Development of Enantiospecific Coupling of Secondary and Tertiary Boronic Esters with Aromatic Compounds

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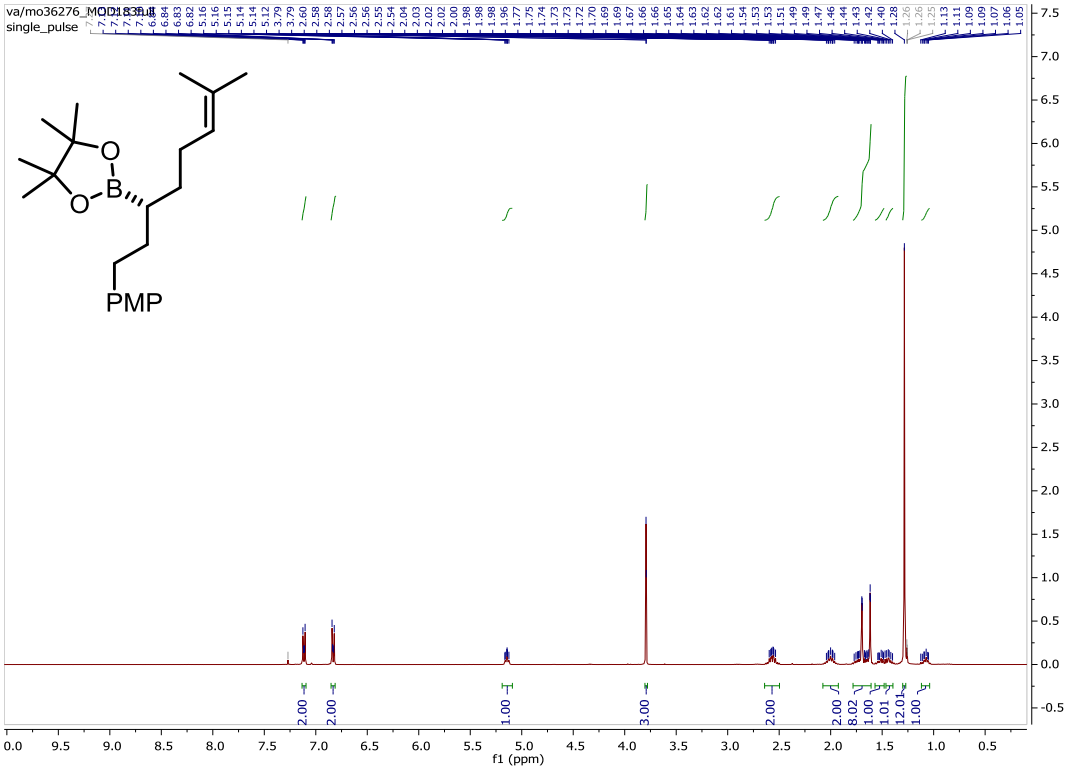
Supporting Material II

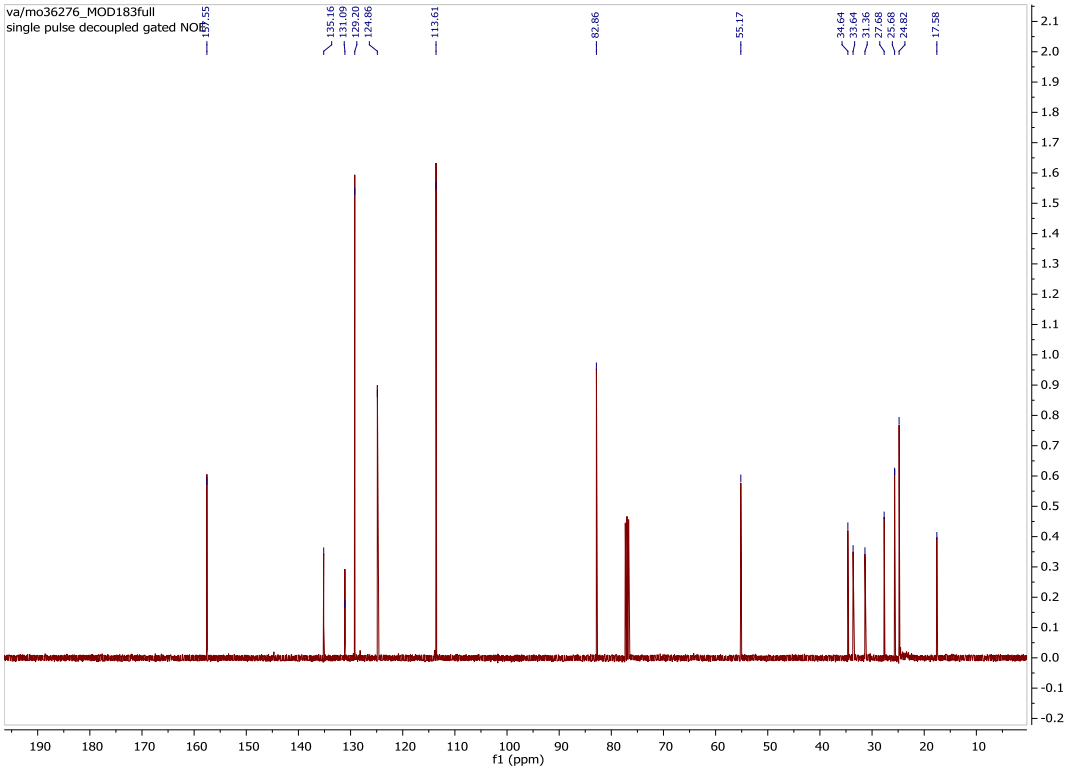
NMR spectra, GC, SFC & HPLC chromatograms

1e

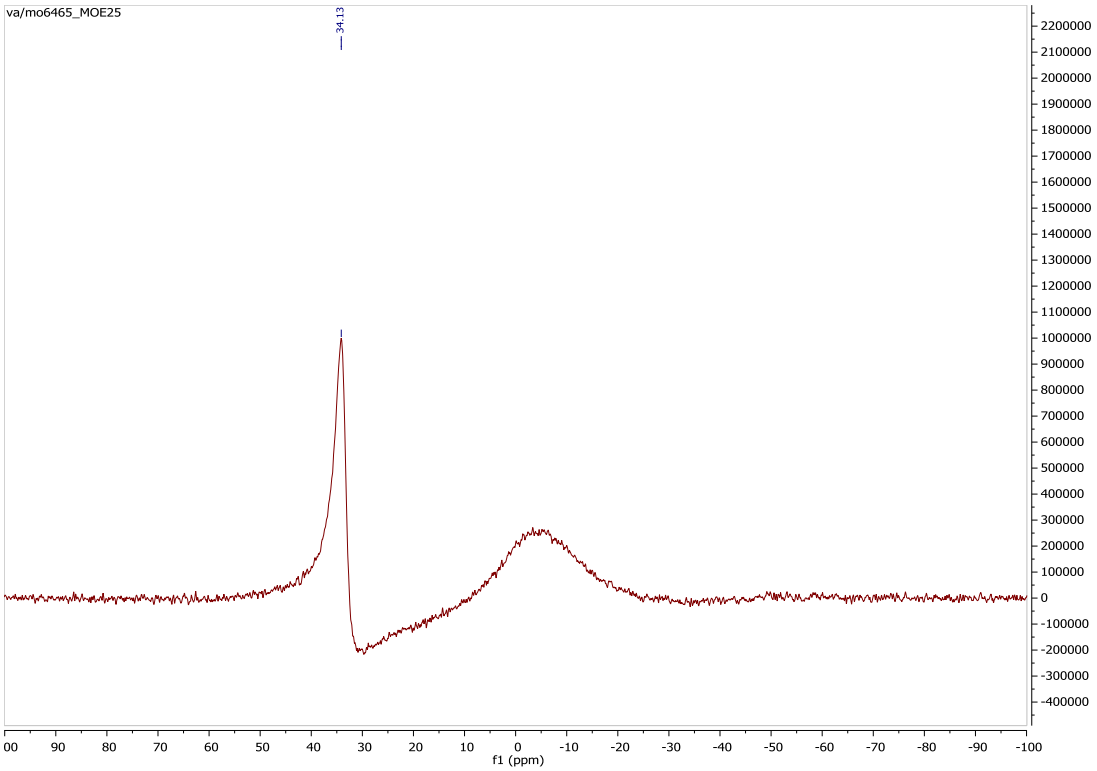
^{1}H NMR (400 MHz, $CDCl_3$)



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

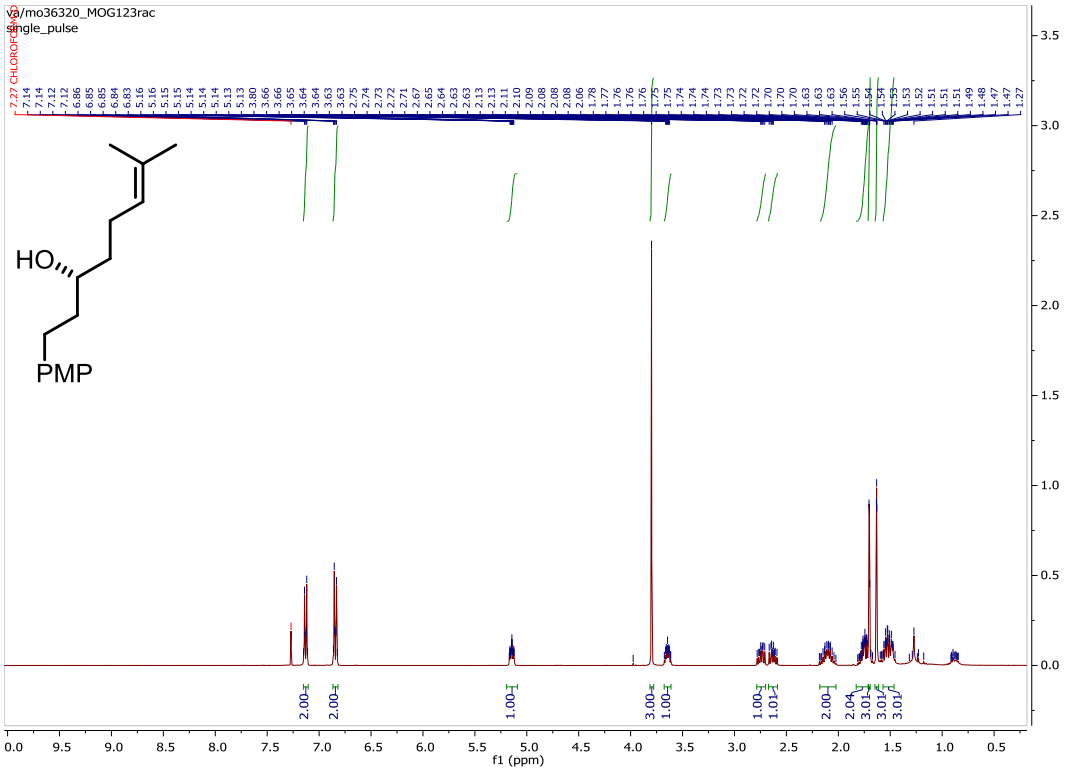


^{11}B NMR (96 MHz, NONE)[1]



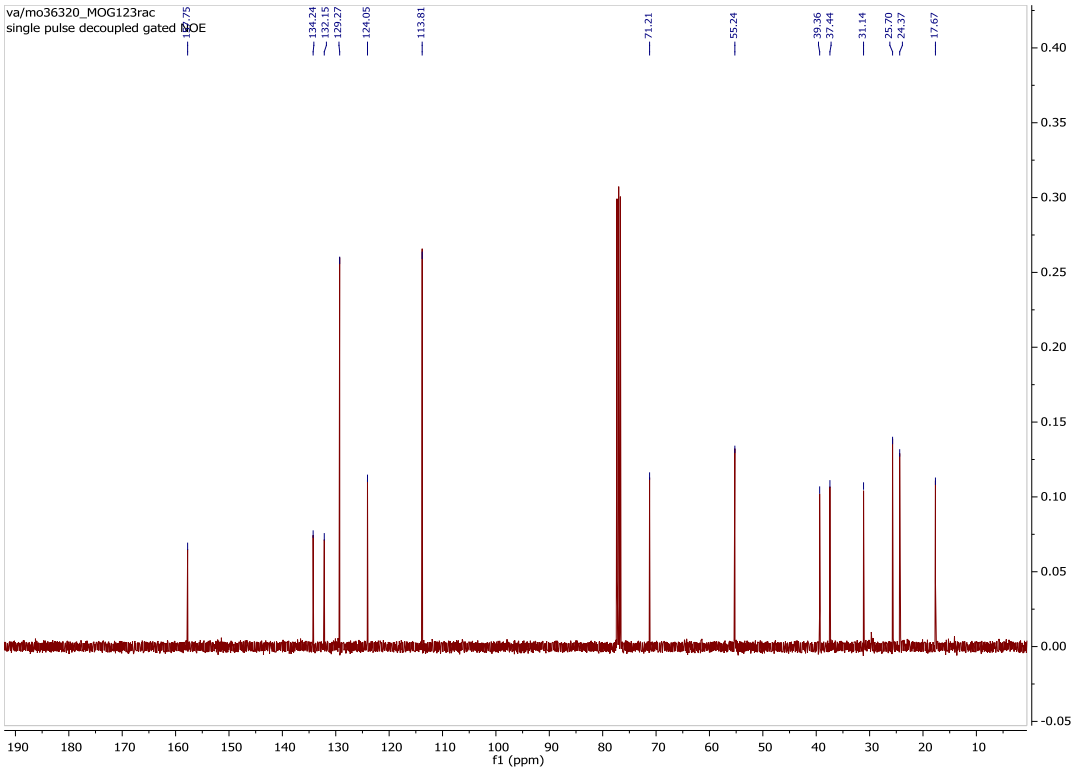
1f-oxidised

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

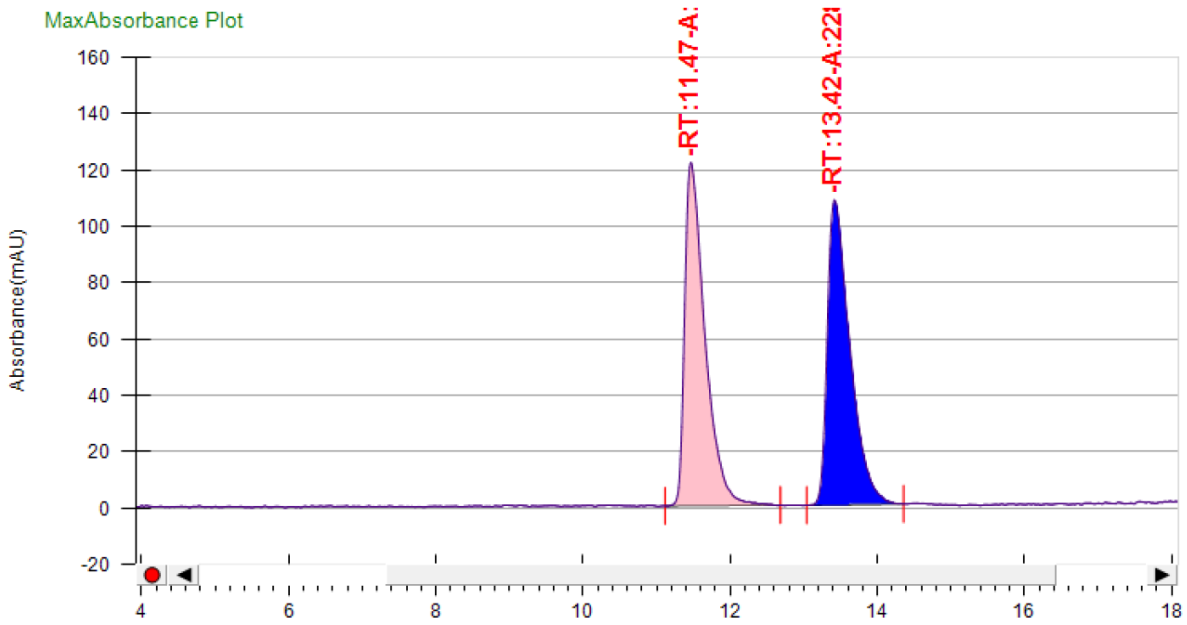


[1] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

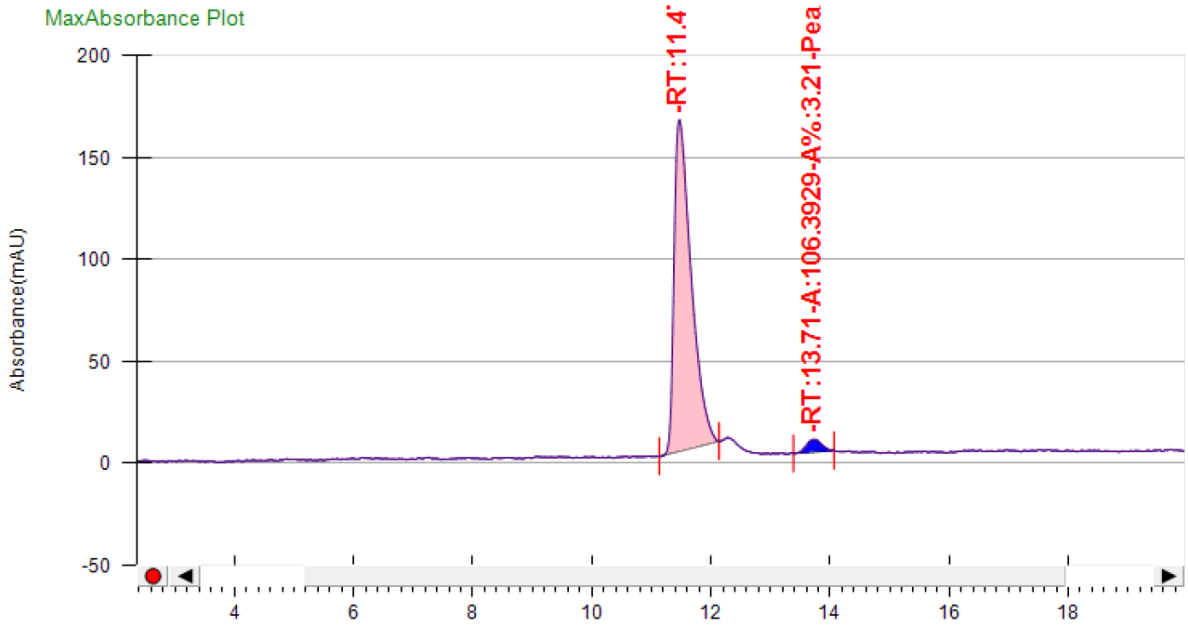
^{13}C-NMR (100 MHz, $CDCl_3$)



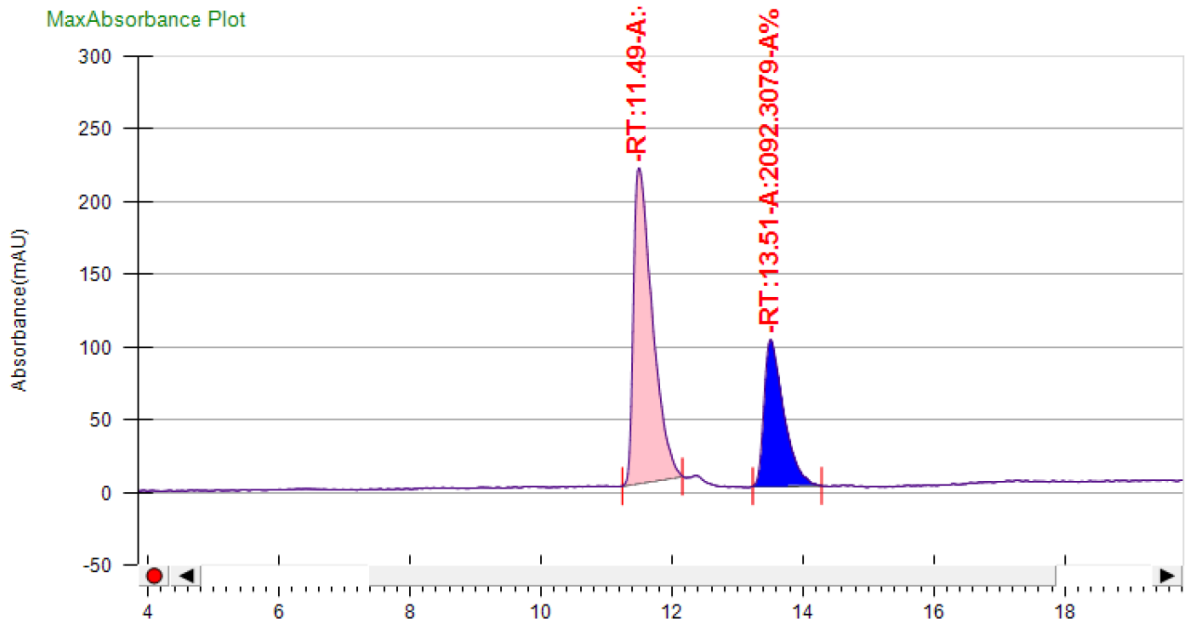
Chiral SFC traces: racemic



Chiral SFC traces: enantioenriched

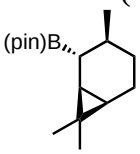


Chiral SFC traces: racemic + enantioenriched

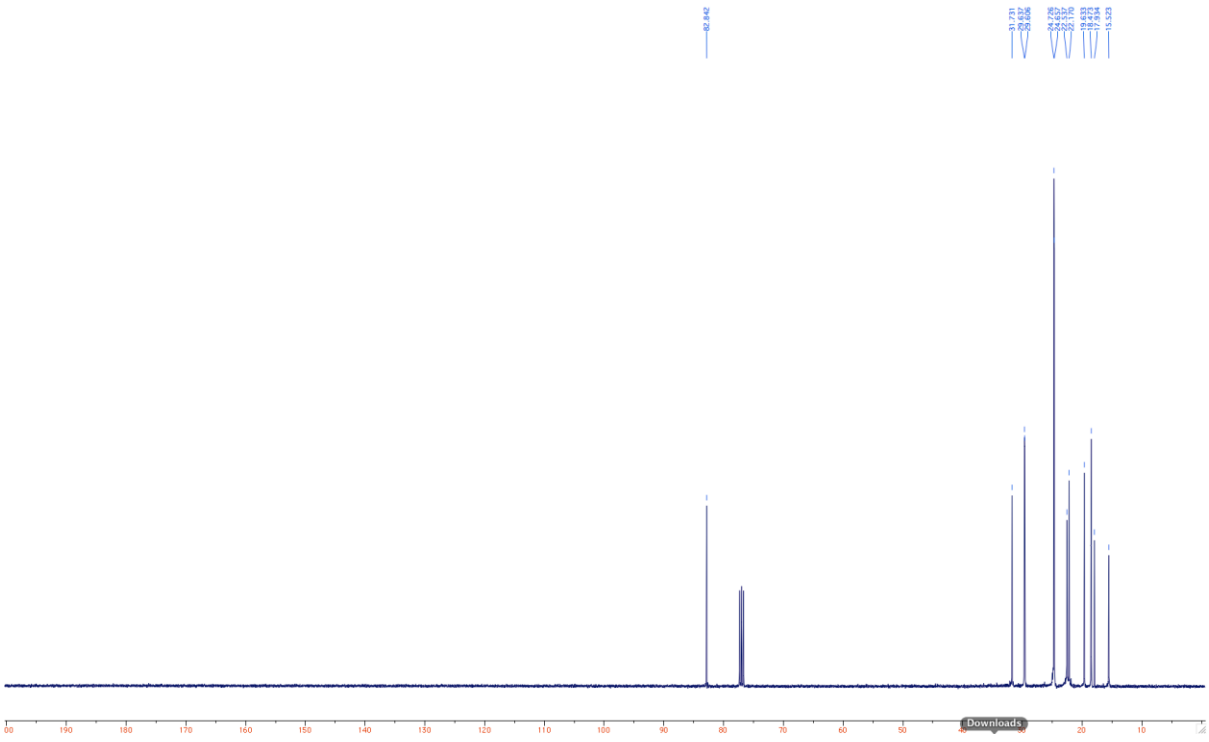


1m

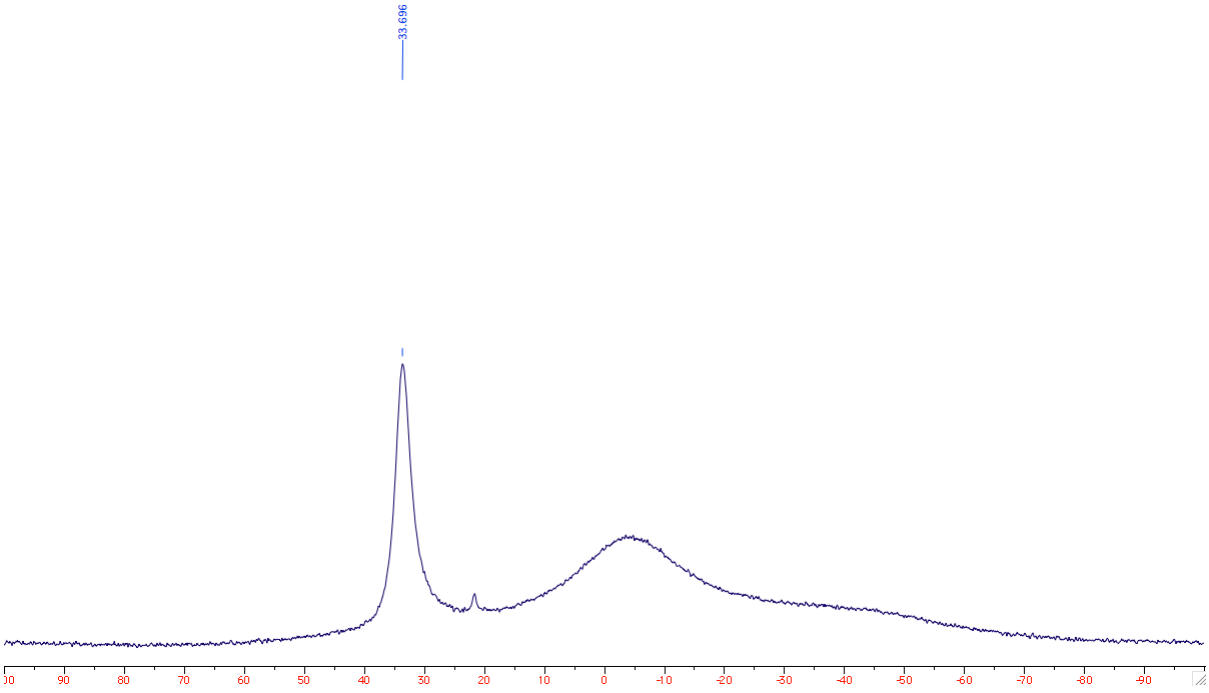
^{1}H NMR (400 MHz, $CDCl_3$)



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



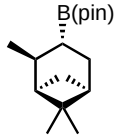
^{11}B NMR (96 MHz, $CDCl_3$)[2]



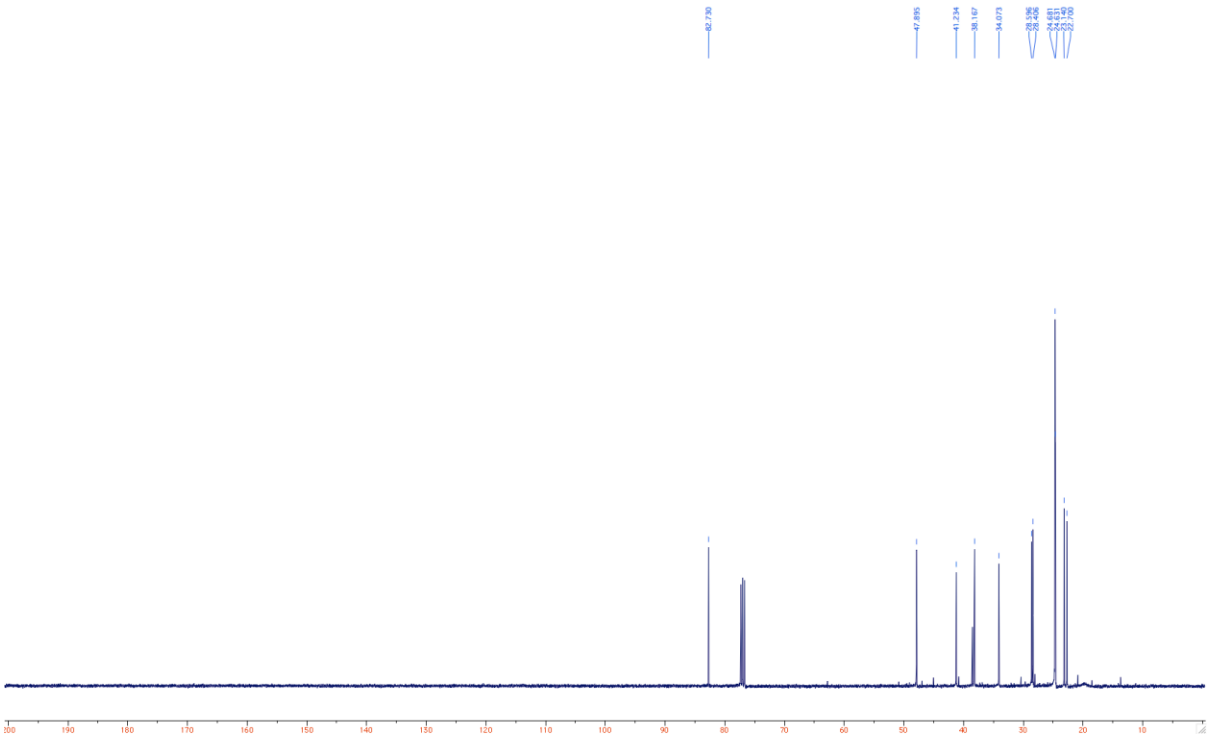
[2] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

1n

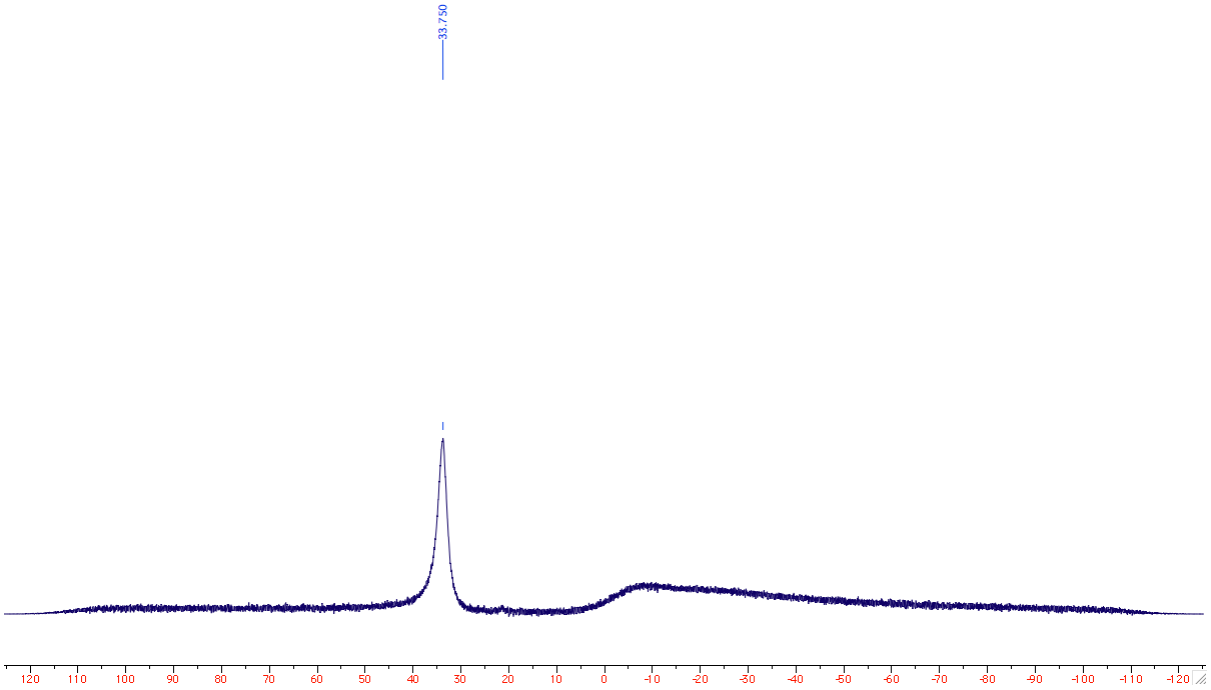
^{1}H NMR (400 MHz, $CDCl_3$)



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



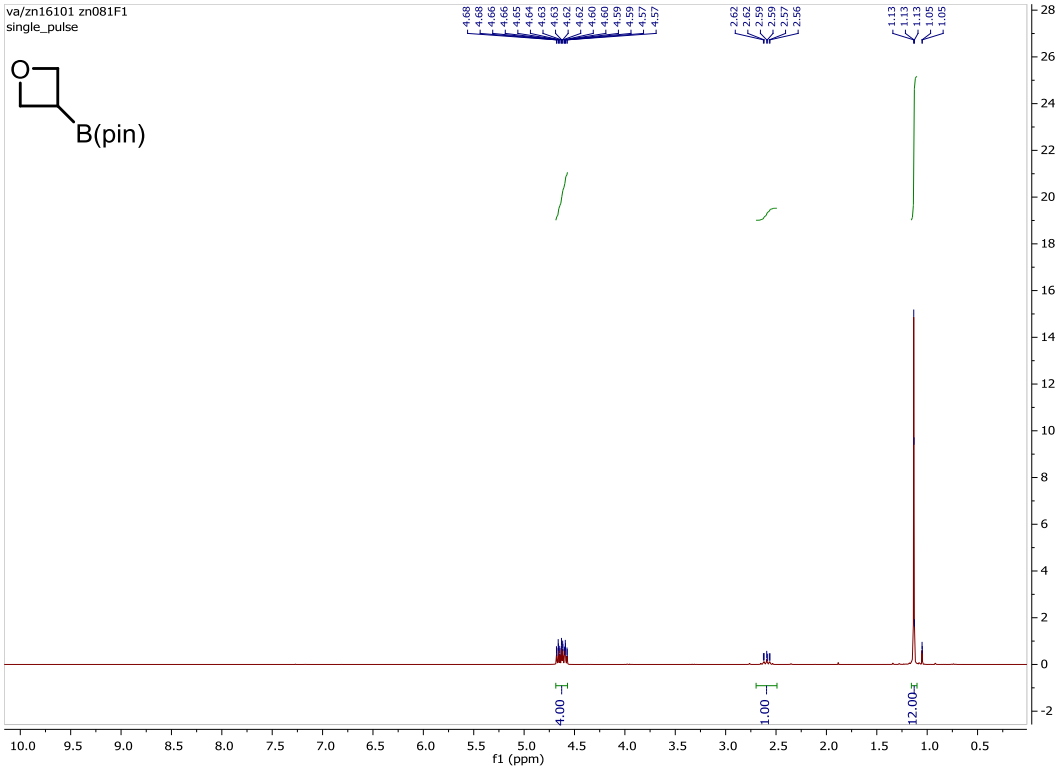
^{11}B NMR (96 MHz, $CDCl_3$)[3]



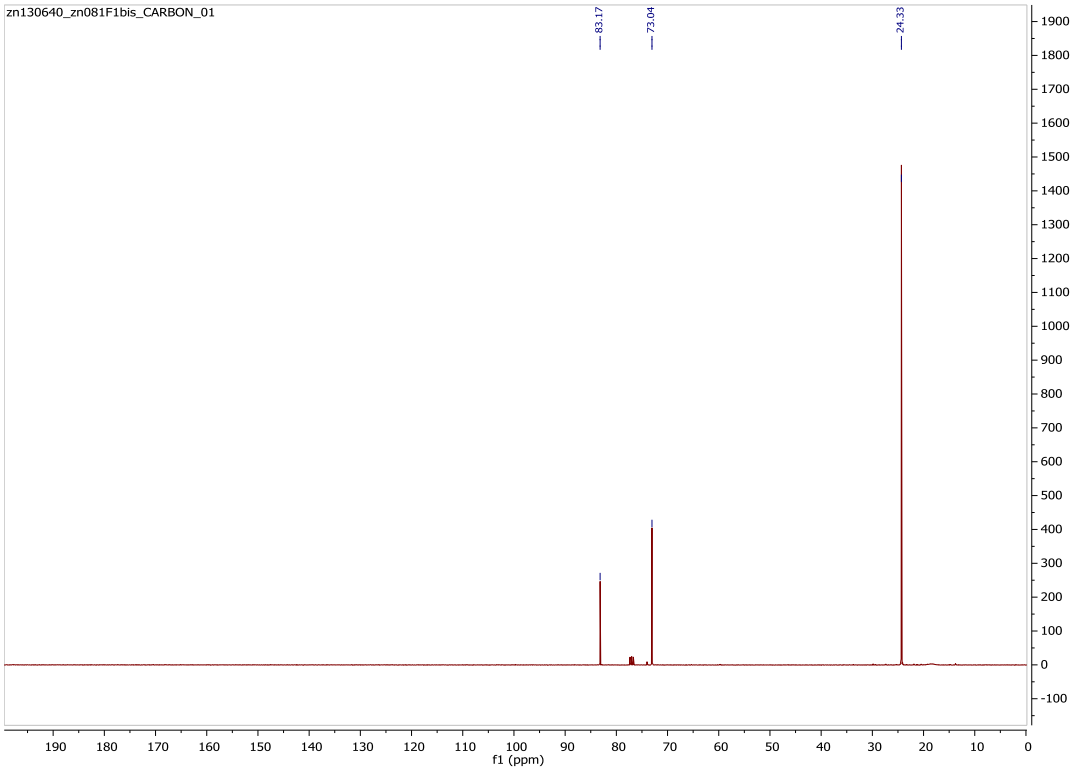
[3] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

1r

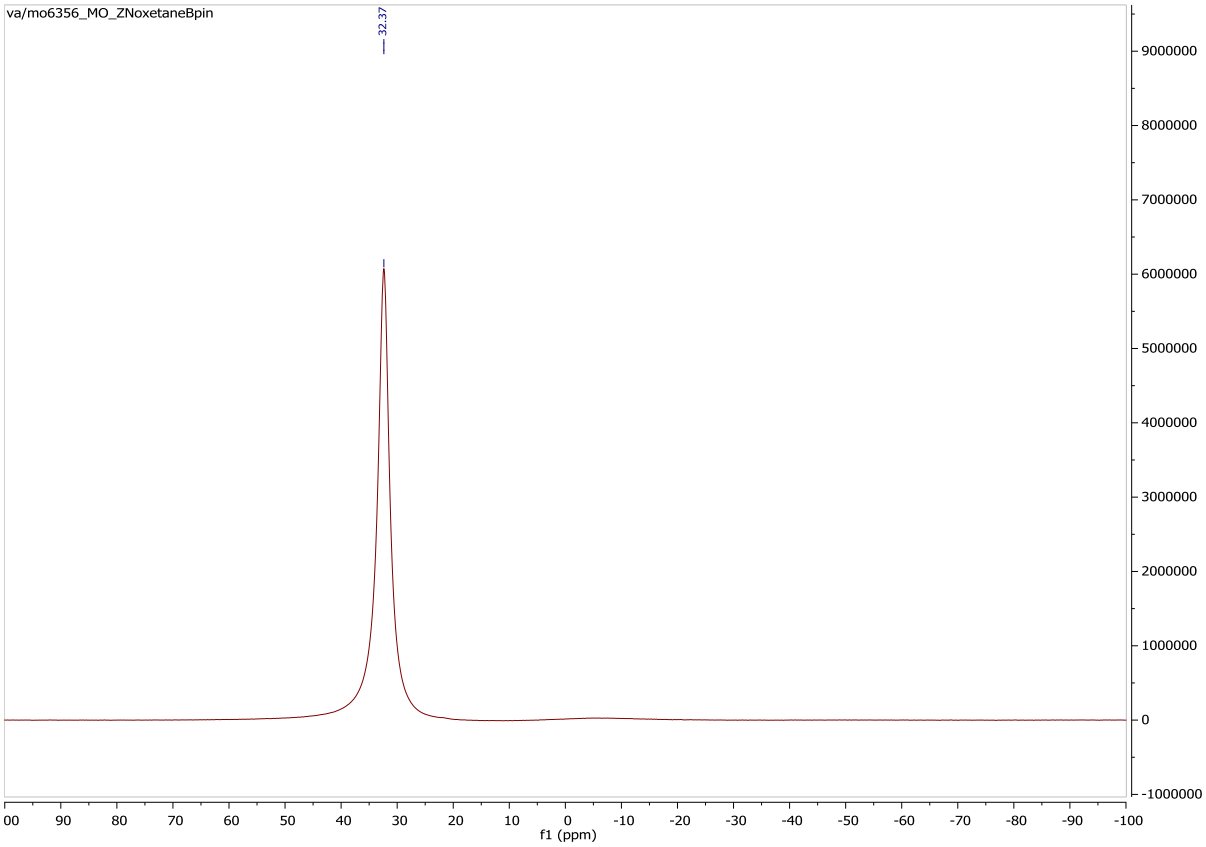
^{1}H NMR (400 MHz, $CDCl_3$)



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

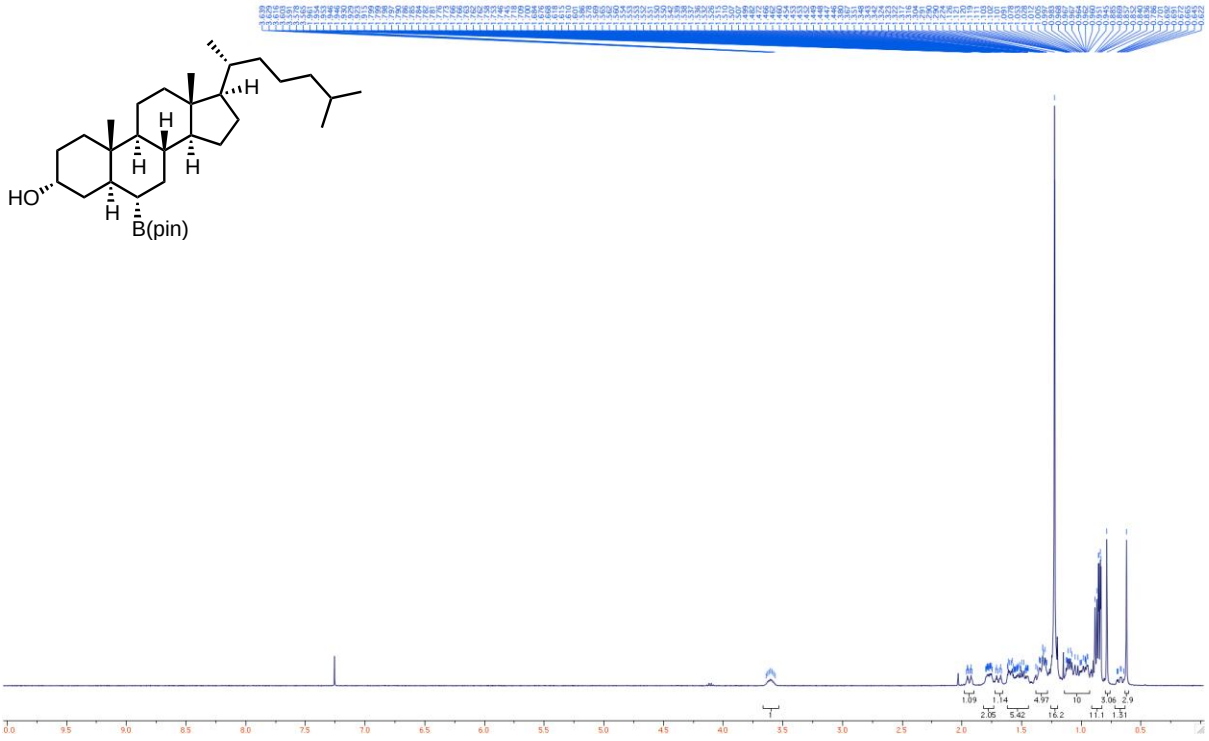


^{11}B NMR (96 MHz, NONE)

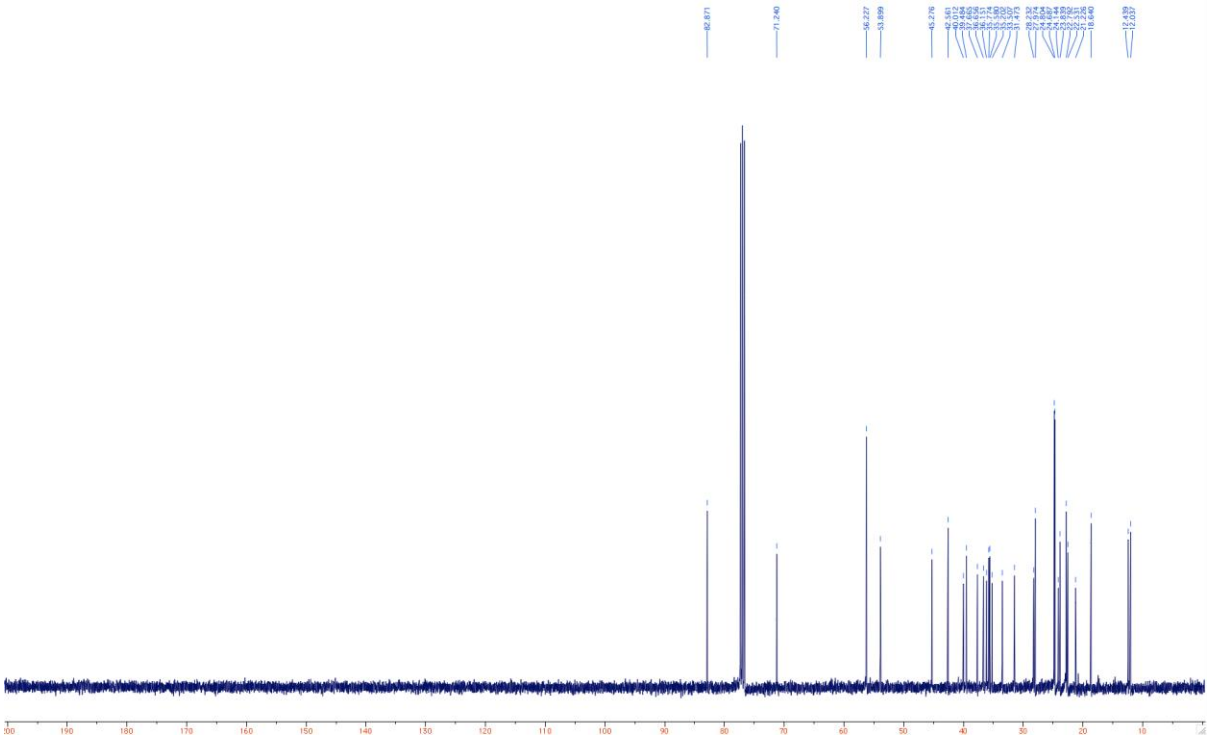


1o

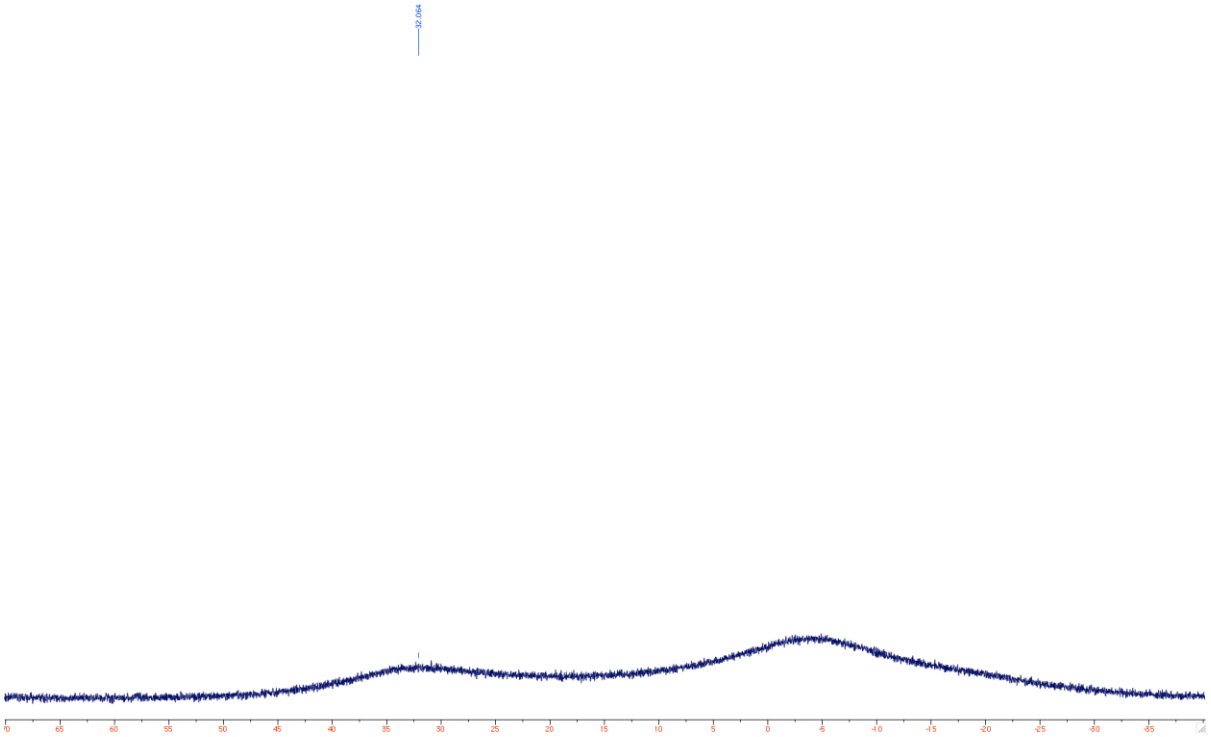
^{1}H NMR (400 MHz, $CDCl_3$)



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



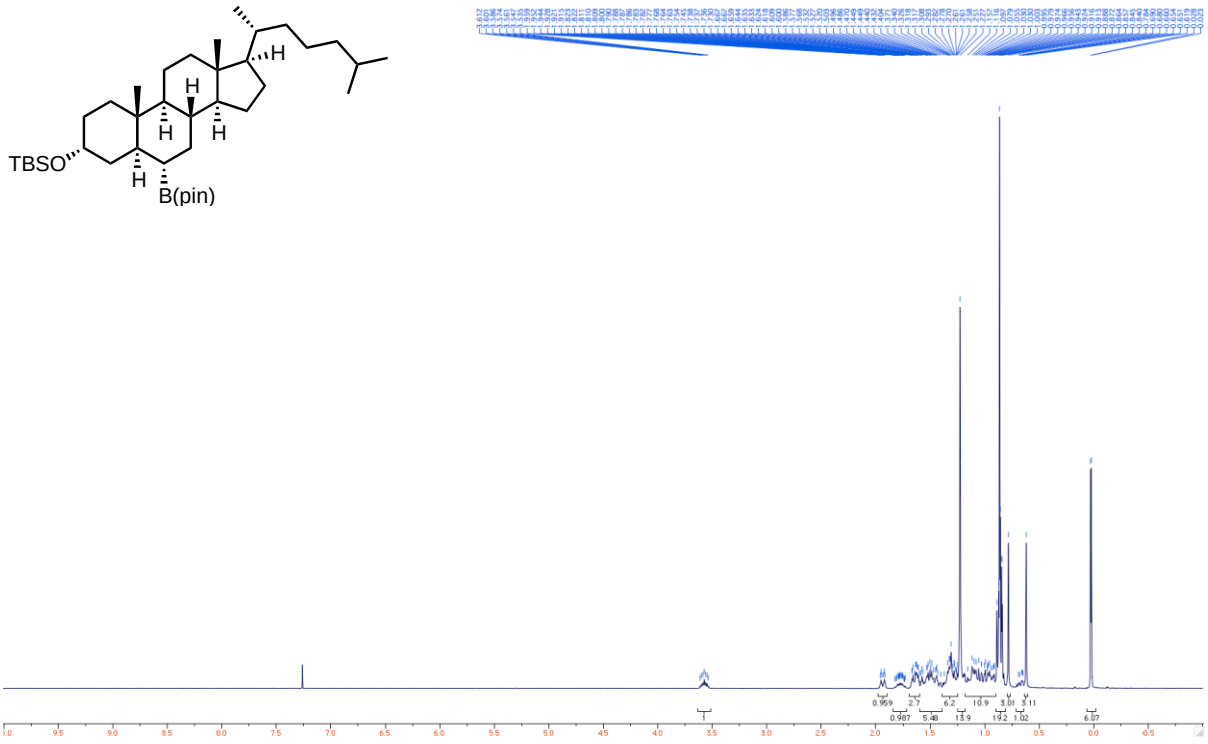
^{11}B NMR (96 MHz, $CDCl_3$)[4]



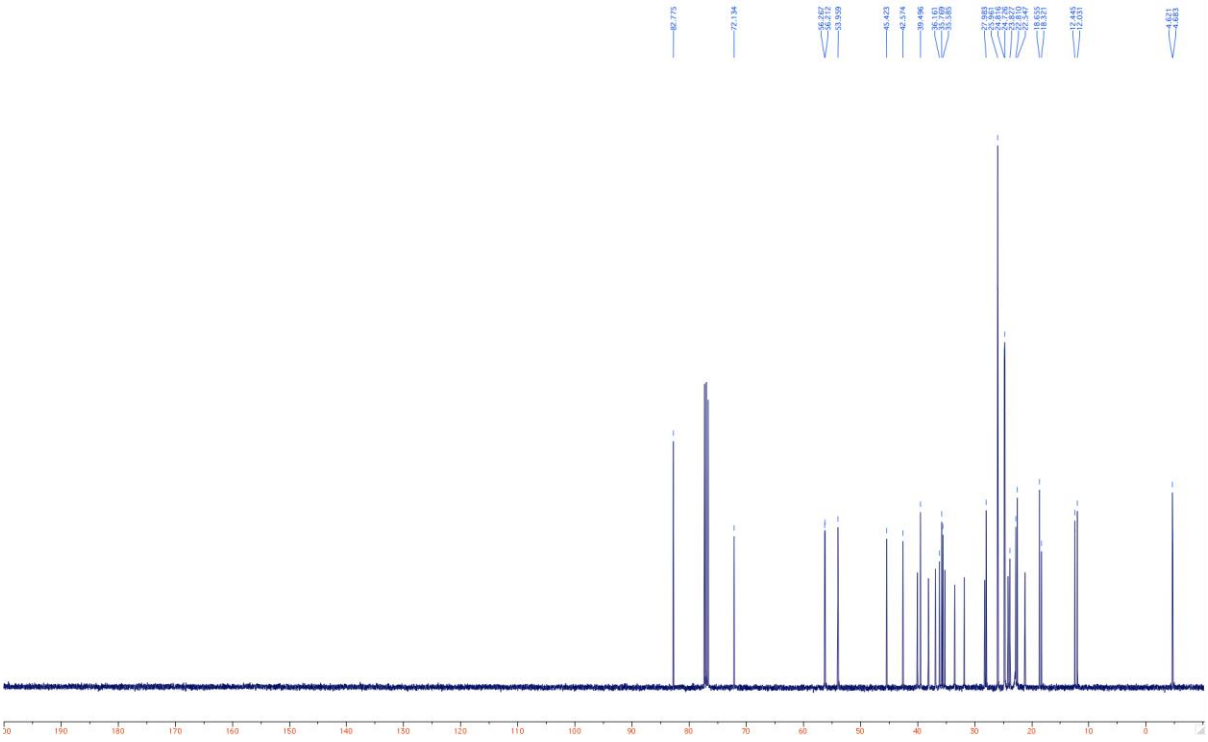
[4] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

1p

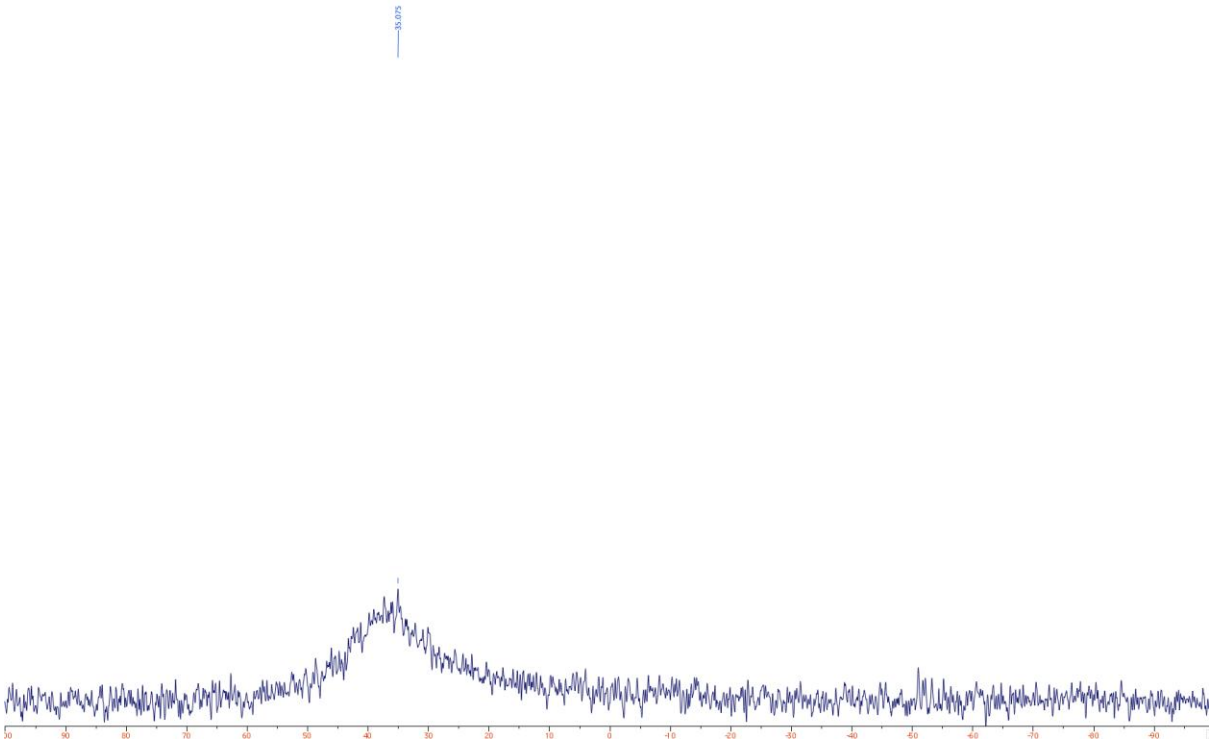
^{1}H NMR (400 MHz, $CDCl_3$)



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



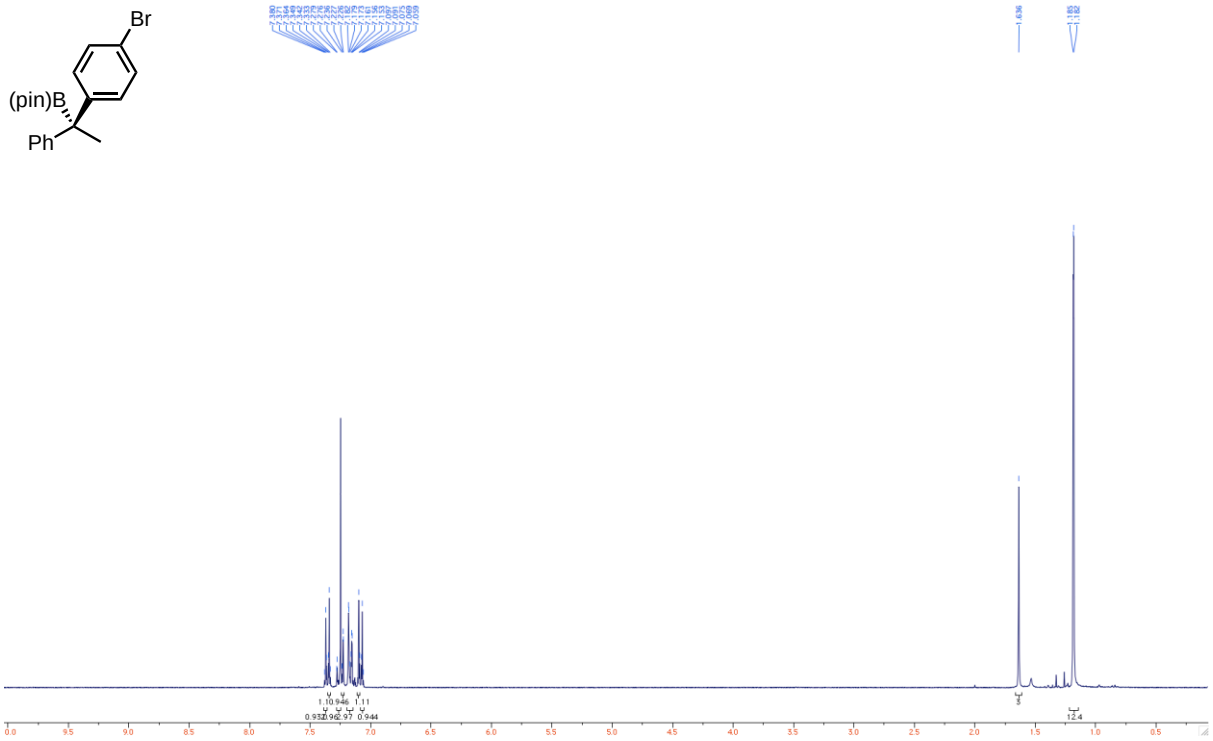
^{11}B NMR (96Mhz, $CDCl_3$)[5]



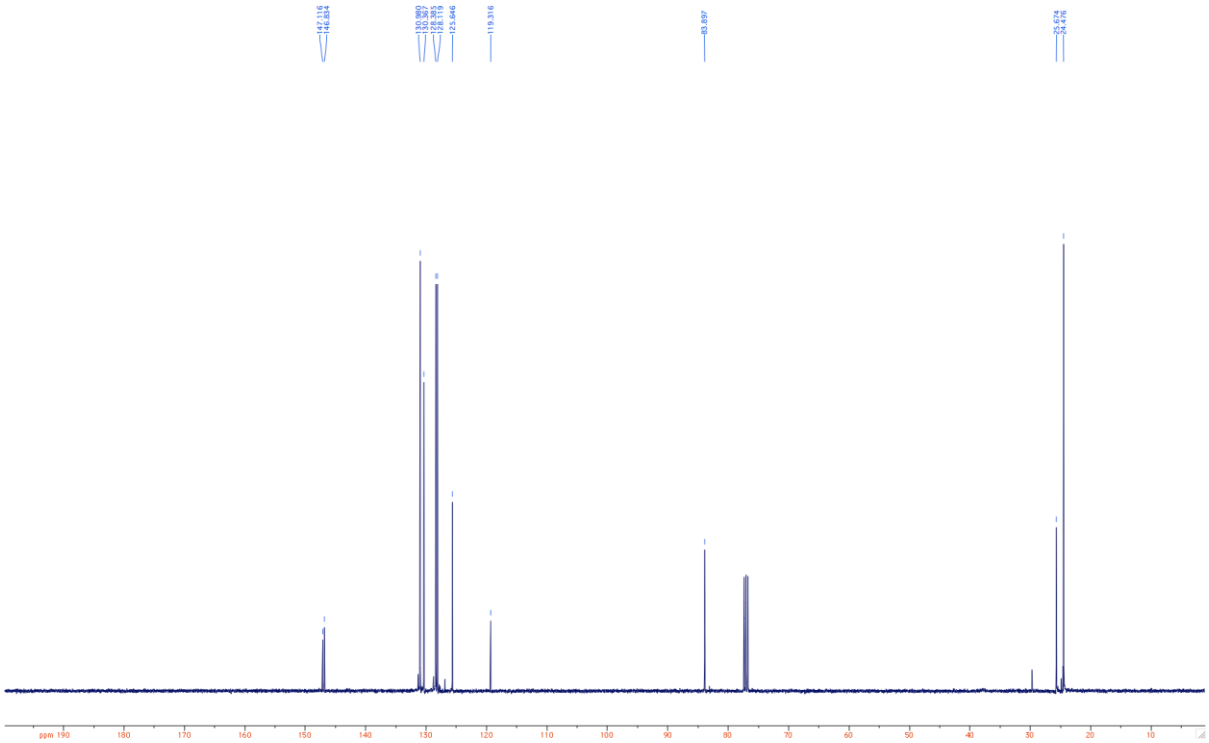
[5] The ^{11}B NMR of steroid **1o** is believed to be weak due to possible aggregation effects.

1j

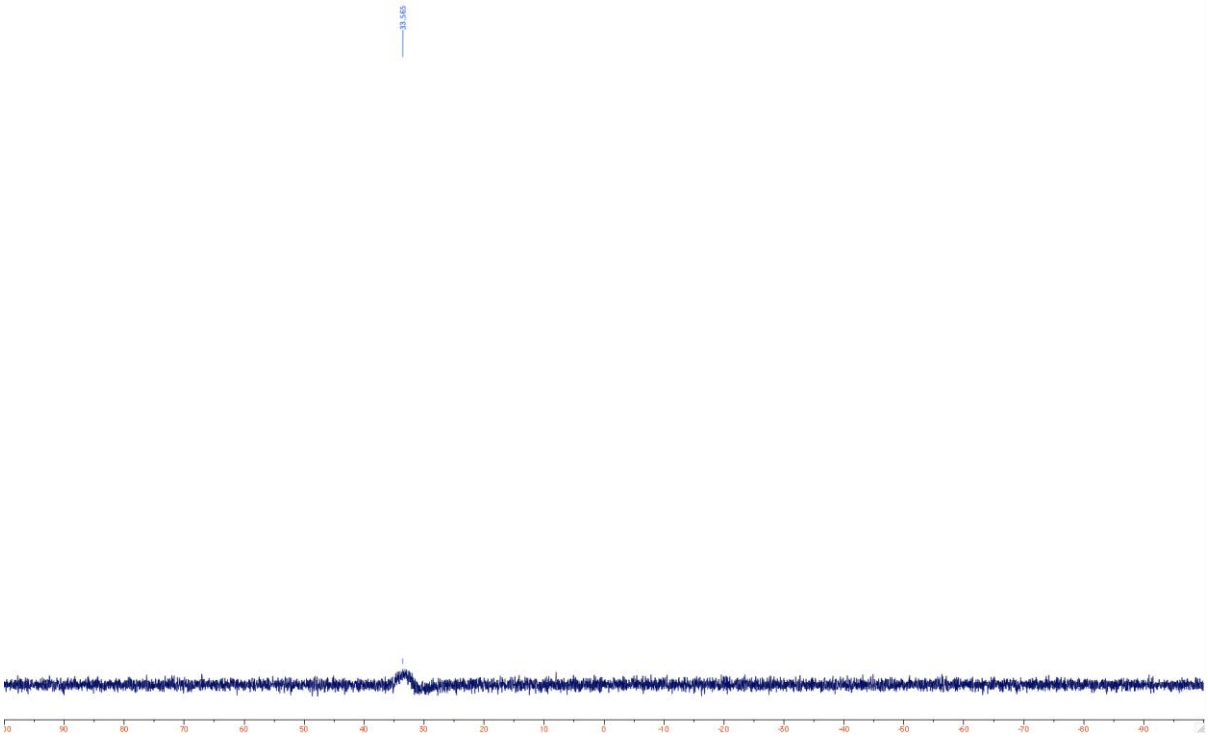
^{1}H NMR (400 MHz, $CDCl_3$)



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

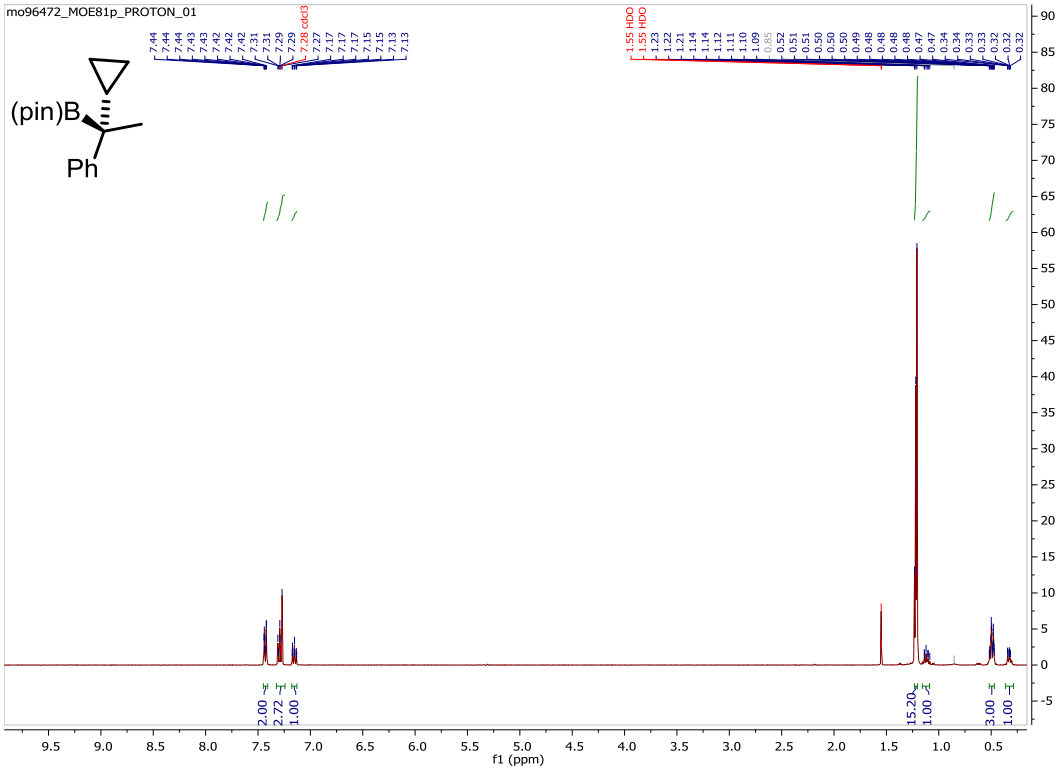


^{11}B NMR (96 MHz, $CDCl_3$)

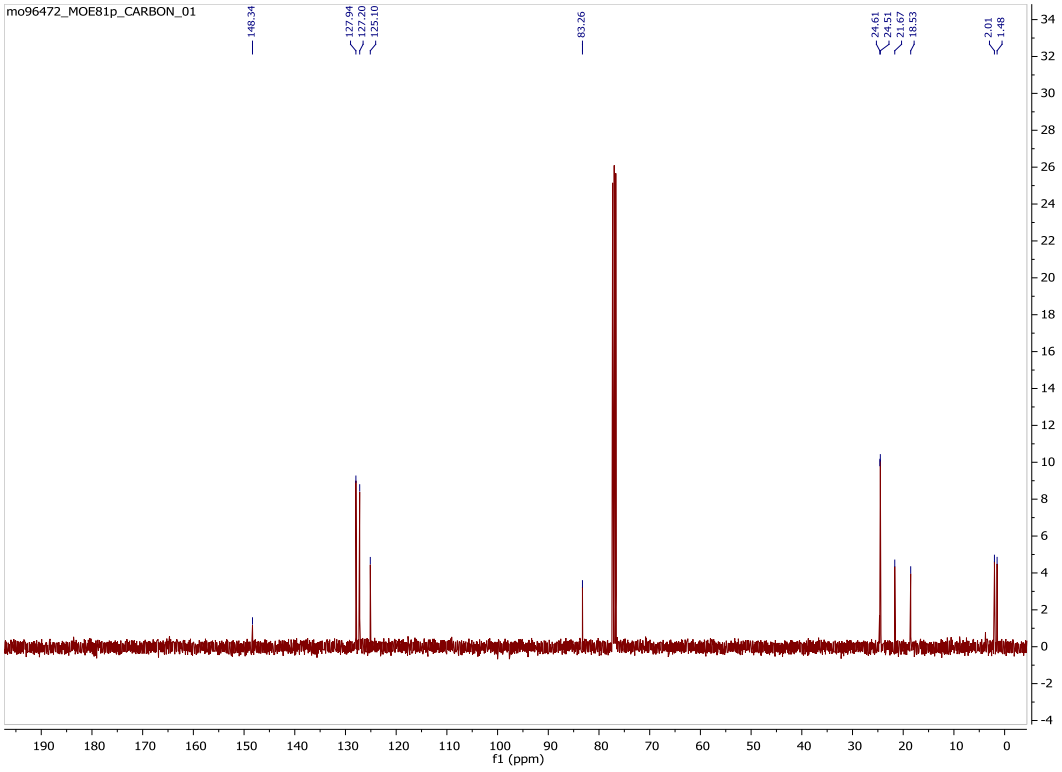


1k

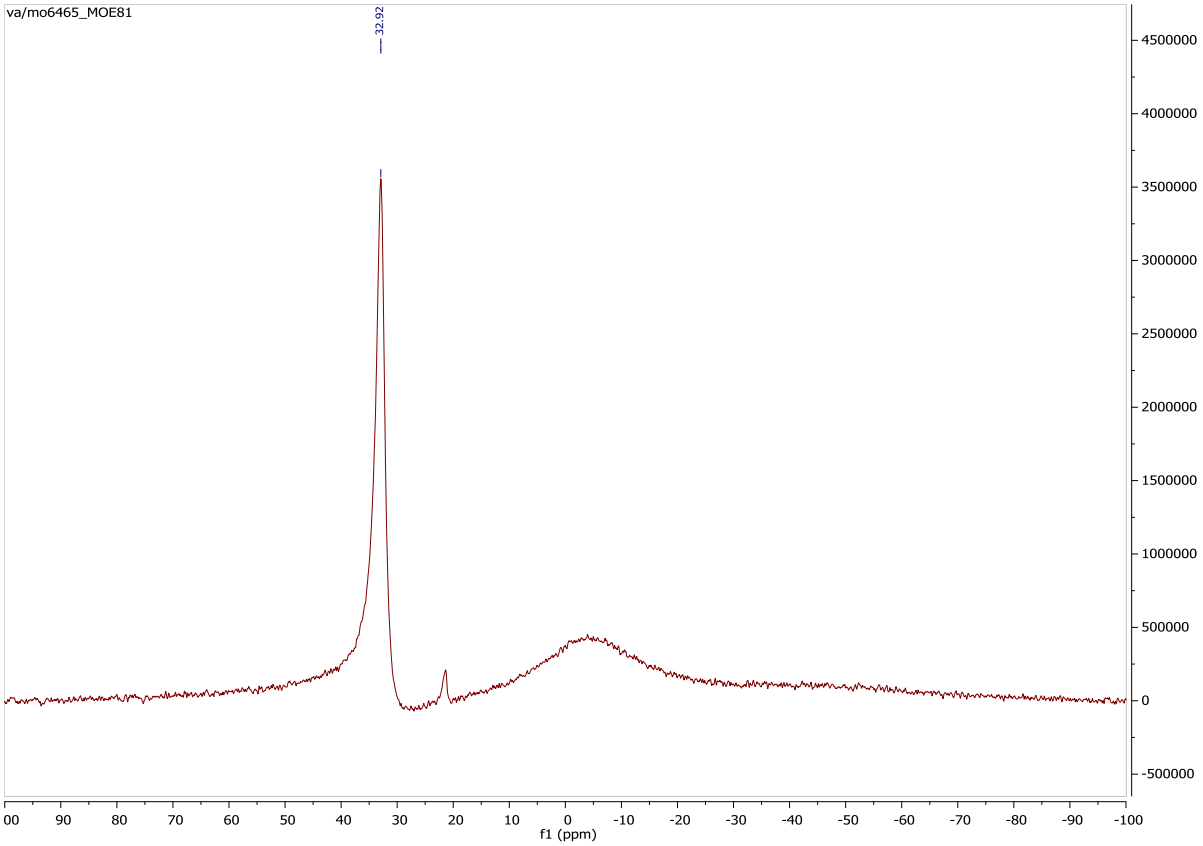
^{1}H NMR (400 MHz, $CDCl_3$)



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



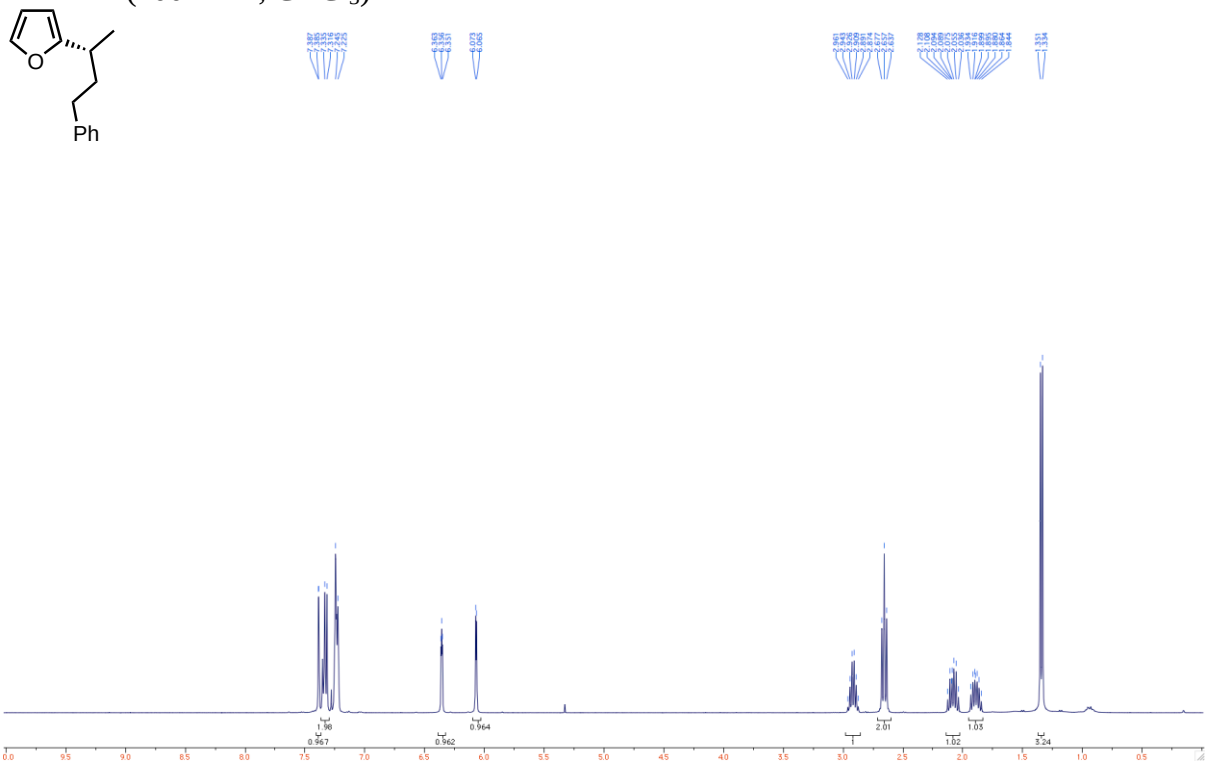
^{11}B NMR (96 MHz, NONE)[6]



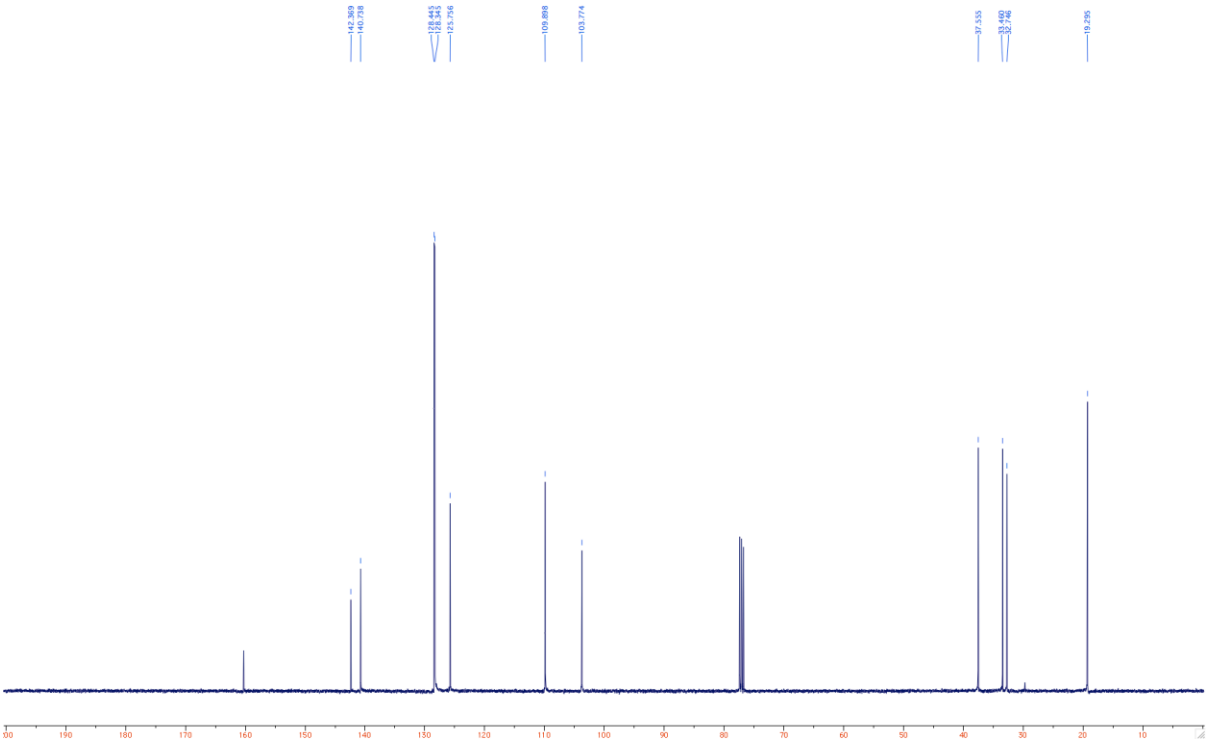
[6] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

2a

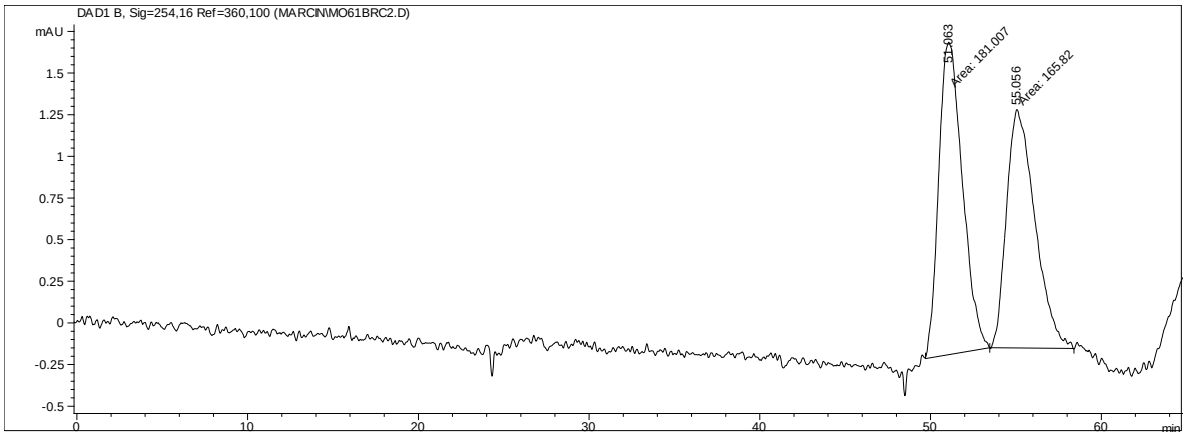
^{1}H NMR (400 MHz, $CDCl_3$)



