



Supporting Information

for

Hoveyda–Grubbs catalysts with an N→Ru coordinate bond in a six-membered ring. Synthesis of stable, industrially scalable, highly efficient ruthenium metathesis catalysts and 2-vinylbenzylamine ligands as their precursors

Kirill B. Polyanskii, Kseniia A. Alekseeva, Pavel V. Raspertov, Pavel A. Kumandin, Eugeniya V. Nikitina, Atash V. Gurbanov and Fedor I. Zubkov

Beilstein J. Org. Chem. **2019**, *15*, 769–779. doi:10.3762/bjoc.15.73

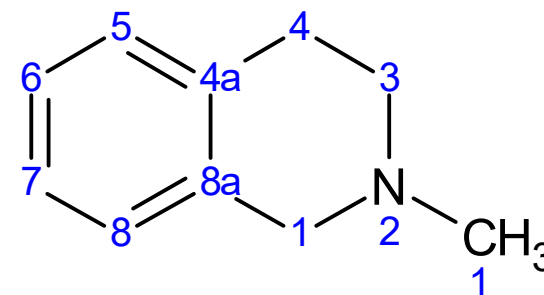
Copies of NMR spectra of synthesised compounds and selected GC–MS data of the metathesis products. Check-cif reports for compounds 11a–c

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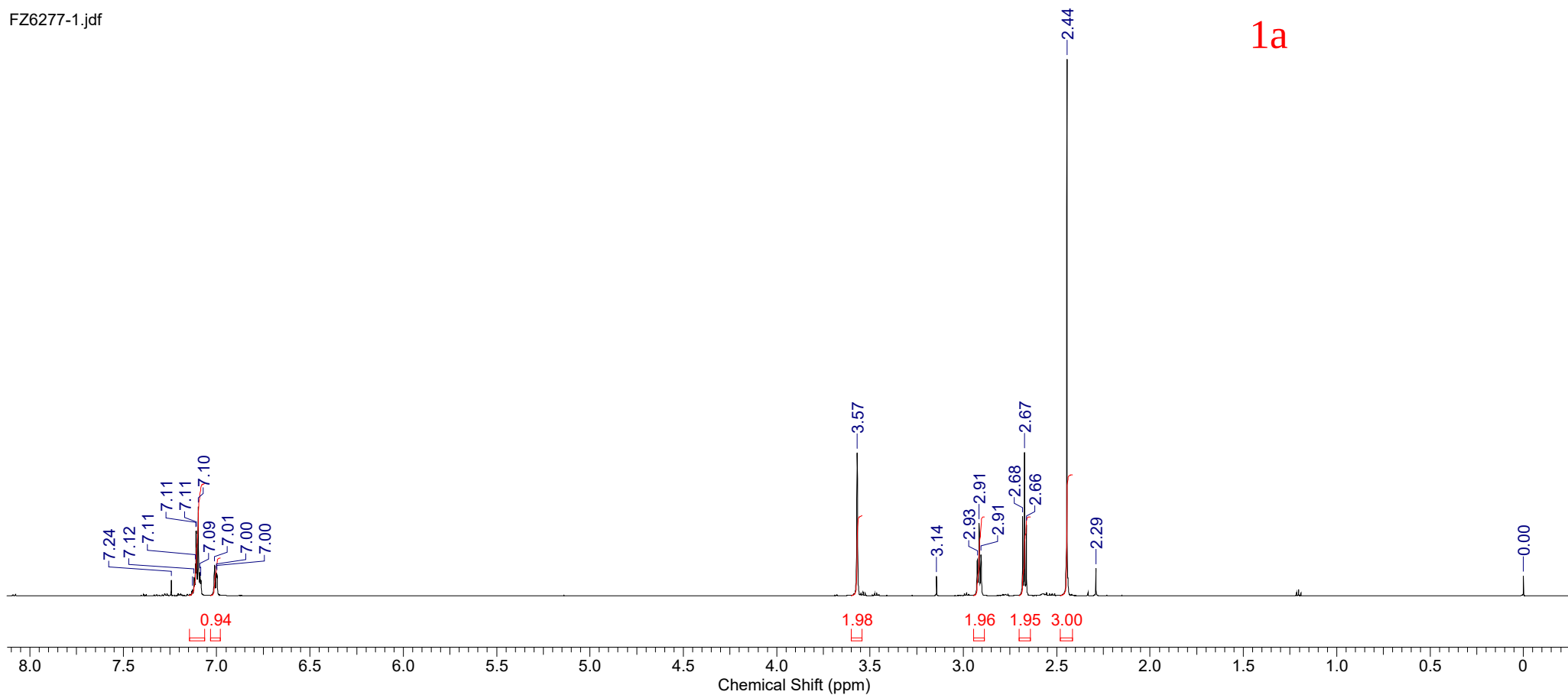
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1. Copies of ^1H and ^{13}C NMR spectra for compounds **1, 3-5, 7, 11, 13, 15, 18**

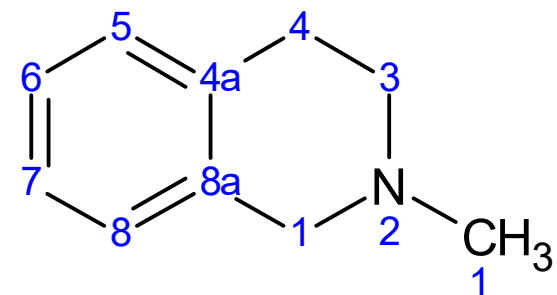
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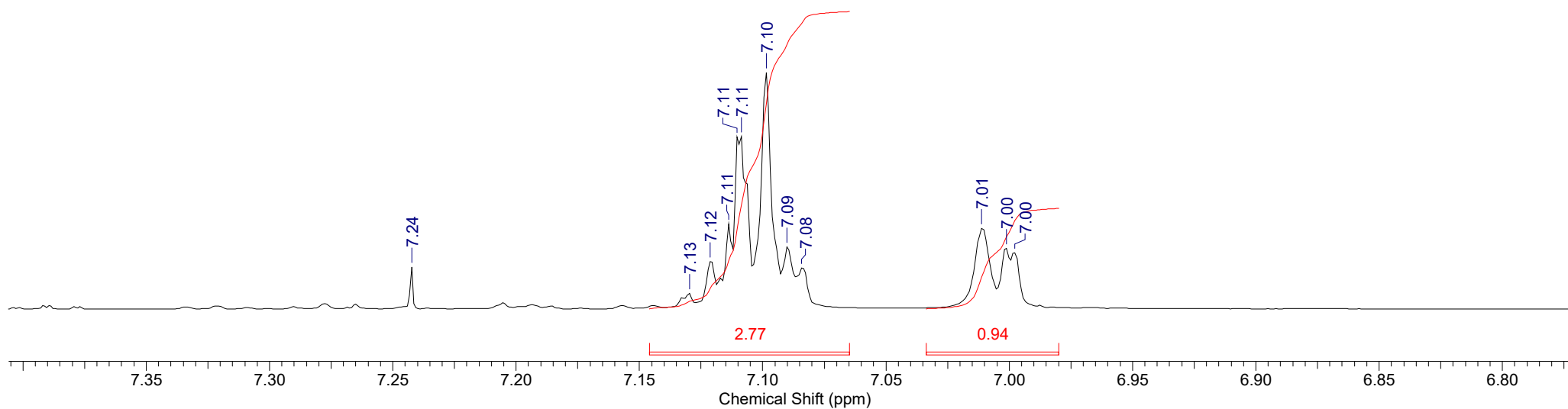


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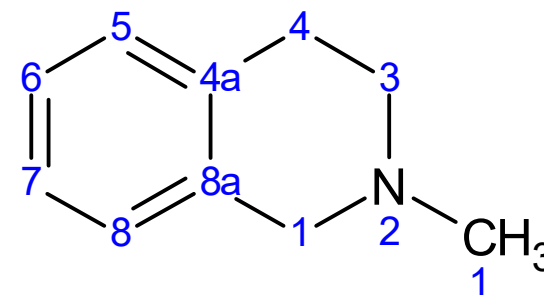


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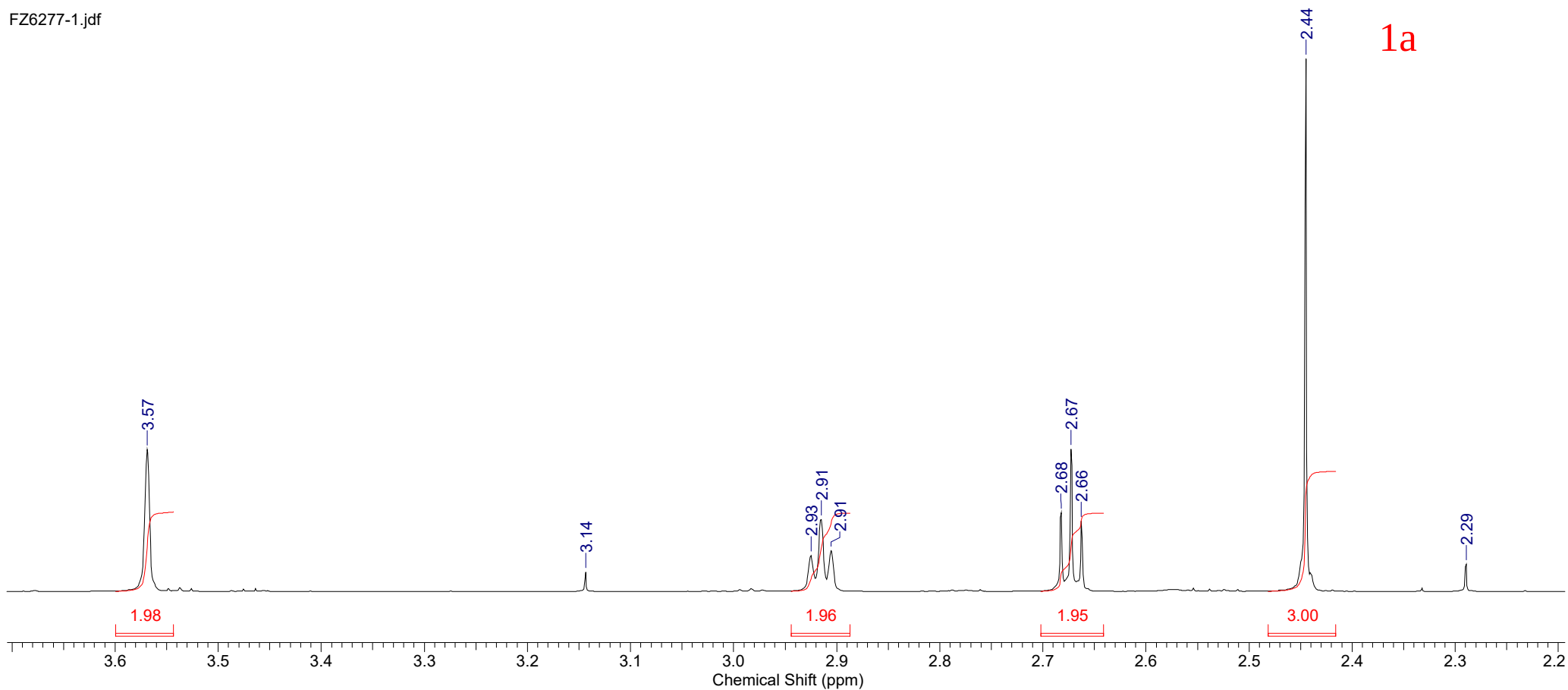
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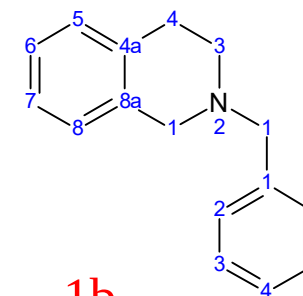
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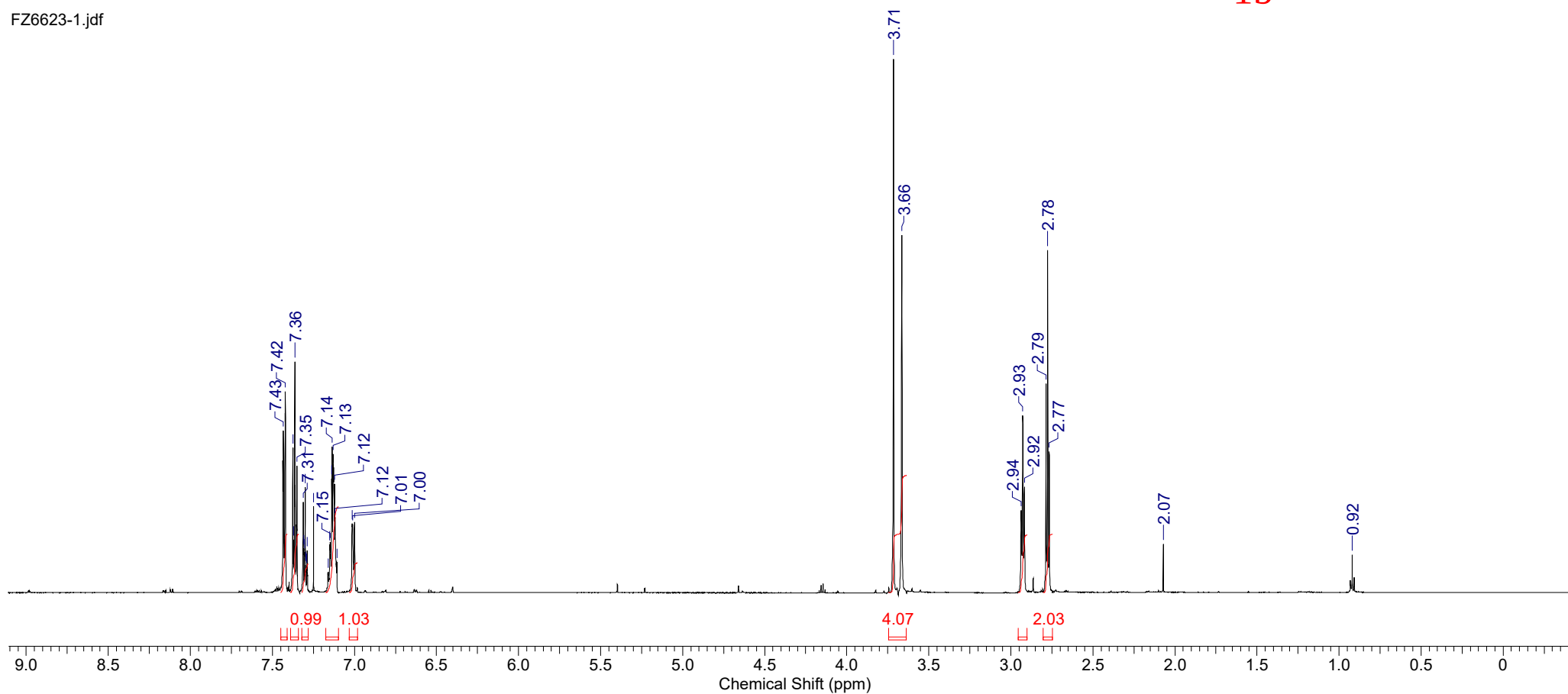


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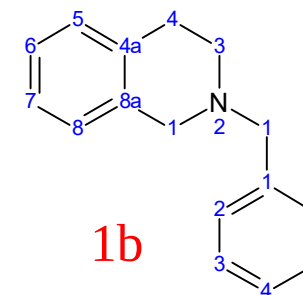


