

**Synthesis of optically active 2-substituted azetidine-2-carbonitriles
from chiral 1-arylethylamine via α -alkylation of *N*-borane complexes**

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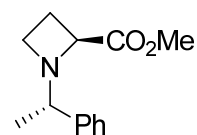
E-mail: tayama@chem.sc.niigata-u.ac.jp

Electronic Supplementary Information

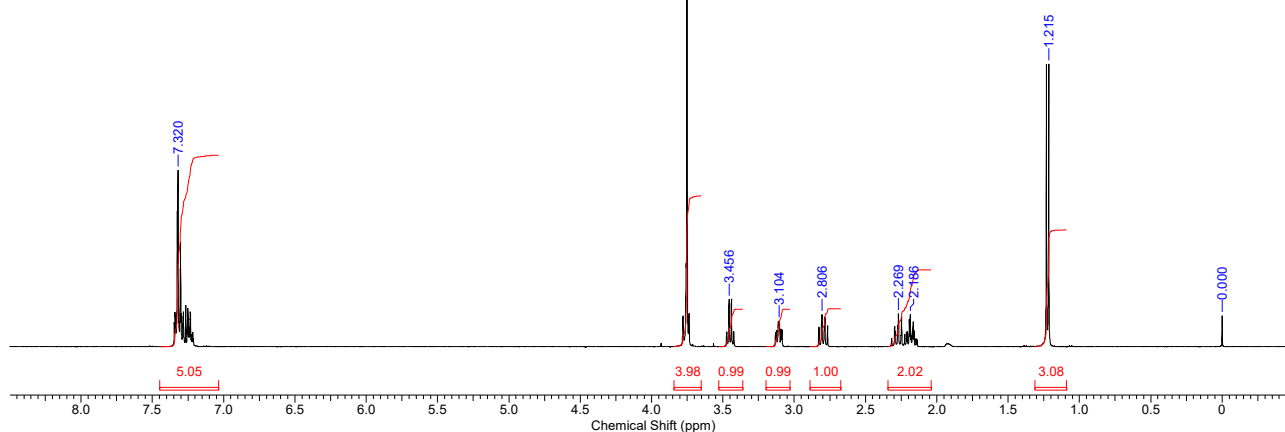
Copies of ^1H , ^{13}C and ^{11}B NMR spectra of substrates and products

Acquisition Time (sec)	3.5000	Date	Jul 18 2020	Date Stamp	Jul 18 2020	Frequency (MHz)	399.83	Nucleus	¹ H
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Solvent	CHLOROFORM-d								

2S,1'S-1a_1H.esp

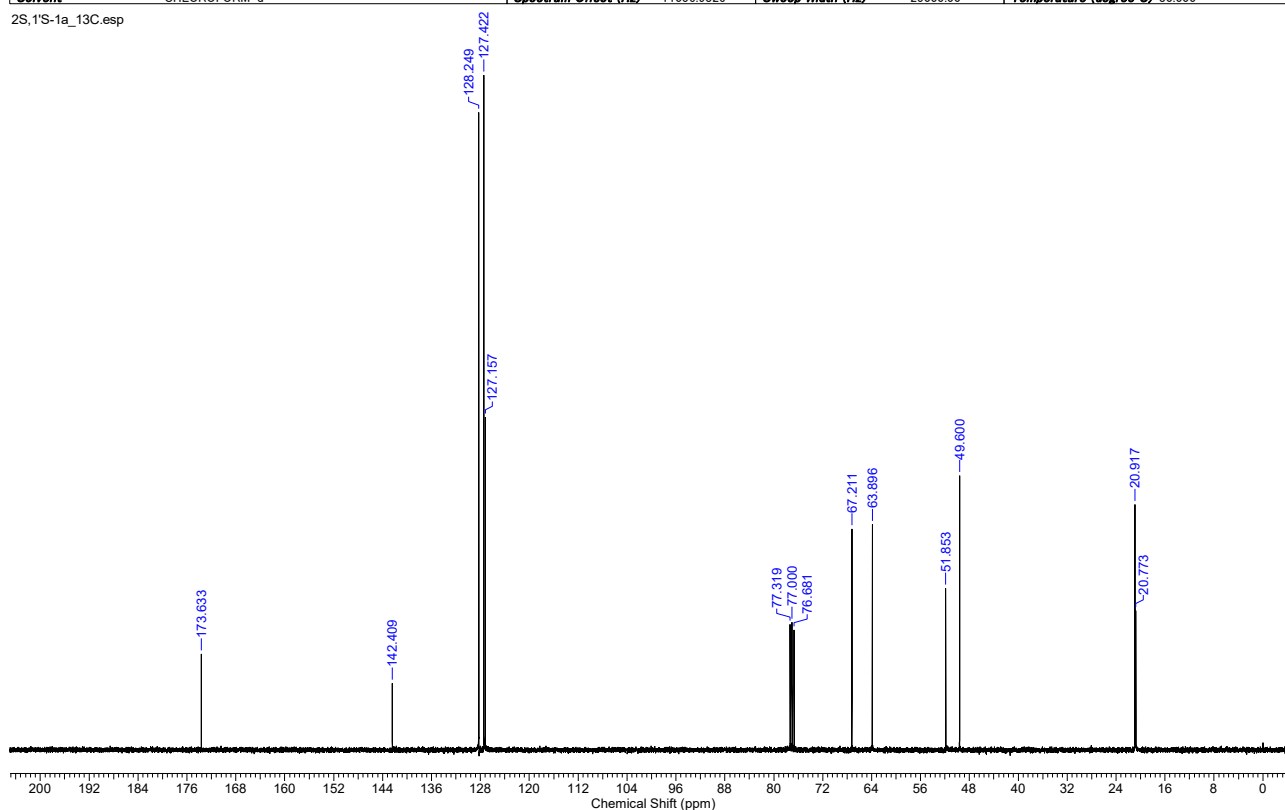


(2S,1'S)-1a
¹H: CDCl₃, ¹³C: CDCl₃



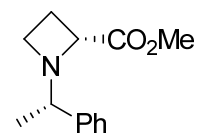
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2S,1'S-1a_13C.esp



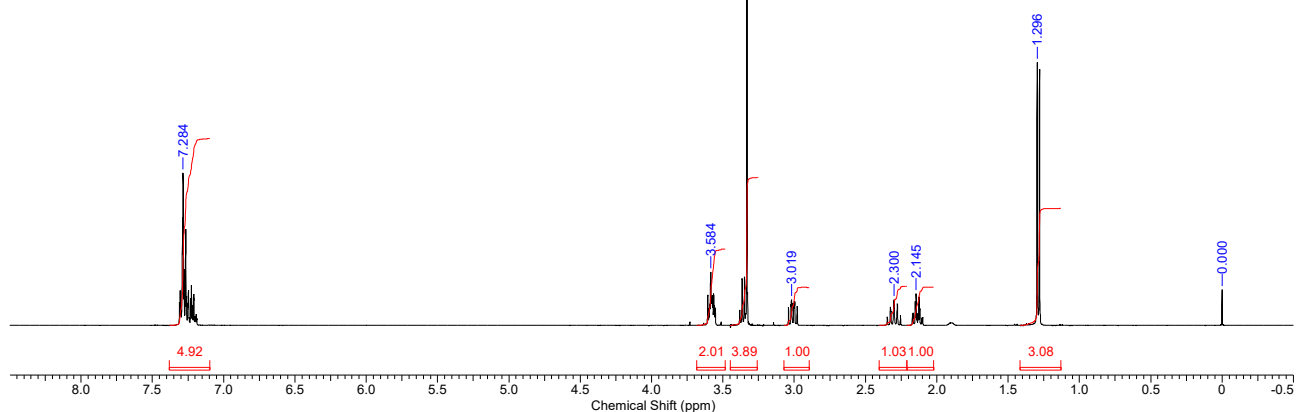
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2R,1'S-1a_1H.esp



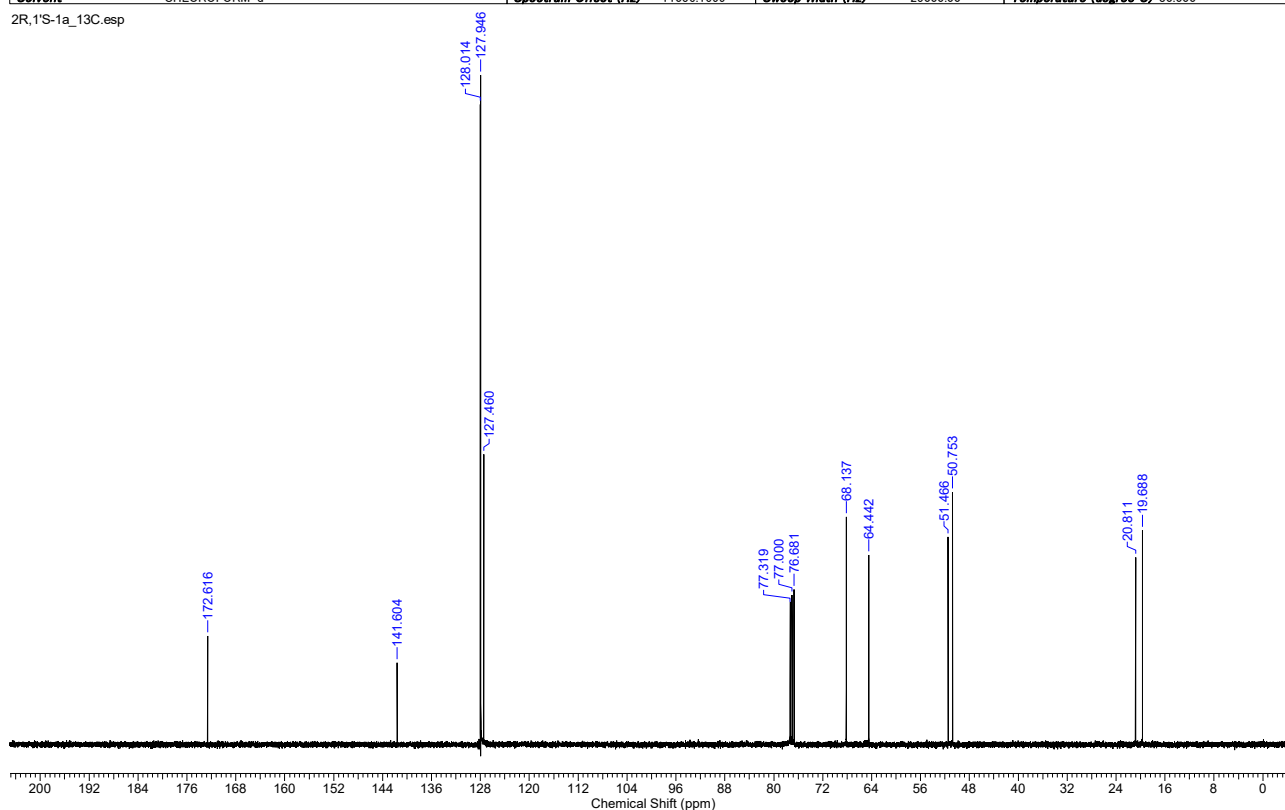
(2R,1'S)-1a

¹H: CDCl₃, ¹³C: CDCl₃



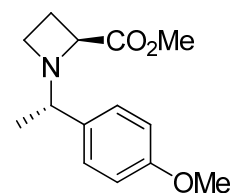
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Solvent	CHLOROFORM-d								

2R,1'S-1a_13C.esp

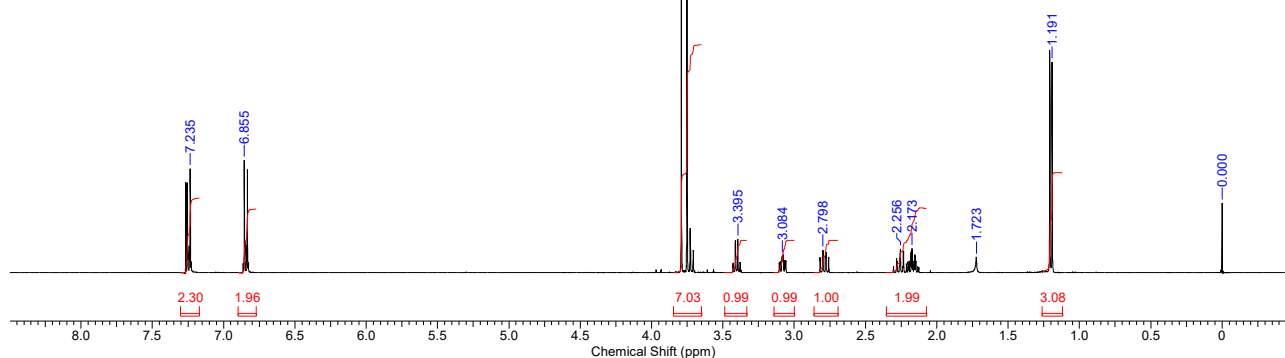


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Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2408.1255	Sweep Width (Hz)	6410.26
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2S,1'S-1b_1H.esp

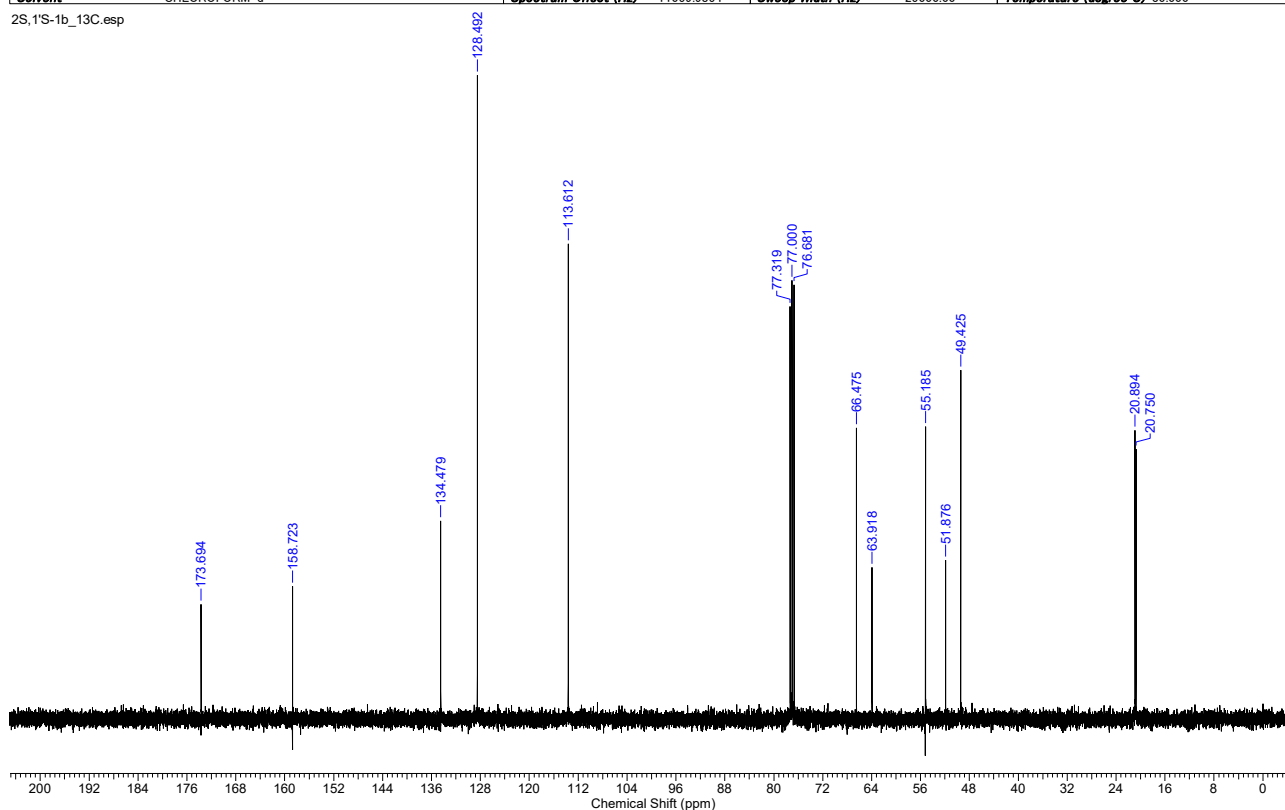


(2S,1'S)-1b
¹H: CDCl₃, ¹³C: CDCl₃



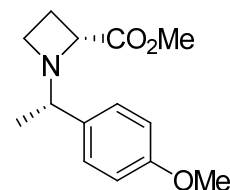
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Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	11059.9854	Sweep Width (Hz)	25000.00
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2S,1'S-1b_13C.esp

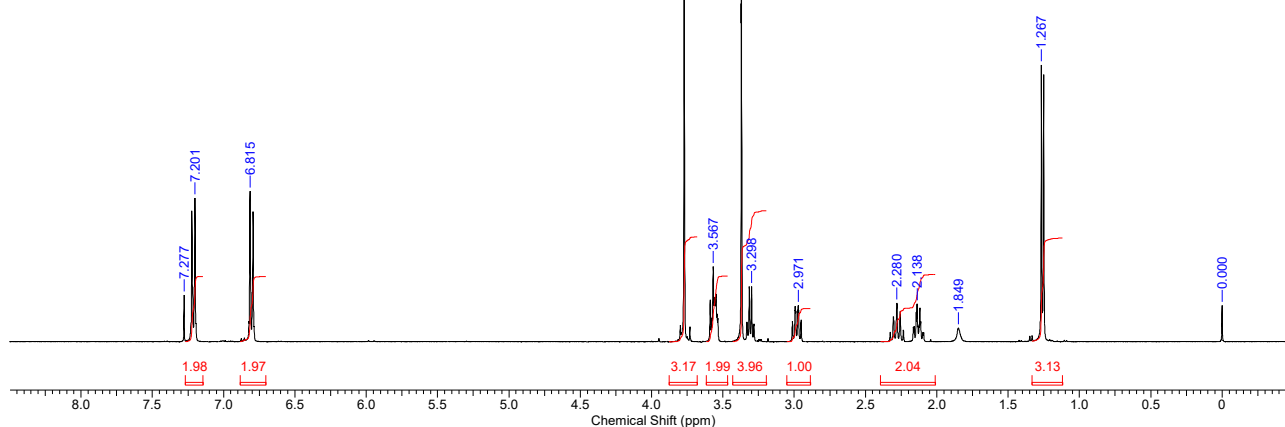


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Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2413.0164	Sweep Width (Hz)	6410.26
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2R,1'S-1b_1H.esp

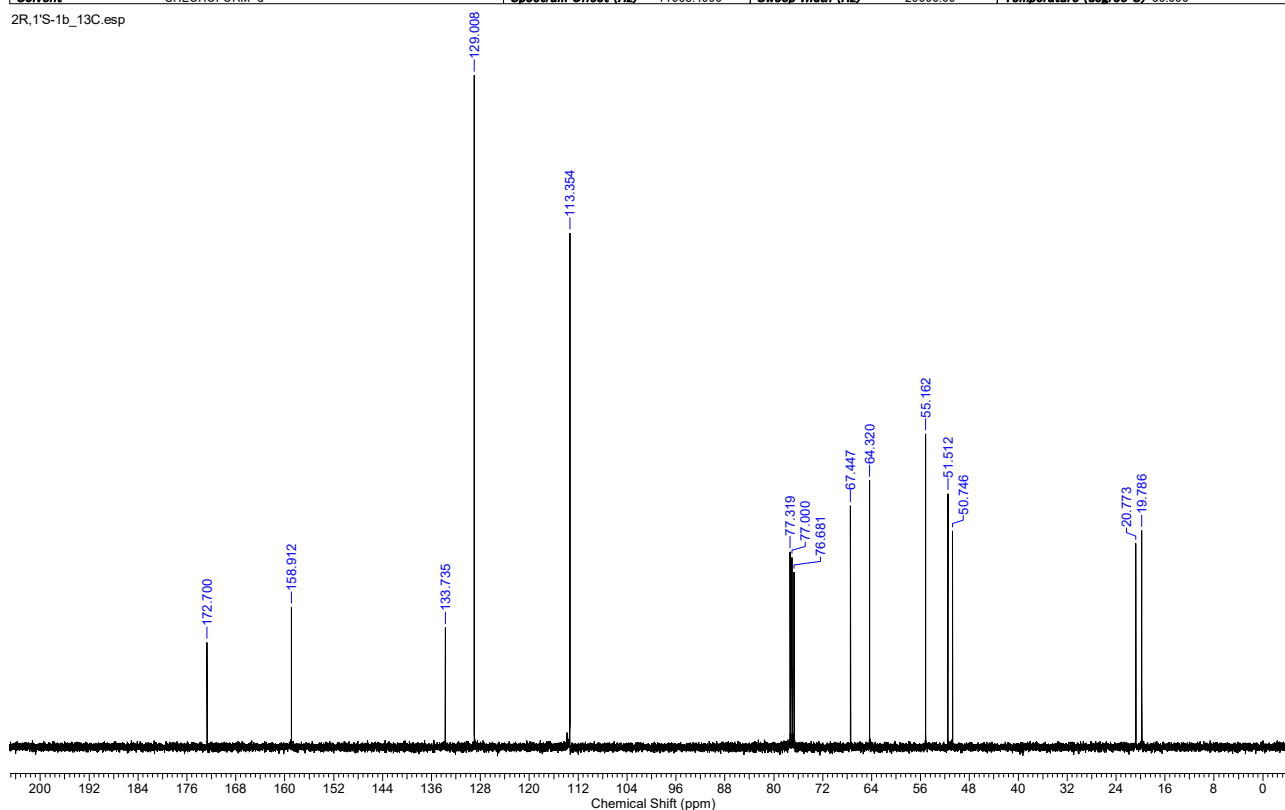


(2R,1'S)-1b
¹H: CDCl₃, ¹³C: CDCl₃



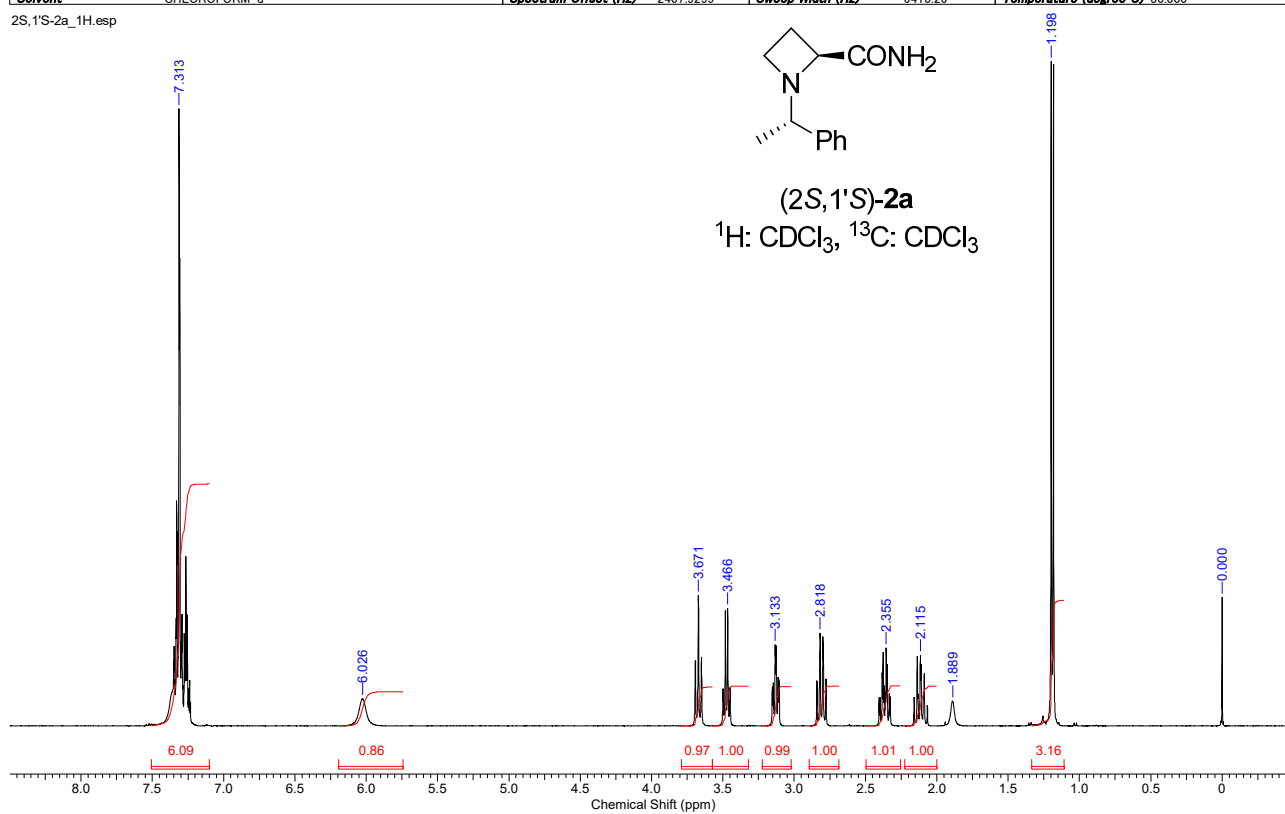
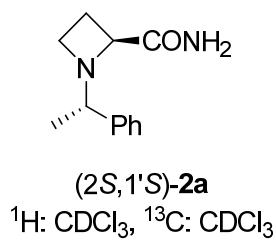
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Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	11058.4590	Sweep Width (Hz)	25000.00
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2R,1'S-1b_13C.esp



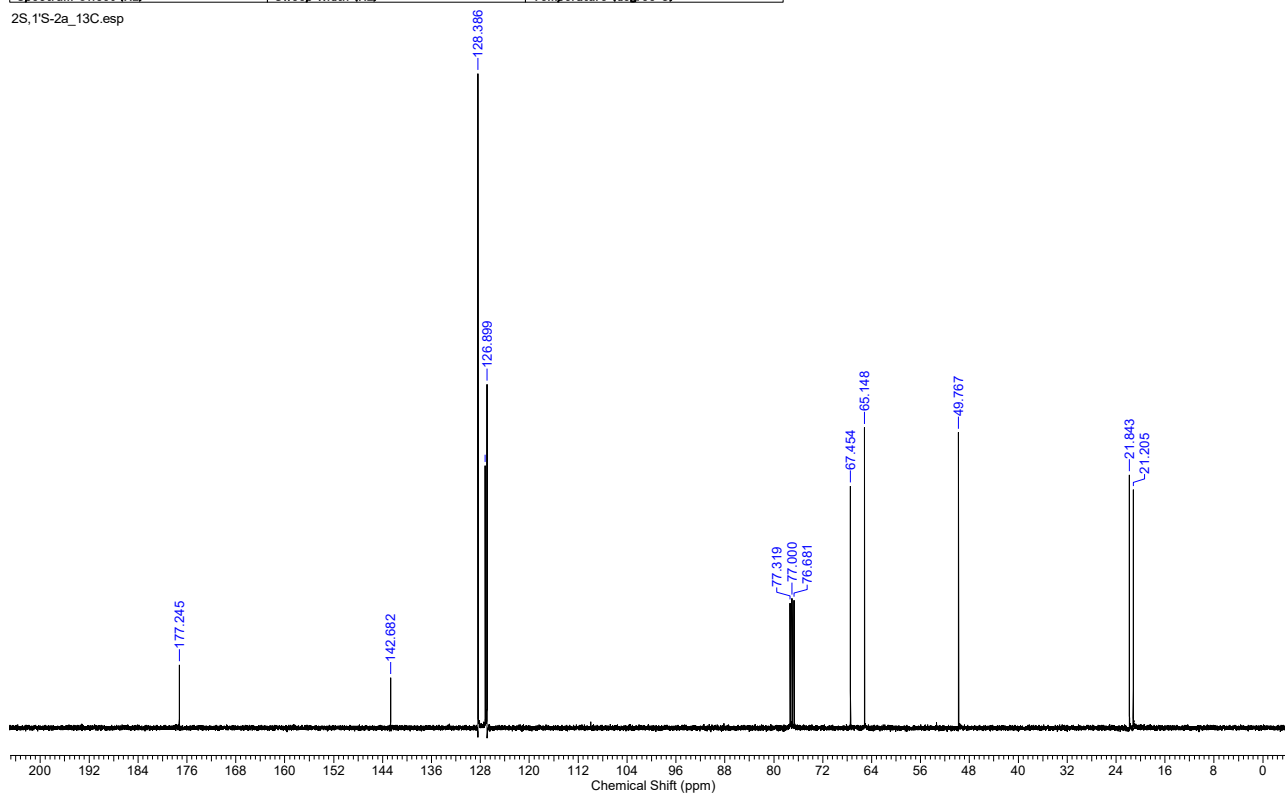
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Number of Transients	16	Spectrum Offset (Hz)	2407.9299	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000		
Solvent	CHLOROFORM-d								

2S,1'S-2a_1H.esp

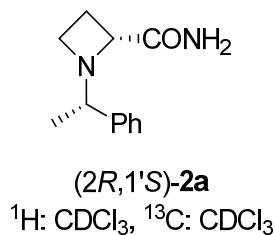


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Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	60.00
Spectrum Offset (Hz)	11053.1172	Sweep Width (Hz)	25000.00	Temperature (degree C)	30.000
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2S,1'S-2a_13C.esp

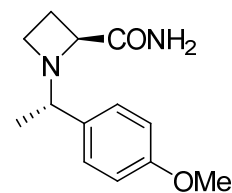


2R,1'S-2a 1H.esp

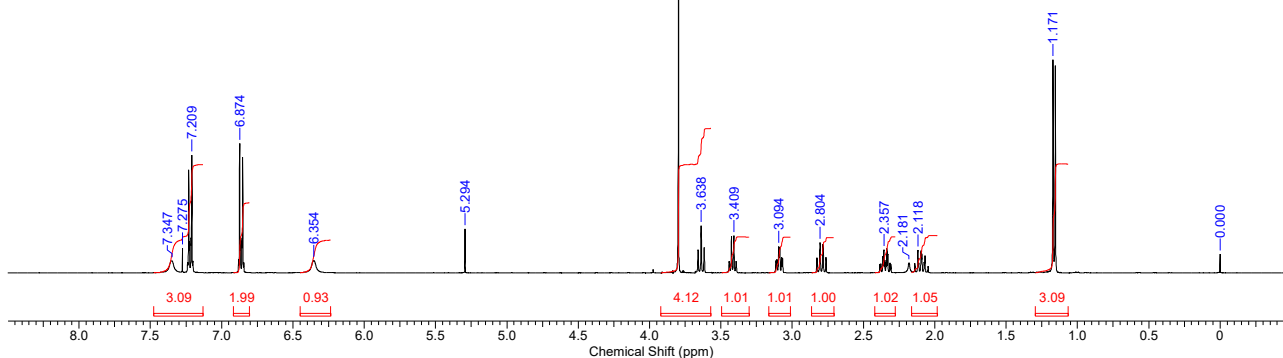
2R,1'S-2a_13C.esp

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Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	34.00
Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	2412.0381	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000	

