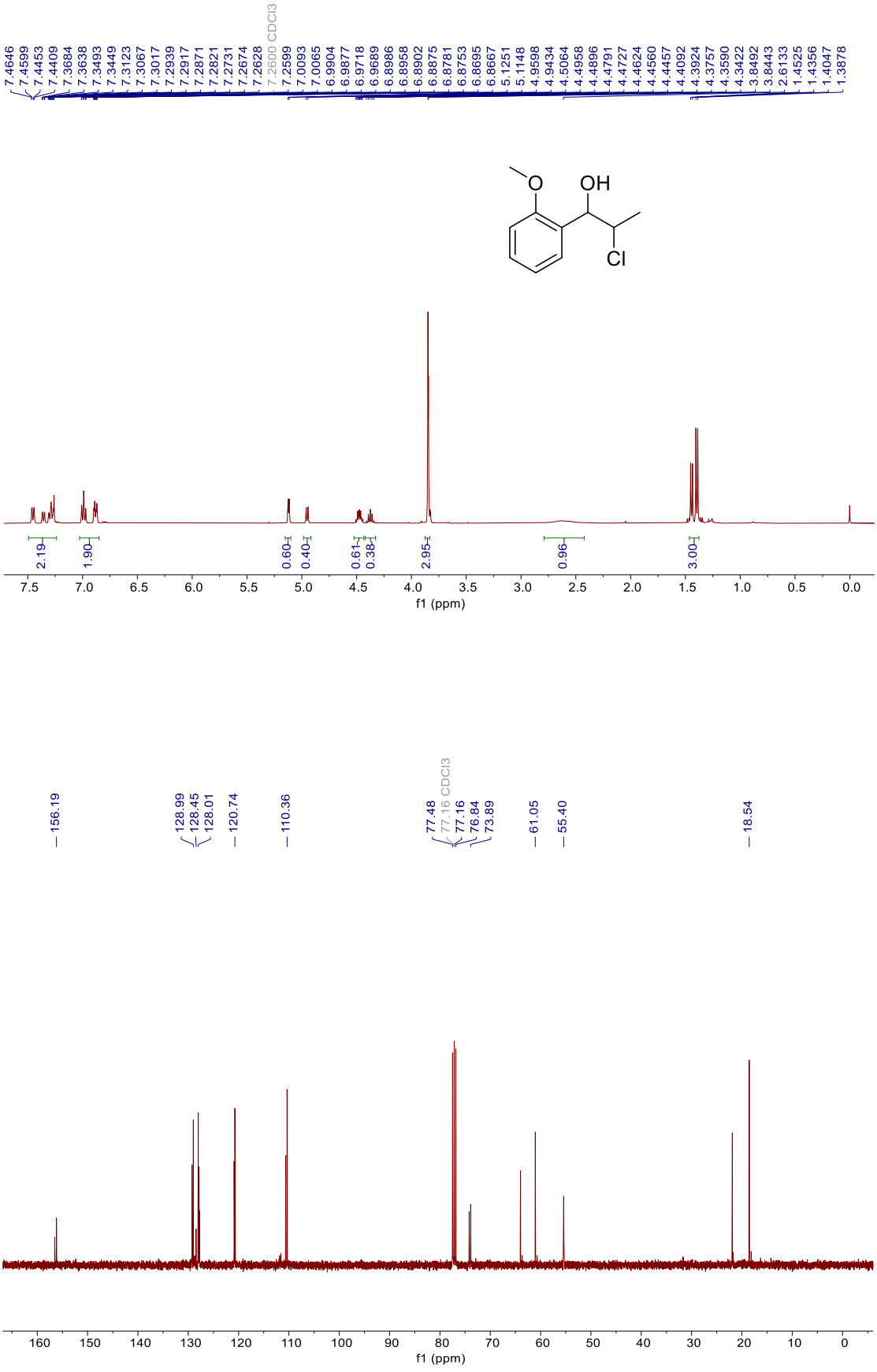
^{1}H and ^{13}C NMR of compound **2j**



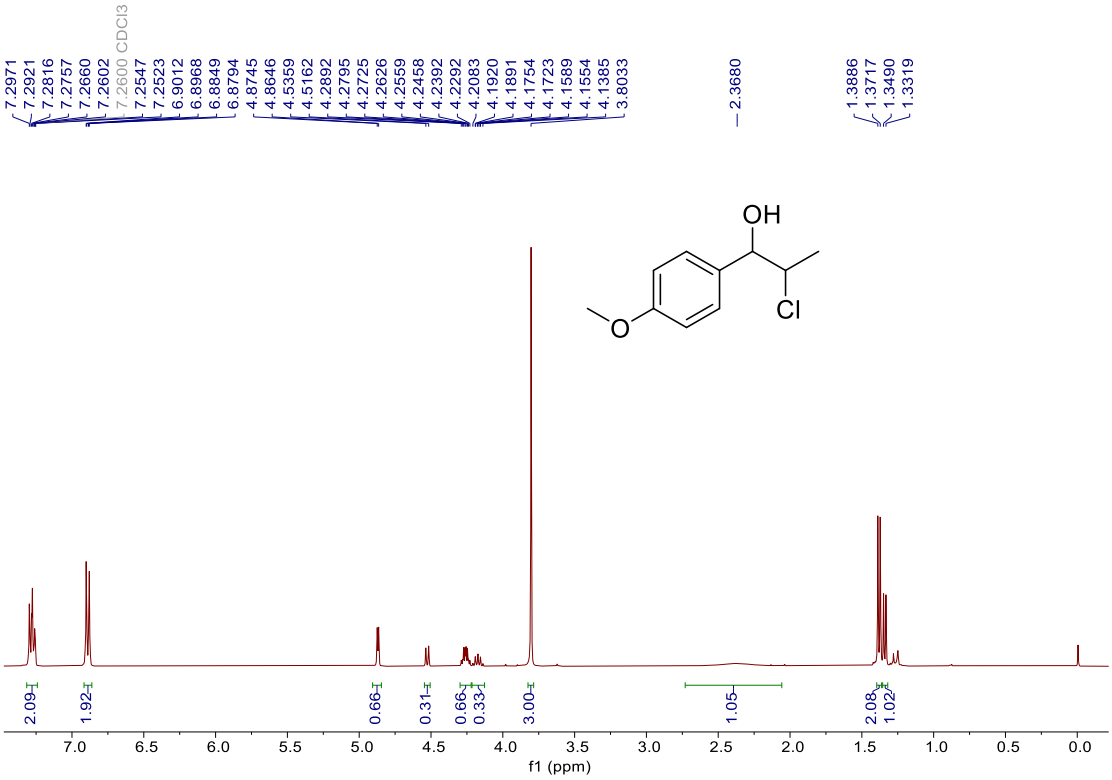
^{1}H and ^{13}C NMR of compound **2k**

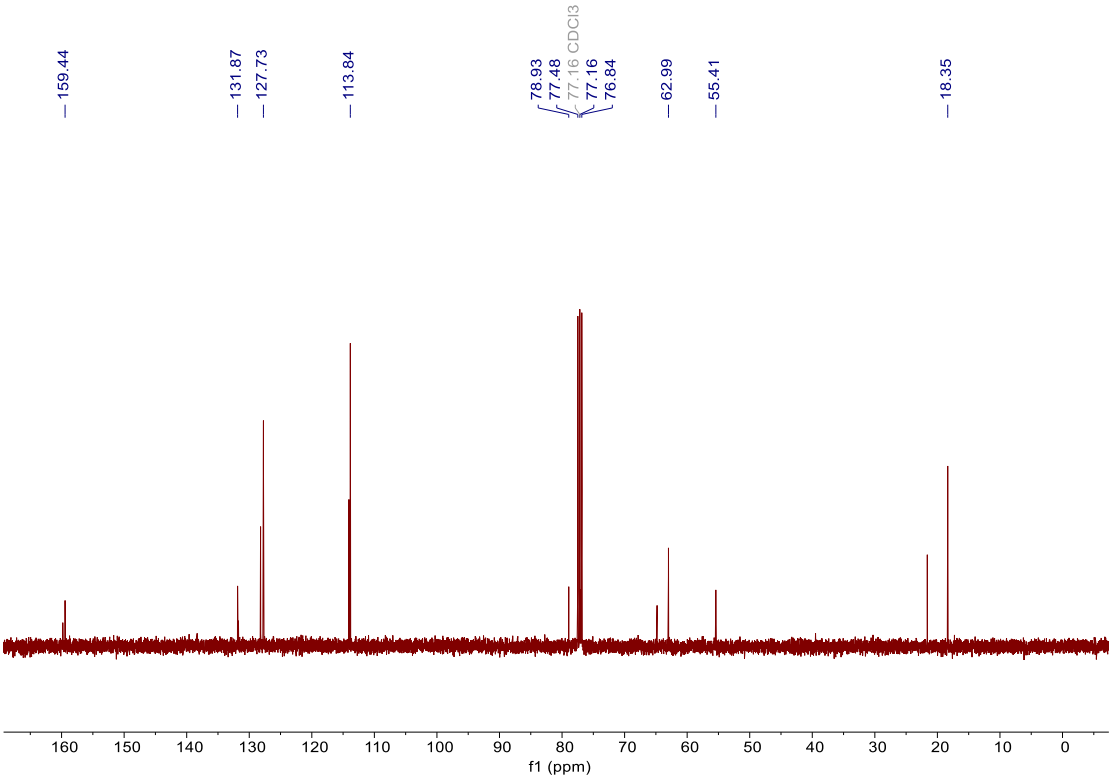


^{1}H and ^{13}C NMR of compound **2l**

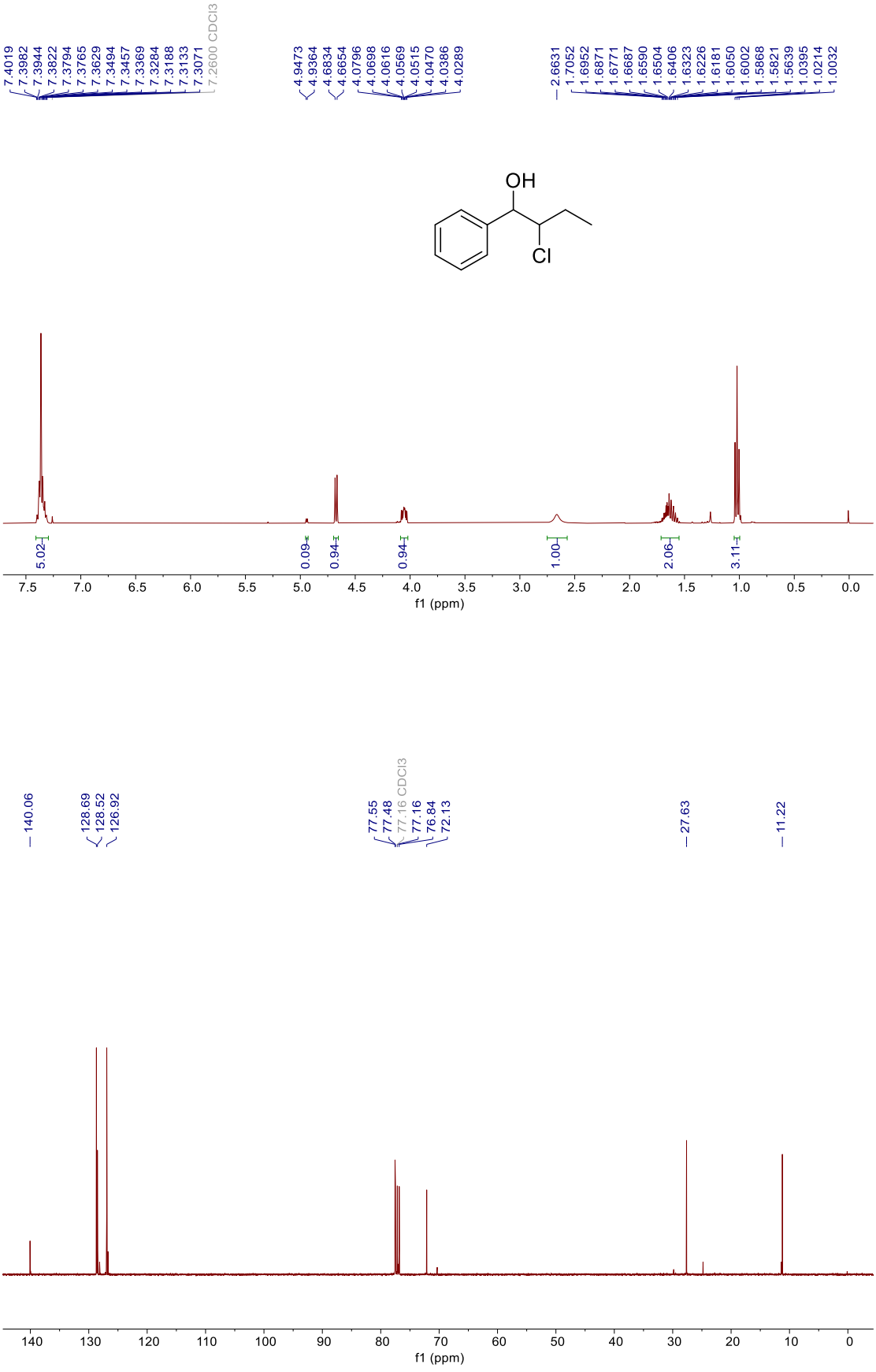


^{1}H and ^{13}C NMR of compound **2m**

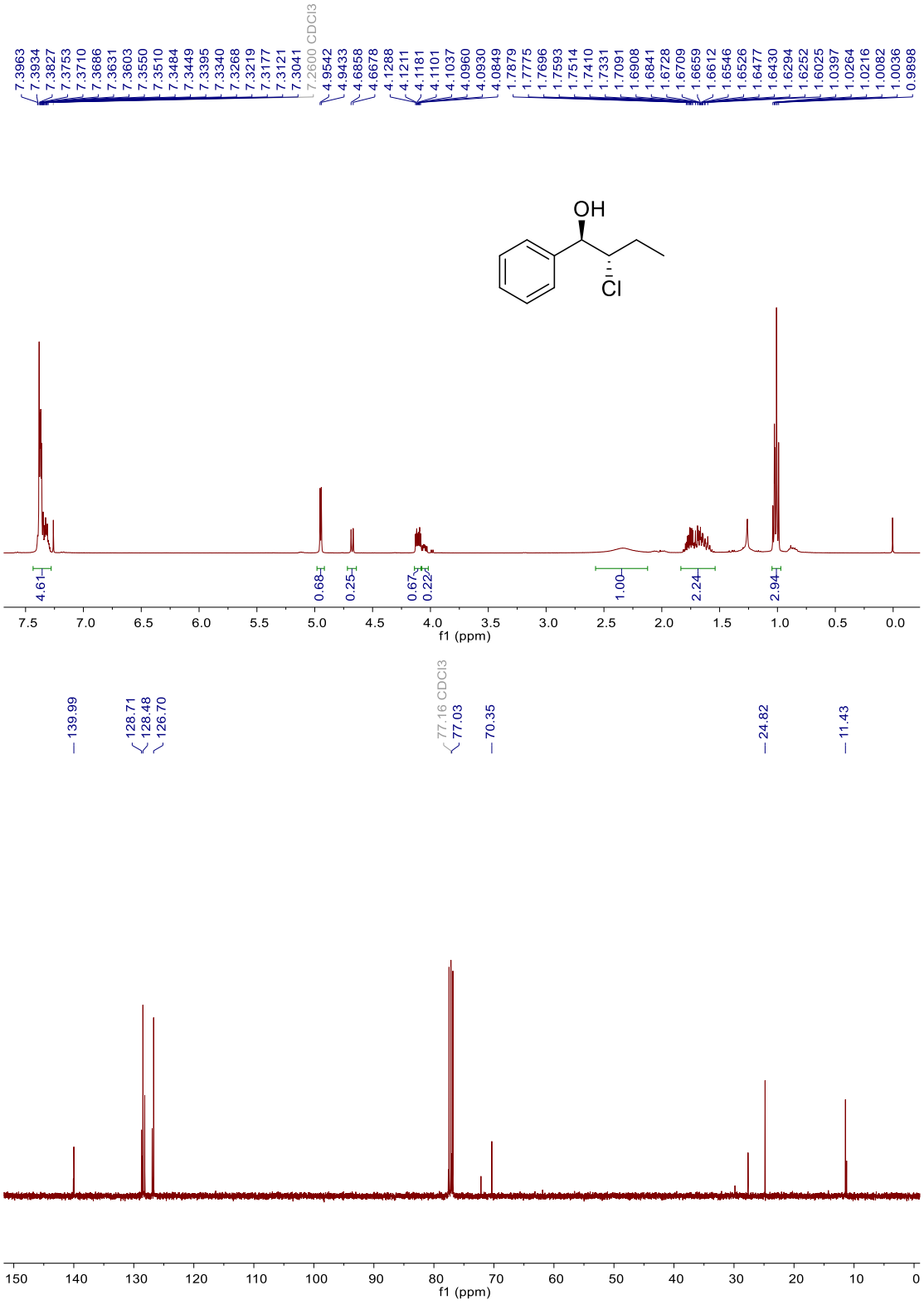




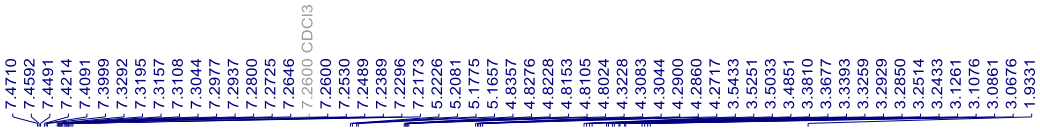
^{1}H and ^{13}C NMR of compound **2n**

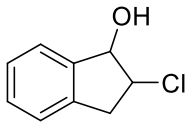


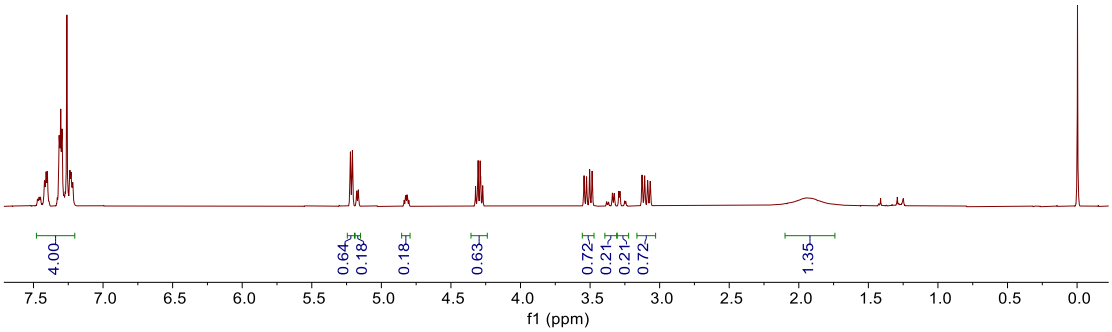
^{1}H and ^{13}C NMR of compound (1*R*,2*S*)-**2n**

