

Supplementary Materials

3-(((1S,3S)-3-((R)-Hydroxy(4-(trifluoromethyl)phenyl)methyl)-4-oxocyclohexyl)methyl)pentane-2,4-dione: Design and Synthesis of New Stereopure Multi-Target Antidiabetic Agent

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Figure S1. ^1H NMR of the purified compound (mixture of diastereomers).

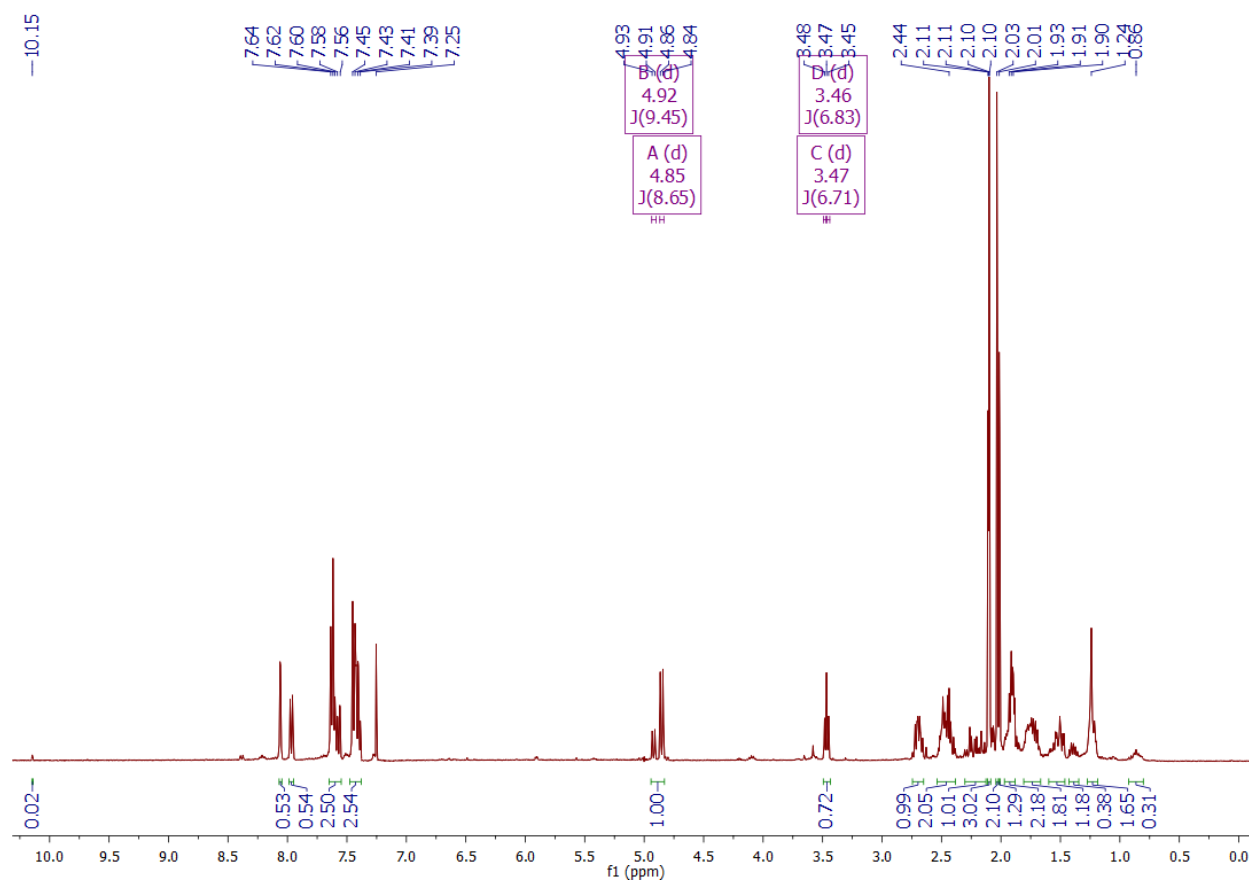


Figure S2. ^{13}C NMR of the purified compound (mixture of diastereomers).