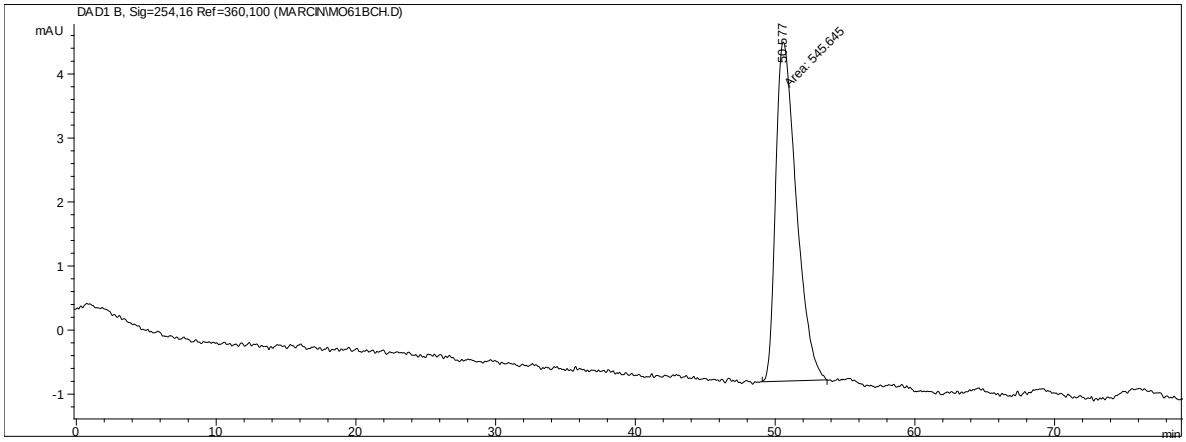
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

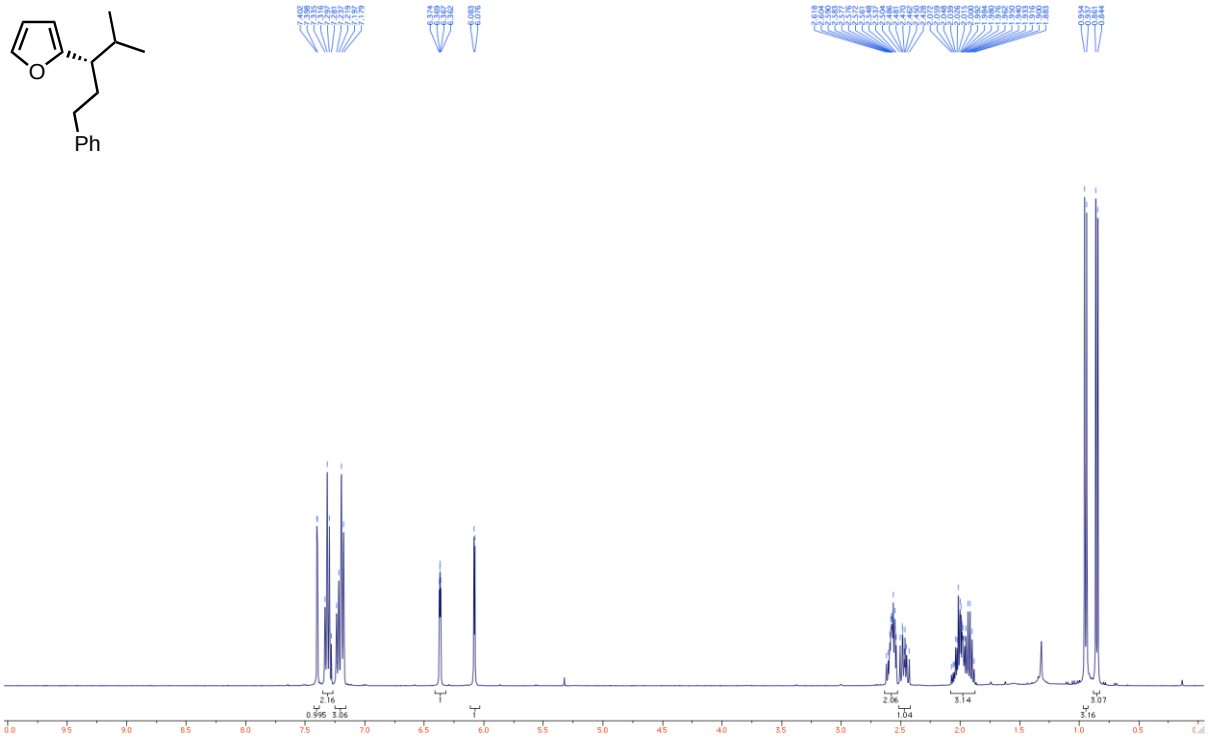


Chiral HPLC traces: enantioenriched

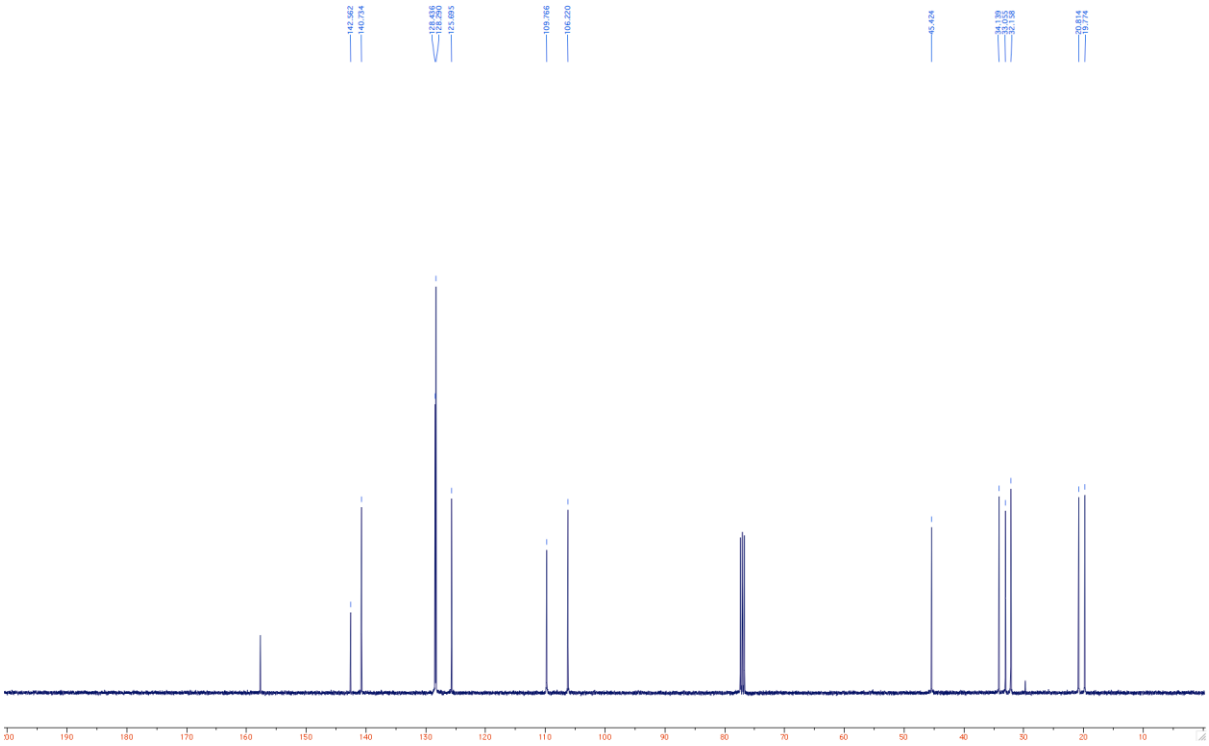


2c

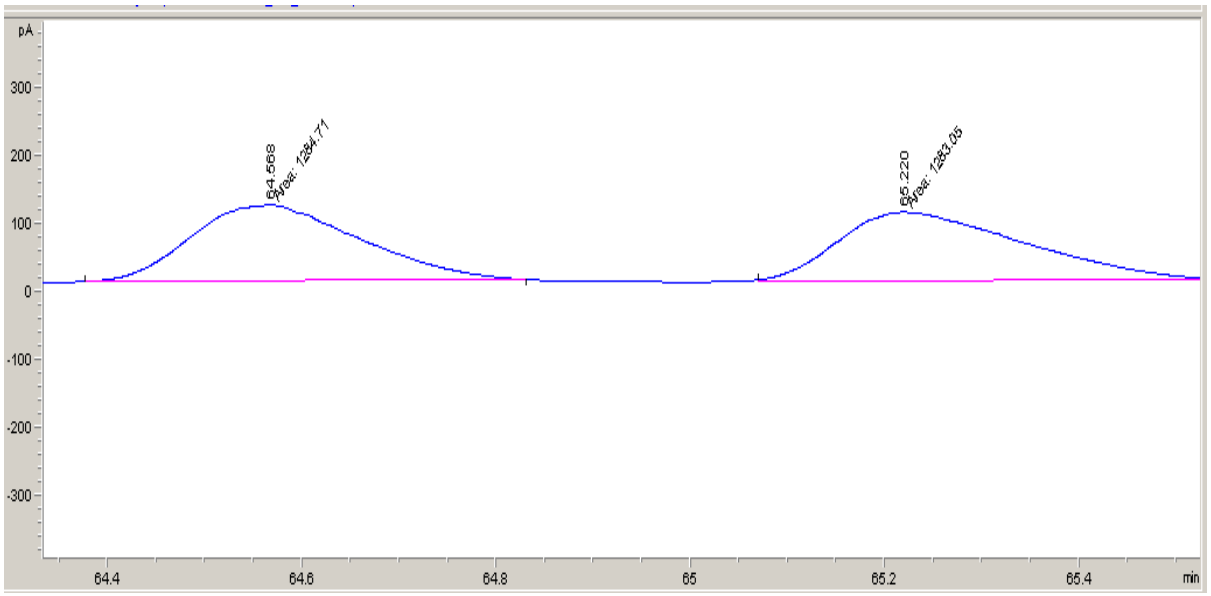
^{1}H NMR (400 MHz, $CDCl_3$)



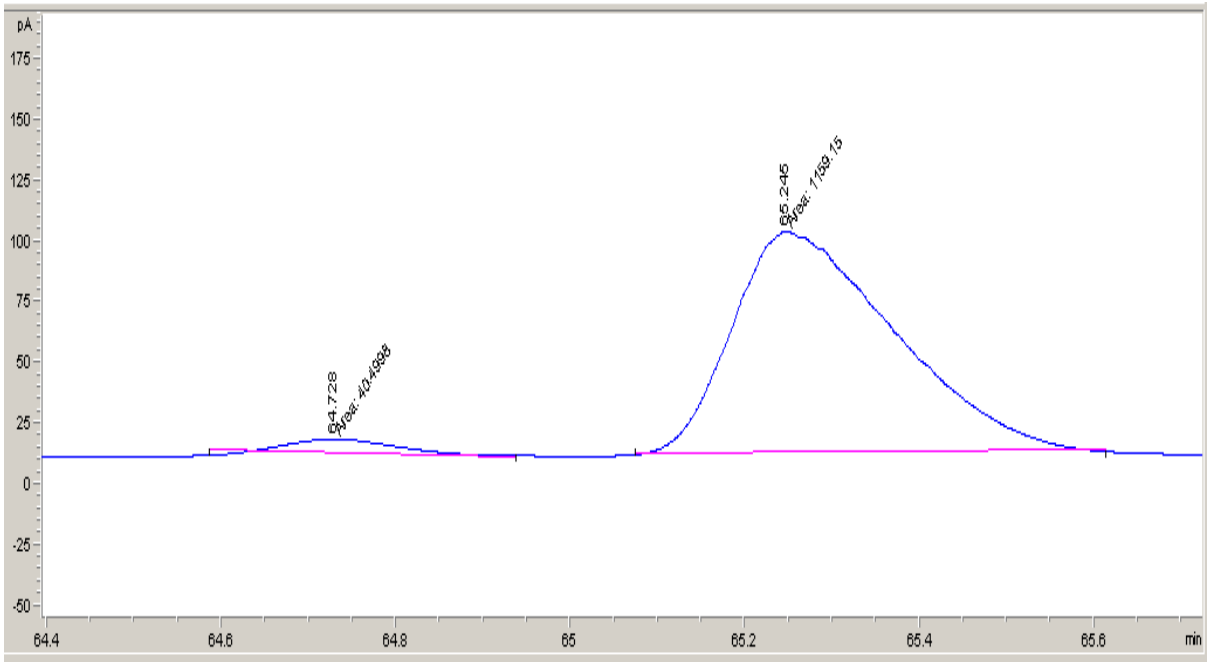
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral GC traces: racemic

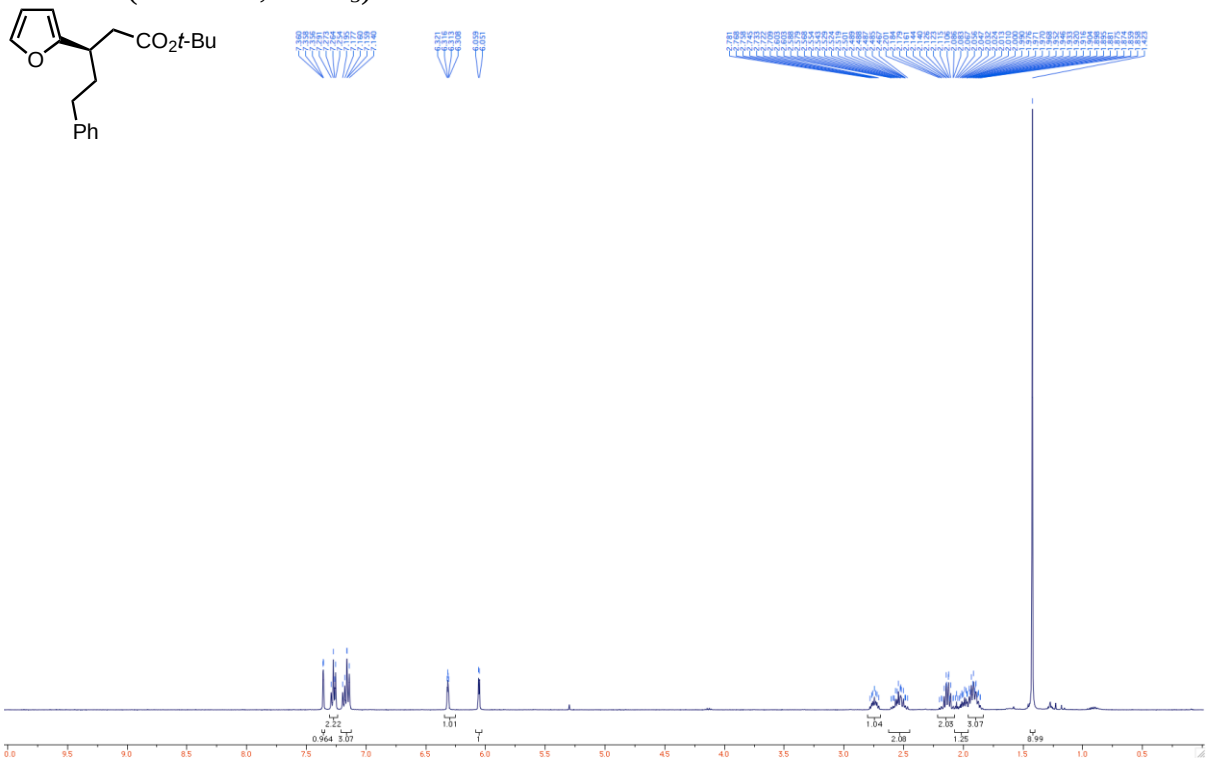


Chiral GC traces: enantioenriched

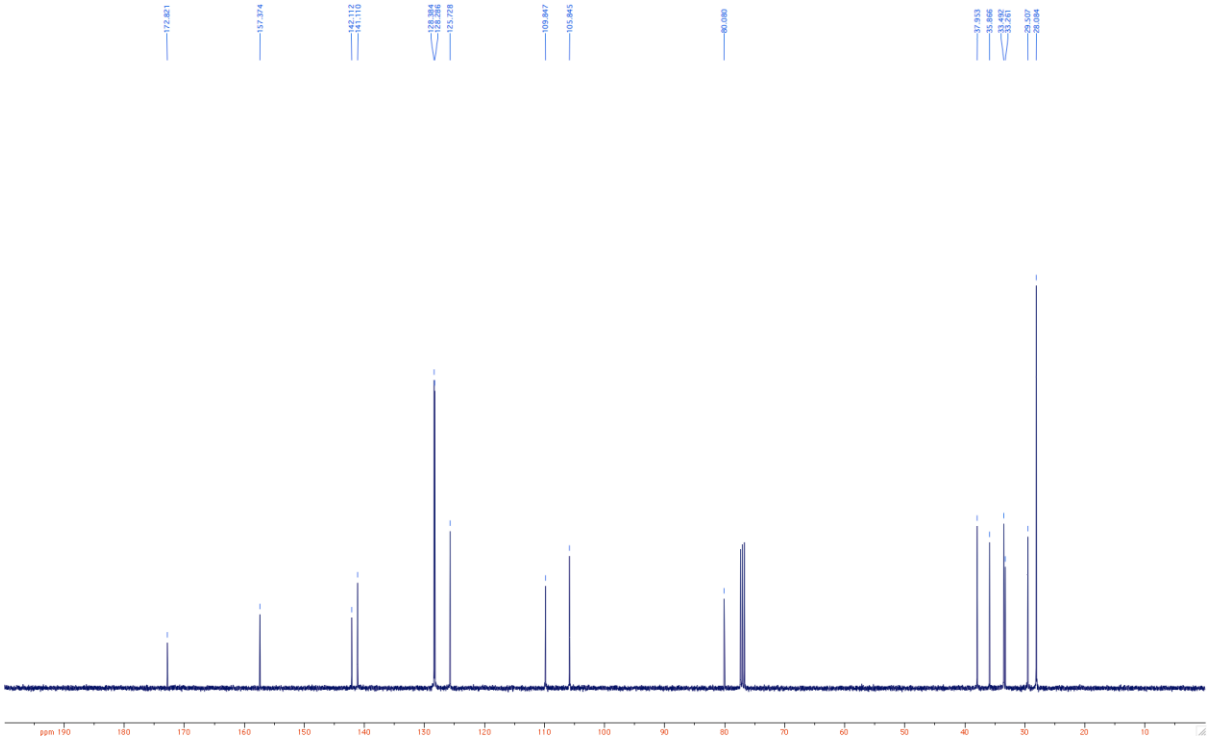


2e

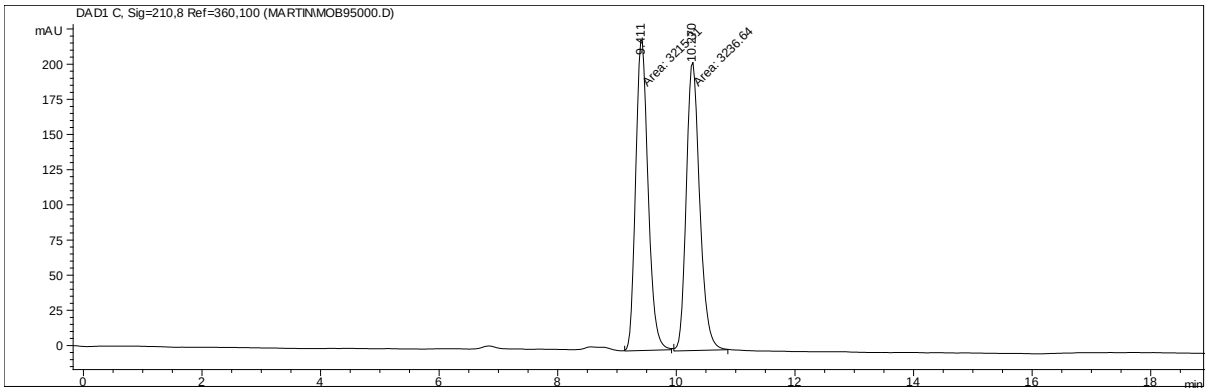
^{1}H NMR (400 MHz, $CDCl_3$)



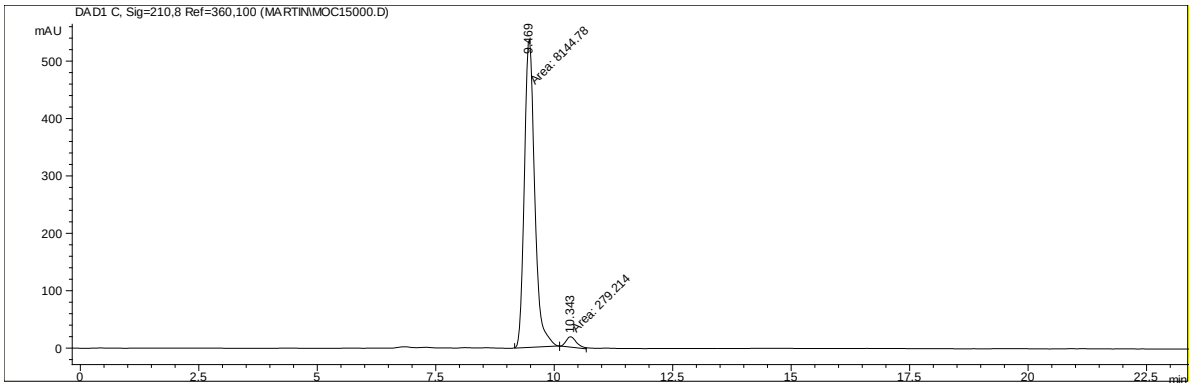
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

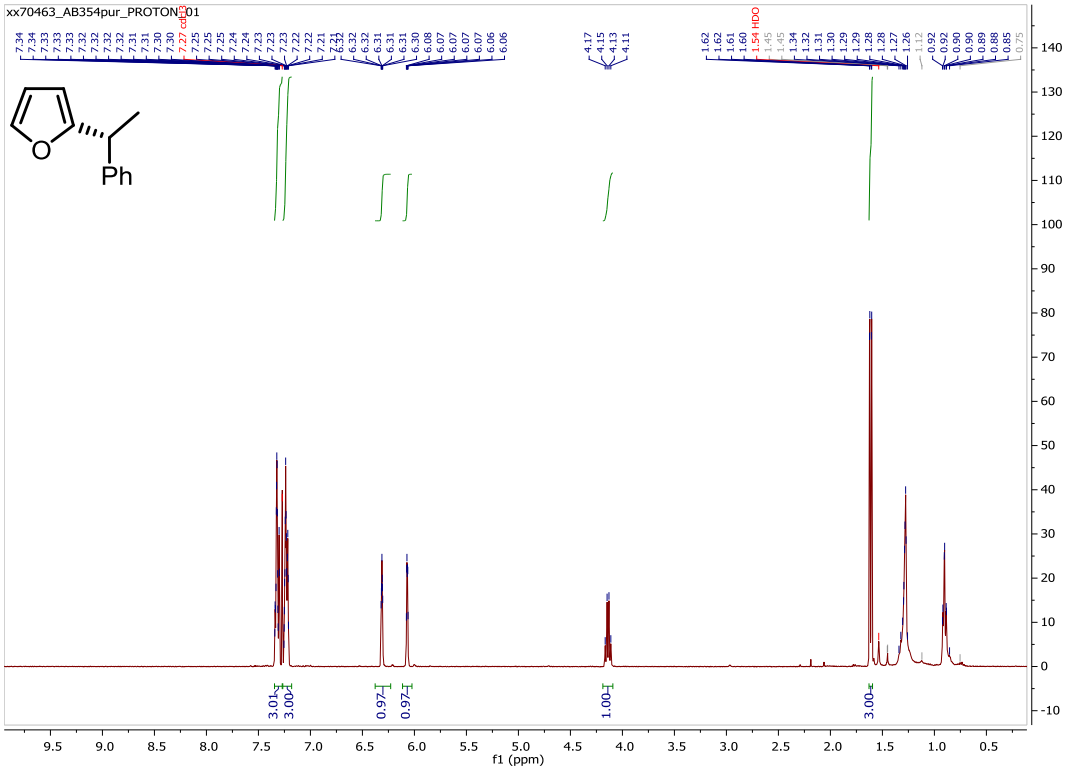


Chiral HPLC traces: enantioenriched

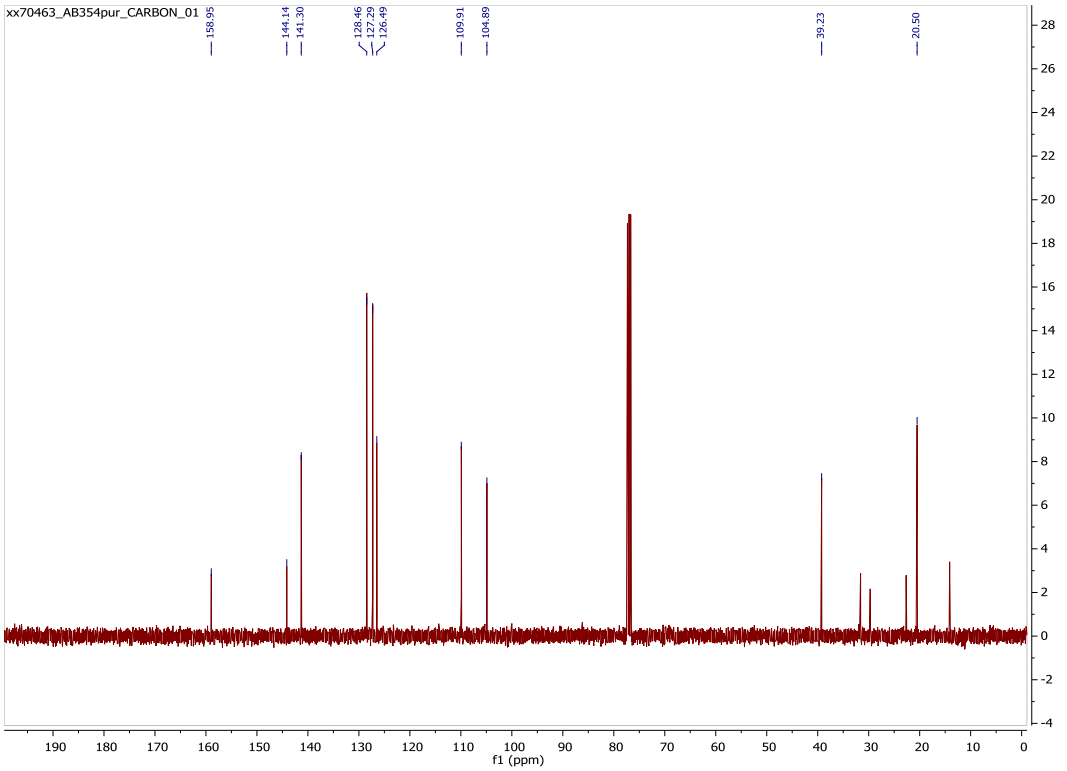


2l

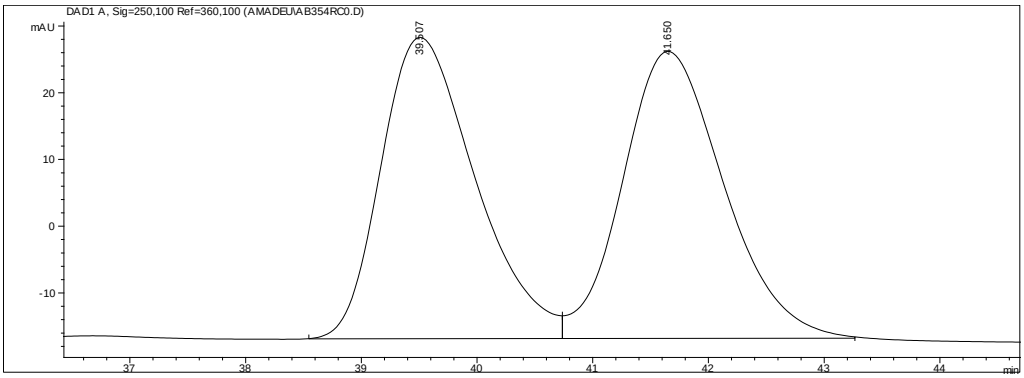
^{1}H NMR (400 MHz, $CDCl_3$)



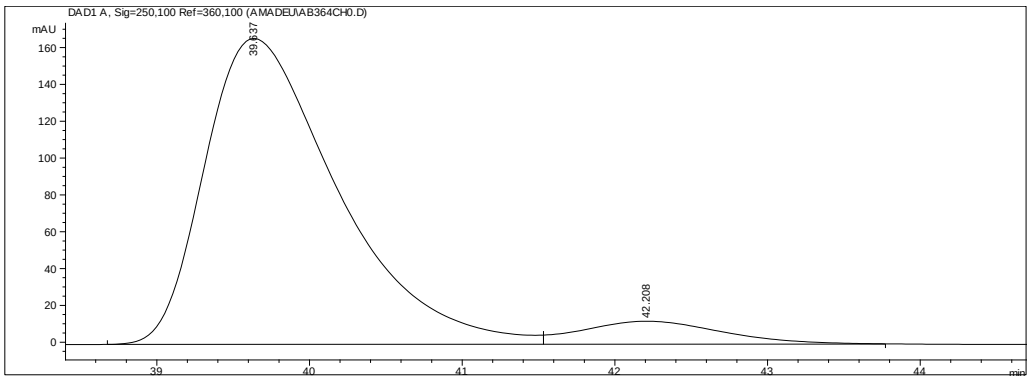
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

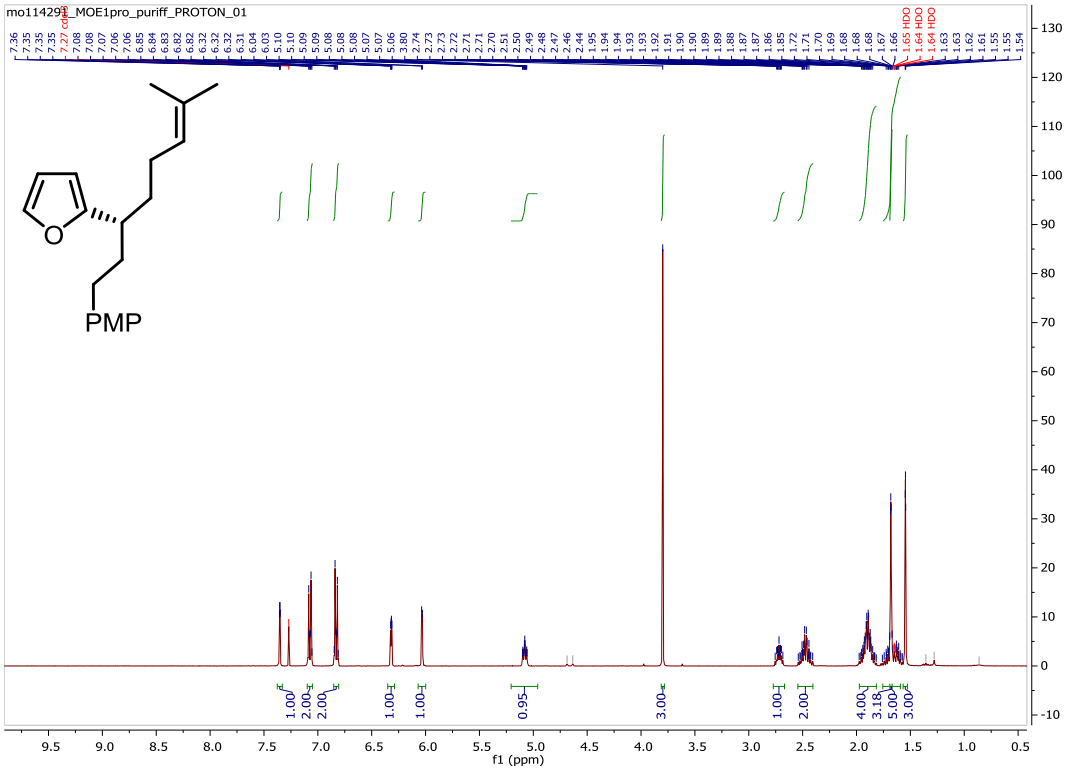


Chiral HPLC traces: enantioenriched

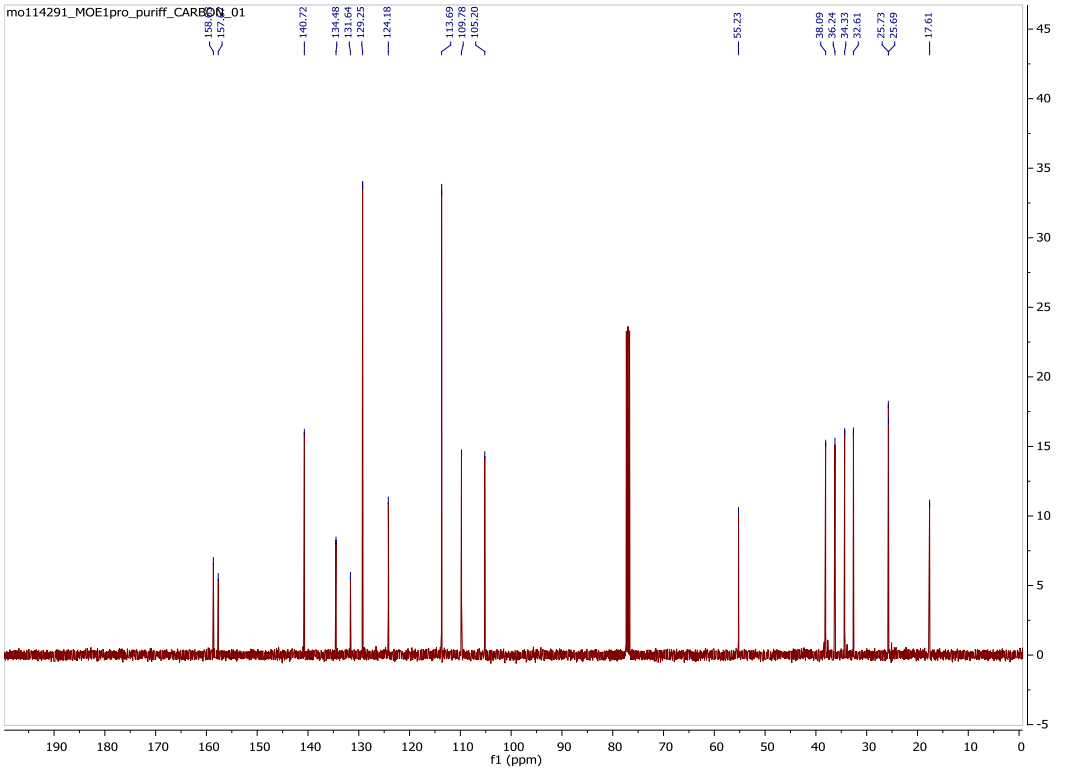


2d

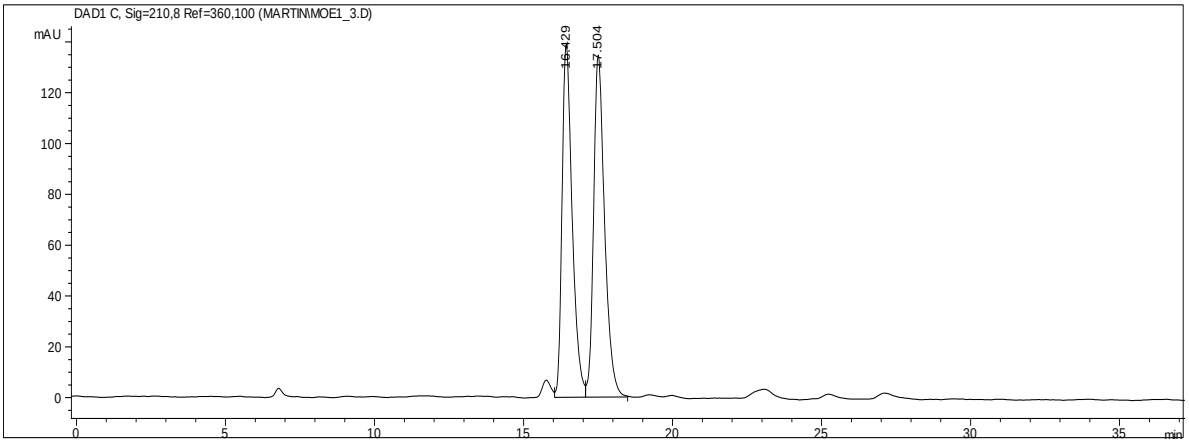
^{1}H NMR (400 MHz, $CDCl_3$)



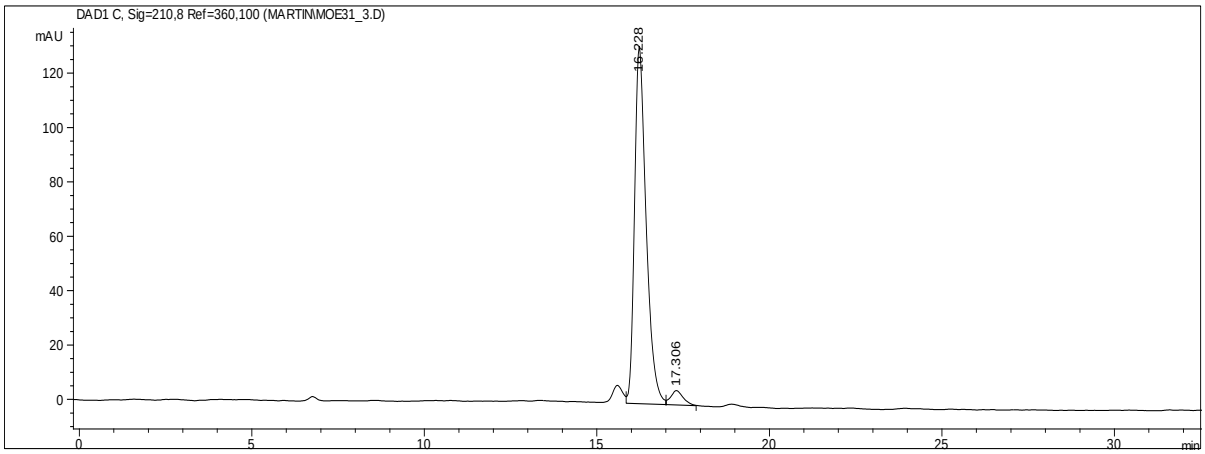
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

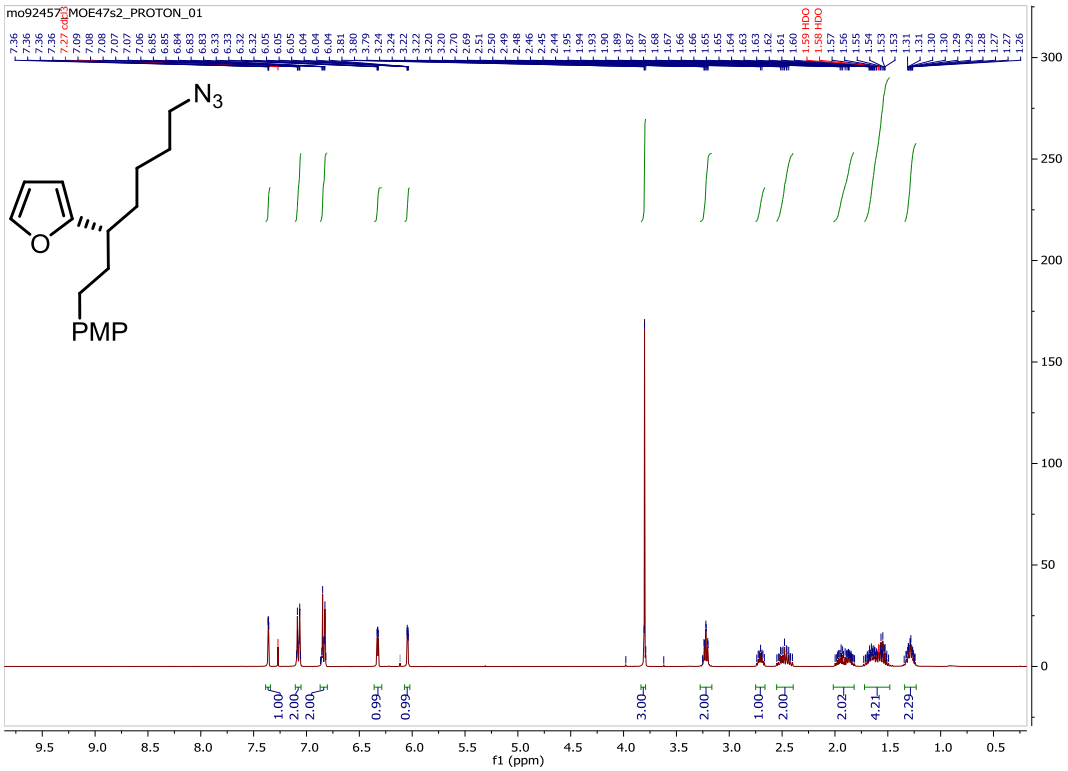


Chiral HPLC traces: enantioenriched

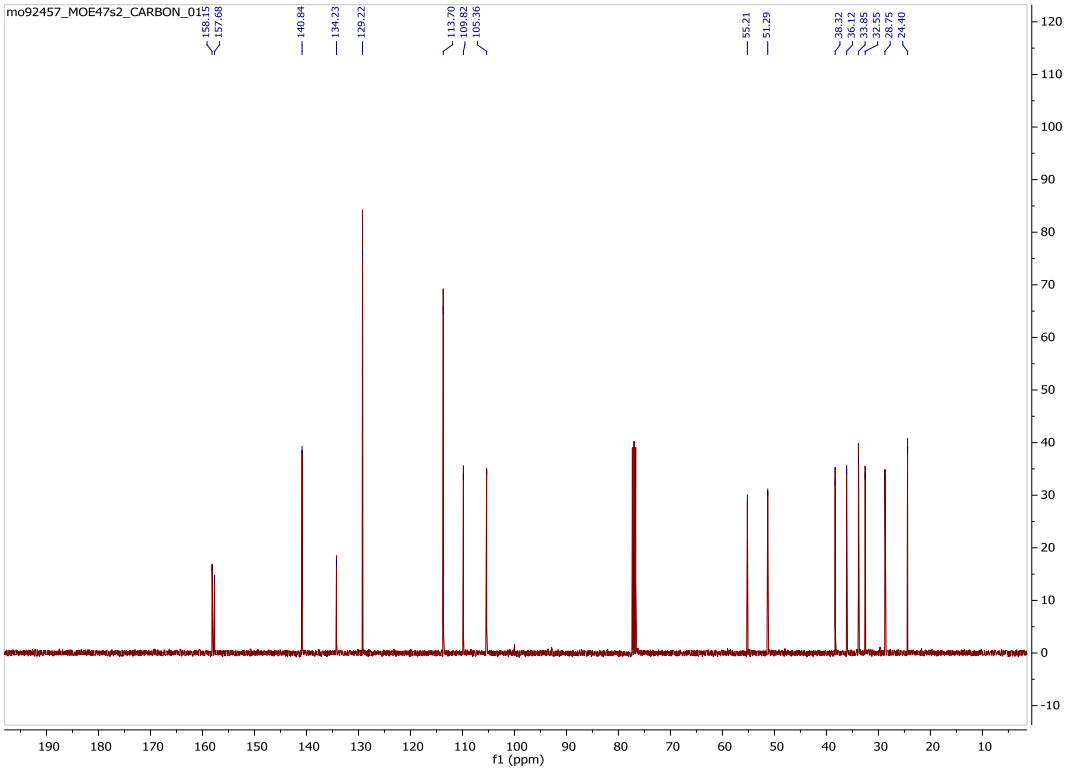


2f

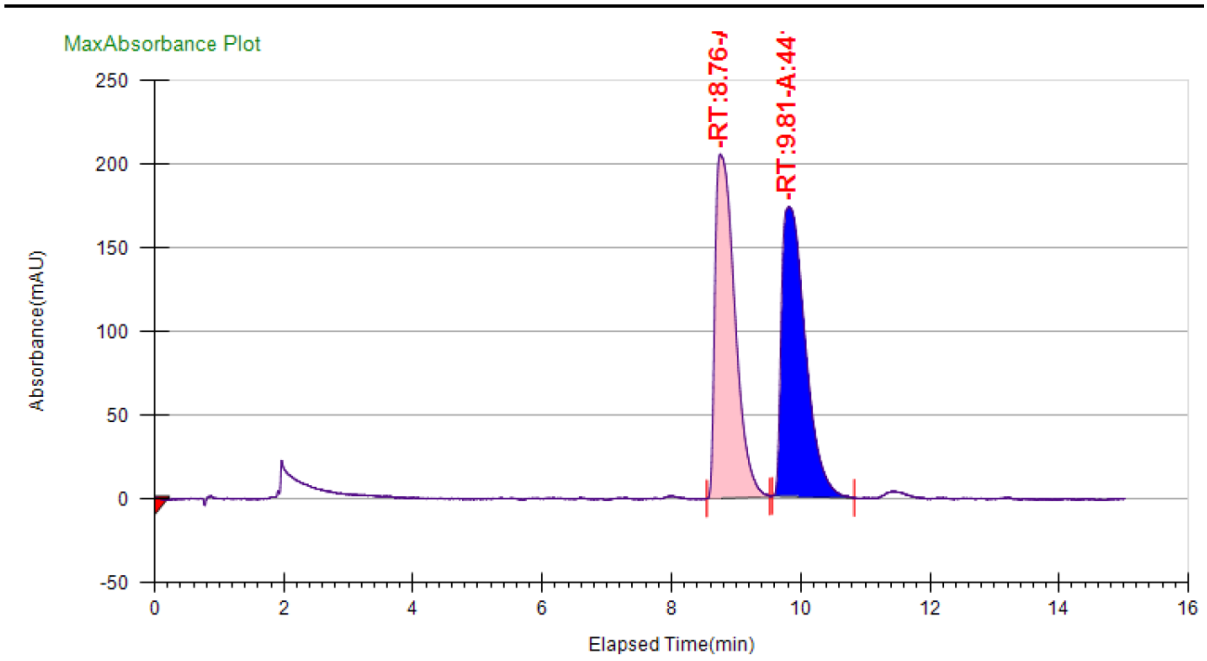
^{1}H NMR (400 MHz, $CDCl_3$)



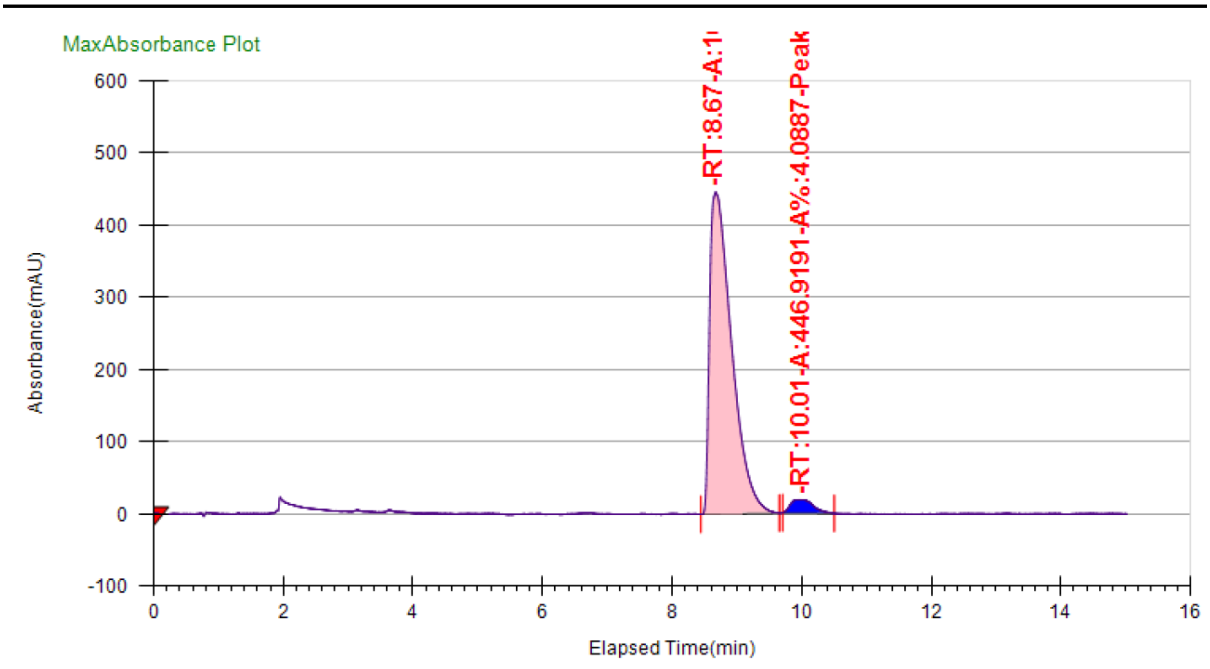
^{13}C-NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

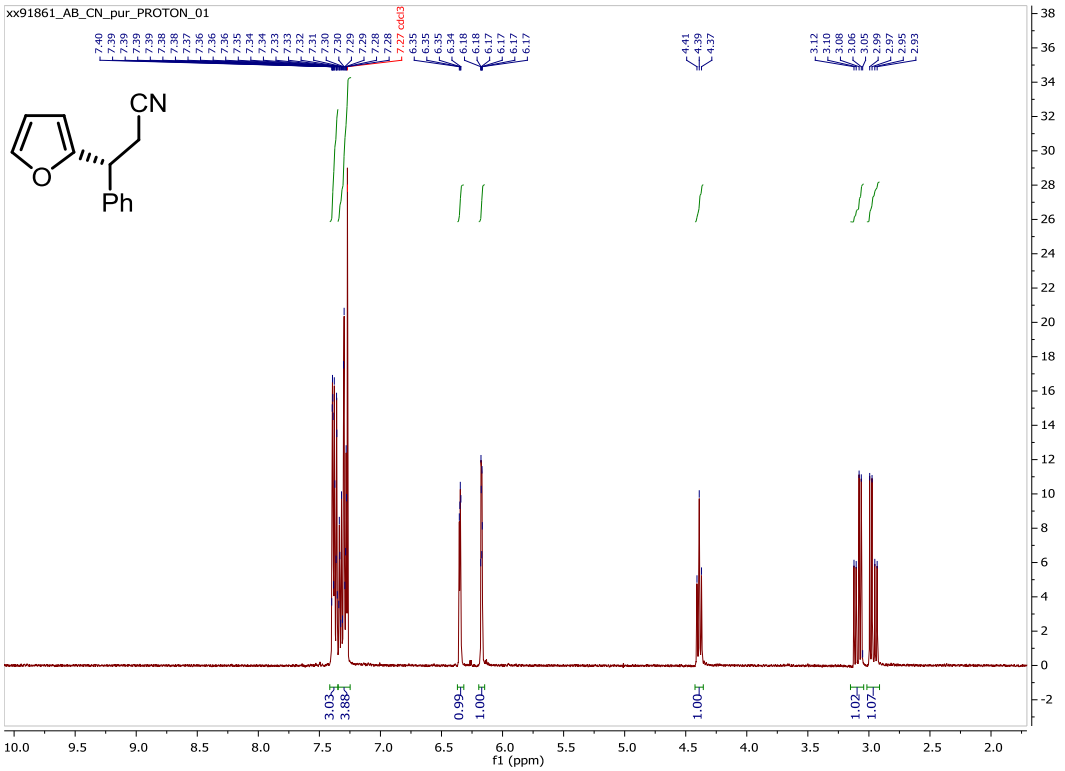


Chiral SFC traces: enantioenriched

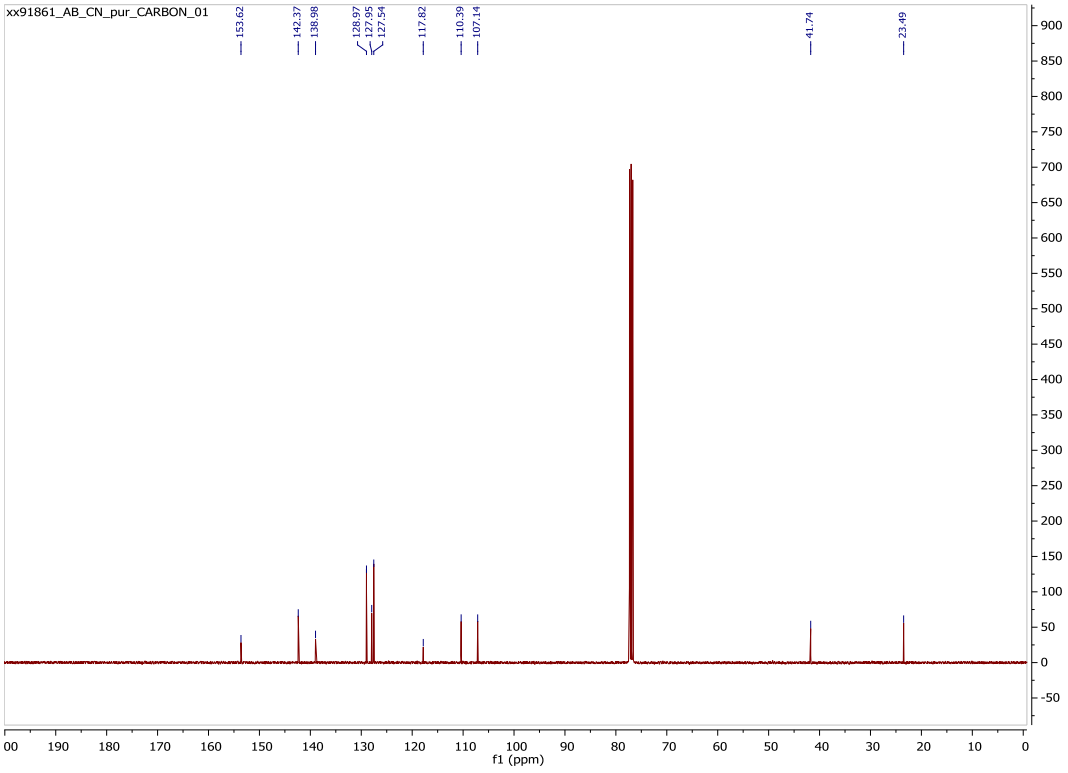


2s

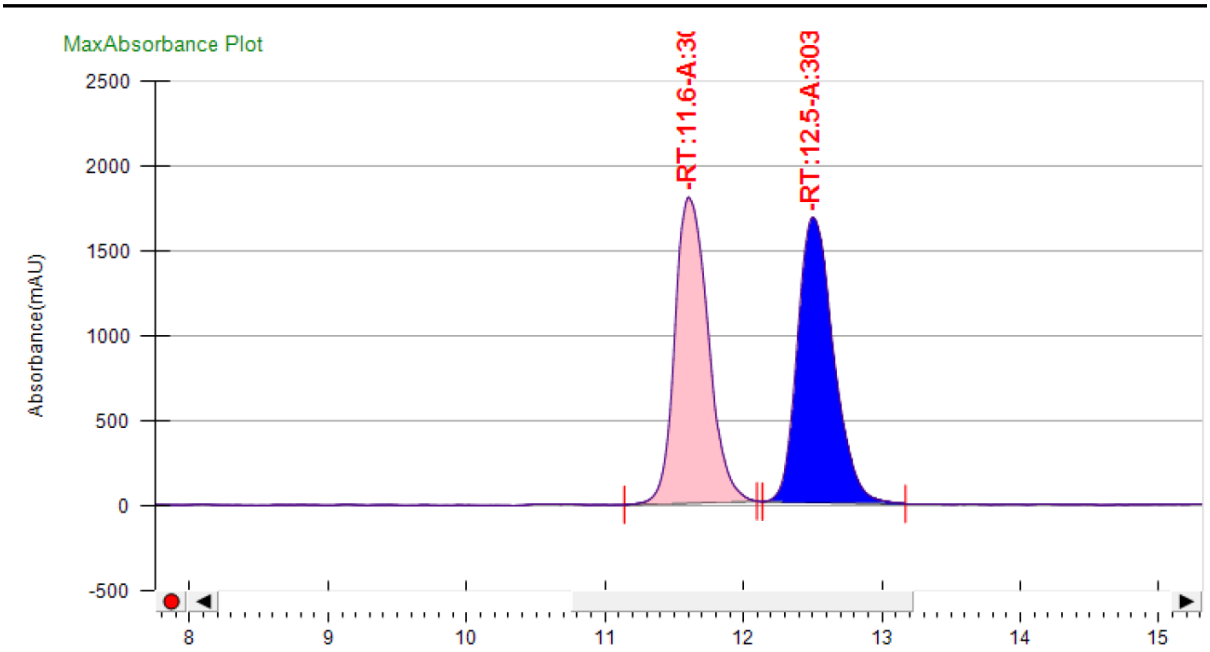
^{1}H NMR (400 MHz, $CDCl_3$)



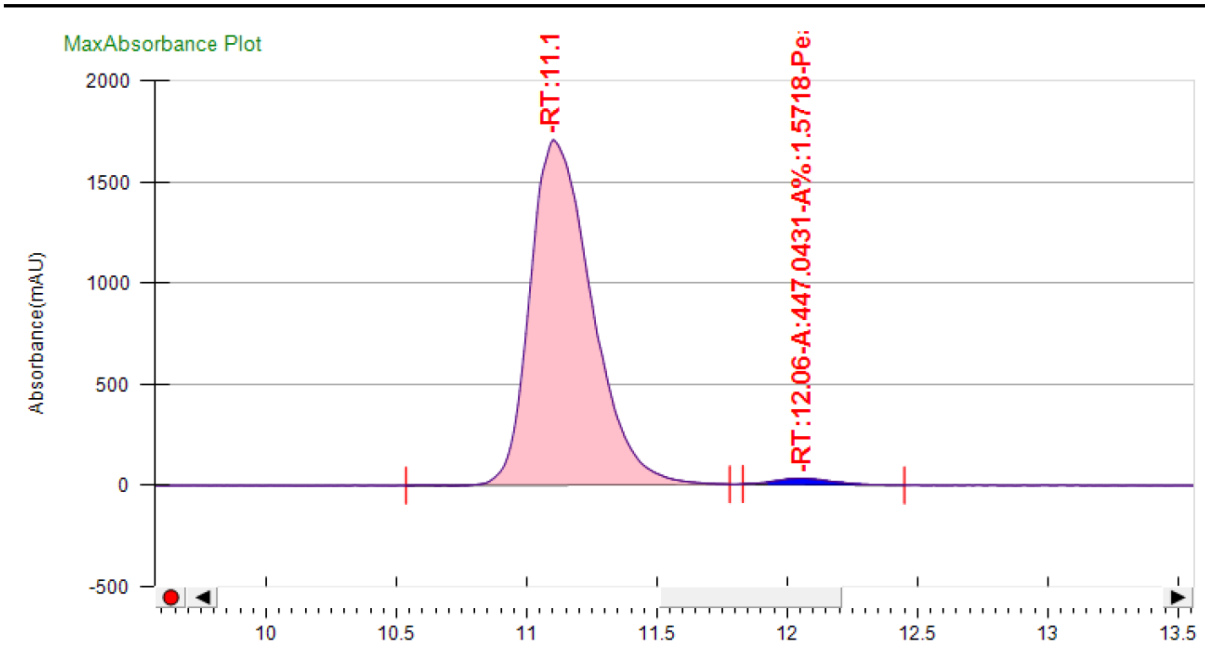
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

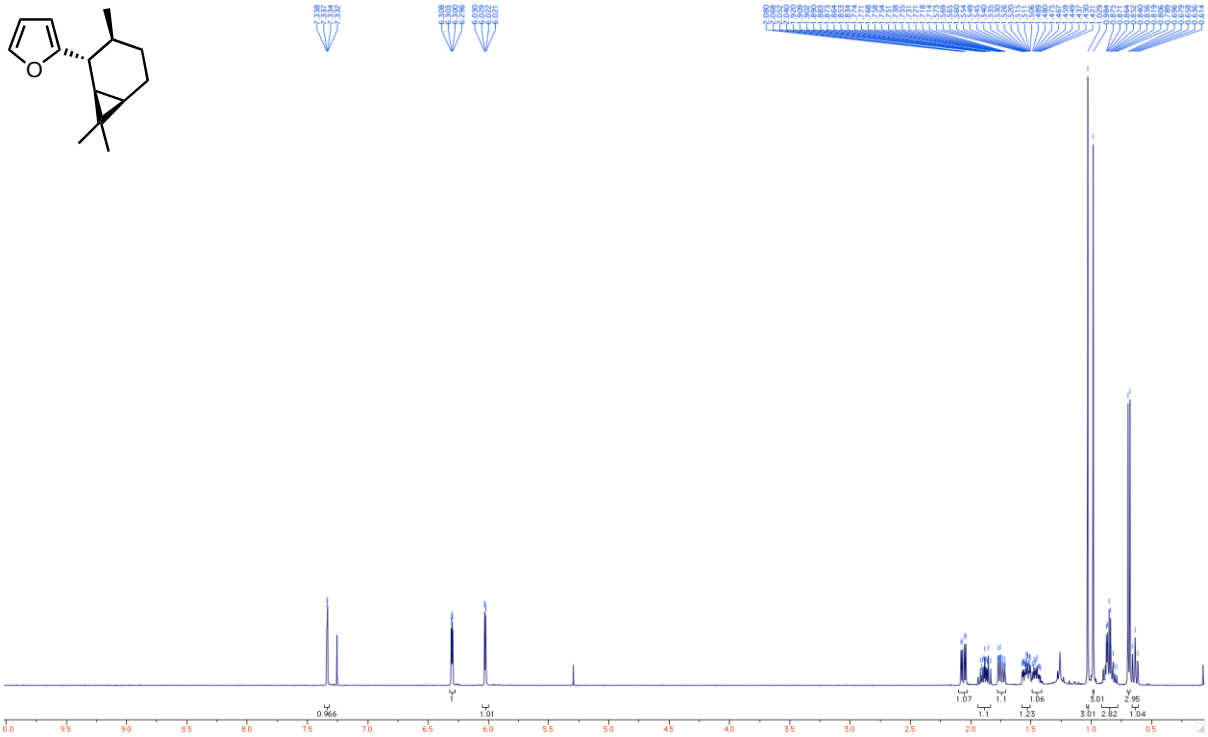


Chiral SFC traces: enantioenriched

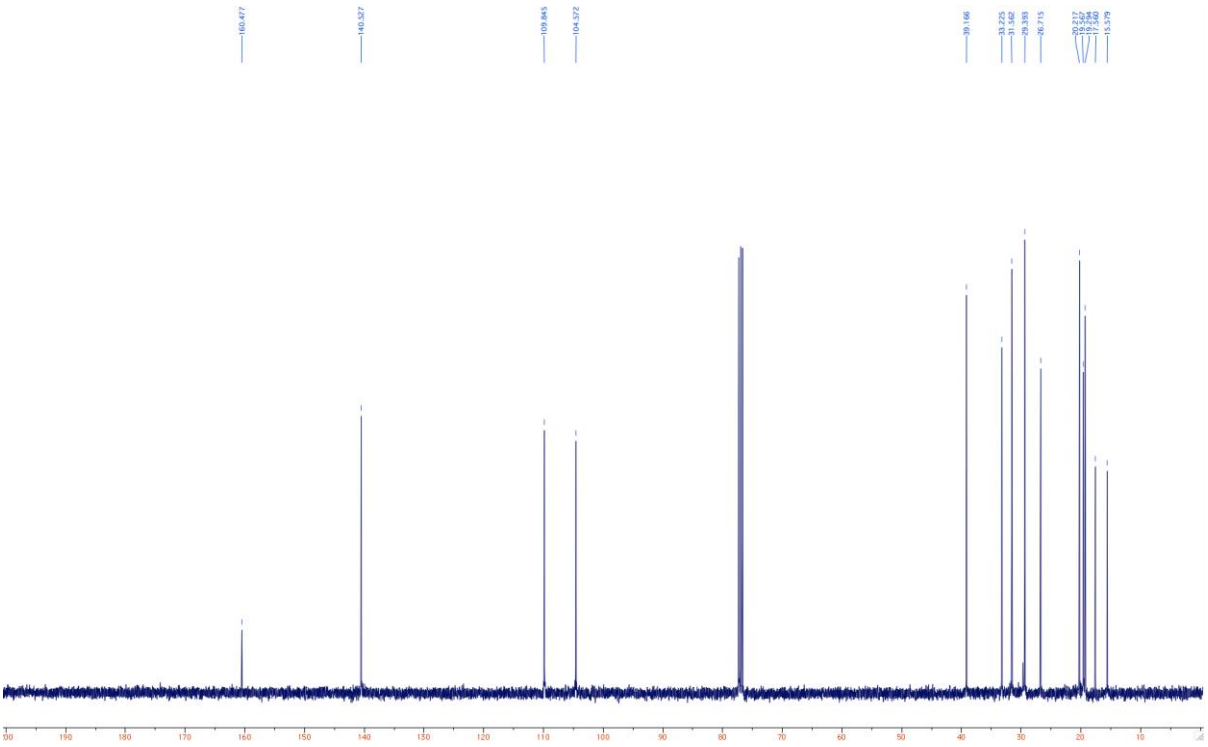


2m

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

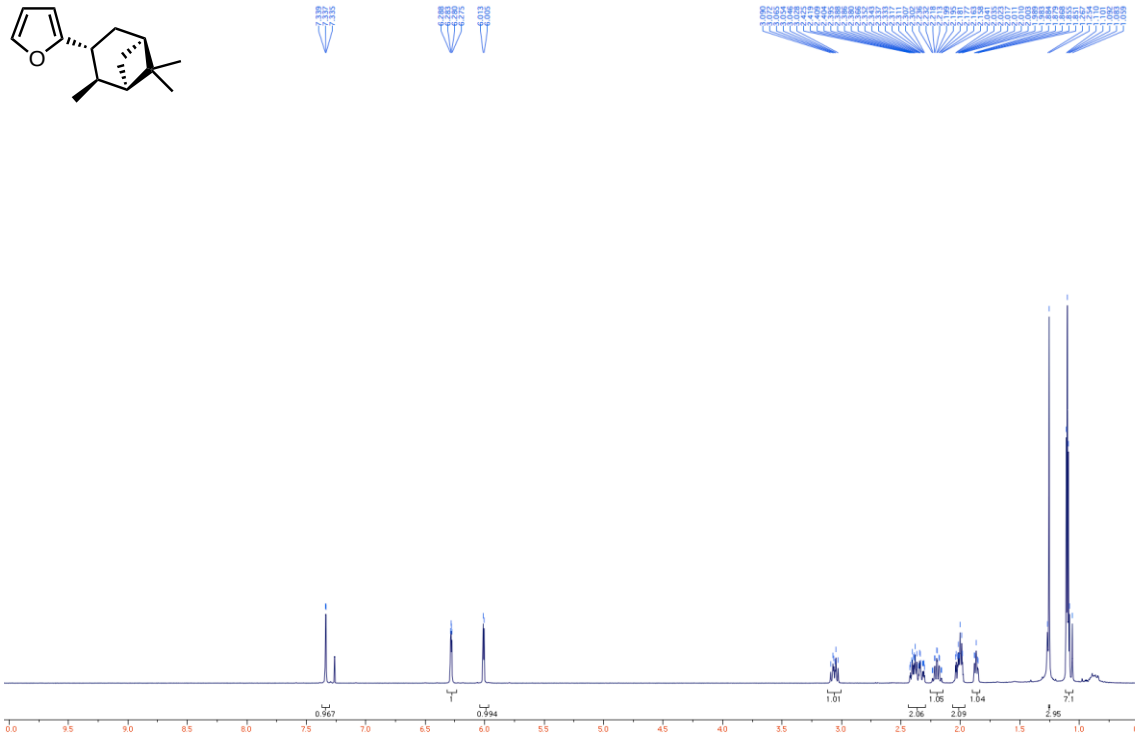


^{13}C NMR (100 MHz, $CDCl_3$)

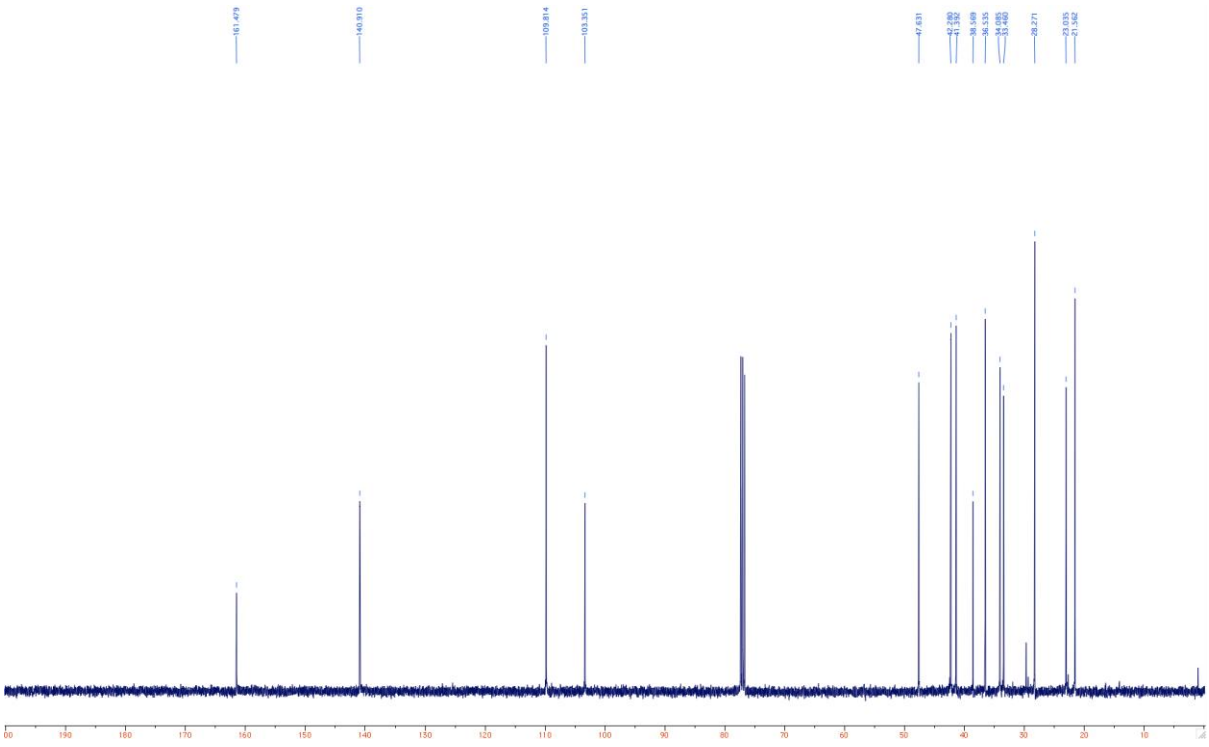


2n

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

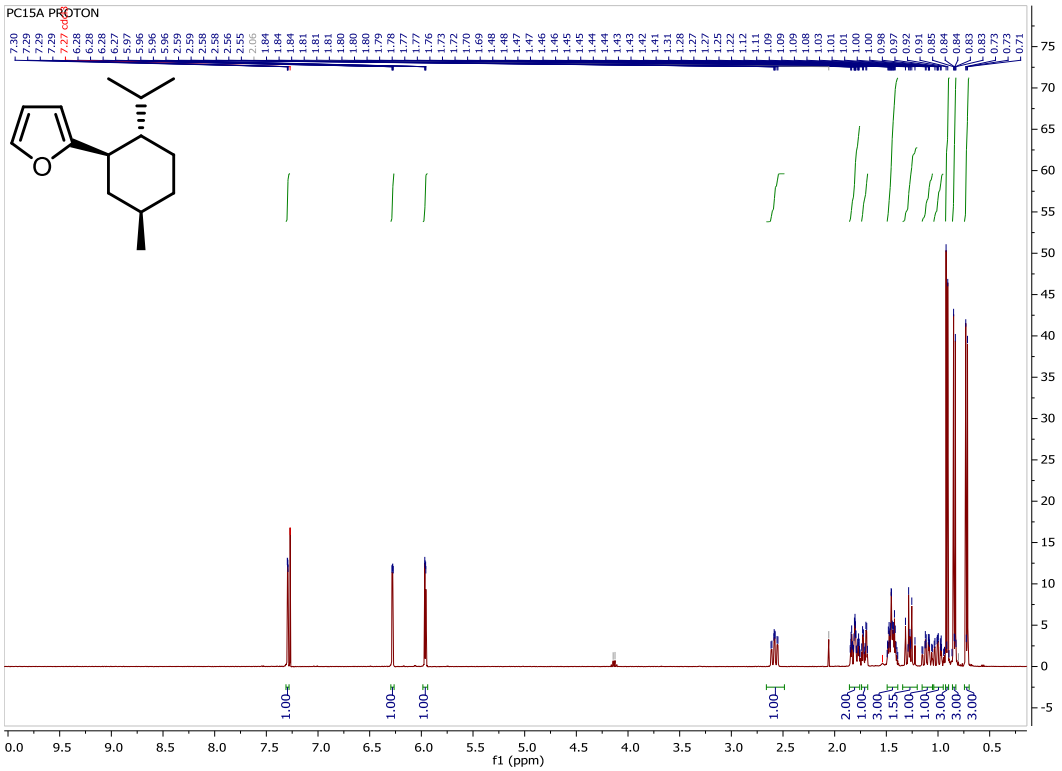


^{13}C NMR (100 MHz, $CDCl_3$)

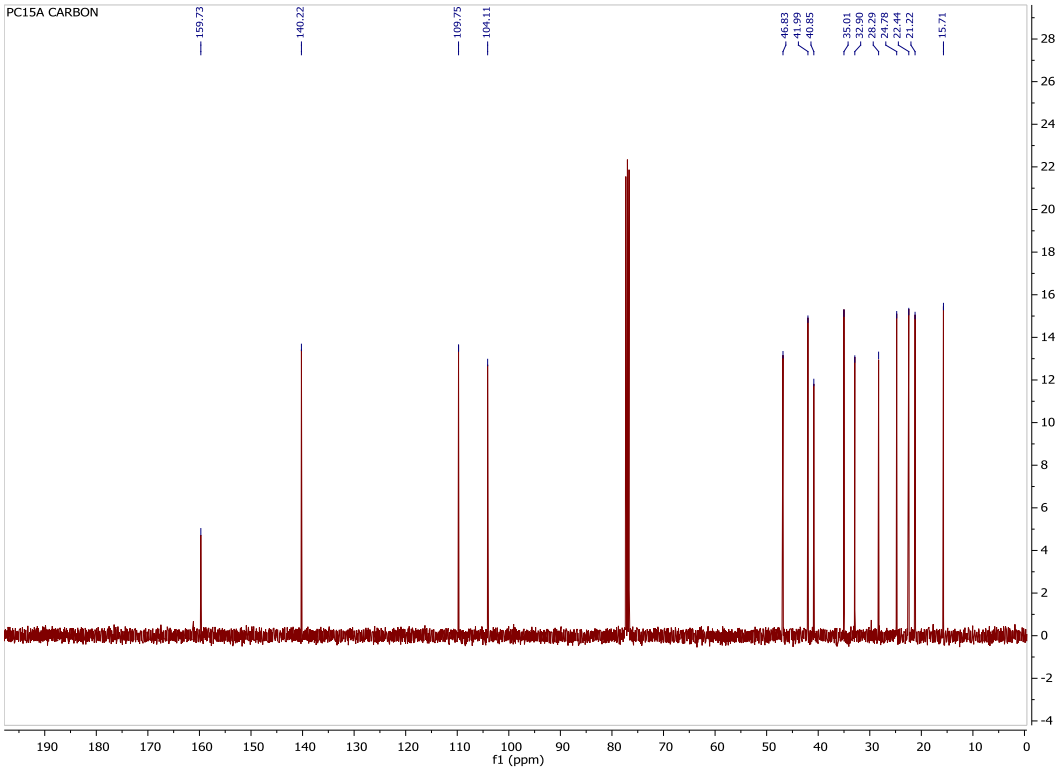


2q

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

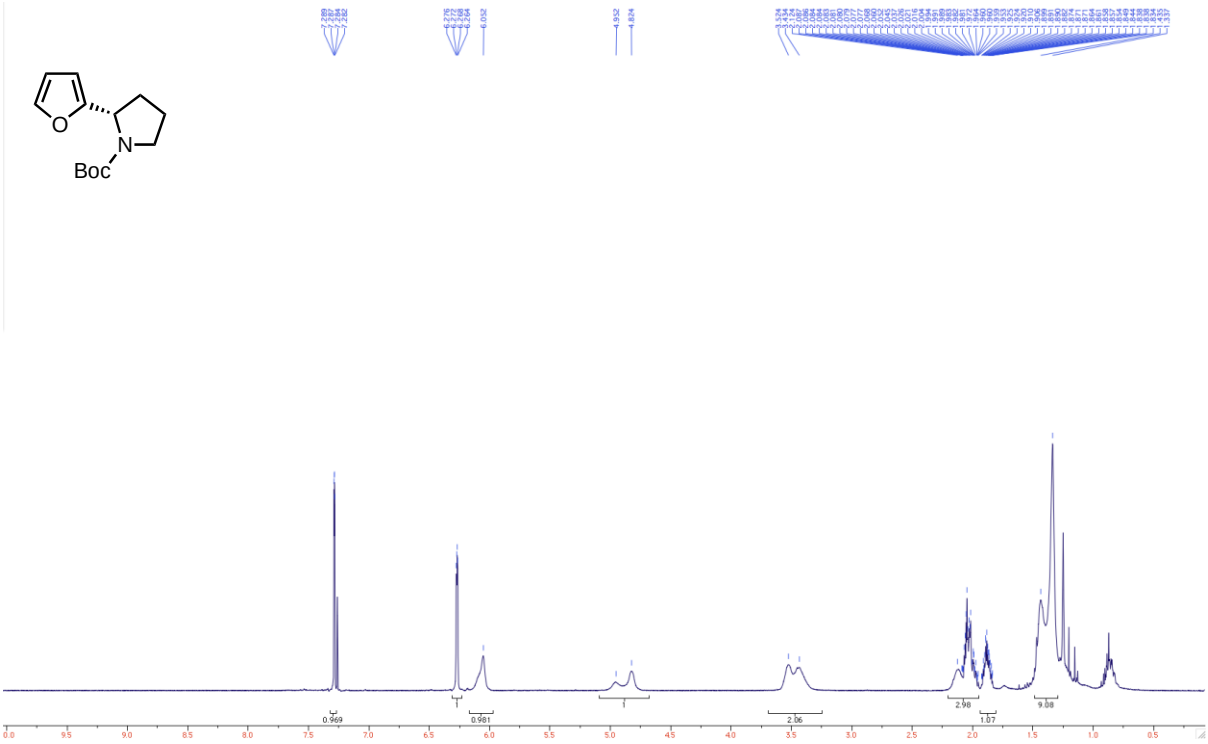


^{13}C NMR (100 MHz, $CDCl_3$)

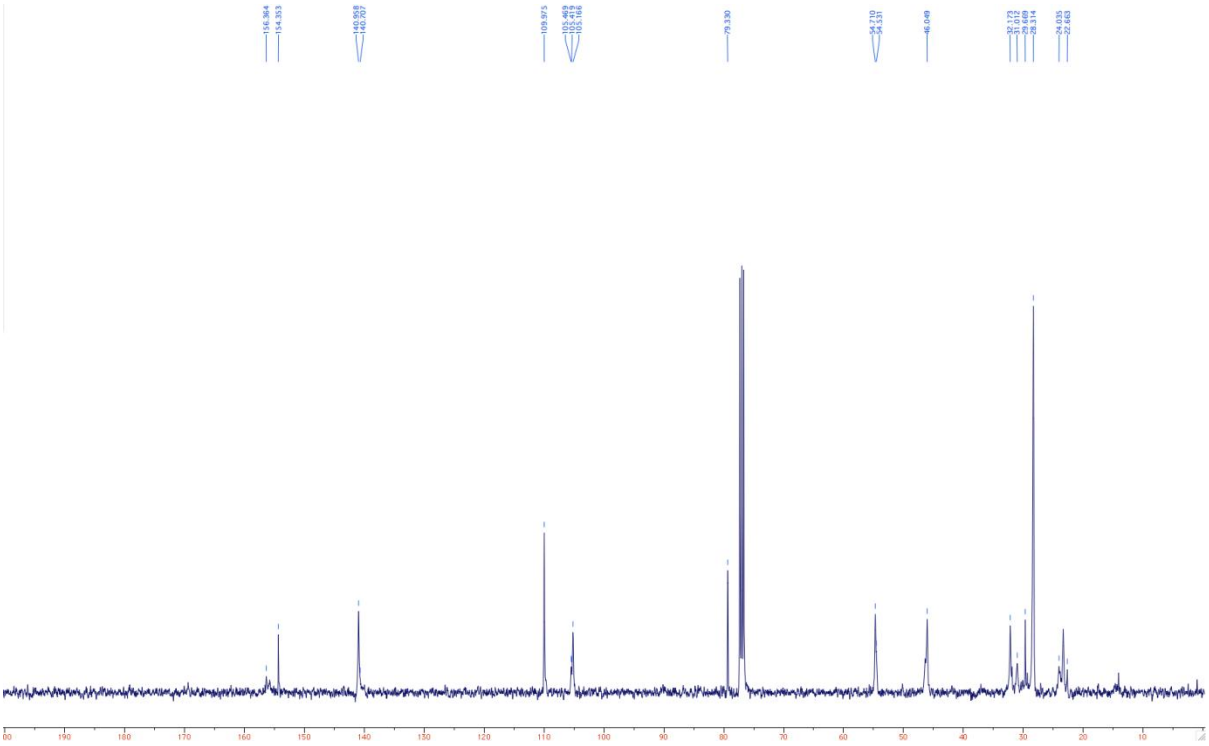


2t

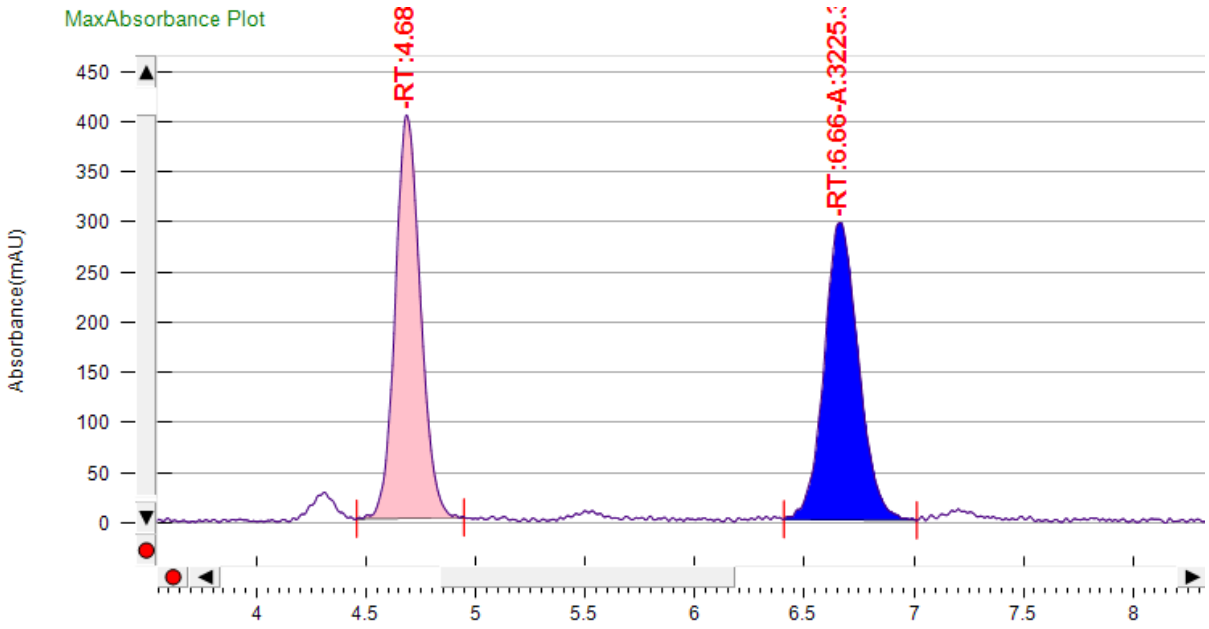
^{1}H NMR (400 MHz, $CDCl_3$)