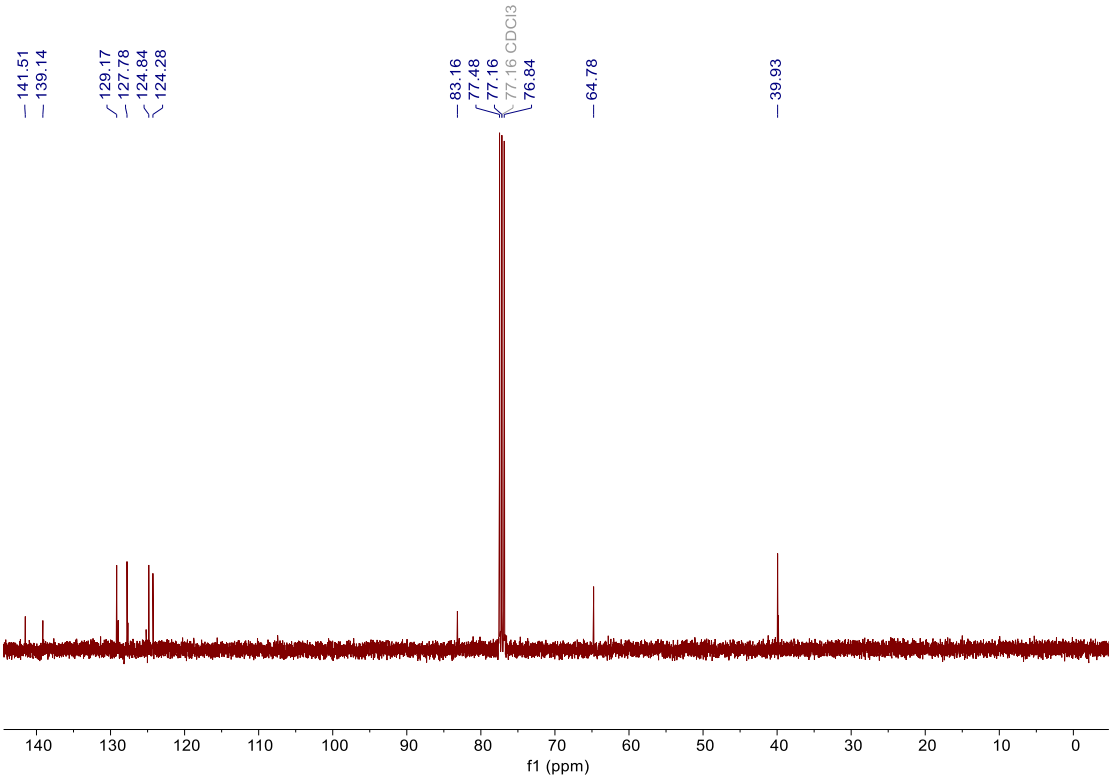


^{1}H and ^{13}C NMR of compound **2o**

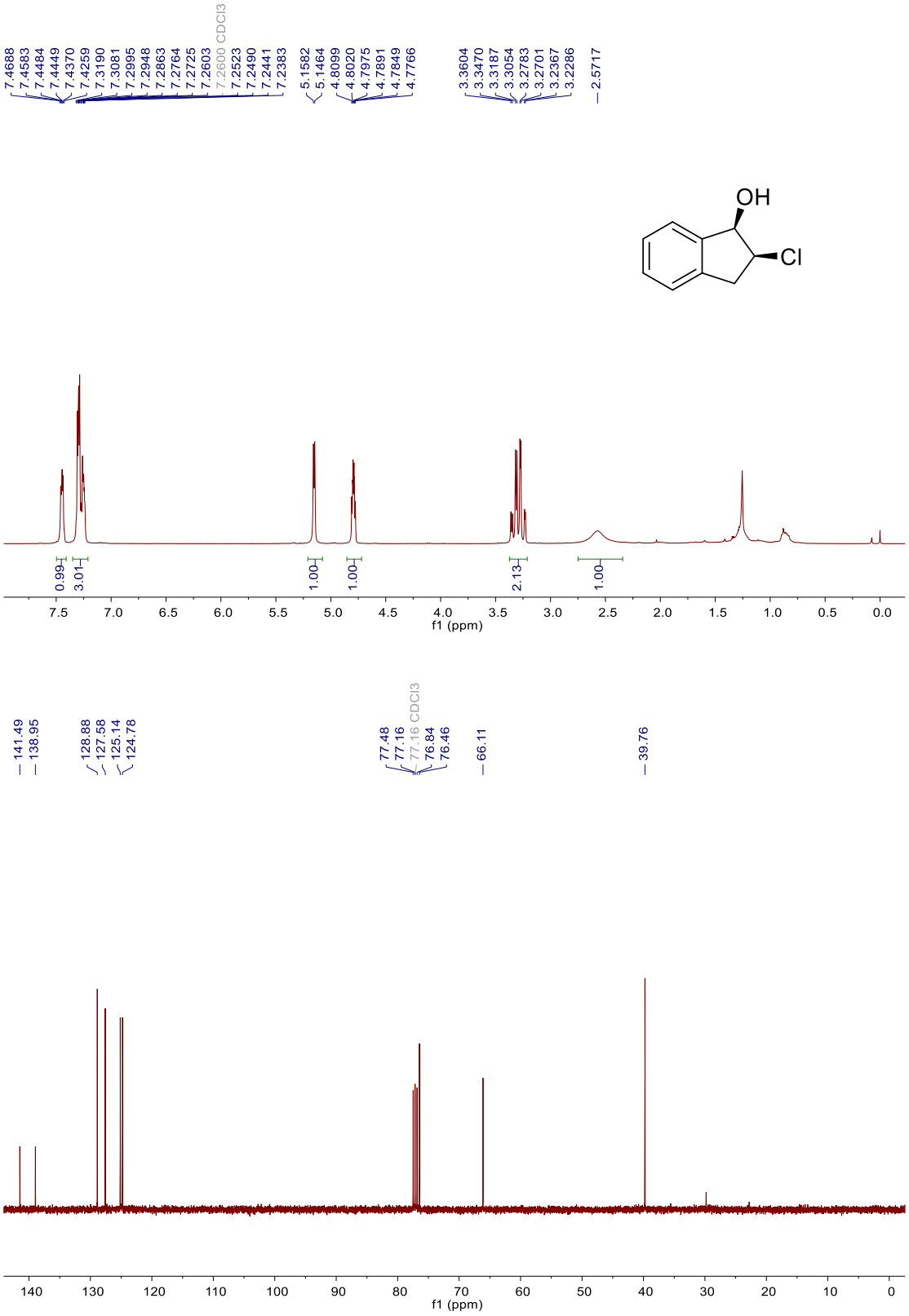




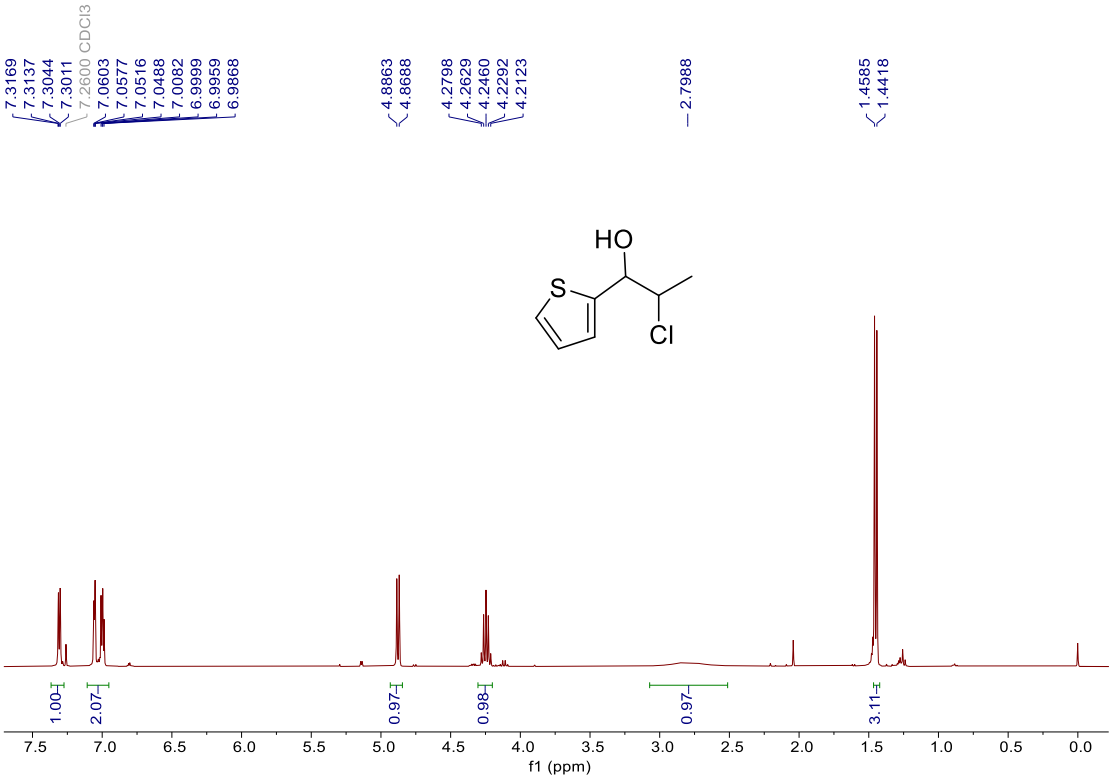


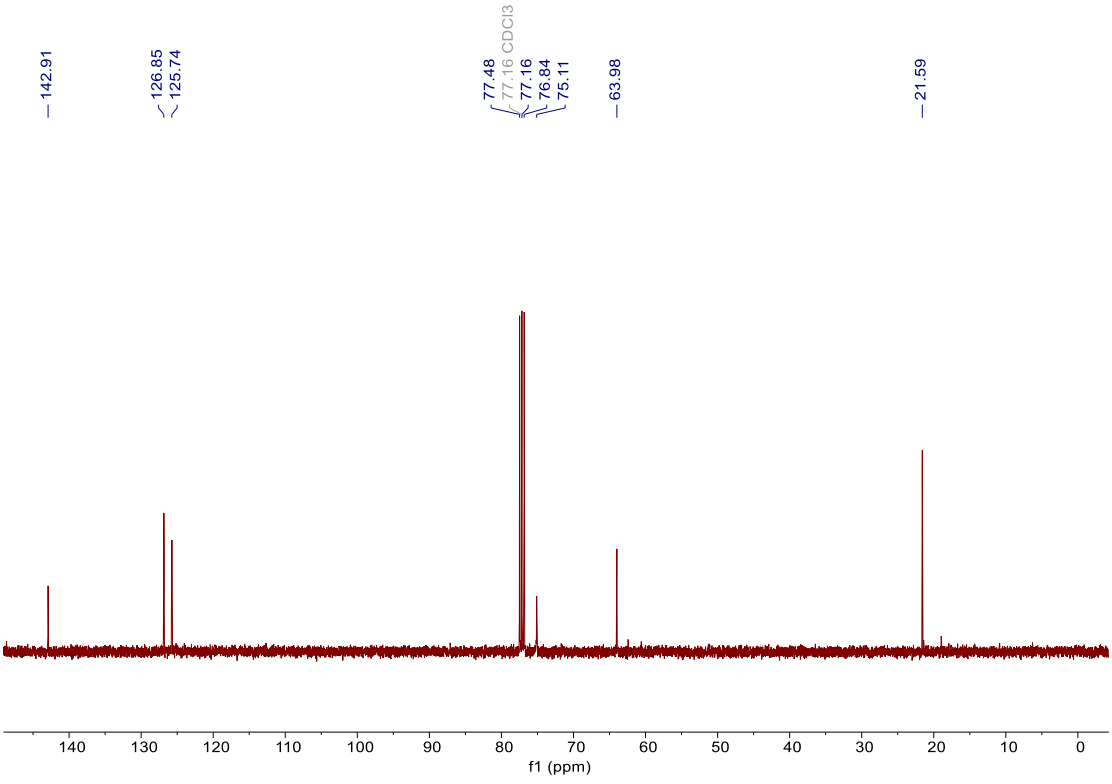


^{1}H and ^{13}C NMR of compound (1*R*,2*S*)-**2o**

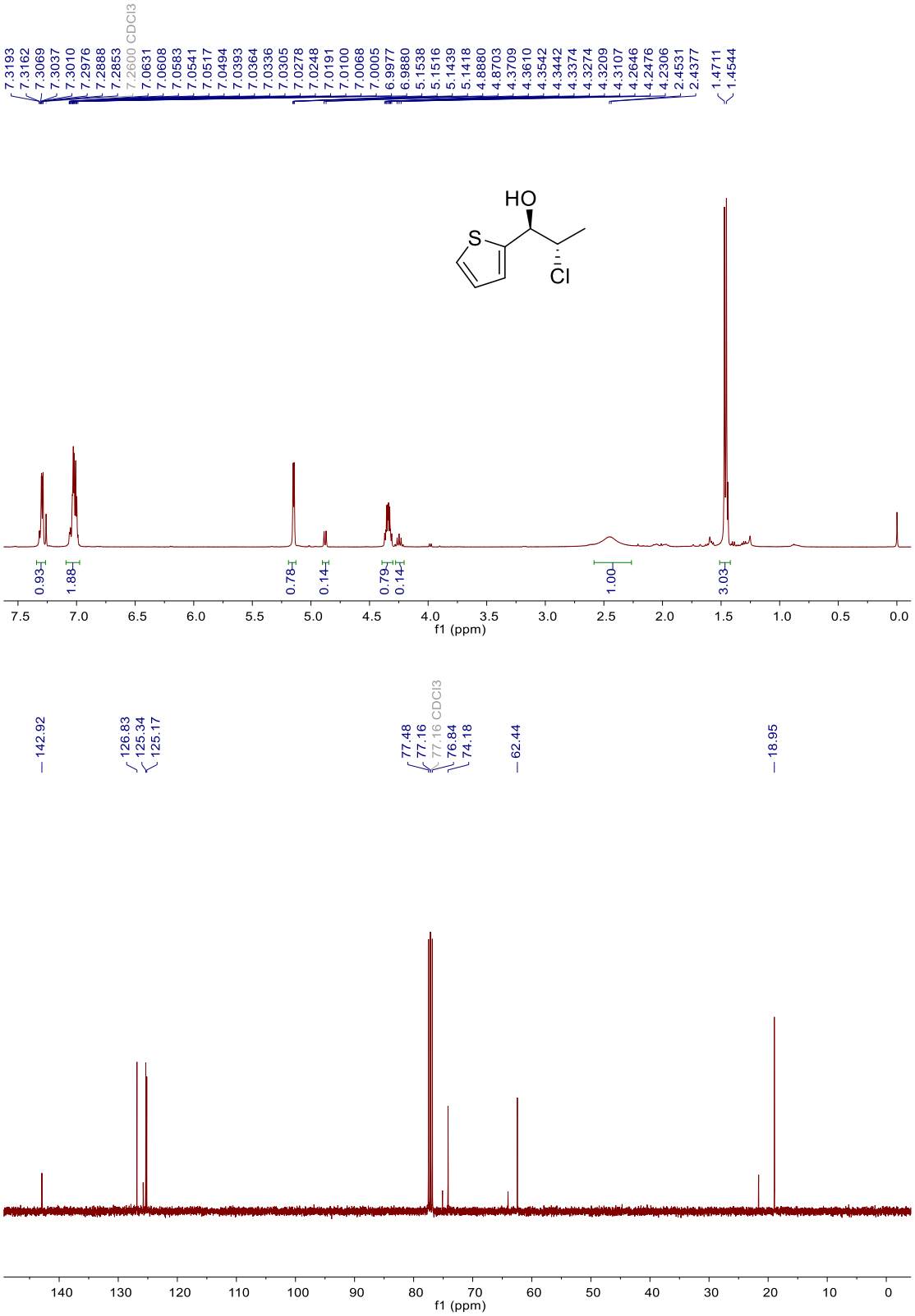