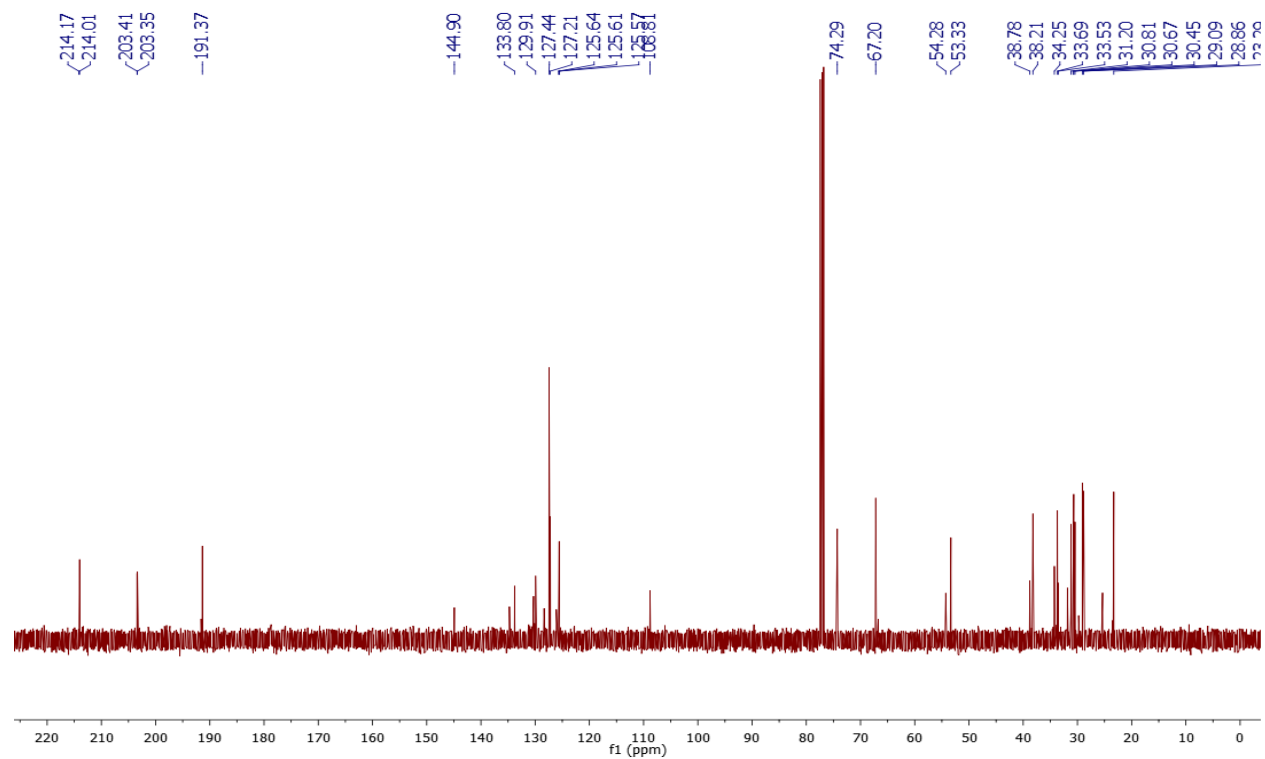


Figure S3. ^1H NMR of the stereopure compound S,S,R -5.

