

Supporting Information

STEREOINVERSION OF A TERTIARY ALCOHOL ON A THP RING: A RECOVERY ROUTE TO AN INTERMEDIATE FOR GYMNOICIN-A

*Takeo Sakai, Kayo Aoyama, Rie Oshima, Kyoko Furukawa, Yuji Mori**

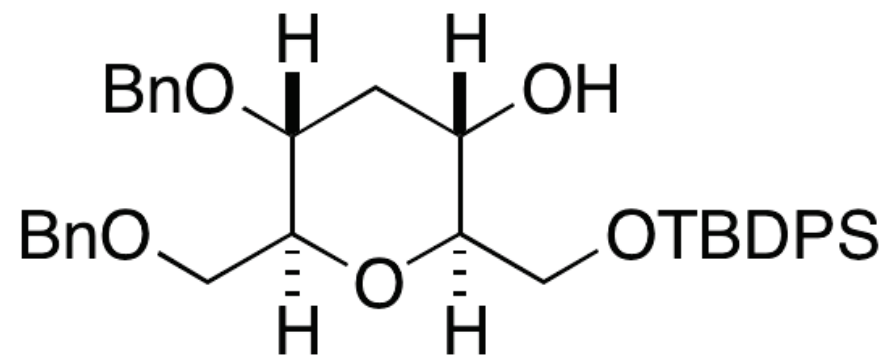
*Faculty of Pharmacy, Meijo University, 150 Yagotoyama, Tempaku-ku, Nagoya
468-8503, Japan*

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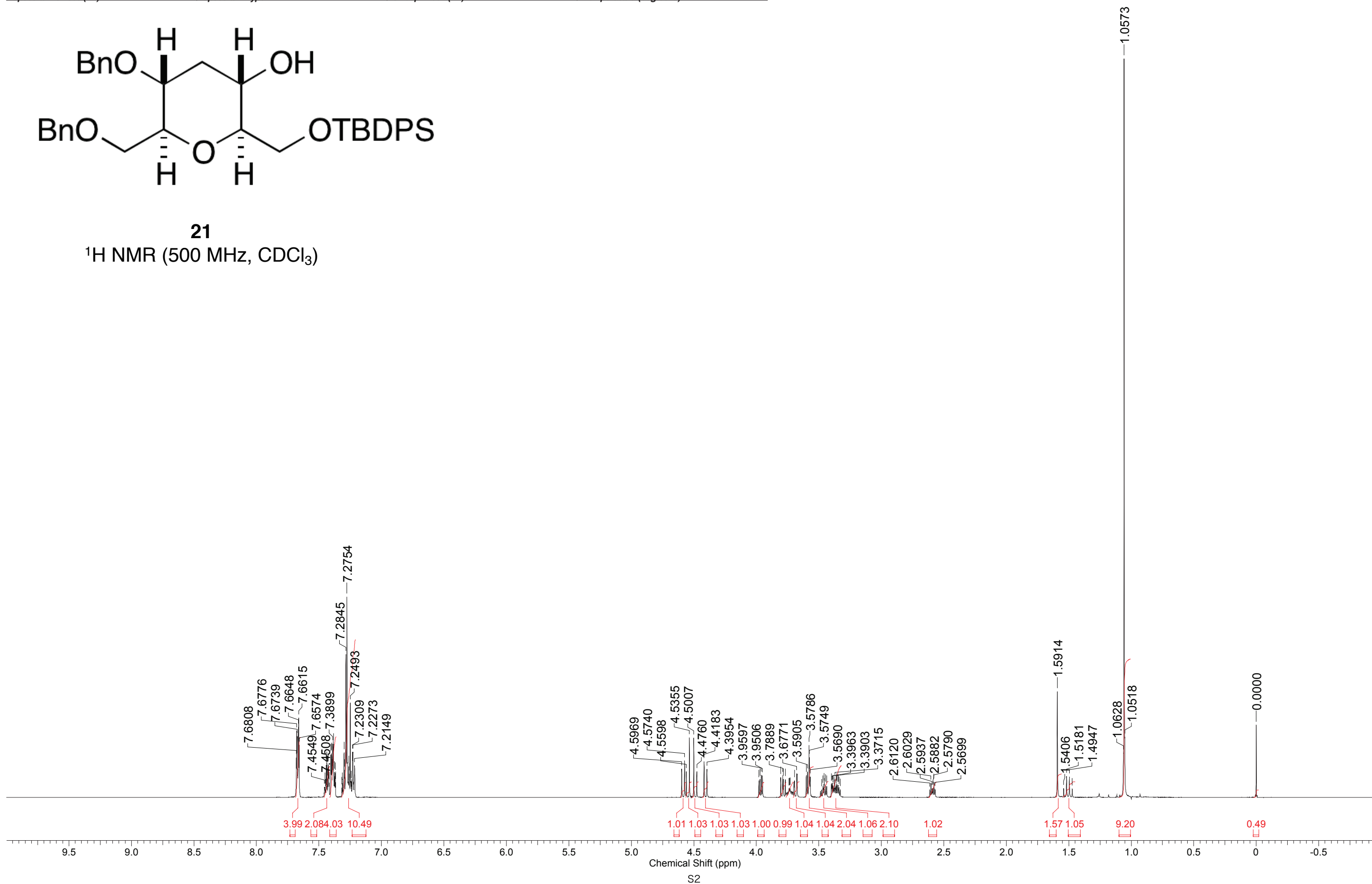
Copies of ^1H and ^{13}C NMR spectra	S 2
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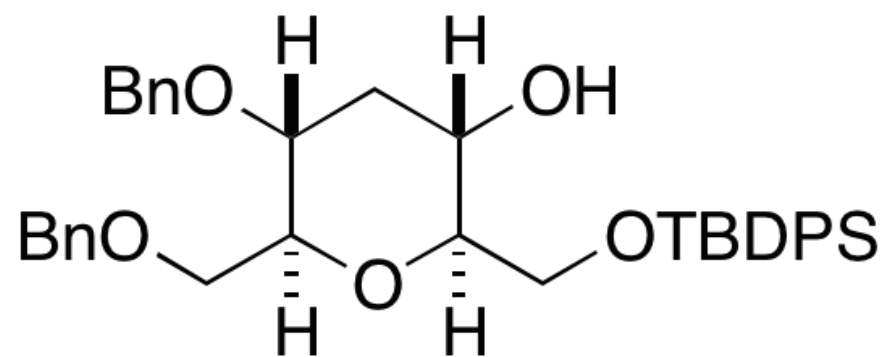


21

¹H NMR (500 MHz, CDCl₃)

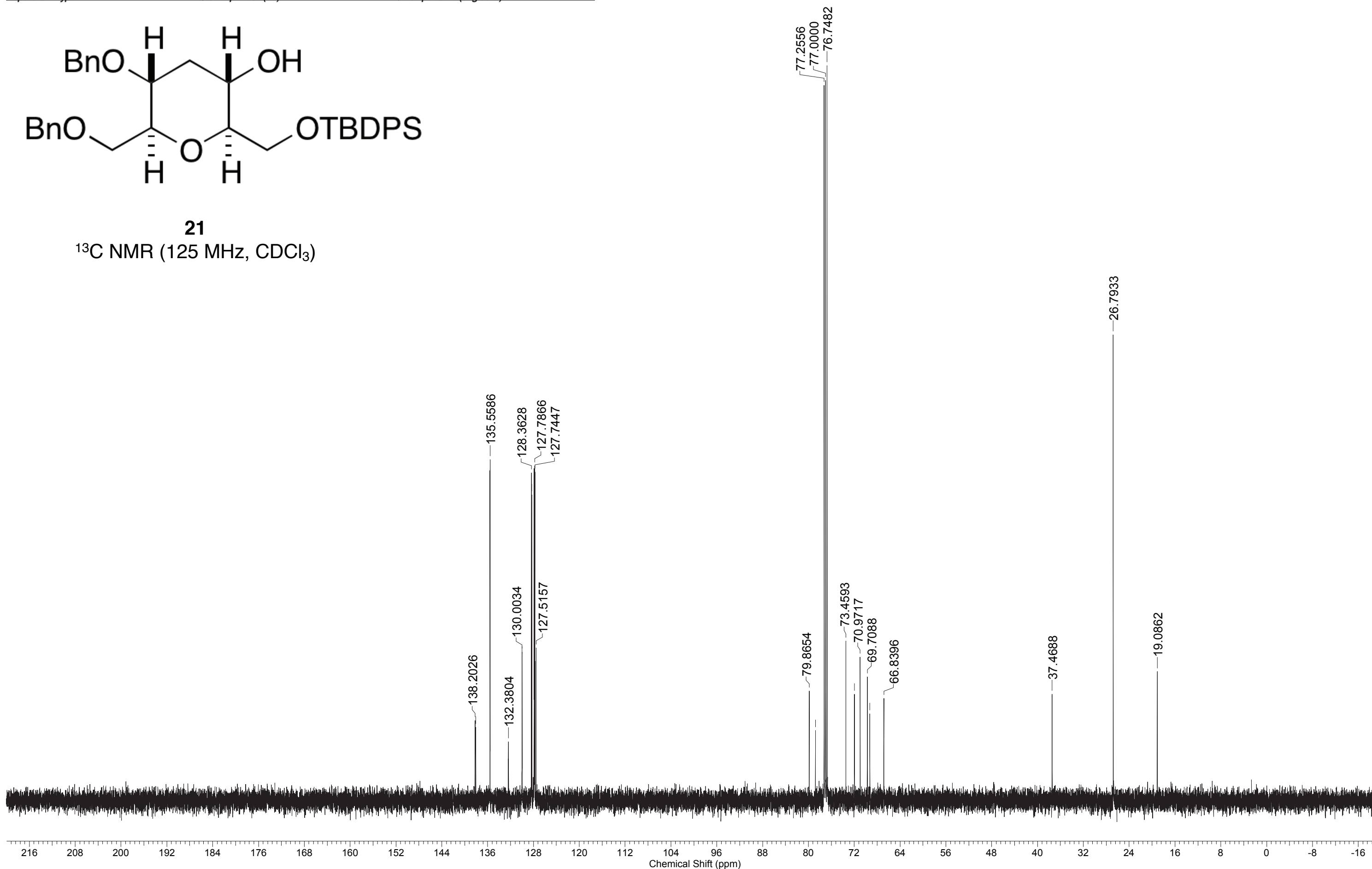


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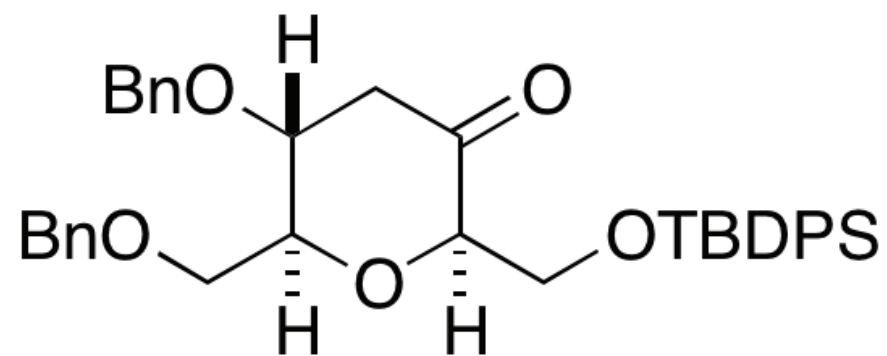


21

¹³C NMR (125 MHz, CDCl₃)

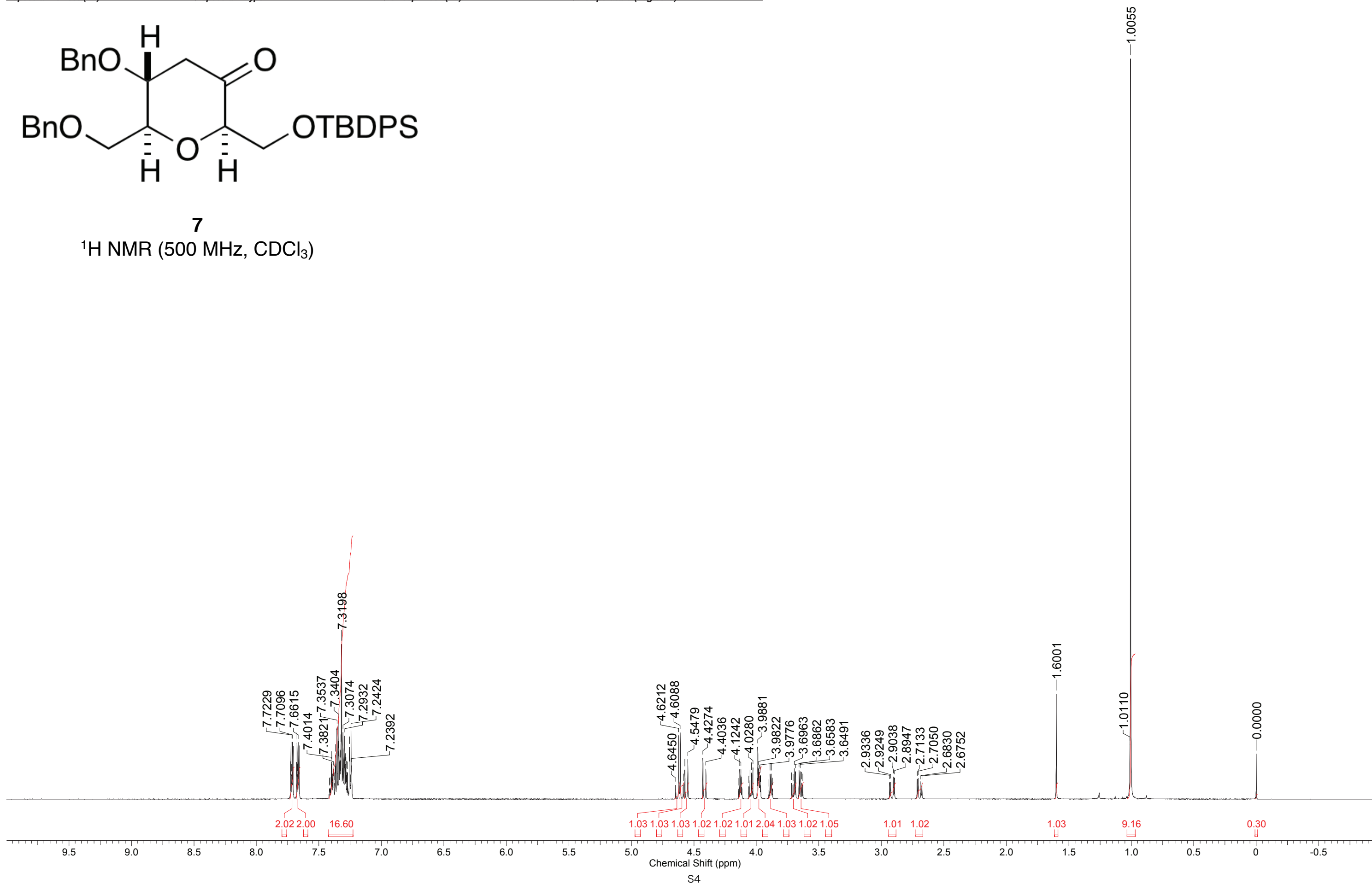


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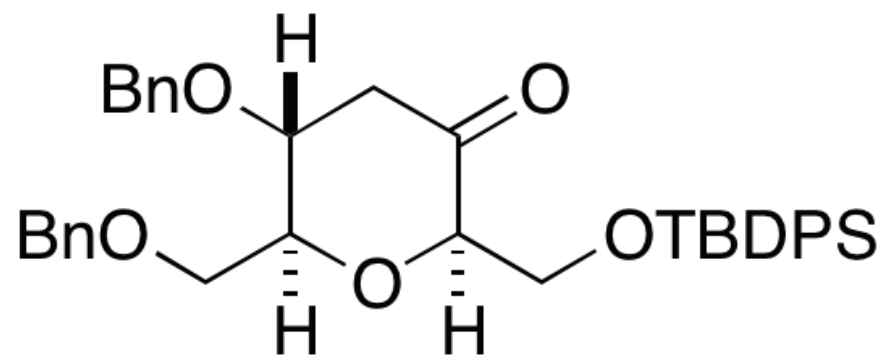


7

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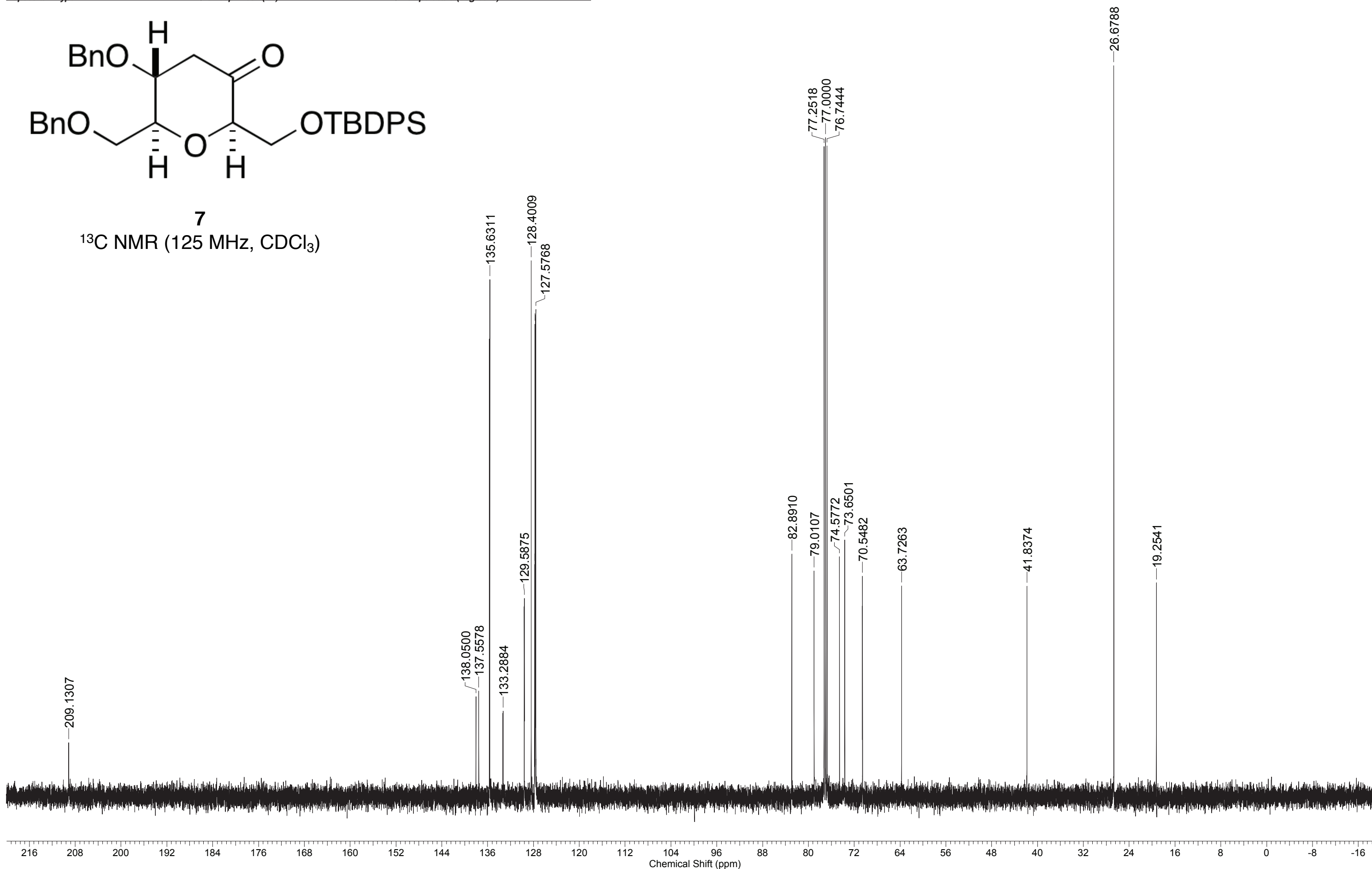