^{1}H and ^{13}C NMR of compound **2p**

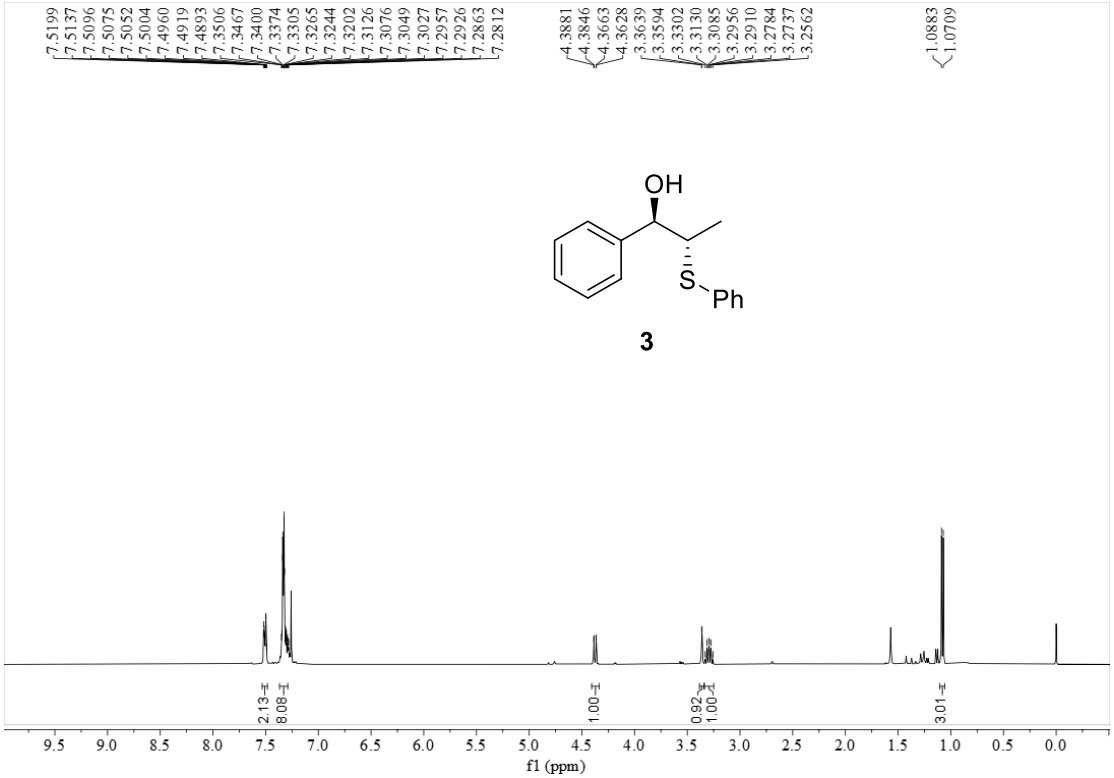




^{1}H and ^{13}C NMR of compound (1*R*,2*S*)-**2p**



^{1}H and ^{13}C NMR of compound **3**



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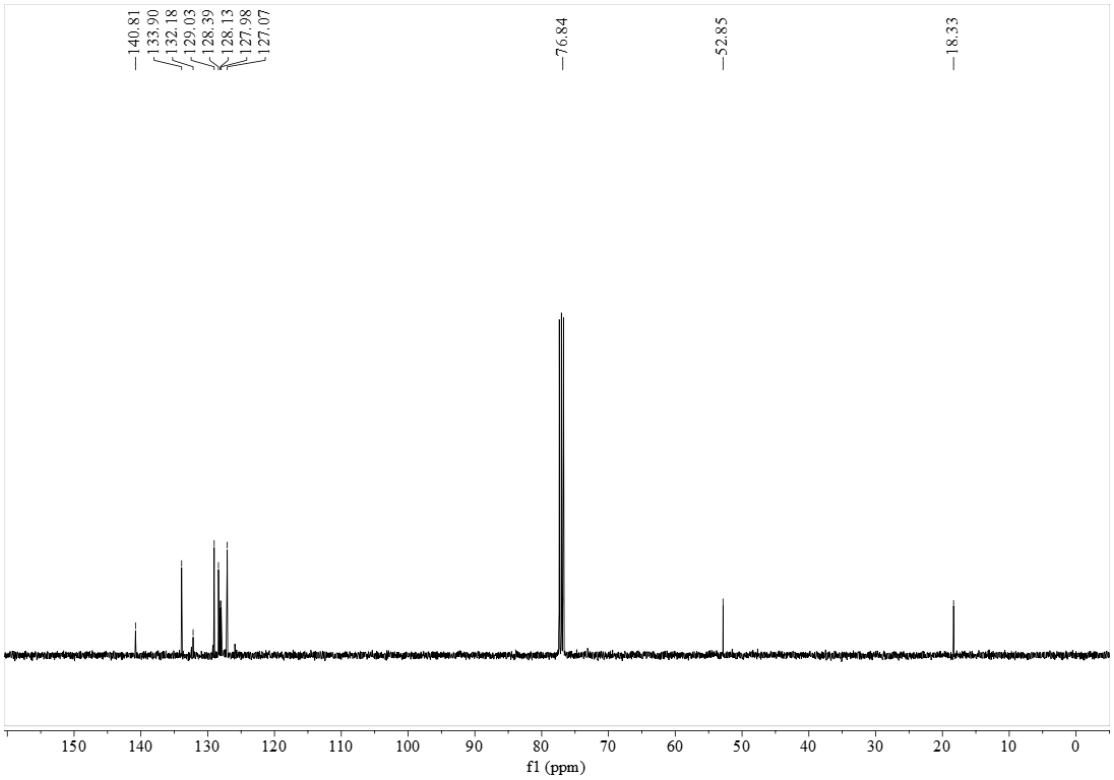
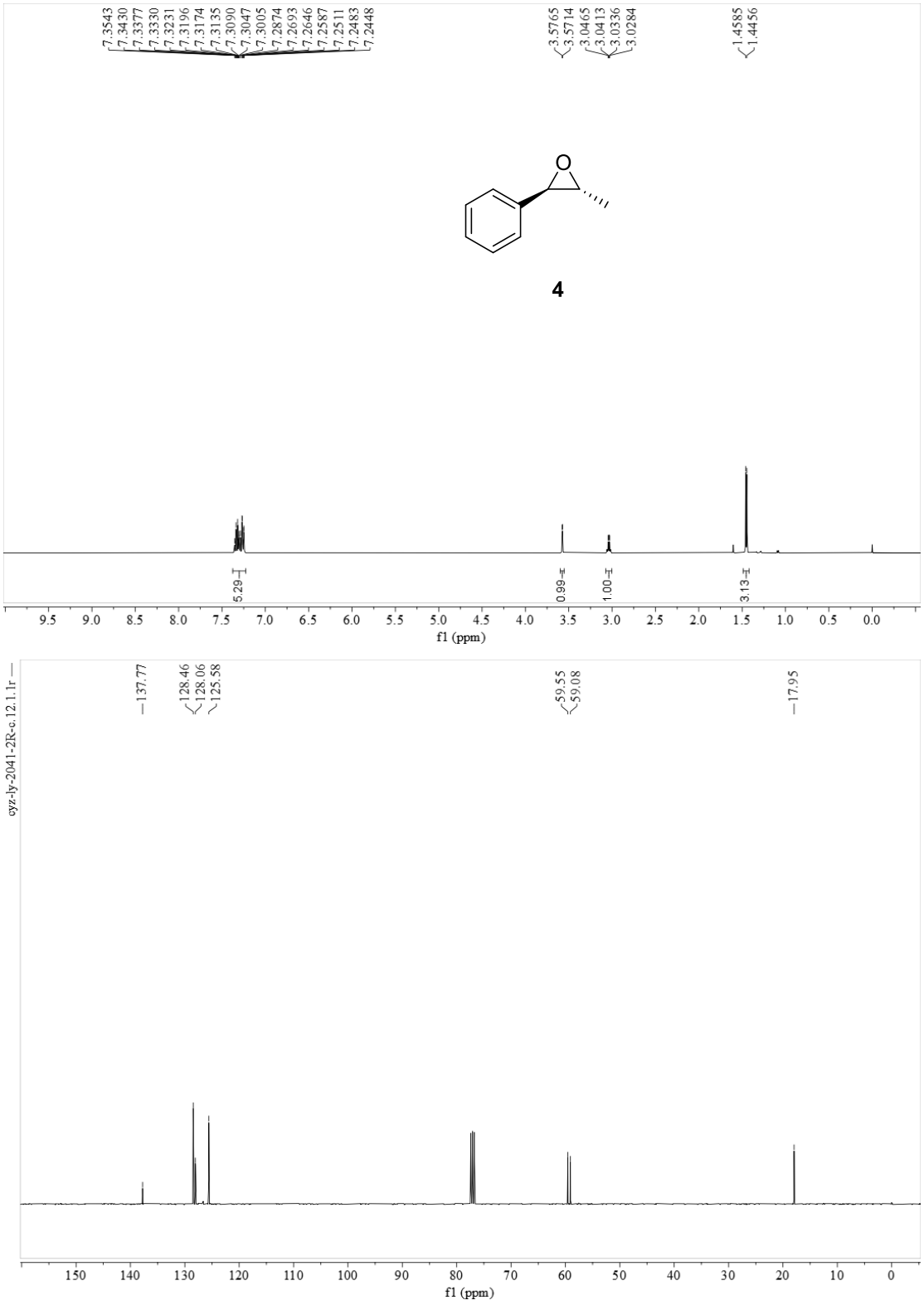