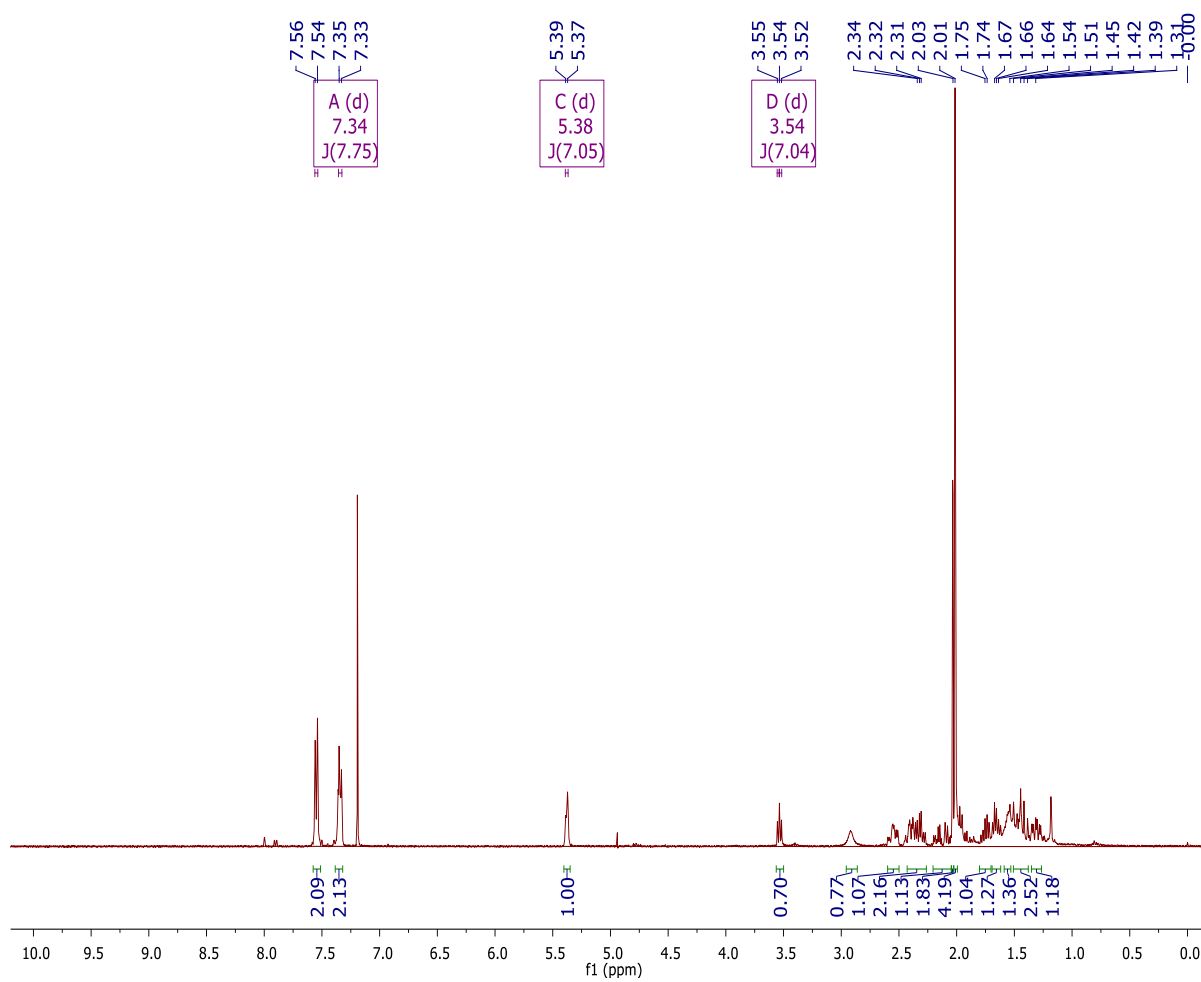


Figure S4. Expansions of the stereopure ^1H NMR of compound S,S,R -5.