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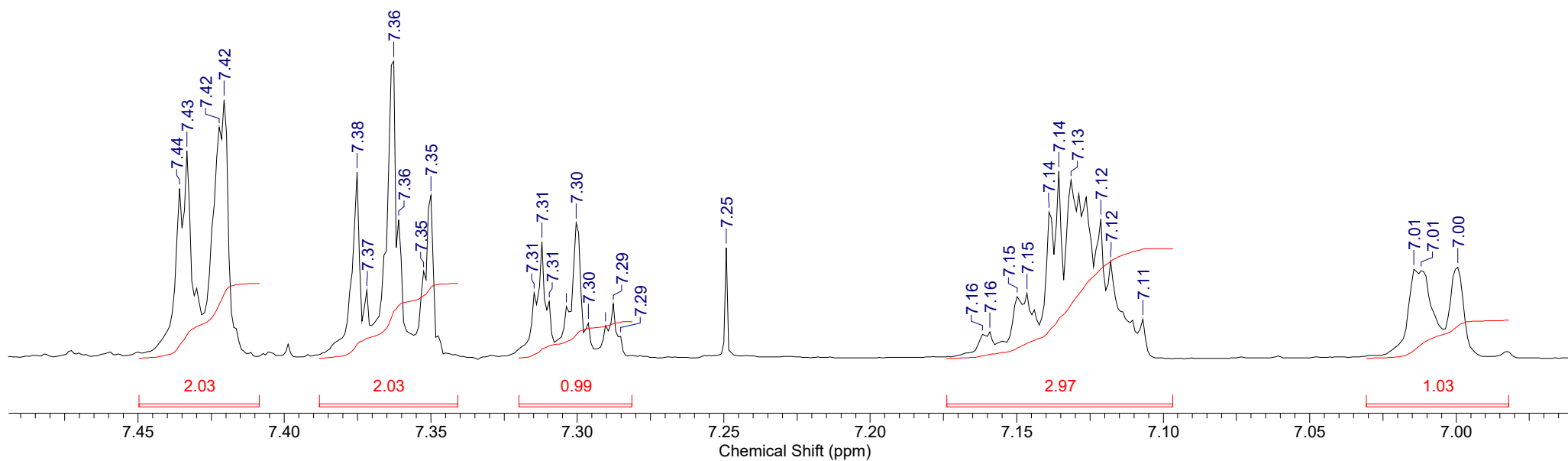
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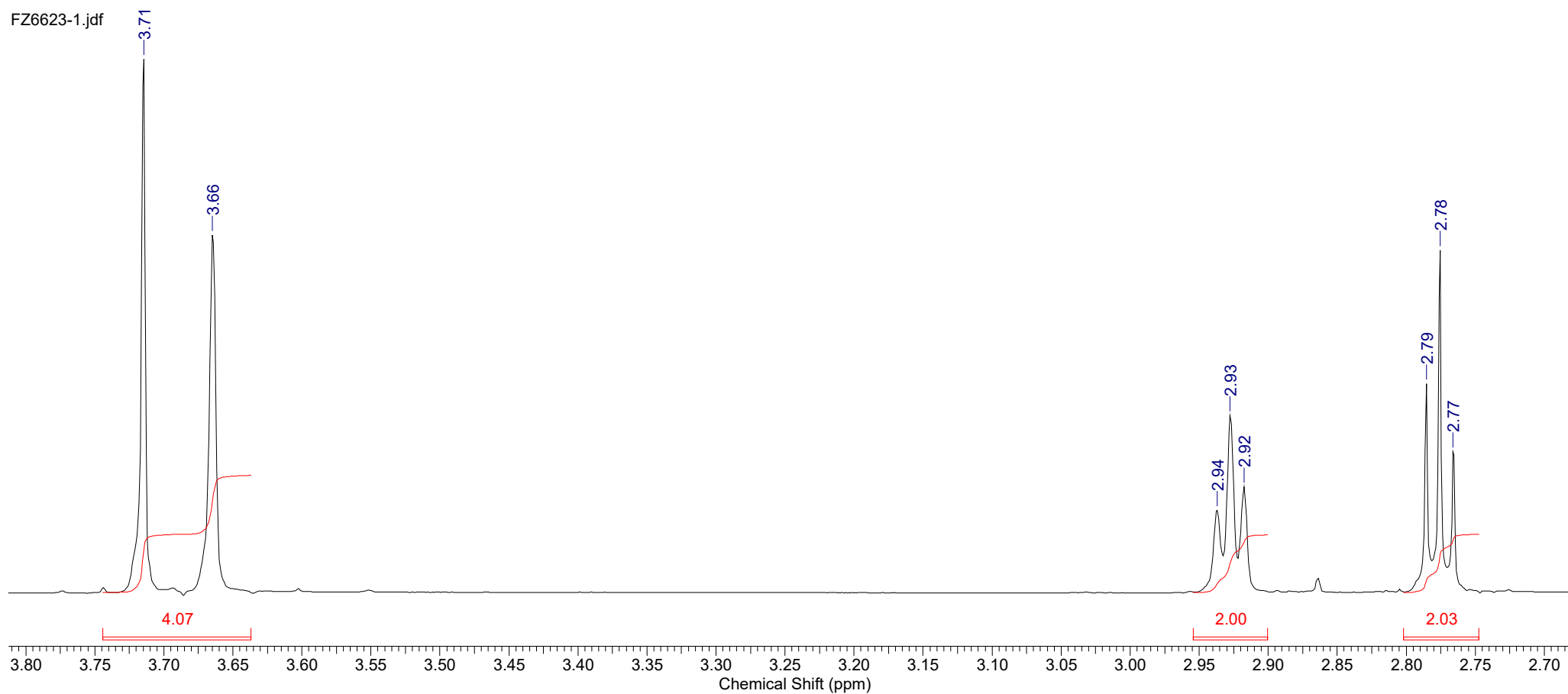
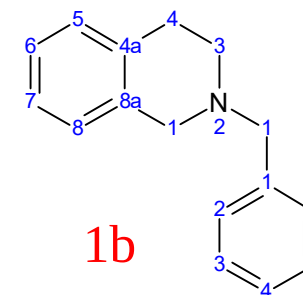
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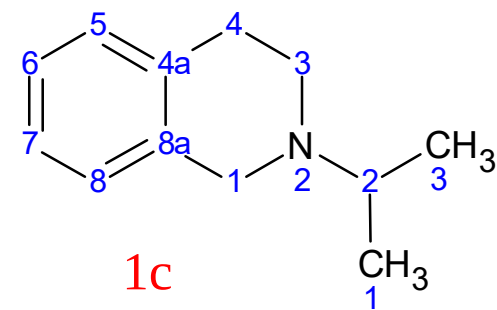
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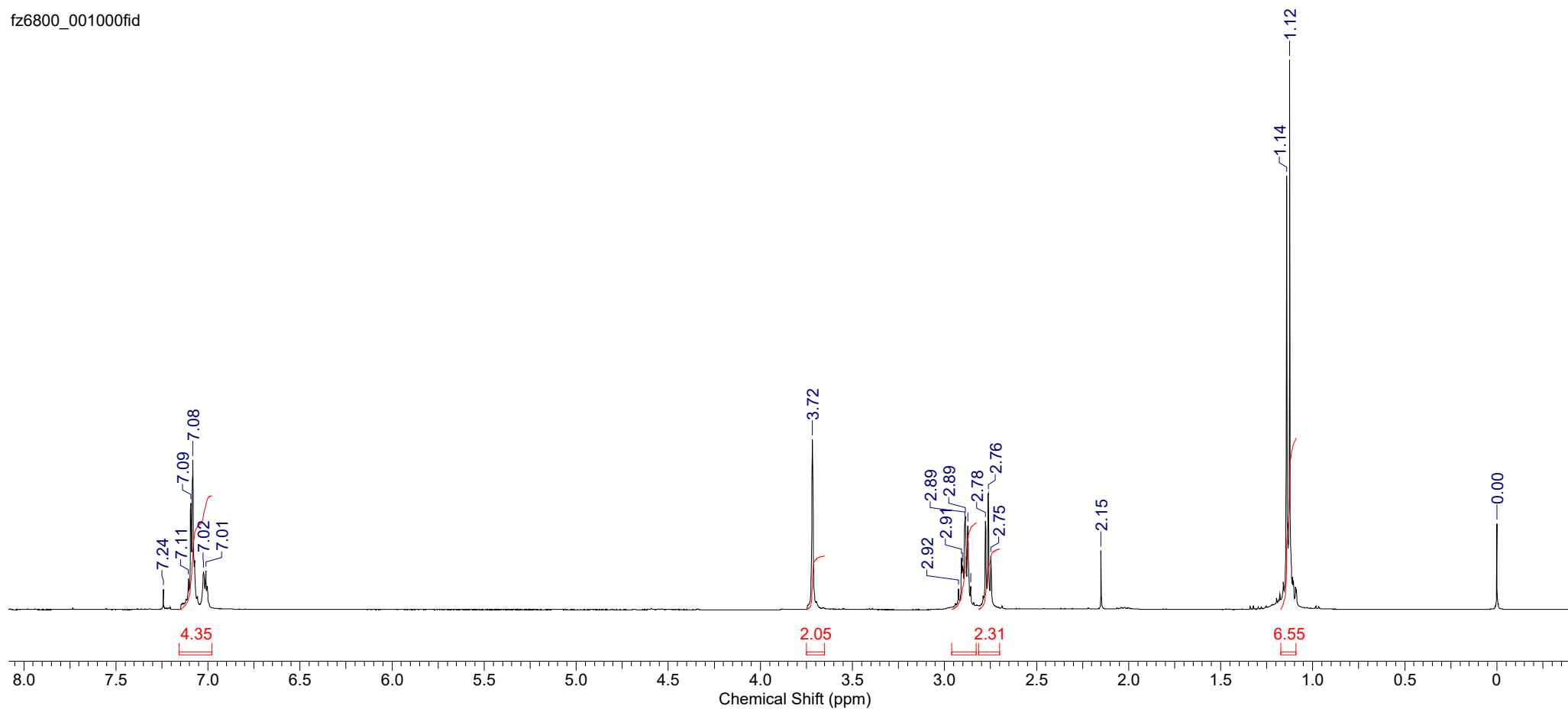
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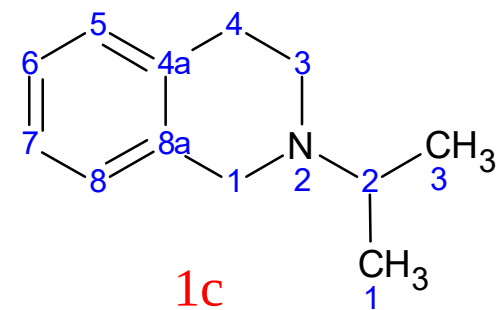
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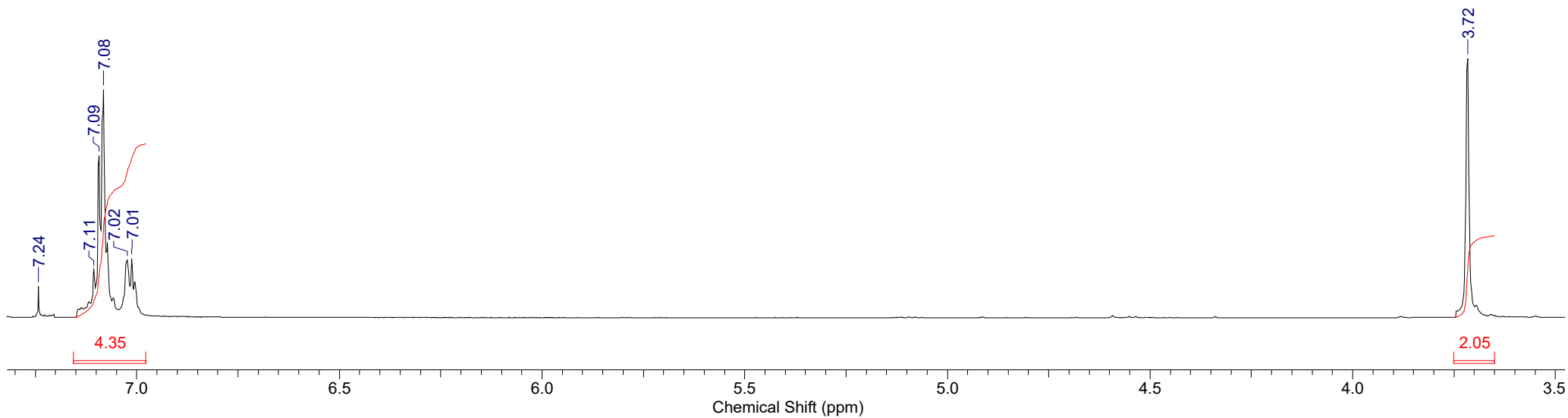
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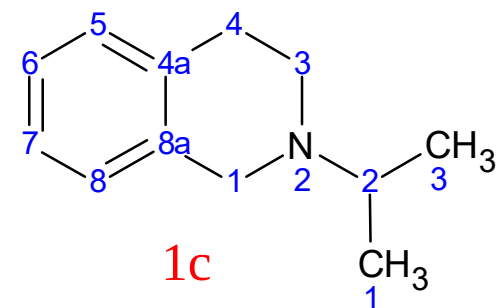
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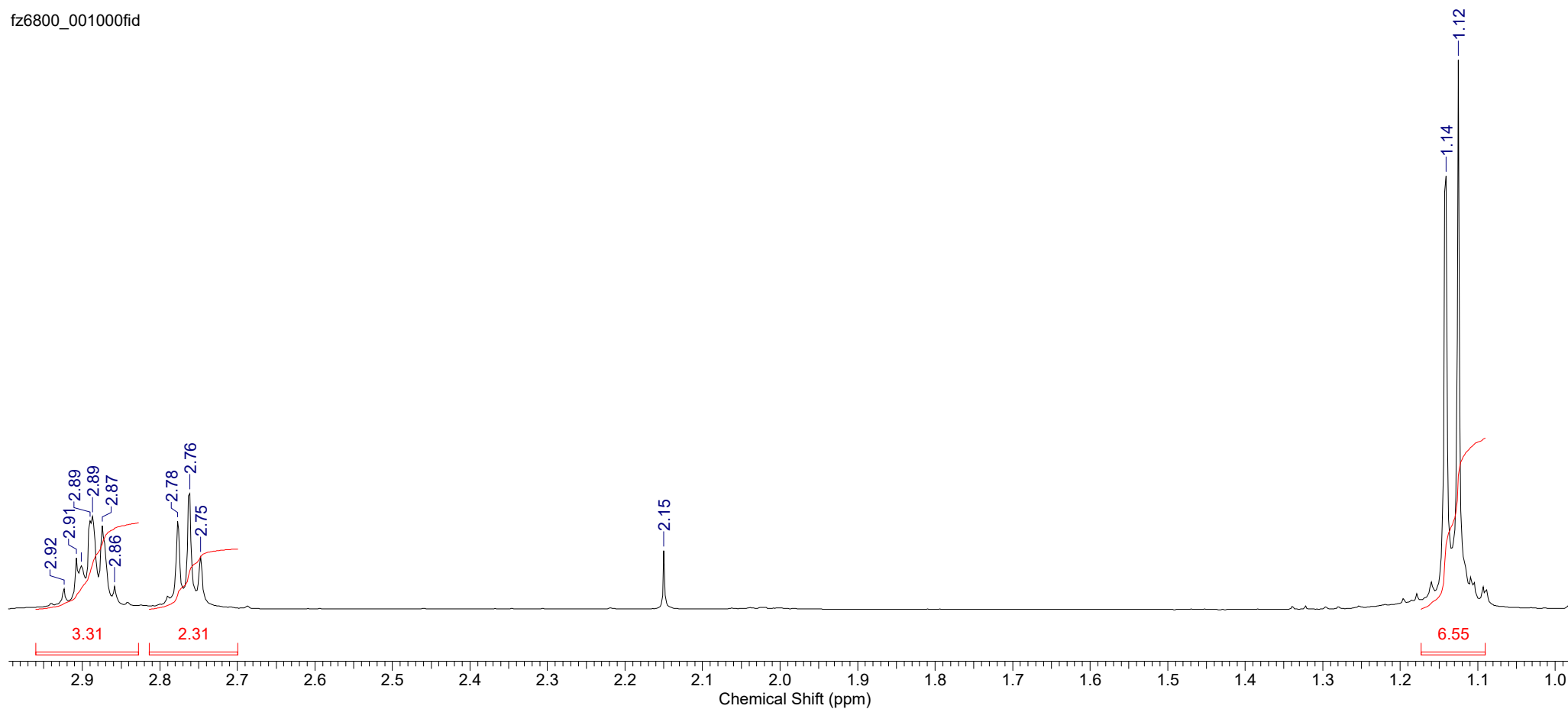
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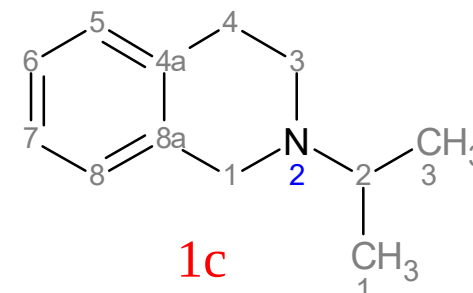
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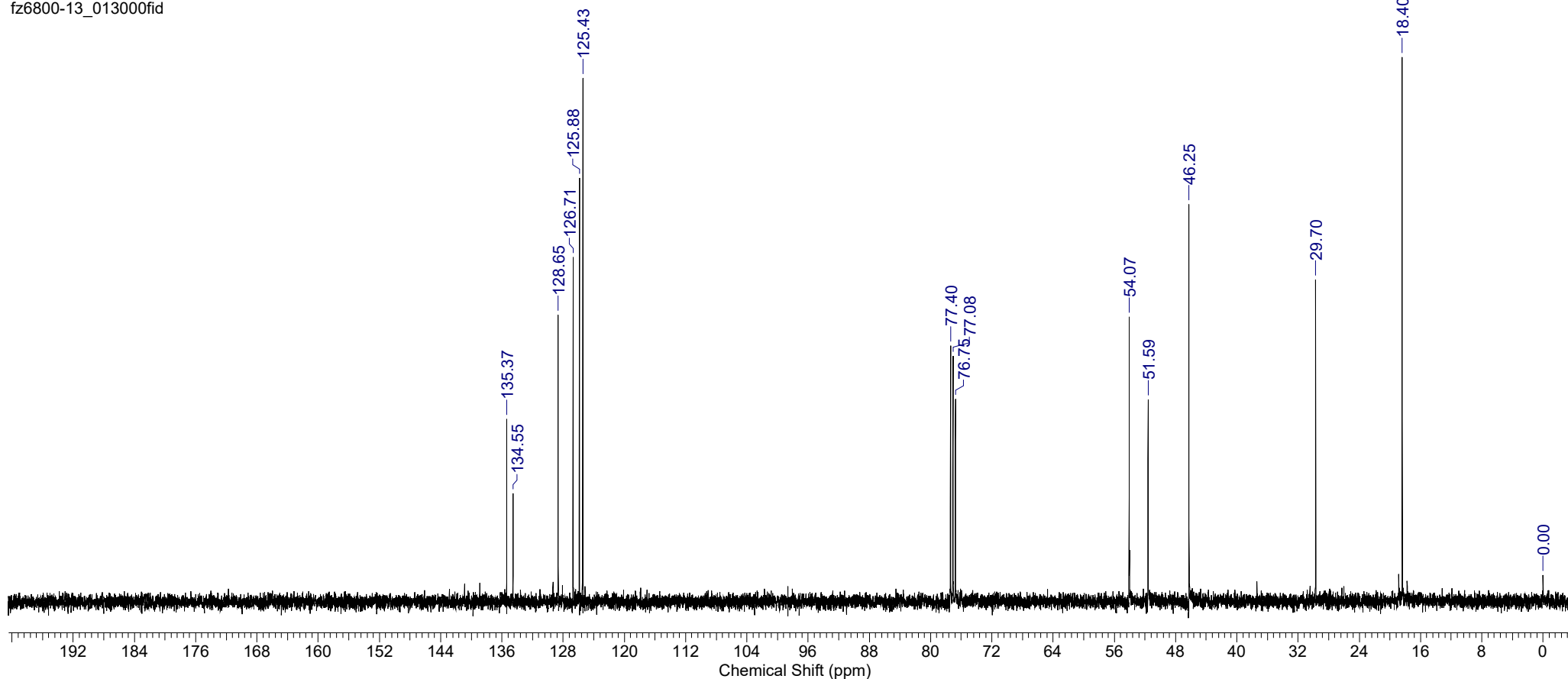
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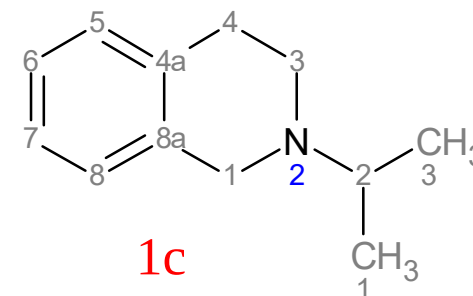
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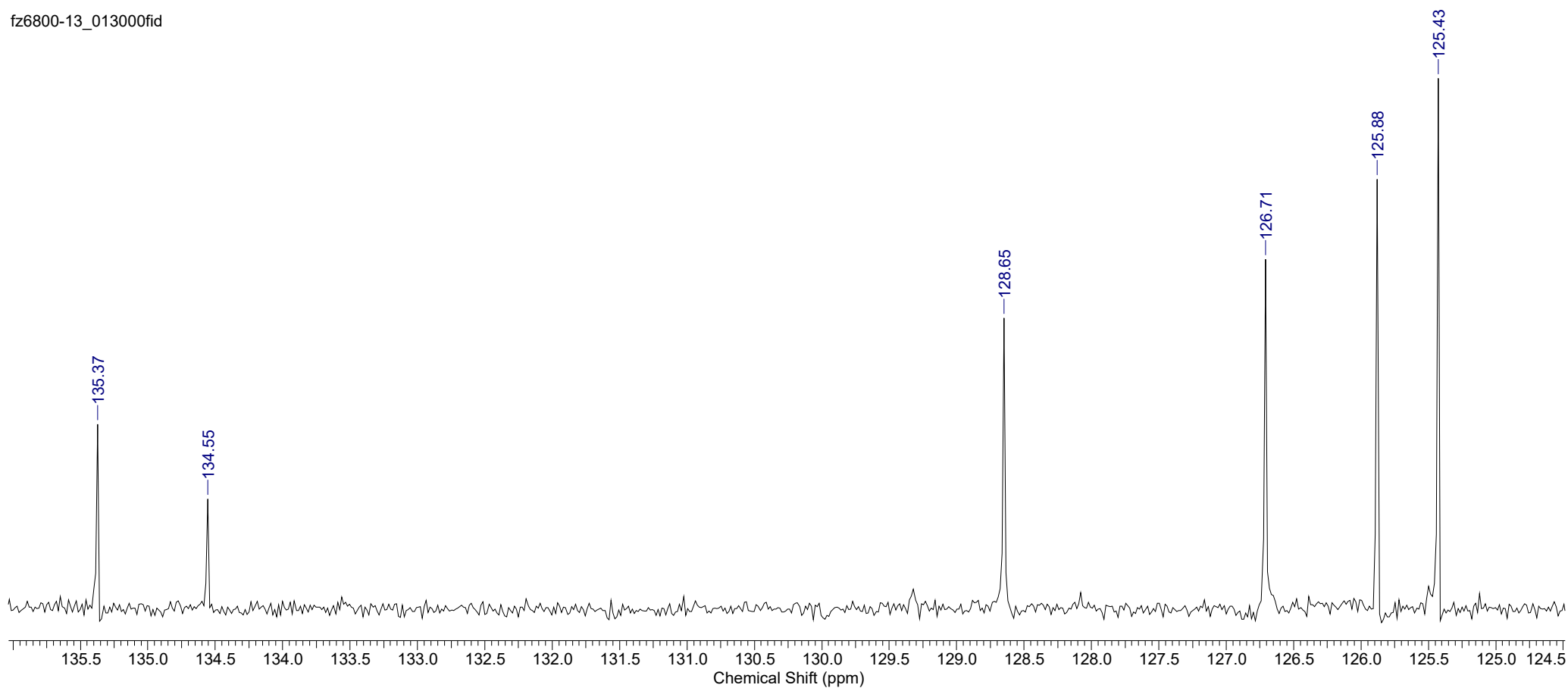
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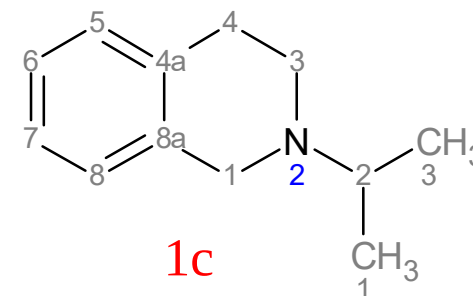
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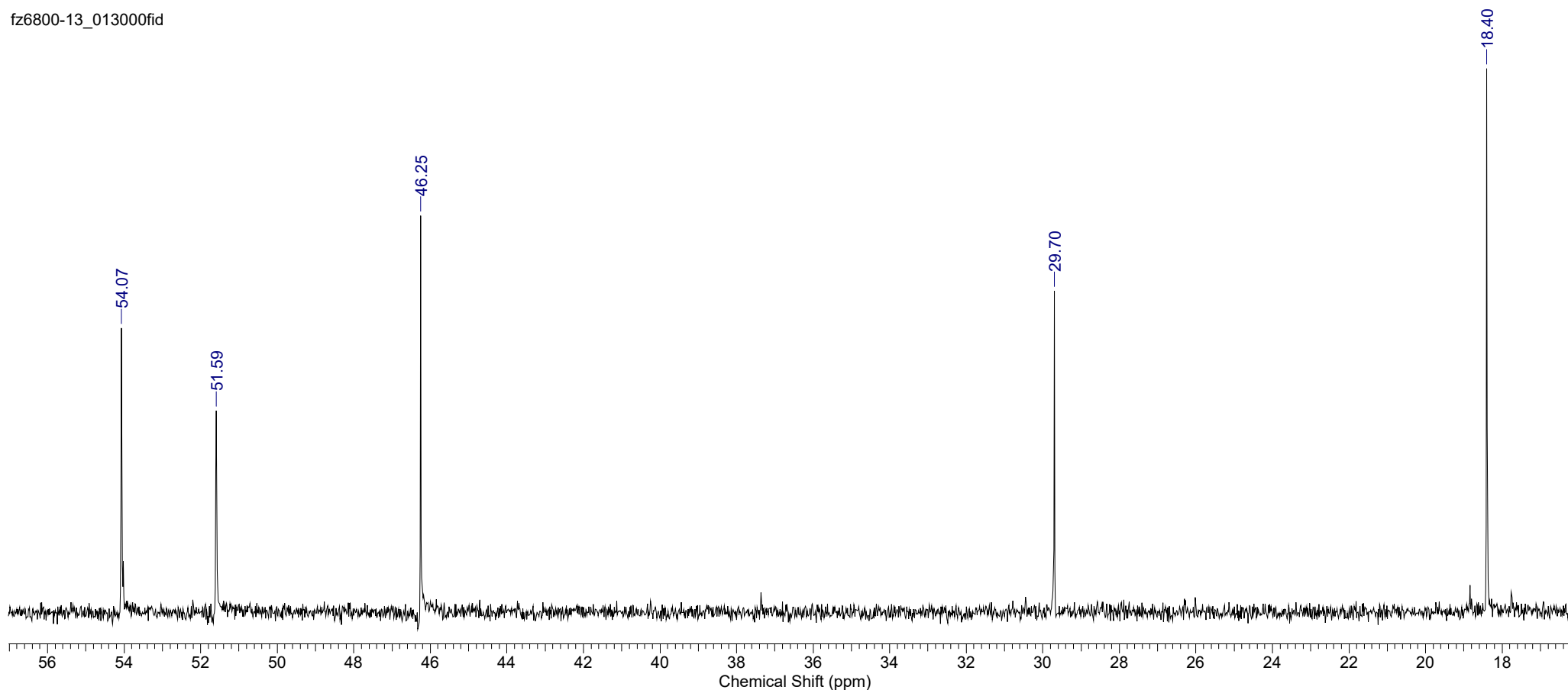
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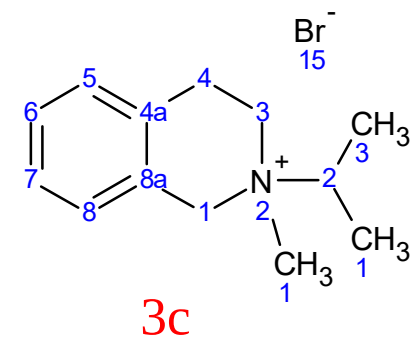
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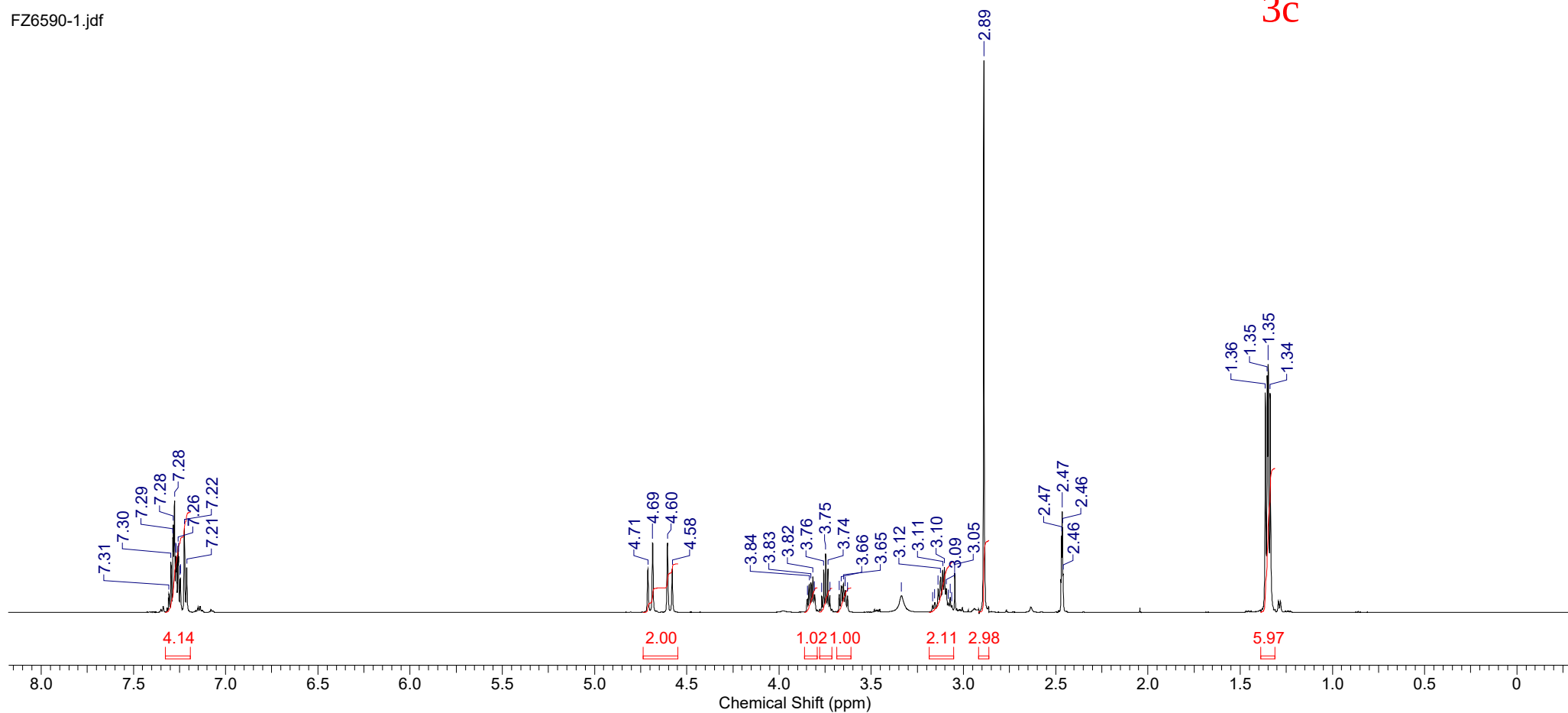
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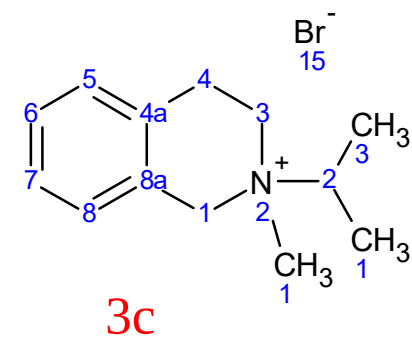
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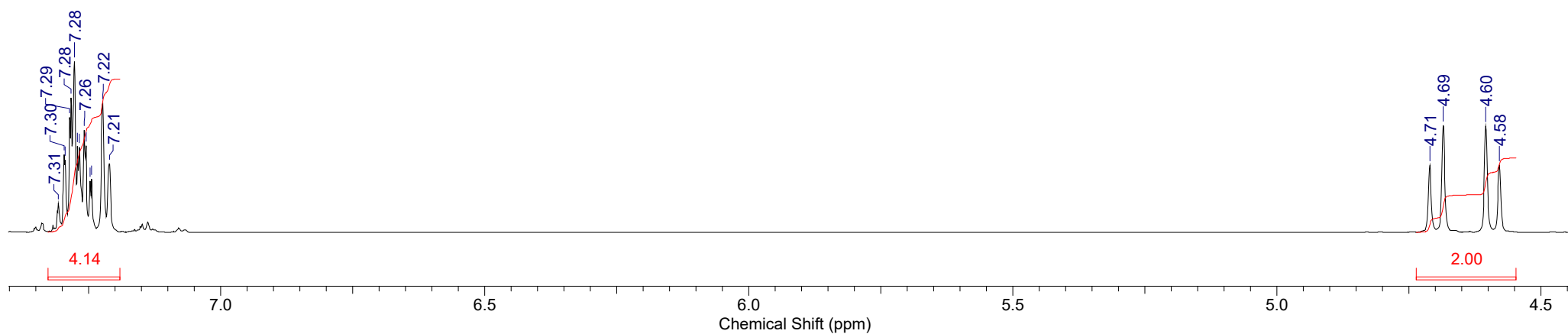
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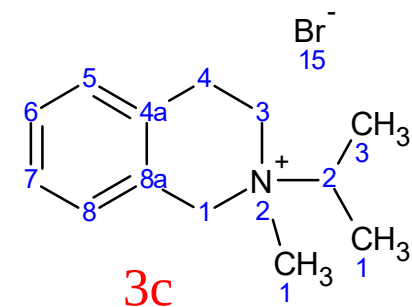
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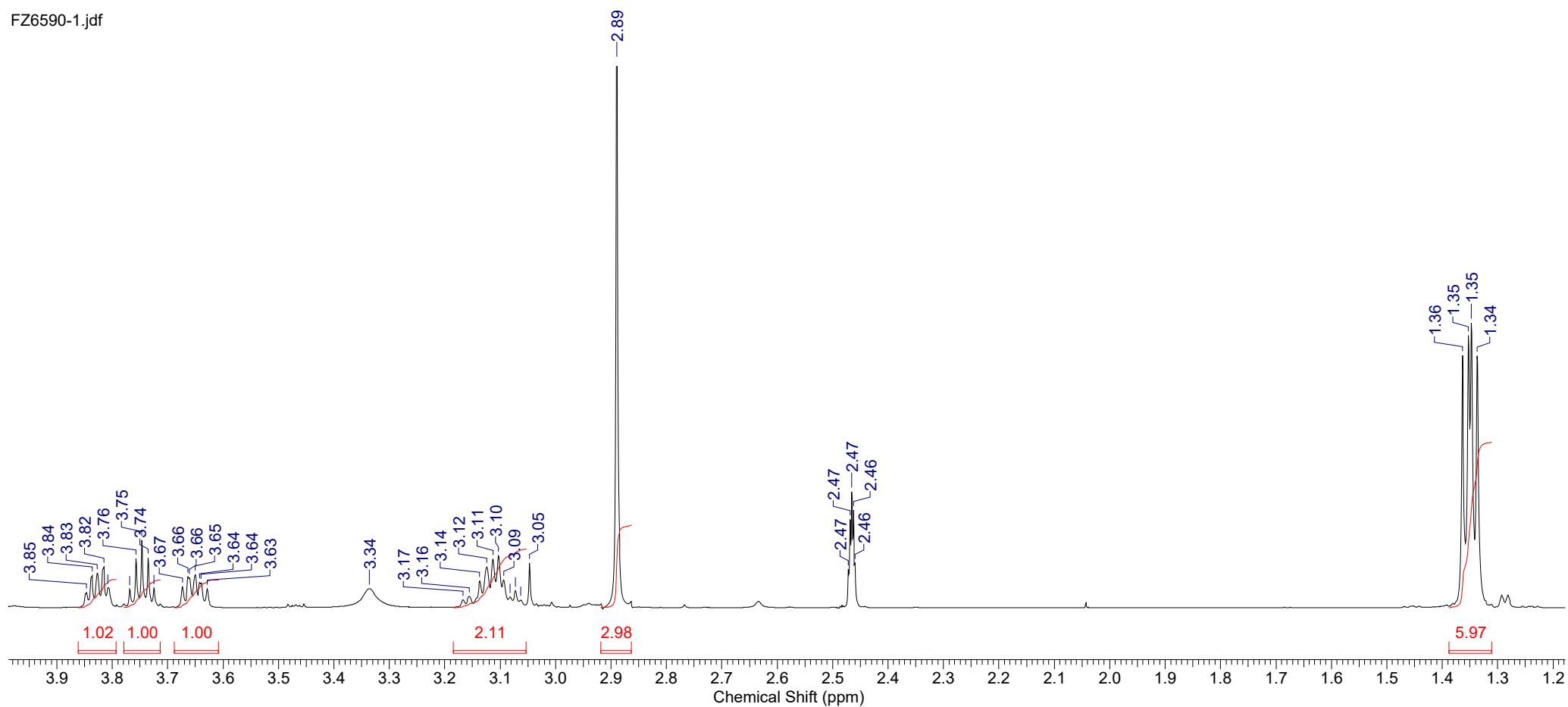
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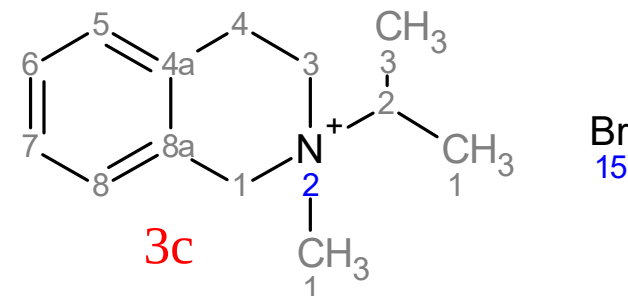
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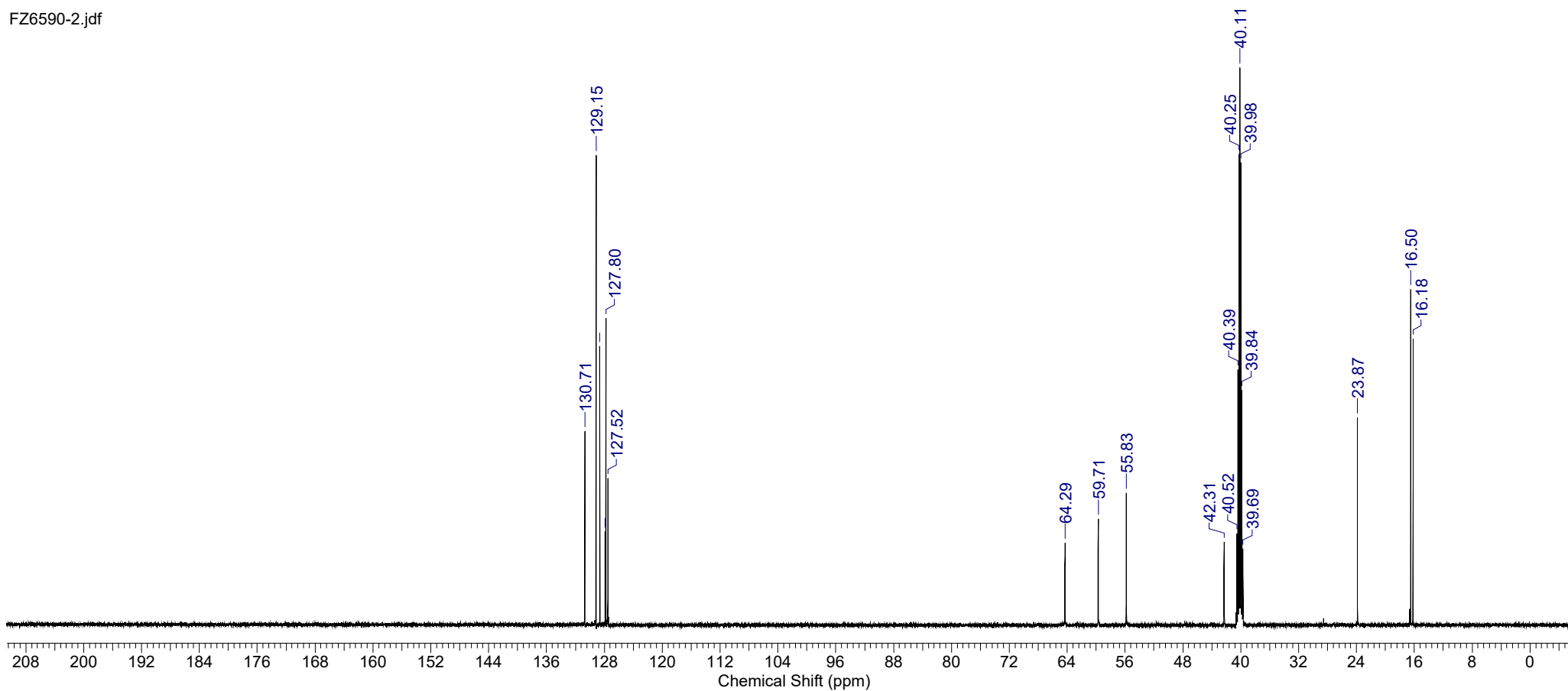
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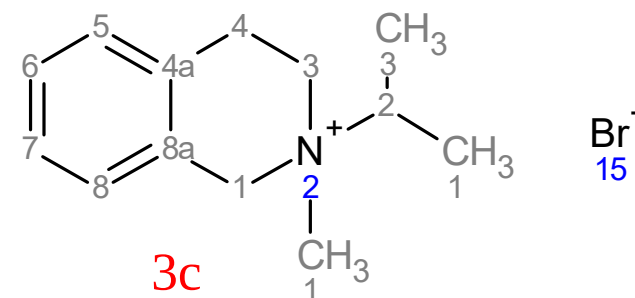
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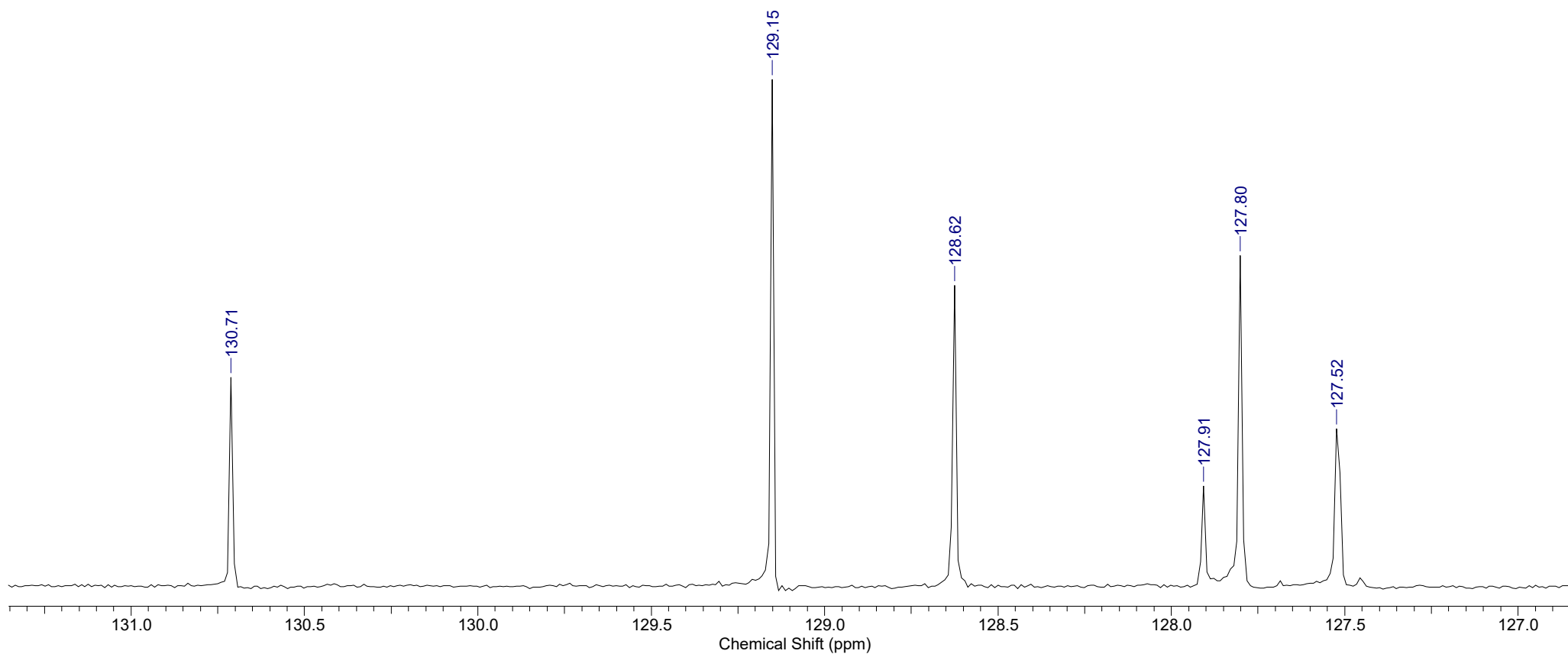
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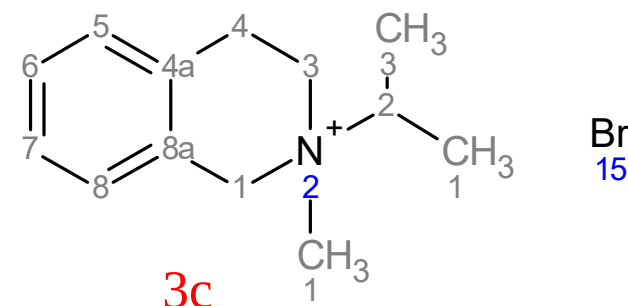
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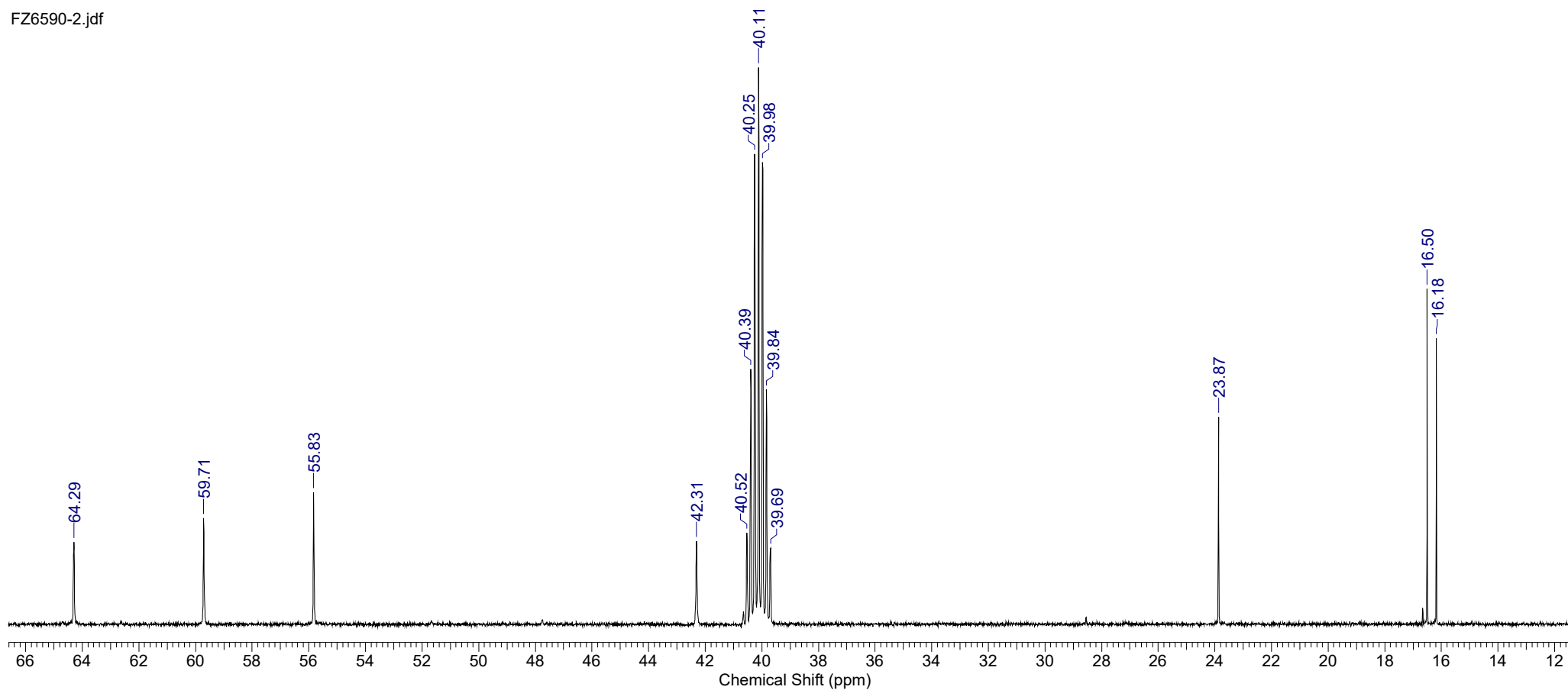
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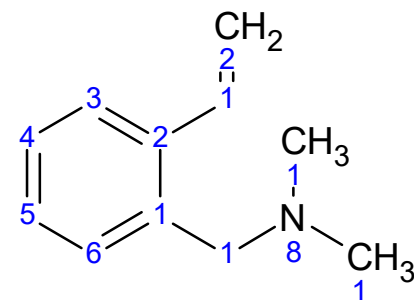
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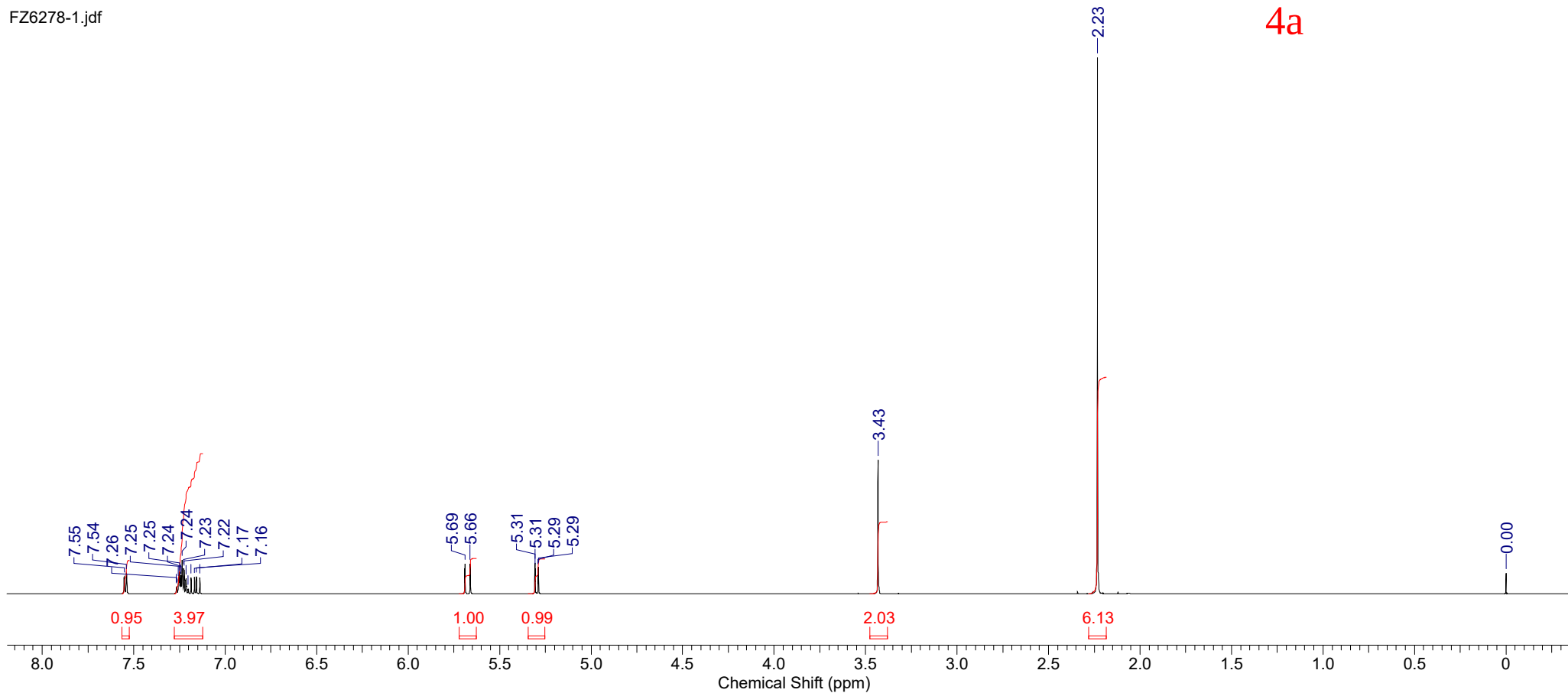
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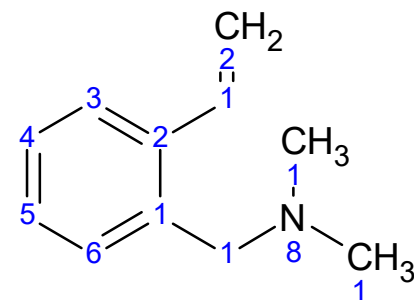
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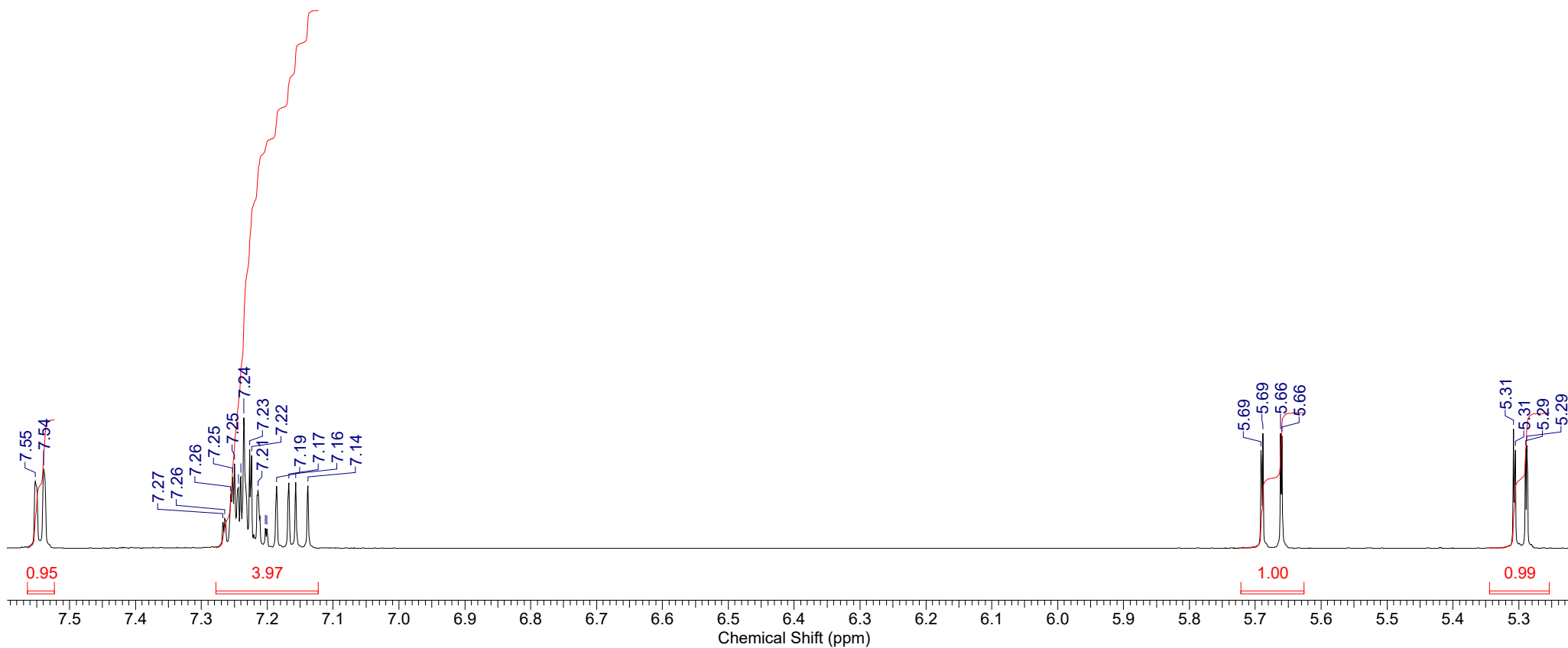


