

New Nitrogen, Sulfur-, and Selenium-donating Ligands Derived from Chiral Pyridine Amino Alcohols. Synthesis and Catalytic Activity in Asymmetric Allylic Alkylation.

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Supporting information

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1. Copies of NMR spectra

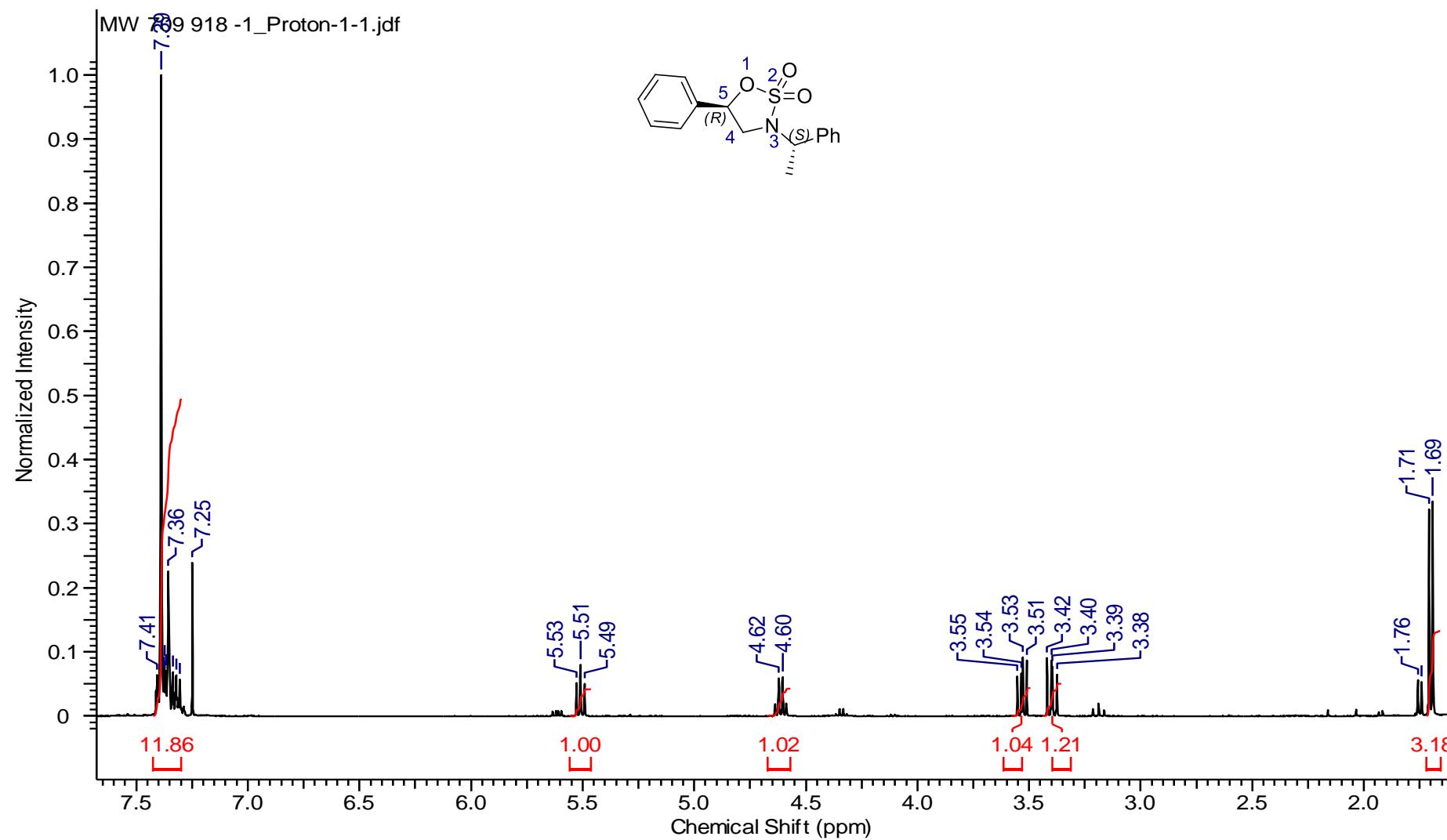


Figure S1. ^1H NMR spectrum (400 MHz, CDCl_3) for (5*R*,1'*S*)-12

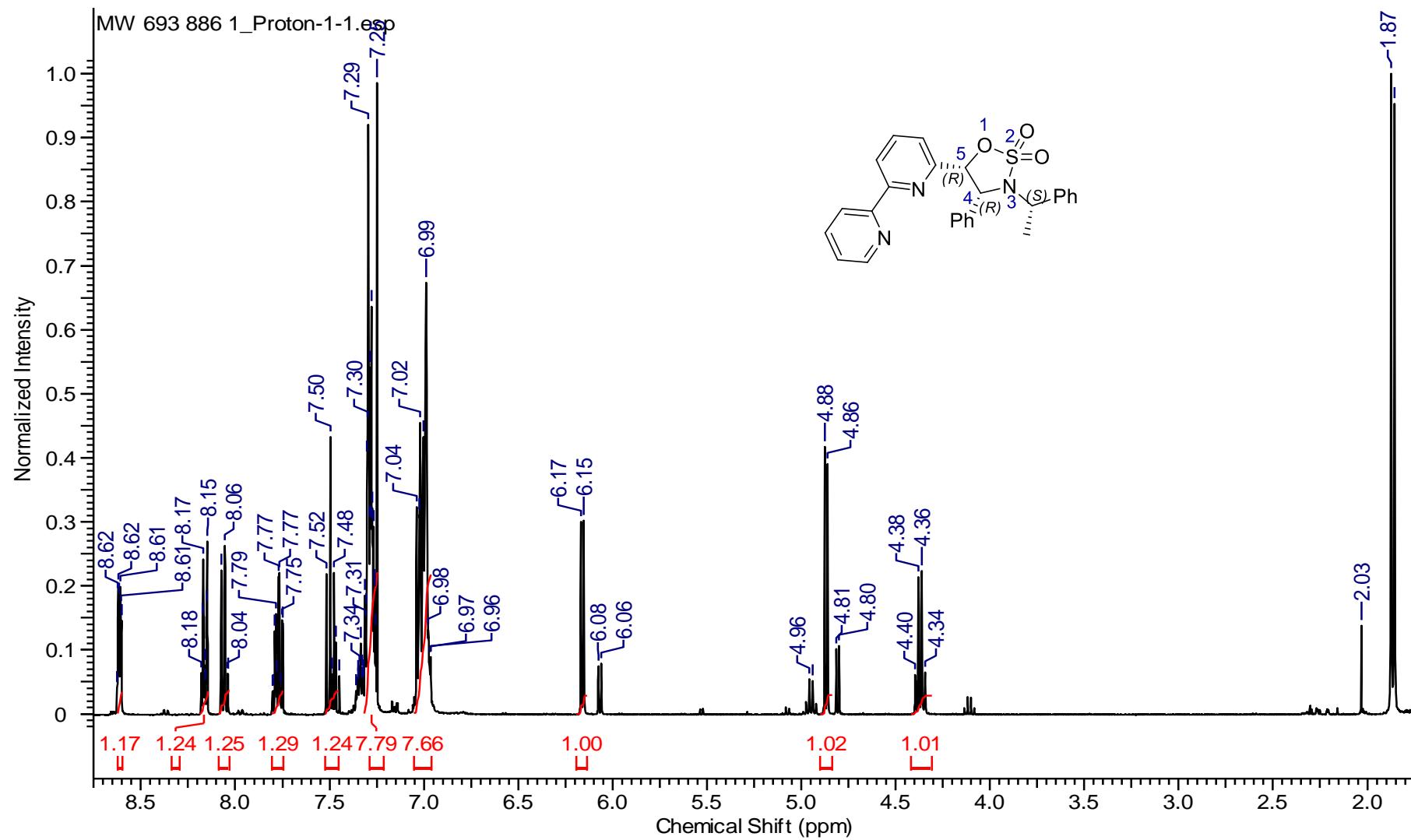


Figure S3. ^1H NMR spectrum (400 MHz, CDCl_3) for (4*R*,5*R*,1'*S*)-14

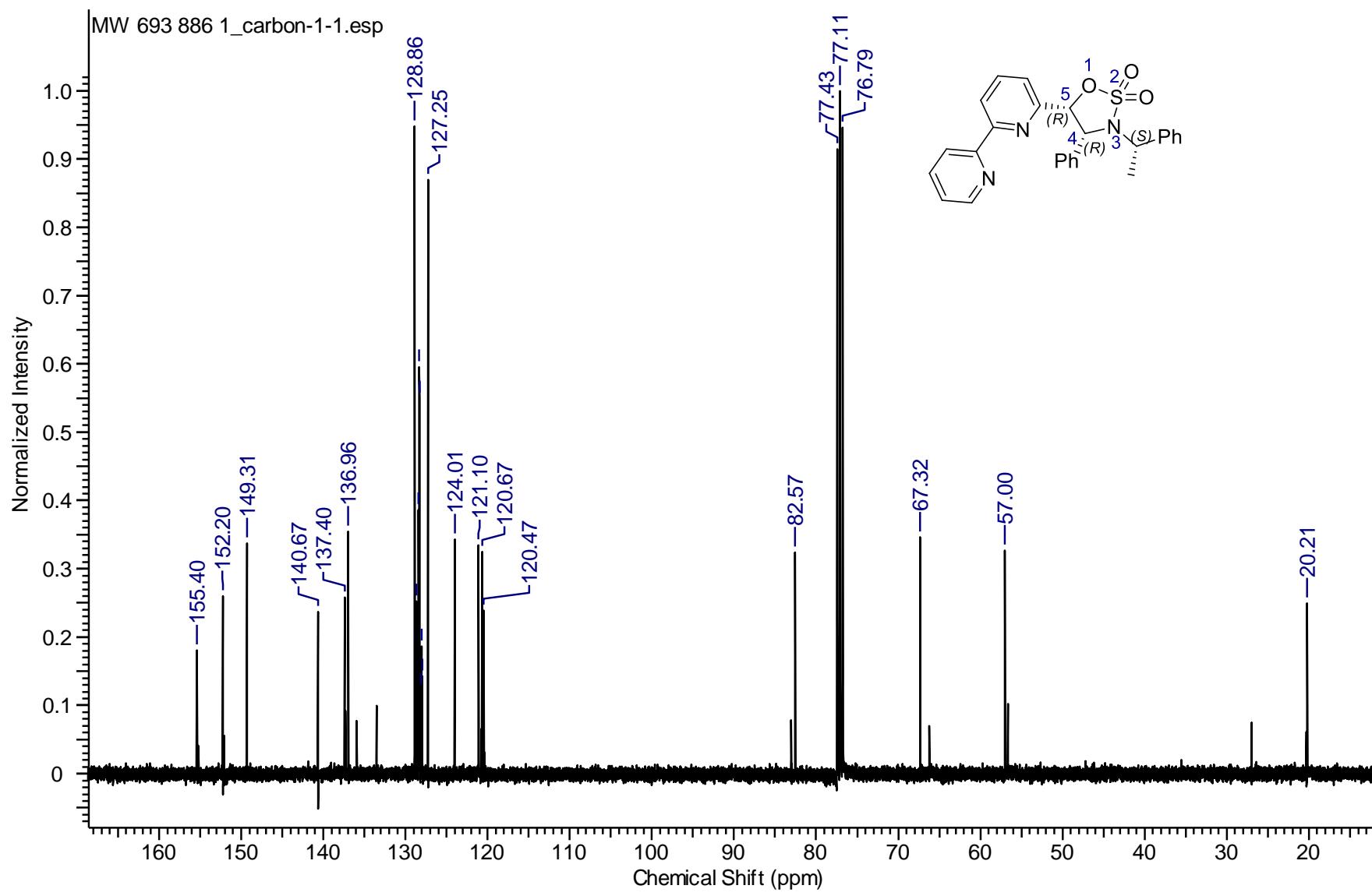


Figure S4. ^{13}C NMR spectrum (101 MHz, CDCl_3) for ($4\text{R},5\text{R},1'\text{S}$)-14