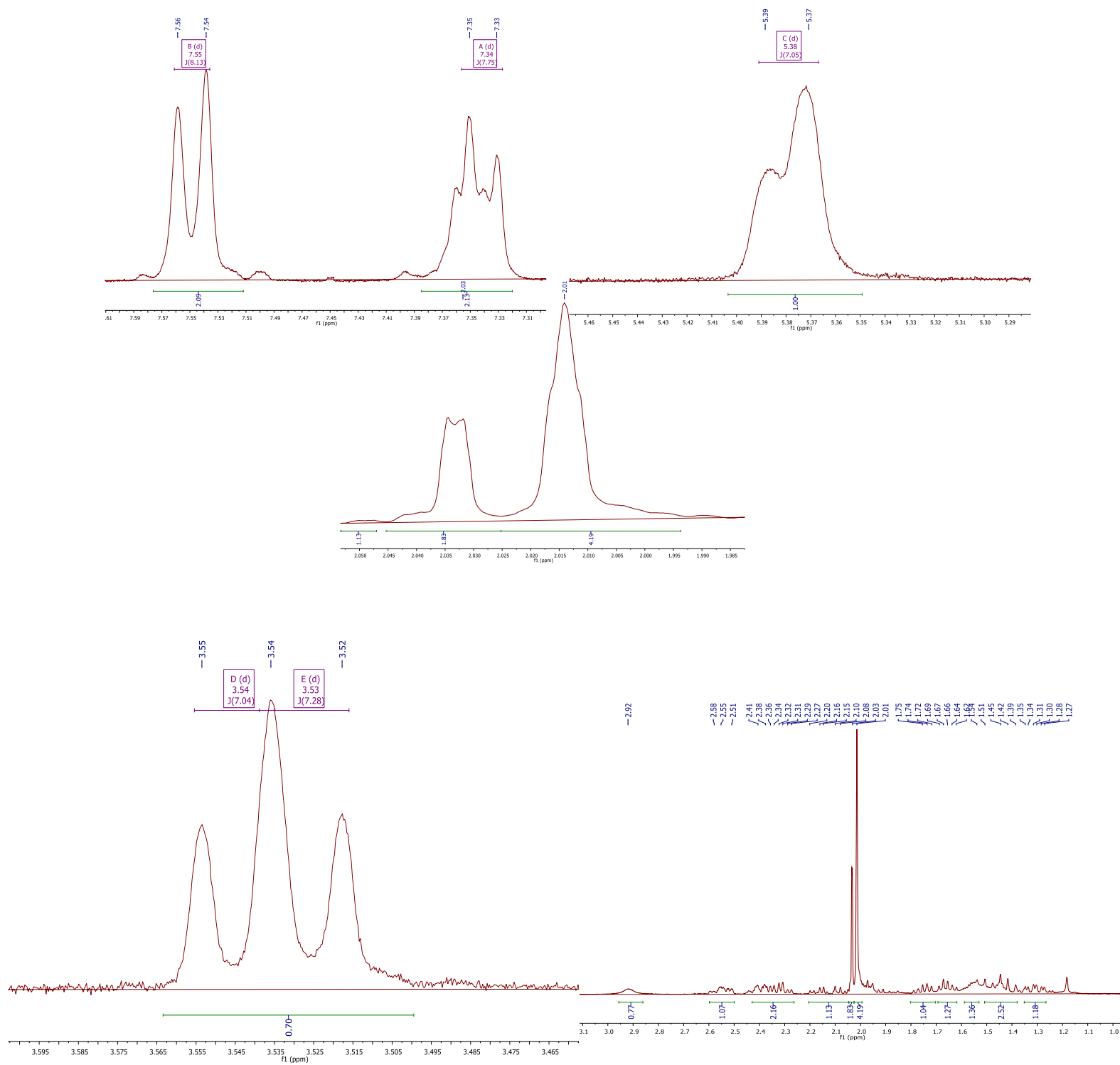


Figure S5. ^{13}C NMR of the stereopure compound *S,S,R*-5.