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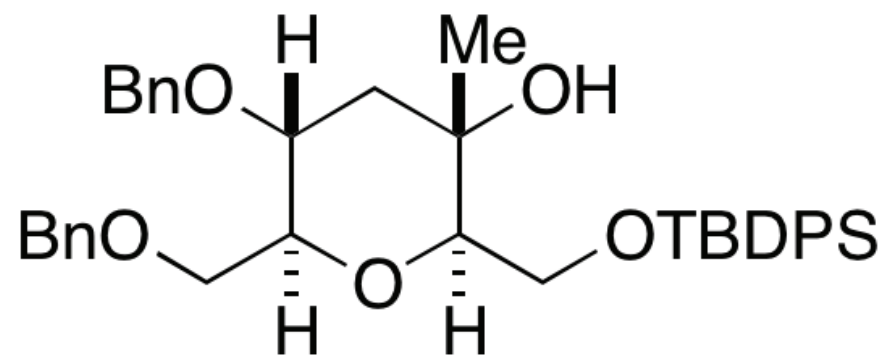


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¹³C NMR (125 MHz, CDCl₃)

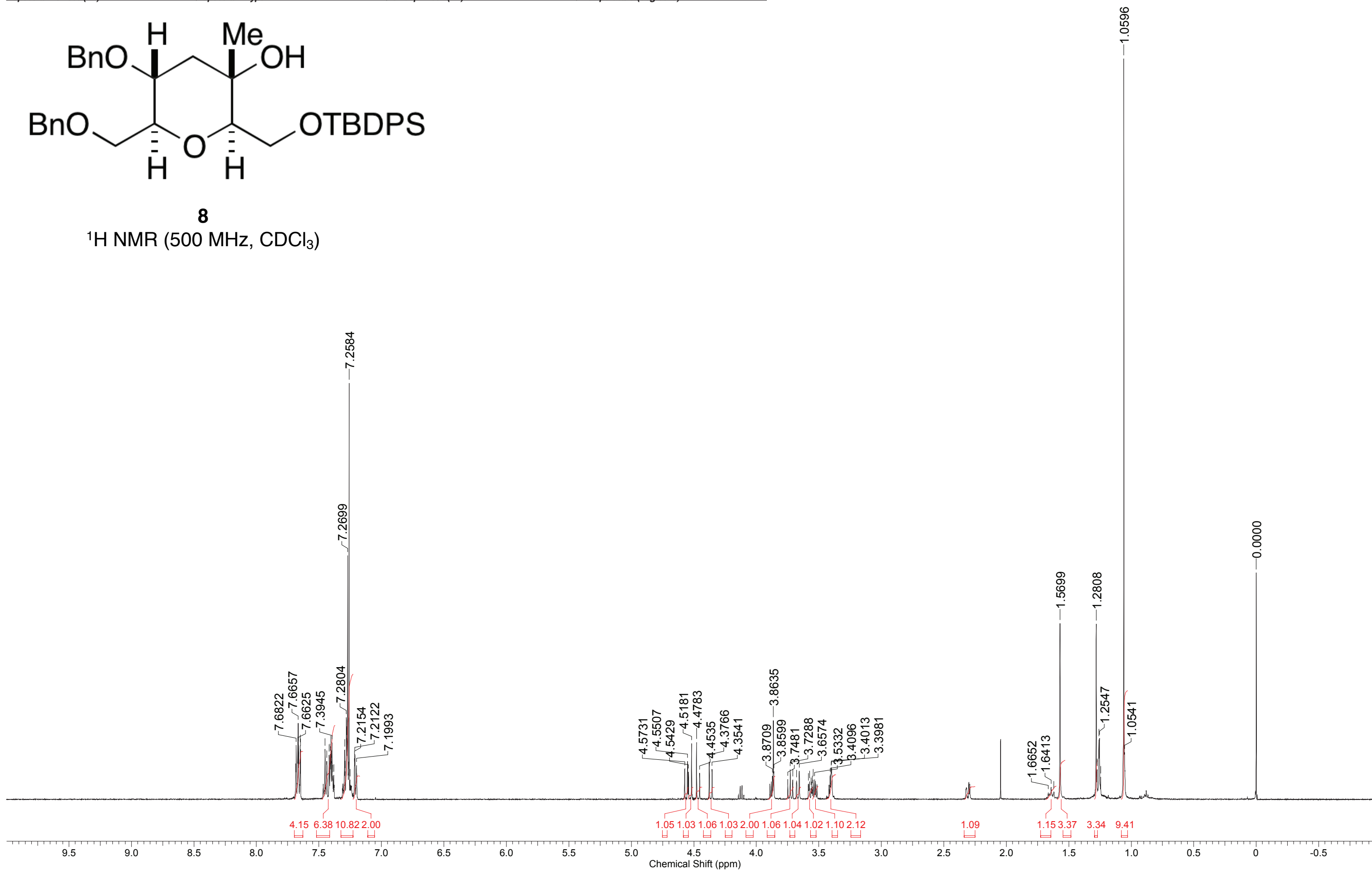


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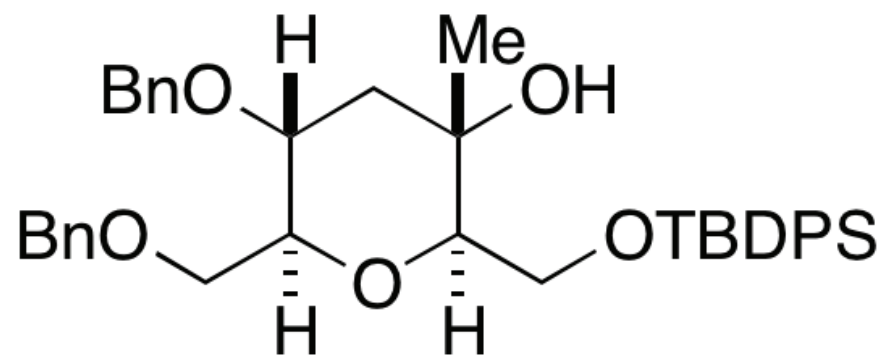


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¹H NMR (500 MHz, CDCl₃)

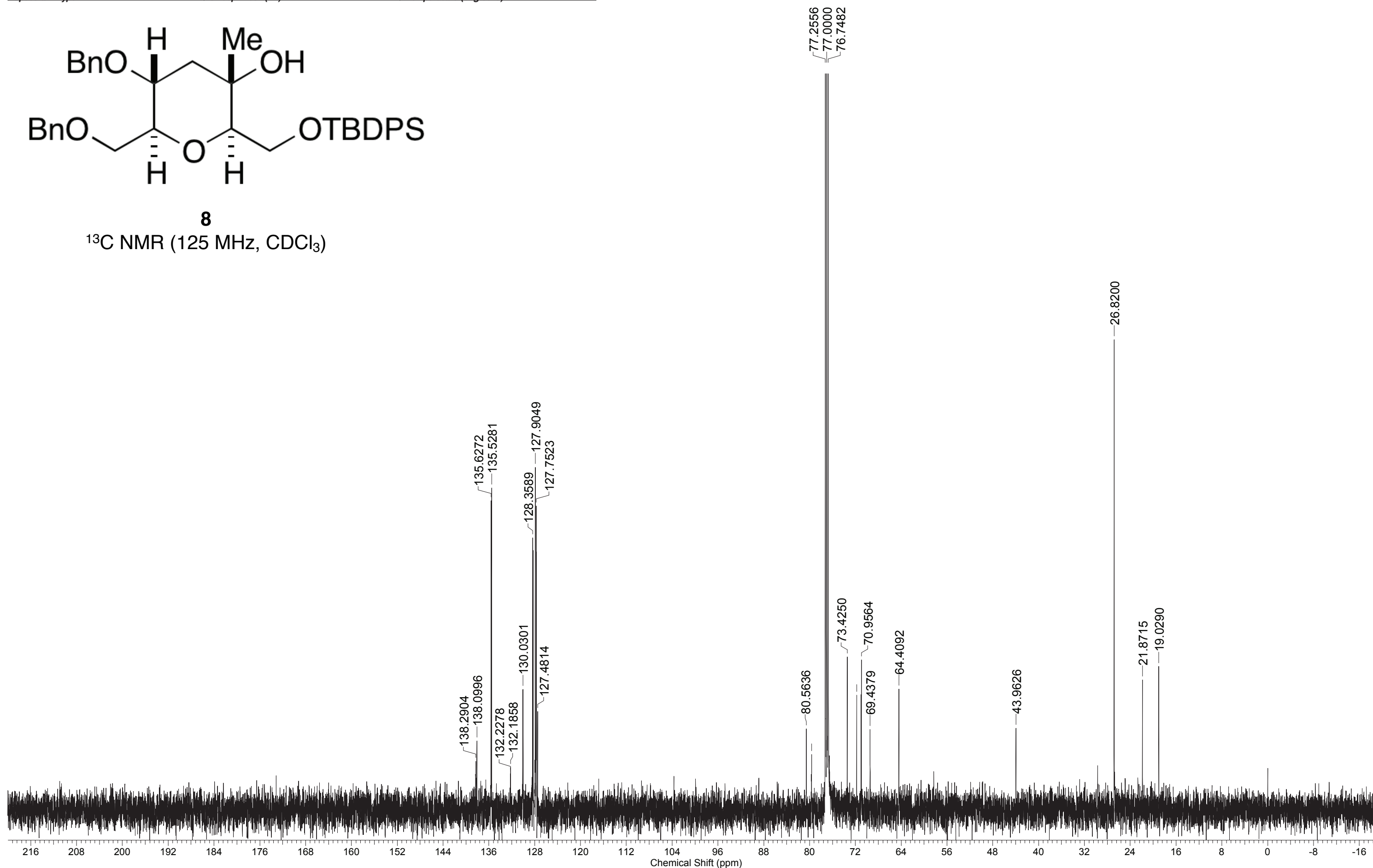


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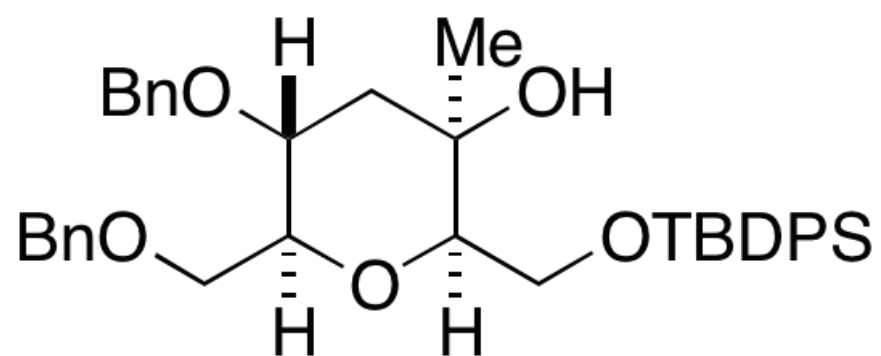


8

¹³C NMR (125 MHz, CDCl₃)

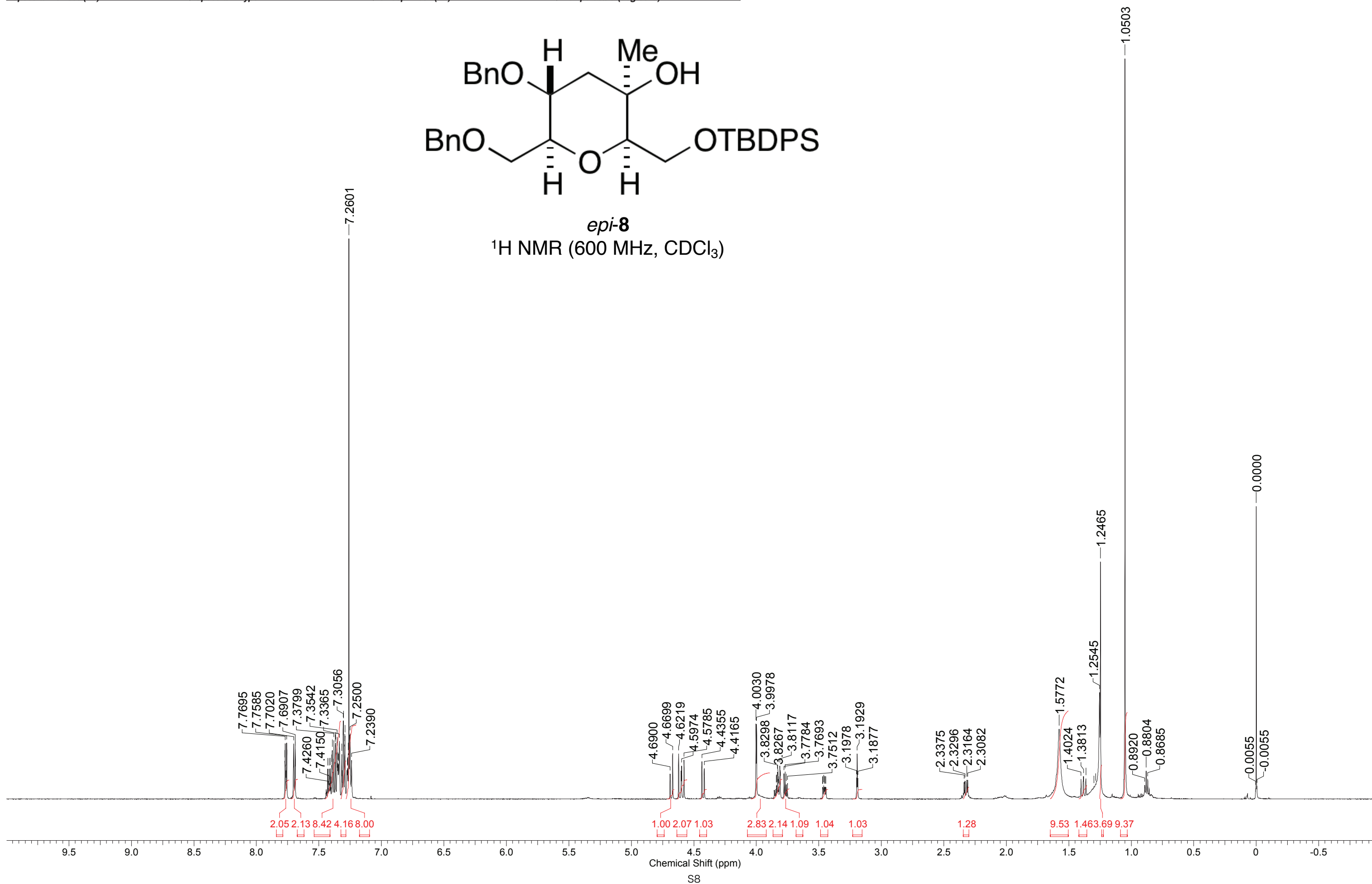


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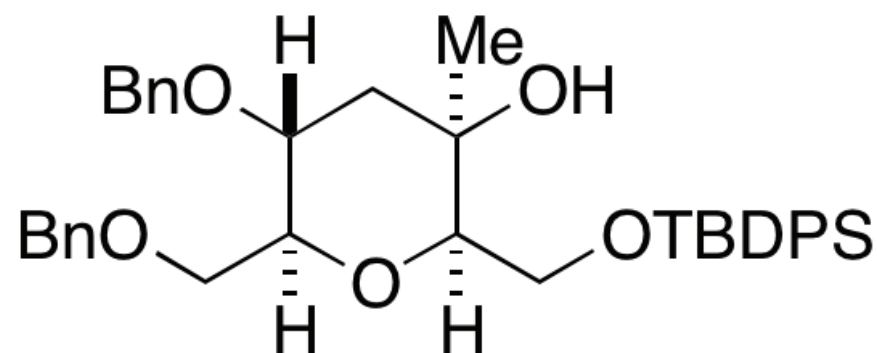


epi-8

¹H NMR (600 MHz, CDCl₃)

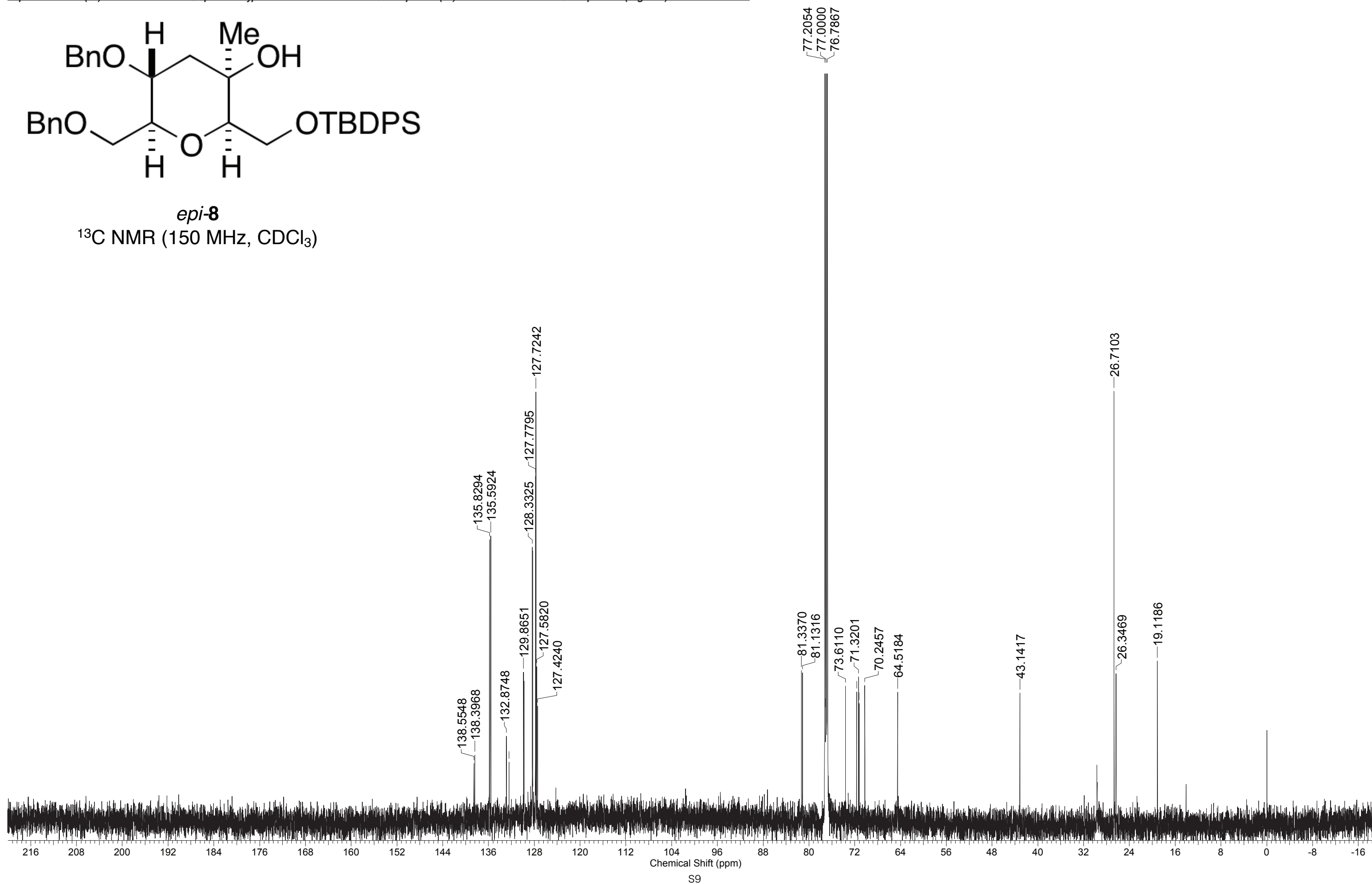


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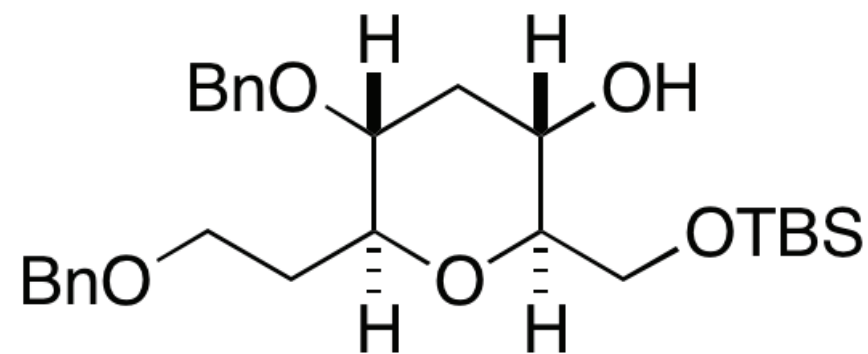


epi-8

¹³C NMR (150 MHz, CDCl₃)