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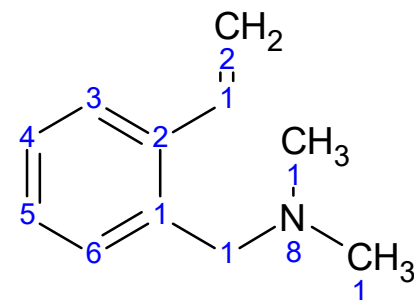


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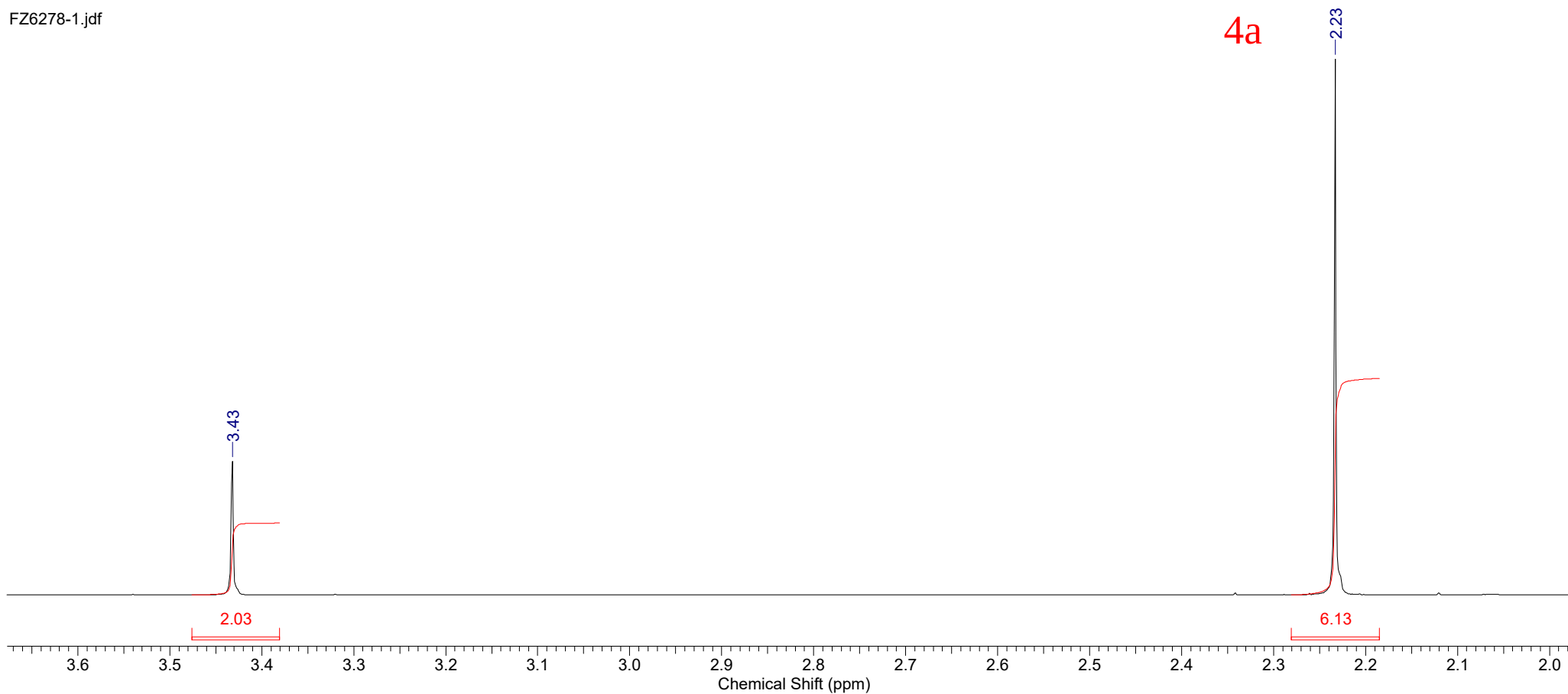
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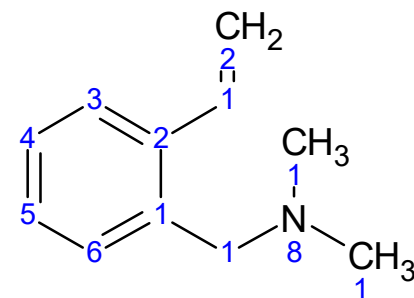
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Nucleus	1H	Number of Transients	8	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse.ex2			Receiver Gain	34.00
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	19.400	Solvent	CHLOROFORM-d



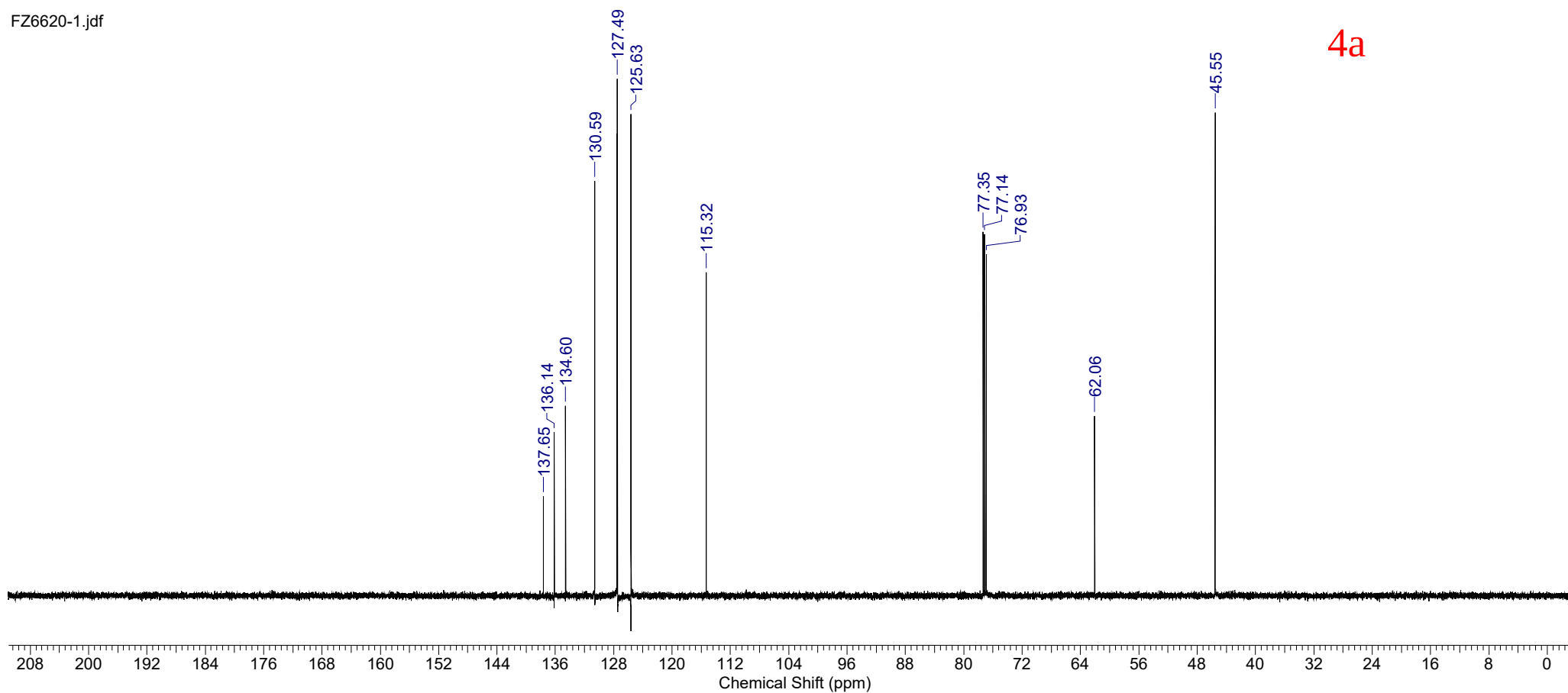
FZ6278-1.jdf



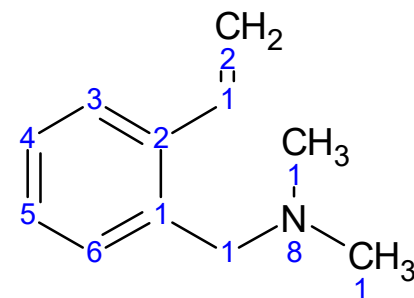
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	22 Apr 1990 08:17:52	
Date Stamp	18 Apr 2018 13:05:31	File Name	C:\Users\Fedor\Desktop\17.04.18\FZ6620-1.jdf				
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	235	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	23.200				



