

Supporting information

Regioselective and stereodivergent synthesis of enantiomerically pure vic-diamines from chiral β -amino alcohols with 2-pyridyl and 6-(2,2'-bipyridyl) moieties

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1. Structure of ring opening products

The structures of the azides (1*R*,1'*S*)-**3a**, (1*R*,2*R*,1'*S*)-**13**, (1*S*,2*S*,1'*S*)-**14**, (1*S*,2*R*,1'*S*)-**19** and (1*R*,2*S*,1'*S*)-**19** and thus the regiochemistry of the reactions was determined by a set of NMR experiments, where the ^1H , ^{13}C HMBC proved to be most revealing.

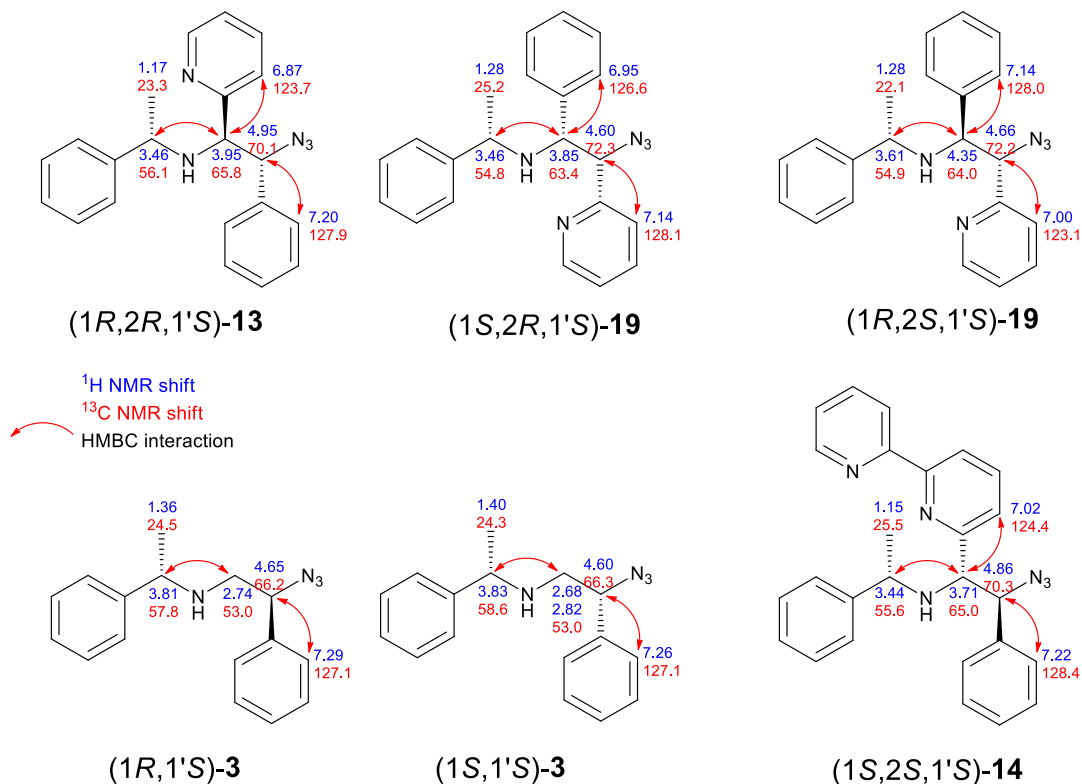


Figure S1. Assignment of selected ^1H and ^{13}C NMR signals and ^1H , ^{13}C HMBC correlations for the establishment of regiochemistry.

2. DFT computations for aziridines **10** and **12**

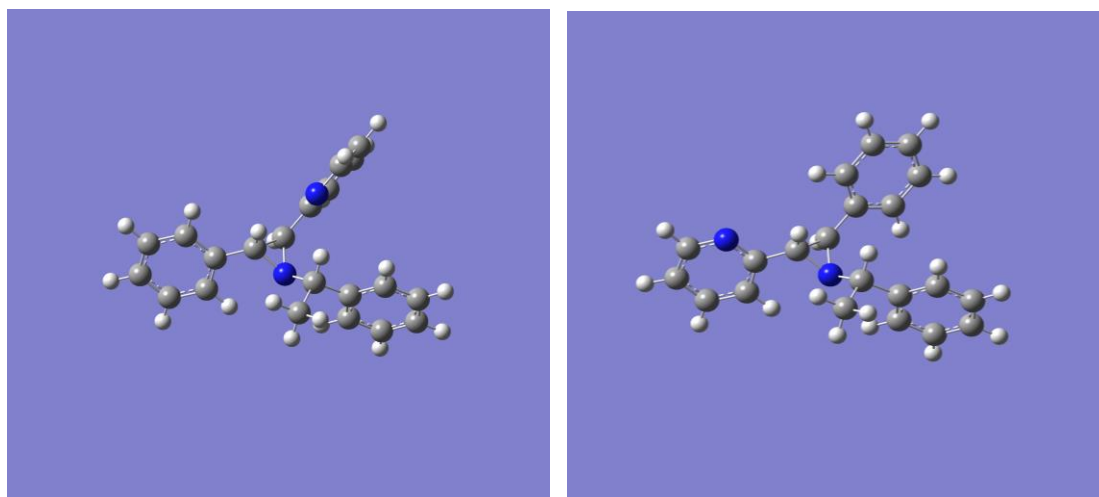


Figure S2. Molecular geometry of lowest energy structures optimized at the DFT/B3LYP/CC-pVDZ level for (1*S*,2*S*,3*R*)-**10**(left) and (1*R*,2*S*,3*R*)-**10** (right).

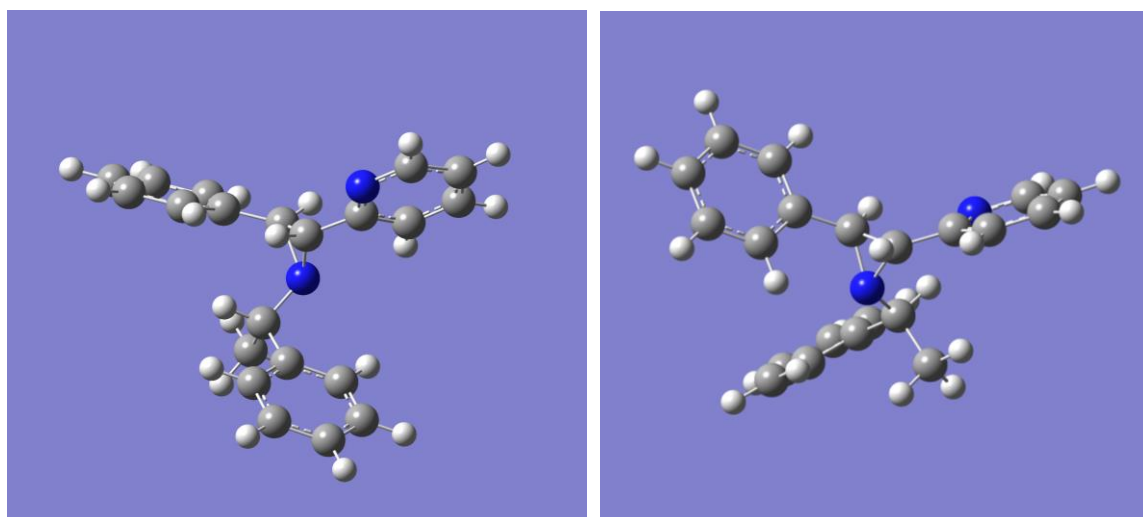


Figure S3. Molecular geometry of lowest energy structures optimized at the DFT/B3LYP/CC-pVDZ level for (1*S*,2*R*,3*S*)-**10** (left) and (1*S*,2*R*,3*S*)-**10** (right).

Table S1. Comparison of experimental and DFT calculated NMR chemical shifts (GIAO DFT/mPW1PW91/6-311+G(2d,p)) for (2*S*,3*R*,1'*S*)-**10**

2 <i>S</i> ,3 <i>R</i> - 10 Signal	DFT δ , ppm		Experiment δ , ppm	
	1 <i>S</i> ^N	1 <i>R</i> ^N	Major (52%)	Minor (48%)
H-2	3.68	3.36	3.45	3.34
H-3	3.76	3.89	3.79	3.78
H-1'	3.56	4.62	3.99	3.24
1'-CH ₃	1.21	1.22	1.06	1.18

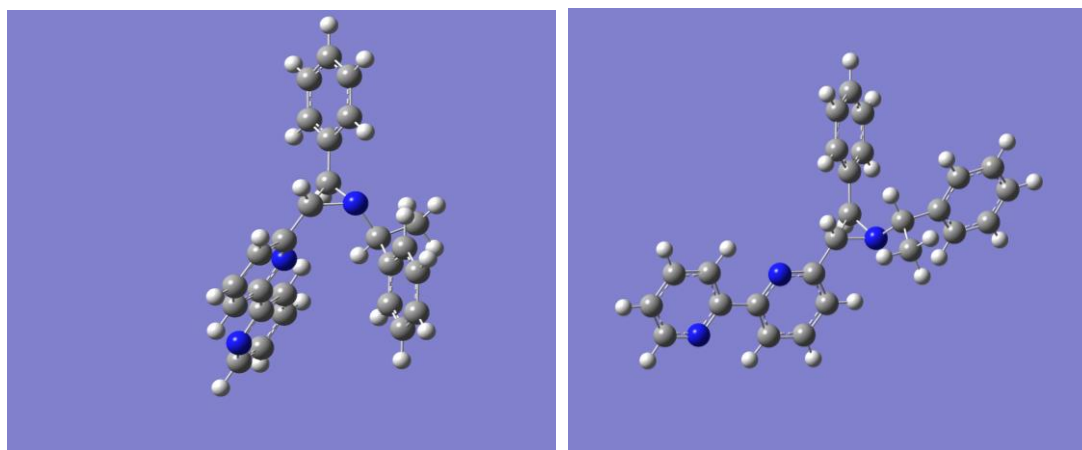


Figure S4. Molecular geometry of lowest energy structures optimized at the DFT/B3LYP/CC-pVDZ level for (1*S*,2*S*,3*R*)-**12** (left) and (1*R*,2*S*,3*R*)-**12** (right).

Table S2. Comparison of experimental and DFT calculated NMR chemical shifts (GIAO DFT/mPW1PW91/6-311+G(2d,p)) for (2*S*,3*R*,1'*S*)-**12**

2 <i>R</i> ,3 <i>S</i> - 12 Signal	DFT δ , ppm		Experiment δ , ppm	
	1 <i>S</i> ^N	1 <i>R</i> ^N	Major (76%)	Minor (24%)
H-2	3.29	4.03	3.33	3.64
H-3	4.32	3.53	4.09	3.56
H-1'	4.52	3.61	4.05	3.17
1'-CH ₃	1.63	1.59	1.55	1.48

Table S3. Comparison of experimental and DFT calculated NMR chemical shifts (GIAO DFT/mPW1PW91/6-311+G(2d,p)) for 2*S*,3*R*-**10**·Zn(OAc)₂

	DFT, δ (ppm)	Experiment, δ (ppm)
H-2	3.41	4.00
H-3	4.52	4.74
H-1'	5.87	3.64
1'-CH ₃	1.70	1.61

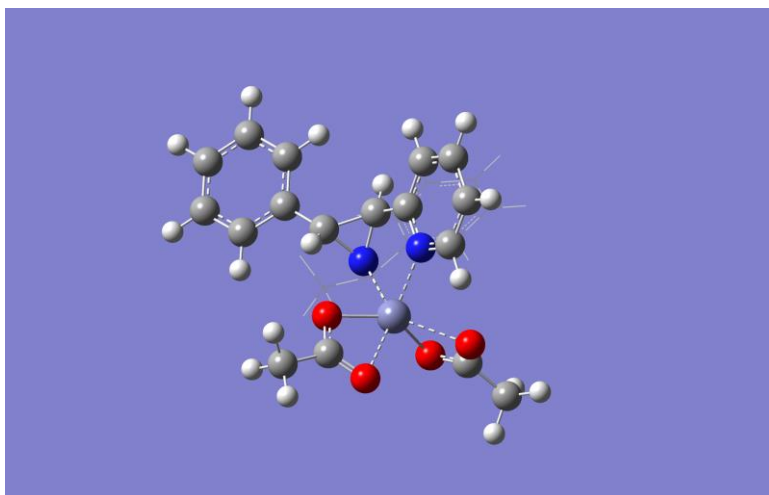


Figure S5. DFT computed structure of zinc ligand (1*S*,2*S*,3*R*)-**10** acetate complex. For clarity, methylbenzyl group is shown as wireframe, Zn-heteroatom distances of 2.15-2.51 Å are shown as dashed lines.

3. NMR spectra for titration of (1*S*/1*R*,2*S*,3*R*)-**10** and (1*S*/1*R*,2*R*,3*S*)-**12** with zinc acetate

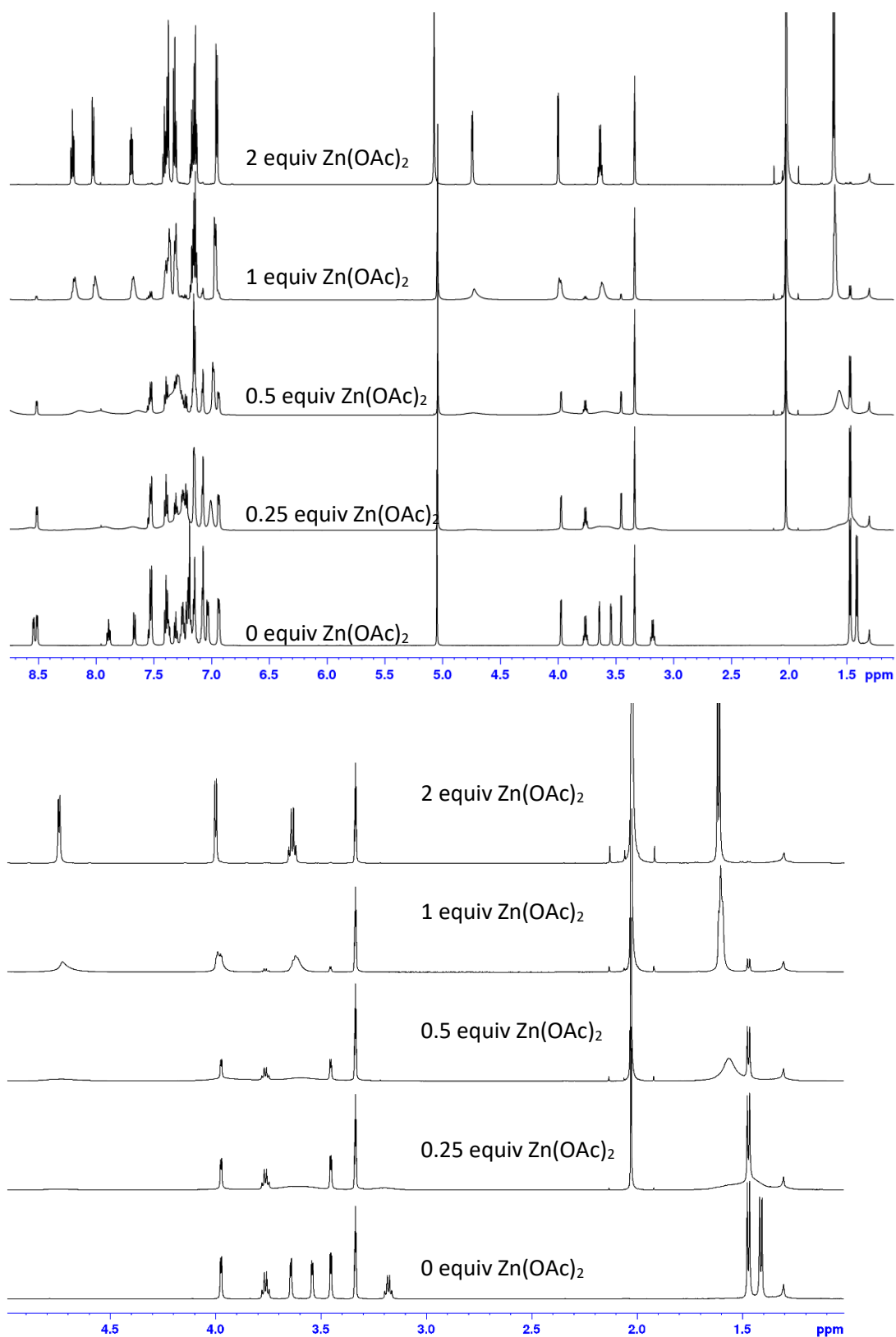


Figure S6. NMR spectra (600 MHz, CD₃OD) collected during titration of (1*S*/1*R*,2*S*,3*R*)-**10** with zinc acetate: full view (top) and expanded aliphatic region (bottom); signal intensity is maintained versus internal standard (dichloromethane).

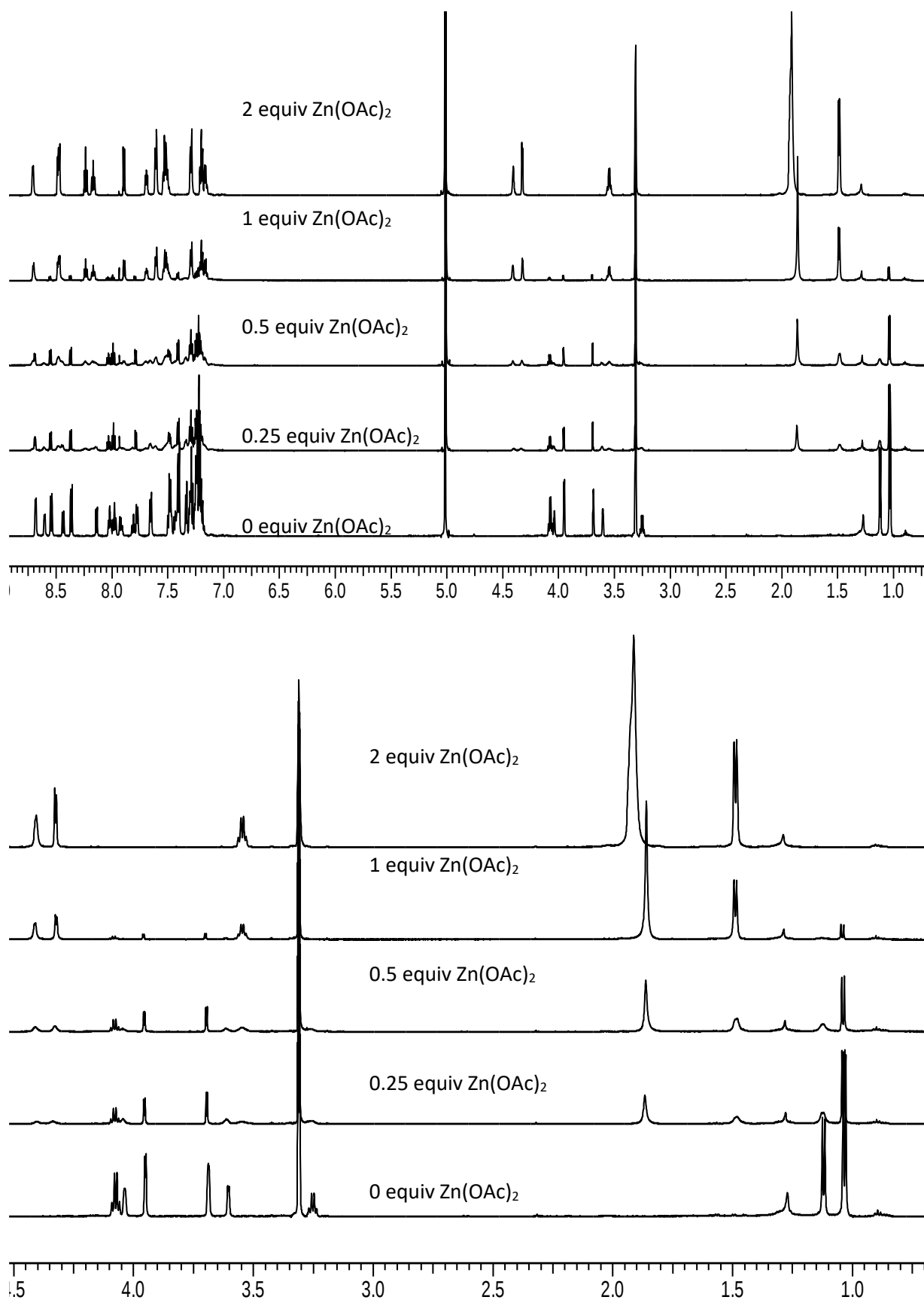


Figure S7. NMR spectra (600 MHz, CD_3OD) collected during titration of (1*S*/1*R*,2*R*,3*S*)-12 with zinc acetate: full view (top) and expanded aliphatic region (bottom). signal intensity is maintained versus internal standard (dichloromethane).

4. EXSY experiment for (2*S*,3*R*,1'*S*)-**10** and ^1H , ^{13}C HSQC and HMBC spectra for azides **3**, **13**, **14** and **19**

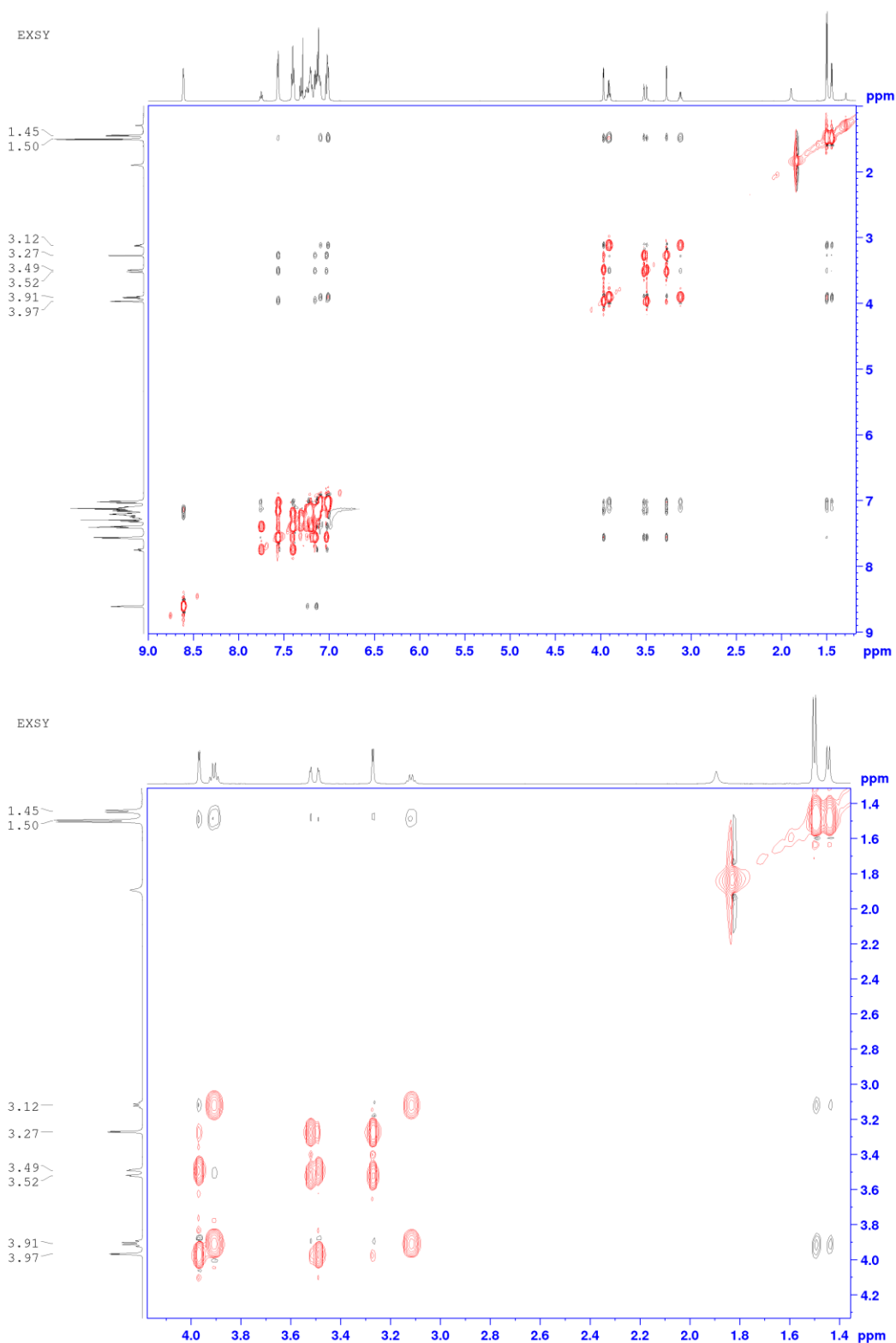


Figure S8. EXSY experiment for (2*S*,3*R*,1'*S*)-**10**, full (top) and expanded view (bottom). Positive phase correlations are drawn in red.

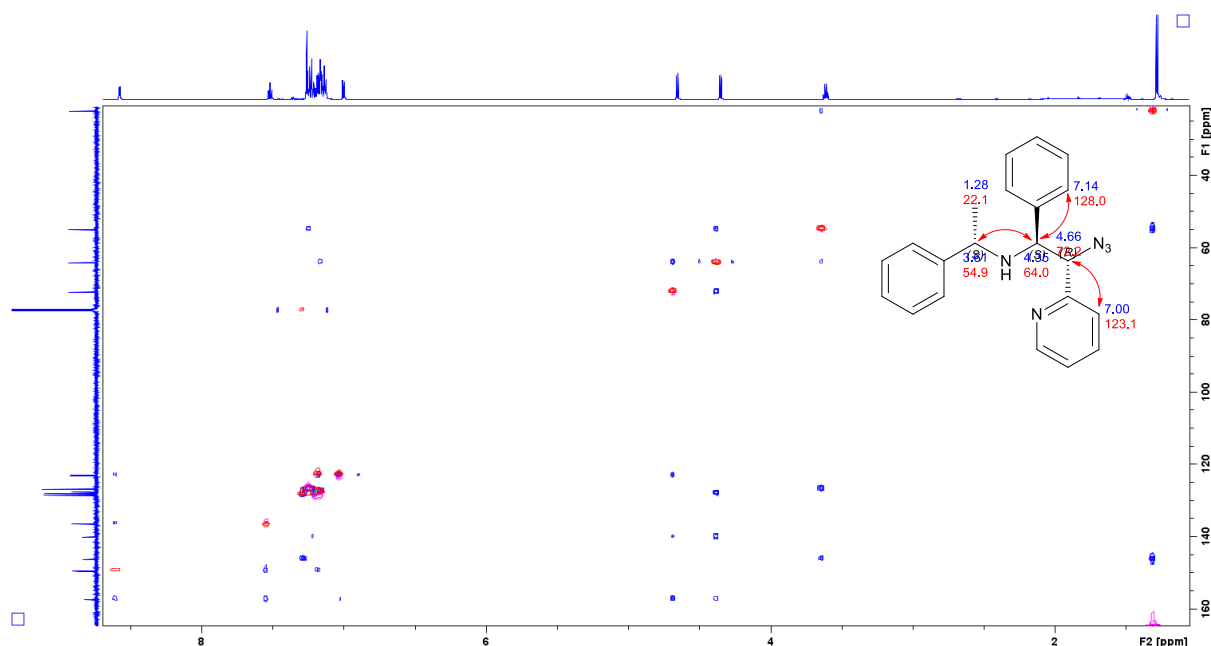


Figure S9. Overlay of ^1H , ^{13}C HSQC (red) and HMBC (blue) experiments for (1R,2S,1'S)-**19** in CDCl_3 (600, 151 MHz). Inset structure drawing shows the assignment of selected ^1H NMR shifts in blue, ^{13}C NMR shifts in red, and HMBC correlations as arrows.

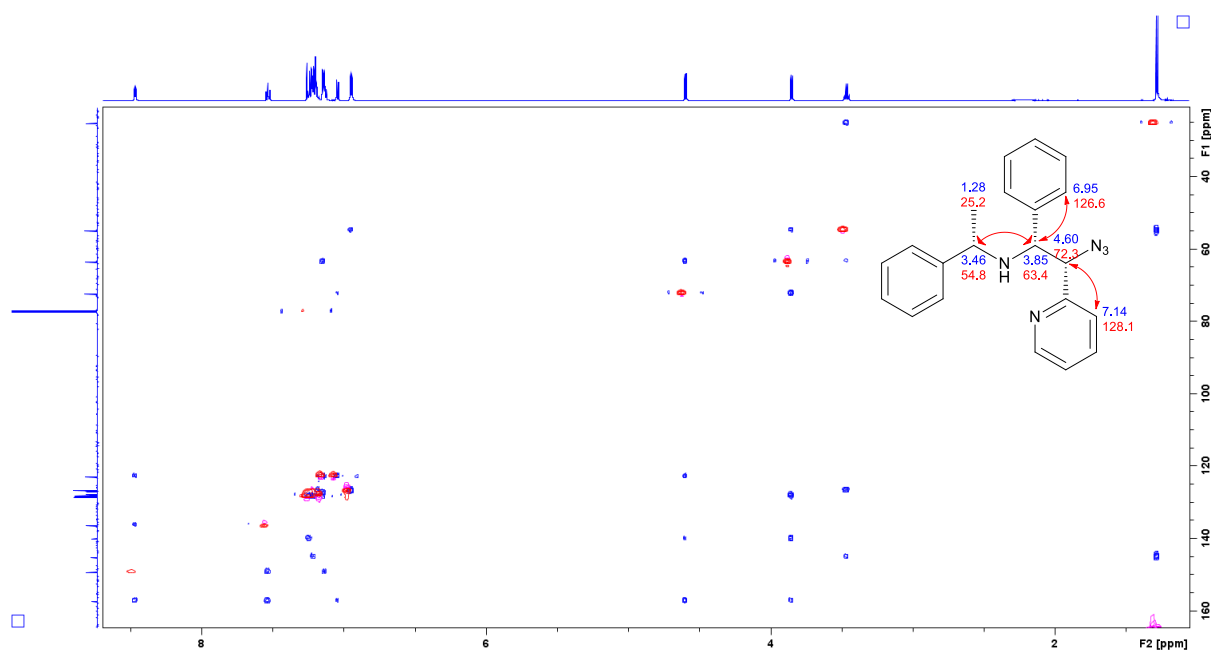


Figure S10. Overlay of ^1H , ^{13}C HSQC (red) and HMBC (blue) experiments for (1S,2R,1'S)-**19** in CDCl_3 (600, 151 MHz). Inset structure drawing shows the assignment of selected ^1H NMR shifts in blue, ^{13}C NMR shifts in red, and HMBC correlations as arrows.

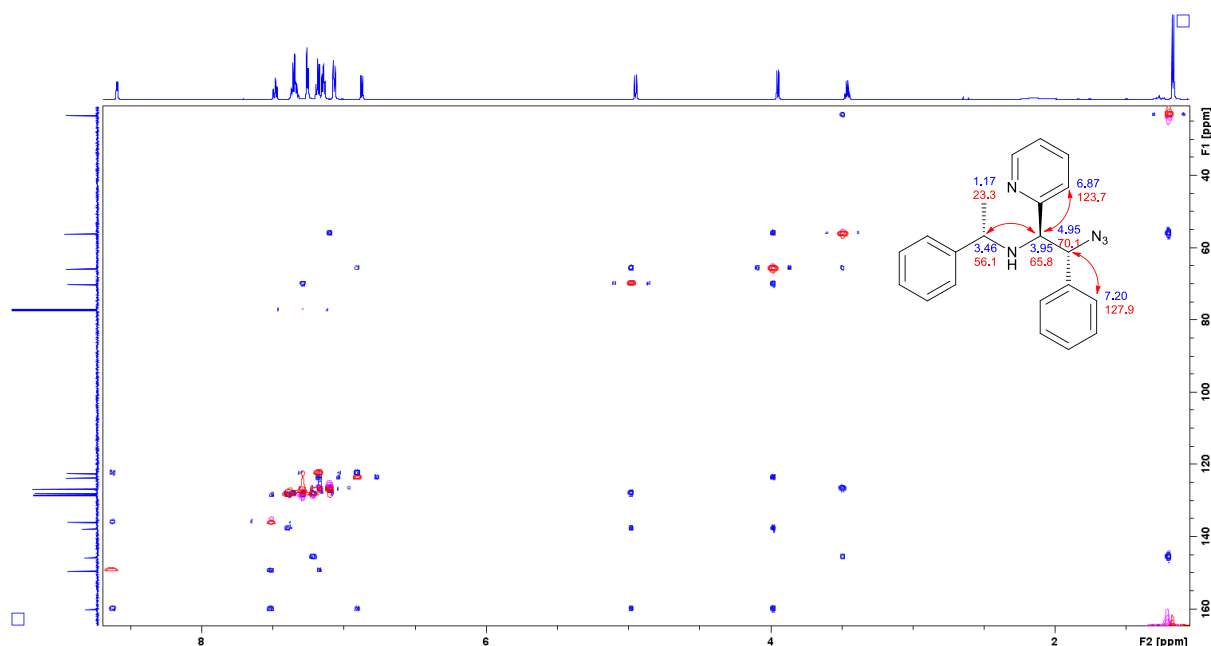


Figure S11. Overlay of ^1H , ^{13}C HSQC (red) and HMBC (blue) experiments for (1R,2R,1'S)-**13** in CDCl_3 (600, 151 MHz). Inset structure drawing shows the assignment of selected ^1H NMR shifts in blue, ^{13}C NMR shifts in red, and HMBC correlations as arrows.