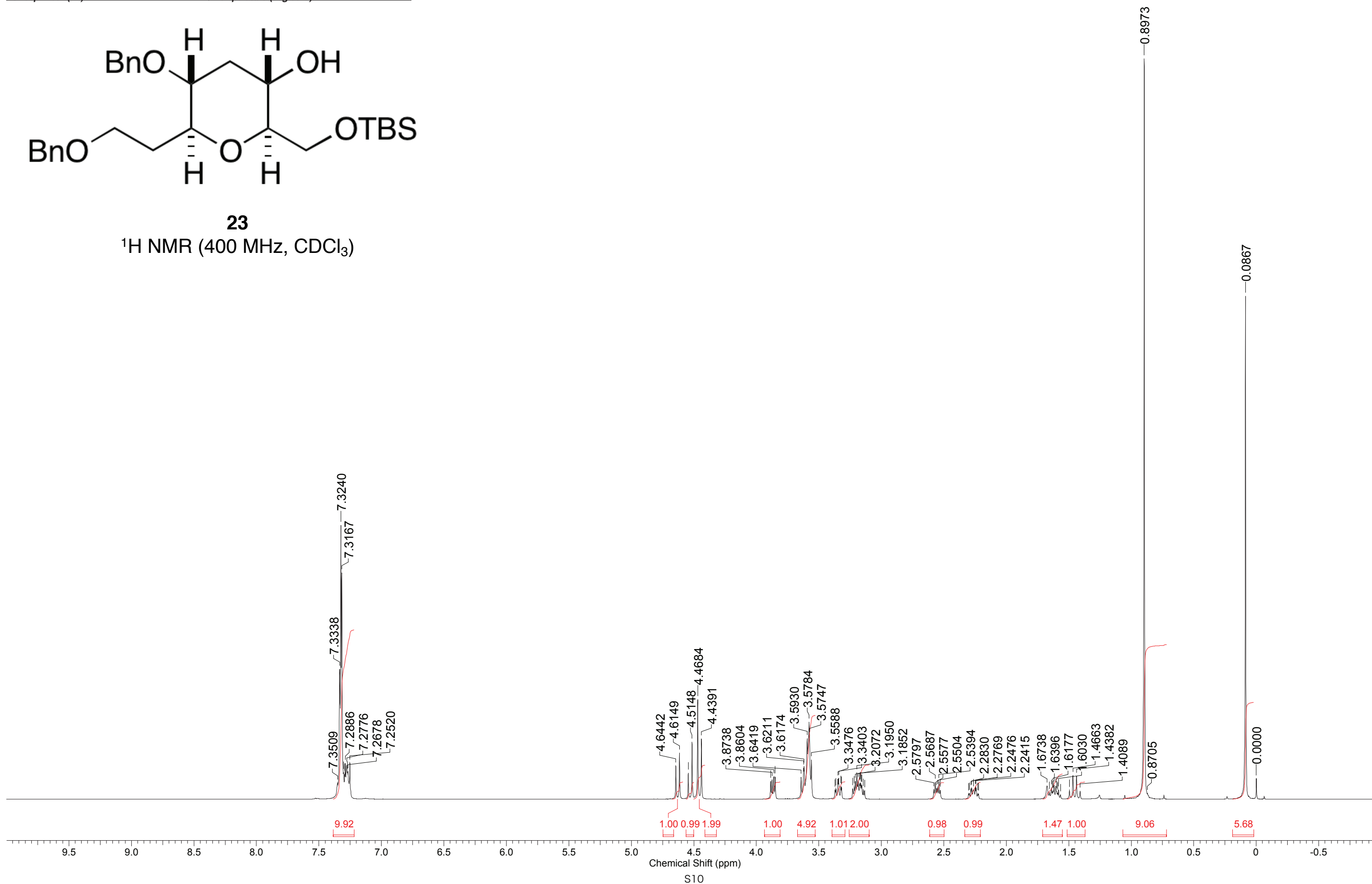


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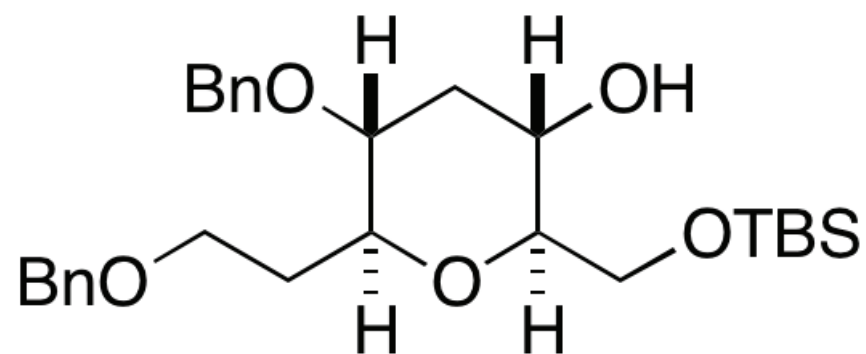


23

¹H NMR (400 MHz, CDCl₃)

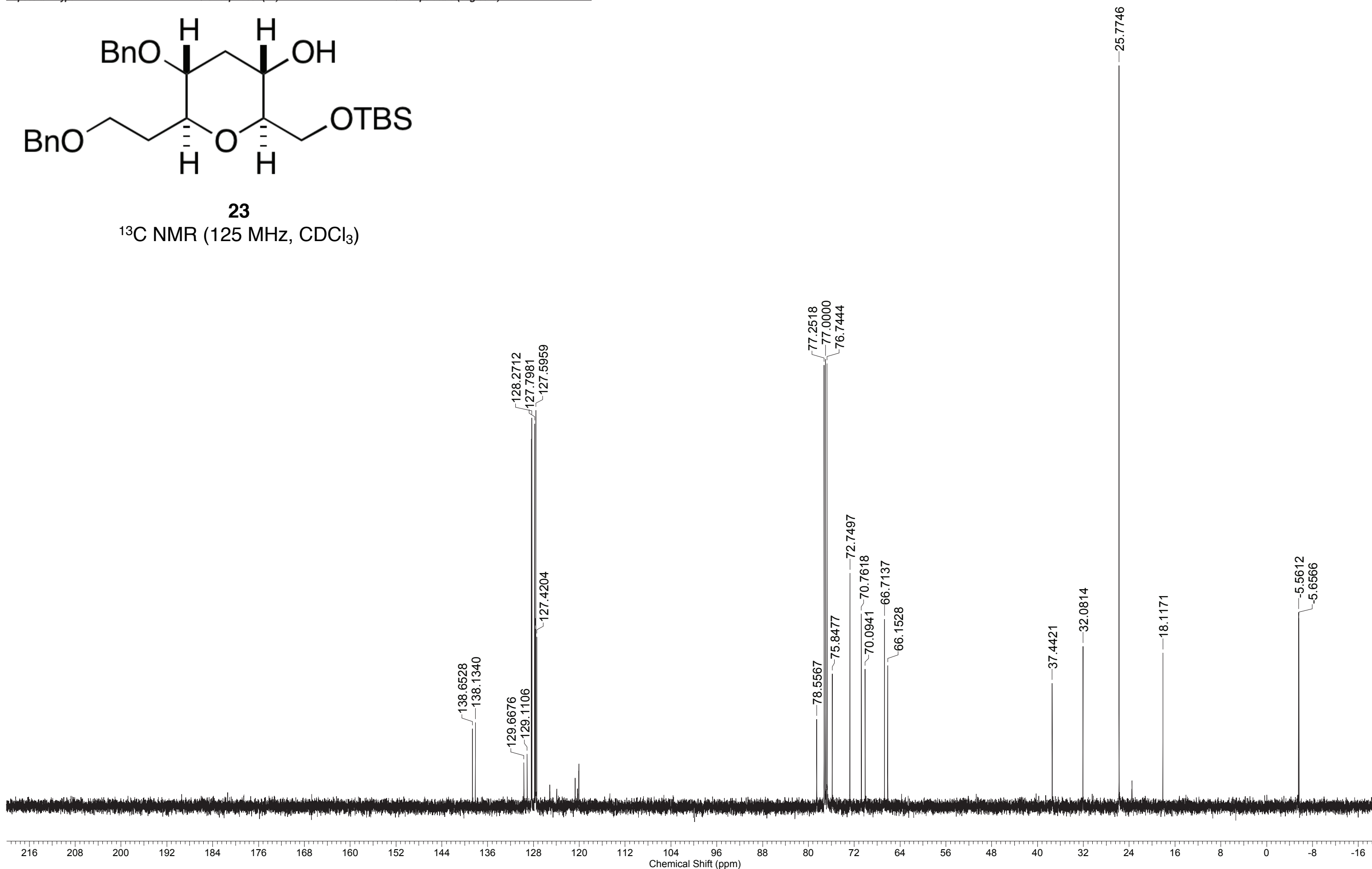


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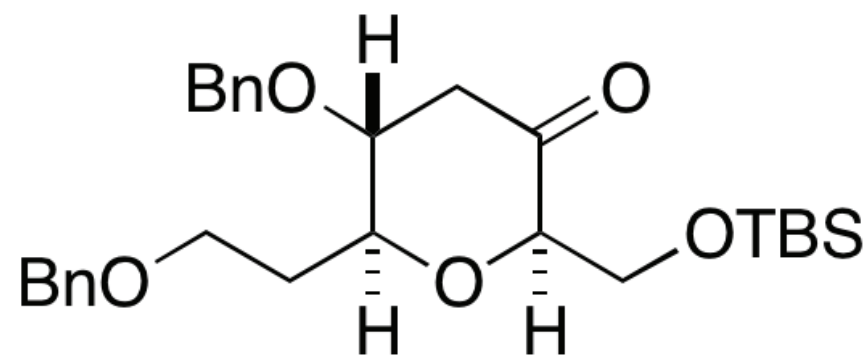


23

¹³C NMR (125 MHz, CDCl₃)

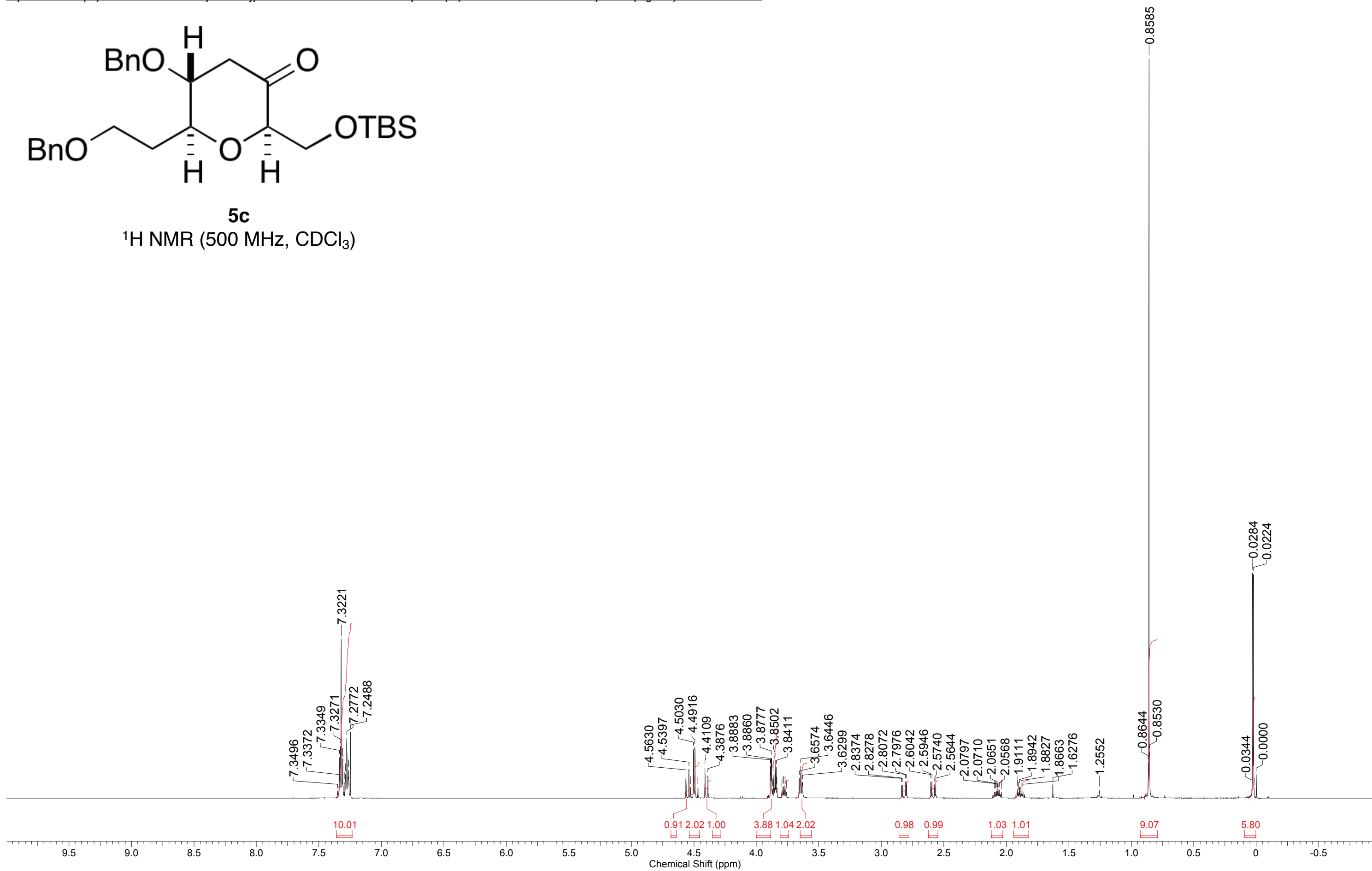


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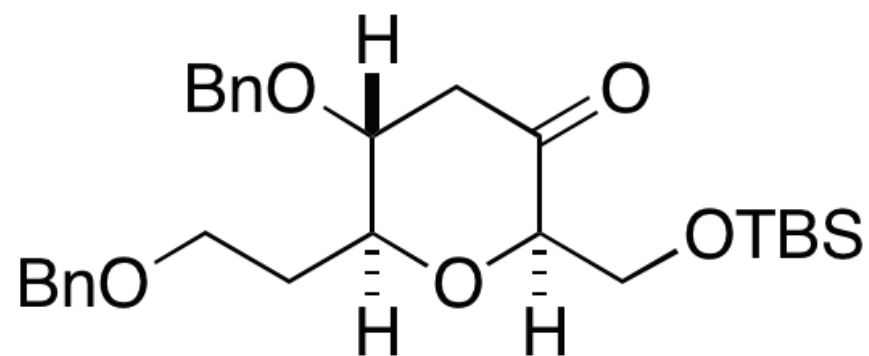


5c

¹H NMR (500 MHz, CDCl₃)