2S,1'S-2b_1H.esp

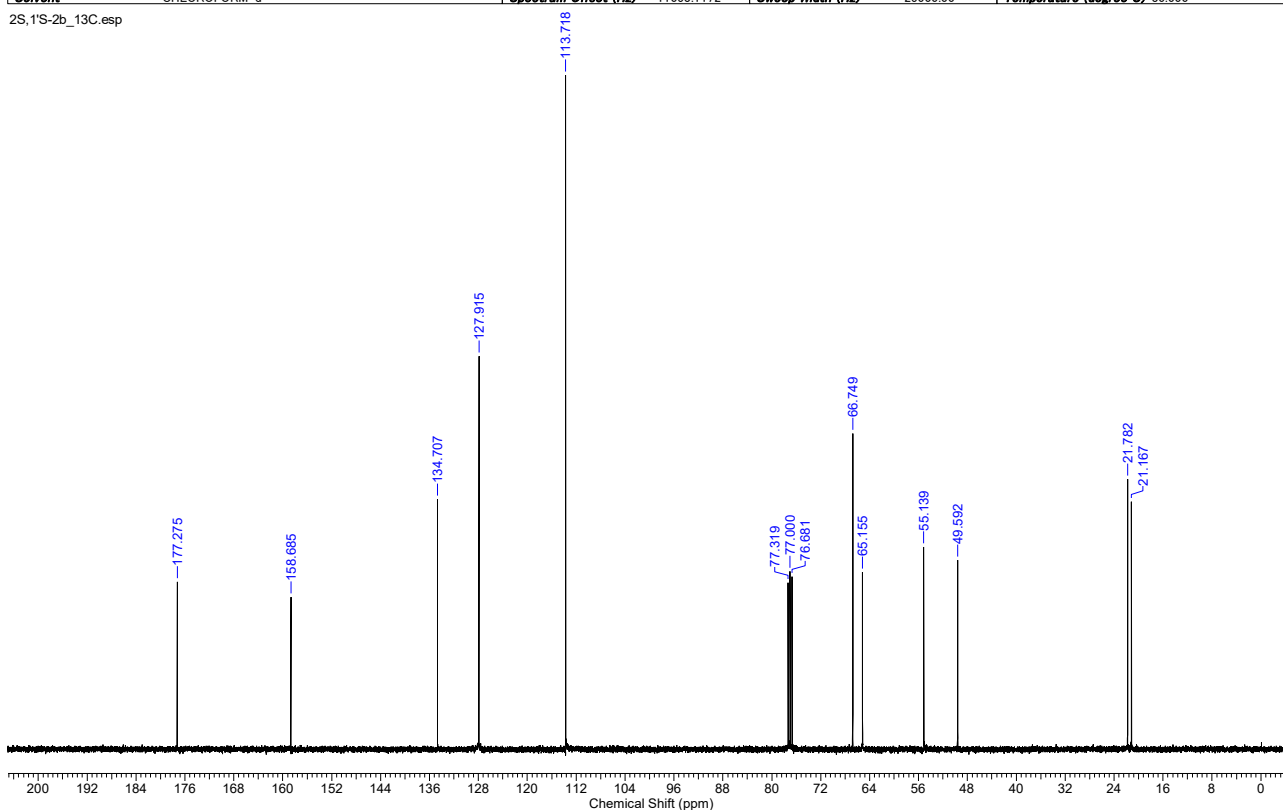


(2S,1'S)-2b
¹H: CDCl₃, ¹³C: CDCl₃



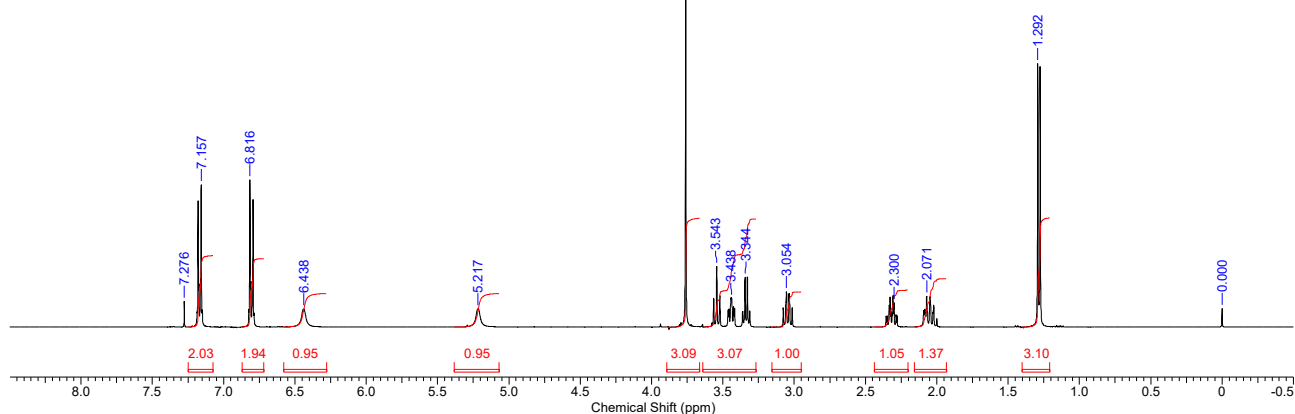
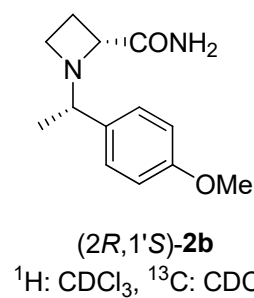
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Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	11053.1172	Sweep Width (Hz)	25000.00	Temperature (degree C)	30.000	

2S,1'S-2b_13C.esp



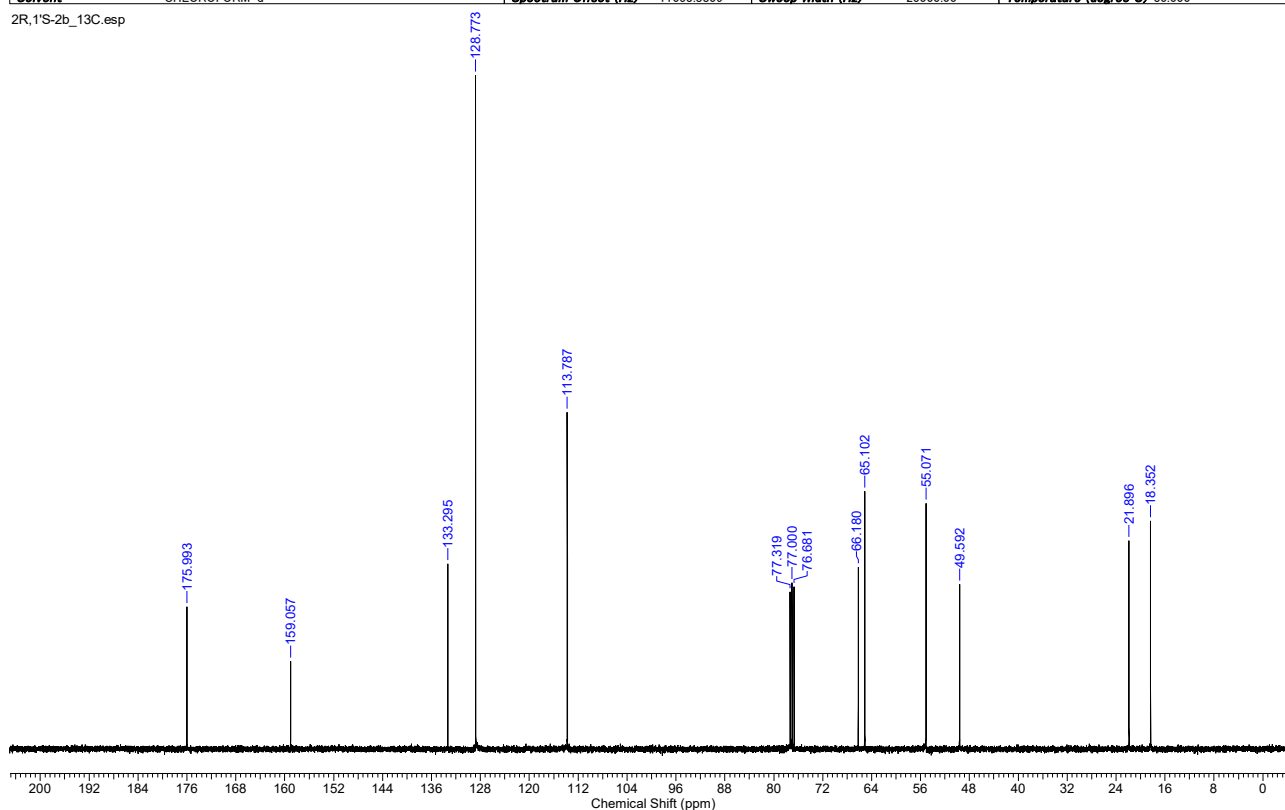
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Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2412.2339	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000

2R,1'S-2b_1H.esp



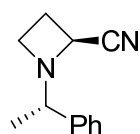
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Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	11053.8809	Sweep Width (Hz)	25000.00	Temperature (degree C)	30.000

2R,1'S-2b_13C.esp



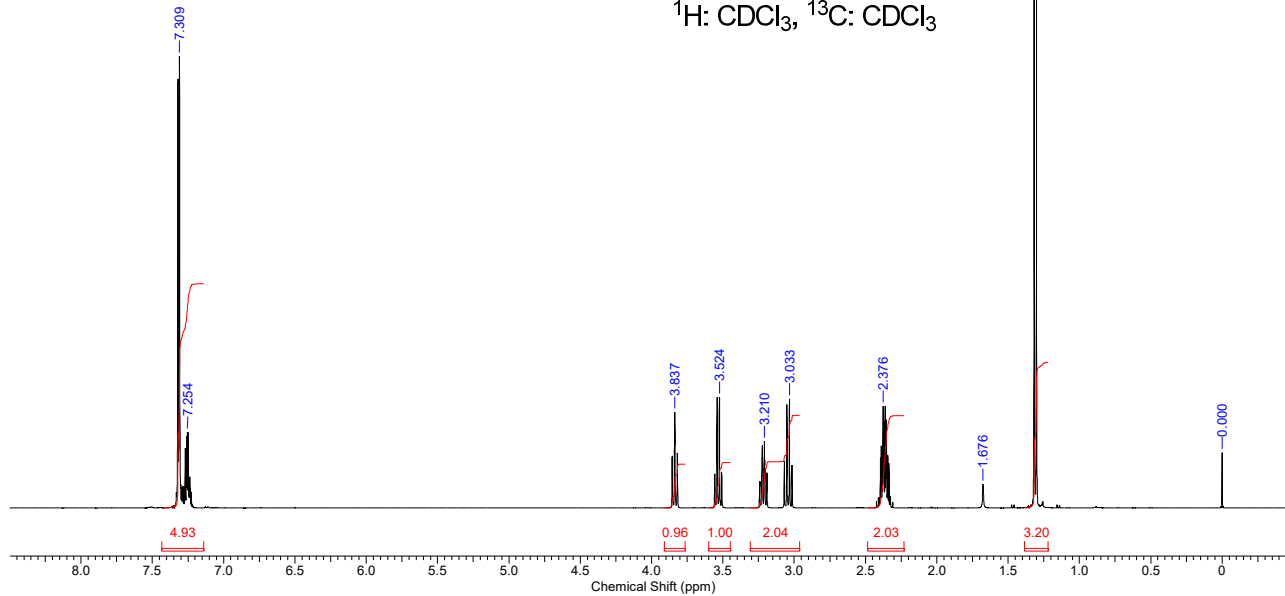
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Number of Transients	16	Spectrum Offset (Hz)	2403.4304	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000		
Solvent	CHLOROFORM-d								

2S,1'S-3a_1H.esp



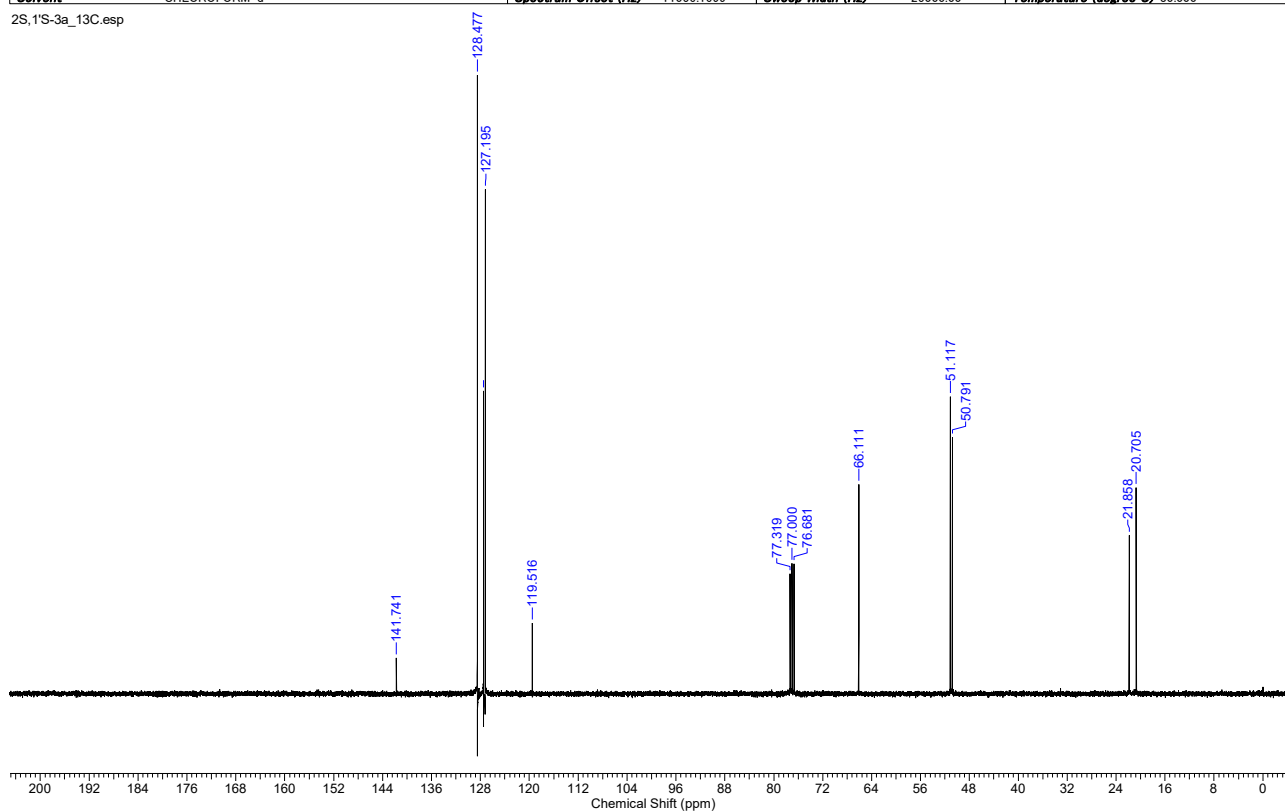
(2S,1'S)-3a

¹H: CDCl₃, ¹³C: CDCl₃



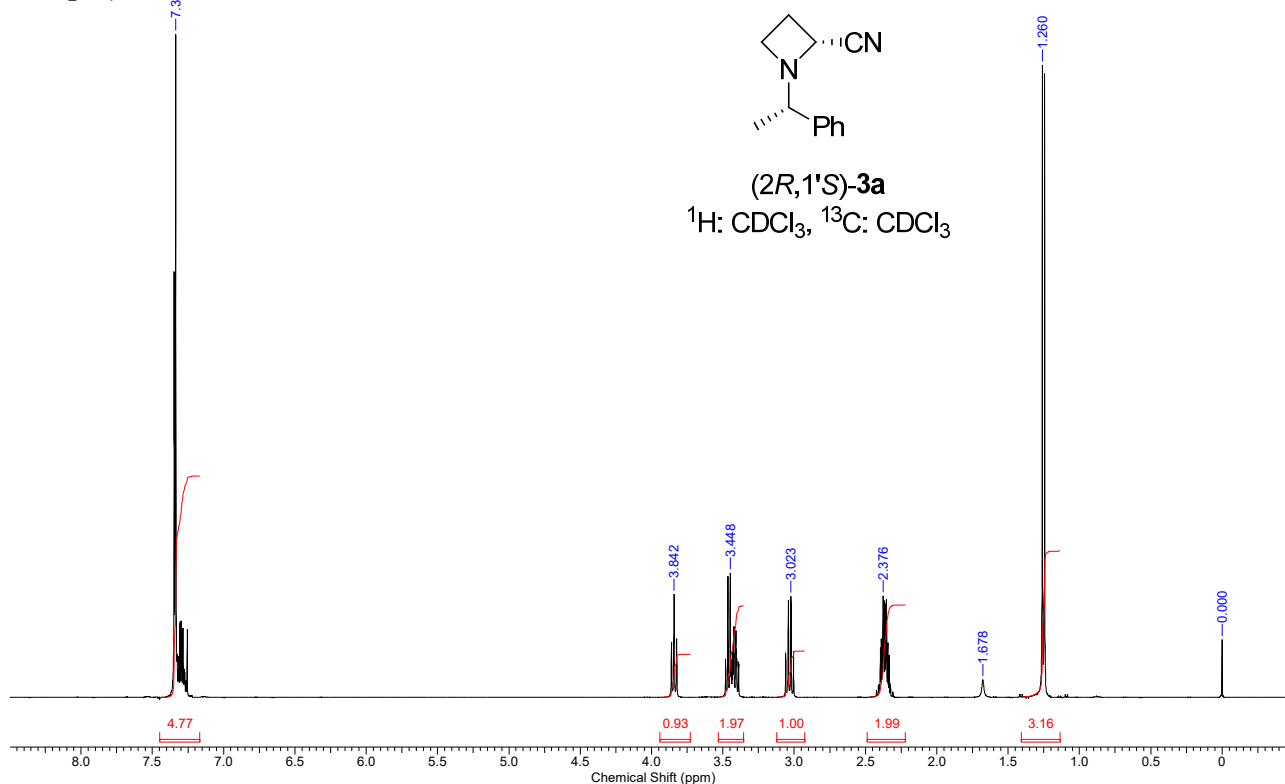
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Solvent	CHLOROFORM-d								

2S,1'S-3a_13C.esp



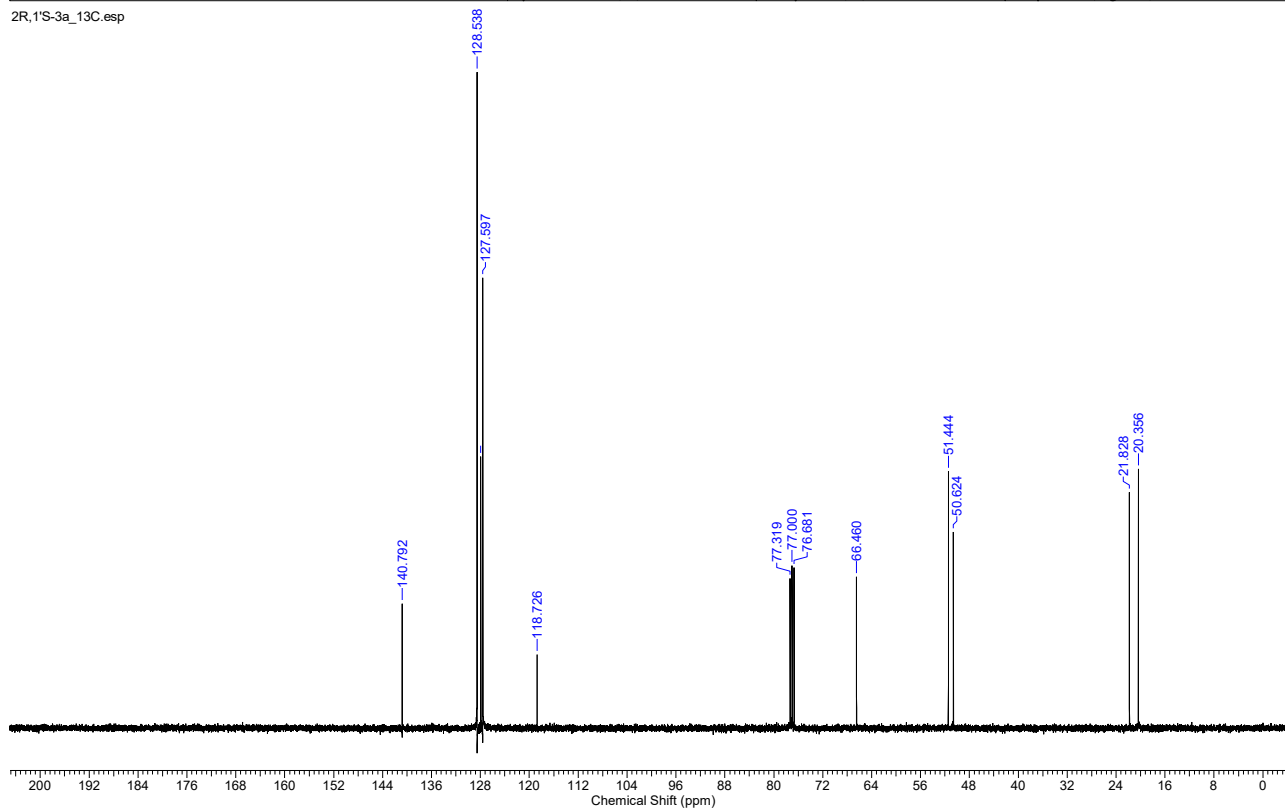
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Solvent	CHLOROFORM-d								

2R,1'S-3a_1H.esp



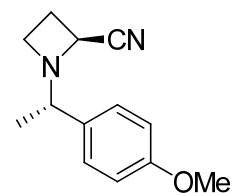
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Solvent	CHLOROFORM-d								

2R,1'S-3a_13C.esp

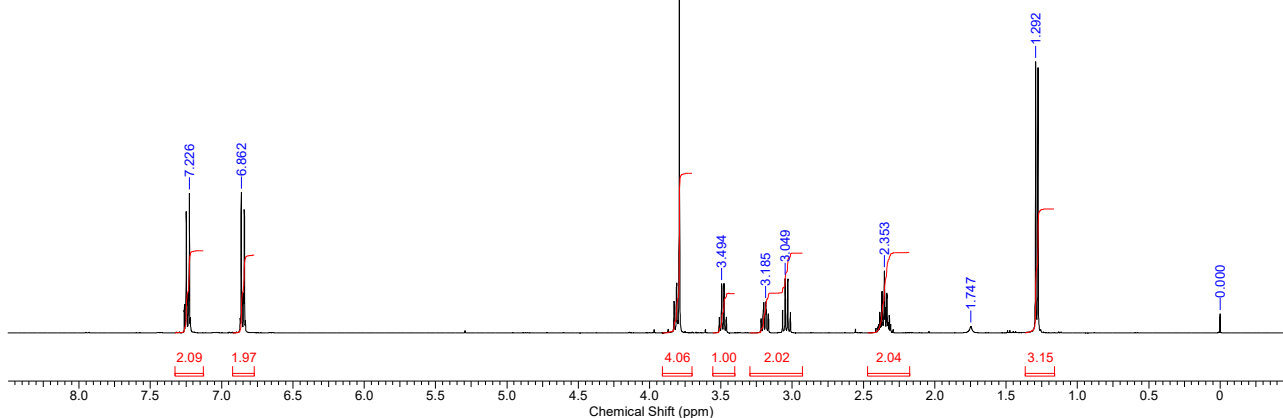


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Solvent	CHLOROFORM-d								

2S,1'S-3b_1H.esp

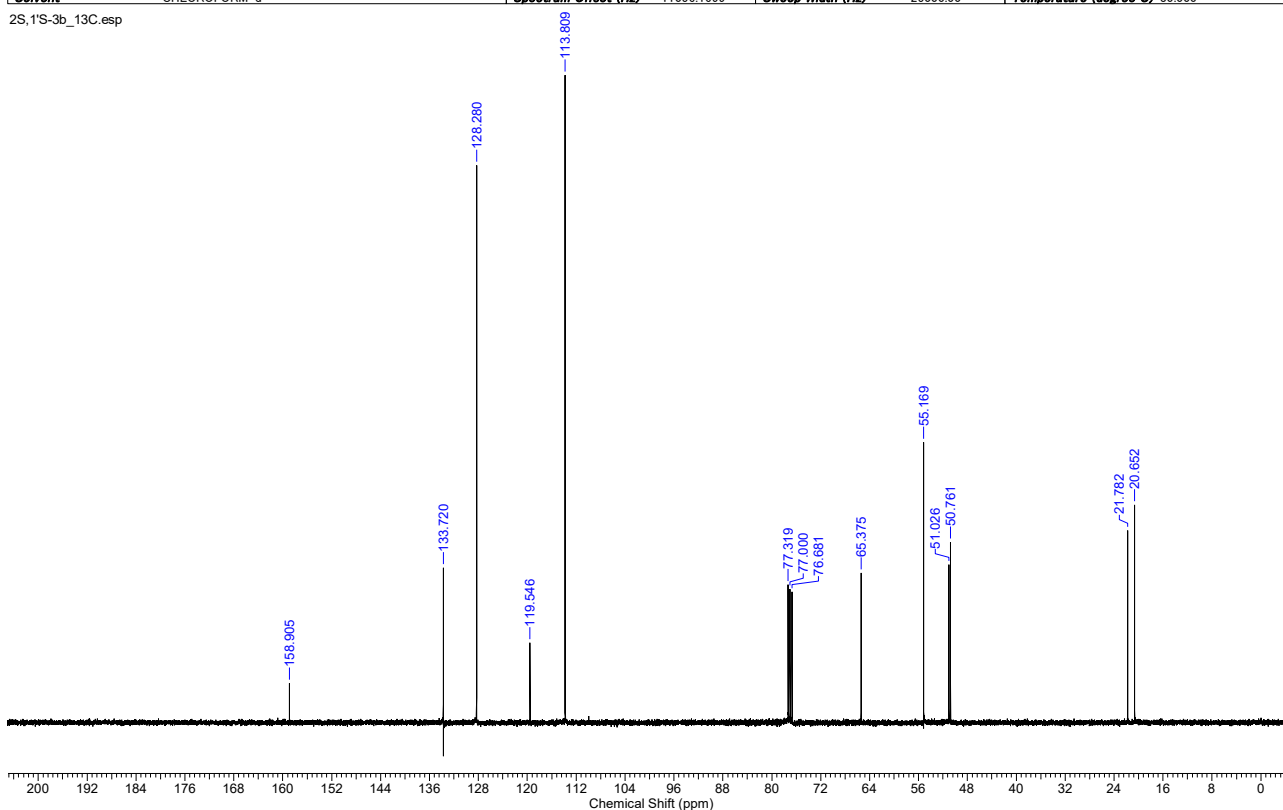


(2S,1'S)-3b
¹H: CDCl₃, ¹³C: CDCl₃



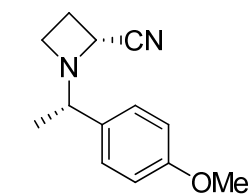
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Number of Transients	512	Spectrum Offset (Hz)	11056.1699	Sweep Width (Hz)	25000.00	Temperature (degree C)	30.000		
Solvent	CHLOROFORM-d								

2S,1'S-3b_13C.esp

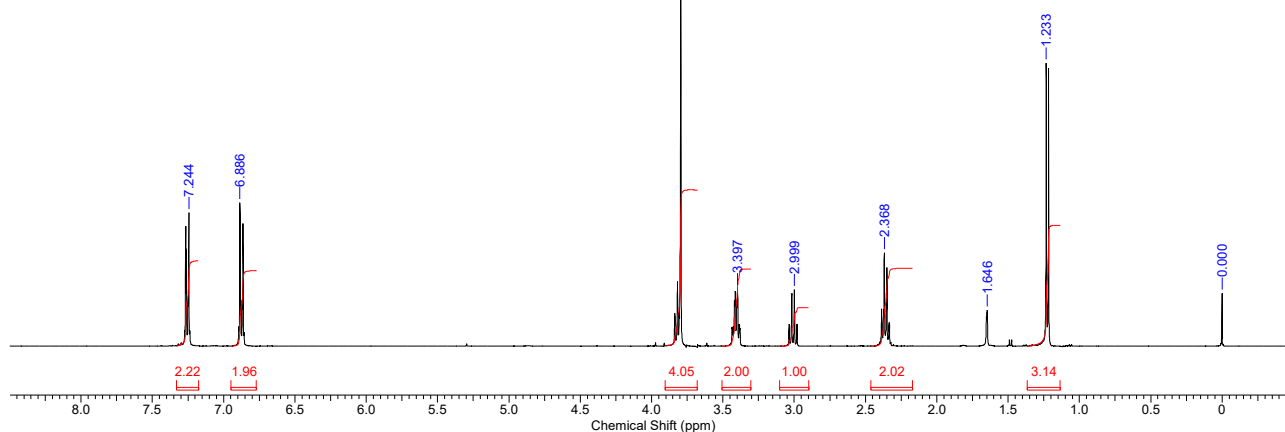


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2R,1'S-3b_1H.esp

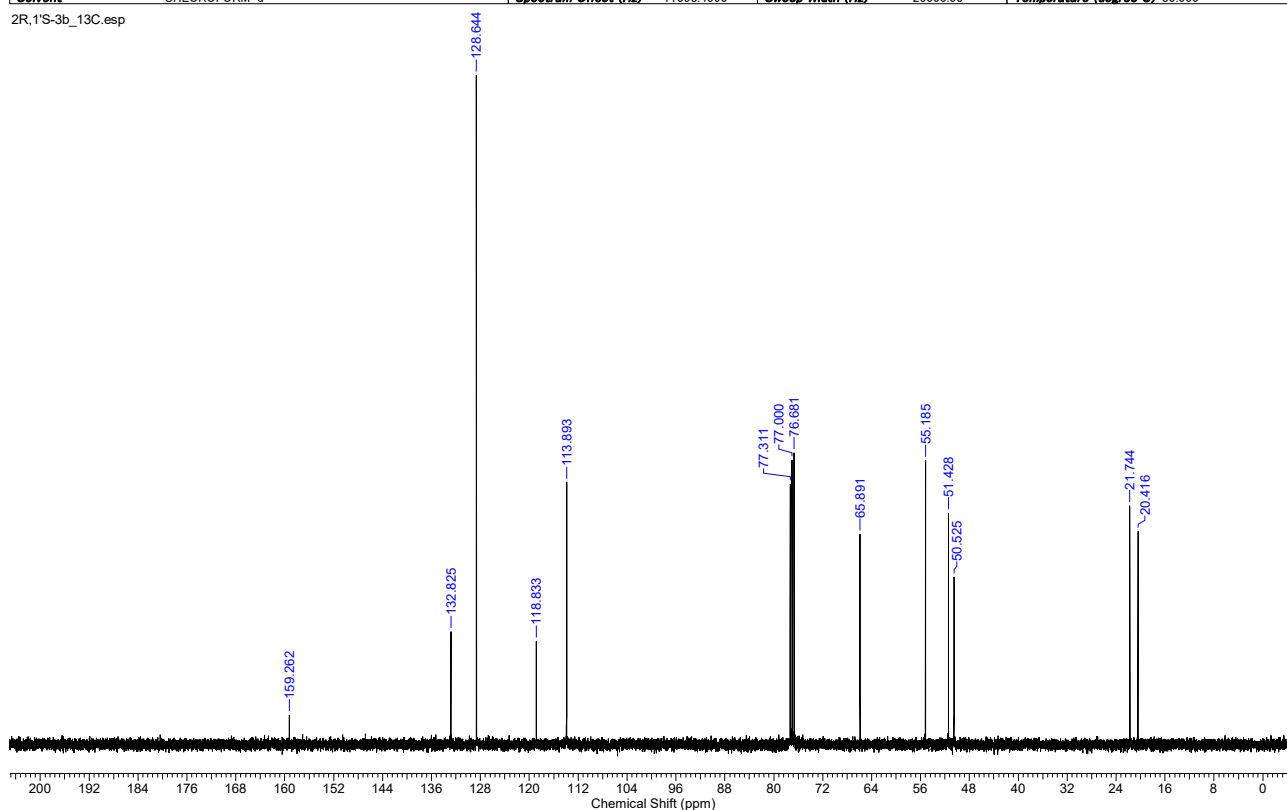


(2R,1'S)-3b
¹H: CDCl₃, ¹³C: CDCl₃



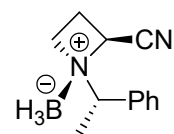
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Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	11058.4590				

2R,1'S-3b_13C.esp

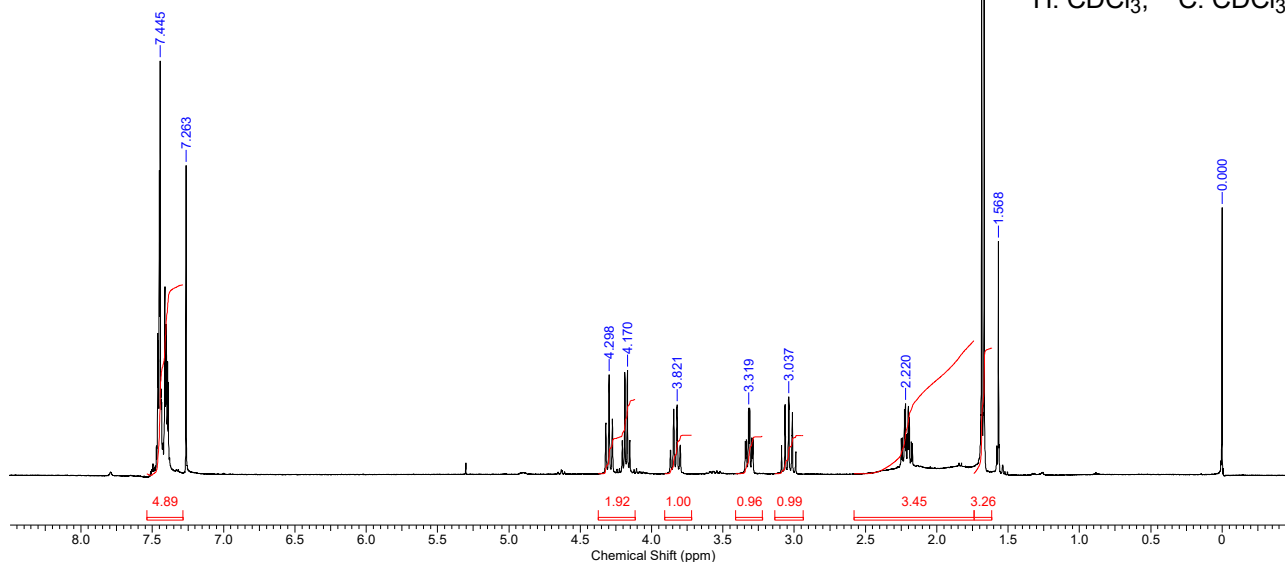


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Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2407.3430	Sweep Width (Hz)	6410.26
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1S,2S,1'S-4a_1H.esp