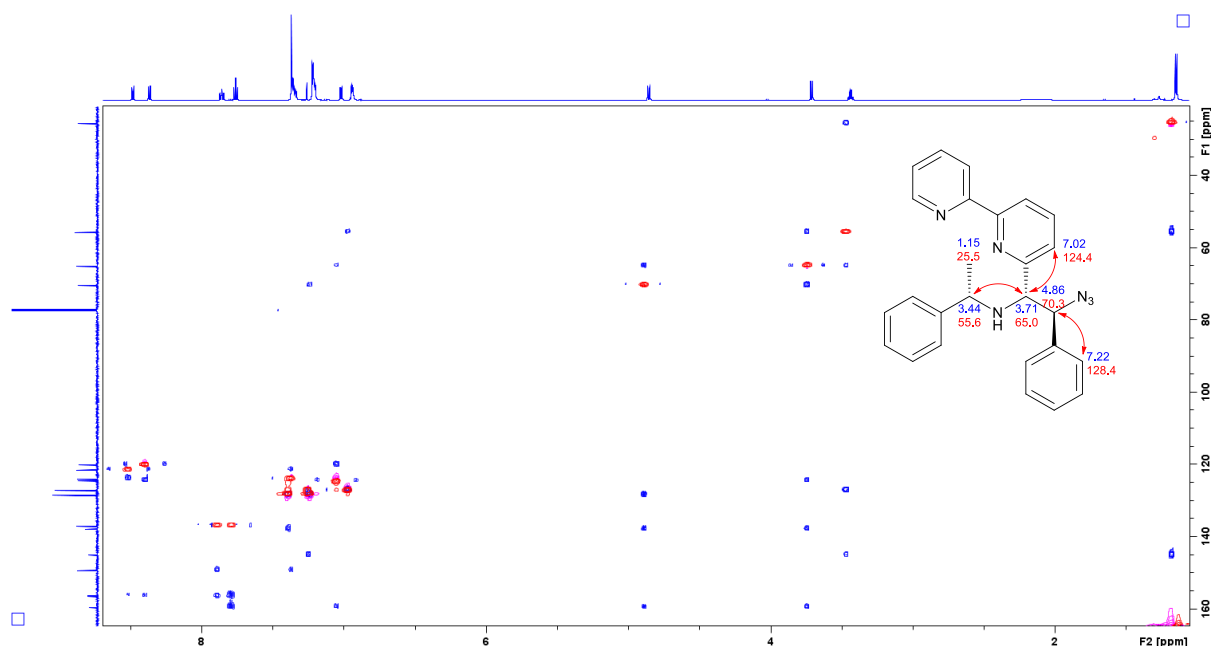


Figure S12. Overlay of ^1H , ^{13}C HSQC (red) and HMBC (blue) experiments for (1S,2S,1'S)-**14** in CDCl_3 (600, 151 MHz). Inset structure drawing shows the assignment of selected ^1H NMR shifts in blue, ^{13}C NMR shifts in red, and HMBC correlations as arrows.

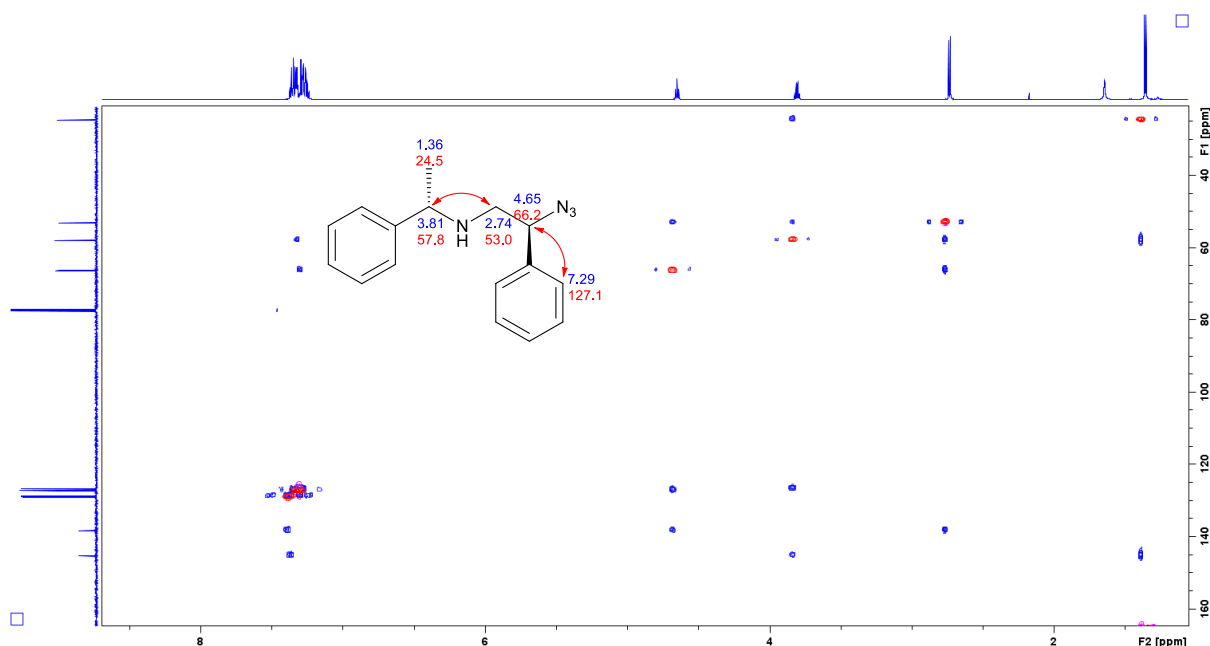


Figure S13. Overlay of ^1H , ^{13}C HSQC (red) and HMBC (blue) experiments for (1*R*, *I'**S*)-**3** in CDCl_3 (600, 151 MHz). Inset structure drawing shows the assignment of selected ^1H NMR shifts in blue, ^{13}C NMR shifts in red, and HMBC correlations as arrows.

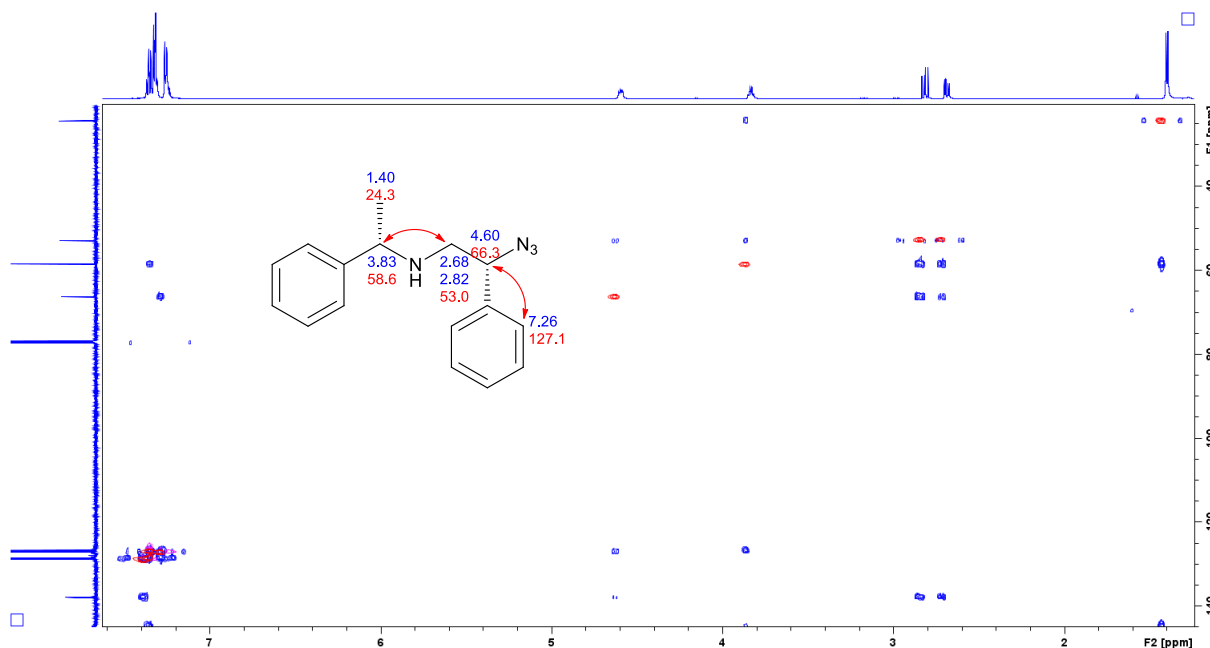


Figure S14. Overlay of ^1H , ^{13}C HSQC (red) and HMBC (blue) experiments for (1*S*, *I'**S*)-**3** in CDCl_3 (600, 151 MHz). Inset structure drawing shows the assignment of selected ^1H NMR shifts in blue, ^{13}C NMR shifts in red, and HMBC correlations as arrows.

5. Copies of NMR Spectra

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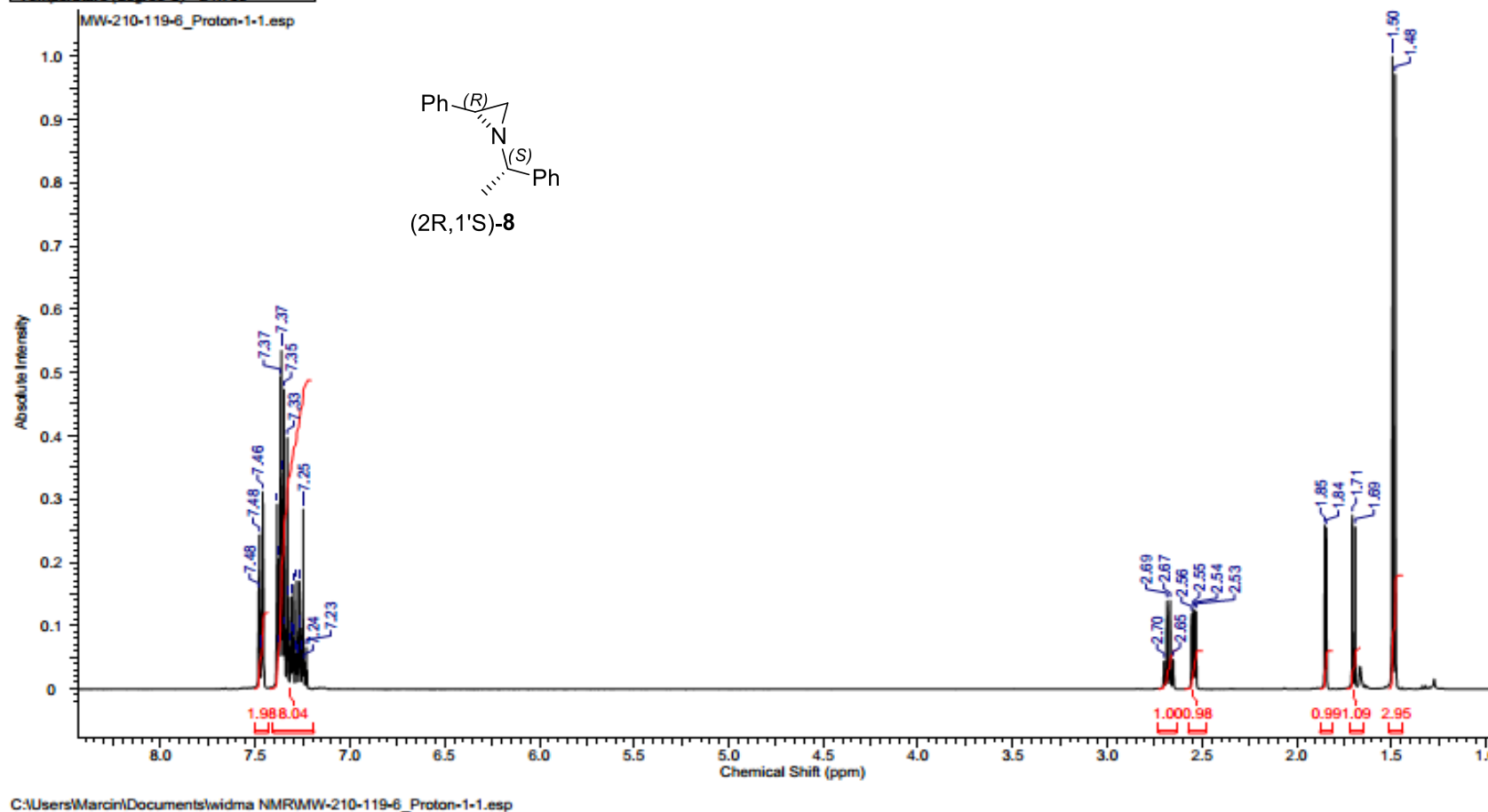
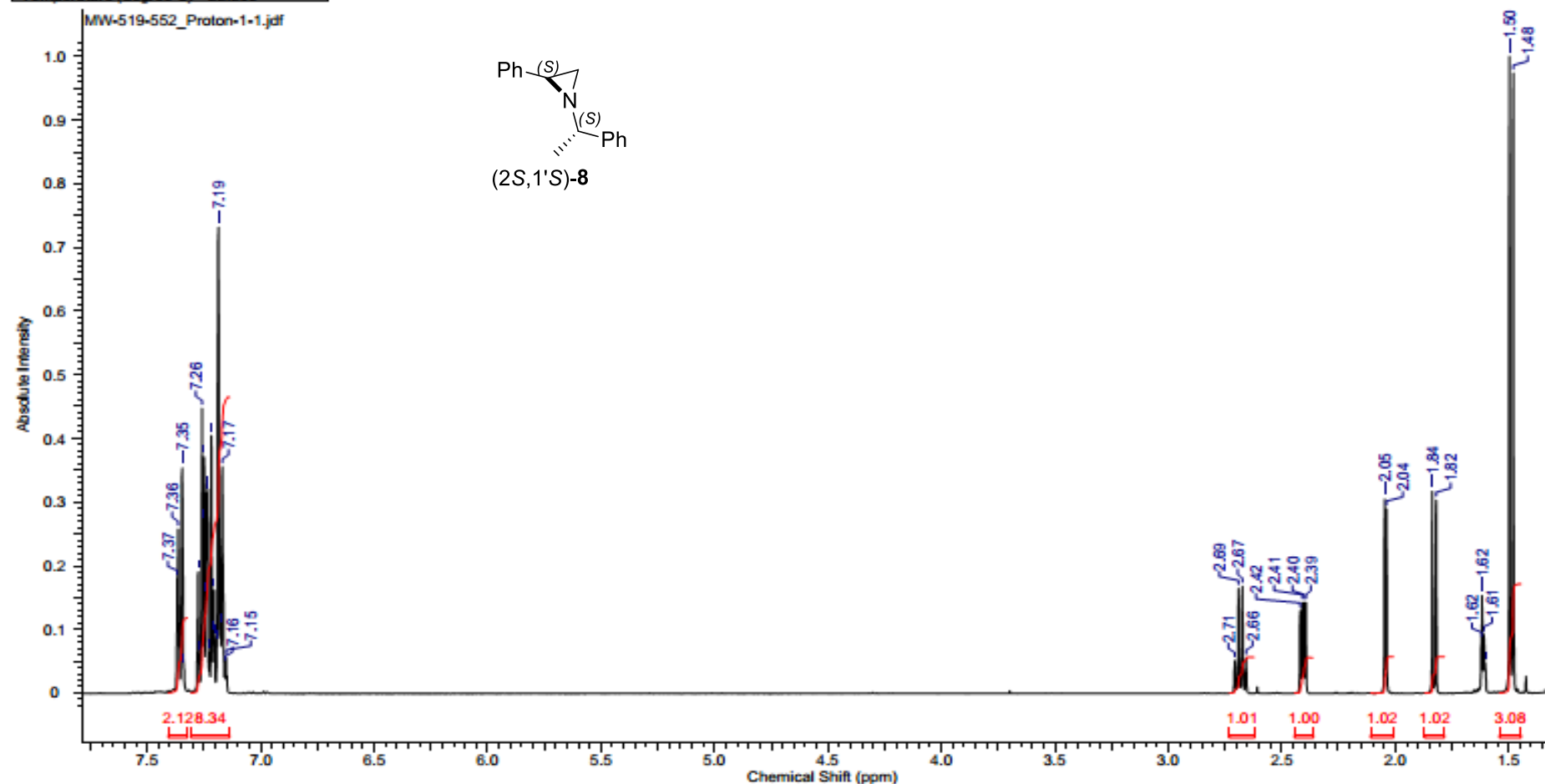


Figure S15. ¹H NMR spectrum (400 MHz, CDCl₃) for (2R,1'S)-8

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Acquisition Time (sec)	3.2716	Comment	single pulse	Date	14 Nov 2019 09:19:47
Date Stamp	14 Nov 2019 09:16:17	File Name	C:\Users\Marcin\Documents\widma NMR\MW-519-552 Proton-1-1.jdf		
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Solvent	CHLOROFORM-d	Pulse Sequence	proton.jxp		
Temperature (degree C)	22.200	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	10016.03



C:\Users\Marcin\Documents\widma NMR\MW-519-552_Proton-1-1.jdf

Figure S16. ¹H NMR spectrum (400 MHz, CDCl₃) for (2S,1'S)-8

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.2716	Comment	single pulse	Date	21 May 2018 09:04:36
Date Stamp	21 May 2018 09:02:46	File Name	C:\Users\Marcin\Documents\widma NMRMW-220-231 Proton-1-1.jdf		
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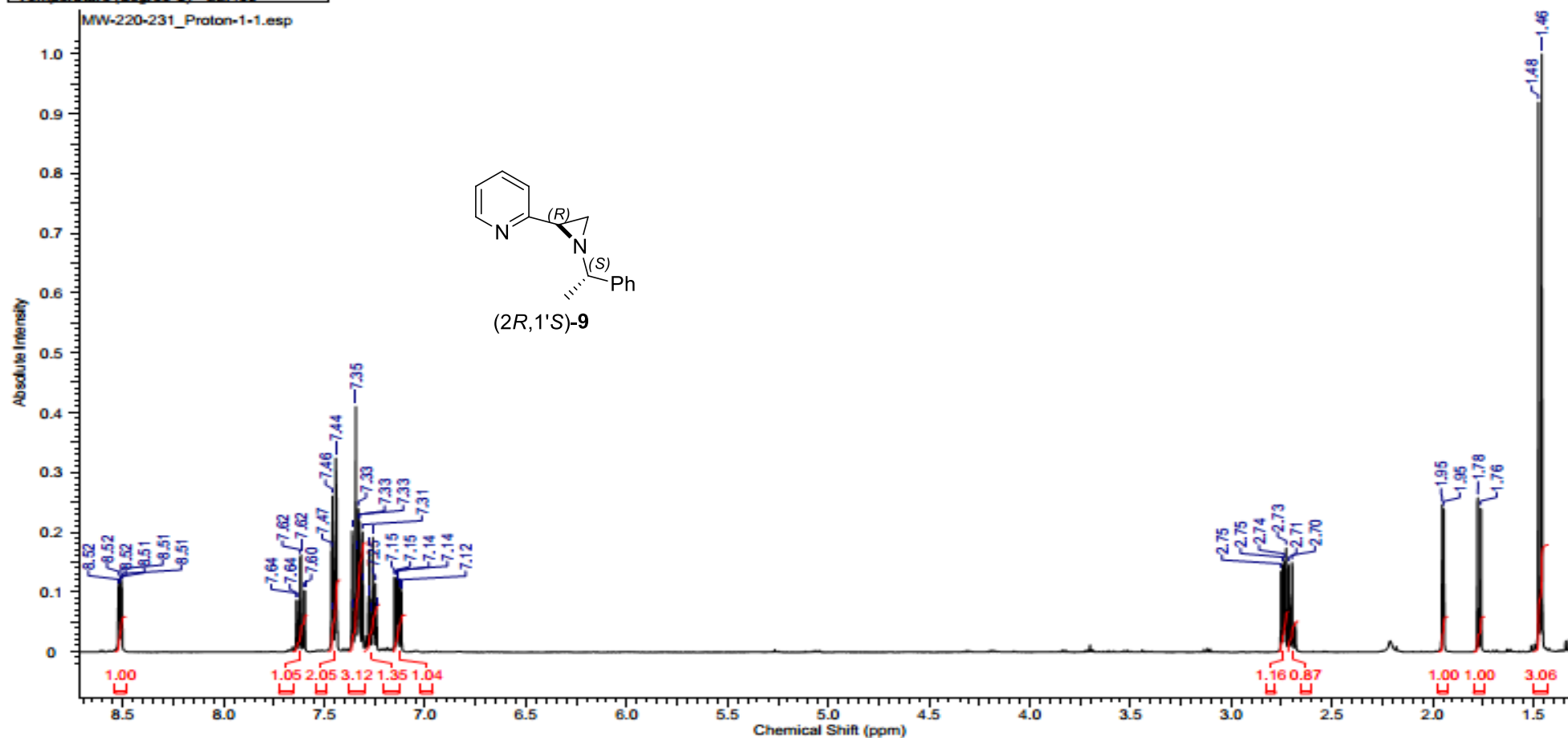
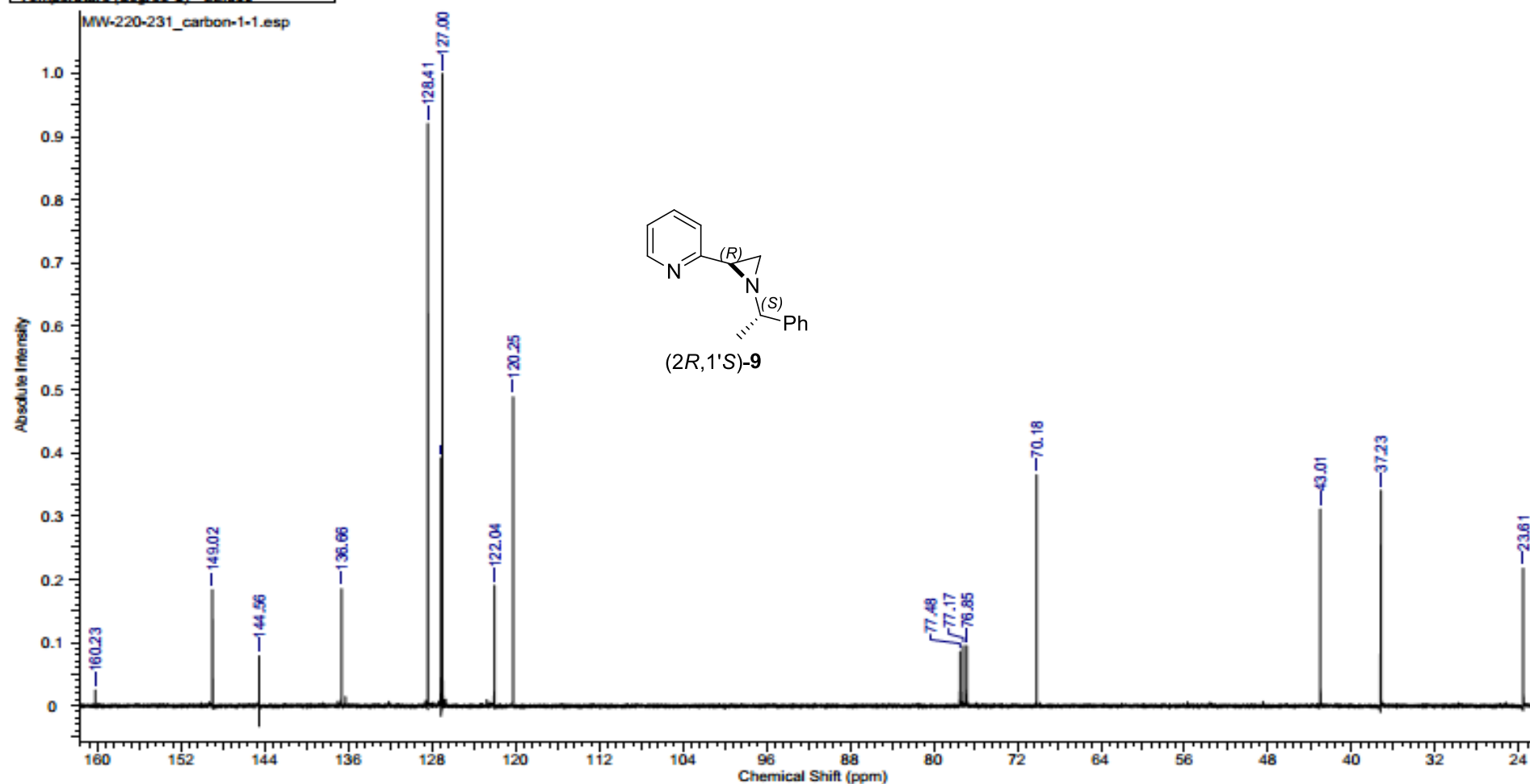


Figure S17. ^1H NMR spectrum (400 MHz, CDCl_3) for (2R,1'S)-9

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This report was created by ACD/NAME Processor Academic Edition. For more information go to www.acdlabs.com/name/proc/

Acquisition Time (sec)	1.7406	Comment	single pulse decoupled gated NOE		Date	23 May 2018 08:36:25	
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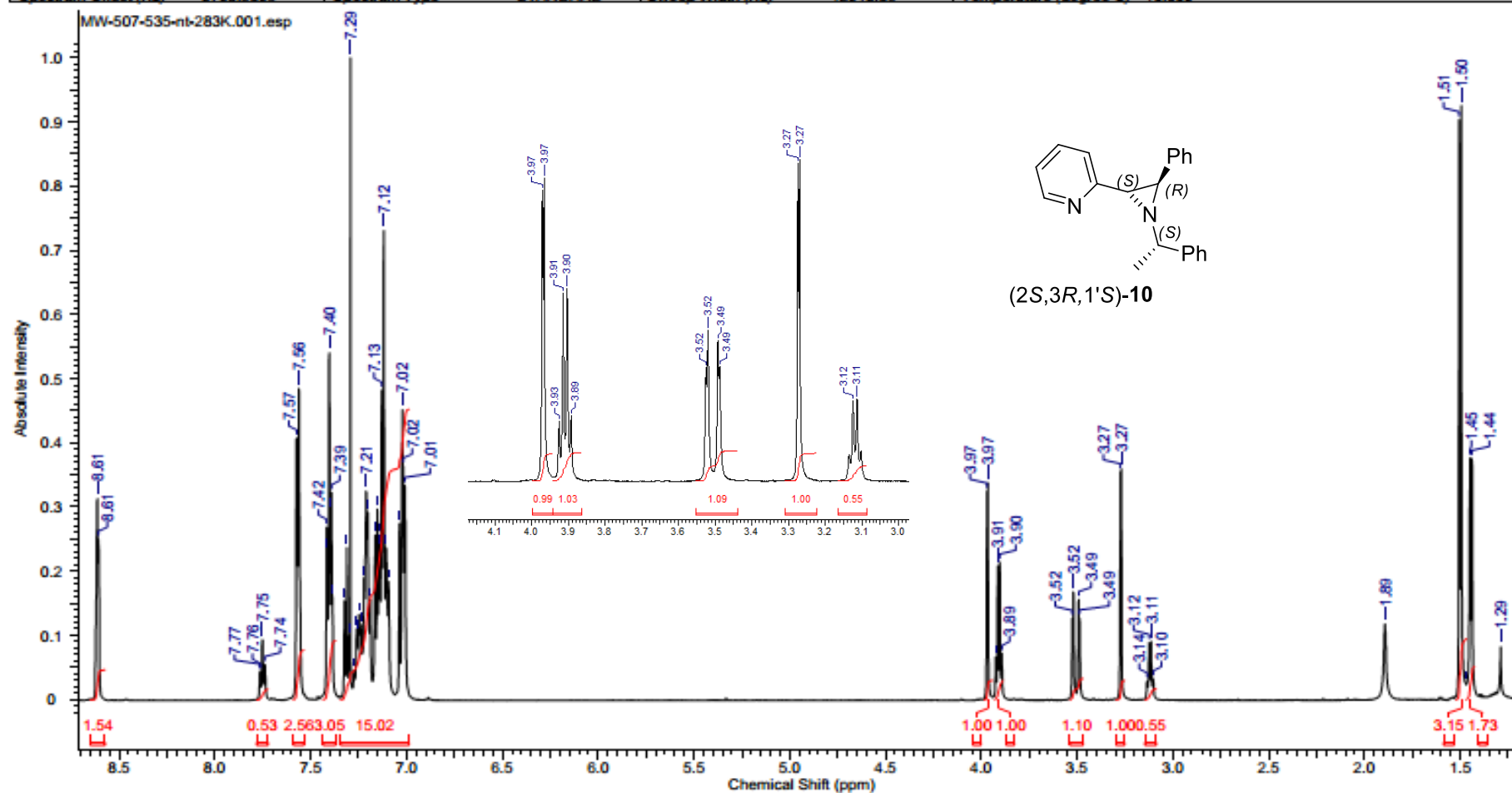


C:\Users\Marcin\Documents\widma NMRMW-220-231_carbon-1-1.esp

Figure S18. ^{13}C NMR spectrum (101 MHz, CDCl_3) for (2R,1'S)-8

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	2.7263	Comment	5 mm PABBO BB-1H/D Z-GRD Z847801/0325	Date	13 Nov 2019 10:16:48
Date Stamp	13 Nov 2019 10:16:48	File Name	C:\Users\Marcin\Documents\widma NMR\MW-507-535-nt-283K\1Vid		
Frequency (MHz)	600.58	Nucleus	1H	Number of Transients	32
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Receiver Gain	114.00	SW(cyclical) (Hz)	12019.23	Solvent	CHLOROFORM-d
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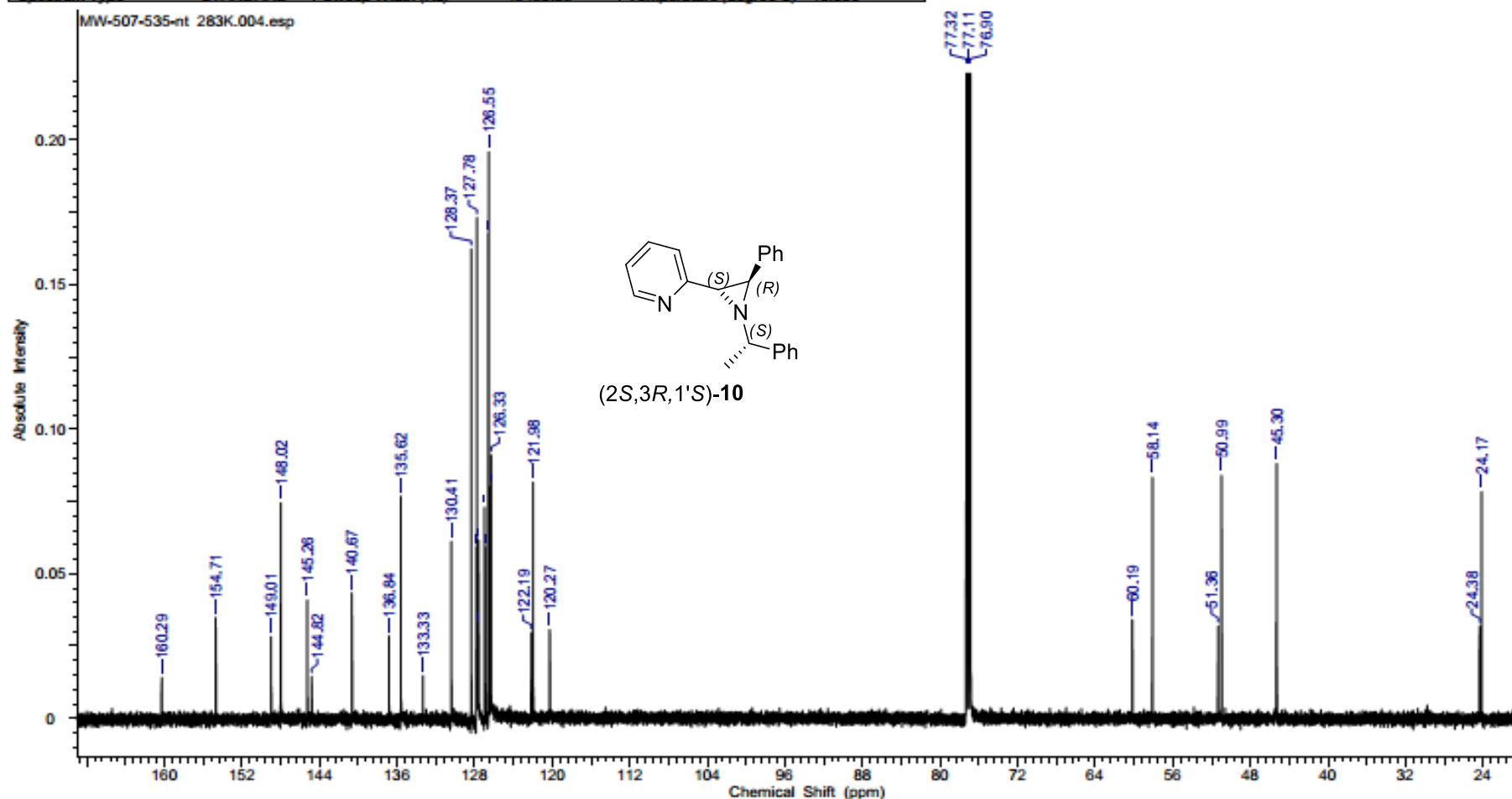