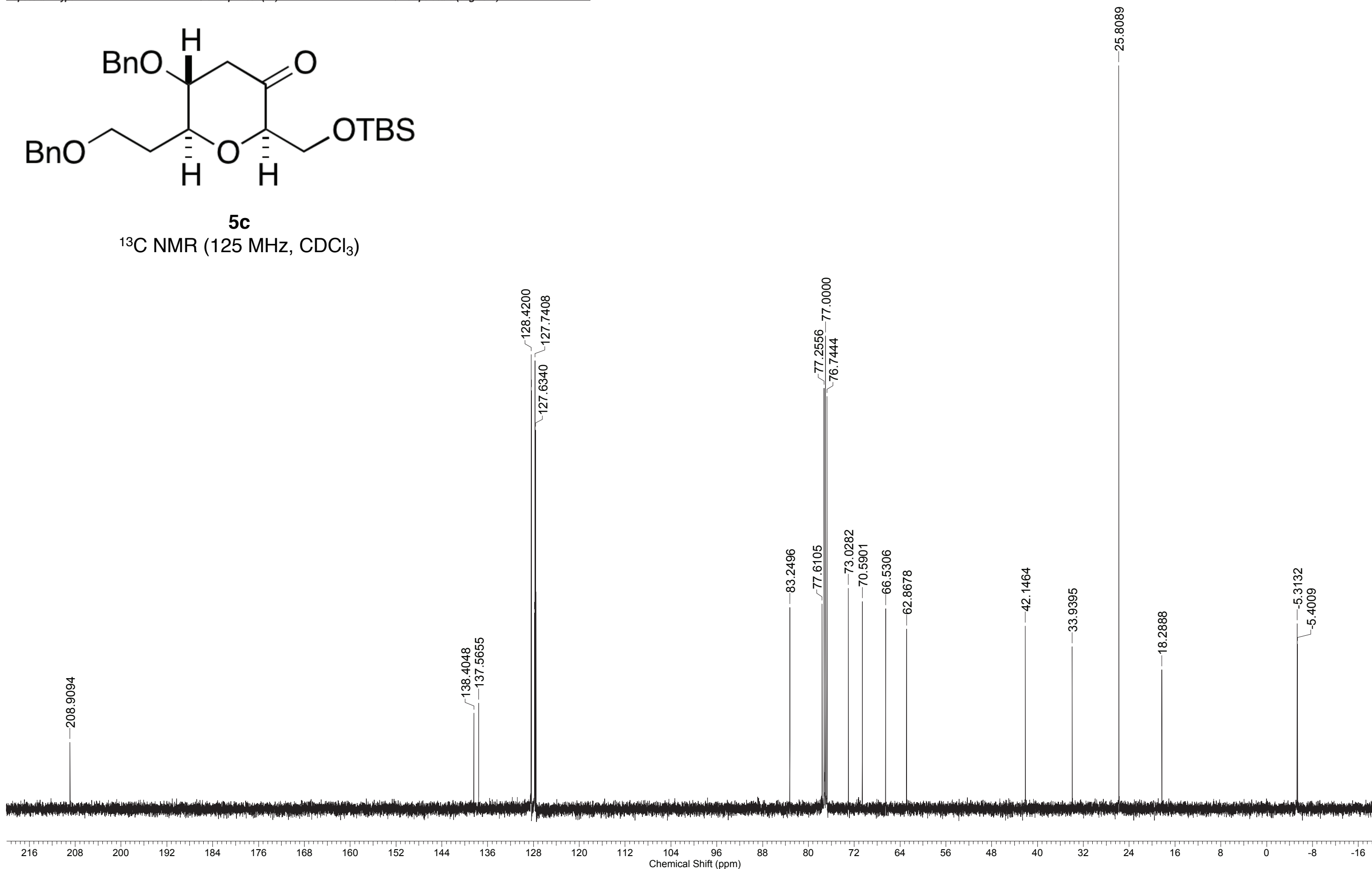


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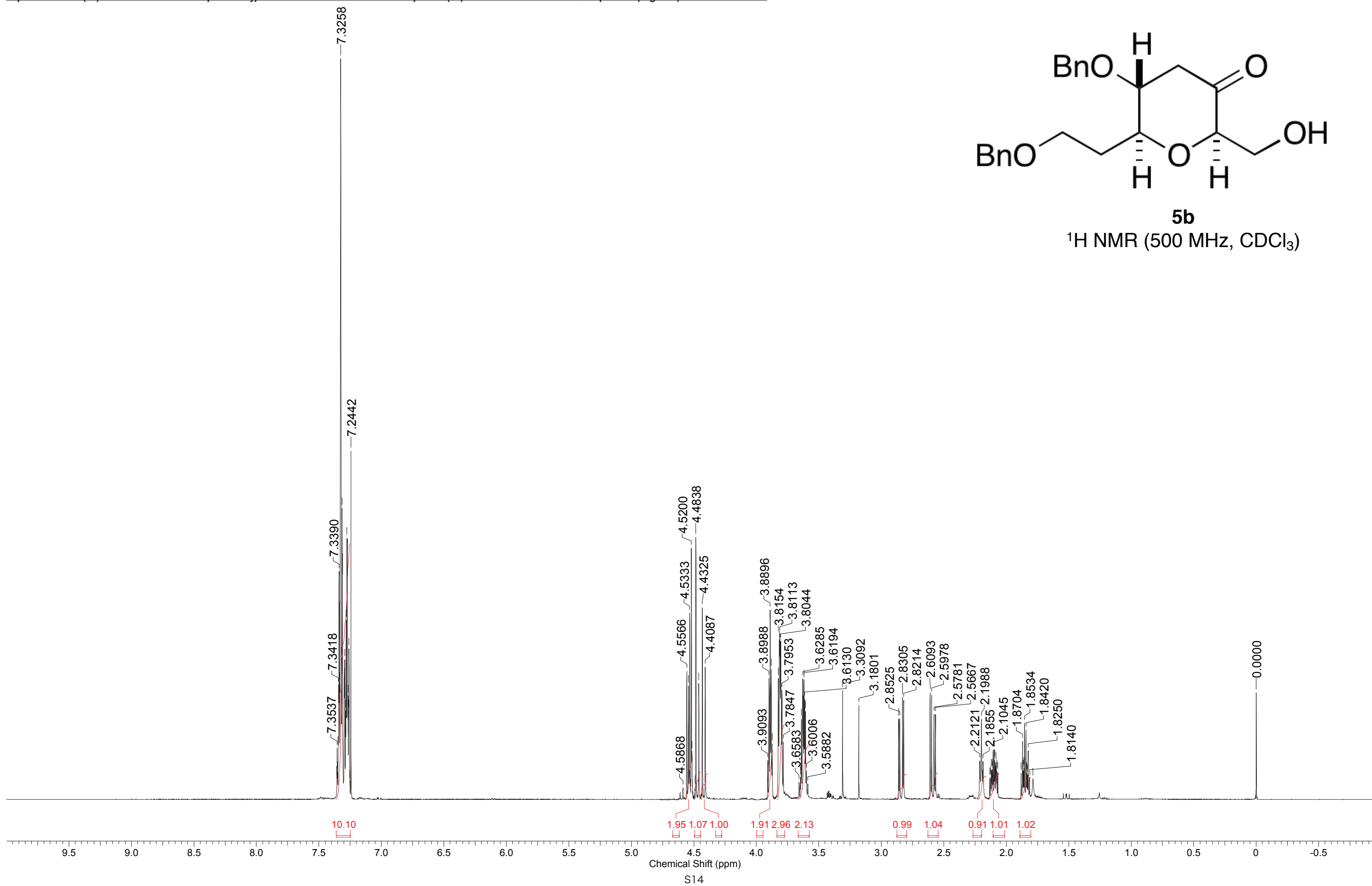


5c

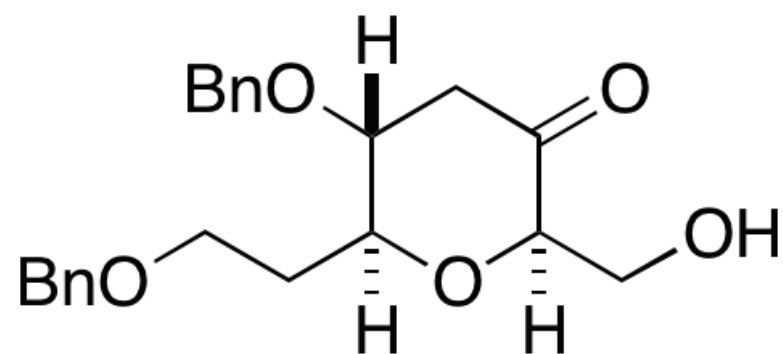
¹³C NMR (125 MHz, CDCl₃)



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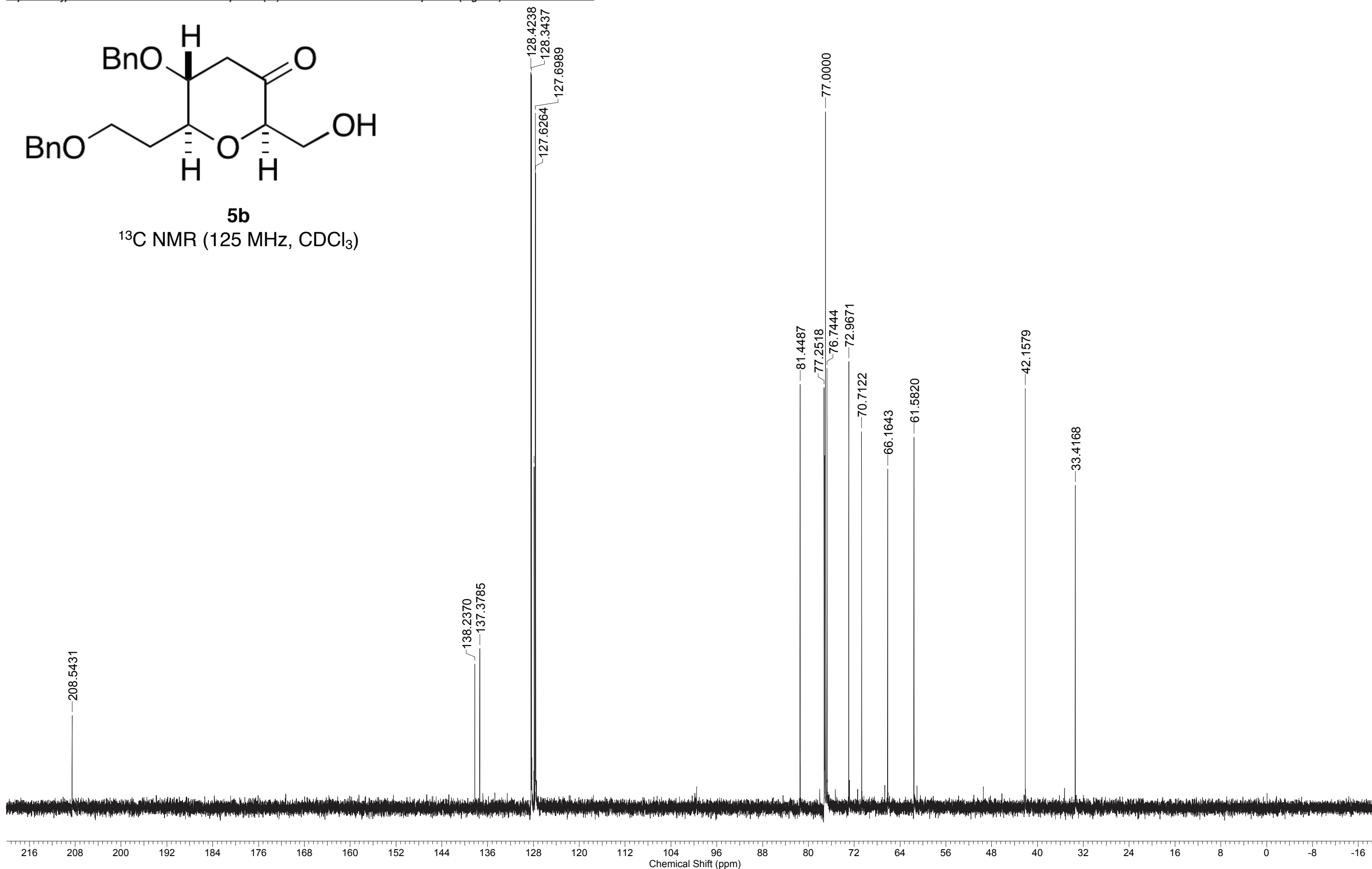


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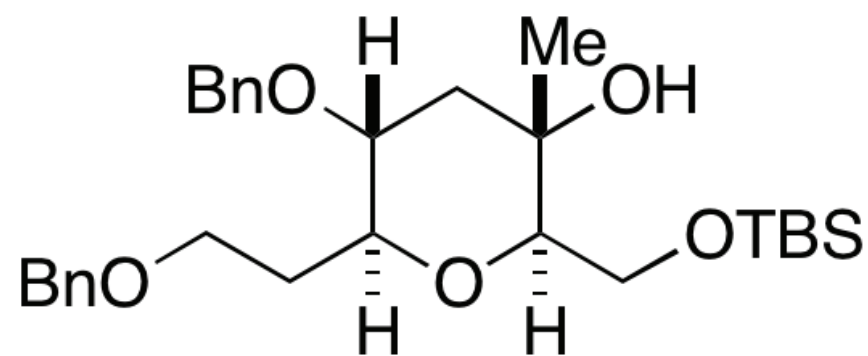


5b

¹³C NMR (125 MHz, CDCl₃)

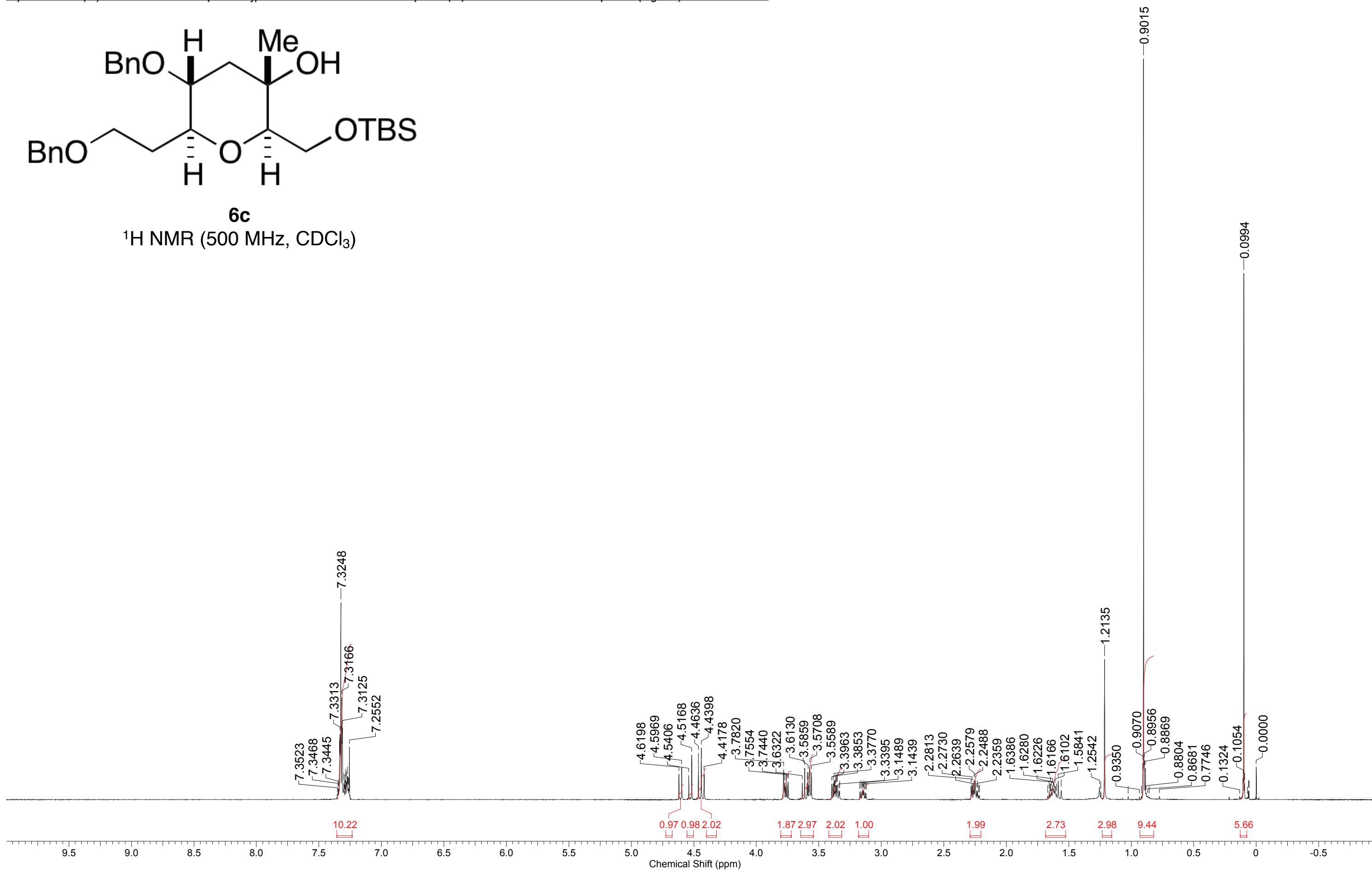


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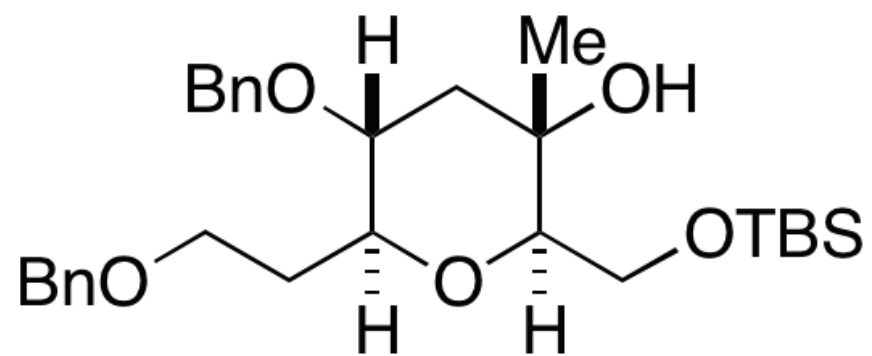


6c

¹H NMR (500 MHz, CDCl₃)

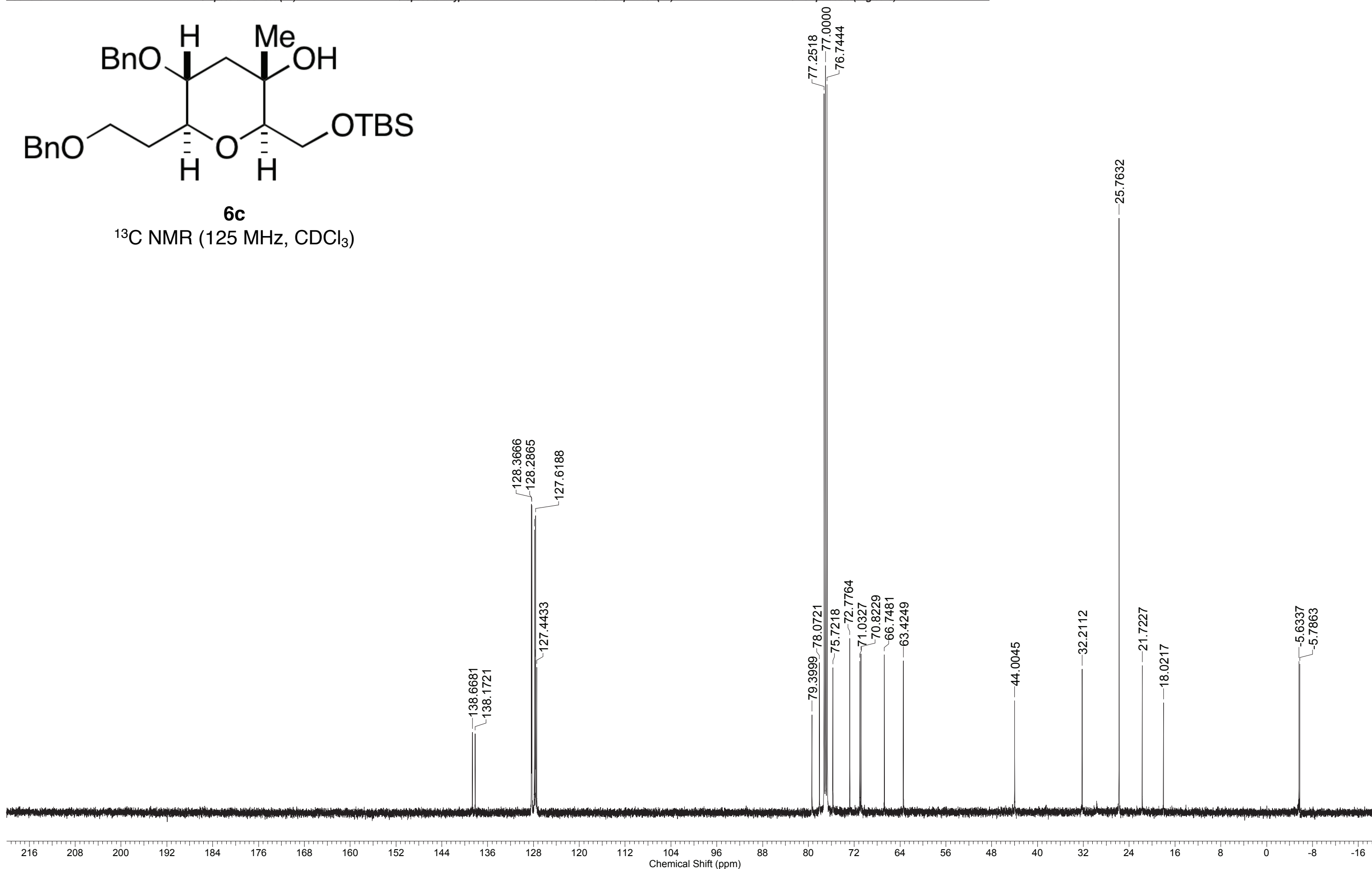


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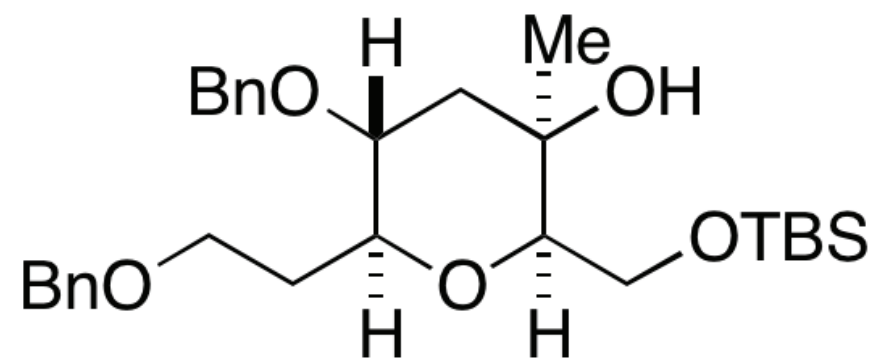