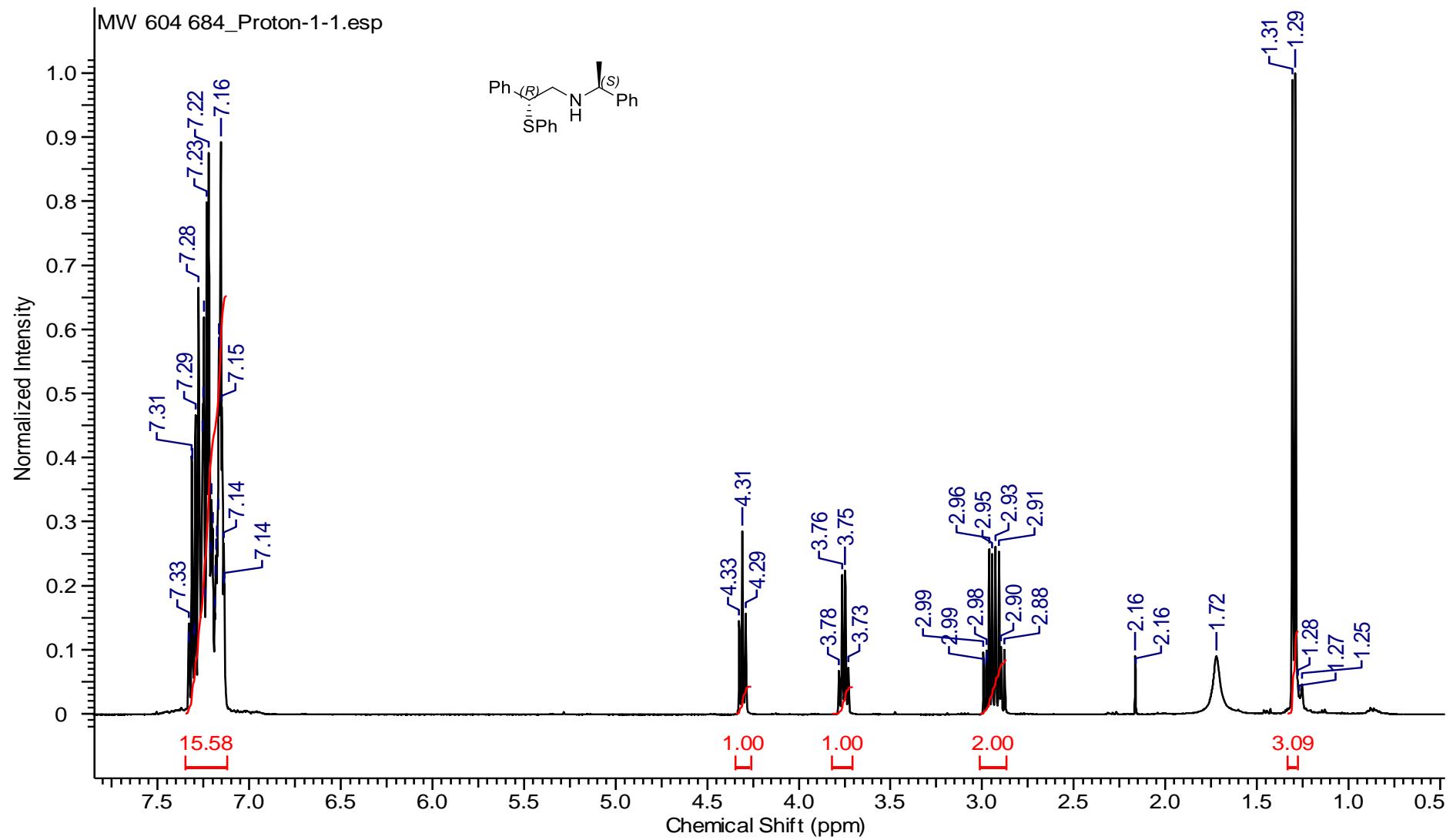


Figure S5. ^1H NMR spectrum (400 MHz, CDCl_3) for ($2R,1'S$)-15

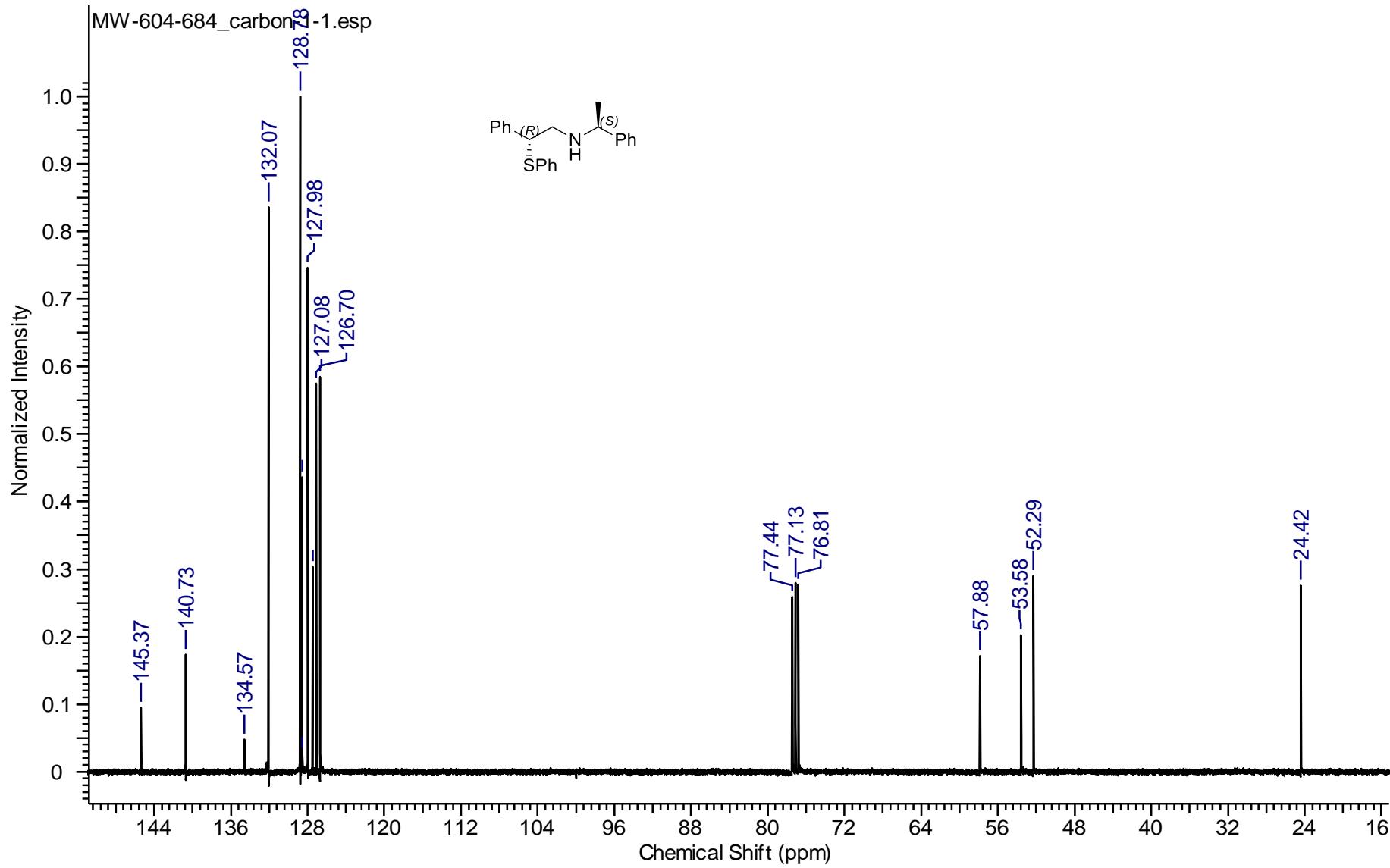


Figure S6. ^{13}C NMR spectrum (101 MHz, CDCl_3) for (2*R*,1'*S*)-15

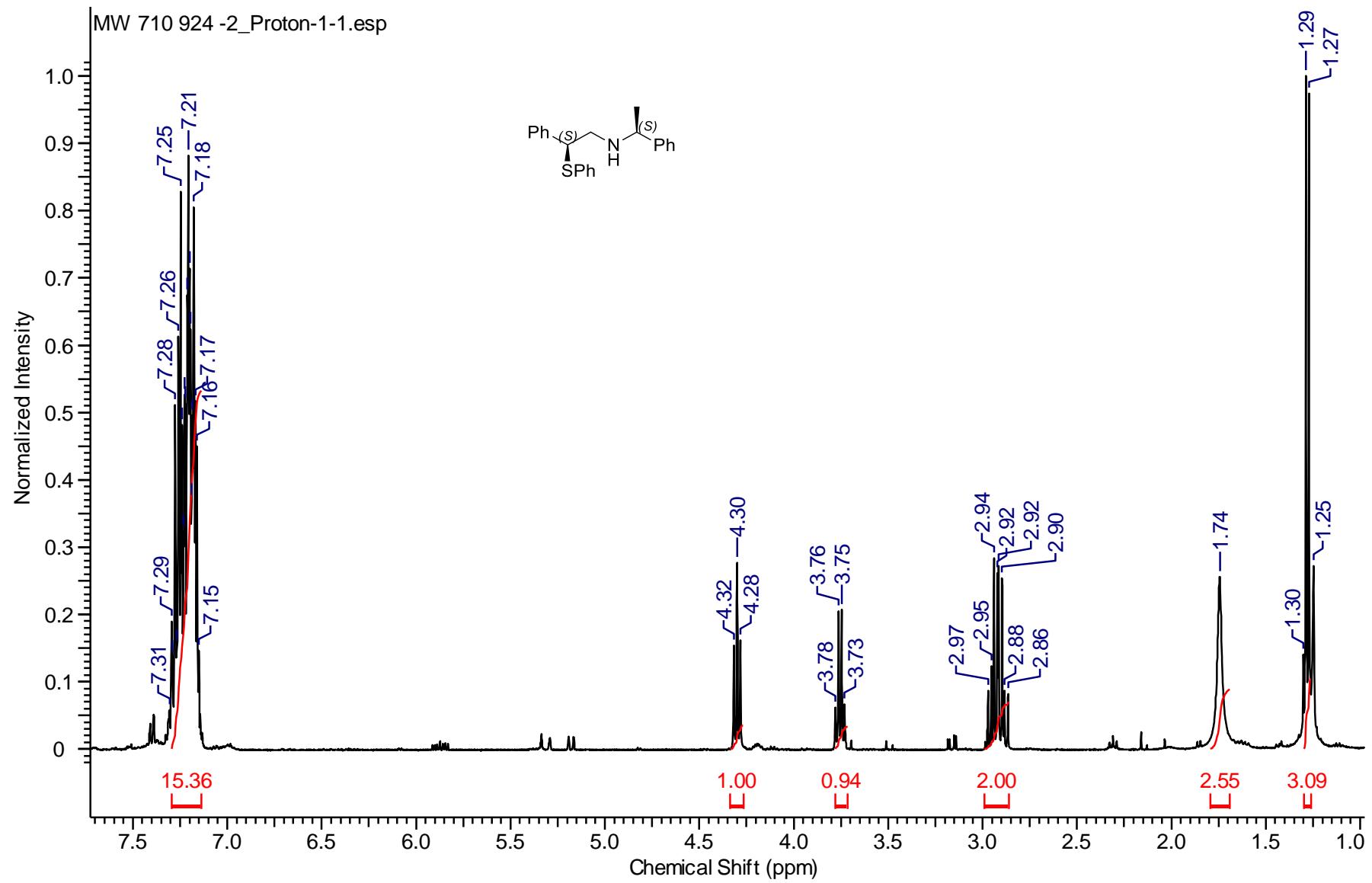


Figure S7. ^{13}C NMR spectrum (101 MHz, CDCl_3) for (2*S*,1'*S*)-15

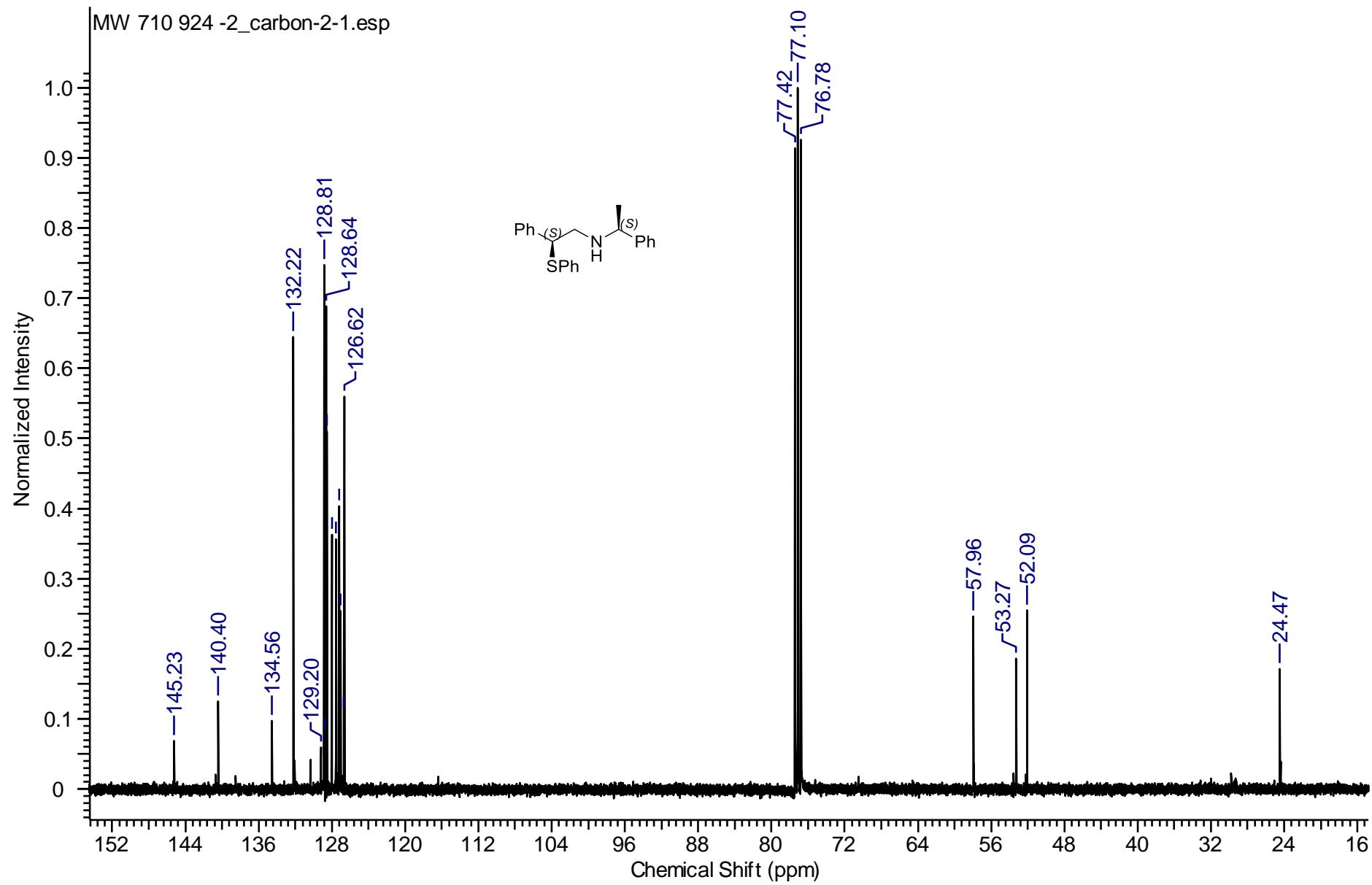