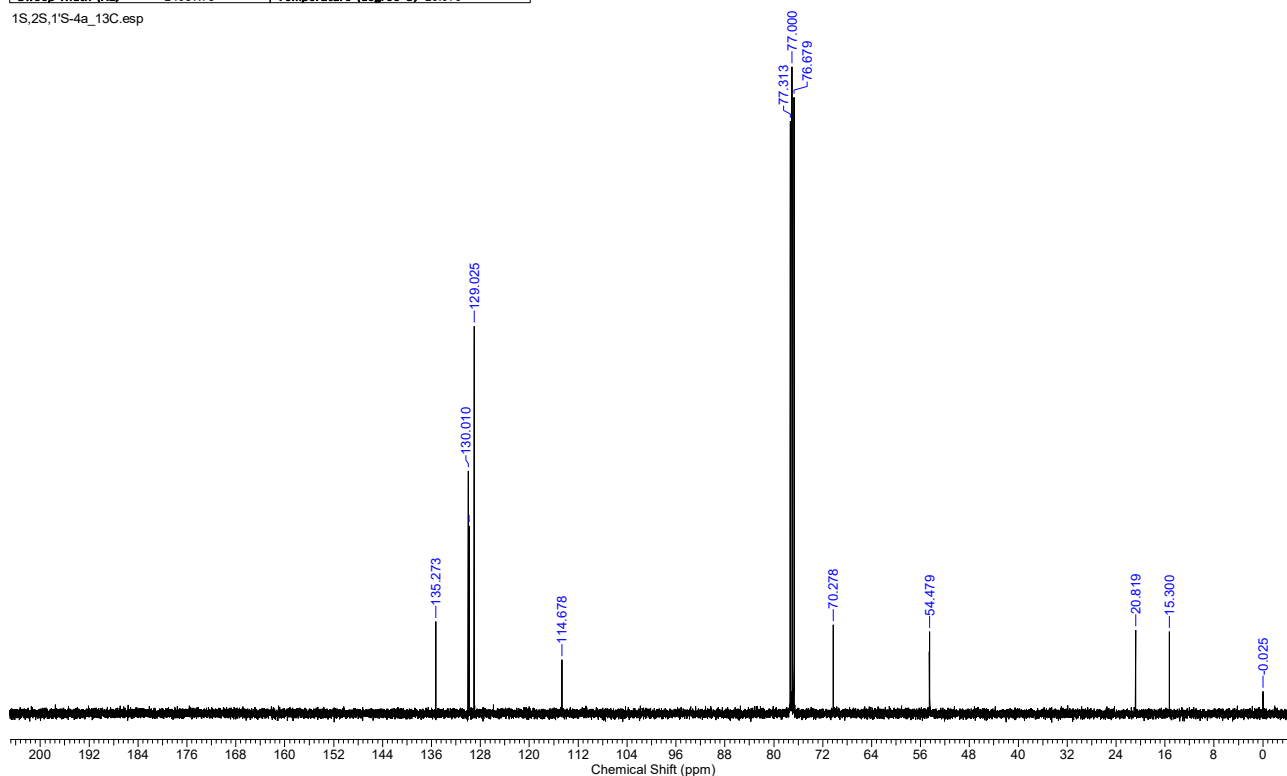


(1S,2S,1'S)-4a
¹H: CDCl₃, ¹³C: CDCl₃



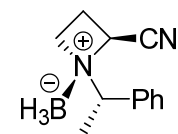
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Nucleus	13C	Number of Transients	1024	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (vocal) (Hz)	24038.46	Solvent	CHLOROFORM-d	Receiver Gain	199.87
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1S,2S,1'S-4a_13C.esp

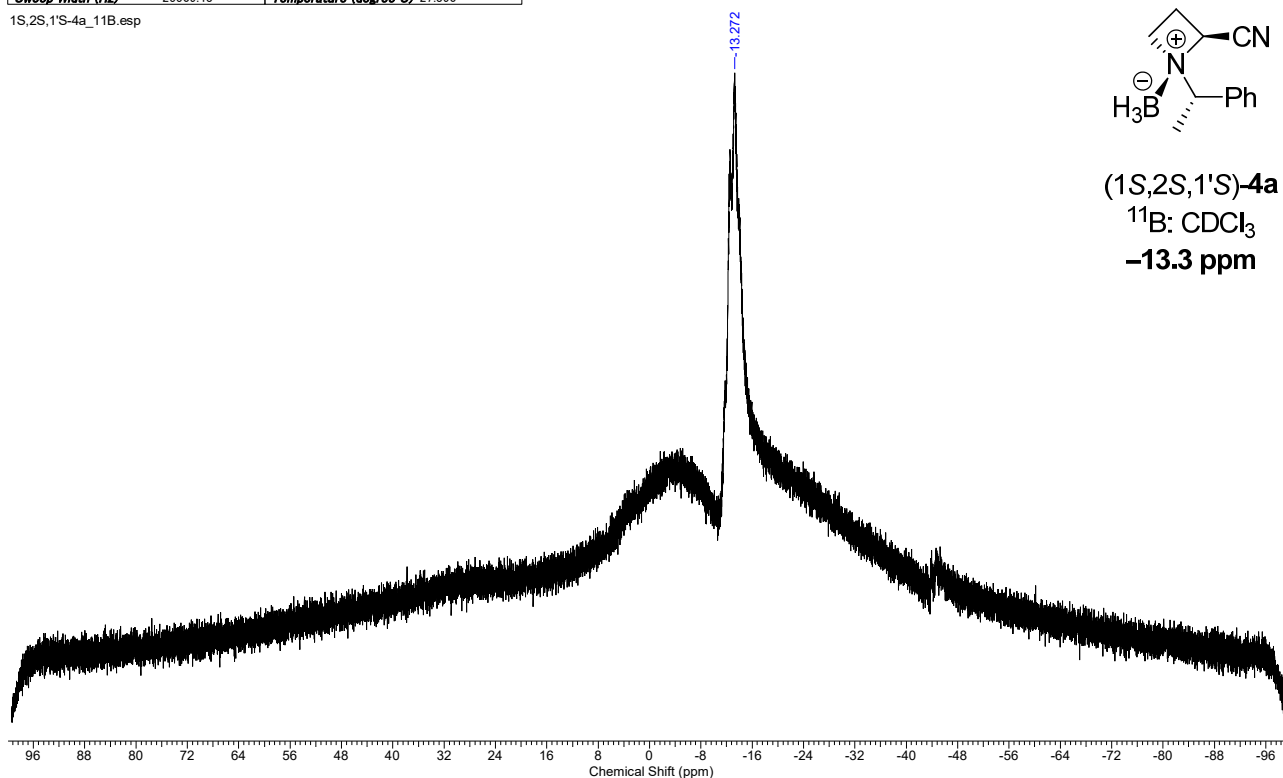


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Nucleus	11B	Number of Transients	128	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zg
SW (vocalist) (Hz)	25510.21	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	25509.43	Temperature (degree C)	27.390	Spectrum Offset (Hz)	0.0002

1S,2S,1'S-4a_11B.esp



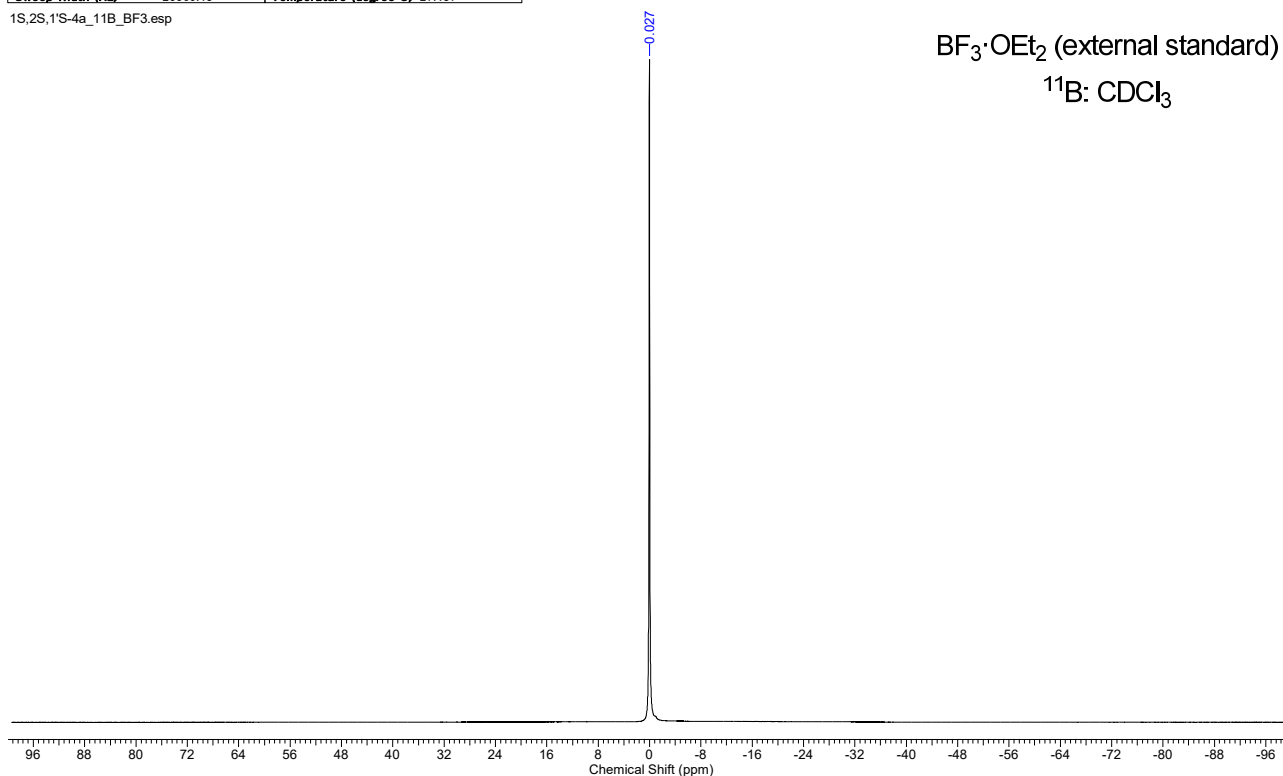
(1S,2S,1'S)-4a
¹¹B: CDCl₃
 -13.3 ppm



Acquisition Time (sec)	1.2845	Date	06 Aug 2020 11:50:24	Date Stamp	06 Aug 2020 11:50:24
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4236\4236_010000fid	Frequency (MHz)	128.38	Original Points Count	32768
Nucleus	11B	Number of Transients	128	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zg
SW (vocalist) (Hz)	25510.21	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	25509.43	Temperature (degree C)	27.437	Spectrum Offset (Hz)	0.0002

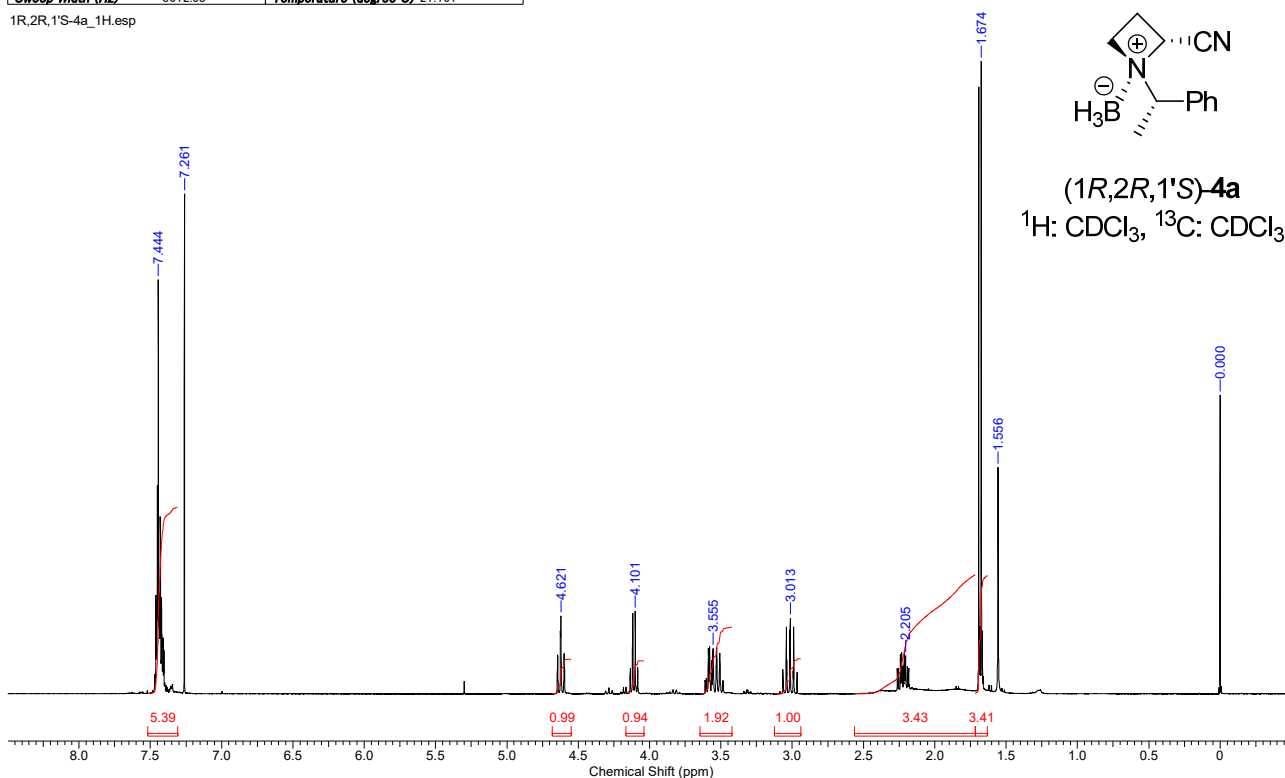
1S,2S,1'S-4a_11B_BF3.esp

BF₃·OEt₂ (external standard)
¹¹B: CDCl₃



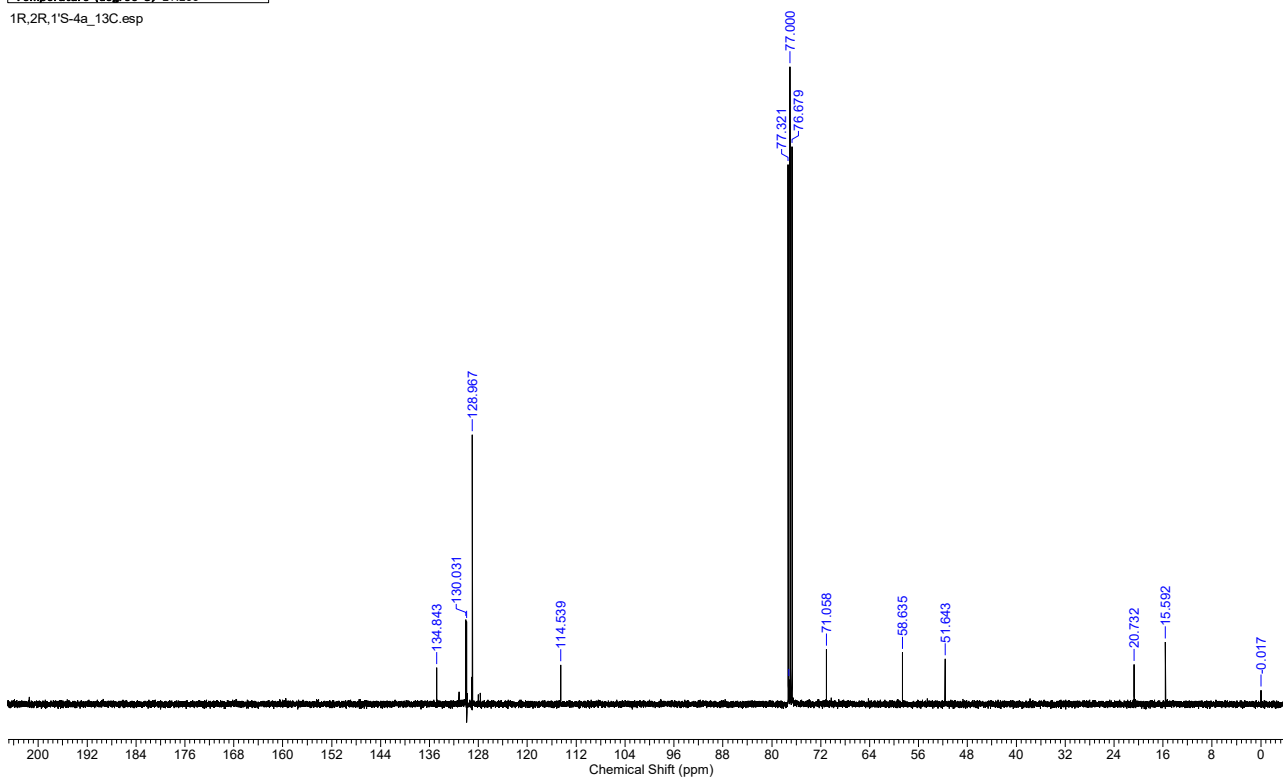
Acquisition Time (sec)	4.0894	Date	07 Aug 2020 09:40:16	Date Stamp	07 Aug 2020 09:40:16
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4246\4246_010000fid	Frequency (MHz)	400.13	Original Points Count	32768
Nucleus	¹ H	Number of Transients	16	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zg30
SW (vocal) (Hz)	8012.82	Solvent	CHLOROFORM-d	Receiver Gain	136.03
Sweep Width (Hz)	8012.58	Temperature (degree C)	27.161	Spectrum Offset (Hz)	2461.7627

1R,2R,1'S-4a_1H.esp



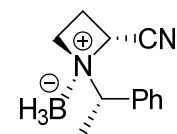
Acquisition Time (sec)	1.3631	Date	07 Aug 2020 11:46:08	Date Stamp	07 Aug 2020 11:46:08
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4248\4248_010000fid	Frequency (MHz)	100.62	Original Points Count	32768
Nucleus	¹³ C	Number of Transients	2048	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (vocal) (Hz)	24038.46	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10059.1514
Temperature (degree C)	27.233	Sweep Width (Hz)	24037.73		

1R,2R,1'S-4a_13C.esp

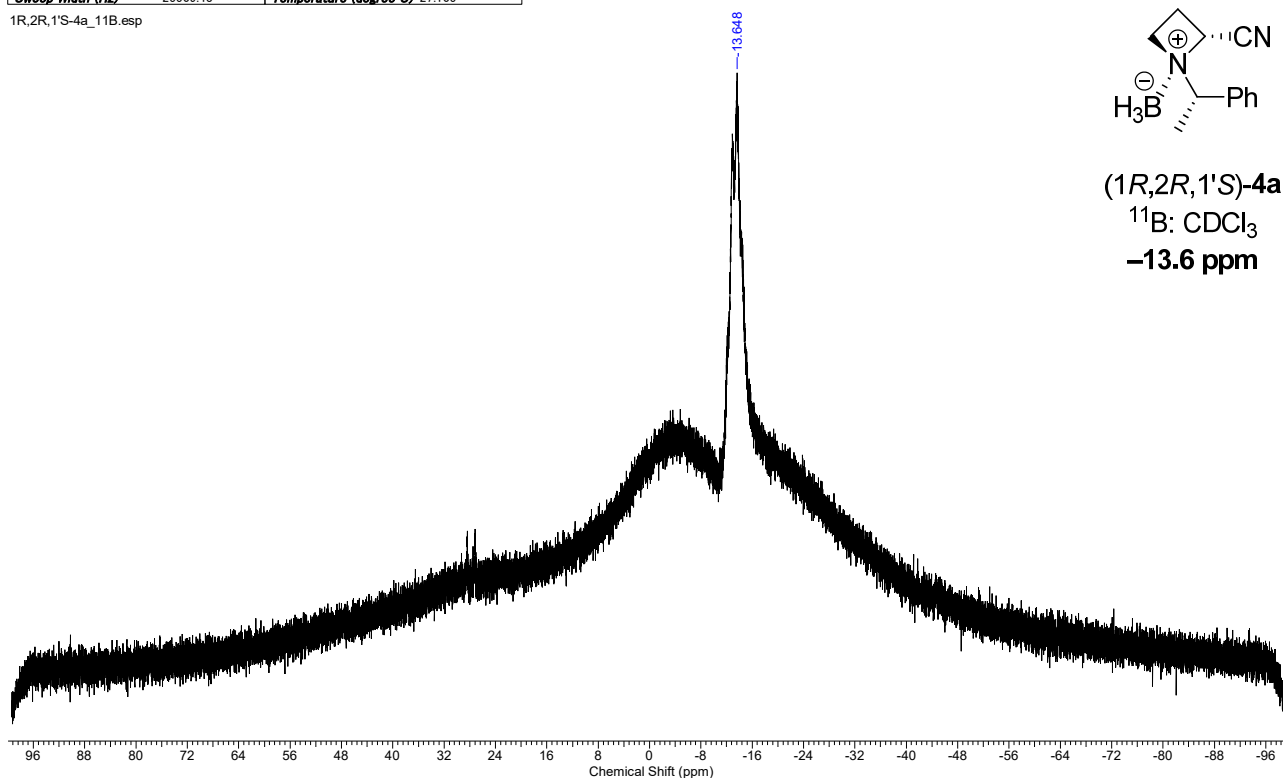


Acquisition Time (sec)	1.2845	Date	07 Aug 2020 09:46:40	Date Stamp	07 Aug 2020 09:46:40
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4247\4247_010000fid	Frequency (MHz)	128.38	Original Points Count	32768
Nucleus	11B	Number of Transients	128	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zg
SW (Hz)	25510.21	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	25509.43	Temperature (degree C)	27.105	Spectrum Offset (Hz)	0.0002

1R,2R,1'S-4a_11B.esp



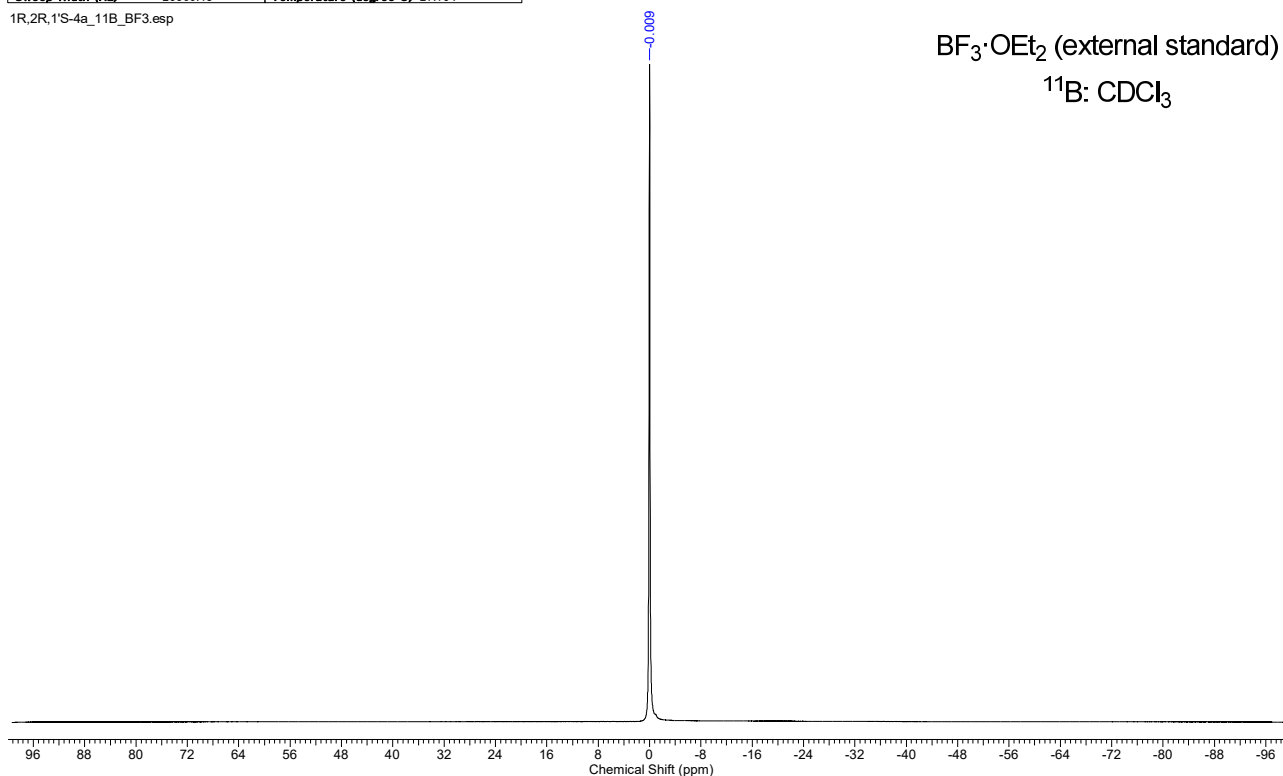
(1R,2R,1'S)-4a
¹¹B: CDCl₃
 -13.6 ppm



Acquisition Time (sec)	1.2845	Date	07 Aug 2020 09:33:52	Date Stamp	07 Aug 2020 09:33:52
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4245\4245_010000fid	Frequency (MHz)	128.38	Original Points Count	32768
Nucleus	11B	Number of Transients	128	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zg
SW (Hz)	25510.21	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	25509.43	Temperature (degree C)	27.154	Spectrum Offset (Hz)	0.0002

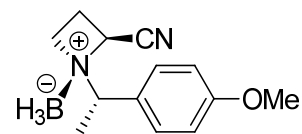
1R,2R,1'S-4a_11B_BF3.esp

BF₃·OEt₂ (external standard)
¹¹B: CDCl₃

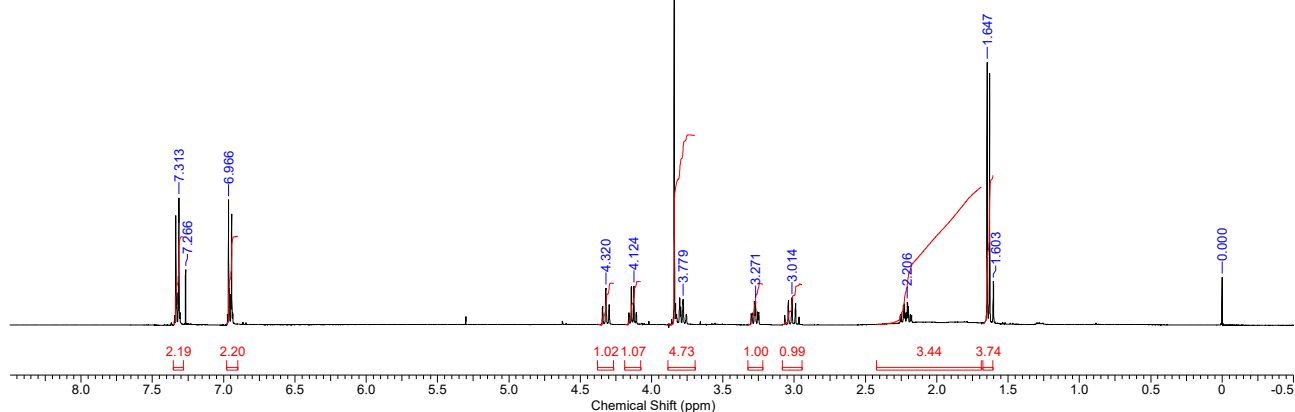


Acquisition Time (sec)	3.5000	Comment	Z0 4103	Date	Aug 4 2020	Date Stamp	Aug 4 2020
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4226					Frequency (MHz)	399.83
Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2408.7124	Sweep Width (Hz)	6410.26
						Temperature (degree C)	30.000

1S,2S,1'S-4b_1H.esp

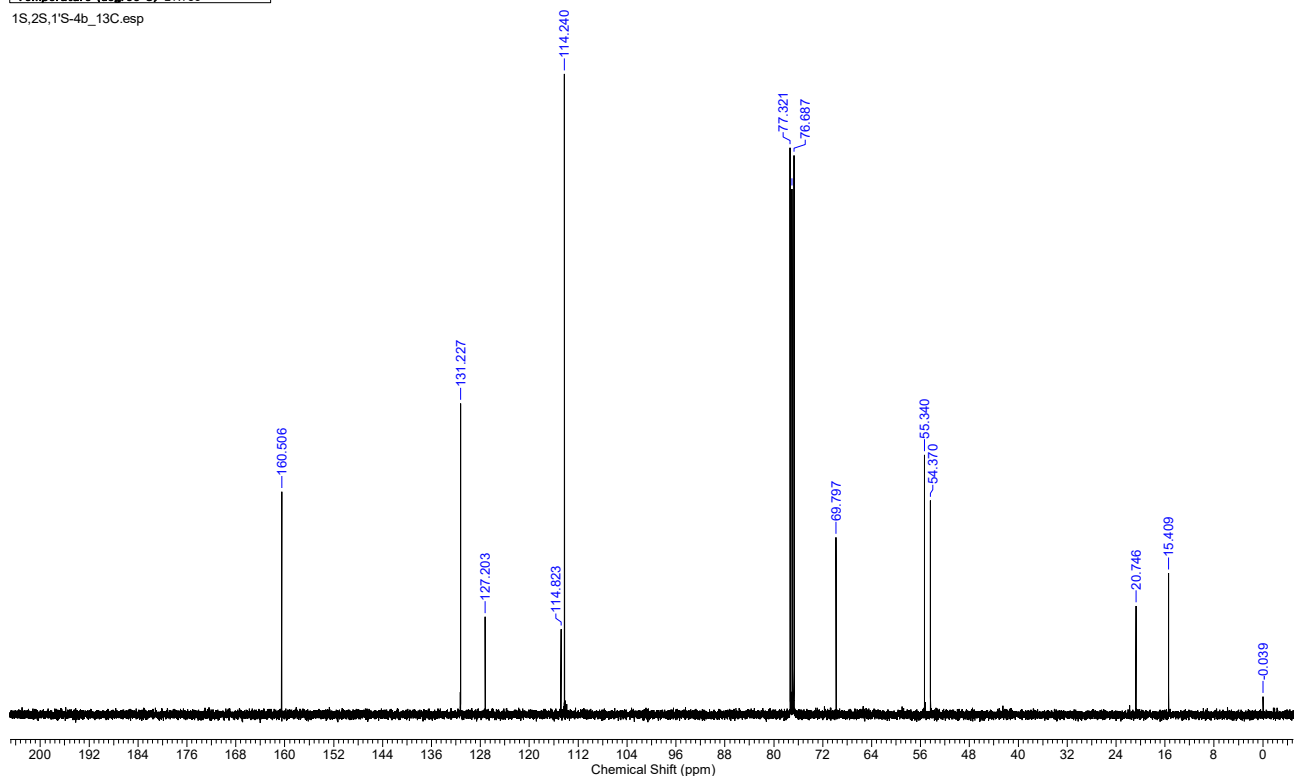


(1S,2S,1'S)-4b
¹H: CDCl₃, ¹³C: CDCl₃



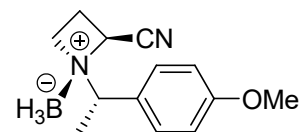
Acquisition Time (sec)	1.3631	Date	04 Aug 2020 12:24:32	Date Stamp	04 Aug 2020 12:24:32
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4234\4234_010000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	1024	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (Hz)	24038.46	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10056.9502
Temperature (degree C)	27.783			Receiver Gain	199.87
				Sweep Width (Hz)	24037.73