6c

¹³C NMR (125 MHz, CDCl₃)

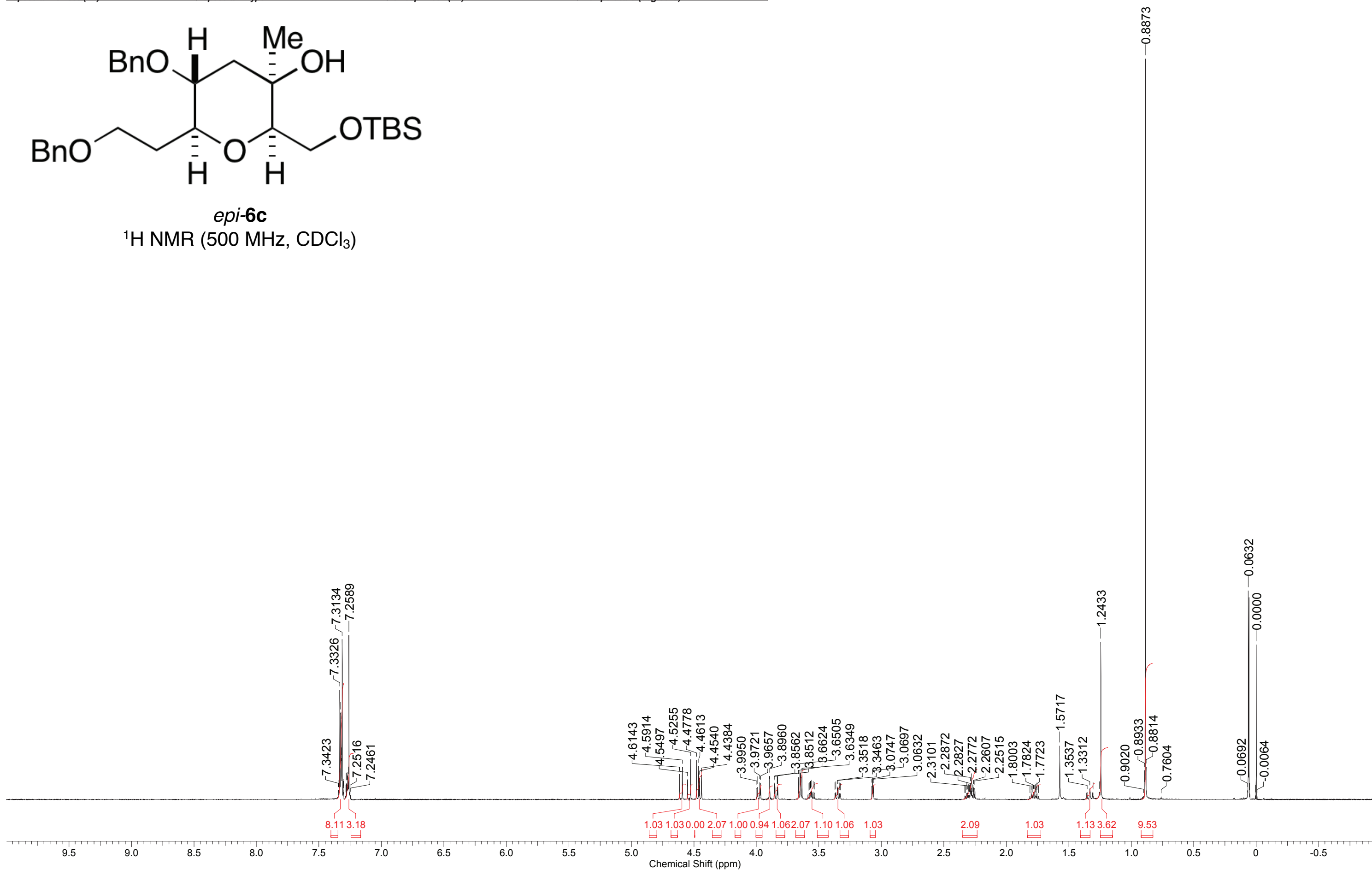


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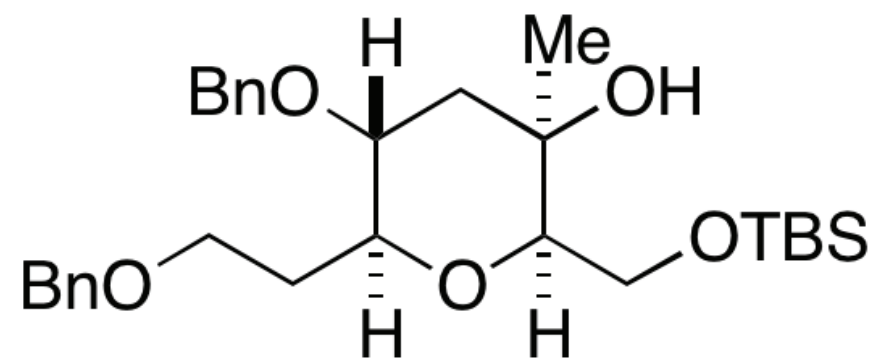


epi-6c

¹H NMR (500 MHz, CDCl₃)

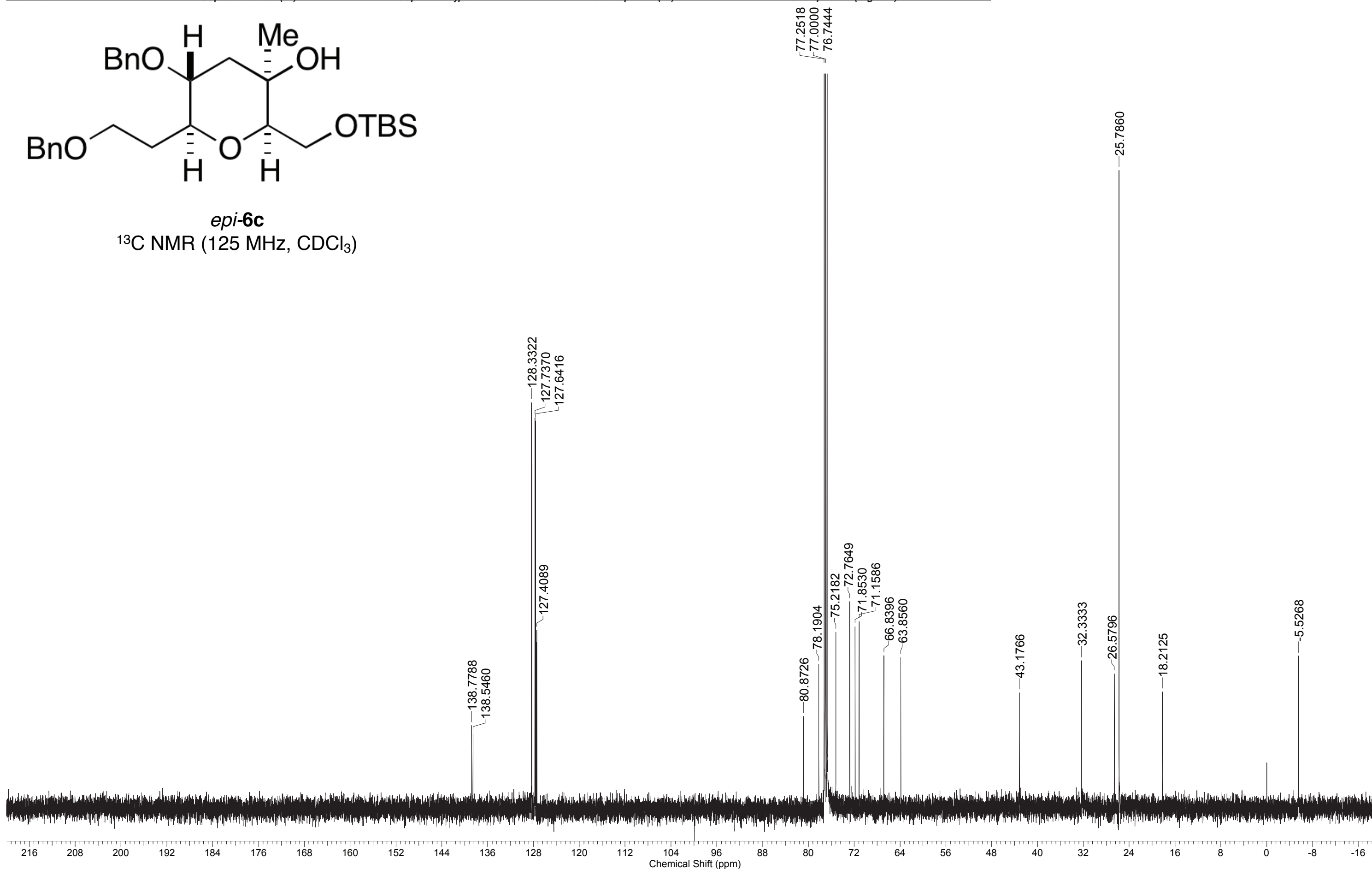


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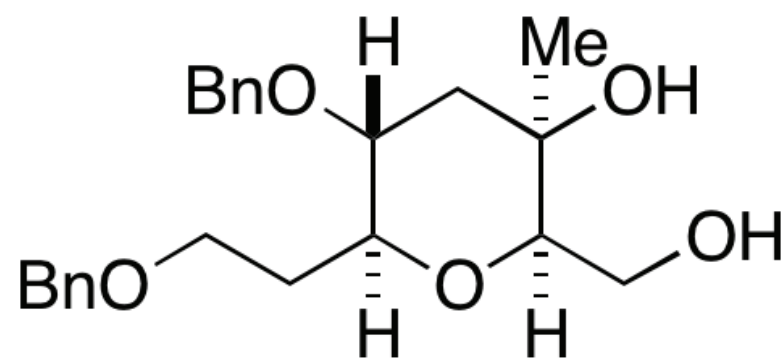


epi-6c

¹³C NMR (125 MHz, CDCl₃)

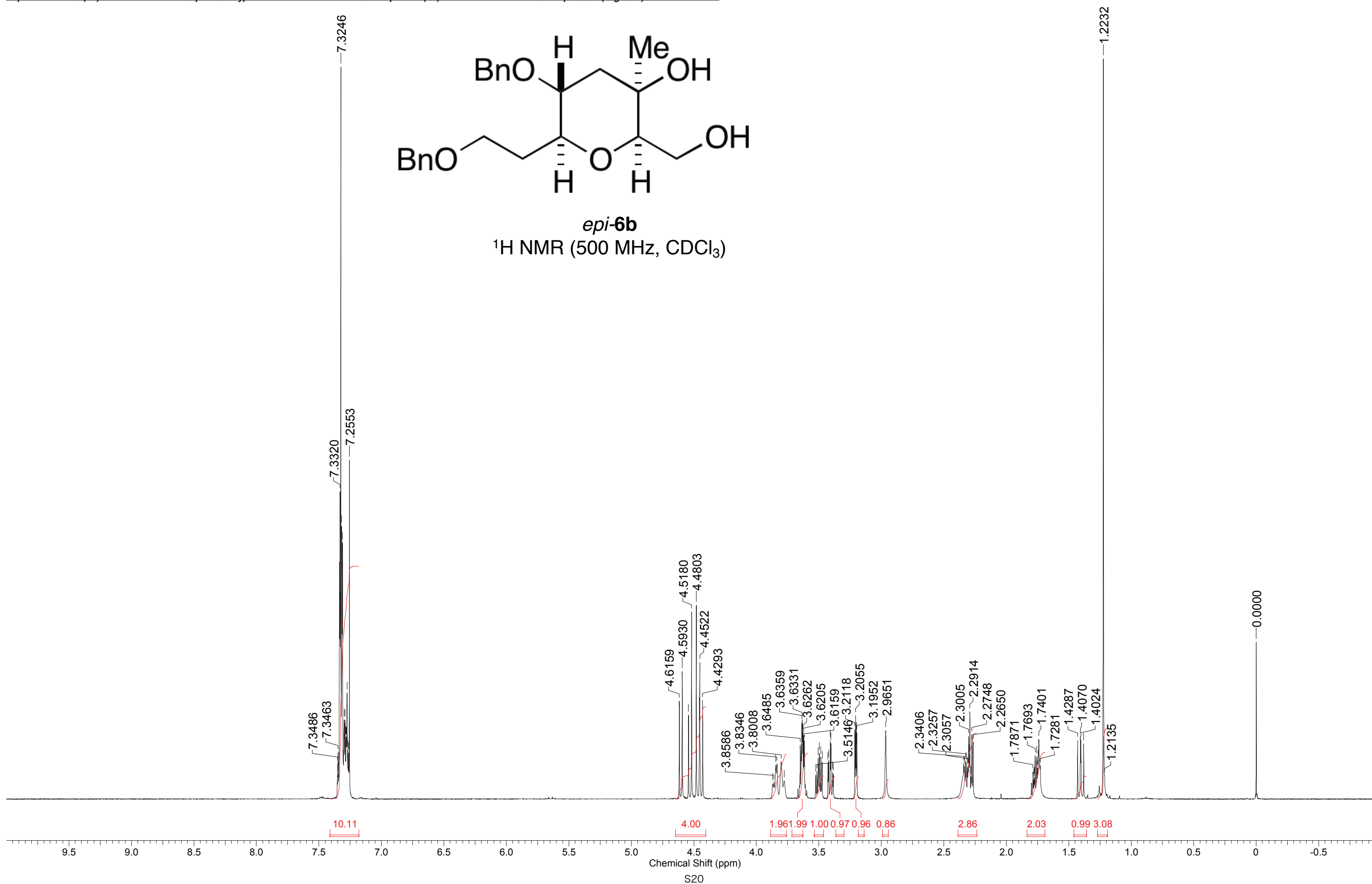


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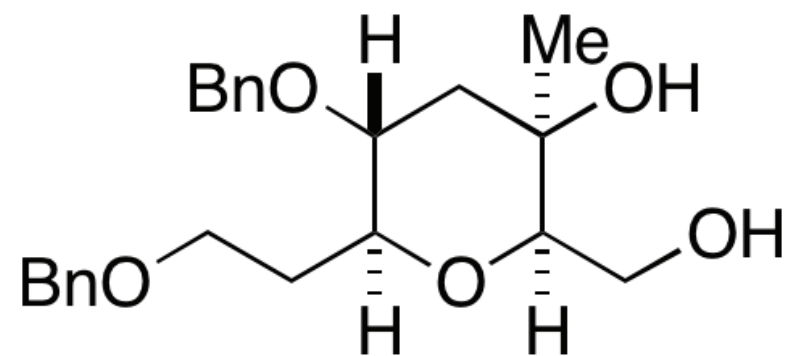


epi-6b

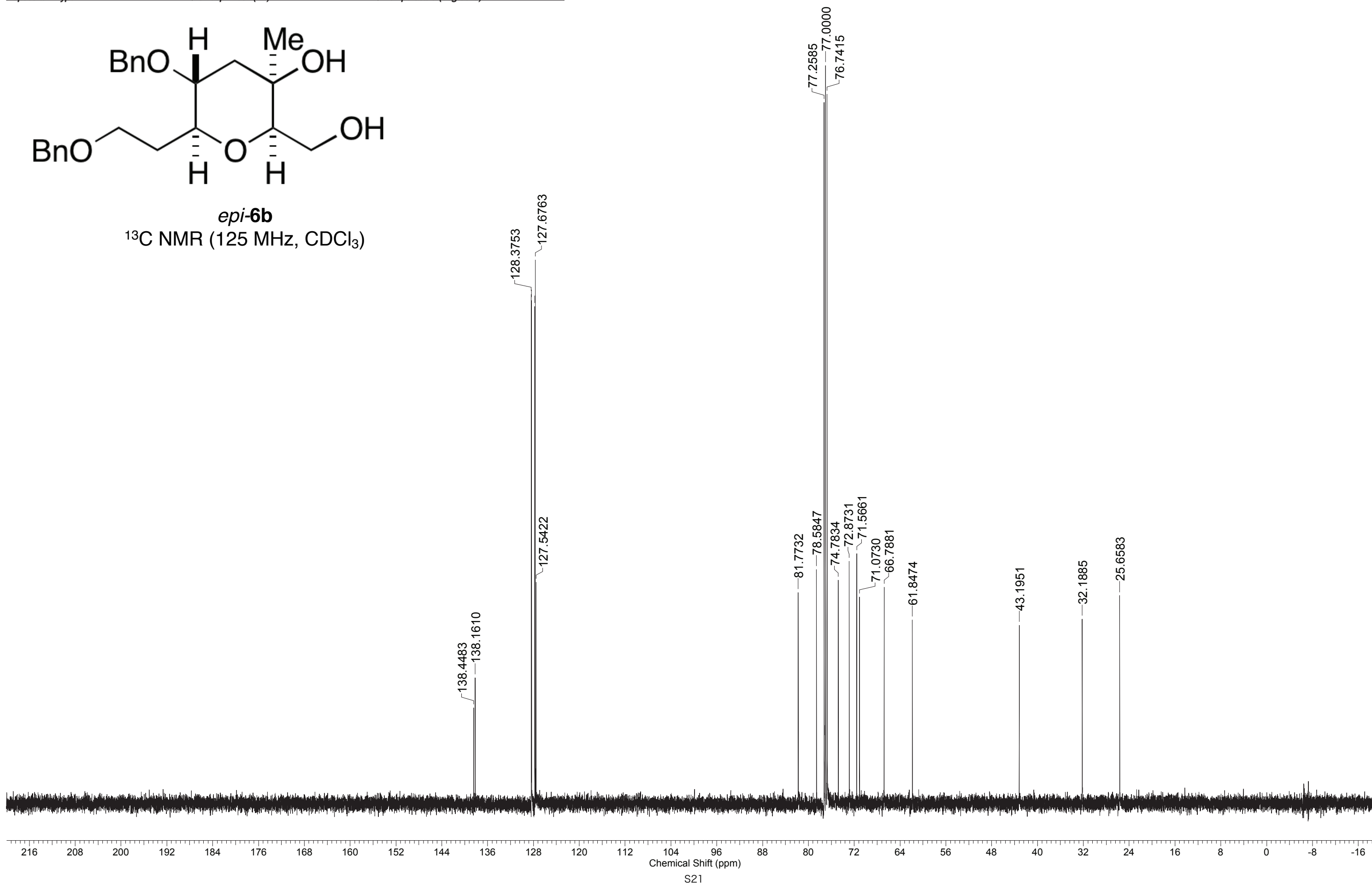
¹H NMR (500 MHz, CDCl₃)