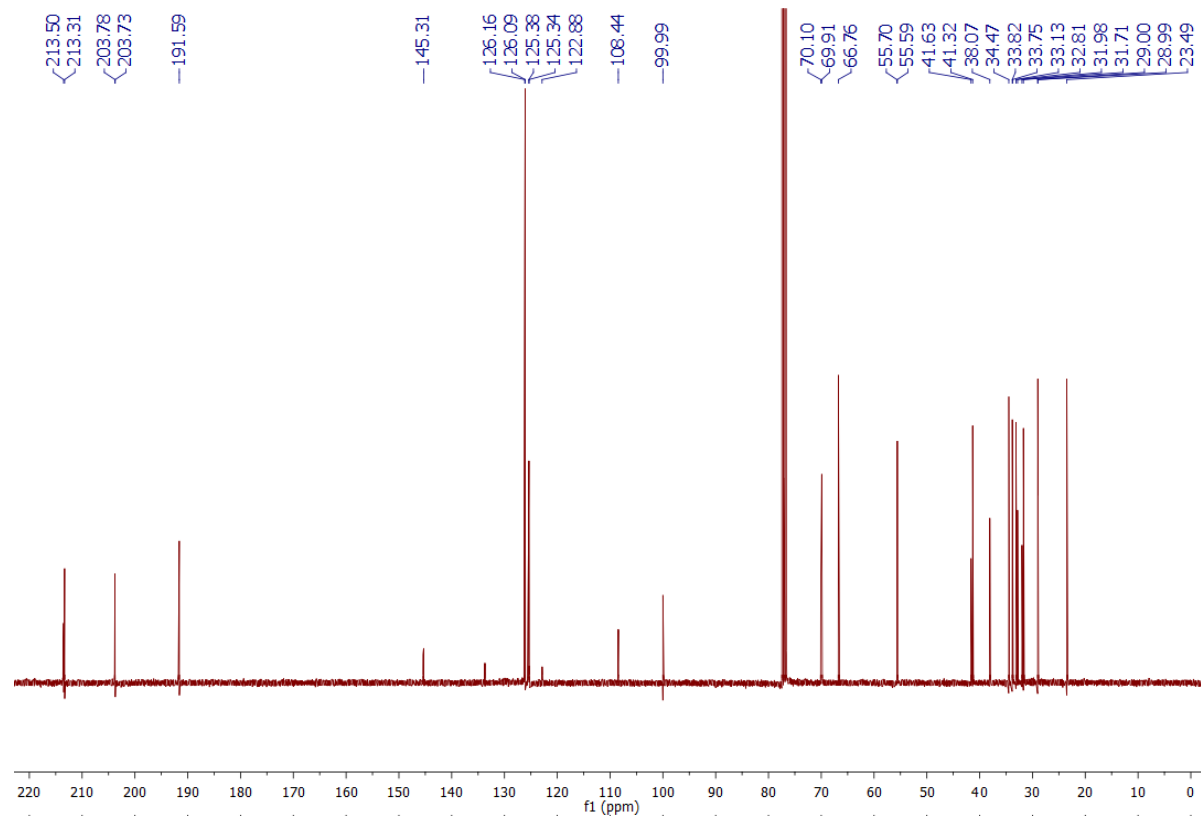


Figure S6. HRMS of the stereopure compound *S,S,R*-5.

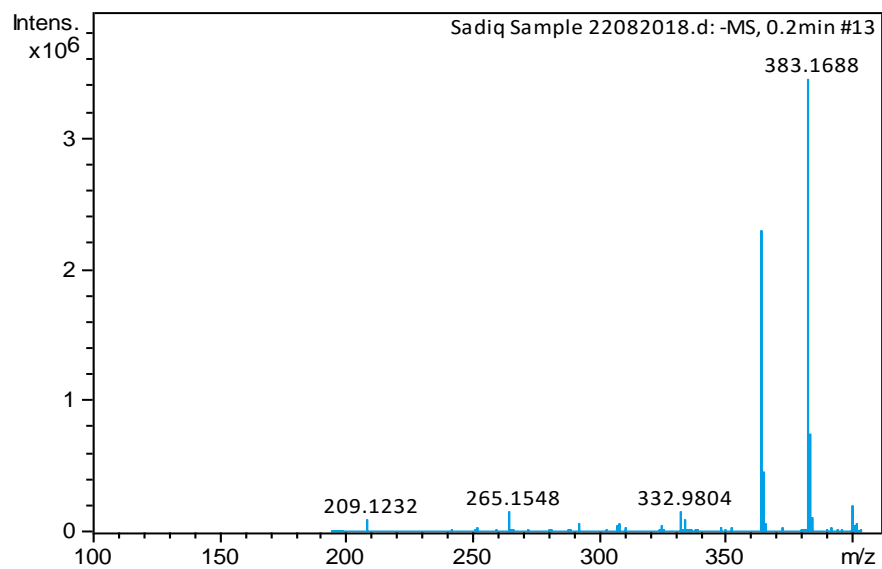


Figure S7. MS data of the stereopure compound *S,S,R*-5.