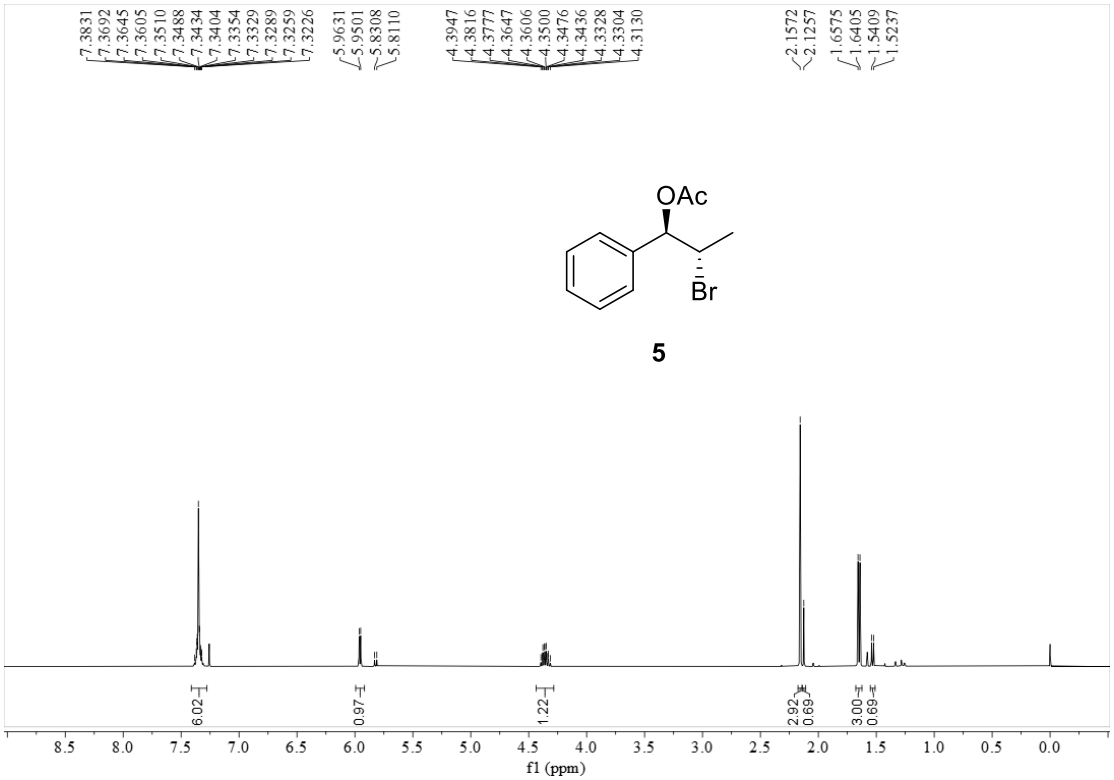


^{1}H and ^{13}C NMR of compound **4**



^{1}H and ^{13}C NMR of compound **5**



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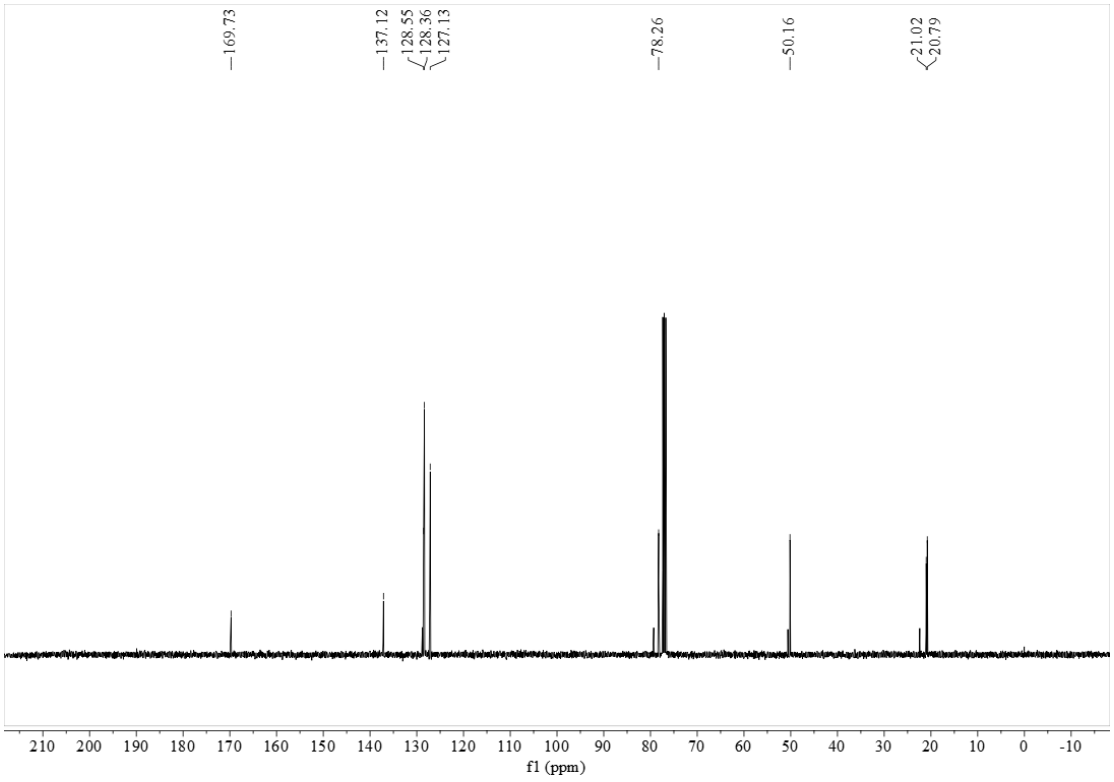
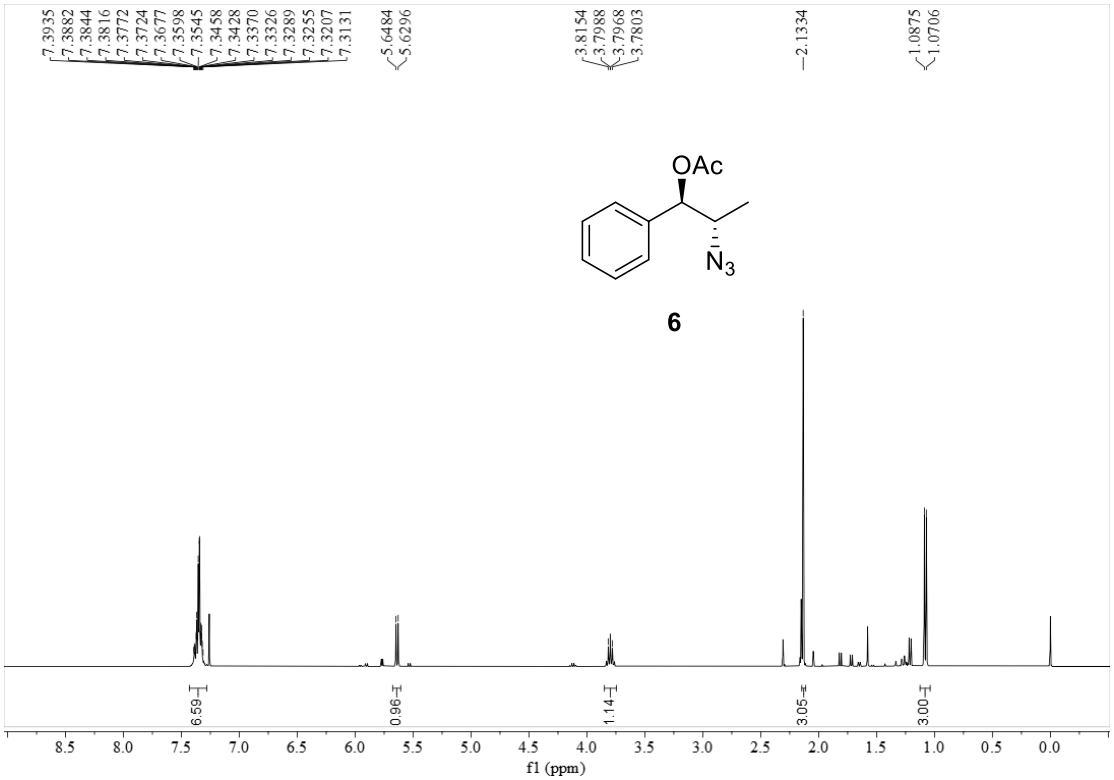
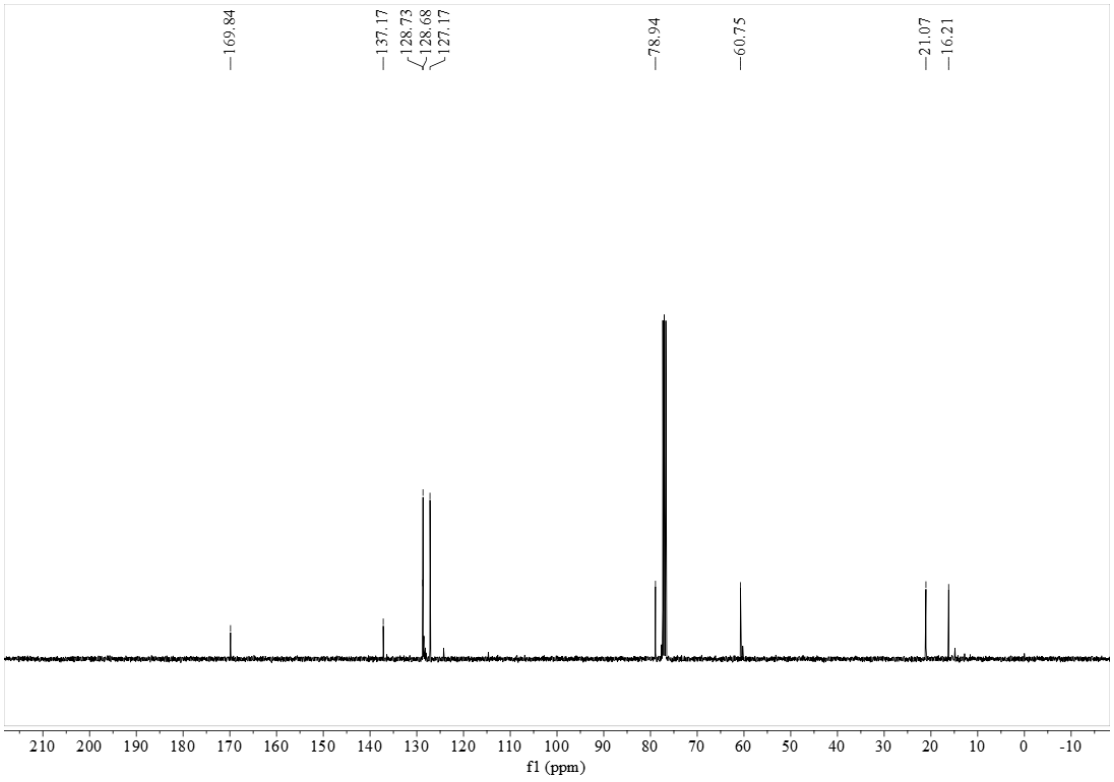
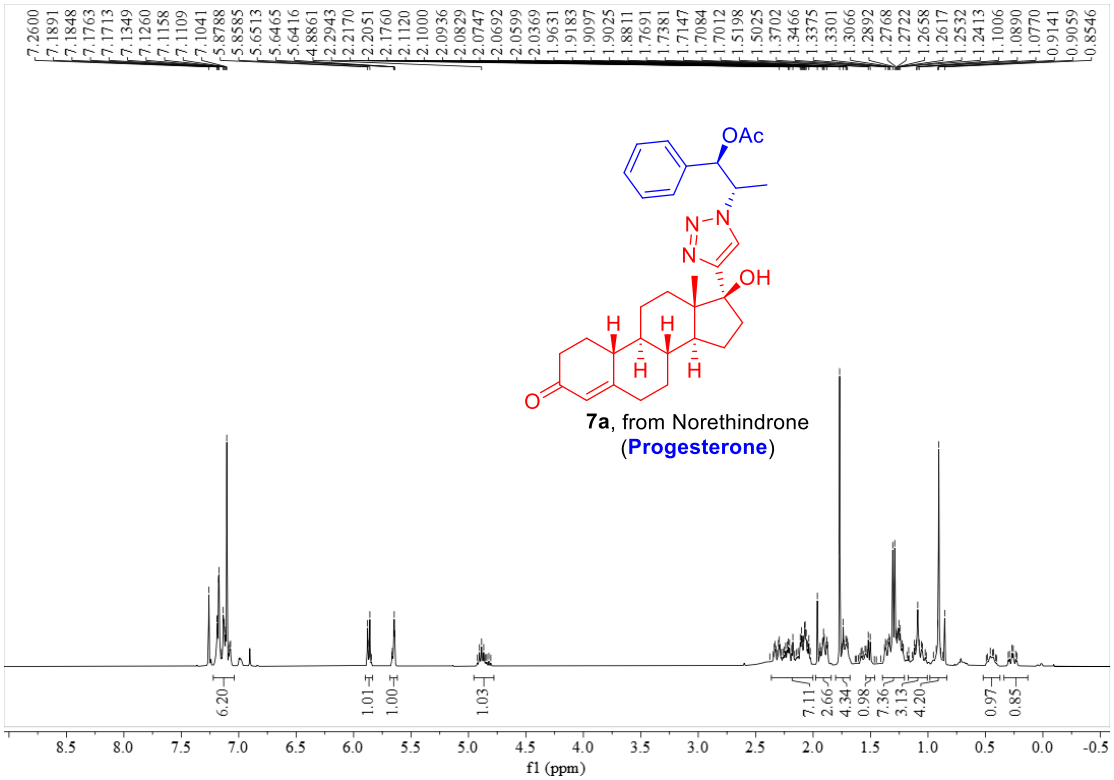