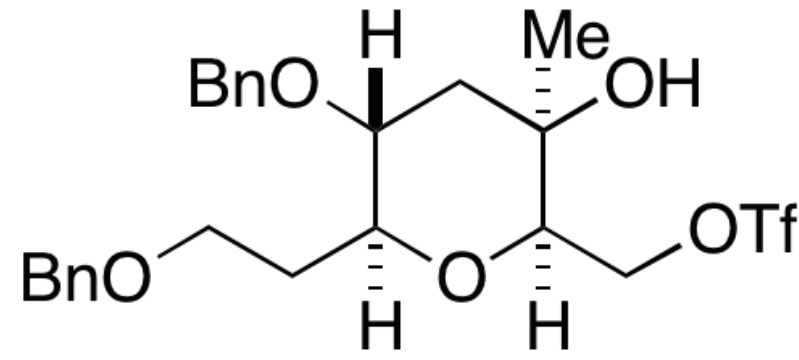
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epi-6b
¹³C NMR (125 MHz, CDCl₃)

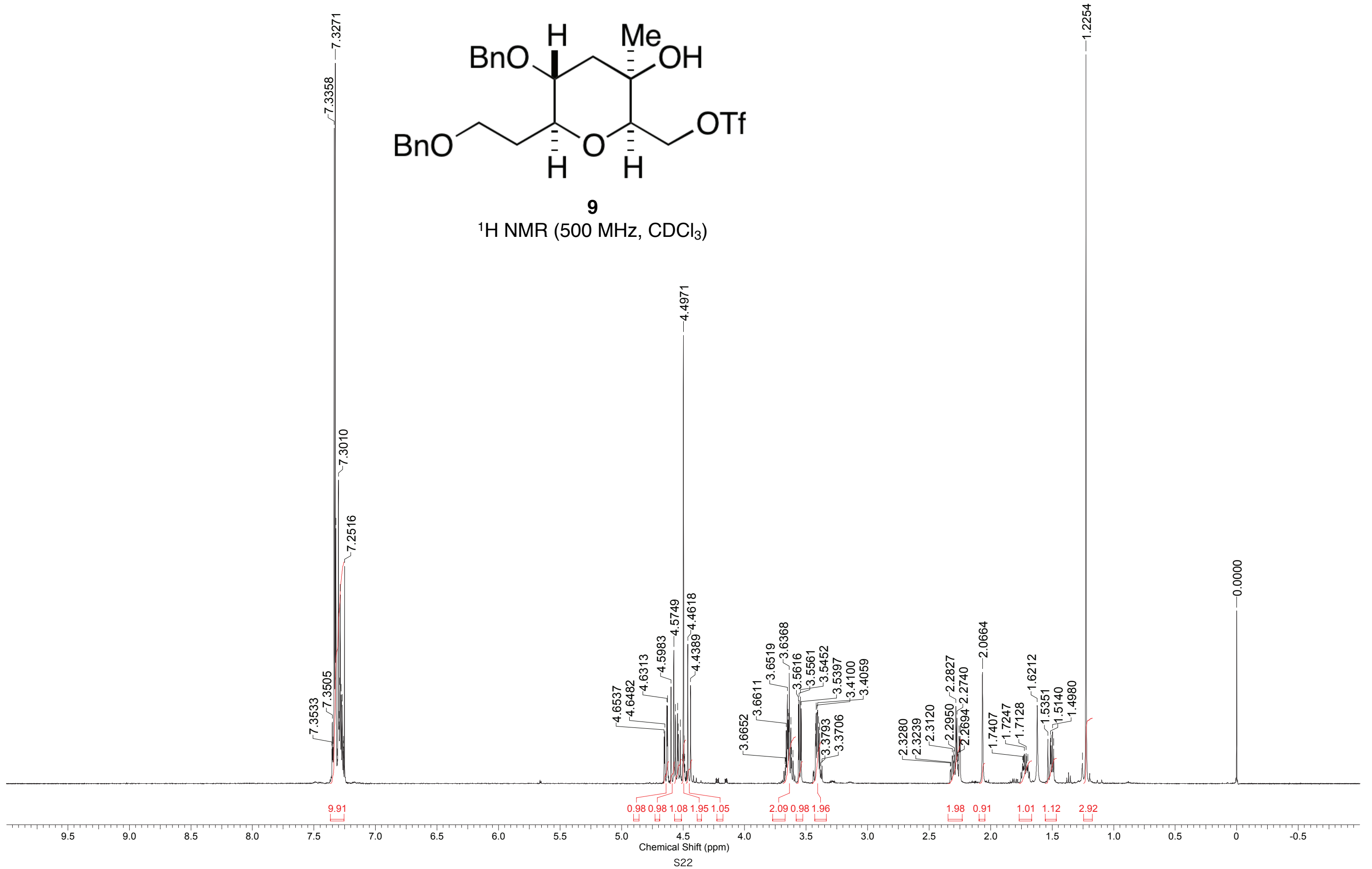


Acquisition Time (sec)	2.1823	Comment	Single Pulse Experiment	Date	27 Aug 2013 11:52:44	Date Stamp	27 Aug 2013 11:52:44
File Name	¥¥psf¥Home¥Desktop¥在在在在¥yoshida01029H1.1	Frequency (MHz)	500.16	Nucleus	1H	Number of Transients	8
Owner	JEOL LTD.	Points Count	32768	Pulse Sequence	single_pulse.exp	Receiver Gain	18.00
Spectrum Offset (Hz)	2499.1038	Spectrum Type	STANDARD	Sweep Width (Hz)	7507.51	Temperature (degree C)	25.500
						Origin	ECP500
						Solvent	CHLOROFORM-d
						Original Points Count	16384

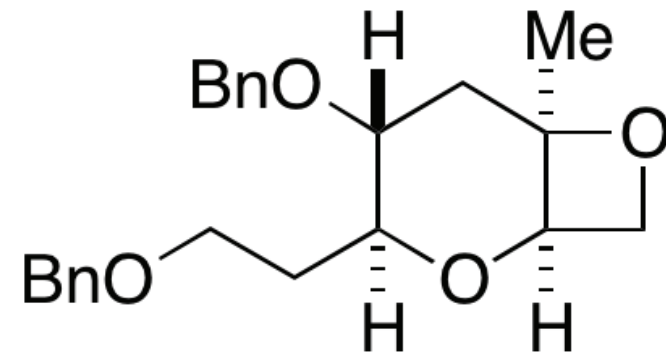


9

¹H NMR (500 MHz, CDCl₃)

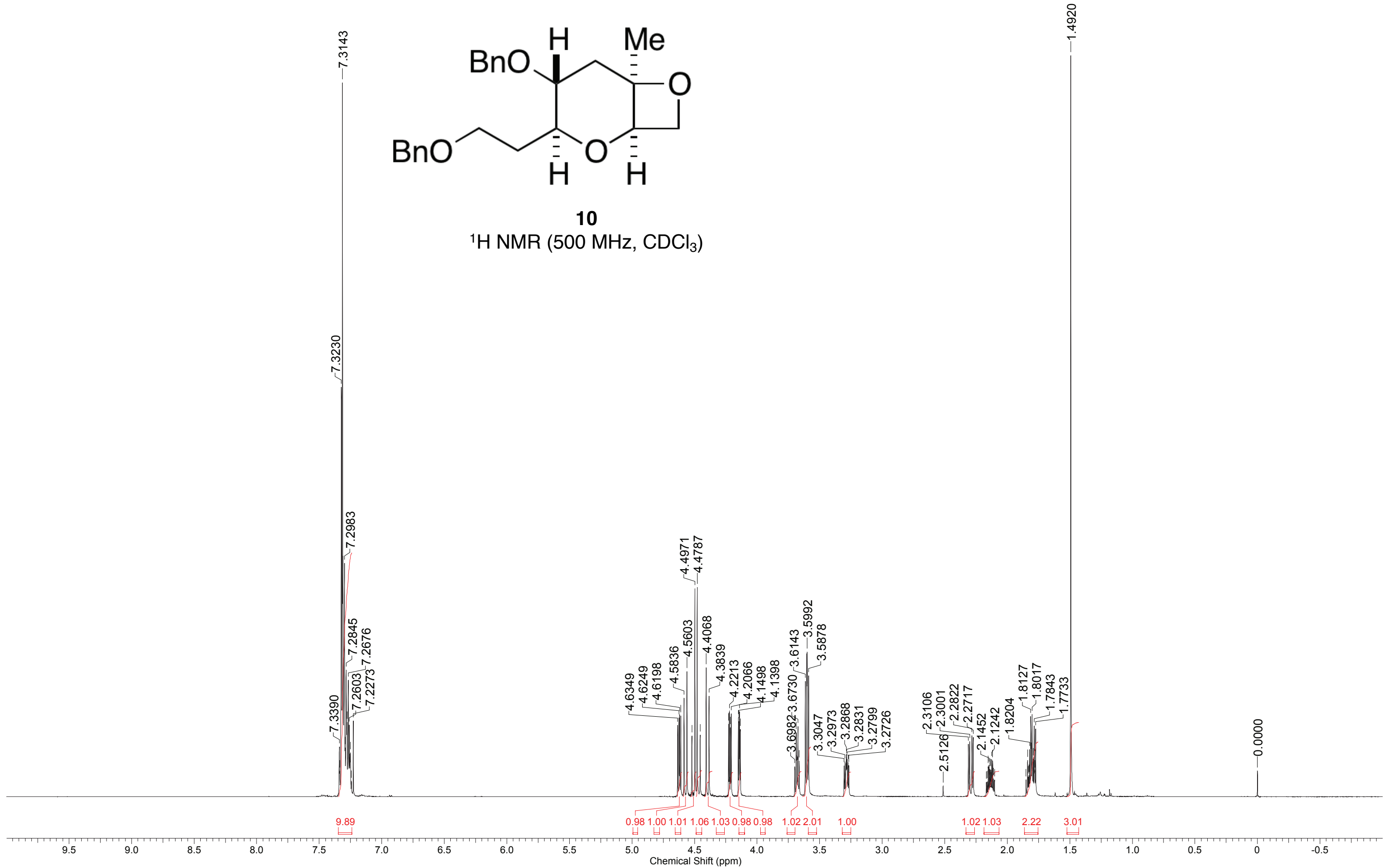


Acquisition Time (sec)	2.1823	Comment	Single Pulse Experiment	Date	28 Aug 2013 11:56:13	Date Stamp	28 Aug 2013 11:56:13
File Name	¥¥psf¥Home¥Desktop¥车车车¥yoshida01030H1.1	Frequency (MHz)	500.16	Nucleus	1H	Number of Transients	8
Owner	JEOL LTD.	Points Count	32768	Pulse Sequence	single_pulse.exp	Receiver Gain	14.00
Spectrum Offset (Hz)	2486.9607	Spectrum Type	STANDARD	Sweep Width (Hz)	7507.51	Temperature (degree C)	24.800
						Origin	ECP500
						Original Points Count	16384
						Solvent	CHLOROFORM-d

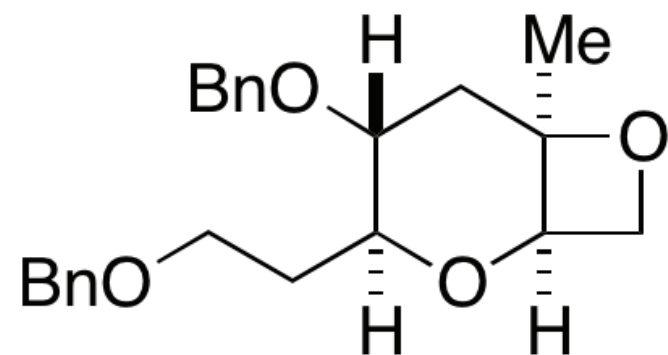


10

¹H NMR (500 MHz, CDCl₃)

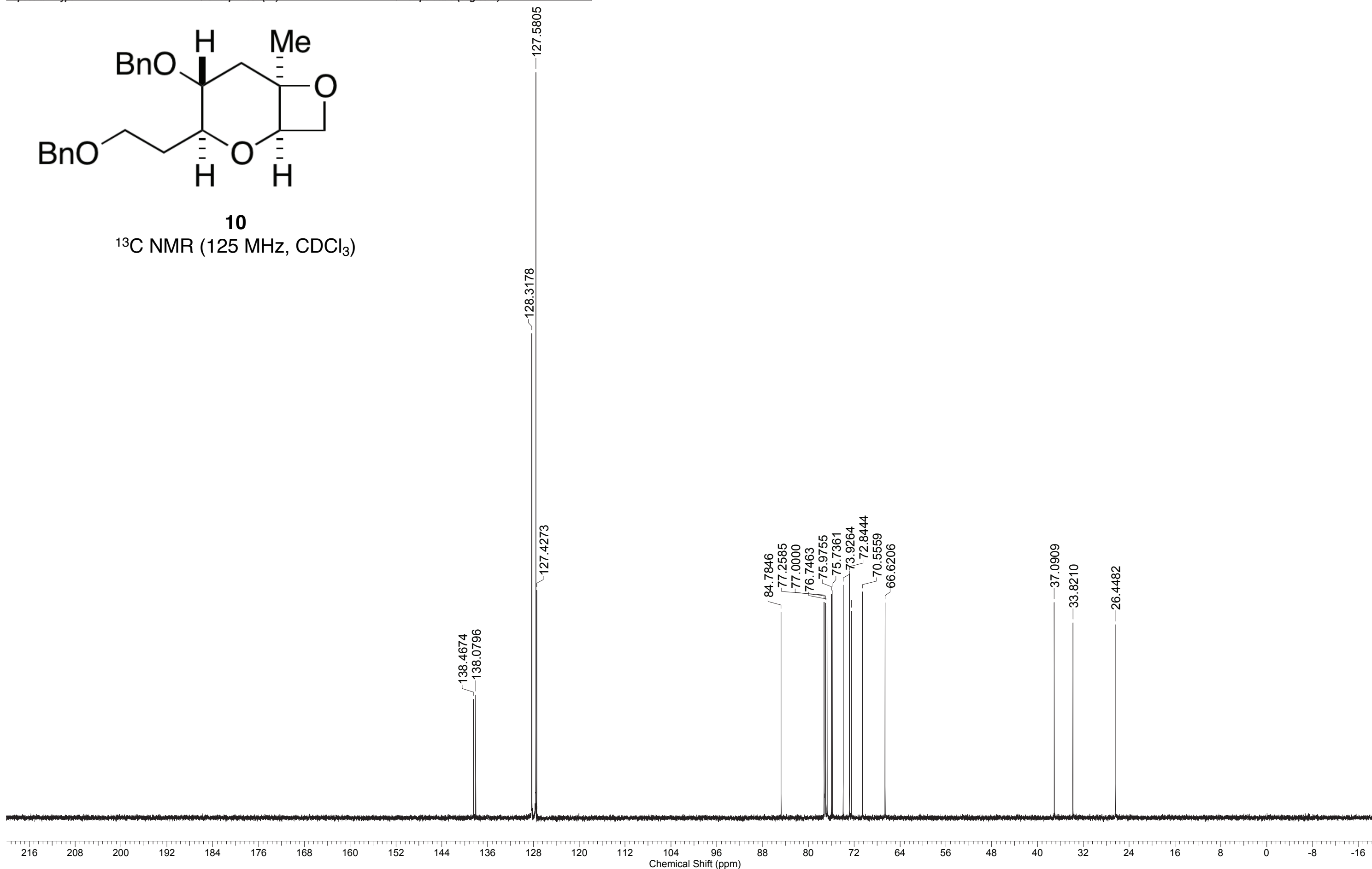


Acquisition Time (sec)	0.8389	Comment	single_pulse_decoupled gated NOE	Date	28 Aug 2013 12:52:19	Date Stamp	28 Aug 2013 12:50:52
File Name	¥¥psf¥Home¥Desktop¥mori lab NMR¥¥¥¥¥2014¥¥¥¥¥¥01030¥¥voshida01030C13-1.jdf	Owner	delta	Frequency (MHz)	124.50	Nucleus	13C
Original Points Count	32768	Points Count	65536	Pulse Sequence	single_pulse_dec	Receiver Gain	58.00
Spectrum Type	STANDARD	Sweep Width (Hz)	39062.50	Temperature (degree C)	23.200	Solvent	CHLOROFORM-d
						Spectrum Offset (Hz)	12424.6953

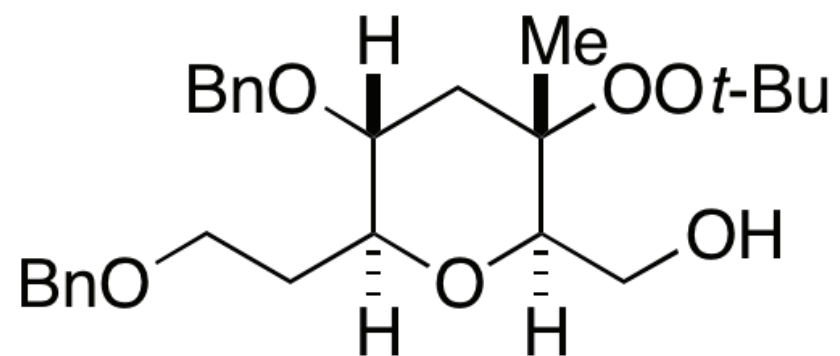


10

¹³C NMR (125 MHz, CDCl₃)