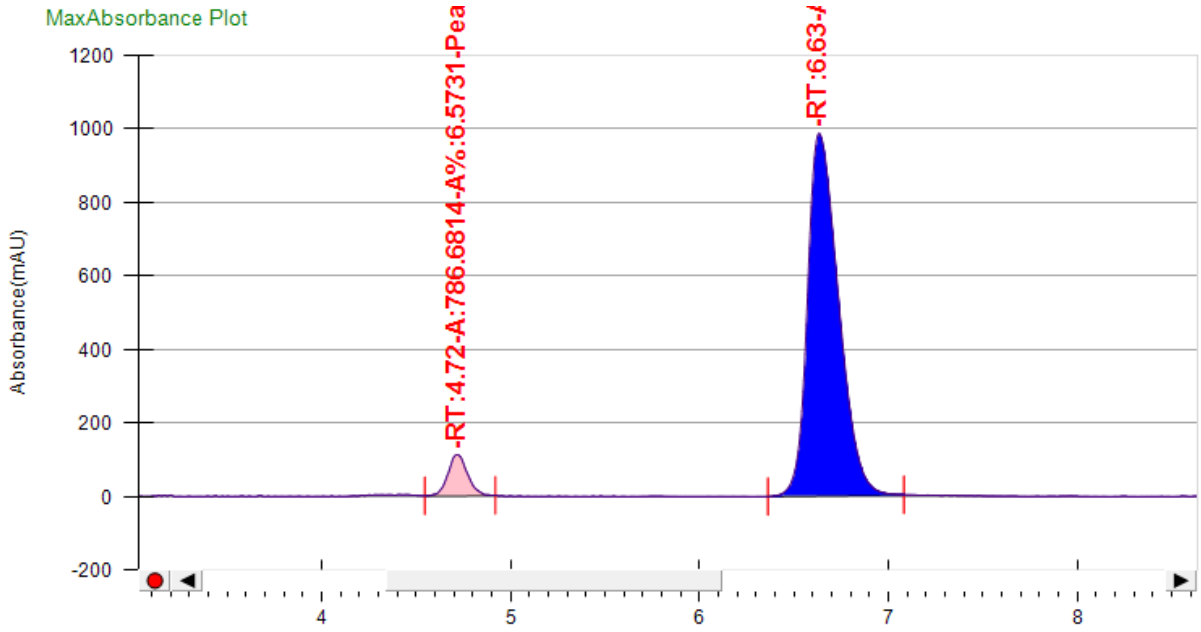
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

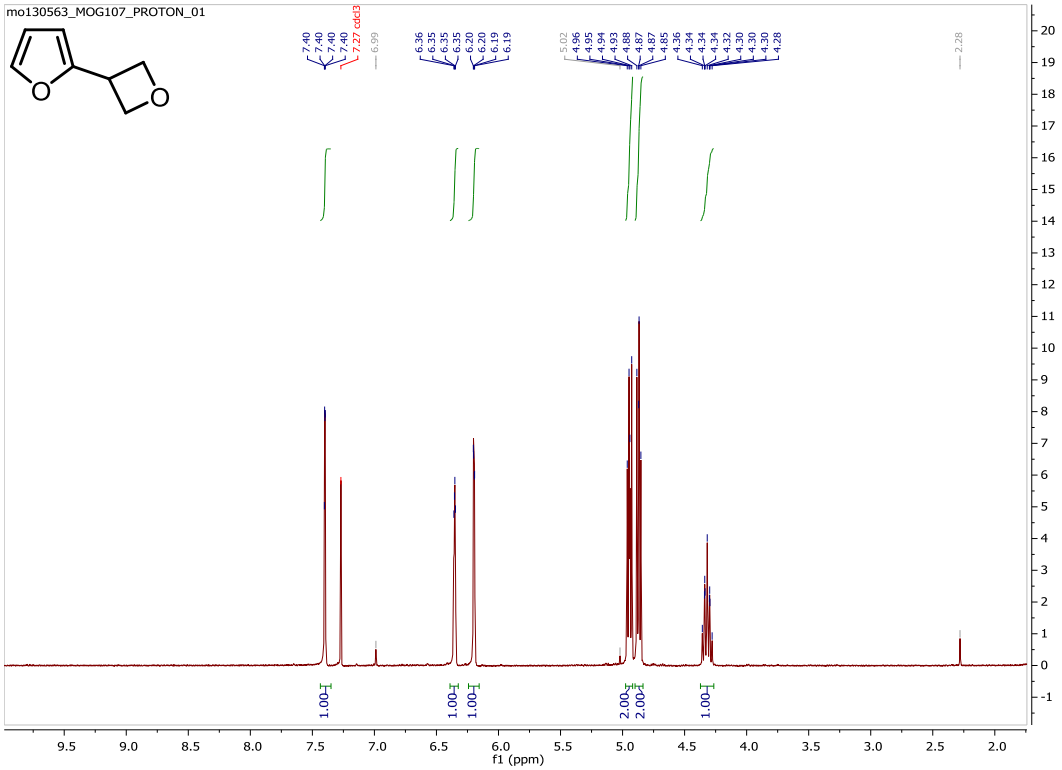


Chiral SFC traces: enantioenriched

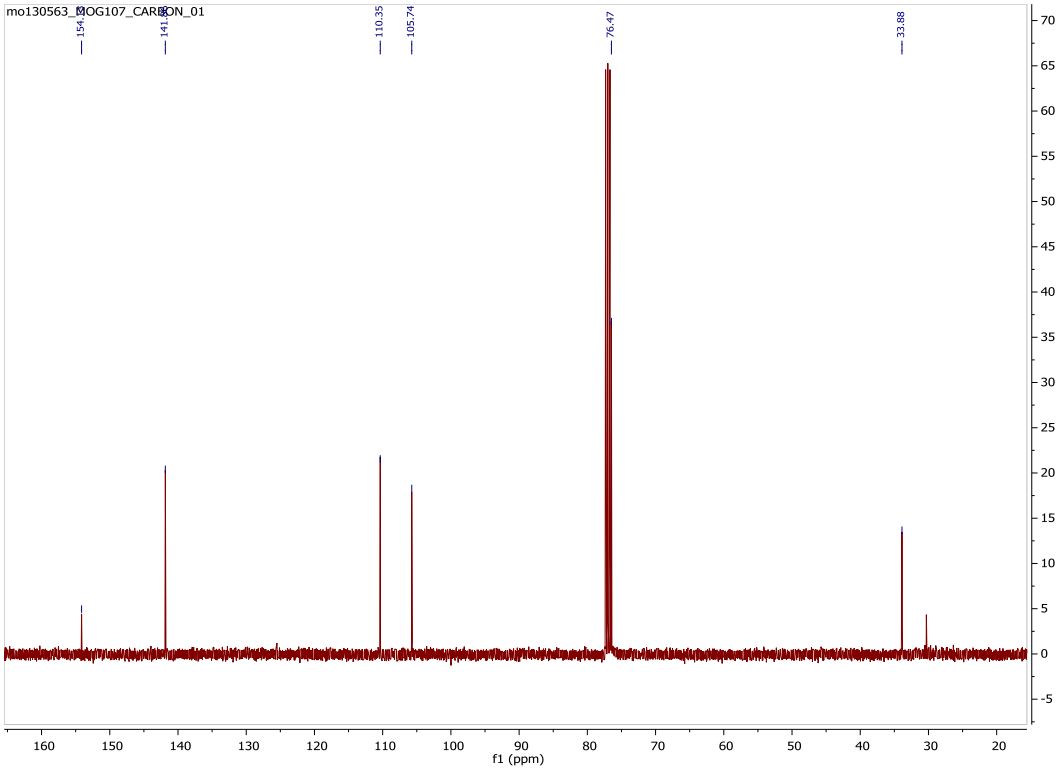


2r

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

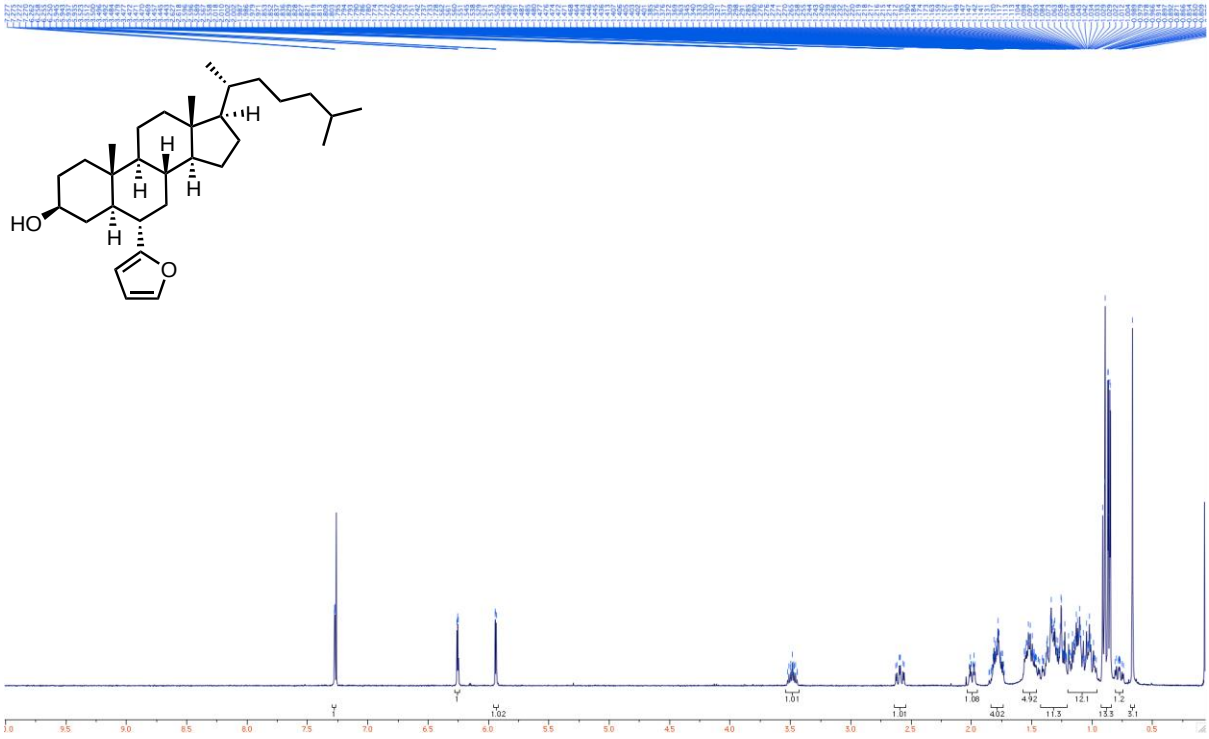


^{13}C NMR (100 MHz, $CDCl_3$)

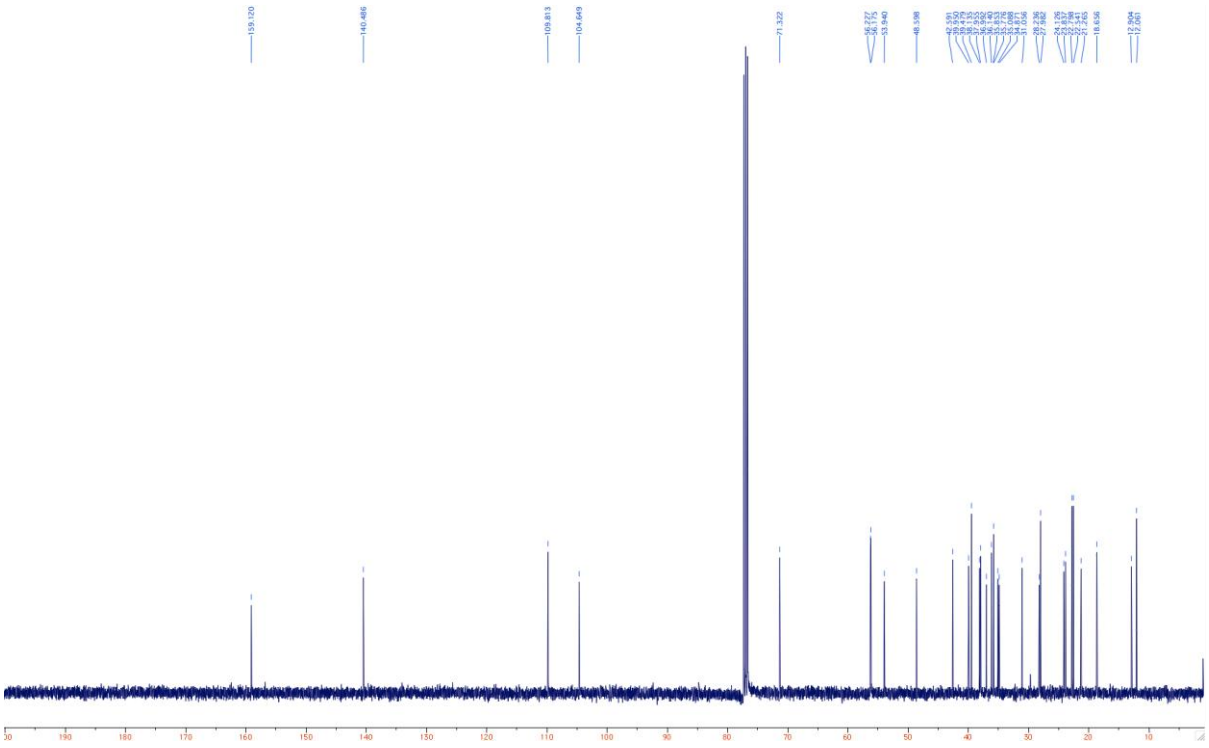


2o

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

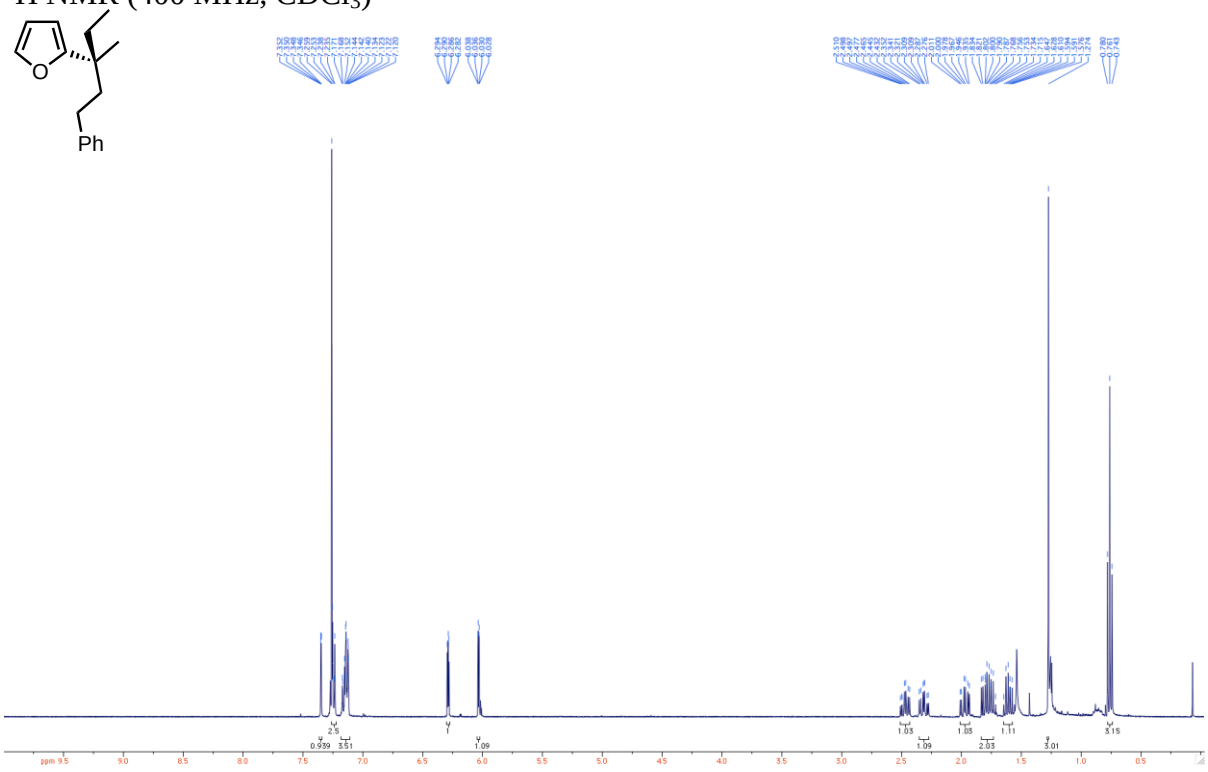


^{13}C NMR (100 MHz, $CDCl_3$)

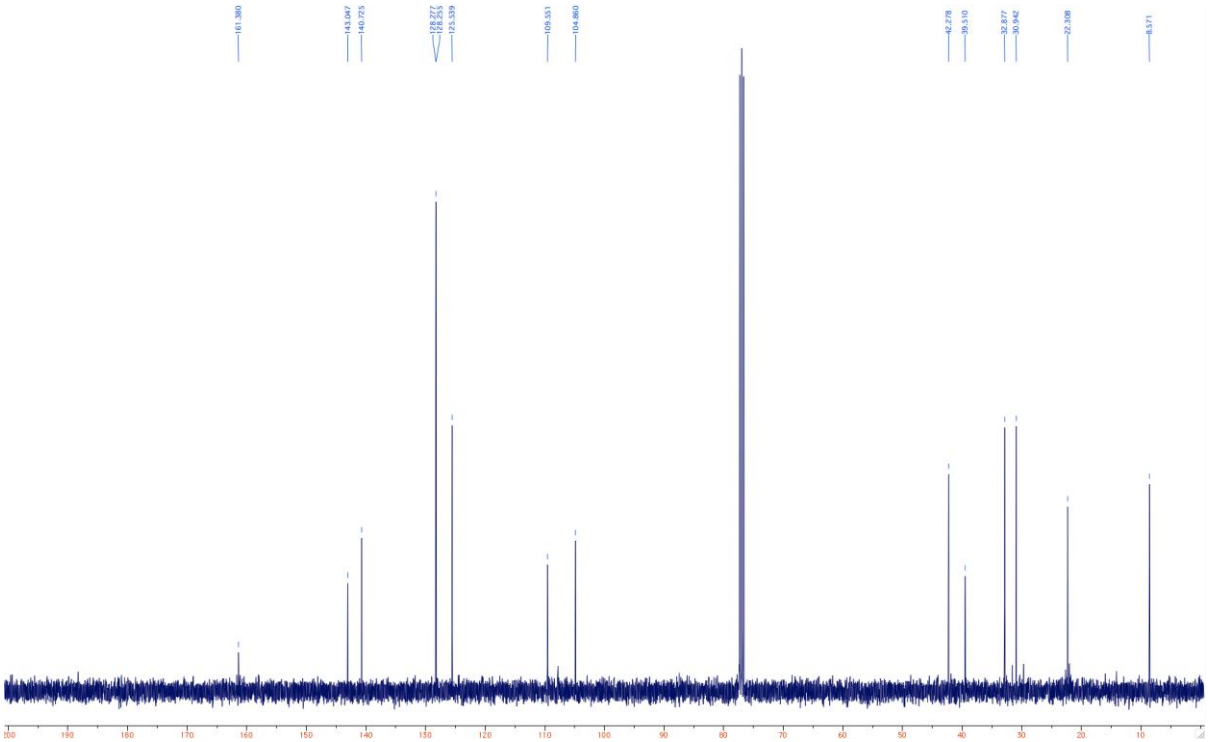


2g

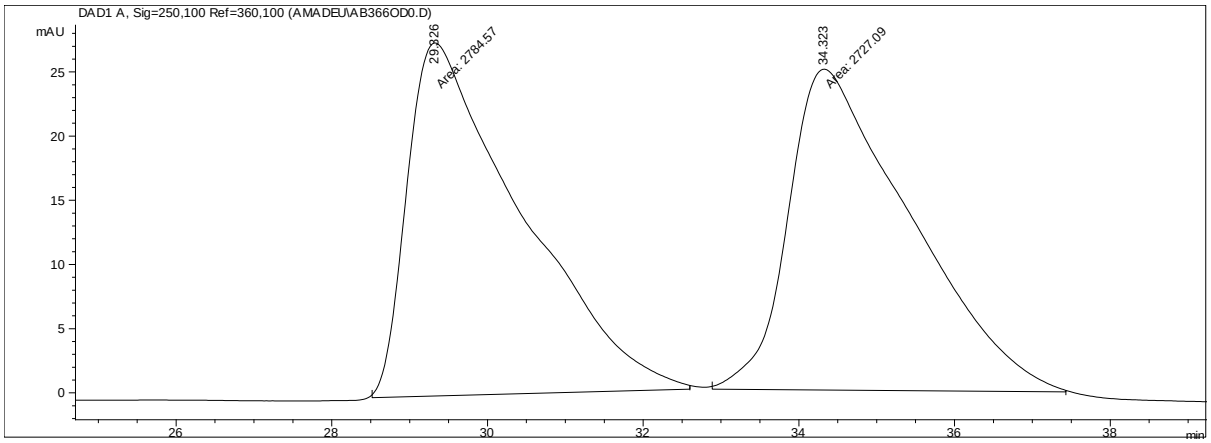
^{1}H NMR (400 MHz, $CDCl_3$)



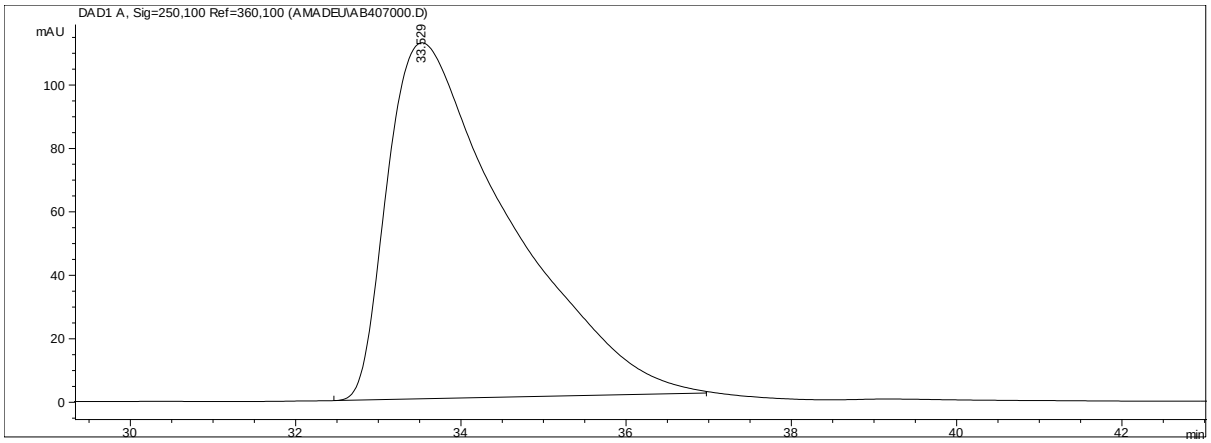
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

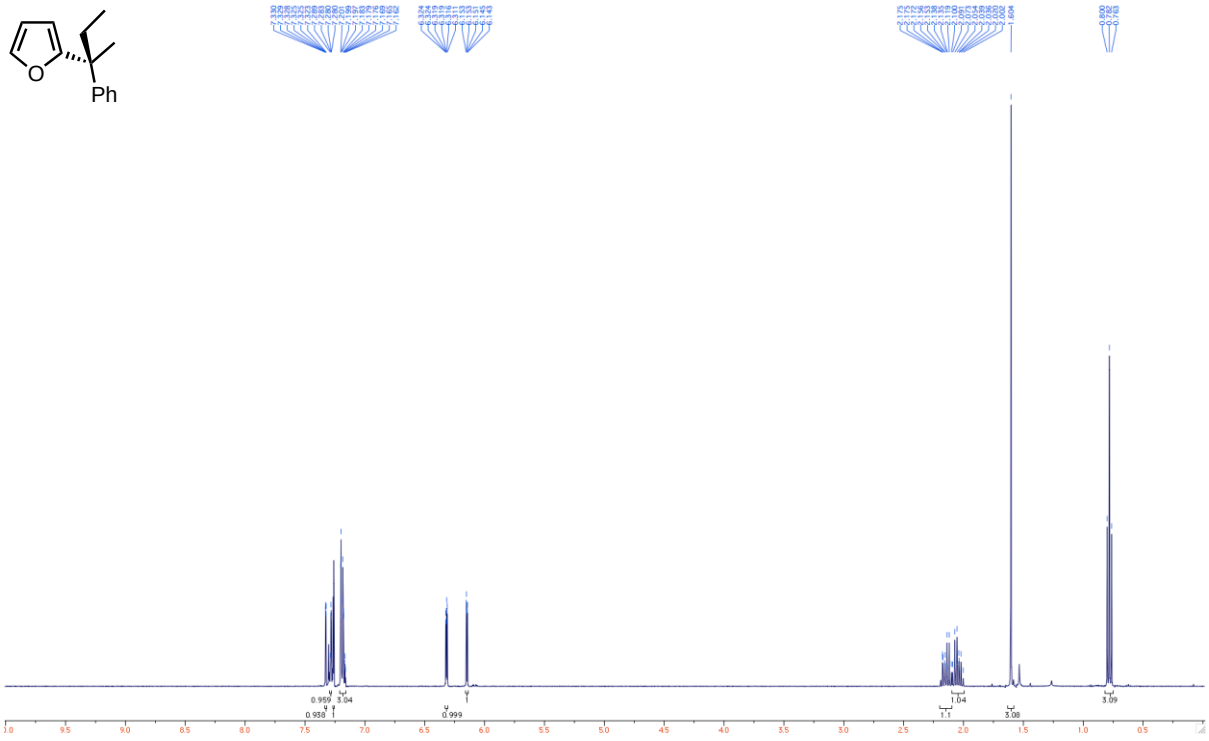


Chiral HPLC traces: enantioenriched

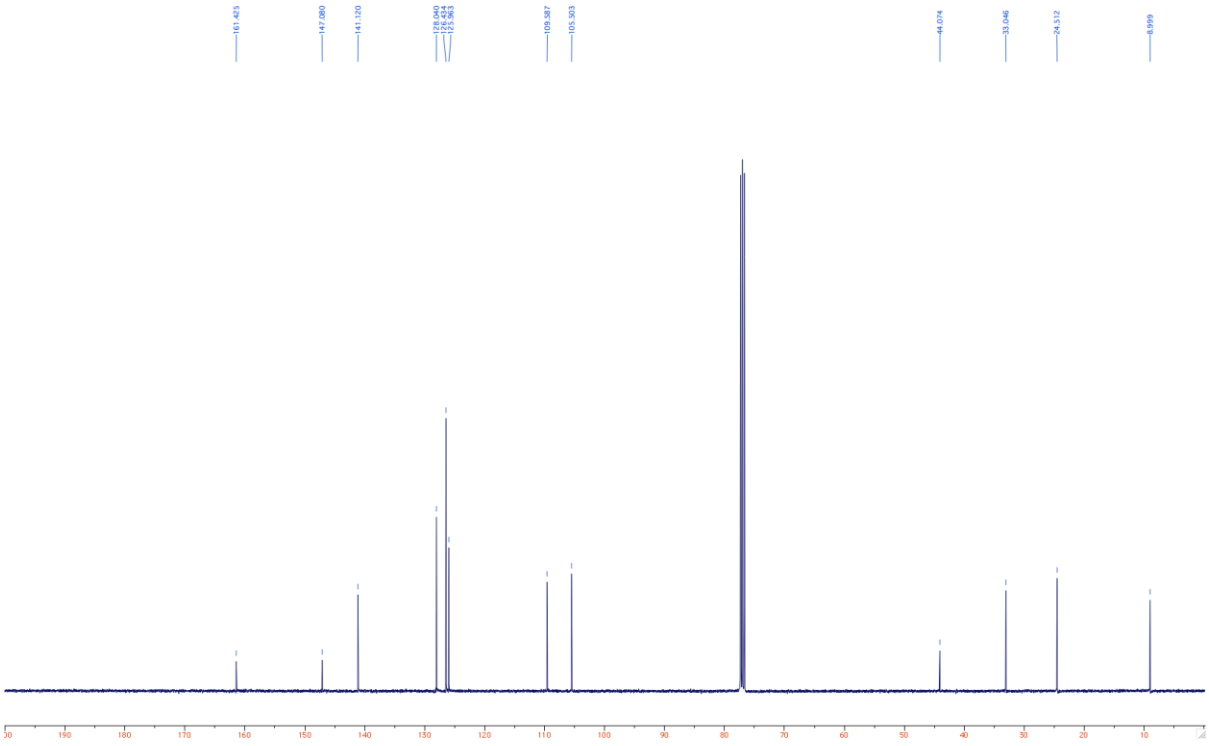


2h

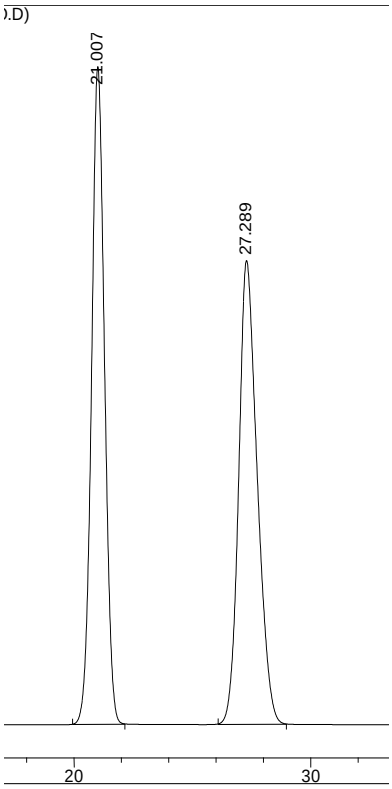
^{1}H NMR (400 MHz, $CDCl_3$)



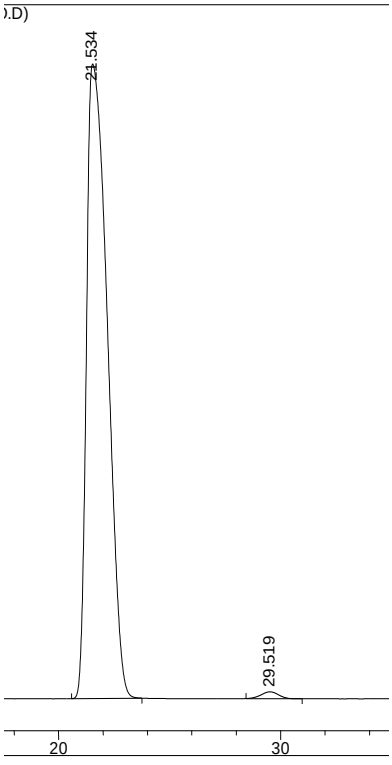
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

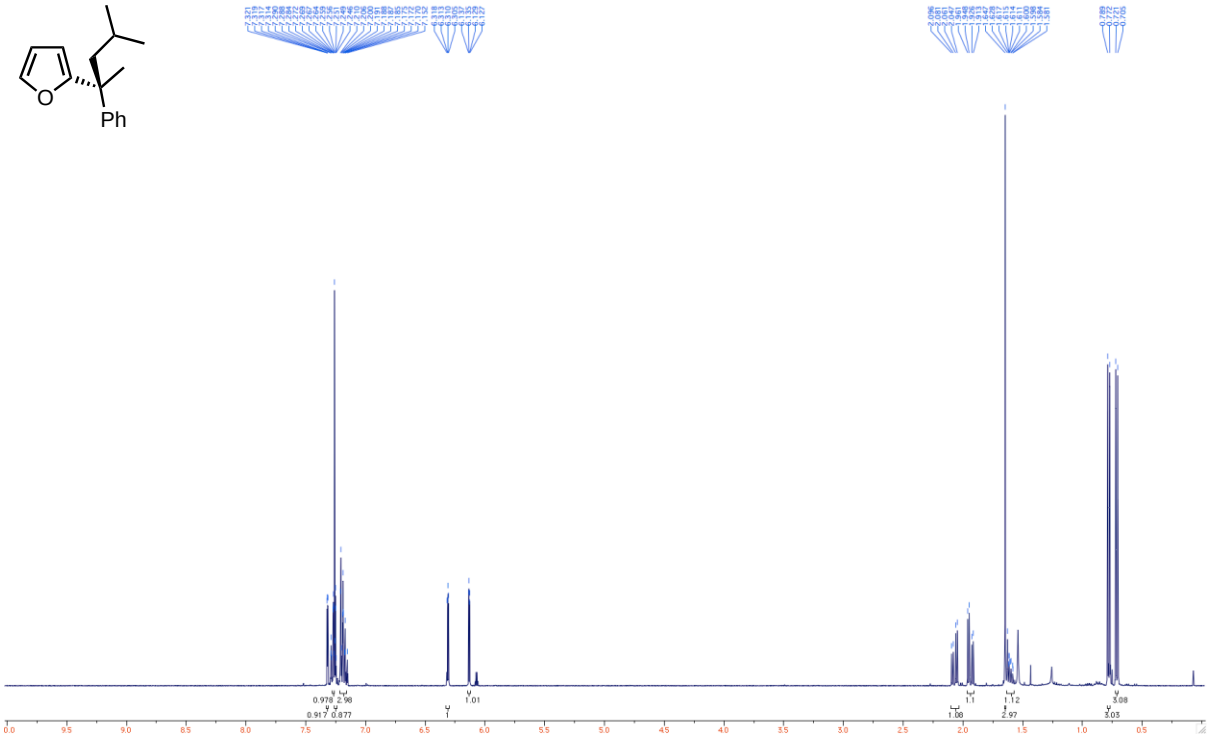


Chiral HPLC traces: enantioenriched

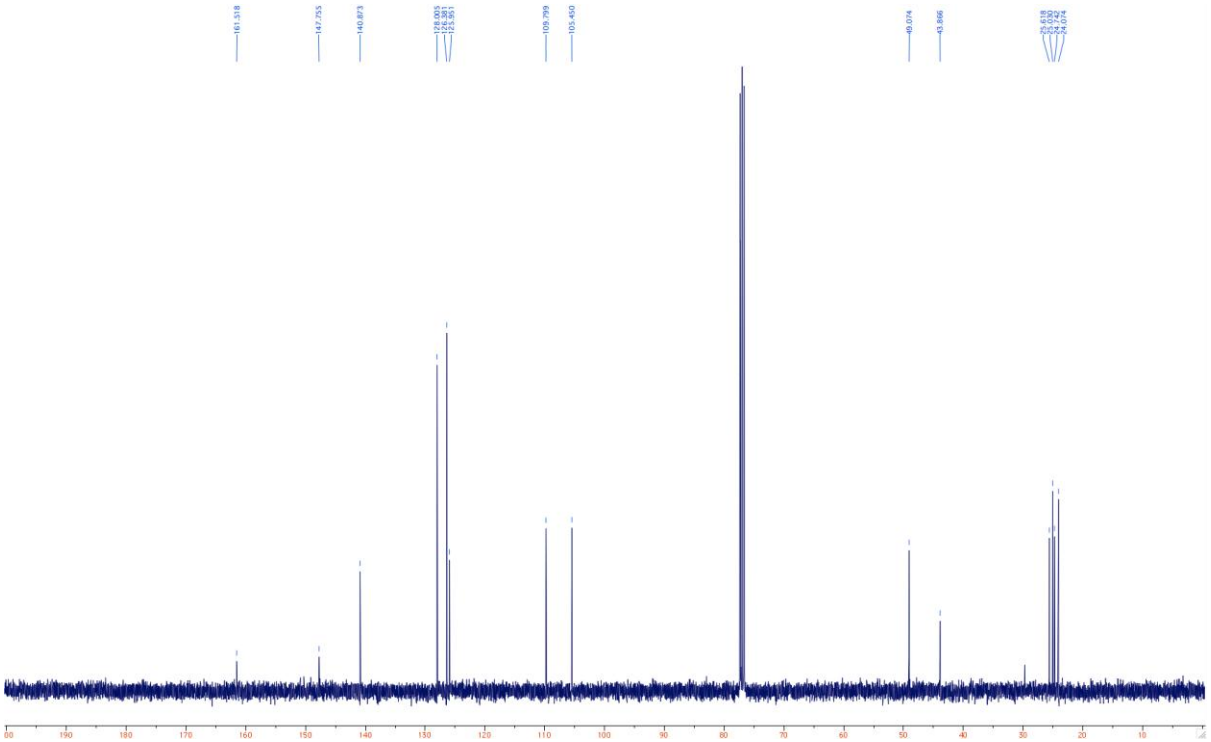


2i

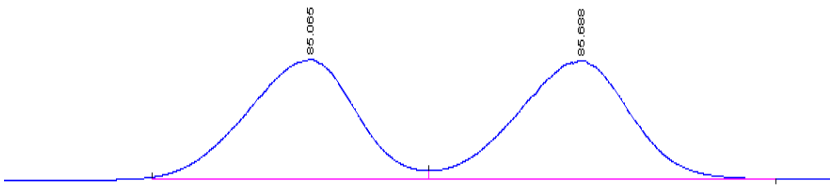
^{1}H NMR (400 MHz, $CDCl_3$)



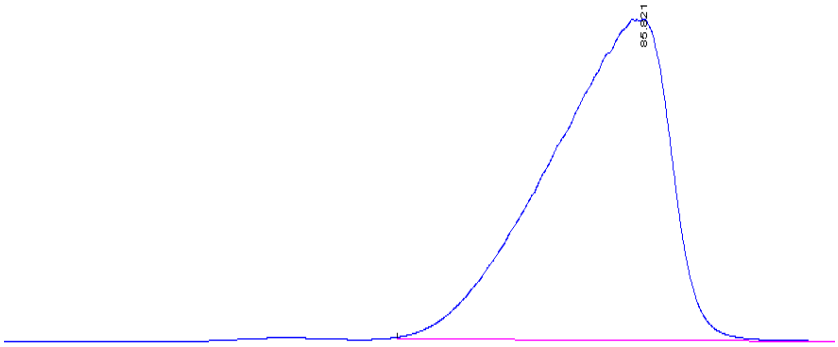
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral GC traces: racemic

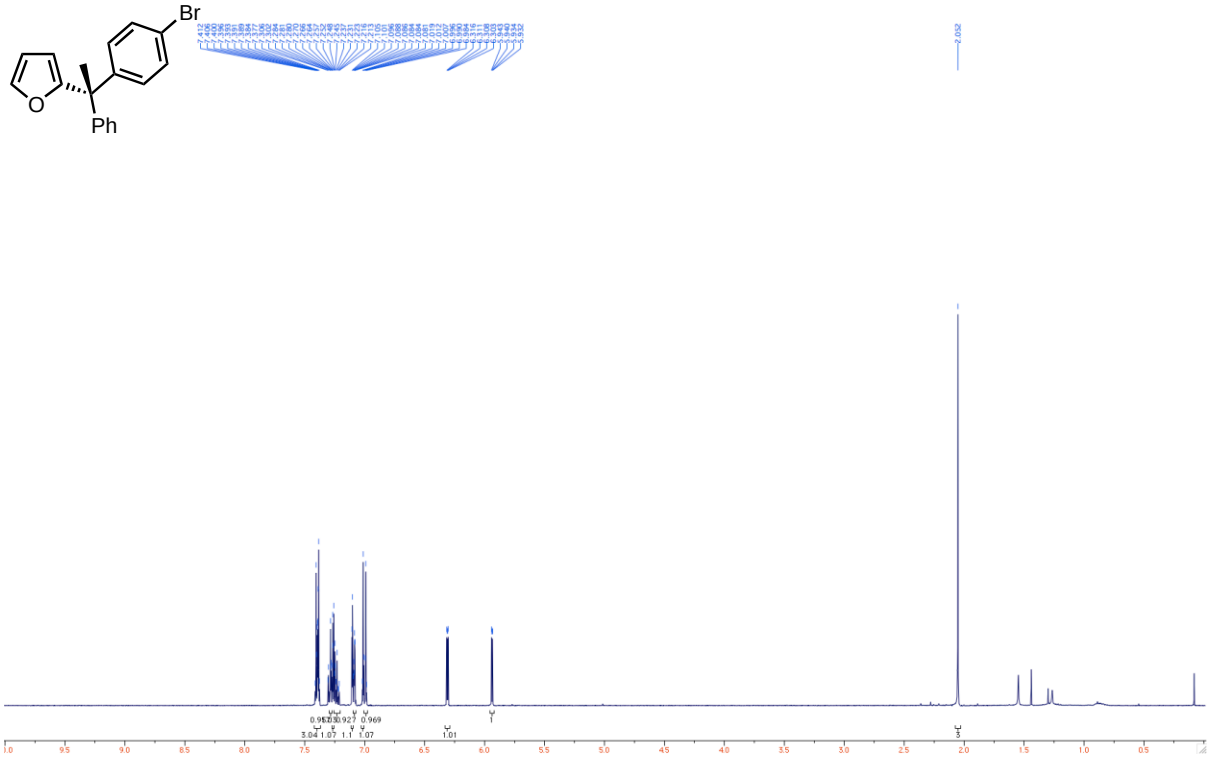


Chiral GC traces: enantioenriched

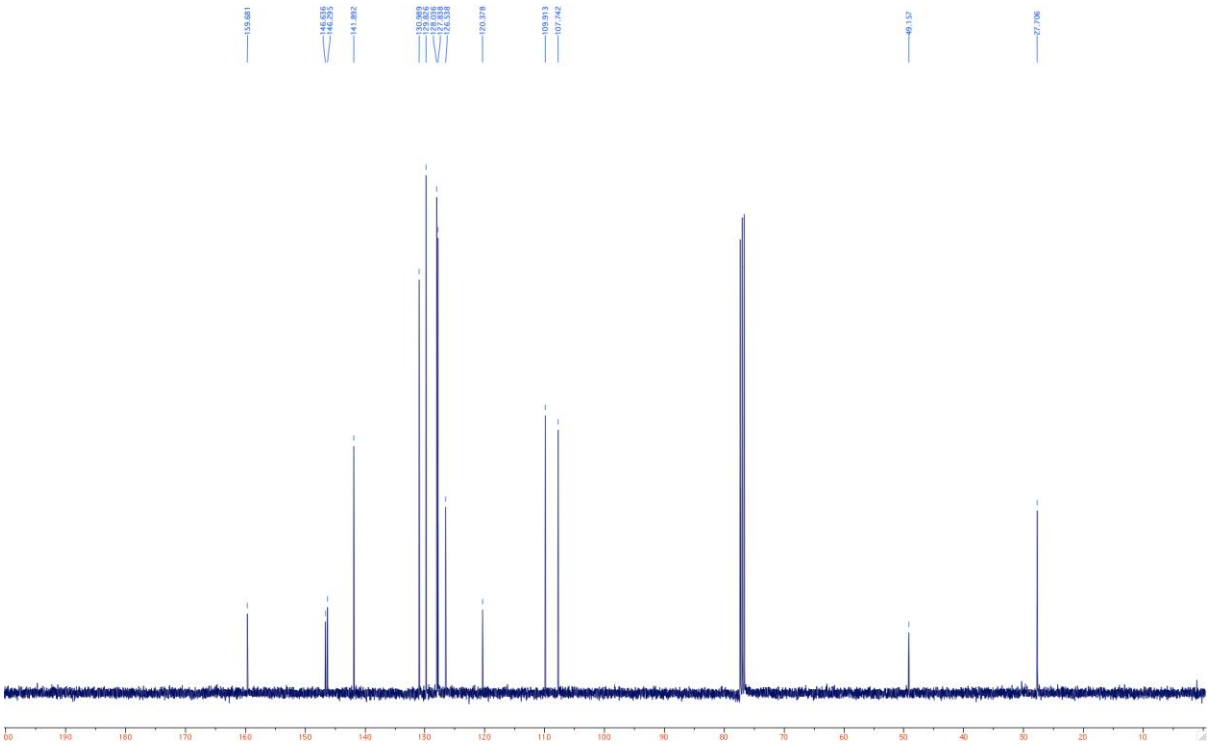


2j

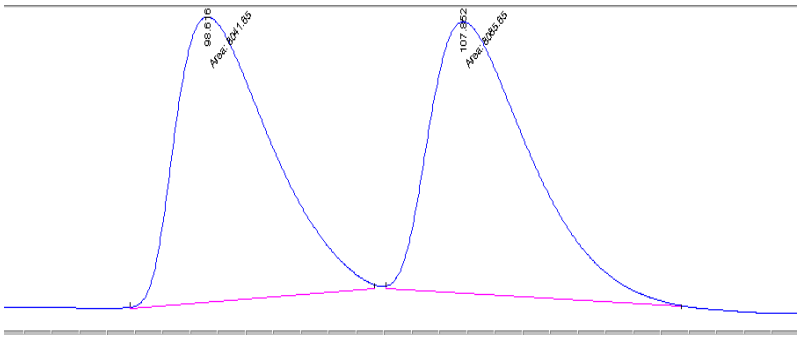
^{1}H NMR (400 MHz, $CDCl_3$)



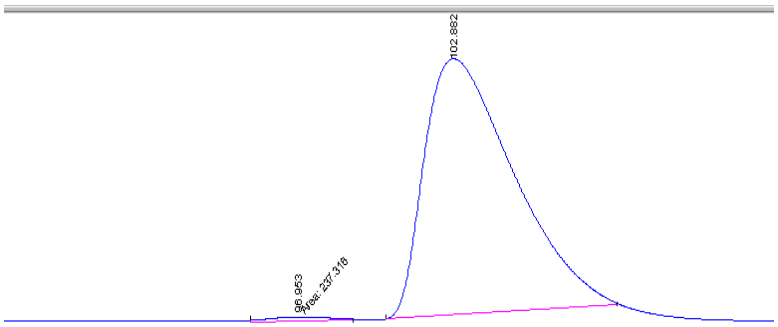
^{13}C NMR (100 MHz, $CDCl_3$)



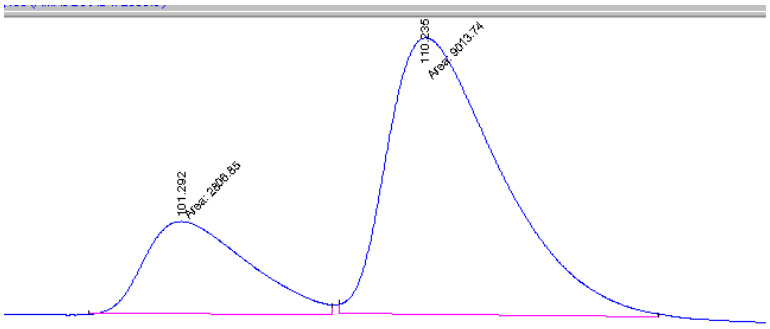
Chiral HPLC traces: racemic



Chiral HPLC traces: enantioenriched

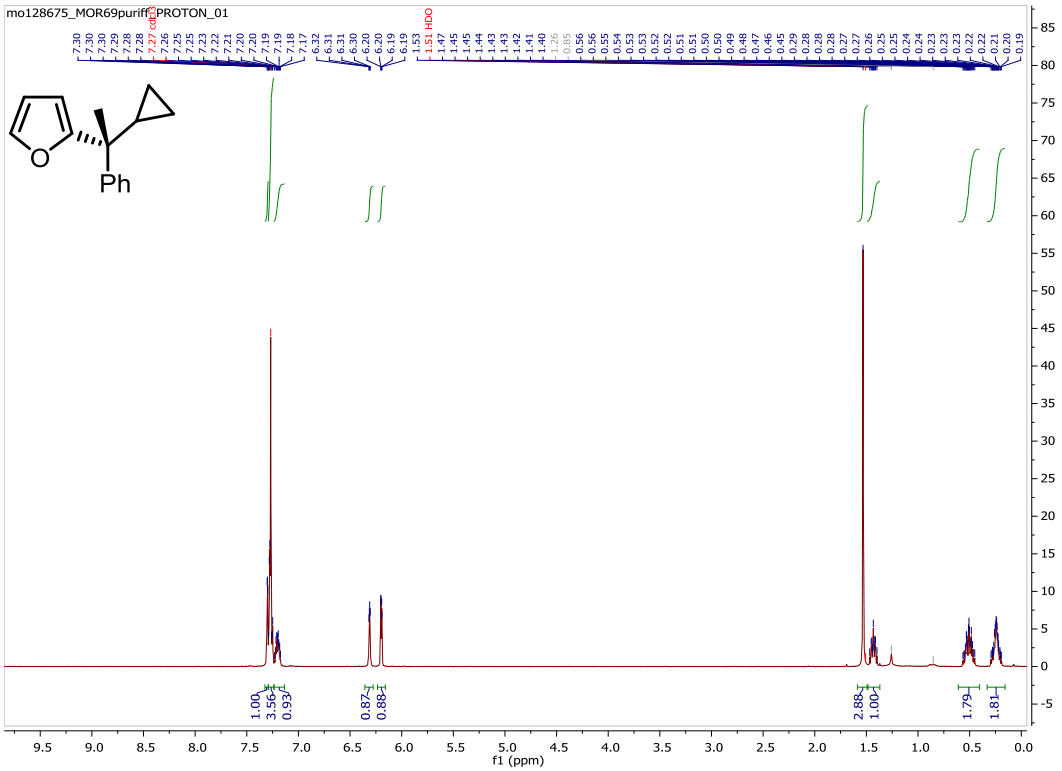


Chiral HPLC traces: racemic + enantioenriched

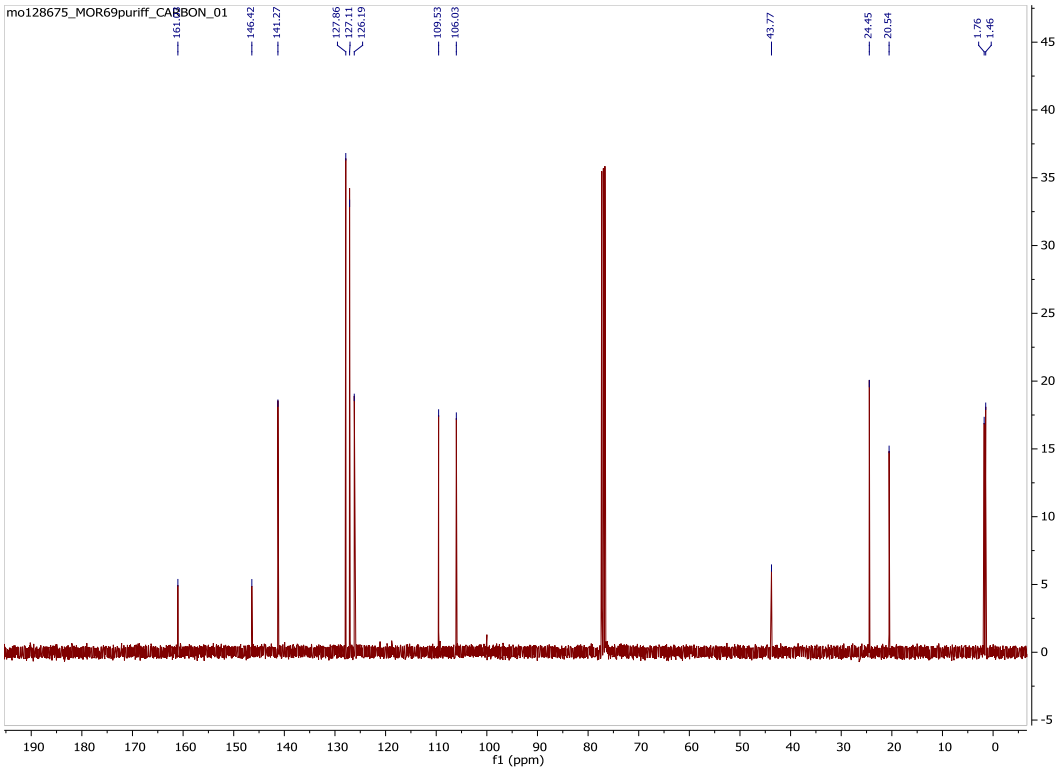


2k

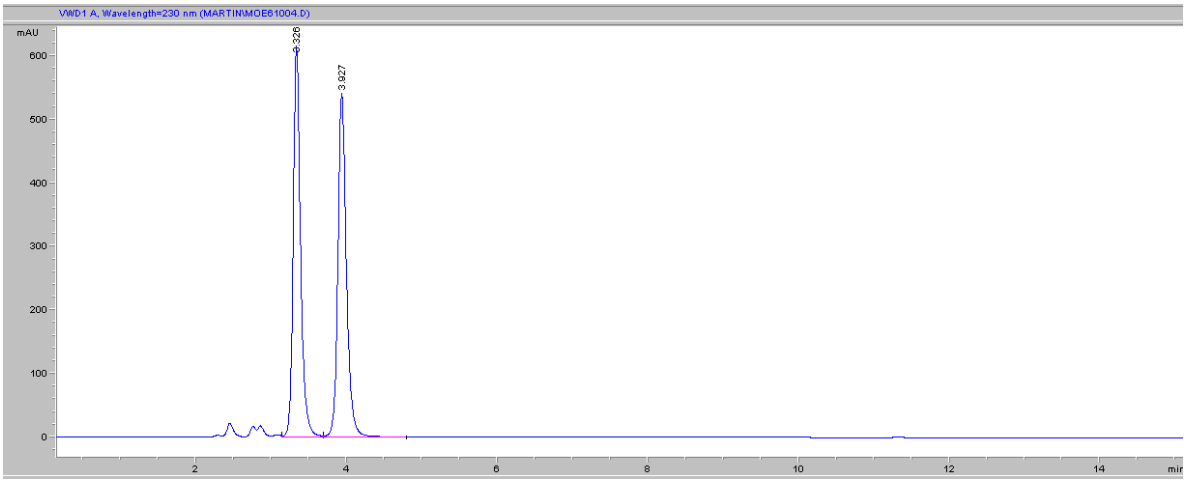
^{1}H NMR (400 MHz, $CDCl_3$)



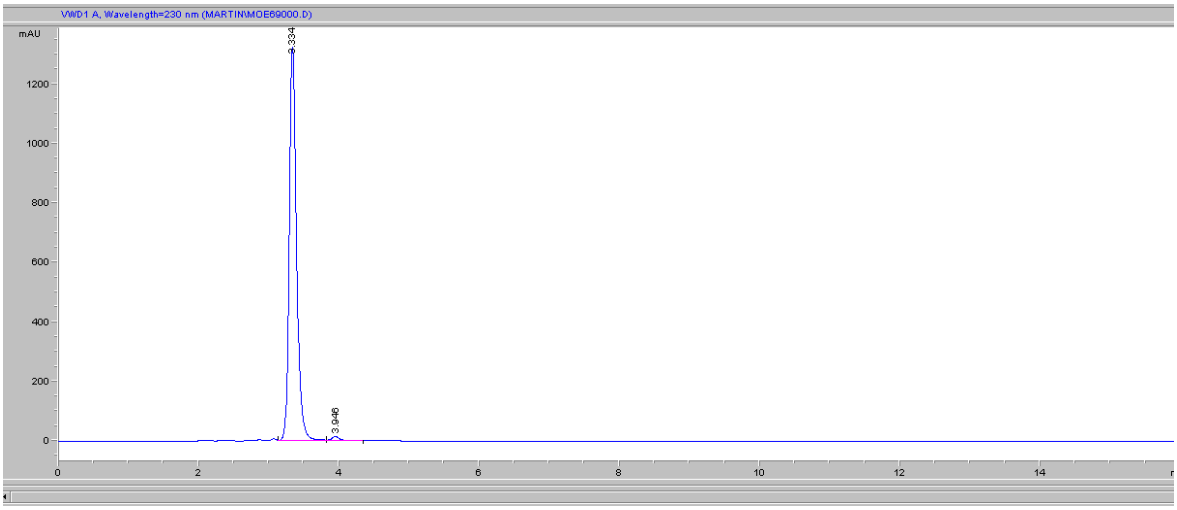
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

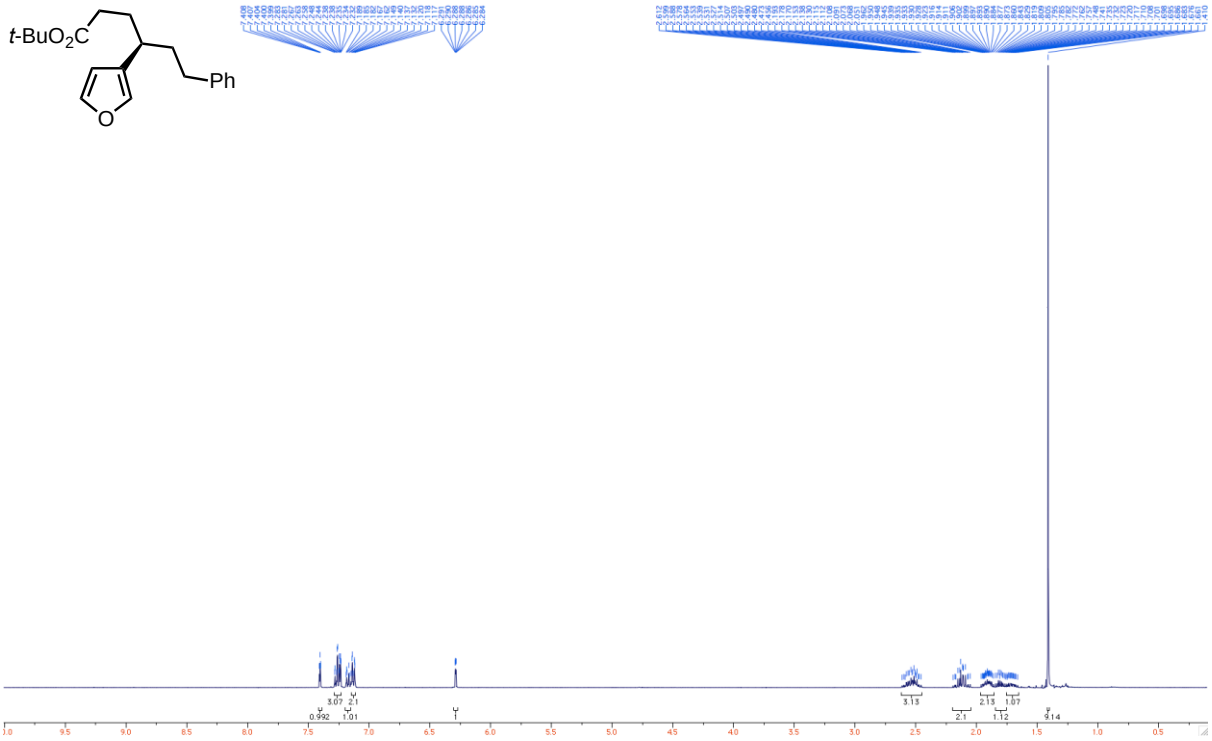


Chiral HPLC traces: enantioenriched

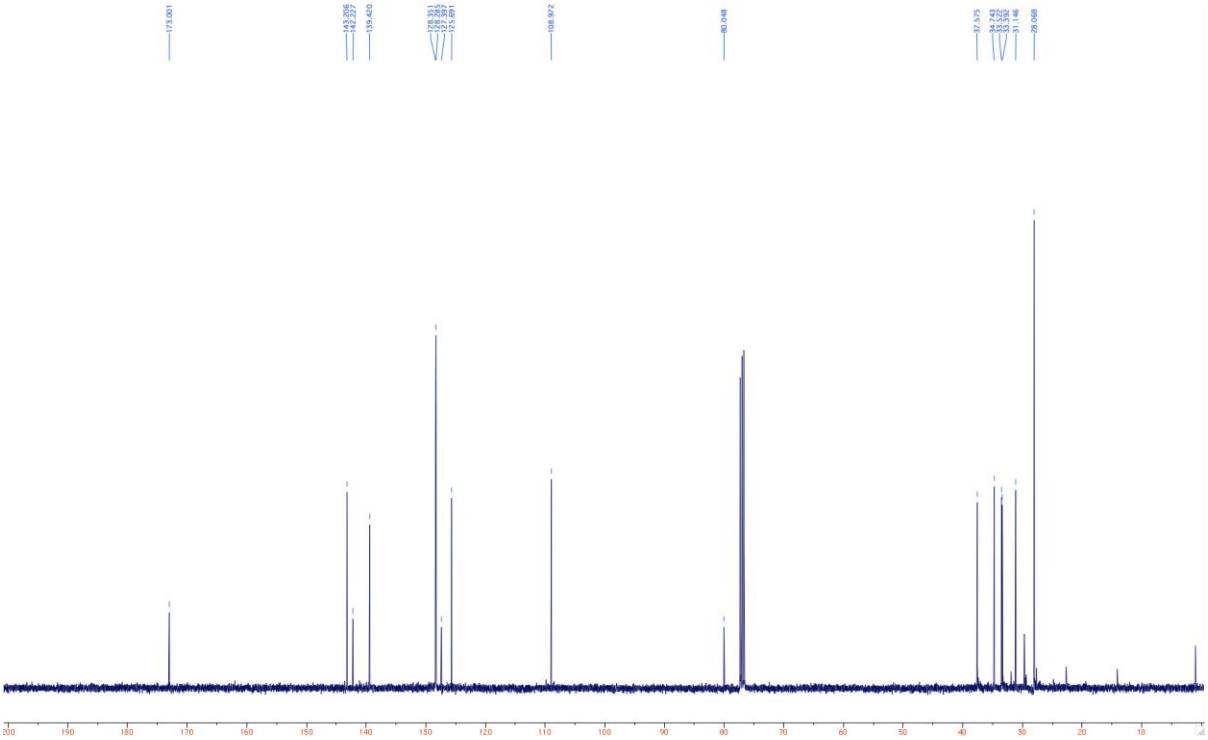


3e

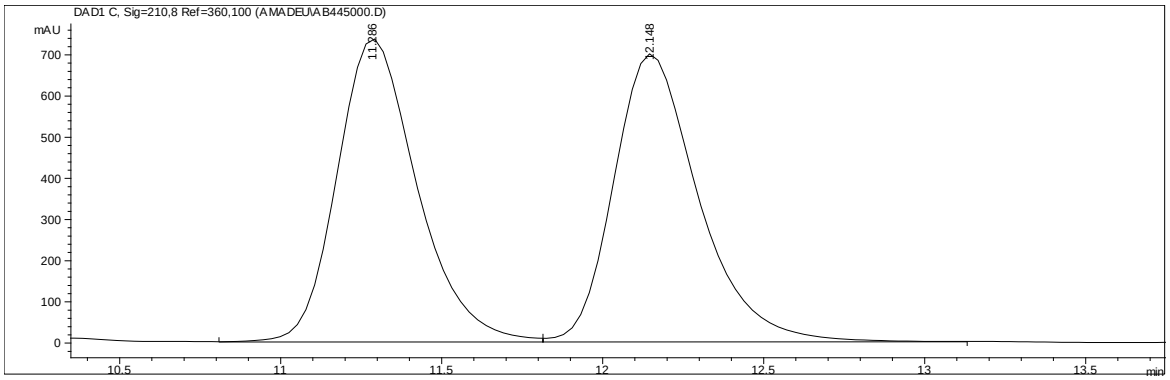
^{1}H NMR (400 MHz, $CDCl_3$)



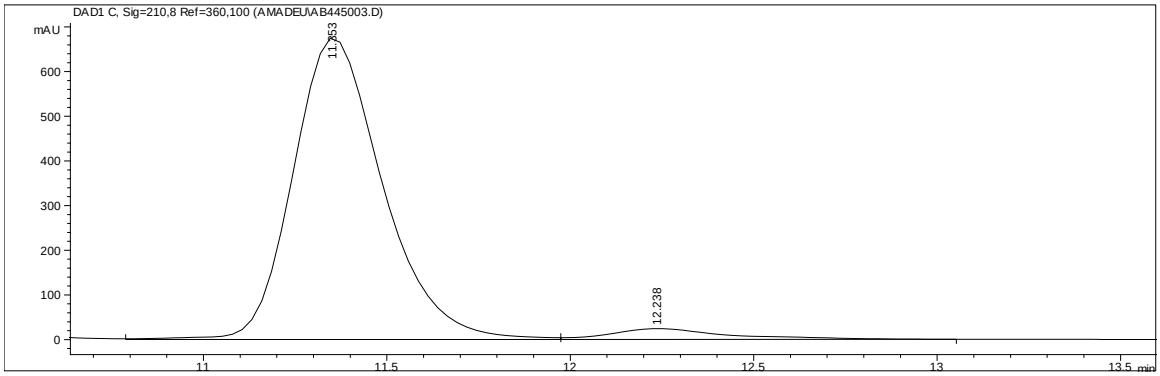
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

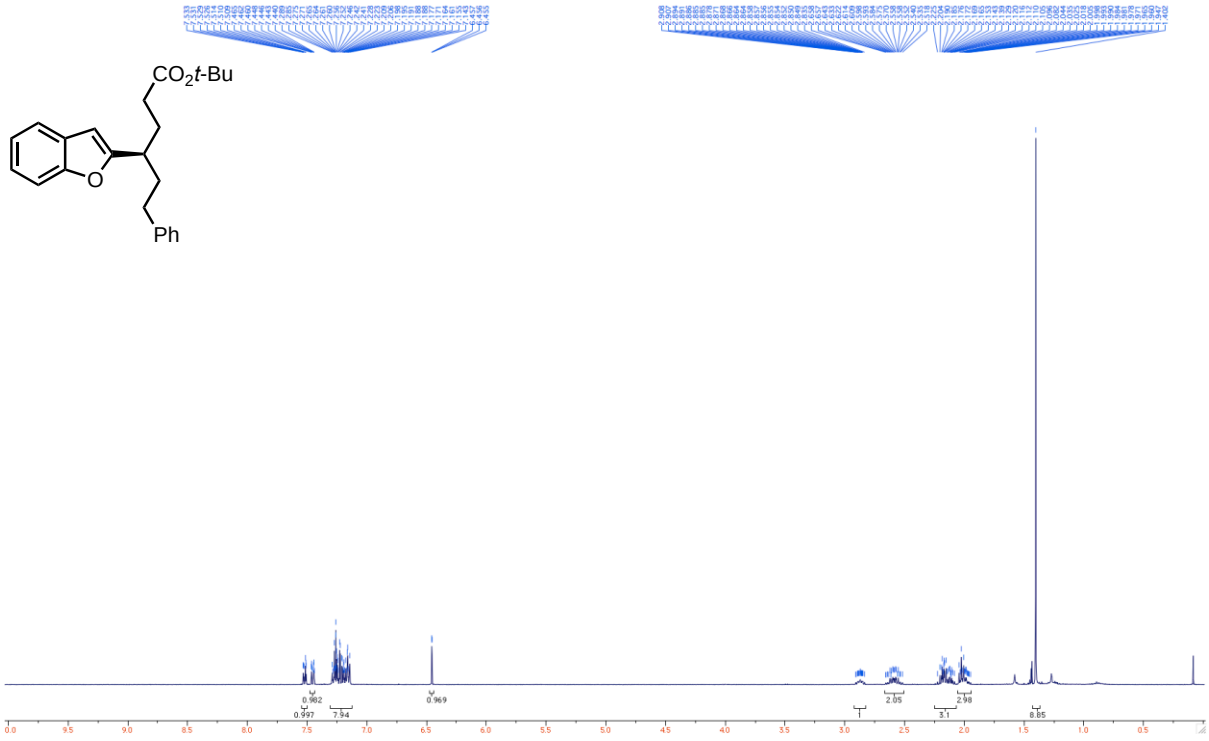


Chiral HPLC traces: enantioenriched

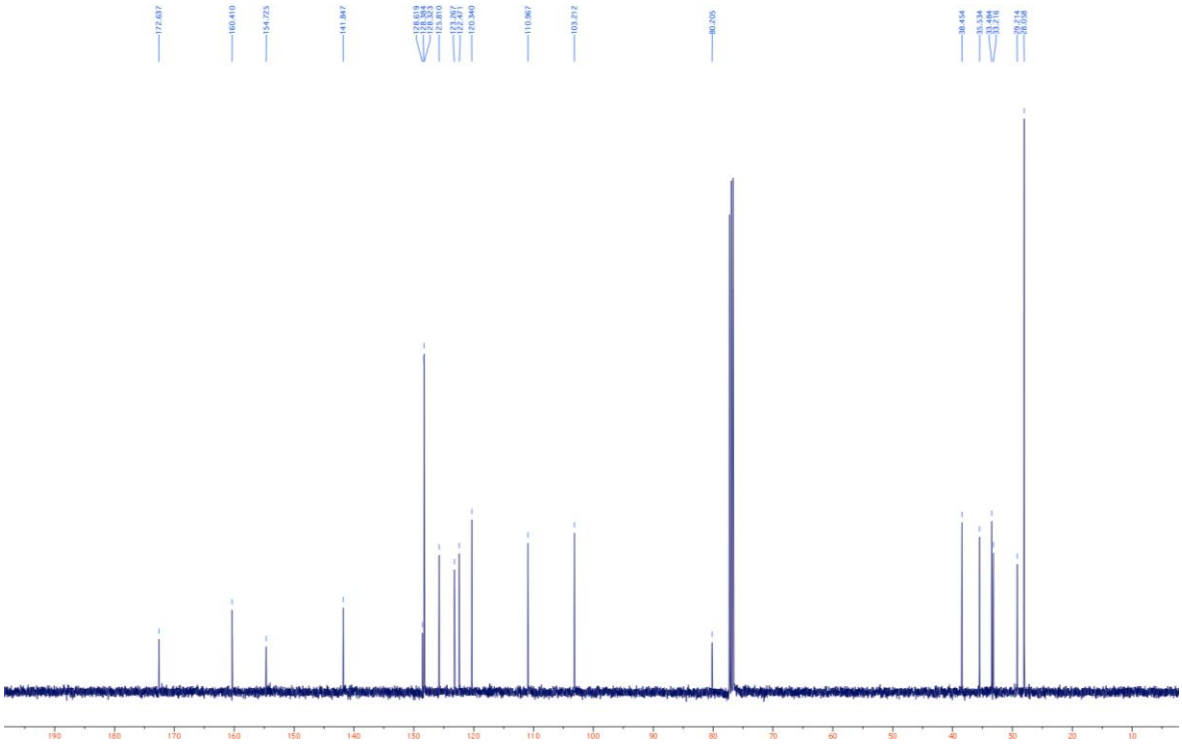


4e

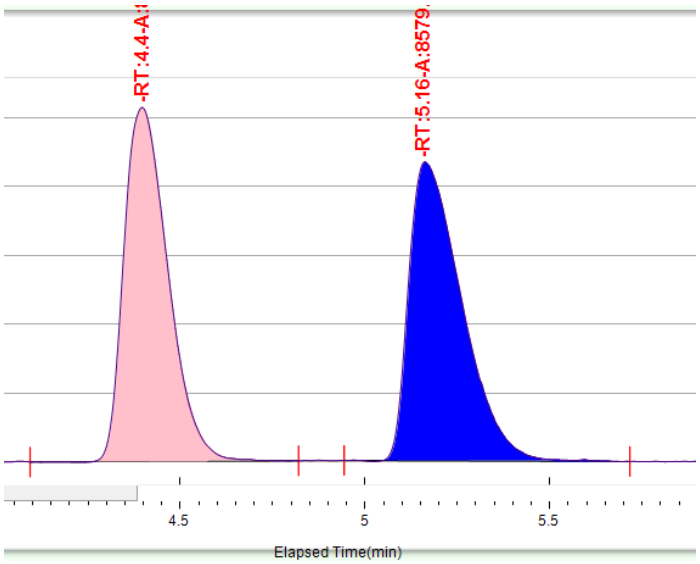
^{1}H NMR (400 MHz, $CDCl_3$)



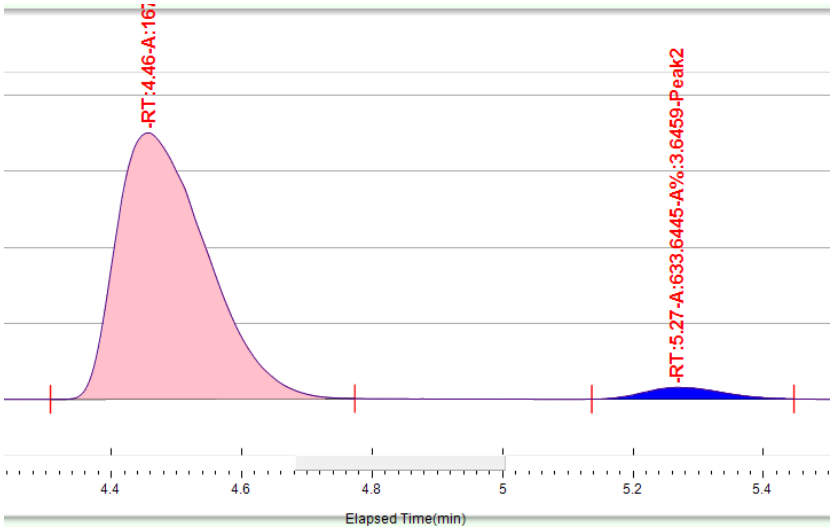
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

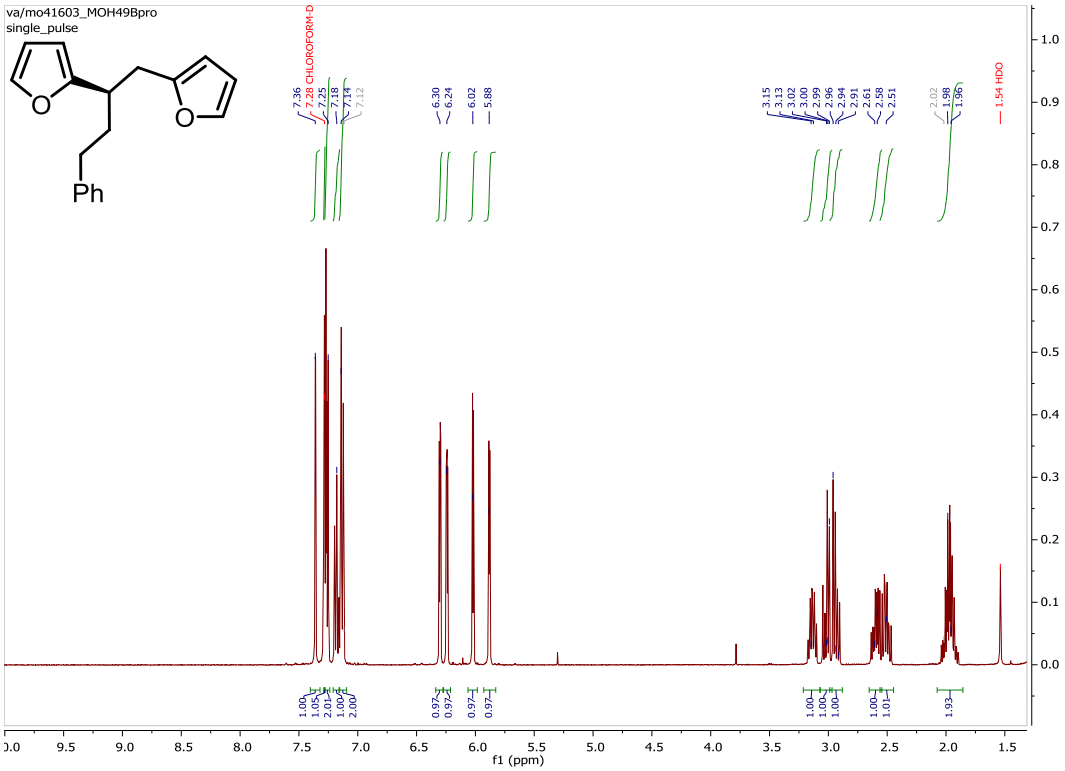


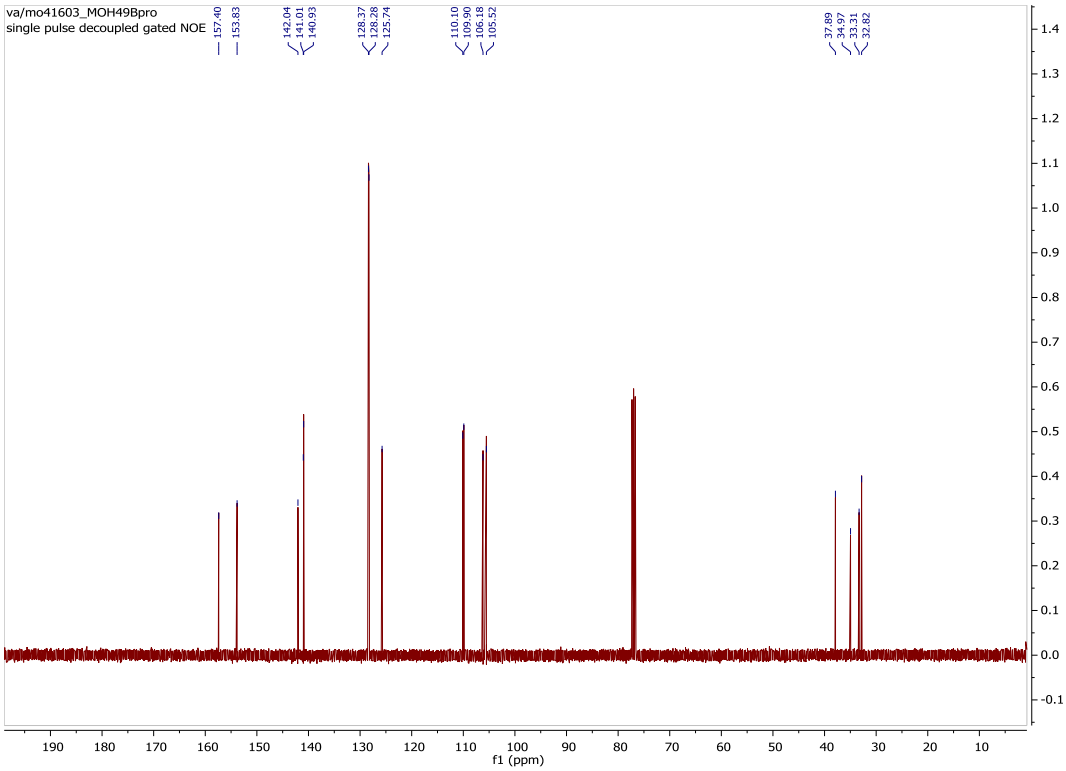
Chiral SFC traces: enantioenriched



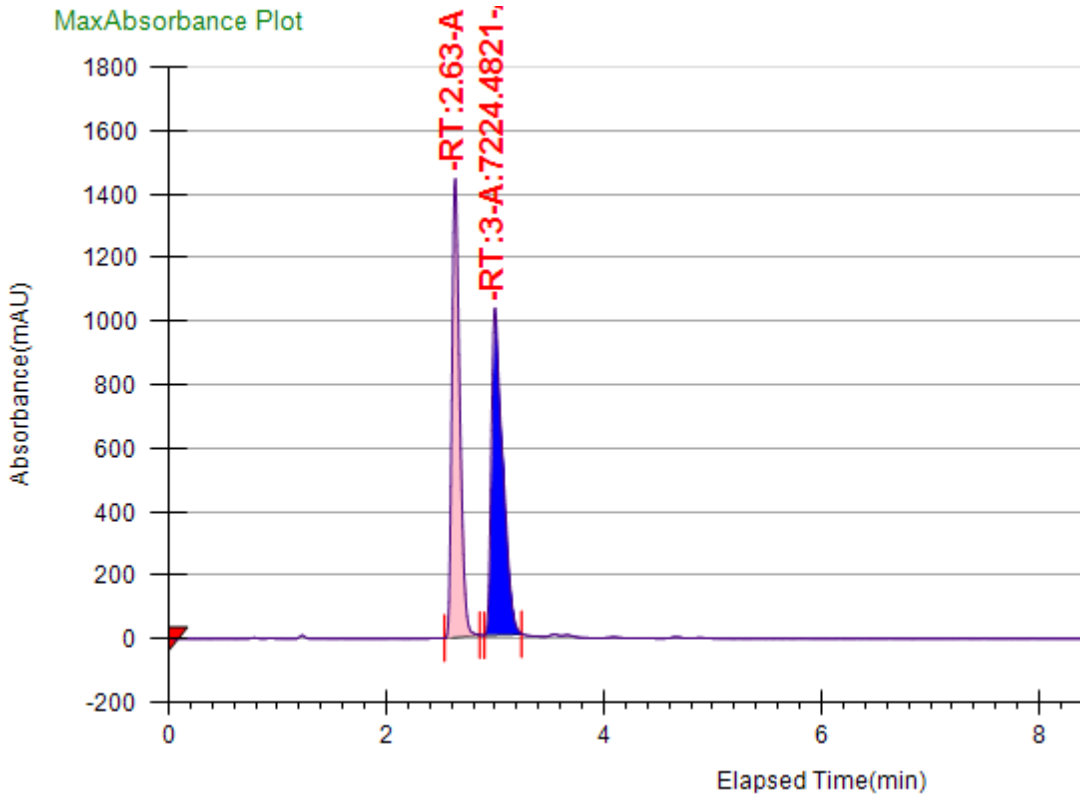
2u

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

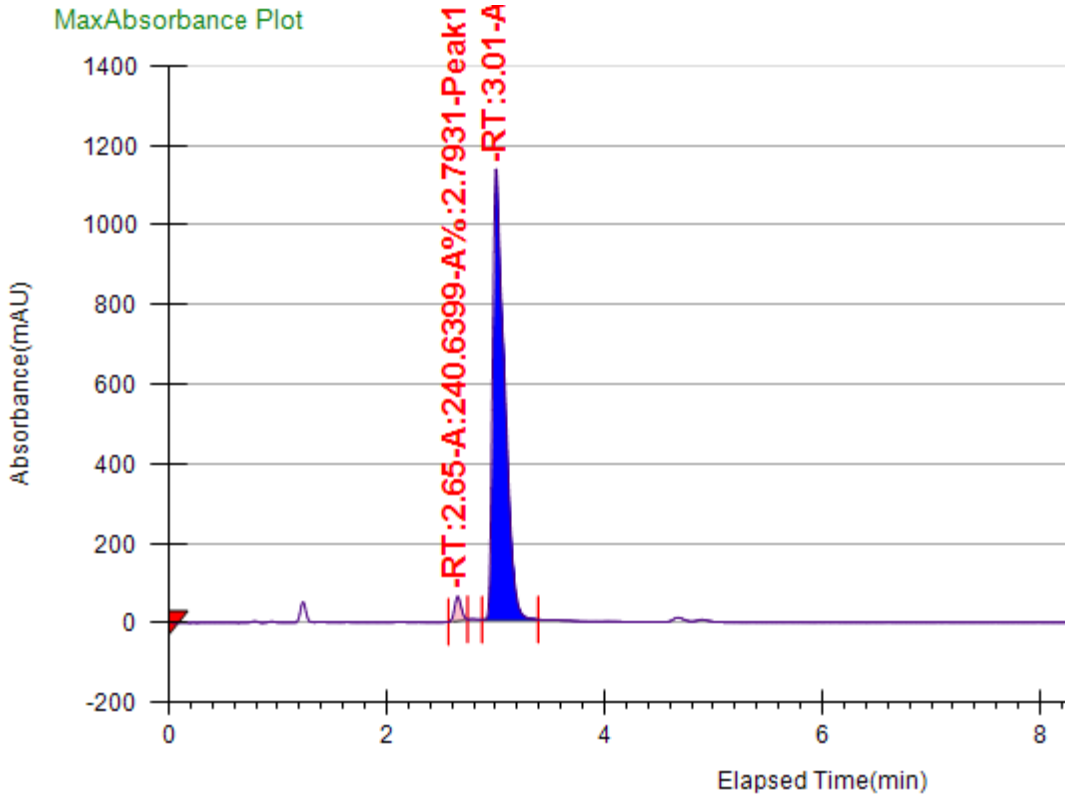




Chiral HPLC traces: racemic

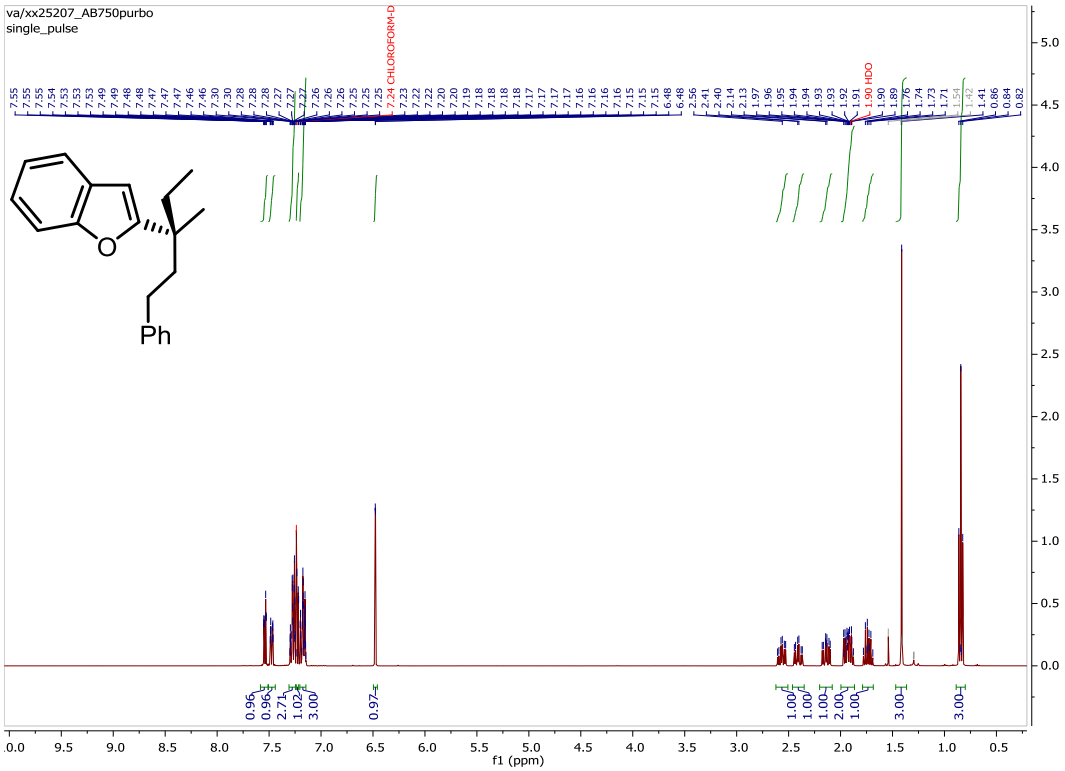


Chiral HPLC traces: enantioenriched

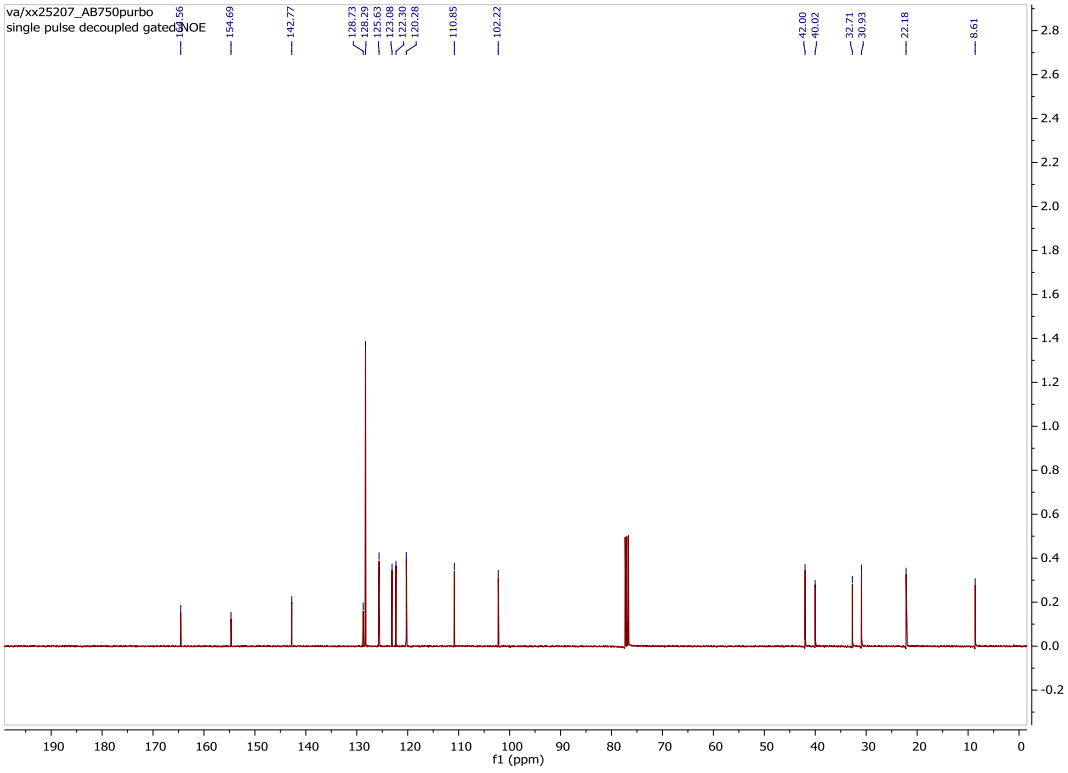


4g

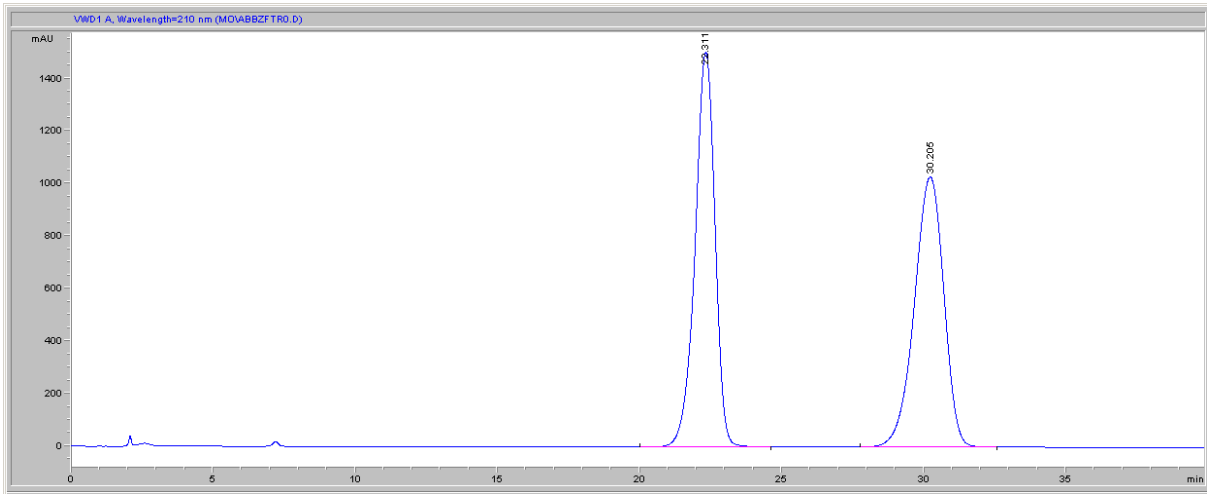
^{1}H NMR (400 MHz, $CDCl_3$)