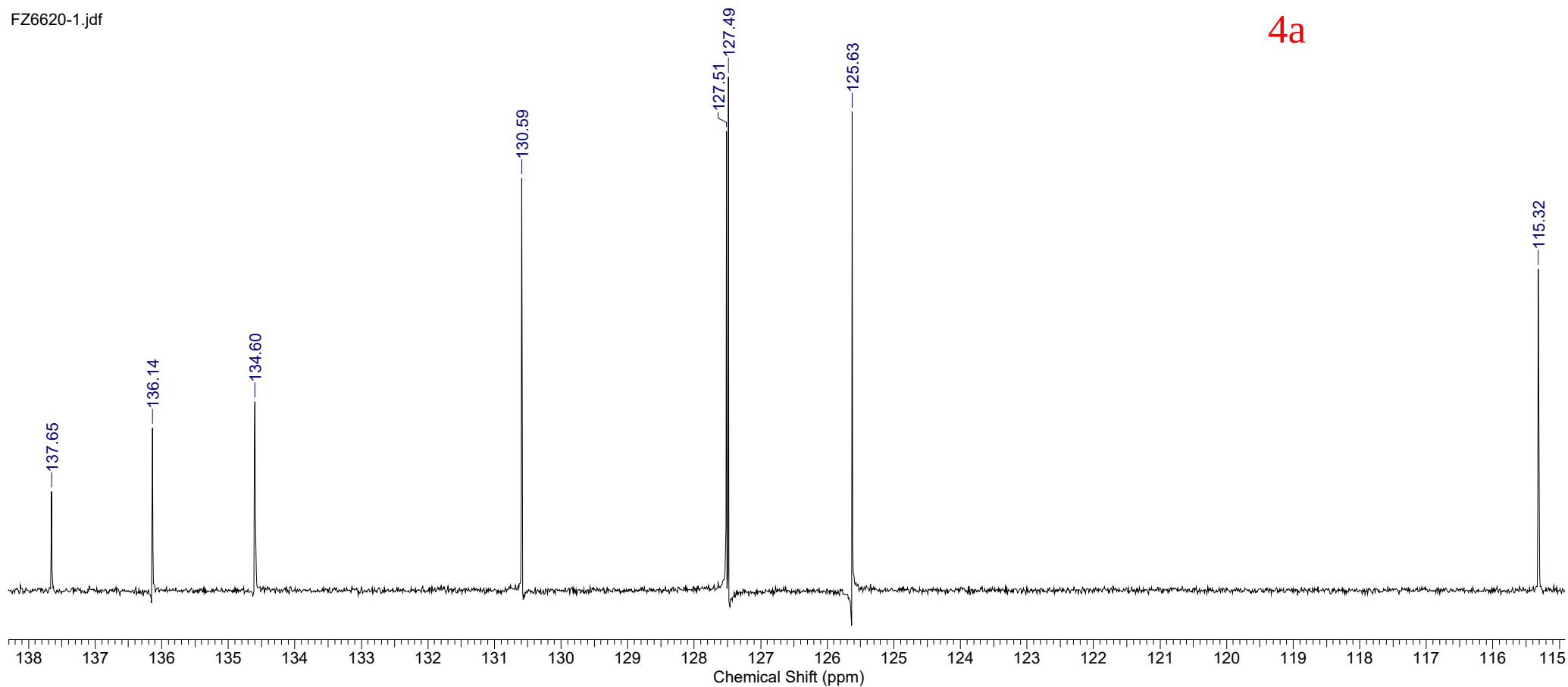
FZ6620-1.jdf



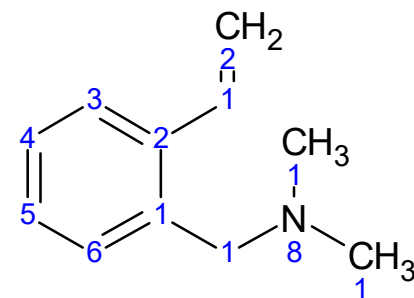
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	22 Apr 1990 08:17:52	
Date Stamp	18 Apr 2018 13:05:31	File Name	C:\Users\Fedor\Desktop\17.04.18\FZ6620-1.jdf				
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	235	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	15091.3428
Sweep Width (Hz)	47348.49	Temperature (degree C)	23.200				



4a

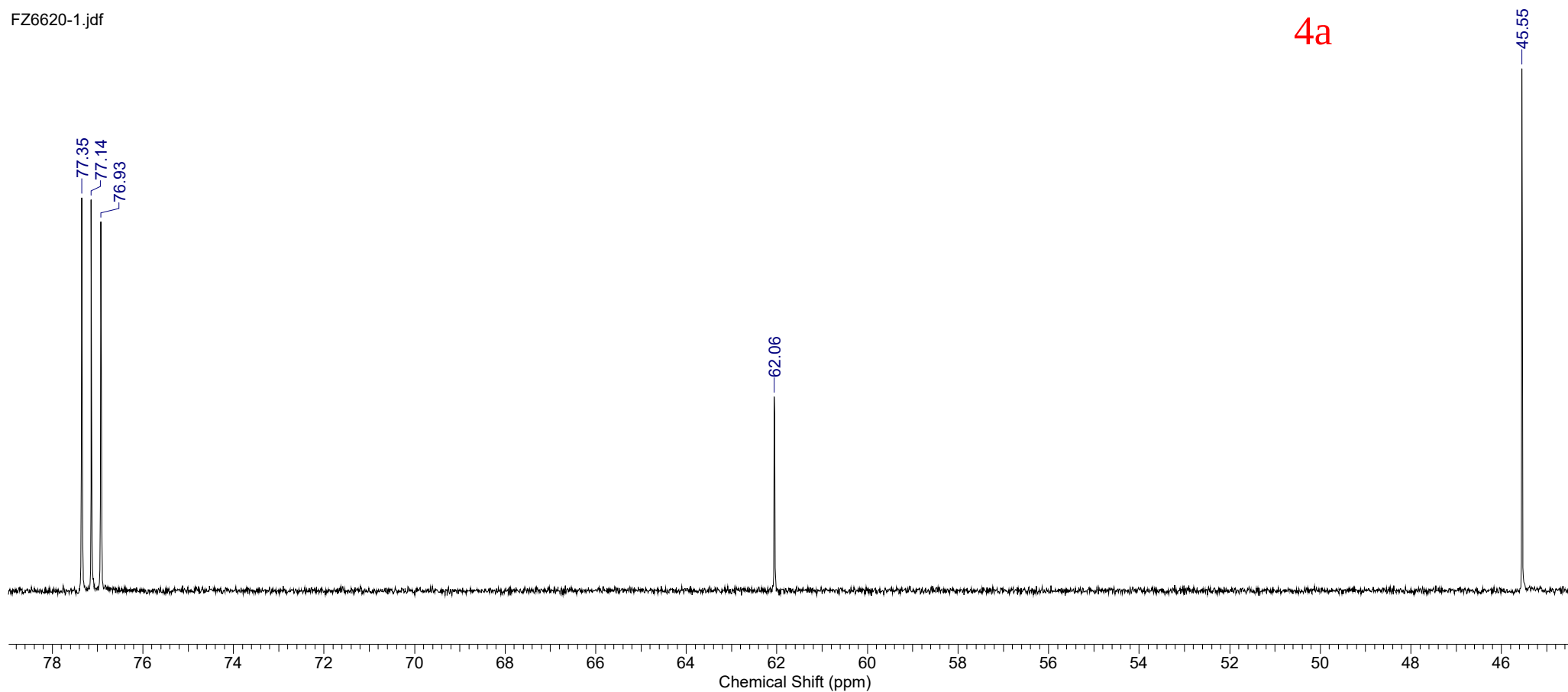


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	22 Apr 1990 08:17:52	
Date Stamp	18 Apr 2018 13:05:31	File Name	C:\Users\Fedor\Desktop\17.04.18\FZ6620-1.jdf				
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	235	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	15091.3428
Sweep Width (Hz)	47348.49	Temperature (degree C)	23.200				

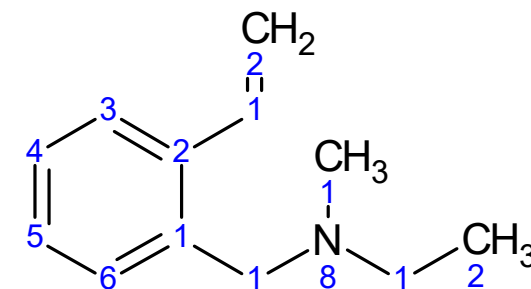


4a

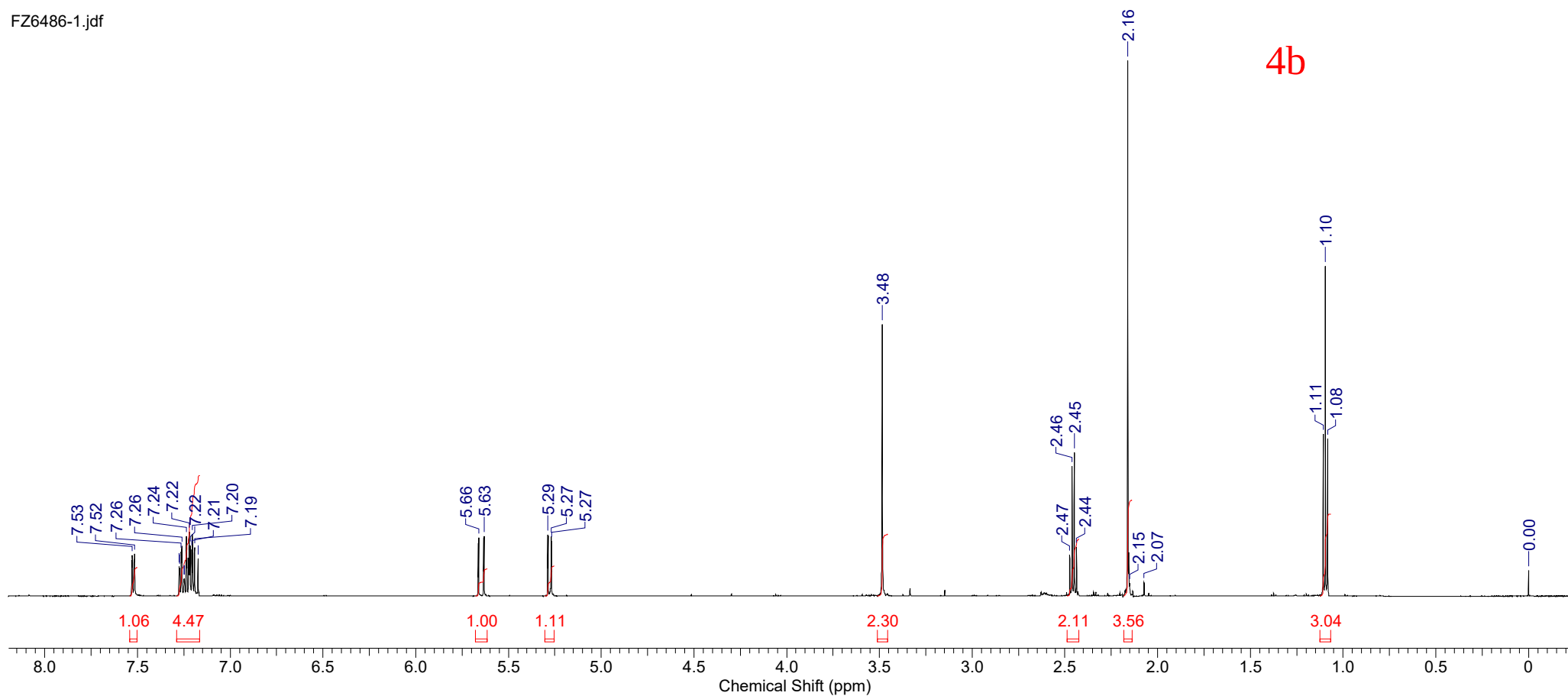
FZ6620-1.jdf



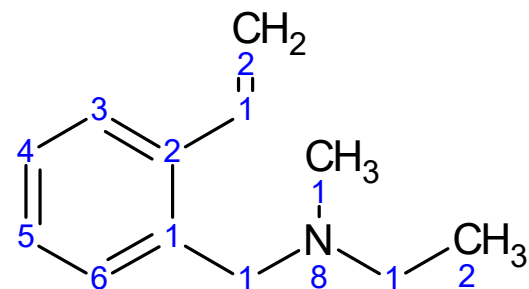
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	11 Mar 1990 03:06:05	
Date Stamp	07 Mar 2018 07:53:44			File Name	C:\Users\Fedor\Desktop\06.03.18\FZ6486-1.jdf	Frequency (MHz) 600.17
Nucleus	¹ H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 28.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5393.9751	Sweep Width (Hz)	16534.39	Temperature (degree C)	22.200	



FZ6486-1.jdf

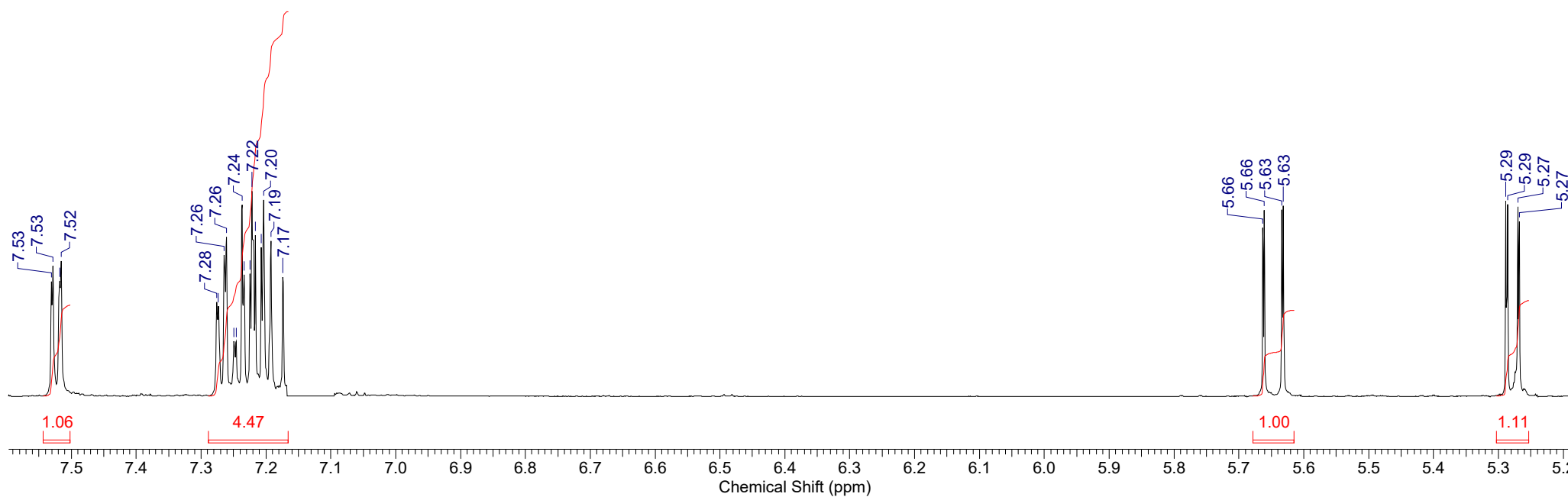


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	11 Mar 1990 03:06:05	
Date Stamp	07 Mar 2018 07:53:44			File Name	C:\Users\Fedor\Desktop\06.03.18\FZ6486-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 28.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5393.9751	Sweep Width (Hz)	16534.39	Temperature (degree C)	22.200	

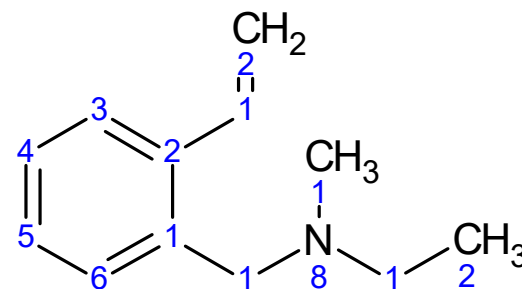


4b

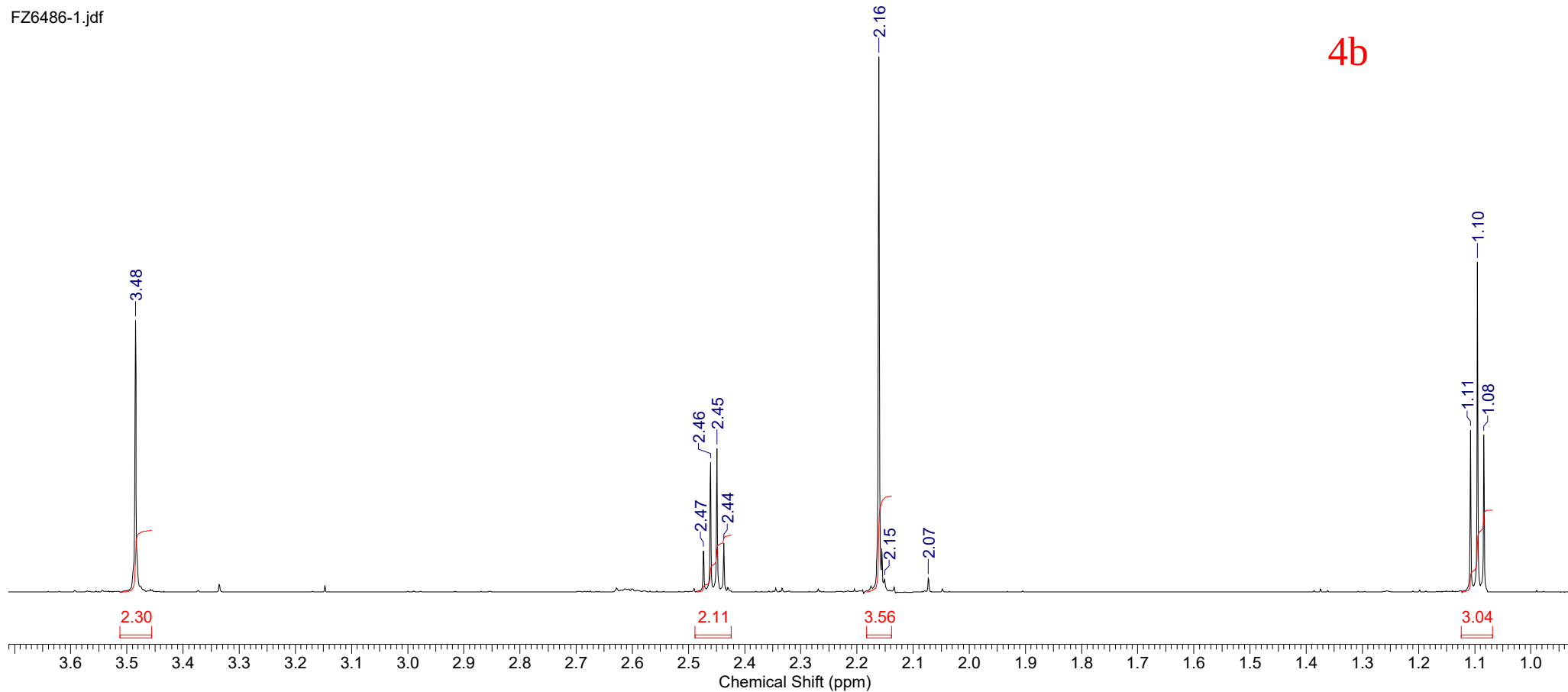
FZ6486-1.jdf



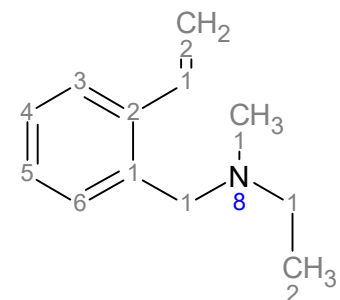
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	11 Mar 1990 03:06:05	
Date Stamp	07 Mar 2018 07:53:44			File Name	C:\Users\Fedor\Desktop\06.03.18\FZ6486-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 28.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5393.9751	Sweep Width (Hz)	16534.39	Temperature (degree C)	22.200	



4b

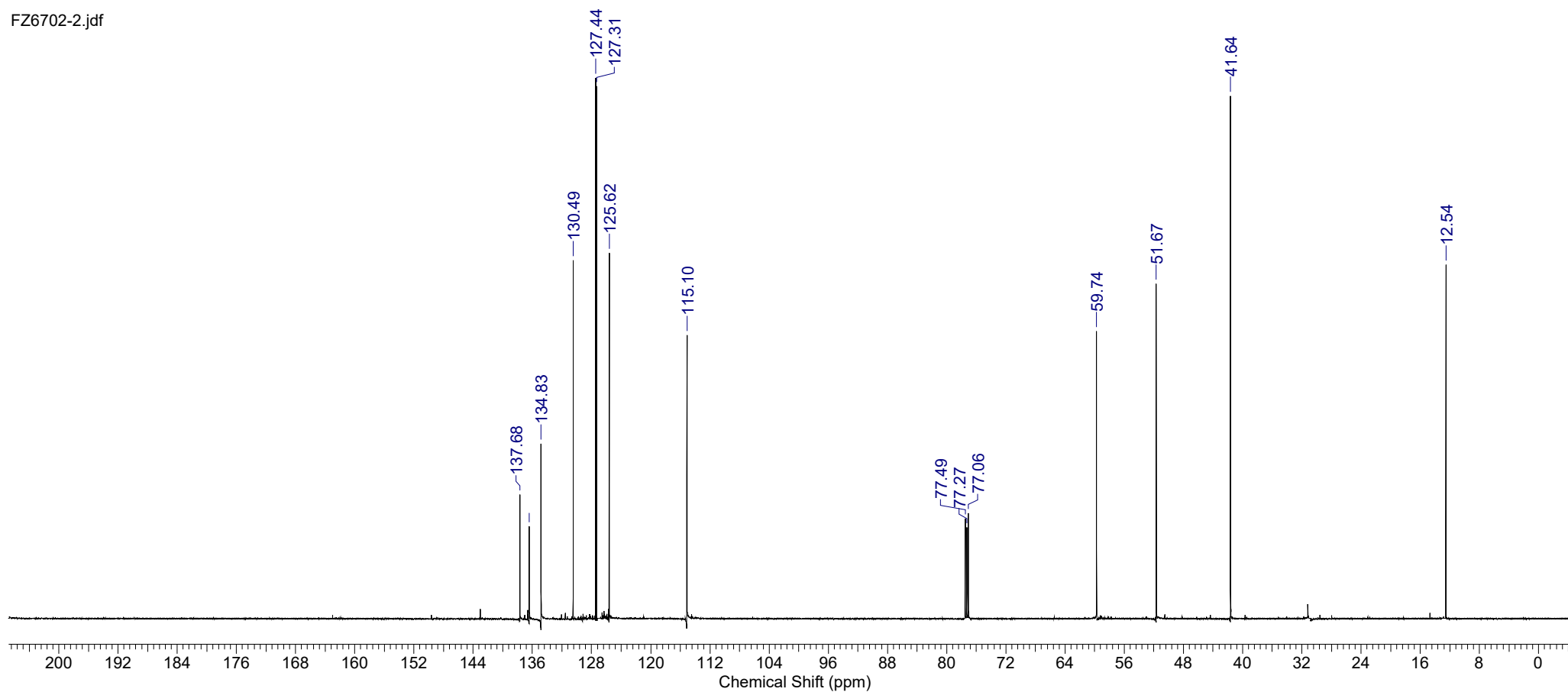


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	18 May 1990 05:49:40	
Date Stamp	14 May 2018 10:36:25		File Name	C:\Users\Fedor\Desktop\FZ6702-2.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	2000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.100				

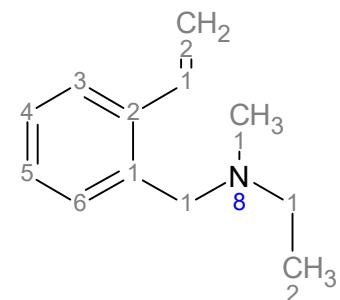


4b

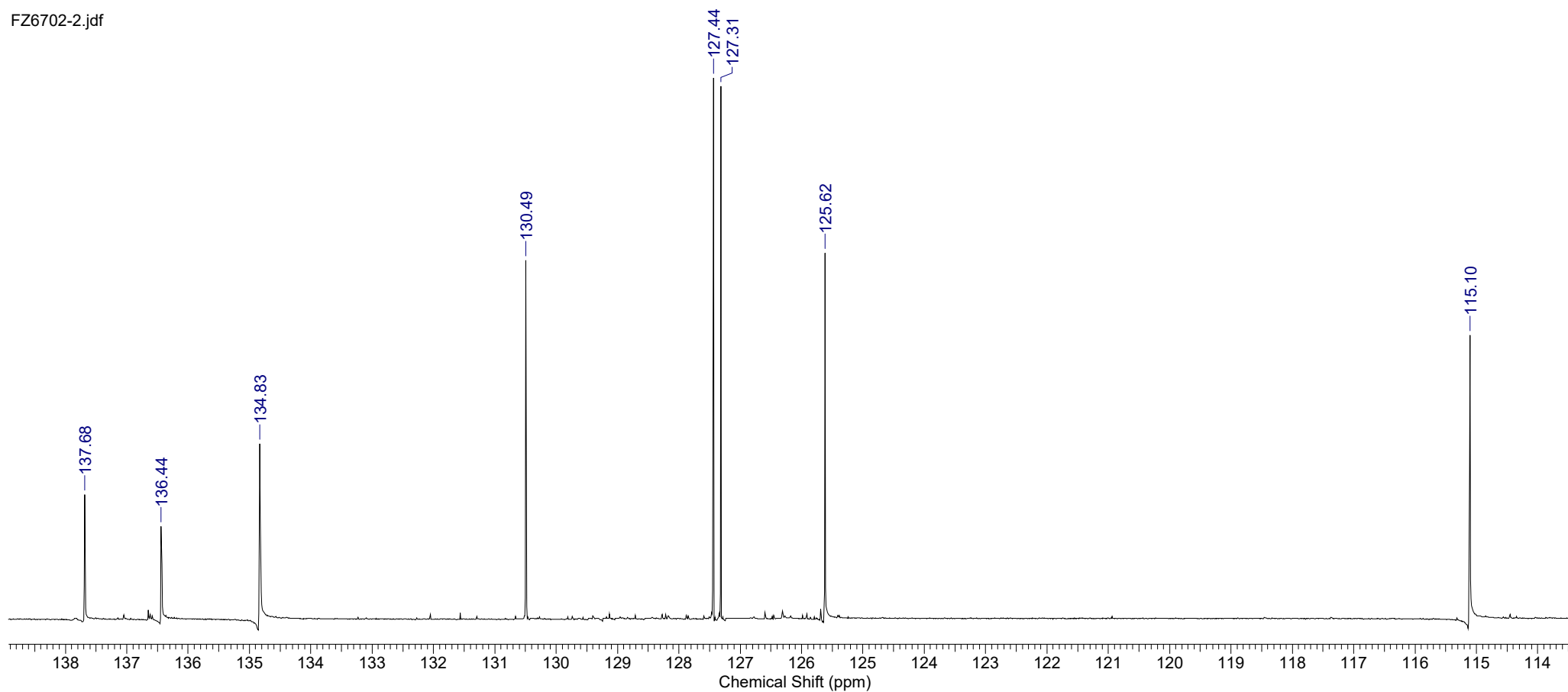
FZ6702-2.jdf



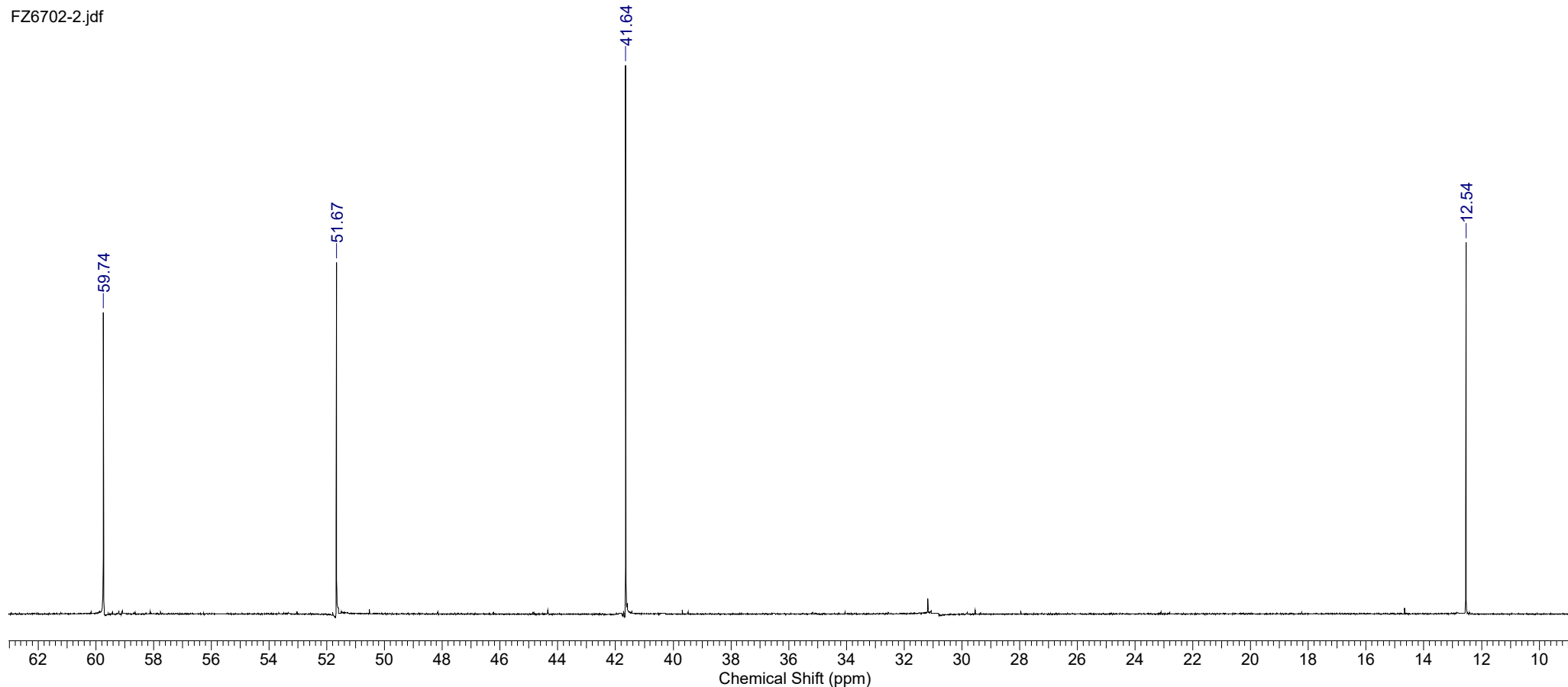
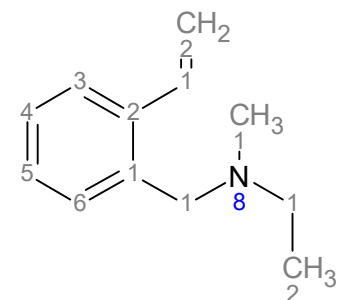
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	18 May 1990 05:49:40	
Date Stamp	14 May 2018 10:36:25		File Name	C:\Users\Fedor\Desktop\FZ6702-2.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	2000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.100				