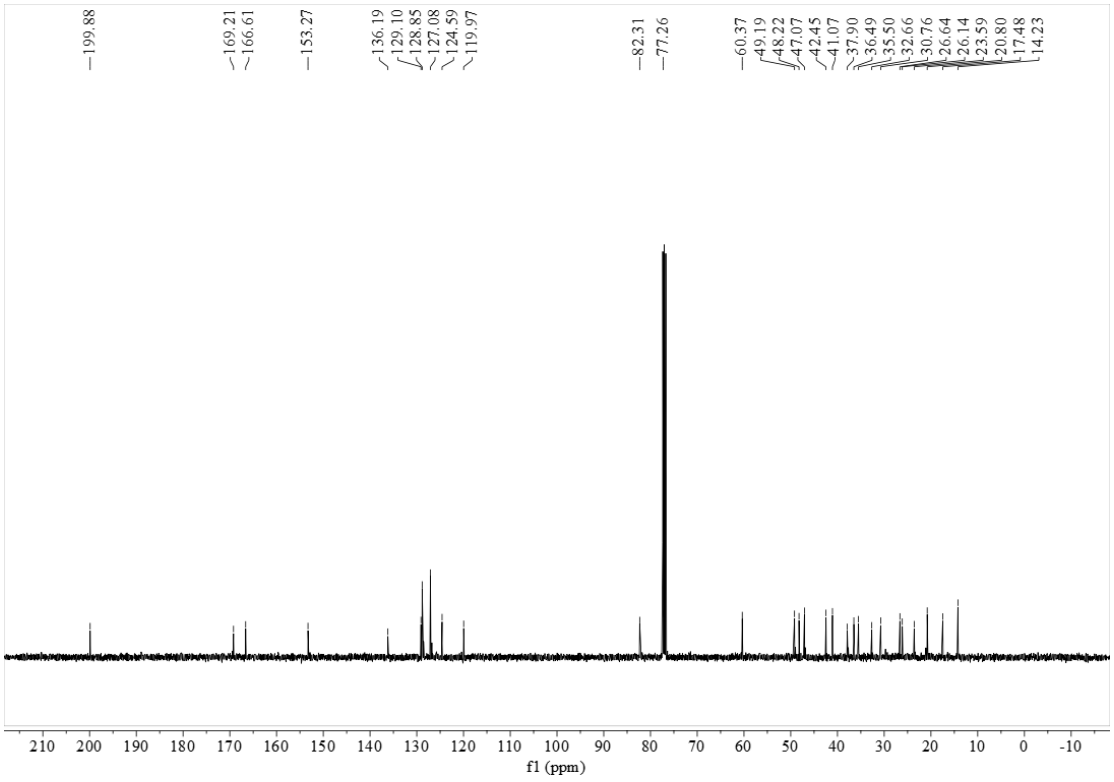
^{1}H and ^{13}C NMR of compound **6**



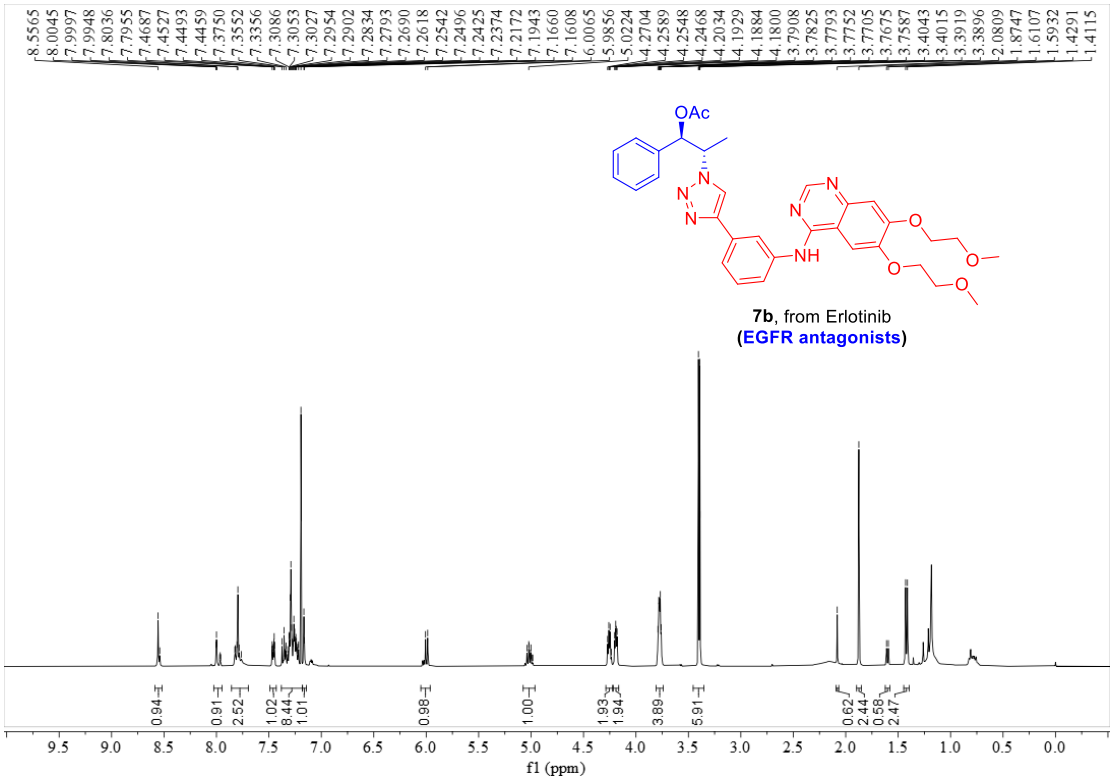


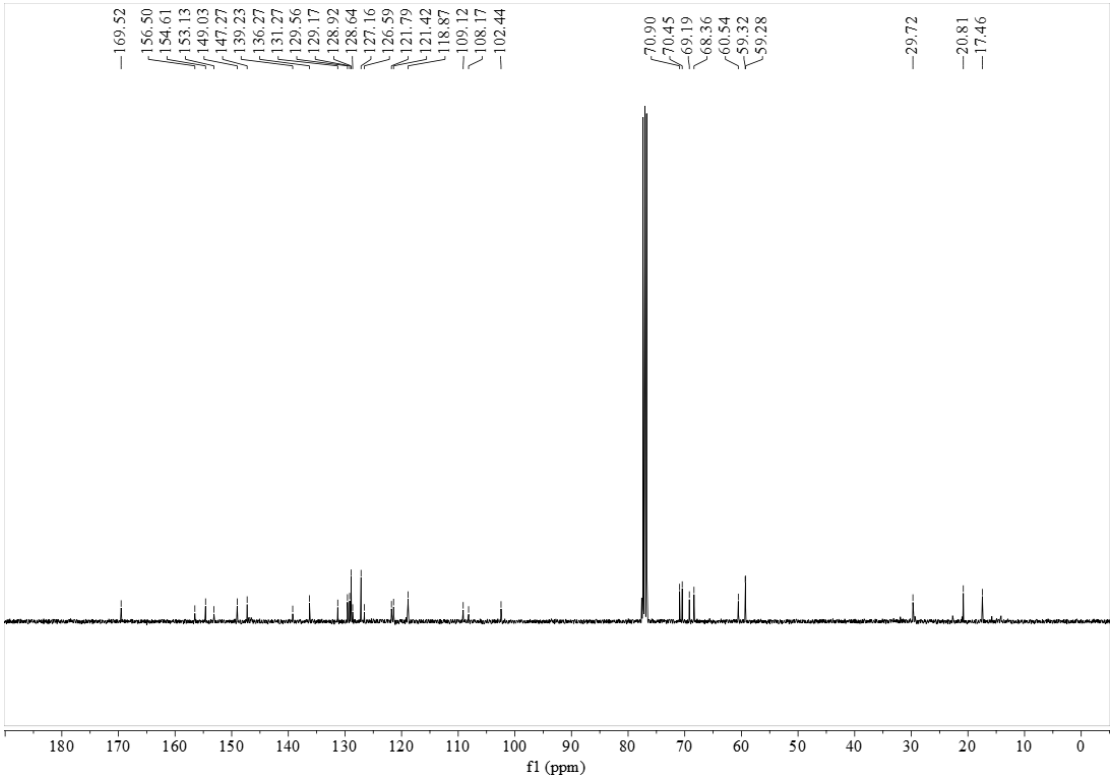
^{1}H and ^{13}C NMR of compound **7a**





^{1}H and ^{13}C NMR of compound **7b**





8. References

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9. Cartesian Coordinates of Geometries Optimized

cI

Fe 0.41589650 1.09981514 0.00000000
N 2.19058150 0.16054114 0.22062100
N -0.51485050 -0.69090486 0.10021600
N 1.33155650 2.87973314 0.23742200
N -1.37604350 2.02335714 0.07190000
C 3.42552250 0.75268714 0.31712100
C -1.87079750 -0.92002686 0.03413100
C 2.42378450 -1.18819686 0.15783900
C 0.07979250 -1.93484486 0.06179000
C 2.67838850 3.10369214 0.33603800
C -2.60957150 1.43461514 -0.01282000
C 0.74493050 4.11658014 0.20167900
C -1.60206550 3.37836814 0.04717900
C 4.46248450 -0.25114686 0.32544400
C -2.13481950 -2.33731786 -0.01233600
C 3.84060350 -1.45646986 0.22022600
C -0.92726650 -2.96427886 -0.00058100
C 2.95086550 4.52067714 0.37369500
C -3.64331350 2.43929014 -0.08028800
C 1.74794550 5.15101414 0.28667700
C -3.01689550 3.64713714 -0.04357000
H 5.52187950 -0.04161186 0.40073000
H -3.12278450 -2.77744986 -0.05989100
H 4.28188550 -2.44459786 0.19376400
H -0.71871950 -4.02604586 -0.03269300
H 3.93848450 4.95663914 0.45384700
H -4.70335450 2.22979914 -0.14707300
H 1.54011550 6.21341814 0.28166300
H -3.45536450 4.63648814 -0.07396700
C 3.65746950 2.11817114 0.38561000
C -2.84742850 0.06356414 -0.01567800
C -0.62082350 4.35639614 0.11113100
C 1.44391450 -2.17016986 0.07208700