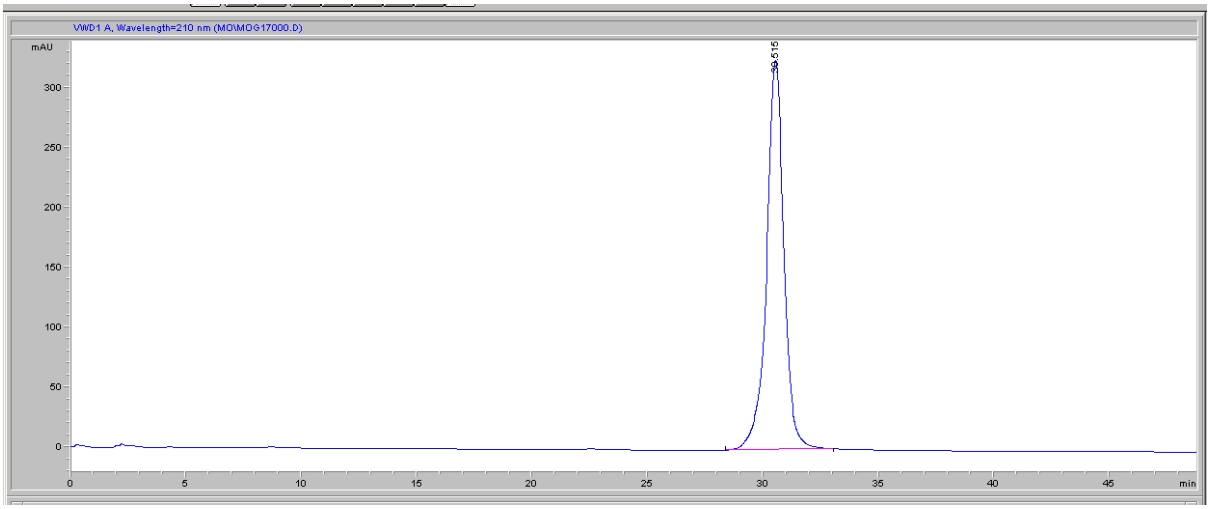
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

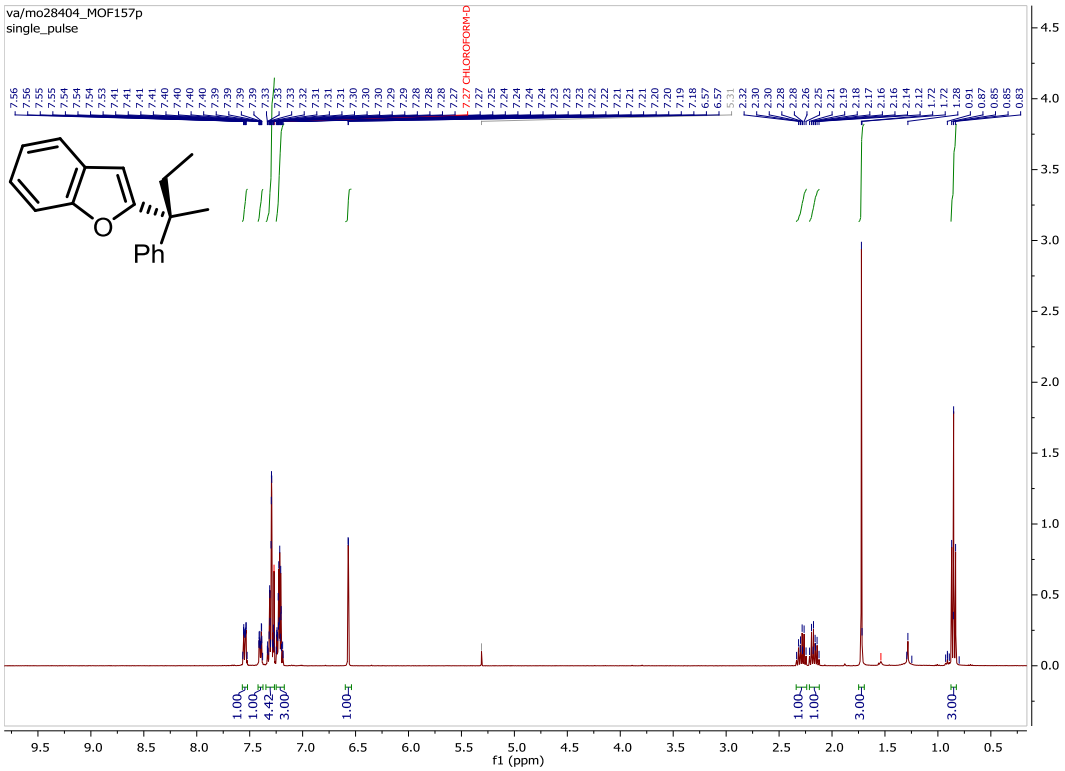


Chiral HPLC traces: enantioenriched

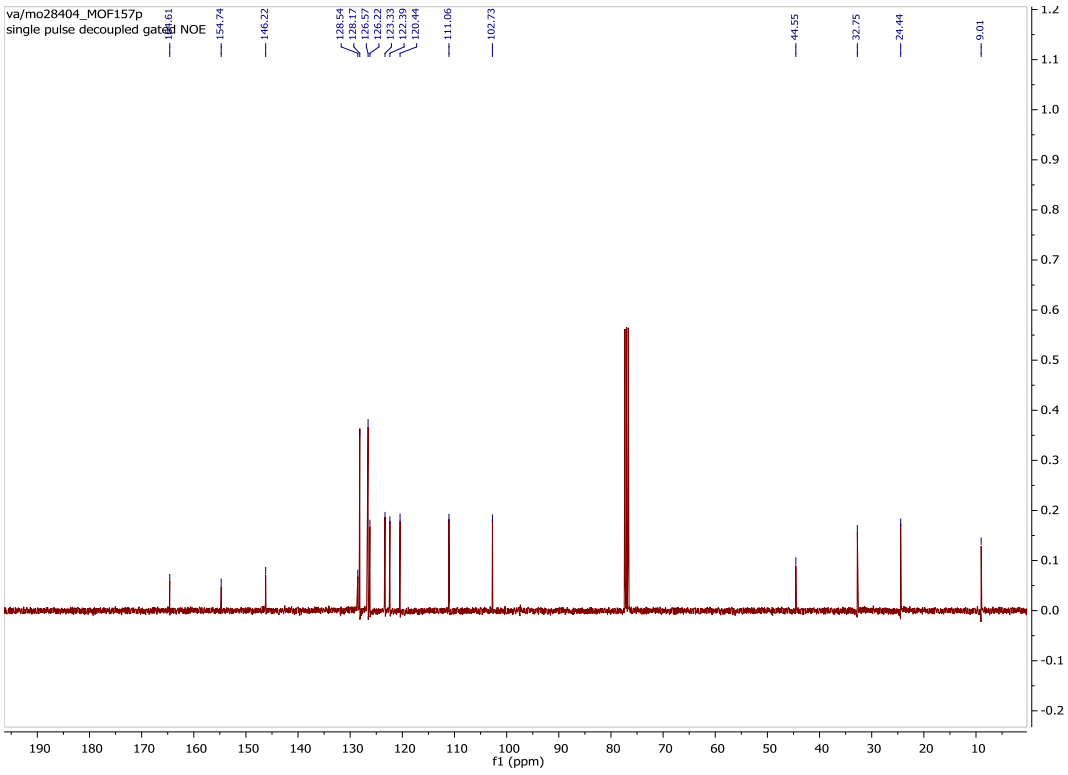


4h

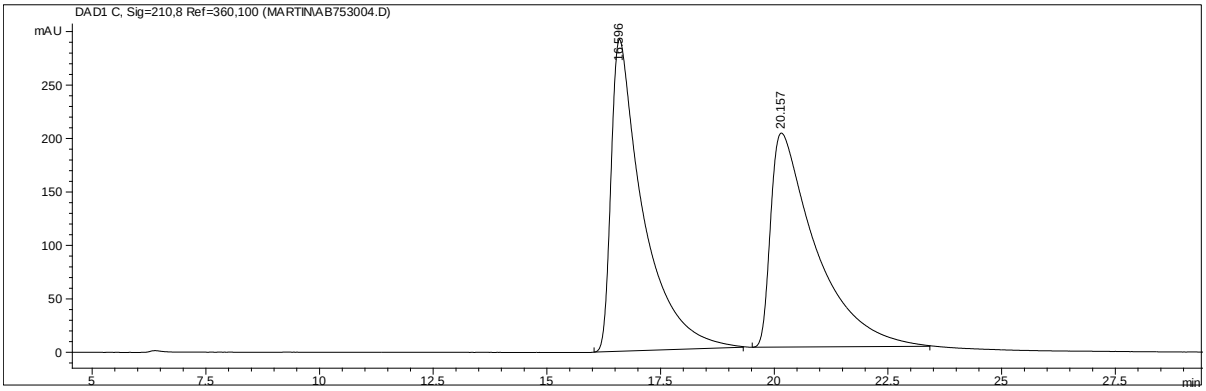
^{1}H NMR (400 MHz, $CDCl_3$)



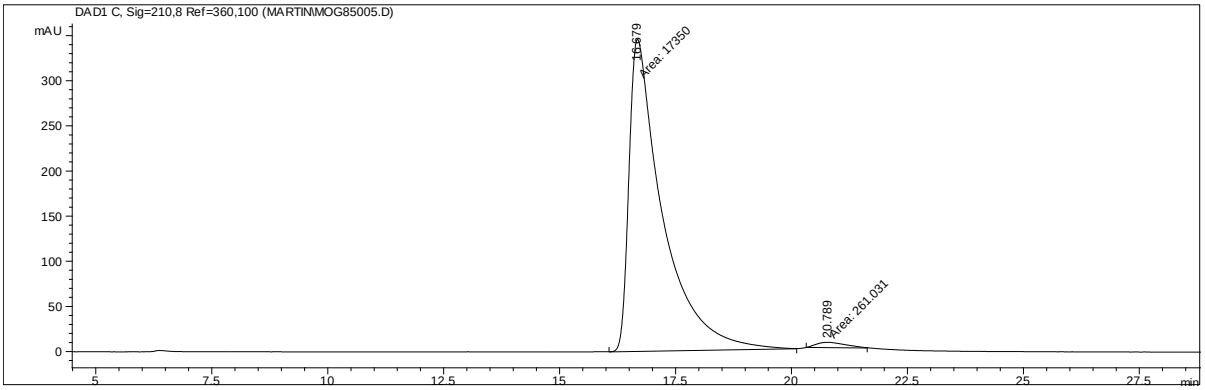
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

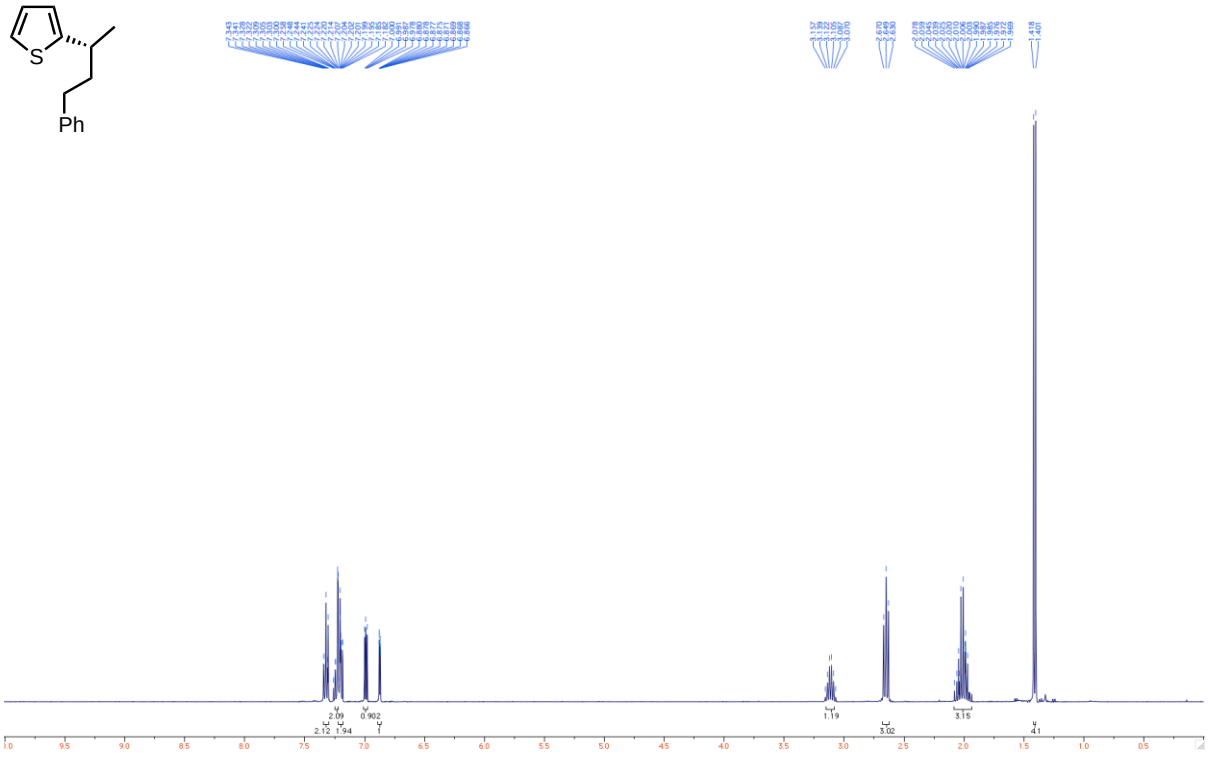


Chiral HPLC traces: enantioenriched

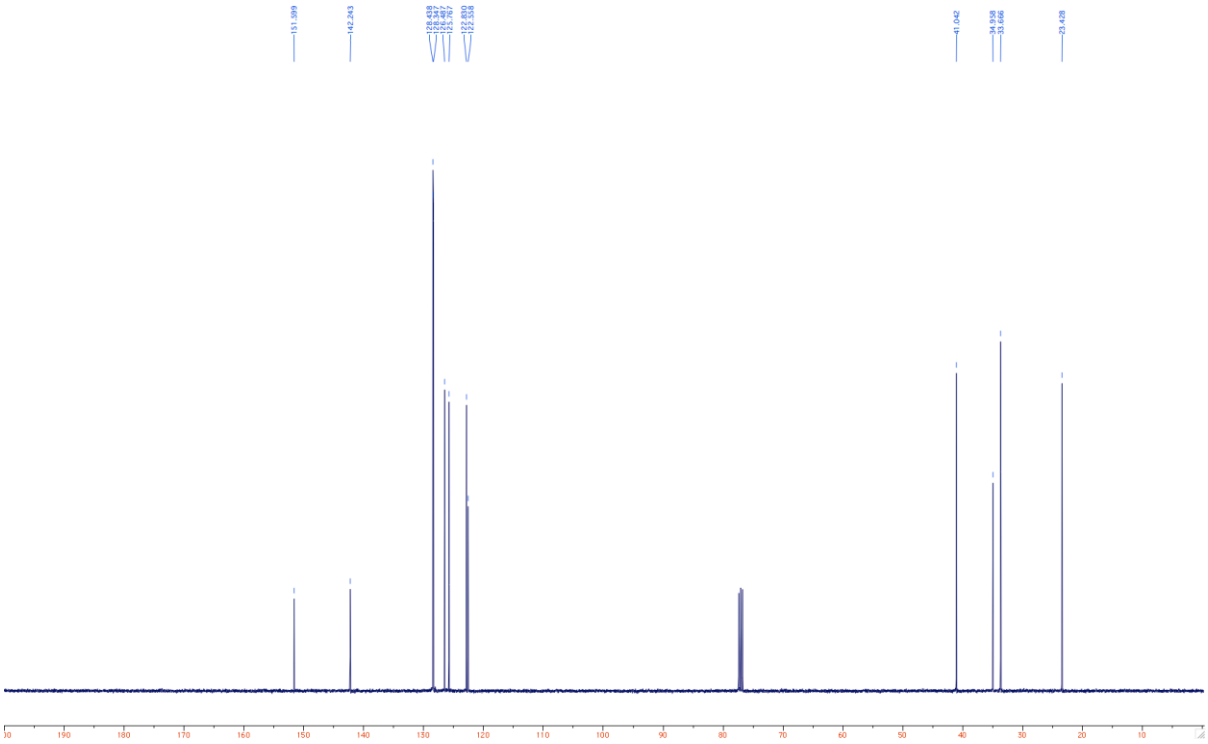


7a

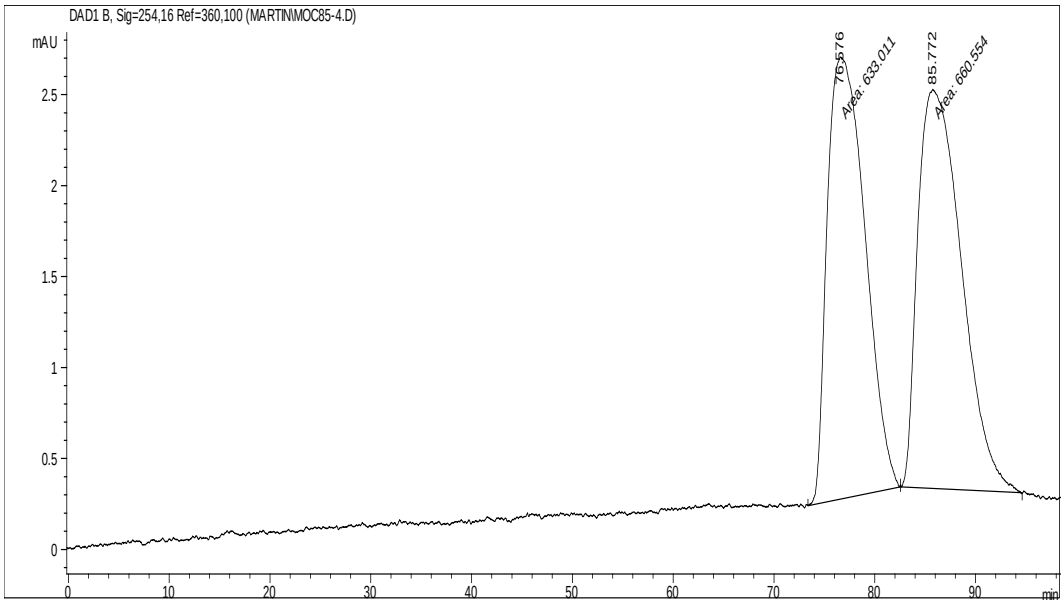
^{1}H NMR (400 MHz, $CDCl_3$)



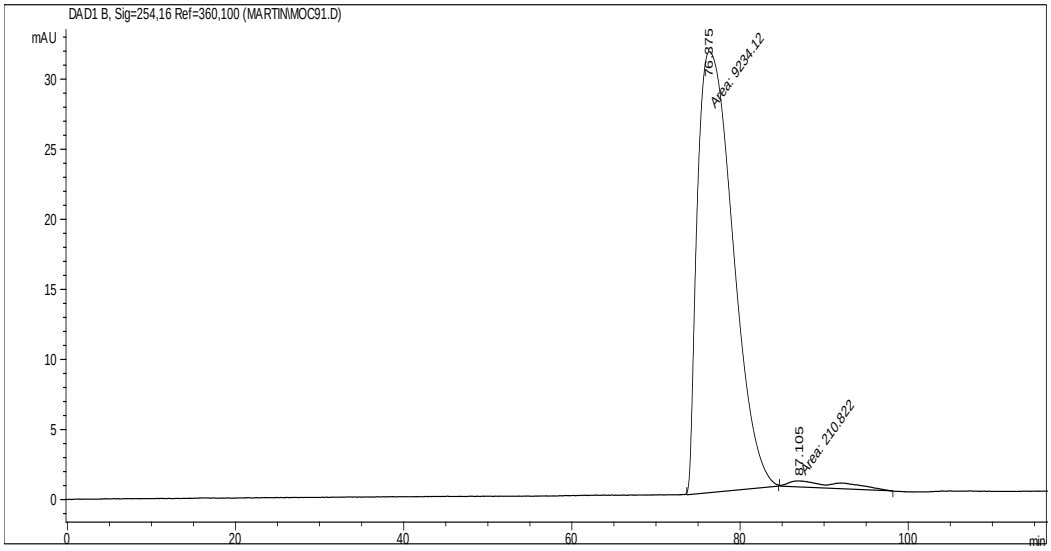
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

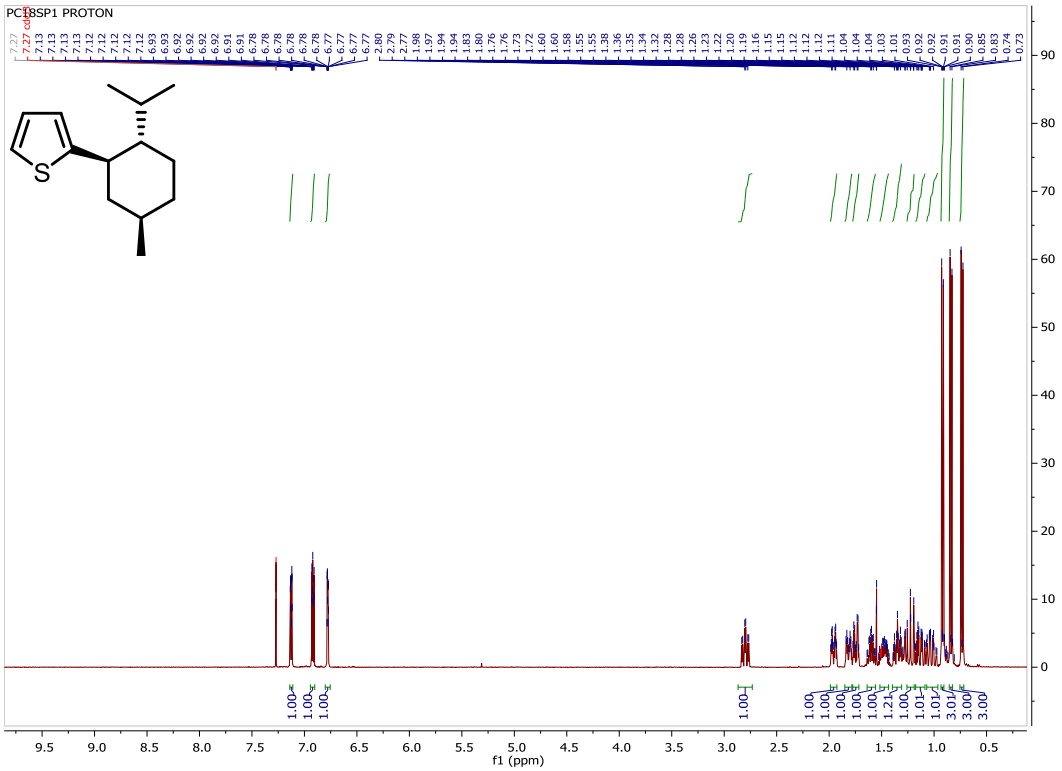


Chiral HPLC traces: enantioenriched

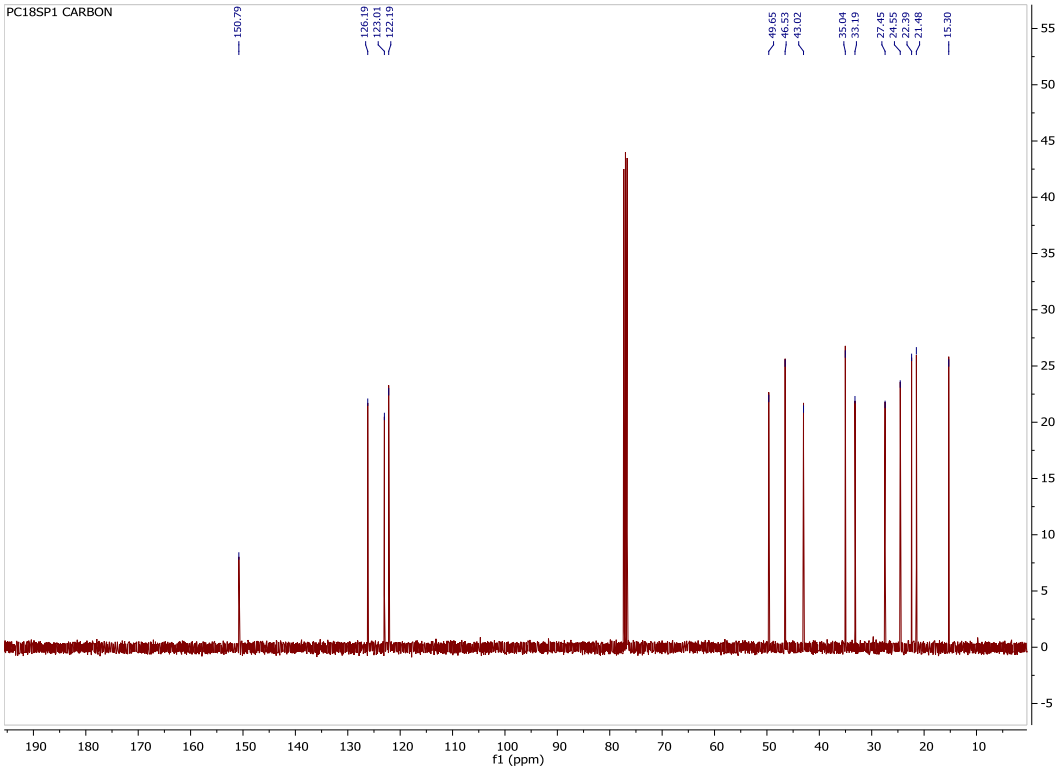


7q

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

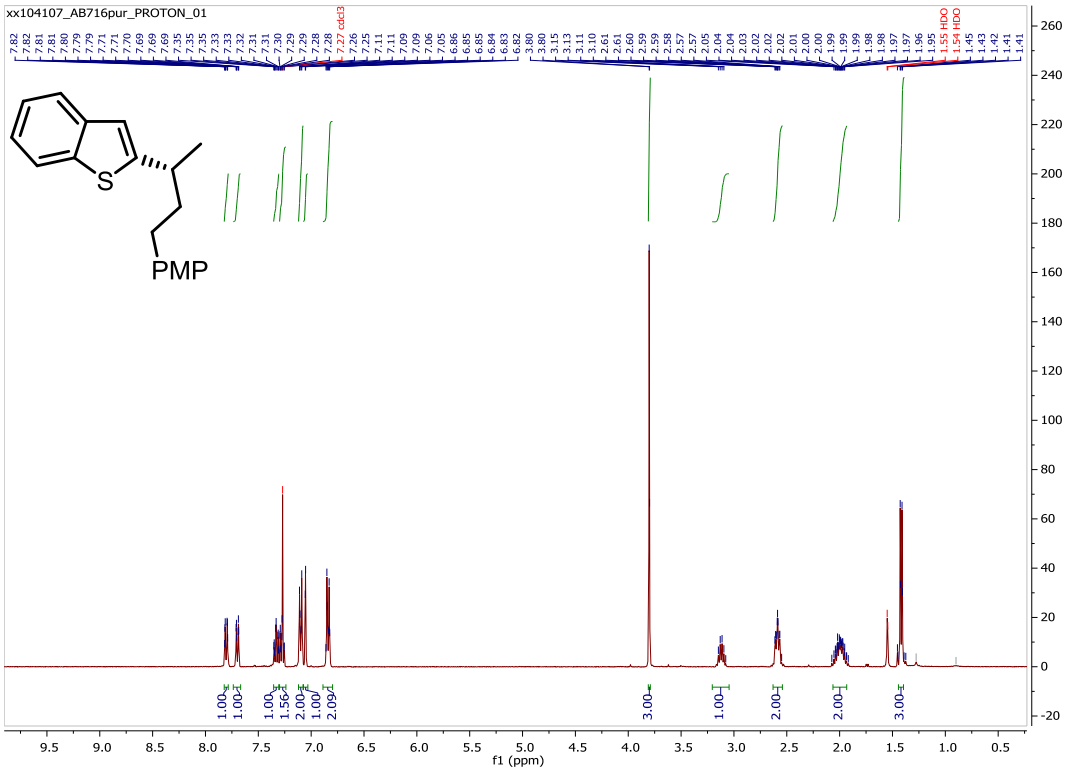


^{13}C NMR (100 MHz, $CDCl_3$)

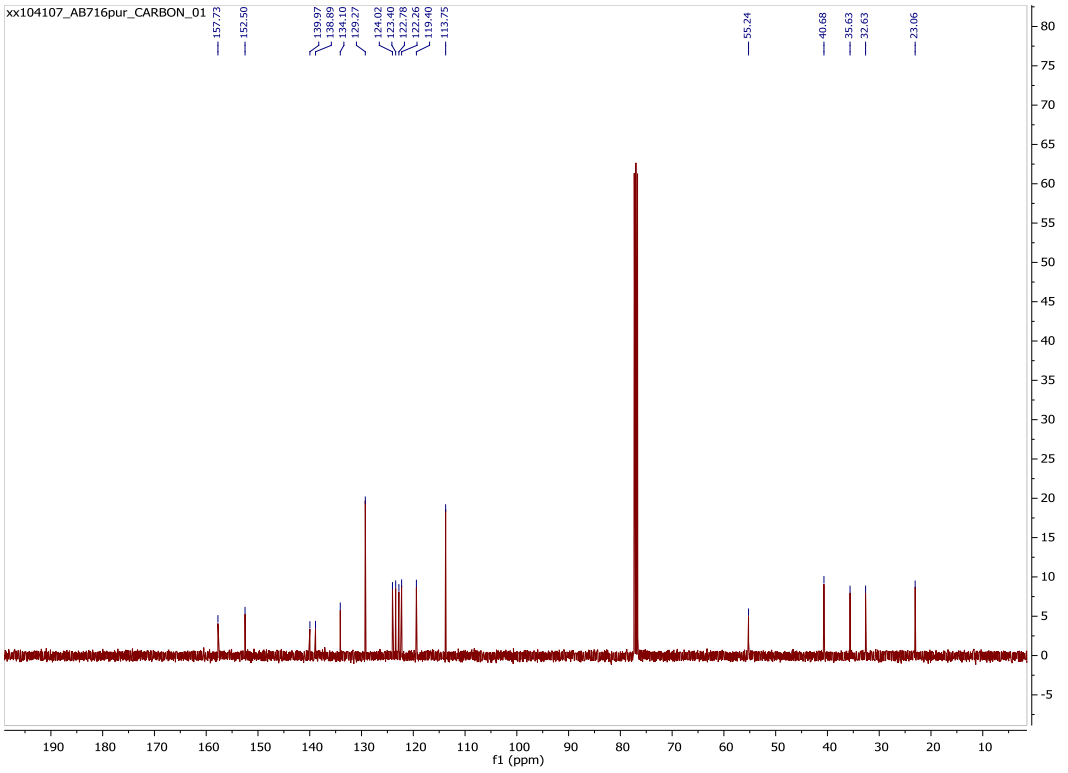


8b

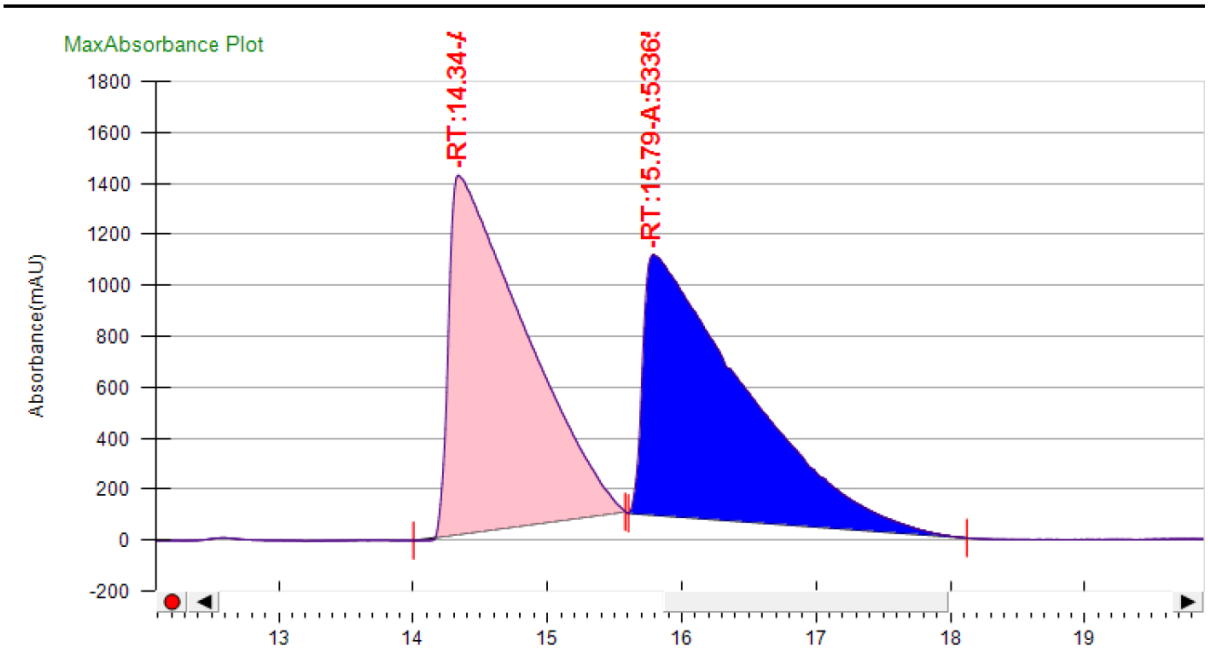
^{1}H NMR (400 MHz, $CDCl_3$)



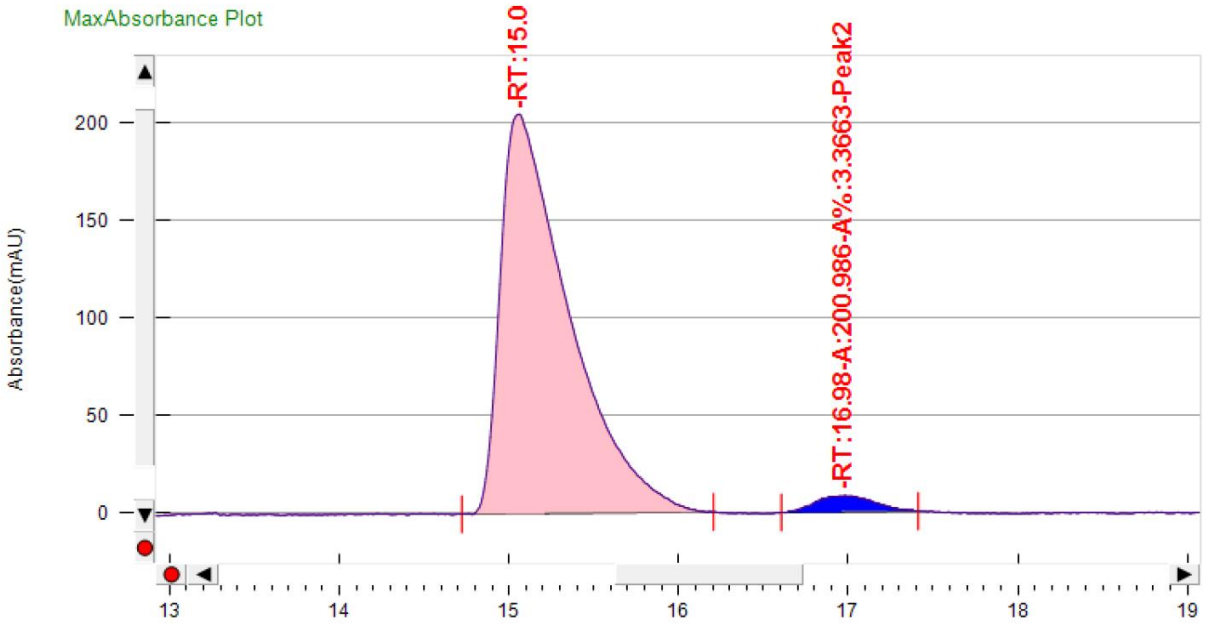
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

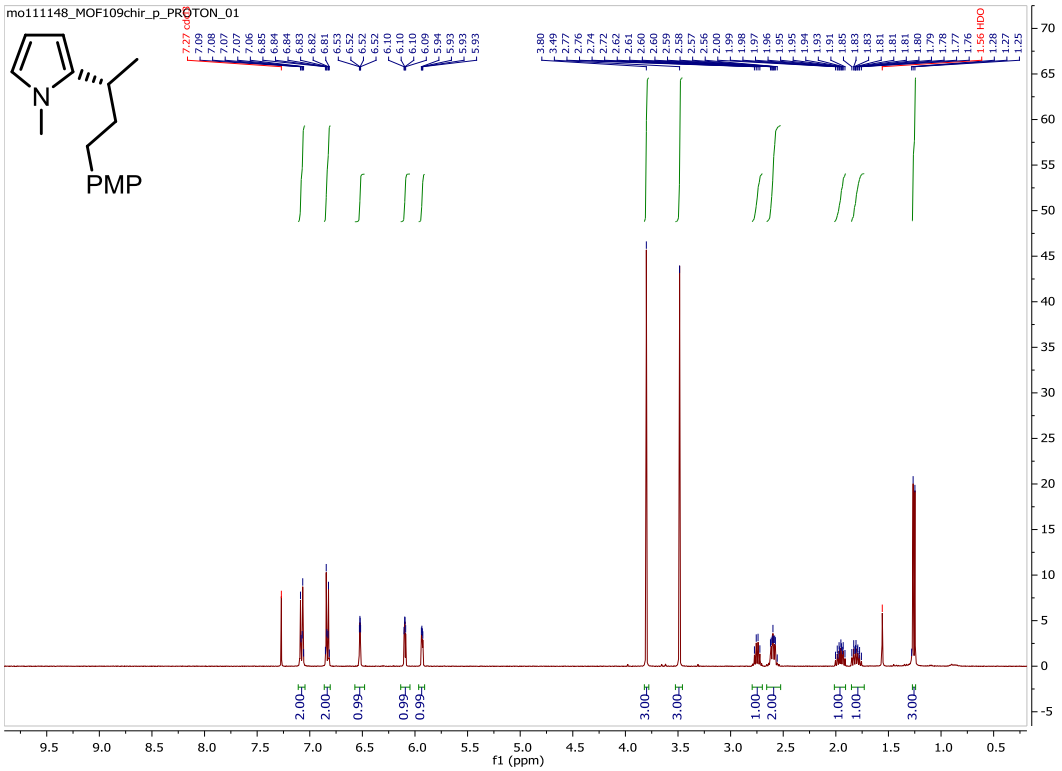


Chiral SFC traces: enantioenriched

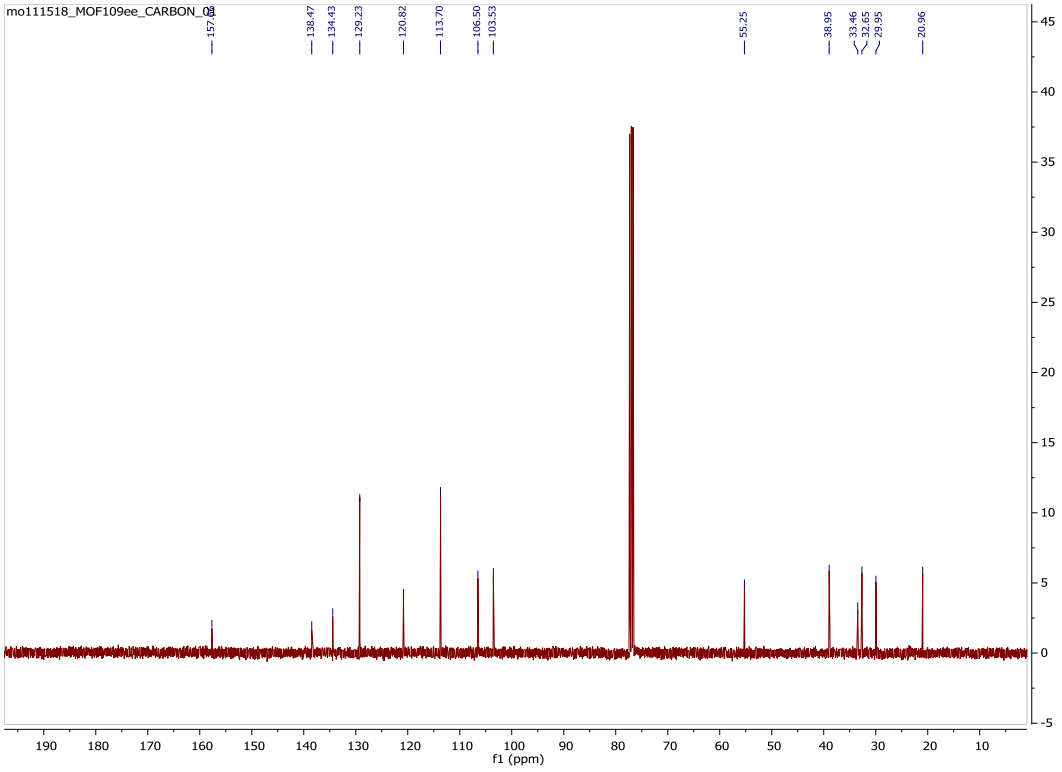


5b

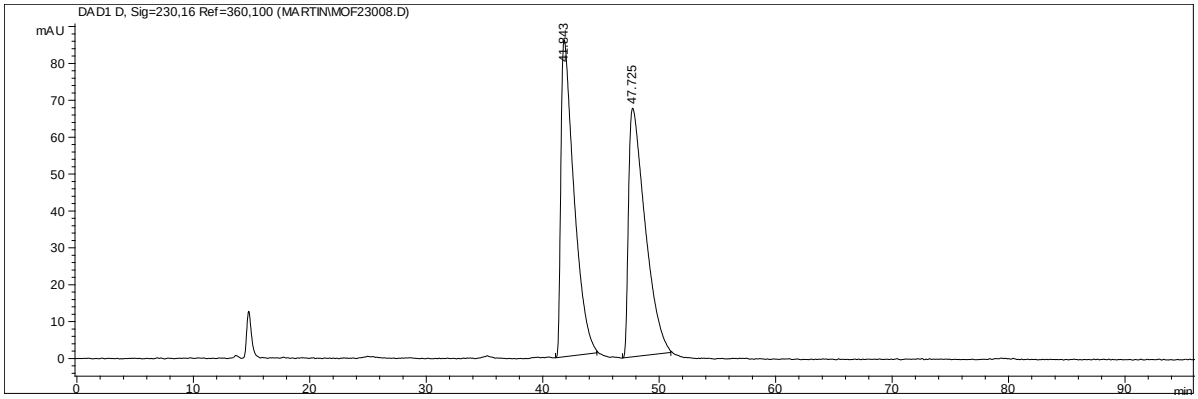
^{1}H NMR (400 MHz, $CDCl_3$)



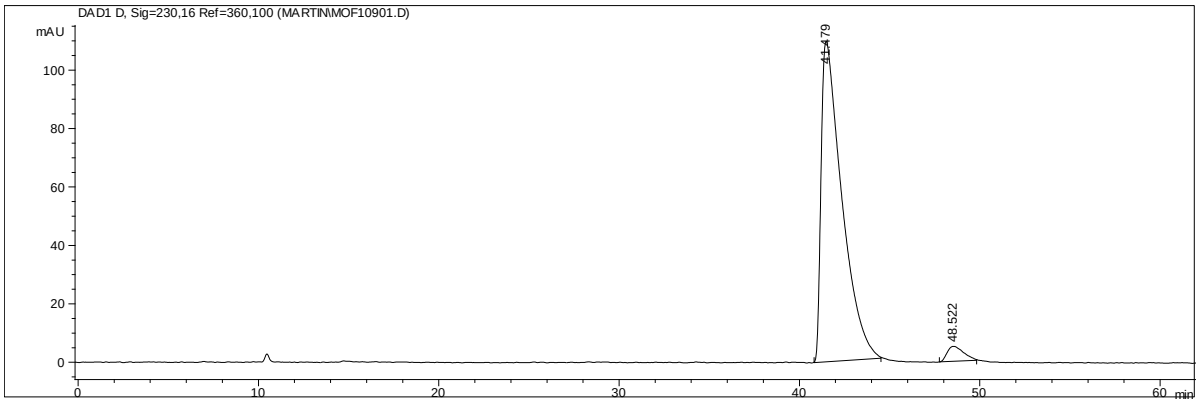
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

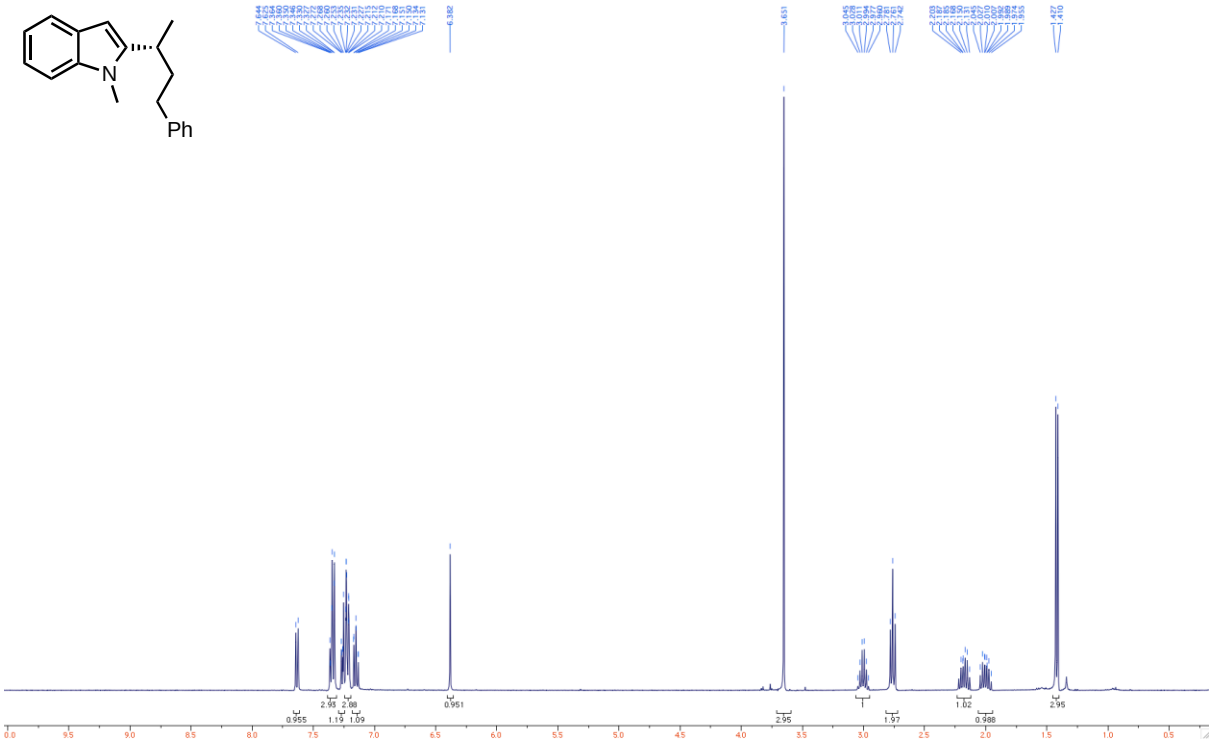


Chiral HPLC traces: enantioenriched

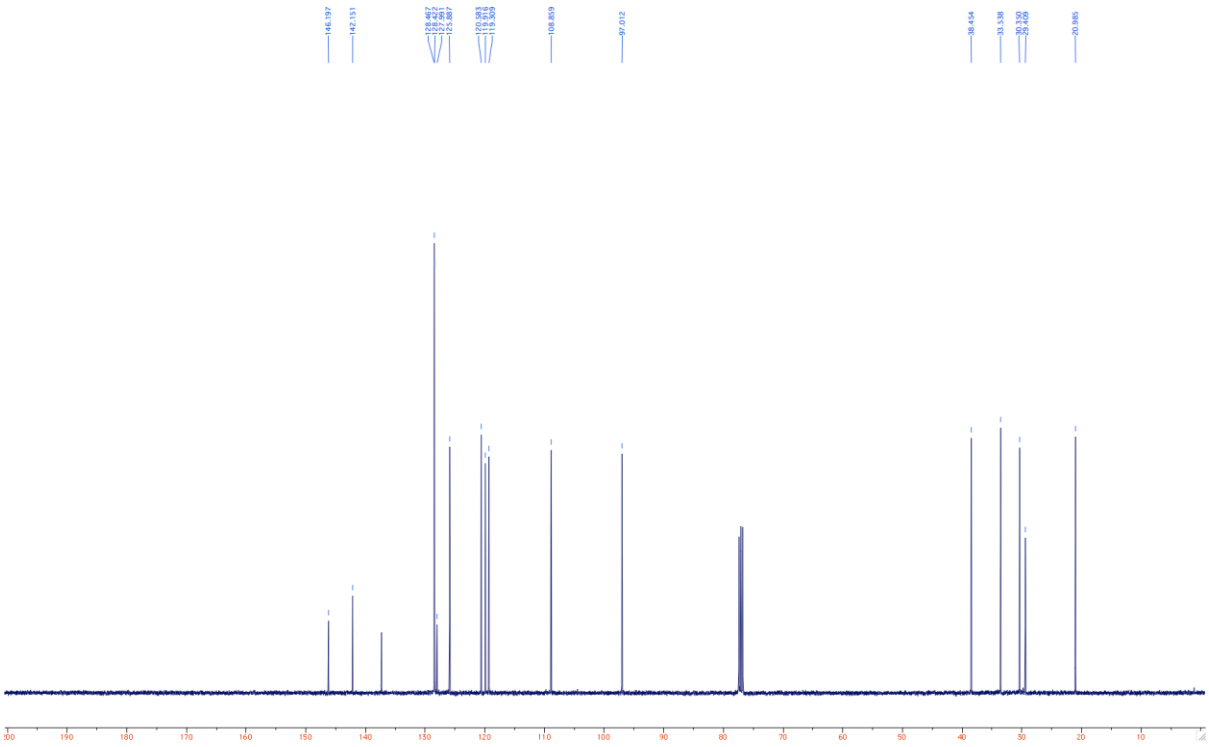


6a

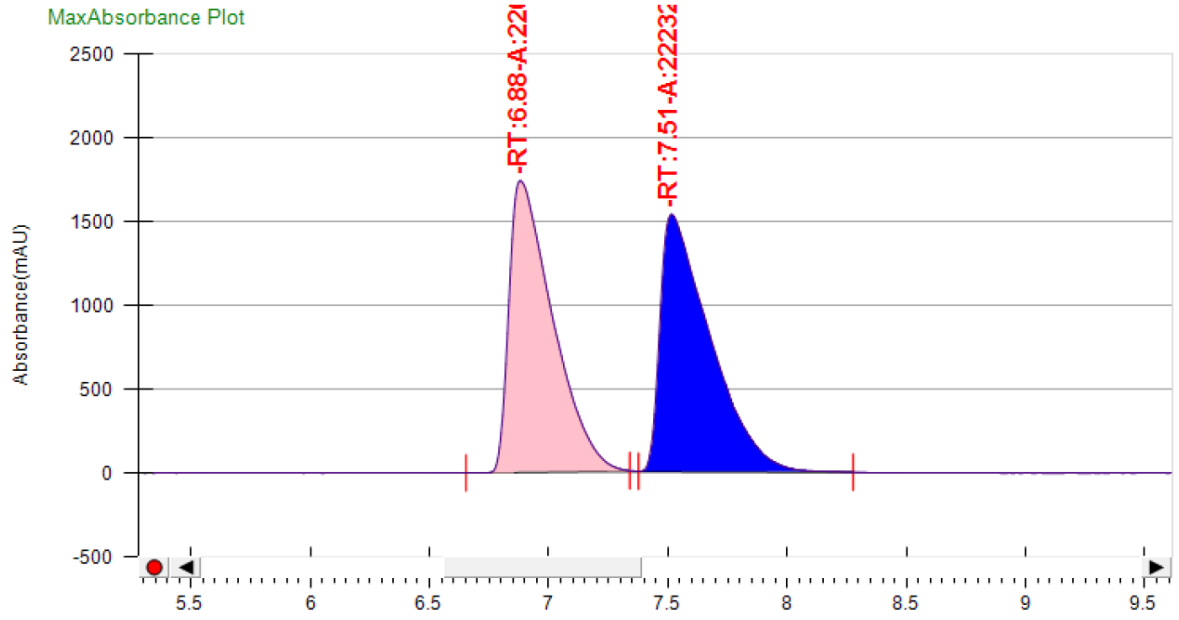
^{1}H NMR (400 MHz, $CDCl_3$)



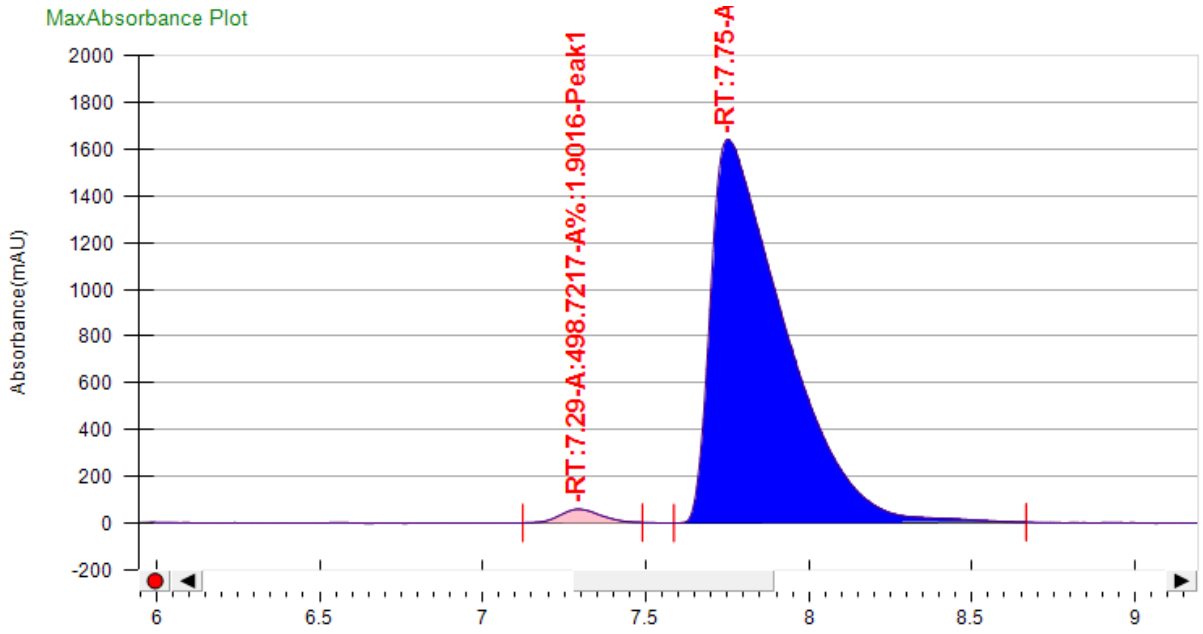
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

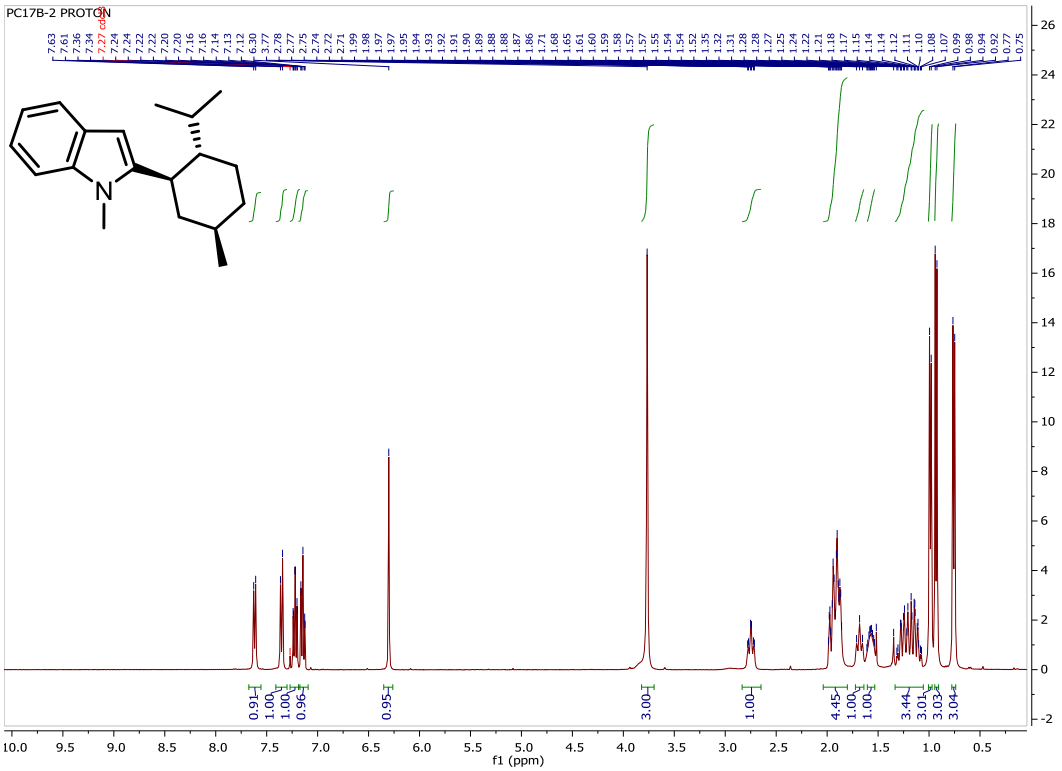


Chiral SFC traces: enantioenriched

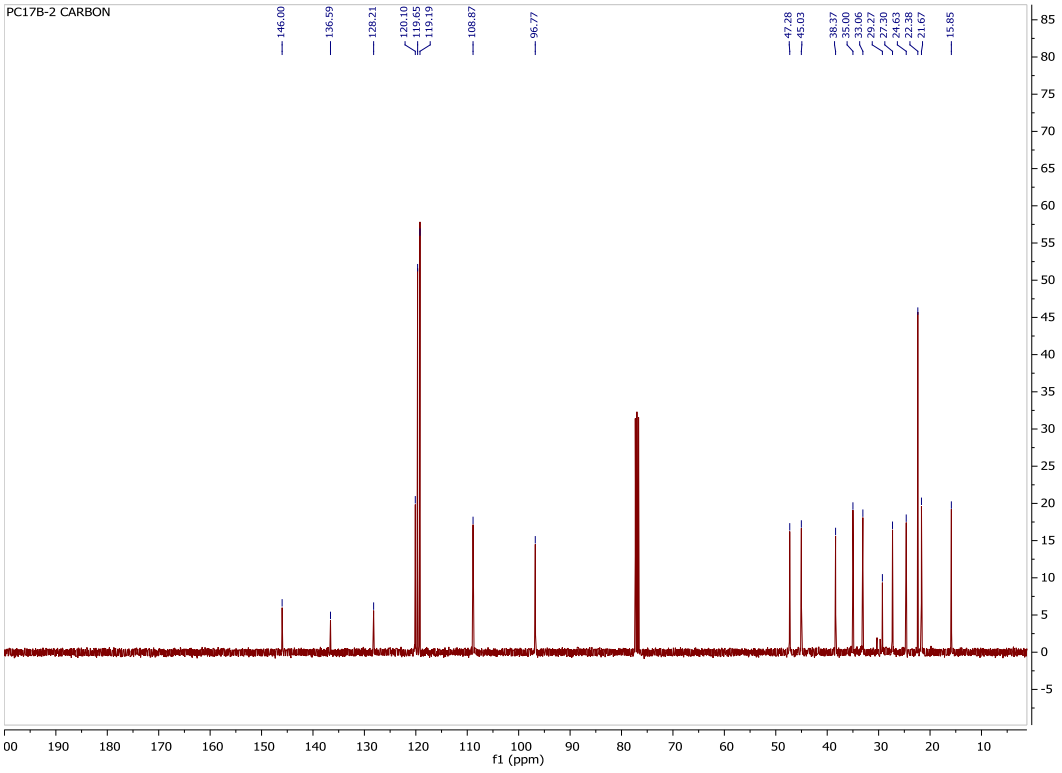


6q

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

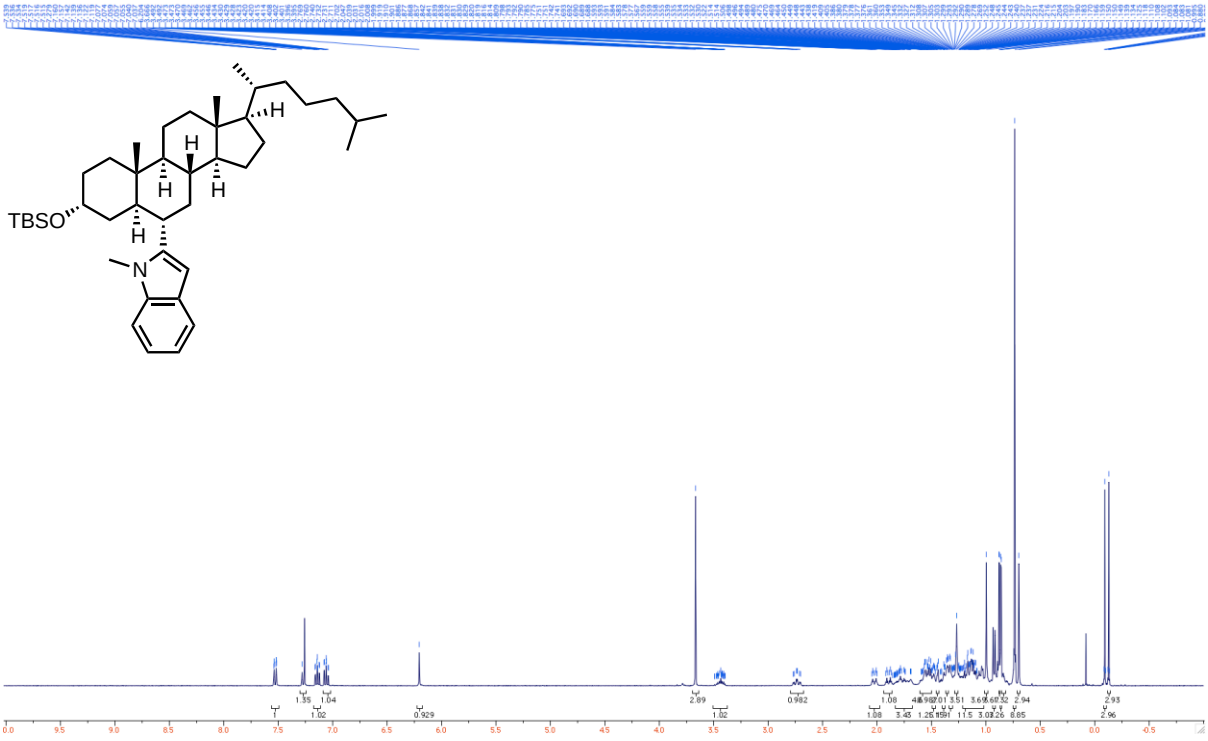


^{13}C NMR (100 MHz, $CDCl_3$)

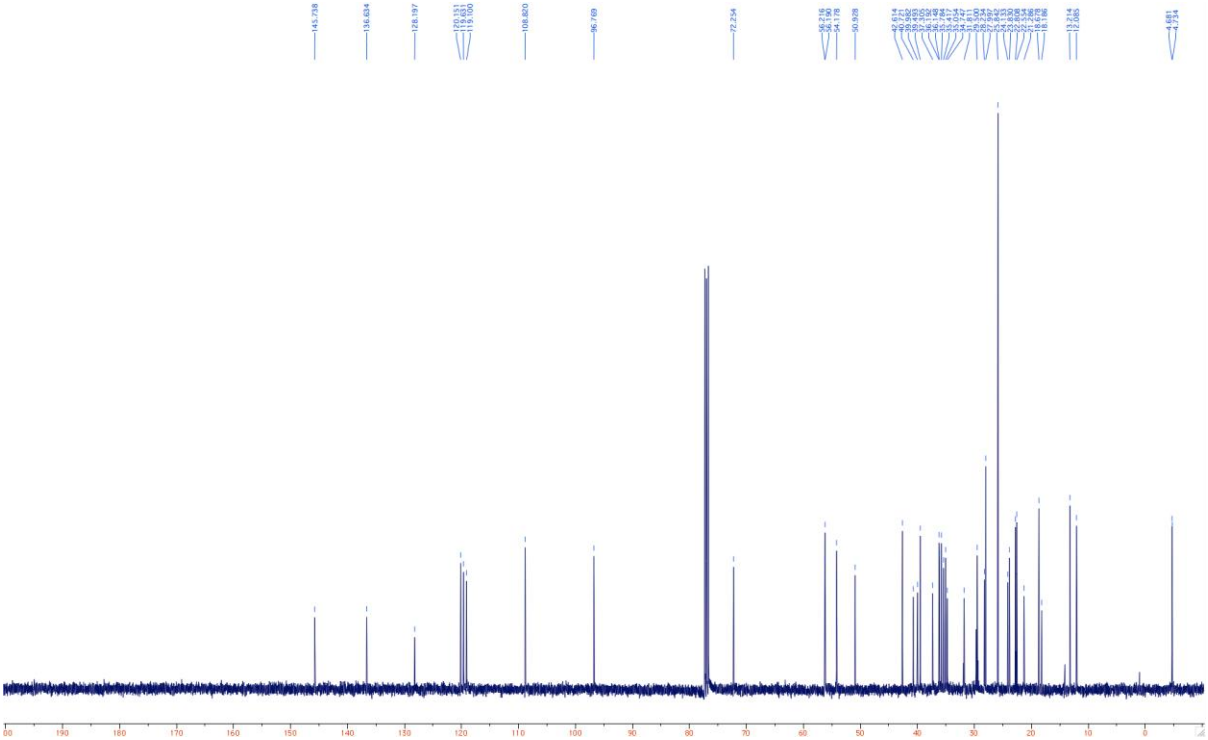


6p

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

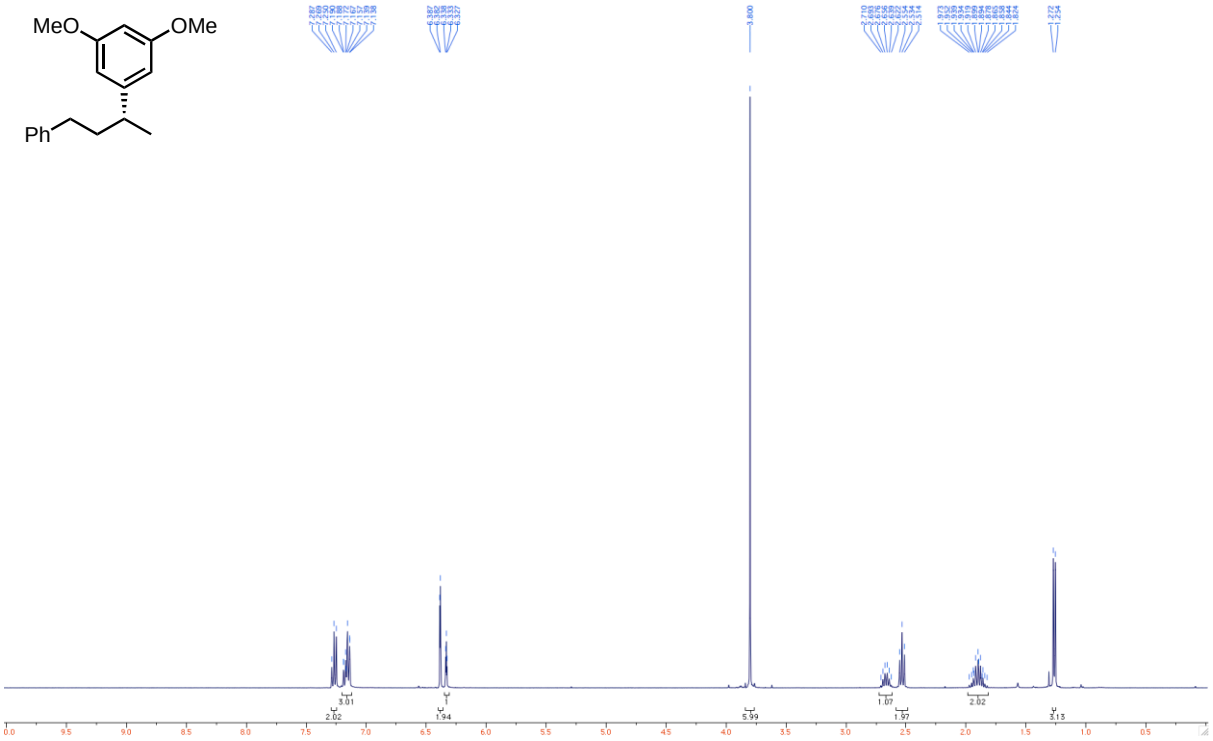


^{13}C NMR (100 MHz, $CDCl_3$)

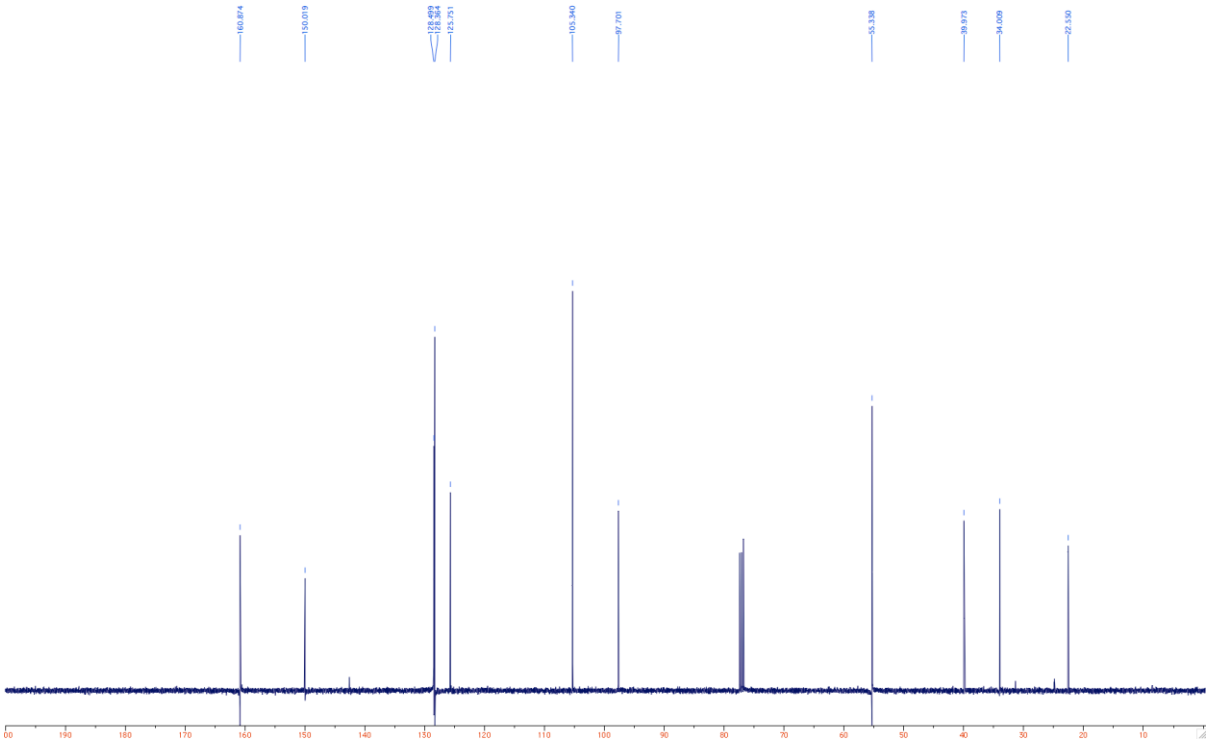


9a

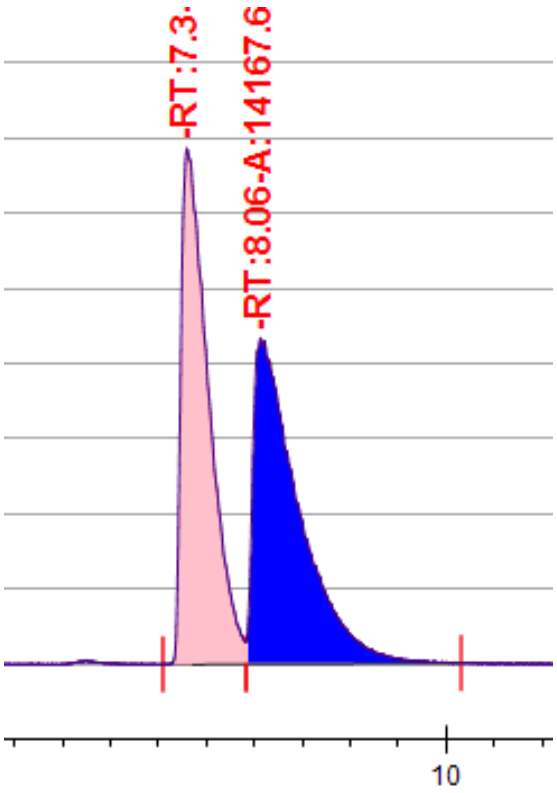
^{1}H NMR (400 MHz, $CDCl_3$)



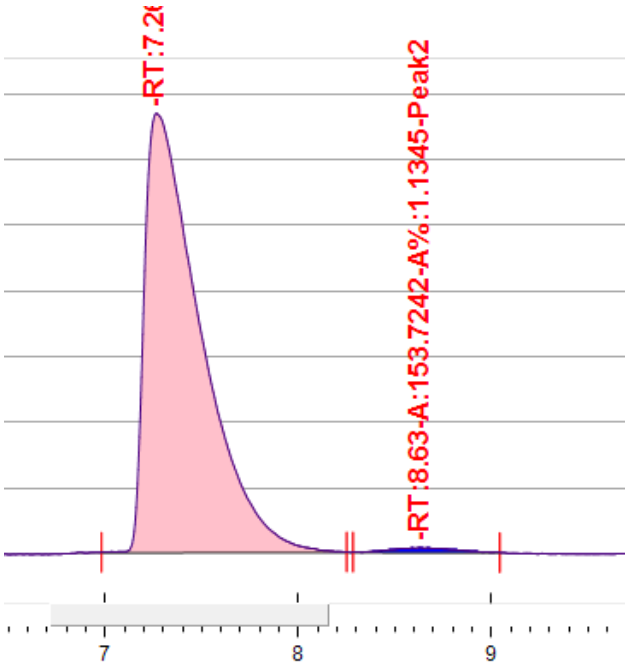
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