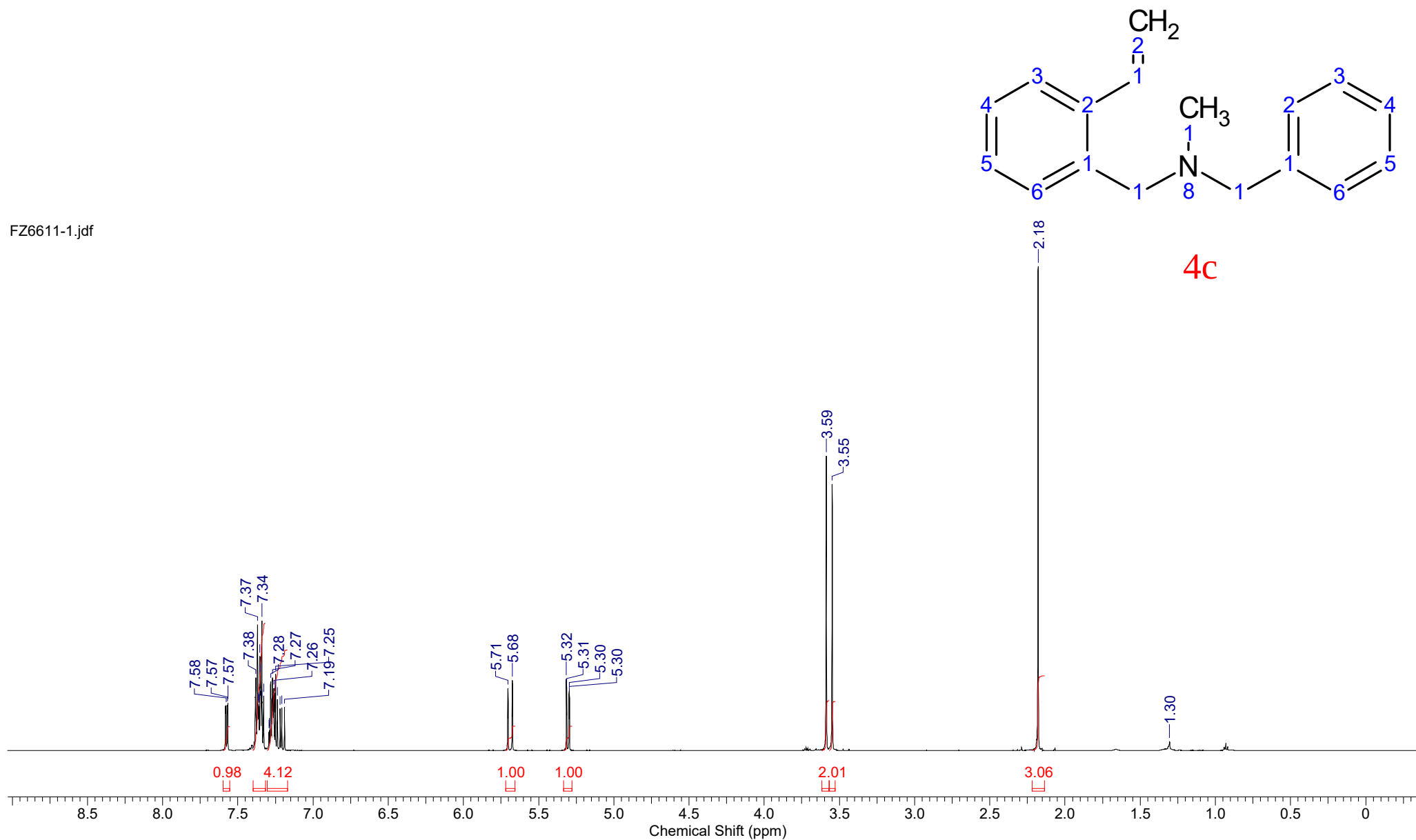
FZ6702-2.jdf



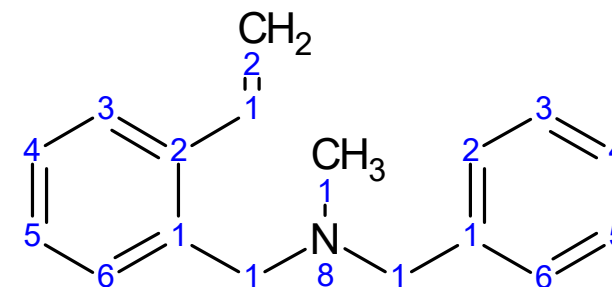
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	18 May 1990 05:49:40	
Date Stamp	14 May 2018 10:36:25		File Name	C:\Users\Fedor\Desktop\FZ6702-2.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	2000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.100				



Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	15 Apr 1990 04:18:56	
Date Stamp	11 Apr 2018 09:06:28			File Name	C:\Users\Fedor\Desktop\10.04.18\FZ6611-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 30.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	21.900	

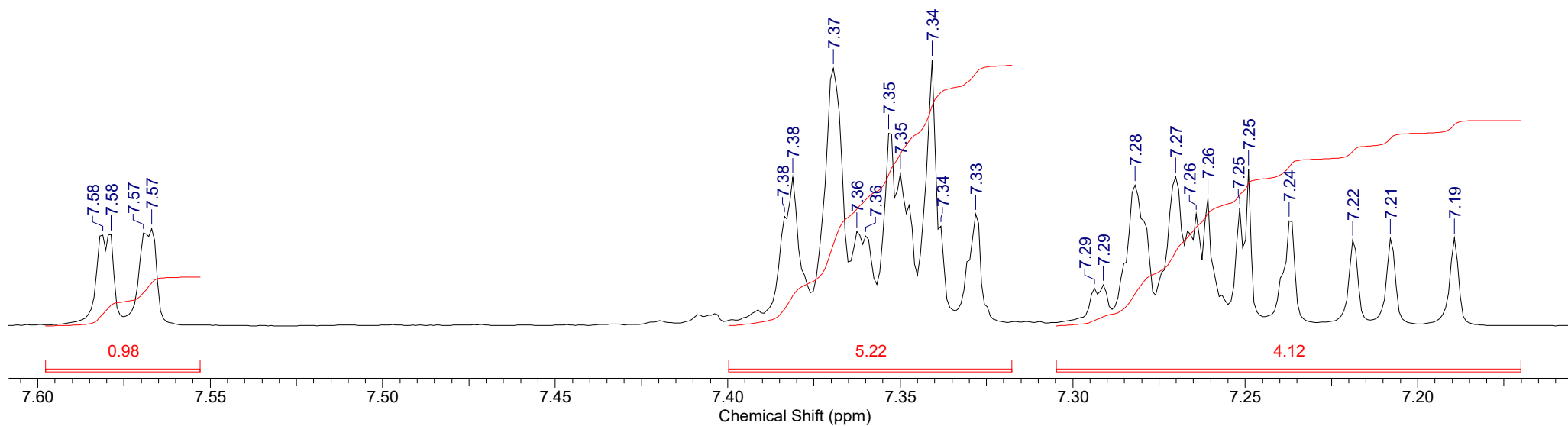


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	15 Apr 1990 04:18:56	
Date Stamp	11 Apr 2018 09:06:28			File Name	C:\Users\Fedor\Desktop\10.04.18\FZ6611-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 30.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	21.900	

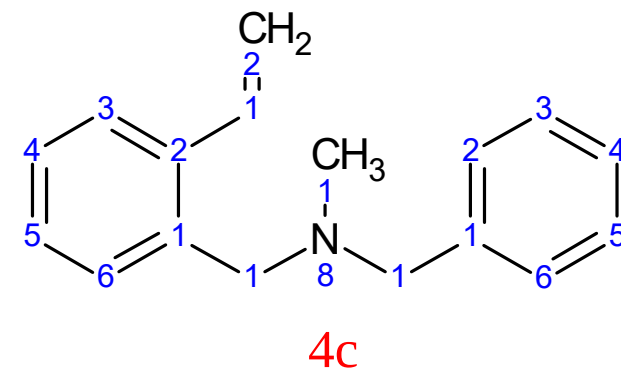


4c

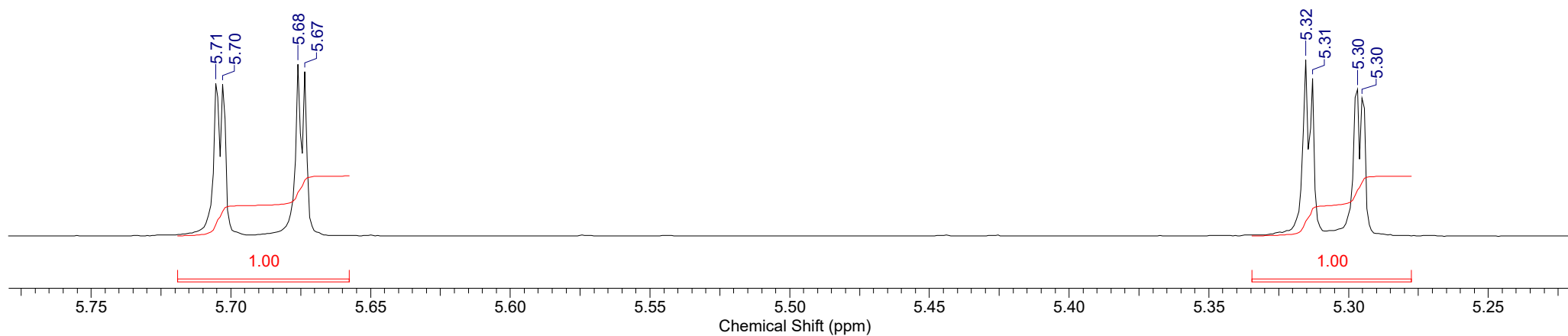
FZ6611-1.jdf



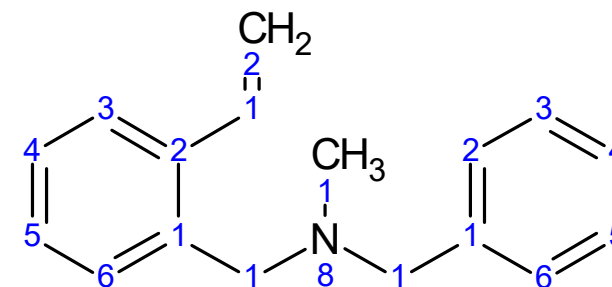
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	15 Apr 1990 04:18:56	
Date Stamp	11 Apr 2018 09:06:28			File Name	C:\Users\Fedor\Desktop\10.04.18\FZ6611-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 30.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	21.900	



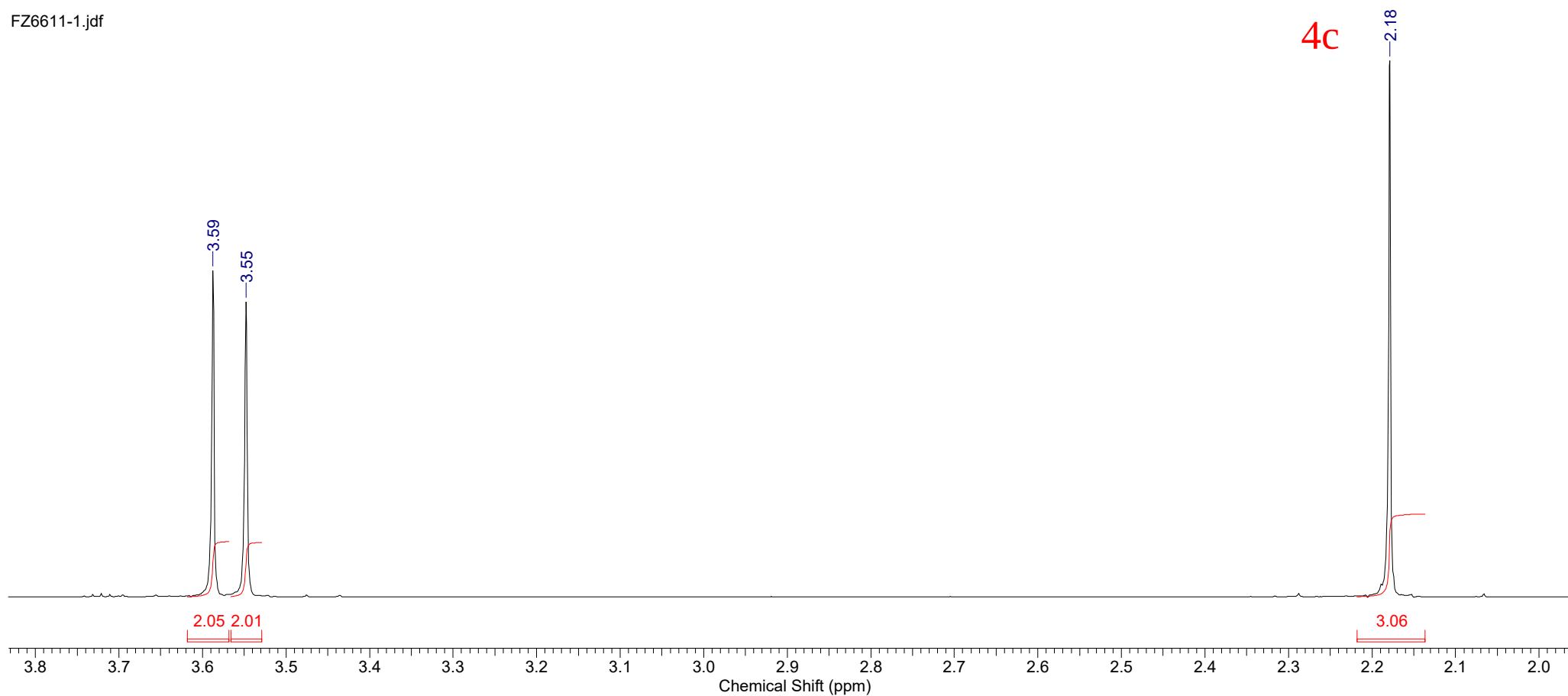
FZ6611-1.jdf



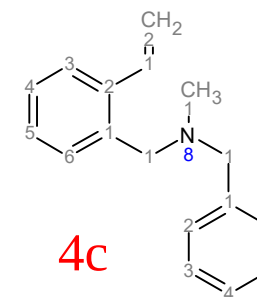
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	15 Apr 1990 04:18:56		
Date Stamp	11 Apr 2018 09:06:28			File Name	C:\Users\Fedor\Desktop\10.04.18\FZ6611-1.jdf	Frequency (MHz)	600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse.ex2			Receiver Gain	30.00
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	21.900	Solvent	CHLOROFORM-d



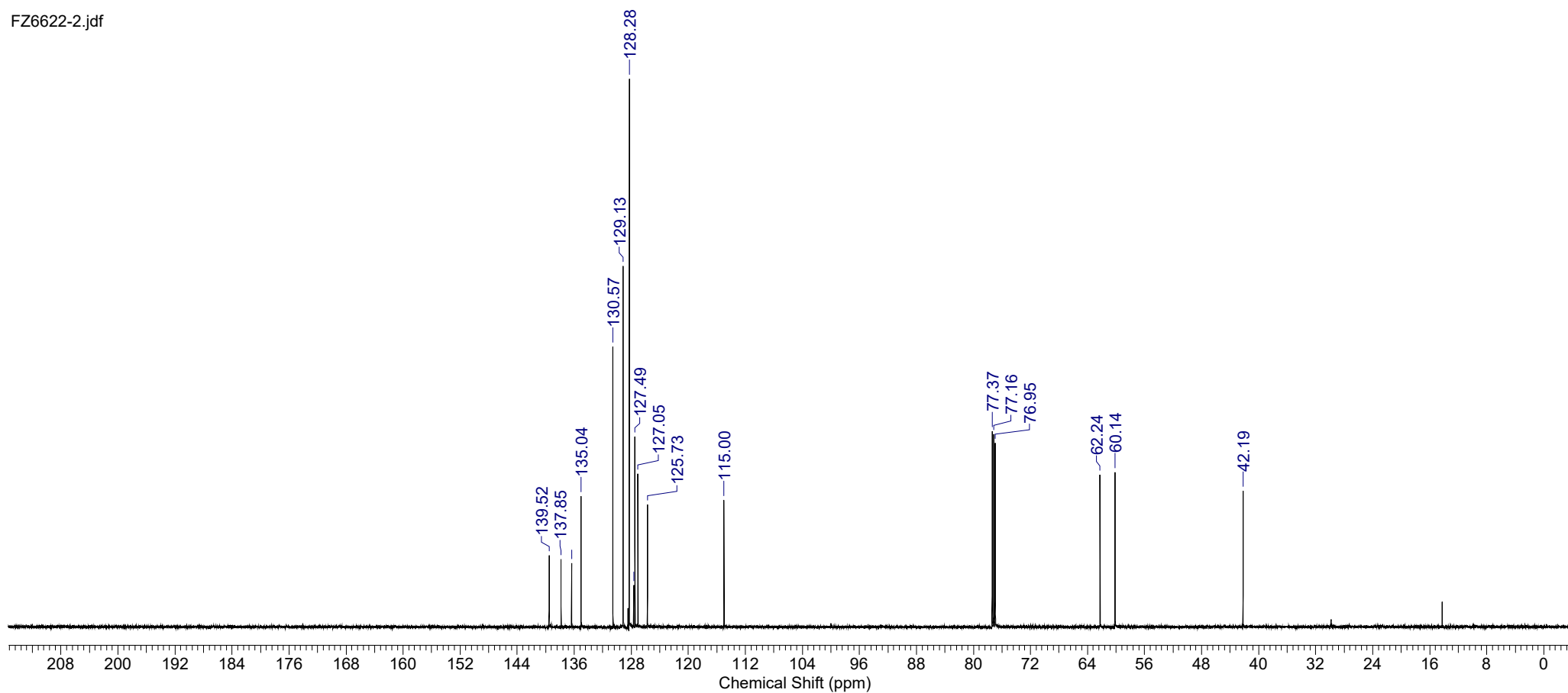
FZ6611-1.jdf



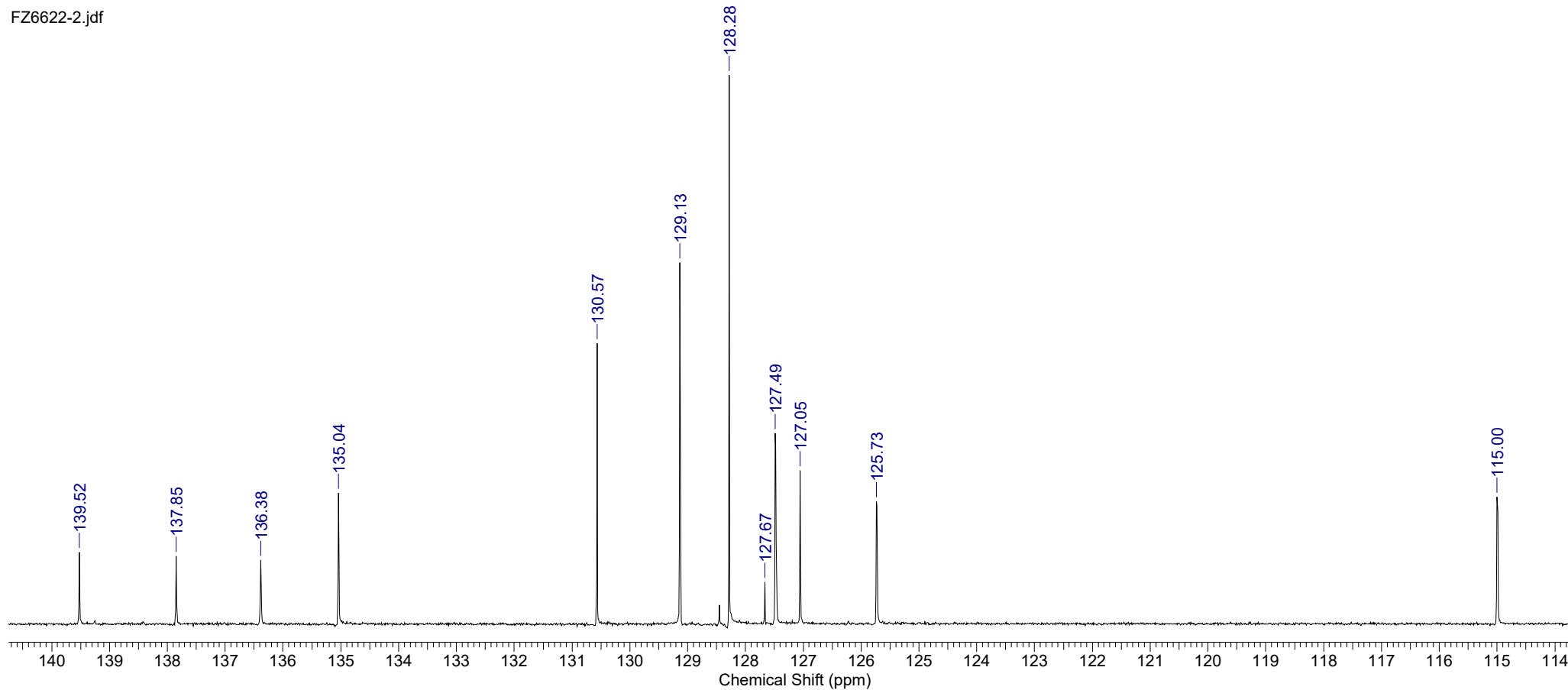
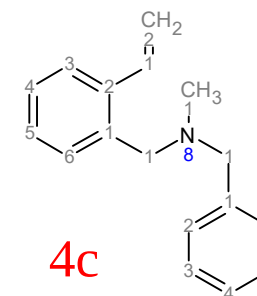
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	27 Apr 1990 04:56:23	
Date Stamp	23 Apr 2018 09:43:28		File Name	C:\Users\Fedor\Desktop\FZ6622-2.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	800	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	54.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	23.400				



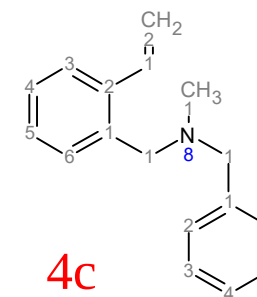
FZ6622-2.jdf



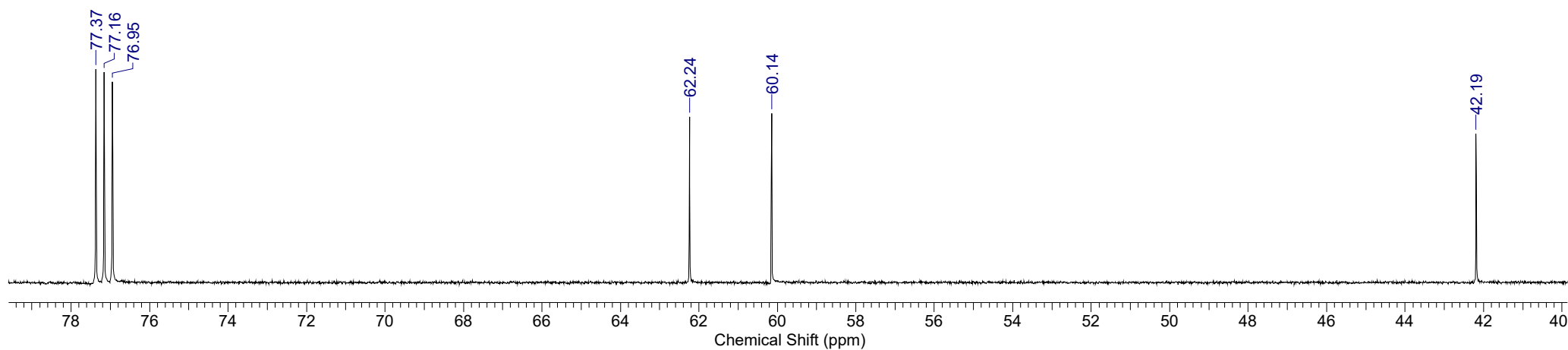
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	27 Apr 1990 04:56:23	
Date Stamp	23 Apr 2018 09:43:28		File Name	C:\Users\Fedor\Desktop\FZ6622-2.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	800	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	54.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	23.400				