1S,2S,1'S-4b_13C.esp

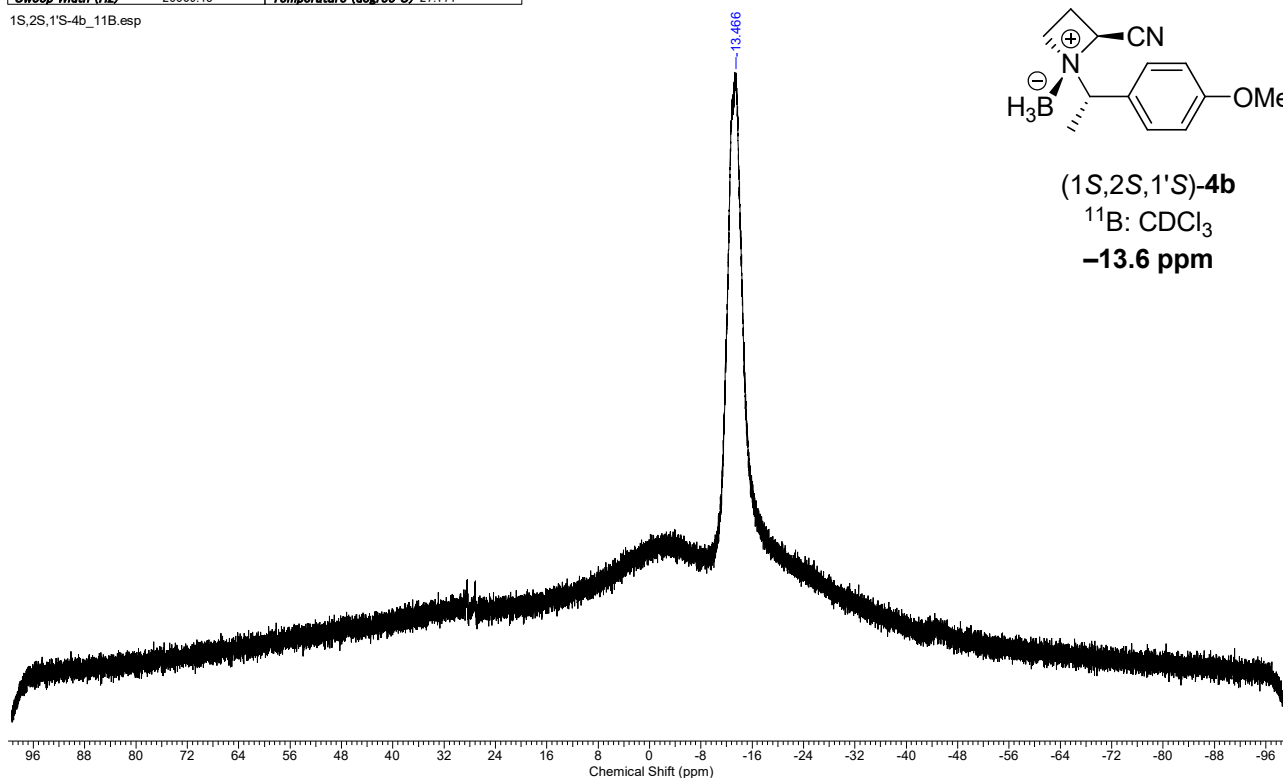


Acquisition Time (sec)	1.2845	Date	04 Aug 2020 11:24:48	Date Stamp	04 Aug 2020 11:24:48
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4233\4233_010000fid	Frequency (MHz)	128.38	Original Points Count	32768
Nucleus	11B	Number of Transients	128	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zg
SW (Hz)	25510.21	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	25509.43	Temperature (degree C)	27.171	Spectrum Offset (Hz)	0.0002

1S,2S,1'S-4b_11B.esp



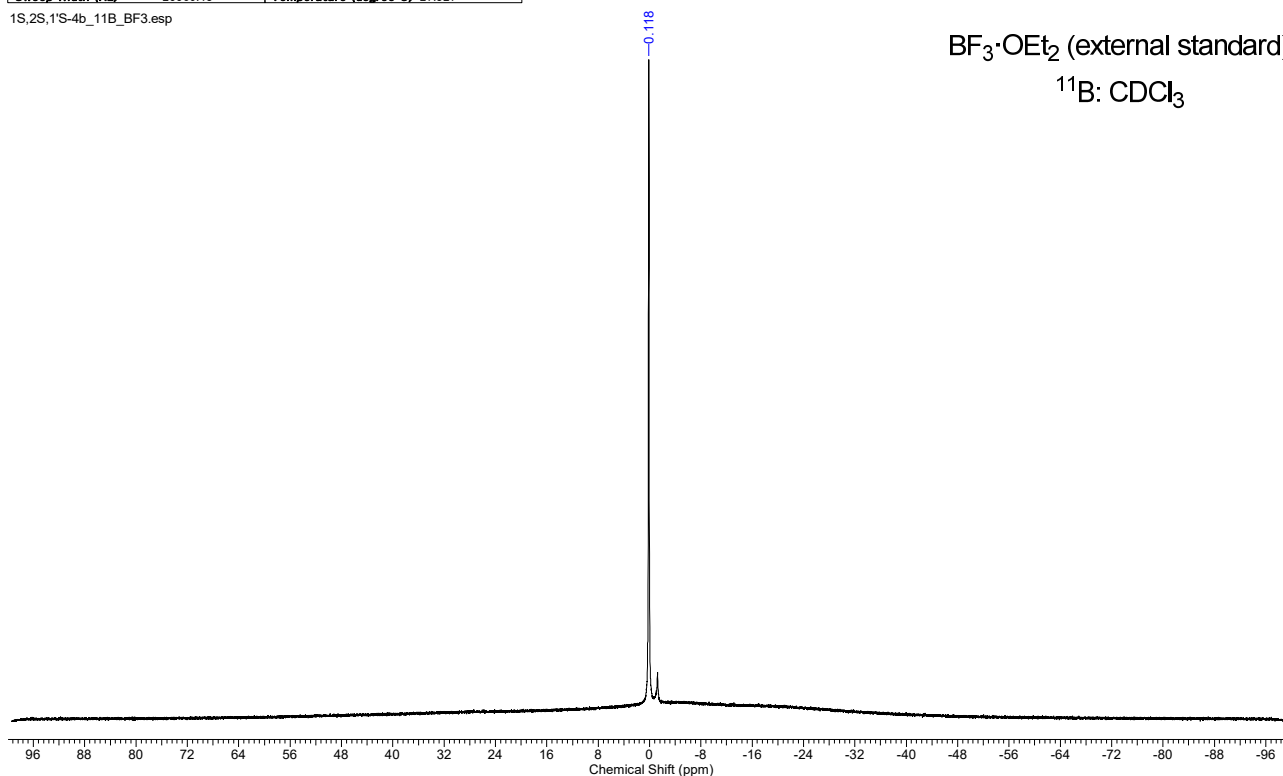
(1S,2S,1'S)-4b
¹¹B: CDCl₃
 -13.6 ppm



Acquisition Time (sec)	1.2845	Date	04 Aug 2020 11:12:00	Date Stamp	04 Aug 2020 11:12:00
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4231\4231_010000fid	Frequency (MHz)	128.38	Original Points Count	32768
Nucleus	11B	Number of Transients	128	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zg
SW (Hz)	25510.21	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	25509.43	Temperature (degree C)	27.327	Spectrum Offset (Hz)	0.0002

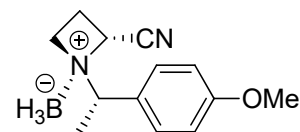
1S,2S,1'S-4b_11B_BF3.esp

BF₃·OEt₂ (external standard)
¹¹B: CDCl₃

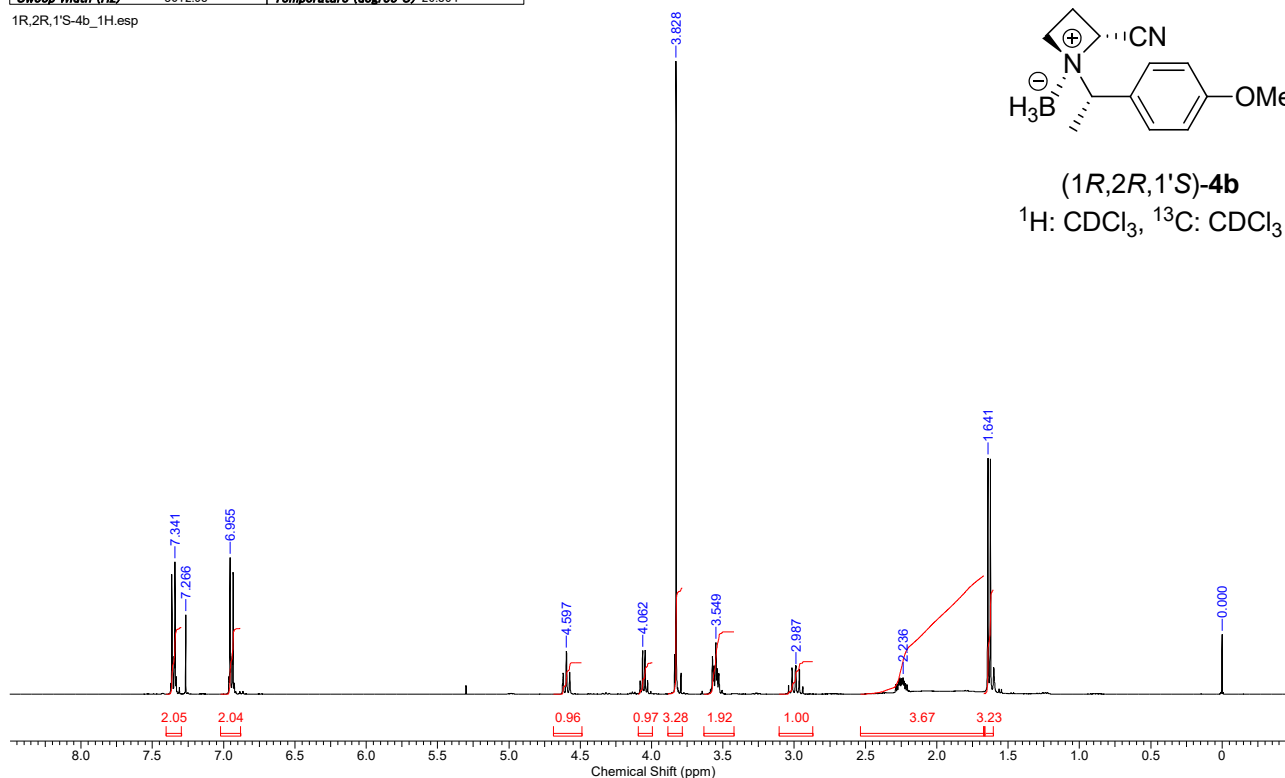


Acquisition Time (sec)	4.0894	Date	26 Aug 2020 04:05:20	Date Stamp	26 Aug 2020 04:05:20
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4249\4249_010000fid	Frequency (MHz)	400.13	Original Points Count	32768
Nucleus	¹ H	Number of Transients	16	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zg30
SW (vocal) (Hz)	8012.82	Solvent	CHLOROFORM-d	Receiver Gain	67.15
Sweep Width (Hz)	8012.58	Temperature (degree C)	26.854	Spectrum Offset (Hz)	2463.6516

1R,2R,1'S-4b_1H.esp

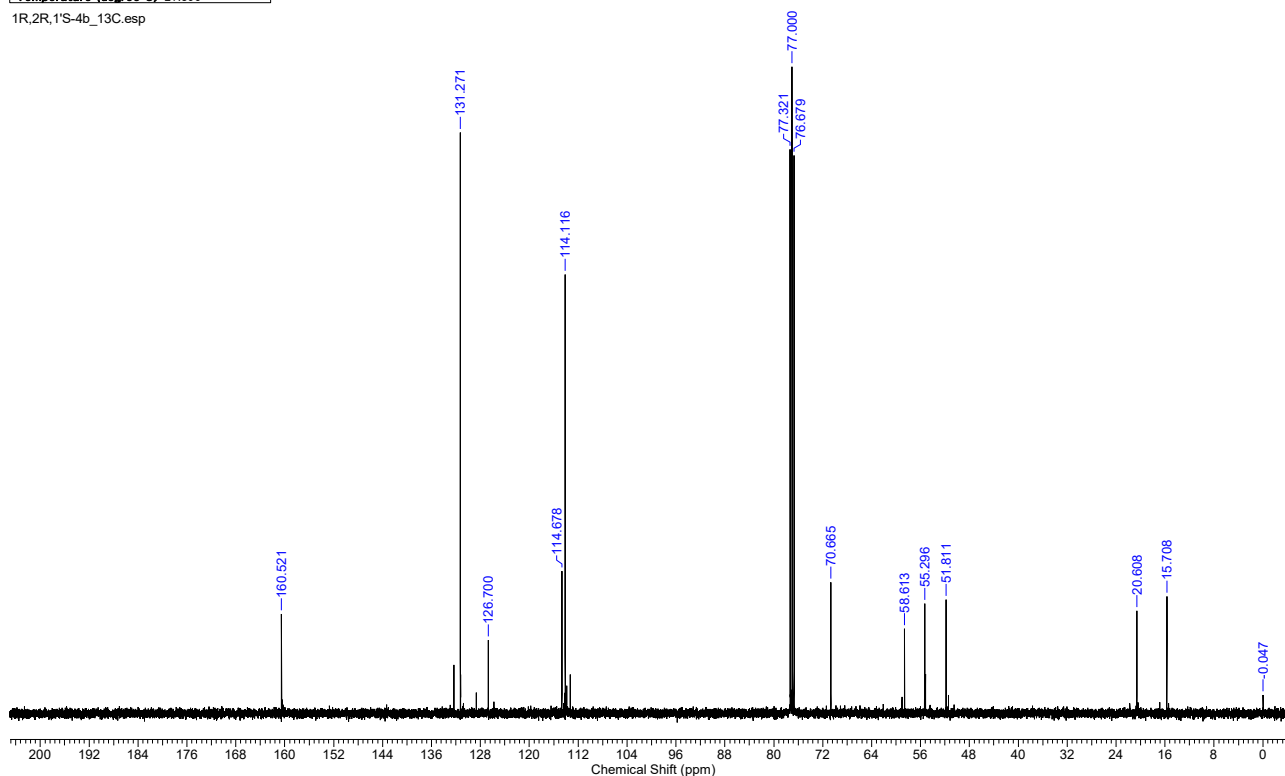


(1R,2R,1'S)-4b
¹H: CDCl₃, ¹³C: CDCl₃



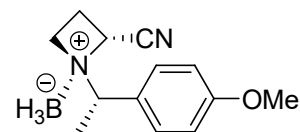
Acquisition Time (sec)	1.3631	Date	26 Aug 2020 10:52:48	Date Stamp	26 Aug 2020 10:52:48
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4255\4255_010000fid	Frequency (MHz)	100.62	Original Points Count	32768
Nucleus	¹³ C	Number of Transients	1024	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (vocal) (Hz)	24038.46	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10056.2168
Temperature (degree C)	27.396	Sweep Width (Hz)	24037.73		

1R,2R,1'S-4b_13C.esp

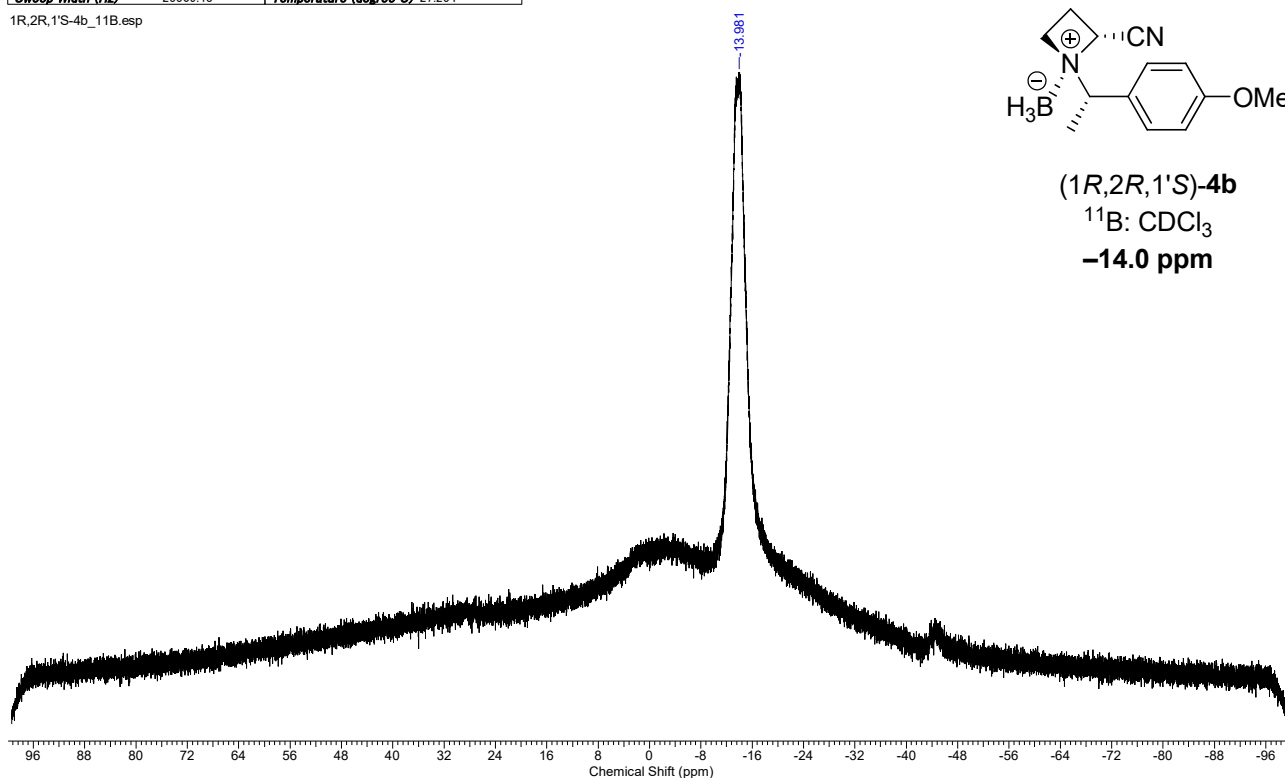


Acquisition Time (sec)	1.2845	Date	26 Aug 2020 09:53:04	Date Stamp	26 Aug 2020 09:53:04
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4254\4254_010000fid	Frequency (MHz)	128.38	Original Points Count	32768
Nucleus	11B	Number of Transients	128	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zg
SW (Hz)	25510.21	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	25509.43	Temperature (degree C)	27.254	Spectrum Offset (Hz)	0.0002

1R,2R,1'S-4b_11B.esp



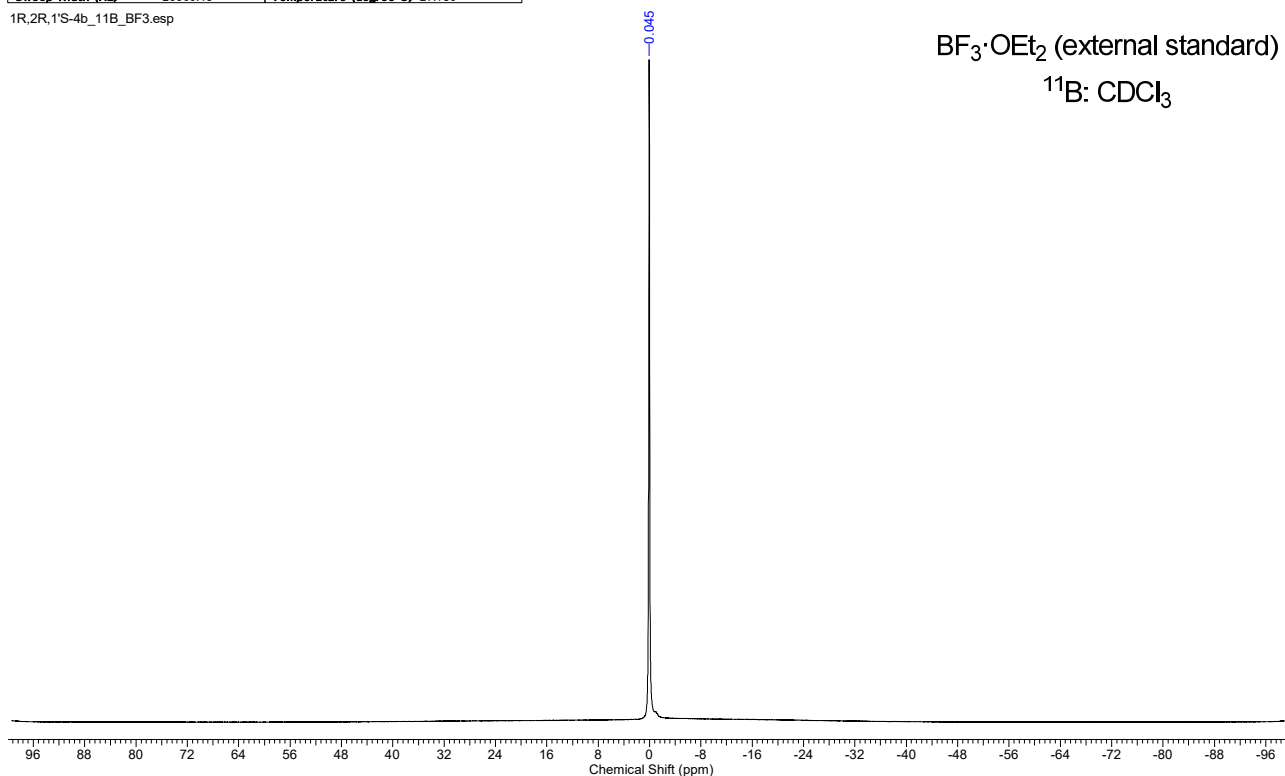
(1R,2R,1'S)-4b
¹¹B: CDCl₃
 -14.0 ppm



Acquisition Time (sec)	1.2845	Date	26 Aug 2020 09:40:16	Date Stamp	26 Aug 2020 09:40:16
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\subs-BH3\4252\4252_010000fid	Frequency (MHz)	128.38	Original Points Count	32768
Nucleus	11B	Number of Transients	128	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zg
SW (Hz)	25510.21	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	25509.43	Temperature (degree C)	27.186	Spectrum Offset (Hz)	0.0002

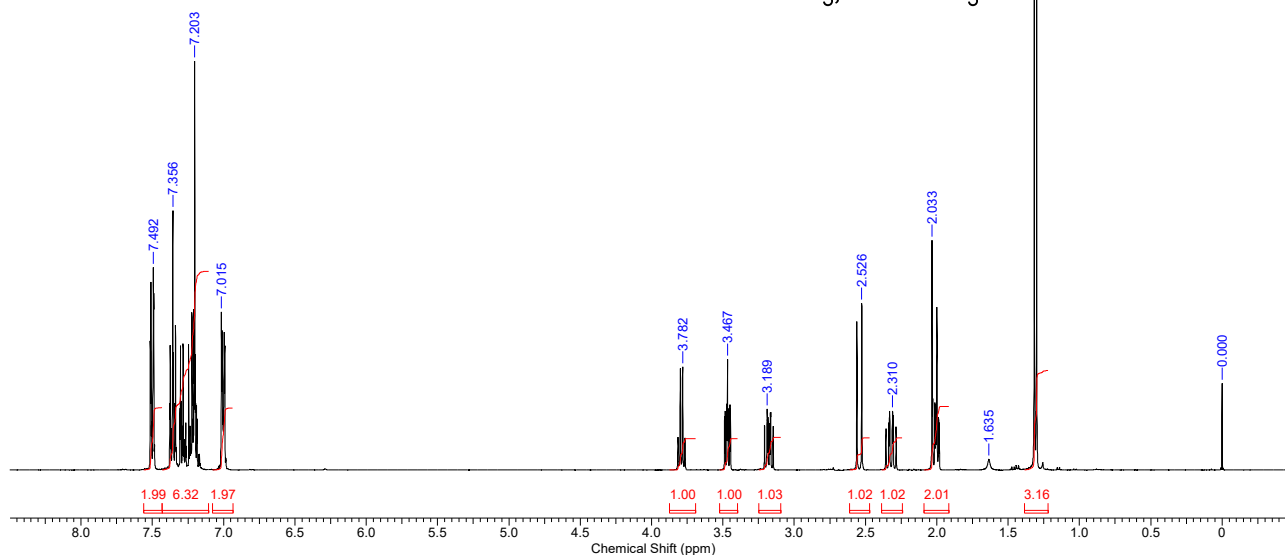
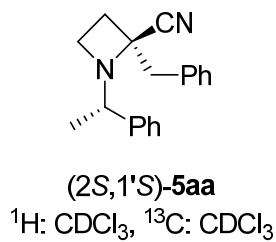
1R,2R,1'S-4b_11B_BF3.esp

BF₃·OEt₂ (external standard)
¹¹B: CDCl₃



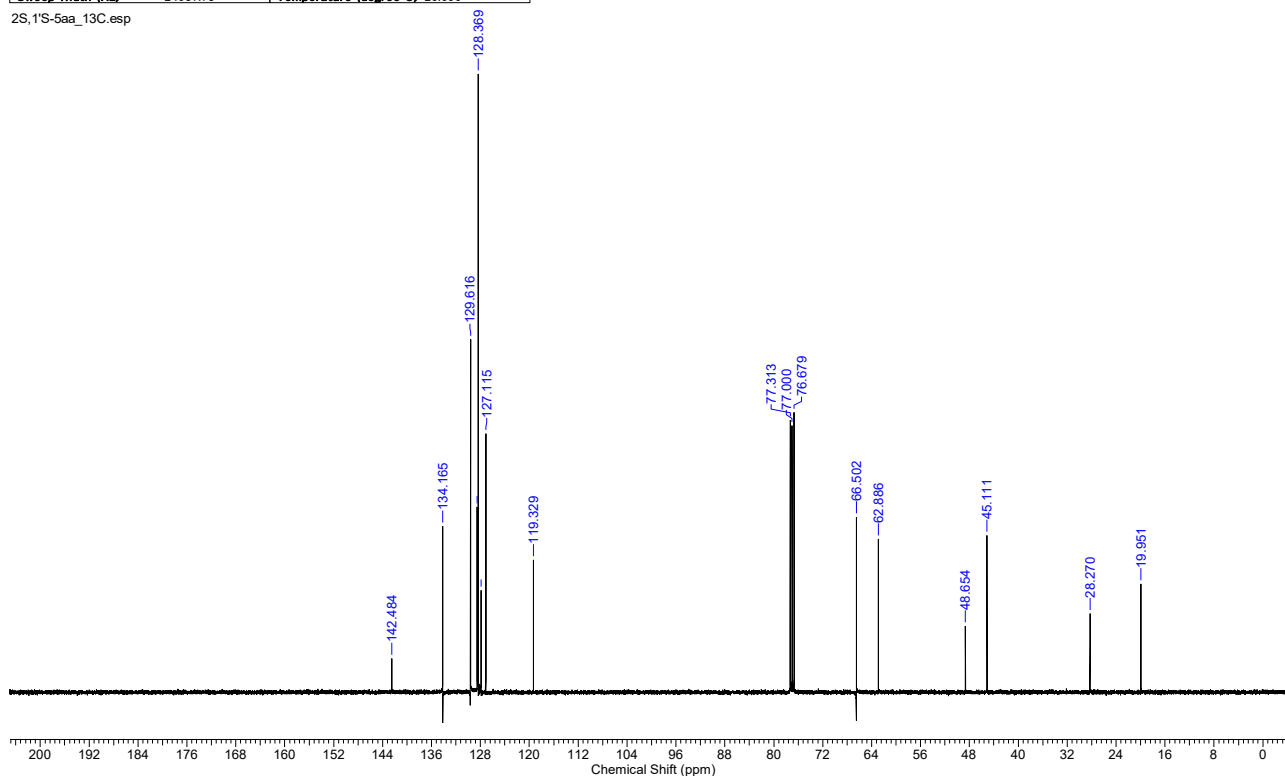
Acquisition Time (sec)	3.5000	Date	Sep 25 2020	Date Stamp	Sep 25 2020	Frequency (MHz)	399.83	Nucleus	¹ H
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\Y4295					Pulse Sequence	s2pul	Receiver Gain	36.00
Number of Transients	16	Original Points Count	22436	Points Count	32768	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000
Solvent	CHLOROFORM-d					Spectrum Offset (Hz)	2400.1047		

2S,1'S-5aa_1H.esp



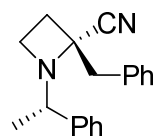
Acquisition Time (sec)	1.3631	Date	25 Sep 2020 10:29:20	Date Stamp	25 Sep 2020 10:29:20	Frequency (MHz)	100.62
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\Yn4276\Yn4276_010000fid					Original Points Count	32768
Nucleus	¹³ C	Number of Transients	1024	Origin	spect	Receiver Gain	199.87
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30	Spectrum Offset (Hz)	10054.7500
SW (vocal) (Hz)	24038.46	Solvent	CHLOROFORM-d				
Sweep Width (Hz)	24037.73	Temperature (degree C)	25.656				

2S,1'S-5aa_13C.esp

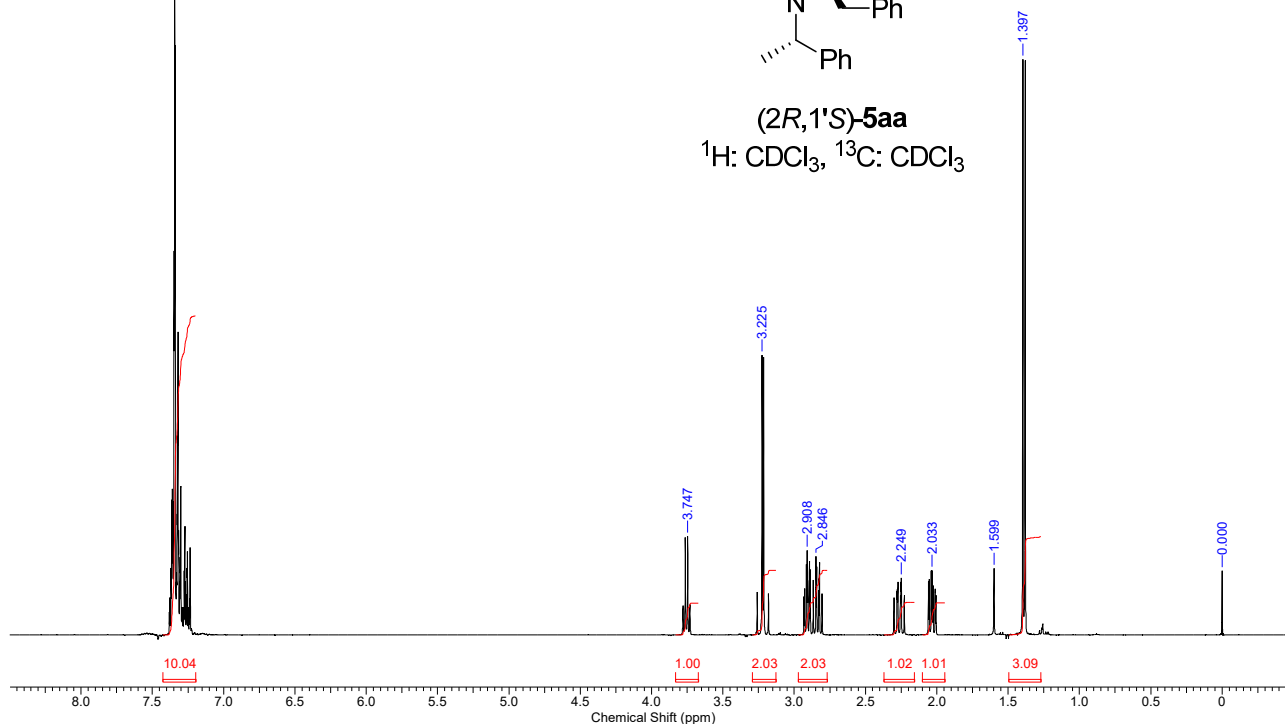


Acquisition Time (sec)	3.5000	Comment	Z0.4103	Date	Jul 22 2020	Date Stamp	Jul 22 2020		
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\4208					Frequency (MHz)	399.83	Nucleus	¹ H
Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	34.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2395.8008	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000