Figure S8. ^{13}C NMR spectrum (101 MHz, CDCl_3) for (2*S*,1'*S*)-15

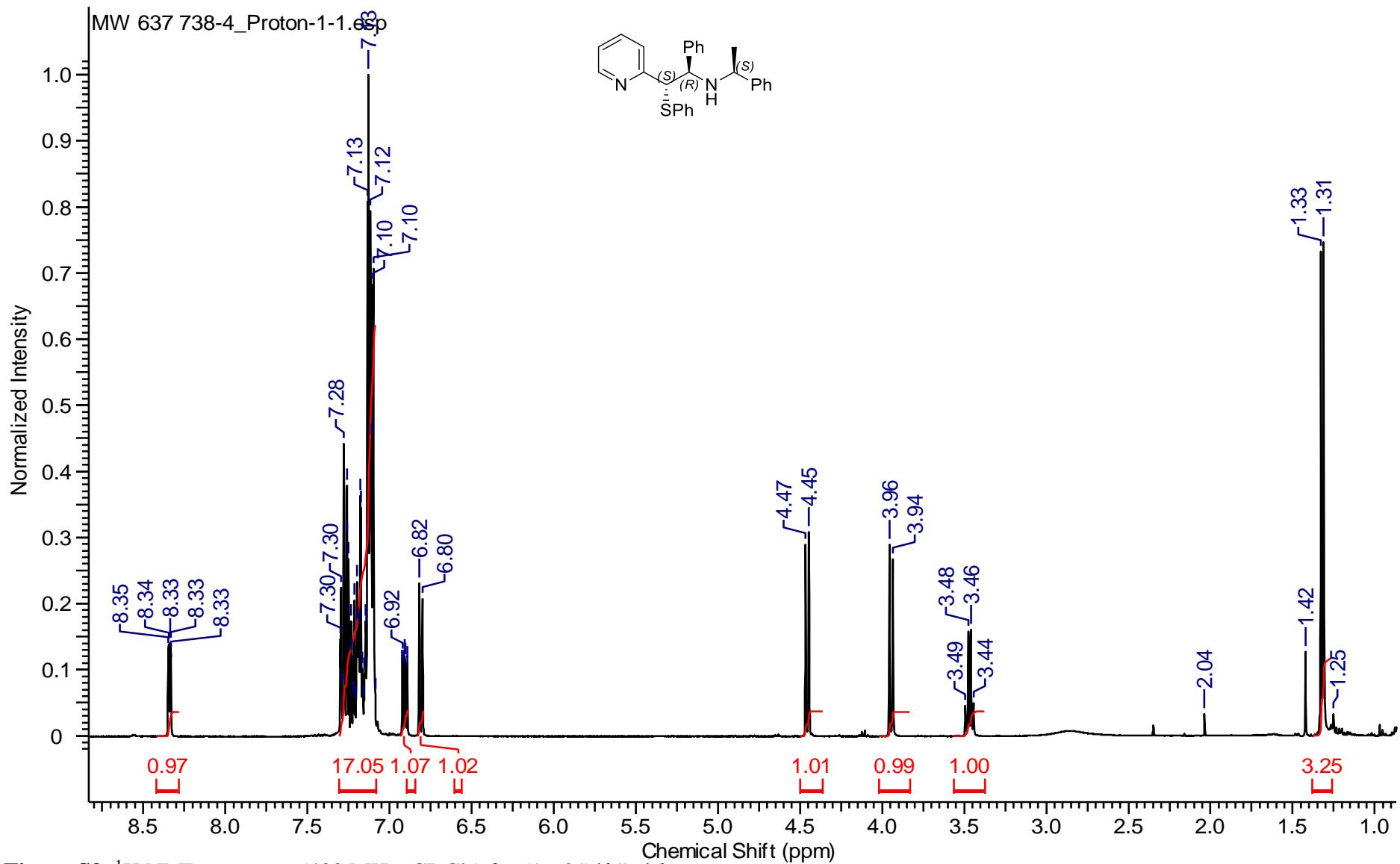


Figure S9. ^1H NMR spectrum (400 MHz, CDCl_3) for (*1R,2S,1'S*)-**16**

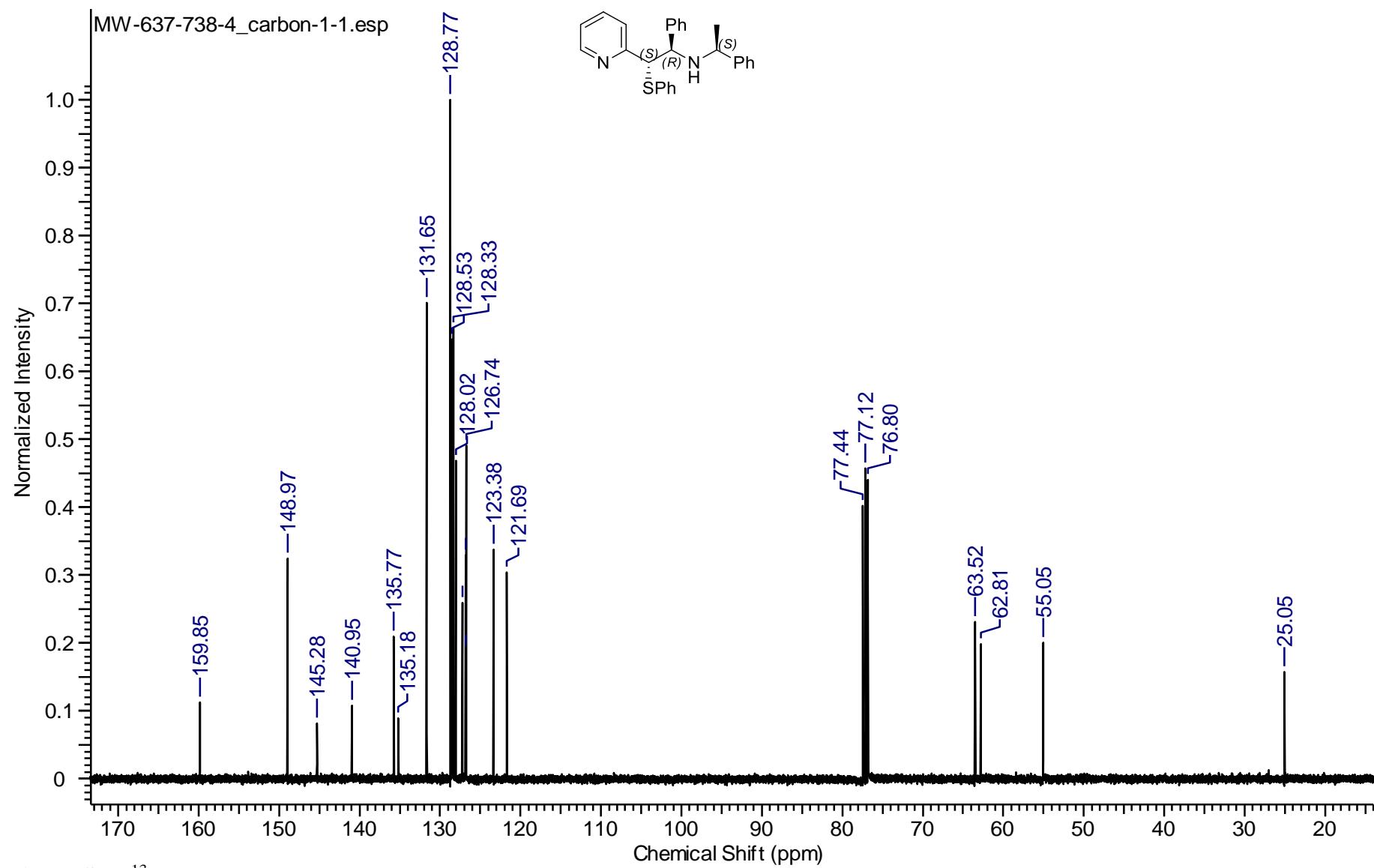


Figure S10. ¹³C NMR spectrum (101 MHz, CDCl₃) for (1*R*,2*S*,1'*S*)-**16**

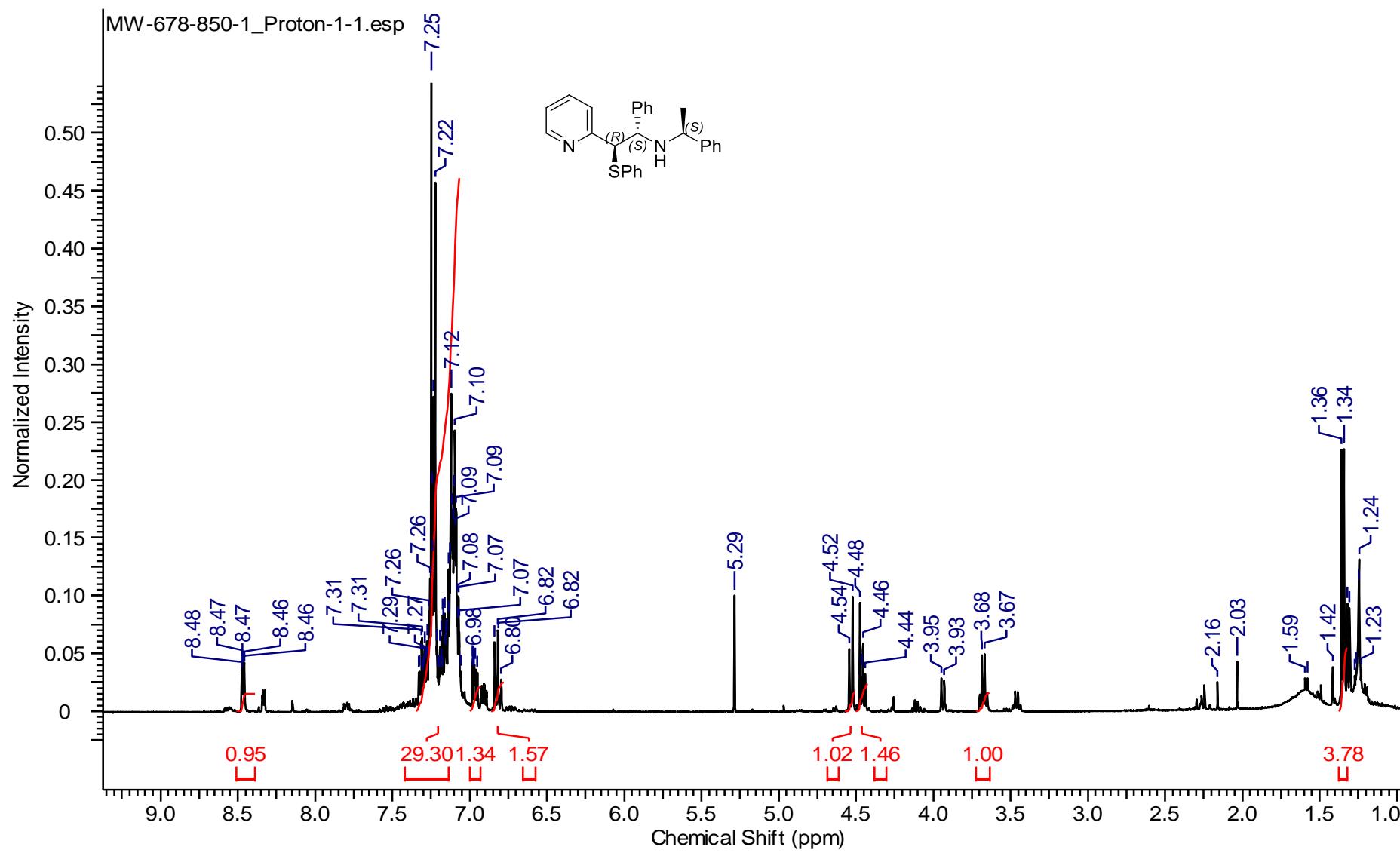


Figure S11. ^1H NMR spectrum (400 MHz, CDCl_3) for $(1\text{S},2\text{R},1'\text{S})\text{-16}$