C:\Users\Marcin\Documents\widma NMR\MW-507-535-nt-283K\MW-507-535-nt-283K.001.esp

Figure S19. ¹H NMR spectrum (283K, 600 MHz, CDCl₃) for (2S,3R,1'S)-10

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Acquisition Time (sec)	1.4418	Date	23 Nov 2019 02:42:24		Date Stamp	23 Nov 2019 02:42:24	
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Spectrum Type	STANDARD	Sweep Width (Hz)	45453.85	Temperature (degree C)	10.000		



C:\Users\Marcin\Documents\widma NMR\MW-507-535-nt 283K\MW-507-535-nt 283K.004.esp

Figure S20. ¹³C NMR spectrum (283K, 151 MHz, CDCl₃) for (2S,3R,1'S)-10

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

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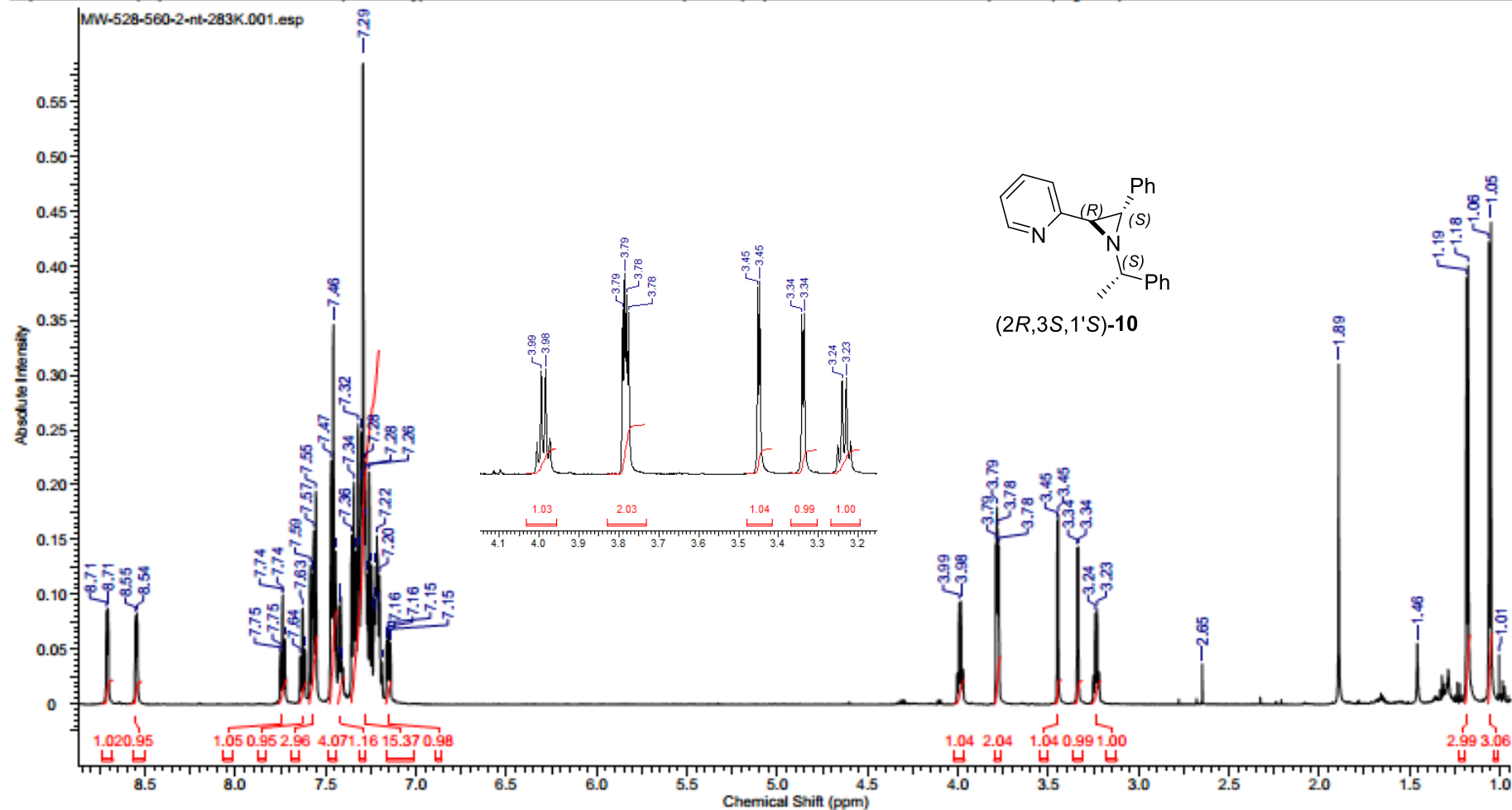
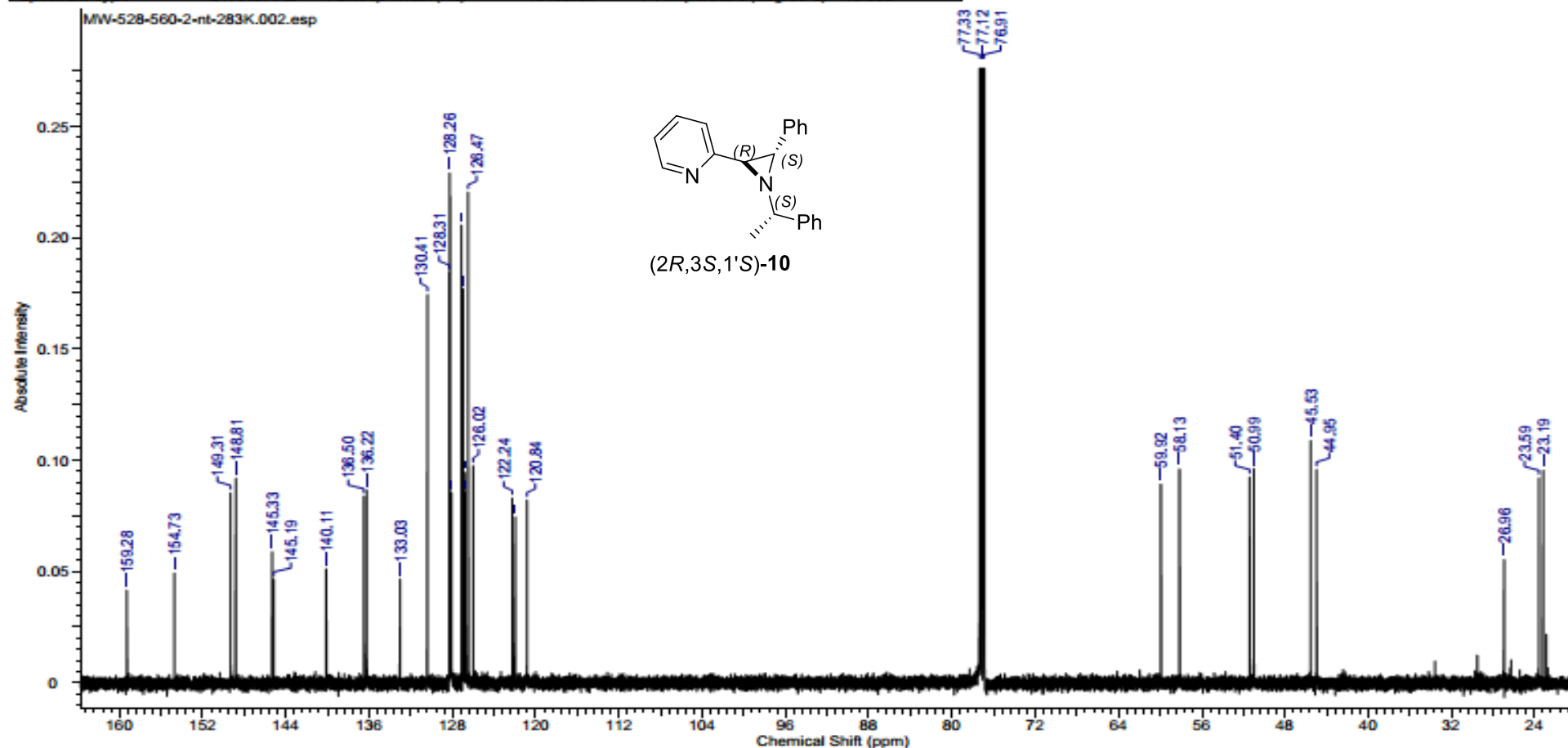


Figure S21. ¹H NMR spectrum (283K, 600 MHz, CDCl₃) for (2R,3S,1'S)-10

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Acquisition Time (sec)	1.4418	Date	25 Nov 2019 09:46:56	Date Stamp	25 Nov 2019 09:46:56
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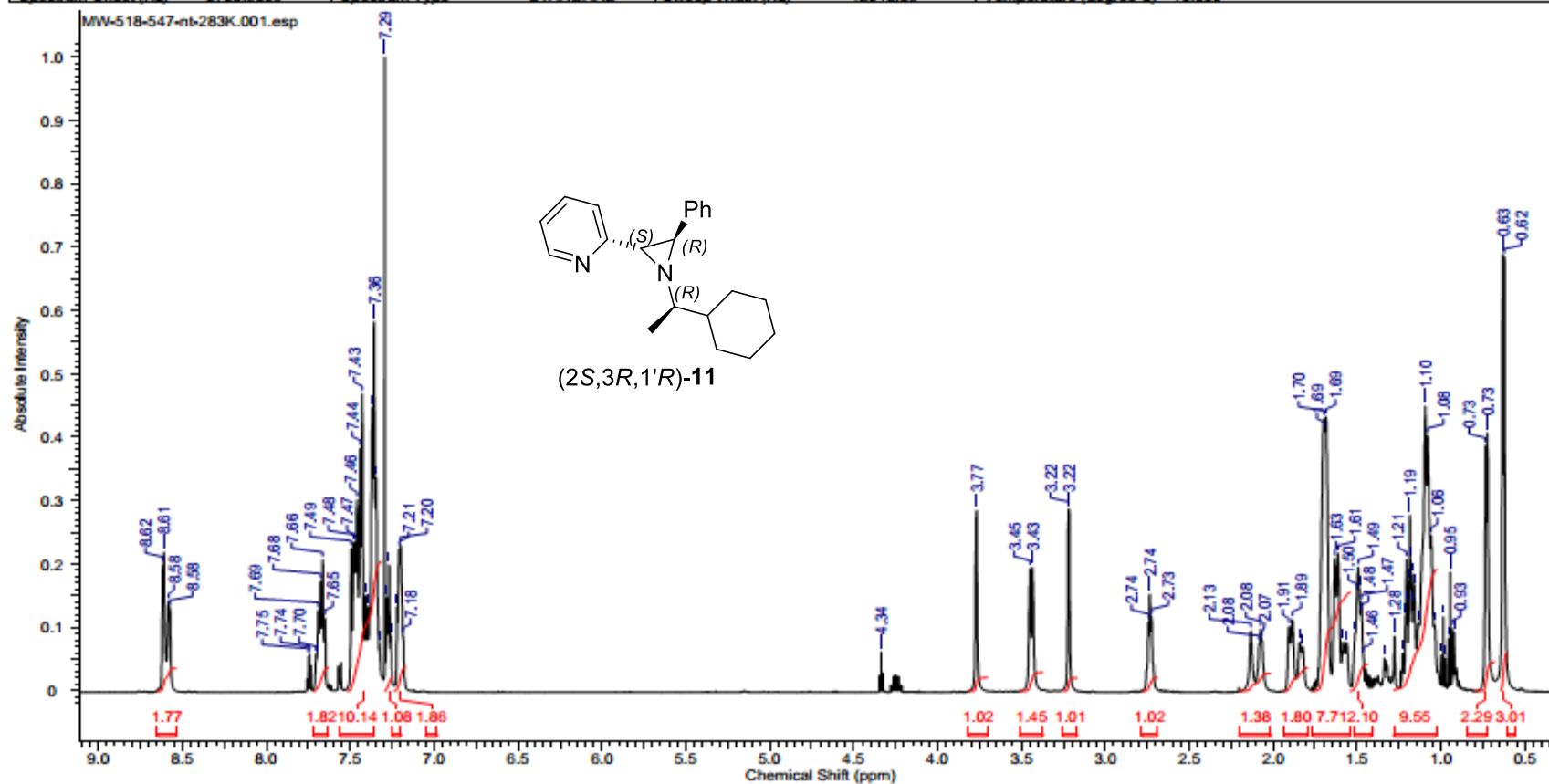


C:\Users\Marcin\Documents\widma NMR\MW-528-560-2-nt-283K\MW-528-560-2-nt-283K.002.esp

Figure S22. ¹³C NMR spectrum (283K, 151 MHz, CDCl₃) for (2R,3S,1'S)-10

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

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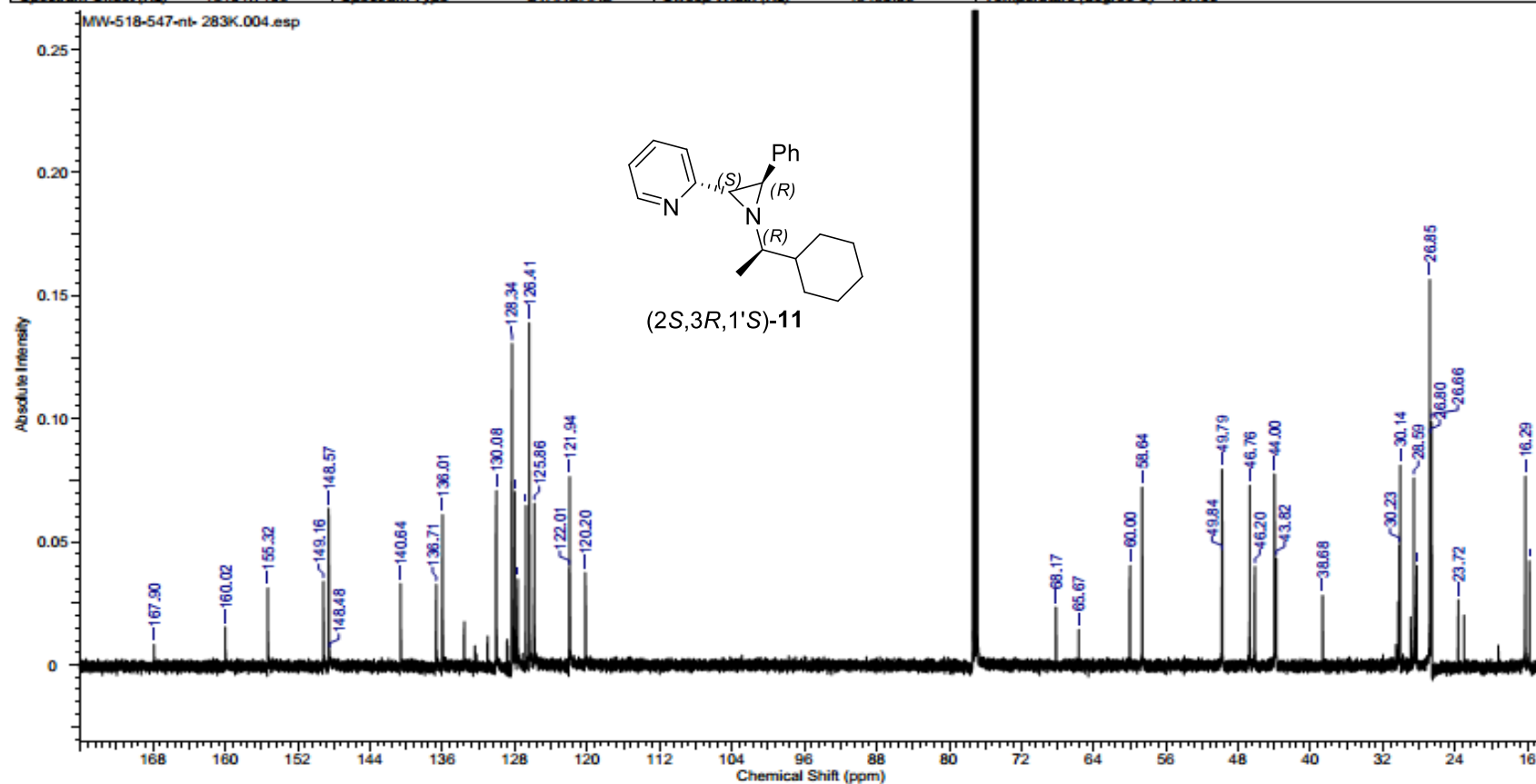


C:\Users\Marcin\Documents\widma NMR\MW-518-547-nt-283K\MW-518-547-nt-283K.001.esp

Figure S23. ¹H NMR spectrum (283K, 600 MHz, CDCl₃) for (2S,3R,1'R)-11

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

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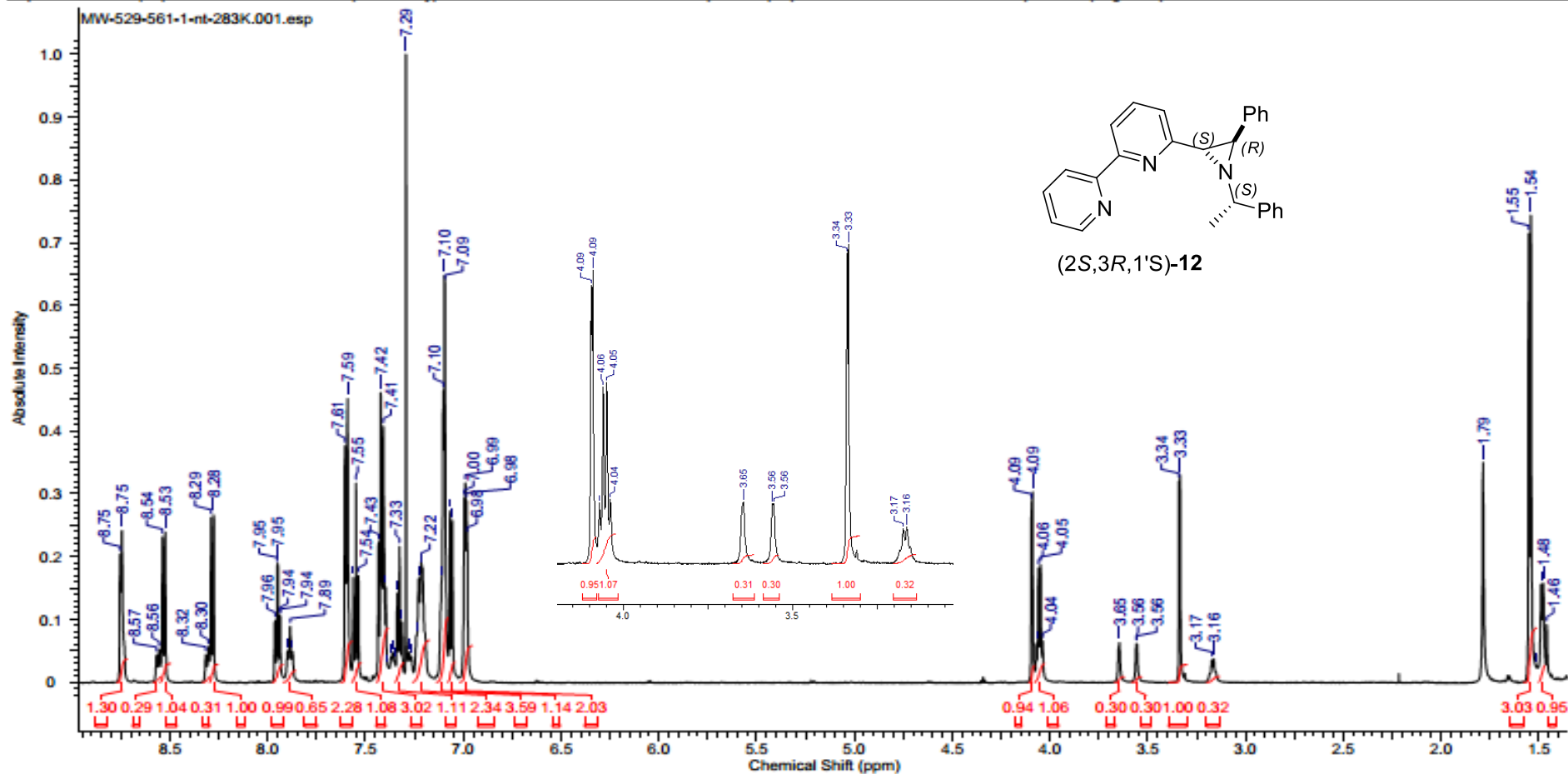


C:\Users\Marcin\Documents\widma NMR\MW-518-547-nt- 283K\MW-518-547-nt- 283K.004.esp

Figure S24. ^{13}C NMR spectrum (283K, 151 MHz, CDCl_3) for (2S,3R,1'R)-11

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

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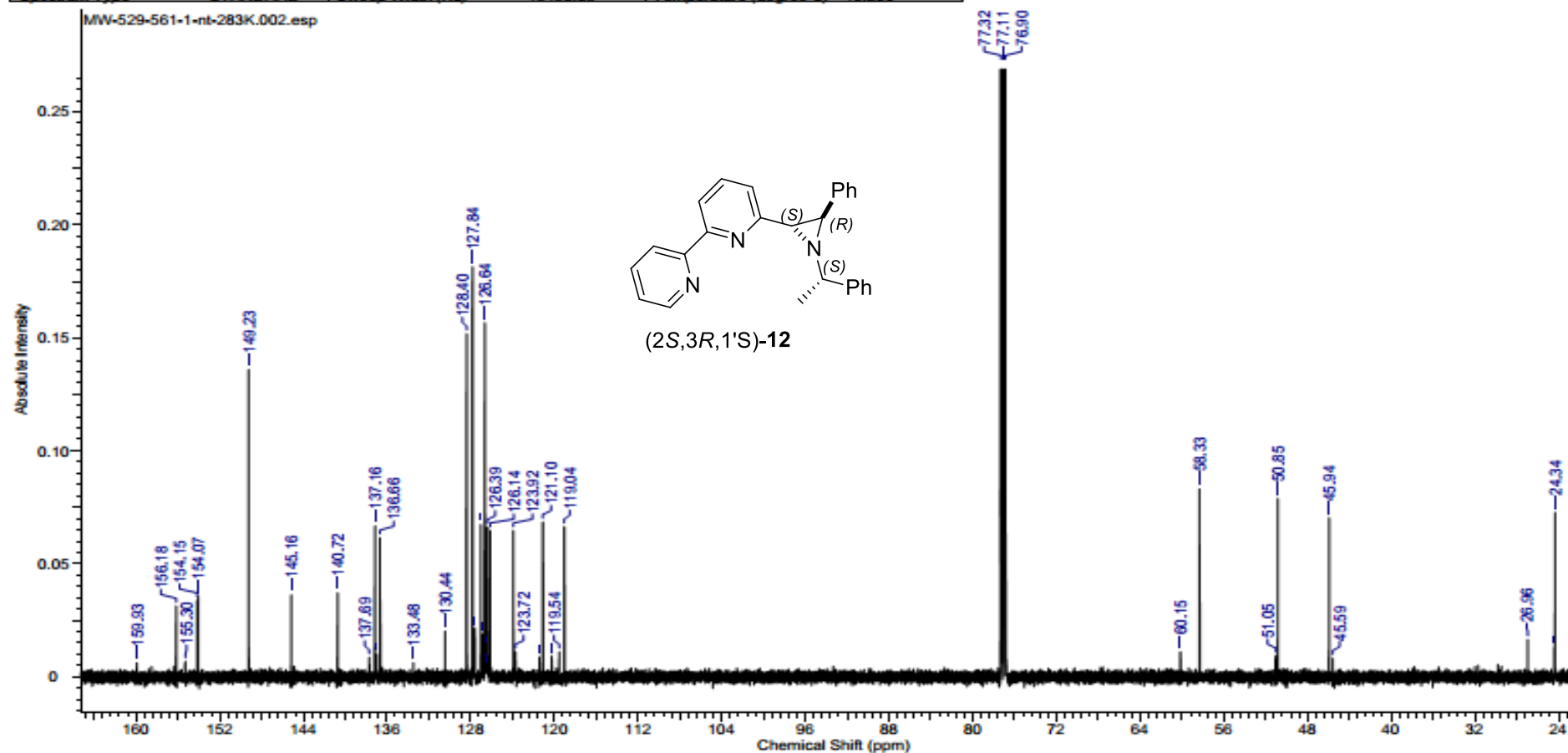


C:\Users\Marcin\Documents\widma NMR\MW-529-561-1-nt-283K\MW-529-561-1-nt-283K.001.esp

Figure S25. ¹H NMR spectrum (283K, 600 MHz, CDCl₃) for (2S,3R,1'S)-12

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

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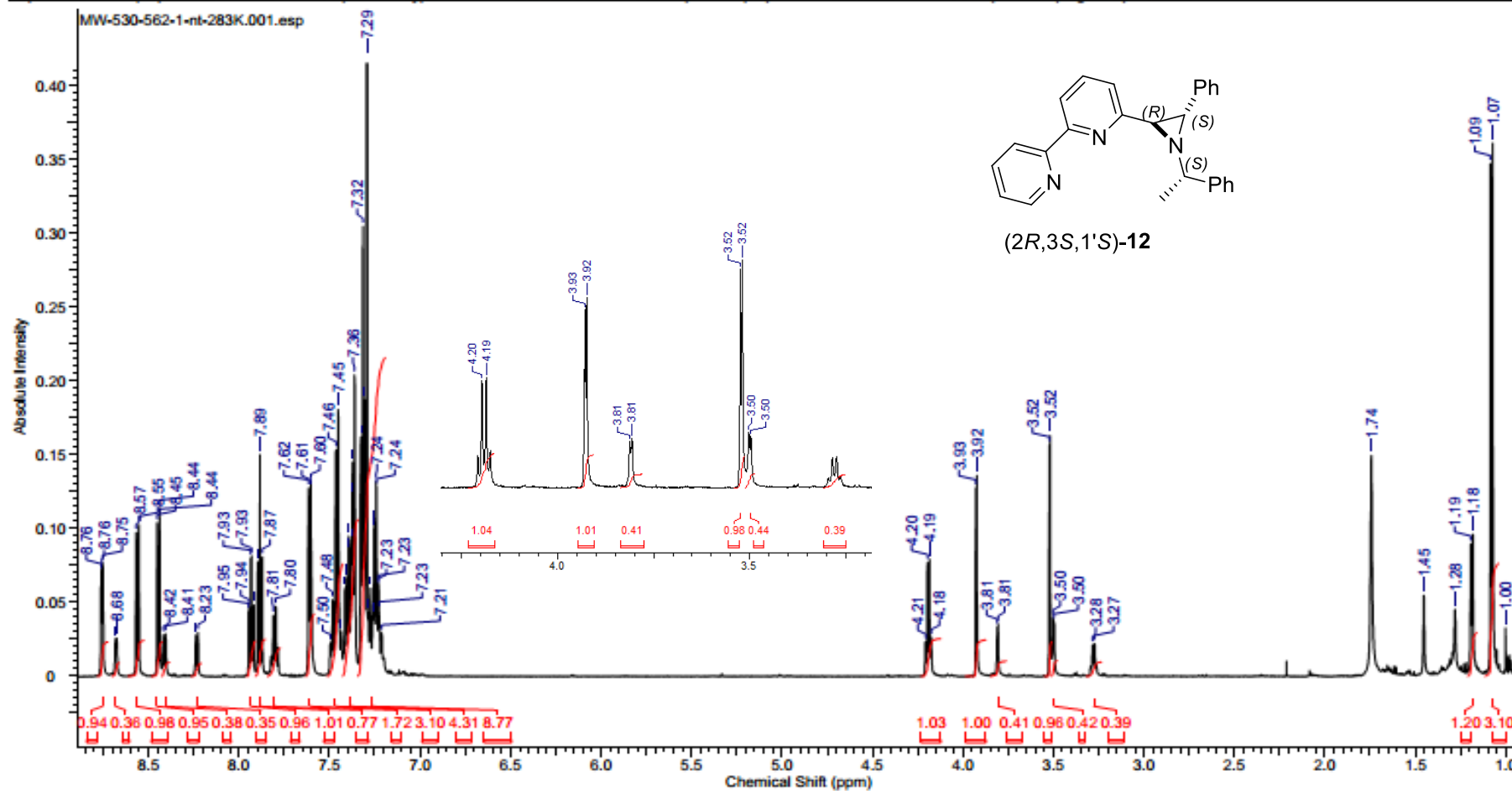


C:\Users\Marcin\Documents\widma NMR\MW-529-561-1-nt-283K\MW-529-561-1-nt-283K.002.esp

Figure S26. ¹³C NMR spectrum (283K, 151 MHz, CDCl₃) for (2S,3R,1'S)-12

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	2.7263	Comment	5 mm PABBO BB-1H/D Z-GRD Z847801/0325	Date	25 Nov 2019 10:53:04
Date Stamp	25 Nov 2019 10:53:04	File Name	C:\Users\Marcin\Documents\widma NMR\MW-530-562-1-nt-283K\1Vid	Origin	spect
Frequency (MHz)	600.58	Nucleus	¹ H	Number of Transients	32
Original Points Count	32768	Owner	nmsu	Points Count	32768
Receiver Gain	181.00	SW(cyclical) (Hz)	12019.23	Pulse Sequence	zg30
Spectrum Offset (Hz)	3708.5806	Spectrum Type	STANDARD	Solvent	CHLOROFORM-d
		Sweep Width (Hz)	12018.86	Temperature (degree C)	10.000

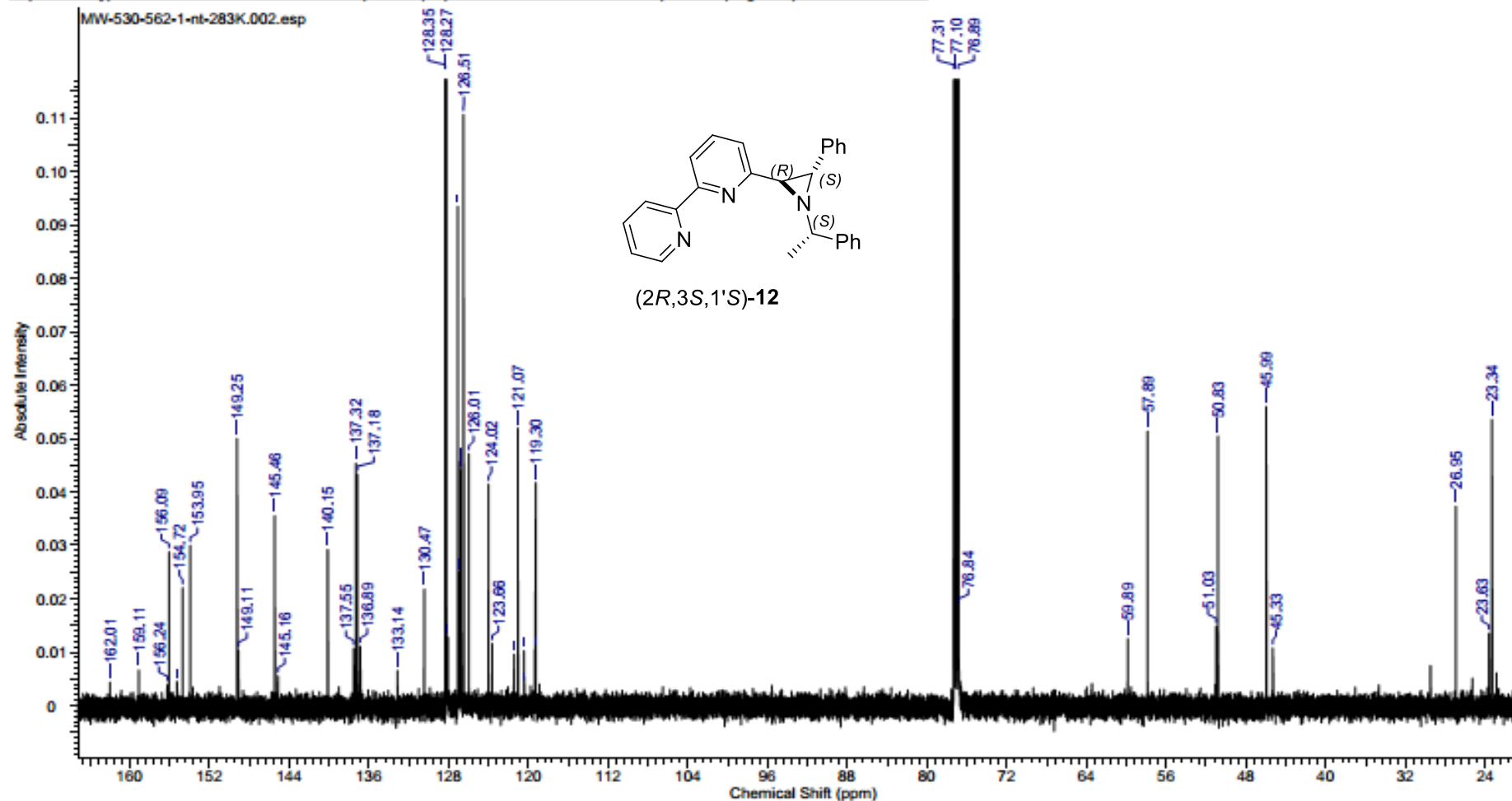


C:\Users\Marcin\Documents\widma NMR\MW-530-562-1-nt-283K\MW-530-562-1-nt-283K.001.esp