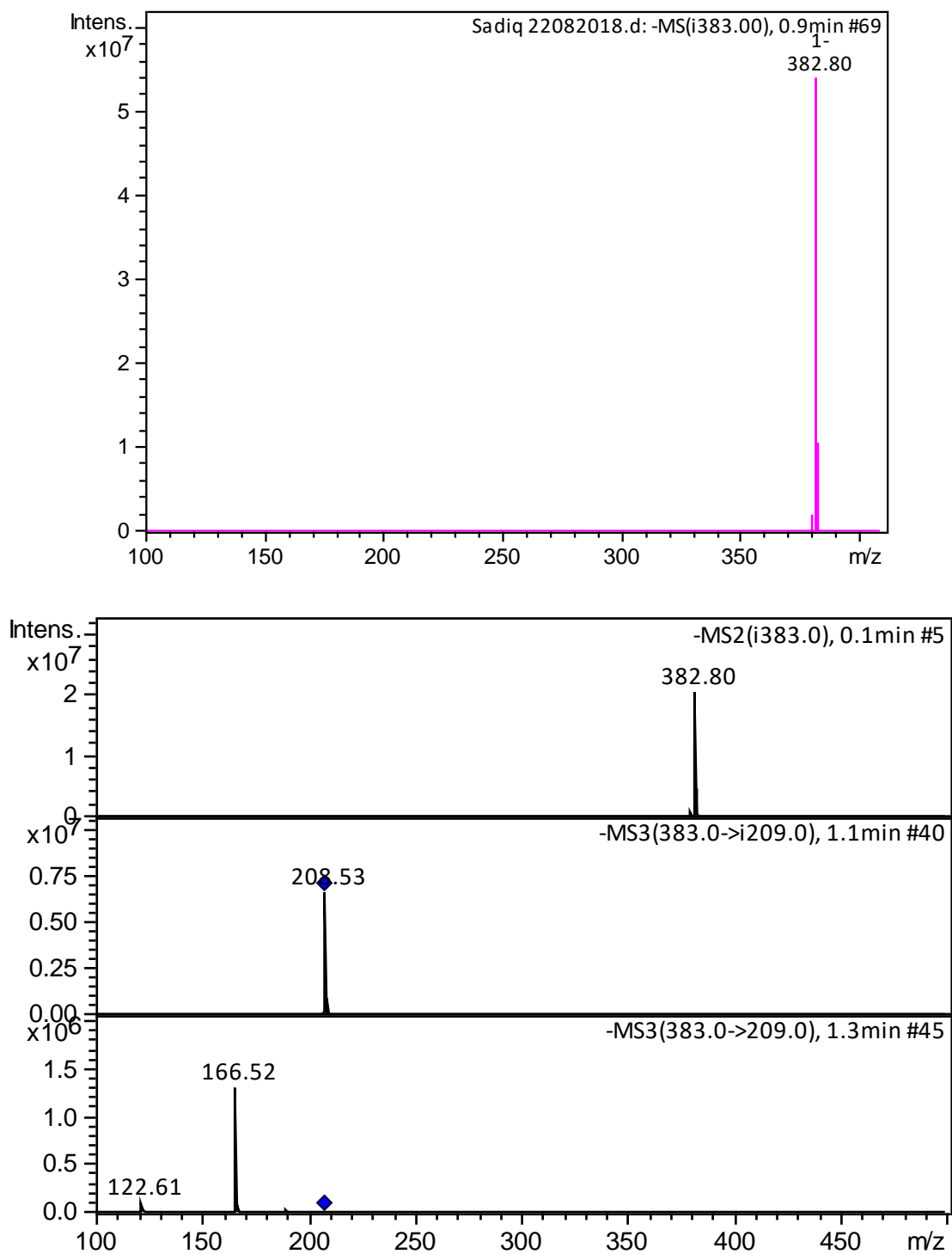


Figure S8. FT-IR analysis of the compound *S,S,R*-5.