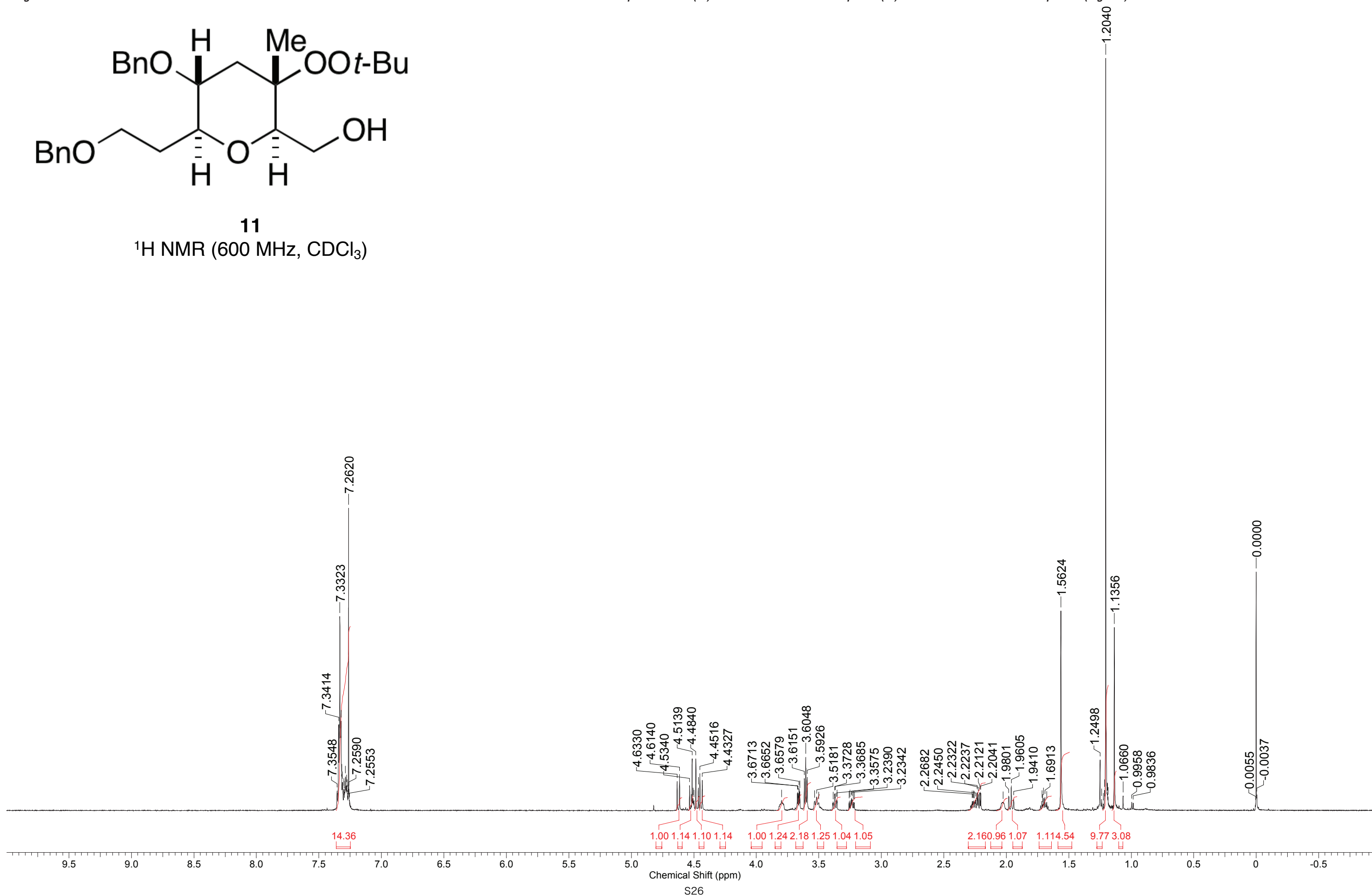


Acquisition Time (sec)	1.3648	Comment	1H SINGL NON SAKAI01095NAKA EN1	Date	06 Dec 2013 09:00:06
File Name	¥¥psf¥Home¥Desktop¥mori lab NMR¥sakaiNMR¥sakai01095¥sakai01095naka1non e1.nmf	Points Count	32768	Frequency (MHz)	600.05
Original Points Count	16384	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2995.2473
				Nucleus	1H
				Sweep Width (Hz)	12004.80
				Number of Transients	4
				Temperature (degree C)	24.000

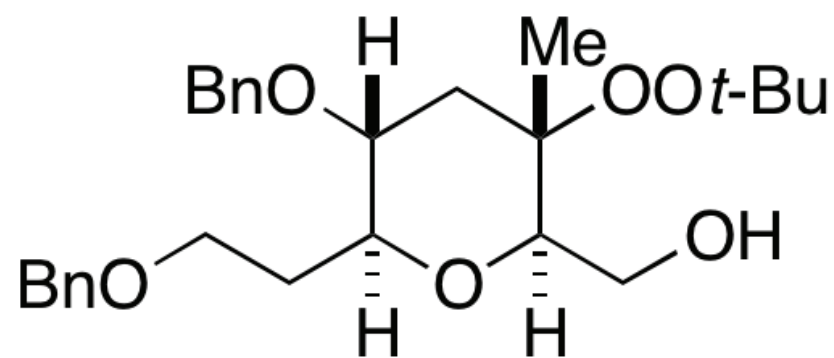


11

¹H NMR (600 MHz, CDCl₃)

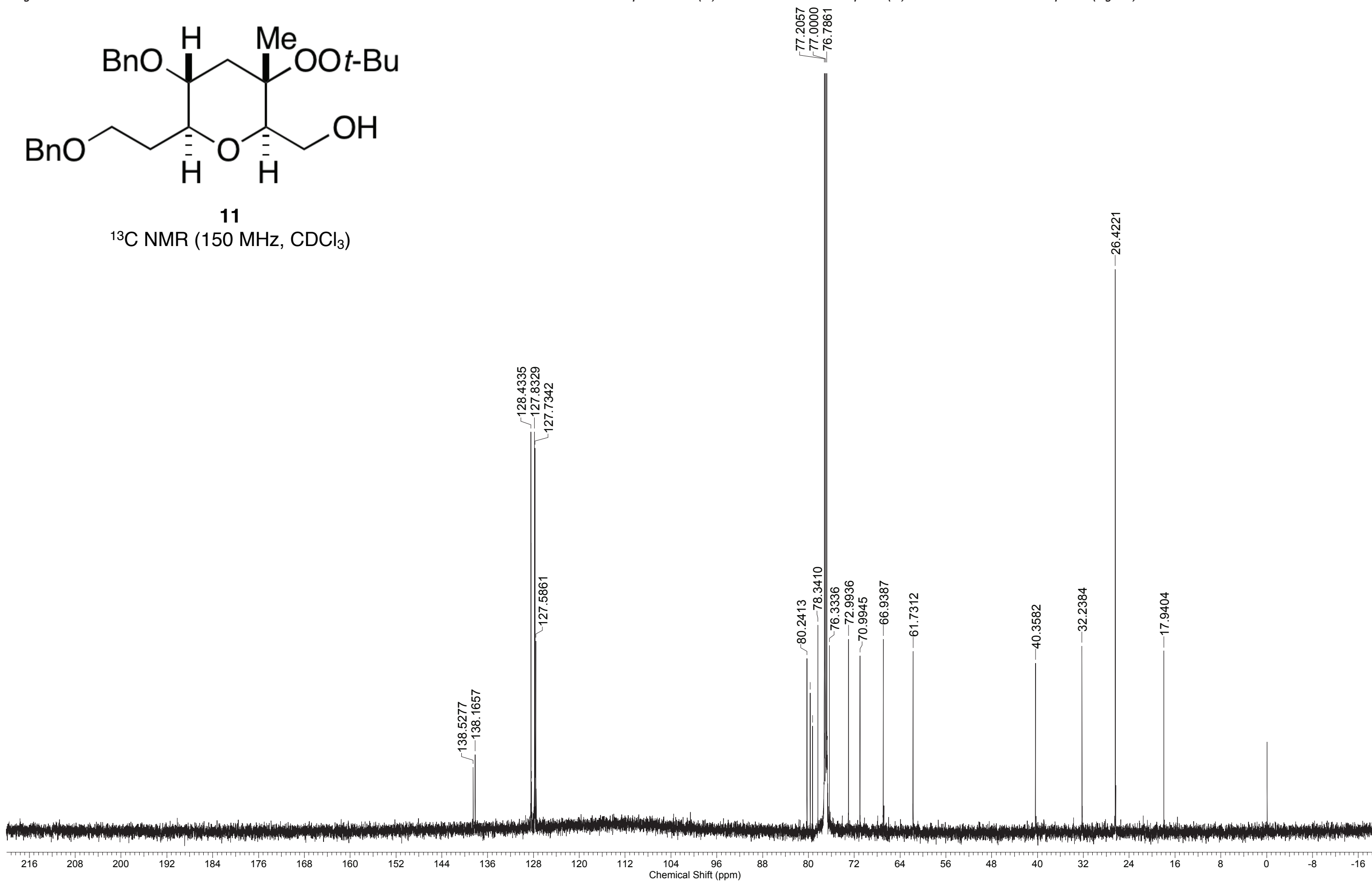


Acquisition Time (sec)	0.4030	Comment	13C SINGL BCM SAKAI01095NAKA EN1	Date	06 Dec 2013 09:00:06
File Name	¥¥psf¥Home¥Desktop¥mori lab NMR¥sakaiNMR¥sakai01095¥sakai01095naka2bcm.e1.nmf	Frequency (MHz)	150.80	Nucleus	13C
Original Points Count	16384	Points Count	32768	Solvent	CHLOROFORM-d
		Spectrum Offset (Hz)	15167.7520	Sweep Width (Hz)	40650.41
				Temperature (degree C)	24.000

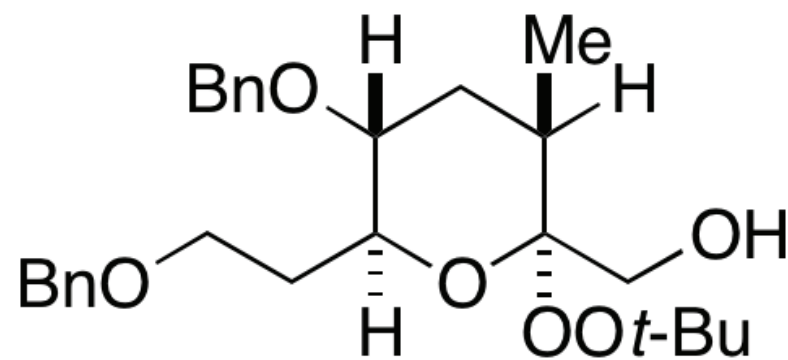


11

¹³C NMR (150 MHz, CDCl₃)

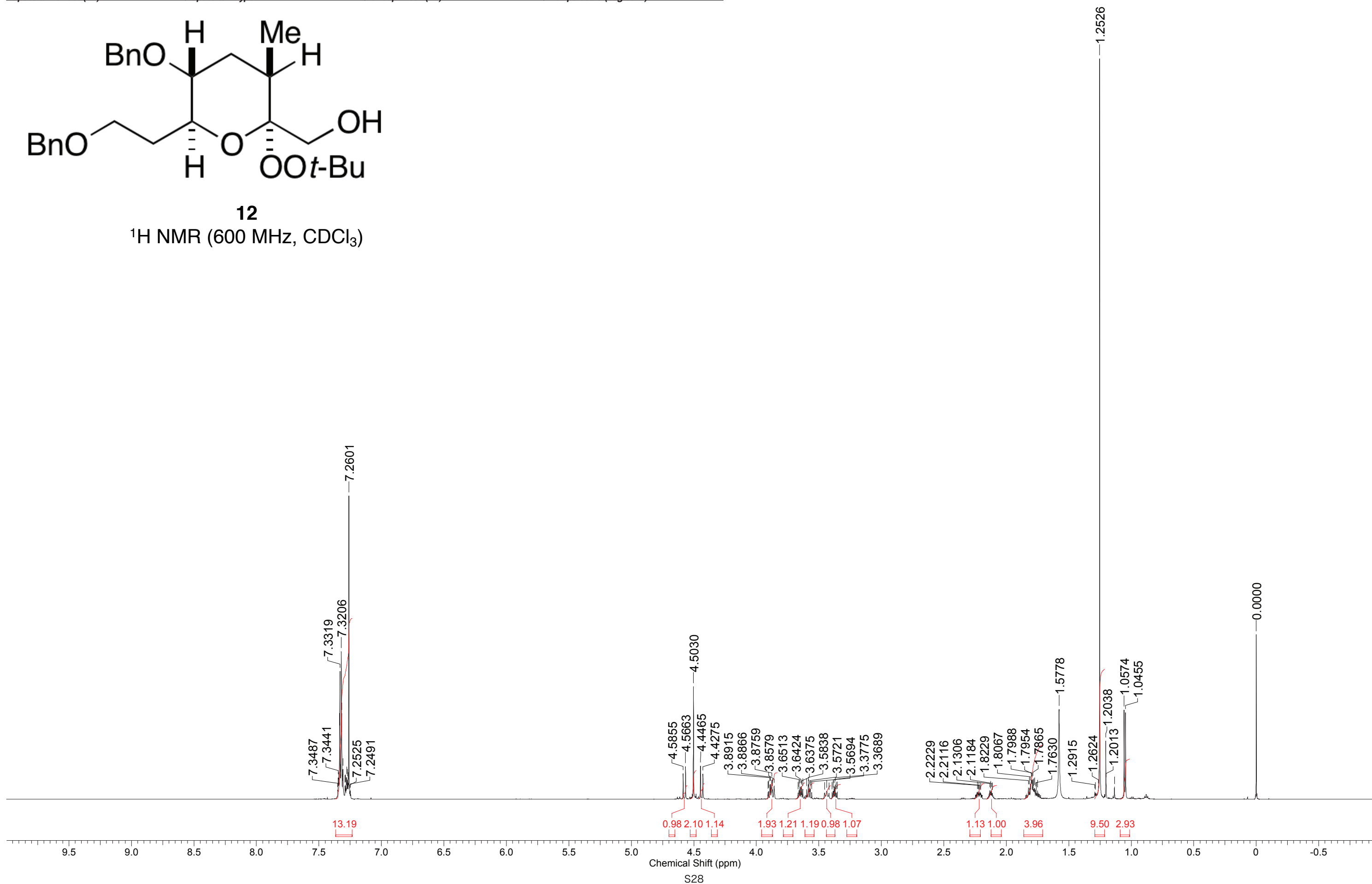


Acquisition Time (sec)	2.7263	Comment	proton	Date	14 Oct 2017 18:50:56	Date Stamp	14 Oct 2017 18:50:56
File Name	¥¥psf¥Home¥Desktop¥mori lab NMR¥sakaiNMR¥sakai01094ue 2¥1¥pdata¥1¥1r	Owner	nmsu	Frequency (MHz)	600.13	Nucleus	1H
Original Points Count	32768	Spectrum Type	STANDARD	Points Count	65536	Receiver Gain	30.91
Spectrum Offset (Hz)	3691.5447	Sweep Width (Hz)	12019.05	Pulse Sequence	zg30	Number of Transients	8
		Temperature (degree C)	25.141			SW(cyclical) (Hz)	12019.23
						Origin	spect
						Solvent	CHLOROFORM-d

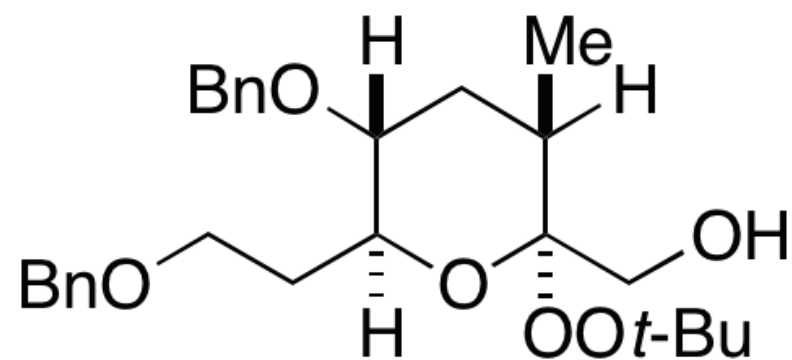


12

¹H NMR (600 MHz, CDCl₃)

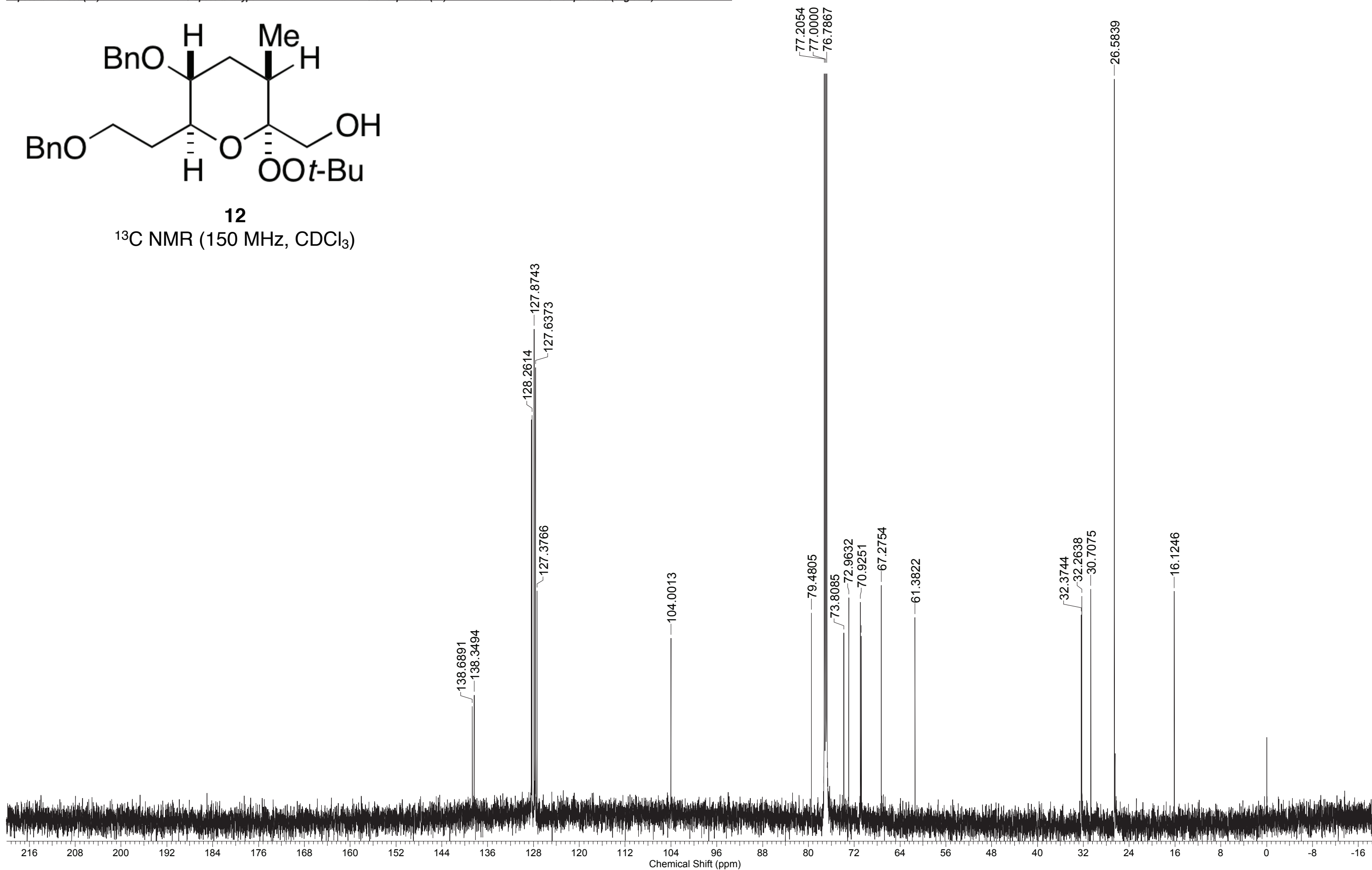


Acquisition Time (sec)	0.8389	Comment	carbon	Date	14 Oct 2017 19:01:36	Date Stamp	14 Oct 2017 19:01:36
File Name	¥¥psf¥Home¥Desktop¥mori lab NMR¥sakaiNMR¥sakai01094ue 2¥2¥pdata¥1¥1r	Frequency (MHz)	150.90	Nucleus	13C	Number of Transients	128
Original Points Count	32768	Owner	nmsu	Points Count	32768	Pulse Sequence	zgpg30
Spectrum Offset (Hz)	15085.5254	Spectrum Type	STANDARD	Sweep Width (Hz)	39061.31	Receiver Gain	193.26
				Temperature (degree C)	25.158	SW(cyclical) (Hz)	39062.50
						Origin	spect
						Solvent	CHLOROFORM-d