Figure S27. ¹H NMR spectrum (283K, 600 MHz, CDCl₃) for (2R,3S,1'S)-12

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.4418	Date	25 Nov 2019 11:48:32	Date Stamp	25 Nov 2019 11:48:32
File Name	C:\Users\Marcin\Documents\widma NMR\MW-530-562-1-nt-283K2\fid	Frequency (MHz)	151.02	Original Points Count	65536
Nucleus	¹³ C	Number of Transients	3680	Origin	spect
Owner	nmsu	Points Count	65536	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	45454.55	Solvent	CHLOROFORM-d	Receiver Gain	2050.00
Spectrum Type	STANDARD	Sweep Width (Hz)	45453.85	Temperature (degree C)	10.000
				Spectrum Offset (Hz)	15101.7109

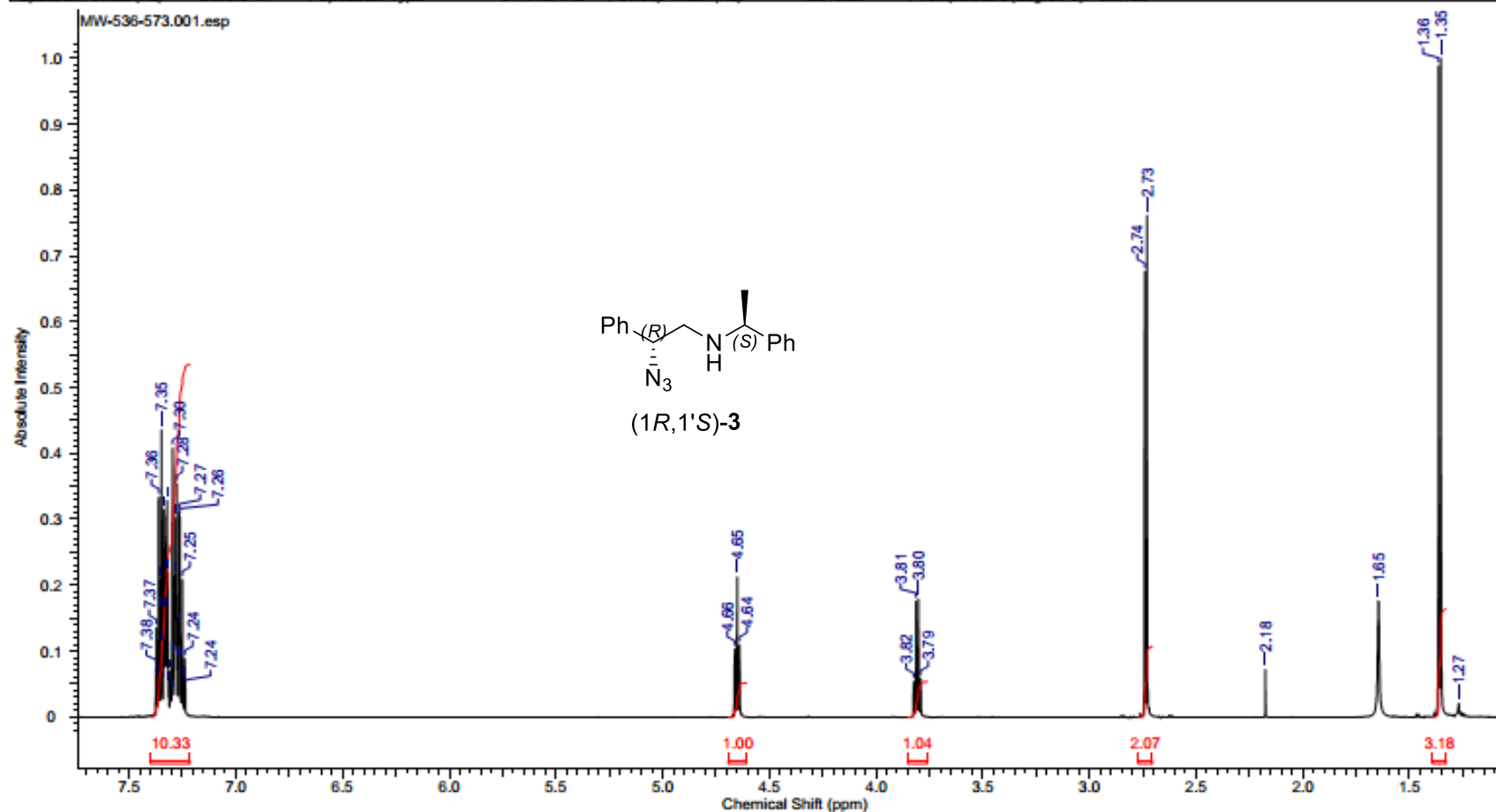


C:\Users\Marcin\Documents\widma NMR\MW-530-562-1-nt-283K\MW-530-562-1-nt-283K.002.esp

Figure S28. ¹³C NMR spectrum (283K, 151 MHz, CDCl₃) for (2R,3S,1'S)-12

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	2.7263	Comment	MBA-NH-CH(Ph)-CH ₂ -N ₃	Date	28 Nov 2019 16:47:12
Date Stamp	28 Nov 2019 16:47:12	File Name	C:\Users\Marcin\Documents\widma NMR\MW-536-573\1\fid		
Frequency (MHz)	600.58	Nucleus	¹ H	Number of Transients	32
Original Points Count	32768	Owner	nmrsu	Points Count	32768
Receiver Gain	203.00	SW(cyclical) (Hz)	12019.23	Pulse Sequence	zg30
Spectrum Offset (Hz)	3690.0164	Spectrum Type	STANDARD	Solvent	CHLOROFORM-d
		Sweep Width (Hz)	12018.86	Temperature (degrees C)	25.100

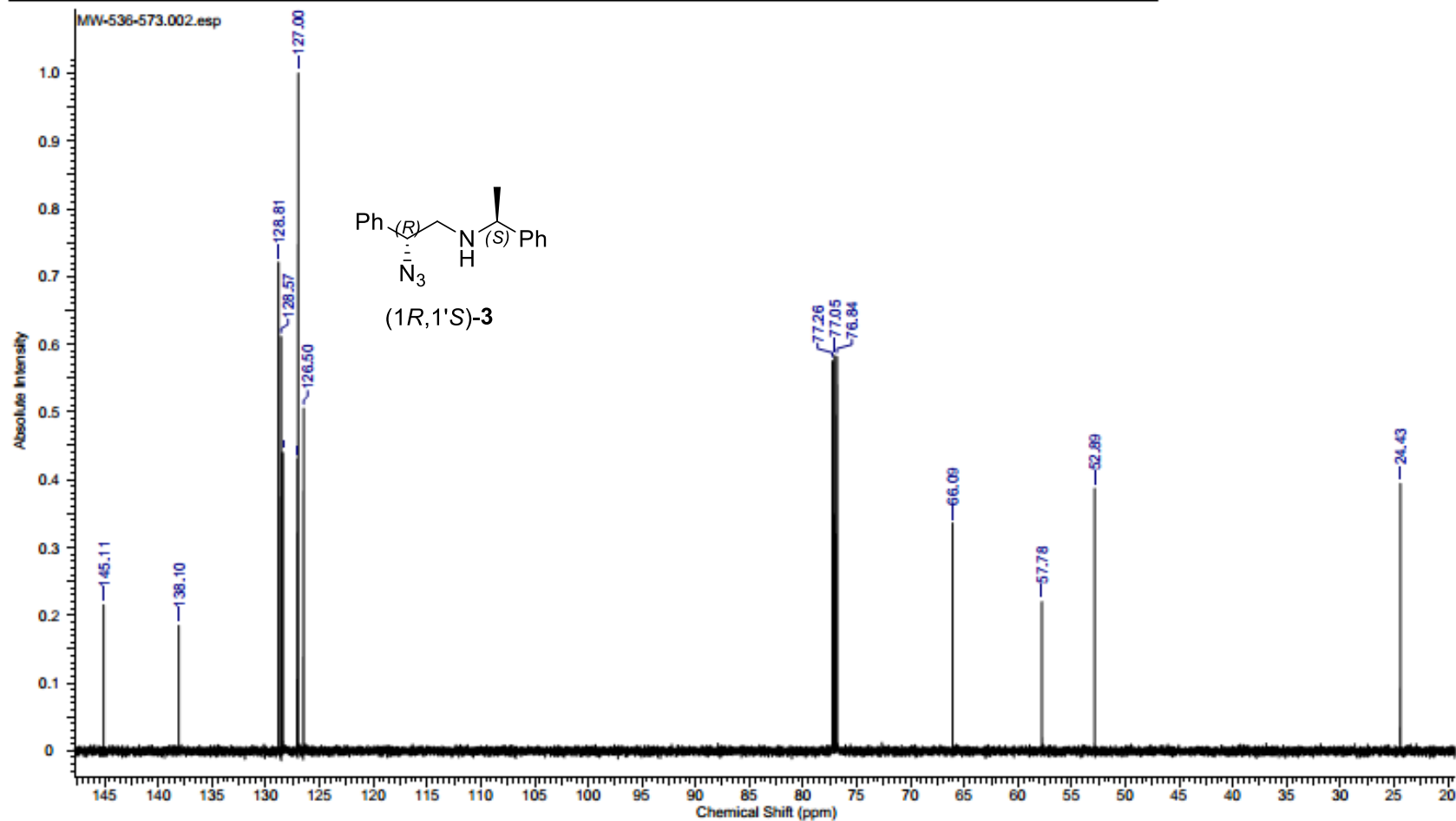


C:\Users\Marcin\Documents\widma NMR\MW-536-573\MW-536-573.001.esp

Figure S29. ¹H NMR spectrum (600 MHz, CDCl₃) for (1R,1'S)-3

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.4418	Date	28 Nov 2019 17:04:16	Date Stamp	28 Nov 2019 17:04:16
File Name	C:\Users\Marcin\Documents\widma NMR\MW-536-573\2\fid	Frequency (MHz)	151.03	Nucleus	13C
Number of Transients	256	Origin	spect	Original Points Count	65536
Pulse Sequence	zgpg30	Receiver Gain	2050.00	SW(cyclical) (Hz)	45454.55
Spectrum Offset (Hz)	15101.7100	Spectrum Type	STANDARD	Sweep Width (Hz)	45453.85
				Solvent	CHLOROFORM-d
				Temperature (degree C)	25.000

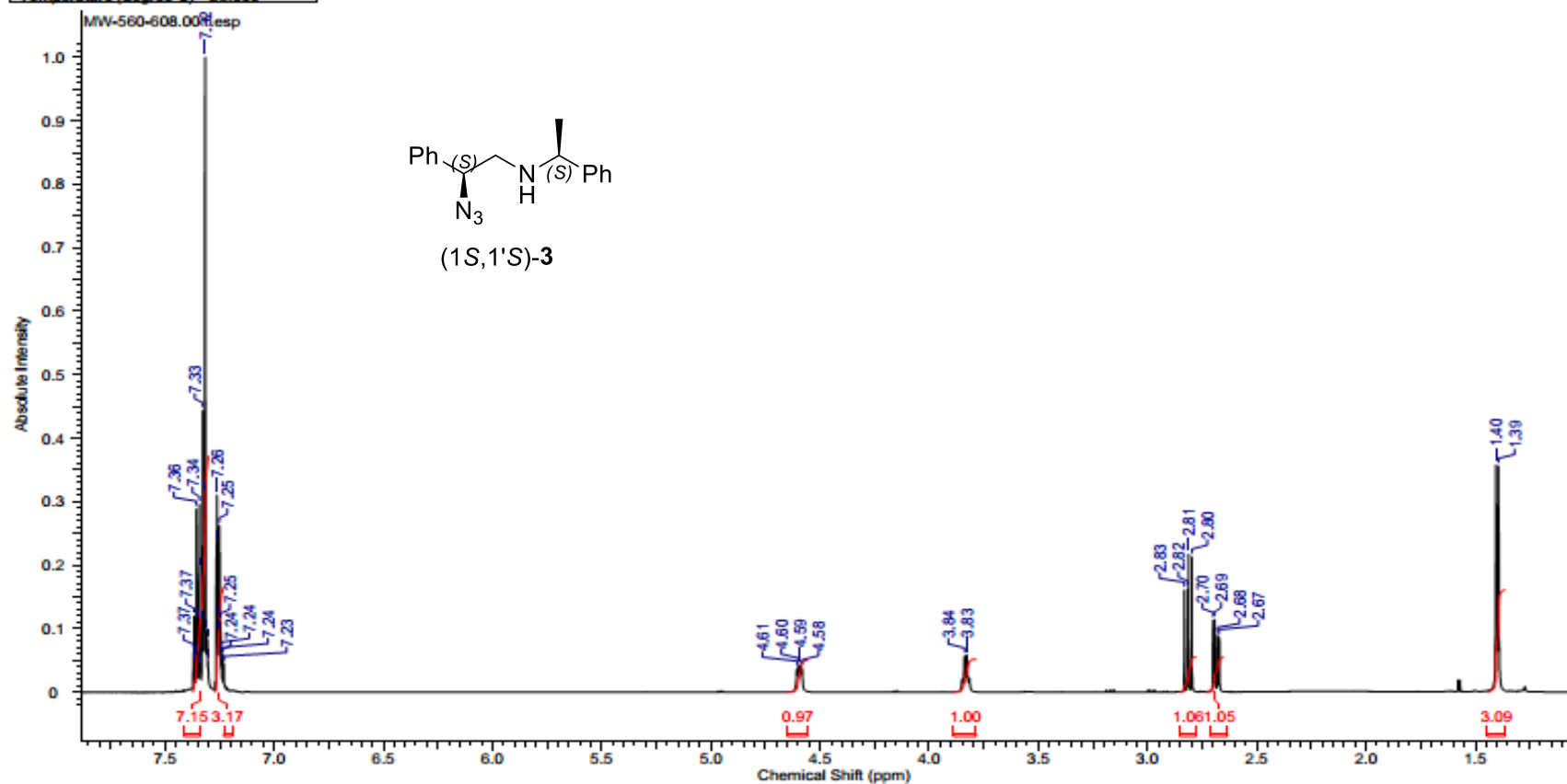


C:\Users\Marcin\Documents\widma NMR\MW-536-573\MW-536-573.002.esp

Figure S30. ^{13}C NMR spectrum (151 MHz, CDCl_3) for (1R,1'S)-3

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

This report was created by ACD/NAME Processor Academic Edition. For more information go to www.aculabs.com/nmr/prod/									
Acquisition Time (sec)	2.7263	Comment	3b ?	Date	31 Jan 2020 08:42:56				
Date Stamp	31 Jan 2020 08:42:56			File Name	C:\Users\Marcin\Documents\widma NMR\MW-560-608\1\fid				
Frequency (MHz)	600.58	Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmsu	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	181.00	SW(cyclical) (Hz)	12019.23
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	3690.0164	Spectrum Type	STANDARD	Sweep Width (Hz)	12018.86
Temperature (degree C)	25.000								



C:\Users\Marcin\Documents\widma NMR\MW-560-608\MW-560-608.001.esp

Figure S31. ¹H NMR spectrum (600 MHz, CDCl₃) for (1S,1'S)-3

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.4418	Date	31 Jan 2020 08:45:04	Date Stamp	31 Jan 2020 08:45:04
File Name	C:\Users\Marcin\Documents\widma NMR\MW-560-608\2\fid	Frequency (MHz)	151.02	Nucleus	13C
Number of Transients	256	Origin	spect	Original Points Count	65536
Pulse Sequence	zgpg30	Receiver Gain	2050.00	SW(cyclical) (Hz)	45454.55
Spectrum Offset (Hz)	15101.7109	Spectrum Type	STANDARD	Sweep Width (Hz)	45453.85
				Temperature (degree C)	25.100

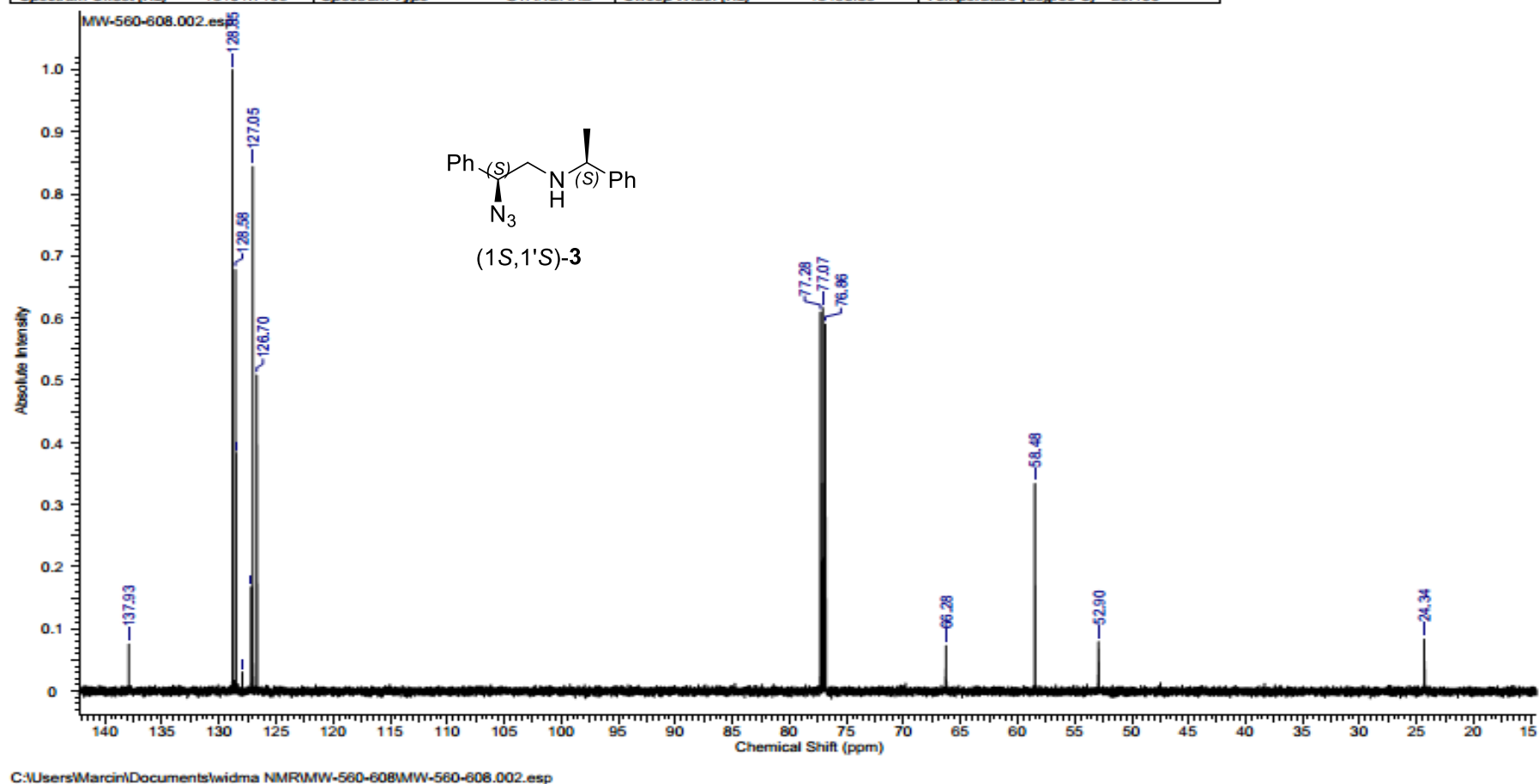


Figure S32. ^{13}C NMR spectrum (151 MHz, CDCl_3) for (1S,1'S)-3

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.2716	Comment	single pulse	Date	04 Dec 2019 10:53:46
Date Stamp	04 Dec 2019 10:51:57	File Name	C:\Users\Marcin\Documents\widma NMR\MW-538-578-3 Proton-1-1.jdf		
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Owner	Delta	Points Count	32768
Solvent	CHLOROFORM-d	Pulse Sequence	proton.jxp		
Temperature (degree C)	22.400	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	10016.03

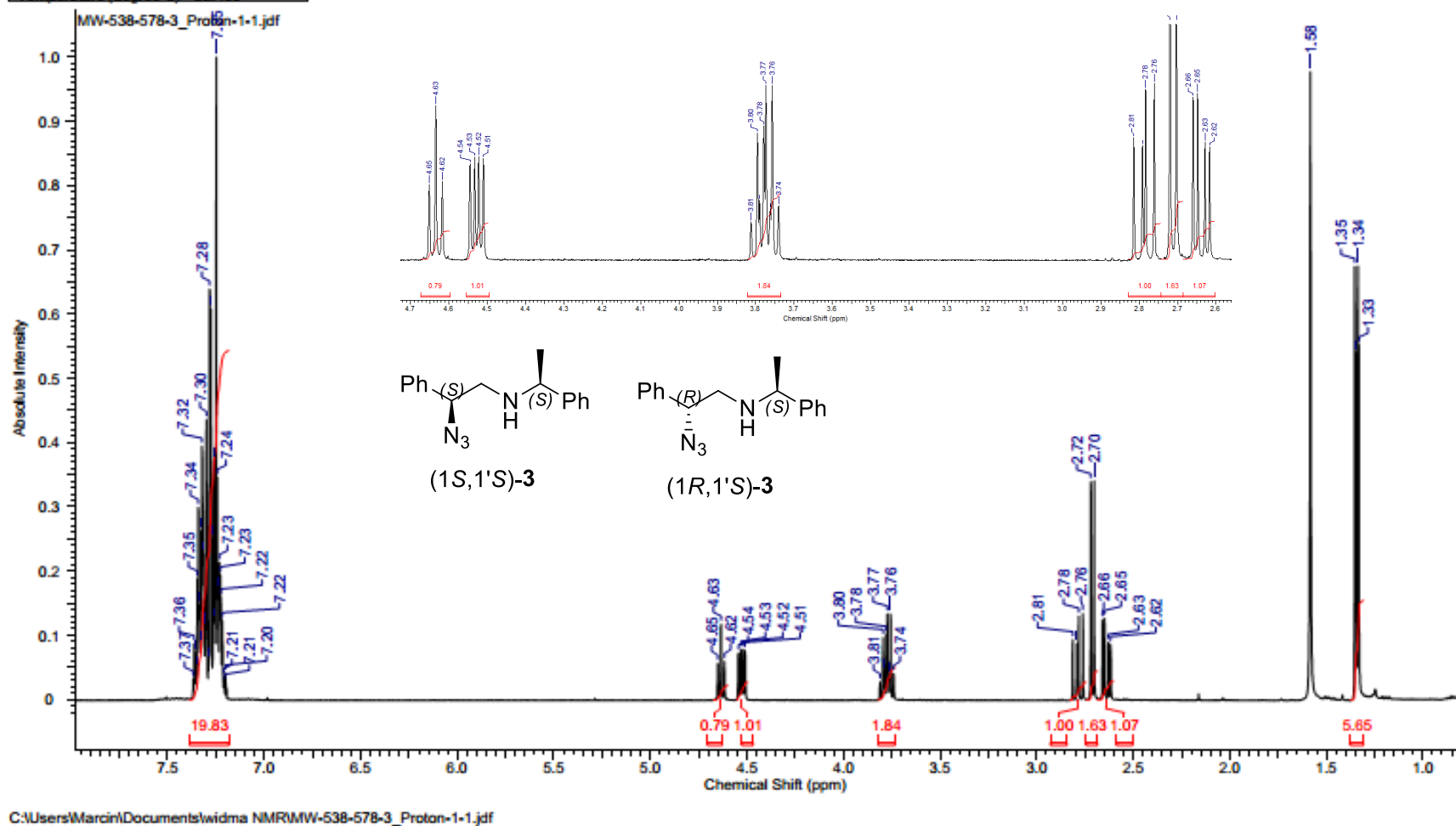


Figure S33. ^1H NMR spectrum (400 MHz, CDCl_3) for (1R,1'S)-3 and (1S,1'S)-3

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.2716	Comment	single pulse	Date	11 Dec 2019 11:20:13
Date Stamp	11 Dec 2019 11:18:23	File Name	C:\Users\Marcin\Documents\widma NMR\MW-546-587-1 Proton-2-1.jdf		
Frequency (MHz)	399.78	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Owner	Delta	Points Count	32768
Solvent	CHLOROFORM-d	Pulse Sequence	proton.jxp		
Temperature (degree C)	22.700	Spectrum Offset (Hz)	2398.6931	Sweep Width (Hz)	10016.03

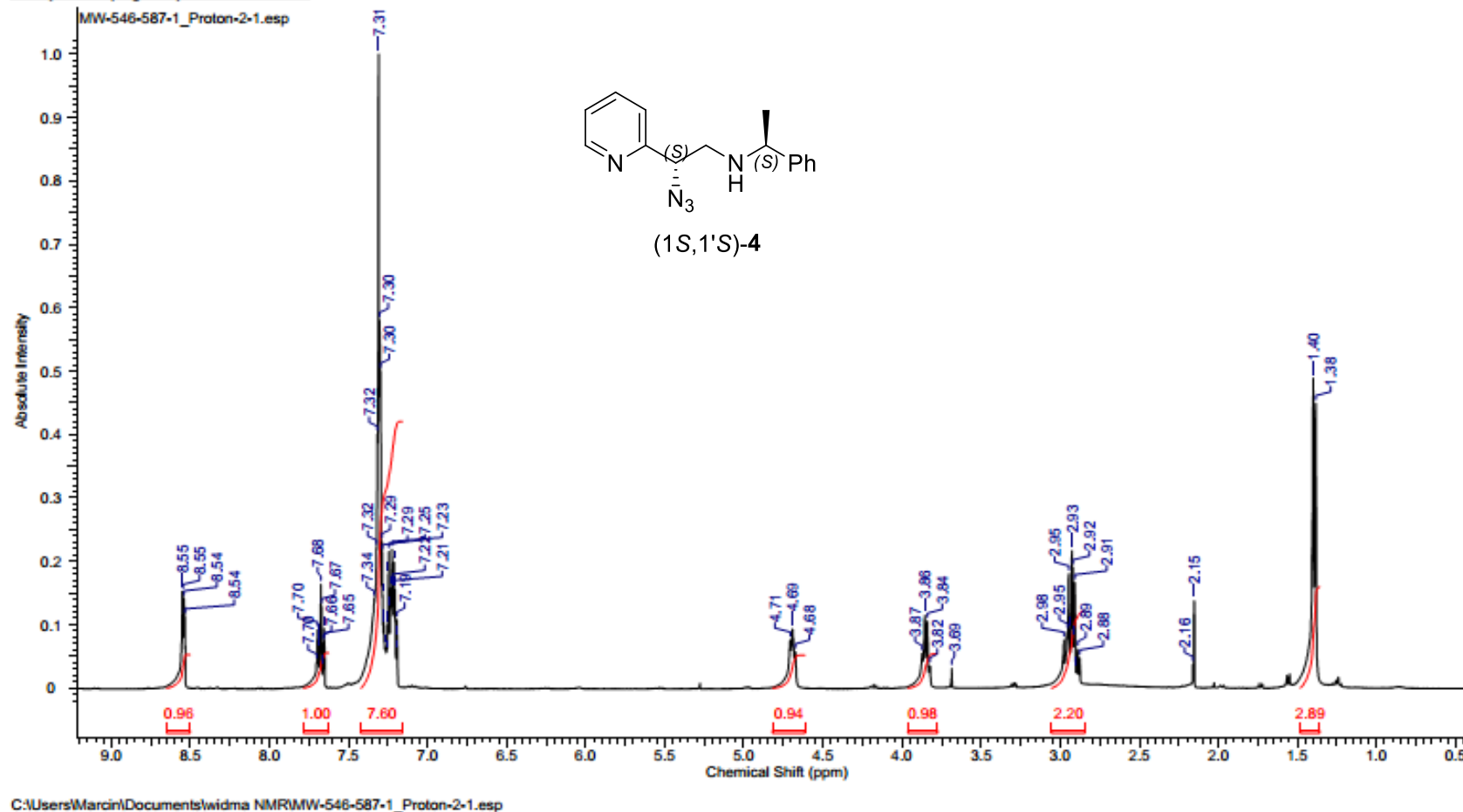
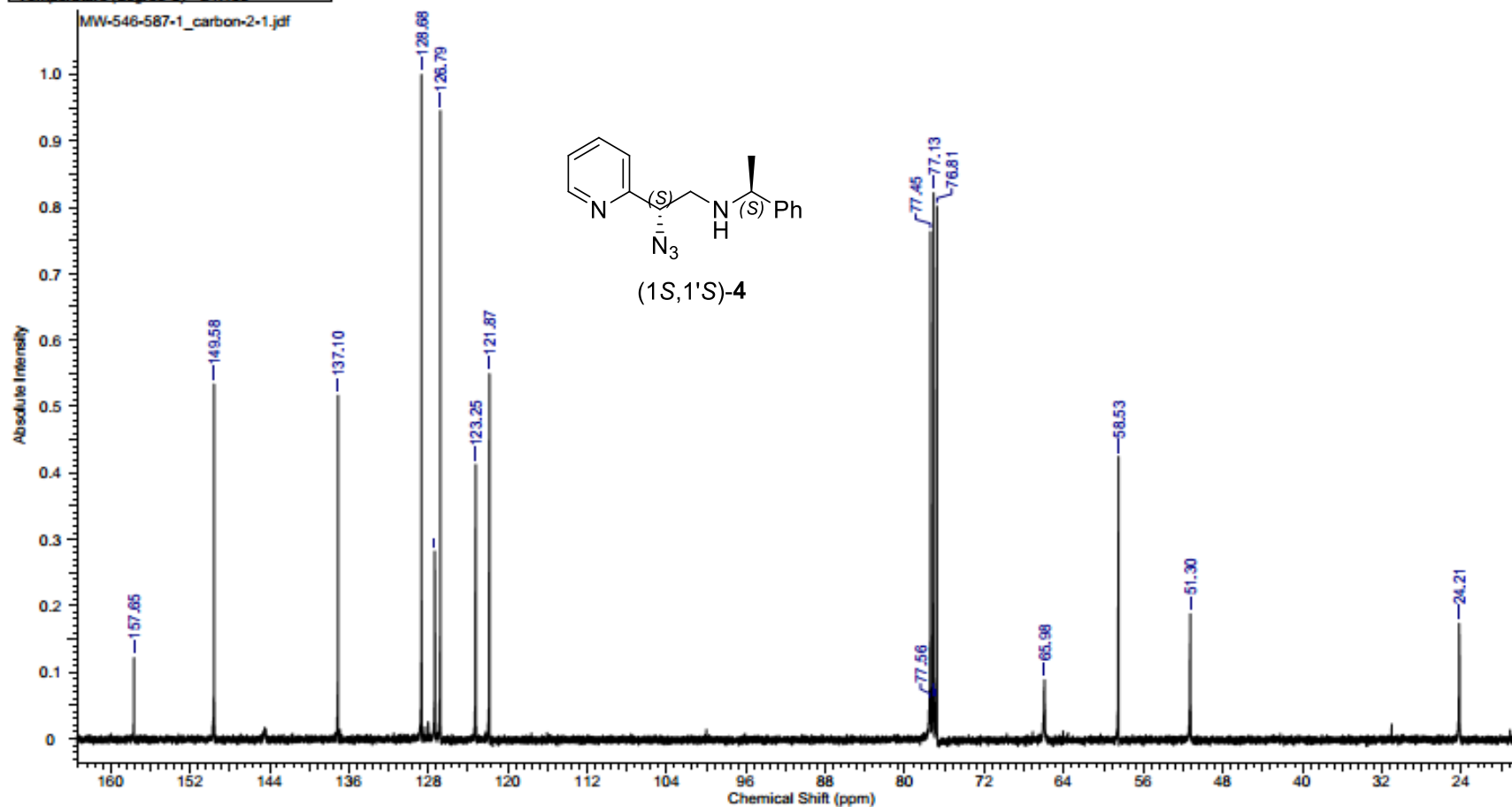


Figure S34. ¹H NMR spectrum (400 MHz, CDCl₃) for (1S,1'S)-4

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.7406	Comment	single pulse decoupled gated NOE	Date	13 Dec 2019 05:42:39
Date Stamp	12 Dec 2019 17:52:50	File Name	C:\Users\Marcin\Documents\widma NMRMW-546-587-1 carbon-2-1.jdf	Origin	ECA
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	7631
Original Points Count	65536	Owner	Delta	Points Count	65536
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10052.5303	Pulse Sequence	carbon.jxp
Temperature (degree C)	21.100	Sweep Width (Hz)	37650.60		



C:\Users\Marcin\Documents\widma NMRMW-546-587-1 carbon-2-1.jdf

Figure S35. ¹³C NMR spectrum (101 MHz, CDCl₃) for (1S,1'S)-4

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	2.7263	Comment	aziridine attempted opening with HN3 (298K)		Date	26 Nov 2019 15:17:36	
Date Stamp	26 Nov 2019 15:17:36		File Name	C:\Users\Marcin\Documents\widma NMR\MW-553-571\11Vid			
Frequency (MHz)	600.58	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	32768	Owner	nmrsu	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	161.00	SW(cyclical) (Hz)	12019.23	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	3690.0164	Spectrum Type	STANDARD	Sweep Width (Hz)	12018.86	Temperature (degree C)	25.000