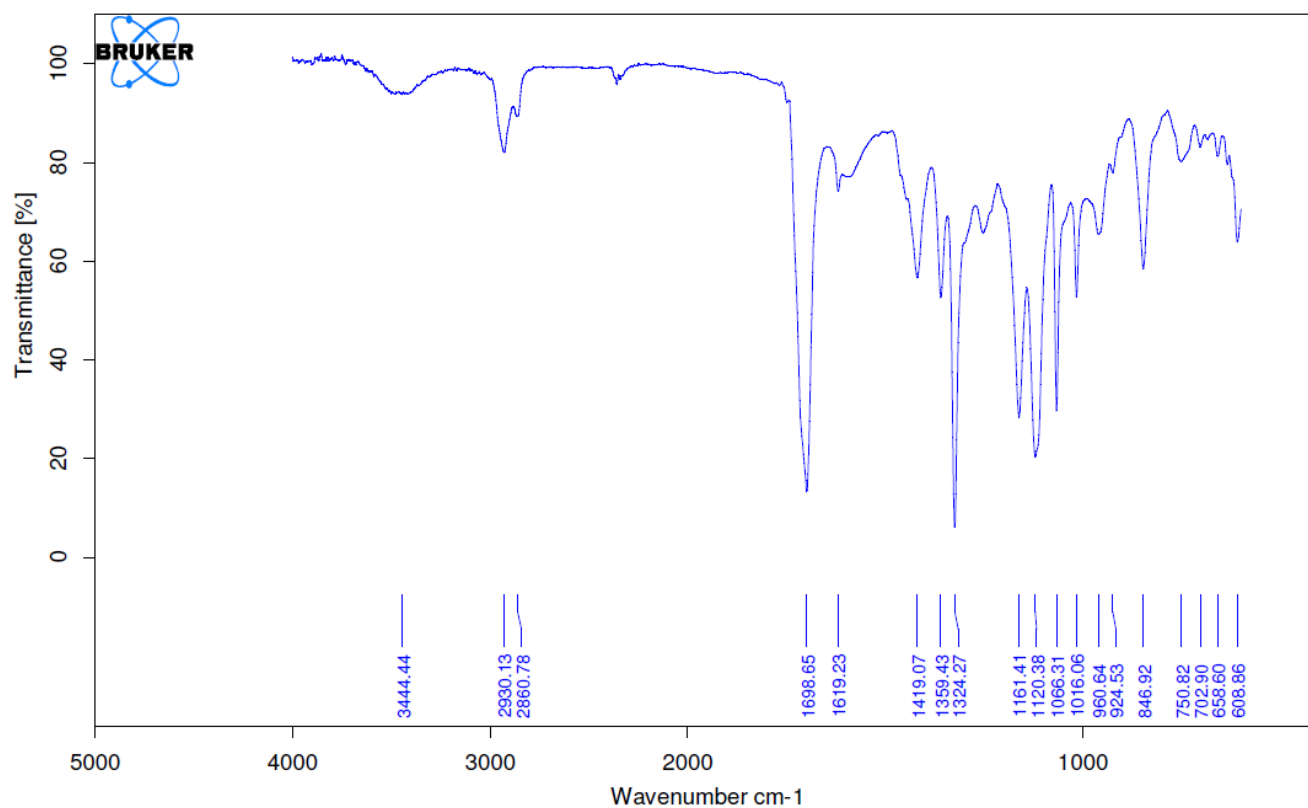
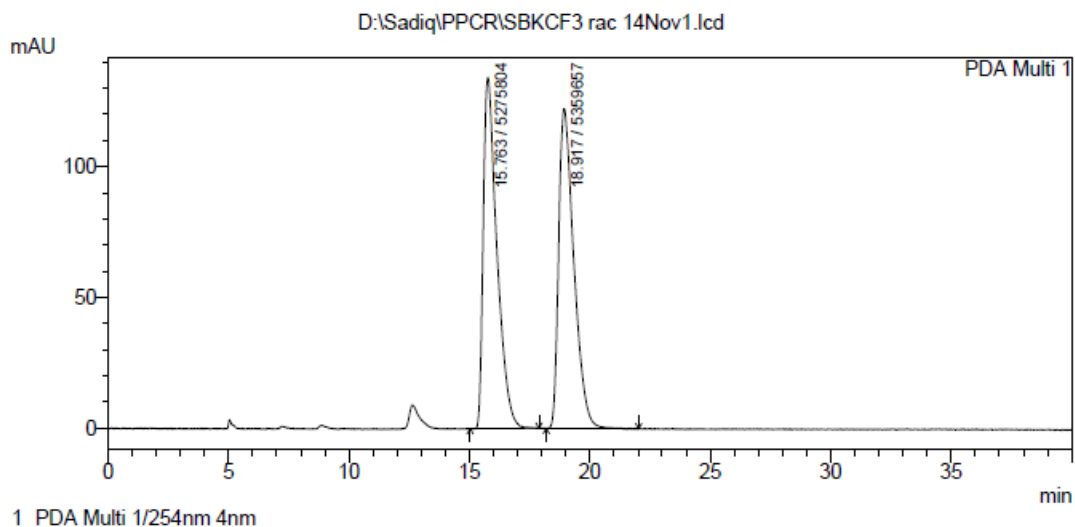