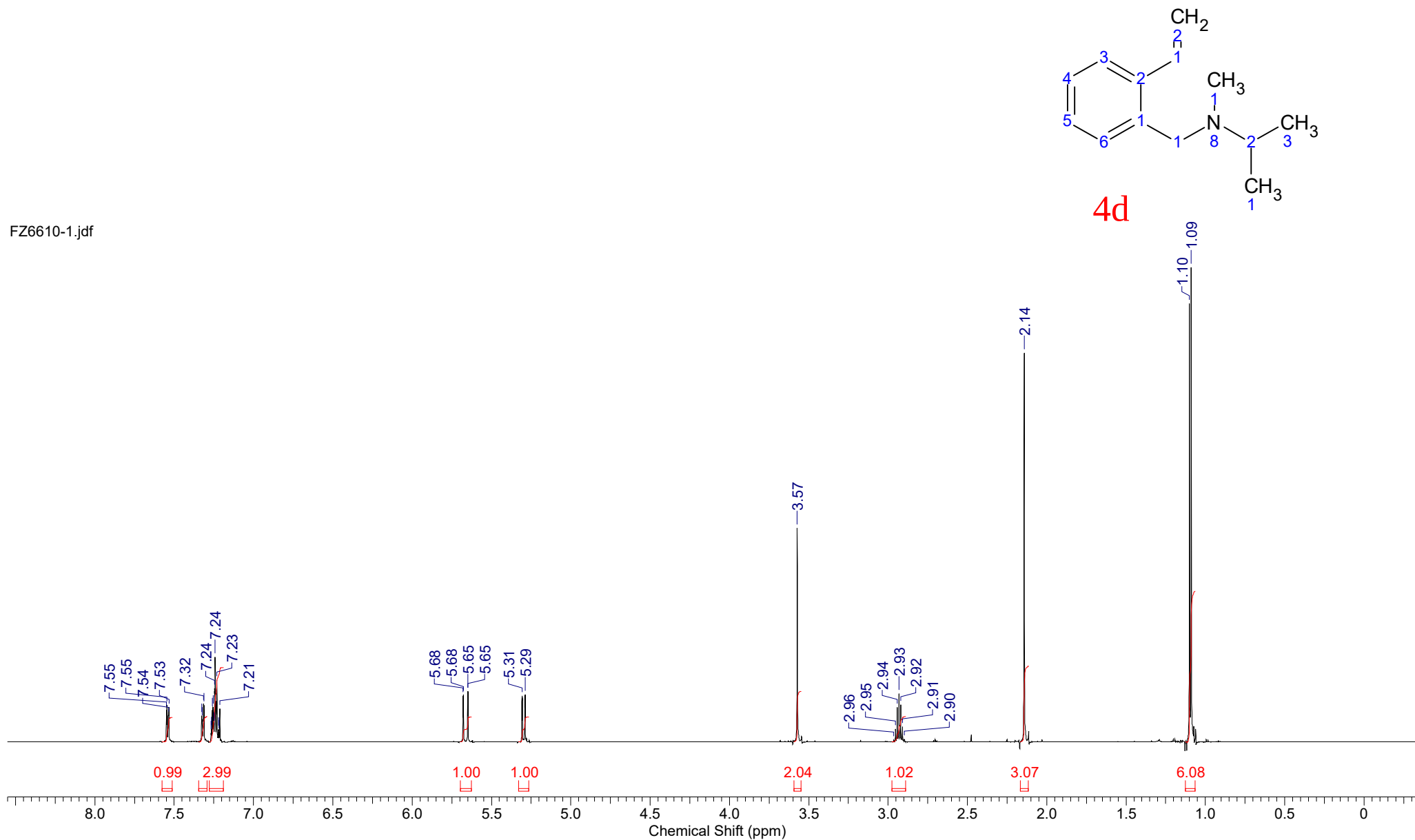
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	27 Apr 1990 04:56:23	
Date Stamp	23 Apr 2018 09:43:28		File Name	C:\Users\Fedor\Desktop\FZ6622-2.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	800	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	54.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	23.400				



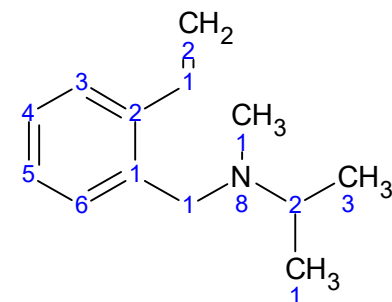
FZ6622-2.jdf



Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	15 Apr 1990 04:13:18	
Date Stamp	11 Apr 2018 09:00:50			File Name	C:\Users\Fedor\Desktop\10.04.18\FZ6610-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 26.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	22.000	

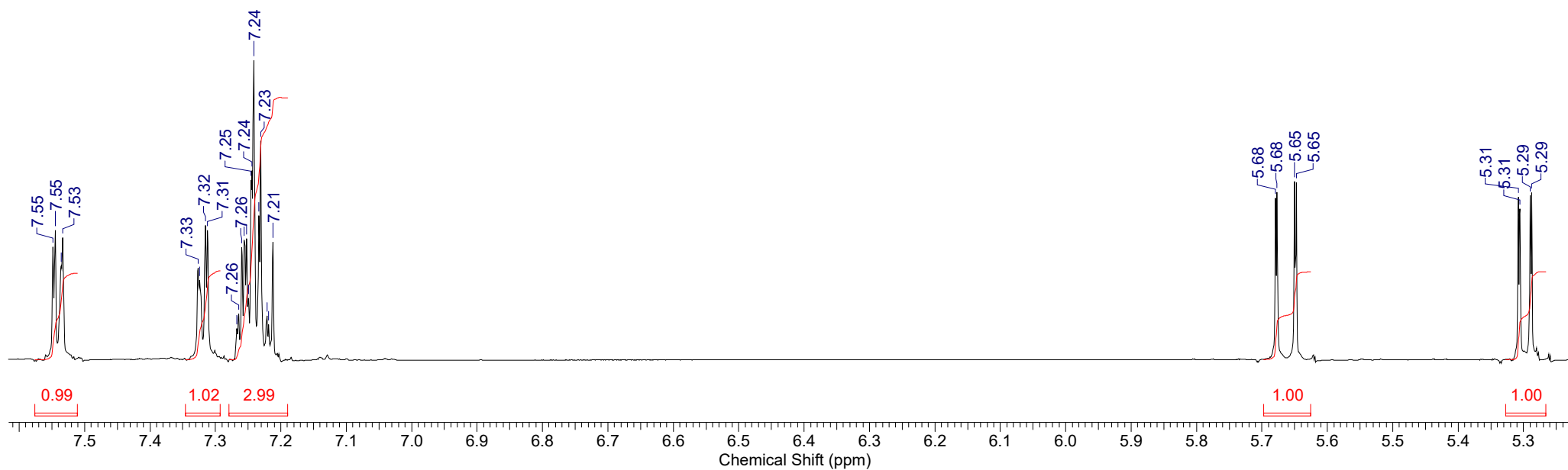


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	15 Apr 1990 04:13:18	
Date Stamp	11 Apr 2018 09:00:50			File Name	C:\Users\Fedor\Desktop\10.04.18\FZ6610-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 26.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	22.000	

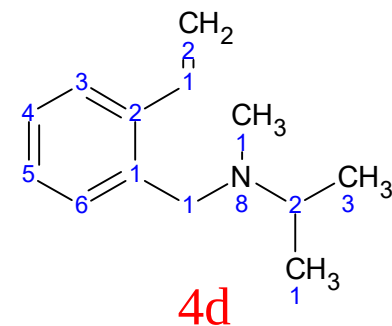


4d

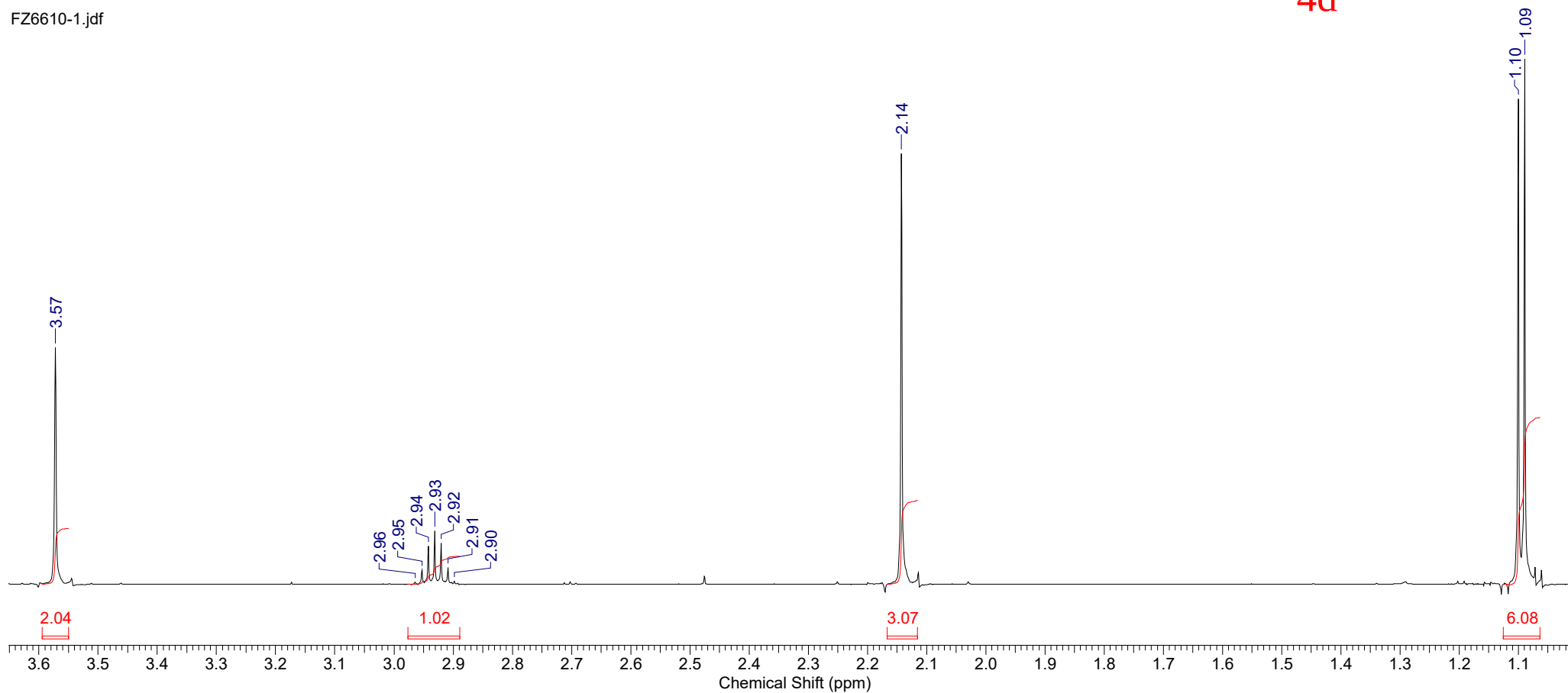
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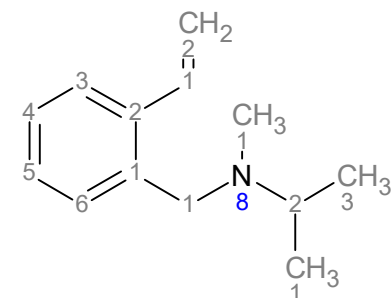
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	15 Apr 1990 04:13:18	
Date Stamp	11 Apr 2018 09:00:50			File Name	C:\Users\Fedor\Desktop\10.04.18\FZ6610-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 26.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	22.000	



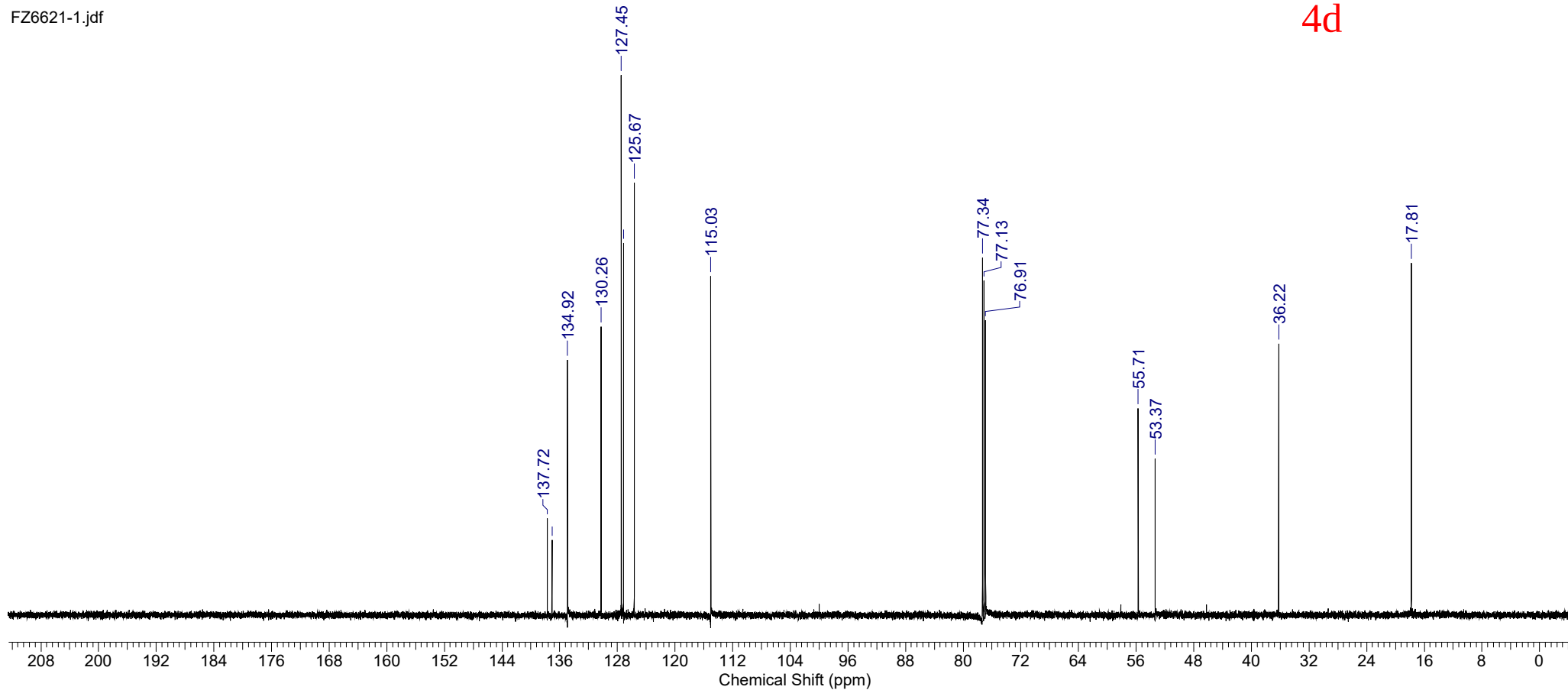
FZ6610-1.jdf



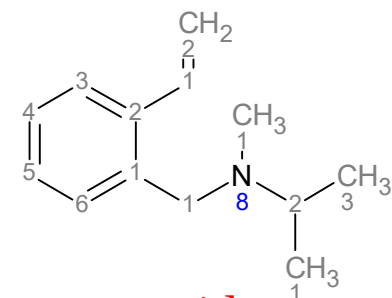
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	22 Apr 1990 08:30:36	
Date Stamp	18 Apr 2018 13:18:15	File Name	C:\Users\Fedor\Desktop\17.04.18\FZ6621-1.jdf				
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	246	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.700				



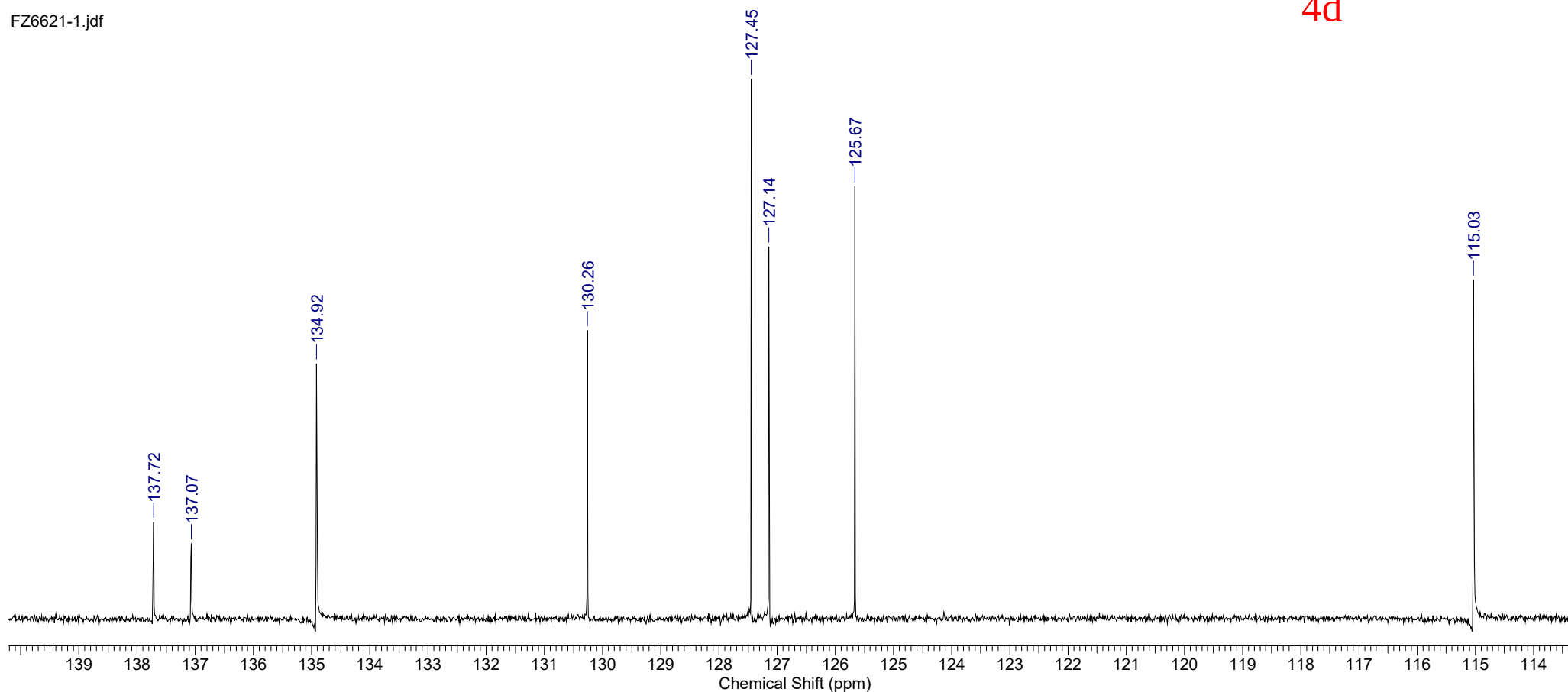
4d



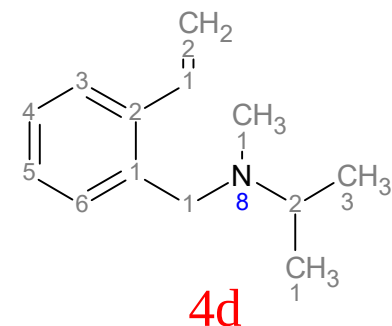
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	22 Apr 1990 08:30:36	
Date Stamp	18 Apr 2018 13:18:15		File Name	C:\Users\Fedor\Desktop\17.04.18\FZ6621-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	246	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.700				



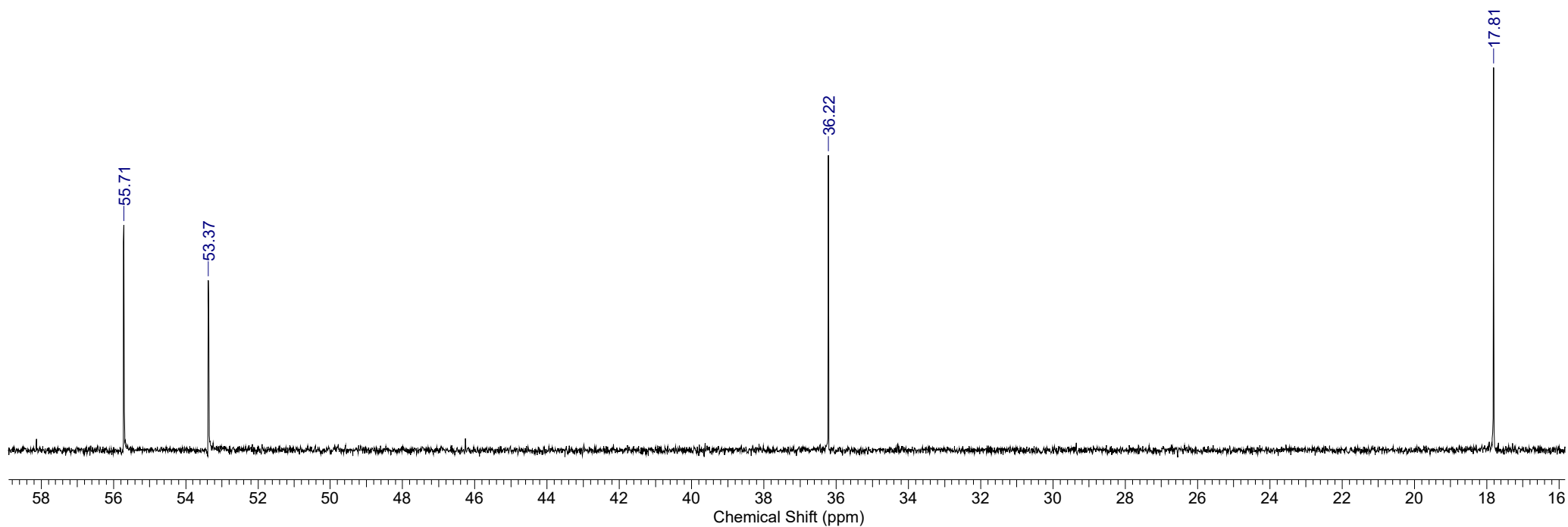
FZ6621-1.jdf



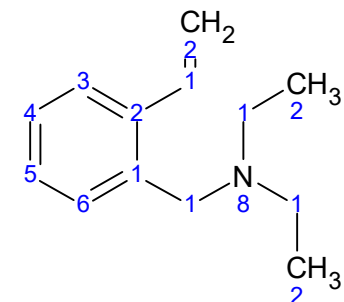
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	22 Apr 1990 08:30:36	
Date Stamp	18 Apr 2018 13:18:15		File Name	C:\Users\Fedor\Desktop\17.04.18\FZ6621-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	246	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.700				



FZ6621-1.jdf

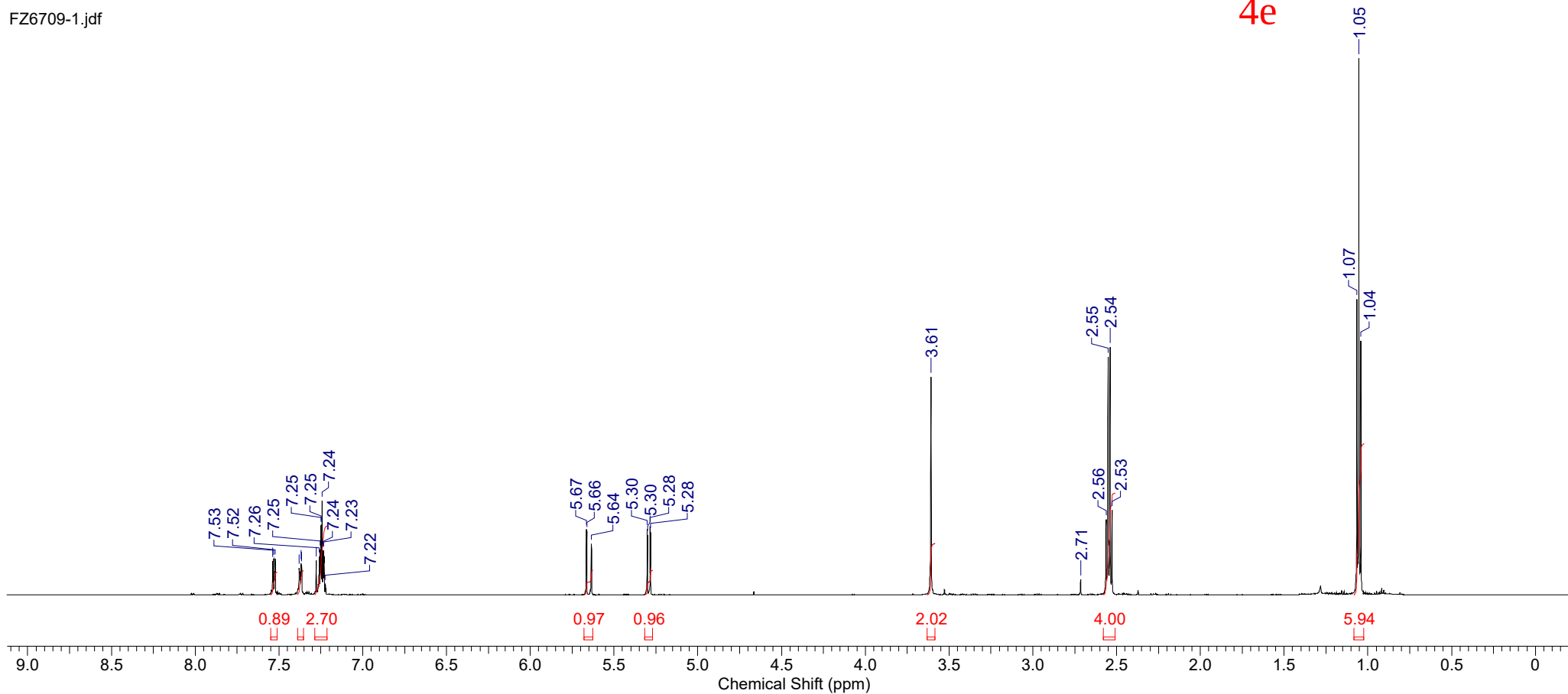


Acquisition Time (sec)	1.9818	Comment	single pulse	Date	21 May 1990 06:49:43	
Date Stamp	17 May 2018 11:36:26			File Name	C:\Users\Fedor\Desktop\15.05.18\FZ6709-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 26.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	19.600	