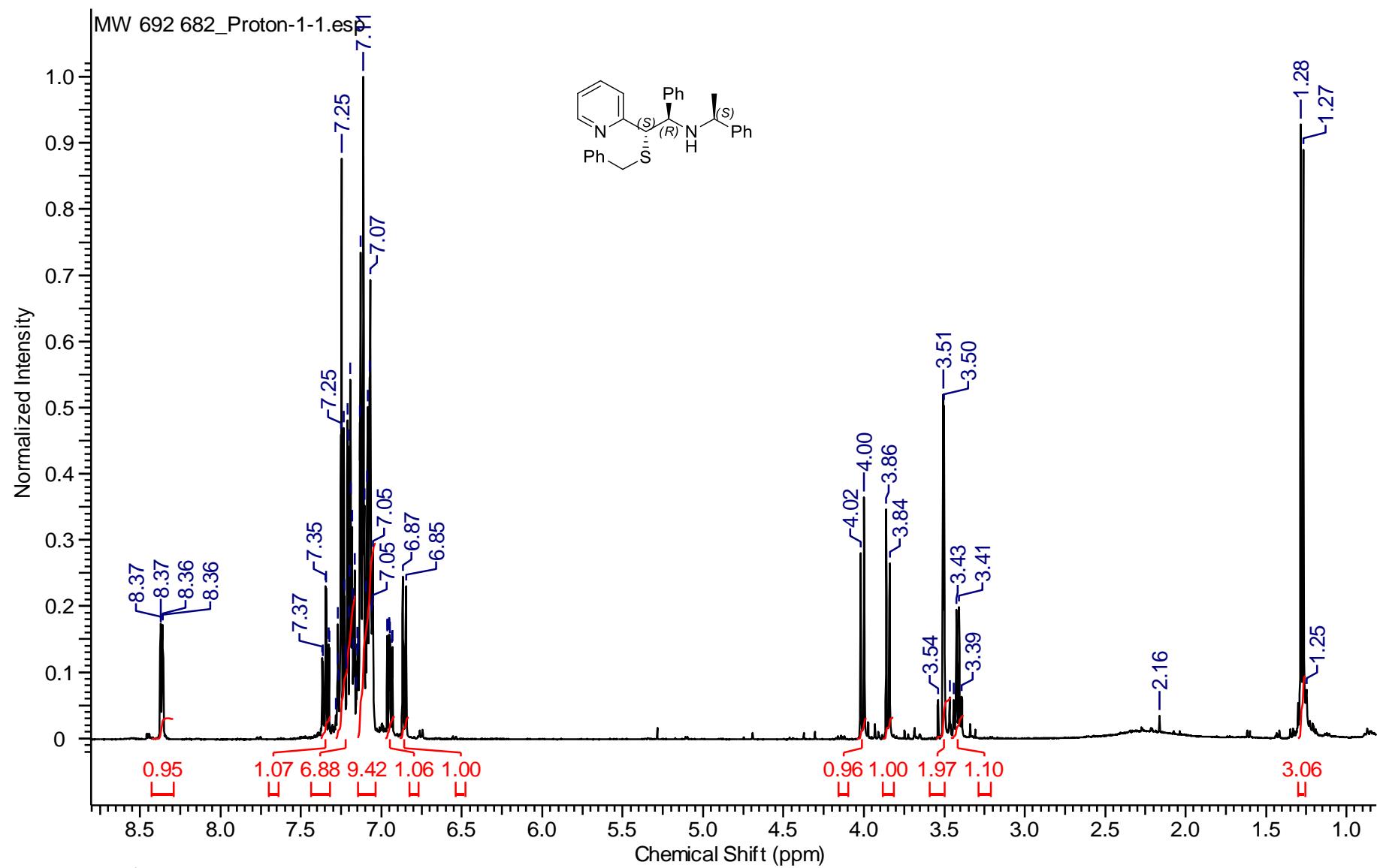


Figure S12. ^1H NMR spectrum (400 MHz, CDCl_3) for $(1\text{R},2\text{S},1'\text{S})\text{-17}$