H 4.68969550 2.44524914 0.46521300
H -3.88088750 -0.26296686 -0.08147600
H -0.94553350 5.39222414 0.08911400
H 1.77376350 -3.20348386 0.02852800
O 0.49916550 1.14308714 -1.61897600
S 0.30495350 0.66143514 2.59038600
C -1.38147850 0.98705614 3.17989500
H -2.07221350 0.29558114 2.68152400
H -1.42990250 0.80356814 4.25734700
H -1.69476150 2.00905814 2.95184600

R-R-IRC-S

Fe	-1.12139800	-0.15785400	0.19283100
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N	-2.15276100	-1.16988000	-1.22040400
N	-0.39378700	0.80323100	1.79374200
N	-1.95177800	1.55492700	-0.44764700
C	0.17660500	-2.10247700	2.14457600
C	-2.90281700	-0.62993300	-2.24209600
C	-0.68923600	-3.16314000	0.43637700
C	-2.07794800	-2.52232000	-1.48965900
C	0.30660700	0.25721800	2.83955500
C	-2.70933400	1.73567600	-1.57649400
C	-0.37849700	2.15870000	2.00418700
C	-1.71510300	2.81692900	0.04584500
C	0.50699300	-3.49538700	2.31173200
C	-3.34018100	-1.66528100	-3.14416000
C	-0.02435200	-4.15355000	1.24622000
C	-2.82383600	-2.83537500	-2.68118900
C	0.76288300	1.29012100	3.73510900
C	-2.97356100	3.13705600	-1.78935300
C	0.34152400	2.47409000	3.21231400
C	-2.35280900	3.80893100	-0.78289100
H	1.07487900	-3.89791300	3.14068000
H	-3.95218400	-1.49778000	-4.02125900
H	0.00991700	-5.21147000	1.01935300
H	-2.92728500	-3.82950000	-3.09686000
H	1.33241300	1.11406400	4.63863900
H	-3.55489000	3.53584000	-2.61081500

H	0.48885300	3.47489400	3.59749600
H	-2.31585100	4.87565200	-0.60349300
C	0.56399900	-1.09626300	3.01546200
C	-3.17308600	0.71987500	-2.40469100
C	-0.98563100	3.10419900	1.18790800
C	-1.38784200	-3.44942700	-0.72977800
H	1.13742300	-1.38562500	3.89064900
H	-3.76761800	1.01032400	-3.26545800
H	-0.88029500	4.14785700	1.46635300
H	-1.40684100	-4.48297200	-1.06105500
O	0.21375100	0.00462300	-0.70882700
S	-3.36530300	-0.78848700	1.41507100
C	-4.69645500	0.31113200	0.85389300
H	-4.85846600	0.15672400	-0.21998200
H	-5.62019300	0.05418200	1.38032000
H	-4.44385000	1.36187700	1.01658300
C	6.06207200	-1.76361700	-0.85604000
C	5.66148500	-0.46679400	-1.18502200
C	4.30640800	-0.14852500	-1.34273100
C	3.35352900	-1.16330600	-1.15977200
C	3.75221500	-2.45773300	-0.82452400
C	5.10689200	-2.76388200	-0.67304700
H	7.11957100	-1.98996300	-0.74364400
H	6.41153100	0.30859500	-1.32637000
H	2.29548700	-0.93643500	-1.26851700
H	2.99902400	-3.22851000	-0.68054200
H	5.41524800	-3.77418000	-0.41577000
C	3.87794700	1.26263900	-1.70383400
H	4.75979400	1.87495800	-1.92639200
H	3.26174500	1.24656000	-2.61018700
Cl	2.55217400	3.61459500	-1.19771200
C	3.06734400	1.94434400	-0.59012700
H	2.12240000	1.41836200	-0.43938900
C	3.81643000	2.11490000	0.72308500
H	4.09910500	1.12909400	1.10893600
H	4.72794700	2.70658400	0.58343000
H	3.18860300	2.60987700	1.46916100

R-R-IRC-2TSH

Fe	0.89418285	0.25741765	0.24253886
N	-0.10510215	1.97171865	0.59959386
N	2.17755385	1.27287465	-0.97059014
N	-0.27924715	-0.69779835	1.56618586
N	2.05542285	-1.38006935	0.08130086
C	-1.16632915	2.15025065	1.45137986
C	3.26176585	0.76142465	-1.63586414
C	0.07860885	3.17411265	-0.03464614
C	2.04254485	2.56949965	-1.40288014
C	-1.30081715	-0.16244935	2.30604686
C	3.14801085	-1.53722235	-0.73037314
C	-0.18846615	-2.01266535	1.94686886
C	1.81846185	-2.61106435	0.63941486
C	-1.65602815	3.50412965	1.36339886
C	3.84250385	1.76880265	-2.49553914
C	-0.88873415	4.13703965	0.43438386
C	3.08256085	2.88777765	-2.35496814
C	-1.89287415	-1.17105835	3.15214586
C	3.63003985	-2.89599435	-0.66372414
C	-1.20550315	-2.32485135	2.92318586
C	2.80349485	-3.56337135	0.18767086
H	-2.48588415	3.89795065	1.93596086
H	4.71191185	1.61793465	-3.12292914
H	-0.95379315	5.16144465	0.09019686
H	3.20055285	3.84833865	-2.84032114
H	-2.71625215	-0.99968635	3.83410986
H	4.48472285	-3.27450235	-1.20996314
H	-1.34545915	-3.29653035	3.37987186
H	2.83677485	-4.60394435	0.48424186
C	-1.71390115	1.16526065	2.26113986
C	3.72311785	-0.54288835	-1.51765014
C	0.77814685	-2.91045635	1.50829586
C	1.06061485	3.45173165	-0.97976214
H	-2.54672815	1.44965765	2.89660886
H	4.59067385	-0.82016435	-2.10918514
H	0.71939785	-3.92808835	1.88217086
H	1.07354085	4.45227865	-1.40148314
O	0.01413985	-0.12288535	-1.18884614
S	2.40579185	1.22880165	1.98162486

C	4.00535685	0.36472665	1.95537286
H	4.48090585	0.50191465	0.97708186
H	4.65358485	0.80548065	2.71871886
H	3.88398885	-0.70665835	2.13452486
C	-4.48611515	2.00688965	-1.62170514
C	-3.54022415	1.05107665	-1.97726714
C	-3.30659015	-0.08497435	-1.17197614
C	-4.05594315	-0.20957535	0.01703086
C	-5.01181015	0.74333165	0.36600286
C	-5.23377615	1.85550865	-0.44919614
H	-4.64824715	2.86879365	-2.26367114
H	-2.96693115	1.17103665	-2.89307714
H	-3.89171215	-1.05803435	0.67424686
H	-5.58649315	0.61599665	1.28016086
H	-5.98069115	2.59583965	-0.17558114
C	-2.29005315	-1.06564835	-1.59719214
H	-2.07255515	-1.00197635	-2.66700014
H	-1.08473415	-0.59955535	-1.18051414
Cl	-1.00374015	-3.48358835	-1.76078614
C	-2.43567015	-2.50874635	-1.14896214
H	-2.37087215	-2.59494135	-0.06192714
C	-3.71224515	-3.18067635	-1.66217514
H	-4.59080815	-2.65234435	-1.27673614
H	-3.74660915	-3.15504135	-2.75589714
H	-3.75735115	-4.22459035	-1.33722814

R-R-IRC-P

Fe	-1.32553503	-0.21967897	0.30245895
N	-0.08880146	-1.62493645	1.04611210
N	-1.94856966	-1.50229751	-1.10322375
N	-0.68188140	1.07628491	1.70142842
N	-2.62282755	1.15413671	-0.36593717
C	0.82843320	-1.46809995	2.05321802
C	-2.82165501	-1.23775369	-2.12968791
C	0.04784433	-2.91605075	0.59883864
C	-1.55264726	-2.80769180	-1.26326862
C	0.30671977	0.86221910	2.63262486
C	-3.40486598	1.06301126	-1.49337800
C	-1.18079824	2.33232489	1.95794583

C	-2.84526458	2.40721780	0.15311622
C	1.55514793	-2.69688860	2.25598745
C	-2.97811344	-2.40613255	-2.95871639
C	1.06588682	-3.59678591	1.35935105
C	-2.19835743	-3.38128859	-2.41650896
C	0.45066448	2.02175550	3.47596203
C	-4.15150403	2.28132094	-1.67522510
C	-0.47571588	2.92827243	3.06411438
C	-3.81238856	3.11034786	-0.64983394
H	2.33178682	-2.83444190	2.99757043
H	-3.61264234	-2.45698557	-3.83434675
H	1.35935741	-4.62756151	1.20687526
H	-2.05558729	-4.39906421	-2.75657417
H	1.16876218	2.10773377	4.28140562
H	-4.84177079	2.46163147	-2.48950635
H	-0.67559345	3.91694851	3.45678908
H	-4.16122067	4.11520288	-0.44959595
C	1.02888158	-0.30993968	2.79023877
C	-3.49429512	-0.04063949	-2.32734431
C	-2.19741958	2.95391495	1.25126450
C	-0.64321438	-3.48092074	-0.46220967
H	1.78757298	-0.33201666	3.56569878
H	-4.15716910	0.02843068	-3.18387327
H	-2.48167172	3.95612995	1.55544100
H	-0.42807567	-4.51602495	-0.70743852
O	-0.04295011	0.36013083	-0.84005607
S	-2.85539674	-1.03775486	1.79736742
C	-4.53031569	-0.89801789	1.08043699
H	-4.60389668	-1.44926928	0.13934437
H	-5.21935021	-1.34199179	1.80543017
H	-4.81244846	0.14431338	0.91420580
C	5.69961352	-1.57500010	0.45079660
C	4.51997383	-1.16553882	-0.15180543
C	4.45201258	0.04704935	-0.89663271
C	5.64041648	0.82560955	-0.98465880
C	6.81480277	0.40815754	-0.37466971
C	6.85808957	-0.79388672	0.34349205
H	5.72333426	-2.50656139	1.01056731
H	3.62268860	-1.77230196	-0.06057519

H	5.62913447	1.76831850	-1.52272293
H	7.70755961	1.02319519	-0.45398161
H	7.78181947	-1.11531884	0.81651380
C	3.22310885	0.40767161	-1.51173506
H	2.35123585	-0.21337213	-1.31867792
H	0.30271816	1.23412944	-0.57962263
Cl	2.31757310	3.00031710	-1.17176603
C	2.97824659	1.60636437	-2.32598496
H	3.89173882	2.06302854	-2.70660189
C	1.94723588	1.41579412	-3.42856105
H	2.33890525	0.69584486	-4.15872572
H	1.01465389	1.02011919	-3.01613461
H	1.74469798	2.35848772	-3.94446238

R-S-IRC-S

Fe	-1.21271000	0.25905000	0.04073100
N	-0.90553400	0.91605700	1.92059600
N	-2.29572200	-1.27553500	0.78672400
N	-0.44830200	1.96769700	-0.67720000
N	-1.80507200	-0.24406800	-1.81274600
C	-0.24074100	2.05925400	2.29573500
C	-2.92490700	-2.27015000	0.06877600
C	-1.16841500	0.24142700	3.08620100
C	-2.37978000	-1.66364900	2.10986700
C	0.14407600	2.97464100	0.04196500
C	-2.48292300	-1.37670000	-2.18553500
C	-0.29008600	2.31142100	-1.99650500
C	-1.45593600	0.38280100	-2.98665300
C	-0.09399600	2.10909900	3.72892100
C	-3.44555200	-3.27717200	0.95830100
C	-0.66473900	0.97667100	4.21966400
C	-3.10275900	-2.90375600	2.22076700
C	0.67780000	3.97973500	-0.84229800
C	-2.57822100	-1.45877400	-3.62183000
C	0.41170700	3.56488500	-2.11075700
C	-1.93878800	-0.36611100	-4.11936700
H	0.38954000	2.91229500	4.26987700
H	-3.99051600	-4.15643500	0.63920300

H	-0.75265400	0.65540100	5.24950500
H	-3.31169700	-3.41081900	3.15394900
H	1.18663800	4.87827200	-0.51694600
H	-3.07206500	-2.25708700	-4.16126000
H	0.65406600	4.05145700	-3.04699000
H	-1.79732600	-0.07787100	-5.15309600
C	0.23420900	3.02864300	1.42684900
C	-3.02150700	-2.31569700	-1.31288000
C	-0.75378500	1.57430500	-3.07785700
C	-1.84787300	-0.96668400	3.17965500
H	0.73748200	3.88687000	1.86141800
H	-3.53642700	-3.16558400	-1.75016200
H	-0.55214300	1.96251200	-4.07143700
H	-1.98270200	-1.38970400	4.17029200
O	0.17132200	-0.57834100	-0.03139400
S	-3.57685700	1.33850400	0.49308700
C	-4.73525800	0.84635900	-0.81522600
H	-4.86811200	-0.24204200	-0.78302800
H	-5.70593600	1.31546100	-0.63051000
H	-4.36132100	1.11899900	-1.80524400
C	6.27409000	0.89873300	0.28631100
C	5.53673200	-0.21840200	0.68348200
C	4.16883000	-0.31213900	0.40103300
C	3.55198000	0.74290400	-0.28738000
C	4.28663800	1.85929500	-0.68782300
C	5.65136000	1.94117900	-0.40177500
H	7.33576800	0.95331400	0.51426900
H	6.02797100	-1.02992700	1.21449100
H	2.48706100	0.68294600	-0.50063500
H	3.78845800	2.66782800	-1.21741200
H	6.22478500	2.81185000	-0.71056000
C	3.35413100	-1.51807100	0.81687800
H	3.83934400	-2.04724800	1.64568100
H	2.37034600	-1.18162400	1.16802200
C	3.06349400	-2.52177400	-0.30670700
H	2.72286800	-1.99166200	-1.19811400
C	2.05299700	-3.58587600	0.09589400
H	1.89615000	-4.30582100	-0.71245800
H	2.38849000	-4.13148300	0.98471400