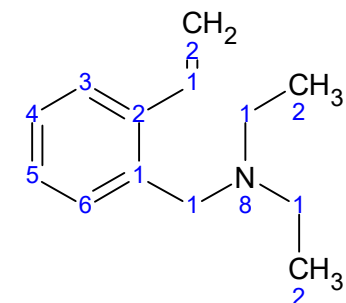


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FZ6709-1.jdf

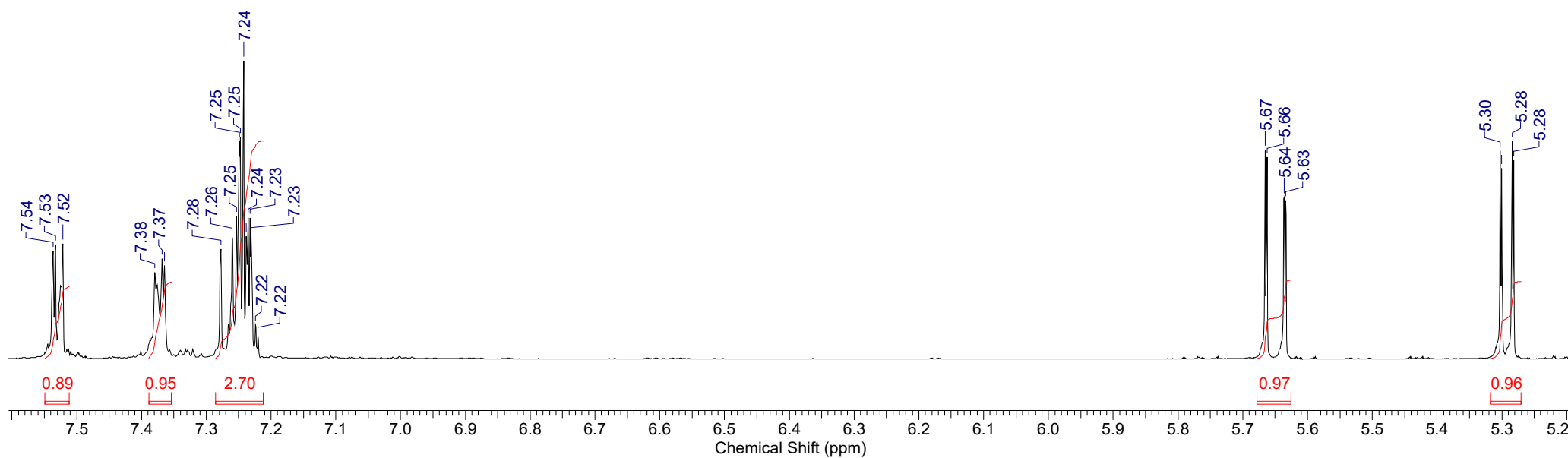


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	21 May 1990 06:49:43	
Date Stamp	17 May 2018 11:36:26			File Name	C:\Users\Fedor\Desktop\15.05.18\FZ6709-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Original Points Count 32768	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	19.600	

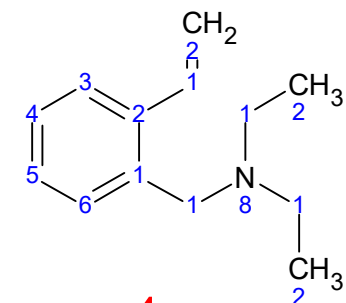


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FZ6709-1.jdf

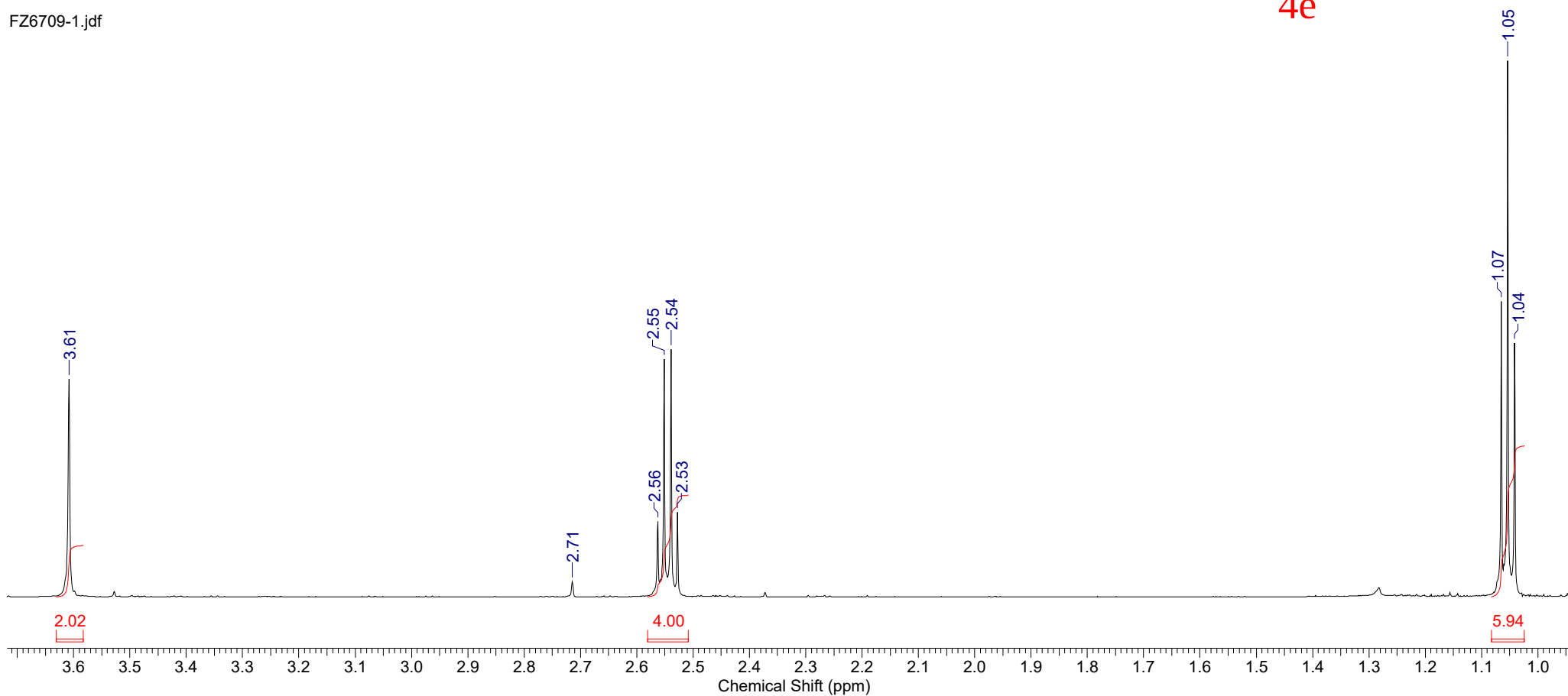


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	21 May 1990 06:49:43	
Date Stamp	17 May 2018 11:36:26			File Name	C:\Users\Fedor\Desktop\15.05.18\FZ6709-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 26.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	19.600	

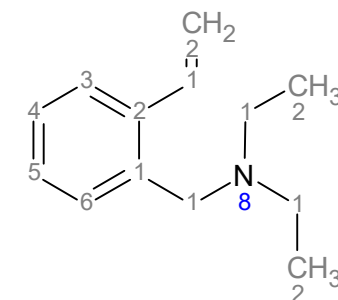


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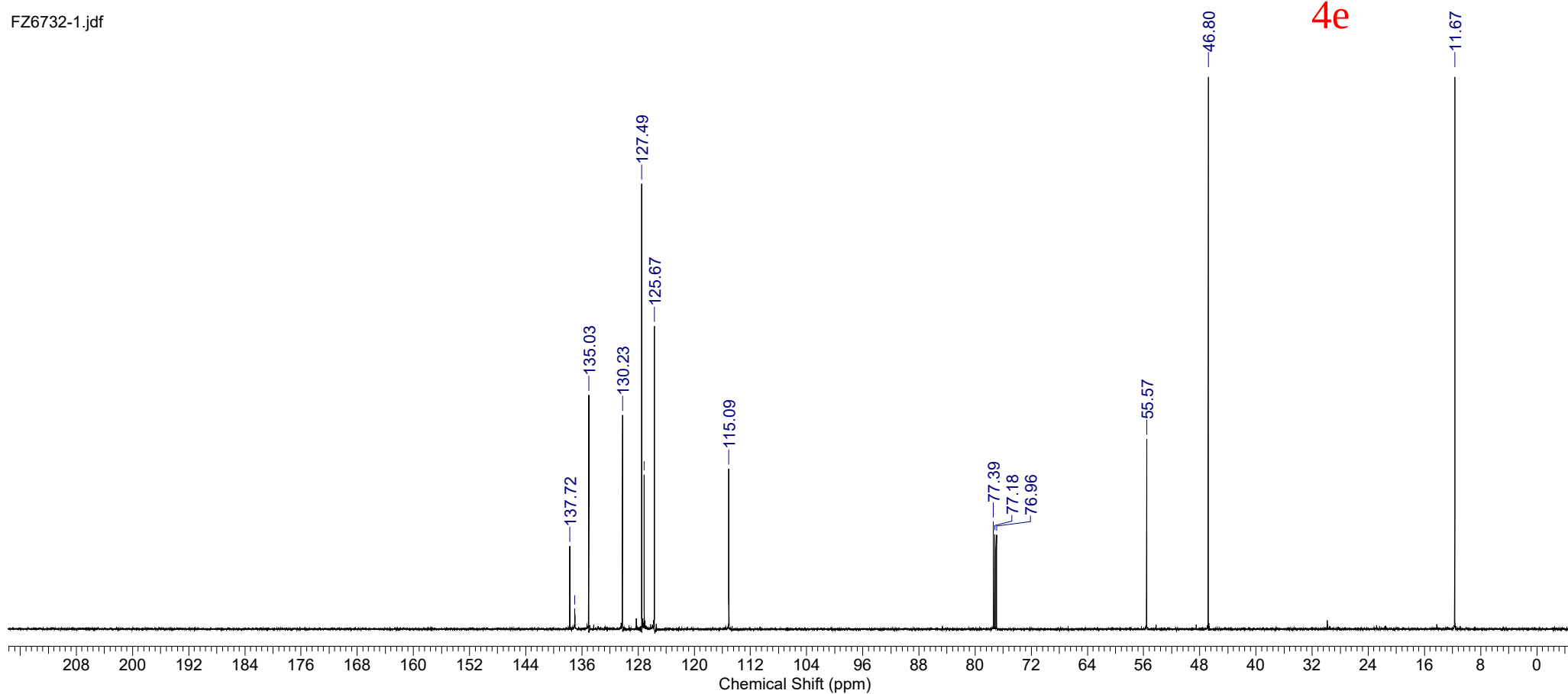
FZ6709-1.jdf



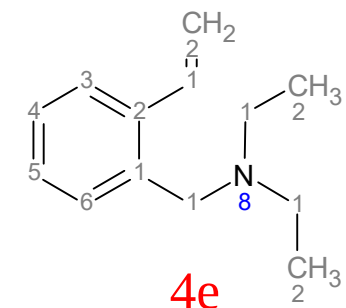
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	28 May 1990 00:10:35	
Date Stamp	24 May 2018 04:57:18		File Name	C:\Users\Fedor\Desktop\22.05.18\FZ6732-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.200				



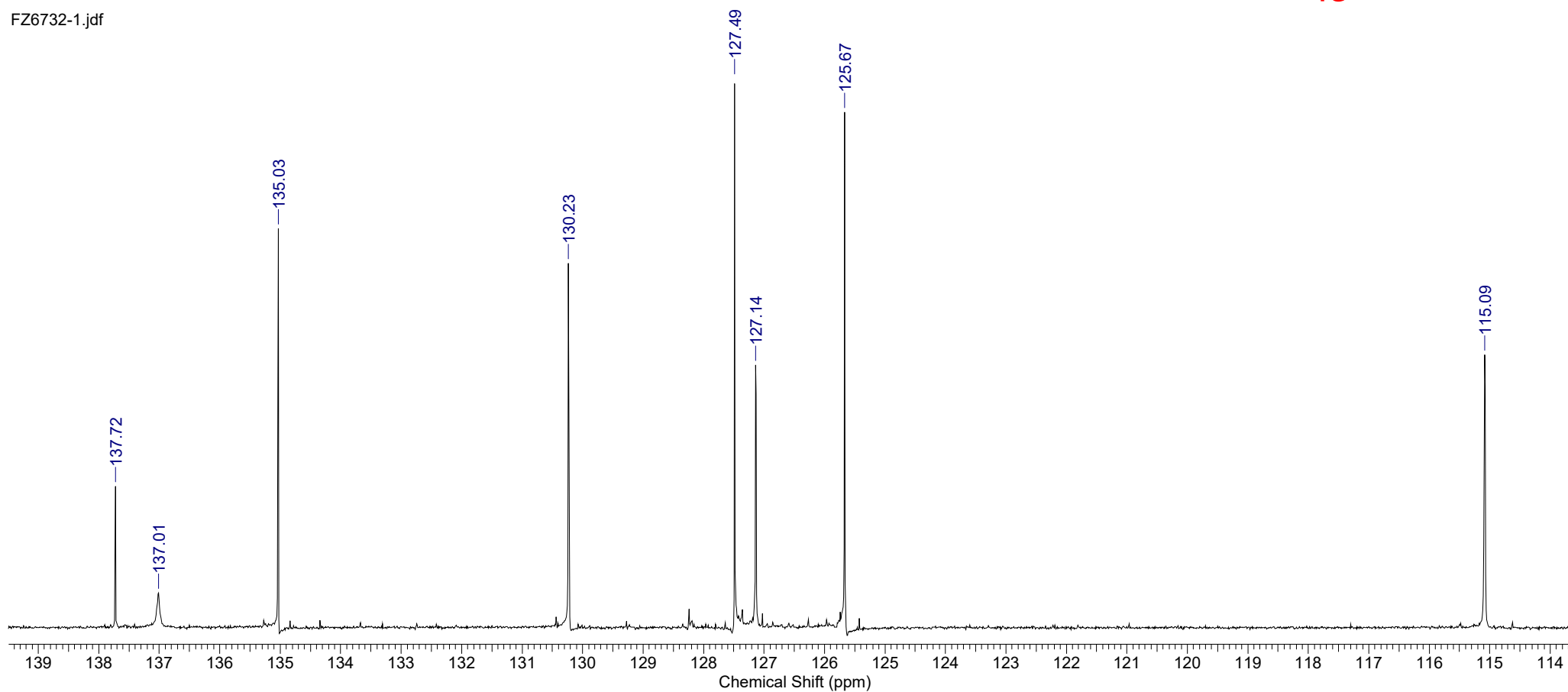
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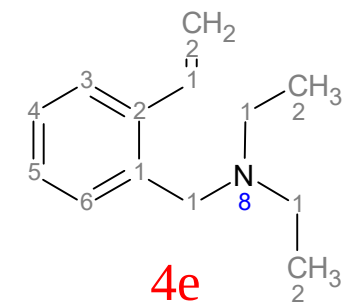
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	28 May 1990 00:10:35	
Date Stamp	24 May 2018 04:57:18		File Name	C:\Users\Fedor\Desktop\22.05.18\FZ6732-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.200				



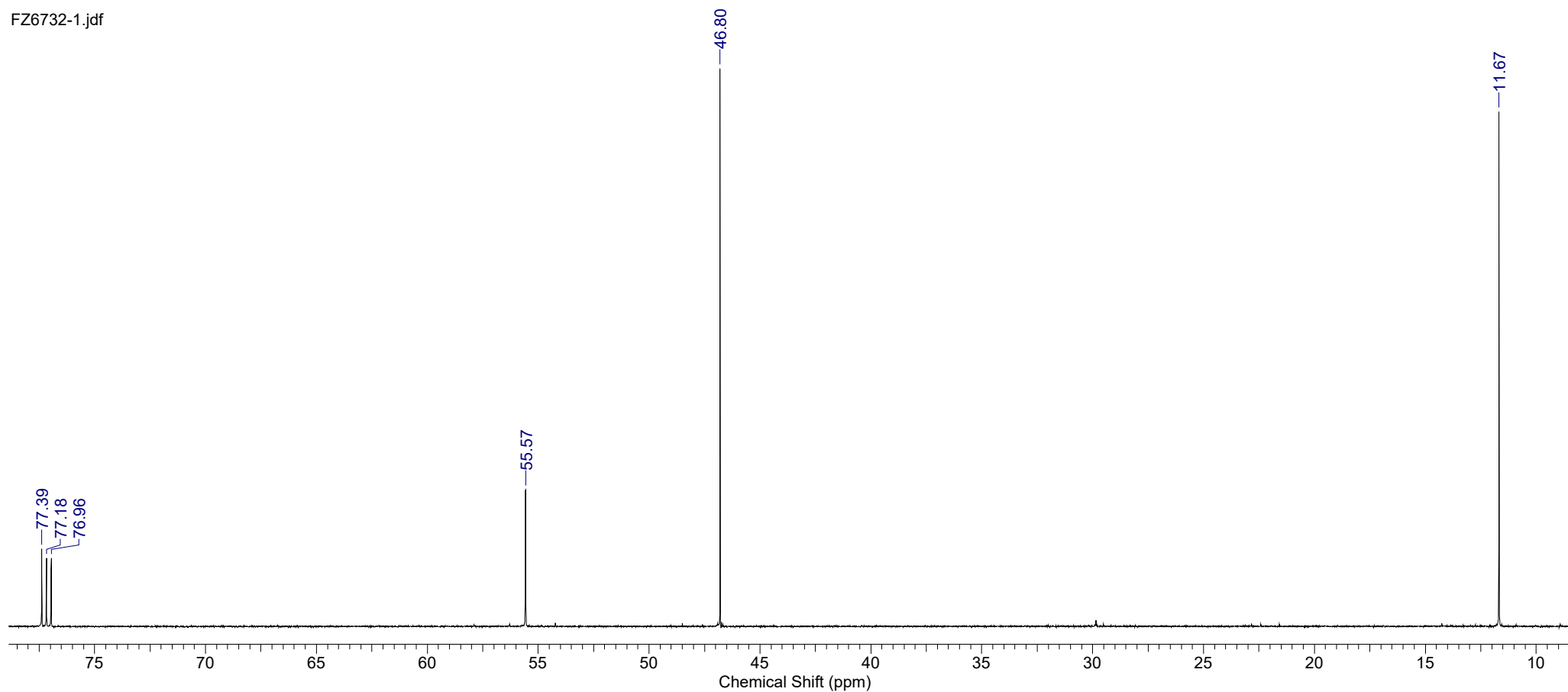
FZ6732-1.jdf



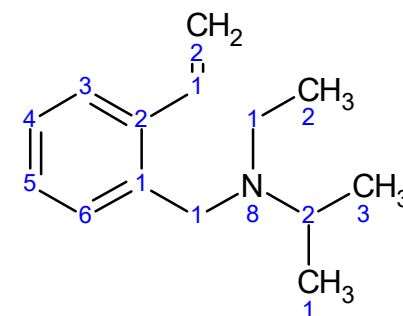
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	28 May 1990 00:10:35	
Date Stamp	24 May 2018 04:57:18		File Name	C:\Users\Fedor\Desktop\22.05.18\FZ6732-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.200				



FZ6732-1.jdf

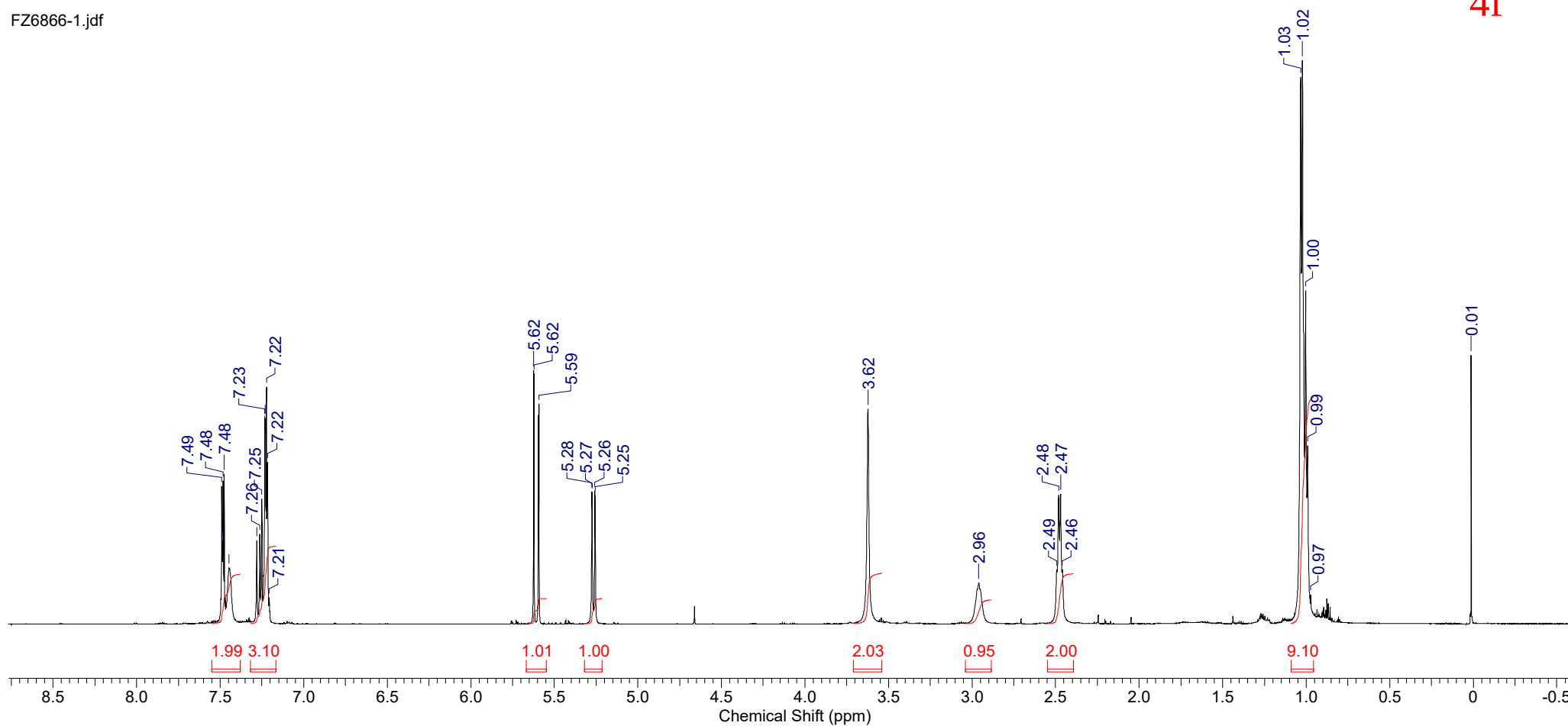


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	01 Mar 1990 00:08:24	Date Stamp	29 Aug 2018 09:38:17
File Name	C:\Users\Fedor\Desktop\28.08.18\FZ6866-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39

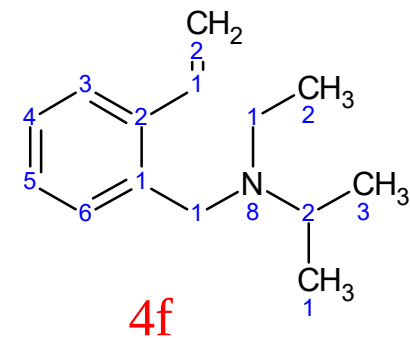


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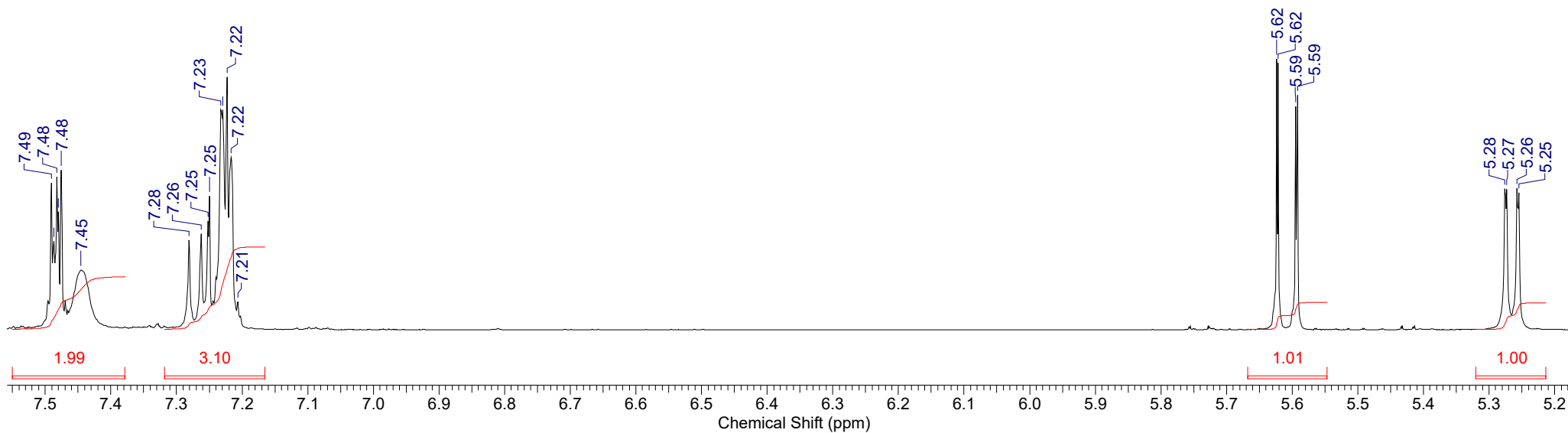
FZ6866-1.jdf



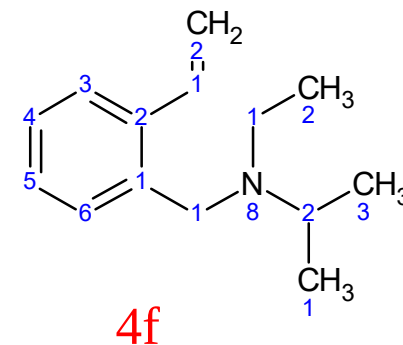
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	01 Mar 1990 00:08:24	Date Stamp	29 Aug 2018 09:38:17
File Name	C:\Users\Fedor\Desktop\28.08.18\FZ6866-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