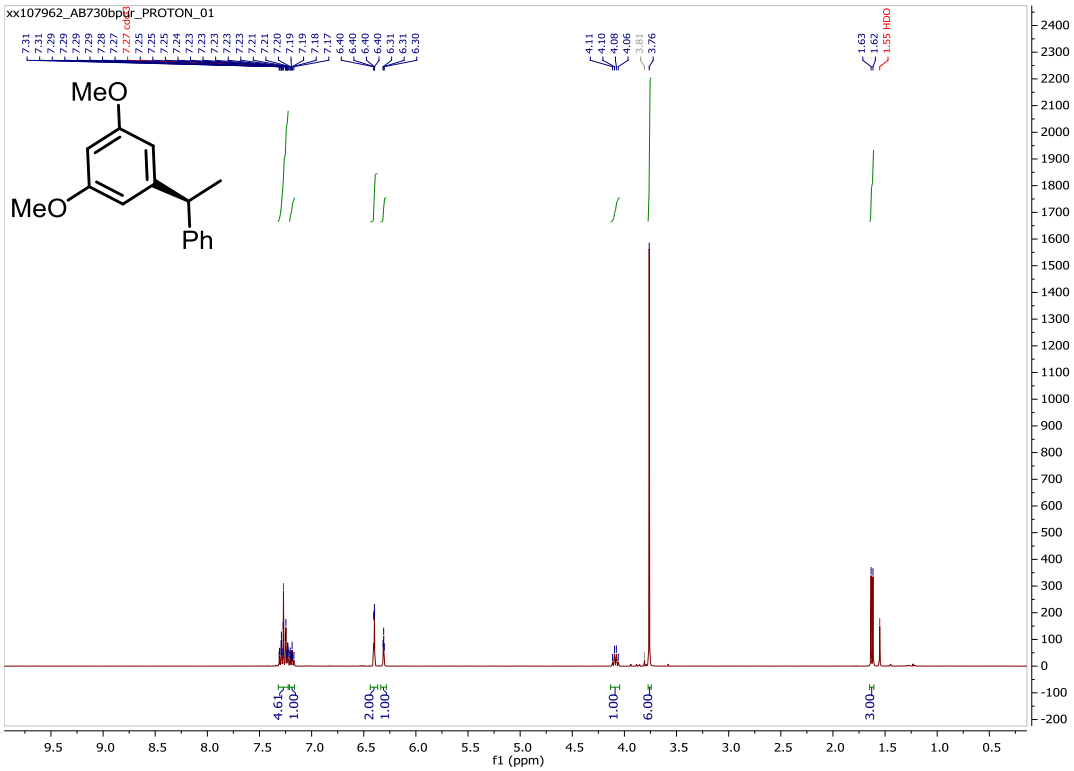


Chiral SFC traces: enantioenriched

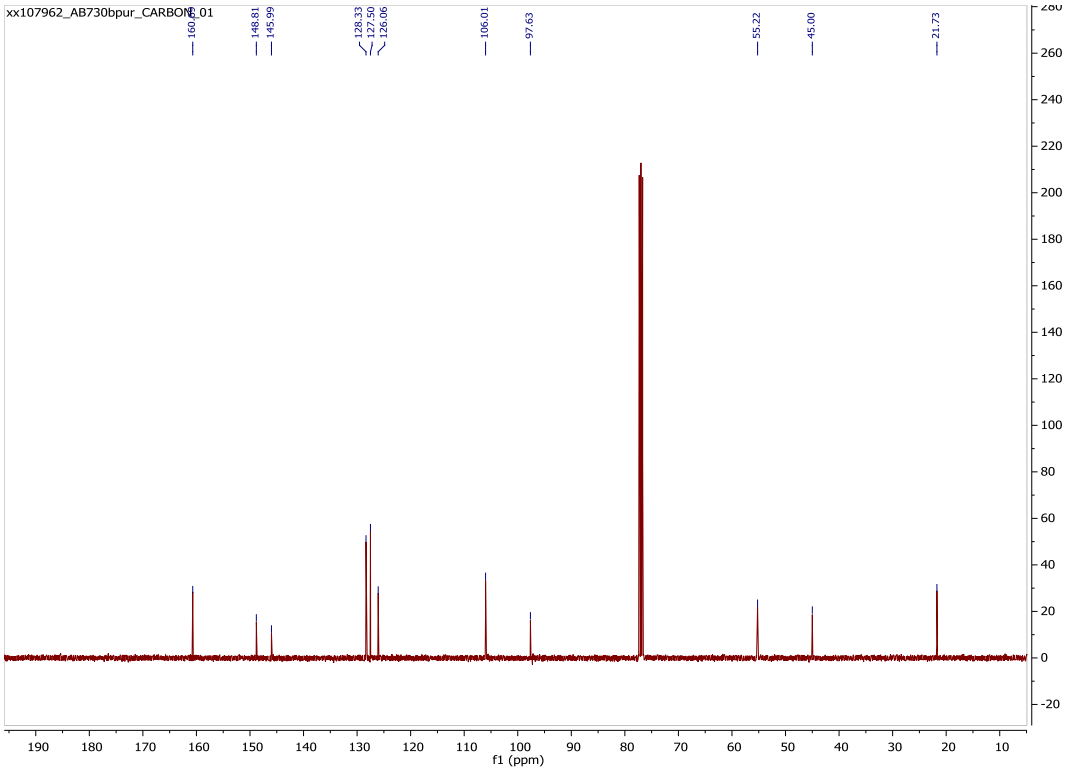


9l

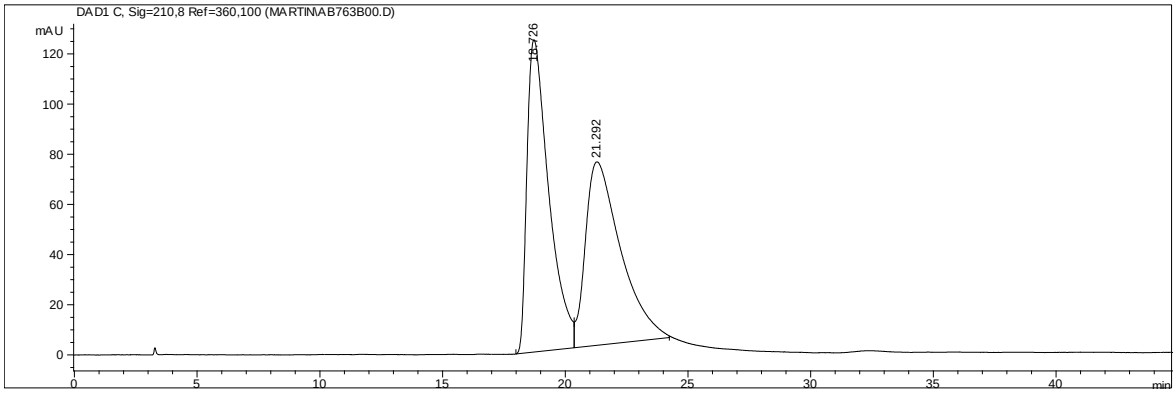
^{1}H NMR (400 MHz, $CDCl_3$)



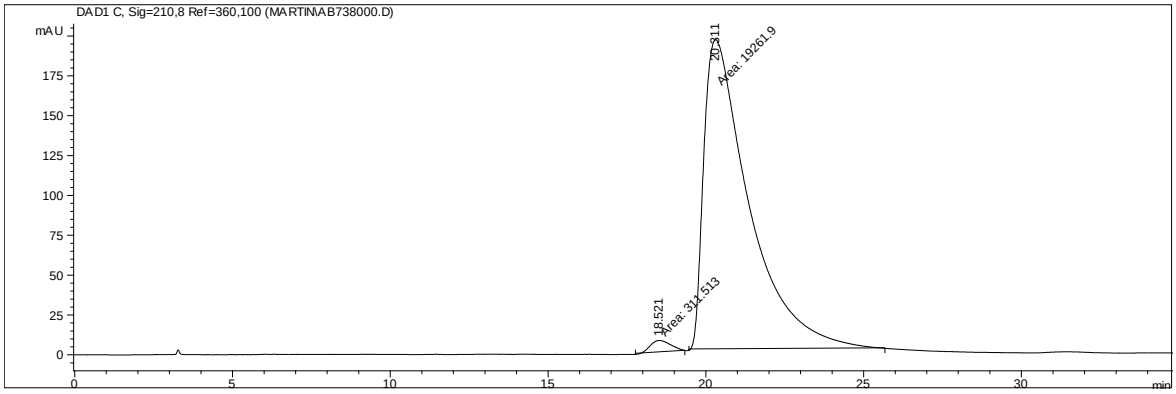
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

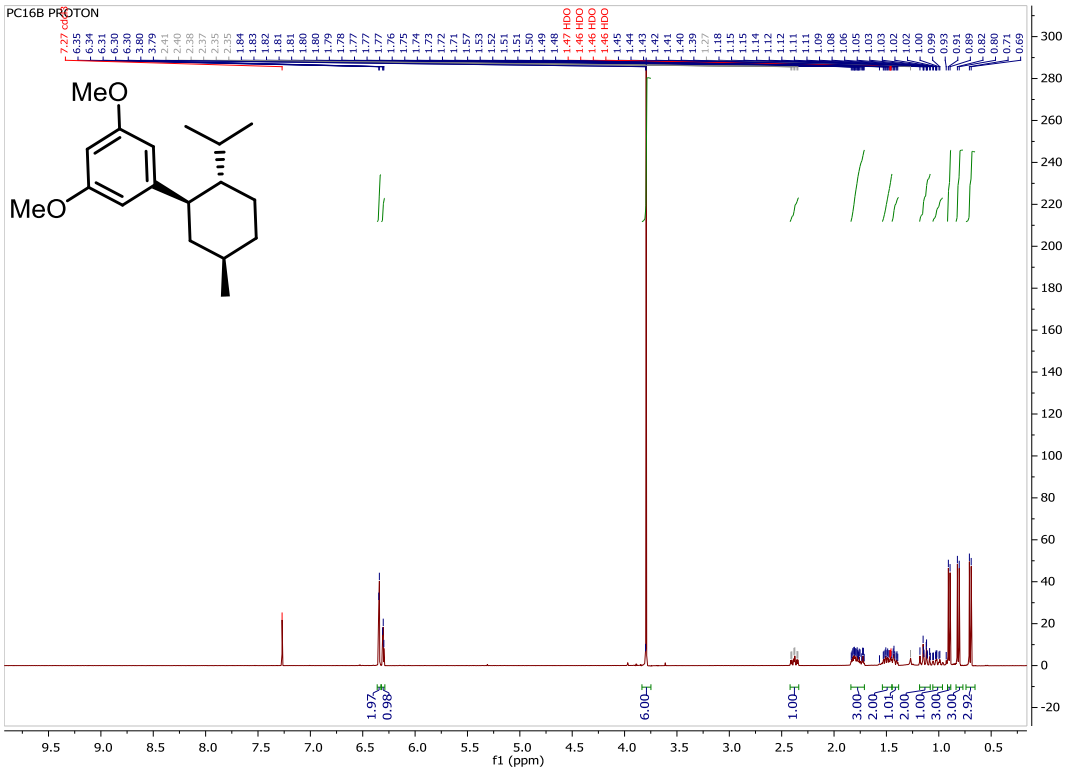


Chiral HPLC traces: enantioenriched

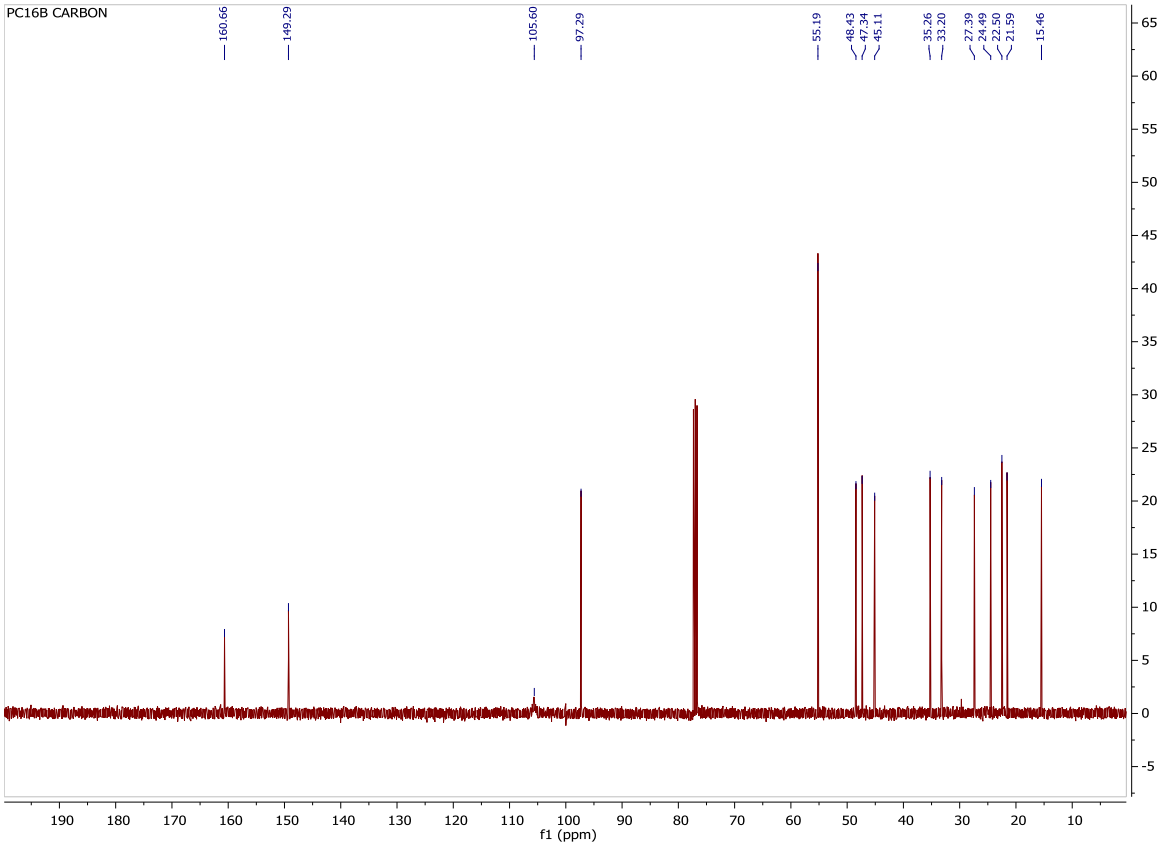


9q

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

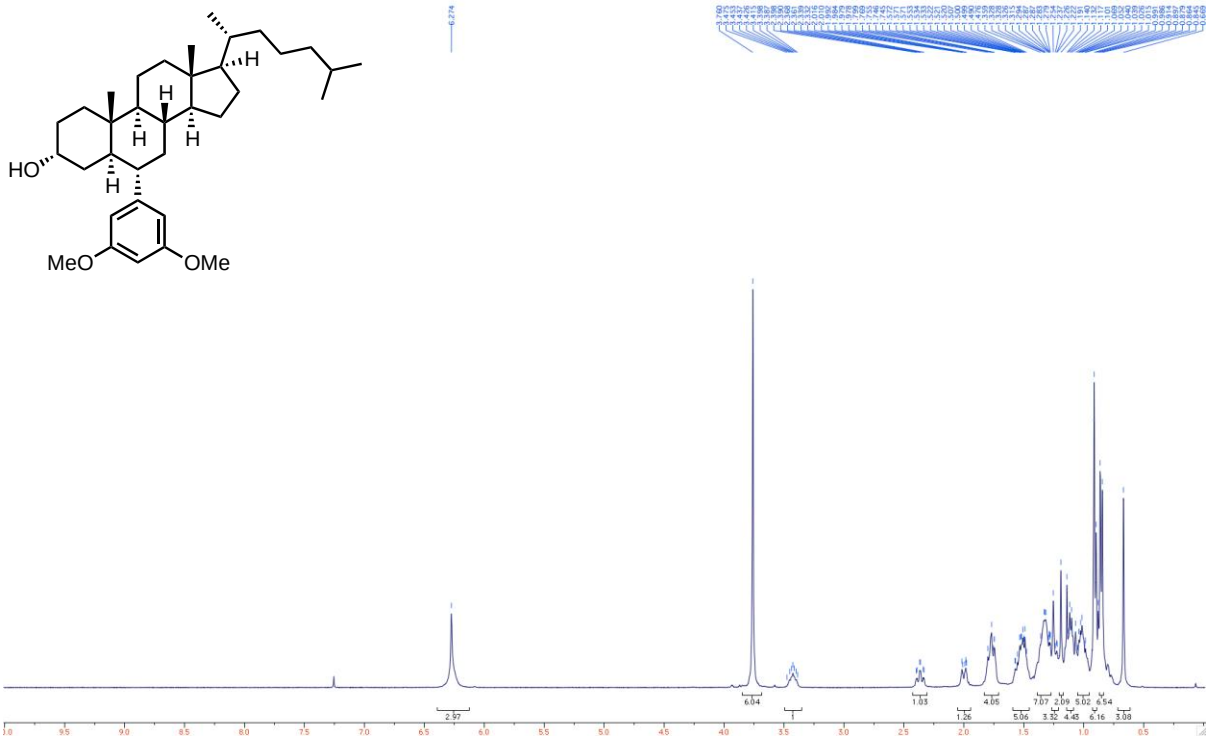


^{13}C NMR (100 MHz, $CDCl_3$)

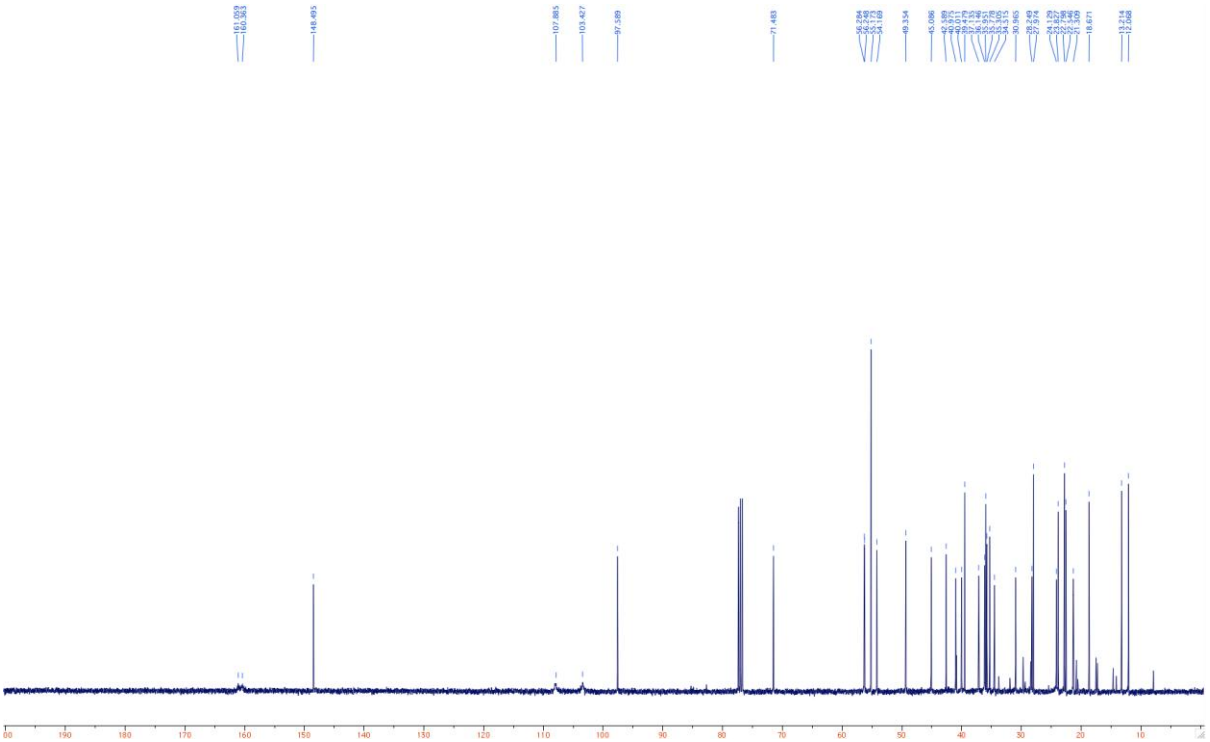


9o

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

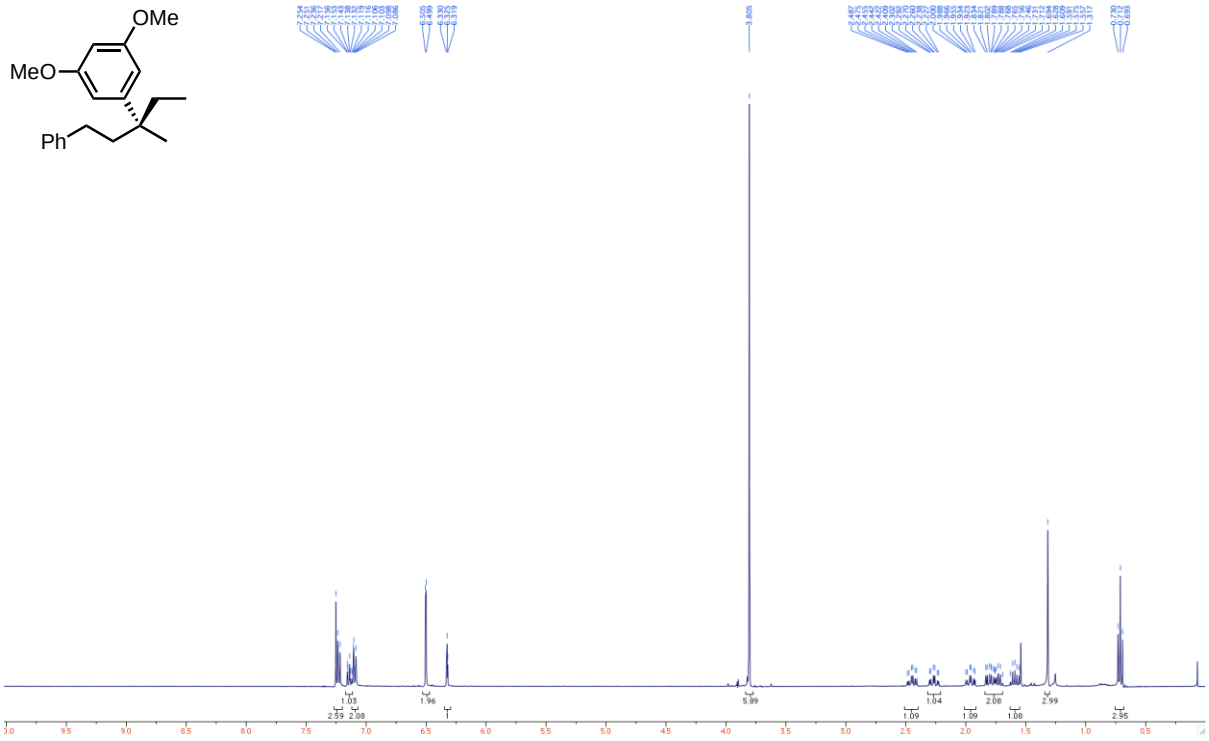


^{13}C NMR (100 MHz, $CDCl_3$)

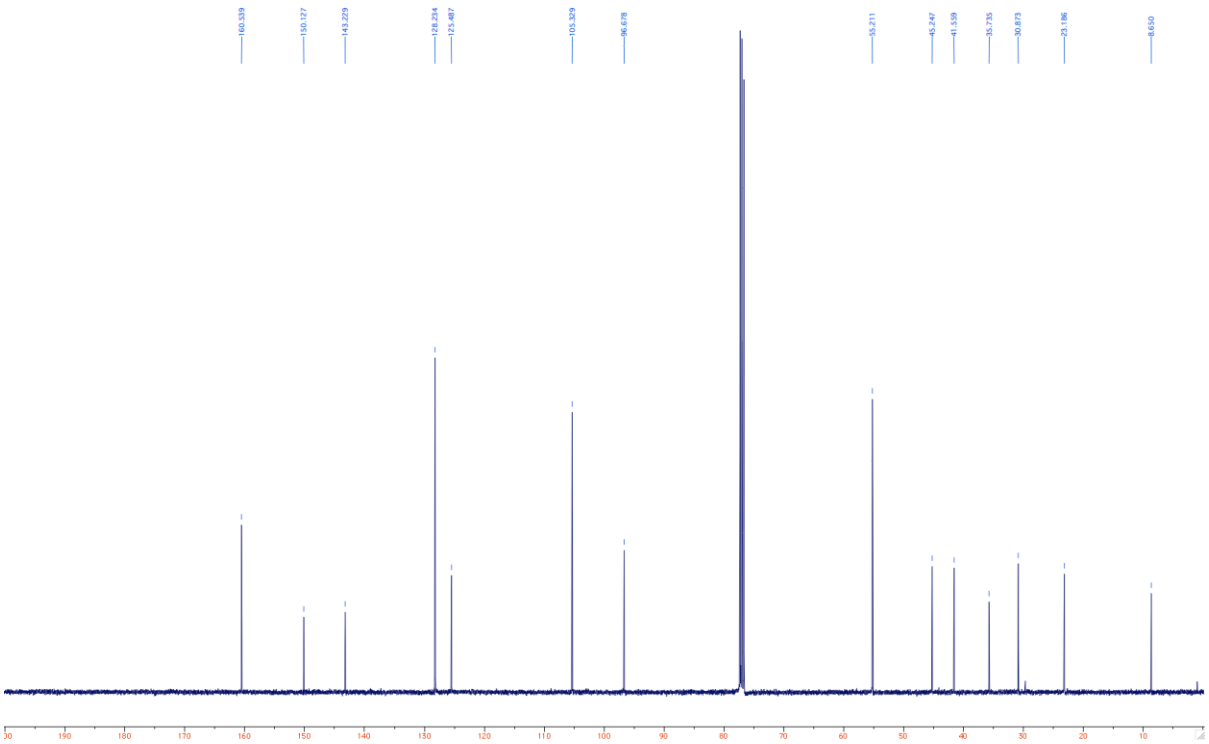


9g

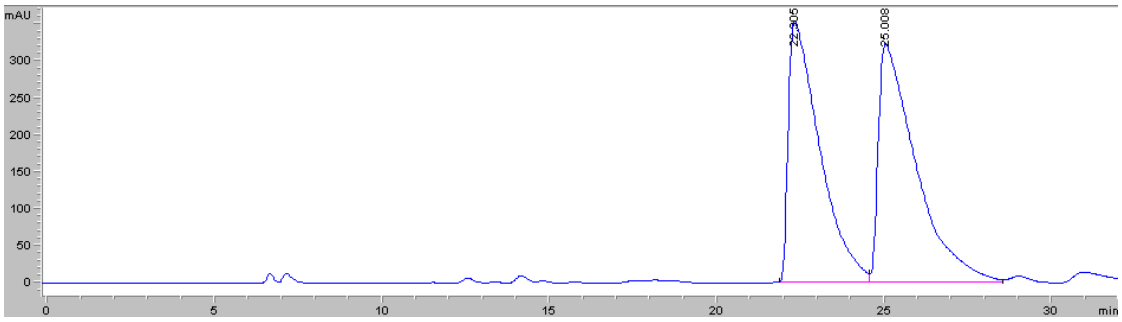
^{1}H NMR (400 MHz, $CDCl_3$)



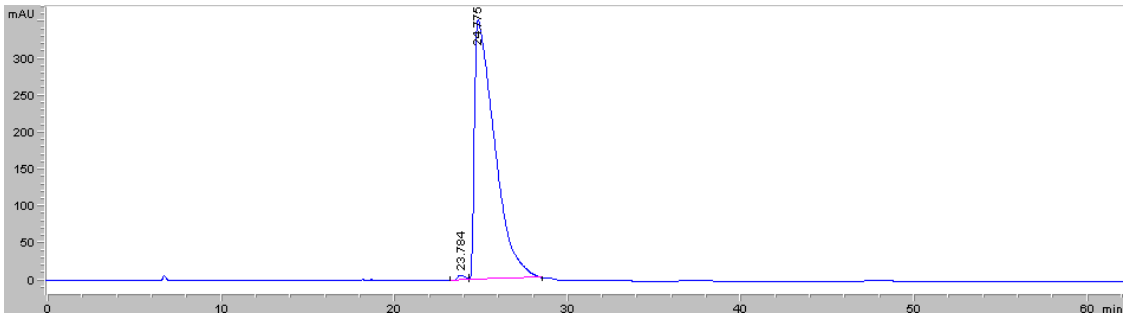
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

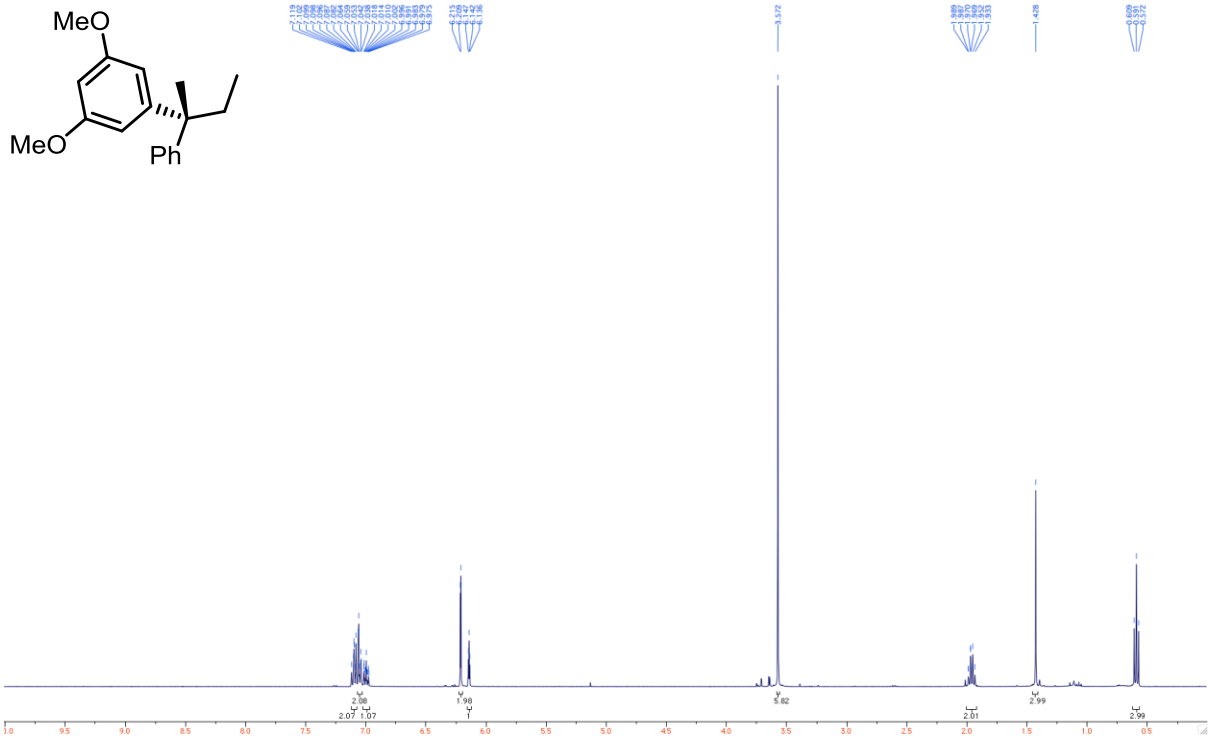


Chiral HPLC traces: enantioenriched

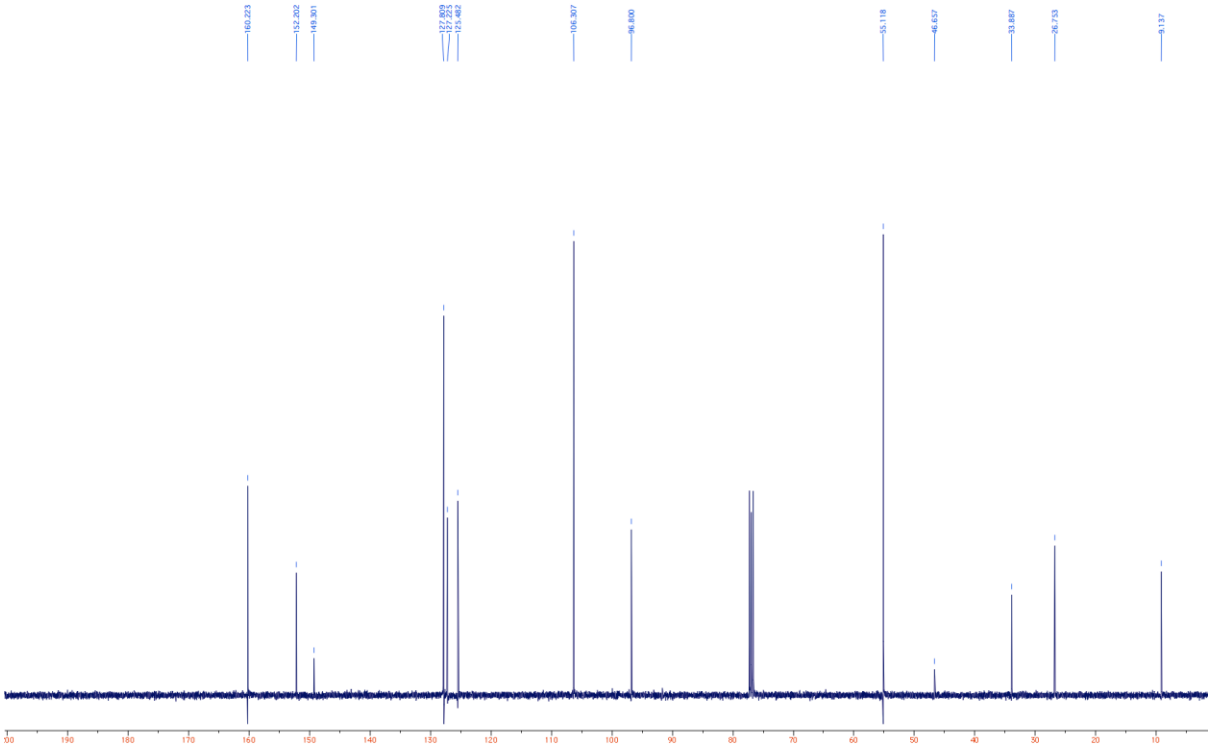


9h

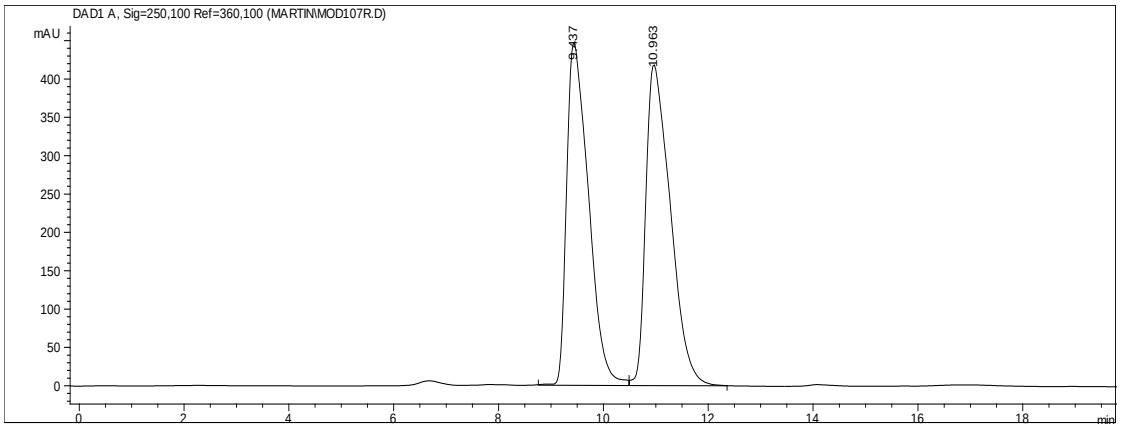
^{1}H NMR (400 MHz, $CDCl_3$)



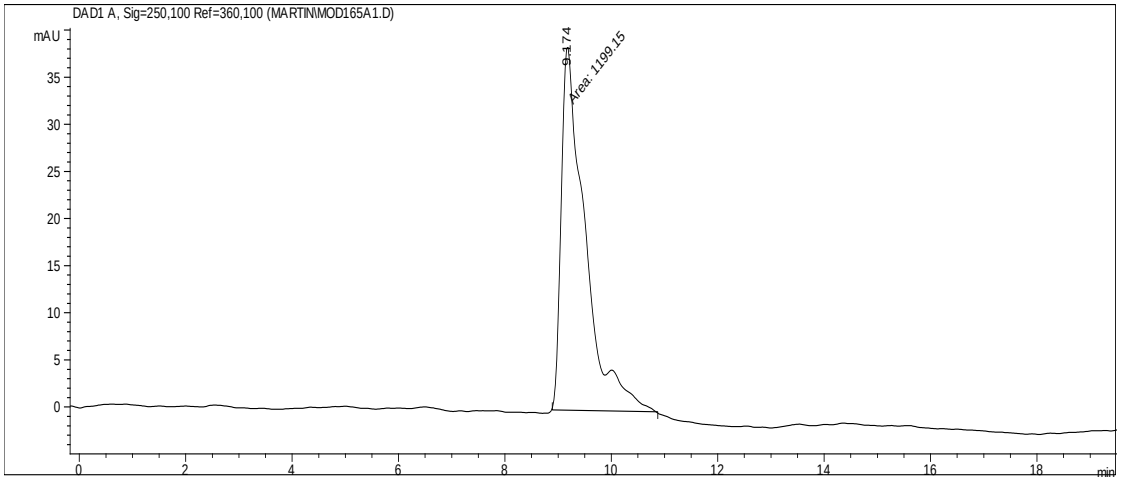
^{13}C NMR (100 MHz, $CDCl_3$)



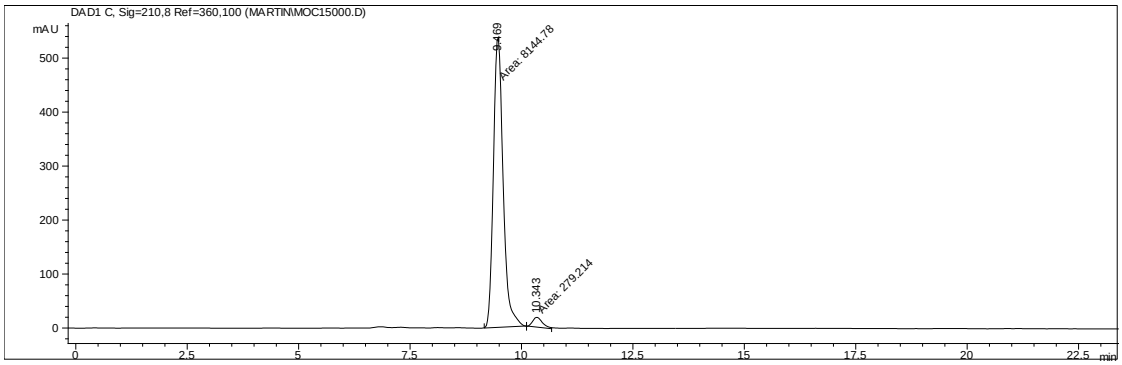
Chiral HPLC traces: racemic



Chiral HPLC traces: enantioenriched

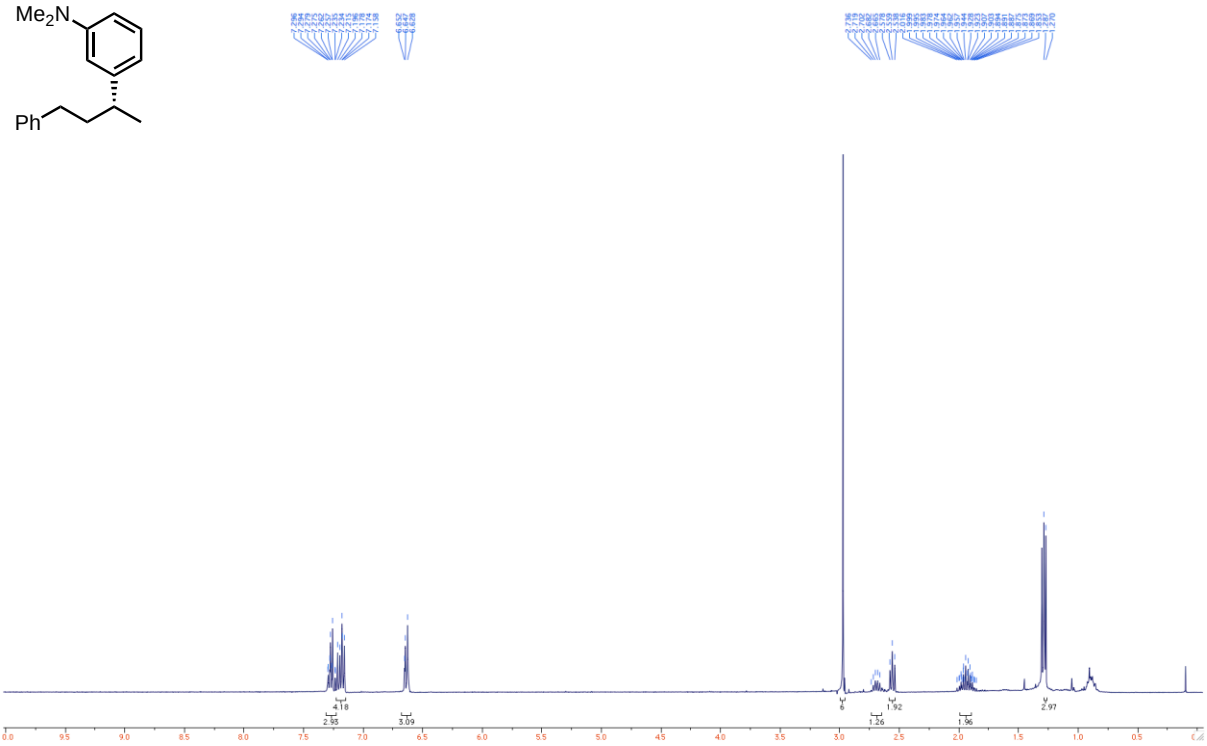


Chiral HPLC traces: enantioenriched + racemic

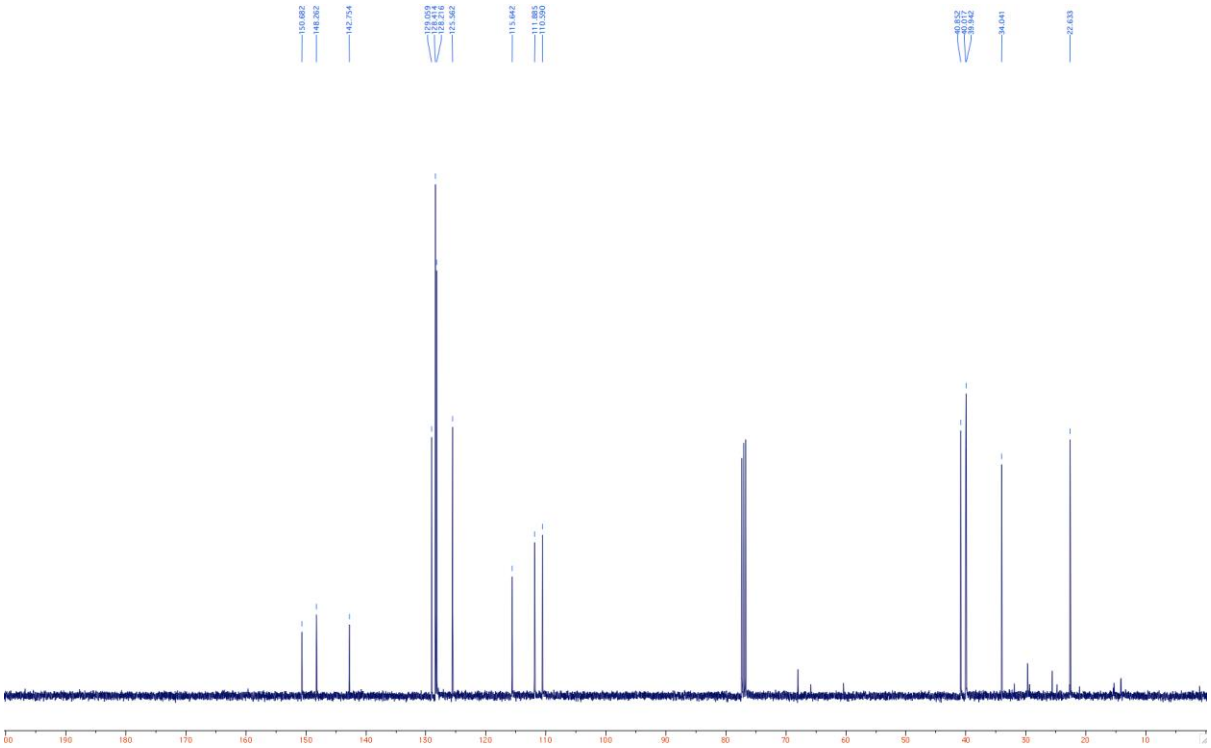


10a

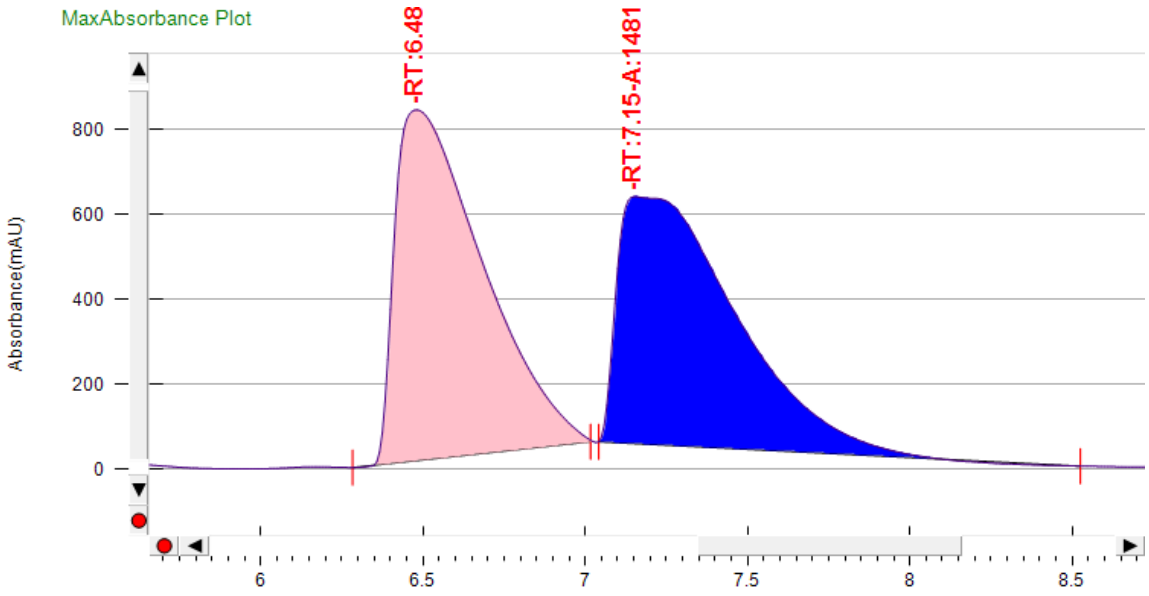
^{1}H NMR (400 MHz, $CDCl_3$)



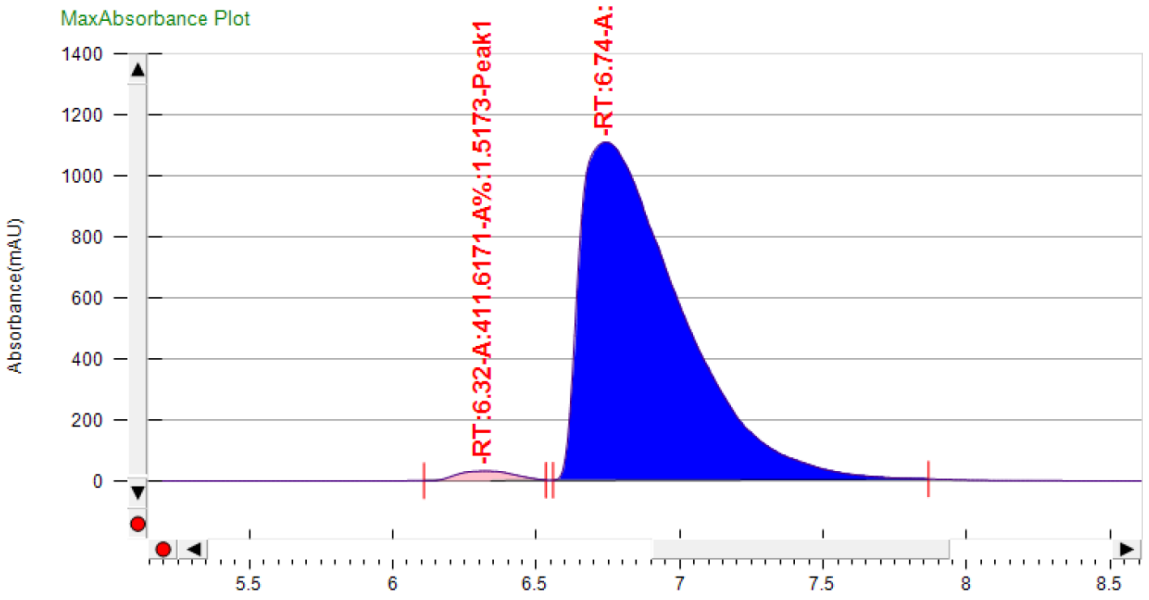
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

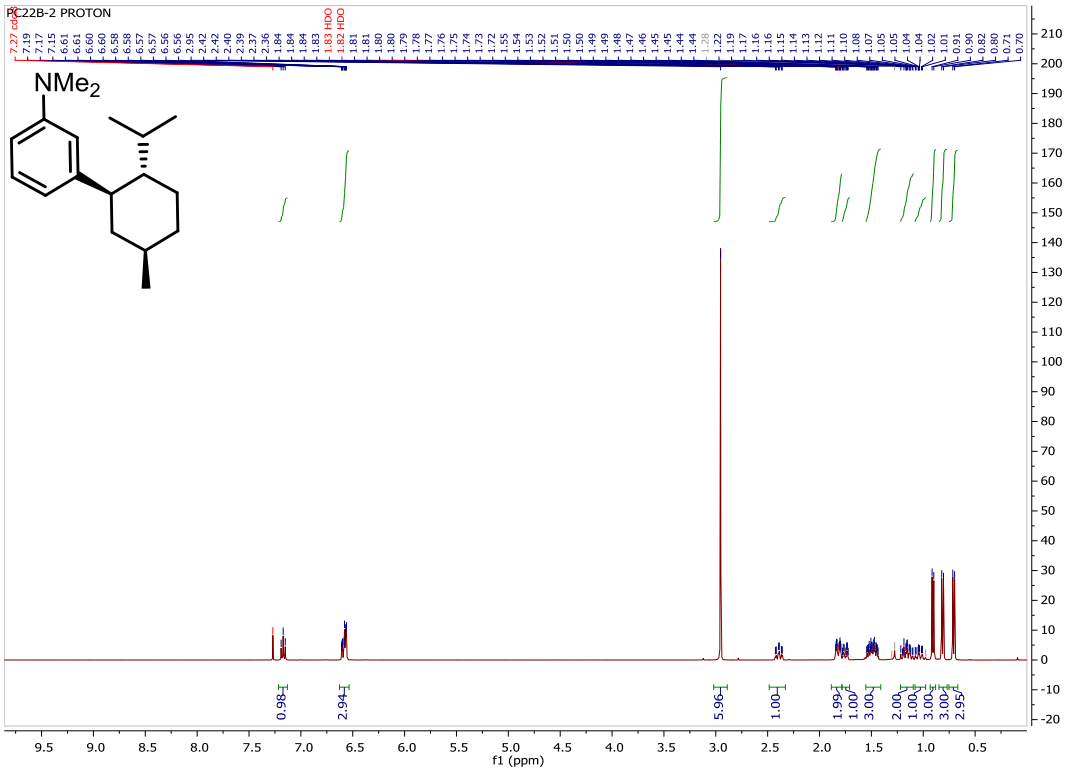


Chiral SFC traces: enantioenriched

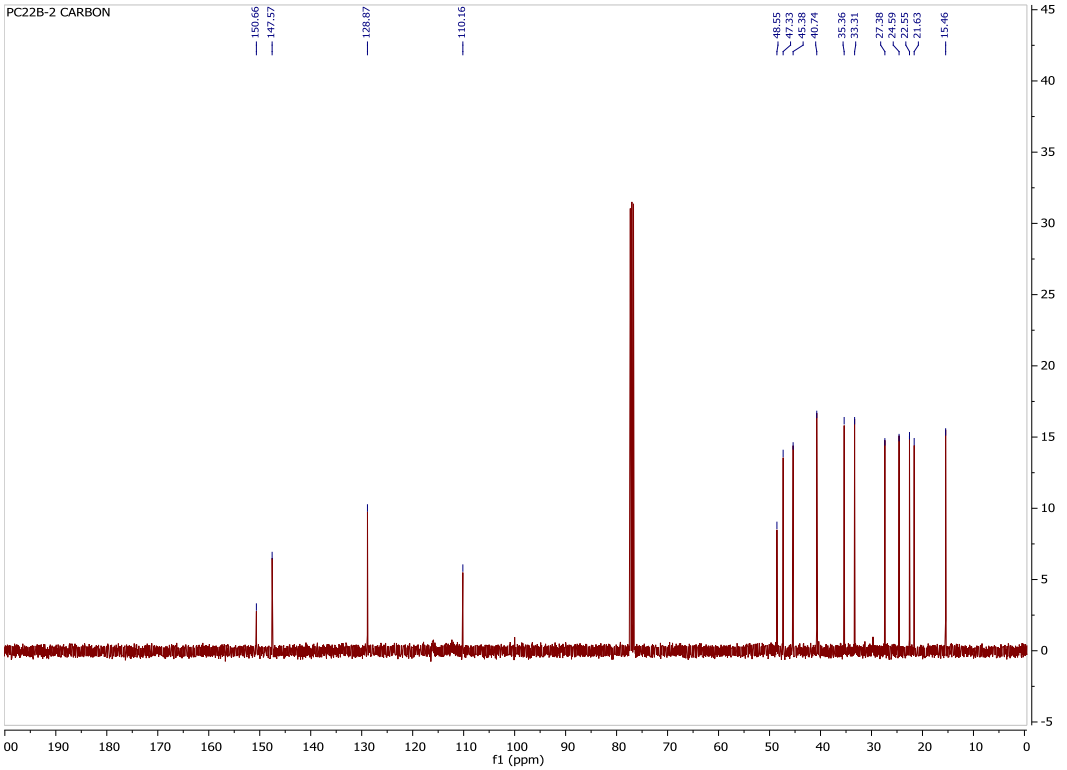


10q

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

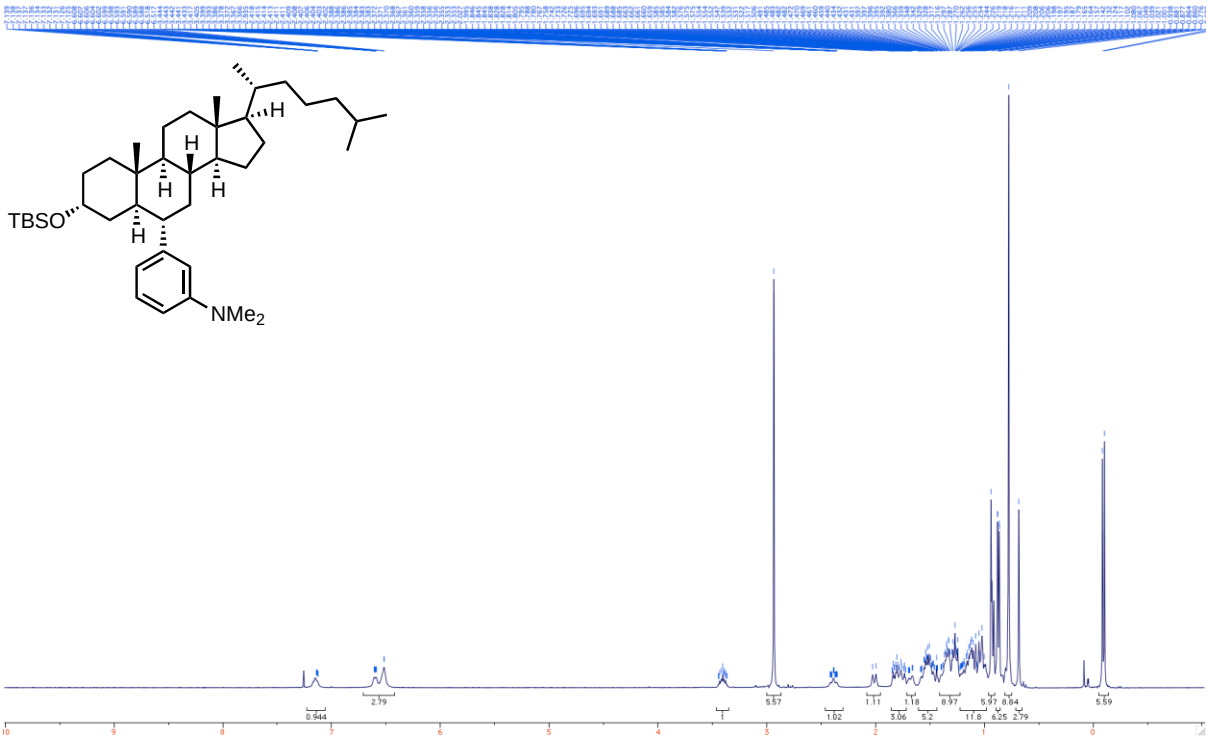


^{13}C NMR (100 MHz, $CDCl_3$)

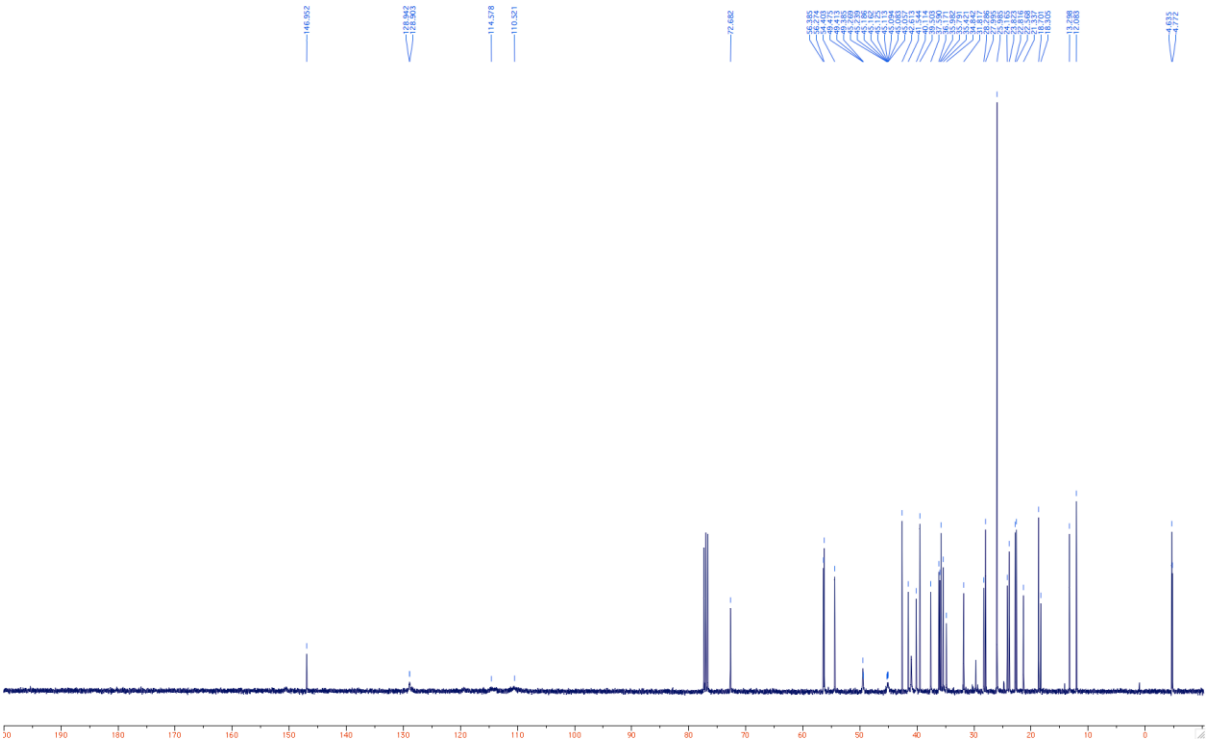


10p

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

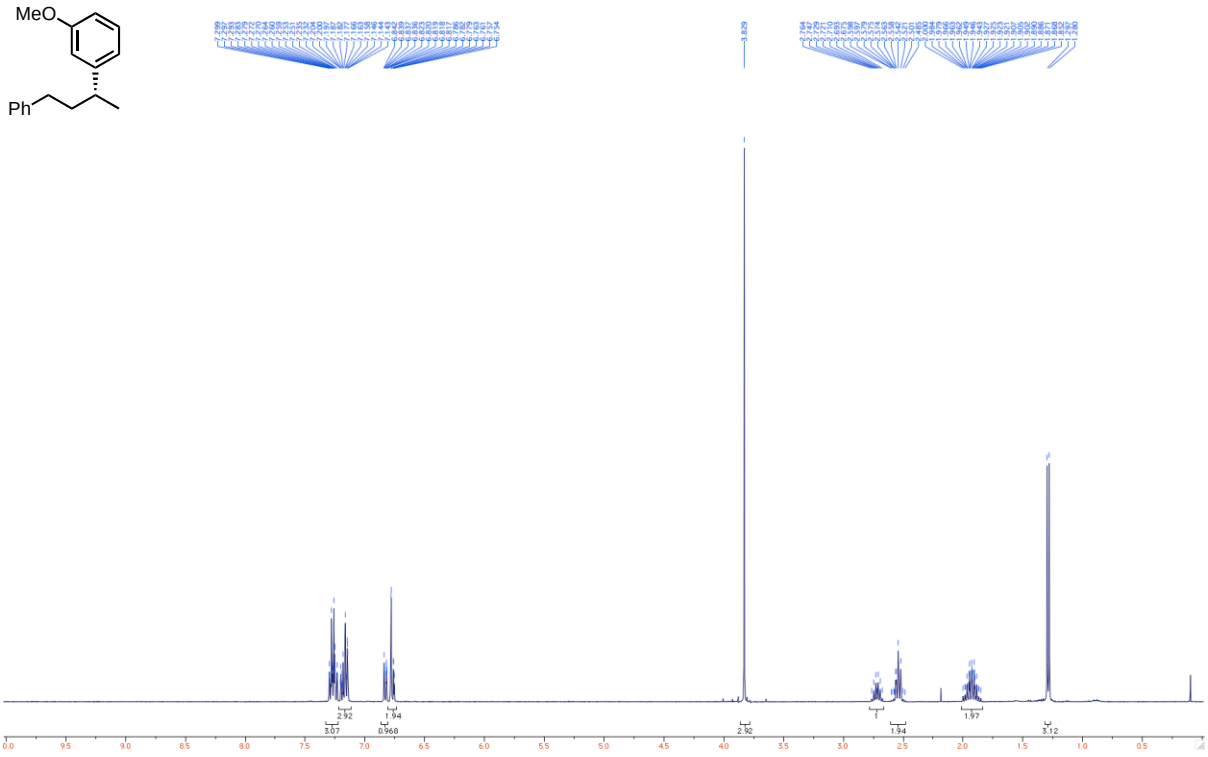


^{13}C NMR (100 MHz, $CDCl_3$)

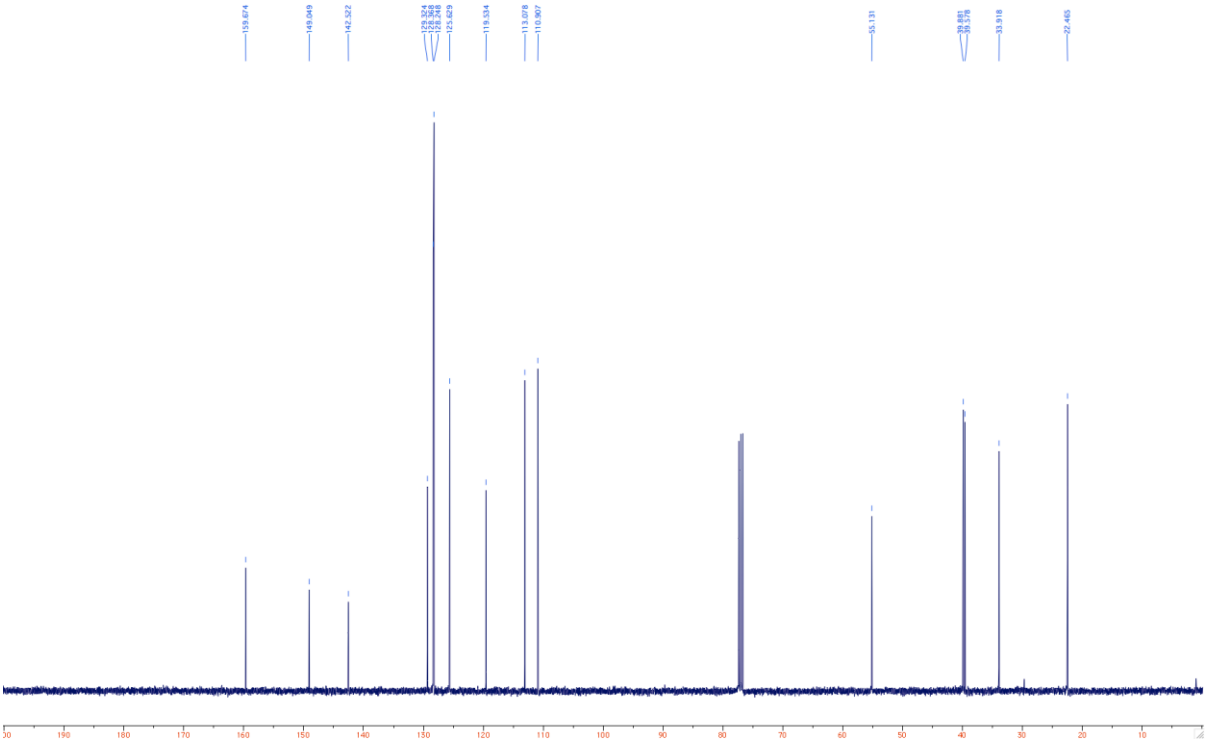


11a

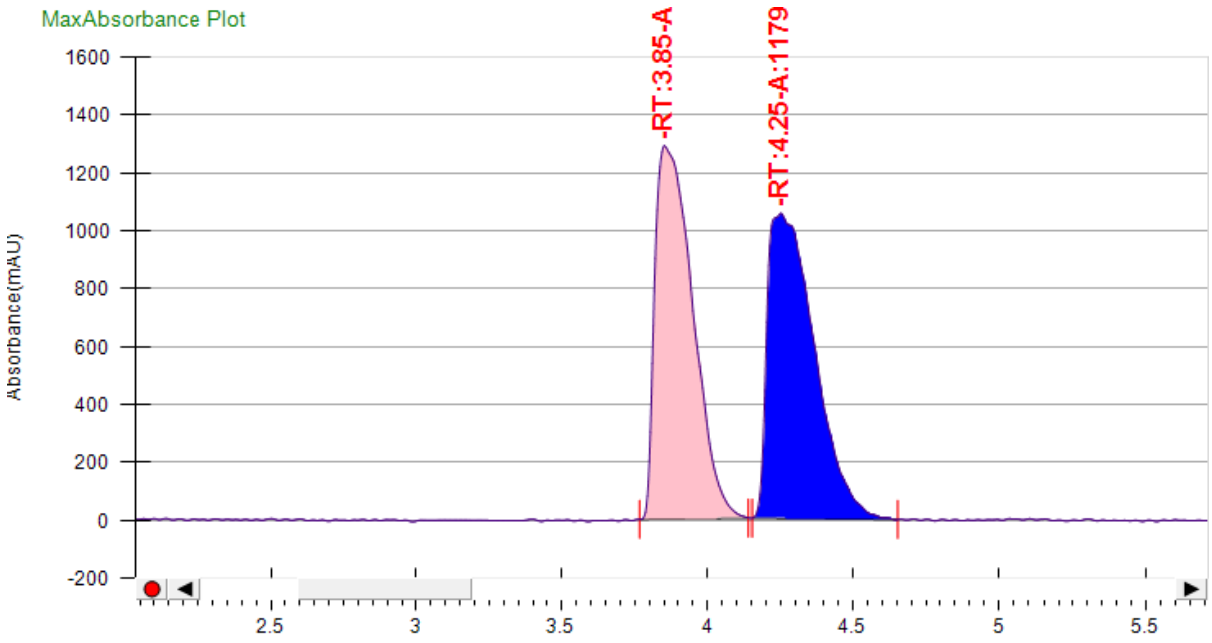
^{1}H NMR (400 MHz, $CDCl_3$)



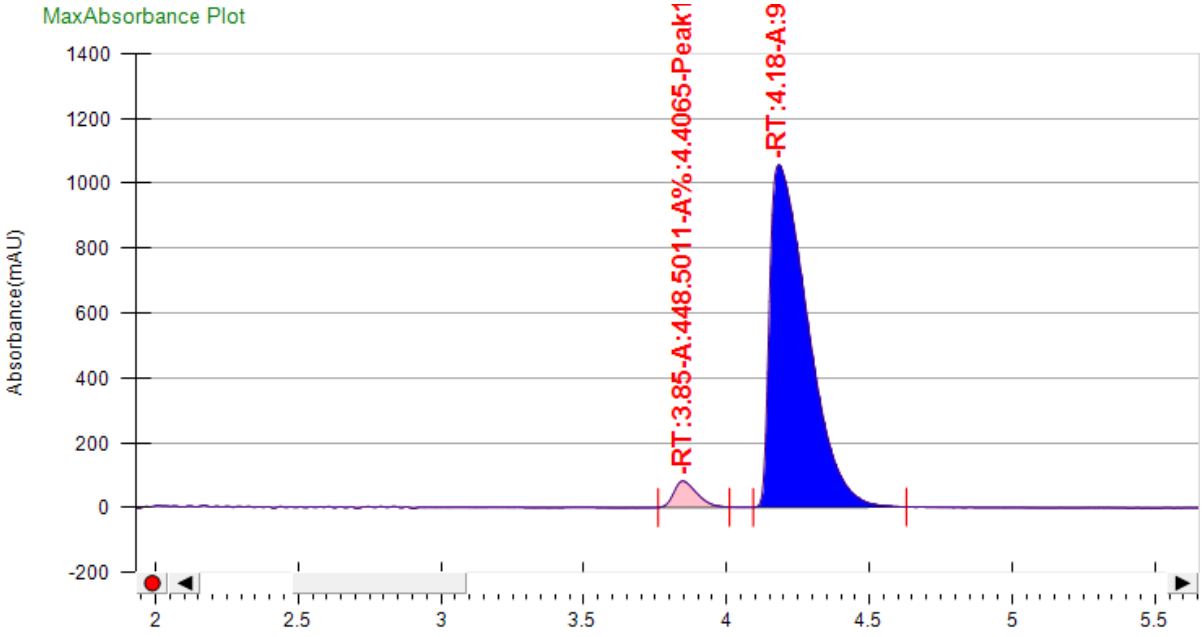
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

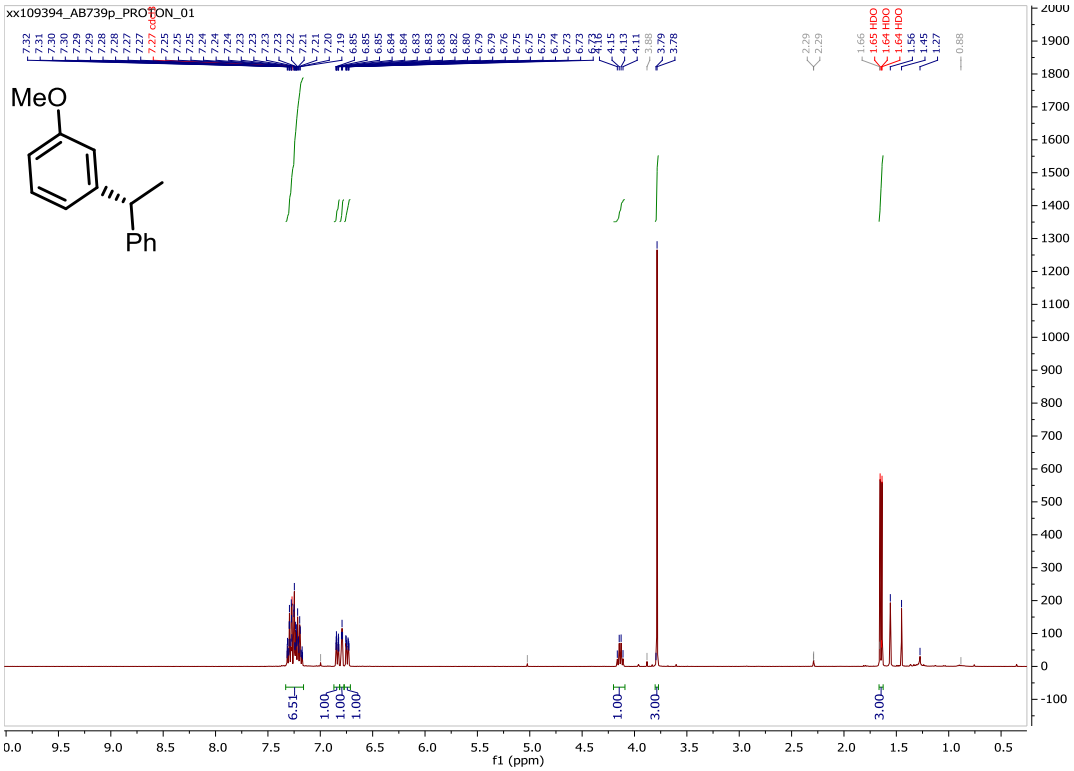


Chiral SFC: enantioenriched

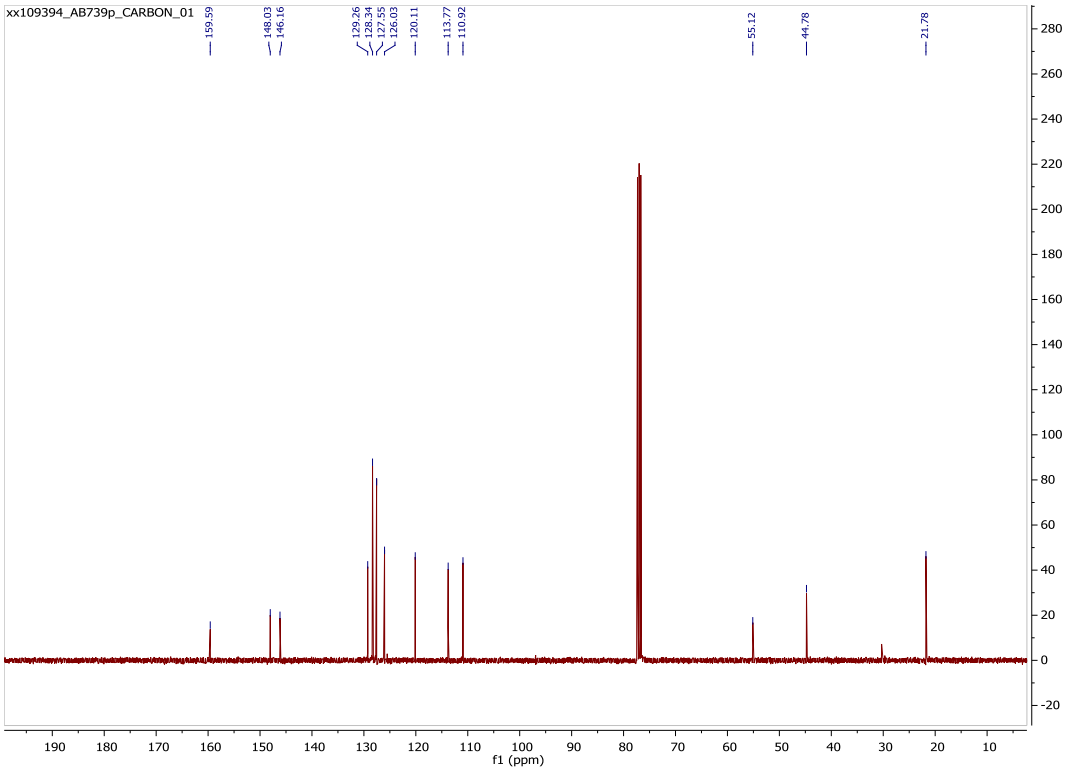


11l

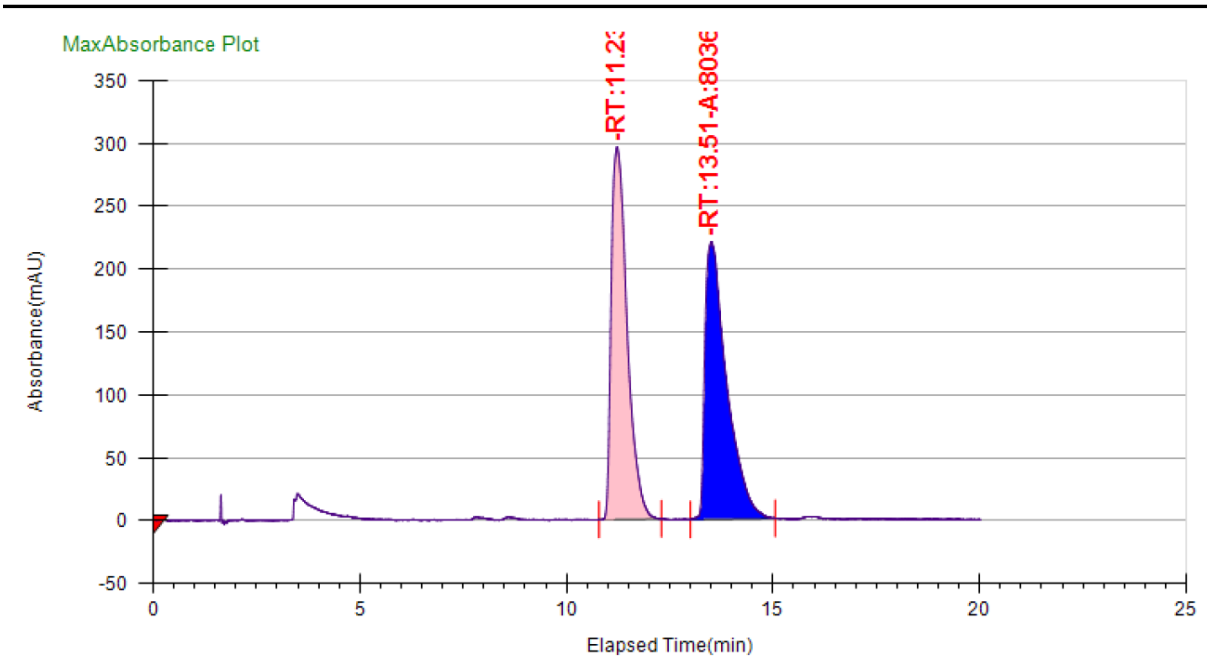
^{1}H NMR (400 MHz, $CDCl_3$)



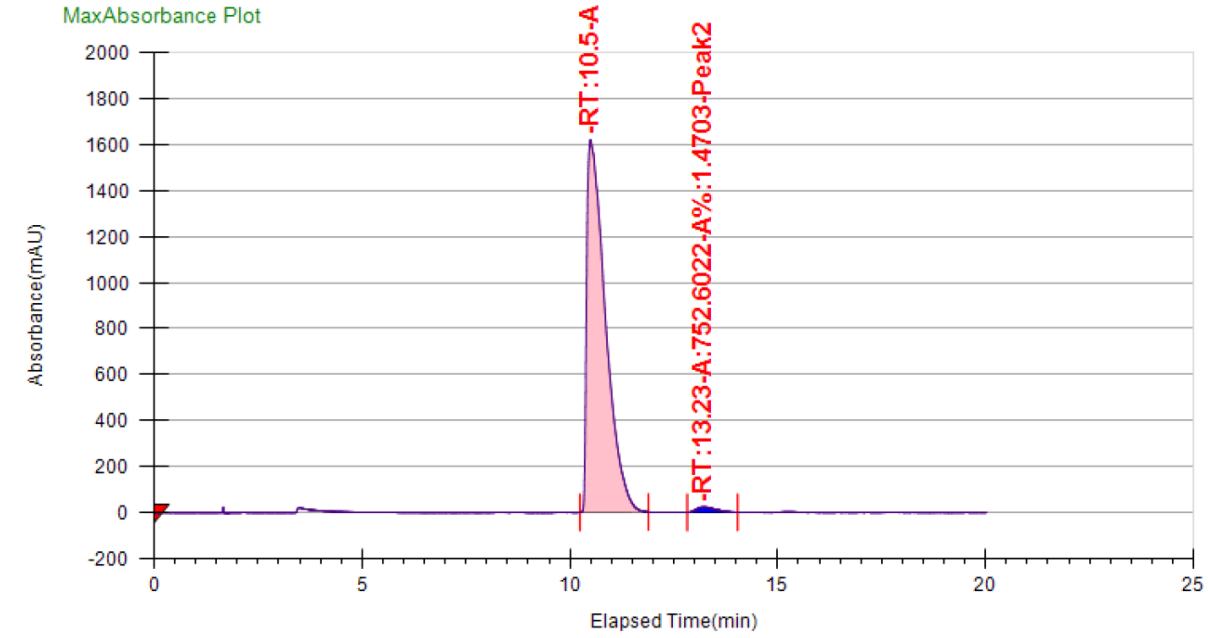
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

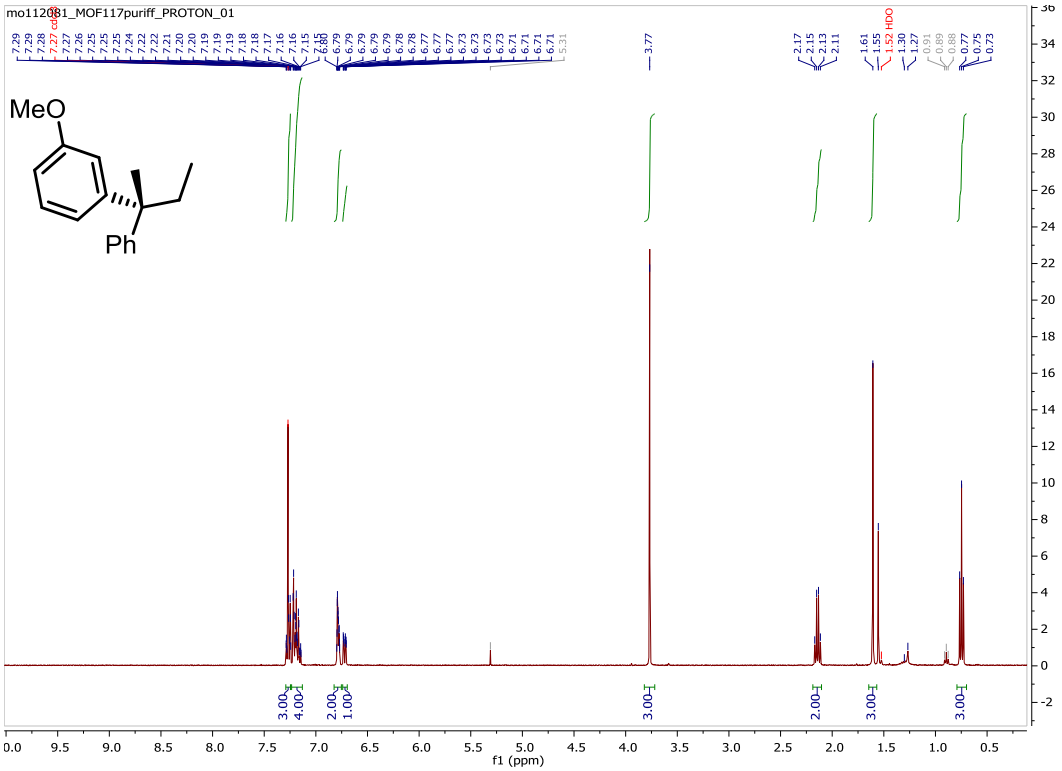


Chiral SFC traces: enantioenriched

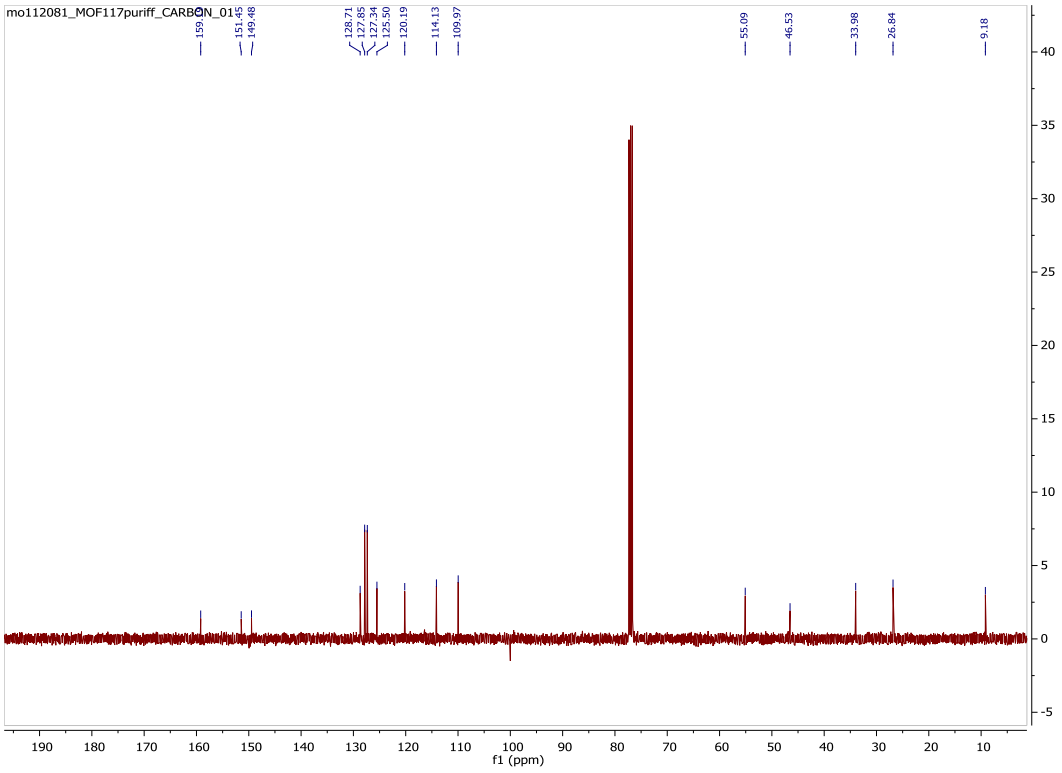


11h

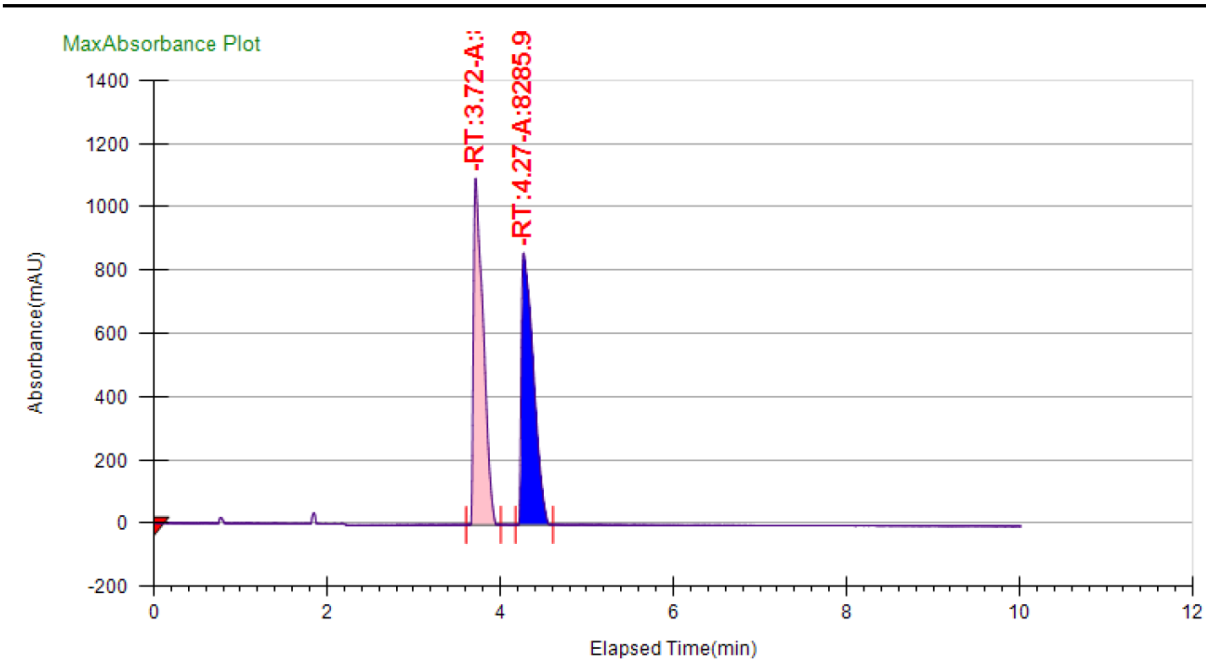
^{1}H NMR (400 MHz, $CDCl_3$)