H	1.09952800	-3.09282300	0.31733800
Cl	4.62692500	-3.34759800	-0.84447000

R-S-IRC-2TSH

Fe	1.02976110	0.16076105	0.20953133
N	0.16235210	1.95673205	0.46835833
N	2.40634010	1.00798305	-1.02739567
N	-0.22111890	-0.63330095	1.56536933
N	2.05871310	-1.57661295	0.12899033
C	-0.88017690	2.26330605	1.30753633
C	3.46198510	0.38601505	-1.64487467
C	0.44292210	3.10706605	-0.22403967
C	2.37215310	2.28695405	-1.52850167
C	-1.19626690	0.01548405	2.27539233
C	3.15278710	-1.85531395	-0.64783267
C	-0.25044890	-1.93766695	1.99124233
C	1.70719110	-2.76099395	0.72777133
C	-1.25992990	3.64574805	1.14837733
C	4.12817910	1.30400605	-2.54122667
C	-0.44511790	4.16670205	0.19105733
C	3.44783010	2.47964505	-2.47404667
C	-1.87620690	-0.90452295	3.15527833
C	3.51711410	-3.24555595	-0.51914867
C	-1.29431390	-2.12191795	2.97210633
C	2.61711910	-3.80922195	0.33383833
H	-2.05601390	4.13257605	1.69650933
H	4.99481310	1.05950605	-3.14233467
H	-0.42771790	5.17422805	-0.20469667
H	3.64253710	3.40242805	-3.00566967
H	-2.68704990	-0.63689095	3.82064433
H	4.35027810	-3.71469695	-1.02695267
H	-1.52429690	-3.06055795	3.46017733
H	2.55925010	-4.83624995	0.67141833
C	-1.50172190	1.36843705	2.16619133
C	3.82160610	-0.94215395	-1.45951367
C	0.63209410	-2.93447095	1.59088533
C	1.45173310	3.25928305	-1.16961667
H	-2.31276590	1.74738905	2.77944233
H	4.67710410	-1.30962895	-2.01850467

H	0.48159510	-3.92734195	2.00428133
H	1.54491410	4.23246405	-1.64209067
O	0.13089810	-0.24214295	-1.20392067
S	2.59958510	1.09400405	1.91557733
C	4.11957710	0.09833105	1.96777033
H	4.62222510	0.14471405	0.99442733
H	4.78928410	0.52197305	2.72211633
H	3.90414510	-0.94832195	2.19741833
C	-4.32720190	2.38519005	-1.09005867
C	-3.43629290	1.45007805	-1.60722367
C	-3.27161190	0.18422705	-1.00642767
C	-4.03514290	-0.10191595	0.14305833
C	-4.93544490	0.83119305	0.65433533
C	-5.08668790	2.07861905	0.04363233
H	-4.43853590	3.35064305	-1.57660667
H	-2.85523890	1.68963605	-2.49454467
H	-3.94364490	-1.06853195	0.62668033
H	-5.52914690	0.57875405	1.52944033
H	-5.79371690	2.80170005	0.44174733
C	-2.31383590	-0.76672295	-1.60114367
H	-2.15315690	-0.57978995	-2.66736767
H	-1.07532890	-0.43989695	-1.20159567
C	-2.38350890	-2.24199295	-1.30056567
H	-2.39647890	-2.42991295	-0.22557567
C	-1.28426090	-3.05342795	-1.97213367
H	-1.38144290	-4.11488495	-1.72823167
H	-1.33321690	-2.94135795	-3.06011567
H	-0.31043690	-2.68883795	-1.63129567
Cl	-4.03072990	-2.92797695	-1.87279967

R-S-IRC-P

Fe	1.41198700	0.14071900	0.29575500
N	0.18040500	1.47061100	1.17509900
N	2.04674300	1.55529900	-0.96862800
N	0.75646700	-1.28750700	1.55459800
N	2.69974300	-1.16786200	-0.50817000
C	-0.73948000	1.21763000	2.16040900
C	2.91710800	1.38981700	-2.01822800
C	0.05614200	2.80253600	0.86512700

C	1.66136000	2.87361000	-0.99451300
C	-0.23343500	-1.16298600	2.50076200
C	3.48321700	-0.96833400	-1.62047600
C	1.24857900	-2.56558300	1.68482800
C	2.91560000	-2.46786000	-0.11685800
C	-1.45608700	2.42507200	2.48929500
C	3.08308600	2.63556300	-2.72352000
C	-0.95762100	3.40909300	1.69137800
C	2.31223100	3.55672400	-2.08343600
C	-0.38582000	-2.40095100	3.22243000
C	4.22323500	-2.16629100	-1.92380200
C	0.53743900	-3.26623600	2.72358200
C	3.87956300	-3.09182200	-0.98662100
H	-2.23118100	2.49205600	3.24207700
H	3.71768200	2.77028400	-3.59016700
H	-1.24194400	4.45270300	1.64708600
H	2.17783700	4.60505400	-2.31757900
H	-1.10658300	-2.56376500	4.01338300
H	4.91284300	-2.26779300	-2.75208800
H	0.73122600	-4.29037900	3.01548700
H	4.22319500	-4.11355300	-0.88791400
C	-0.94934600	-0.00846200	2.77466800
C	3.58010500	0.21385500	-2.33816000
C	2.26334500	-3.11870000	0.92043500
C	0.75513600	3.46848900	-0.12982500
H	-1.70953200	-0.06033600	3.54713500
H	4.24224100	0.22737100	-3.19789700
H	2.54255000	-4.14751500	1.12301800
H	0.54946900	4.52518500	-0.26723900
O	0.12873600	-0.31541000	-0.90052600
S	2.94488400	0.78146500	1.86960900
C	4.61554000	0.73728600	1.13114500
H	4.68011700	1.39685800	0.26185200
H	5.30726000	1.09543900	1.89968200
H	4.90124900	-0.27639000	0.84028500
C	-6.04318300	1.25360400	0.91295200
C	-4.79233300	1.17001000	0.32072200
C	-4.49127300	0.16221100	-0.64070700
C	-5.51878100	-0.77641300	-0.94155800

C	-6.76605400	-0.68661600	-0.33853400
C	-7.04369200	0.32911400	0.58471000
H	-6.24635500	2.03928600	1.63636300
H	-4.01698600	1.88622100	0.58205900
H	-5.31209100	-1.59533400	-1.62061100
H	-7.53074200	-1.42000000	-0.58154000
H	-8.02339200	0.39342700	1.04999600
C	-3.19294400	0.14631500	-1.22075700
H	-2.45275800	0.81173300	-0.78415700
H	-0.19913600	-1.21844100	-0.73820600
C	-2.68571000	-0.68478400	-2.33672400
C	-3.46552600	-0.66257800	-3.64788400
H	-4.50184300	-0.98416600	-3.52806000
H	-3.47233400	0.36553800	-4.03078500
H	-2.98250400	-1.30440200	-4.39010300
H	-1.64277300	-0.42377200	-2.51018700
Cl	-2.51888900	-2.50634300	-1.78567000

S-R-IRC-S

Fe	1.21657000	-0.26442400	-0.00600200
N	0.42008000	-1.85956200	0.93492700
N	1.52285100	0.60464600	1.79315600
N	1.22824000	-1.29126700	-1.72724400
N	2.29778500	1.18892600	-0.87533200
C	-0.02076500	-3.02417500	0.35268900
C	2.09464800	1.83581100	2.02999000
C	0.05783900	-1.94490000	2.25616700
C	1.01334500	0.19245000	3.00881600
C	0.68827200	-2.53177100	-1.95389900
C	2.75423600	2.34308900	-0.29047600
C	1.65819600	-0.84530000	-2.95142500
C	2.57789300	1.31617300	-2.21625400
C	-0.66201400	-3.86519500	1.33236600
C	1.97610600	2.18398700	3.42343200
C	-0.61907100	-3.19159700	2.51372100
C	1.30186500	1.16881100	4.02739700
C	0.78856200	-2.87920900	-3.34930400
C	3.34814200	3.20910700	-1.27799700
C	1.38870600	-1.82840700	-3.97060100

C	3.23748500	2.57126400	-2.47480900
H	-1.08438900	-4.83987300	1.12439000
H	2.35519100	3.09775700	3.86295800
H	-0.99598100	-3.49808400	3.48101800
H	1.01519700	1.07402200	5.06686000
H	0.43764800	-3.80877000	-3.77870000
H	3.78650400	4.17574600	-1.06515300
H	1.63698100	-1.71358600	-5.01793000
H	3.56626200	2.90408800	-3.45099900
C	0.11584900	-3.34867600	-0.98768900
C	2.67650900	2.64294600	1.06498700
C	2.28520800	0.37091900	-3.18677200
C	0.32304400	-0.98648500	3.22578200
H	-0.27550400	-4.30761800	-1.31262300
H	3.08113900	3.59690000	1.38902700
H	2.56990000	0.59784700	-4.20952300
H	-0.02823600	-1.18355000	4.23368800
O	-0.20852300	0.46083400	-0.26088700
S	3.44031400	-1.39381800	0.85039200
C	4.83125000	-0.24481500	0.64841900
H	4.65743900	0.63872600	1.27483700
H	5.75031100	-0.73052900	0.98870600
H	4.93397200	0.08279400	-0.38909100
C	-4.31044200	-1.81145000	0.65170800
C	-3.57085700	-0.76834800	0.09389900
C	-4.19407900	0.20991000	-0.69476800
C	-5.57309700	0.11422400	-0.91567500
C	-6.31541600	-0.93002000	-0.36080500
C	-5.68627000	-1.89612300	0.42574500
H	-3.80748400	-2.56143500	1.25744600
H	-2.49774700	-0.70661700	0.26105400
H	-6.06908000	0.86704200	-1.52330900
H	-7.38571200	-0.98755100	-0.54330900
H	-6.26340000	-2.71038300	0.85711900
C	-3.37442400	1.33834200	-1.28283000
H	-2.41465900	0.93844300	-1.63416700
H	-3.88548600	1.77911900	-2.14709700
C	-3.01306400	2.45854200	-0.29867000
C	-2.00817600	3.44799700	-0.87014900

H	-1.80323400	4.25469100	-0.16049900
H	-1.07267700	2.91456200	-1.07363000
H	-2.37744500	3.89179500	-1.80125100
H	-2.63580900	2.02783100	0.63046800
Cl	-4.53534900	3.37378000	0.21177000

S-R-IRC-2TSH

Fe	-1.02805655	-0.22897507	0.23134565
N	-0.36085955	-2.12979807	0.30617265
N	-2.26887755	-0.74455707	-1.29875735
N	0.09045945	0.23231293	1.83780765
N	-1.88630555	1.59133693	0.31011065
C	0.56125445	-2.64412907	1.18258065
C	-3.15942855	0.07390993	-1.94546135
C	-0.64022755	-3.13543207	-0.58411635
C	-2.28773455	-1.93865407	-1.97728235
C	0.93052845	-0.60390407	2.52475265
C	-2.82200055	2.09464493	-0.55755235
C	0.14685945	1.43847693	2.48959765
C	-1.55118955	2.62645893	1.14867465
C	0.85629045	-4.01655607	0.84946565
C	-3.77179155	-0.62793107	-3.05155035
C	0.11584445	-4.31900707	-0.25149035
C	-3.22727455	-1.87390407	-3.07355535
C	1.55421845	0.09755793	3.62249365
C	-3.10142455	3.47477593	-0.24474235
C	1.07095345	1.36998093	3.59727765
C	-2.31225455	3.80509093	0.81554565
H	1.54997745	-4.64684007	1.39095565
H	-4.51375955	-0.20408107	-3.71641435
H	0.07172545	-5.25152007	-0.79957335
H	-3.43146555	-2.68691007	-3.75865735
H	2.25843945	-0.34367307	4.31640965
H	-3.80766855	4.09745993	-0.77919335
H	1.29525145	2.19116193	4.26615365
H	-2.23670355	4.75453193	1.33022565
C	1.15213045	-1.94395807	2.22513265
C	-3.42527155	1.39180093	-1.59794335
C	-0.60779655	2.55979693	2.16642965

C	-1.52394955	-3.04947407	-1.65417735
H	1.85788645	-2.48326307	2.84923965
H	-4.15212755	1.92862793	-2.20040235
H	-0.45444355	3.45390493	2.76332065
H	-1.63601855	-3.93149207	-2.27734235
O	0.11366345	0.23919193	-0.97250835
S	-2.89169055	-1.23253907	1.55654065
C	-4.31819955	-0.10583307	1.56022565
H	-4.66726455	0.04546893	0.53199865
H	-5.12694455	-0.56562807	2.13580465
H	-4.05713655	0.86738693	1.98387065
C	4.56264345	-1.67225107	-1.74229435
C	3.65068245	-0.62092007	-1.75082635
C	3.38538545	0.11726693	-0.57966235
C	4.05767845	-0.25382407	0.60115565
C	4.97386745	-1.30368407	0.60845865
C	5.23191045	-2.01783207	-0.56383535
H	4.75323345	-2.22600207	-2.65788135
H	3.13125945	-0.37479107	-2.67241735
H	3.86437145	0.30377993	1.51368865
H	5.49249345	-1.56078707	1.52870165
H	5.94700845	-2.83616107	-0.56107135
C	2.41419945	1.22932493	-0.55506935
H	1.20356645	0.66566693	-0.65174935
H	2.36047845	1.73132893	0.41436765
C	2.37455145	2.21452993	-1.69810835
C	1.22117945	3.20436093	-1.63171835
H	1.27684745	3.92052493	-2.45615435
H	0.27917145	2.65061693	-1.69622335
H	1.23690645	3.75885093	-0.68773935
H	2.38435445	1.70403293	-2.66203735
Cl	3.97651345	3.18147593	-1.71426635