2R,1'S-5aa_1H.esp

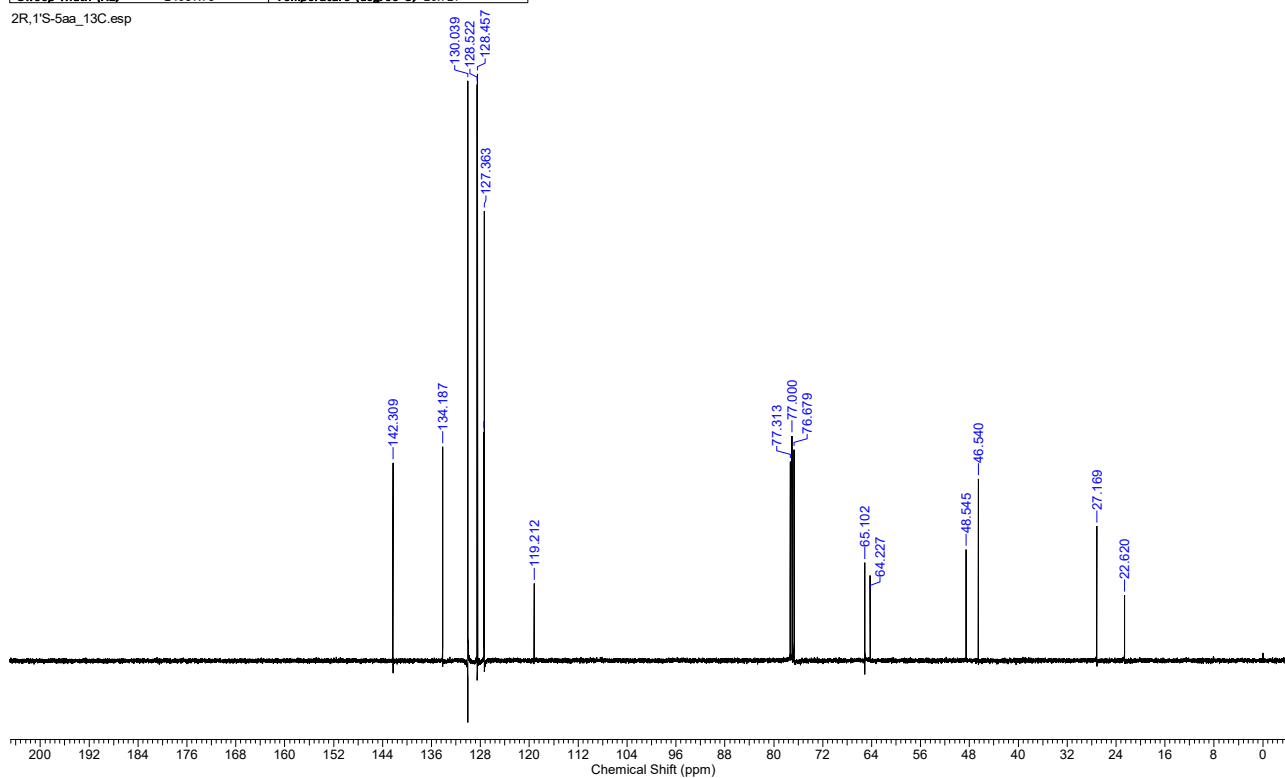


(2R,1'S)-5aa
¹H: CDCl₃, ¹³C: CDCl₃



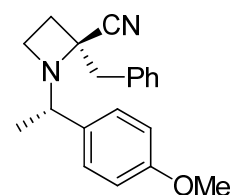
Acquisition Time (sec)	1.3631	Date	22 Jul 2020 09:21:04	Date Stamp	22 Jul 2020 09:21:04
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Nakanome\product\4219\4219_010000fid			Frequency (MHz)	100.62
Nucleus	¹³ C	Number of Transients	512	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (Hz)	24038.46	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	24037.73	Temperature (degree C)	25.727	Spectrum Offset (Hz)	10052.5488

2R,1'S-5aa_13C.esp

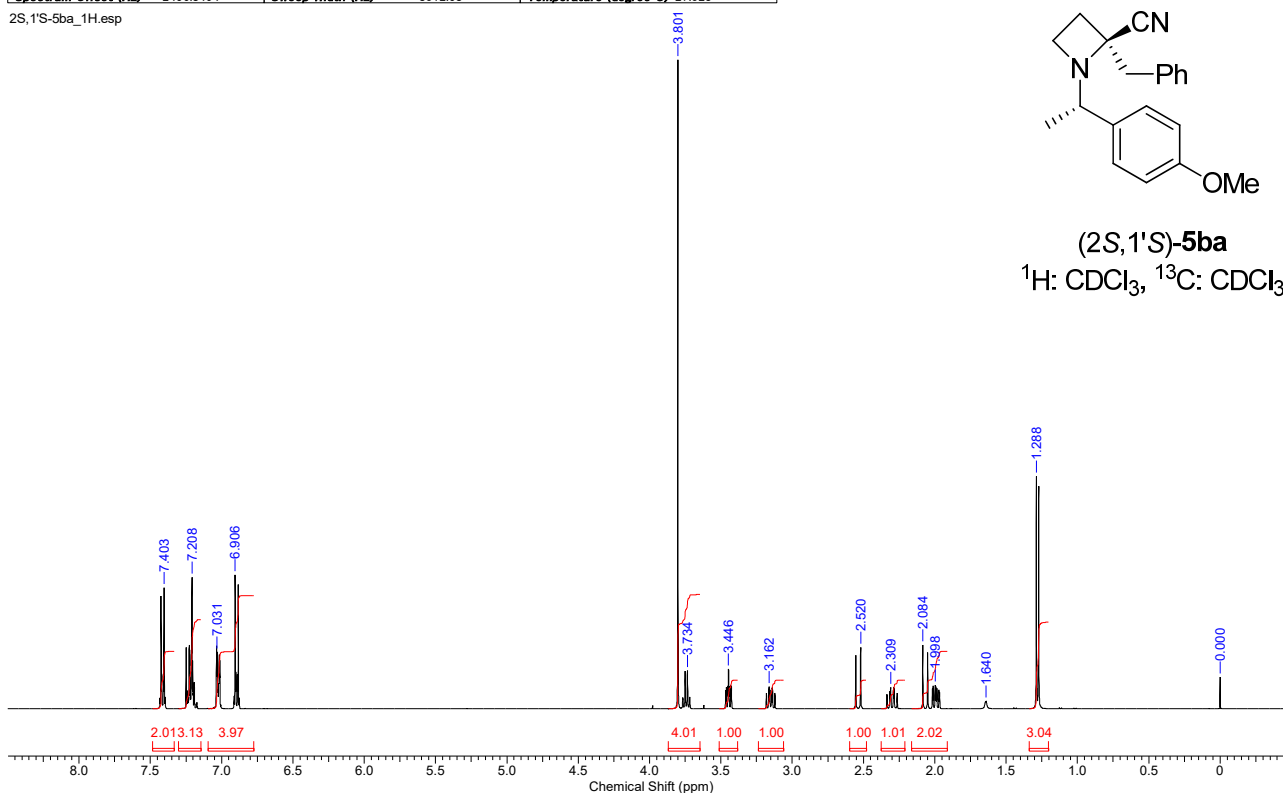


Acquisition Time (sec)	4.0894	Date	17 Sep 2020 09:08:16	Date Stamp	17 Sep 2020 09:08:16
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\N4274\N4274_010000fid	Frequency (MHz)	400.13	Nucleus	¹ H
Number of Transients	16	Origin	spect	Original Points Count	32768
Pulse Sequence	zg30	Receiver Gain	30.60	Owner	BrukerNMR
Spectrum Offset (Hz)	2456.8494	Sweep Width (Hz)	8012.58	SW (cyclical) (Hz)	8012.82
		Temperature (degree C)	27.023	Solvent	CHLOROFORM-d
				Points Count	32768

2S,1'S-5ba_1H.esp

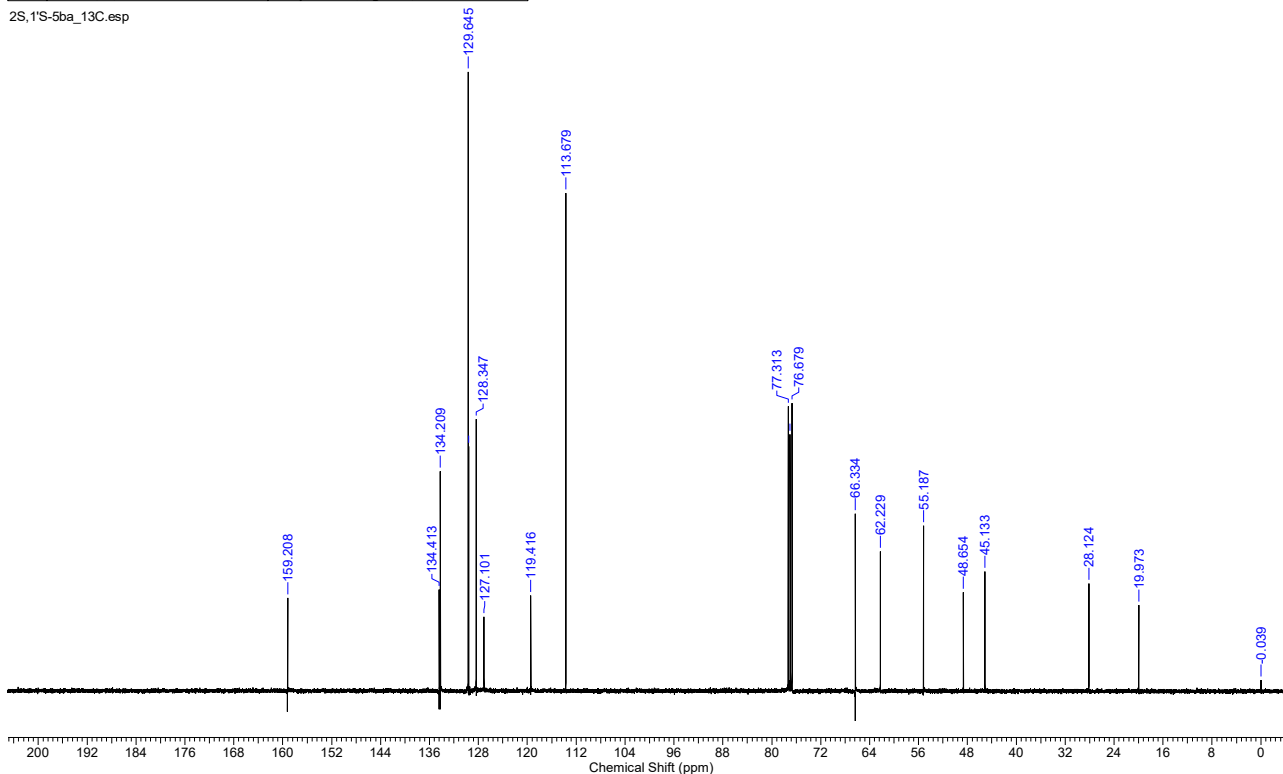


(2S,1'S)-5ba
¹H: CDCl₃, ¹³C: CDCl₃



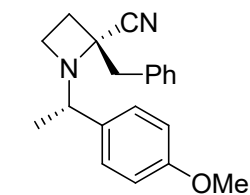
Acquisition Time (sec)	1.3631	Date	17 Sep 2020 10:08:00	Date Stamp	17 Sep 2020 10:08:00
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\N4275\N4275_010000fid	Frequency (MHz)	100.62	Nucleus	¹³ C
Nucleus	¹³ C	Number of Transients	1024	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	24037.73	Temperature (degree C)	27.485	Spectrum Offset (Hz)	10054.7500

2S,1'S-5ba_13C.esp

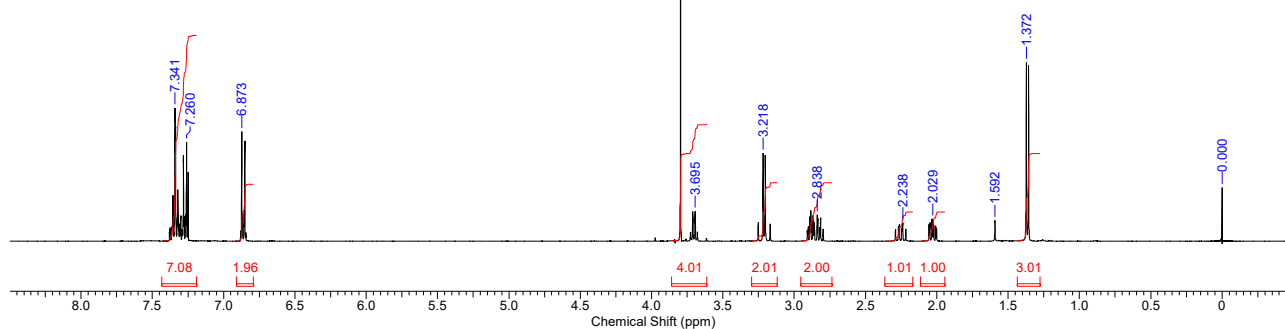


Acquisition Time (sec)	3.5000	Date	Sep 9 2020	Date Stamp	Sep 9 2020	Frequency (MHz)	399.83	Nucleus	¹ H
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\4255	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2oul	Receiver Gain	38.00
Number of Transients	16	Spectrum Offset (Hz)	2401.6697	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000		
Solvent	CHLOROFORM-d								

2R,1'S-5ba_1H.esp

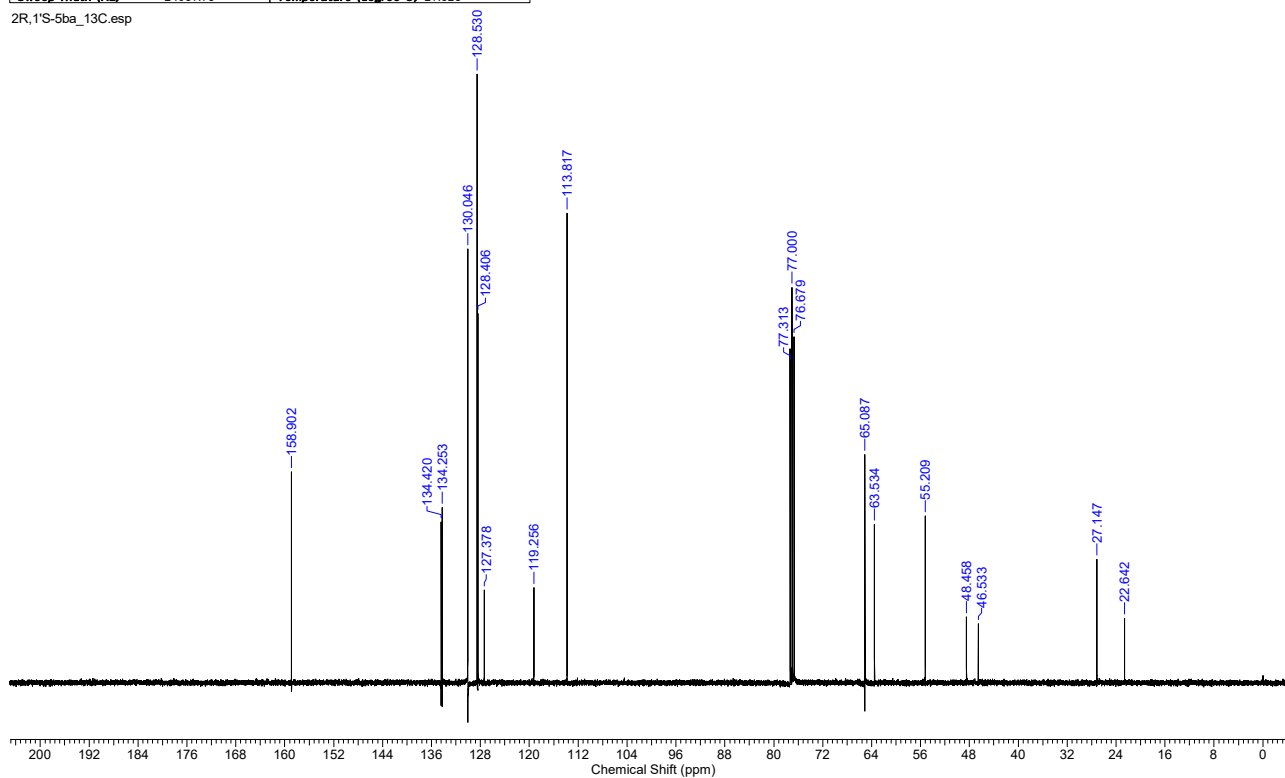


(2R,1'S)-5ba
¹H: CDCl₃, ¹³C: CDCl₃



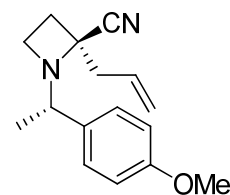
Acquisition Time (sec)	1.3631	Date	09 Sep 2020 10:31:28	Date Stamp	09 Sep 2020 10:31:28	Frequency (MHz)	100.62
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\4261\010000fid	Number of Transients	1024	Origin	spect	Original Points Count	32768
Nucleus	¹³ C	Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	199.87
Owner	BrukerNMR	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10056.2168		
SW (vocal) (Hz)	24038.46	Temperature (degree C)	27.328				
Sweep Width (Hz)	24037.73						

2R,1'S-5ba_13C.esp

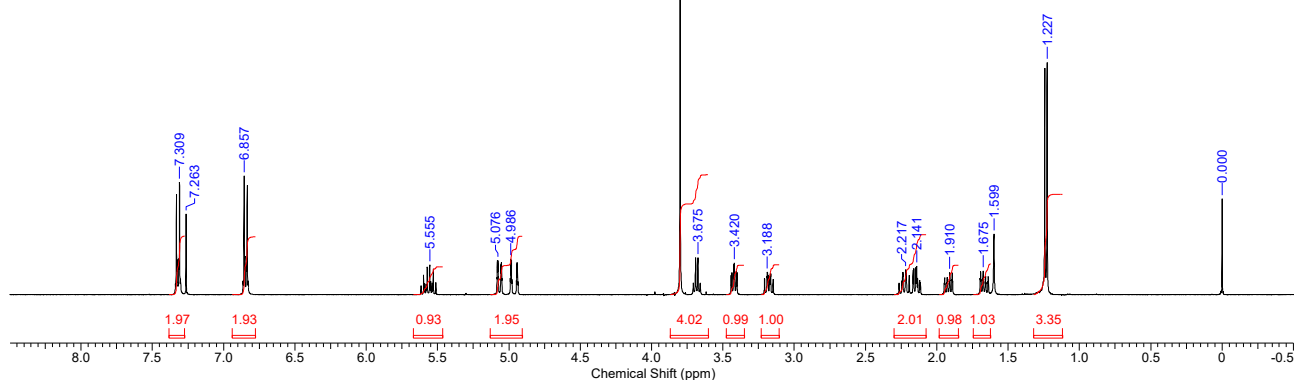


Acquisition Time (sec)	3.5000	Comment	STANDARD 1H OBSERVE - profile	Date	Oct 23 2020
Date Stamp	Oct 23 2020	File Name	C:\Users\ytayam\Documents\Results for Publication\Nakanome\Nakanome\data\product\44387		
Frequency (MHz)	399.83	Nucleus	1H	Number of Transients	16
Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	46.00
Spectrum Offset (Hz)	2407.1475	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000
				Solvent	CHLOROFORM-d

2S,1'S-5bb_1H.esp

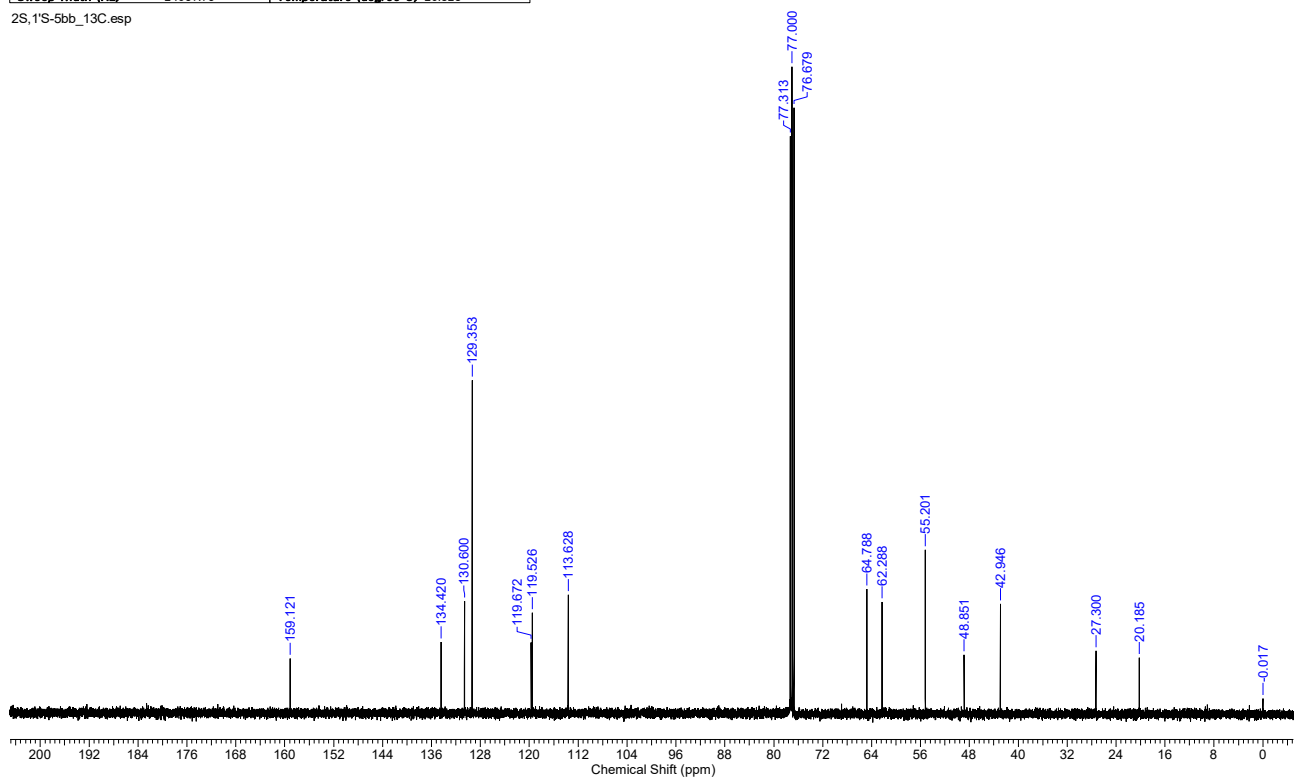


(2S,1'S)-5bb
 ^1H : CDCl_3 , ^{13}C : CDCl_3



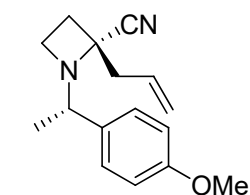
Acquisition Time (sec)	1.3631	Date	23 Oct 2020 09:48:48	Date Stamp	23 Oct 2020 09:48:48
File Name	C:\Users\ytayam\Documents\Results for Publication\Nakanome\Nakanome\data\product\44387\44387_13C	Frequency (MHz)	100.62		
Nucleus	13C	Number of Transients	1024	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (Hz)	24038.46	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Spectrum Offset (Hz)	24037.73	Temperature (degree C)	25.828	Spectrum Offset (Hz)	10058.4180

2S,1'S-5bb_13C.esp

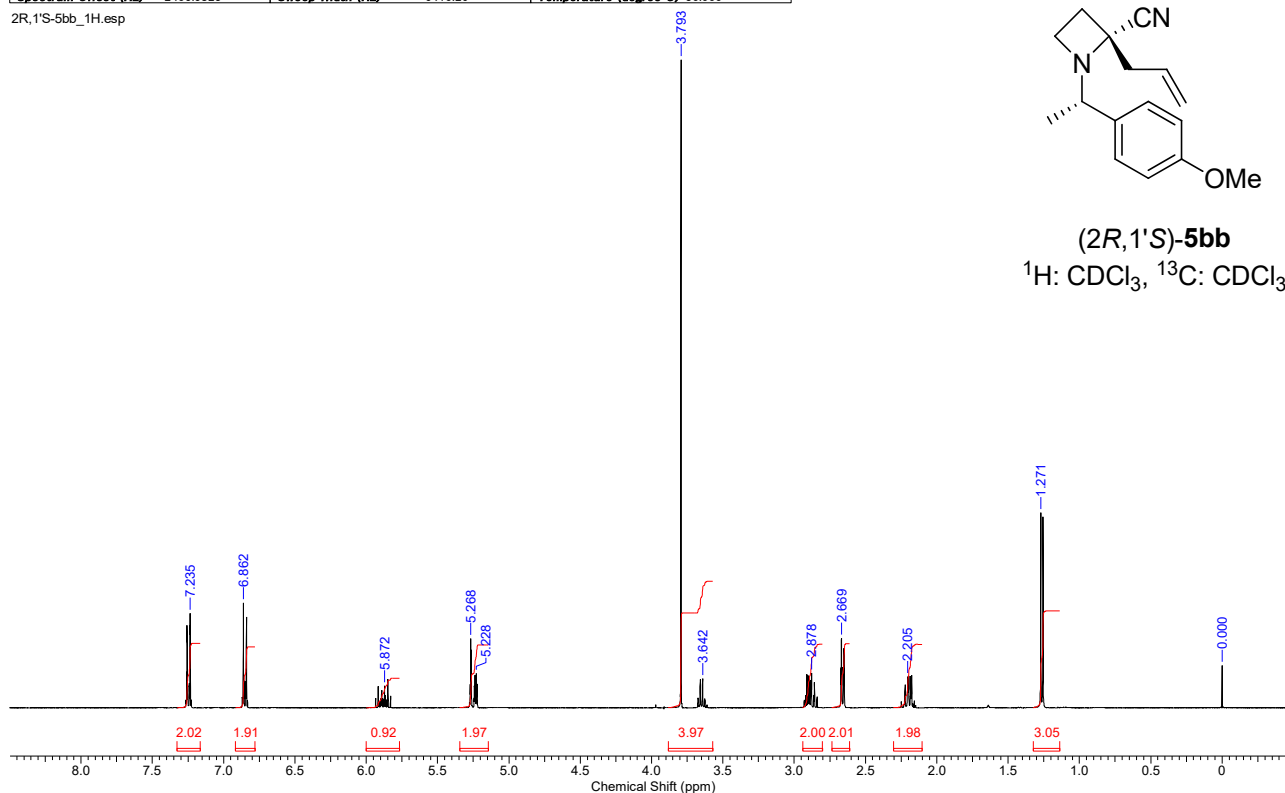


Acquisition Time (sec)	3.5000	Comment	STANDARD 1H OBSERVE - profile	Date	Oct 29 2020
Date Stamp	Oct 29 2020	File Name	C:\Users\ytayam\Documents\Results for Publication\Nakanome\Nakanome\data\product\4397		
Frequency (MHz)	399.83	Nucleus	1H	Number of Transients	16
Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	36.00
Spectrum Offset (Hz)	2405.5823	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000
				Solvent	CHLOROFORM-d

2R,1'S-5bb_1H.esp

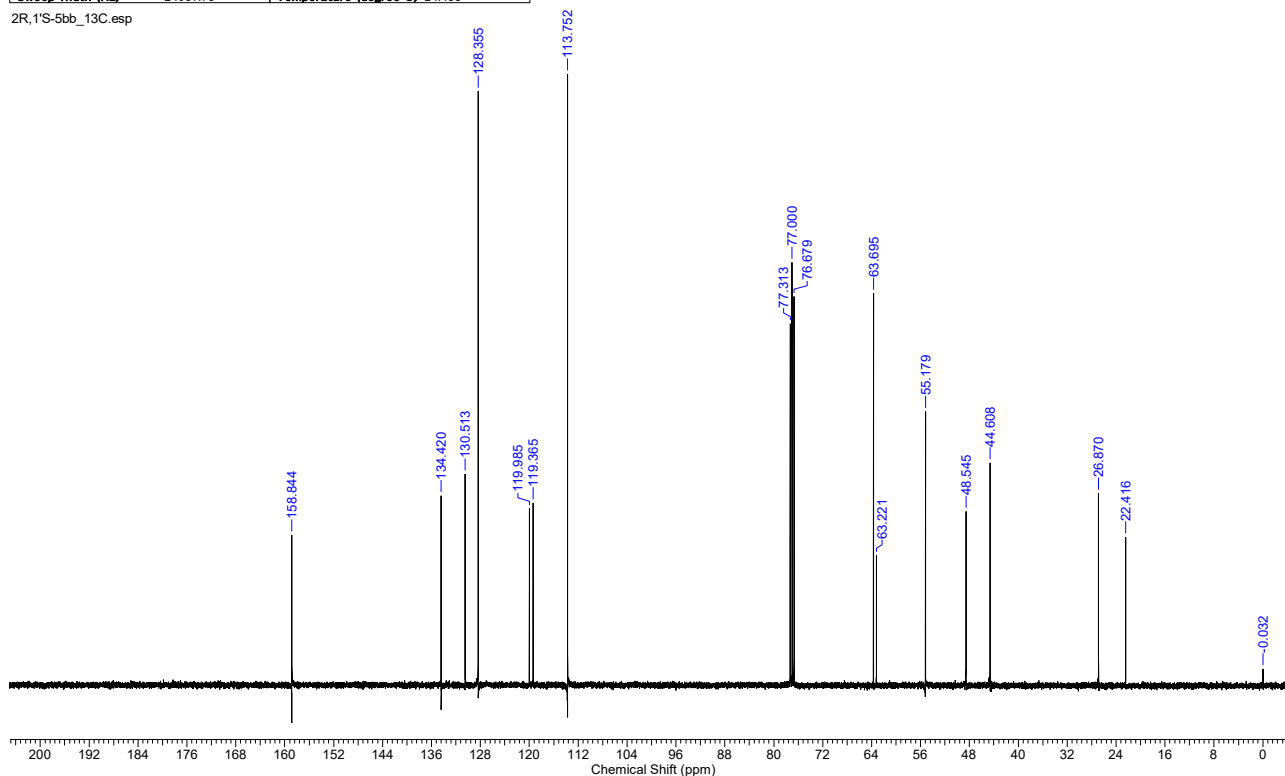


(2R,1'S)-5bb
¹H: CDCl₃, ¹³C: CDCl₃



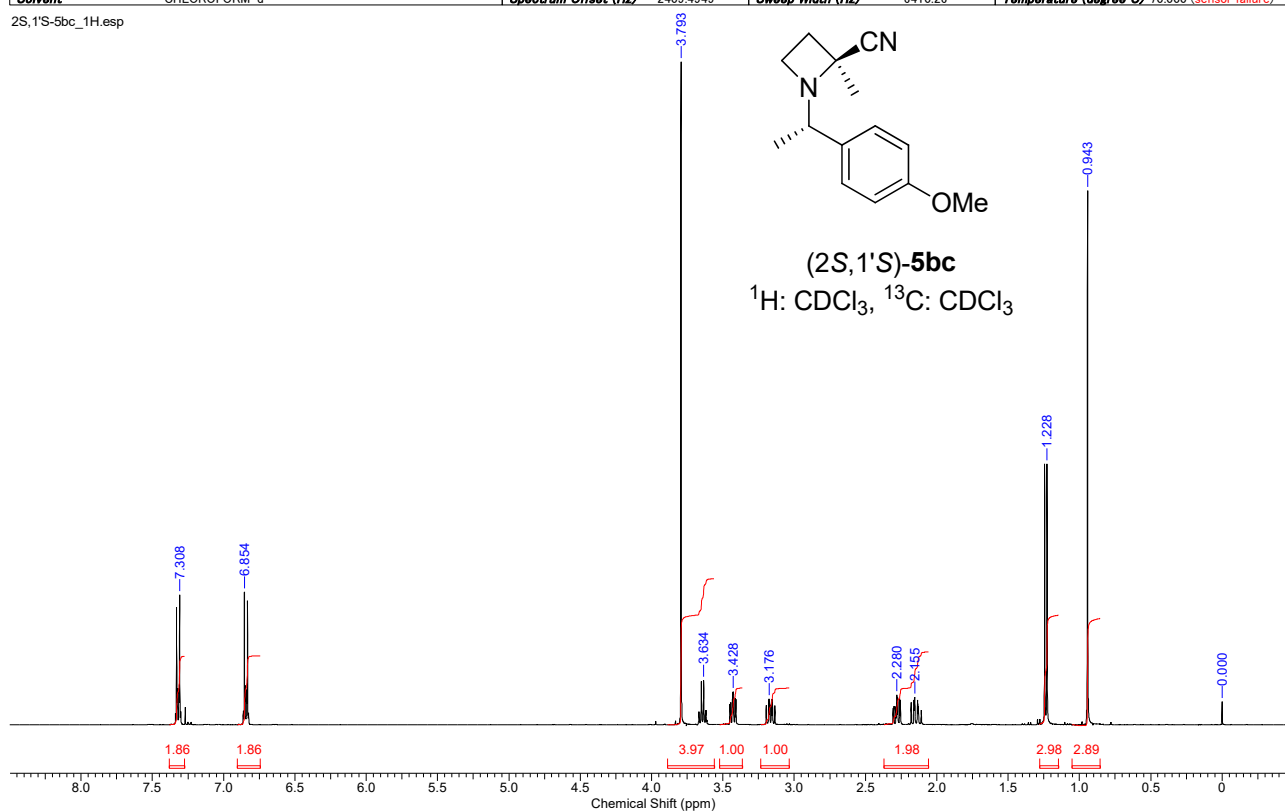
Acquisition Time (sec)	1.3631	Date	29 Oct 2020 13:00:48	Date Stamp	29 Oct 2020 13:00:48
File Name	C:\Users\ytayam\Documents\Results for Publication\Nakanome\Nakanome\data\product\4290\4290_010000fid	Frequency (MHz)	100.62		
Nucleus	13C	Number of Transients	1024	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (Hz)	24038.46	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	24037.73	Temperature (degree C)	24.488	Spectrum Offset (Hz)	10055.4834