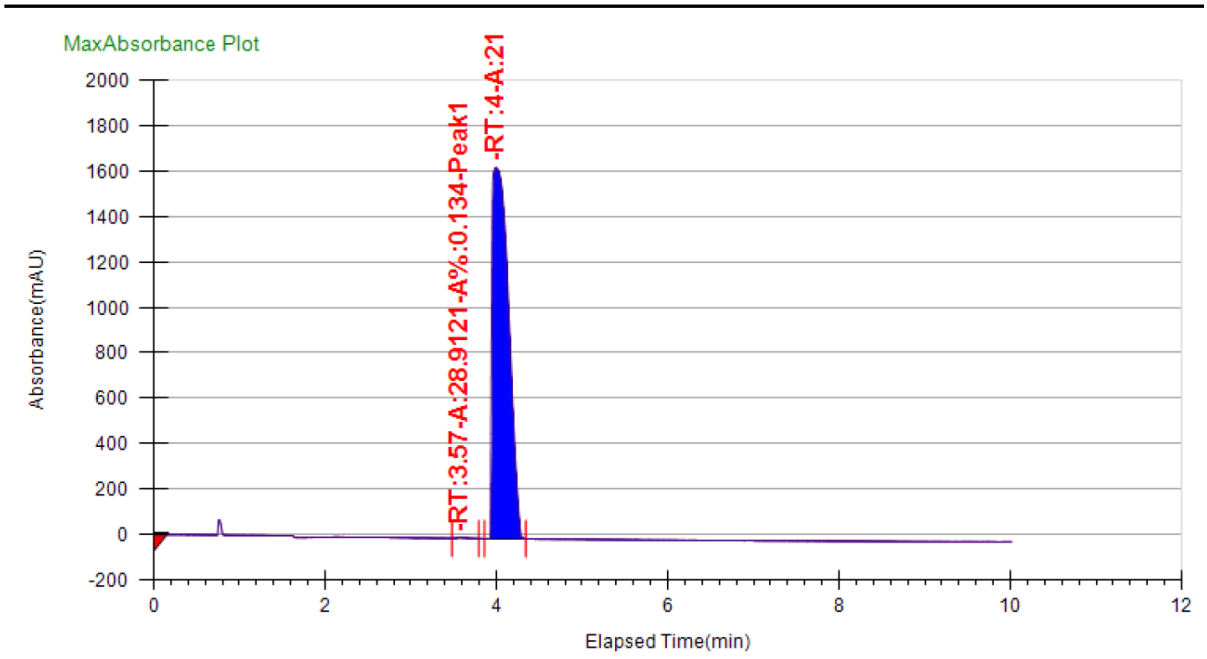
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

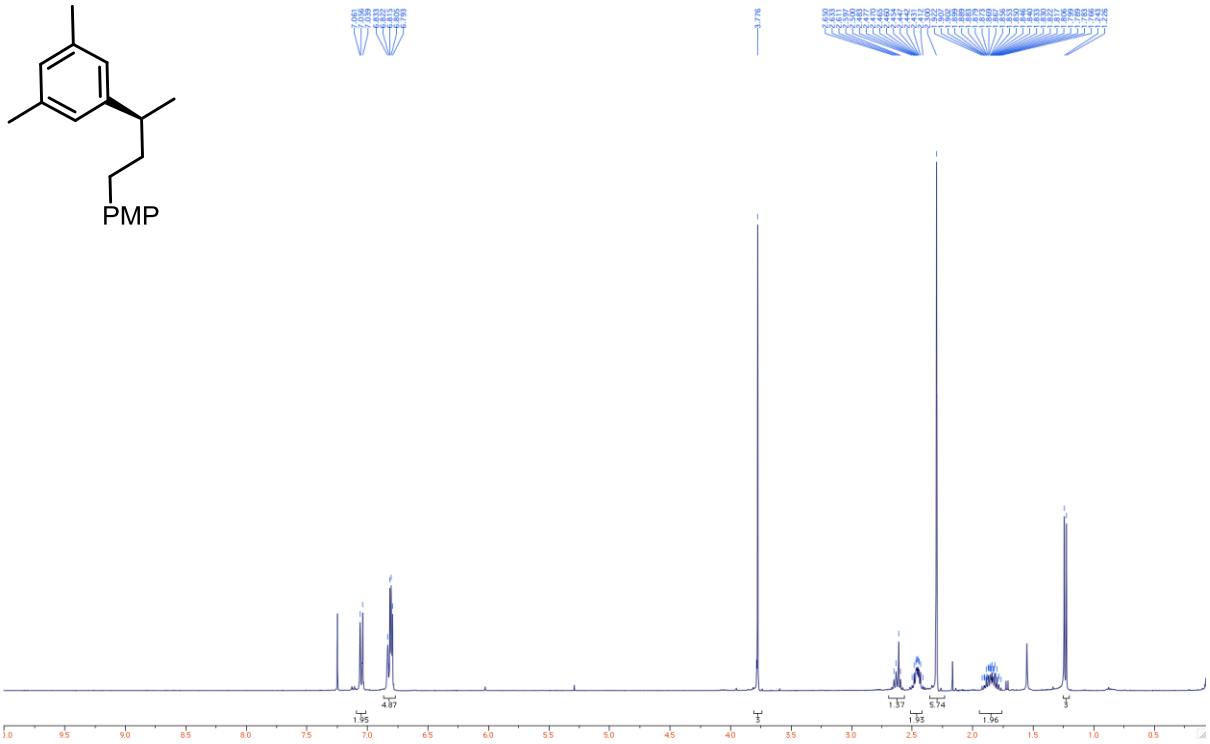


Chiral SFC traces: enantioenriched

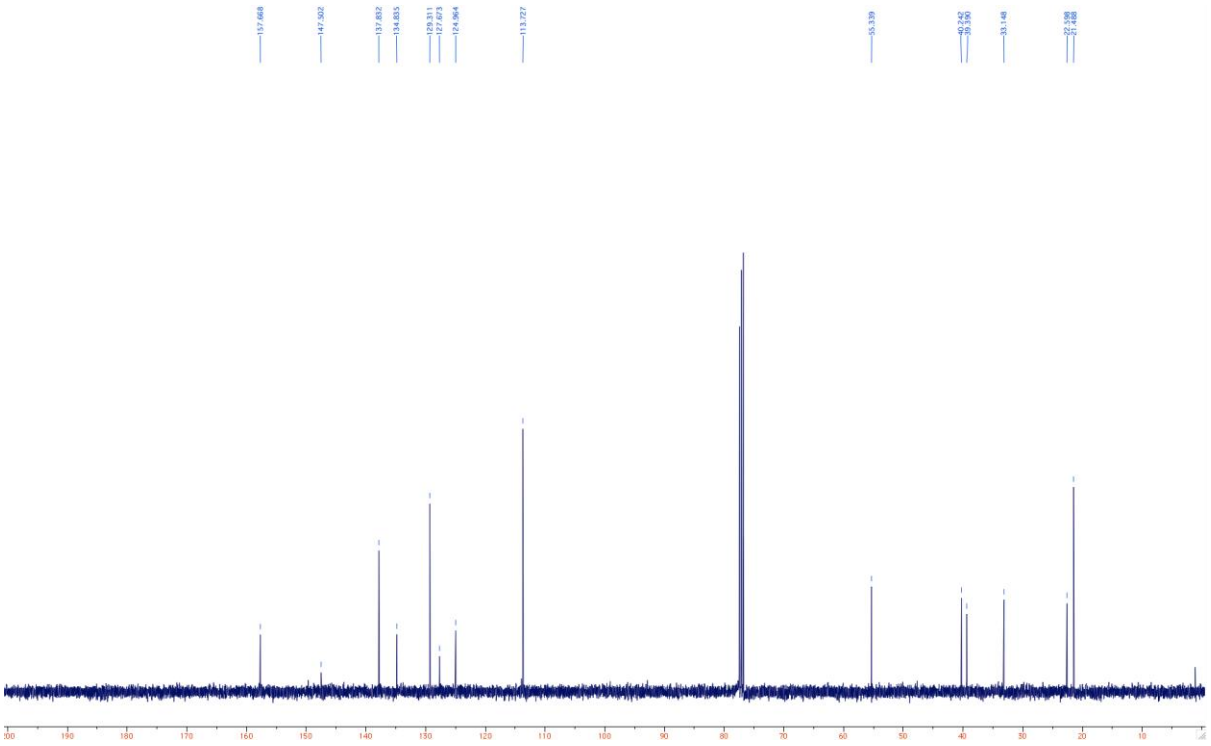


18b

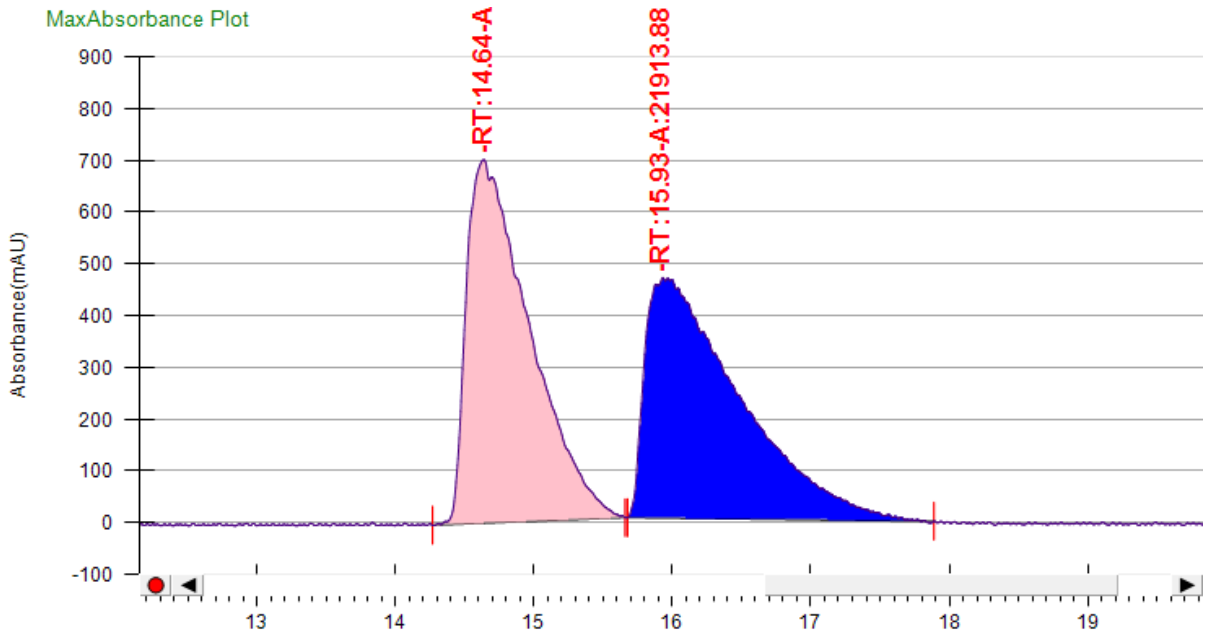
^{1}H NMR (400 MHz, $CDCl_3$)



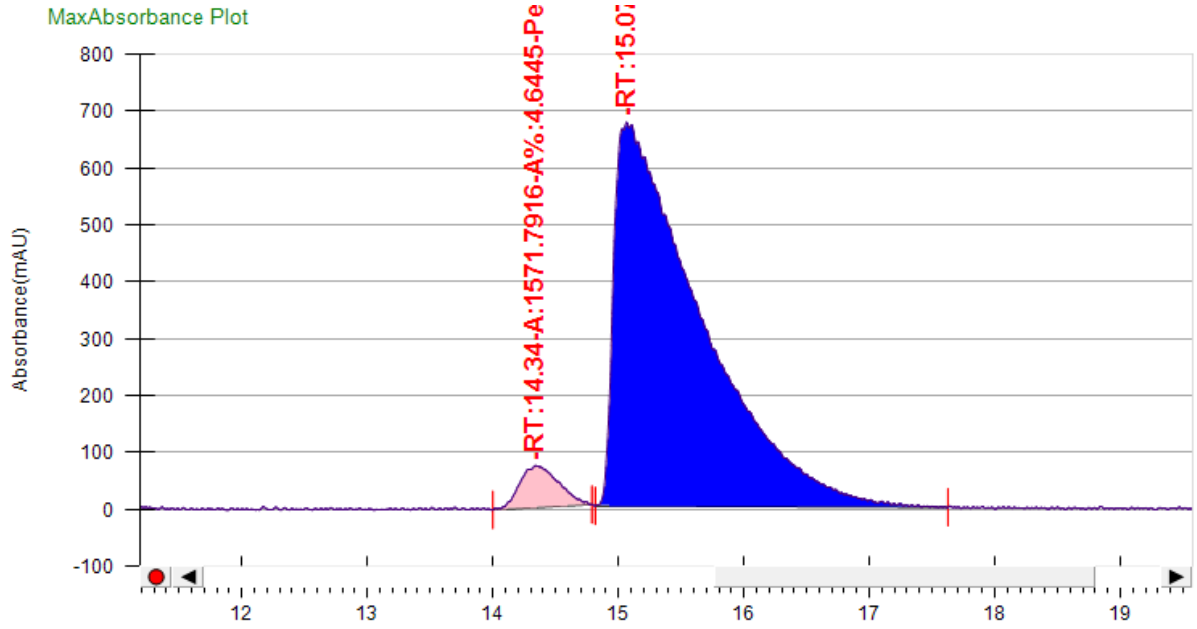
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

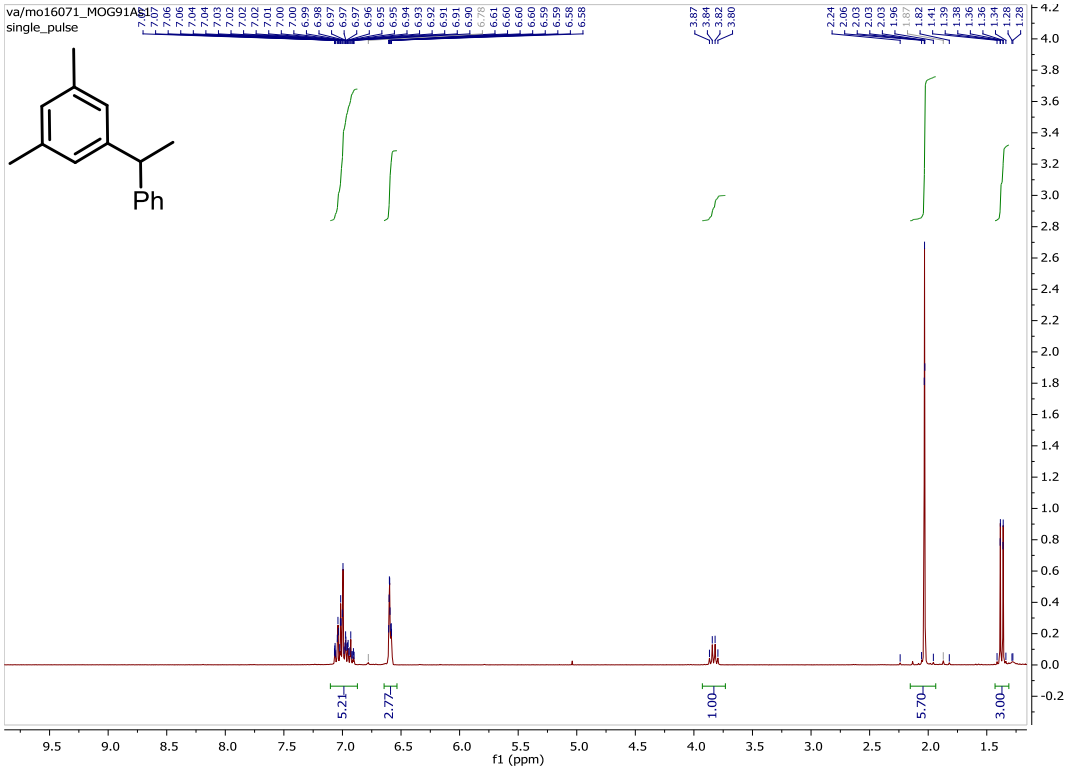


Chiral SFC traces: enantioenriched

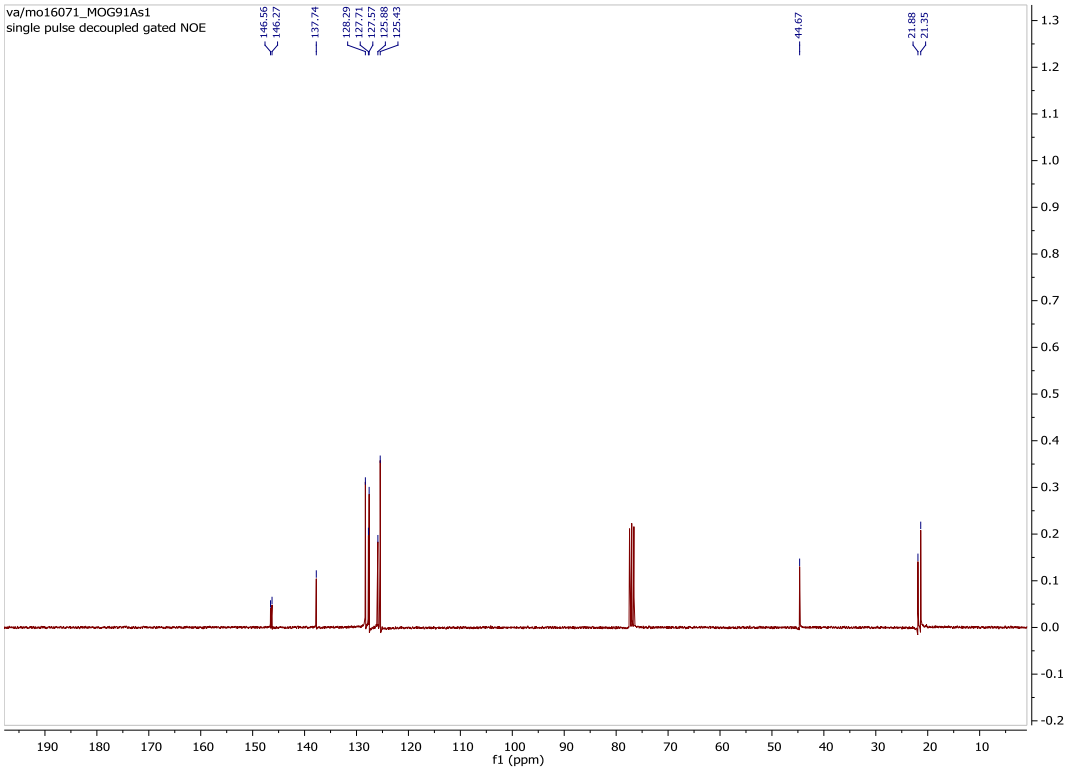


18l

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

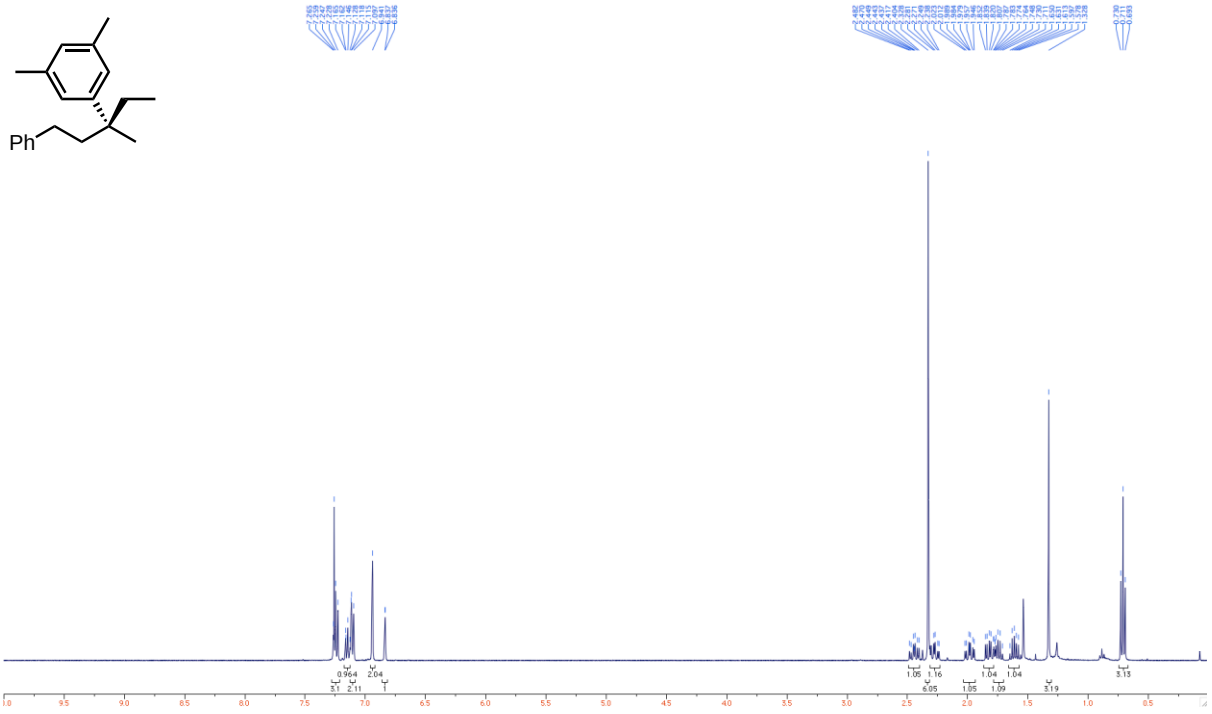


^{13}C NMR (100 MHz, $CDCl_3$)

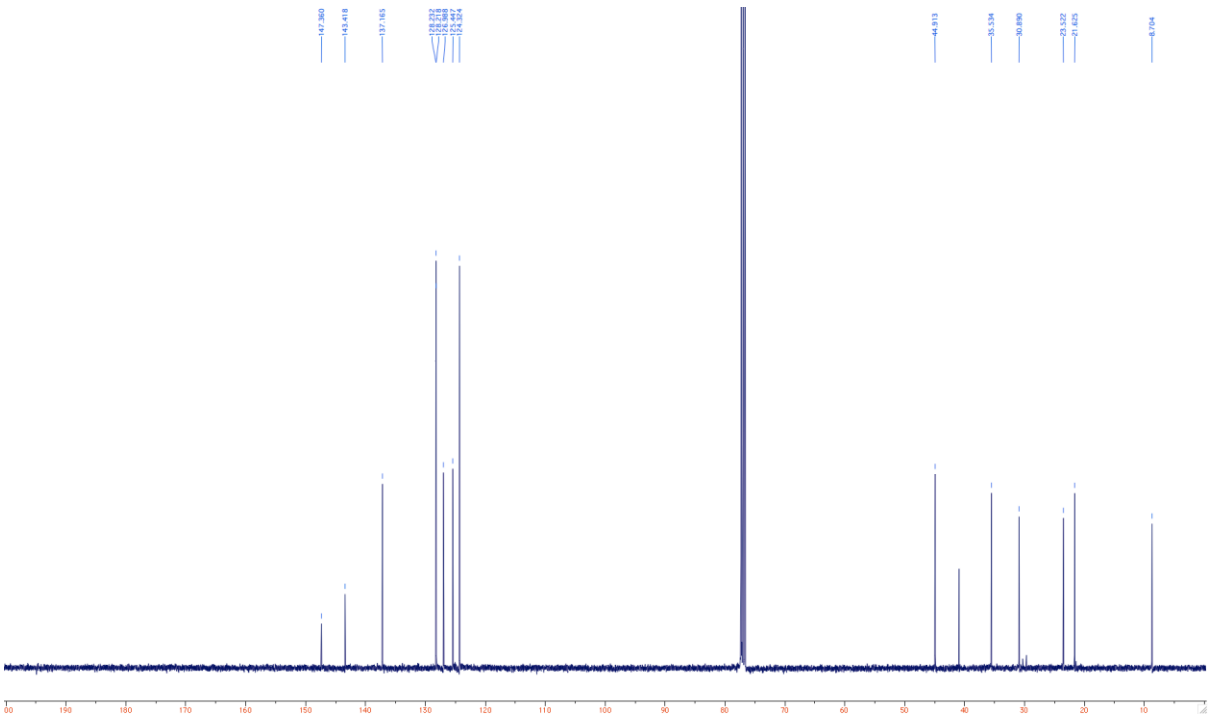


18g[7]

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



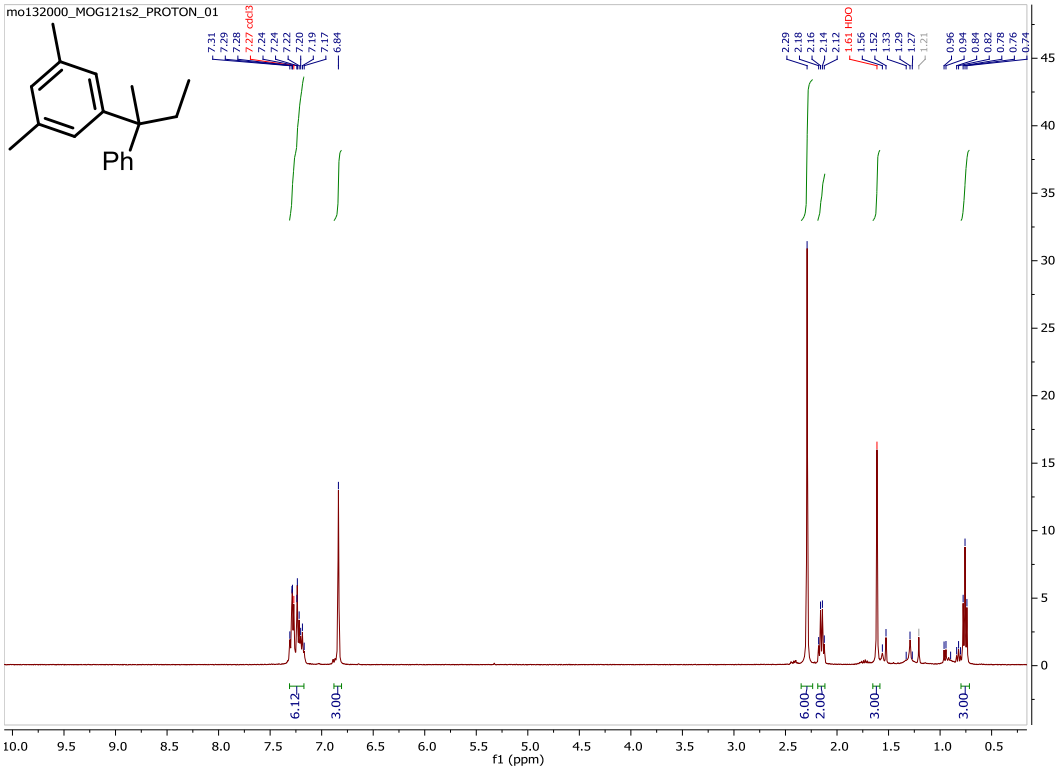
^{13}C NMR (100 MHz, $CDCl_3$)



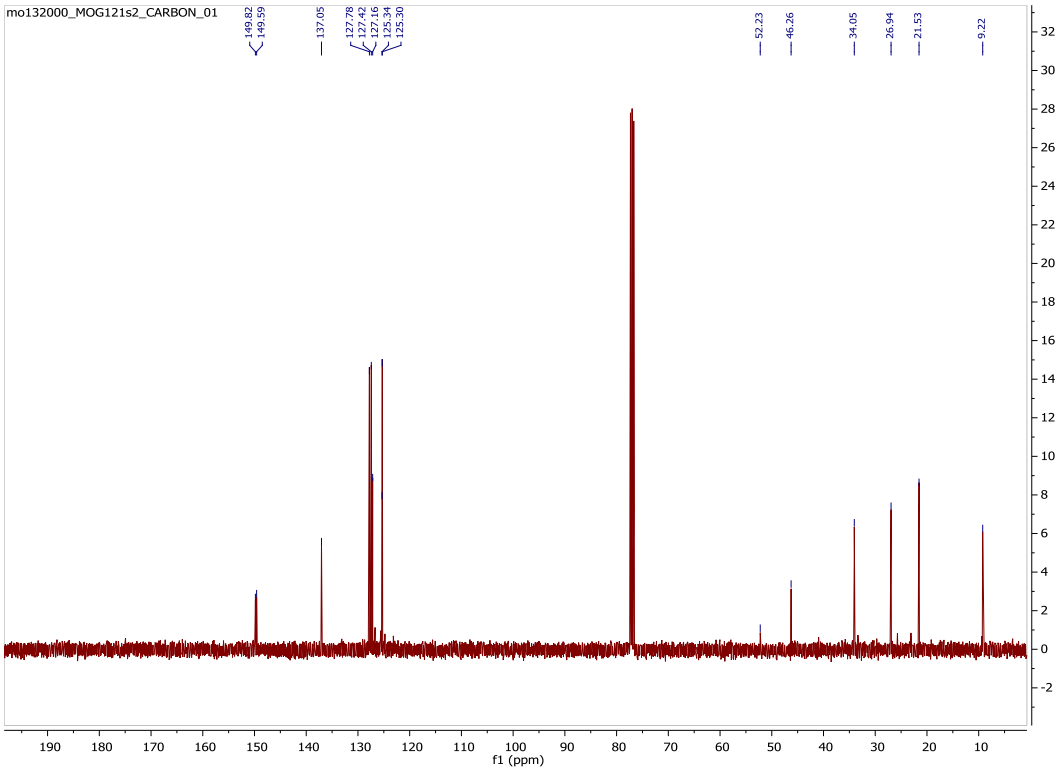
[7] e.r. of **18ga** reflects the e.r. of **18g** (see below).

18h

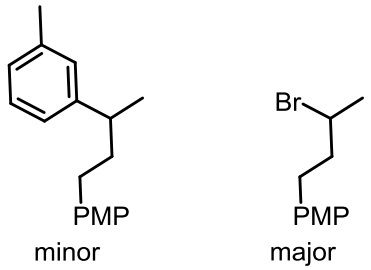
^{1}H NMR (400 MHz, $CDCl_3$)



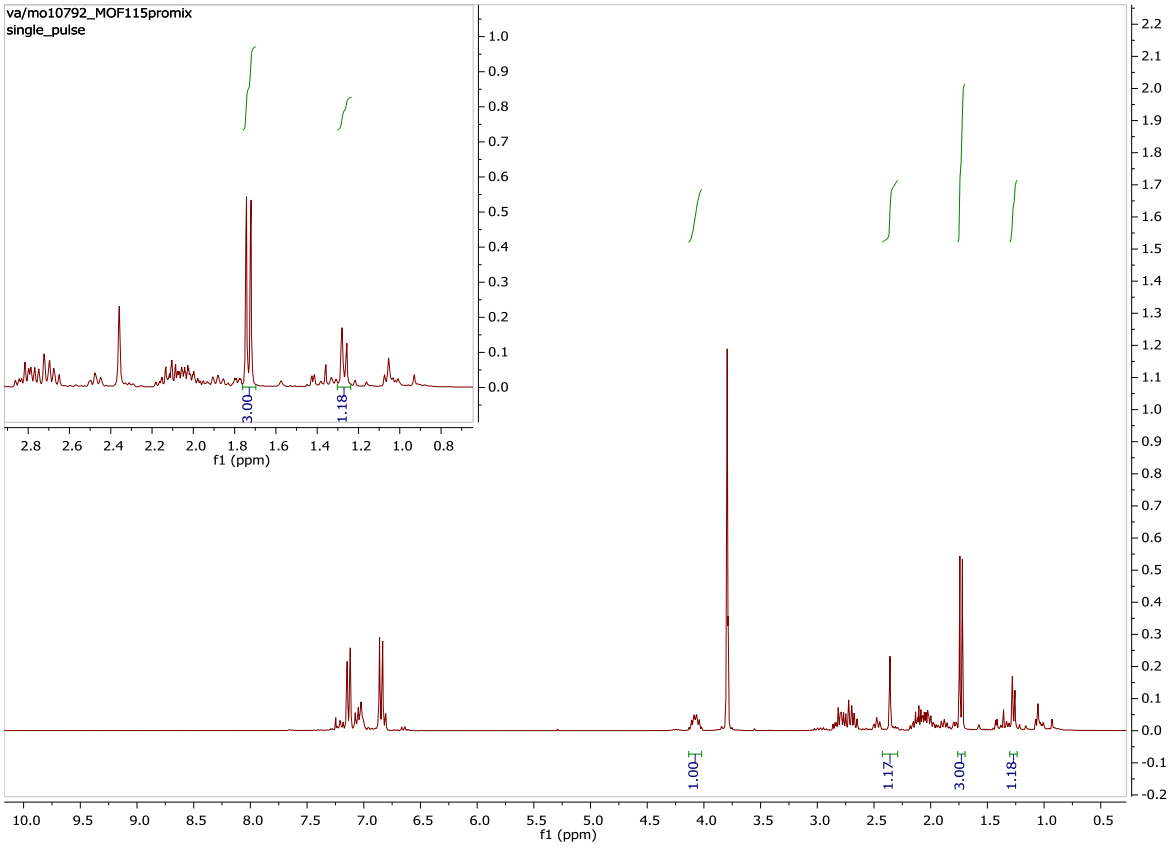
^{13}C NMR (100 MHz, $CDCl_3$)



19b and 21 – unseparable mixture

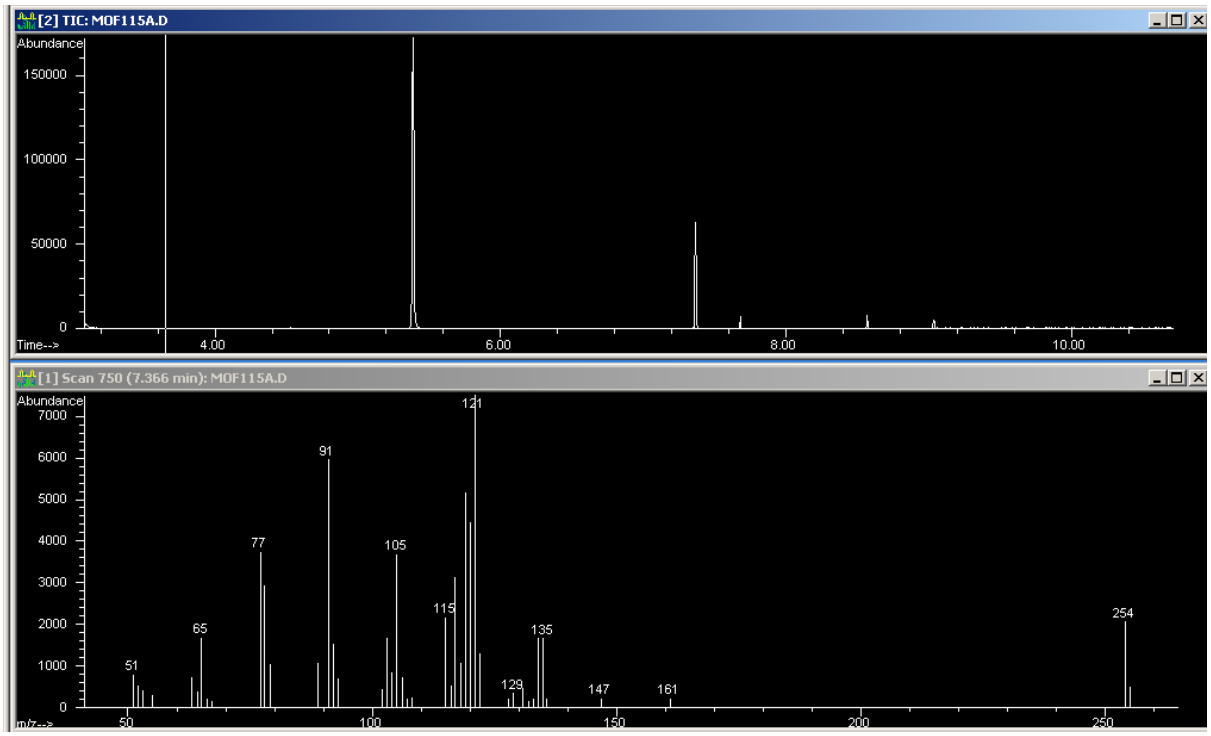


^{1}H NMR (400 MHz, $CDCl_3$)

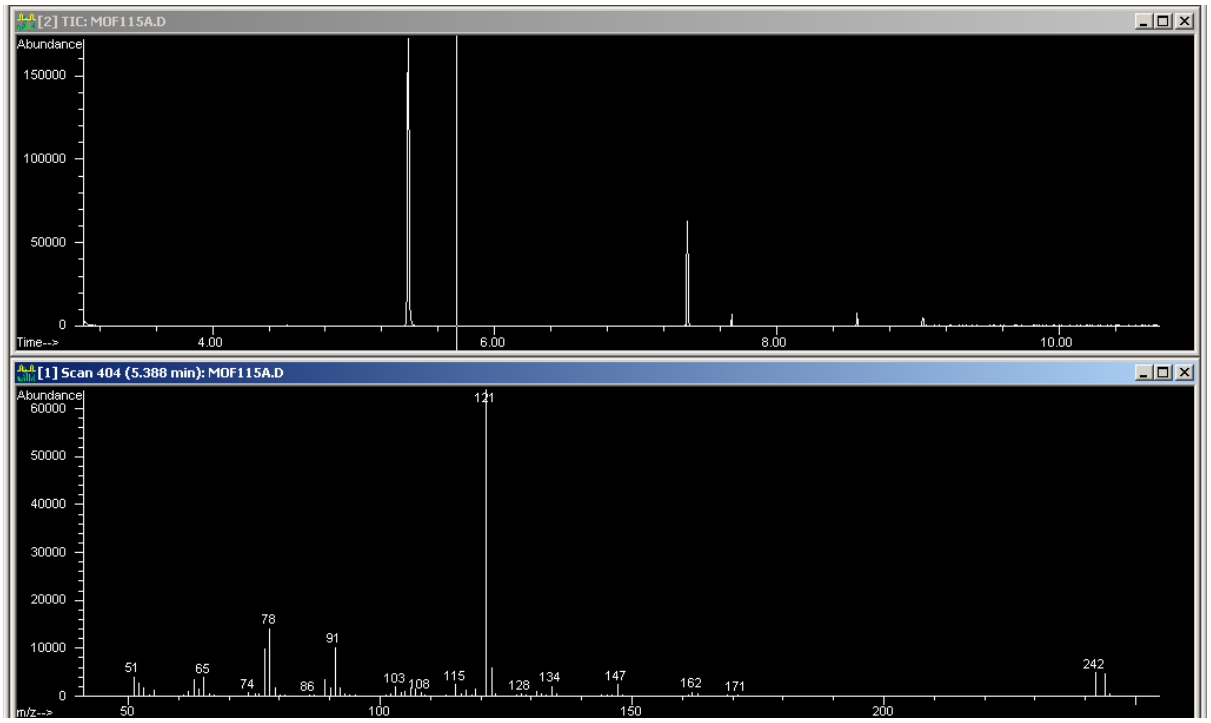


GC-MS chromatogram of inseparable mixture of products:

Coupling product **13b**:

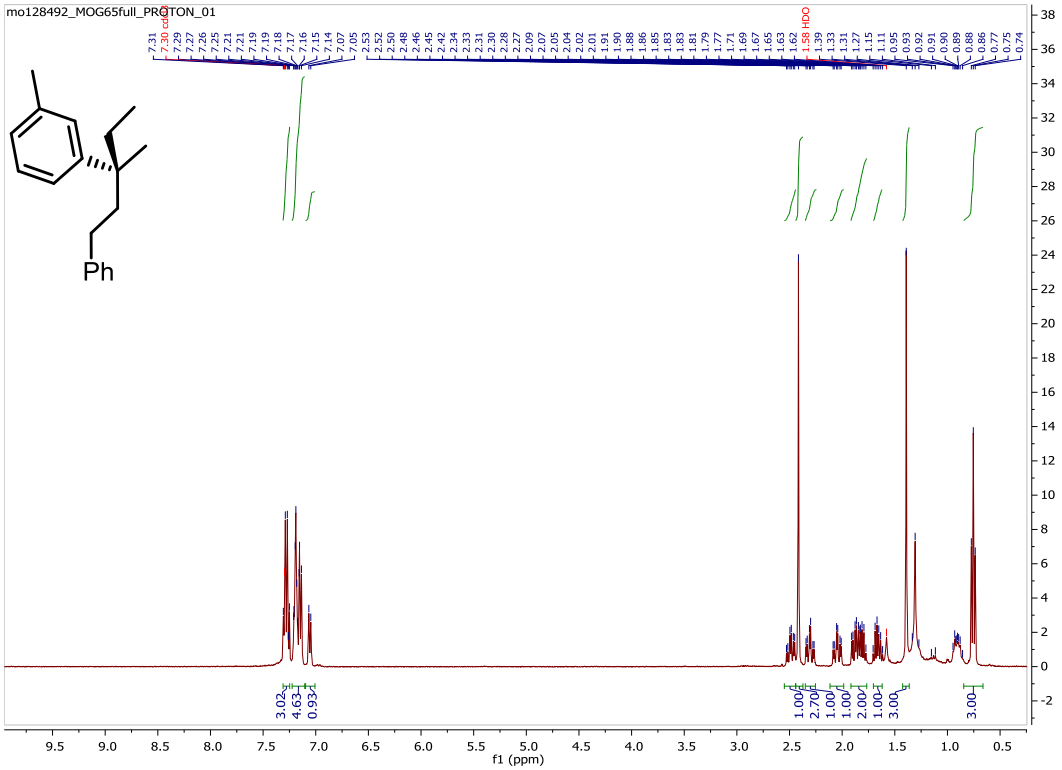


Bromination on C(sp^3) centre:

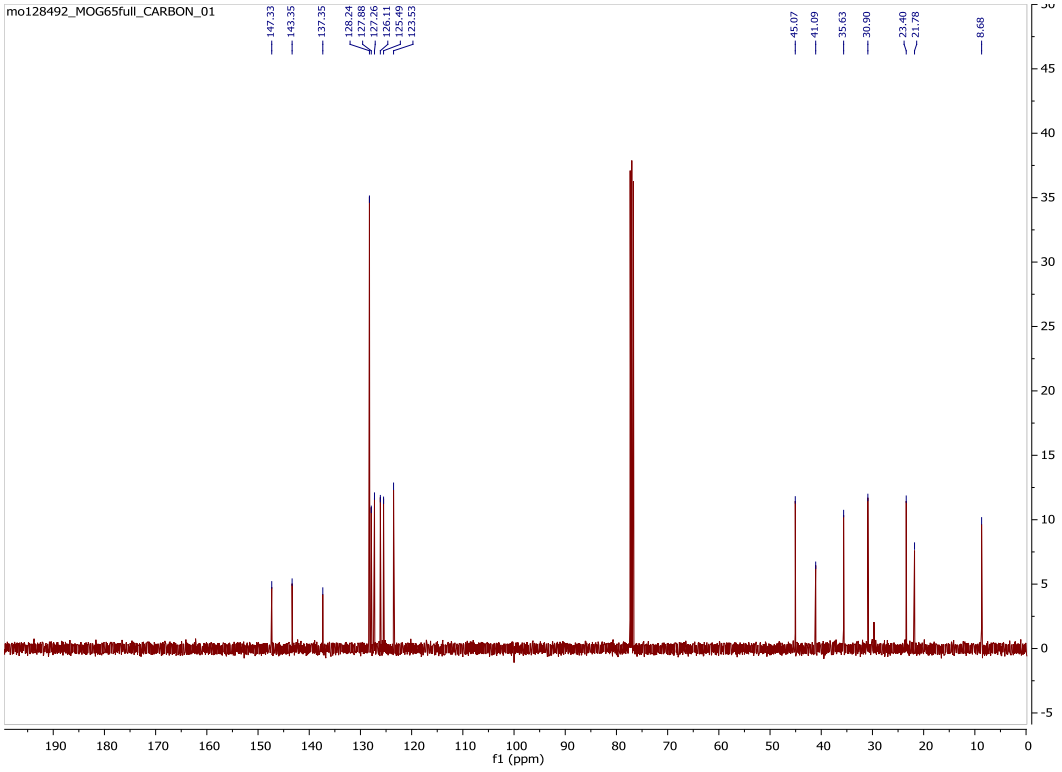


19g

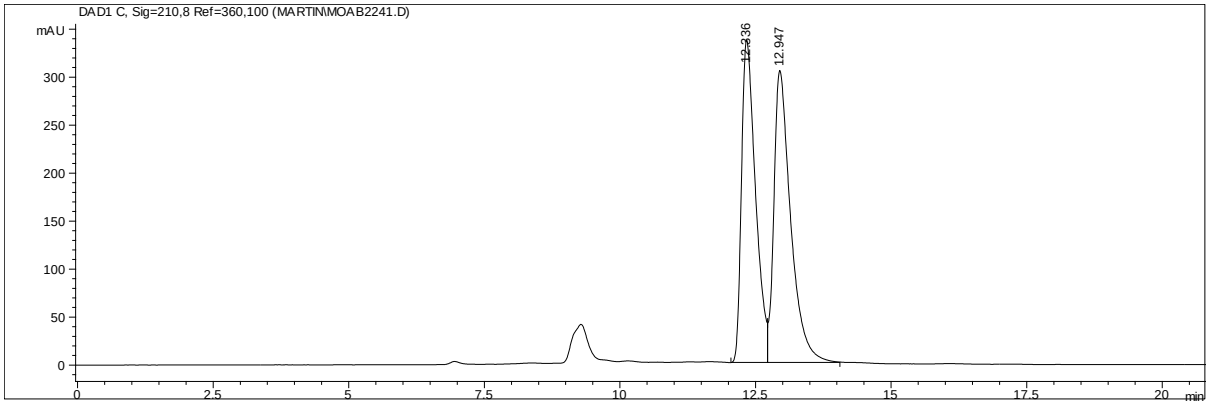
^{1}H NMR (400 MHz, $CDCl_3$)



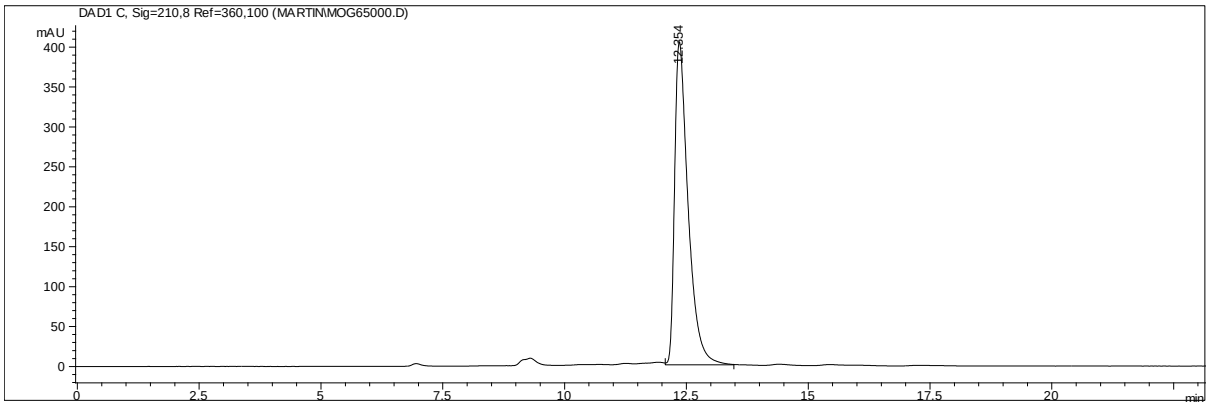
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

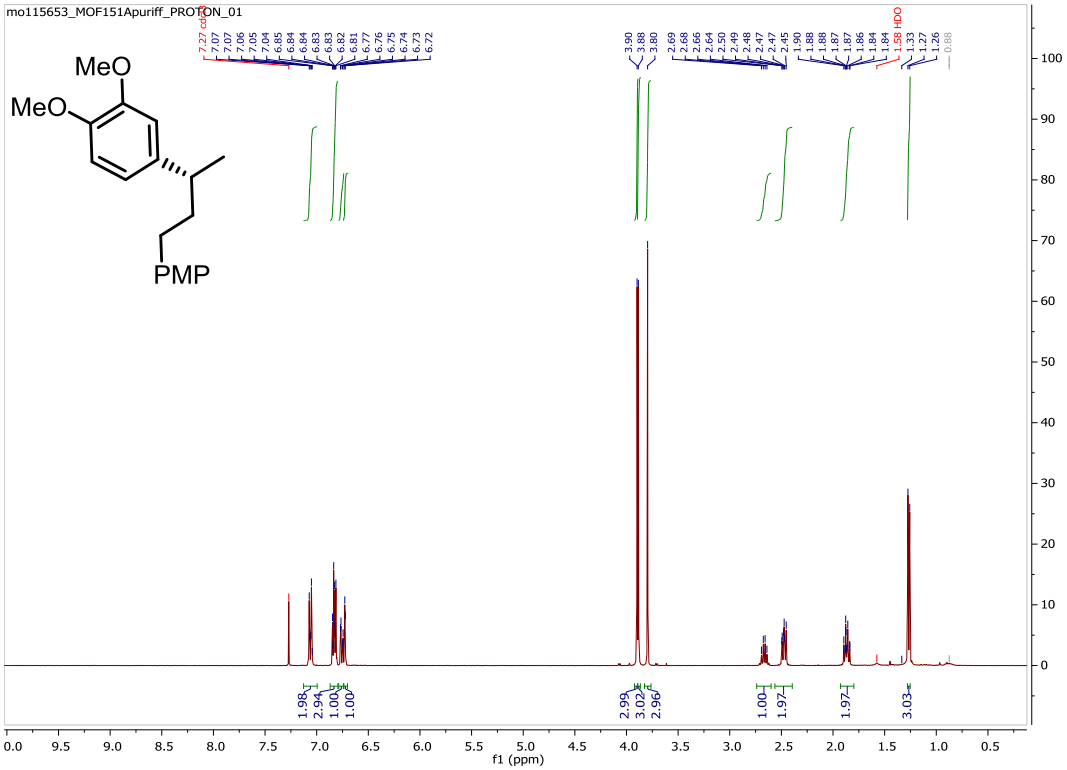


Chiral HPLC traces: enantioenriched

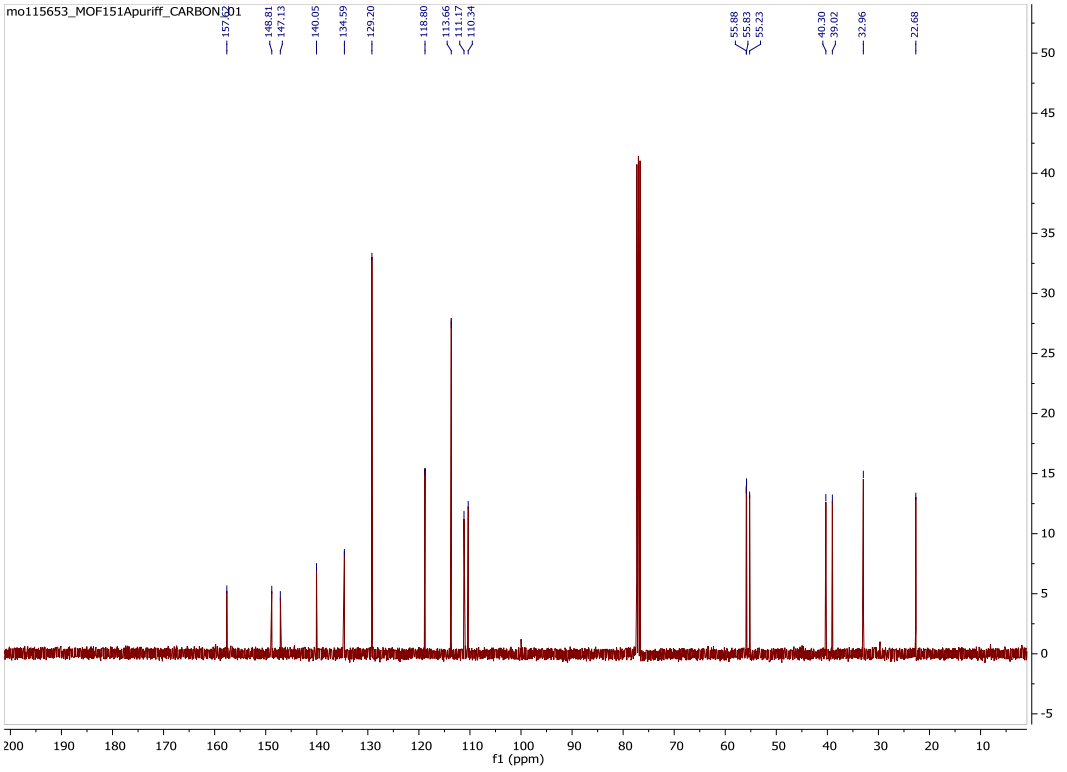


13b

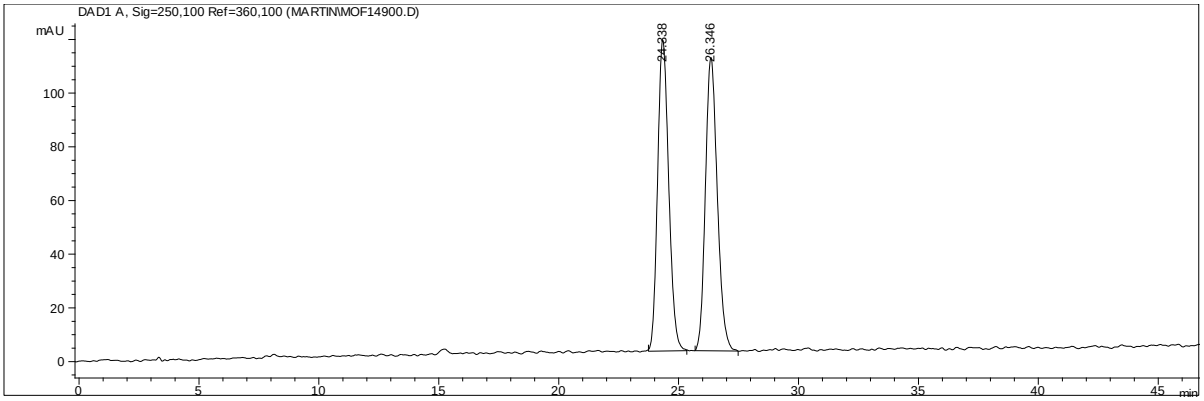
^{1}H NMR (400 MHz, $CDCl_3$)



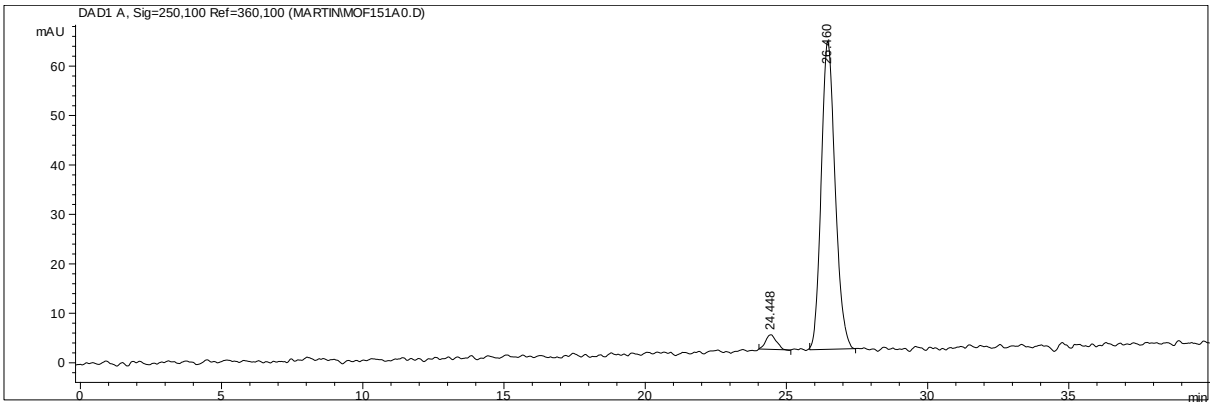
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

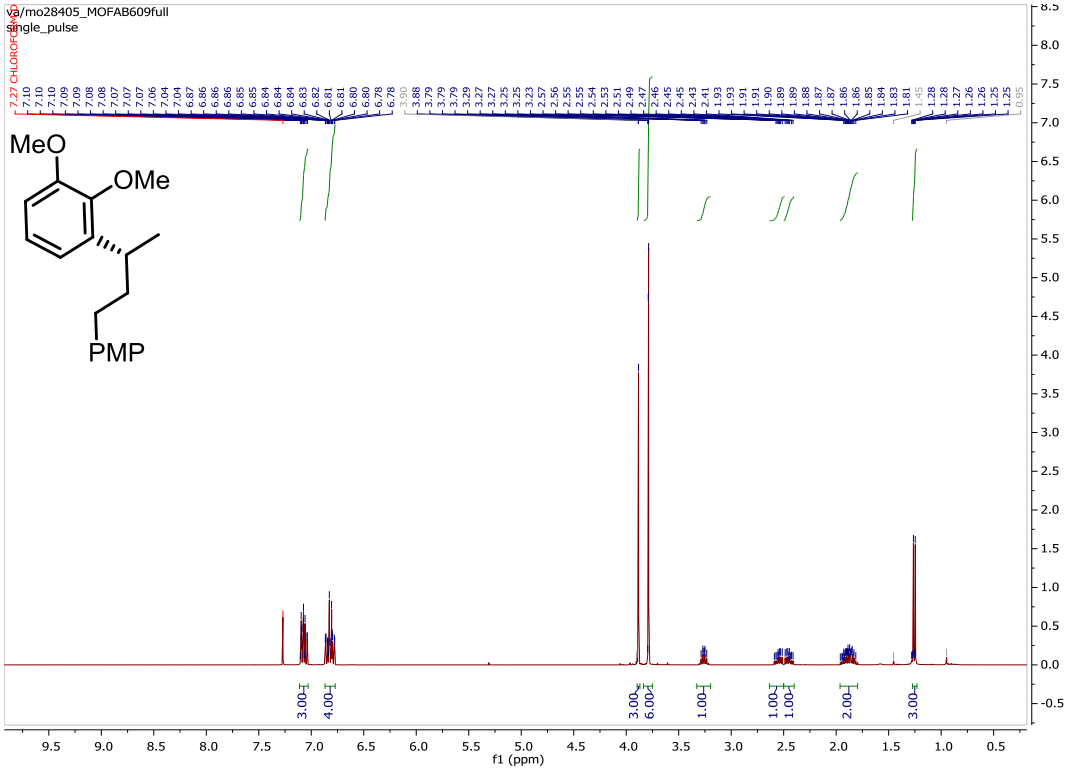


Chiral HPLC traces: enantioenriched

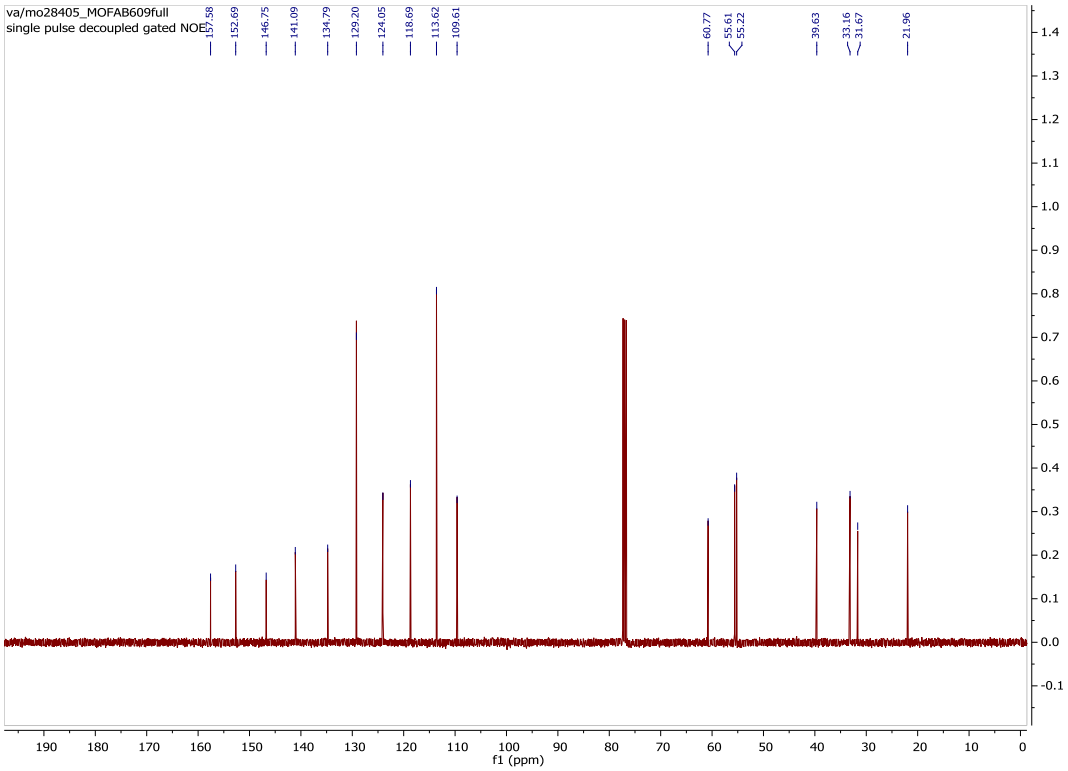


12b

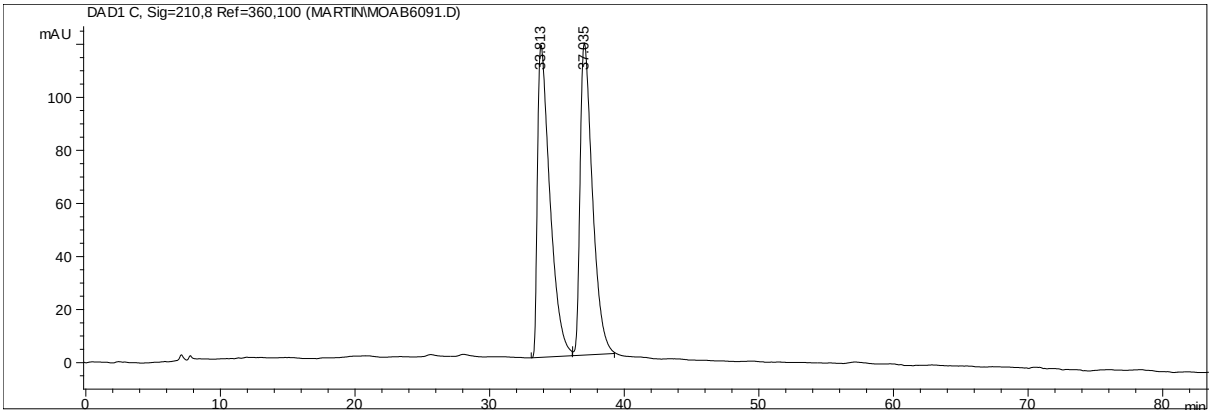
^{1}H NMR (400 MHz, $CDCl_3$)



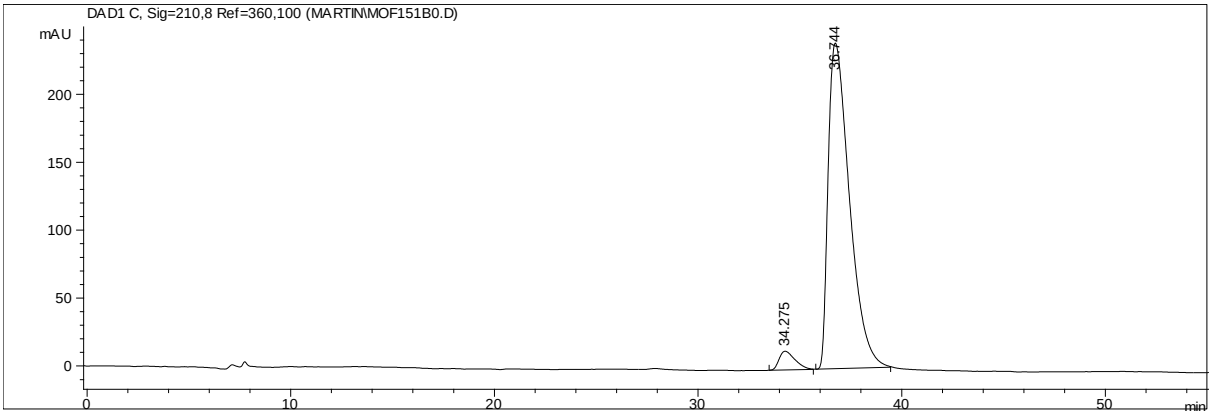
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

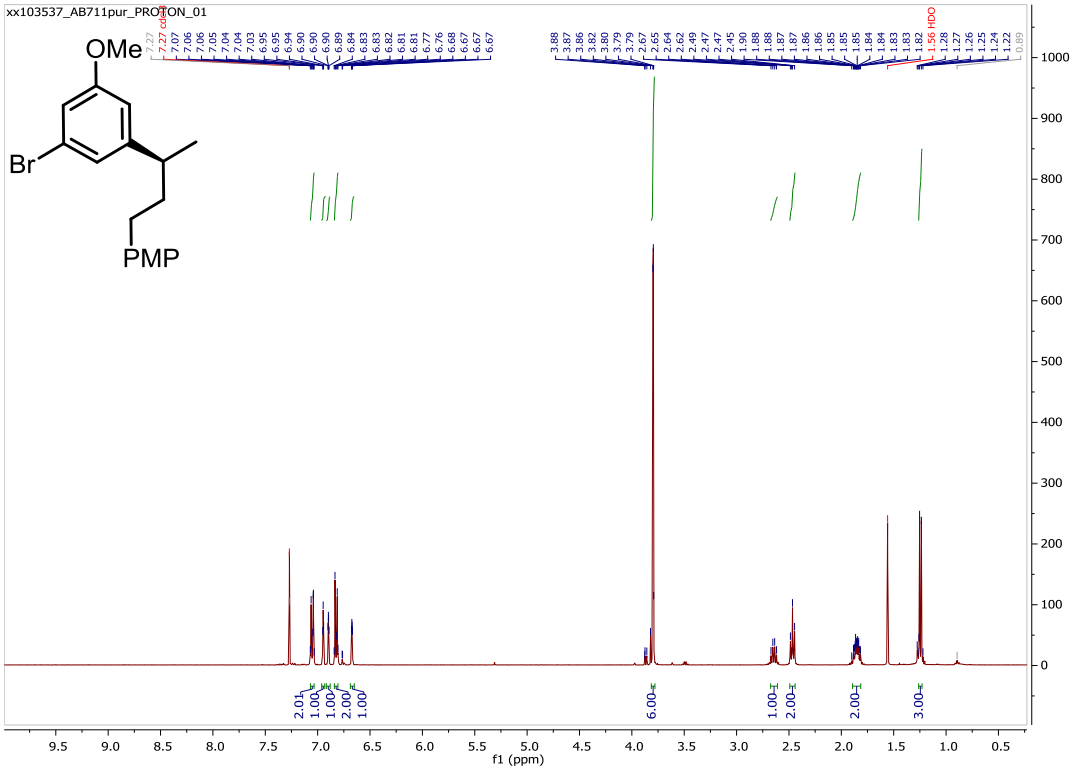


Chiral HPLC traces: enantioenriched

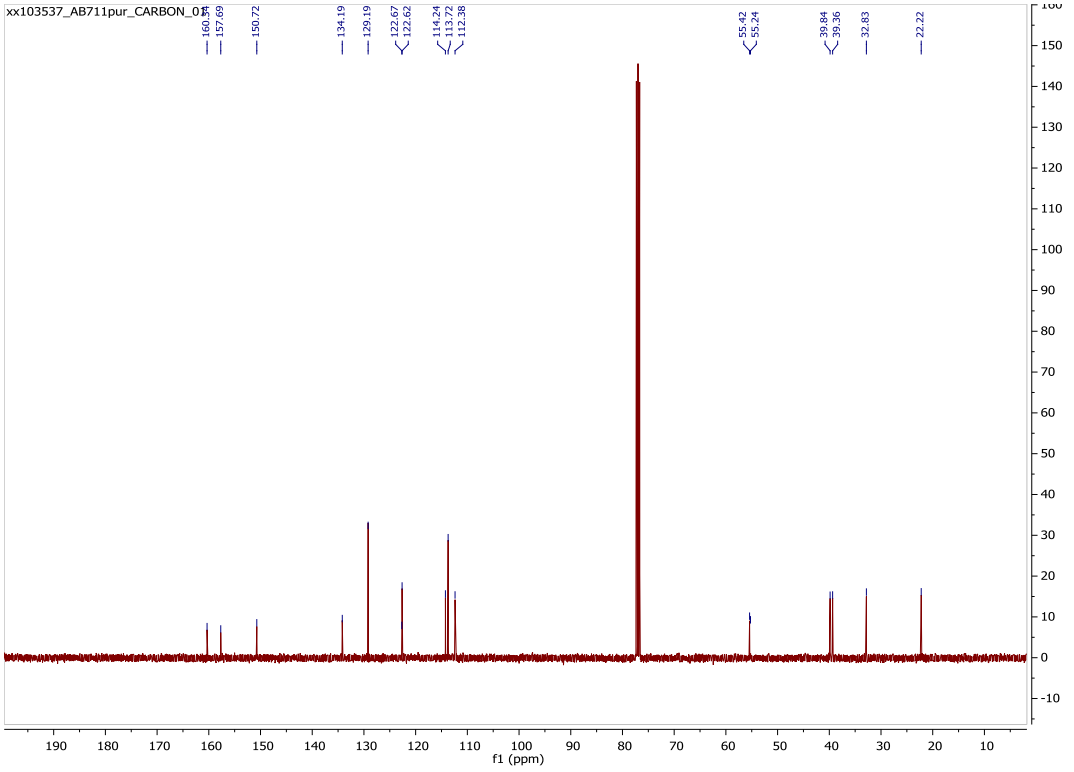


14b

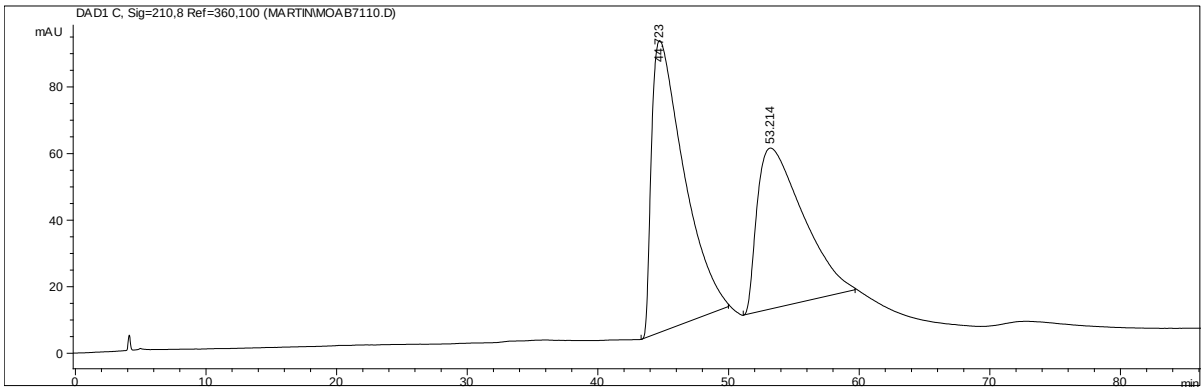
^{1}H NMR (400 MHz, $CDCl_3$)



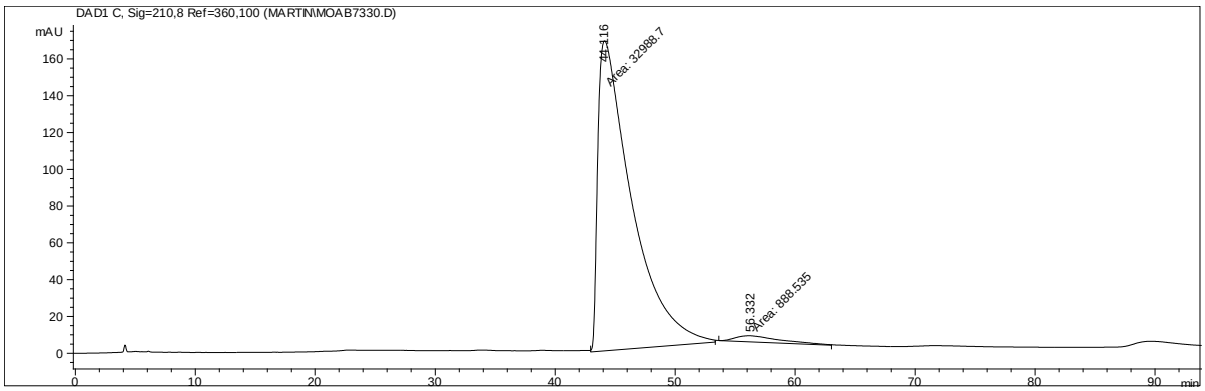
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

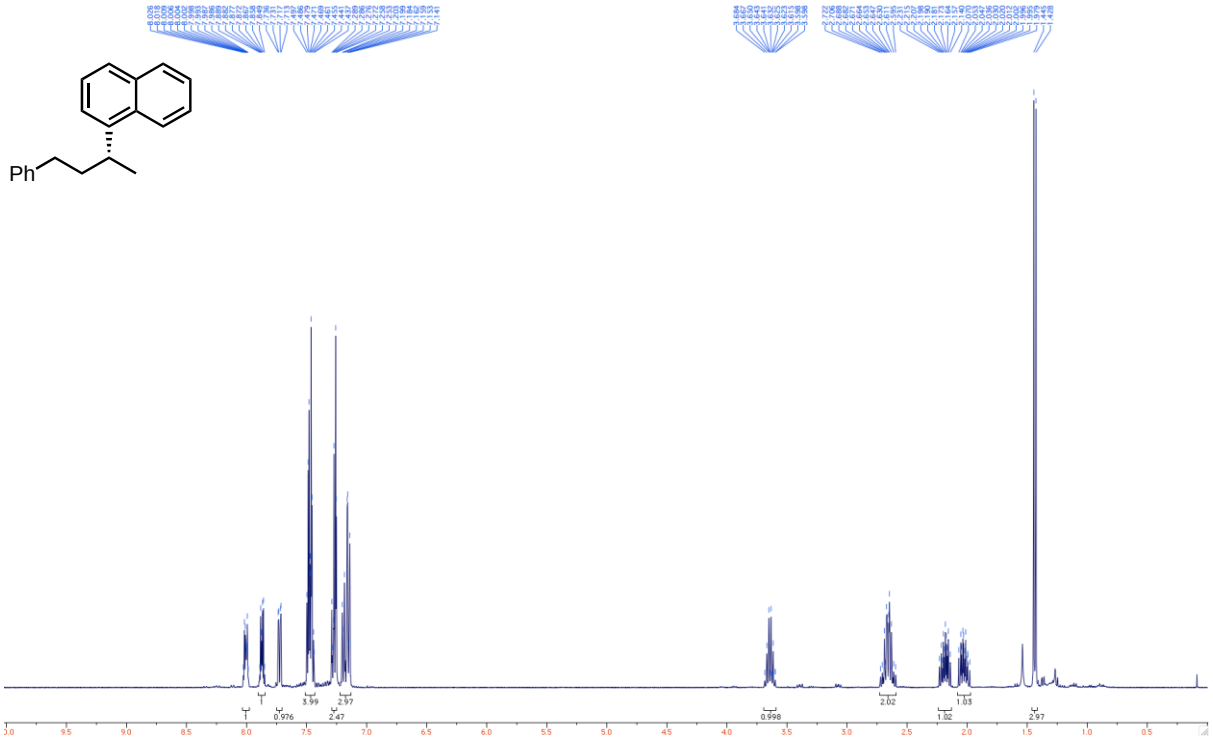


Chiral HPLC traces: enantioenriched

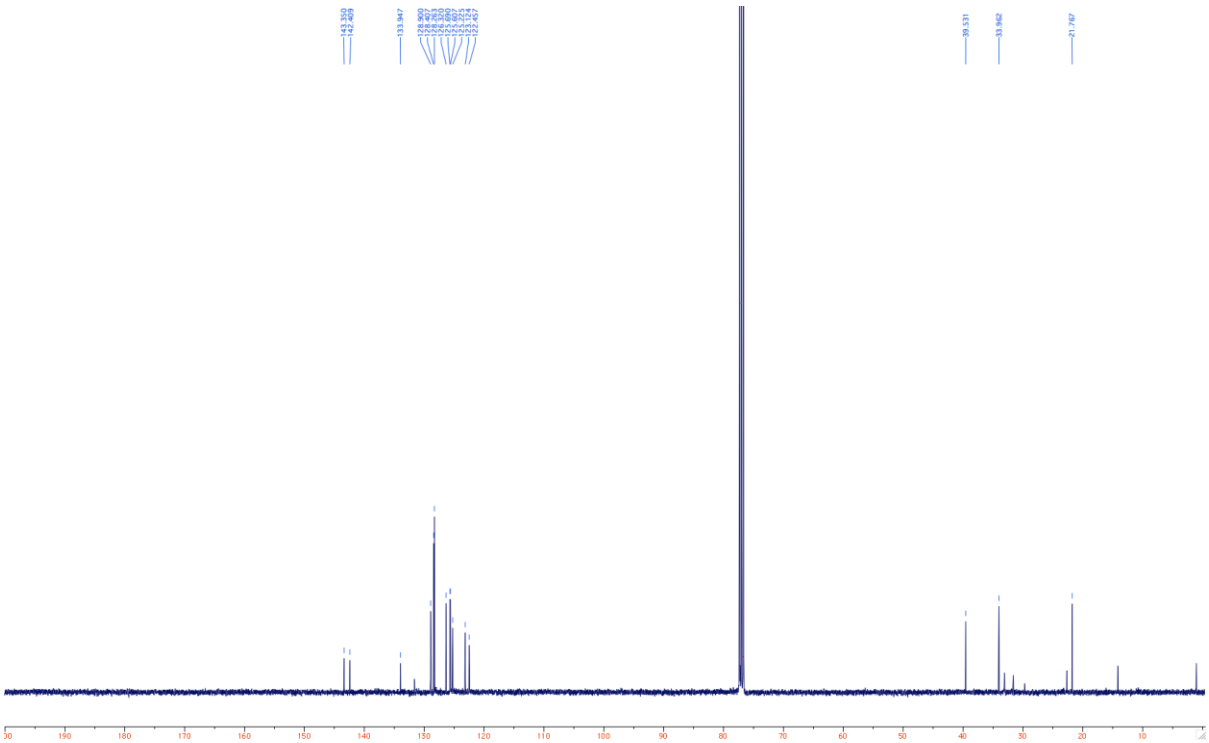


15a

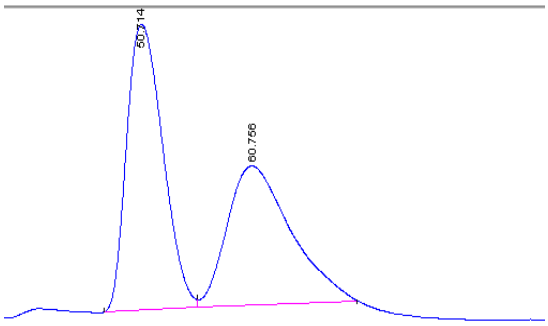
^{1}H NMR (400 MHz, $CDCl_3$)



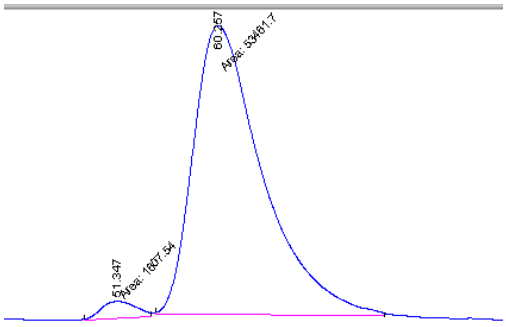
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