S-R-IRC-P

Fe	-1.37610100	-0.18874100	0.14556400
N	-1.93069500	-1.80507800	-0.91798900
N	-2.47528700	0.98649500	-1.04428700
N	-0.23770300	-1.36604700	1.32315200

N	-0.90237300	1.39525800	1.28206800
C	-1.48639200	-3.09284500	-0.76068500
C	-2.58170000	2.35387300	-0.98366600
C	-2.77728100	-1.82101400	-1.99844700
C	-3.24183800	0.58988200	-2.11215800
C	-0.04693700	-2.72268600	1.19654900
C	-1.21391900	2.71028800	1.02680900
C	0.41853100	-0.99585800	2.47474400
C	-0.11973200	1.40183900	2.41264200
C	-2.08234900	-3.94749800	-1.75786200
C	-3.43484400	2.83138500	-2.04324900
C	-2.88691700	-3.16031700	-2.52101000
C	-3.84916200	1.73746200	-2.73799000
C	0.77488100	-3.20918700	2.27469400
C	-0.63029300	3.56063700	2.03185900
C	1.05640200	-2.14179600	3.07134100
C	0.04152800	2.74947700	2.89507200
H	-1.89486500	-5.00995800	-1.84614000
H	-3.67794600	3.87245200	-2.21337300
H	-3.49679800	-3.43905100	-3.37072500
H	-4.50130300	1.69193800	-3.60075900
H	1.07267000	-4.24239800	2.39957300
H	-0.73094400	4.63816800	2.05782800
H	1.63495800	-2.11486500	3.98605700
H	0.61066600	3.02253900	3.77446400
C	-0.60374000	-3.52911300	0.21613400
C	-1.98848800	3.16679000	-0.02887900
C	0.47765900	0.28982000	2.98991000
C	-3.40439200	-0.71525100	-2.55057400
H	-0.35299400	-4.58472800	0.23193100
H	-2.15621600	4.23635900	-0.10367700
H	1.04974200	0.44227100	3.89948000
H	-4.04568800	-0.87938800	-3.41048100
O	0.03546200	0.10378600	-0.95220500
S	-3.20219400	-0.67266500	1.43796800
C	-3.85770400	0.86787200	2.17136100
H	-4.14117800	1.58346100	1.39516300
H	-4.75142200	0.58844700	2.73757500
H	-3.13787200	1.33191600	2.84953400

C	5.51513200	-1.78766000	-1.72018500
C	4.86118000	-0.56907700	-1.61078300
C	4.07166800	-0.26339300	-0.46612300
C	3.99077700	-1.25262700	0.55554700
C	4.64344200	-2.46951900	0.43285000
C	5.41104300	-2.74834400	-0.70559600
H	6.11677000	-1.99485700	-2.60128000
H	4.97132400	0.16710300	-2.40031000
H	3.39516000	-1.04322200	1.44033900
H	4.55725300	-3.20795700	1.22558200
H	5.92492700	-3.70082100	-0.80003600
C	3.37047200	0.96214100	-0.30615400
H	0.86521100	-0.20258700	-0.54537900
H	2.87997700	1.14188800	0.64902500
C	3.31020500	2.06143400	-1.28690300
C	2.05549400	2.91442000	-1.19264000
H	2.08720800	3.73531500	-1.91426900
H	1.18392700	2.28157500	-1.39803900
H	1.94635800	3.33594200	-0.18814200
H	3.46838700	1.71282400	-2.30778700
Cl	4.81875200	3.19859000	-1.02476000

S-S-IRC-S

Fe	-1.23649700	-0.17142500	0.14785700
N	-0.46420900	-1.79115300	1.06654900
N	-1.21638400	-1.19094600	-1.59731000
N	-1.57368600	0.67522400	1.93300200
N	-2.29312100	1.29131400	-0.73591300
C	-0.20964900	-1.93267800	2.41022500
C	-1.63894200	-0.73388200	-2.82699800
C	0.06305600	-2.90882600	0.46929500
C	-0.58573700	-2.39411800	-1.84630300
C	-1.18007600	0.20329600	3.15950100
C	-2.56146700	1.42511700	-2.07488400
C	-2.12465500	1.90896800	2.17061700
C	-2.74042900	2.45277500	-0.14969400
C	0.48123900	-3.17246300	2.66337700
C	-1.30156700	-1.68268500	-3.85770900
C	0.65578800	-3.77611000	1.45667100

C	-0.64477500	-2.70738500	-3.25050800
C	-1.49926400	1.15589700	4.19341600
C	-3.20490900	2.68800700	-2.33728400
C	-2.08354900	2.21861800	3.57767200
C	-3.31498300	3.32700600	-1.14120900
H	0.78536100	-3.51825900	3.64299500
H	-1.53474800	-1.55848800	-4.90749900
H	1.13006900	-4.72392800	1.23679500
H	-0.22902800	-3.60124000	-3.69759100
H	-1.29297500	1.01325400	5.24652000
H	-3.52276000	3.02530000	-3.31563500
H	-2.46044900	3.13271400	4.01841200
H	-3.74240700	4.29906600	-0.93082700
C	-0.55485400	-1.01515600	3.38960400
C	-2.27312700	0.47831400	-3.05137000
C	-2.66766100	2.74437000	1.20330500
C	0.01842100	-3.19052500	-0.89013000
H	-0.29750700	-1.25822500	4.41588400
H	-2.54373800	0.71861900	-4.07488200
H	-3.06703600	3.69848400	1.53279100
H	0.48501200	-4.11104300	-1.22605900
O	0.19907800	0.53678500	-0.09574000
S	-3.41514800	-1.65348900	0.27461800
C	-4.71326000	-0.92888900	-0.76713500
H	-4.38051600	-0.94270600	-1.81247900
H	-5.61832900	-1.53784200	-0.68803100
H	-4.92319900	0.10594800	-0.48551900
C	6.24388700	-1.09114500	-0.54466400
C	5.50313200	-0.02343700	-1.05521000
C	4.15031100	0.13112300	-0.72982500
C	3.55162700	-0.81245400	0.11793500
C	4.29001600	-1.87864300	0.63199300
C	5.63970400	-2.02194100	0.30185800
H	7.29370000	-1.19436800	-0.80822200
H	5.98025100	0.70194200	-1.70950900
H	2.49778100	-0.70582700	0.36556000
H	3.80623500	-2.60031800	1.28590500
H	6.21581700	-2.85398800	0.69929700
C	3.33262400	1.28630900	-1.26619000

H	3.78472800	1.69113000	-2.17951300
H	2.32905900	0.92484000	-1.52429900
C	3.10883200	2.43594400	-0.27480000
H	2.80377000	2.03583700	0.69389600
C	2.09468500	3.45667300	-0.76981700
H	1.98699200	4.28094600	-0.05893100
H	2.39419600	3.87197900	-1.73836900
H	1.12478600	2.95787100	-0.87851900
Cl	4.70699500	3.29549100	0.07593200

S-S-IRC-2TSH

Fe	-0.94519100	-0.26569300	0.26309200
N	0.30400900	-1.06413900	1.63176900
N	-0.95936100	-2.02627100	-0.75244600
N	-1.08791000	1.39397300	1.38848600
N	-2.36029900	0.44209100	-0.99419600
C	0.72897400	-0.49520900	2.80857500
C	-1.64574400	-2.31358700	-1.90519400
C	0.91257800	-2.29099300	1.56333800
C	-0.14456600	-3.10835300	-0.51444100
C	-0.47872800	1.64687600	2.59040900
C	-2.84965400	-0.16517200	-2.11787900
C	-1.83766900	2.50617200	1.10506100
C	-2.90399600	1.70061000	-0.97577500
C	1.62677600	-1.38830100	3.50011700
C	-1.27820800	-3.62410000	-2.39183500
C	1.74729700	-2.49981300	2.72188500
C	-0.34368700	-4.11308200	-1.53345200
C	-0.84009900	2.95817200	3.07200000
C	-3.74362500	0.72529000	-2.82212900
C	-1.68151300	3.49499400	2.14548400
C	-3.77629100	1.88589800	-2.11285400
H	2.09282000	-1.17841300	4.45460600
H	-1.68306800	-4.08686600	-3.28292300
H	2.33213700	-3.39193900	2.90655600
H	0.17558800	-5.06223000	-1.57157000
H	-0.49176900	3.39353900	4.00003300
H	-4.26328400	0.47964700	-3.73957400
H	-2.16763000	4.46232200	2.15541600

H	-4.32844200	2.79233200	-2.32617700
C	0.36213200	0.76500800	3.26243000
C	-2.53689300	-1.45589800	-2.53664900
C	-2.66759800	2.66059200	-0.00132700
C	0.73300800	-3.22911600	0.55073200
H	0.76982500	1.09141700	4.21459000
H	-3.00368500	-1.80797000	-3.45176000
H	-3.18632300	3.60930400	-0.10247800
H	1.30651000	-4.14836400	0.62086400
O	0.27455700	0.28725700	-0.82352500
S	-2.64677000	-1.53027700	1.59297500
C	-4.20269700	-1.64185200	0.65966500
H	-4.03337500	-2.20318500	-0.26700600
H	-4.93555400	-2.18577500	1.26305000
H	-4.58486100	-0.65126300	0.40048400
C	5.17458400	-0.45889900	-2.01747200
C	4.15301100	0.45520500	-1.76771400
C	3.52144400	0.50622800	-0.50728200
C	3.94837900	-0.40796100	0.47934000
C	4.96689300	-1.32176900	0.22614900
C	5.58877700	-1.35155100	-1.02544800
H	5.64862100	-0.47588600	-2.99557100
H	3.83519800	1.12868600	-2.55575300
H	3.47358800	-0.39091400	1.45649200
H	5.28016300	-2.00875200	1.00837600
H	6.38612400	-2.06247600	-1.22554400
C	2.44038800	1.45781700	-0.18189900
H	1.27564600	0.84350500	-0.47075600
H	2.29275200	1.55492100	0.89819400
C	2.41068500	2.82705400	-0.83990100
H	3.43415300	3.18756100	-0.98459700
C	1.59671700	3.85132000	-0.06019800
H	1.60691000	4.82167800	-0.56442100
H	0.56028100	3.52165400	0.04627200
H	2.02657100	3.97587900	0.94154300
Cl	1.74992900	2.77723100	-2.57210800

S-S-IRC-P

Fe	-1.37692400	0.05010000	0.16277700

N	-1.41820100	-1.47819100	1.47387000
N	-2.05797300	-1.17342200	-1.30309000
N	-0.82910600	1.27999100	1.63676700
N	-1.42030300	1.57299500	-1.14307400
C	-1.13626500	-1.43757600	2.81638500
C	-2.34830200	-0.85214700	-2.60911600
C	-1.66543000	-2.79470700	1.18561500
C	-2.22823400	-2.53806100	-1.20709700
C	-0.62839100	0.97184900	2.95626200
C	-1.77422600	1.54559700	-2.47053100
C	-0.52303200	2.61086000	1.51485000
C	-1.02726400	2.86616600	-0.89253700
C	-1.21690200	-2.75953800	3.39100300
C	-2.73882200	-2.03109800	-3.34219400
C	-1.53626700	-3.60451400	2.37520900
C	-2.65631200	-3.07606200	-2.47467300
C	-0.19374600	2.13633700	3.68853800
C	-1.60660700	2.84731700	-3.06640700
C	-0.12223400	3.15571300	2.79014300
C	-1.13859100	3.66750100	-2.08588800
H	-1.04073800	-2.99145700	4.43356400
H	-3.02146100	-2.04212100	-4.38716000
H	-1.68218800	-4.67666400	2.40946400
H	-2.86259000	-4.12252500	-2.65999800
H	0.02794600	2.15197200	4.74798500
H	-1.81705300	3.08409000	-4.10152900
H	0.16763500	4.18522000	2.95767000
H	-0.88539400	4.71805800	-2.14897500
C	-0.79203400	-0.29100500	3.51710100
C	-2.22880400	0.42055400	-3.15317800
C	-0.60693600	3.34987700	0.34036400
C	-2.02743400	-3.29216300	-0.06141400
H	-0.59884500	-0.39304100	4.58074300
H	-2.47510500	0.54067200	-4.20392900
H	-0.33173400	4.39900600	0.39320500
H	-2.19271600	-4.36263500	-0.13846200
O	0.33861100	-0.35889500	-0.25686300
S	-3.71912400	0.15958800	0.66834900
C	-4.58121200	1.14778800	-0.58932200

H	-4.48932000	0.66440500	-1.56912700
H	-5.64095000	1.19850200	-0.32482800
H	-4.16098700	2.15431700	-0.66050500
C	6.01588900	-2.48532200	-0.80168200
C	5.55275700	-1.21900900	-0.47293600
C	4.16753000	-0.98452600	-0.24665700
C	3.27953600	-2.09107900	-0.38212800
C	3.75669600	-3.35198200	-0.70800600
C	5.12642000	-3.56155100	-0.91803200
H	7.07800200	-2.63994900	-0.97473900
H	6.25733700	-0.39547200	-0.40807600
H	2.21720800	-1.92004300	-0.22279400
H	3.06084600	-4.18197900	-0.80280900
H	5.49685000	-4.55037300	-1.17485500
C	3.62827800	0.28162400	0.11010800
H	0.48716500	-0.19748700	-1.20429900
H	2.54414000	0.35721900	0.18190400
C	4.40152500	1.50955200	0.34082500
H	5.43522300	1.31342500	0.62760200
C	3.74310200	2.49149900	1.29799500
H	4.32672000	3.41235400	1.38279200
H	2.73253700	2.74262800	0.96231800
H	3.66699100	2.03036400	2.29070100
Cl	4.64756200	2.43151100	-1.32727300