2R,1'S-5bb_13C.esp



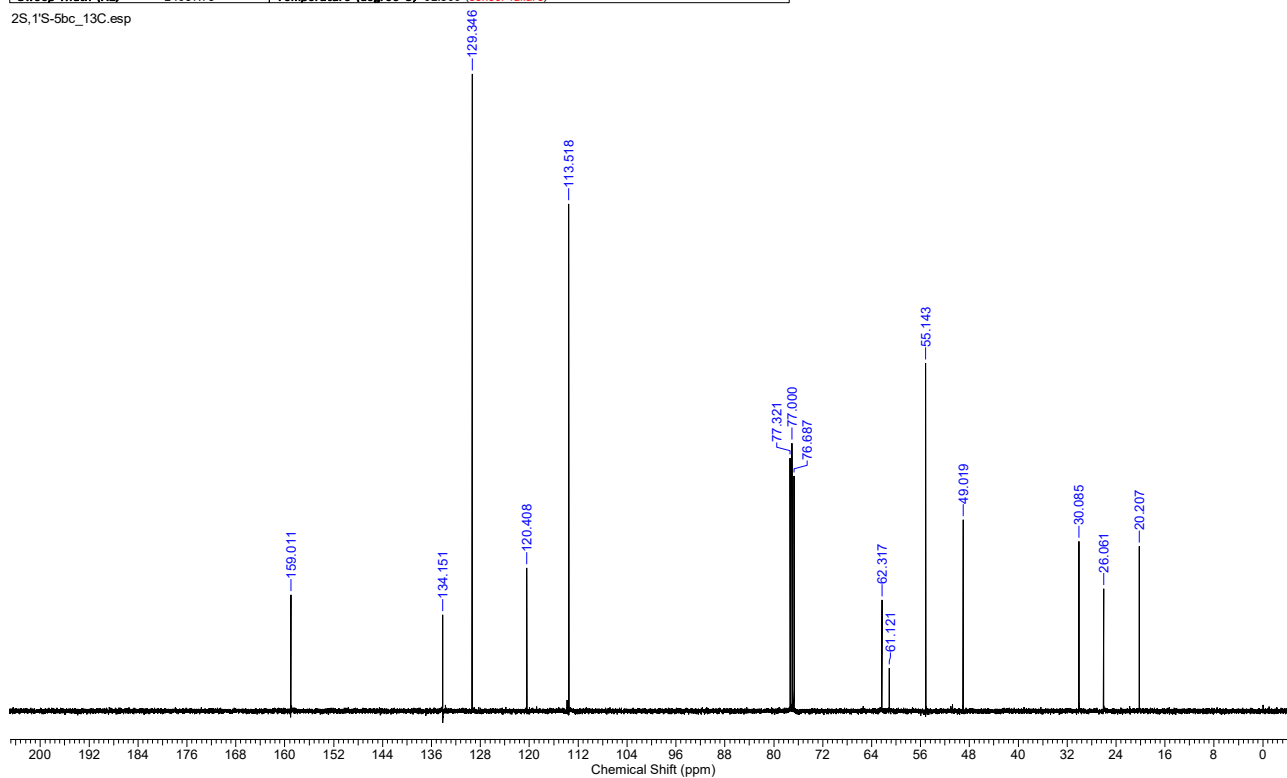
Acquisition Time (sec)	3.5000	Comment	Z0 19875	Date	Jan 12 2021	Date Stamp	Jan 12 2021
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\Y4454					Frequency (MHz)	399.83
Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2409.4949	Sweep Width (Hz)	6410.26
						Temperature (degree C)	70.000 (sensor failure)

2S,1'S-5bc_1H.esp



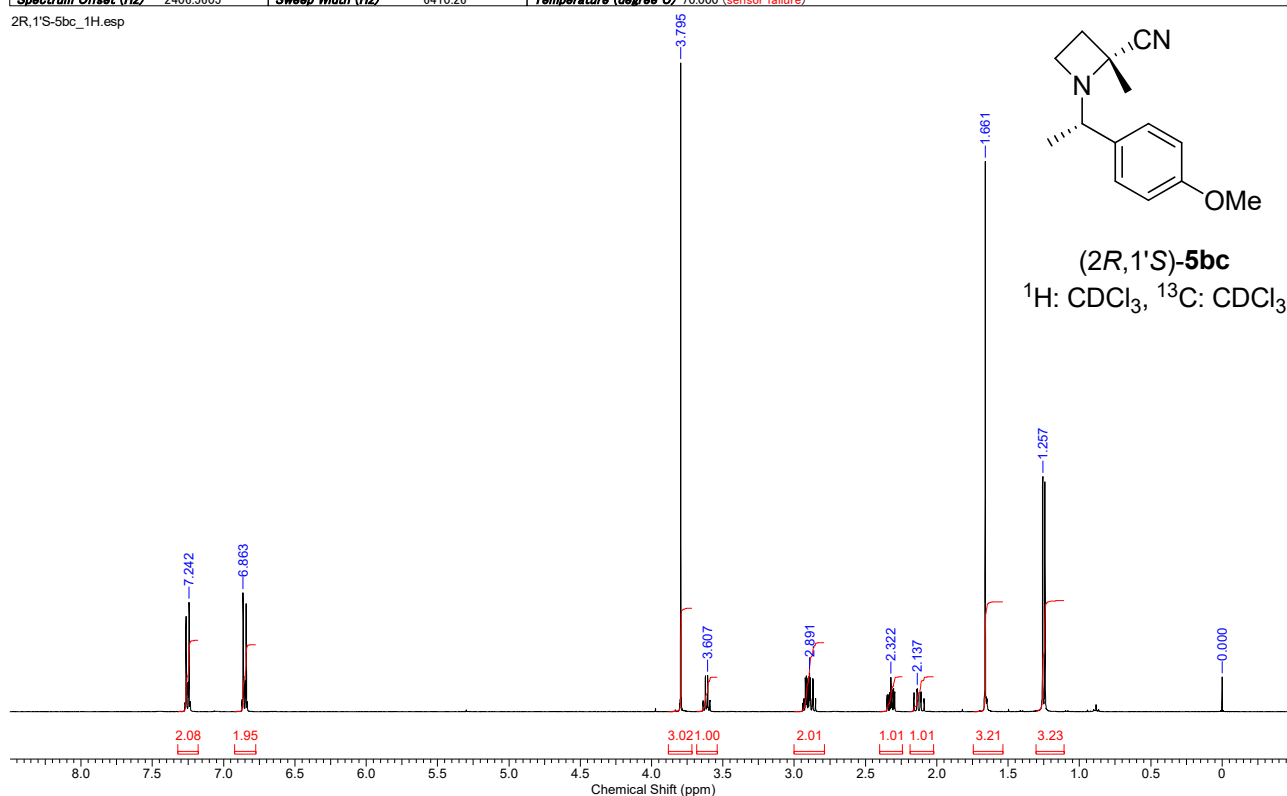
Acquisition Time (sec)	1.3631	Date	12 Jan 2021 05:49:52	Date Stamp	12 Jan 2021 05:49:52
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\Yn4306\Yn4306_010000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	512	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (Hz)	24038.46	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	24037.73	Temperature (degree C)	52.860 (sensor failure)	Spectrum Offset (Hz)	10054.0166

2S,1'S-5bc_13C.esp



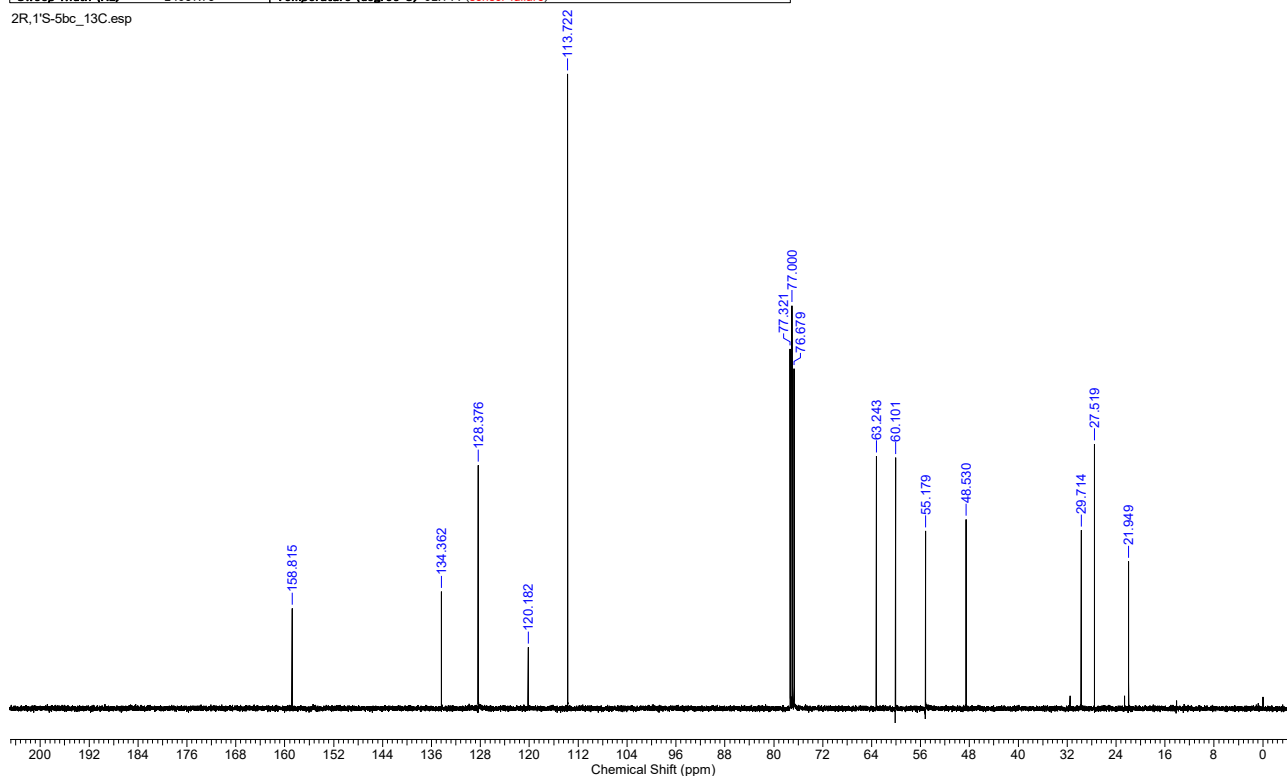
Acquisition Time (sec)	3.5000	Comment	STANDARD FLUORINE PARAMETERS			Date	Jan 27 2021
Date Stamp	Jan 27 2021	File Name	C:\Users\stavam\Documents\Results for Publication\Nakanome\Data\product\4474				
Frequency (MHz)	399.83	Nucleus	¹ H	Number of Transients	16	Original Points Count	22436
Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	38.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2406.5605	Sweep Width (Hz)	6410.26	Temperature (degree C)	70.000 (sensor failure)		

2R,1'S-5bc_1H.esp



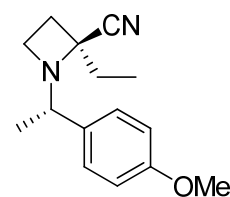
Acquisition Time (sec)	1.3631	Date	27 Jan 2021 06:49:36	Date Stamp	27 Jan 2021 06:49:36
File Name	C:\Users\stavam\Documents\Results for Publication\Nakanome\Data\product\4474\4308_010000fid			Frequency (MHz)	100.62
Nucleus	¹³ C	Number of Transients	1024	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (Hz)	24038.46	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	24037.73	Temperature (degree C)	52.144 (sensor failure)	Spectrum Offset (Hz)	10054.7500

2R,1'S-5bc_13C.esp

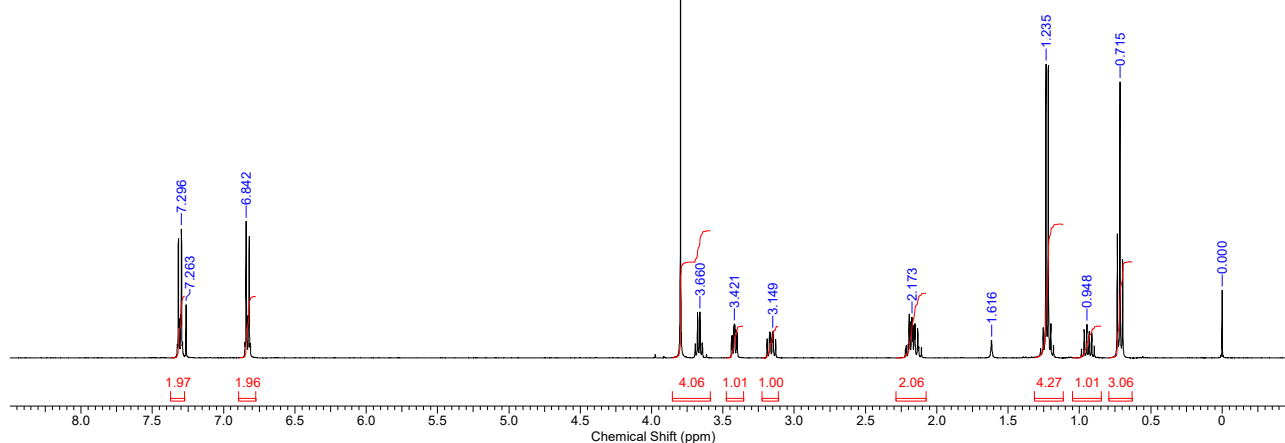


Acquisition Time (sec)	3.5000	Date	Oct 16 2020	Date Stamp	Oct 16 2020	Frequency (MHz)	399.83	Nucleus	¹ H
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\4362	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	42.00
Number of Transients	16	Spectrum Offset (Hz)	2407.3430	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000		
Solvent	CHLOROFORM-d								

2S,1'S-5bd_1H.esp

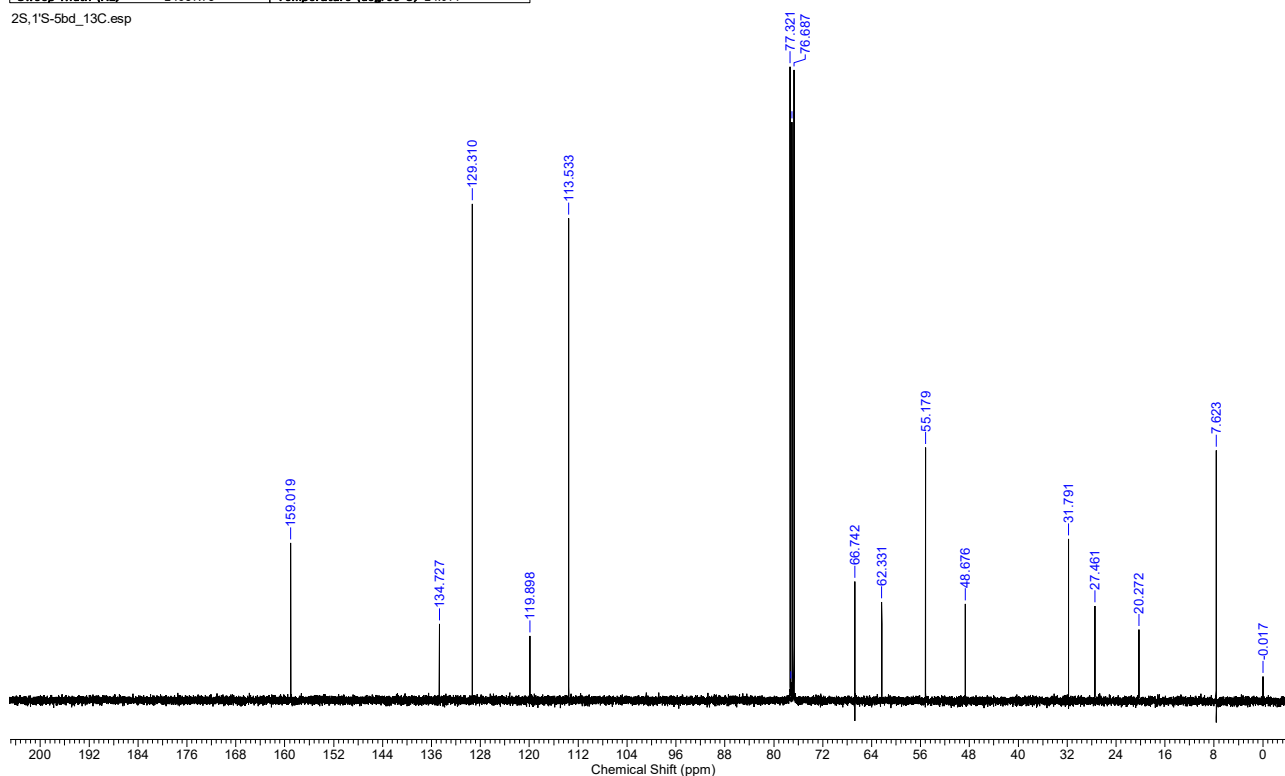


(2S,1'S)-5bd
¹H: CDCl₃, ¹³C: CDCl₃



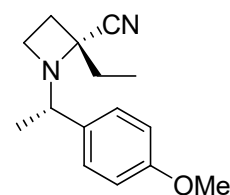
Acquisition Time (sec)	1.3631	Date	19 Oct 2020 06:00:32	Date Stamp	19 Oct 2020 06:00:32	Frequency (MHz)	100.62
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\4287\4287_010000fid	Number of Transients	1024	Origin	spect	Original Points Count	32768
Nucleus	¹³ C	Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	199.87
Owner	BrukerNMR	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10058.4180		
SW (vocal) (Hz)	24038.46	Temperature (degree C)	24.977				
Sweep Width (Hz)	24037.73						

2S,1'S-5bd_13C.esp

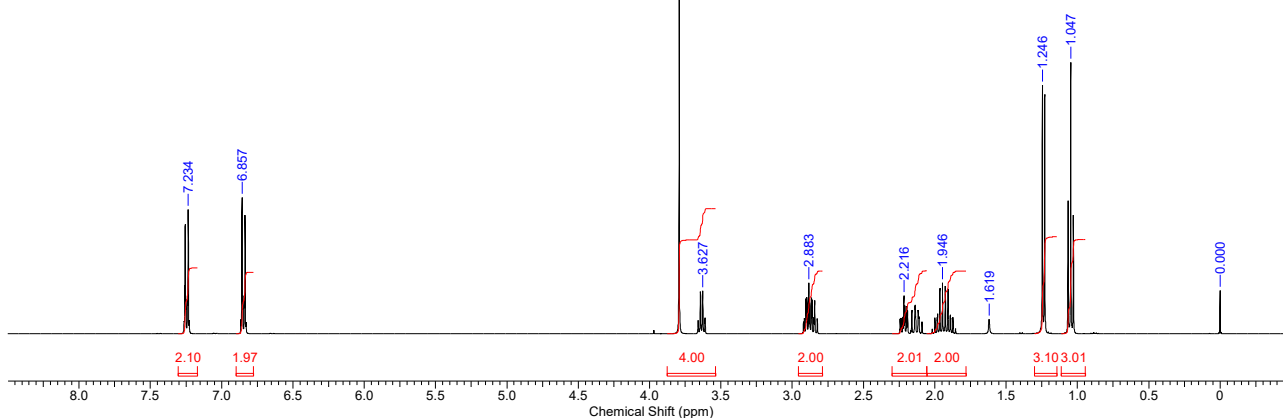


Acquisition Time (sec)	4.0894	Date	10 Oct 2020 03:05:36	Date Stamp	10 Oct 2020 03:05:36
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\4284\4284_010000fid	Frequency (MHz)	400.13	Nucleus	¹ H
Number of Transients	16	Origin	spect	Original Points Count	32768
Pulse Sequence	zg30	Receiver Gain	59.80	SW (cycles)	8012.82
Spectrum Offset (Hz)	2461.0232	Sweep Width (Hz)	8012.58	Temperature (degree C)	26.018
				Solvent	CHLOROFORM-d

2R,1'S-5bd_1H.esp

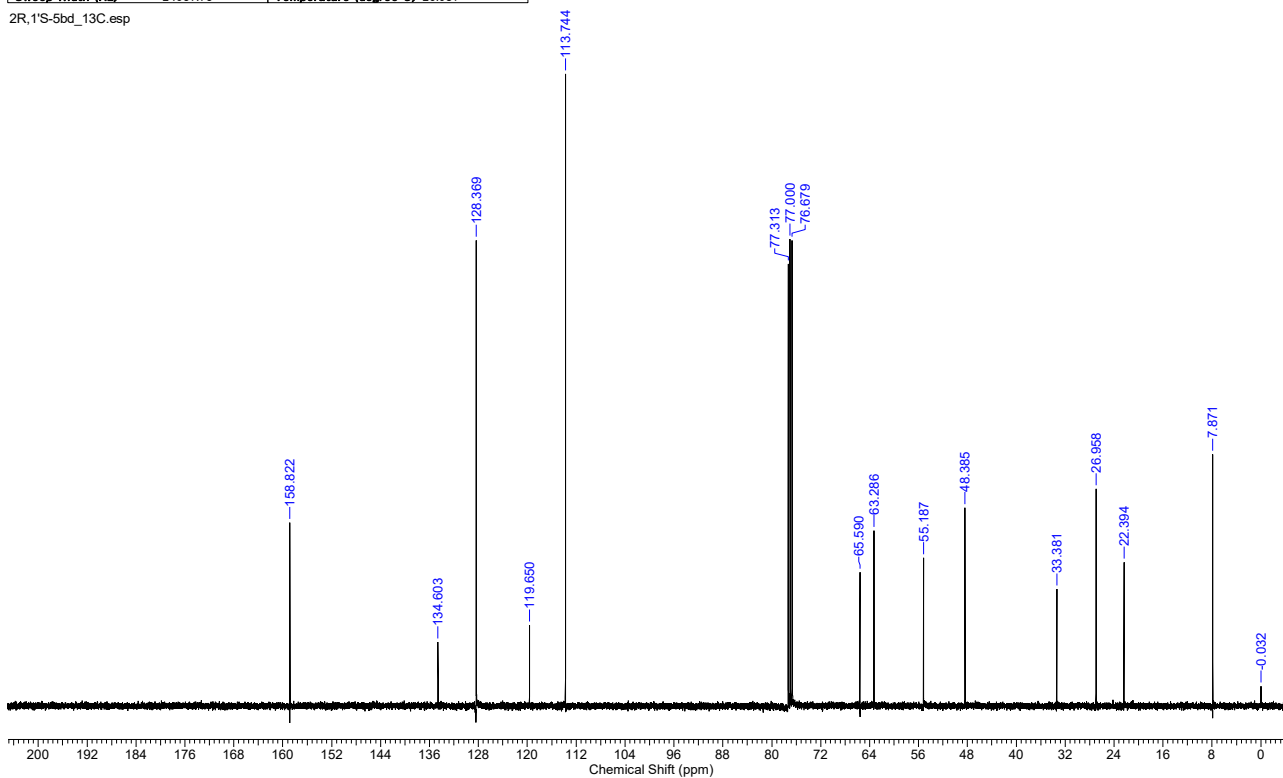


(2R,1'S)-5bd
¹H: CDCl₃, ¹³C: CDCl₃



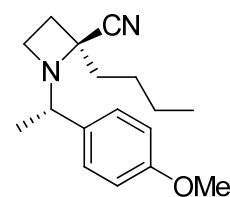
Acquisition Time (sec)	1.3631	Date	10 Oct 2020 04:05:20	Date Stamp	10 Oct 2020 04:05:20
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\4285\4285_010000fid	Frequency (MHz)	100.62	Nucleus	¹³ C
Nucleus	¹³ C	Number of Transients	1024	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (cycles)	24038.46	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	24037.73	Temperature (degree C)	25.987	Spectrum Offset (Hz)	10056.9502

2R,1'S-5bd_13C.esp

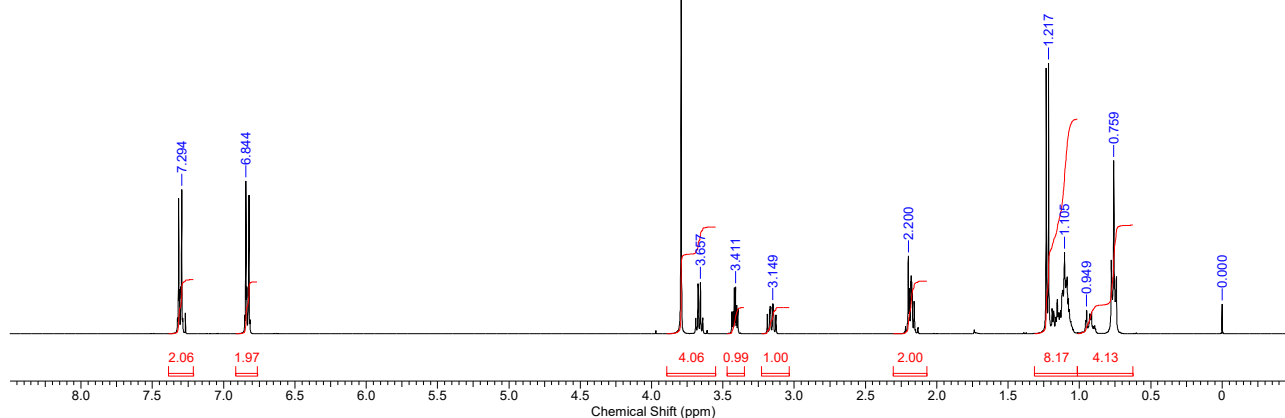


Acquisition Time (sec)	4.0894	Date	19 Dec 2020 04:13:52	Date Stamp	19 Dec 2020 04:13:52
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\N4303\N4303_010000fid	Frequency (MHz)	400.13	Nucleus	¹ H
Number of Transients	16	Origin	spect	Original Points Count	32768
Pulse Sequence	zg30	Receiver Gain	30.60	Points Count	32768
Spectrum Offset (Hz)	2464.1721	Sweep Width (Hz)	8012.58	Solvent	CHLOROFORM-d
		Temperature (degree C)	22.600		

2S,1'S-5be_1H.esp

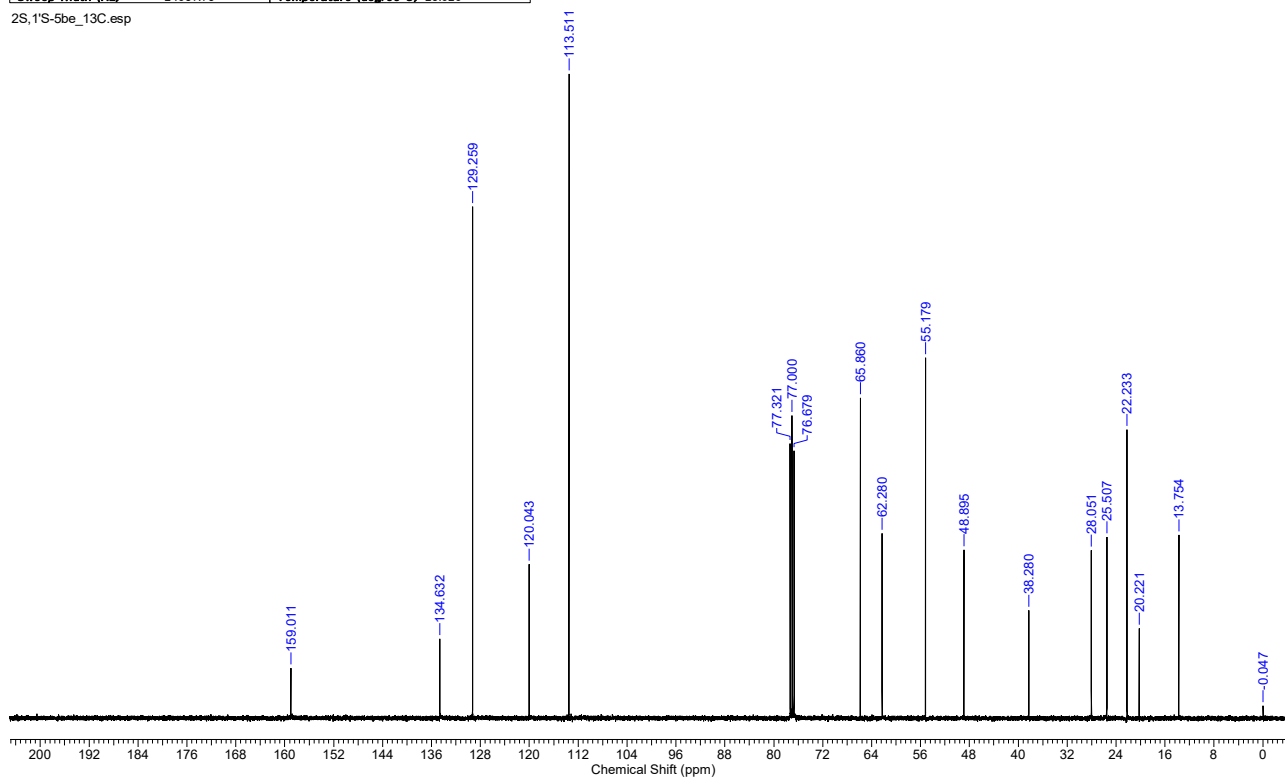


(2S,1'S)-5be
¹H: CDCl₃, ¹³C: CDCl₃



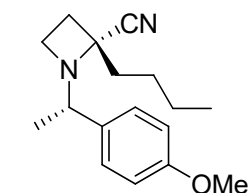
Acquisition Time (sec)	1.3631	Date	19 Dec 2020 05:34:56	Date Stamp	19 Dec 2020 05:34:56
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\N4305\N4305_010000fid	Frequency (MHz)	100.62	Nucleus	¹³ C
Nucleus	¹³ C	Number of Transients	1024	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (Hz)	24038.46	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	24037.73	Temperature (degree C)	23.020	Spectrum Offset (Hz)	10054.7500