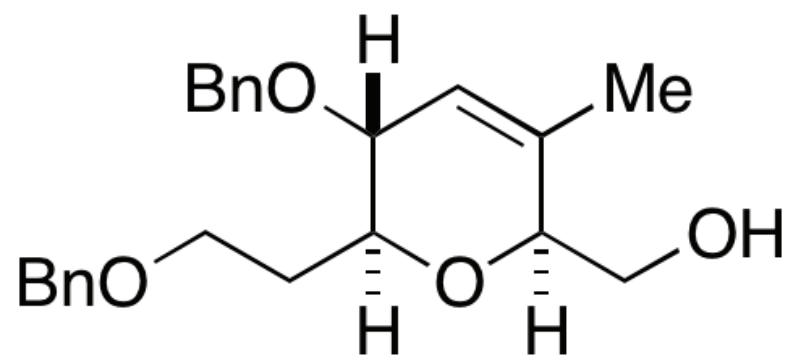


12

¹³C NMR (150 MHz, CDCl₃)

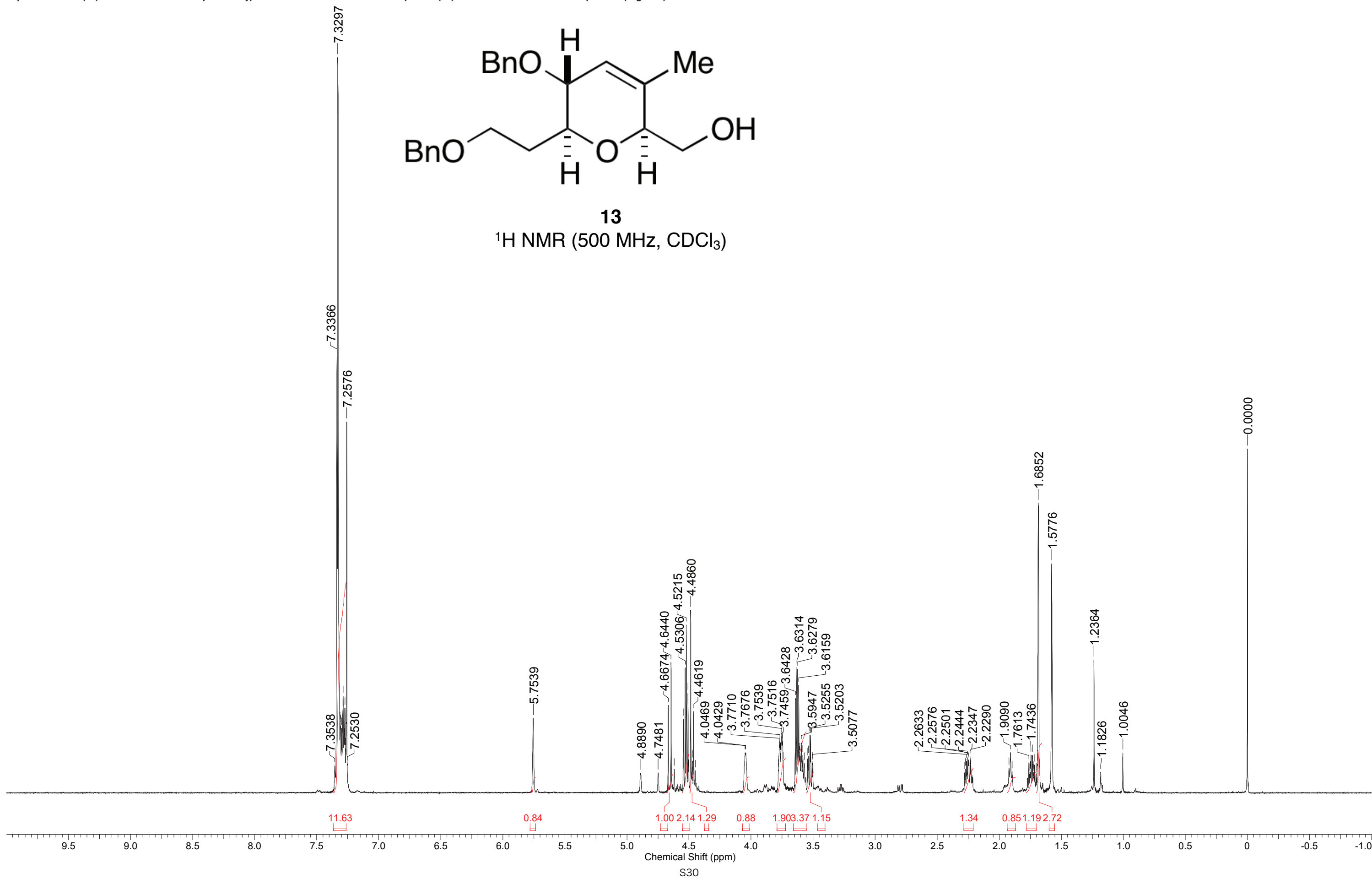


Acquisition Time (sec)	1.7642	Comment	single_pulse	Date	03 Dec 2013 16:06:35	Date Stamp	03 Dec 2013 16:00:28
File Name	¥¥psf¥Home¥Desktop¥mori lab NMR¥sakaiNMR¥sakai01093¥sakai01094shitamajorH-1.jdf			Frequency (MHz)	495.13	Nucleus	1H
Original Points Count	16384	Owner	delta	Points Count	32768	Pulse Sequence	single_pulse.ex2
Spectrum Offset (Hz)	2476.9363	Spectrum Type	STANDARD	Sweep Width (Hz)	9286.78	Receiver Gain	48.00
				Temperature (degree C)	24.000	Solvent	CHLOROFORM-d
						Number of Transients	8
						Origin	ECA 500

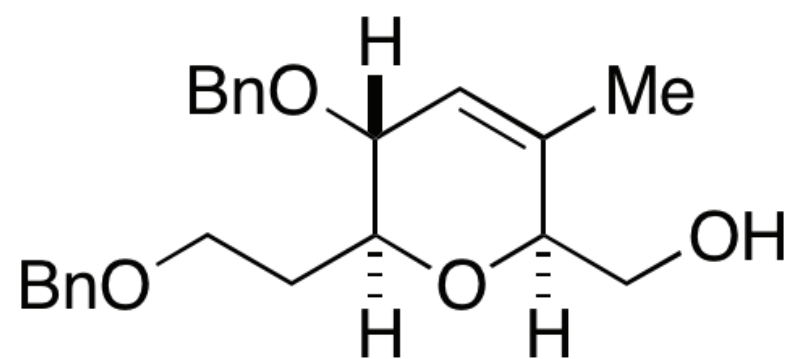


13

¹H NMR (500 MHz, CDCl₃)

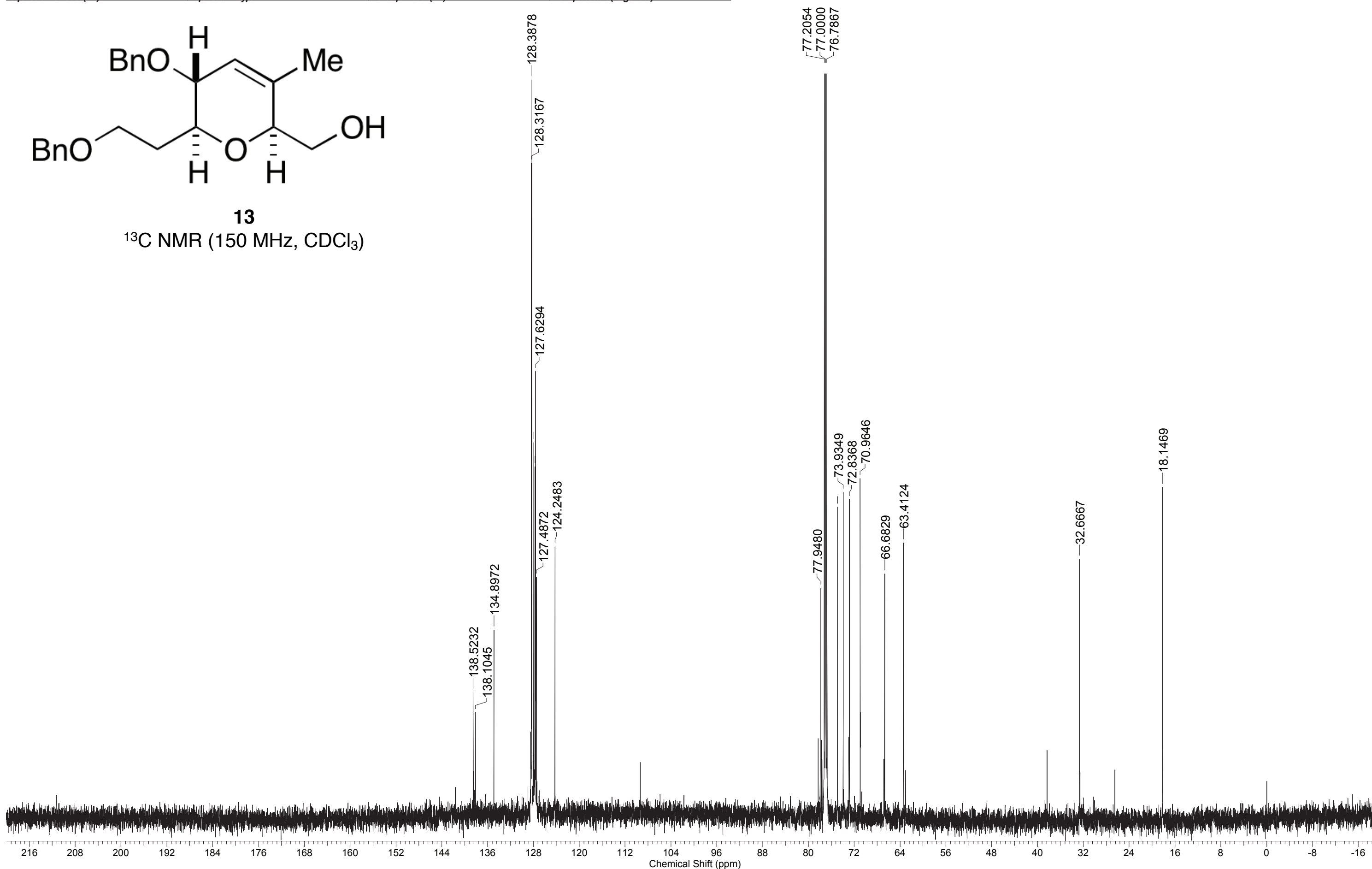


Acquisition Time (sec)	0.8389	Comment	carbon	Date	28 Oct 2017 10:44:32	Date Stamp	28 Oct 2017 10:44:32
File Name	¥¥psf¥Home¥Desktop¥mori lab NMR¥sakaiNMR¥sakai01094shita¥2¥pdata¥1¥1r	Frequency (MHz)	150.90	Nucleus	13C	Number of Transients	64
Original Points Count	32768	Owner	nmsu	Points Count	32768	Pulse Sequence	zgpg30
Spectrum Offset (Hz)	15083.1416	Spectrum Type	STANDARD	Sweep Width (Hz)	39061.31	Receiver Gain	193.26
				Temperature (degree C)	25.160	SW(cyclical) (Hz)	39062.50
						Origin	spect
						Solvent	CHLOROFORM-d

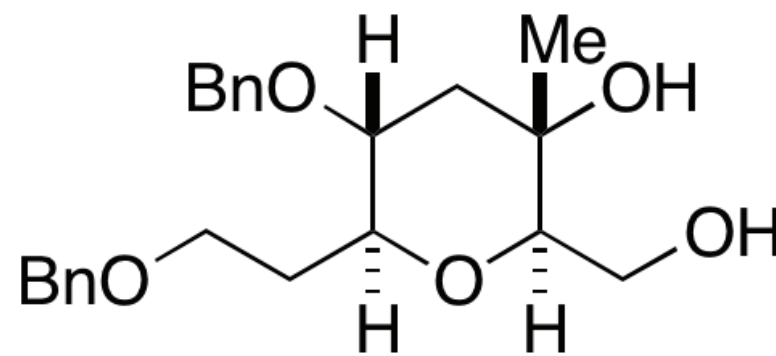


13

¹³C NMR (150 MHz, CDCl₃)

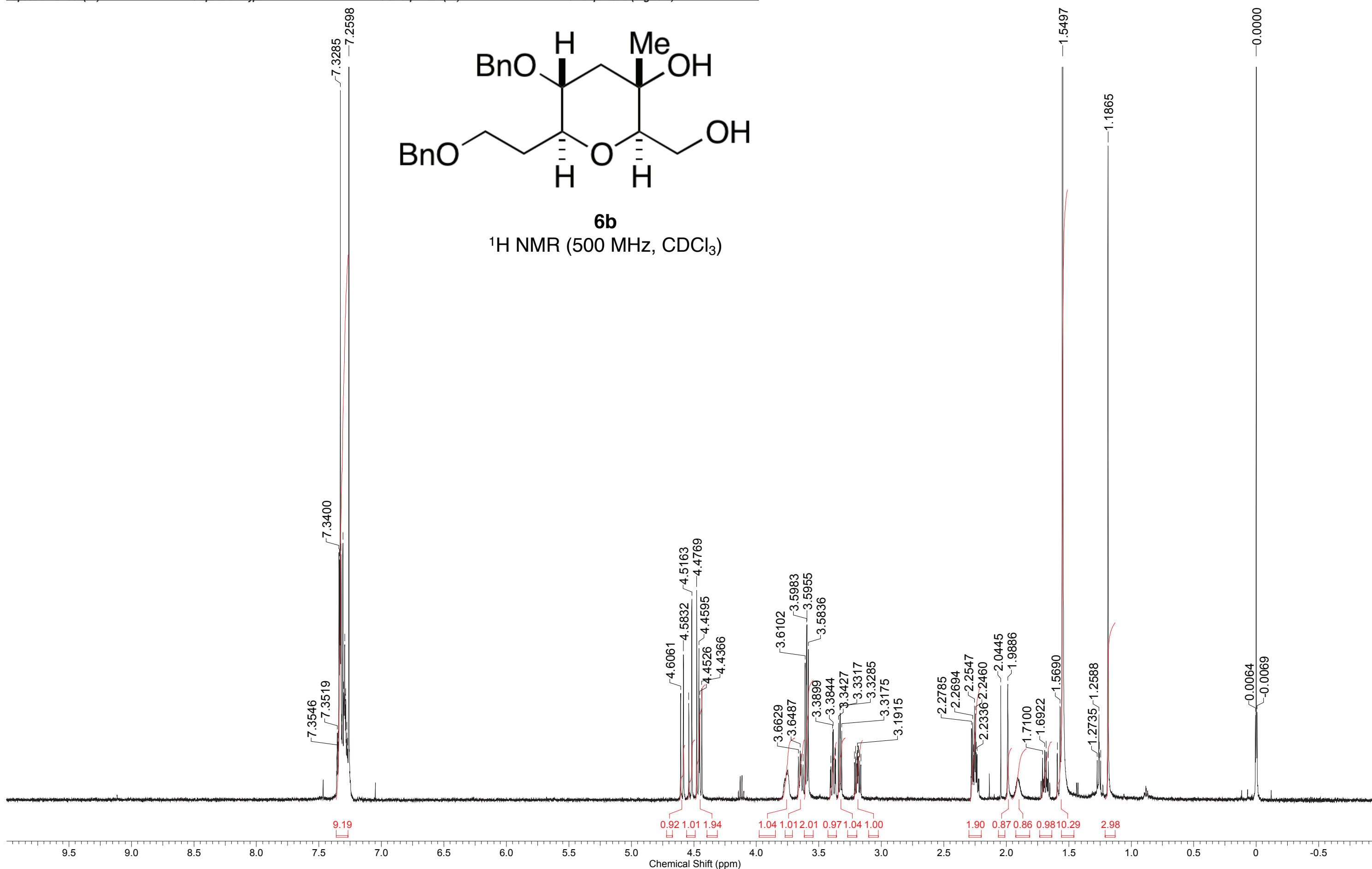


Acquisition Time (sec)	2.1823	Comment	Single Pulse Experiment		Date	07 Dec 2013 15:47:05		Date Stamp	07 Dec 2013 15:47:05		
File Name	¥¥psf¥Home¥Desktop¥mori lab NMR¥sakaiNMR¥sakai01096¥sakai01096.1				Frequency (MHz)	500.16		Nucleus	1H		
Original Points Count	16384	Owner	JEOL LTD.	Points Count	32768	Pulse Sequence	single_pulse.exp	Receiver Gain	25.00	Number of Transients	16
Spectrum Offset (Hz)	2503.9153	Spectrum Type	STANDARD	Sweep Width (Hz)	7507.51	Temperature (degree C)	26.500	Solvent	CHLOROFORM-d		

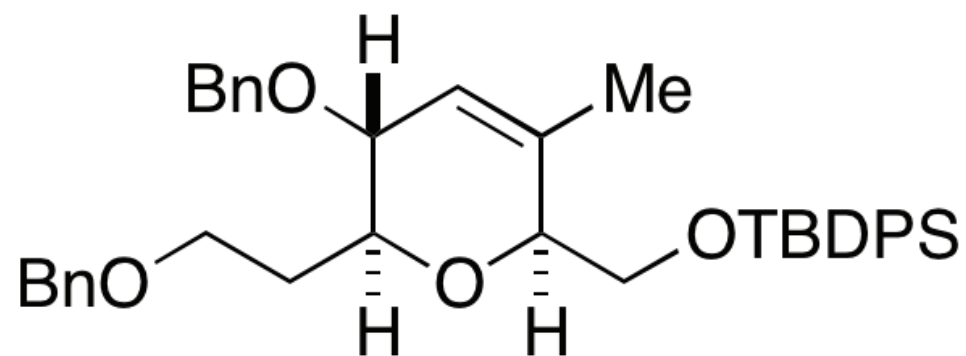


6b

¹H NMR (500 MHz, CDCl₃)



Acquisition Time (sec)	2.7263	Comment	proton	Date	08 Dec 2014 18:16:48	Date Stamp	08 Dec 2014 18:16:48
File Name	Y:\psf\Home\Desktop\mori lab NMR\data\11112015\11112015_10178_sita_aoyama\data\111r	Owner	nmsu	Points Count	65536	Nucleus	¹ H
Original Points Count	32768	Spectrum Type	STANDARD	Pulse Sequence	zg30	Receiver Gain	25.50
Spectrum Offset (Hz)	3683.2917	Sweep Width (Hz)	12019.05	Temperature (degree C)	25.151	Number of Transients	8
						SM(cyclical) (Hz)	12019.23
						Origin	spect
						Solvent	CHLOROFORM-d



14

¹H NMR (600 MHz, CDCl₃)