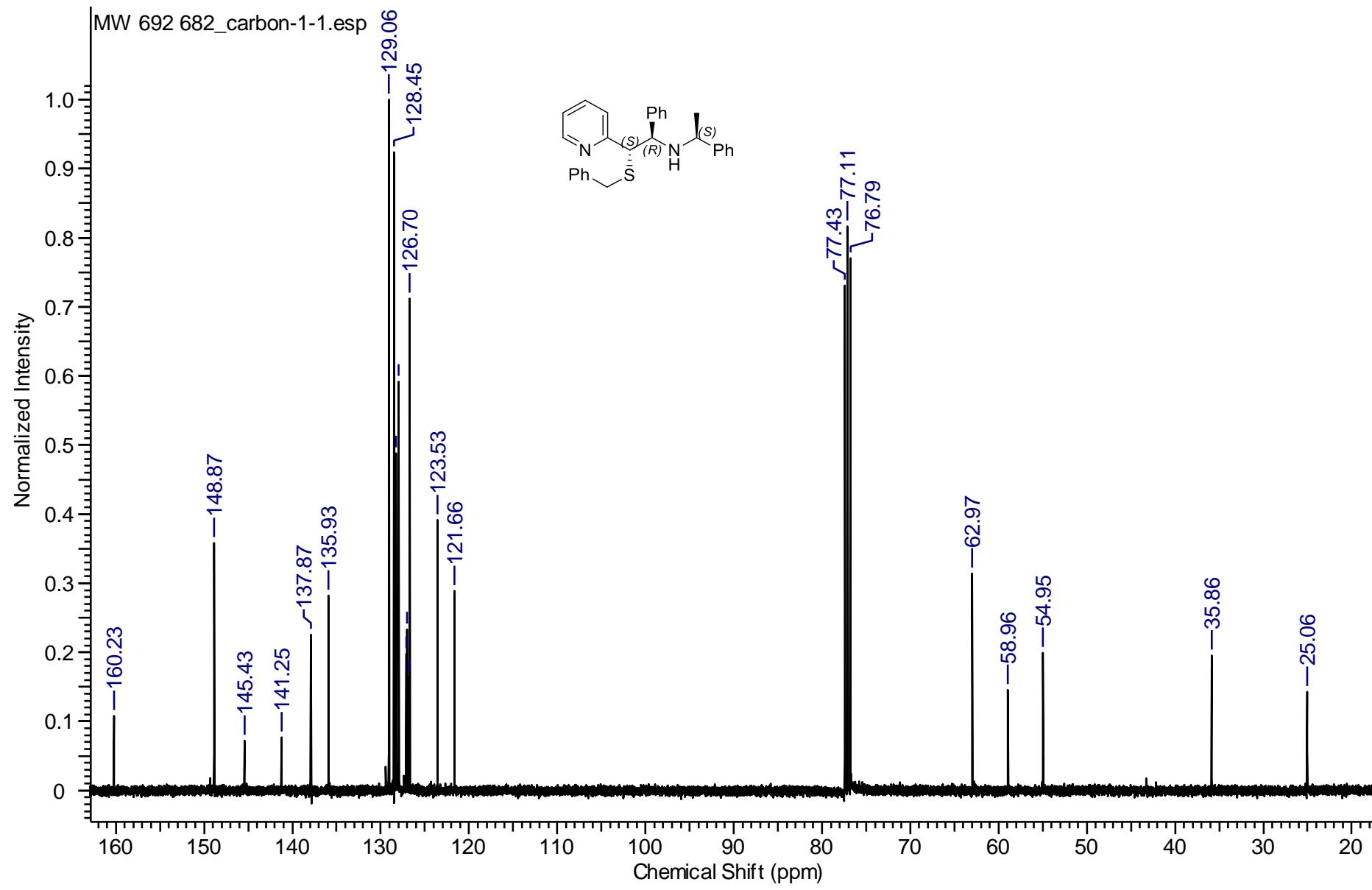


Figure S13. ¹³C NMR spectrum (101 MHz, CDCl₃) for (1*R*,2*S*,1'*S*)-17

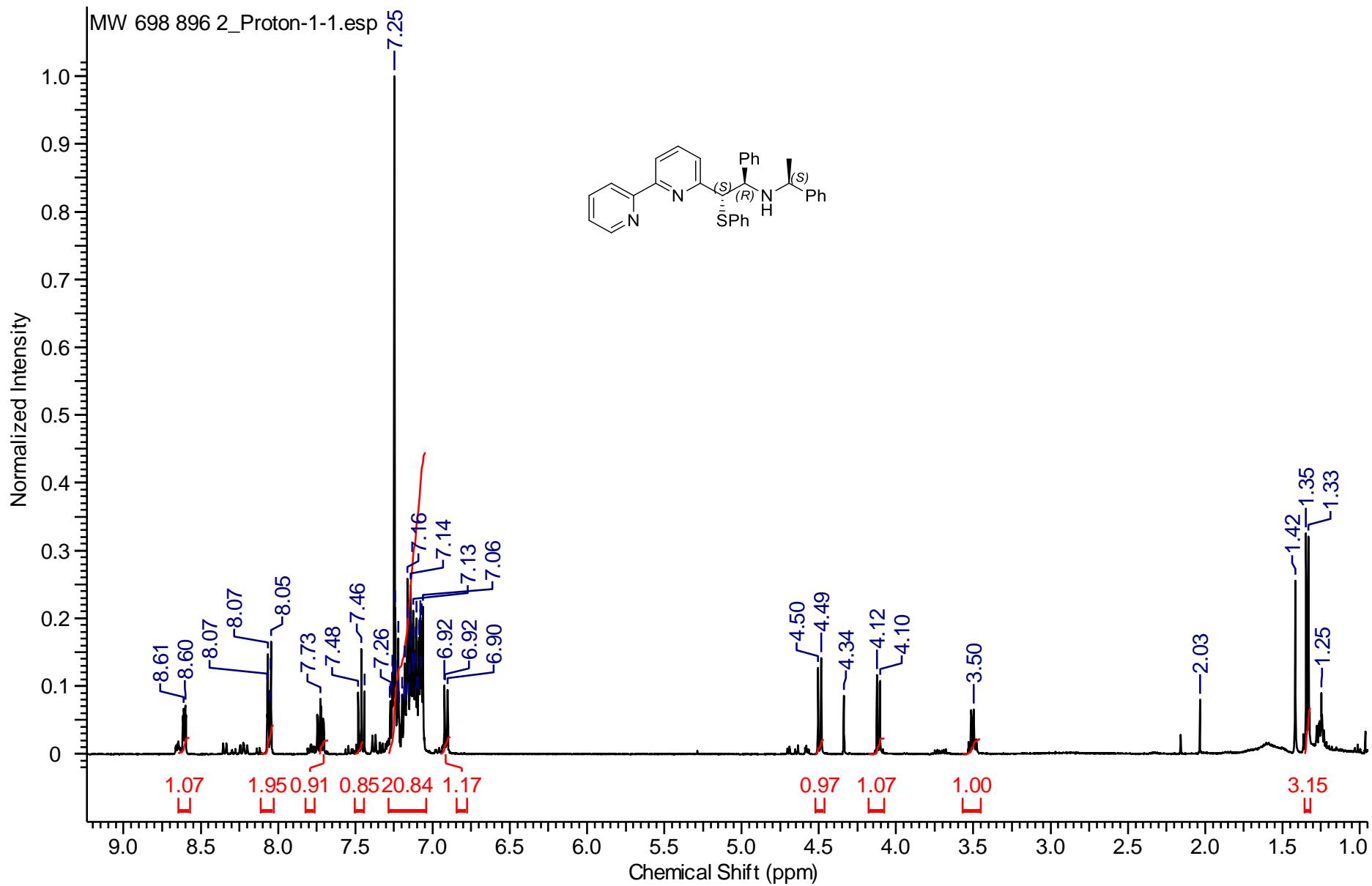


Figure S14. ^1H NMR spectrum (400 MHz, CDCl_3) for (*1R,2S,1'S*)-18

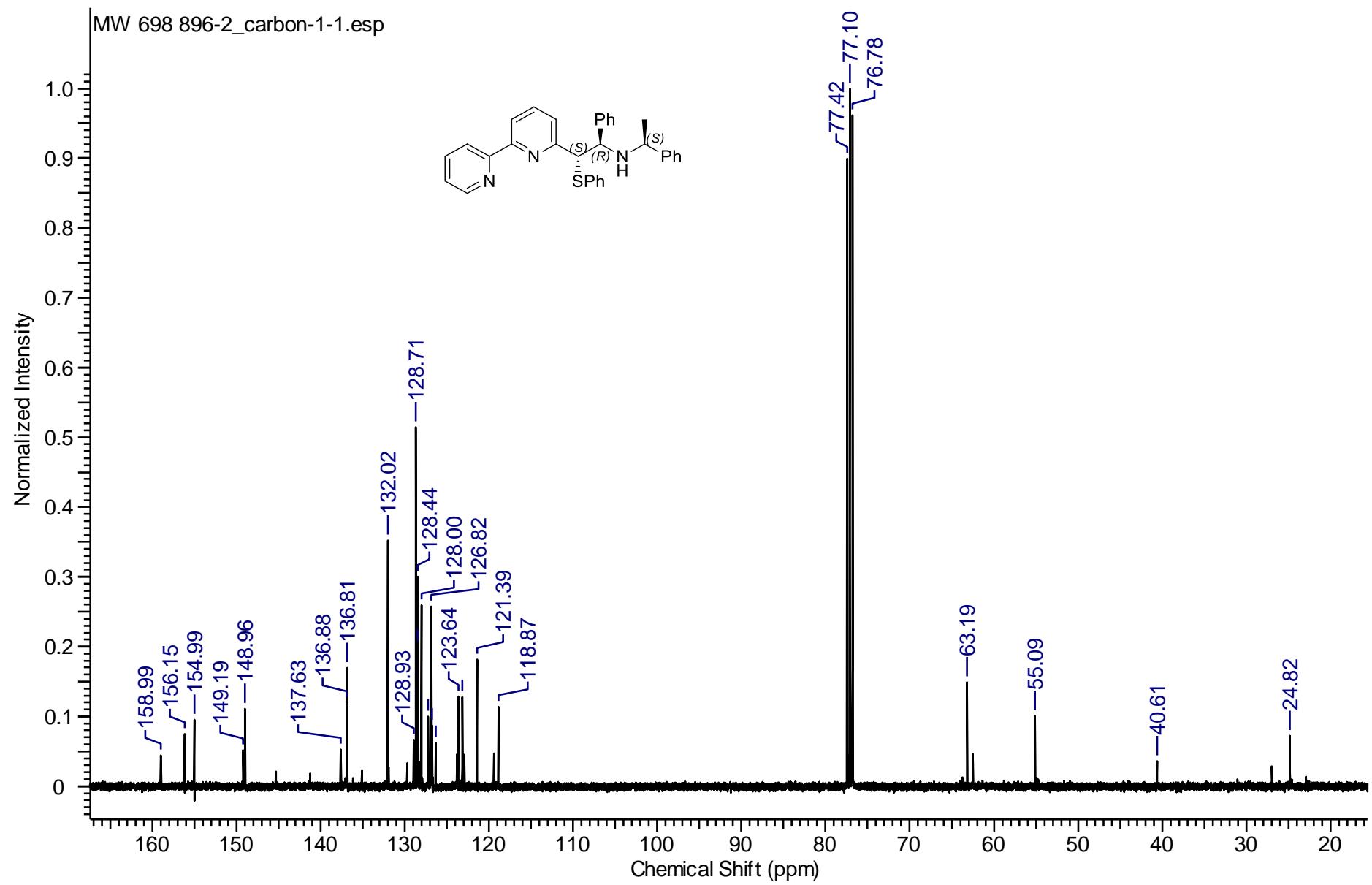


Figure S15. ^{13}C NMR spectrum (101 MHz, CDCl_3) for (1*R*,2*S*,1'*S*)-**18**

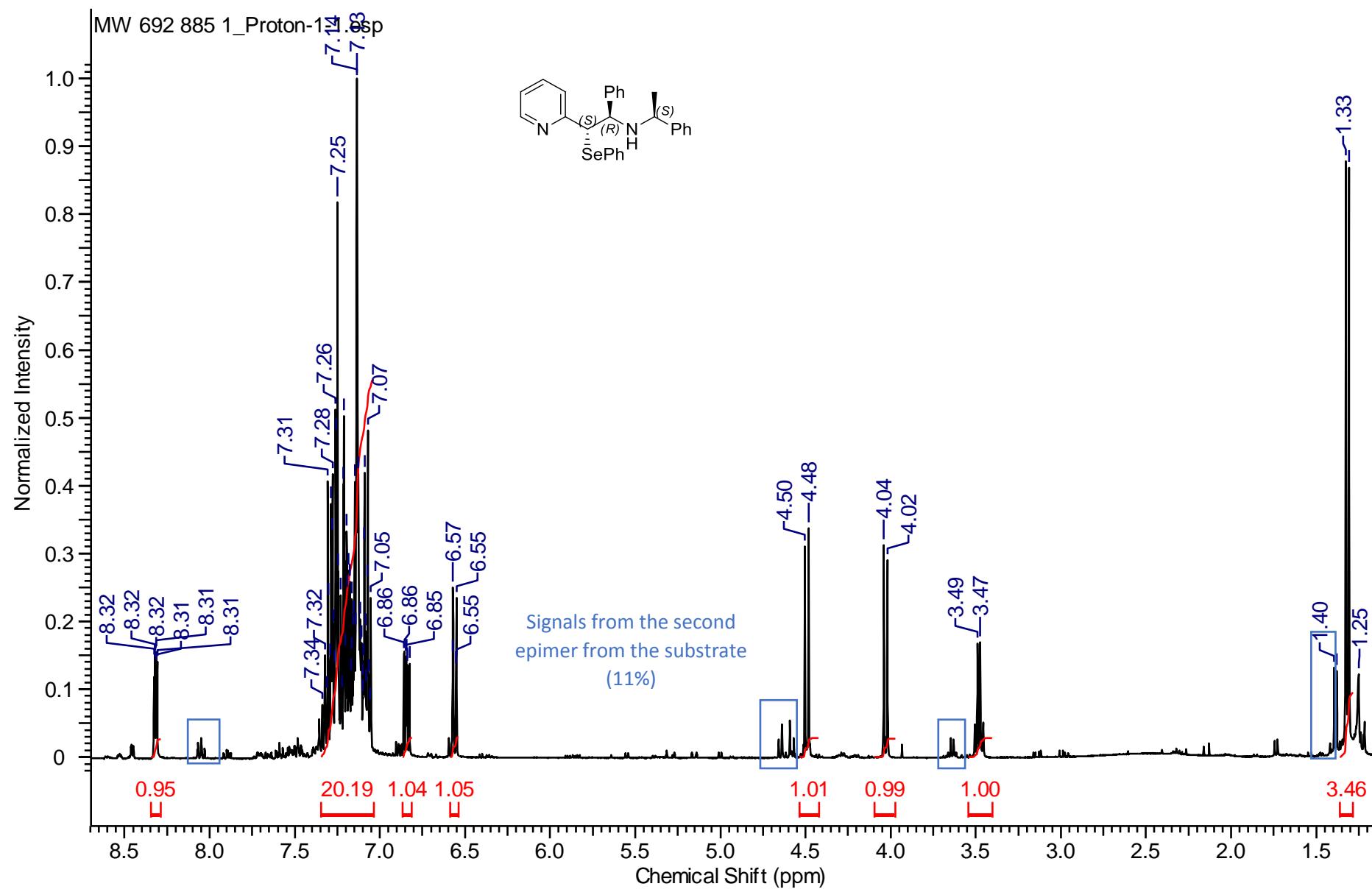


Figure S16. ^1H NMR spectrum (400 MHz, CDCl_3) for ($1R,2S,1'S$)-**19**

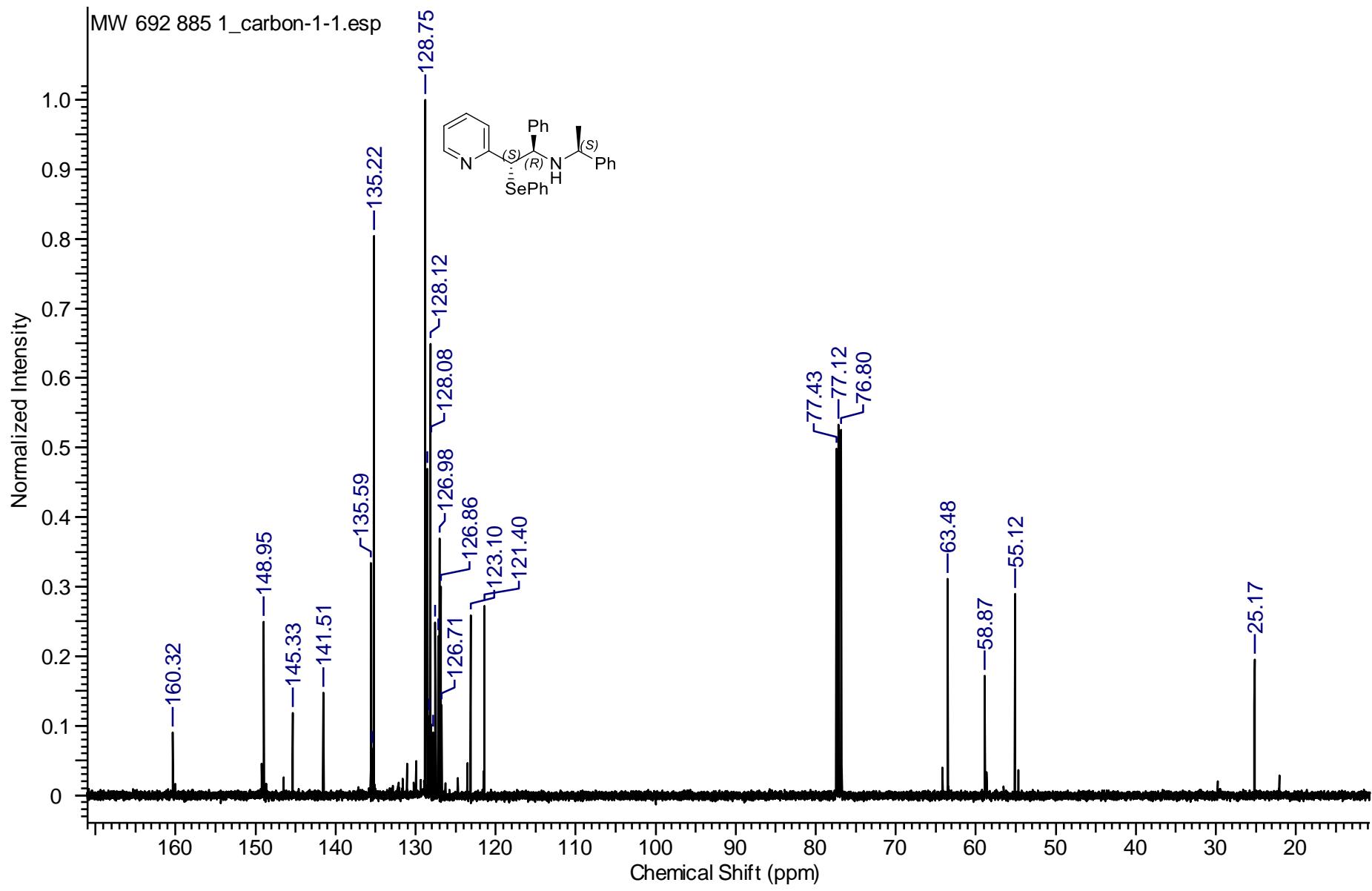