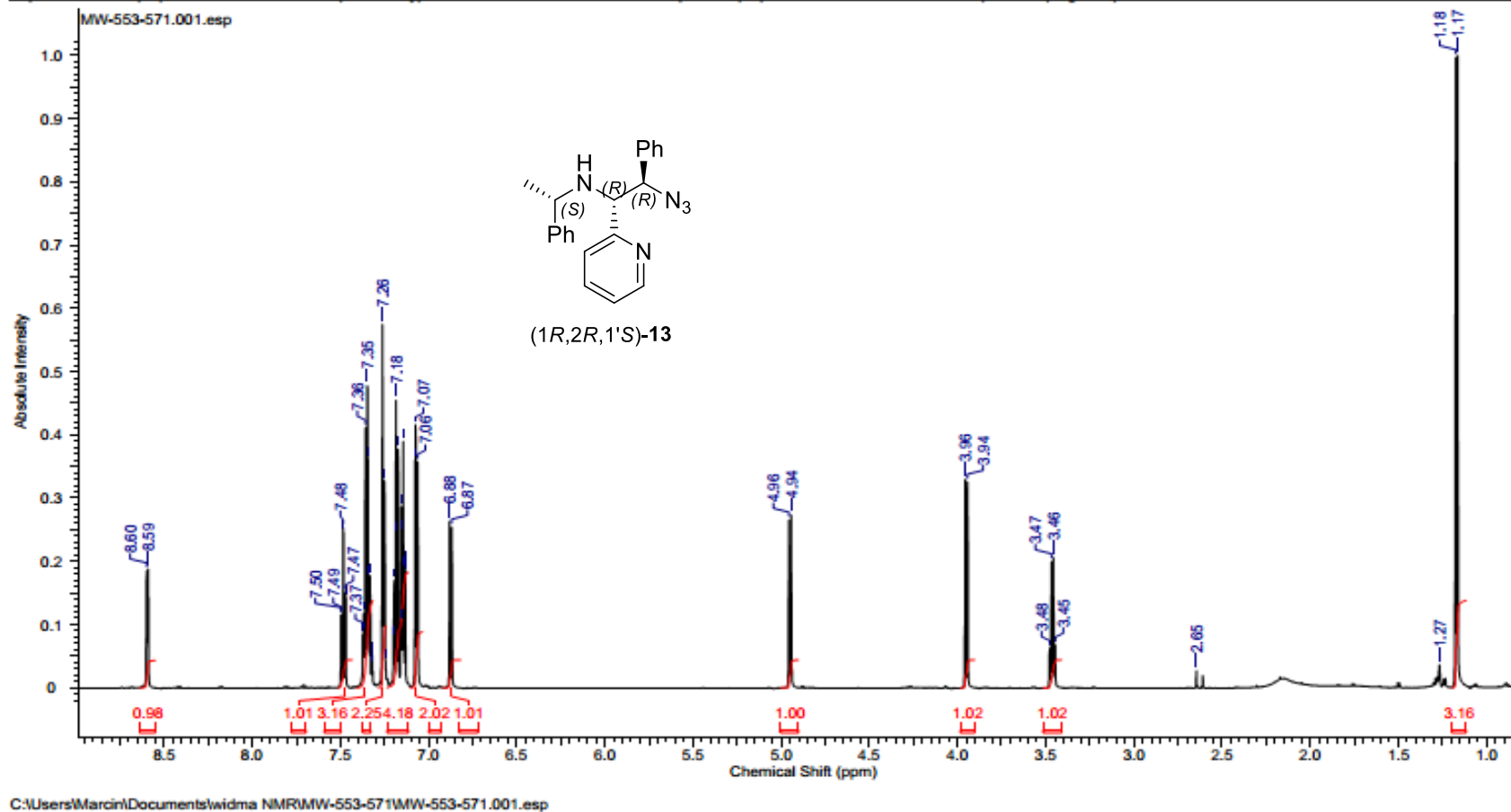
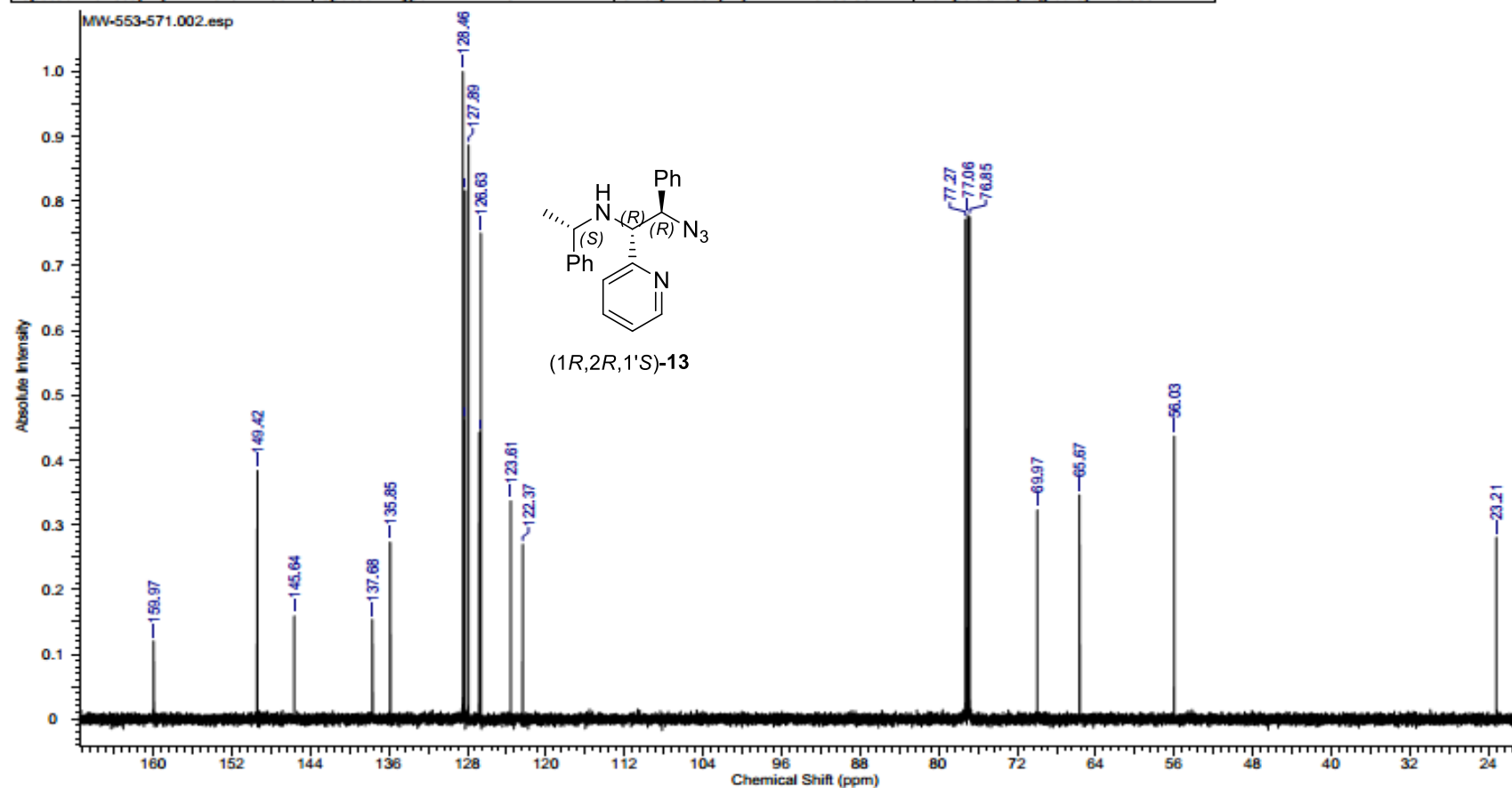


Figure S36. ^1H NMR spectrum (600 MHz, CDCl_3) for (1R,2R,1'S)-13

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.4418	Date	26 Nov 2019 15:32:32	Date Stamp	26 Nov 2019 15:32:32
File Name	C:\Users\Marcin\Documents\widma NMR\MW-553-571\2Mid	Frequency (MHz)	151.02	Nucleus	13C
Number of Transients	256	Origin	spect	Original Points Count	65536
Pulse Sequence	zgpg30	Receiver Gain	2050.00	SW(cyclical) (Hz)	45454.55
Spectrum Offset (Hz)	15101.7109	Spectrum Type	STANDARD	Sweep Width (Hz)	45453.85
				Temperature (degree C)	25.000

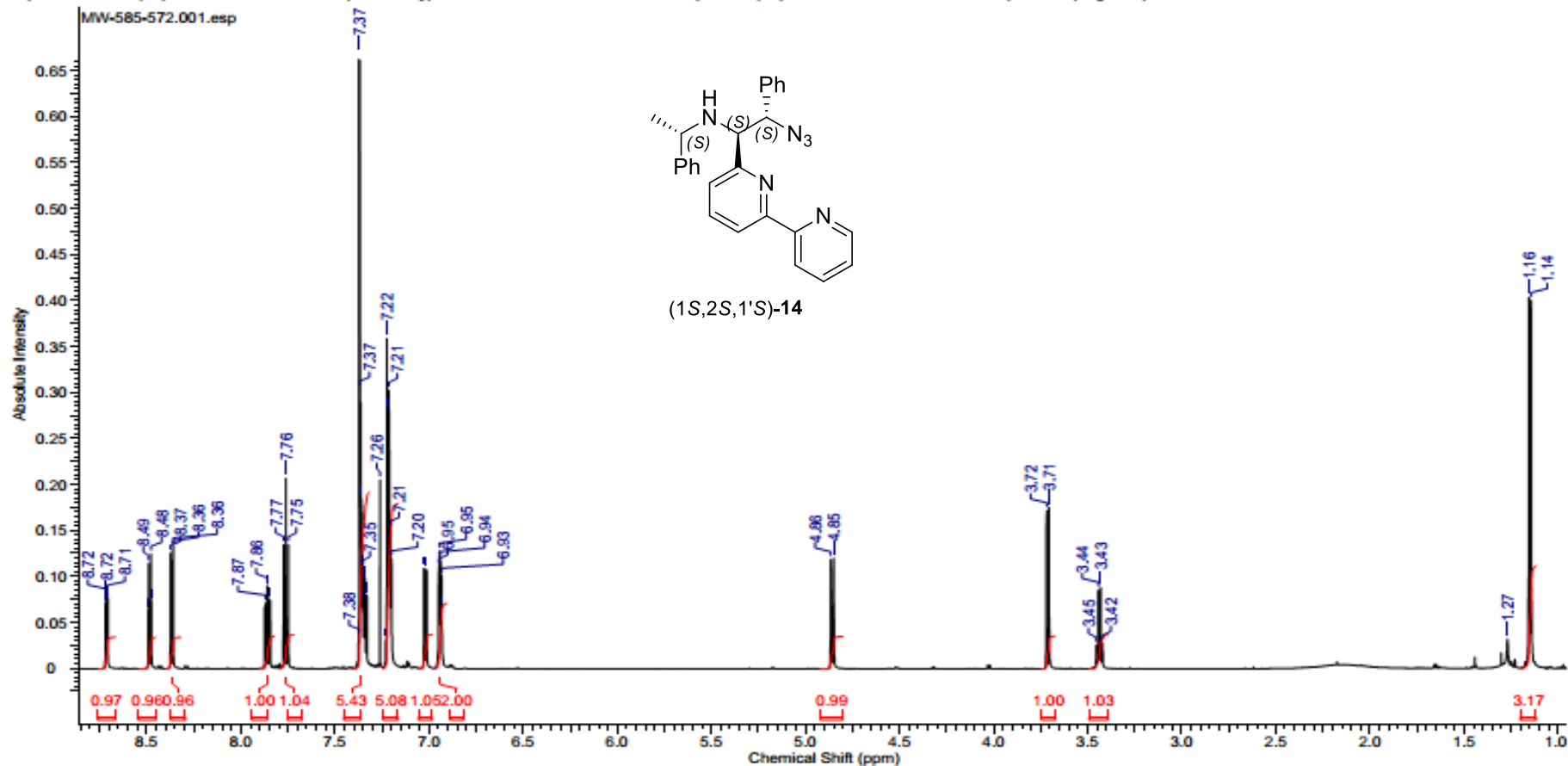


C:\Users\Marcin\Documents\widma NMR\MW-553-571\MW-553-571.002.esp

Figure S37. ^{13}C NMR spectrum (151 MHz, CDCl_3) for (1R,2R,1'S)-13

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

This report was created by ACD/NAME 1 released Academic Edition. For more information go to www.acdlabs.com/mr/prof							
Acquisition Time (sec)	2.7263	Comment	MBA-NH-CH(Bipy)-CH(Ph)-N3 or regioisom.			Date	28 Nov 2019 17:49:04
Date Stamp	28 Nov 2019 17:49:04		File Name	C:\Users\Marcin\Documents\widma NMR\MW-585-572\1Vid			
Frequency (MHz)	600.58	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	32768	Owner	nmrsu	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	203.00	SW(cyclical) (Hz)	12019.23	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	3690.0164	Spectrum Type	STANDARD	Sweep Width (Hz)	12018.86	Temperature (degree C)	25.000

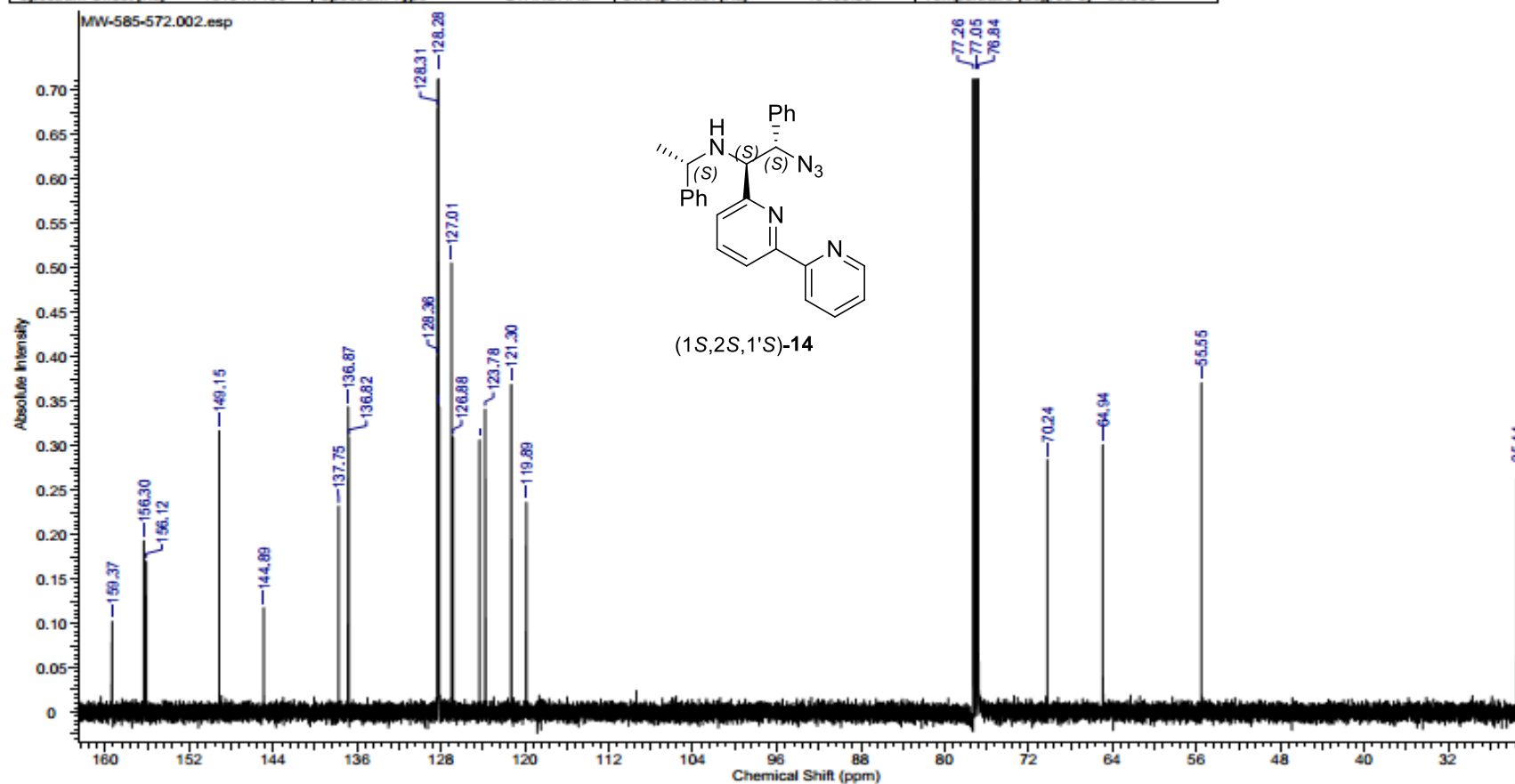


C:\Users\Marcin\Documents\widma NMR\MW-585-572\MW-585-572.001.esp

Figure S38. ^1H NMR spectrum (600 MHz, CDCl_3) for (1S,2S,1'S)-14

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.4418	Date	28 Nov 2019 18:06:08	Date Stamp	28 Nov 2019 18:06:08
File Name	C:\Users\Marcin\Documents\widma NMR\MW-585-572\2Mid	Frequency (MHz)	151.03	Nucleus	13C
Number of Transients	256	Origin	spect	Original Points Count	65536
Pulse Sequence	zpgq30	Receiver Gain	2050.00	SW(cyclical) (Hz)	45454.55
Spectrum Offset (Hz)	15101.7100	Spectrum Type	STANDARD	Sweep Width (Hz)	45453.85
				Solvent	CHLOROFORM-d
				Temperature (degree C)	25.000

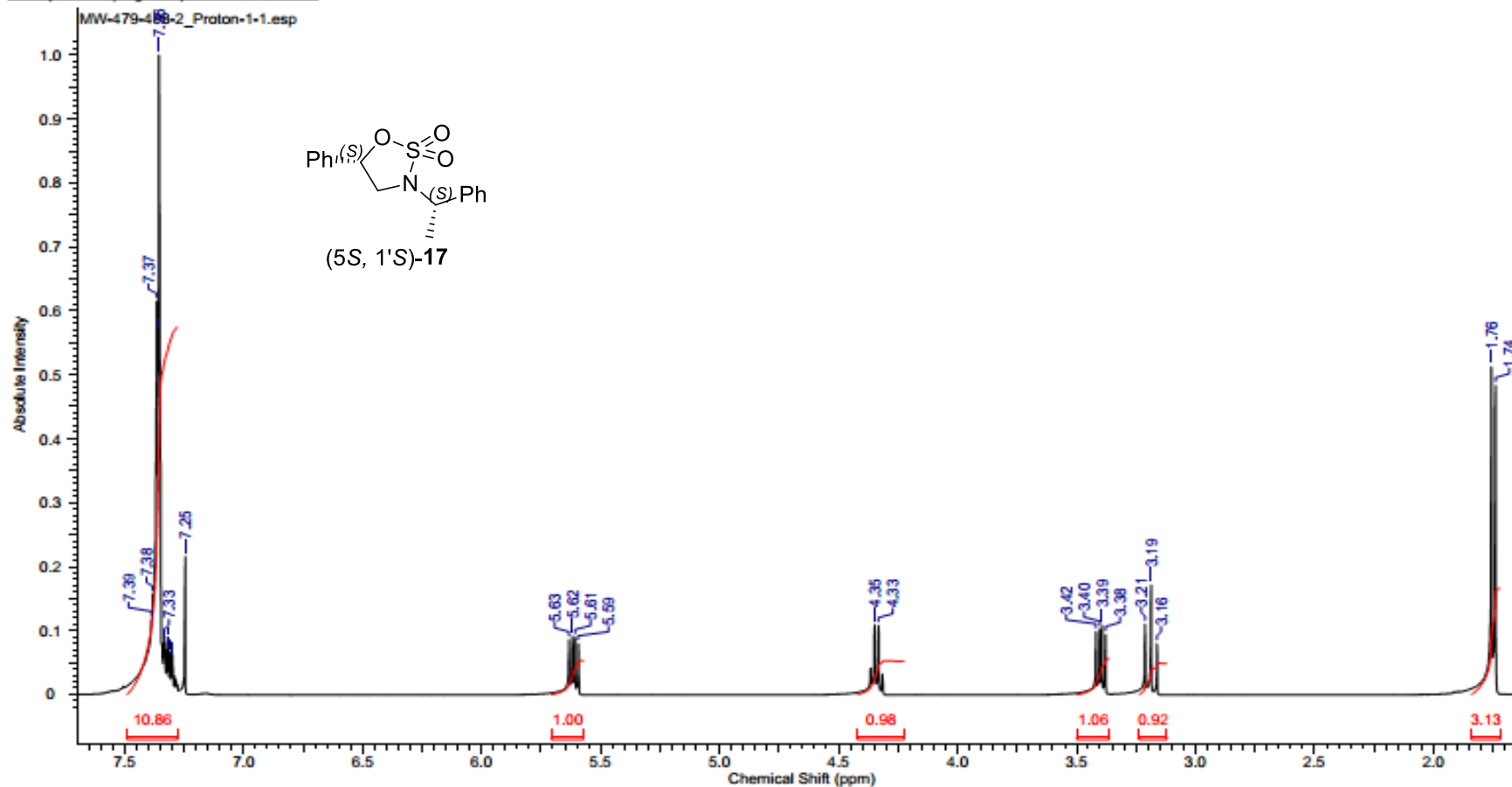


C:\Users\Marcin\Documents\widma NMR\MW-585-572\MW-585-572.002.esp

Figure S39. ^{13}C NMR spectrum (151 MHz, CDCl_3) for (1S,2S,1'S)-14

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.2716	Comment	single pulse	Date	28 Aug 2019 08:00:53
Date Stamp	28 Aug 2019 07:59:04			File Name	C:\Users\Marcin\Documents\widma NMR\MW-479-498-2 Proton-1-1.jdf
Frequency (MHz)	399.78	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Owner	Delta	Points Count	32768
Solvent	CHLOROFORM-d			Pulse Sequence	proton.jxp
Temperature (degrees C)	23.000			Spectrum Offset (Hz)	2398.6931
				Sweep Width (Hz)	10016.03

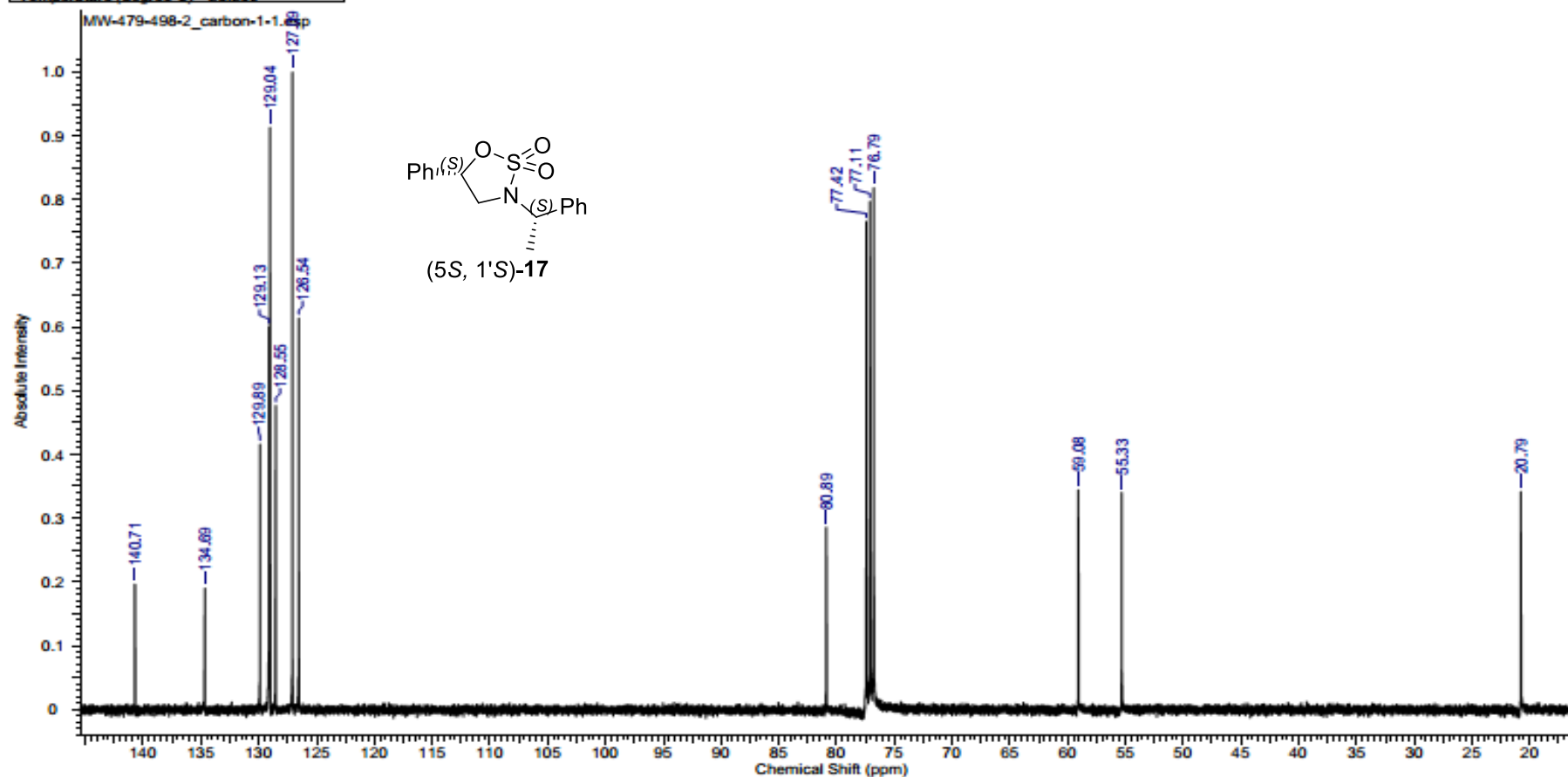


C:\Users\Marcin\Documents\widma NMR\MW-479-498-2_Proton-1-1.esp

Figure S40. ¹H NMR spectrum (400 MHz, CDCl₃) for (5S,1'S)-17

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.7406	Comment	single pulse decoupled gated NOE	Date	28 Aug 2019 16:10:16
Date Stamp	28 Aug 2019 13:00:21	File Name	C:\Users\Marcin\Documents\widma NMR\MW-479-498-2_carbon-1-1.jdf	Origin	ECA
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	4000
Original Points Count	65536	Owner	Delta	Points Count	65536
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10052.5303	Pulse Sequence	carbon.jxp
Temperature (degree C)	23.200	Sweep Width (Hz)	37650.60		

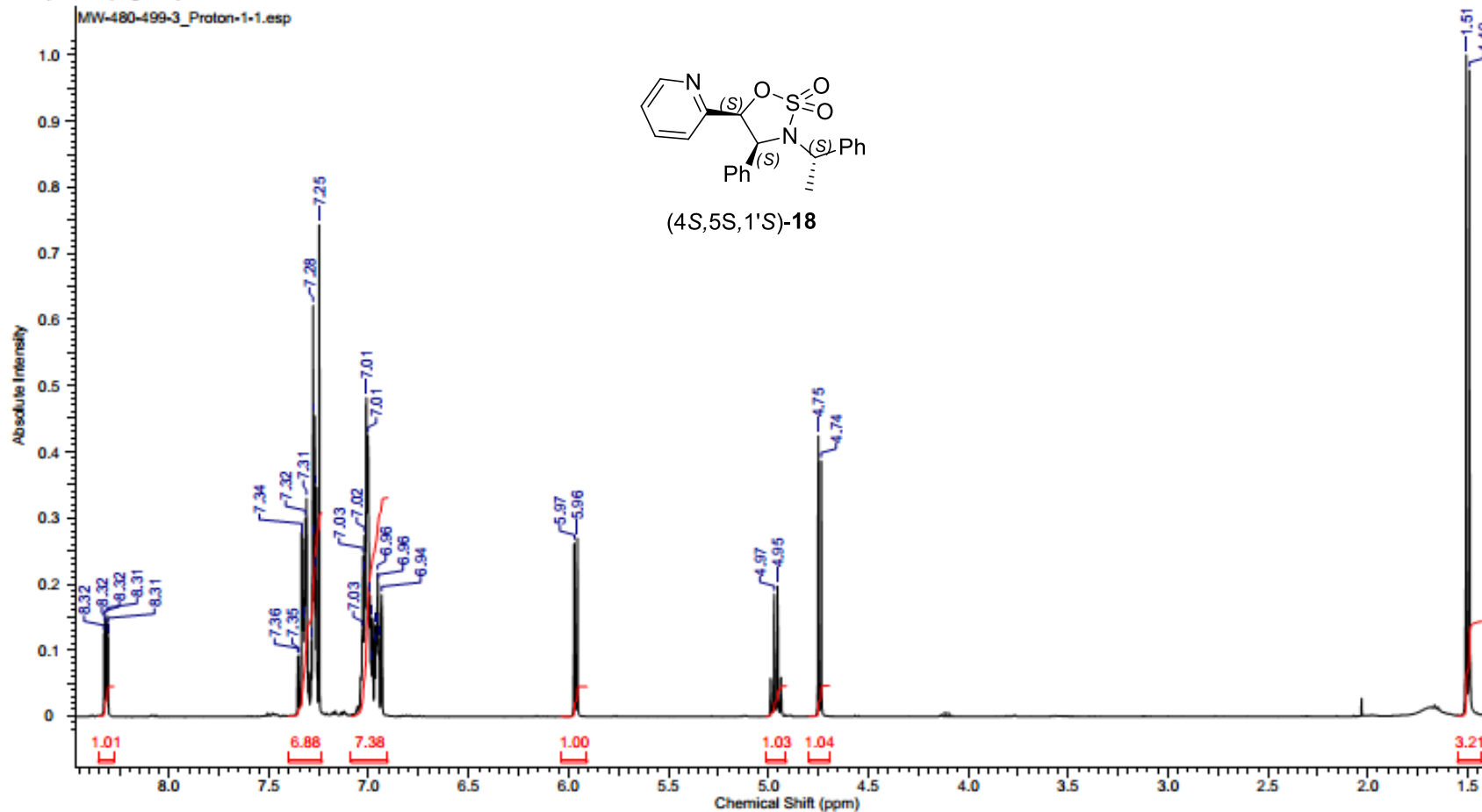


C:\Users\Marcin\Documents\widma NMR\MW-479-498-2_carbon-1-1.esp

Figure S41. ^{13}C NMR spectrum (101 MHz, CDCl_3) for (5S,1'S)-17

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.2716	Comment	single pulse	Date	24 Sep 2019 07:24:37
Date Stamp	24 Sep 2019 07:21:07			File Name	C:\Users\Marcin\Documents\widma NMR\MW-480-499-3 Proton-1-1.jdf
Frequency (MHz)	399.78	Nucleus	¹ H	Number of Transients	32
Original Points Count	32768	Owner	Delta	Points Count	32768
Solvent	CHLOROFORM-d			Pulse Sequence	proton.jxp
Temperature (degree C)	21.000			Spectrum Offset (Hz)	2398.6931
				Sweep Width (Hz)	10016.03