Figure S9. Chiral HPLC analysis of the racemic compound **Rac-5**.

==== Shimadzu LCsolution Analysis Report ====

Acquired by : Admin
Sample Name : SBKCF3 rac 14Nov
Sample ID : SBKCF3 rac 14Nov
Vial # : 1
Injection Volume : 10 uL
Data File Name : SBKCF3 rac 14Nov1.lcd
Method File Name : 10 % 0.6 mL, 60 min.lcm
Batch File Name :
Report File Name : Musterreport.lcr
Data Acquired : 14.11.2018 08:38:53
Data Processed : 14.11.2018 09:18:58
Diese Probe heit: SBKCF3 rac 14Nov

<Chromatogram>



<Results>

PDA Ch1 254nm 4nm

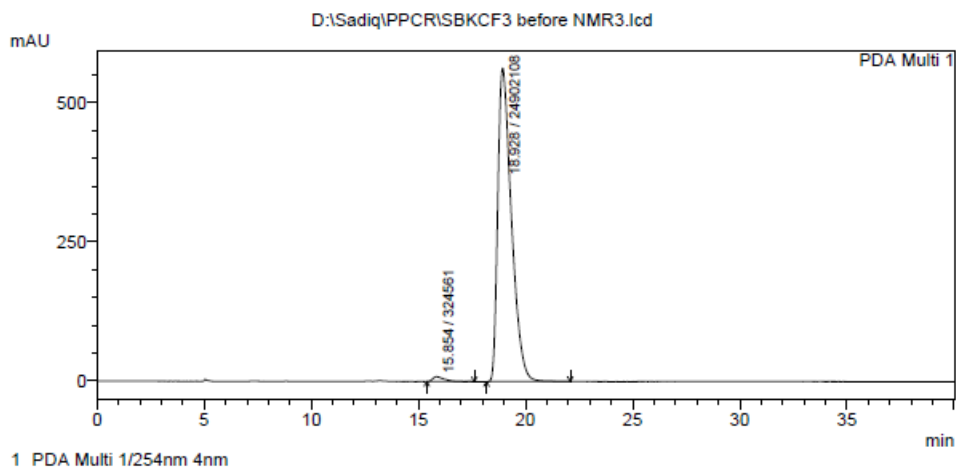
Peak #	Ret. Time	Area	Height	Area %	Height %	Width at 10% Height	Mark
1	15.763	527580.4	134224	49.606	52.342	1.185	
2	18.917	535965.7	122214	50.394	47.658	1.285	
Total		1063546.1	256438	100.000	100.000		

Figure S10. Chiral HPLC analysis of the stereopure compound *S,S,R*-5.

==== Shimadzu Lcsolution Analysis Report ====

Acquired by : Admin
Sample Name : SBKCF3 before NMR
Sample ID : SBKCF3 before NMR
Vial # : 1
Injection Volume : 10 uL
Data File Name : SBKCF3 before NMR3.lcd
Method File Name : 10 % 0.6 mL, 60 min.lcm
Batch File Name :
Report File Name : Musterreport.lcr
Data Acquired : 14.11.2018 07:54:56
Data Processed : 14.11.2018 08:35:01
Diese Probe heit: SBKCF3 before NMR

<Chromatogram>



<Results>

PDA Ch1 254nm 4nm

Peak #	Ret. Time	Area	Height	Area %	Height %	Width at 10% Height	Mark
1	15.854	324561	8754	1.287	1.531	1.131	
2	18.928	24902108	563170	98.713	98.469	1.299	
Total		25226669	571924	100.000	100.000		