Figure S17. ^{13}C NMR spectrum (101 MHz, CDCl_3) for (1*R*,2*S*,1'*S*)-19

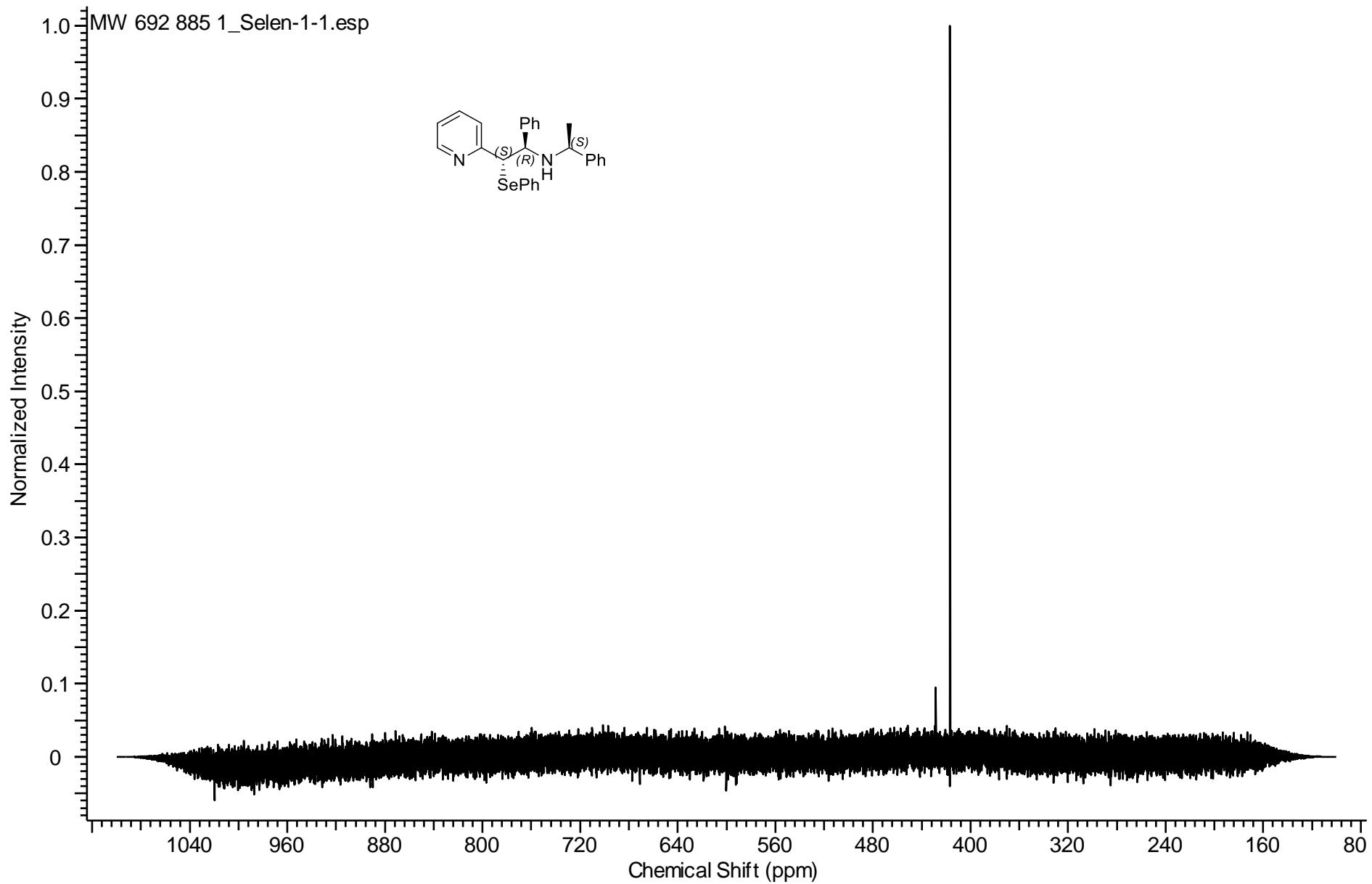


Figure S18. ^{77}Se NMR (38 MHz, CDCl_3): for $(1R,2S,1'S)\text{-19}$

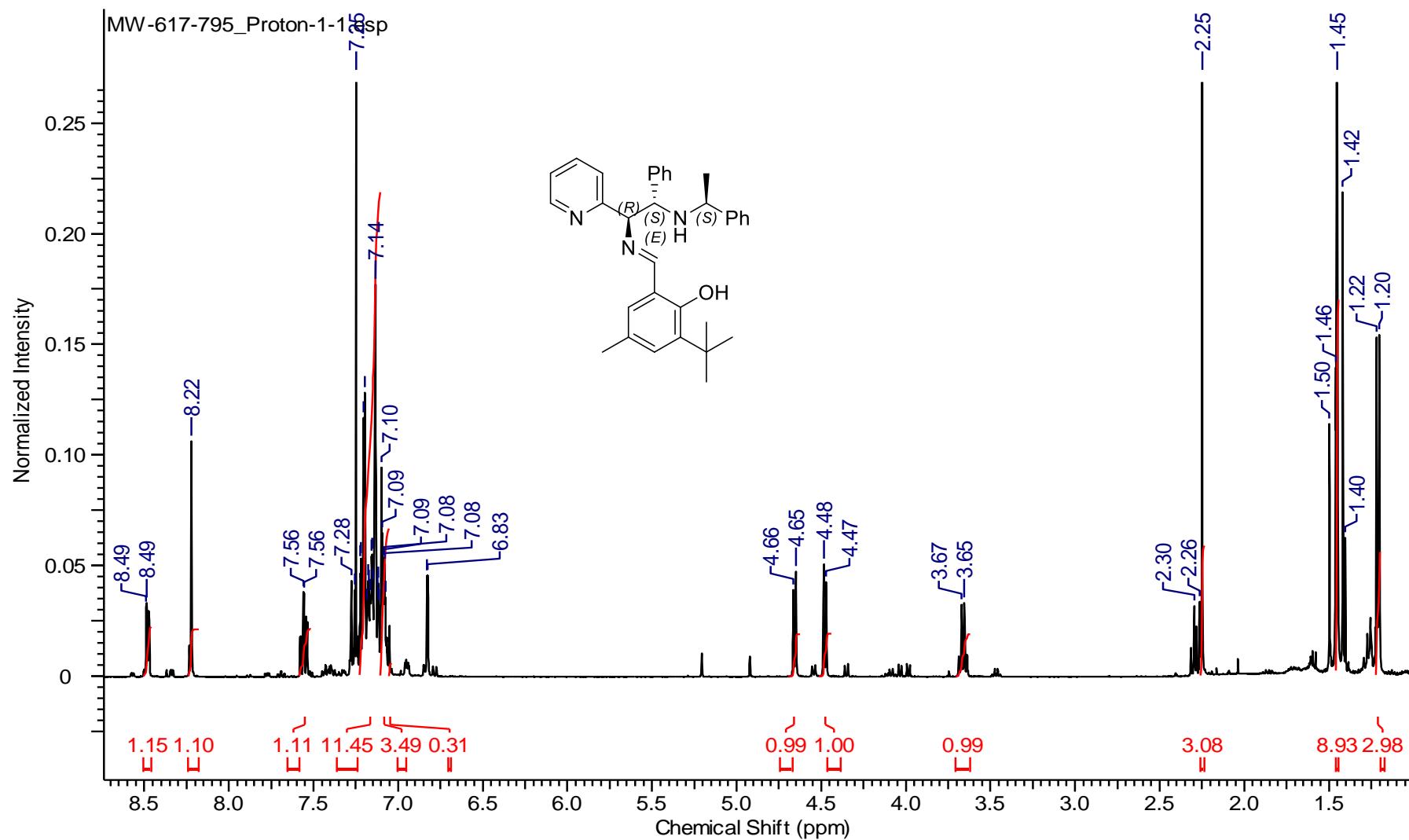


Figure S19. ^1H NMR spectrum (400 MHz, CDCl_3) for $(1\text{S},2\text{R},1'\text{S})\text{-22}$

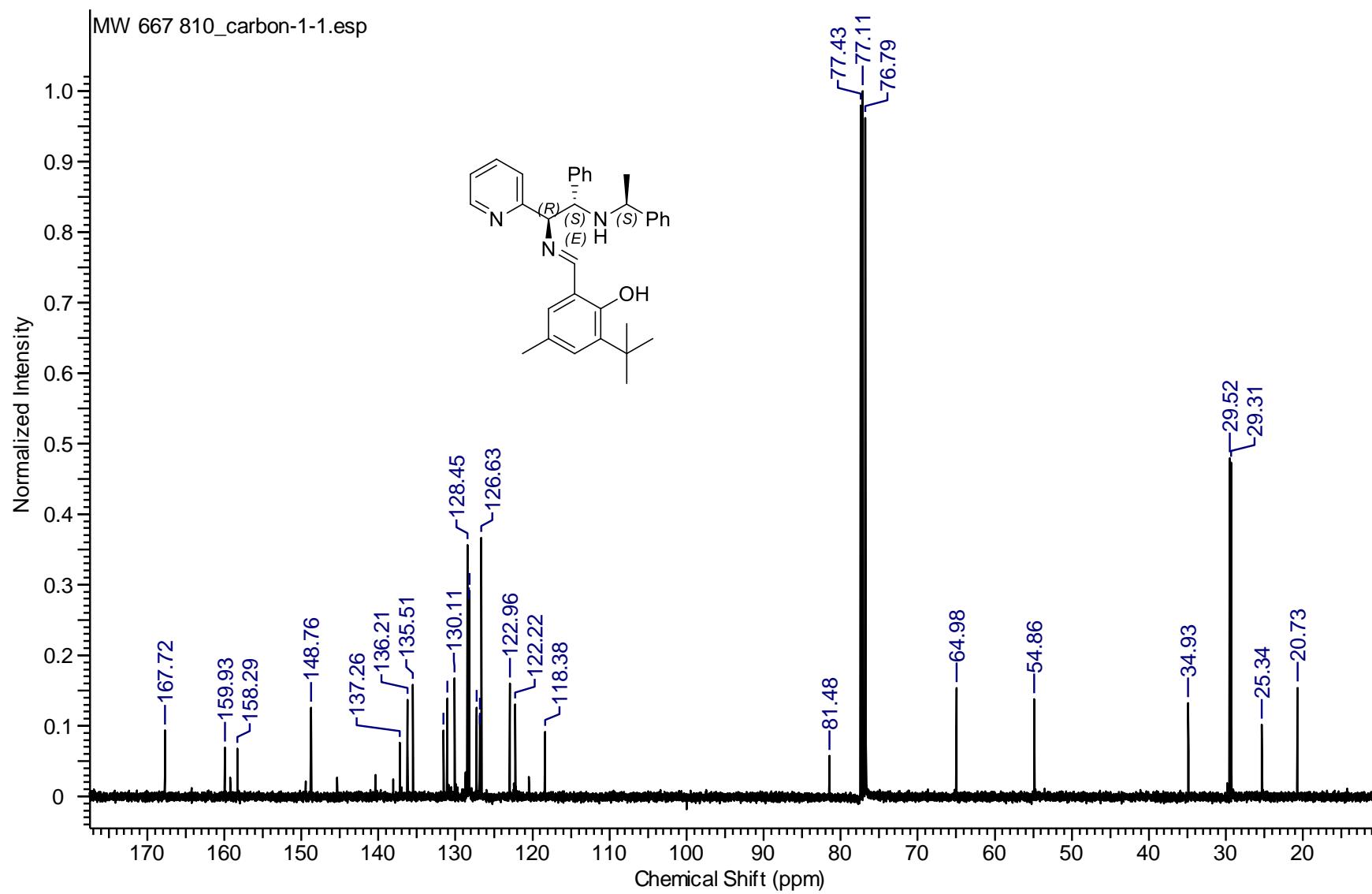


Figure S20. ^{13}C NMR spectrum (101 MHz, CDCl_3) for $(1\text{S},2\text{R},1'\text{S})\text{-22}$