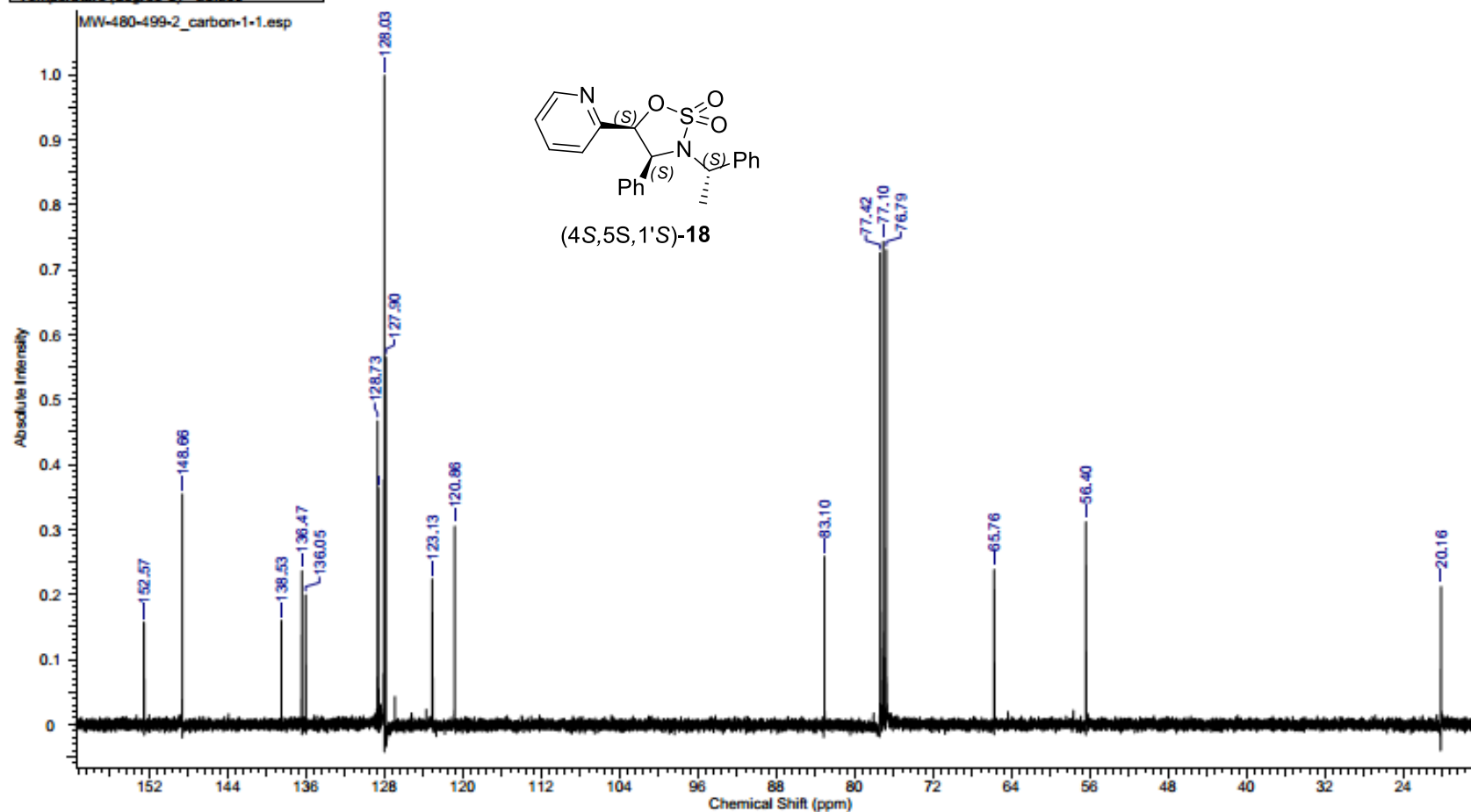


C:\Users\Marcin\Documents\widma NMR\MW-480-499-3_Proton-1-1.esp

Figure S42. ¹H NMR spectrum (400 MHz, CDCl₃) for (4S,5S,1'S)-18

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.7406	Comment	single pulse decoupled gated NOE	Date	28 Aug 2019 12:56:26
Date Stamp	28 Aug 2019 11:45:03	File Name	C:\Users\Marcin\Documents\widma NMR\MW-480-499-2_carbon-1-1.jdf		
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	1500
Original Points Count	65536	Owner	Delta	Points Count	65536
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10052.5303	Pulse Sequence	carbon.jsp
Temperature (degree C)	23.200	Sweep Width (Hz)	37650.60		

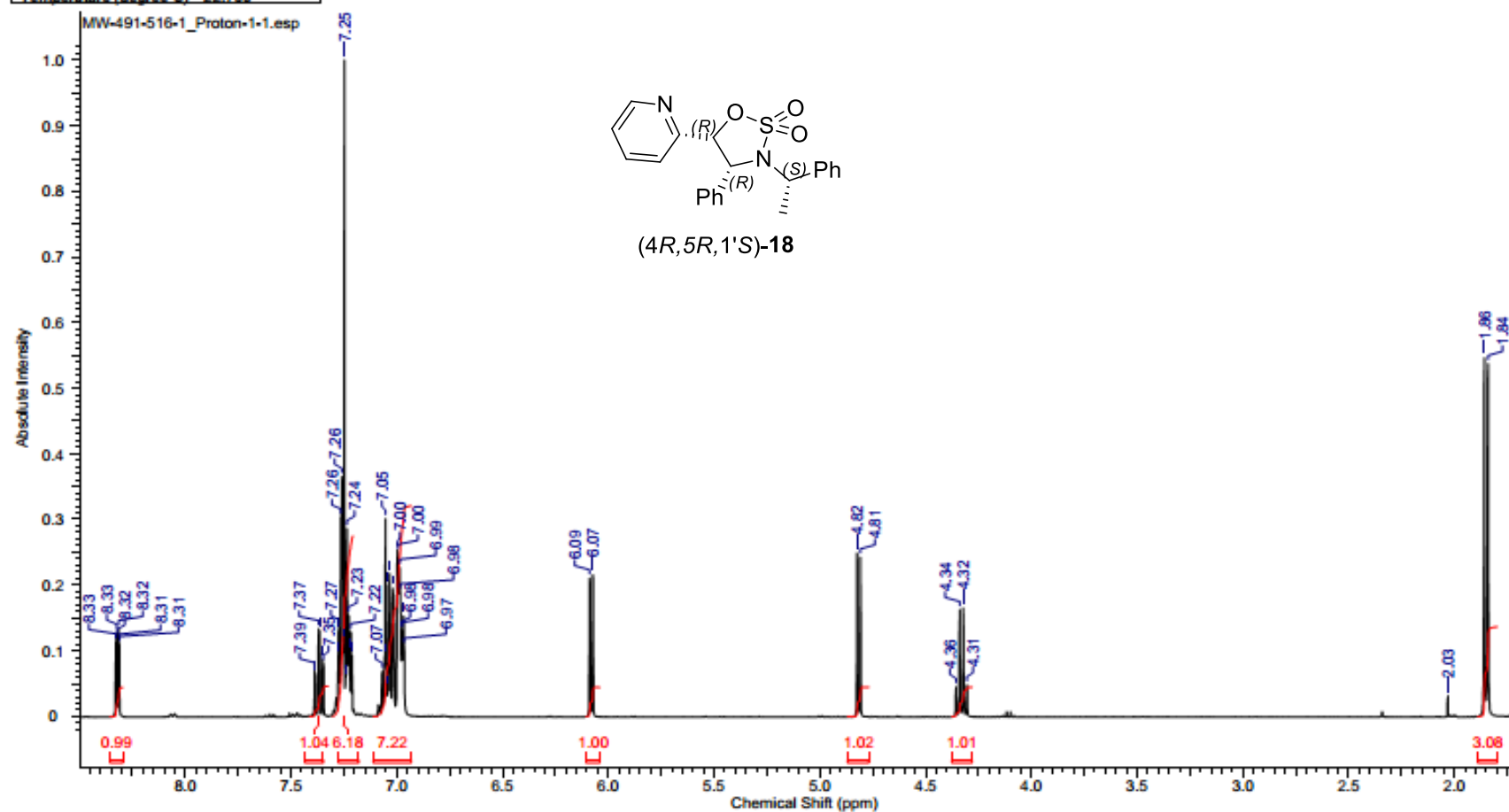


C:\Users\Marcin\Documents\widma NMR\MW-480-499-2_carbon-1-1.esp

Figure S43. ¹³C NMR spectrum (101 MHz, CDCl₃) for (4S,5S,1'S)-18

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.2716	Comment	single pulse	Date	03 Oct 2019 08:44:45
Date Stamp	03 Oct 2019 08:41:15			File Name	C:\Users\Marcin\Documents\widma NMR\MW-491-516-1 Proton-1-1.jdf
Frequency (MHz)	399.78	Nucleus	¹ H	Number of Transients	32
Original Points Count	32768	Owner	Delta	Points Count	32768
Solvent	CHLOROFORM-d			Pulse Sequence	proton.jxp
Temperature (degree C)	22.700			Spectrum Offset (Hz)	2398.6931
				Sweep Width (Hz)	10016.03



C:\Users\Marcin\Documents\widma NMR\MW-491-516-1_Proton-1-1.esp

Figure S44. ¹H NMR spectrum (400 MHz, CDCl₃) for (4R,5R,1'S)-18

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.7408	Comment	single pulse decoupled gated NOE	Date	07 Oct 2019 15:13:29
Date Stamp	07 Oct 2019 13:38:24	File Name	C:\Users\Marcin\Documents\widma NMR\MW-491-516-1_carbon-1-1.jdf		
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	2000
Original Points Count	65536	Owner	Delta	Points Count	65536
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10052.5303	Pulse Sequence	carbon.jsp
Temperature (degree C)	22.900	Sweep Width (Hz)	37650.60		

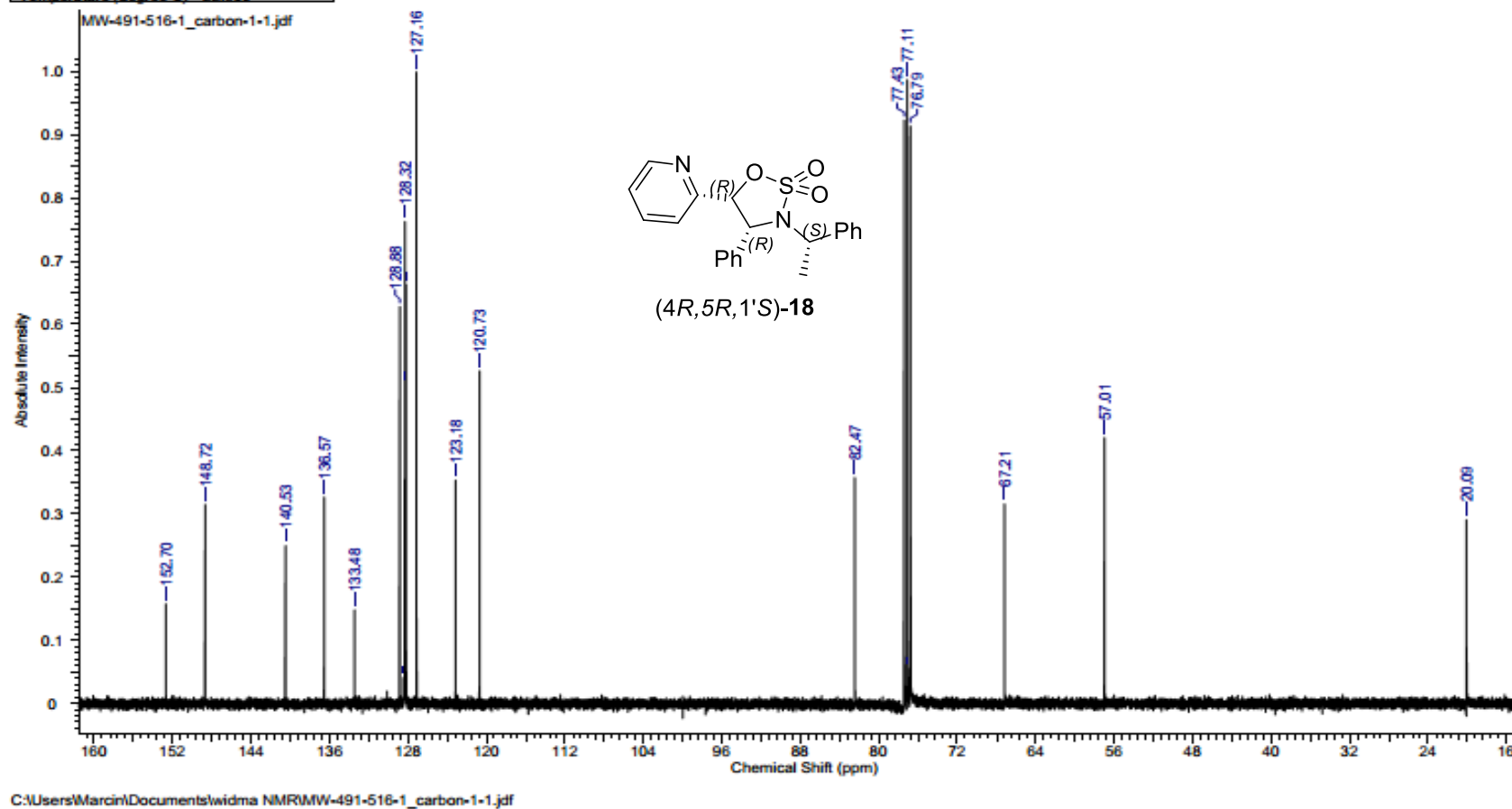


Figure S45. ^{13}C NMR spectrum (101 MHz, CDCl_3) for (4R,5R,1'S)-18

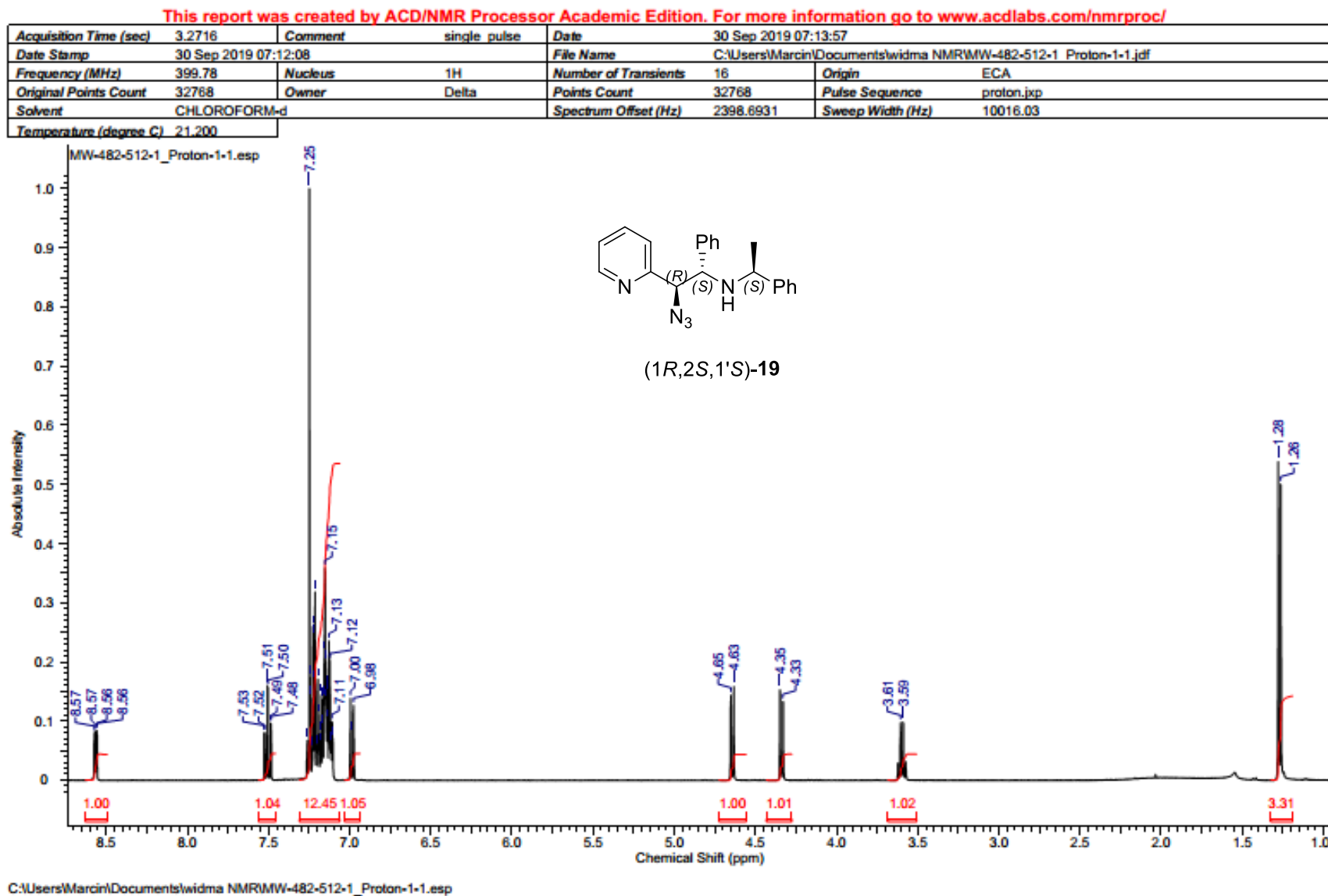


Figure S46. ¹H NMR spectrum (400 MHz, CDCl₃) for (1R,2S,1'S)-19

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.7406	Comment	single pulse decoupled gated NOE	Date	01 Oct 2019 10:16:13
Date Stamp	01 Oct 2019 07:47:13	File Name	C:\Users\Marcin\Documents\widma NMR\MW-482-512-1 carbon-1-1.jdf	Origin	ECA
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	3137
Original Points Count	65536	Owner	Delta	Points Count	65536
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10052.5303	Pulse Sequence	carbon.jxp
Temperature (degree C)	21.500	Sweep Width (Hz)	37650.60		

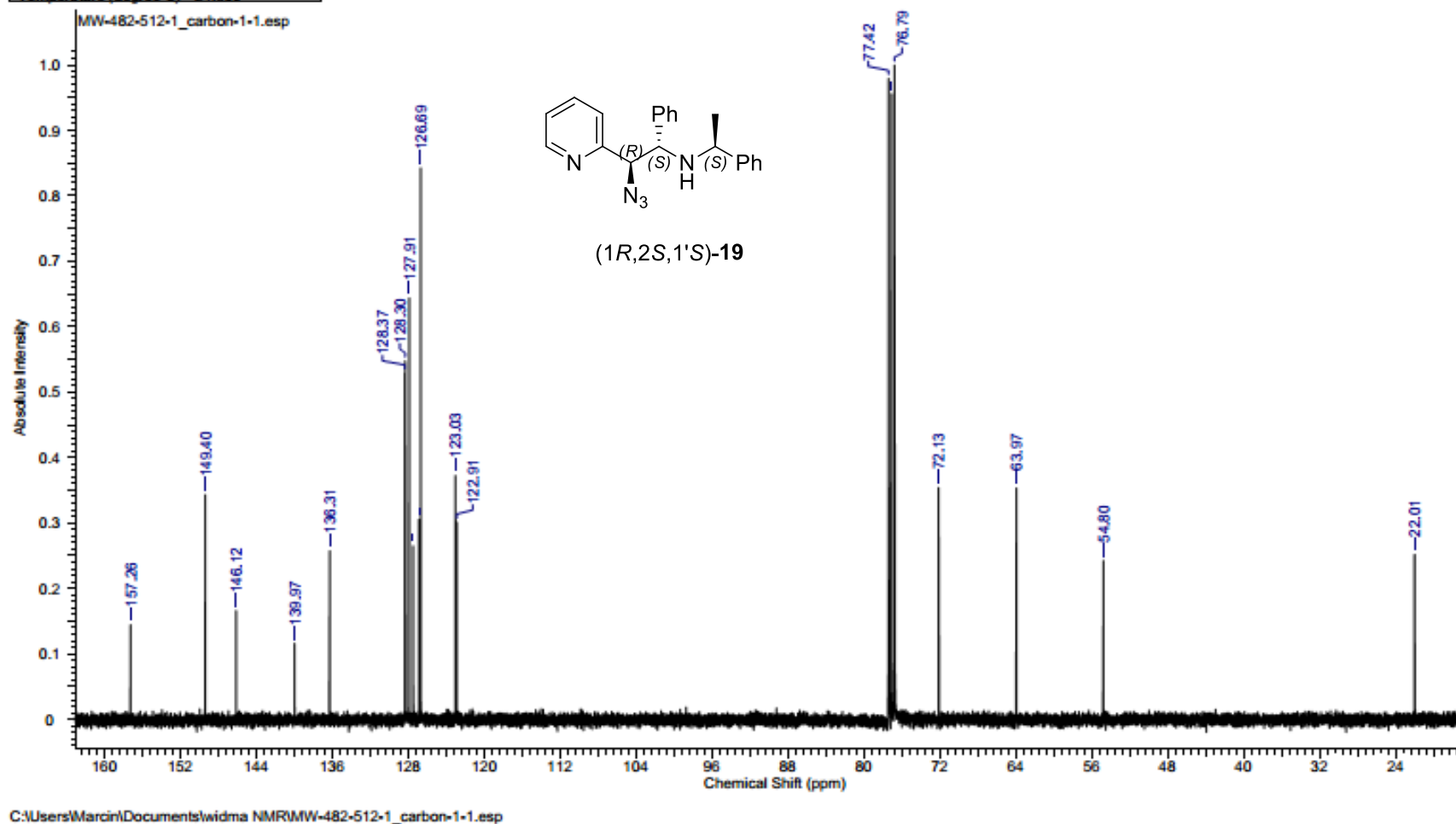


Figure S47. ¹³C NMR spectrum (101 MHz, CDCl₃) for (1R,2S,1'S)-19

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	2.7263	Comment	5 mm PABBO BB-1HVD Z-GRD Z847801/0325	Date	28 Nov 2019 15:43:12
Date Stamp	28 Nov 2019 15:43:12	File Name	C:\Users\Marcin\Documents\widma NMR\MW-492-517-1\1\1\fid	Origin	spect
Frequency (MHz)	600.58	Nucleus	1H	Number of Transients	32
Original Points Count	32768	Owner	nmsu	Points Count	32768
Receiver Gain	287.00	SW(cyclical) (Hz)	12019.23	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	3690.0164	Spectrum Type	STANDARD	Sweep Width (Hz)	12018.86
				Temperature (degree C)	25.000

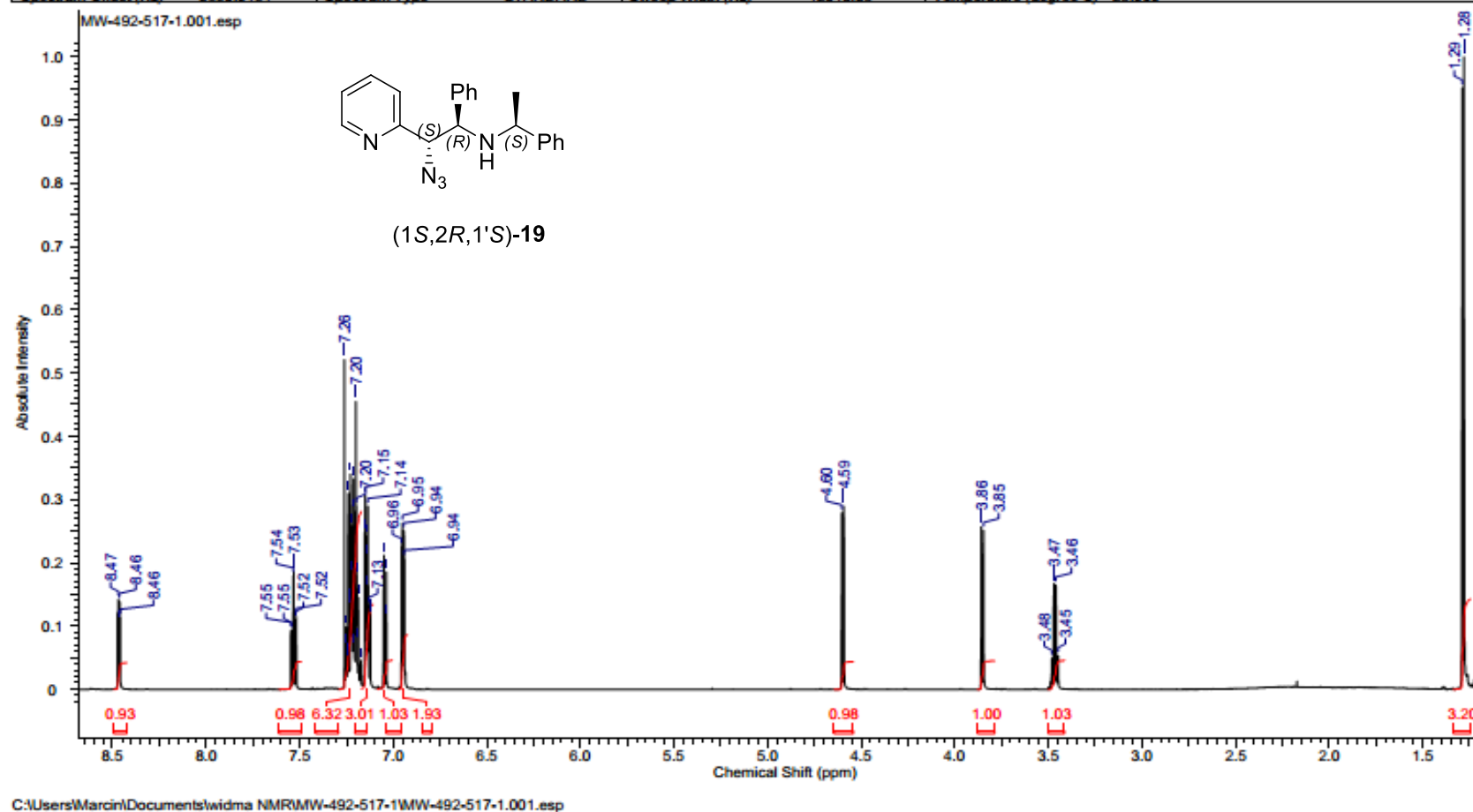
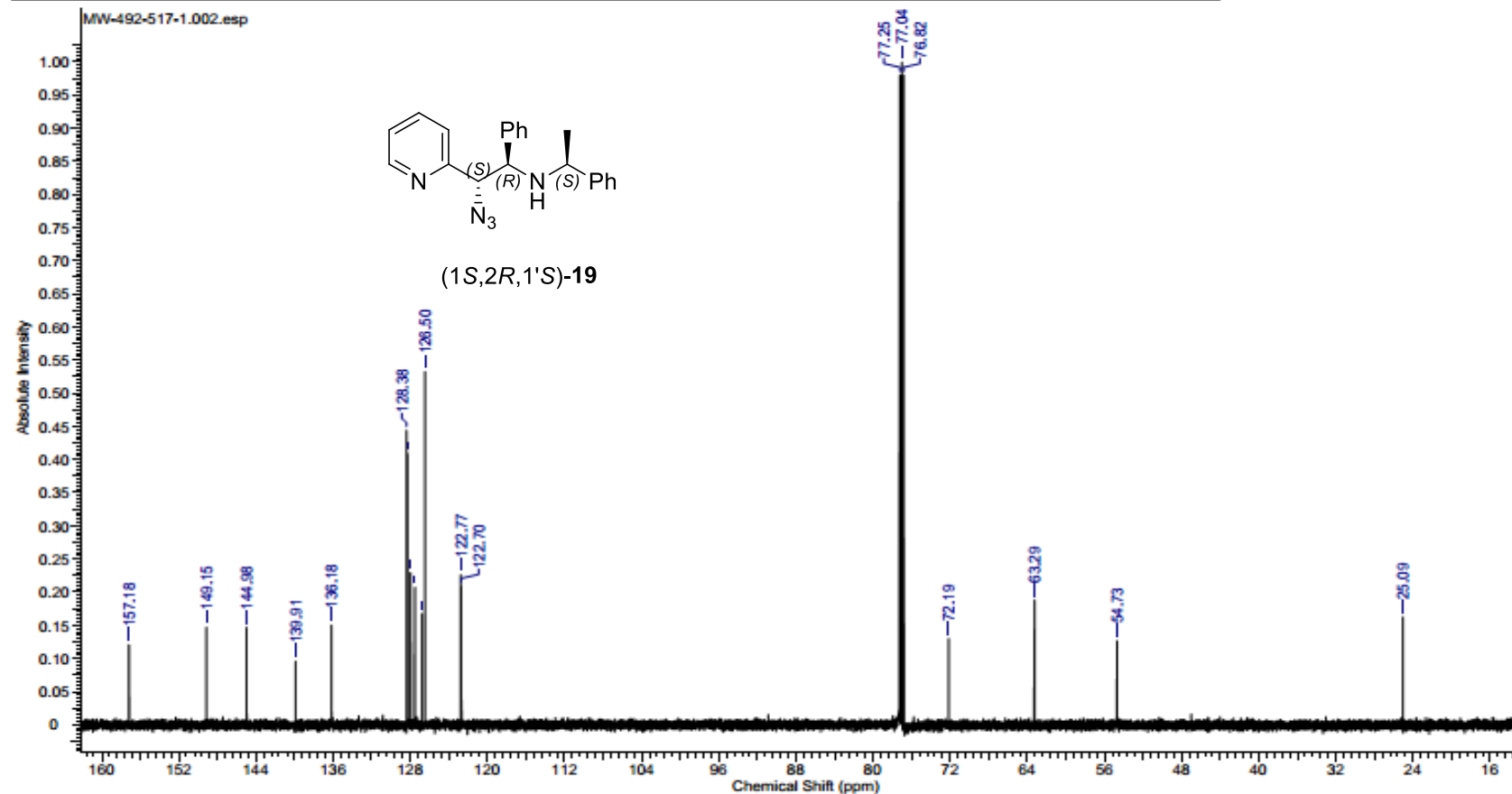


Figure S48. ^1H NMR spectrum (600 MHz, CDCl_3) for (1S,2R,1'S)-19

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.4418	Date	28 Nov 2019 16:00:16	Date Stamp	28 Nov 2019 16:00:16
File Name	C:\Users\Marcin\Documents\widma NMR\MW-492-517-1\2\wid	Frequency (MHz)	151.03	Nucleus	¹³ C
Number of Transients	256	Origin	spect	Original Points Count	65536
Pulse Sequence	zgpg30	Receiver Gain	2050.00	SW(cyclical) (Hz)	45454.55
Spectrum Offset (Hz)	15101.7100	Spectrum Type	STANDARD	Sweep Width (Hz)	45453.85
				Solvent	CHLOROFORM-d
				Temperature (degree C)	25.000



C:\Users\Marcin\Documents\widma NMR\MW-492-517-1\MW-492-517-1.002.esp

Figure S49. ¹³C NMR spectrum (151 MHz, CDCl₃) for (1S,2R,1'S)-19

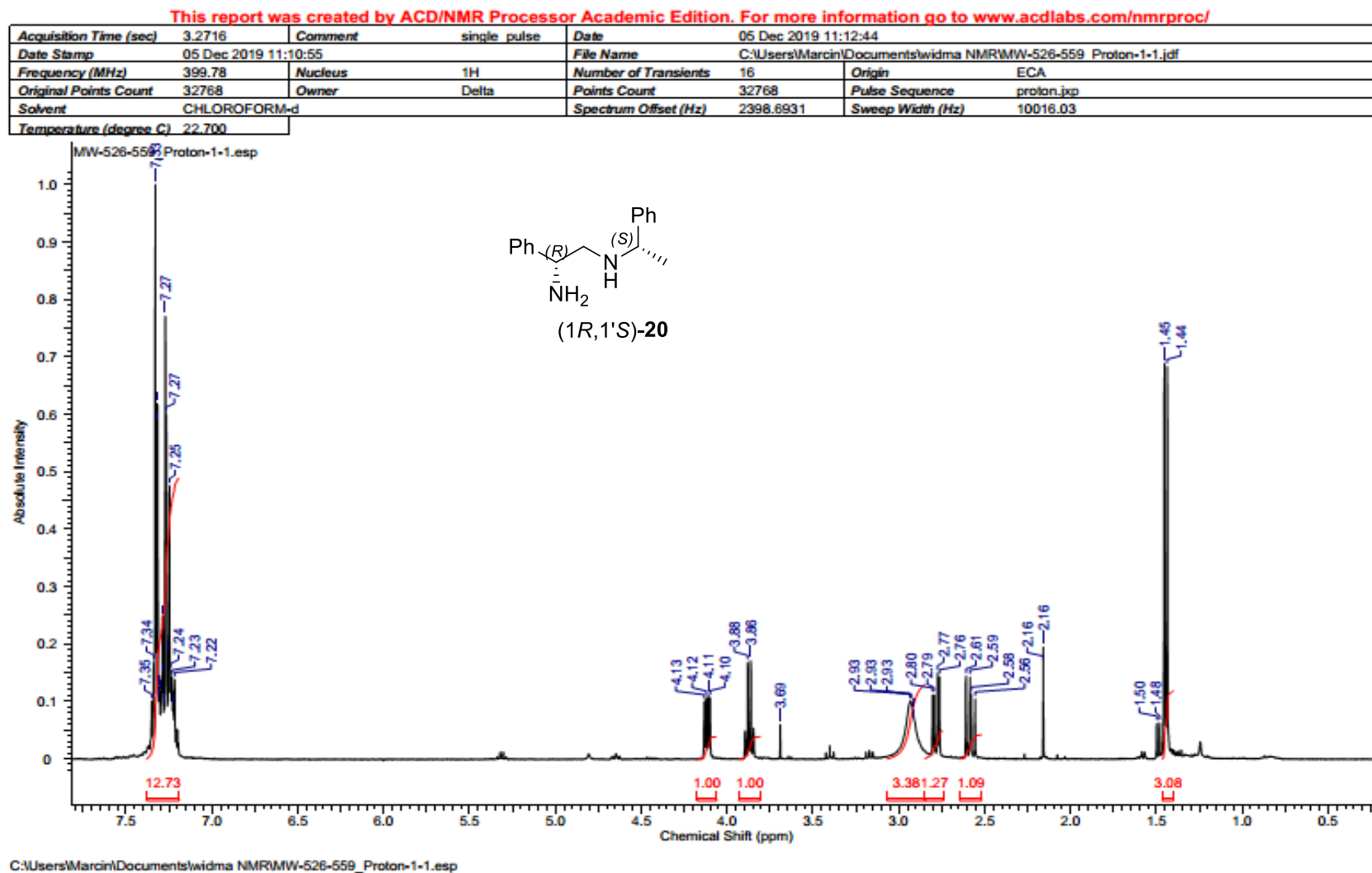


Figure S50. ¹H NMR spectrum (400 MHz, CDCl₃) for (1R,1'S)-20

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.7406	Comment	single pulse decoupled gated NOE	Date	14 Dec 2019 03:58:24
Date Stamp	13 Dec 2019 16:30:31	File Name	C:\Users\Marcin\Documents\widma NMR\MW-526-559_carbon-1-1.jdf		
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	7168
Original Points Count	65536	Owner	Delta	Points Count	65536
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10052.5303	Pulse Sequence	carbon.jxp
Temperature (degree C)	21.800	Sweep Width (Hz)	37650.60		