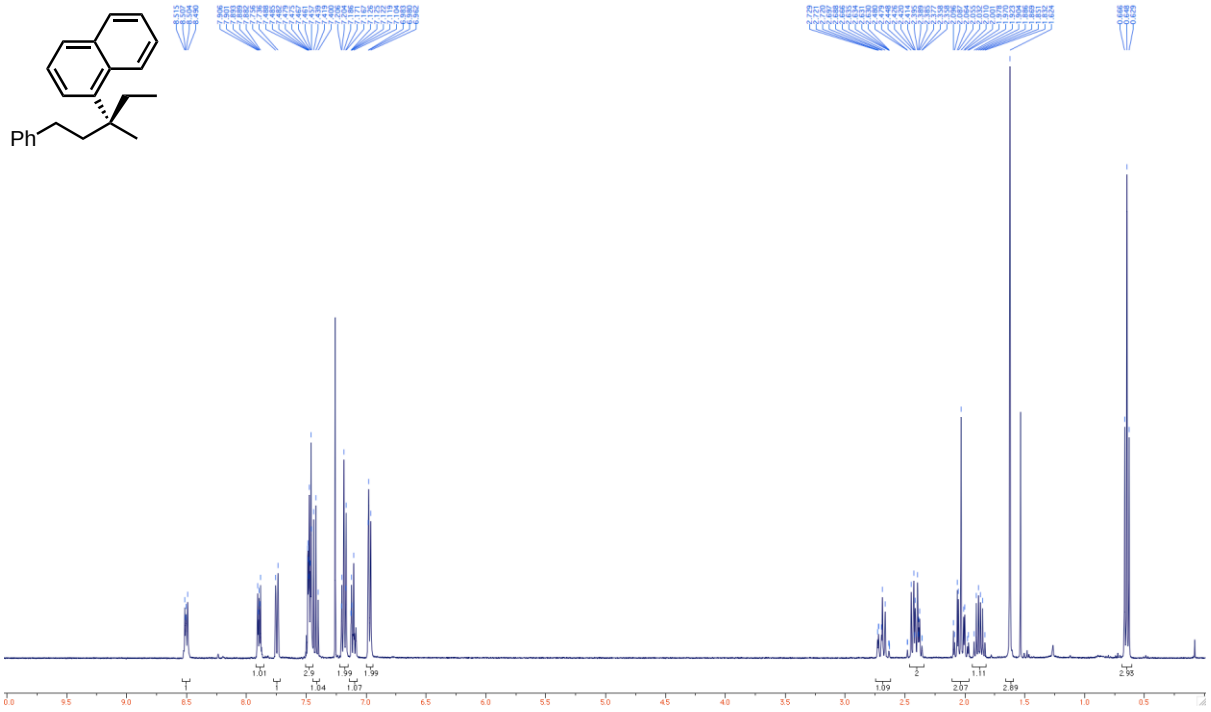


Chiral HPLC traces: enantioenriched

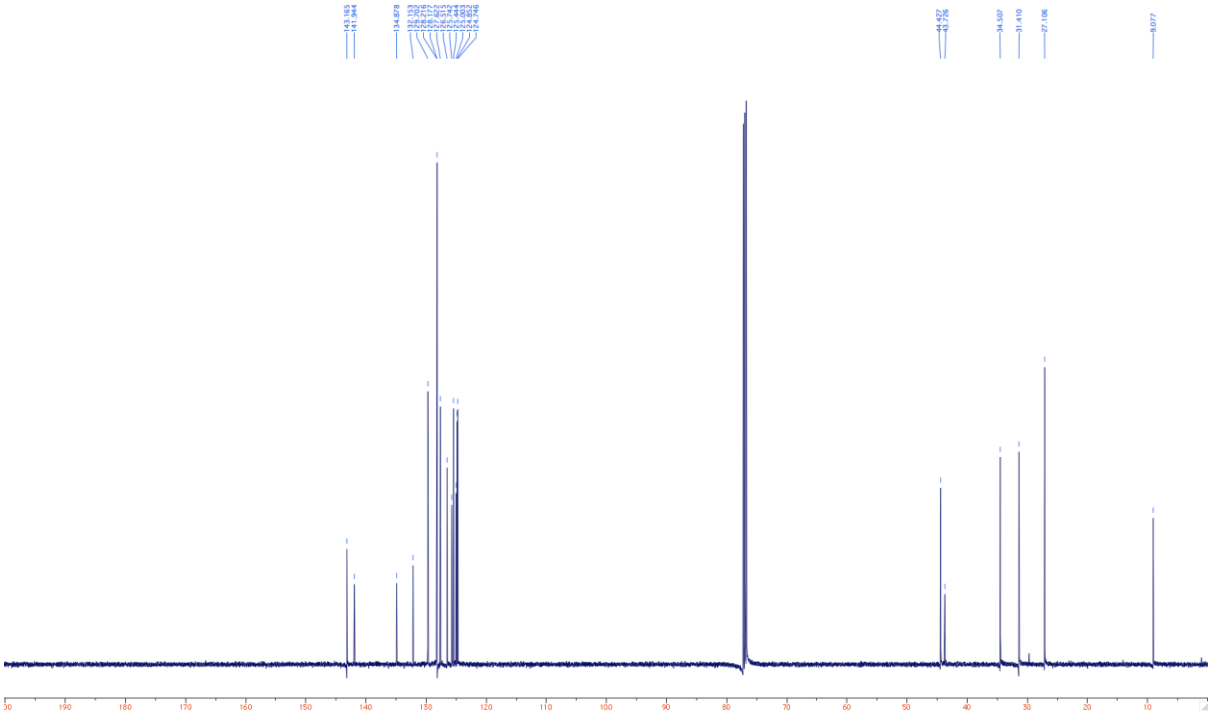


15g

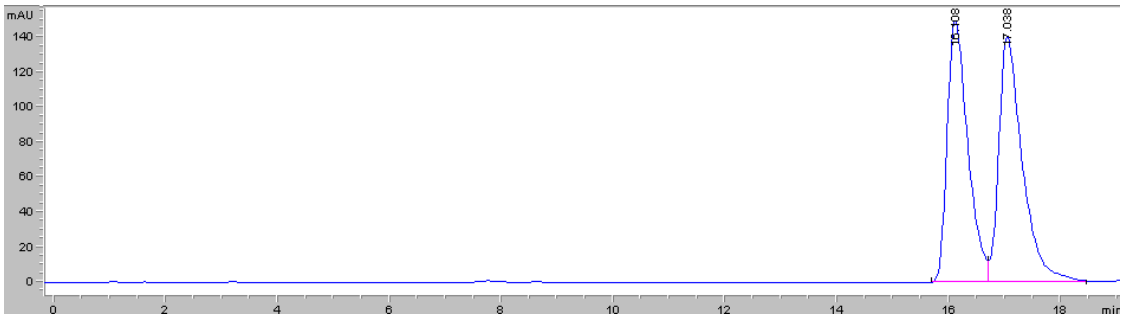
^{1}H NMR (400 MHz, $CDCl_3$)



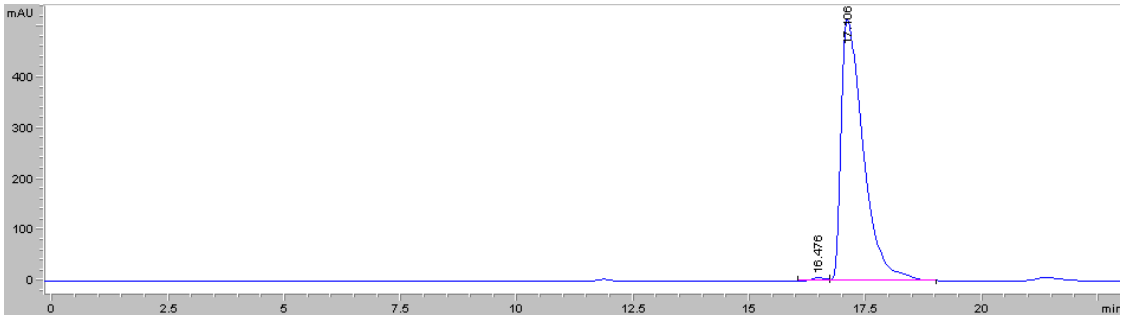
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

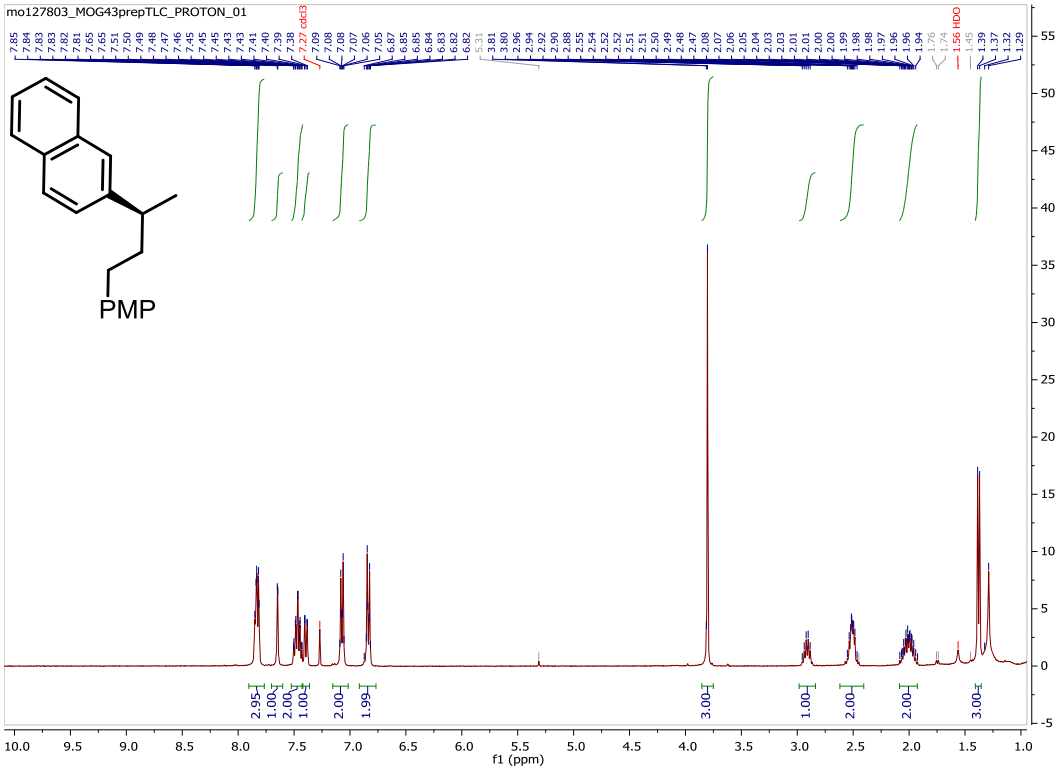


Chiral HPLC traces: enantioenriched

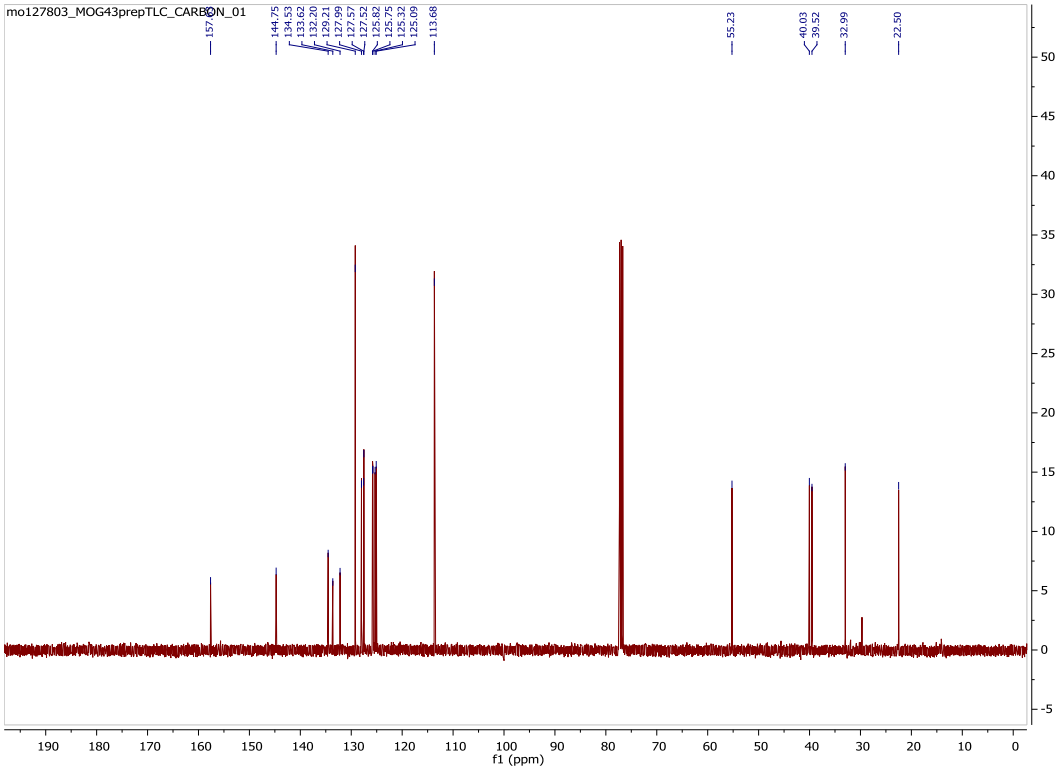


16b

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

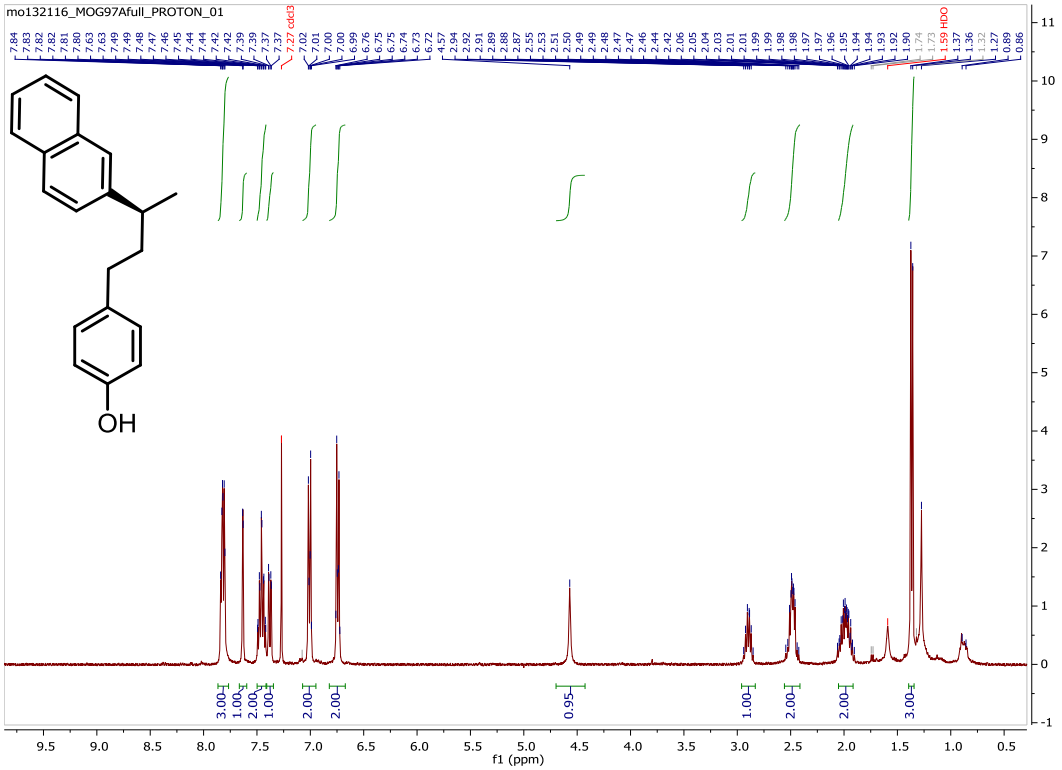


^{13}C NMR (100 MHz, $CDCl_3$)

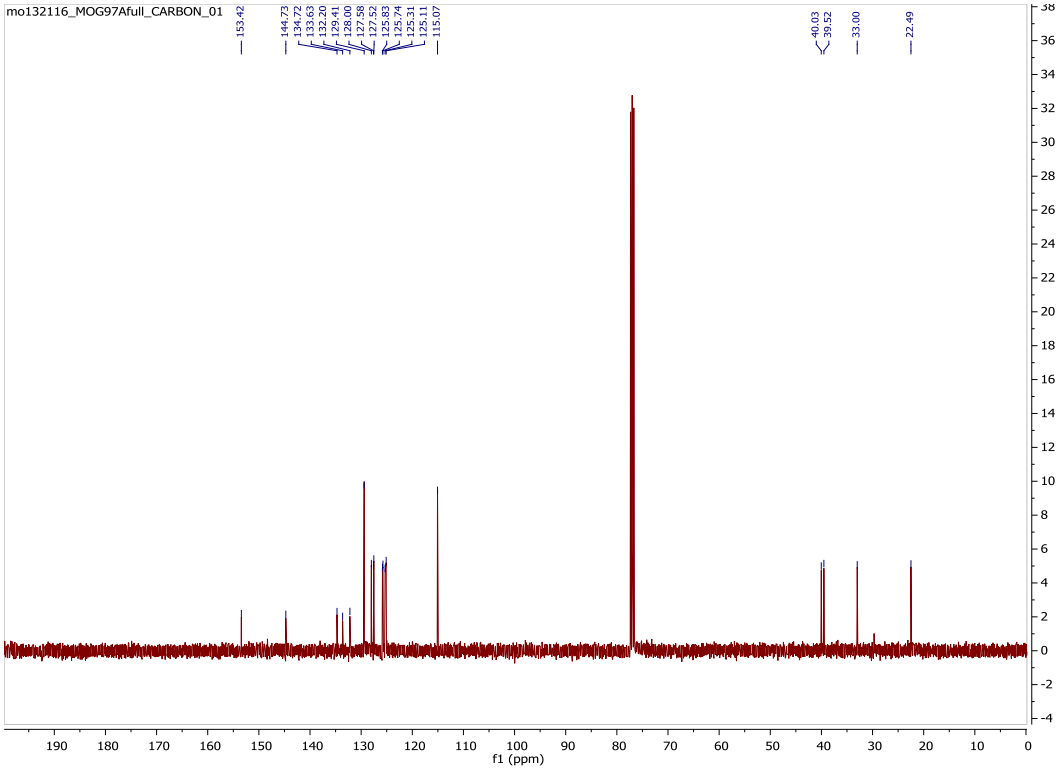


16b-[OH]

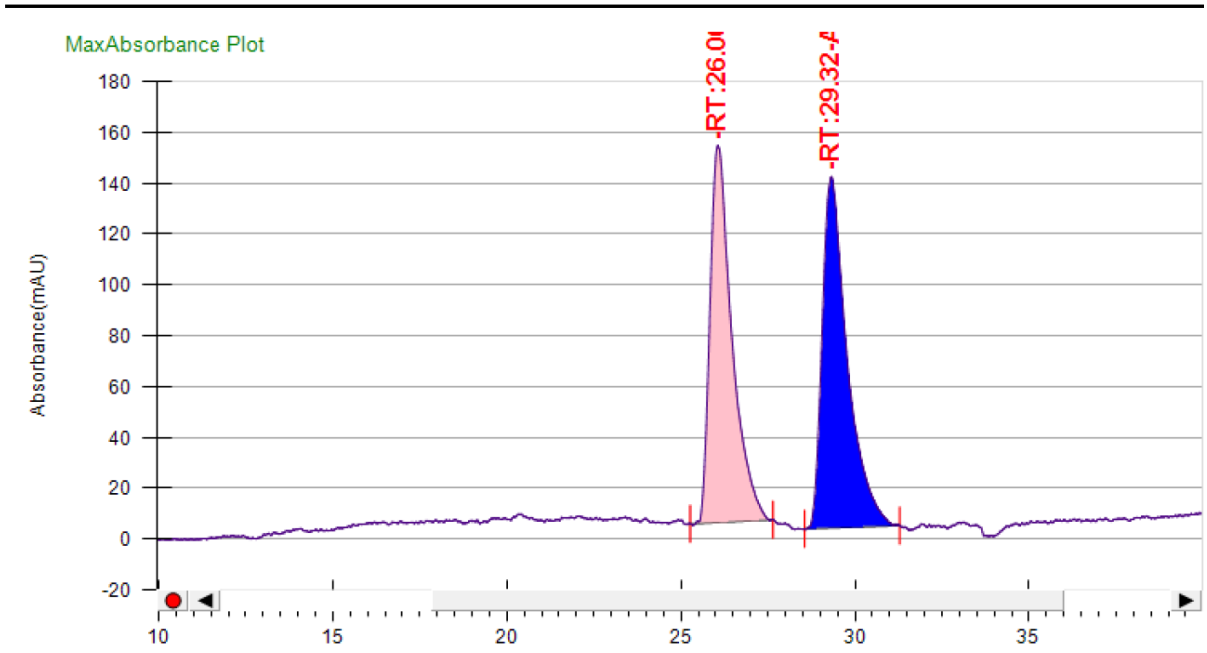
^{1}H NMR (400 MHz, $CDCl_3$)



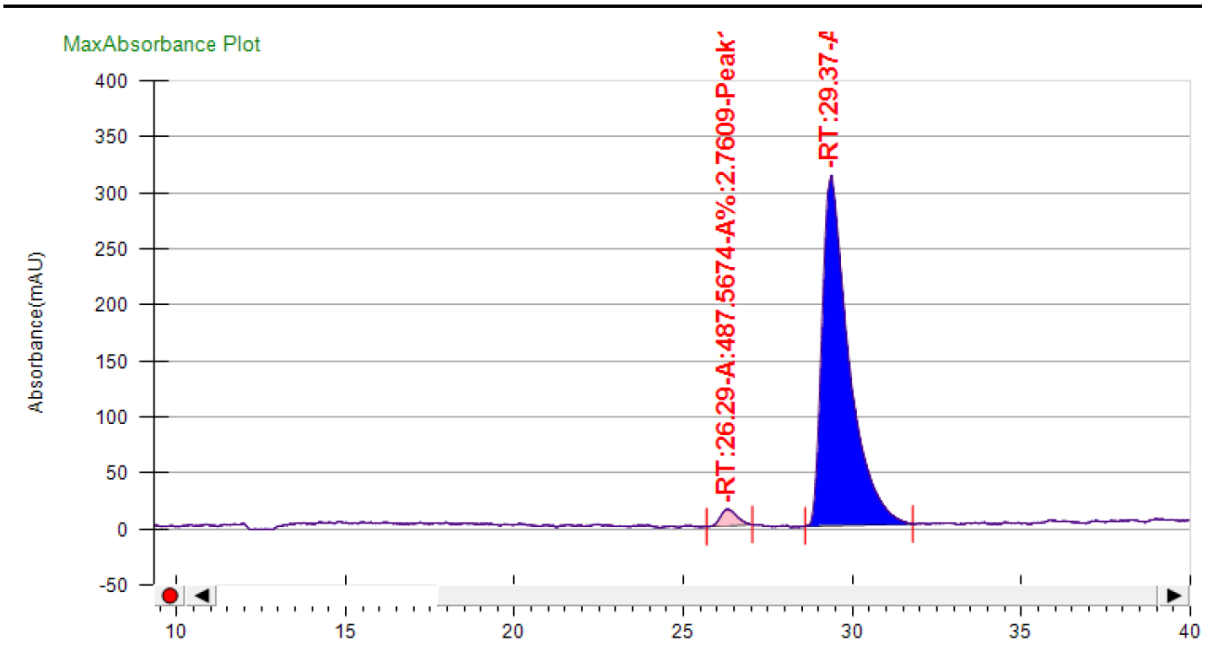
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

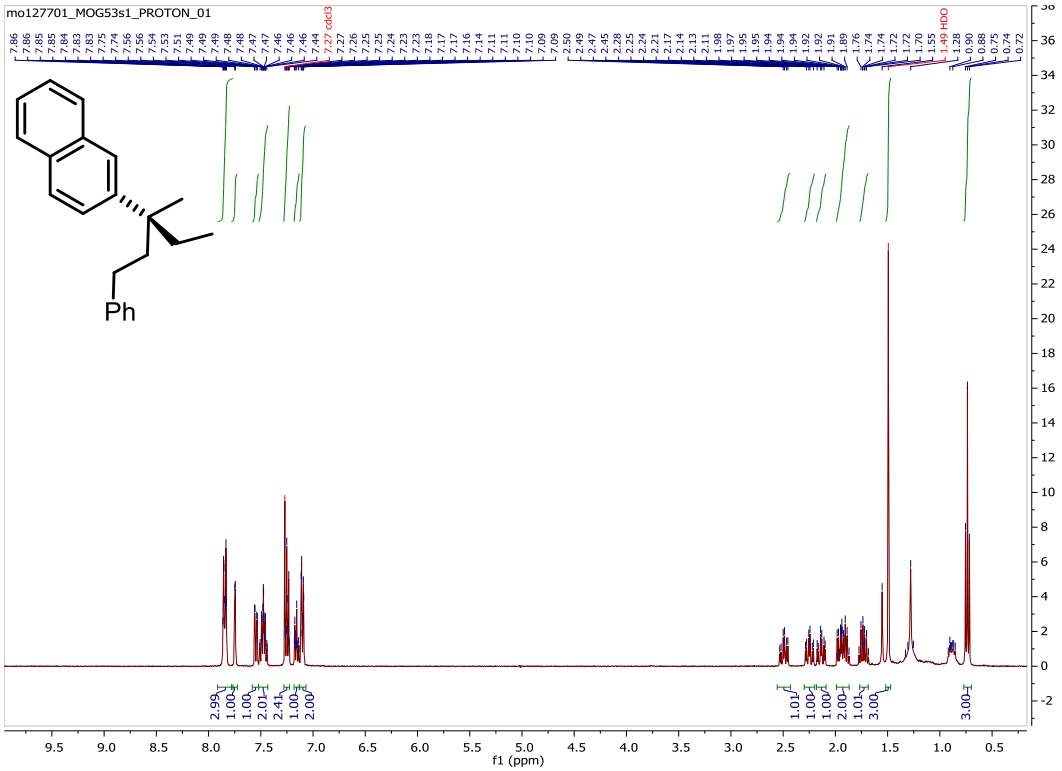


Chiral SFC traces: enantioenriched

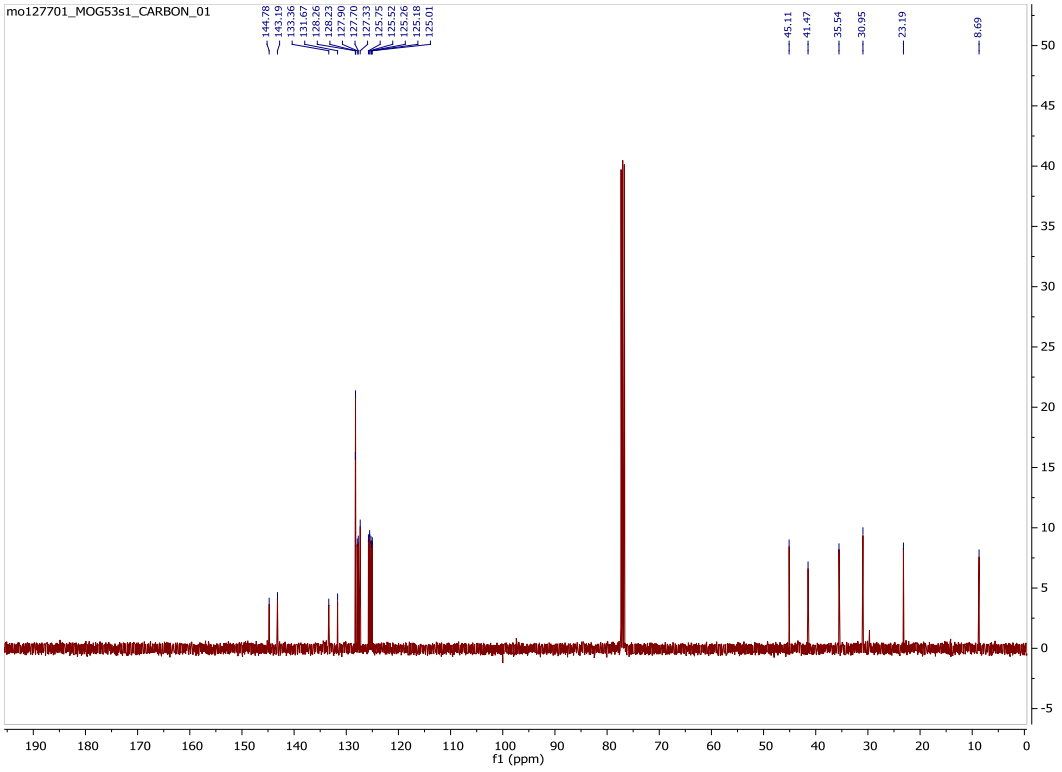


16g

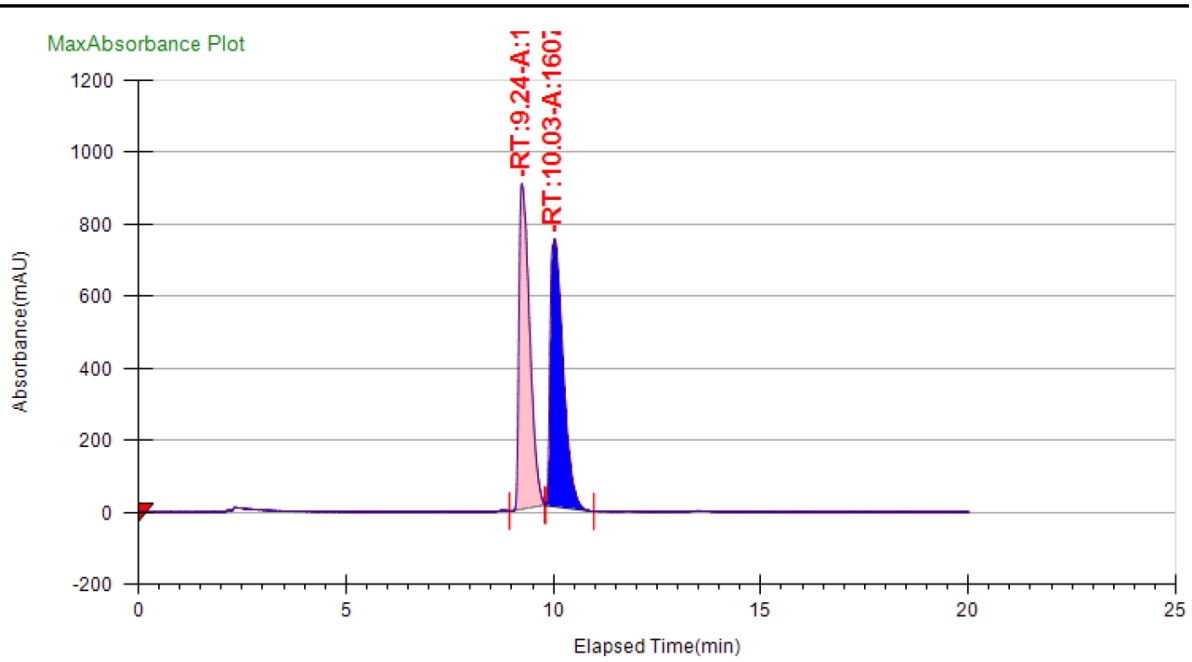
^{1}H NMR (400 MHz, $CDCl_3$)



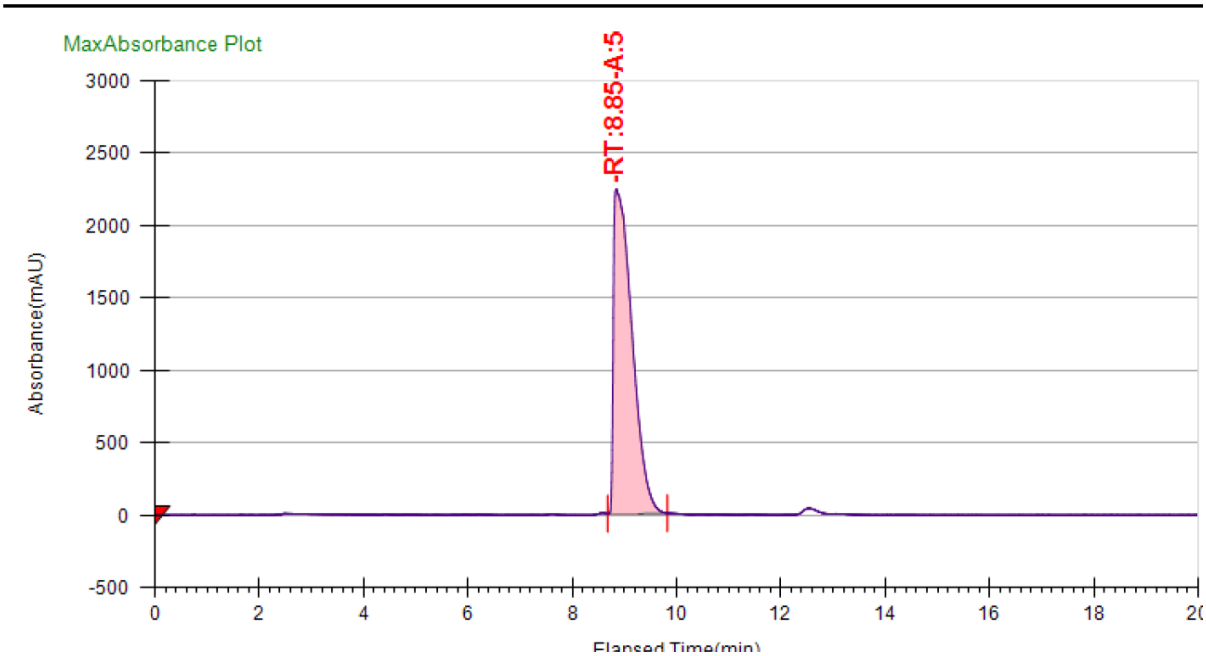
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral SFC traces: racemic

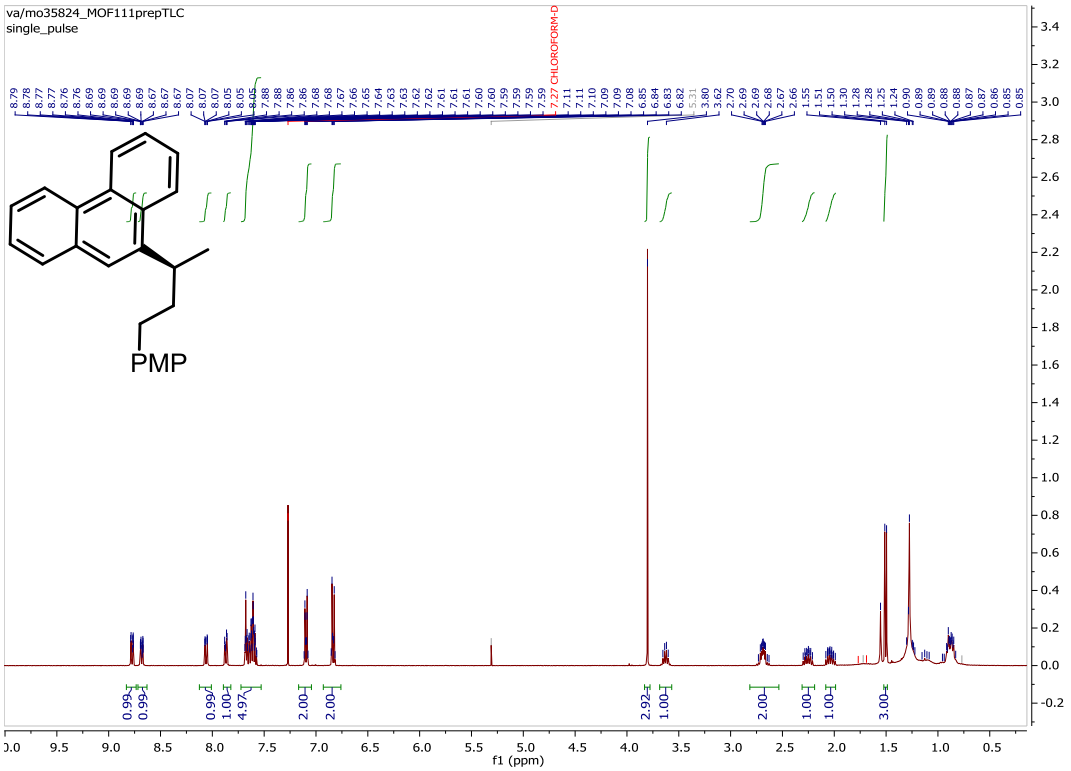


Chiral SFC traces: enantioenriched

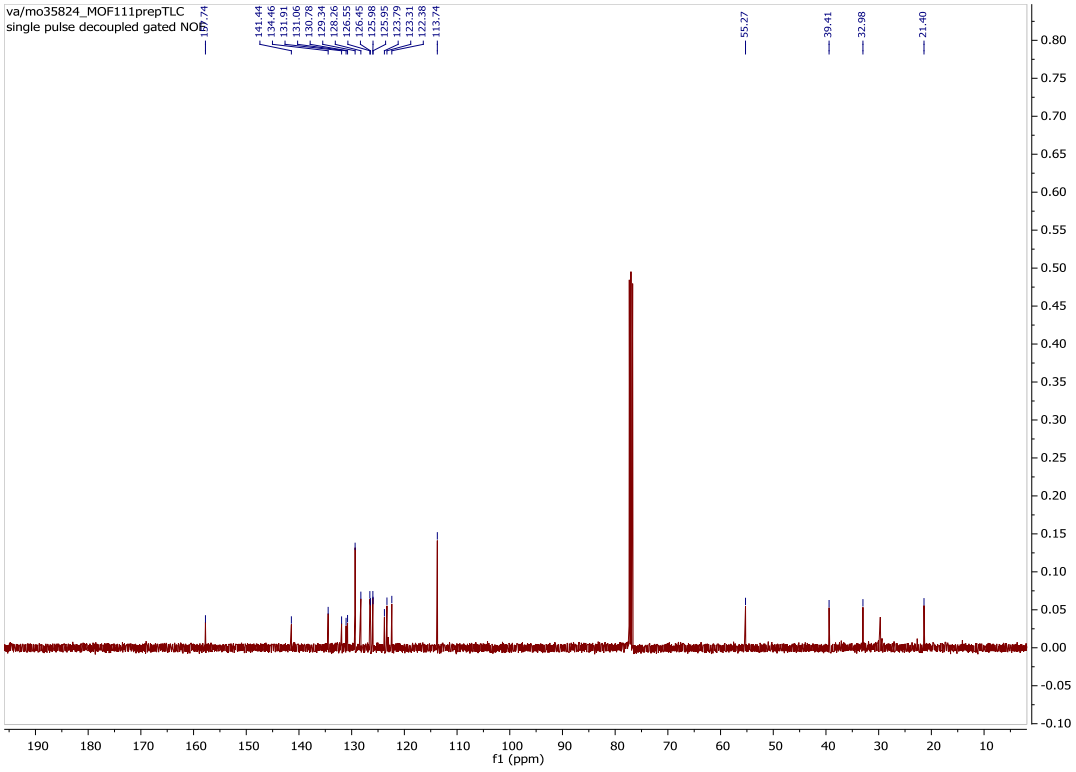


17b

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

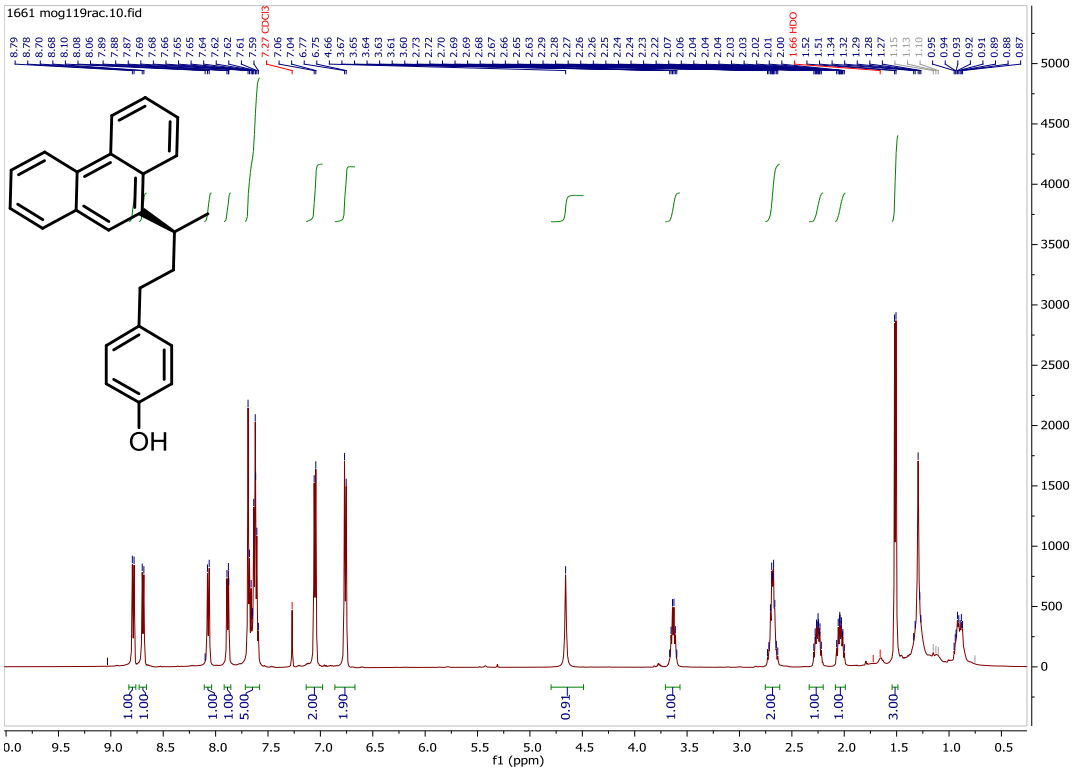


^{13}C NMR (100 MHz, $CDCl_3$)

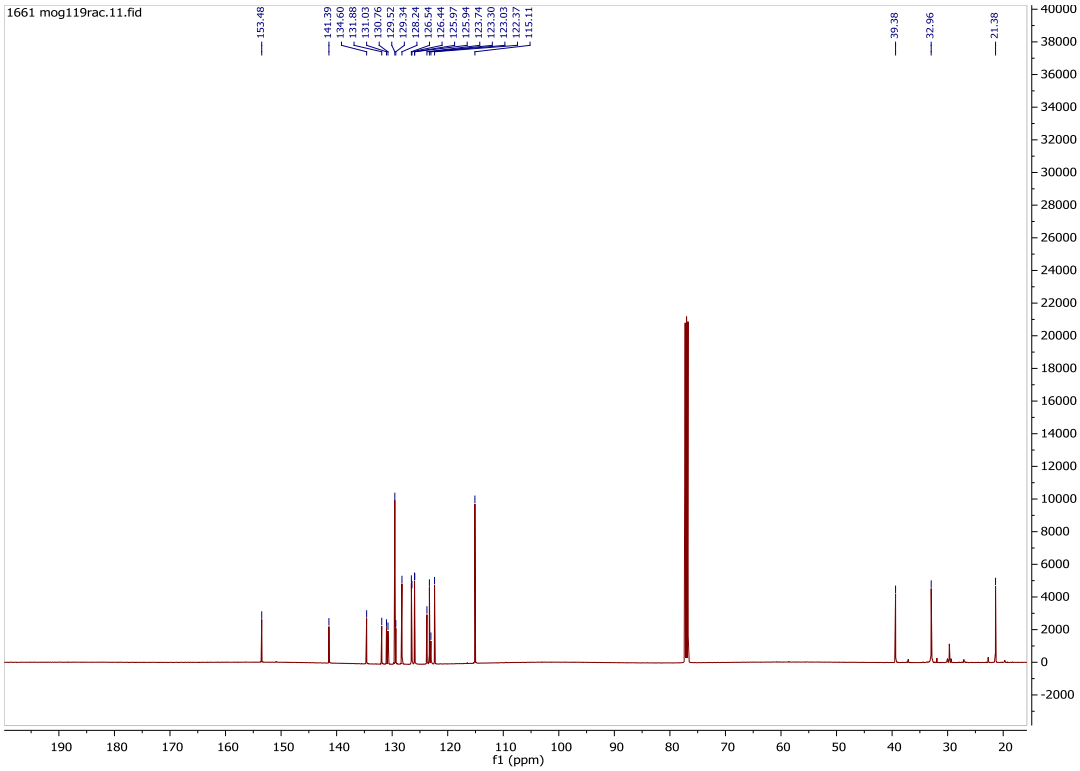


17b-[OH]

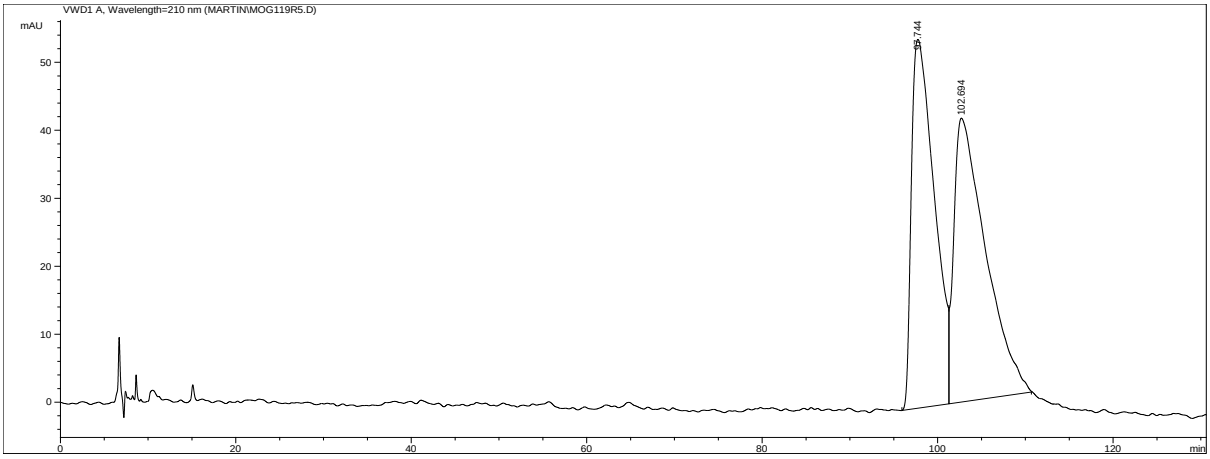
^{1}H NMR (400 MHz, $CDCl_3$)



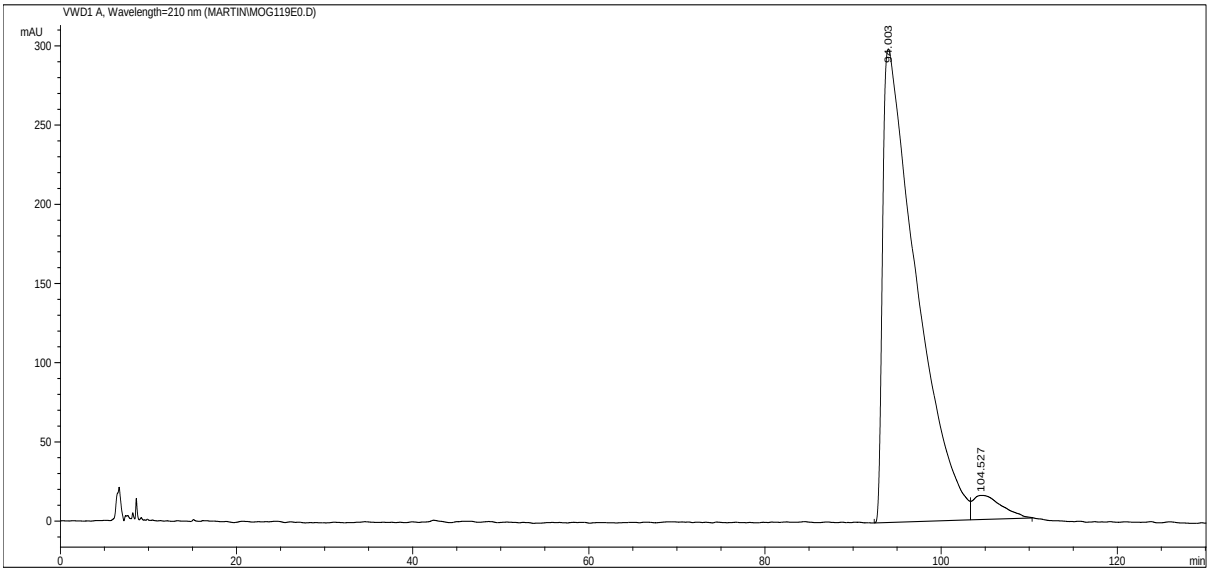
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

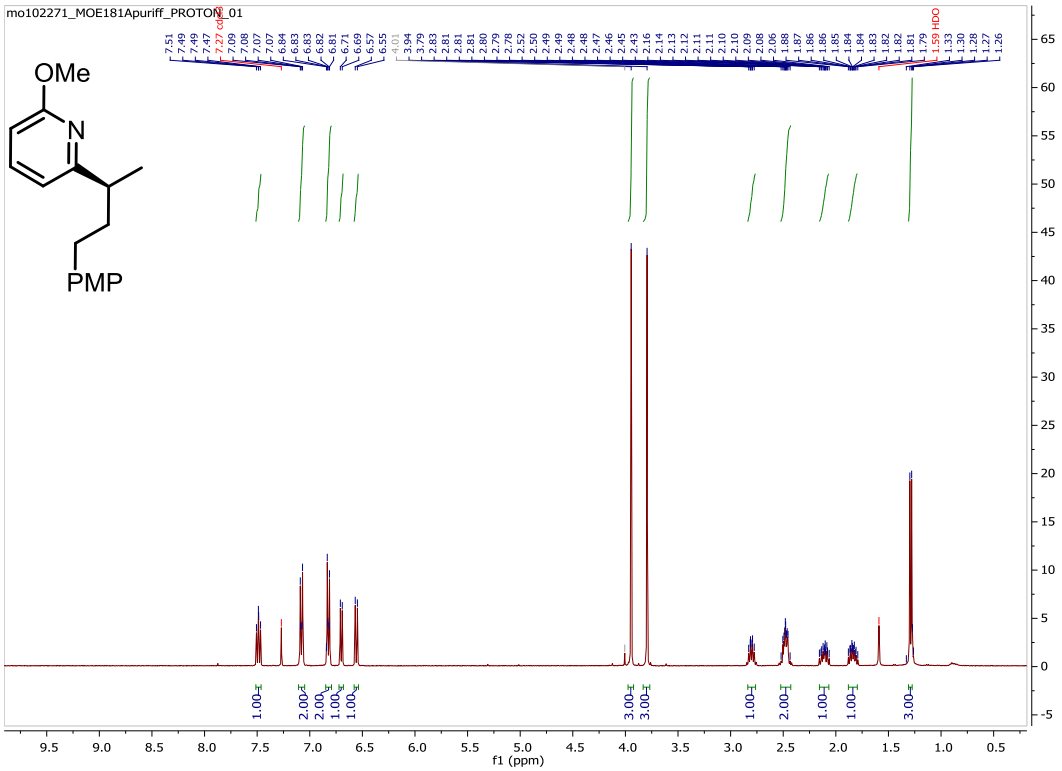


Chiral HPLC traces: enantioenriched

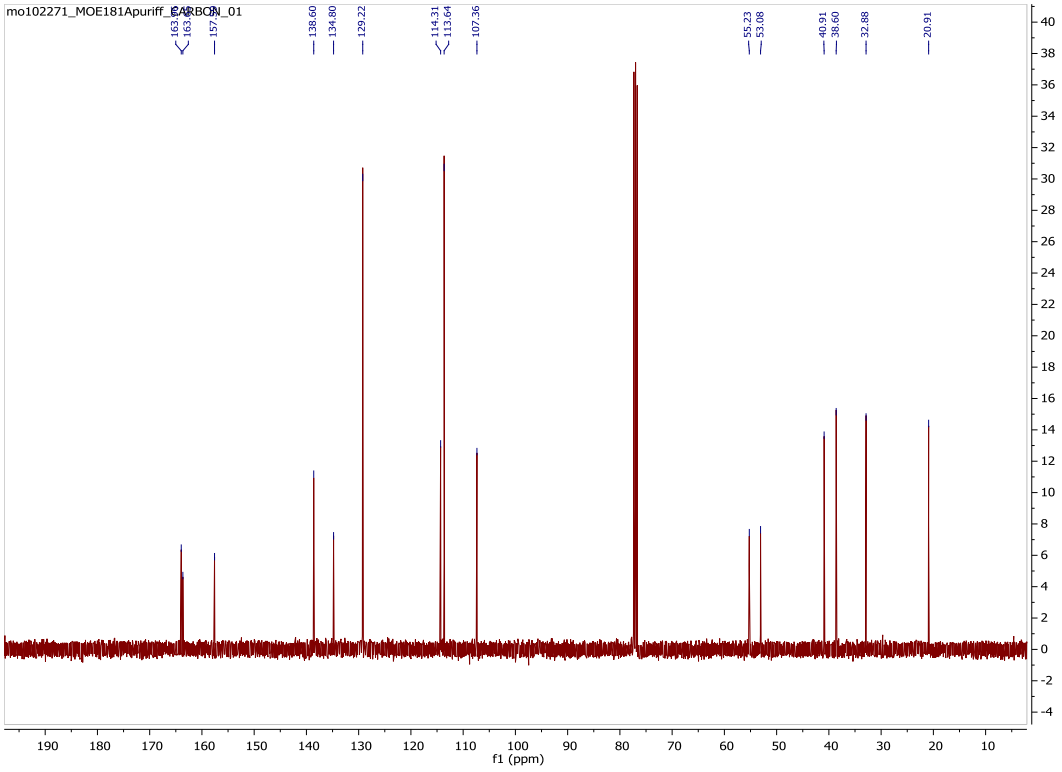


20b

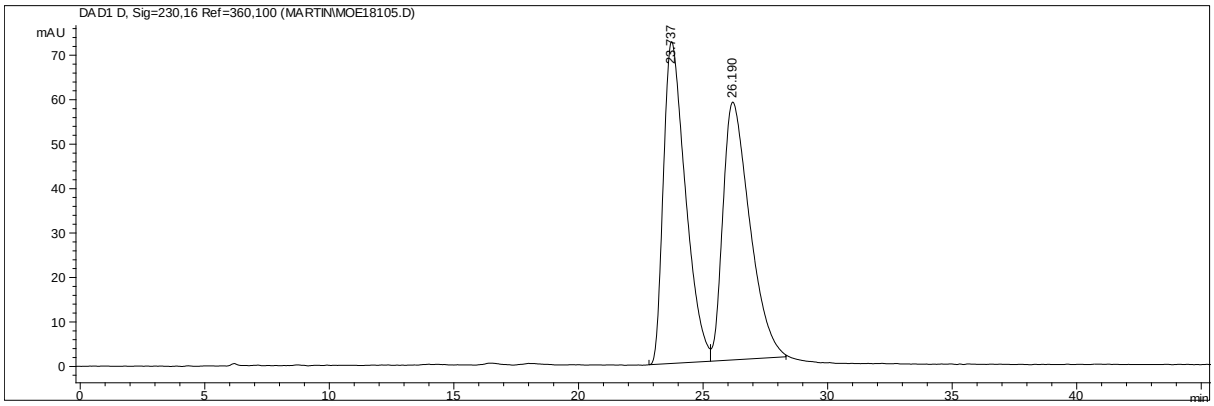
^{1}H NMR (400 MHz, $CDCl_3$)



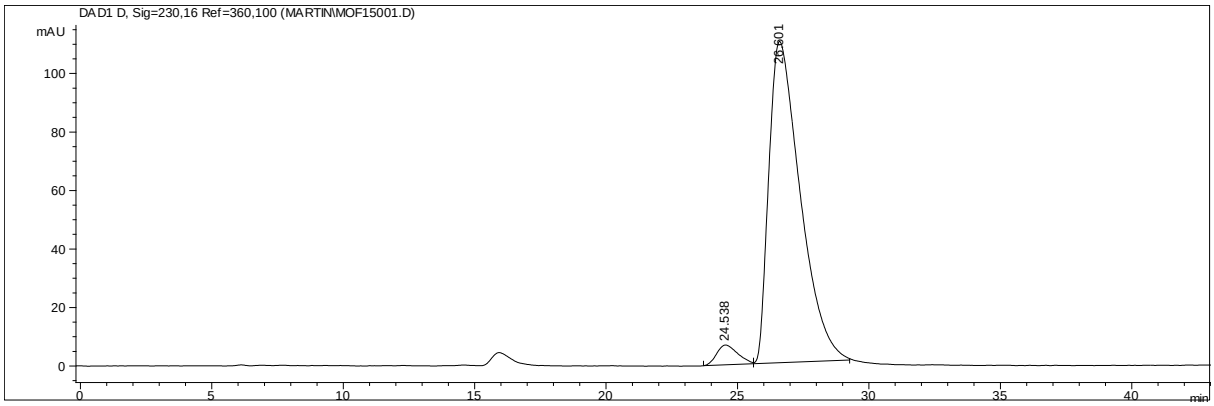
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

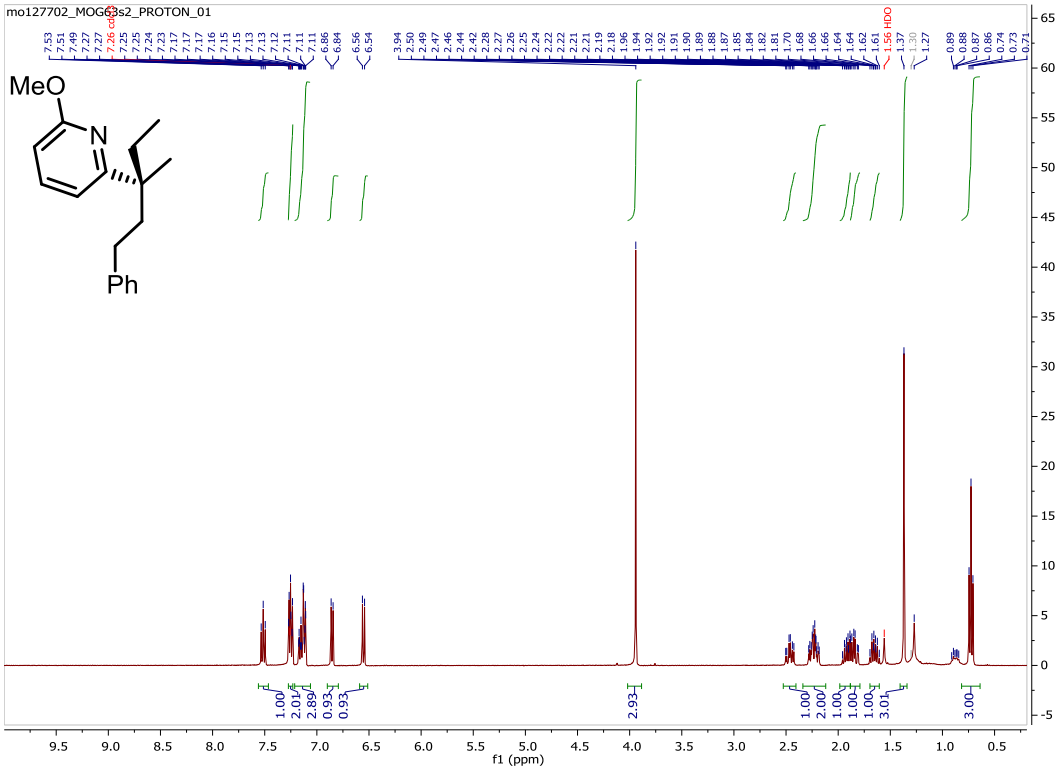


Chiral HPLC traces: enantioenriched

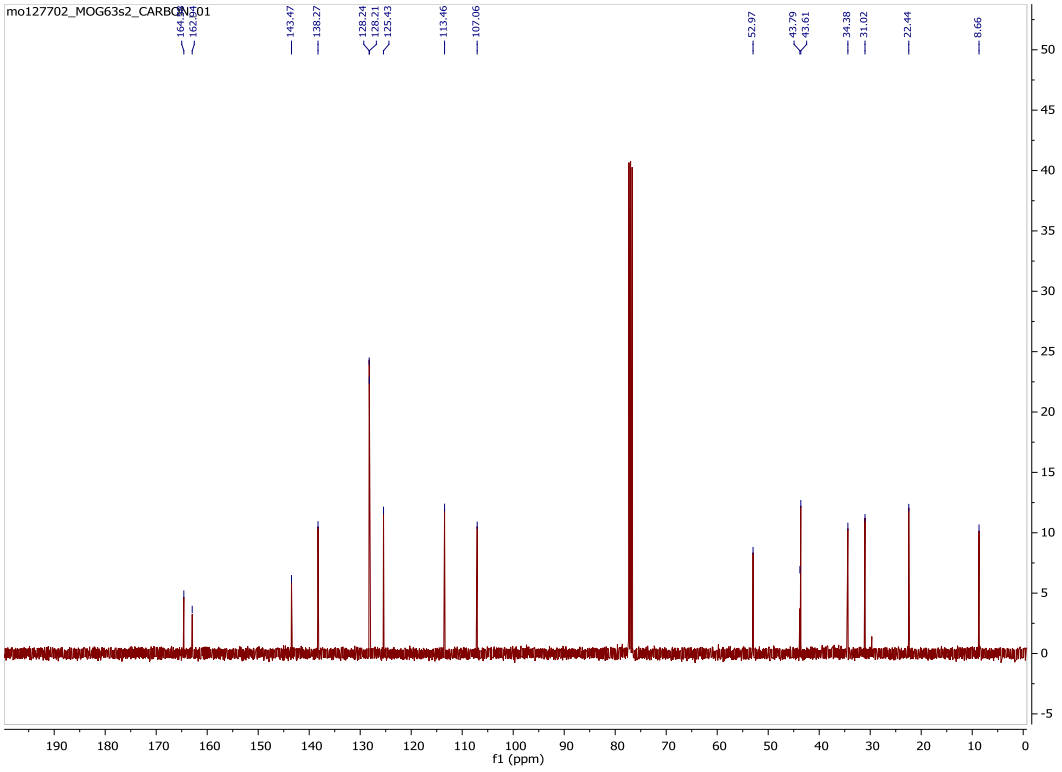


20g

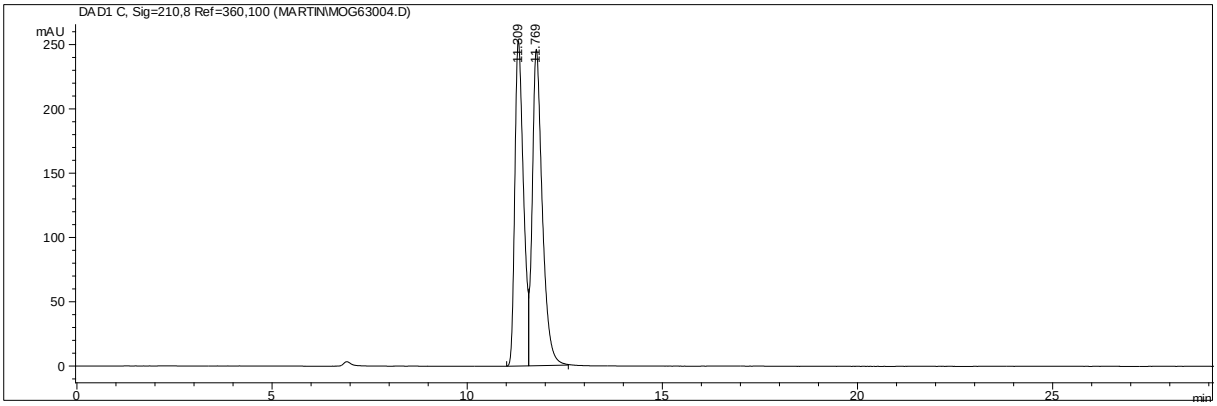
^{1}H NMR (400 MHz, $CDCl_3$)



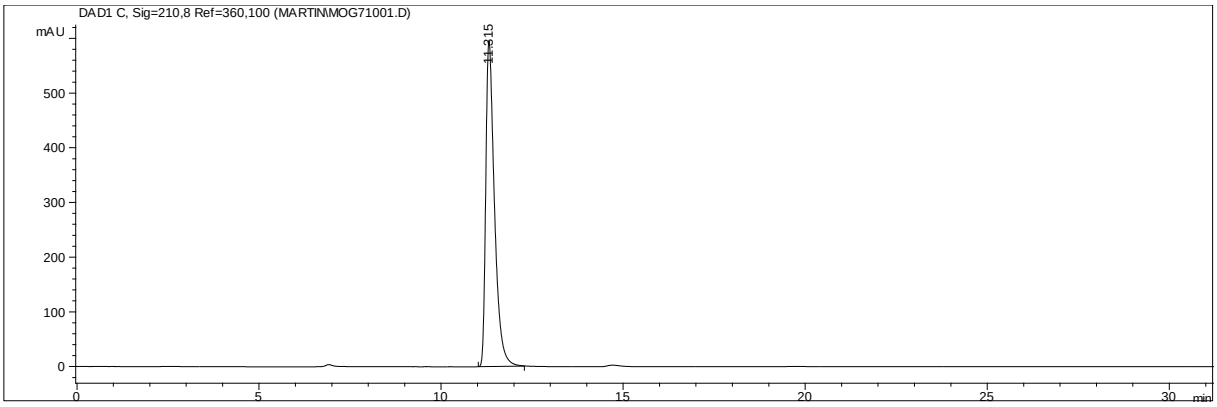
^{13}C NMR (100 MHz, $CDCl_3$)



Chiral HPLC traces: racemic

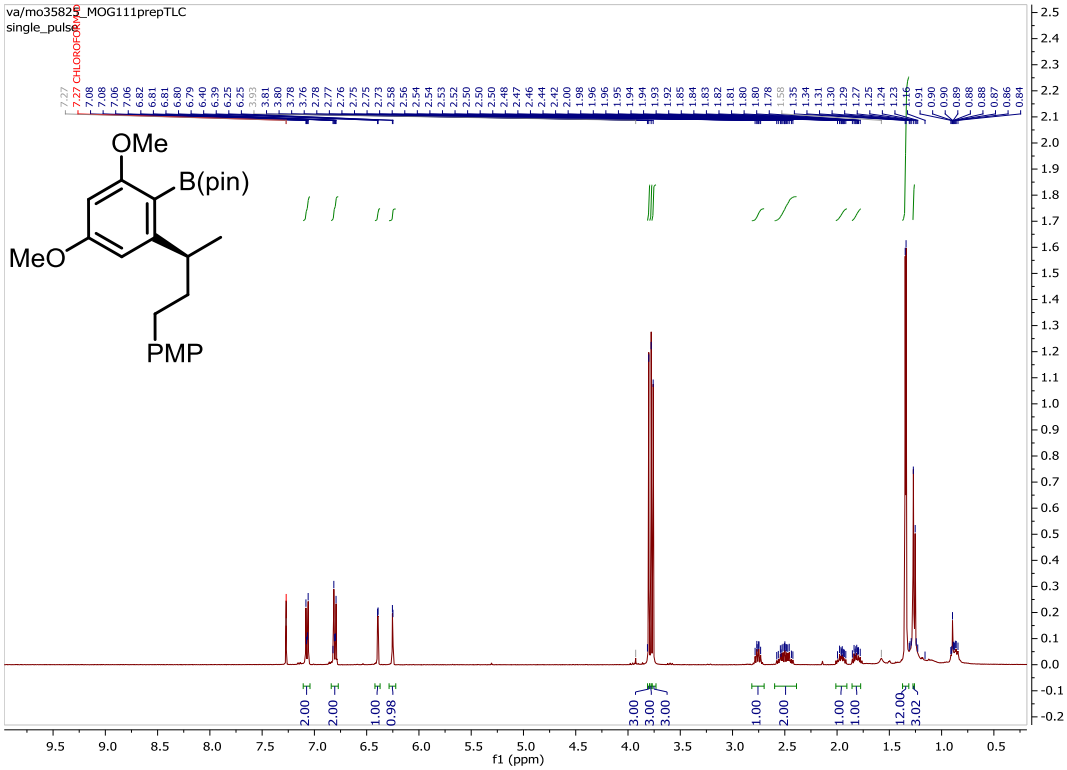


Chiral HPLC traces: enantioenriched

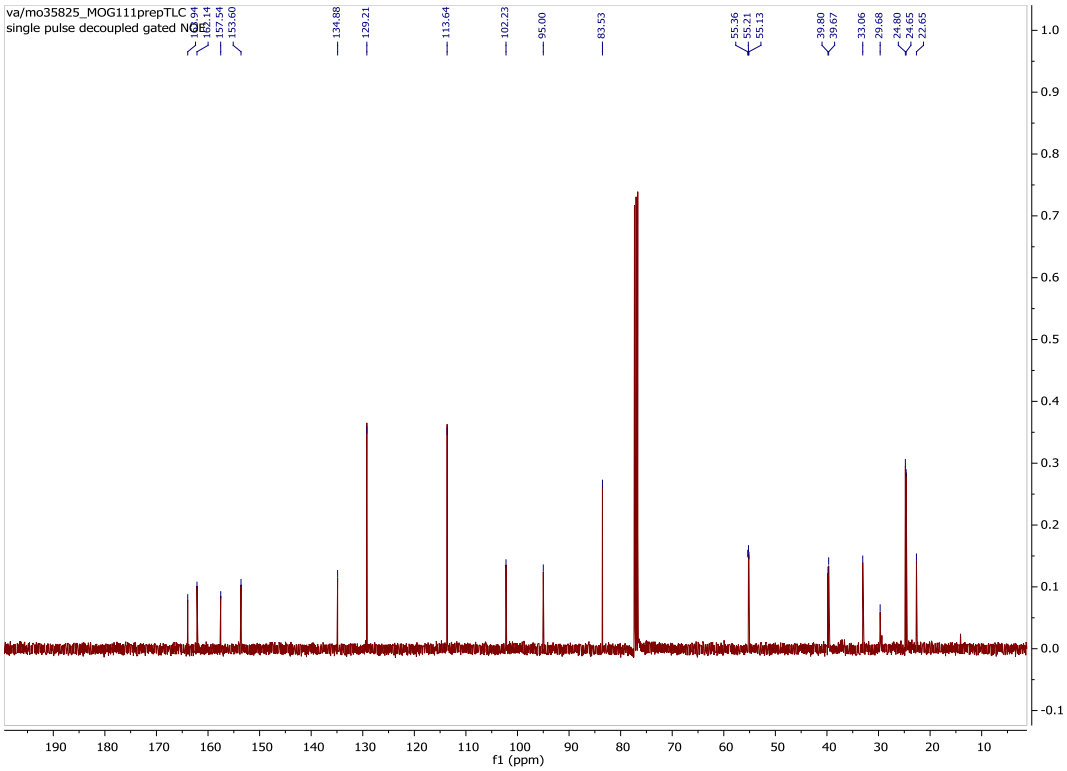


9ba

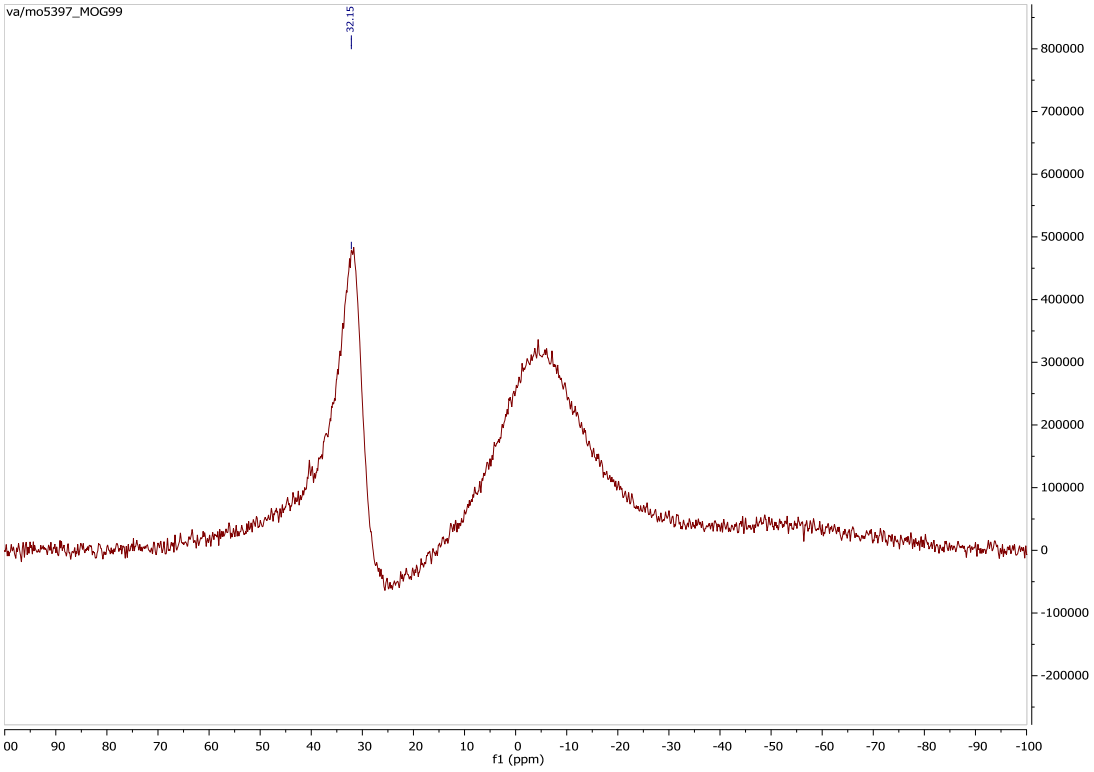
^{1}H NMR (400 MHz, $CDCl_3$)



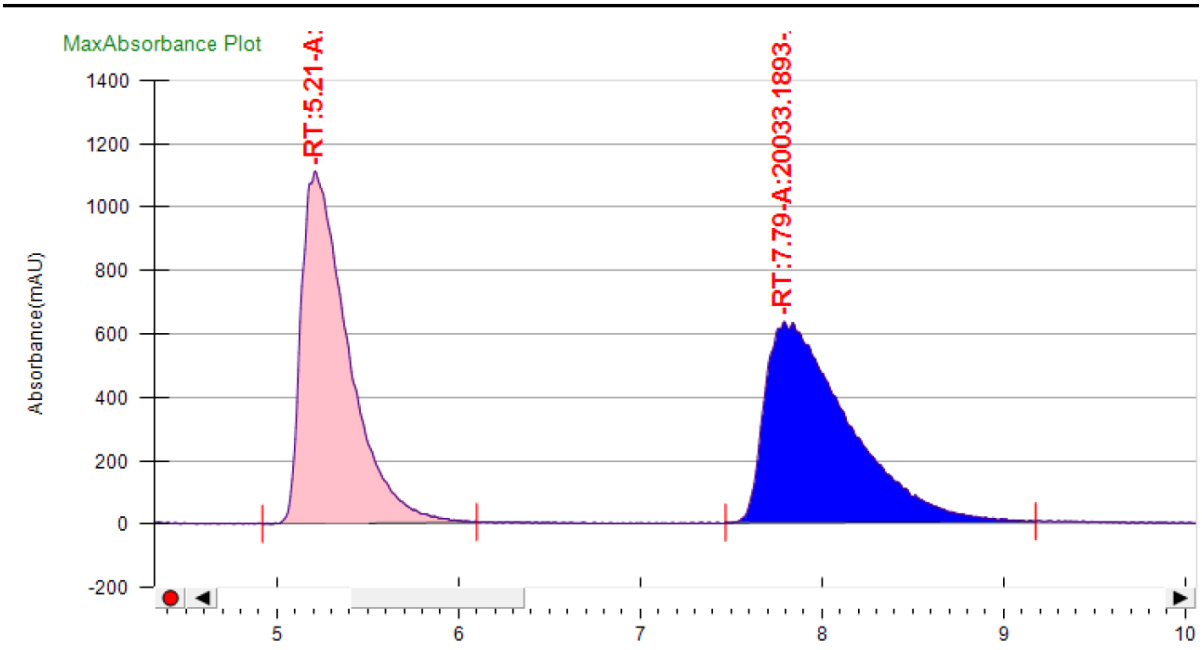
^{13}C NMR (100 MHz, $CDCl_3$)



^{11}B NMR (96 MHz, NONE)[8]

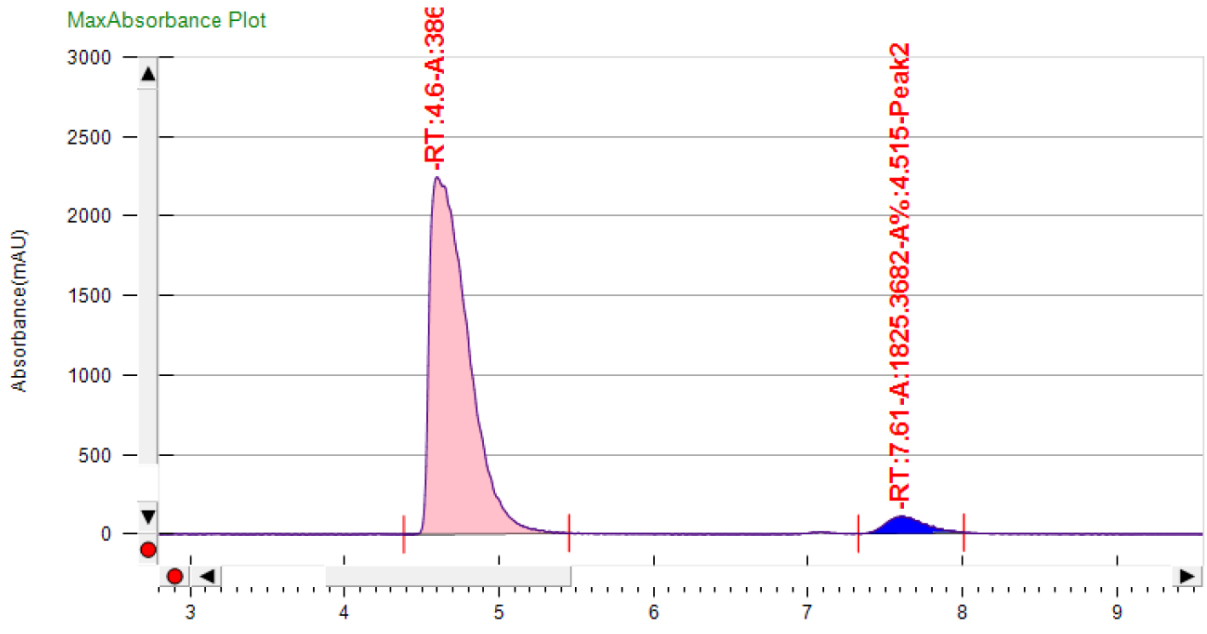


Chiral HPLC traces: racemic



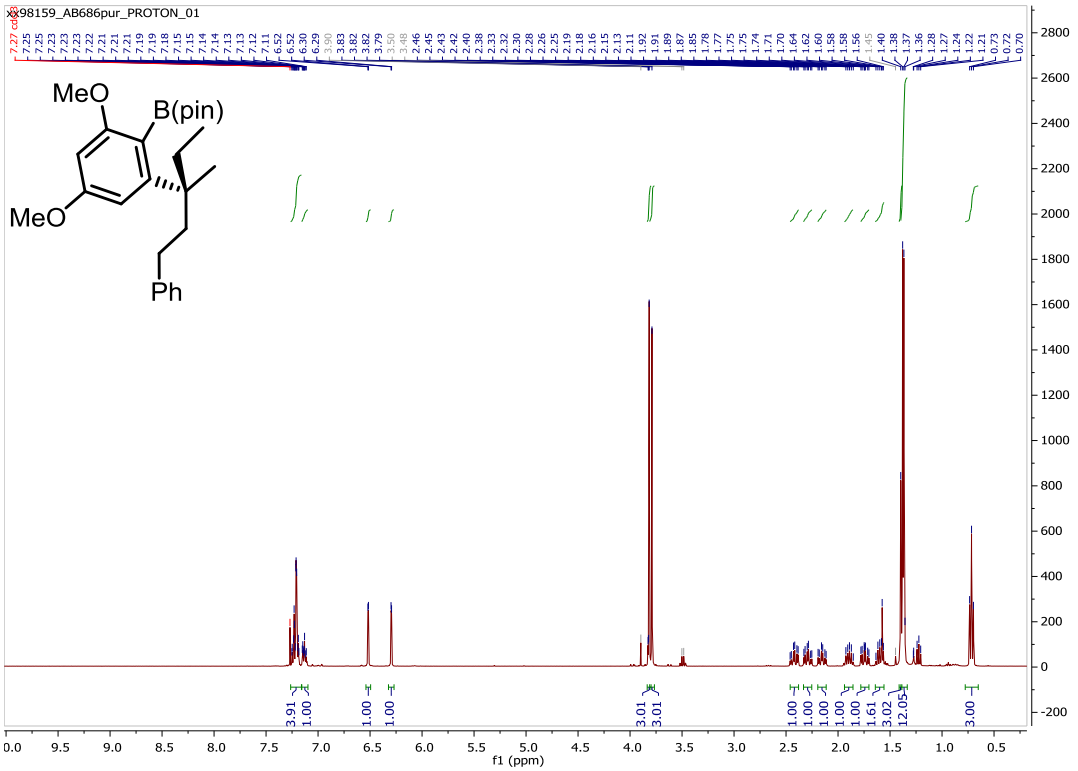
[8] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