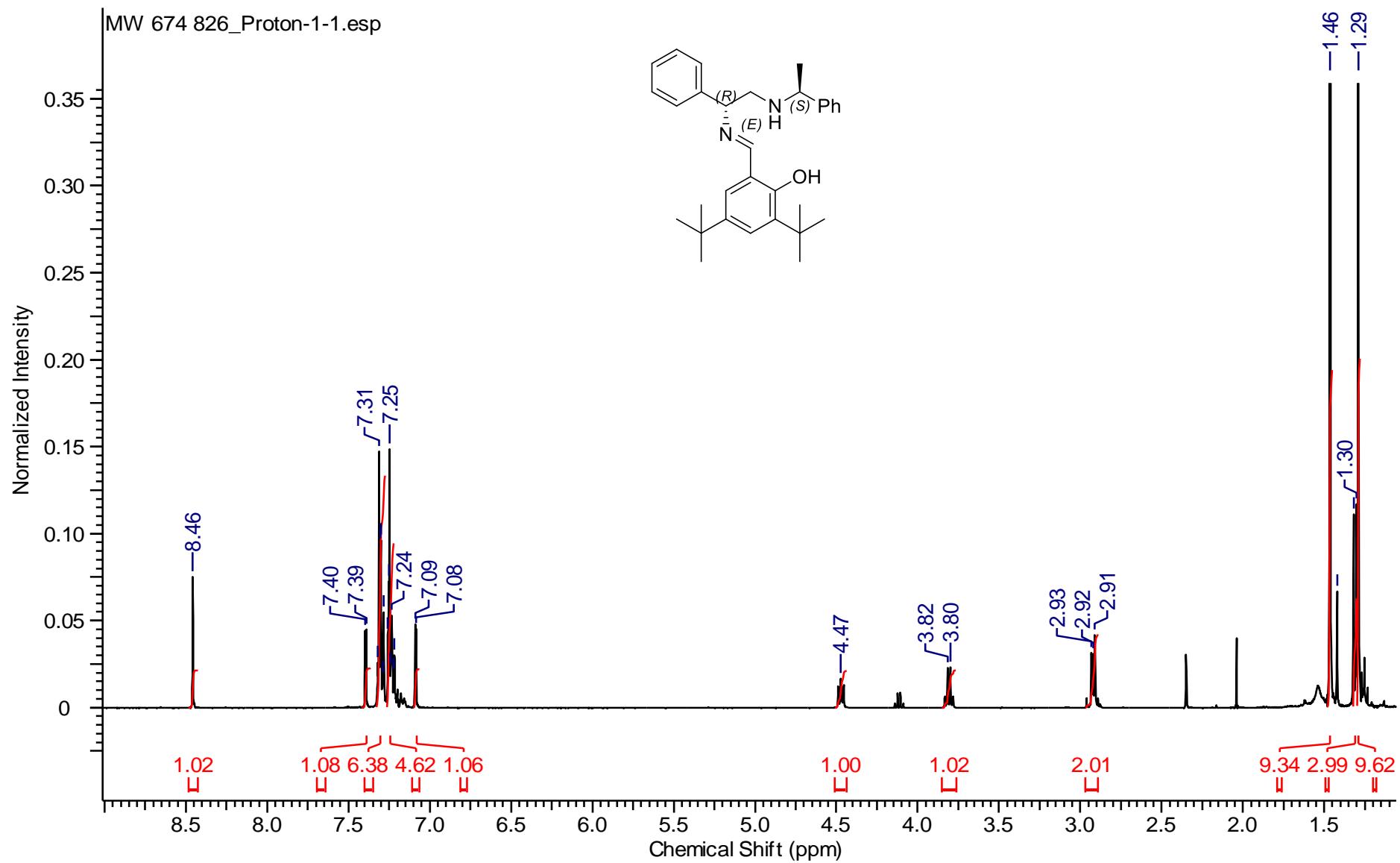


Figure S21. ^1H NMR spectrum (400 MHz, CDCl_3) for ($2R,1'S$)-23

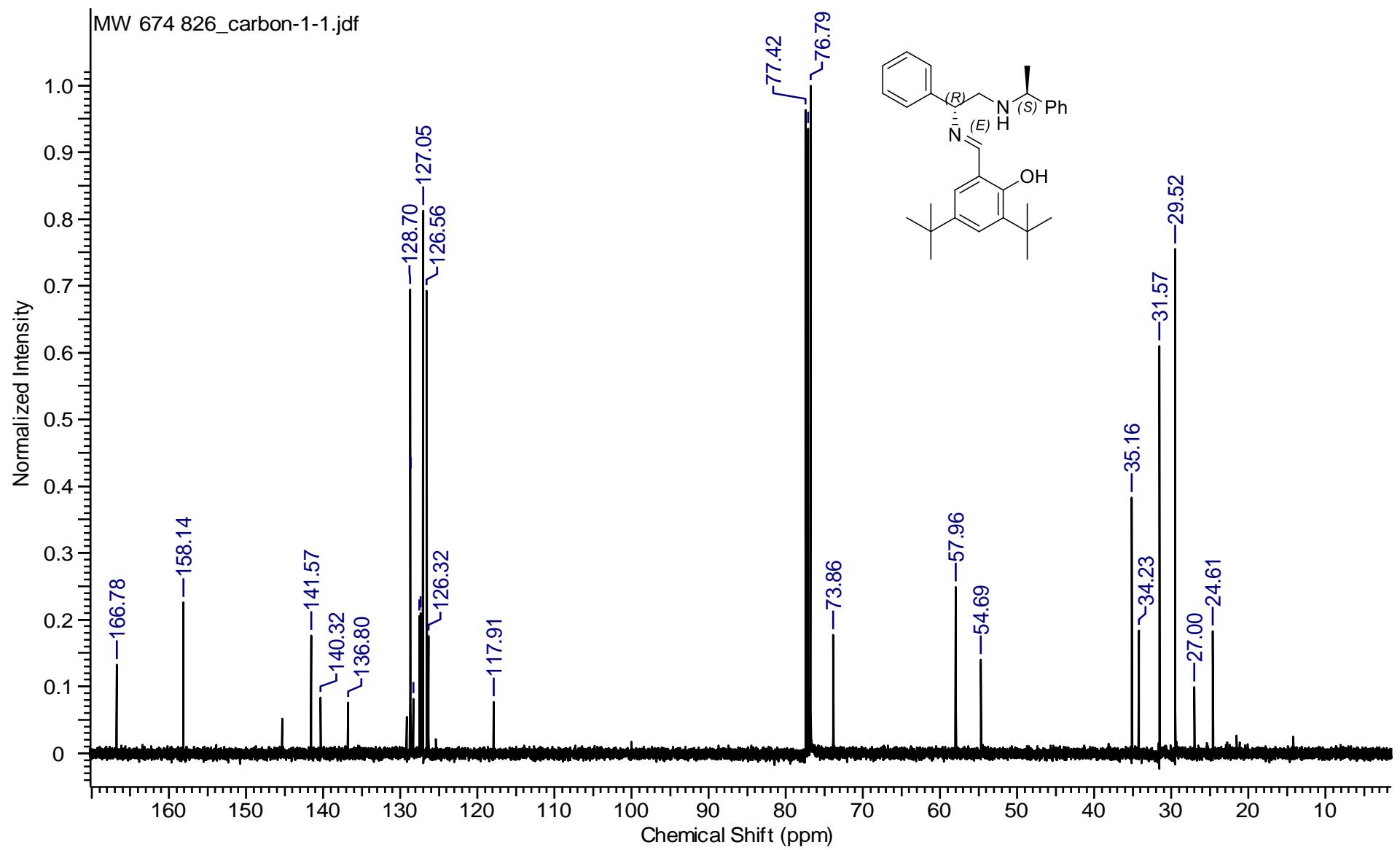


Figure S22. ^{13}C NMR spectrum (101 MHz, CDCl_3) for $(2\text{R},1'\text{S})\text{-23}$