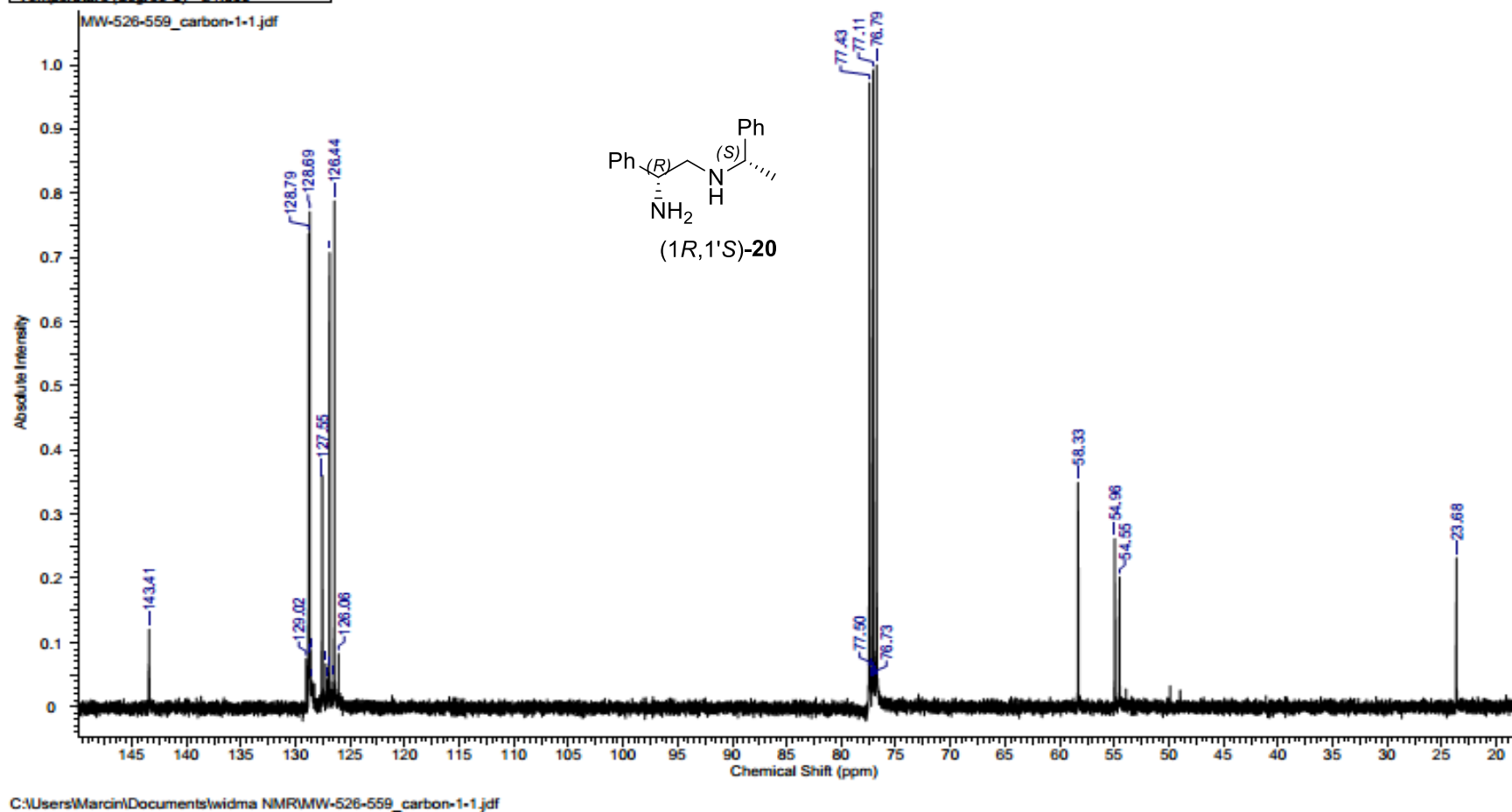


Figure S51. ¹³C NMR spectrum (101 MHz, CDCl₃) for (1R,1'S)-20

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	2.7263	Comment	5 mm PABBO BB-1H/D Z-GRD Z847801/0325	Date	20 Dec 2019 08:57:52
Date Stamp	20 Dec 2019 08:57:52	File Name	C:\Users\Marcin\Documents\widma NMR\MW-540-593\1\fid		
Frequency (MHz)	600.58	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Owner	nrmrsu	Points Count	32768
Receiver Gain	256.00	SW(cyclical) (Hz)	12019.23	Pulse Sequence	zg30
Spectrum Offset (Hz)	3708.5806	Spectrum Type	STANDARD	Solvent	CHLOROFORM-d
				Sweep Width (Hz)	12018.86
				Temperature (degree C)	25.000

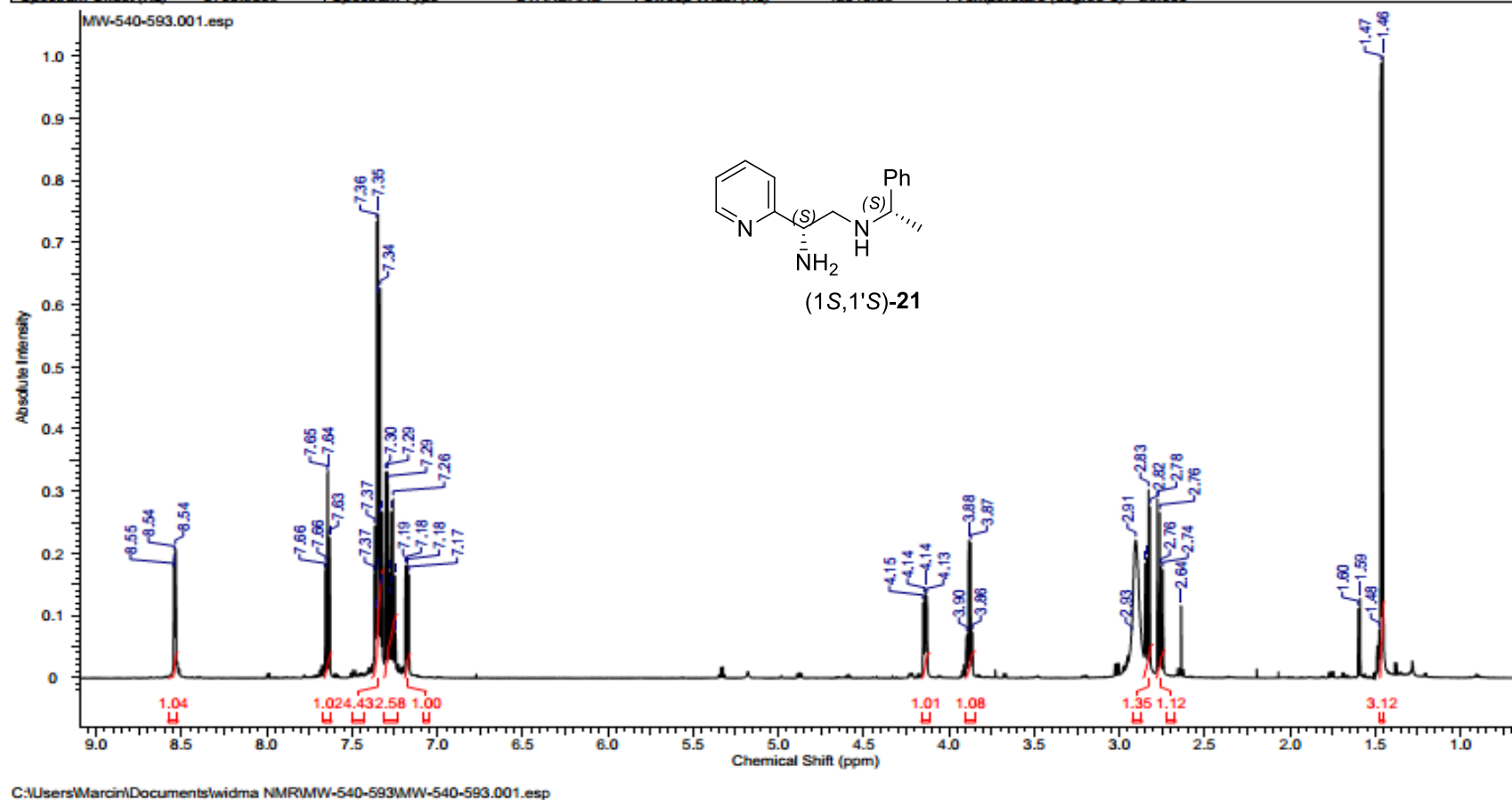
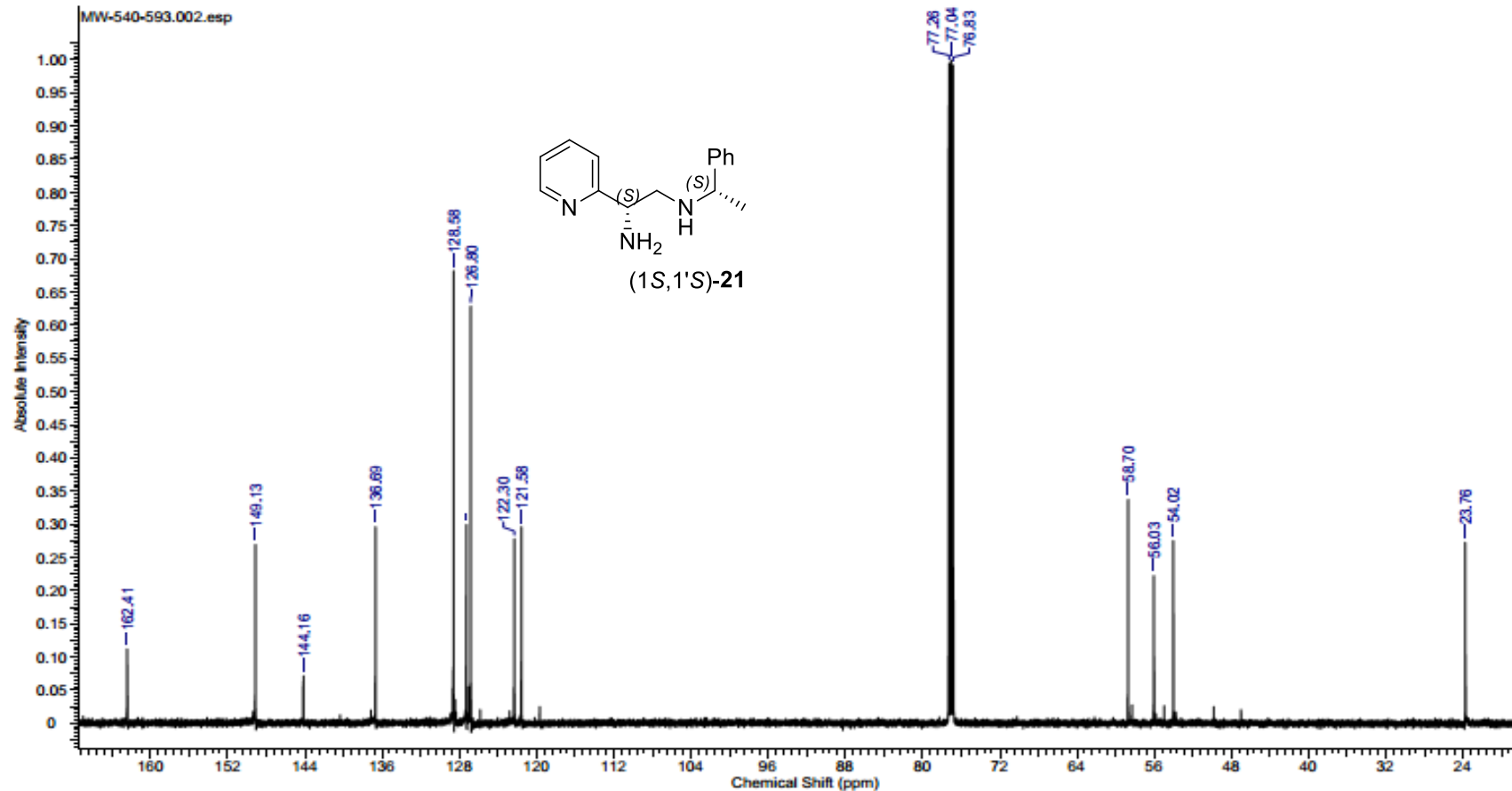


Figure S52. ^1H NMR spectrum (600 MHz, CDCl_3) for (1S,1'S)-21

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.4418	Date	20 Dec 2019 18:57:20	Date Stamp	20 Dec 2019 18:57:20
File Name	C:\Users\Marcin\Documents\widma NMR\MW-540-593\2\fid	Frequency (MHz)	151.02	Nucleus	13C
Number of Transients	8192	Origin	spect	Original Points Count	65536
Pulse Sequence	zgpg30	Receiver Gain	2050.00	Owner	nmr-su
Spectrum Offset (Hz)	15101.7109	Spectrum Type	STANDARD	SW(cyclical) (Hz)	45454.55
				Solvent	CHLOROFORM-d
				Temperature (degree C)	25.000



C:\Users\Marcin\Documents\widma NMR\MW-540-593\MW-540-593.002.esp

Figure S53. ^{13}C NMR spectrum (151 MHz, CDCl_3) for (1S,1'S)-21

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.2716	Comment	single pulse	Date	04 Dec 2019 10:49:12
Date Stamp	04 Dec 2019 10:47:23			File Name	C:\Users\Marcin\Documents\widma NMR\MW-541-582 Proton-1-1.jdf
Frequency (MHz)	399.78	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Owner	Delta	Points Count	32768
Solvent	CHLOROFORM-d			Pulse Sequence	proton.jxp
Temperature (degree C)	22.400			Spectrum Offset (Hz)	2398.6931
				Sweep Width (Hz)	10016.03

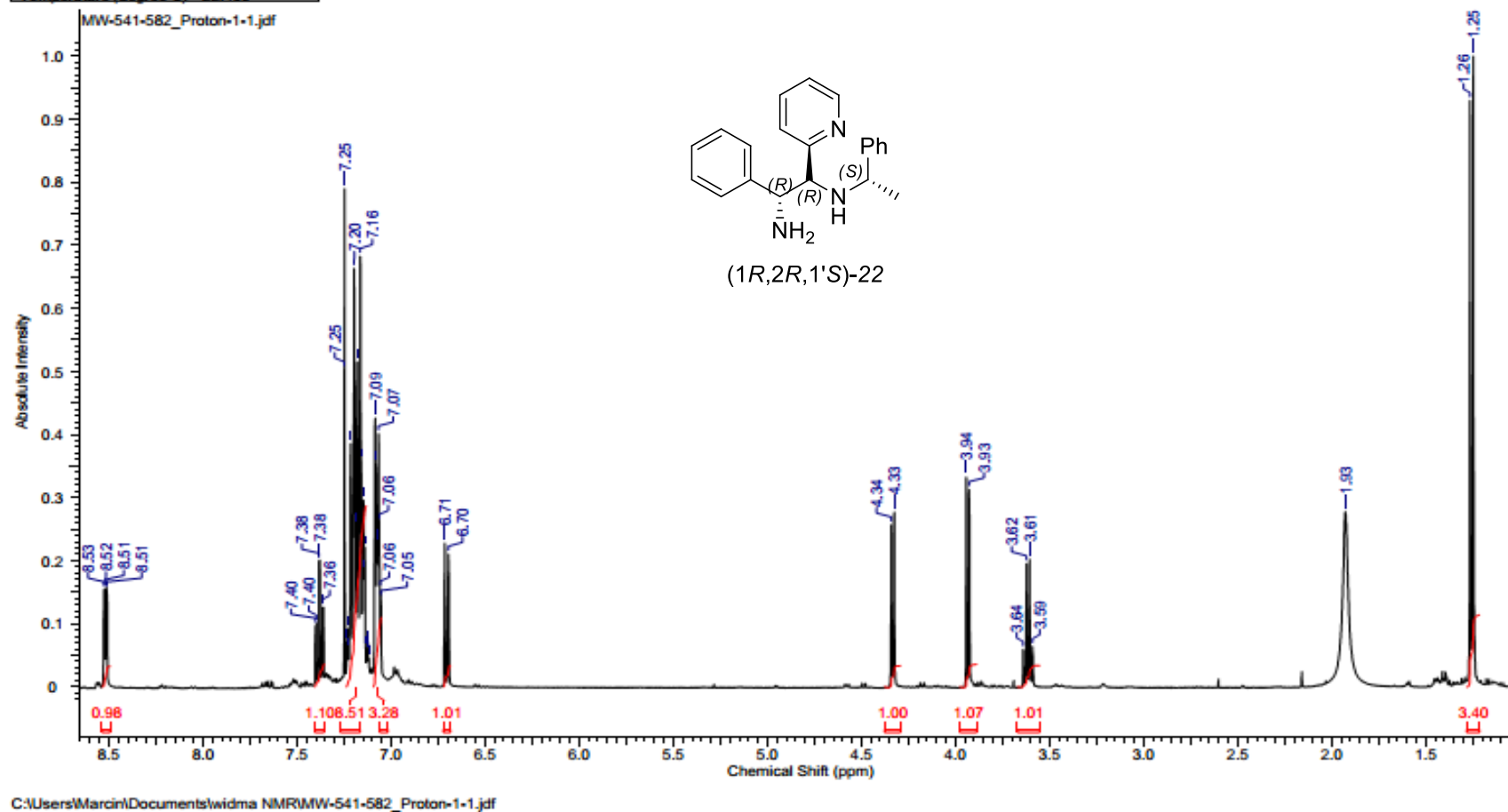
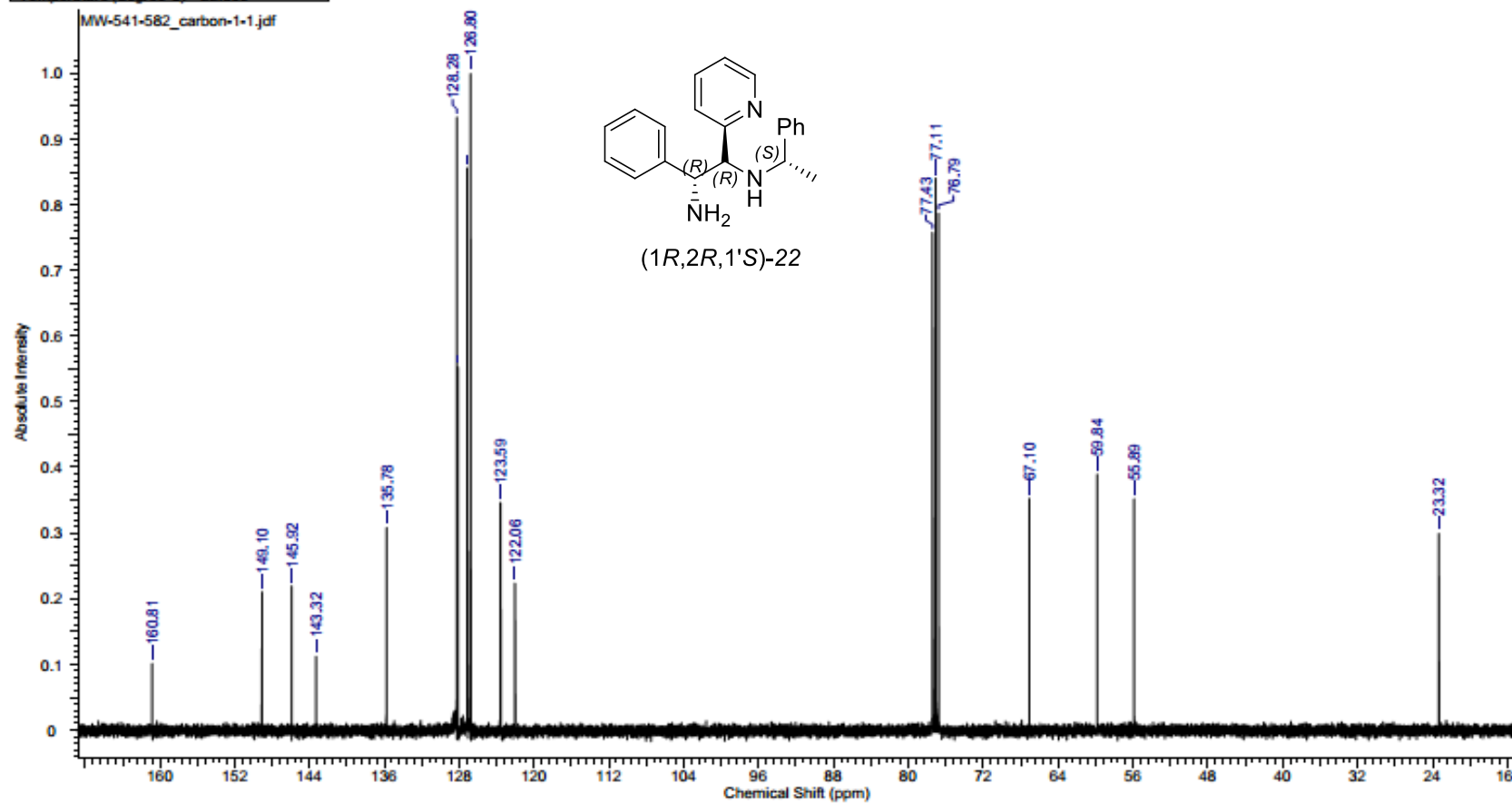


Figure S54. ¹H NMR spectrum (400 MHz, CDCl₃) for (1R,2R,1'S)-22

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.7406	Comment	single pulse decoupled gated NOE	Date	05 Dec 2019 17:31:02
Date Stamp	05 Dec 2019 15:55:57	File Name	C:\Users\Marcin\Documents\widma NMR\MW-541-582_carbon-1-1.jdf		
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	2000
Original Points Count	65536	Owner	Delta	Points Count	65536
Solvent	CHLOROFORM-d			Pulse Sequence	carbon.jxp
Temperature (degree C)	22.300			Spectrum Offset (Hz)	10052.5303
				Sweep Width (Hz)	37650.60



C:\Users\Marcin\Documents\widma NMR\MW-541-582_carbon-1-1.jdf

Figure S55. ¹³C NMR spectrum (101 MHz, CDCl₃) for (1R,2R,1'S)-22

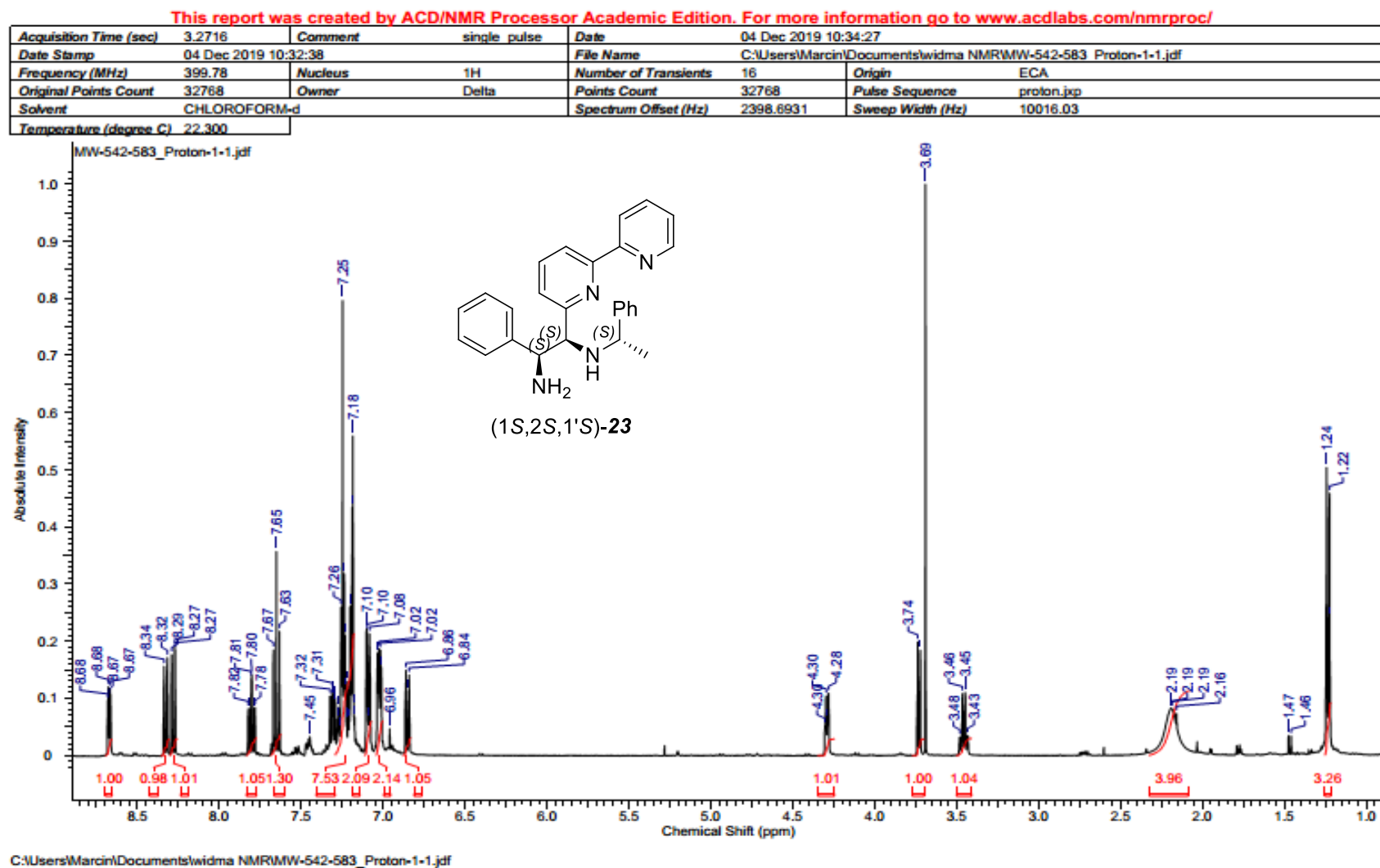
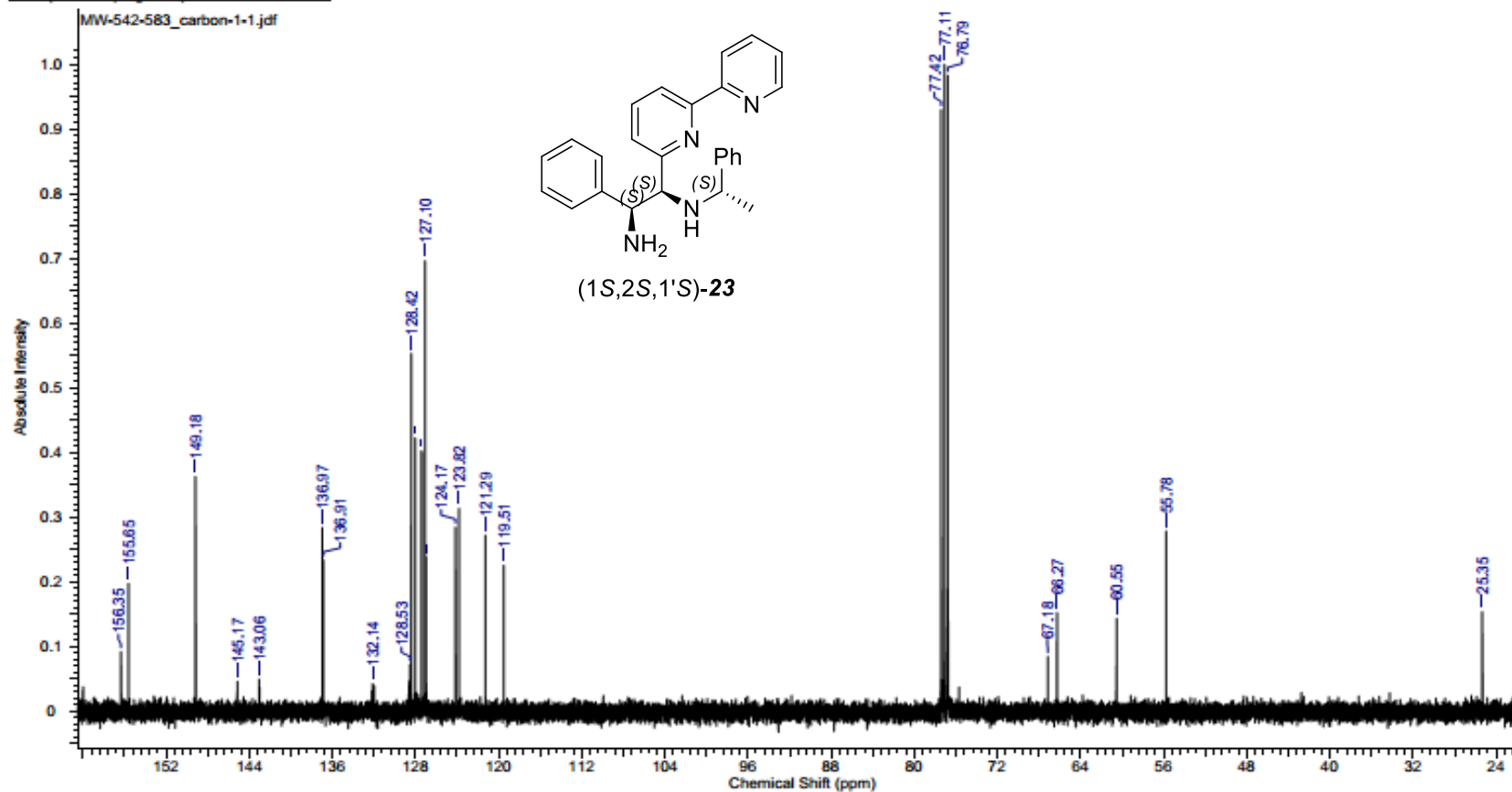


Figure S56. ¹H NMR spectrum (400 MHz, CDCl₃) for (1S,2S,1'S)-23

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.7406	Comment	single pulse decoupled gated NOE	Date	05 Dec 2019 10:22:40
Date Stamp	05 Dec 2019 09:35:23	File Name	C:\Users\Marcin\Documents\widma NMR\MW-542-583_carbon-1-1.jdf		
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	992
Original Points Count	65536	Owner	Delta	Points Count	65536
Solvent	CHLOROFORM-d			Pulse Sequence	carbon.jxp
Temperature (degree C)	22.500			Spectrum Offset (Hz)	10052.5303
				Sweep Width (Hz)	37650.60