2S,1'S-5be_13C.esp

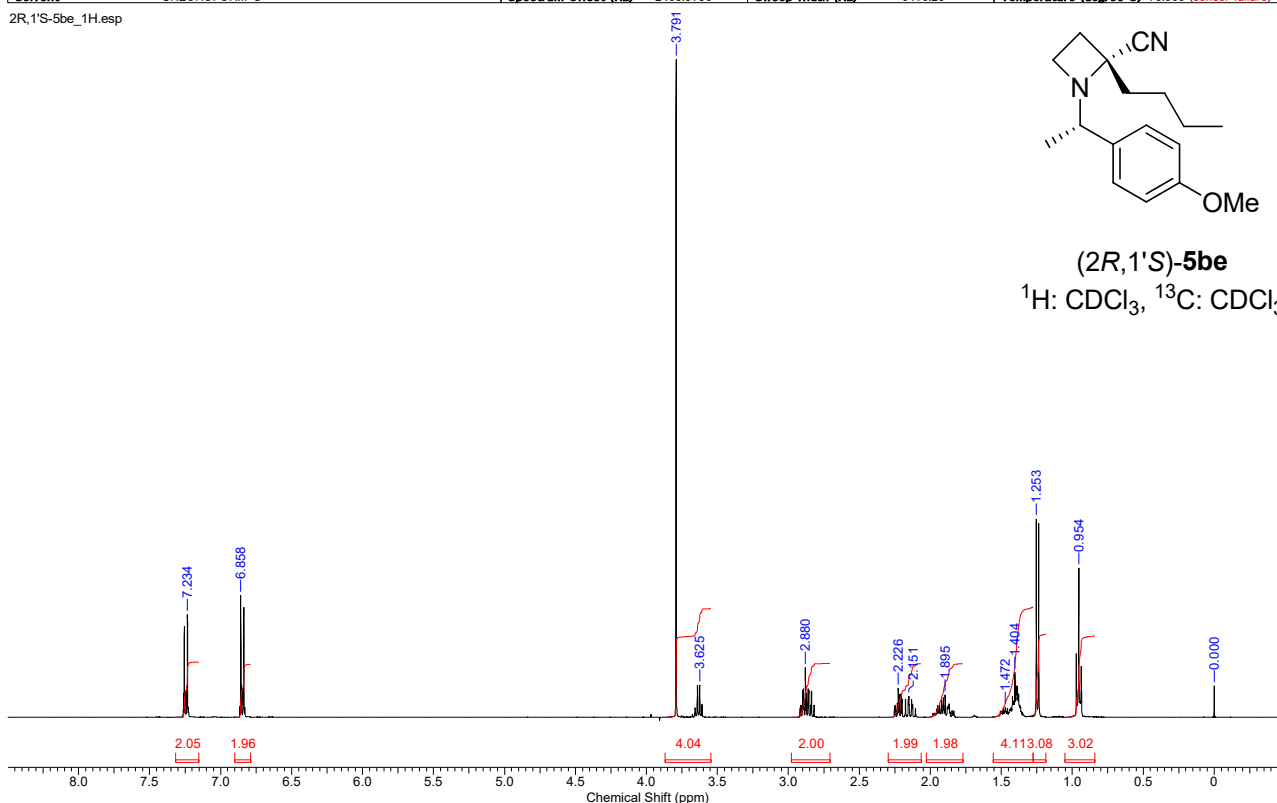


Acquisition Time (sec)	3.5000	Date	Jan 20 2021	Date Stamp	Jan 20 2021	Frequency (MHz)	399.83	Nucleus	¹ H
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\4459	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	32.00
Number of Transients	16	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2405.9736	Sweep Width (Hz)	6410.26	Temperature (degree C)	70.000 (sensor failure)

2R,1'S-5be_1H.esp

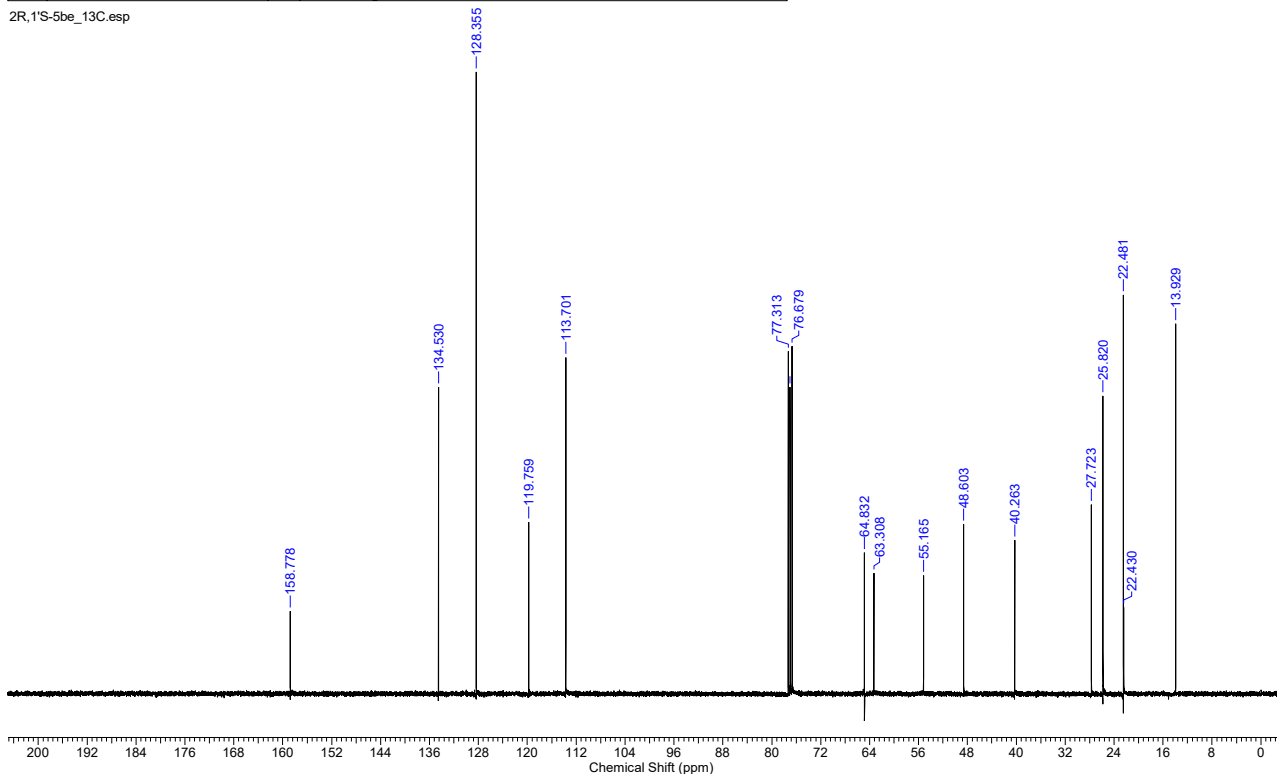


(2R,1'S)-5be
¹H: CDCl₃, ¹³C: CDCl₃



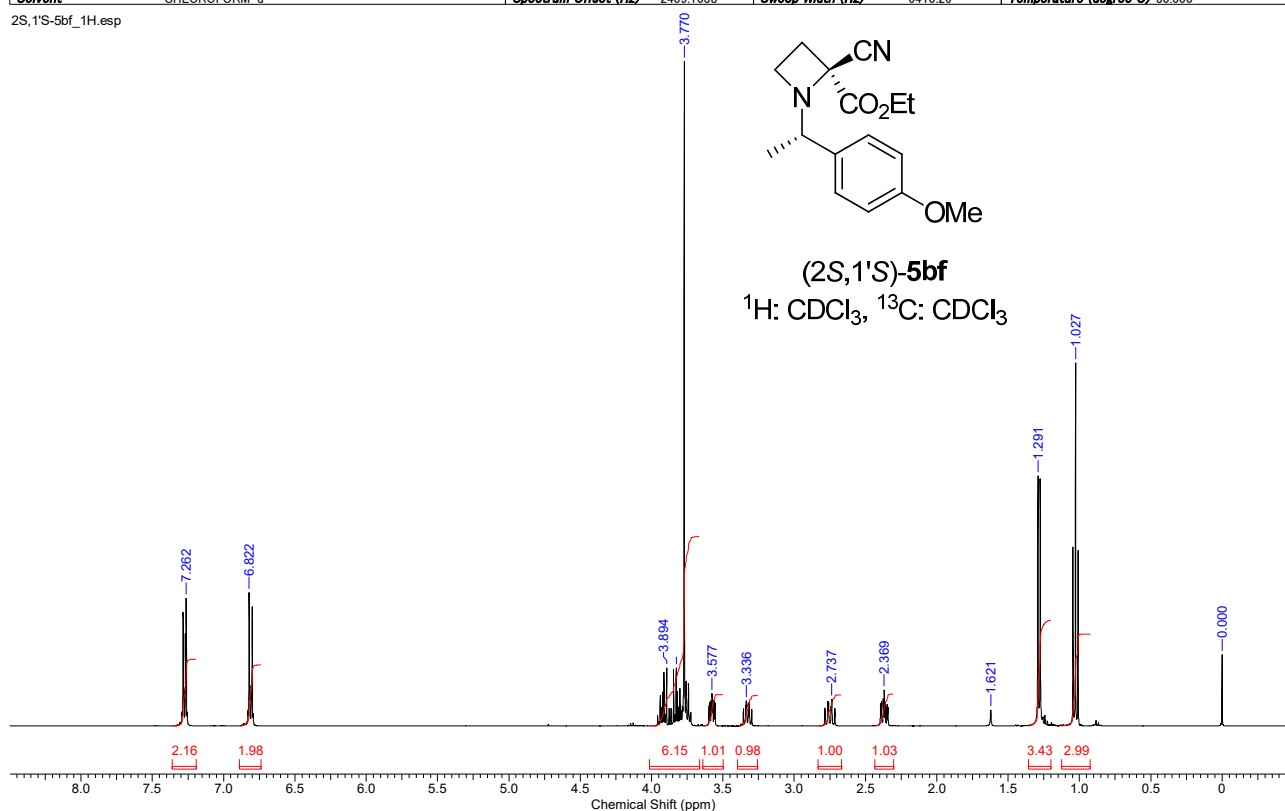
Acquisition Time (sec)	1.3631	Date	21 Jan 2021 08:10:40	Date Stamp	21 Jan 2021 08:10:40	Frequency (MHz)	100.62
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\4307\010000fid	Number of Transients	1024	Origin	spect	Original Points Count	32768
Nucleus	¹³ C	Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	199.87
Owner	BrukerNMR	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10054.0166	Temperature (degree C)	53.061 (sensor failure)
SW (Hz)	24038.46						
Sweep Width (Hz)	24037.73						

2R,1'S-5be_13C.esp



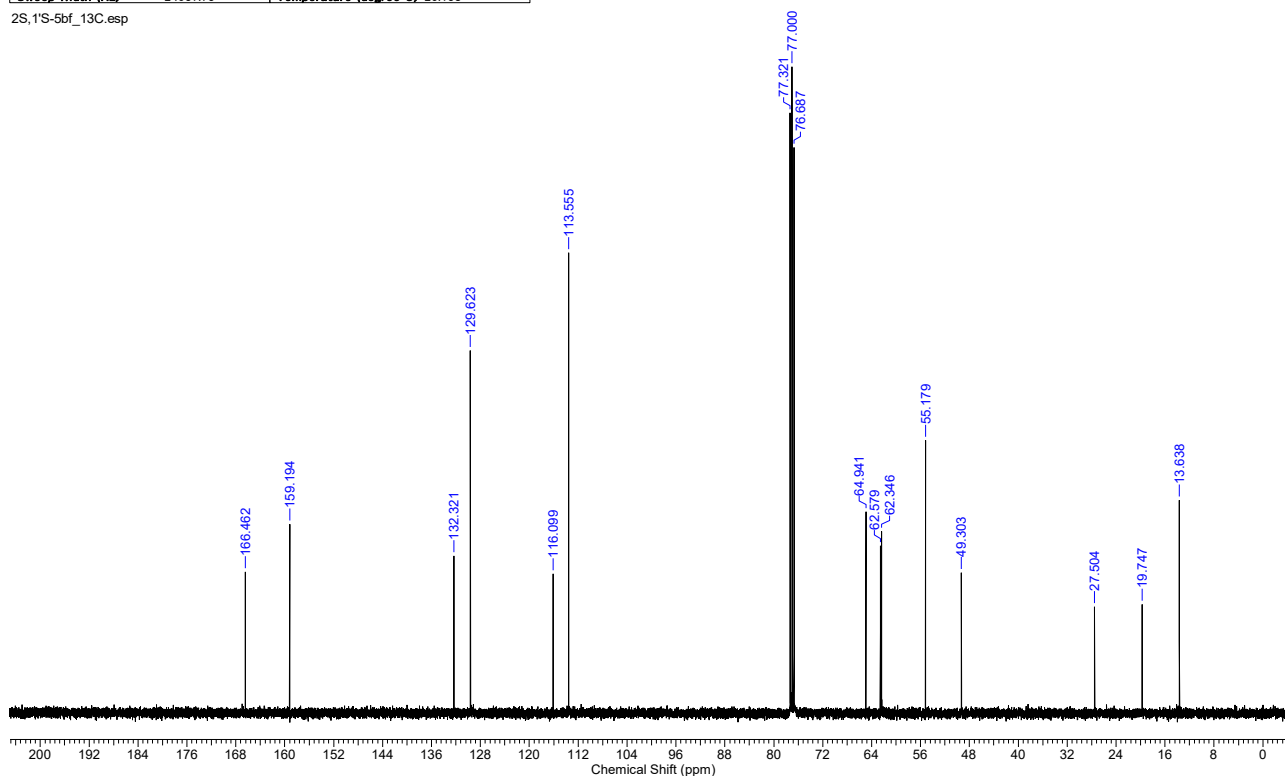
Acquisition Time (sec)	3.5000	Date	Oct 21 2020	Date Stamp	Oct 21 2020	Frequency (MHz)	399.83	Nucleus	¹ H
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\Y4374	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	42.00
Number of Transients	16	Spectrum Offset (Hz)	2409.1038	Sweep Width (Hz)	6410.26	Temperature (degree C)	30.000		
Solvent	CHLOROFORM-d								

2S,1'S-5bf_1H.esp



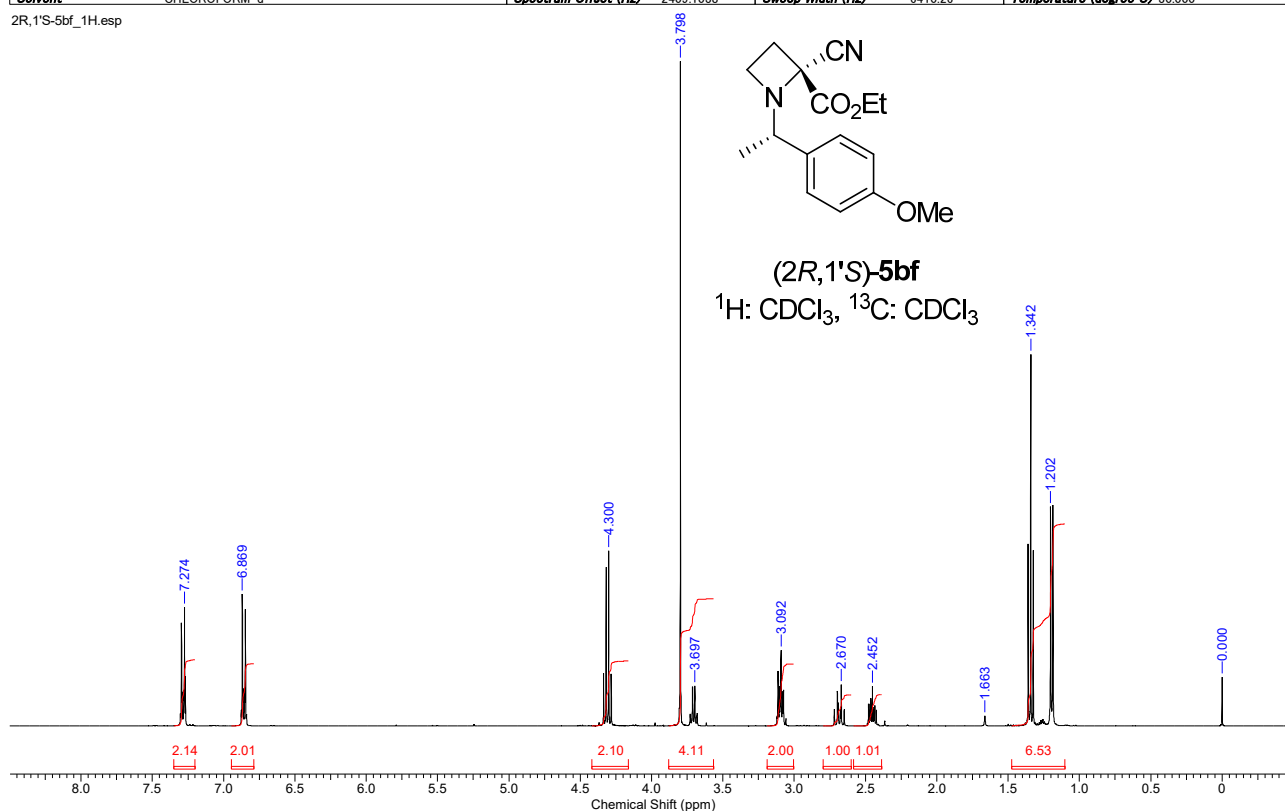
Acquisition Time (sec)	1.3631	Date	21 Oct 2020 09:33:52	Date Stamp	21 Oct 2020 09:33:52	Frequency (MHz)	100.62
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\Yn4288\Yn4288_010000fid	Number of Transients	1024	Origin	spect	Original Points Count	32768
Nucleus	¹³ C	Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	199.87
Owner	BrukerNMR	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10057.6836		
SW (vocal) (Hz)	24038.46	Temperature (degree C)	25.138				
Sweep Width (Hz)	24037.73						

2S,1'S-5bf_13C.esp



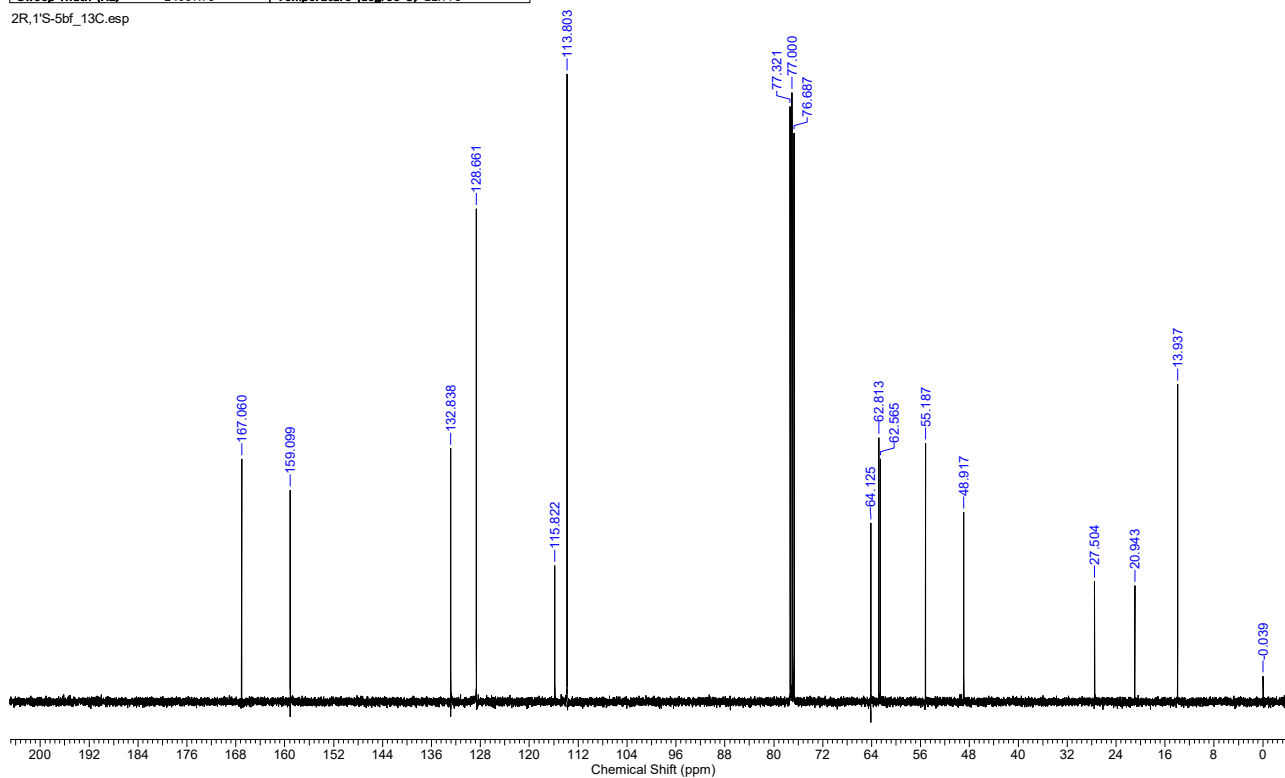
Acquisition Time (sec)	3.5000	Comment	N15 OBSERVE	Date	Nov 6 2020	Date Stamp	Nov 6 2020
File Name	C:\Users\stavam\Documents\Results for Publication\Nakanome\Data\product\Y4408					Frequency (MHz)	399.83
Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2409.1038	Sweep Width (Hz)	6410.26
						Receiver Gain	38.00
						Temperature (degree C)	30.000

2R,1'S-5bf_1H.esp



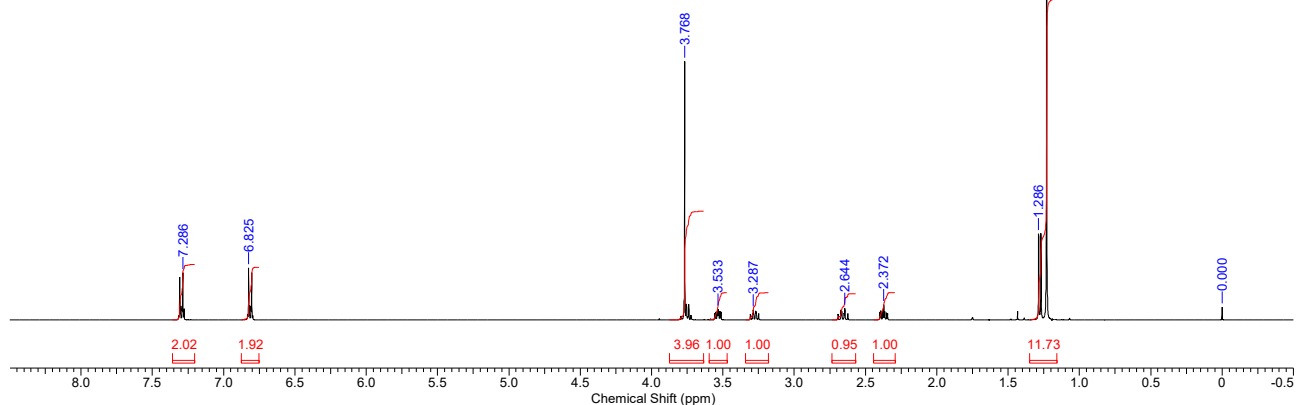
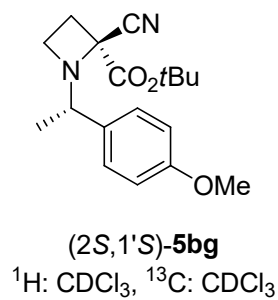
Acquisition Time (sec)	1.3631	Date	05 Nov 2020 17:48:48	Date Stamp	05 Nov 2020 17:48:48
File Name	C:\Users\stavam\Documents\Results for Publication\Nakanome\Data\product\Yn4291\Yn4291_010000fid			Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	1024	Origin	spect
Owner	BrukerNMR	Points Count	32768	Pulse Sequence	zgpg30
SW (Hz)	24038.46	Solvent	CHLOROFORM-d	Receiver Gain	199.87
Sweep Width (Hz)	24037.73	Temperature (degree C)	22.778	Spectrum Offset (Hz)	10055.4834

2R,1'S-5bf_13C.esp



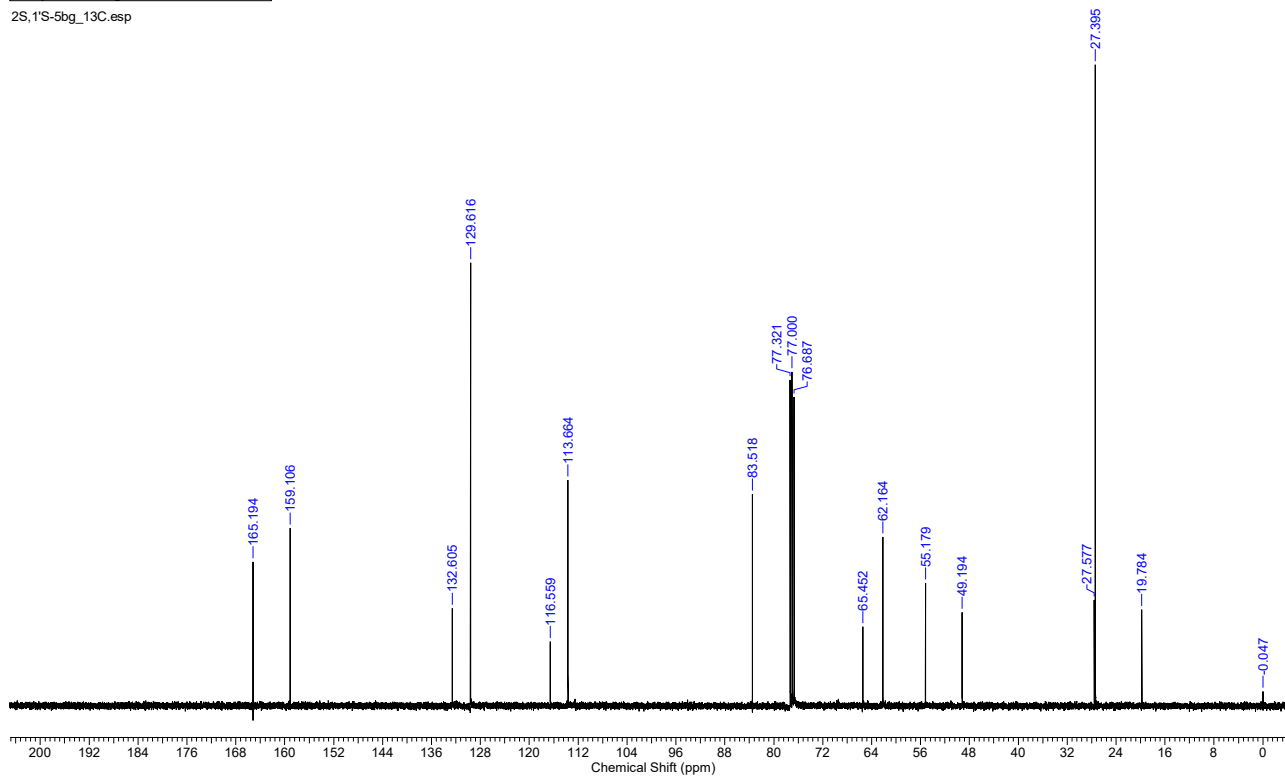
Acquisition Time (sec)	3.5000	Date	Feb 4 2021	Date Stamp	Feb 4 2021	Frequency (MHz)	399.83	Nucleus	¹ H
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\NMR\4487	Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2405.7781	Sweep Width (Hz)	6410.26	Temperature (degree C)	25.000	Receiver Gain	34.00

2S,1'S-5bg_1H.esp



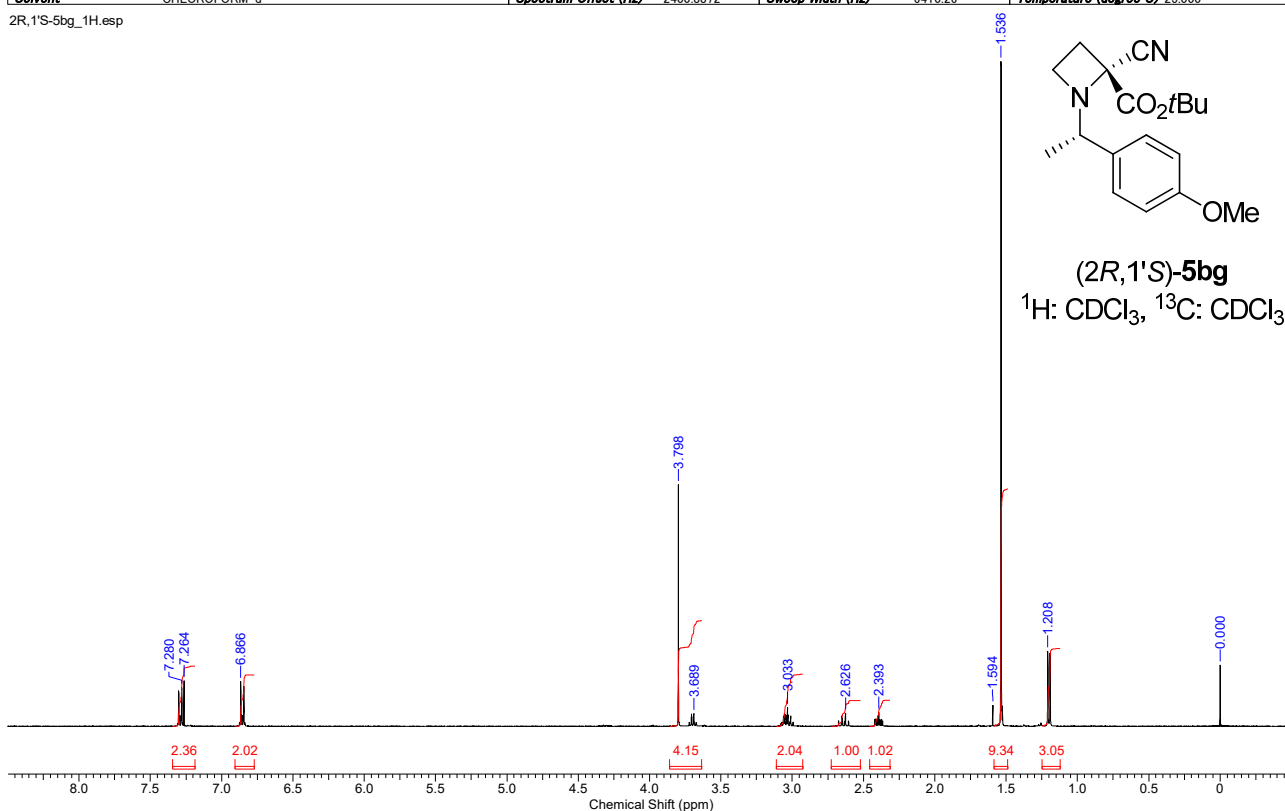
Acquisition Time (sec)	1.3631	Date	06 Feb 2021 02:31:28	Date Stamp	06 Feb 2021 02:31:28	Frequency (MHz)	100.62
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\NMR\4309\4309_010000fid	Number of Transients	512	Origin	spect	Original Points Count	32768
Nucleus	¹³ C	Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	199.87
Owner	BrukerNMR	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10054.7500	Sweep Width (Hz)	24037.73
SW (Hz)	24038.46	Temperature (degree C)	22.170				

2S,1'S-5bg_13C.esp



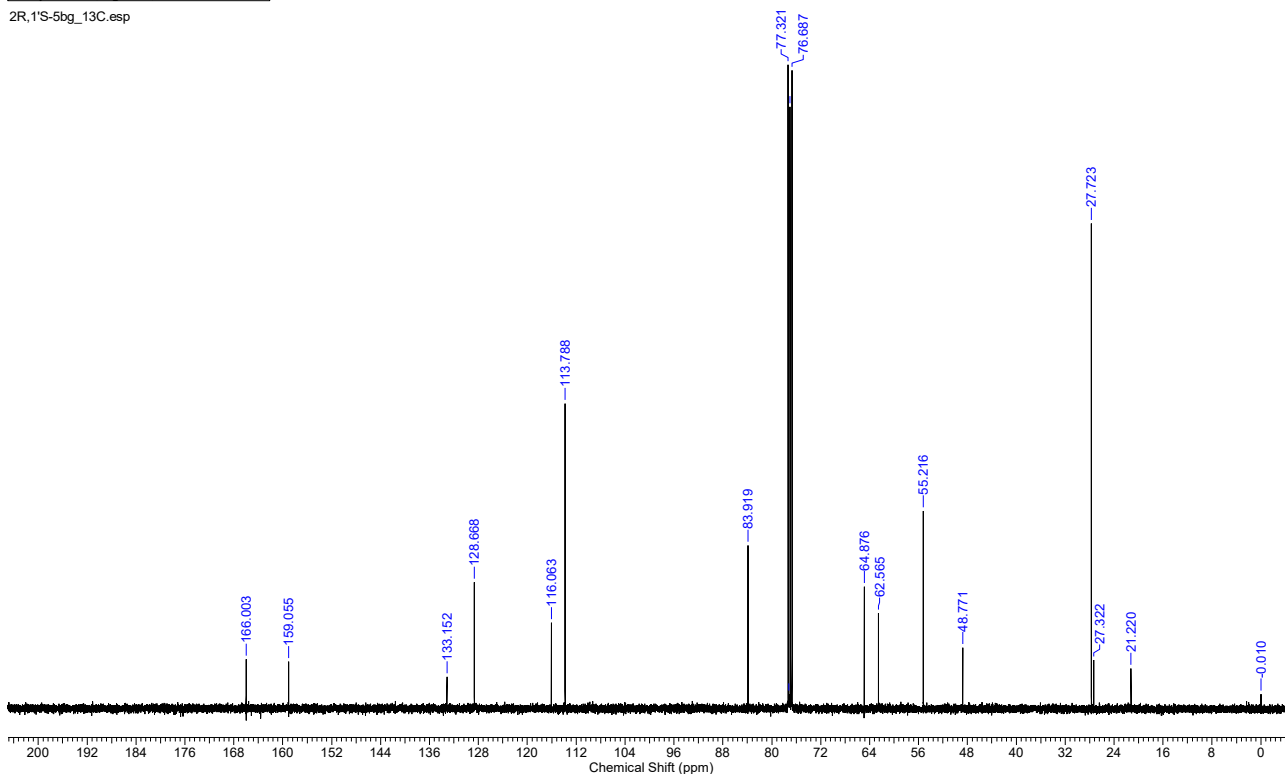
Acquisition Time (sec)	3.5000	Date	Feb 19 2021	Date Stamp	Feb 19 2021	Frequency (MHz)	399.83	Nucleus	¹ H
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\NMR\4506	Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2400.8872	Sweep Width (Hz)	6410.26	Temperature (degree C)	25.000	Receiver Gain	44.00