Chiral HPLC traces: enantioenriched

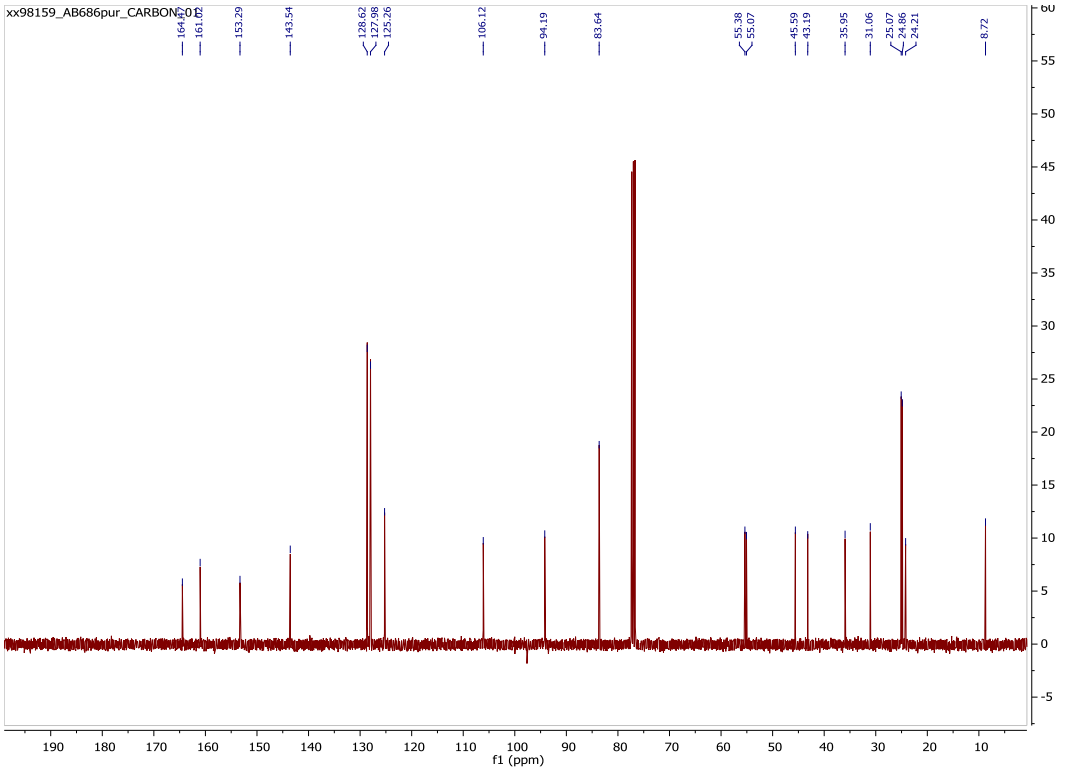


9ga

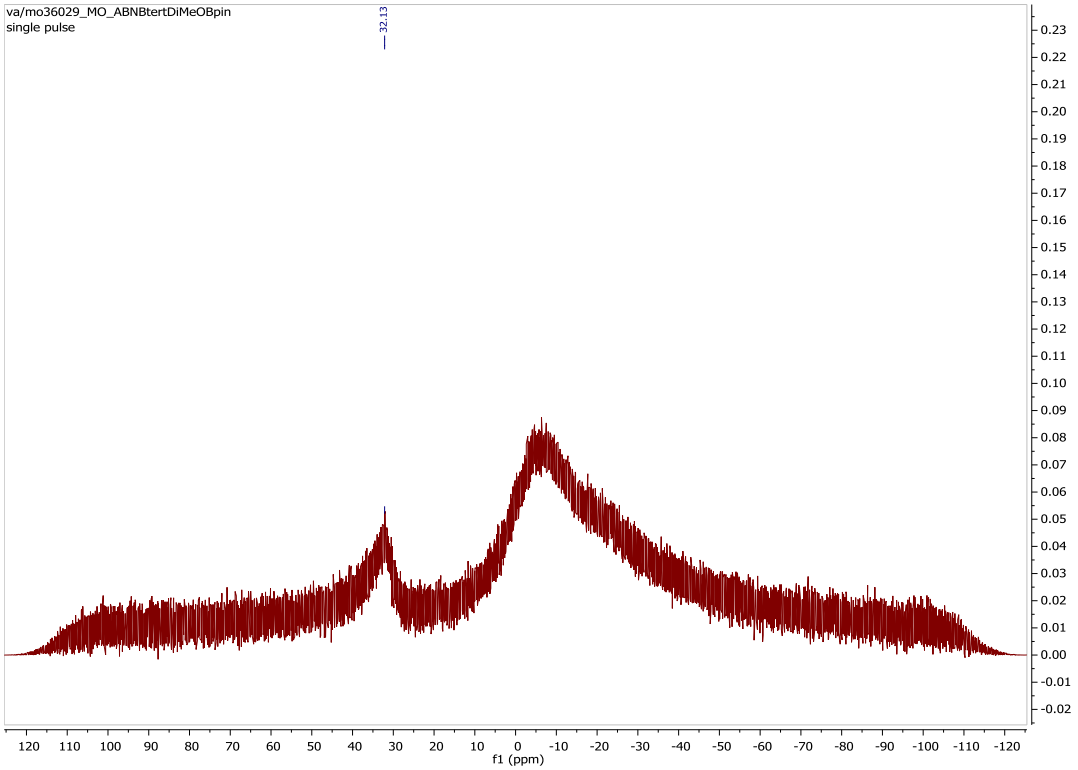
^{1}H NMR (400 MHz, $CDCl_3$)



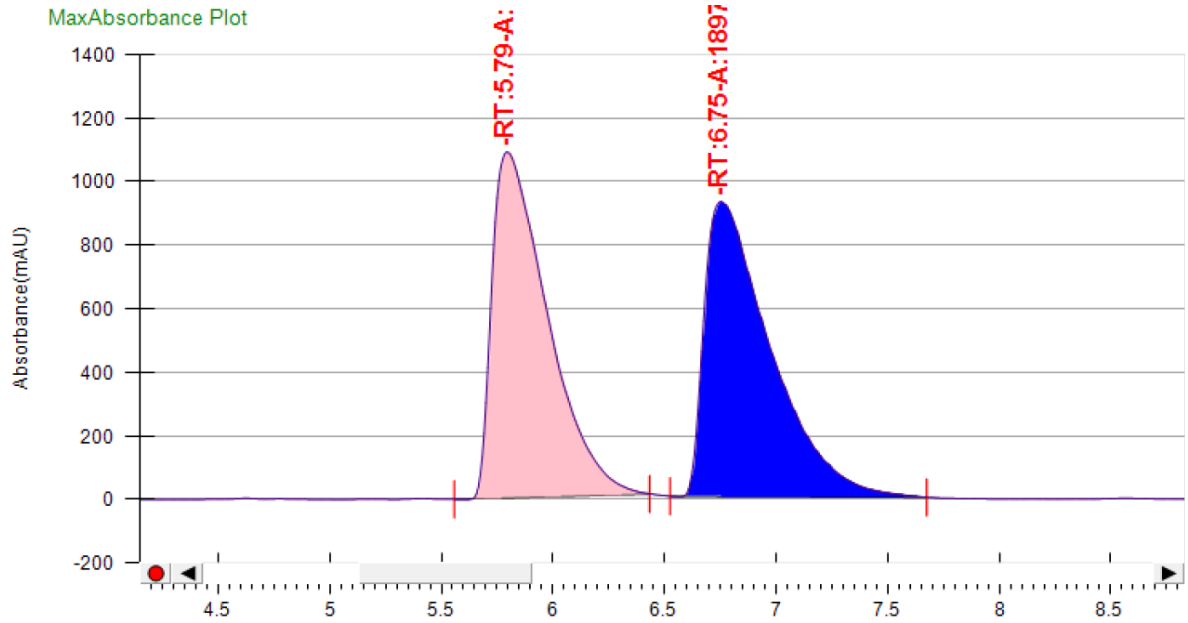
^{13}C NMR (100 MHz, $CDCl_3$)



^{11}B NMR (96 MHz, $CDCl_3$)[9]

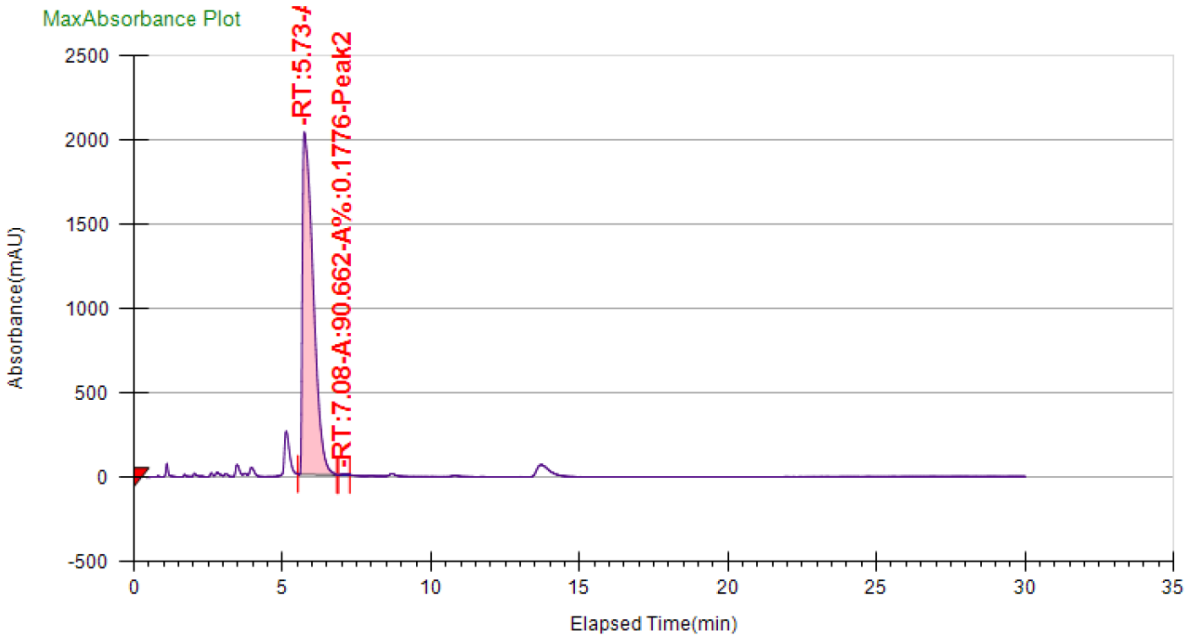


Chiral SFC traces: racemic

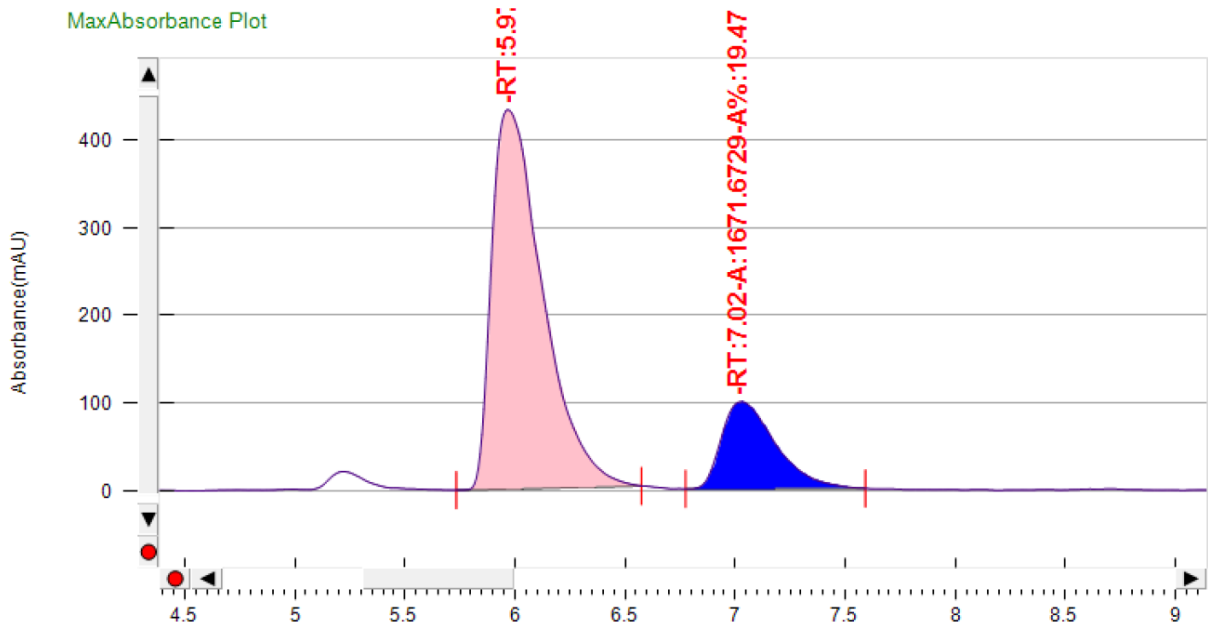


[9] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

Chiral SFC traces: enantioenriched

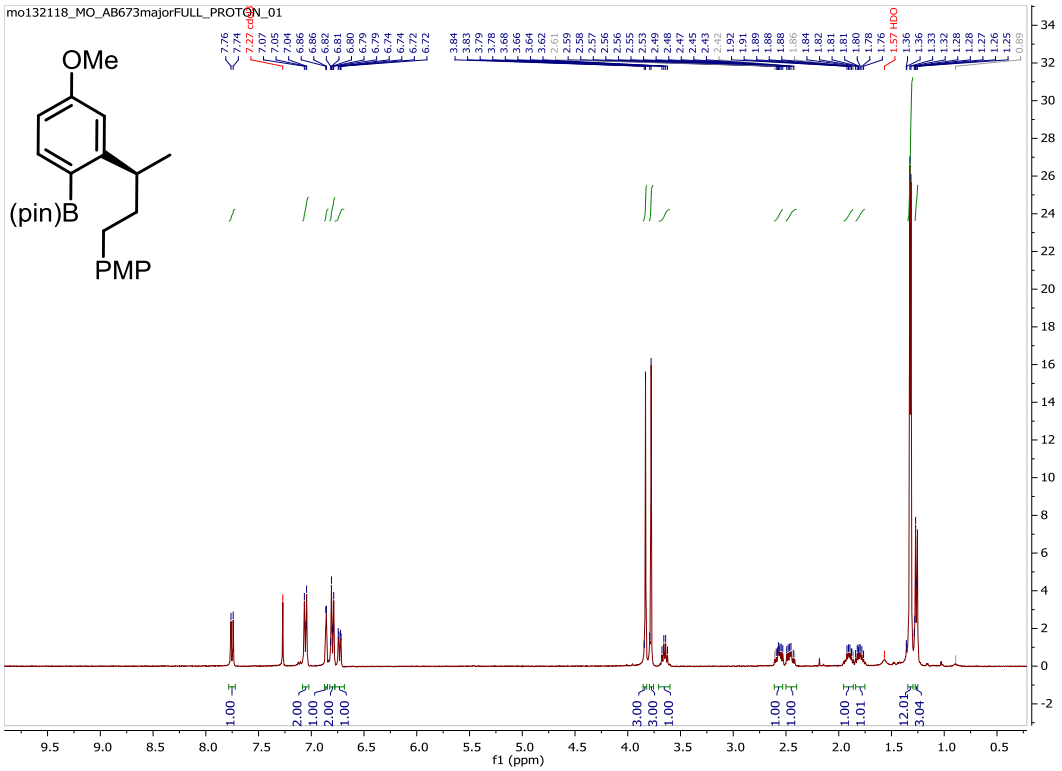


Chiral SFC traces: racemic + enantioenriched

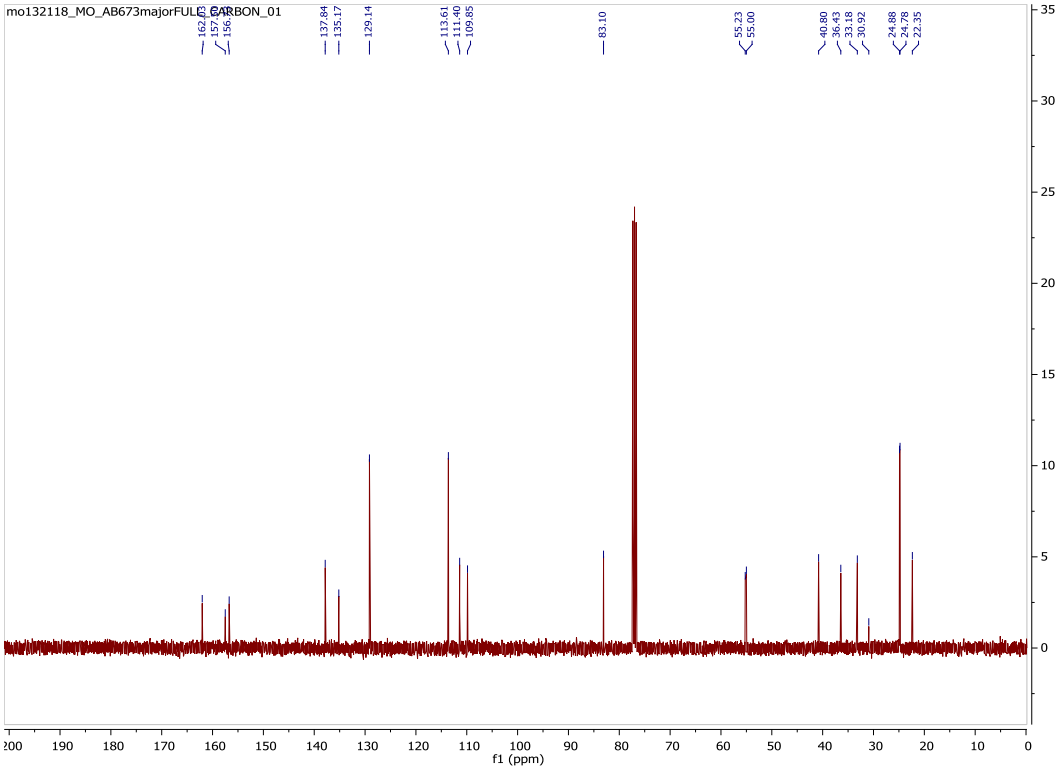


11ba-major

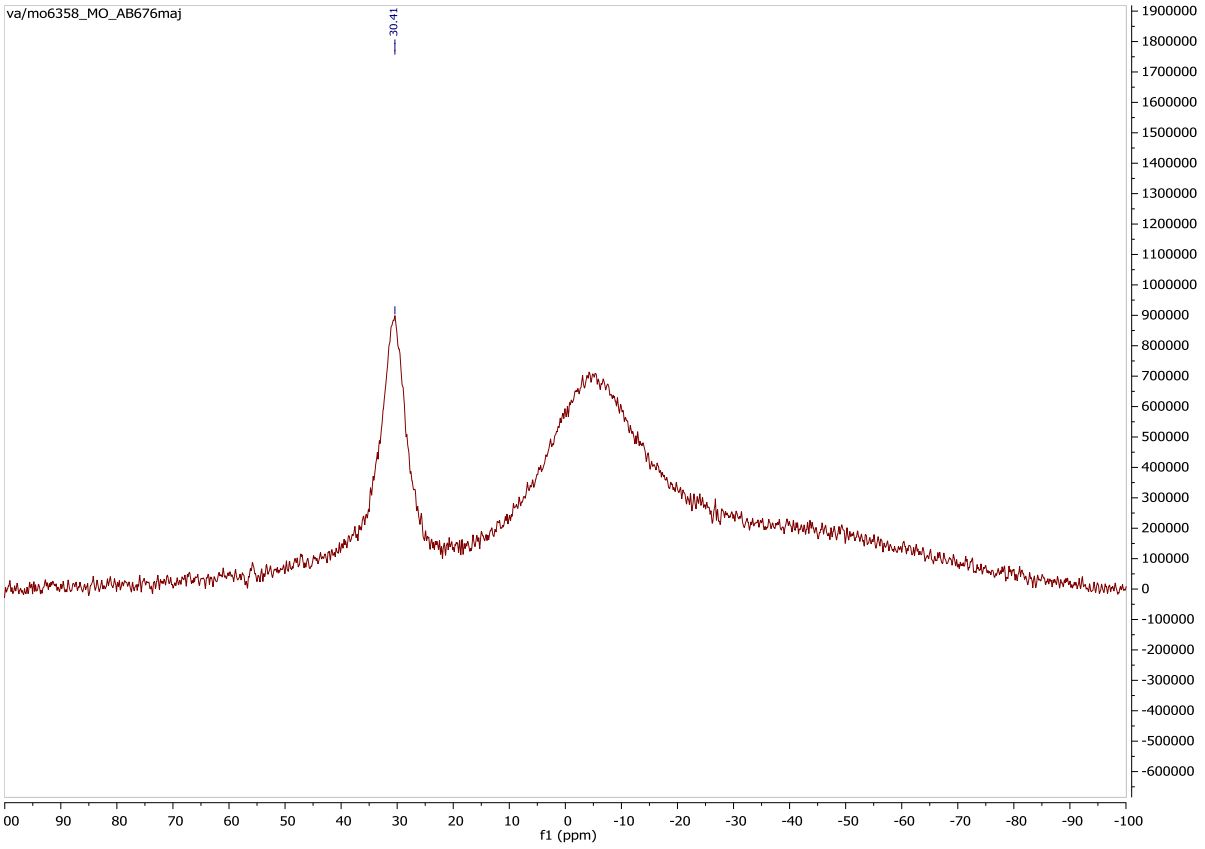
^{1}H NMR (400 MHz, $CDCl_3$)



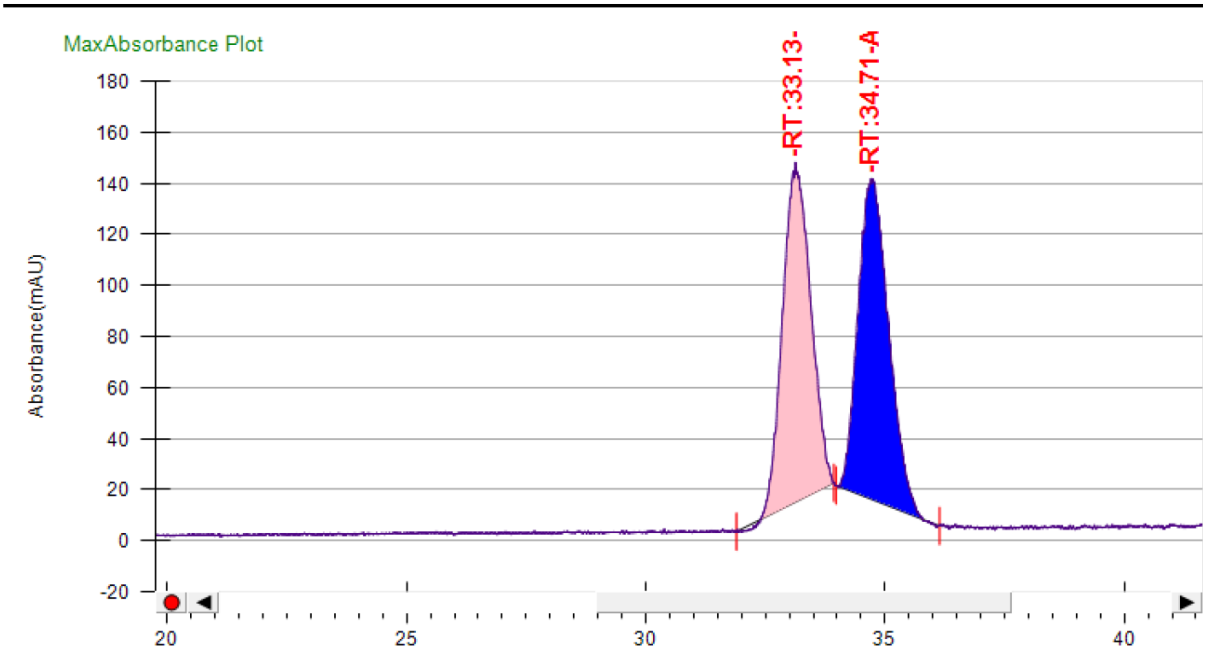
^{13}C NMR (100 MHz, $CDCl_3$)



^{11}B NMR (96 MHz, $CDCl_3$)[10]

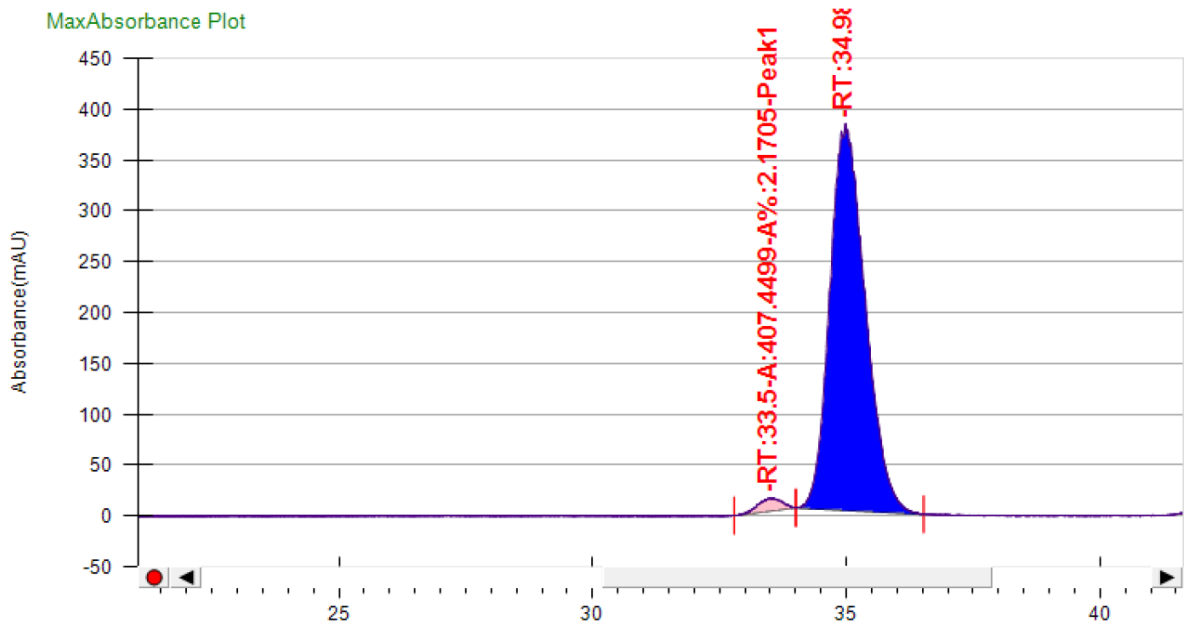


Chiral SFC traces: racemic



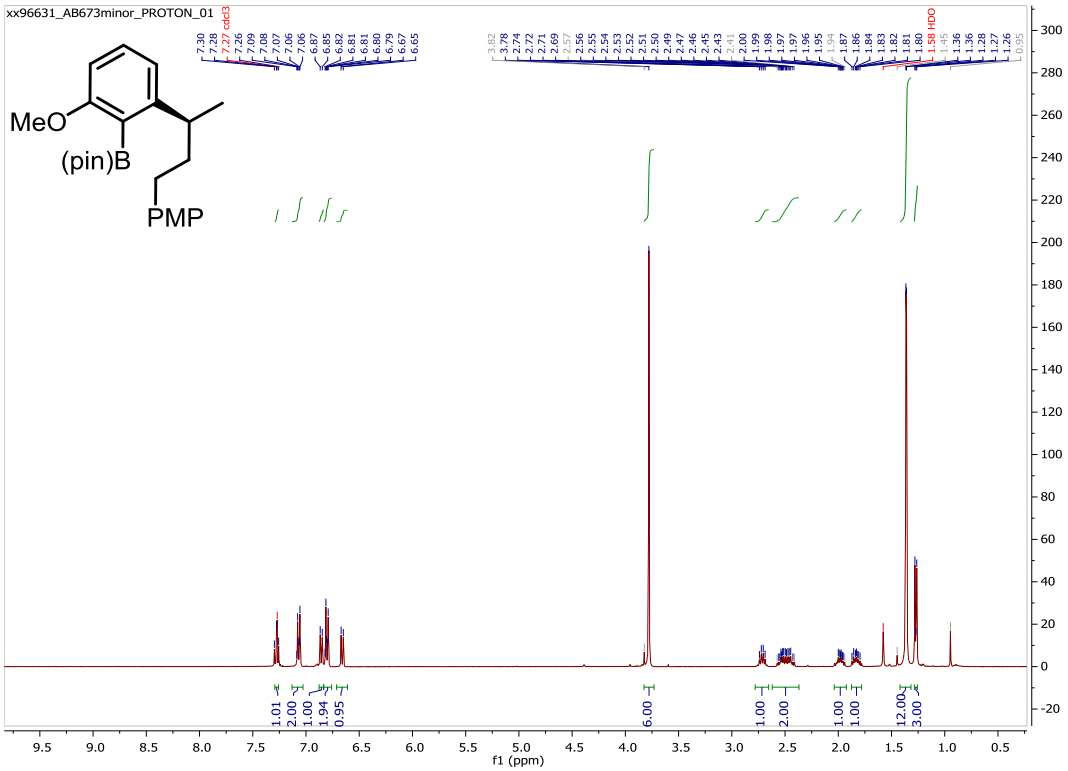
[10] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

Chiral SFC traces: enantioenriched

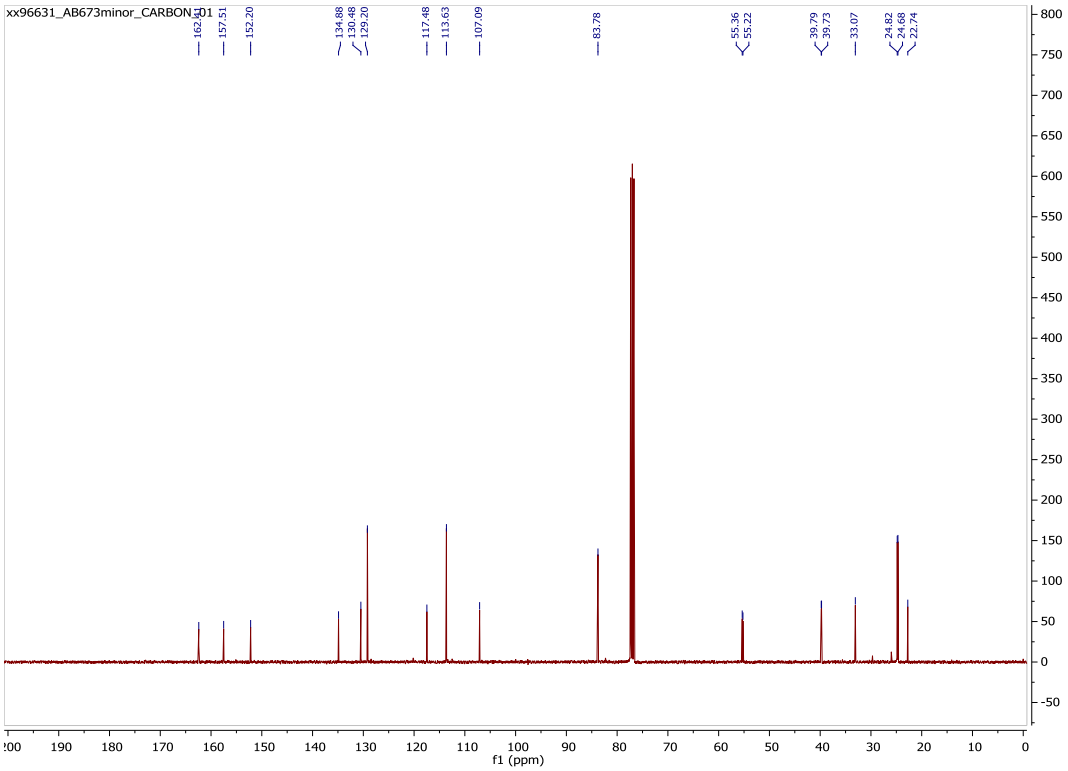


11ba-minor

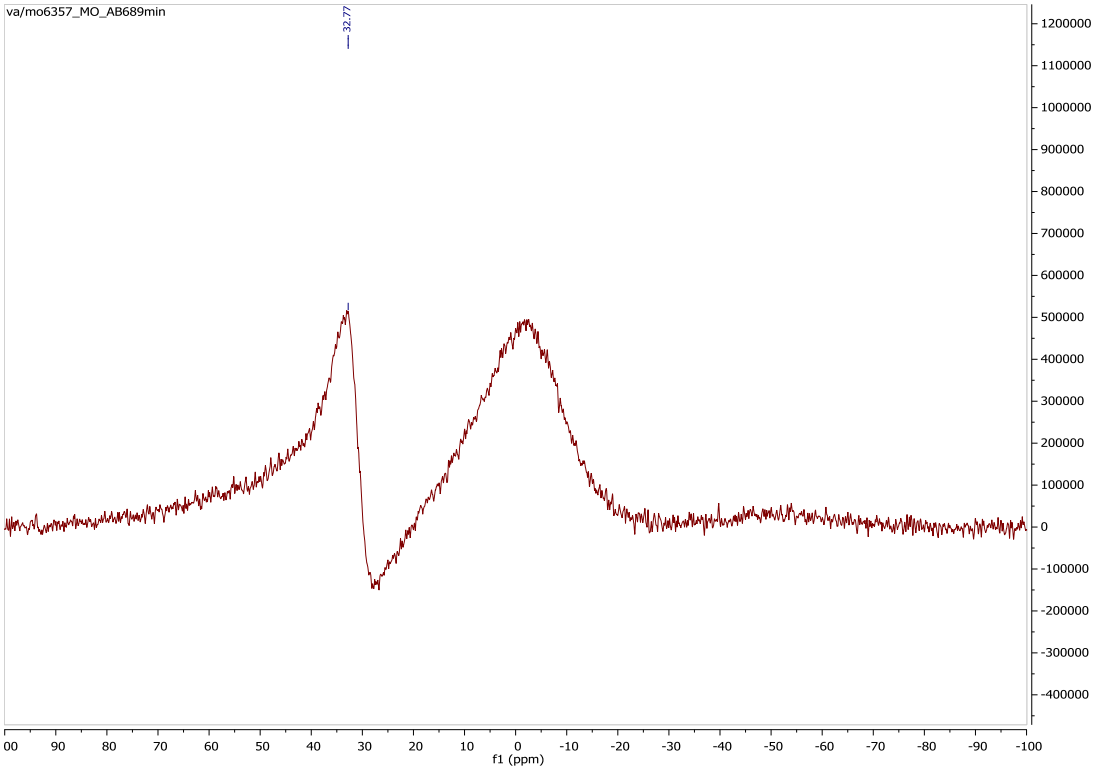
^{1}H NMR (400 MHz, $CDCl_3$)



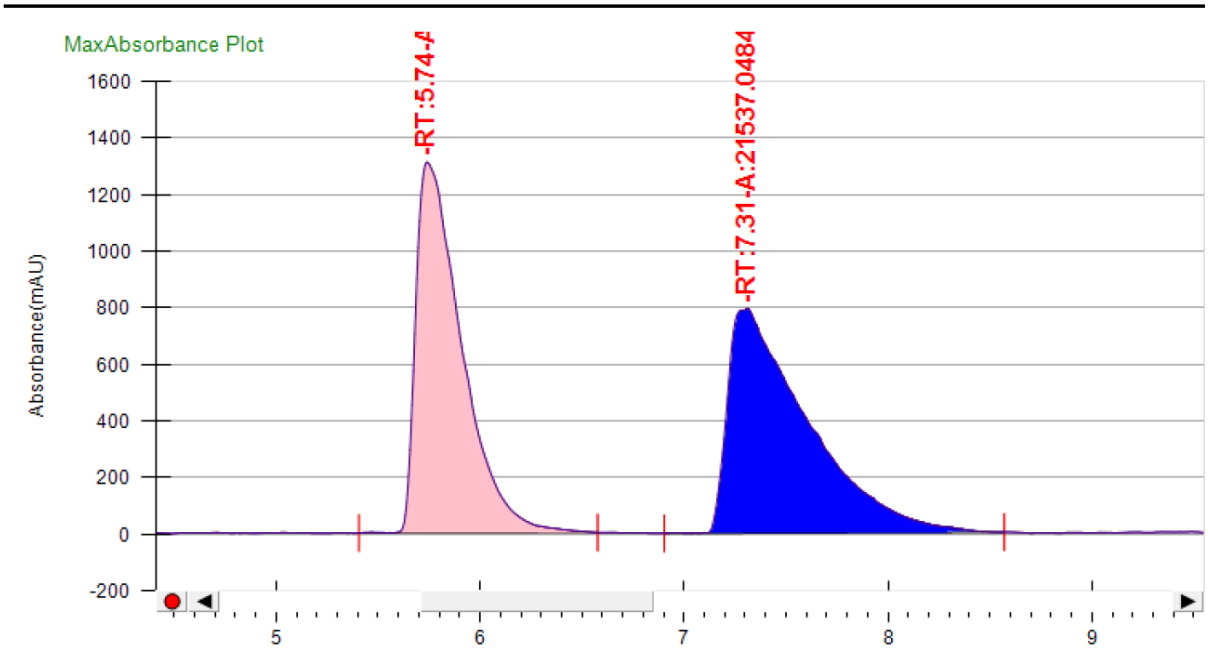
^{13}C NMR (100 MHz, $CDCl_3$)



^{11}B NMR (96 MHz, NONE)[11]

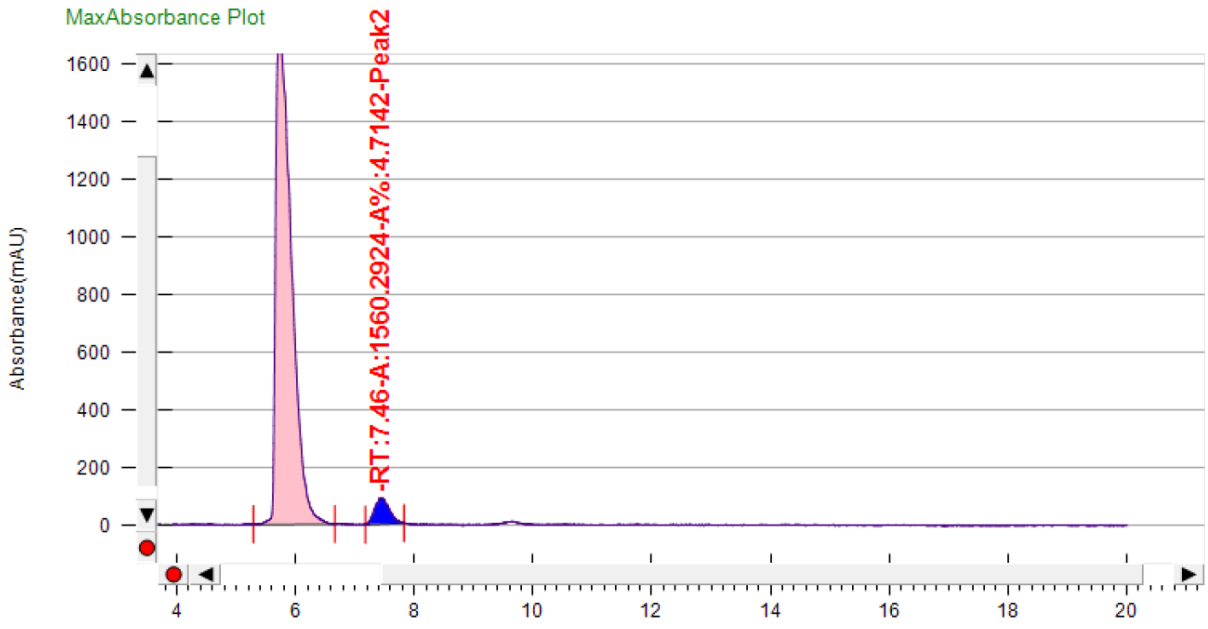


Chiral SFC traces: racemic



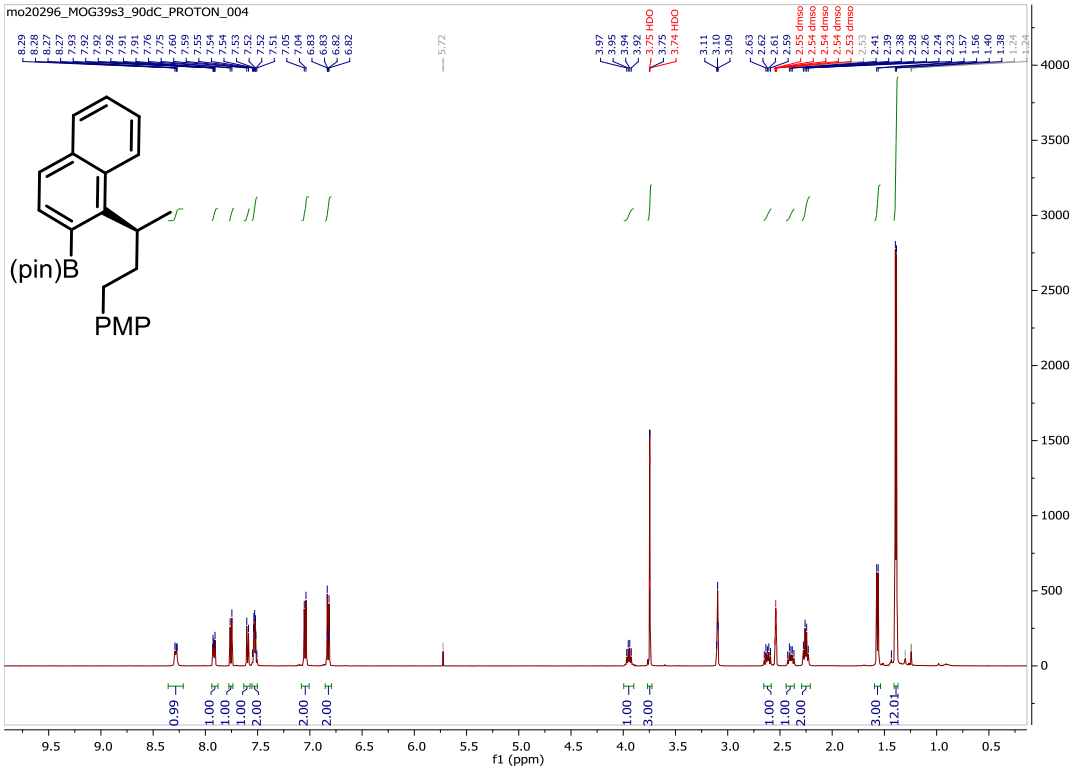
[11] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

Chiral SFC traces: enantioenriched

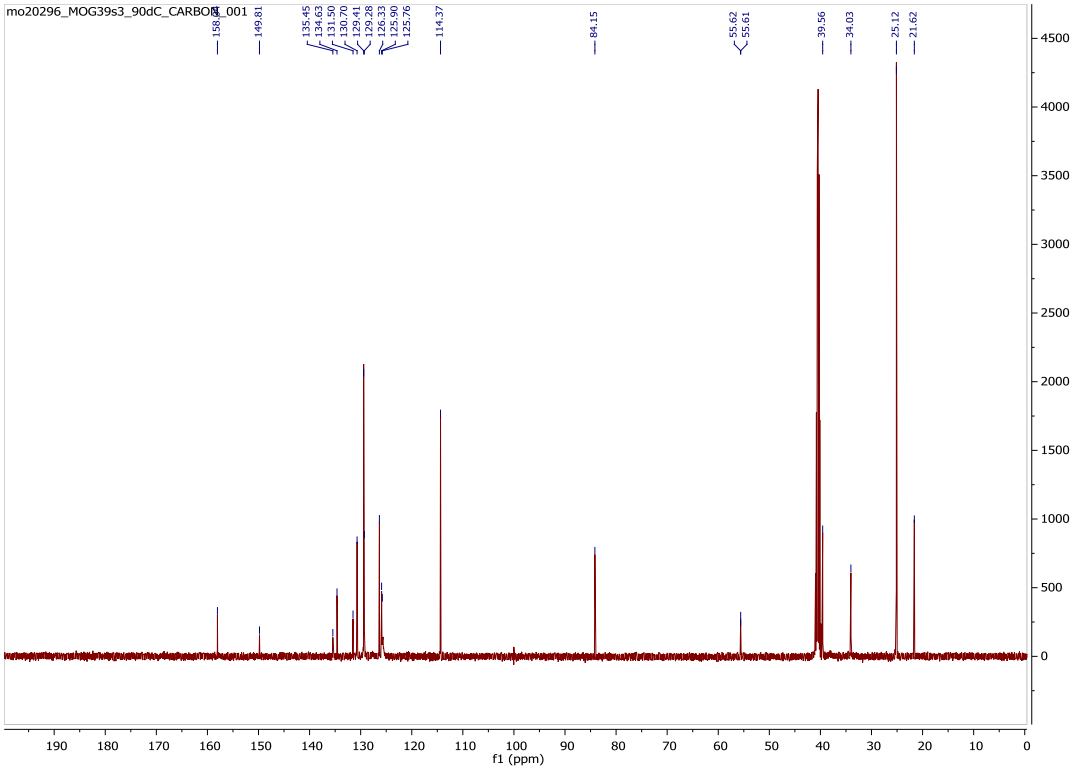


15ba

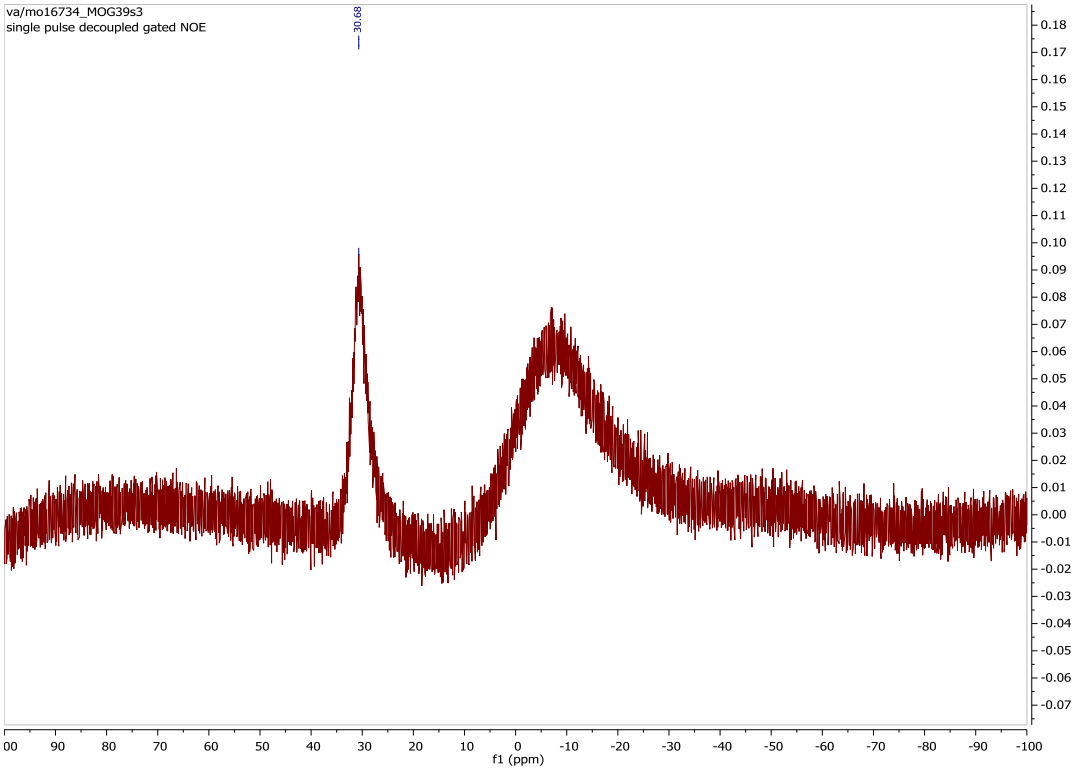
^{1}H NMR (500 MHz, DMSO)



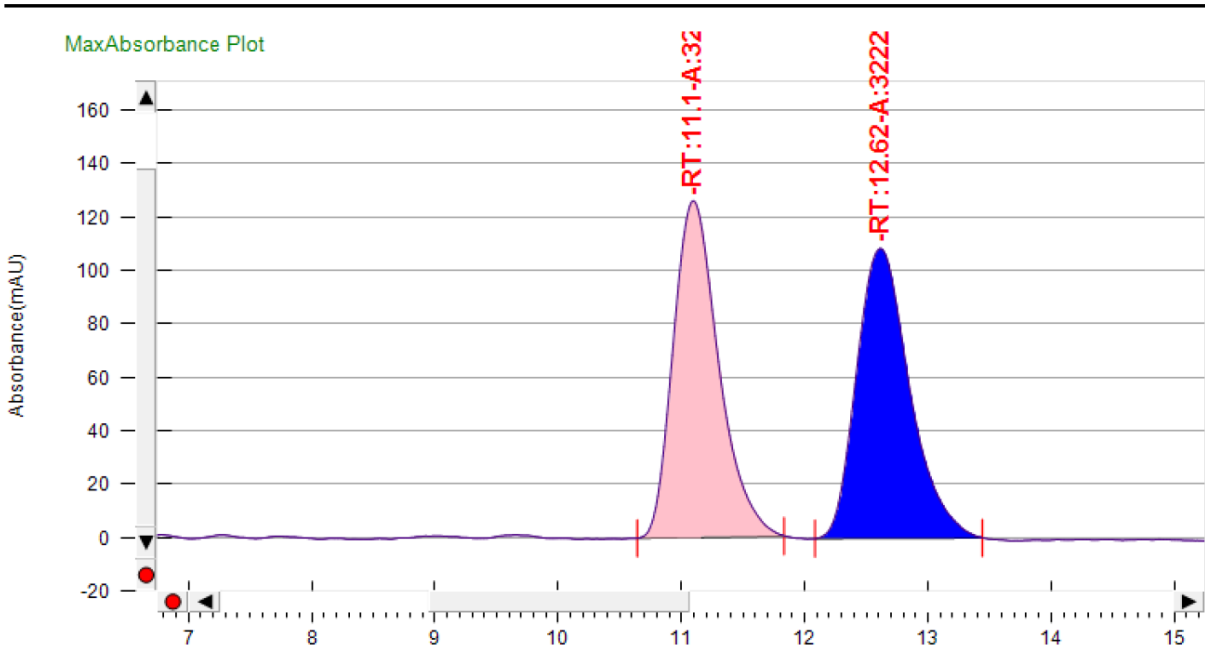
^{13}C NMR (125 MHz, DMSO)



^{11}B NMR (96 MHz, NONE)[12]

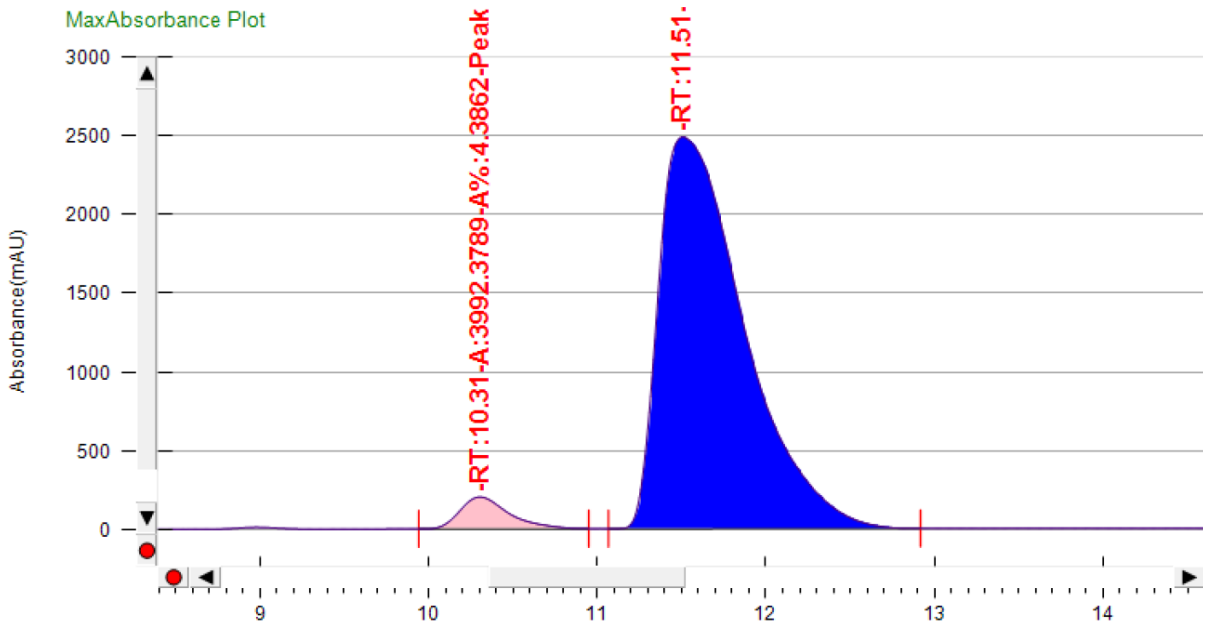


Chiral SFC traces: racemic



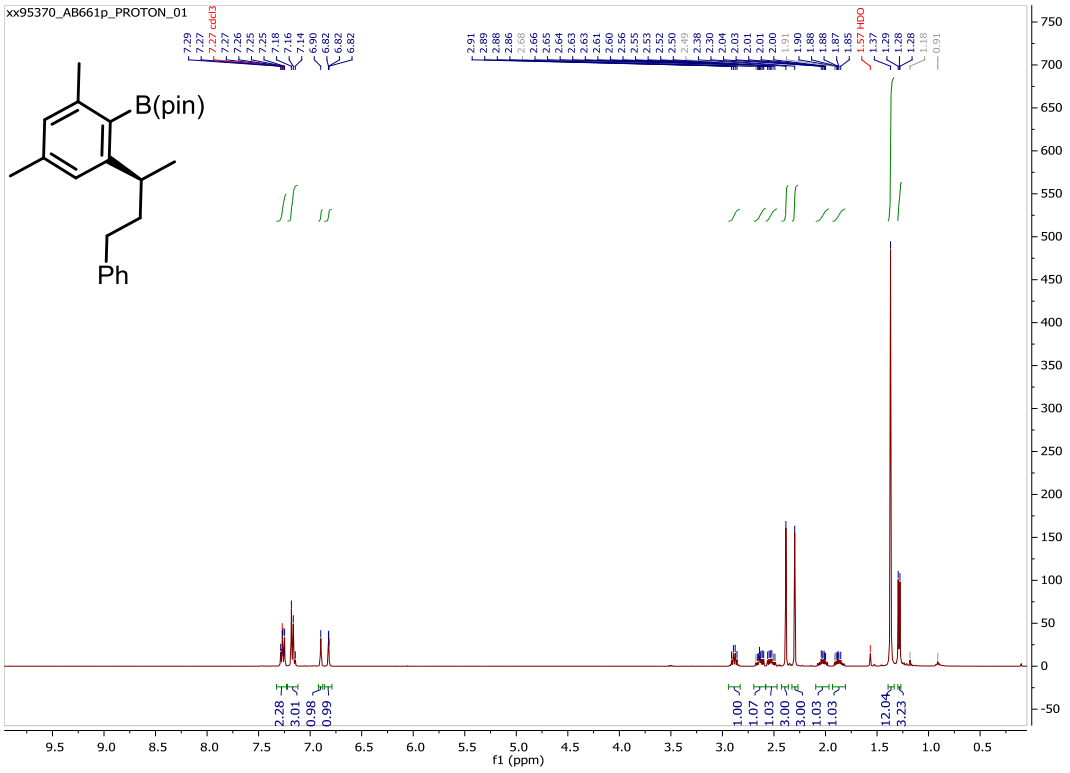
[12] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

Chiral SFC traces: enantioenriched

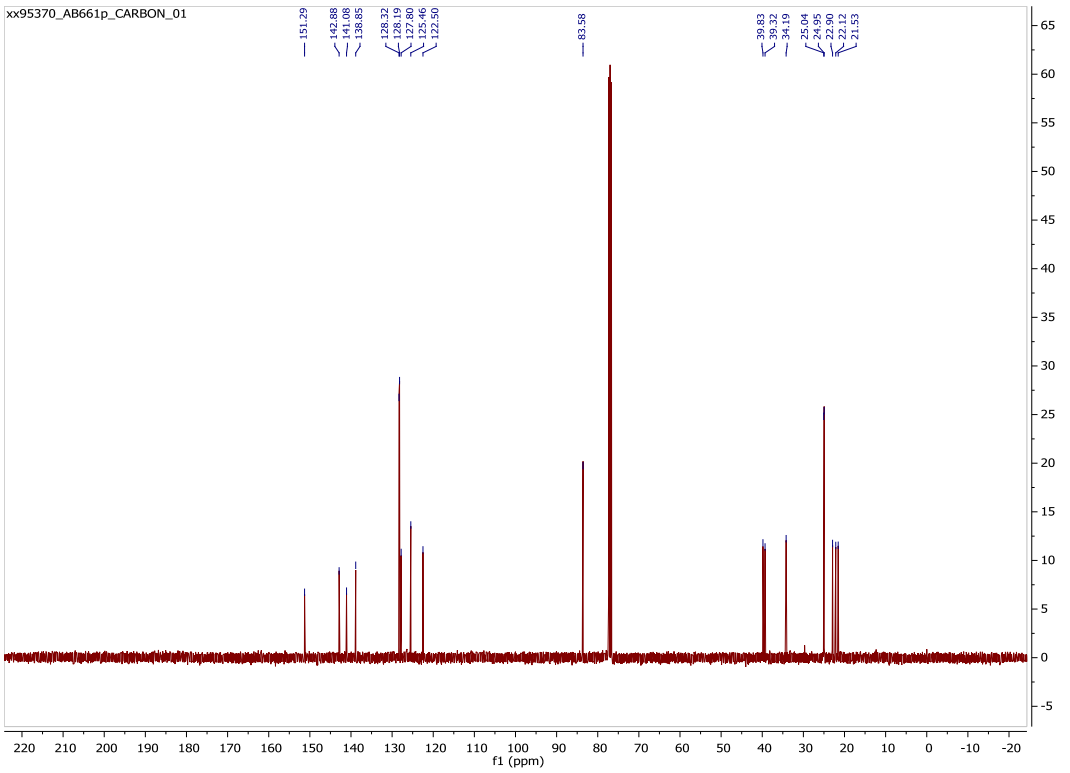


18aa

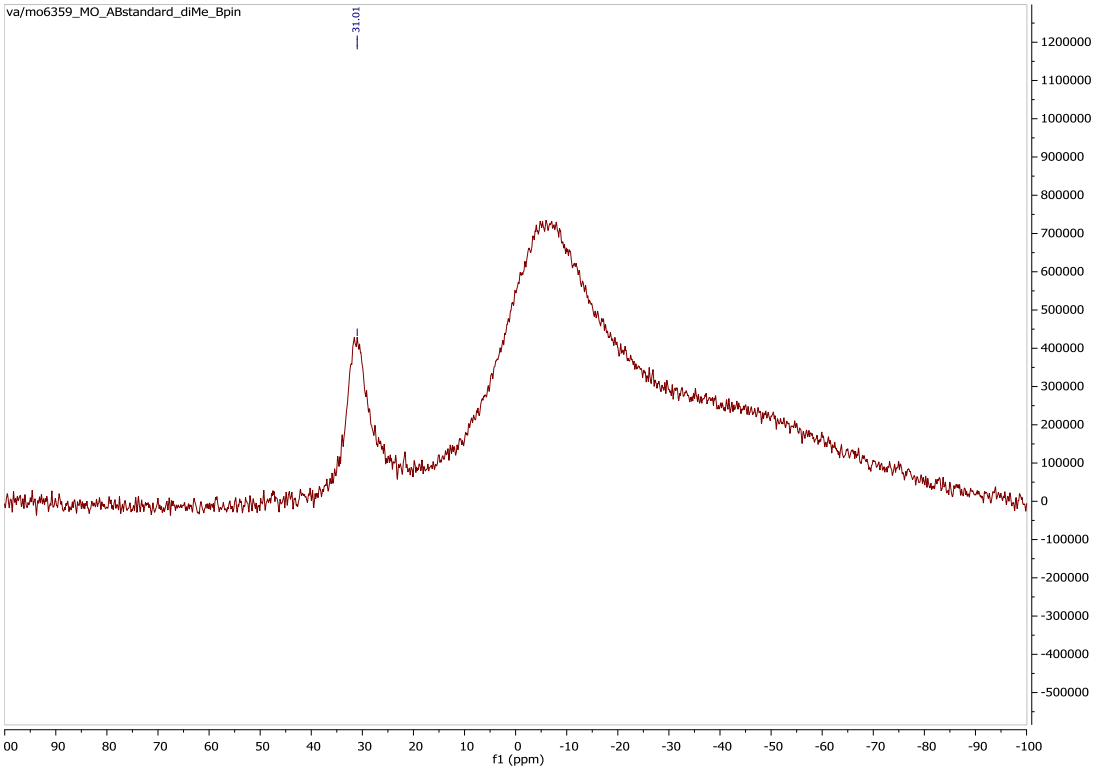
^{1}H NMR (400 MHz, $CDCl_3$)



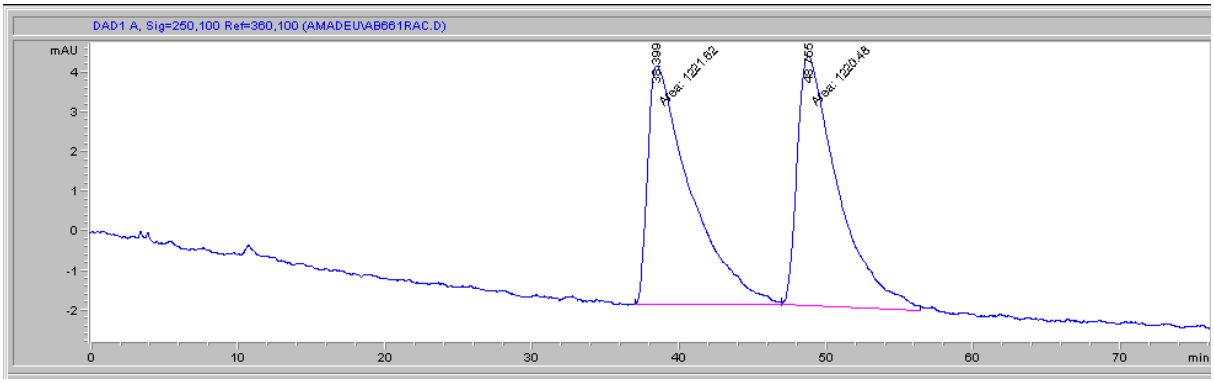
^{13}C NMR (100 MHz, $CDCl_3$)



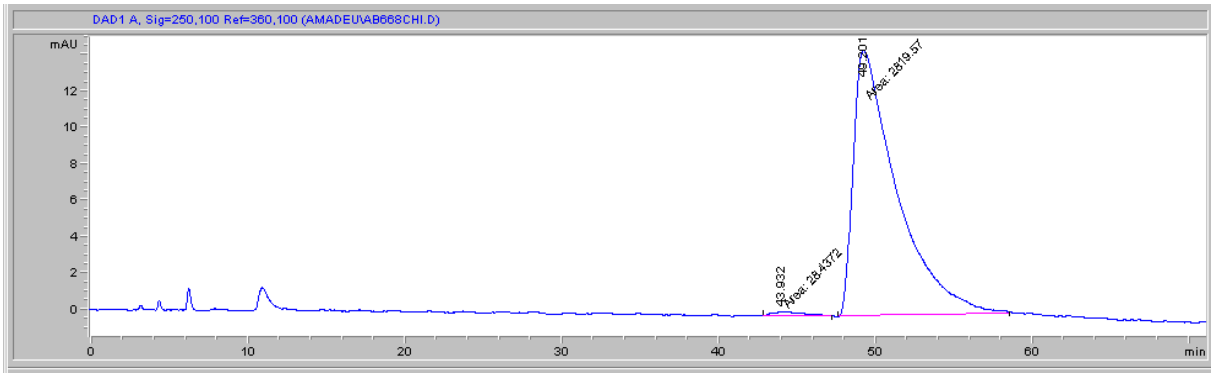
^{11}B NMR (96 MHz, NONE)[13]



Chiral SFC traces: racemic



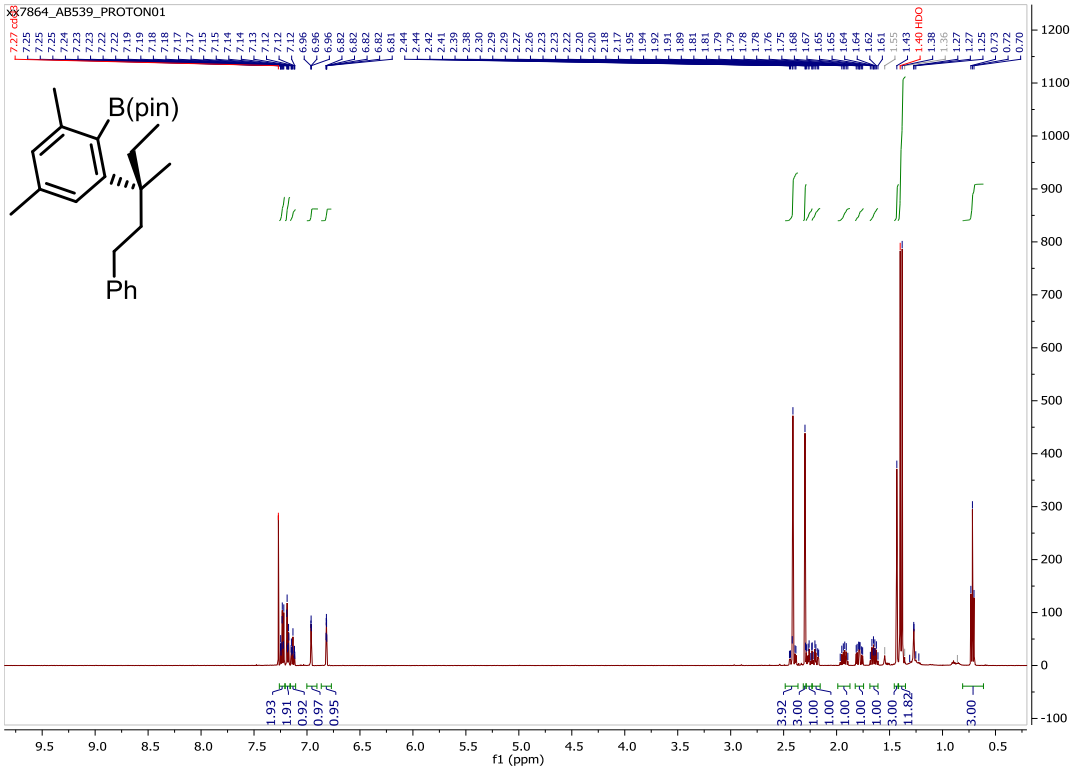
Chiral HPLC traces: enantioenriched



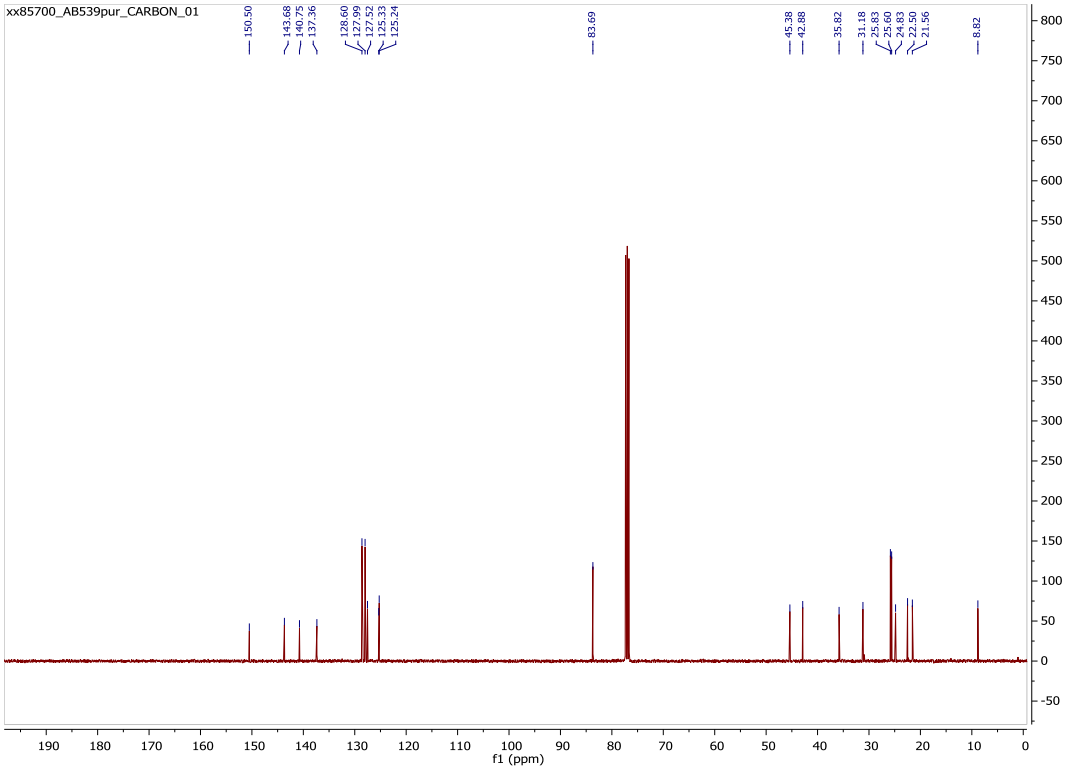
[13] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

18ga

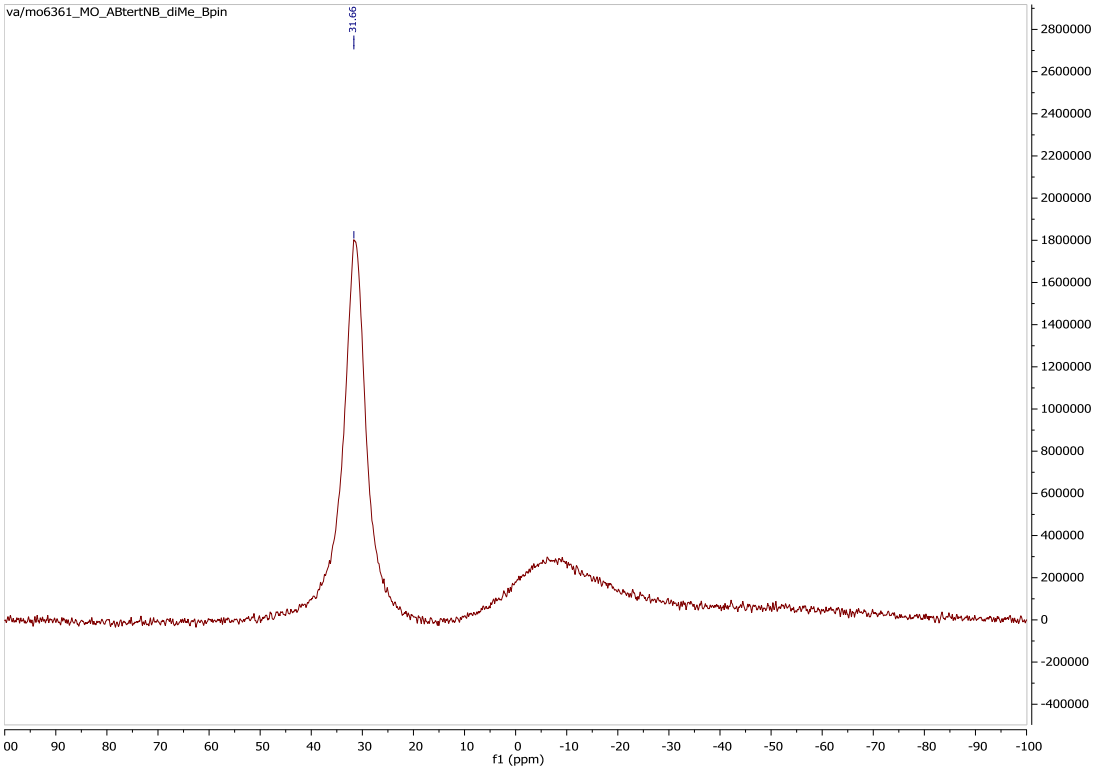
^{1}H NMR (500 MHz, $CDCl_3$)



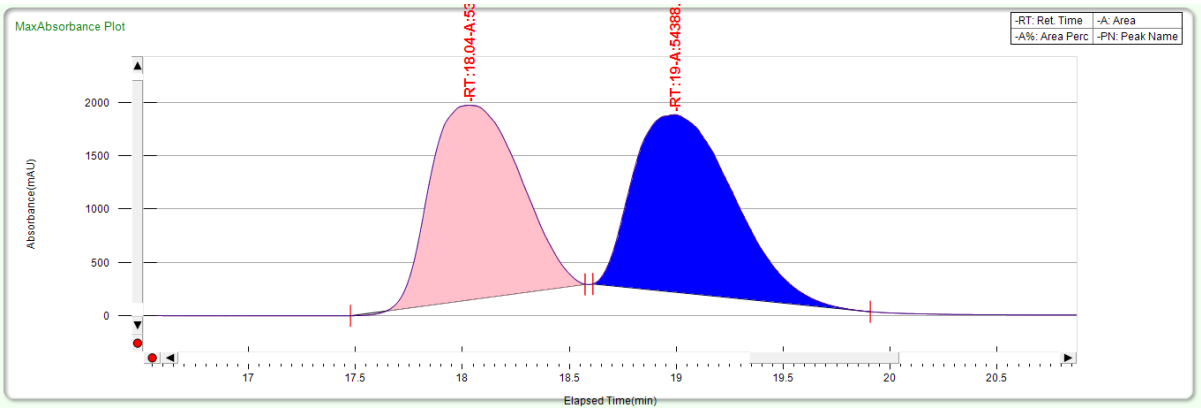
^{13}C NMR (100 MHz, $CDCl_3$)



^{11}B NMR (96 MHz, $CDCl_3$)[14]

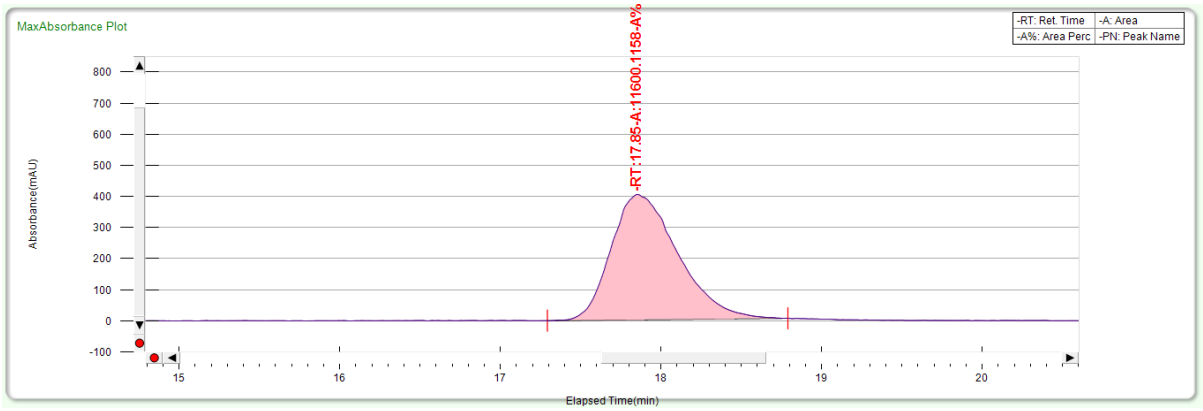


Chiral SFC traces: racemic



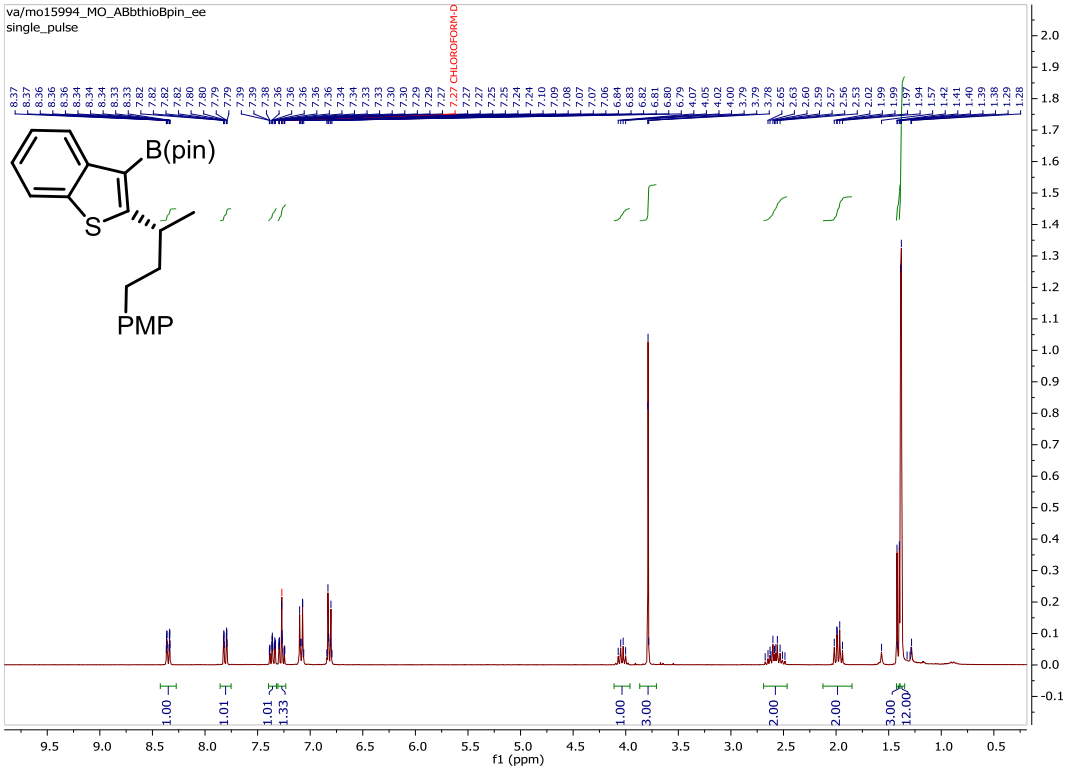
[14] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

Chiral HPLC traces: enantioenriched

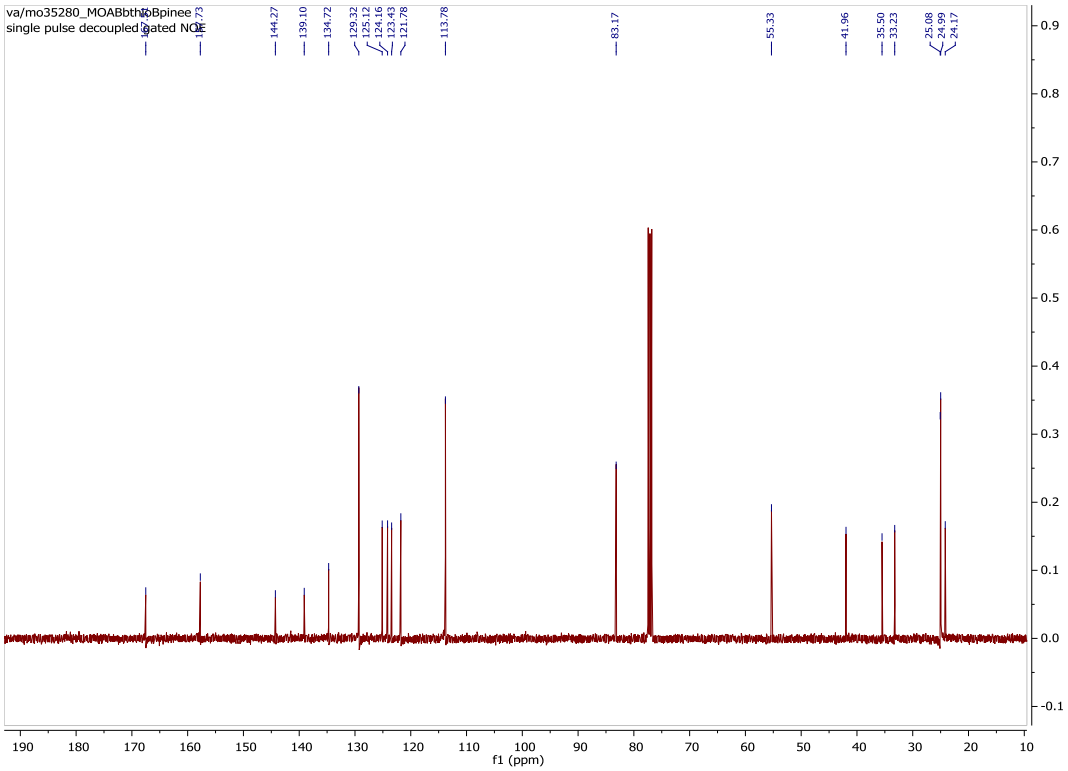


8ba

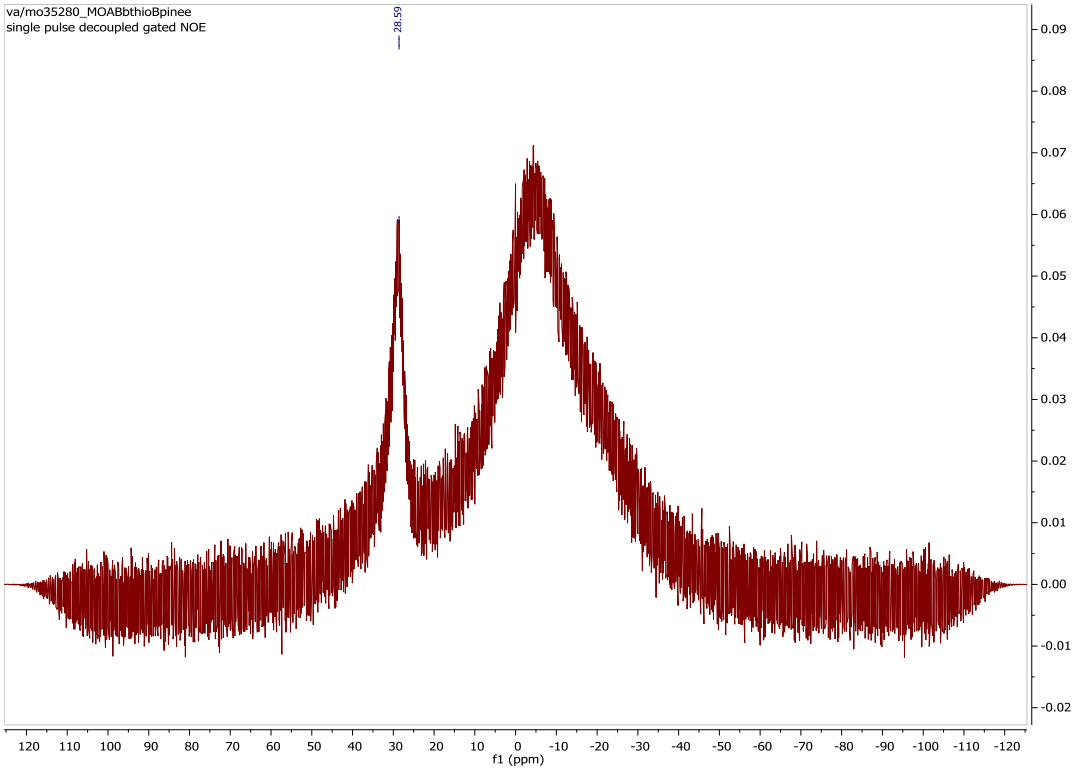
^{1}H NMR (400 MHz, $CDCl_3$)



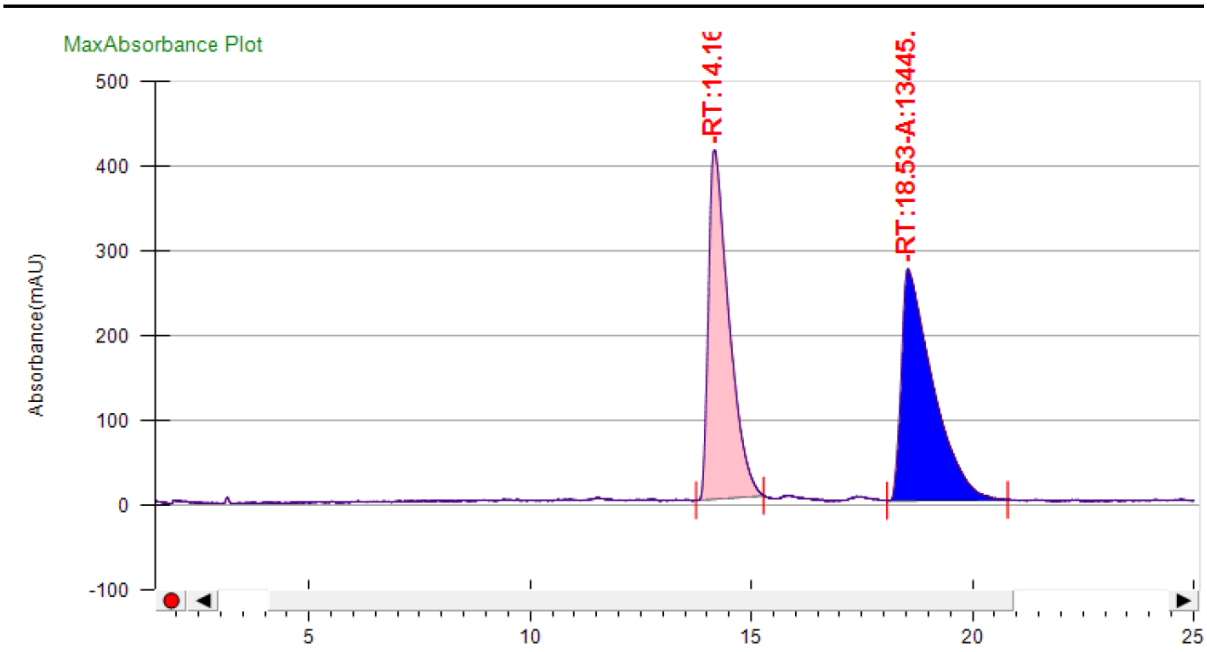
^{13}C NMR (100 MHz, $CDCl_3$)



^{11}B NMR (96 MHz, $CDCl_3$)[15]



Chiral SFC traces: racemic



[15] The broad peak at –5 ppm is due to the use of standard NMR tube (contains borosilicates).

Chiral SFC traces: enantioenriched