C:\Users\Marcin\Documents\widma NMR\MW-542-583_carbon-1-1.jdf

Figure S57. ¹³C NMR spectrum (101 MHz, CDCl₃) for (1S,2S,1'S)-23

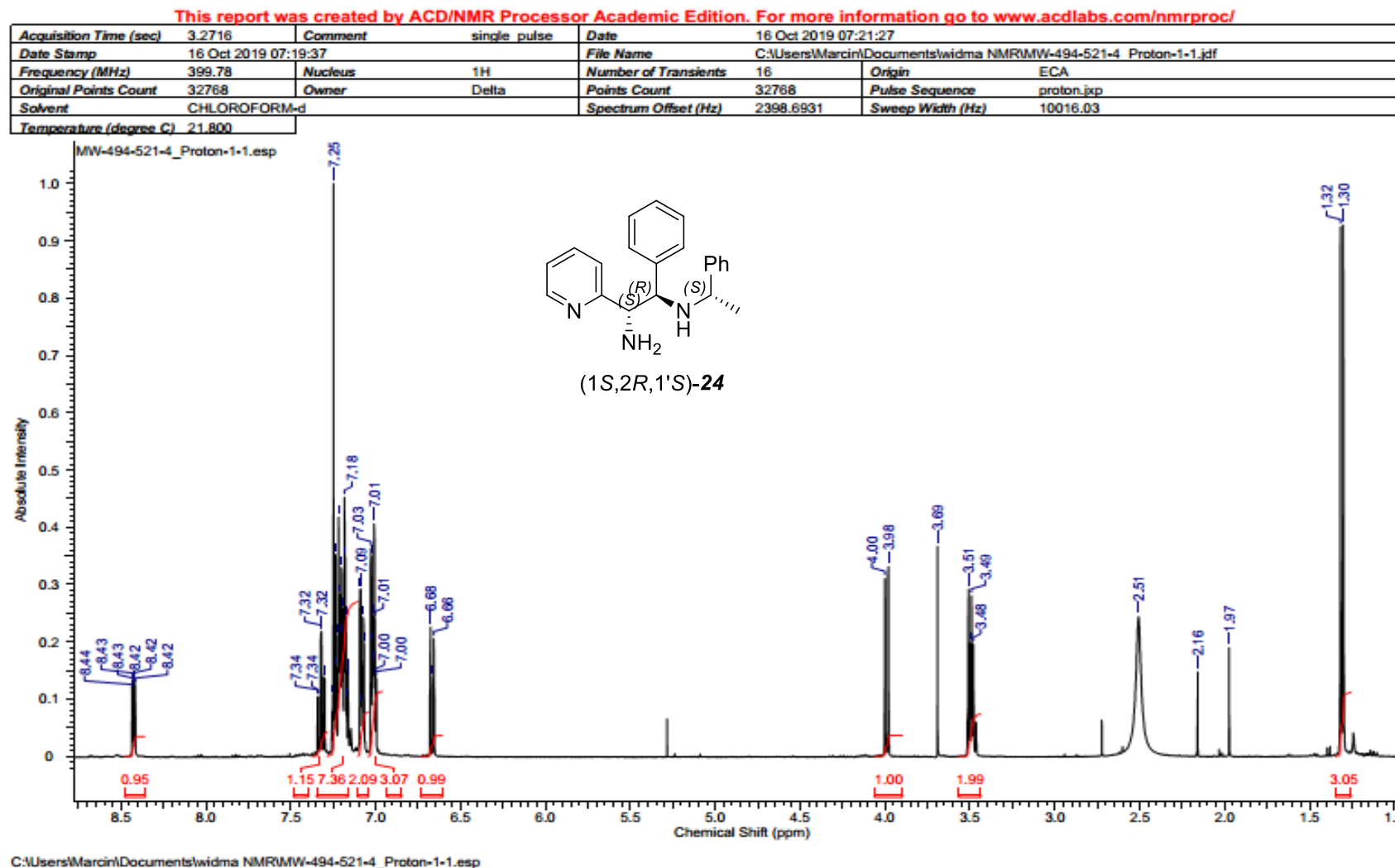
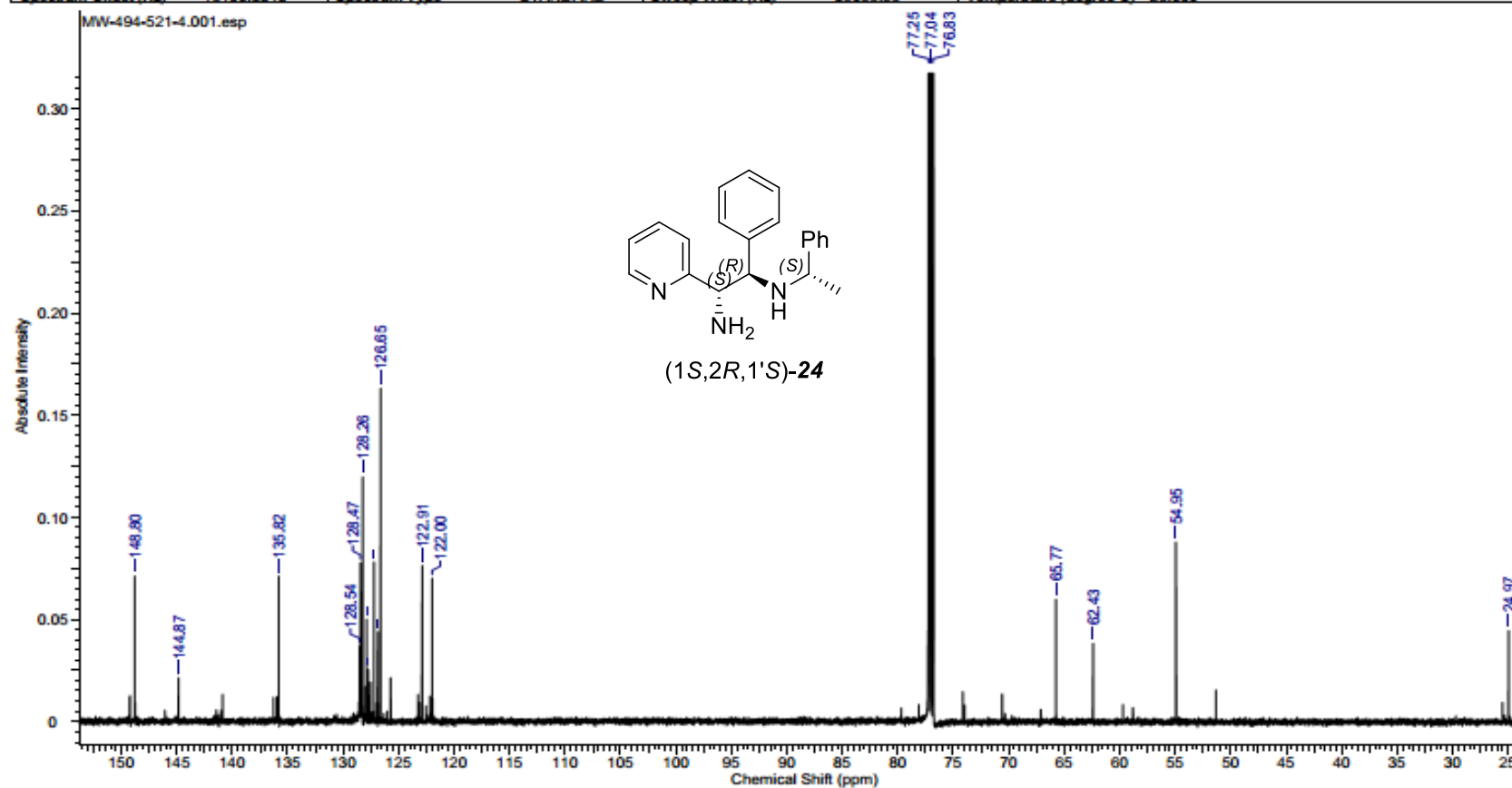


Figure S58. ¹H NMR spectrum (400 MHz, CDCl₃) for (1S,2R,1'S)-**24**

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	0.9088	Comment	5 mm PABBO BB-1H/D Z-GRD Z847801/0325	Date	24 Oct 2019 14:35:12
Date Stamp	24 Oct 2019 14:35:12		File Name	C:\Users\Marcin\Documents\widma NMR\MW-494-521-4\1\fid	
Frequency (MHz)	151.02	Nucleus	¹³ C	Number of Transients	5941
Original Points Count	32768	Owner	nmrsl	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	36057.69	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	15100.8848	Spectrum Type	STANDARD	Sweep Width (Hz)	36056.59
				Temperature (degree C)	25.000

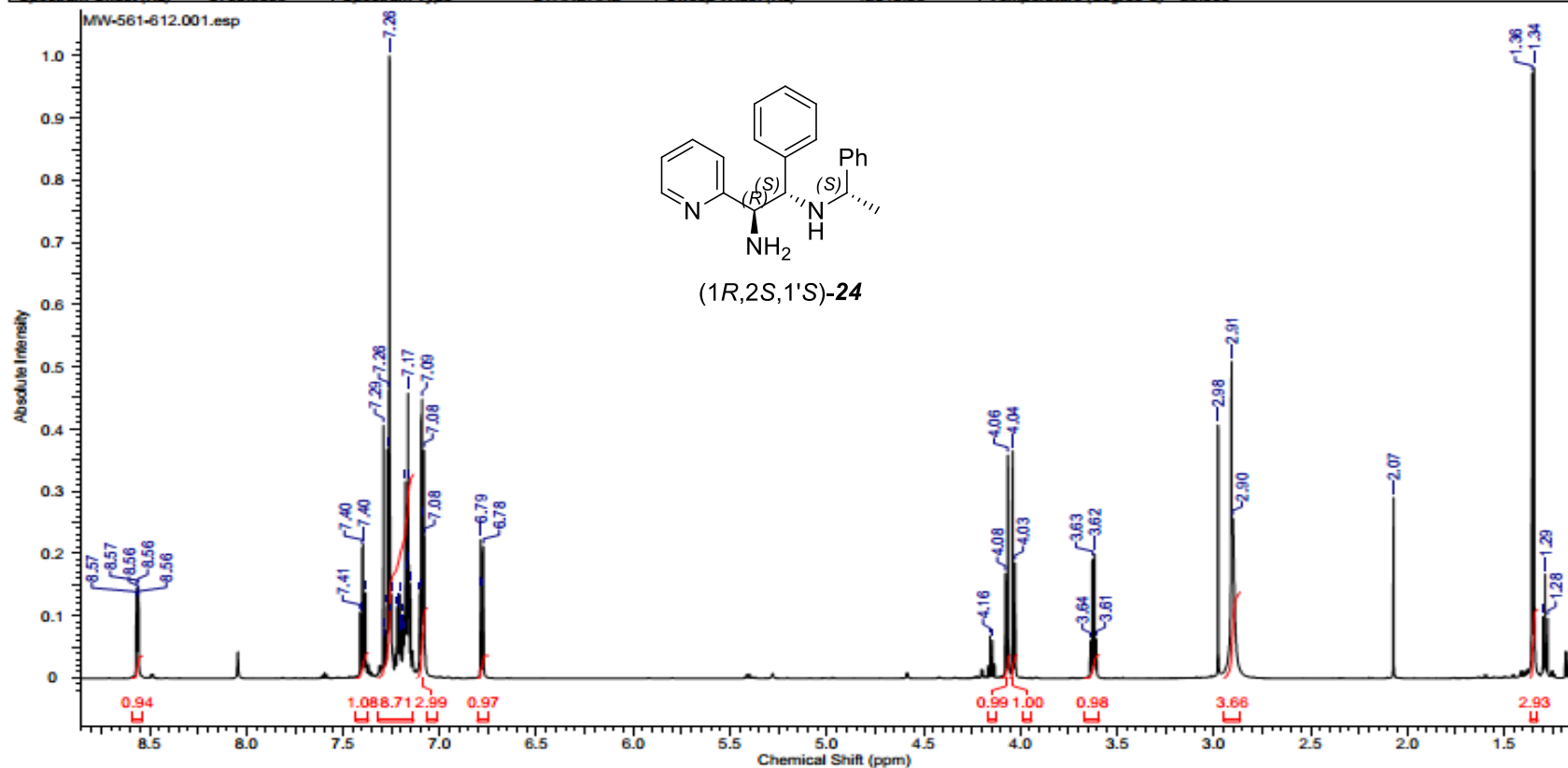


C:\Users\Marcin\Documents\widma NMR\MW-494-521-4\MW-494-521-4.001.esp

Figure S59. ¹³C NMR spectrum (151 MHz, CDCl₃) for (1S,2R,1'S)-24

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

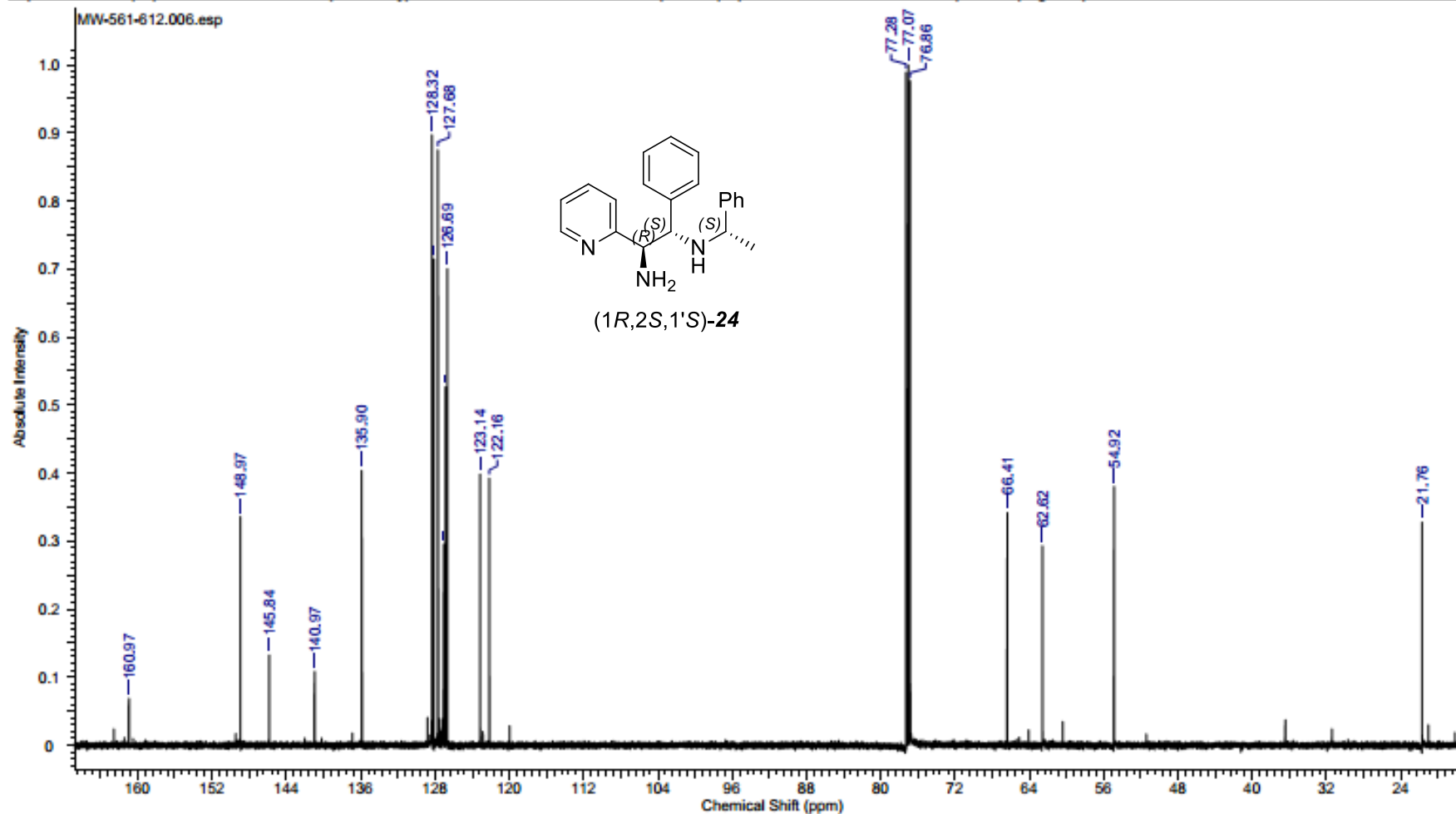
Acquisition Time (sec)	2.7263	Comment	5 mm PABBO BB-1H/D Z-GRD Z847801/0325	Date	29 Jan 2020 12:52:32
Date Stamp	29 Jan 2020 12:52:32			File Name	C:\Users\Marcin\Documents\widma NMR\MW-561-612\1f1d
Frequency (MHz)	600.58	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Owner	nmrsu	Points Count	32768
Receiver Gain	114.00	SW(cyclical) (Hz)	12019.23	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	3708.5806	Spectrum Type	STANDARD	Sweep Width (Hz)	12018.86
				Temperature (degree C)	25.000



C:\Users\Marcin\Documents\widma NMR\MW-561-612\MW-561-612.001.esp

Figure S60. ¹H NMR spectrum (600 MHz, CDCl₃) for (1R,2S,1'S)-24

Acquisition Time (sec)	1.4418	Comment	5 mm PABBO BB-1H/D Z-GRD ZB47801/0325	Date	29 Jan 2020 12:54:40
Date Stamp	29 Jan 2020 12:54:40	File Name	C:\Users\Marcin\Documents\widma NMR\MW-561-612\612	Number of Transients	1673
Frequency (MHz)	151.02	Nucleus	¹³ C	Origin	spect
Original Points Count	65536	Owner	nmsu	Points Count	65536
Receiver Gain	2050.00	SW(cyclical) (Hz)	45454.55	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	15101.7109	Spectrum Type	STANDARD	Sweep Width (Hz)	45453.85
				Temperature (degree C)	25.300



C:\Users\Marcin\Documents\widma NMR\MW-561-612\MW-561-612.006.esp

Figure S61. ¹H NMR spectrum (151 MHz, CDCl₃) for (1R,2S,1'S)-24

6. DFT/B3LYP/CC-pVDZ geometries listings

(1S,2S,3R)-10

C	-0.459858	0.635679	-0.599285
C	-1.474910	0.261520	0.459101
H	-0.765139	0.524180	-1.645123
H	-1.340591	0.829318	1.387878
N	-0.409632	-0.661744	0.102340
C	-2.889451	-0.087217	0.122907
C	-3.199445	-1.185723	-0.692964
C	-3.936528	0.705541	0.618290
C	-4.527296	-1.477438	-1.013788
H	-2.383997	-1.812875	-1.057391
C	-5.264502	0.414434	0.296657
H	-3.706965	1.558978	1.262452
C	-5.564769	-0.678074	-0.522859
H	-4.754683	-2.338542	-1.647204
H	-6.068358	1.040954	0.690786
H	-6.602902	-0.908449	-0.773286
C	0.503028	1.757469	-0.381726
C	1.123507	2.354039	-1.492806
C	1.588101	3.195473	1.054127
C	2.001228	3.417928	-1.293056
H	0.915874	1.981578	-2.497817
C	2.243547	3.853991	0.011151
H	1.751694	3.504839	2.092044
H	2.491092	3.898315	-2.143283
H	2.921746	4.683568	0.219155
N	0.735391	2.179342	0.876142
C	0.639240	-0.949836	1.096398
H	0.884434	-0.051160	1.688320
C	0.098368	-2.025422	2.050422
H	-0.158875	-2.942466	1.497525
H	0.854054	-2.277575	2.810285
H	-0.806091	-1.667508	2.568357
C	1.909700	-1.415039	0.398595
C	3.163130	-1.088519	0.936413
C	1.862541	-2.209059	-0.757609
C	4.341866	-1.548978	0.342645
H	3.215807	-0.461116	1.830635
C	3.039425	-2.667060	-1.356088
H	0.891478	-2.457275	-1.189138
C	4.283792	-2.341035	-0.807540
H	5.308773	-1.282220	0.776478
H	2.984611	-3.282624	-2.257633
H	5.203448	-2.699161	-1.276318

Number of imaginary frequencies:

0

Zero-point correction=

0.356222

(Hartree/Particle)

Thermal correction to Energy=

0.375467

Thermal correction to Enthalpy=

0.376411

Thermal correction to Gibbs Free Energy=

0.305772

Sum of electronic and zero-point Energies=	-921.446668
Sum of electronic and thermal Energies=	-921.427423
Sum of electronic and thermal Enthalpies=	-921.426479
Sum of electronic and thermal Free Energies=	-921.497118

(1R,2S,3R)-10

C	-1.506830	0.240225	0.402129
C	-0.502521	0.644604	-0.642542
H	-1.441923	0.788039	1.348958
H	-0.803044	0.507113	-1.688533
N	-0.402441	-0.652174	0.059707
C	0.446730	1.790958	-0.435840
C	0.123004	2.893226	0.370278
C	1.675715	1.795888	-1.118504
C	1.010889	3.965851	0.503848
H	-0.839663	2.922743	0.884398
C	2.563806	2.864559	-0.983705
H	1.938751	0.947809	-1.754676
C	2.234734	3.953425	-0.169441
H	0.739833	4.816774	1.133269
H	3.517087	2.847130	-1.517086
H	2.928275	4.791075	-0.065079
C	-2.907213	-0.163489	0.070950
C	-3.184636	-1.248854	-0.773297
C	-5.141701	0.288204	0.343771
C	-4.515206	-1.550894	-1.058718
H	-2.358956	-1.837527	-1.174650
C	-5.521818	-0.764631	-0.492211
H	-5.901635	0.921370	0.814622
H	-4.765055	-2.391799	-1.710491
H	-6.577586	-0.964021	-0.686042
N	-3.868943	0.592198	0.629733
C	0.634330	-0.850788	1.084822
H	0.877917	0.102288	1.594558
C	0.096276	-1.832434	2.137060
H	-0.160117	-2.795746	1.669028
H	0.854638	-2.015664	2.913554
H	-0.807127	-1.431237	2.623949
C	1.915183	-1.379922	0.451772
C	3.159731	-1.049944	1.008140
C	1.881954	-2.239648	-0.656324
C	4.343507	-1.569361	0.477475
H	3.202566	-0.370761	1.864248
C	3.065202	-2.756924	-1.192185
H	0.917706	-2.491942	-1.100150
C	4.300267	-2.425904	-0.626711
H	5.303381	-1.297796	0.923551
H	3.021687	-3.422993	-2.057664
H	5.224533	-2.829895	-1.046434

Number of imaginary frequencies: 0

Zero-point correction=	0.356123
(Hartree/Particle)	
Thermal correction to Energy=	0.375379
Thermal correction to Enthalpy=	0.376323
Thermal correction to Gibbs Free Energy=	0.305543
Sum of electronic and zero-point Energies=	-921.442962
Sum of electronic and thermal Energies=	-921.423707
Sum of electronic and thermal Enthalpies=	-921.422762
Sum of electronic and thermal Free Energies=	-921.493542

Complex of (1S,2S,3R)-**10** with zinc acetate

C	-0.267721	-1.839760	-0.762913
C	-1.125293	-1.307844	0.354854
H	-0.822767	-2.313371	-1.576978
H	-0.653593	-1.226963	1.339627
N	-0.426019	-0.397934	-0.595366
C	-2.605705	-1.569601	0.411362
C	-3.180316	-2.722383	-0.152940
C	-3.434041	-0.692313	1.133456
C	-4.549178	-2.978685	-0.025979
H	-2.553775	-3.437399	-0.691845
C	-4.802430	-0.944070	1.256384
H	-3.002731	0.200000	1.593287
C	-5.366510	-2.086456	0.674354
H	-4.975669	-3.882084	-0.472539
H	-5.430633	-0.243699	1.812918
H	-6.436748	-2.283905	0.772741
C	1.088656	-2.438749	-0.559215
C	1.316400	-3.798185	-0.810825
C	3.318296	-2.125064	0.022380
C	2.593897	-4.319796	-0.615452
H	0.497113	-4.431546	-1.156669
C	3.618059	-3.468203	-0.192218
H	4.077017	-1.397529	0.316212
H	2.791644	-5.377874	-0.801859
H	4.635450	-3.831400	-0.040704
N	2.078949	-1.630020	-0.145812
C	-1.066396	0.453524	-1.642891
H	-0.193712	0.777266	-2.243287
C	-2.055269	-0.258261	-2.590702
H	-2.976404	-0.583018	-2.078475
H	-2.342380	0.424505	-3.402389
H	-1.588924	-1.130512	-3.082251
C	-1.646526	1.733510	-1.018864
C	-2.354673	2.661489	-1.836184
C	-1.439640	2.065012	0.332184
C	-2.860670	3.860187	-1.318957
H	-2.507851	2.463416	-2.902348
C	-1.948428	3.265825	0.851370
H	-0.859824	1.404385	0.994647
C	-2.666026	4.166720	0.034066
H	-3.406101	4.559693	-1.981722

H	-1.767663	3.497658	1.906423
H	-3.059239	5.104485	0.441505
Zn	1.647065	0.434378	0.263075
C	3.085792	1.694184	-1.328818
O	3.723719	0.829920	-0.679861
C	1.633926	1.007650	2.799454
O	2.629481	1.547515	2.295205
O	1.810215	1.821630	-1.186377
O	0.809382	0.305164	2.076147
C	3.788574	2.639787	-2.276118
H	3.874004	3.625670	-1.786479
H	4.795480	2.271239	-2.515228
H	3.194818	2.779915	-3.193114
C	1.309127	1.124248	4.276033
H	0.301954	1.553903	4.403546
H	1.290851	0.120024	4.731236
H	2.051444	1.751053	4.785906

(1S,2R,3S)-13

C	0.026440	0.883443	0.263839
C	-1.207018	0.862766	-0.601543
H	-0.091246	0.495076	1.280180
H	-1.259755	1.630925	-1.381263
N	-0.073645	-0.063679	-0.845273
C	-2.564758	0.453215	-0.113435
C	-2.835393	0.005145	1.191575
C	-3.639131	0.547094	-1.018282
C	-4.133309	-0.353297	1.570458
H	-2.035119	-0.051792	1.930959
C	-4.936159	0.192244	-0.640553
H	-3.450962	0.906684	-2.033550
C	-5.188178	-0.263691	0.657596
H	-4.320007	-0.695576	2.591259
H	-5.752901	0.275342	-1.361805
H	-6.201647	-0.540045	0.957899
C	1.028366	1.990472	0.188173
C	1.592405	2.401064	-1.029812
C	2.210831	3.588721	1.346762
C	2.500542	3.458419	-1.027791
H	1.323549	1.883446	-1.951646
C	2.819081	4.072504	0.186950
H	2.440307	4.038535	2.318778
H	2.957424	3.797521	-1.960801
H	3.525654	4.903277	0.237858
N	1.335942	2.571949	1.362162
C	-0.214094	-1.495595	-0.513693
H	-0.887813	-1.645323	0.349388
C	-0.820218	-2.217491	-1.724187
H	-0.177231	-2.098923	-2.611183
H	-0.929550	-3.293618	-1.516396
H	-1.816195	-1.811571	-1.962264
C	1.141719	-2.078547	-0.135139

C	1.257377	-2.924081	0.978248	
C	2.289584	-1.821167	-0.903156	
C	2.484833	-3.504643	1.316704	
H	0.373868	-3.131512	1.588730	
C	3.518098	-2.394802	-0.564466	
H	2.219214	-1.158316	-1.767568	
C	3.620595	-3.240758	0.545942	
H	2.553053	-4.159970	2.188749	
H	4.401839	-2.179519	-1.170679	
H	4.581756	-3.688631	0.810005	
Number of imaginary frequencies:				0
Zero-point correction=				0.356095
(Hartree/Particle)				
Thermal correction to Energy=				0.375321
Thermal correction to Enthalpy=				0.376265
Thermal correction to Gibbs Free Energy=				0.305986
Sum of electronic and zero-point Energies=				-921.468019
Sum of electronic and thermal Energies=				-921.448793
Sum of electronic and thermal Enthalpies=				-921.447848
Sum of electronic and thermal Free Energies=				-921.518128

(1R,2R,3S)-10

C	-1.260653	0.768308	-0.672420
C	-0.070229	0.865462	0.254287
H	-1.330145	1.513919	-1.471413
H	-0.272170	0.477373	1.258827
N	-0.078595	-0.106621	-0.833154
C	0.885713	2.013782	0.204515
C	1.493434	2.417037	-0.995933
C	1.173989	2.727029	1.379221
C	2.363102	3.510173	-1.020155
H	1.287945	1.855670	-1.909595
C	2.043725	3.821557	1.355586
H	0.713276	2.418052	2.321613
C	2.640953	4.218471	0.154833
H	2.830842	3.809098	-1.961805
H	2.258620	4.363448	2.280110
H	3.322755	5.072142	0.134897
C	-2.600317	0.326047	-0.175946
C	-3.747036	0.667638	-0.914028
C	-3.886267	-0.742279	1.412789
C	-5.001319	0.282491	-0.441803
H	-3.648856	1.230975	-1.844166
C	-5.078362	-0.440963	0.750339
H	-3.903826	-1.308933	2.349788
H	-5.905340	0.543006	-0.997369
H	-6.036475	-0.764058	1.161623
N	-2.675502	-0.370174	0.975628
C	-0.156343	-1.544259	-0.496255
H	-0.812301	-1.712542	0.373719
C	-0.740909	-2.295115	-1.699016
H	-0.119406	-2.146051	-2.596839

H	-0.794306	-3.375267	-1.489937
H	-1.759938	-1.941020	-1.924393
C	1.232089	-2.056064	-0.133692
C	1.411919	-2.847619	1.010331
C	2.348956	-1.782704	-0.941114
C	2.671379	-3.361532	1.339698
H	0.553455	-3.064338	1.652266
C	3.608809	-2.290135	-0.612654
H	2.229946	-1.158427	-1.828695
C	3.775168	-3.083476	0.528640
H	2.789608	-3.975656	2.236108
H	4.467209	-2.063589	-1.250401
H	4.760979	-3.479332	0.784997
Number of imaginary frequencies:			0
Zero-point correction=			0.355913
(Hartree/Particle)			
Thermal correction to Energy=			0.375183
Thermal correction to Enthalpy=			0.376127
Thermal correction to Gibbs Free Energy=			0.305374
Sum of electronic and zero-point Energies=			-921.471695
Sum of electronic and thermal Energies=			-921.452426
Sum of electronic and thermal Enthalpies=			-921.451482
Sum of electronic and thermal Free Energies=			-921.522235

(1S,2S,3R)-12

C	-1.238589	-0.051912	1.038778
C	-1.774221	-0.871897	-0.111469
H	-1.918288	0.138080	1.875518
H	-0.993817	-1.430504	-0.640170
N	-1.715106	0.580719	-0.210419
C	-3.106027	-1.551890	-0.062912
C	-4.293712	-0.834840	0.153245
C	-3.177405	-2.945708	-0.221529
C	-5.522053	-1.498300	0.217602
H	-4.244377	0.250696	0.256701
C	-4.405776	-3.609736	-0.156133
H	-2.260205	-3.514426	-0.398668
C	-5.583540	-2.888127	0.065557
H	-6.438393	-0.925867	0.383291
H	-4.443247	-4.694676	-0.282697
H	-6.544714	-3.405462	0.114902
C	0.194373	-0.130258	1.463921
C	0.548227	0.365886	2.730282
C	2.385143	-0.753485	1.028243
C	1.878943	0.284860	3.137364
H	-0.212668	0.807303	3.376419
C	2.818034	-0.280648	2.277370
H	2.182014	0.660625	4.117370
H	3.869270	-0.368107	2.546663
N	1.099228	-0.680550	0.636437
C	-0.767941	1.181447	-1.168378

H	0.182346	0.621835	-1.195934
C	-1.401344	1.119342	-2.565491
H	-2.359030	1.664052	-2.588588
H	-0.728105	1.570287	-3.311406
H	-1.590656	0.075064	-2.863256
C	-0.452468	2.616820	-0.766114
C	0.845645	3.122314	-0.934894
C	-1.446154	3.474957	-0.267189
C	1.145674	4.452366	-0.622221
H	1.633064	2.464087	-1.312731
C	-1.148359	4.803573	0.050029
H	-2.457638	3.091940	-0.120025
C	0.148327	5.298711	-0.128057
H	2.163863	4.825526	-0.758979
H	-1.933783	5.456560	0.439677
H	0.380509	6.337157	0.120867
C	3.354351	-1.375924	0.075864
C	2.929249	-1.935407	-1.140716
N	4.649174	-1.374817	0.449632
C	3.877417	-2.503484	-1.990618
H	1.871900	-1.922295	-1.399757
C	5.547769	-1.922909	-0.375367
C	5.219841	-2.499179	-1.605951
H	3.570760	-2.945606	-2.941494
H	6.588679	-1.901193	-0.035814
H	5.997024	-2.931968	-2.238720

Number of imaginary frequencies:

0

Zero-point correction=

0.424698

(Hartree/Particle)

Thermal correction to Energy=

0.448577

Thermal correction to Enthalpy=

0.449521

Thermal correction to Gibbs Free Energy=

0.367040

Sum of electronic and zero-point Energies=

-1168.525306

Sum of electronic and thermal Energies=

-1168.501427

Sum of electronic and thermal Enthalpies=

-1168.500483

Sum of electronic and thermal Free Energies=

-1168.582964

(1R,2S,3R)-12

C	-0.059946	-0.148413	0.109148
C	0.993630	0.347871	-0.848065
H	-0.228058	0.473060	0.994735
H	0.864915	0.061185	-1.897557
N	1.217306	-0.846266	0.001694
C	1.714069	1.654241	-0.694347
C	1.491125	2.561981	0.355812
C	2.657936	1.998120	-1.679851
C	2.201998	3.764722	0.425120
H	0.746730	2.344273	1.123275
C	3.366321	3.199716	-1.613648
H	2.838271	1.308646	-2.508727

C	3.142823	4.088392	-0.556786
H	2.010014	4.456513	1.248967
H	4.094349	3.443096	-2.391326
H	3.693712	5.030372	-0.502730
C	-1.305931	-0.833290	-0.357073
C	-1.265554	-1.995770	-1.141819
C	-3.620960	-0.800447	-0.383159
C	-2.472334	-2.559960	-1.553344
H	-0.304624	-2.439888	-1.402342
C	-3.672210	-1.957830	-1.175329
H	-2.479264	-3.466901	-2.162810
H	-4.638821	-2.362050	-1.471724
N	-2.457016	-0.254937	0.017676
C	2.126295	-0.781864	1.159315
H	2.121996	0.222353	1.622049
C	1.639277	-1.787956	2.212097
H	1.624184	-2.809737	1.799827
H	2.305817	-1.778390	3.088680
H	0.621728	-1.537463	2.553893
C	3.556185	-1.085405	0.727589
C	4.629430	-0.424463	1.344369
C	3.837462	-2.055264	-0.247963
C	5.951463	-0.727544	1.003428
H	4.426937	0.341702	2.098094
C	5.158221	-2.357230	-0.594023
H	3.011578	-2.568779	-0.743274
C	6.220922	-1.696437	0.031609
H	6.772977	-0.199285	1.493983
H	5.358232	-3.113050	-1.358068
H	7.252866	-1.932091	-0.239941
C	-4.873102	-0.116066	0.058005
C	-4.824373	1.056518	0.830471
N	-6.037586	-0.676911	-0.323206
C	-6.020083	1.660277	1.216149
H	-3.856973	1.470642	1.110989
C	-7.176976	-0.086633	0.054437
C	-7.228239	1.080098	0.822550
H	-6.008831	2.573175	1.816389
H	-8.102146	-0.571916	-0.274252
H	-8.189229	1.517138	1.100568

Number of imaginary frequencies:	0
Zero-point correction=	0.424650
(Hartree/Particle)	
Thermal correction to Energy=	0.448595
Thermal correction to Enthalpy=	0.449539
Thermal correction to Gibbs Free Energy=	0.365924
Sum of electronic and zero-point Energies=	-1168.522832
Sum of electronic and thermal Energies=	-1168.498888
Sum of electronic and thermal Enthalpies=	-1168.497943
Sum of electronic and thermal Free Energies=	-1168.581558