2R,1'S-5bg_1H.esp



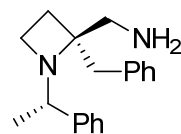
Acquisition Time (sec)	1.3631	Date	19 Feb 2021 04:43:44	Date Stamp	19 Feb 2021 04:43:44	Frequency (MHz)	100.62
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\product\NMR\4313\4313_010000fid	Number of Transients	1024	Origin	spect	Original Points Count	32768
Nucleus	¹³ C	Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	199.87
Owner	BrukerNMR	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10057.6836	Sweep Width (Hz)	24037.73
SW (vocal) (Hz)	24038.46	Temperature (degree C)	21.969				

2R,1'S-5bg_13C.esp

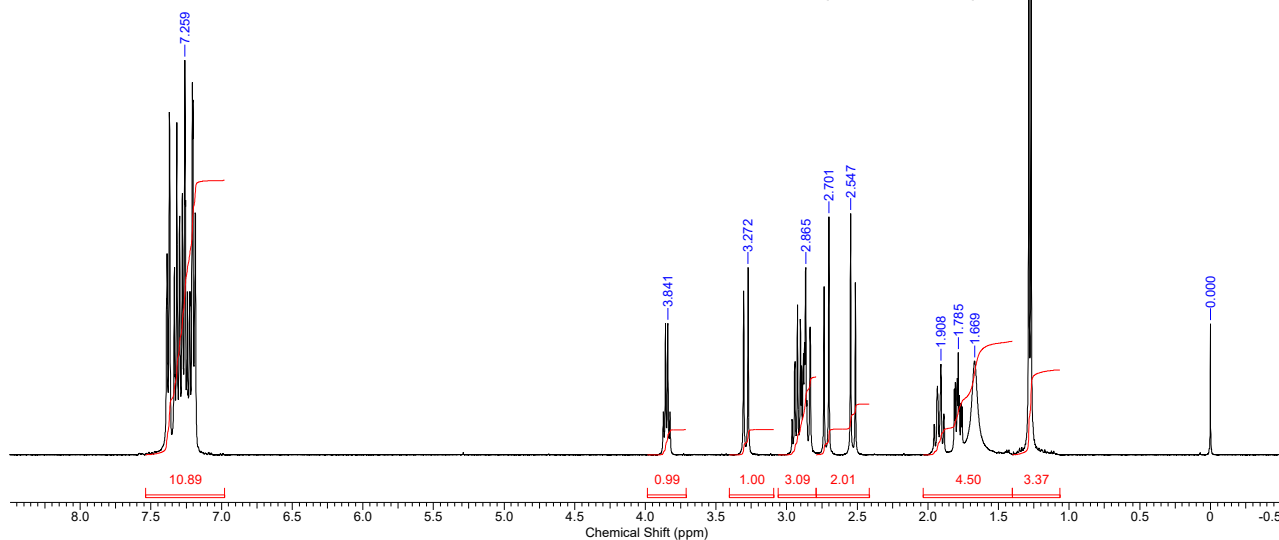


Acquisition Time (sec)	3.5000	Date	Jan 21 2021	Date Stamp	Jan 21 2021	Frequency (MHz)	399.83	Nucleus	¹ H
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\stereochem\43815	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	38.00
Number of Transients	16	Spectrum Offset (Hz)	2403.8218	Sweep Width (Hz)	6410.26	Temperature (degree C)	70.000 (sensor failure)		
Solvent	CHLOROFORM-d								

2S,1'S-6aa_1H.esp

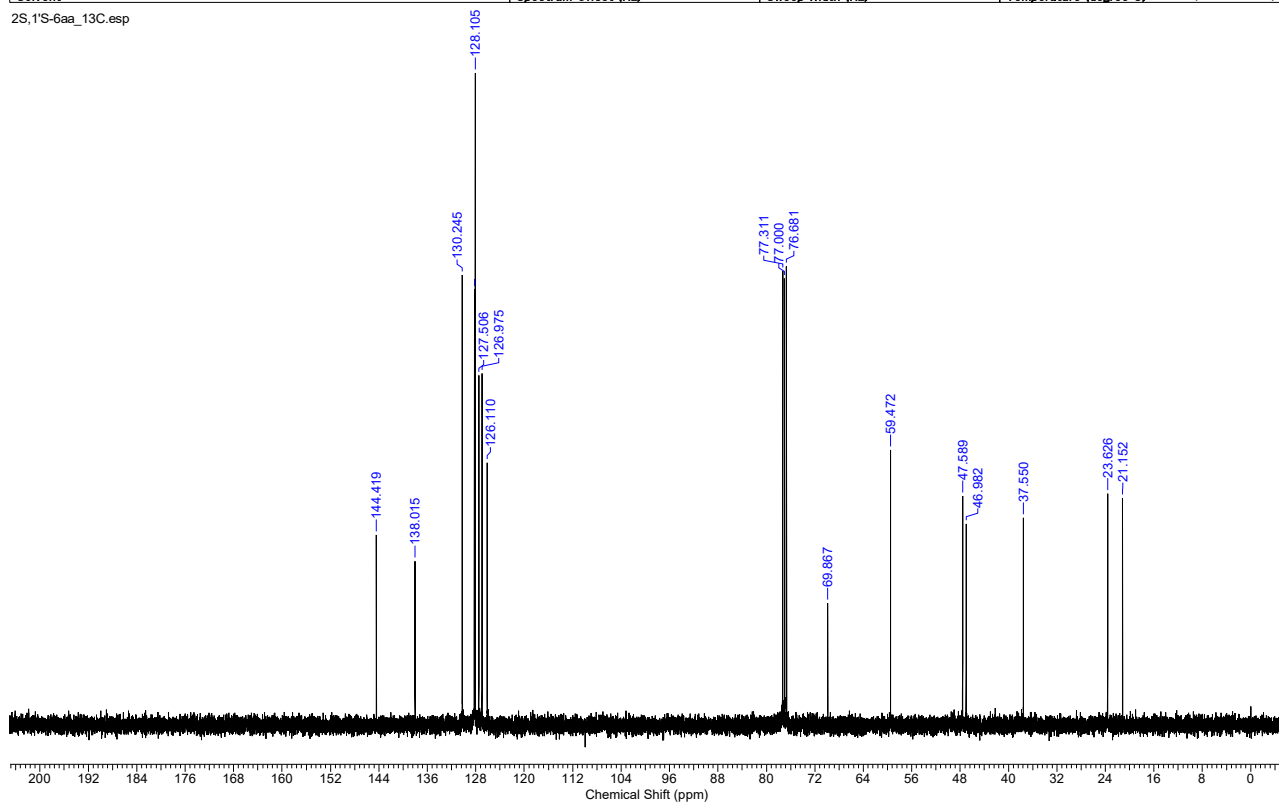


(2S,1'S)-6aa
¹H: CDCl₃, ¹³C: CDCl₃



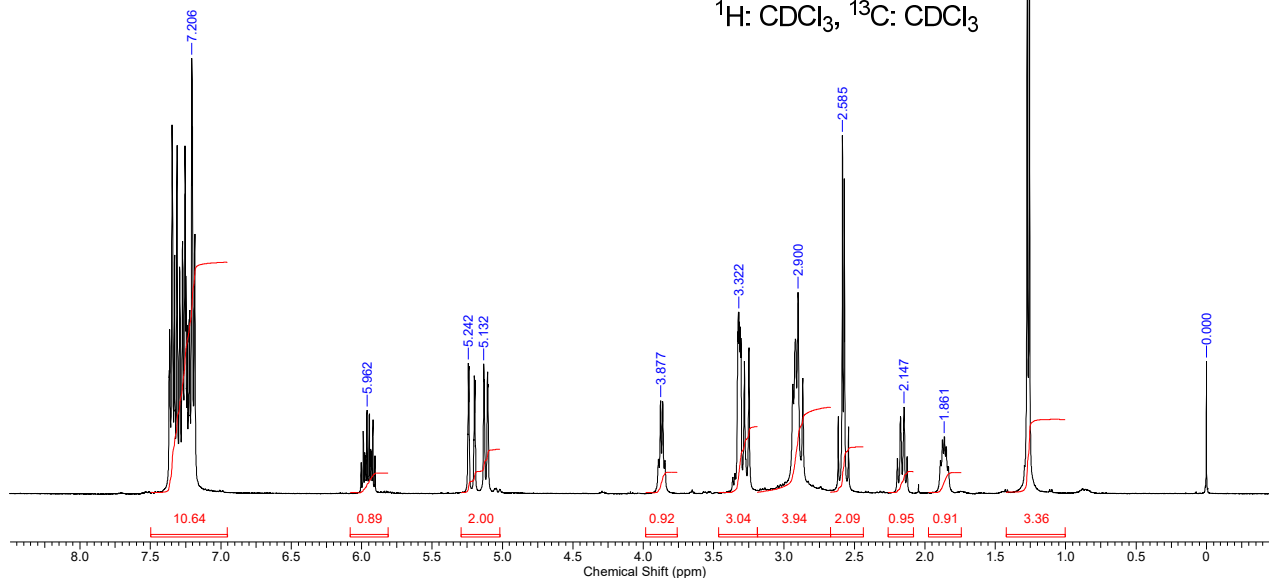
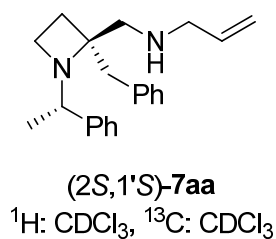
Acquisition Time (sec)	1.3107	Date	Jan 21 2021	Date Stamp	Jan 21 2021	Frequency (MHz)	100.55	Nucleus	¹³ C
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\stereochem\43816	Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	60.00
Number of Transients	512	Spectrum Offset (Hz)	11056.1699	Sweep Width (Hz)	25000.00	Temperature (degree C)	70.000 (sensor failure)		
Solvent	CHLOROFORM-d								

2S,1'S-6aa_13C.esp



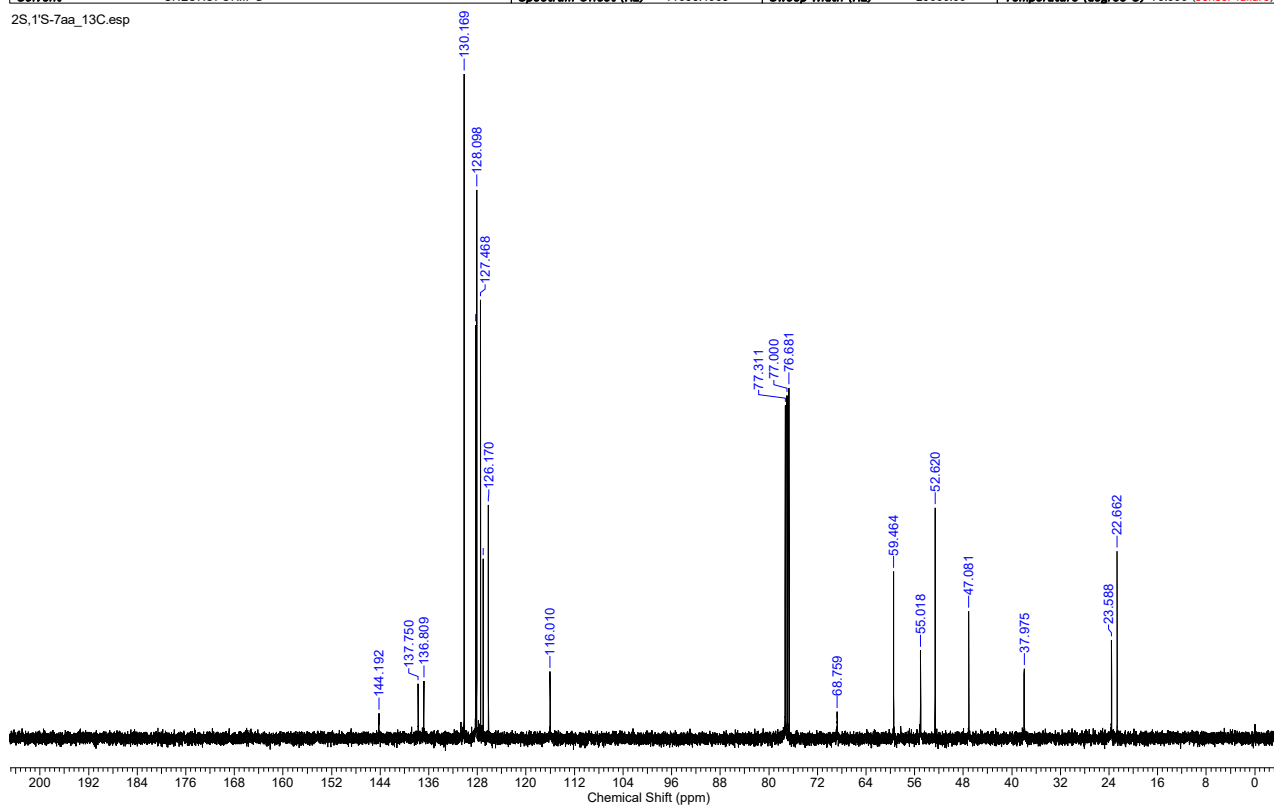
Acquisition Time (sec)	3.5000	Date	Jan 25 2021	Date Stamp	Jan 25 2021				
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\stereochem\43827					Frequency (MHz)	399.83	Nucleus	¹ H
Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	36.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2401.0828	Sweep Width (Hz)	6410.26	Temperature (degree C)	70.000 (sensor failure)

2S,1'S-7aa_1H.esp



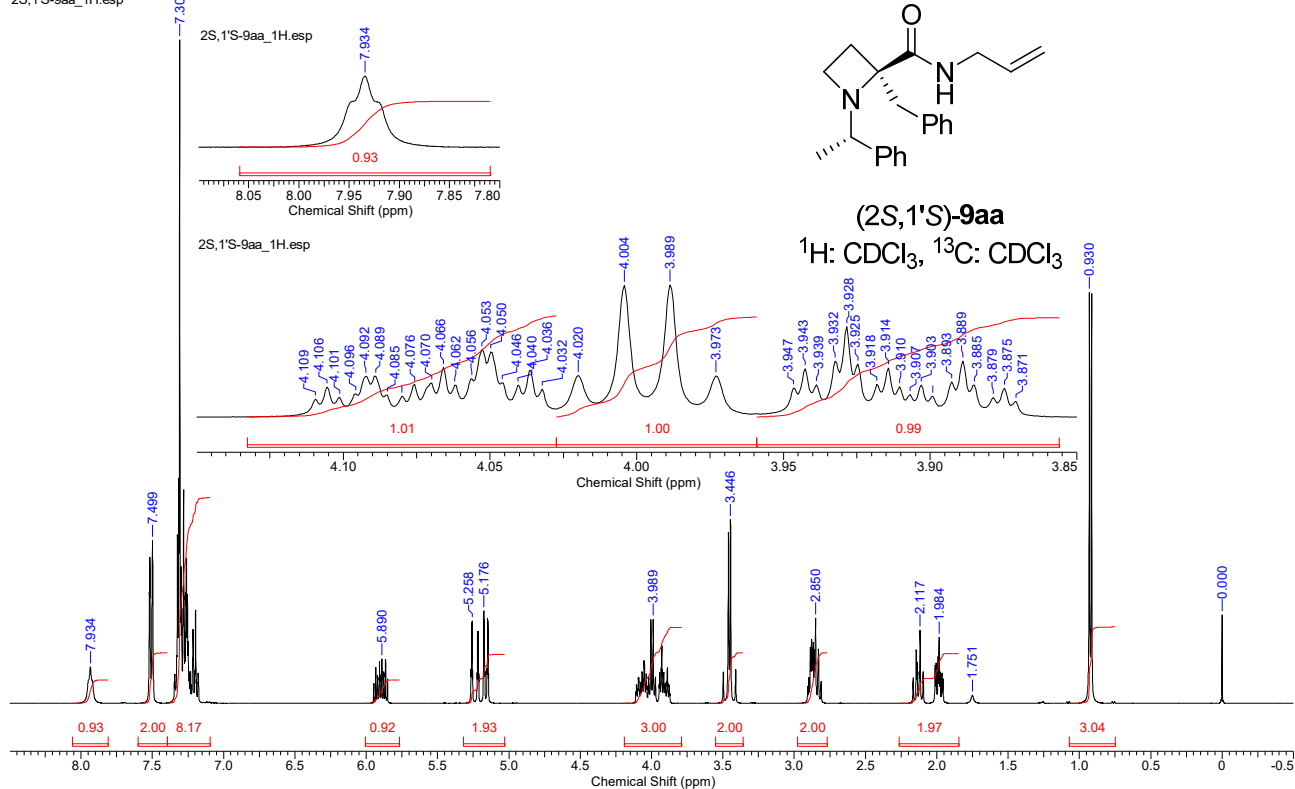
Acquisition Time (sec)	1.3107	Date	Jan 25 2021	Date Stamp	Jan 25 2021				
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\stereochem\43828					Frequency (MHz)	100.55	Nucleus	¹³ C
Number of Transients	512	Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	60.00
Solvent	CHLOROFORM-d		Spectrum Offset (Hz)		11055.4063	Sweep Width (Hz)	25000.00	Temperature (degree C)	70.000 (sensor failure)

2S,1'S-7aa_13C.esp



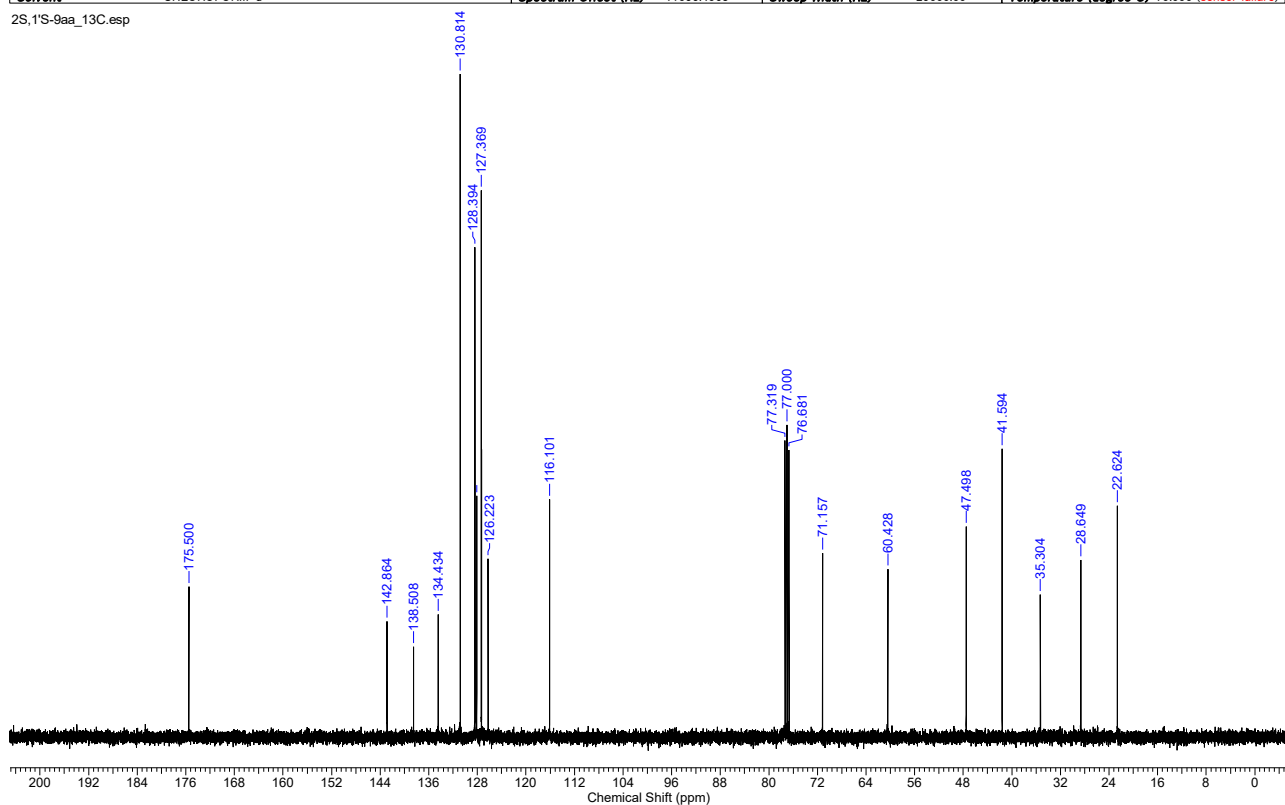
Acquisition Time (sec)	3.5000	Date	Jan 25 2021	Date Stamp	Jan 25 2021
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\stereochem\43825	Frequency (MHz)	399.83	Nucleus	¹ H
Number of Transients	16	Original Points Count	22436	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2403.2349	Sweep Width (Hz)	6410.26
				Receiver Gain	36.00
				Temperature (degree C)	70.000 (sensor failure)

2S,1'S-9aa_1H.esp



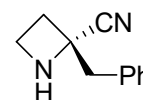
Acquisition Time (sec)	1.3107	Date	Jan 25 2021	Date Stamp	Jan 25 2021
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\stereochem\43826	Frequency (MHz)	100.55	Nucleus	¹³ C
Number of Transients	512	Original Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	11055.4063	Sweep Width (Hz)	25000.00
				Receiver Gain	60.00
				Temperature (degree C)	70.000 (sensor failure)

2S,1'S-9aa_13C.esp

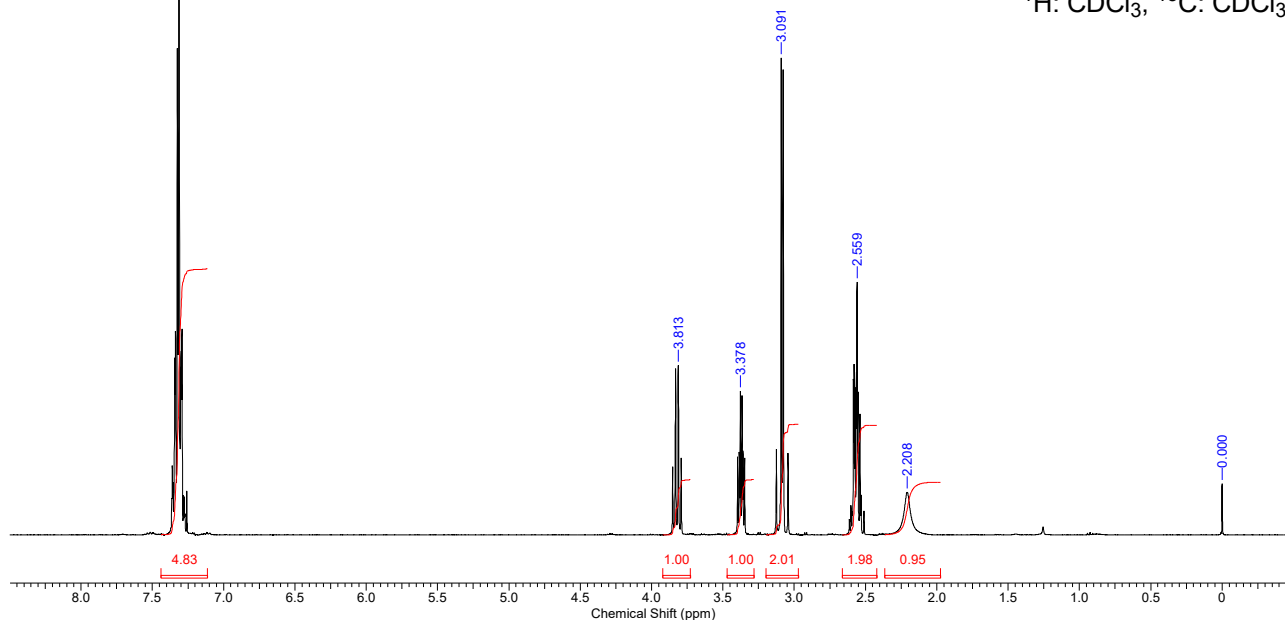


Acquisition Time (sec)	3.5000	Date	Apr 10 2021	Date Stamp	Apr 10 2021	File Name	C:\Users\tayam\Documents\NMR\43901-44000\43909
Frequency (MHz)	399.83	Nucleus	¹ H	Number of Transients	16	Original Points Count	22436
Pulse Sequence	s2pul	Receiver Gain	36.00	Solvent	CHLOROFORM-d	Points Count	32768
Sweep Width (Hz)	6410.26	Temperature (degree C)	25.000			Spectrum Offset (Hz)	2398.7354

R-10a_1H.esp

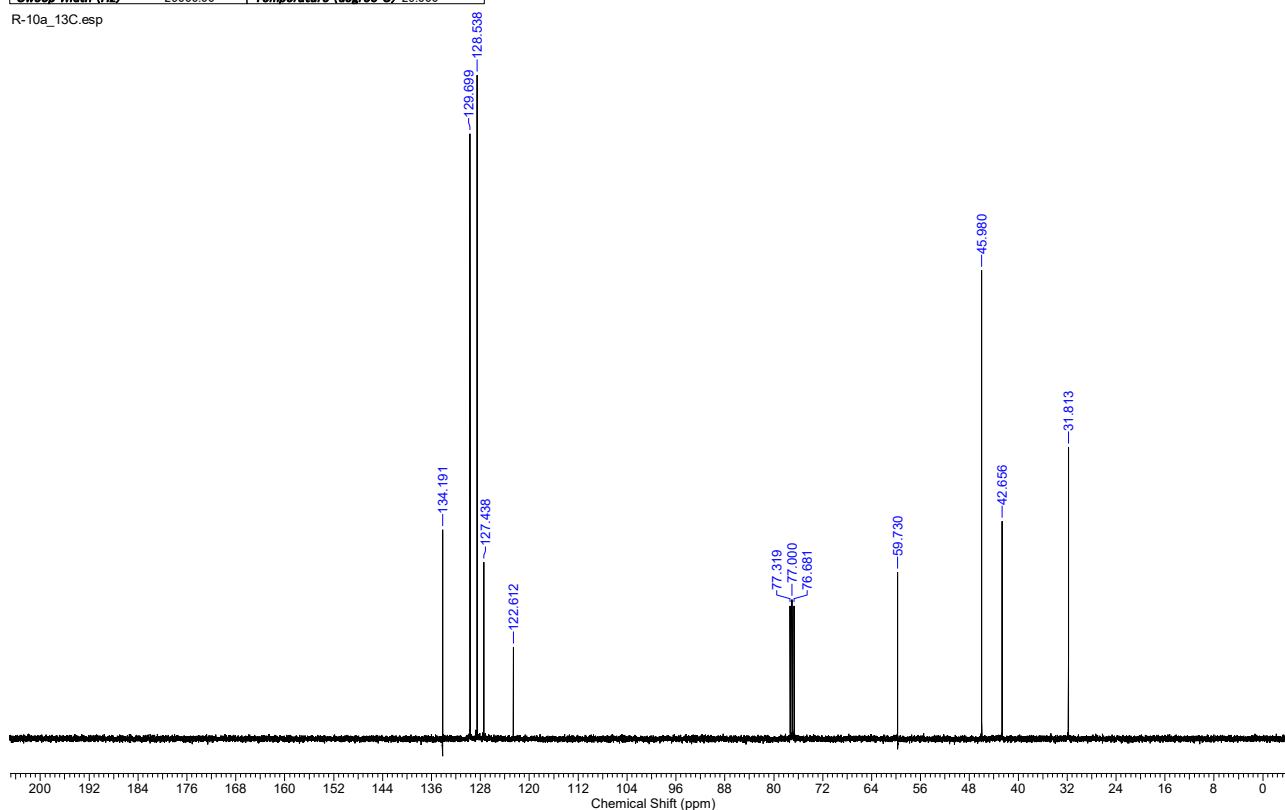


(*R*)-10a
¹H: CDCl₃, ¹³C: CDCl₃



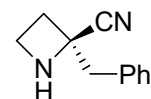
Acquisition Time (sec)	1.3107	Date	Apr 10 2021	Date Stamp	Apr 10 2021	File Name	C:\Users\tayam\Documents\NMR\43901-44000\43910
Frequency (MHz)	100.55	Nucleus	¹³ C	Number of Transients	512	Original Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	60.00	Solvent	CHLOROFORM-d	Points Count	32768
Sweep Width (Hz)	25000.00	Temperature (degree C)	25.000			Spectrum Offset (Hz)	11050.0156

R-10a_13C.esp

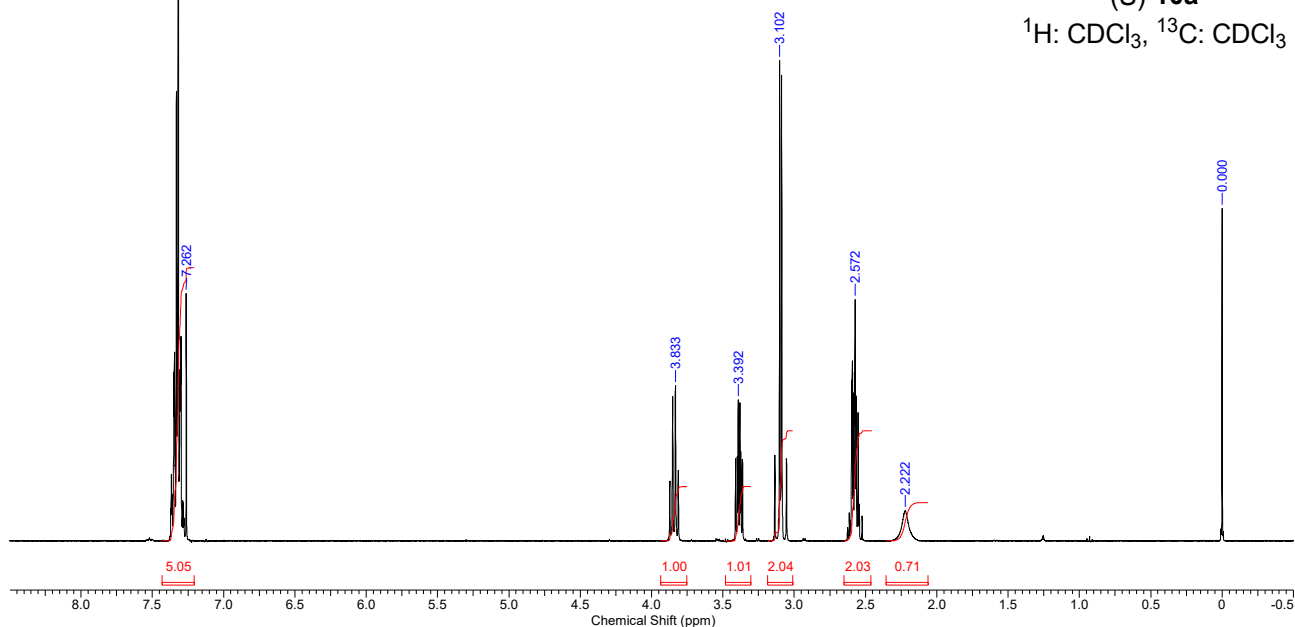


Acquisition Time (sec)	3.5000	Date	Apr 12 2021	Date Stamp	Apr 12 2021				
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\application\NMR\43914					Frequency (MHz)	399.83	Nucleus	¹ H
Number of Transients	16	Original Points Count	22436	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	48.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2400.1047	Sweep Width (Hz)	6410.26	Temperature (degree C)	25.000

S-10a_1H.esp



(S)-10a
¹H: CDCl₃, ¹³C: CDCl₃



Acquisition Time (sec)	1.3107	Date	Apr 13 2021	Date Stamp	Apr 13 2021				
File Name	C:\Users\tayam\Documents\Results for Publication\Nakanome\Data\application\NMR\43916					Frequency (MHz)	100.55	Nucleus	¹³ C
Number of Transients	512	Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul	Receiver Gain	60.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	11051.5410	Sweep Width (Hz)	25000.00	Temperature (degree C)	25.000

S-10a_13C.esp