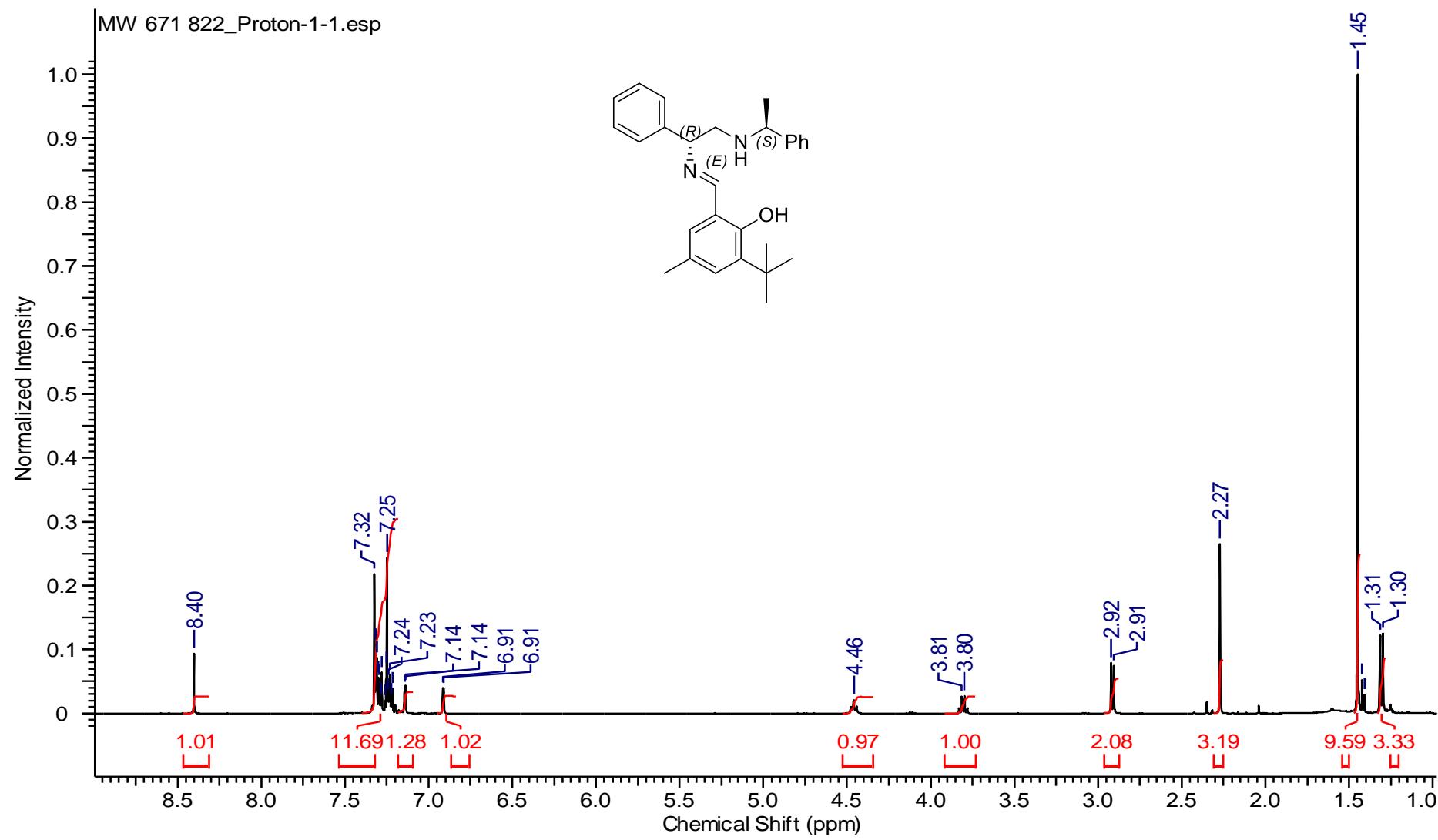


Figure S23. ^1H NMR spectrum (400 MHz, CDCl_3) for (2*R*,1'*S*)-24

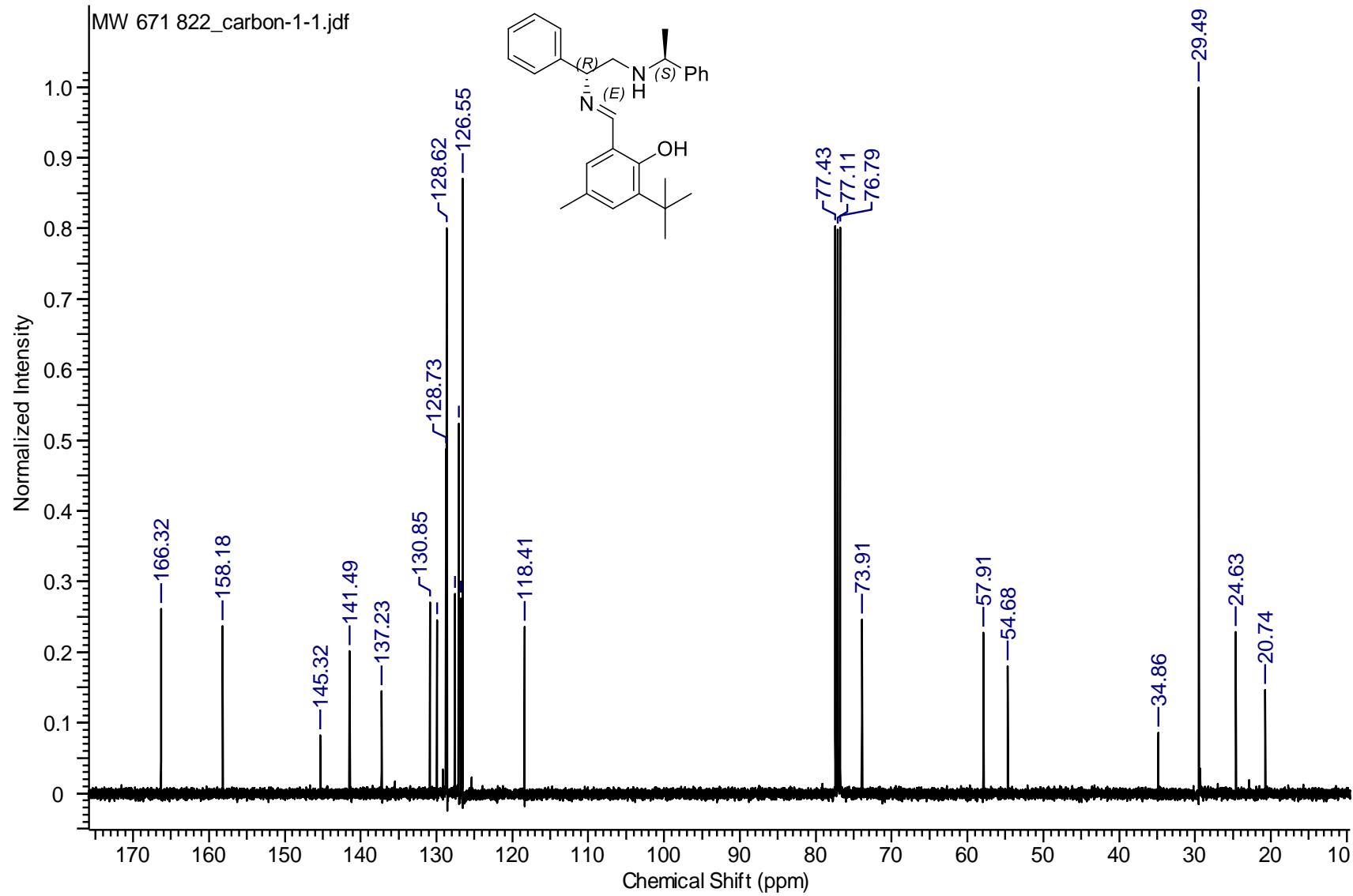


Figure S24. ^{13}C NMR spectrum (101 MHz, CDCl_3) for ($2R,1'S$)-24

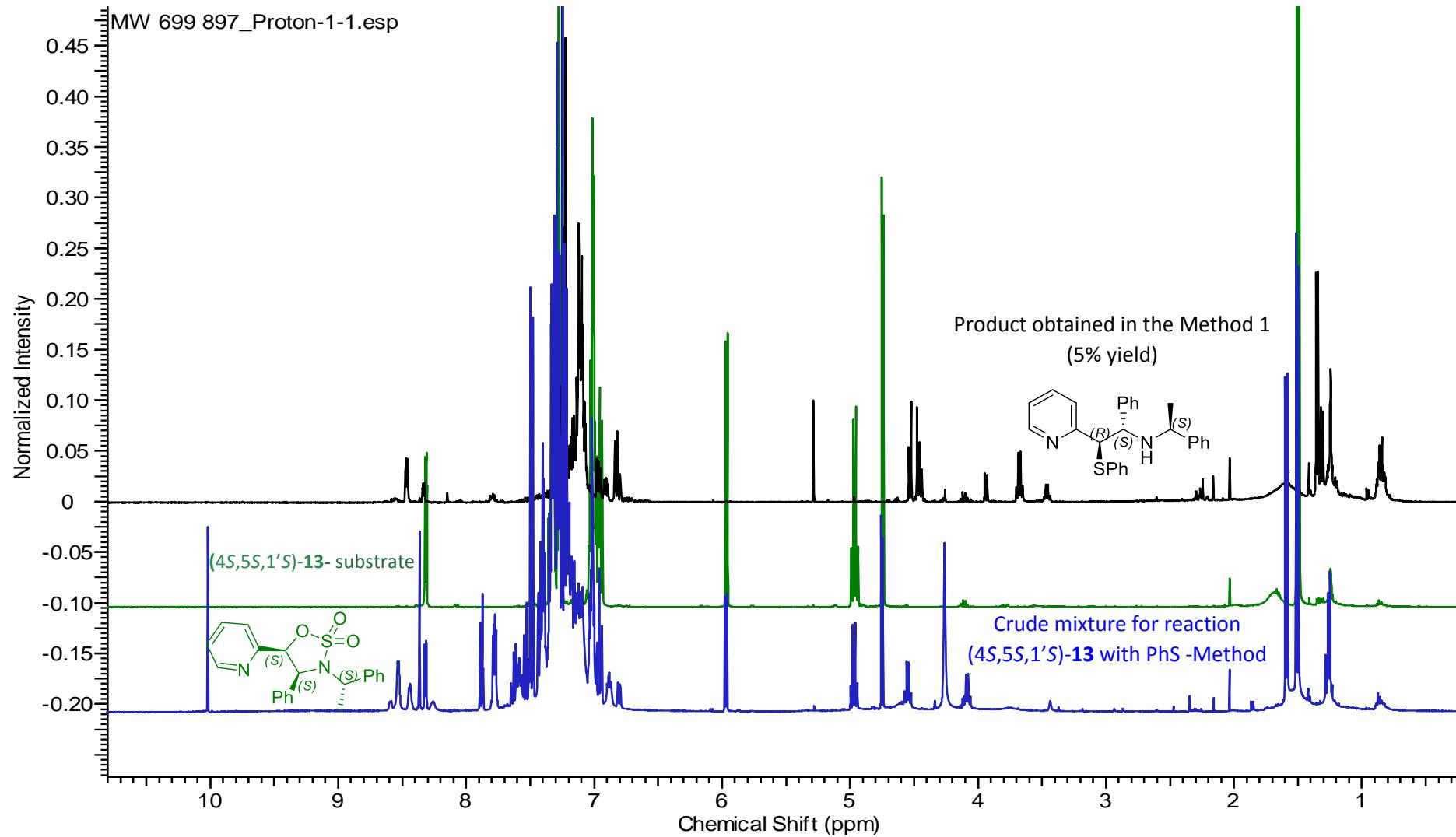


Figure S25. ^1H NMR spectra (400 MHz, CDCl_3) for crude mixture for reaction (4S,5S,1'S)-13 with PhS -Method 2 (blue), substrate (green) and product (1S,2R,1'S)-16 from Method 1 (black)

1. HPLC data

Alkylation of of *rac*-1,3-diphenyl-2-propenyl acetate (Enantiomeric excess was determined using a Chiralpak AD-H column (n-hexane/isopropanol 90/10, 1.0 mL/min, 254 nm)

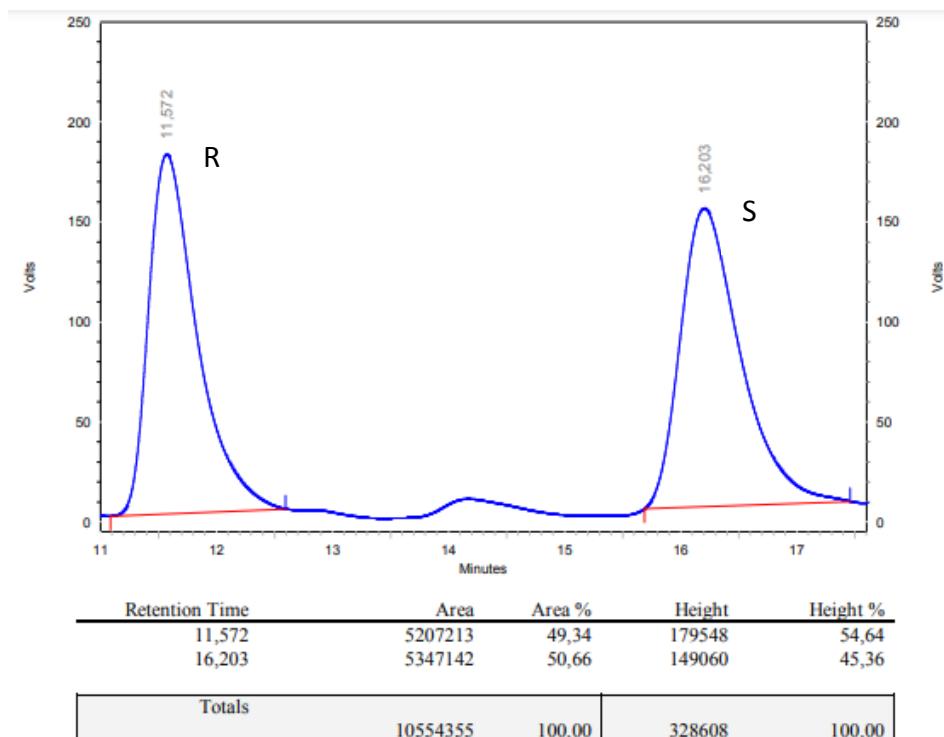


Figure S26. HPLC chromatogram for *rac*-dimethyl [(2E)-1,3-diphenylprop-2-en-1-yl]propanedioate

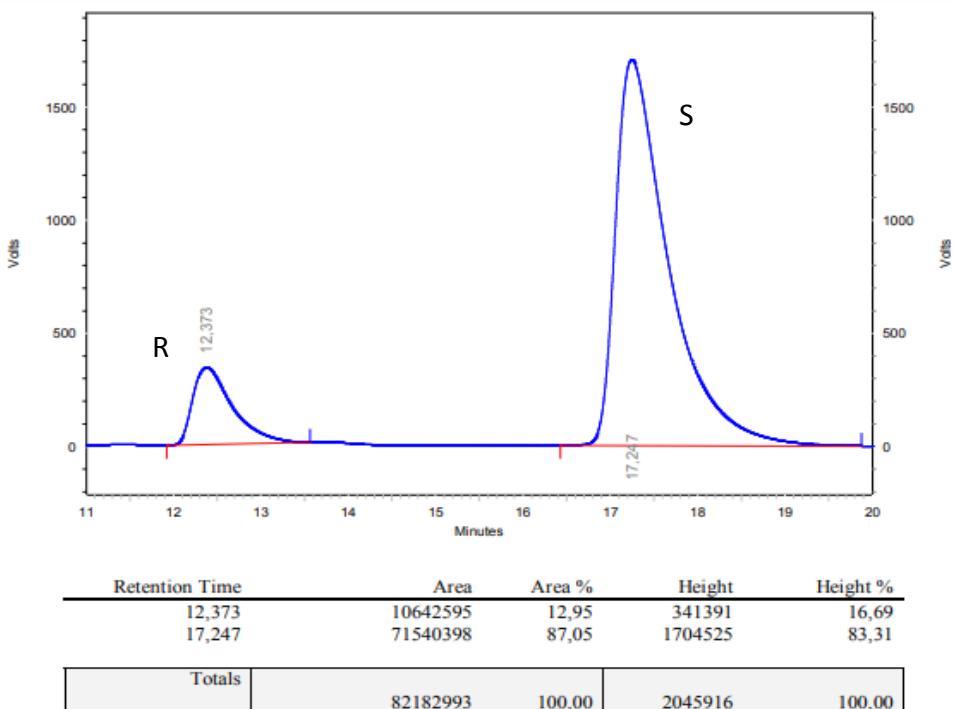


Figure S27. HPLC chromatogram for dimethyl [(2E)-1,3-diphenylprop-2-en-1-yl]propanedioate obtained with catalyst (1*R*,2*S*,1'*S*)-**16**

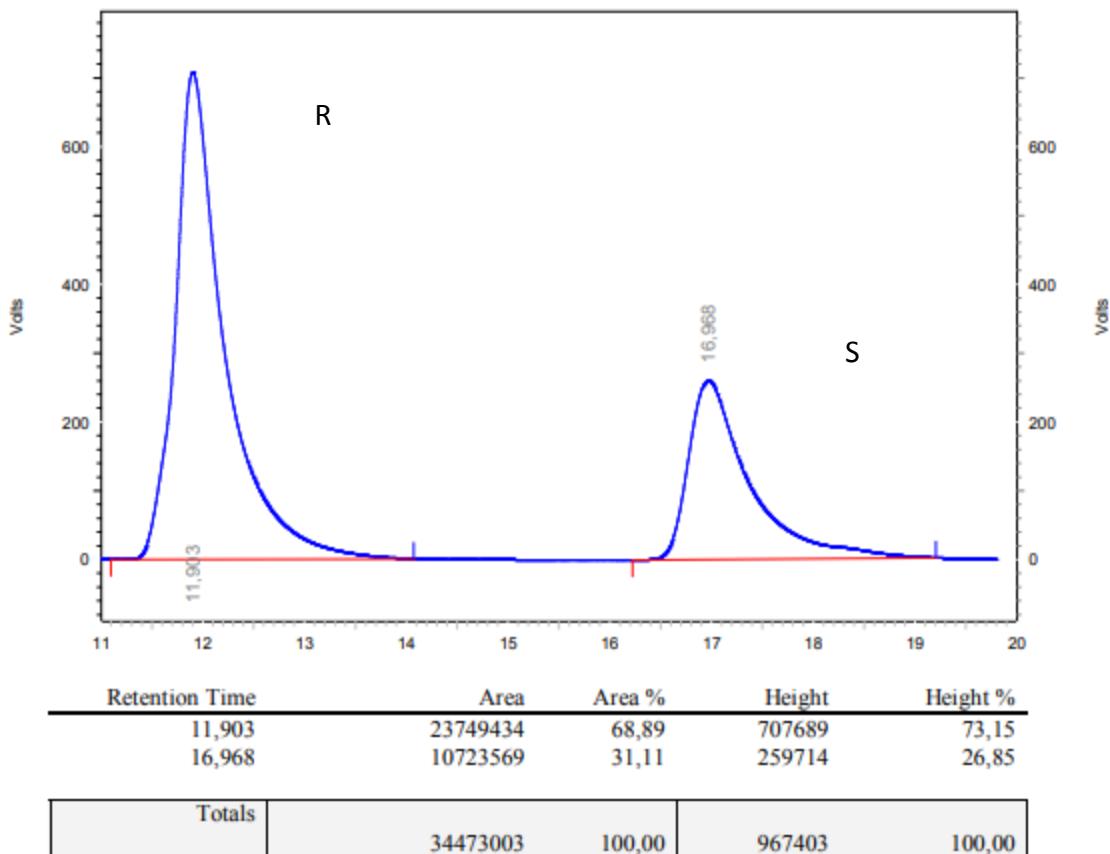


Figure S28. HPLC chromatogram for dimethyl [(*2E*)-1,3-diphenylprop-2-en-1-yl]propanedioate obtained with catalyst (*2R,1'S*)-**24**

2. DFT calculation

Table S1. Comparison of experimental and DFT calculated ^1H NMR chemical shifts (GIAO DFT/mPW1PW91/6-311+G(2d,p)) for (*1R, 2S,1'S*)-**16** and (*1S, 2R,1'S*)-**16**

Sygnal	(1 <i>R</i> , 2 <i>S</i> ,1' <i>S</i>)- 16		(1 <i>S</i> , 2 <i>R</i> ,1' <i>S</i>)- 16	
	DFT δ , ppm	Experiment δ , ppm	DFT δ , ppm	Experiment δ , ppm
H-2	4.37	4.46	5,15	4,54
H-3	4.49	3.95	4,43	4,48
1-CH	3.63	3.46	4,49	3,68
CH ₃	1.44	1.33	1,54	1,36