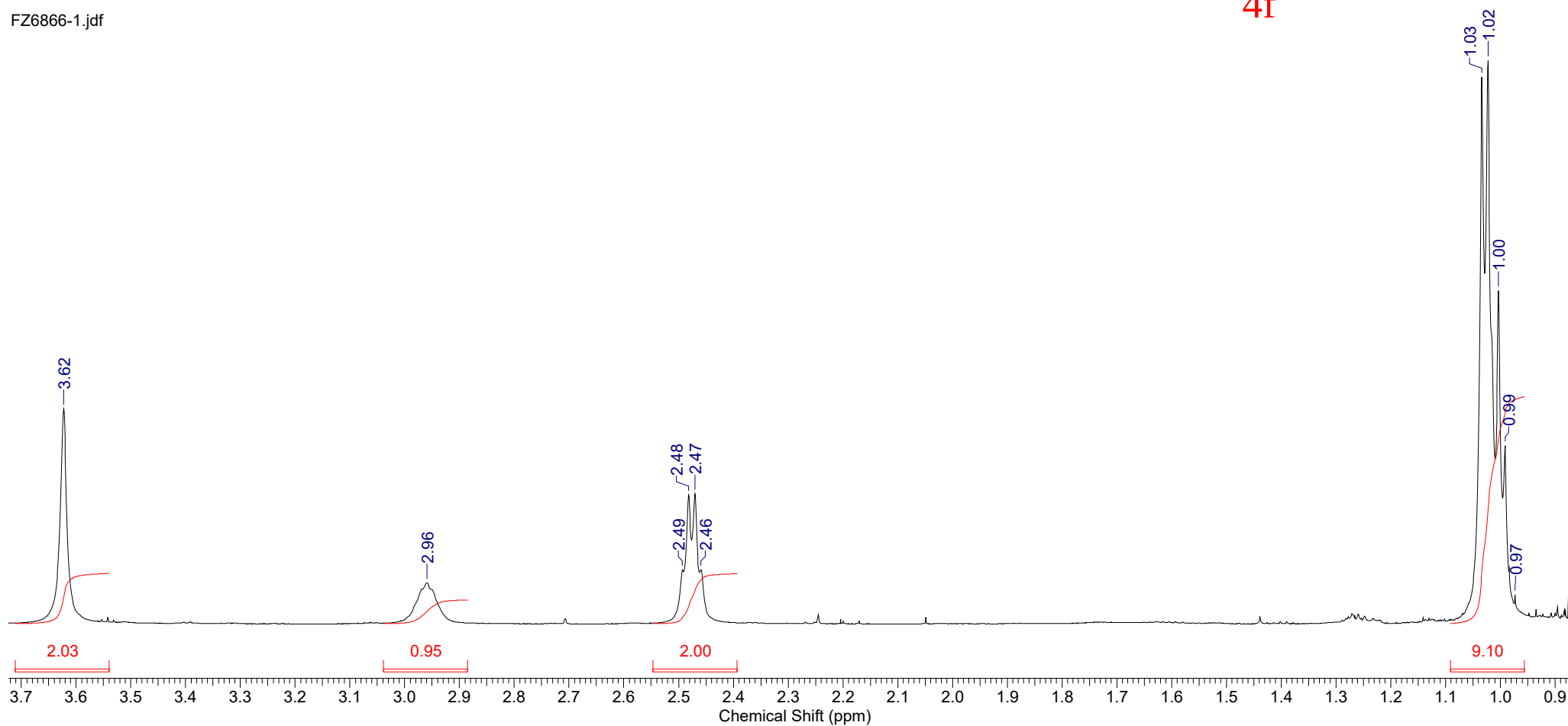
FZ6866-1.jdf



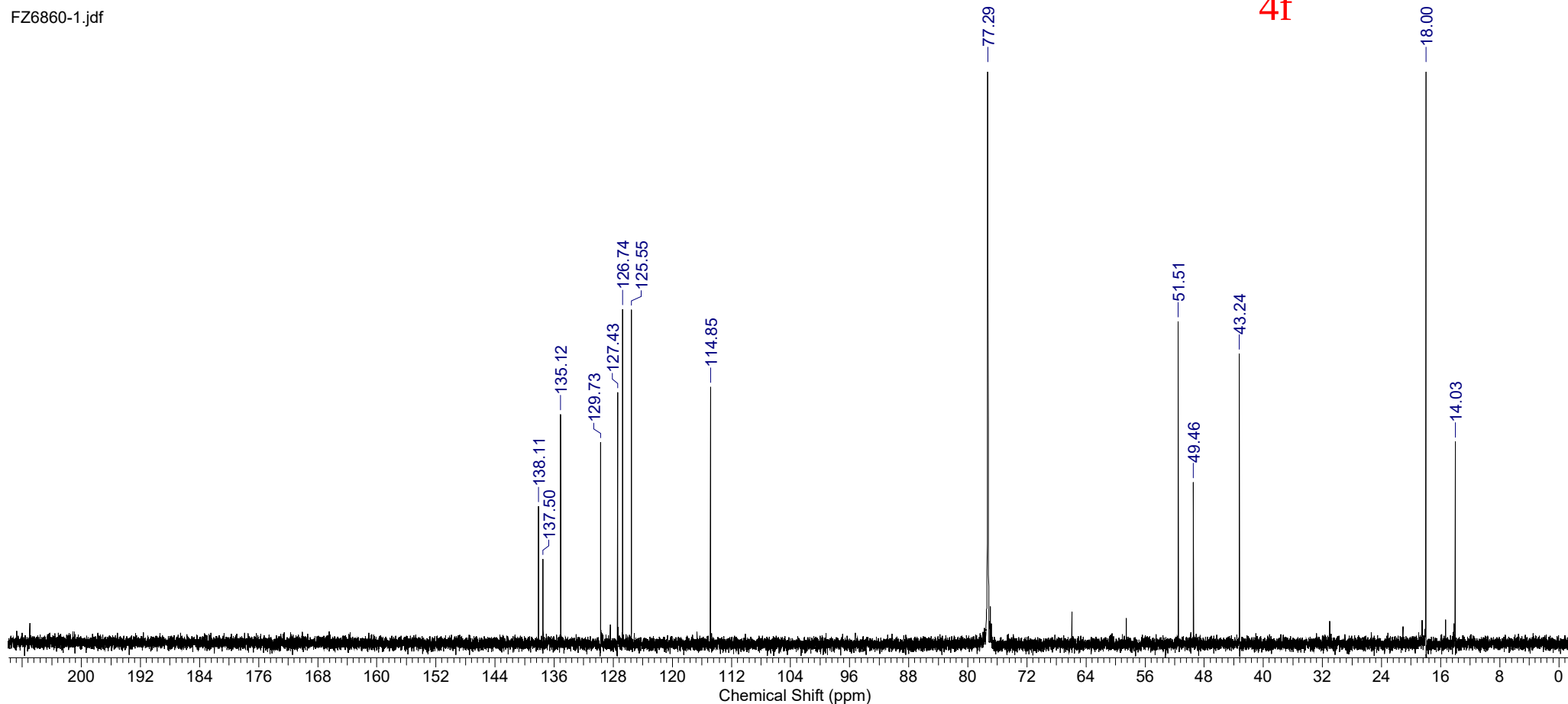
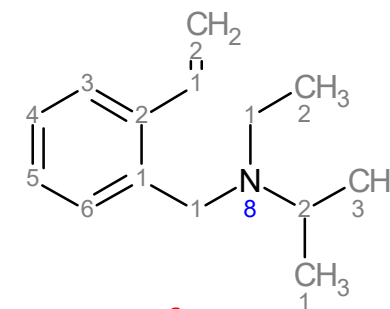
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	01 Mar 1990 00:08:24	Date Stamp	29 Aug 2018 09:38:17
File Name	C:\Users\Fedor\Desktop\28.08.18\FZ6866-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



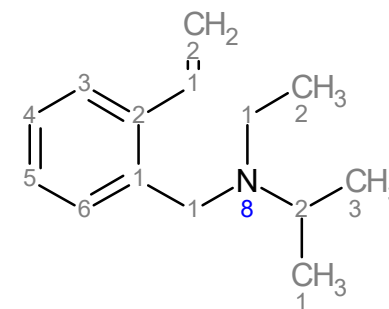
FZ6866-1.jdf



Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	16 Feb 1990 04:58:32	
Date Stamp	15 Aug 2018 14:28:51	File Name	C:\Users\Fedor\Desktop\16.08.18\FZ6860-1.jdf			Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	2000	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single pulse dec	Receiver Gain	56.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49				

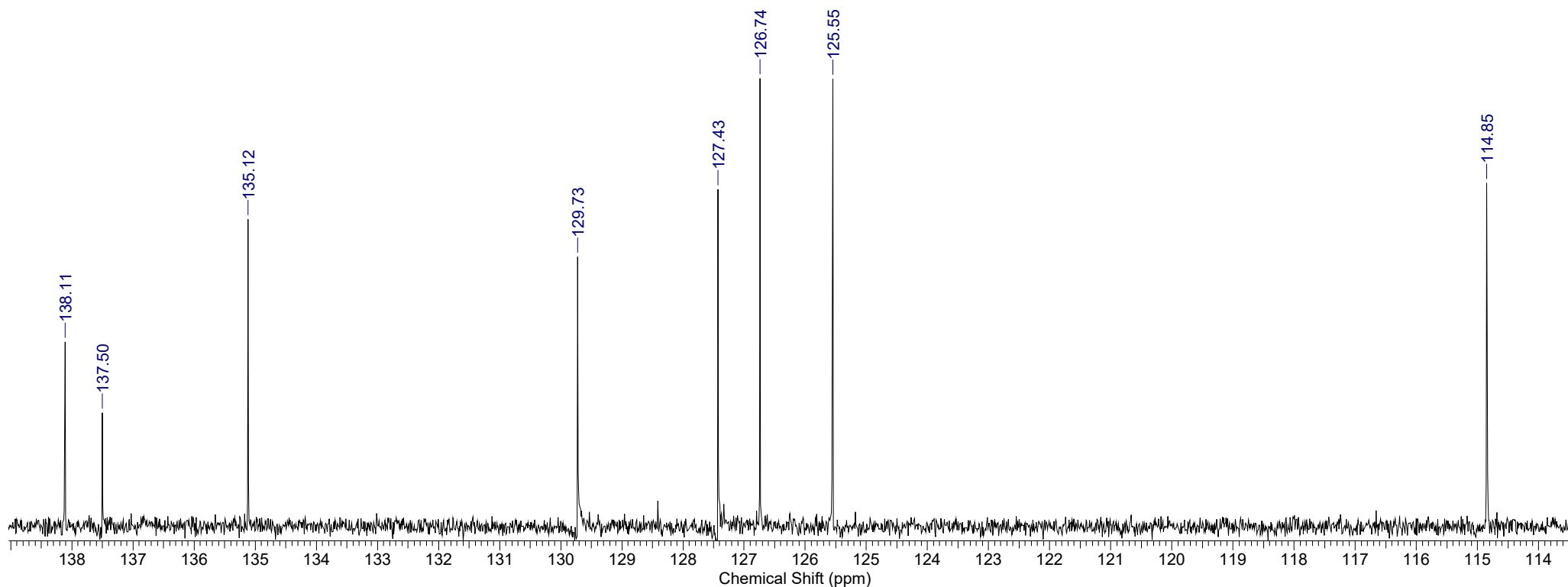


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	16 Feb 1990 04:58:32			
Date Stamp	15 Aug 2018 14:28:51	File Name	C:\Users\Fedor\Desktop\16.08.18\FZ6860-1.jdf			Frequency (MHz)	150.91		
Nucleus	13C	Number of Transients	2000	Origin	ECA 600	Original Points Count	32768		
Points Count	32768	Pulse Sequence	single pulse dec		Receiver Gain	56.00	Owner	delta	
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49					Solvent	CHLOROFORM-c

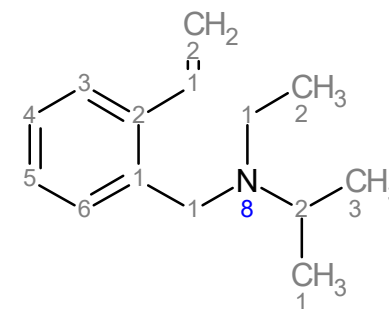


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FZ6860-1.jdf

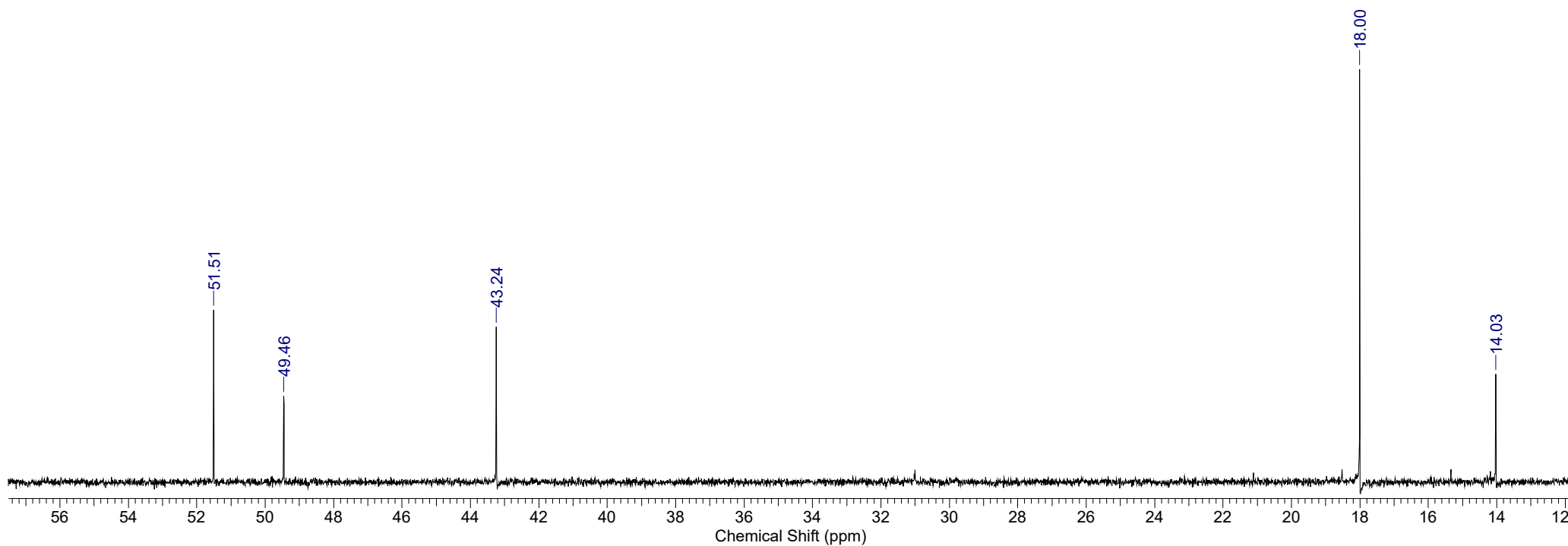


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	16 Feb 1990 04:58:32	
Date Stamp	15 Aug 2018 14:28:51	File Name	C:\Users\Fedor\Desktop\16.08.18\FZ6860-1.jdf		Frequency (MHz)	150.91	
Nucleus	¹³ C	Number of Transients	2000	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse_dec		Receiver Gain	56.00	Owner delta
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49		Solvent	CHLOROFORM-d	

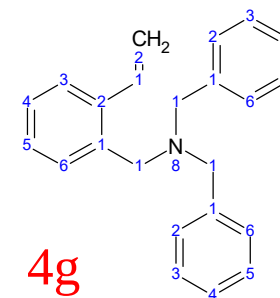


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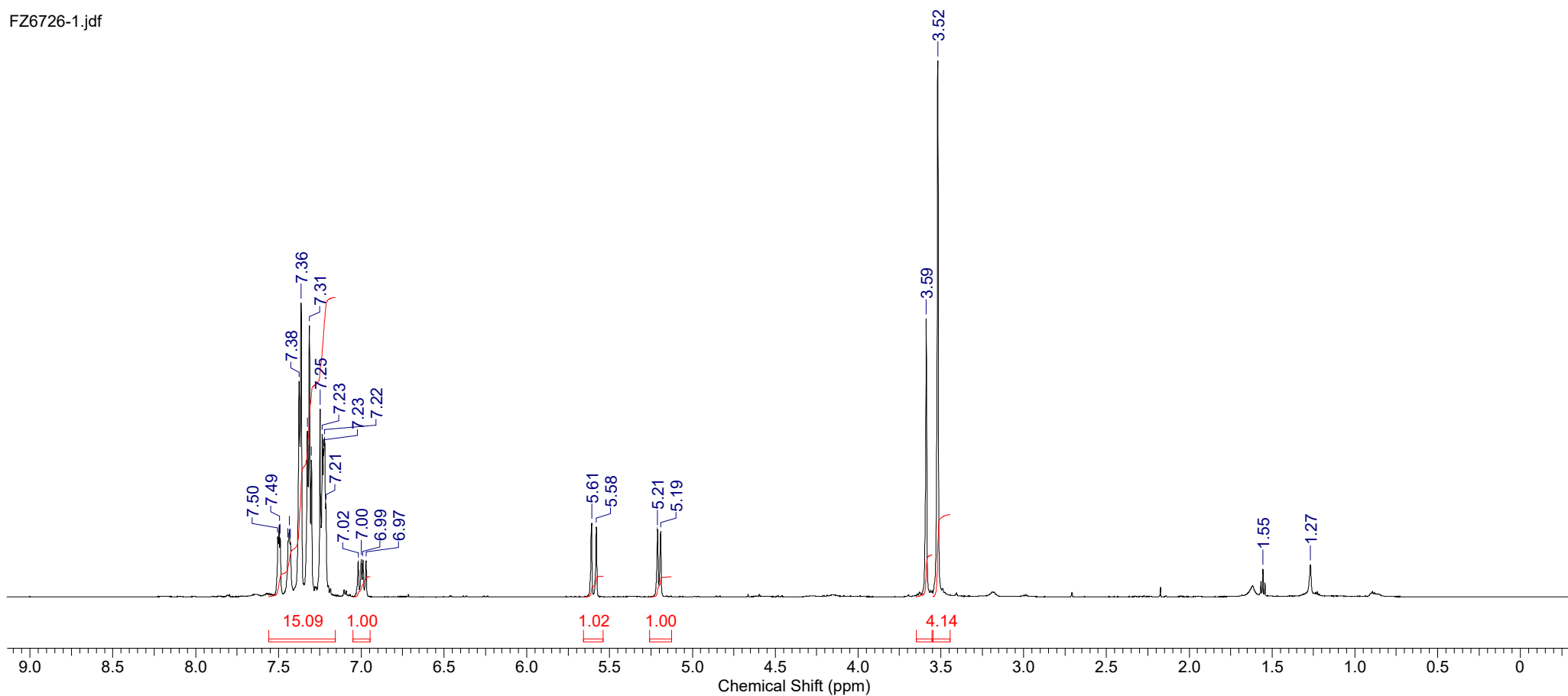
FZ6860-1.jdf



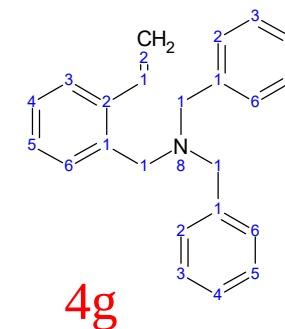
Acquisition Time (sec)	1.9818	Comment	single pulse	Date	21 May 1990 06:44:21		
Date Stamp	17 May 2018 11:31:05			File Name	C:\Users\Fedor\Desktop\15.05.18\FZ6726-1.jdf	Frequency (MHz)	600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse.ex2			Receiver Gain	36.00
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	19.700	Solvent	CHLOROFORM-d



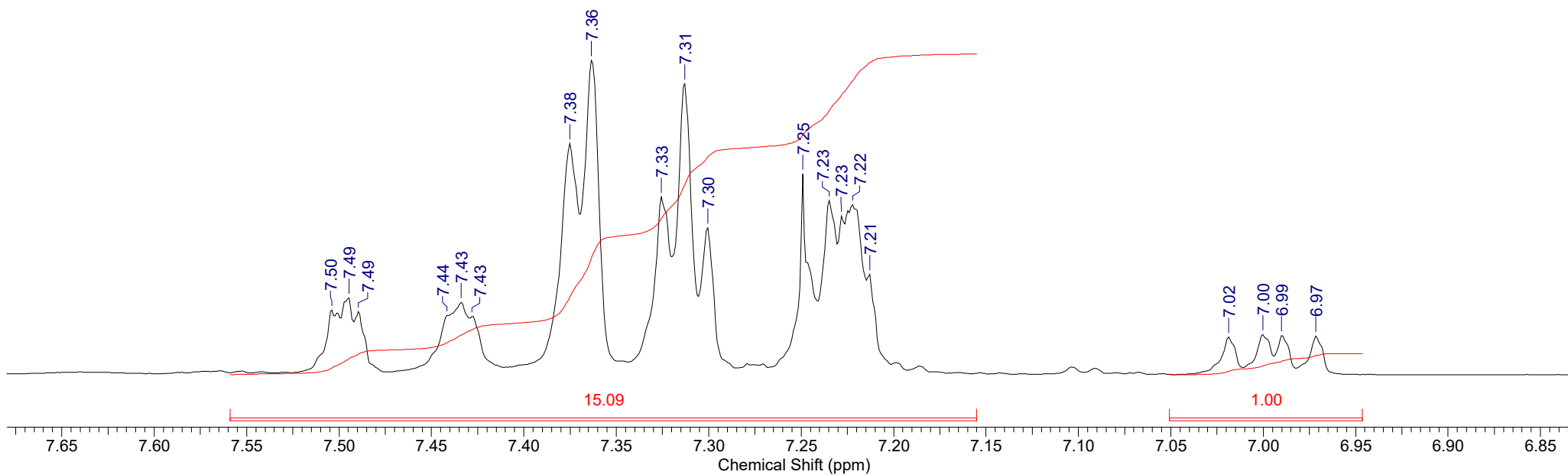
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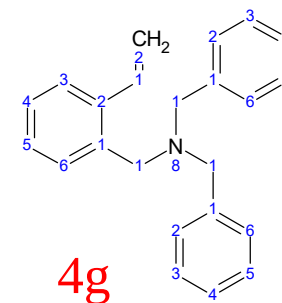
Acquisition Time (sec)	1.9818	Comment	single pulse	Date	21 May 1990 06:44:21	
Date Stamp	17 May 2018 11:31:05			File Name	C:\Users\Fedor\Desktop\15.05.18\FZ6726-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Original Points Count 32768	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	19.700	



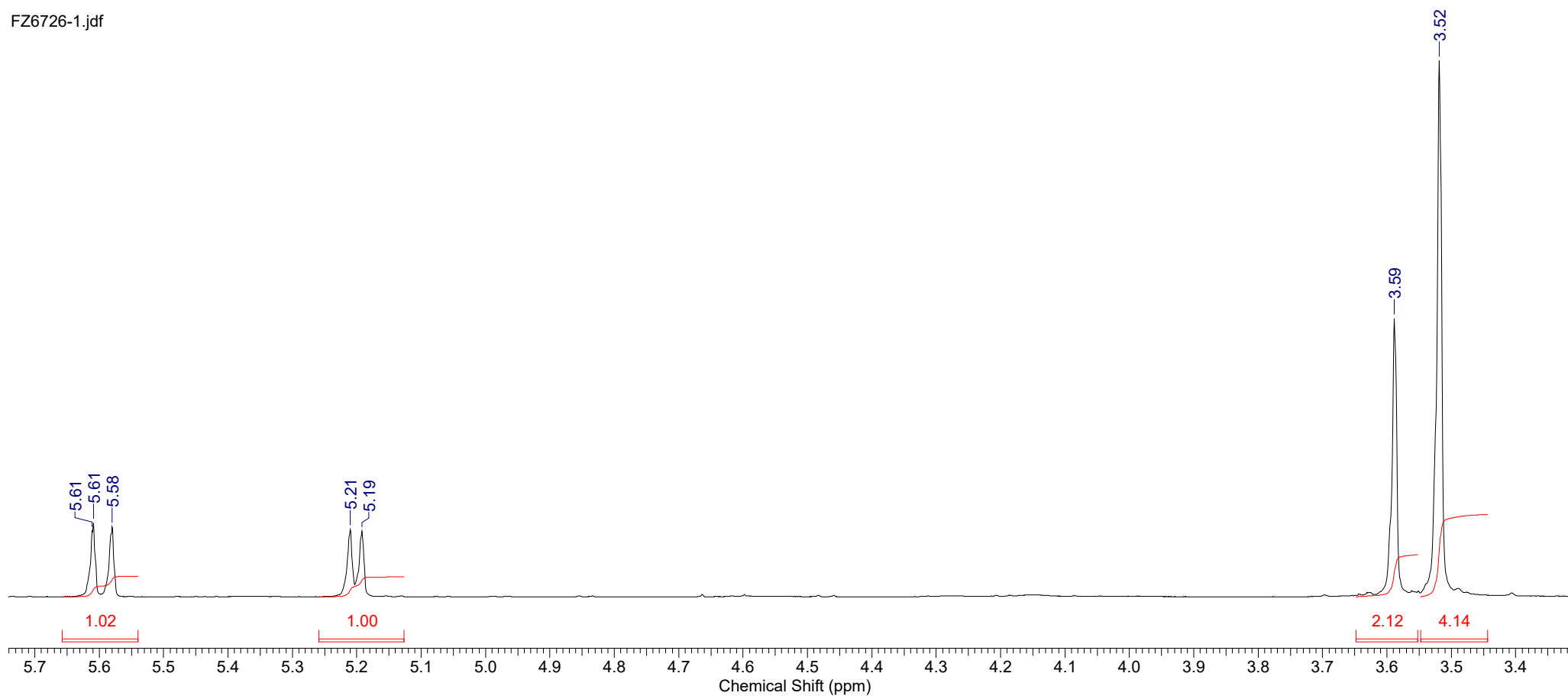
FZ6726-1.jdf



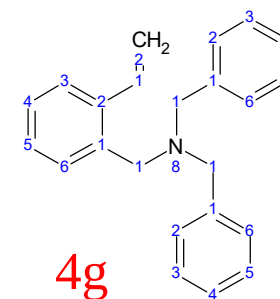
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	21 May 1990 06:44:21	
Date Stamp	17 May 2018 11:31:05			File Name	C:\Users\Fedor\Desktop\15.05.18\FZ6726-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 36.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	19.700	



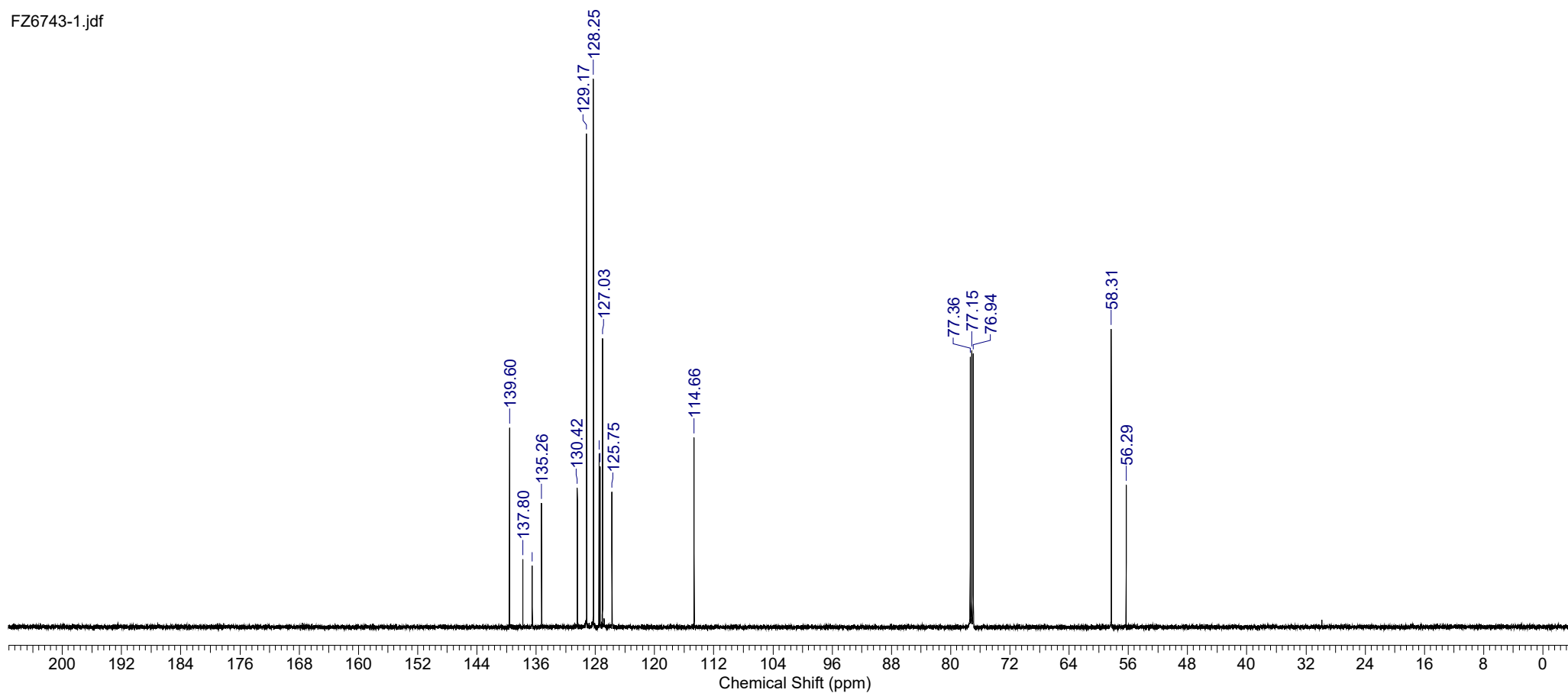
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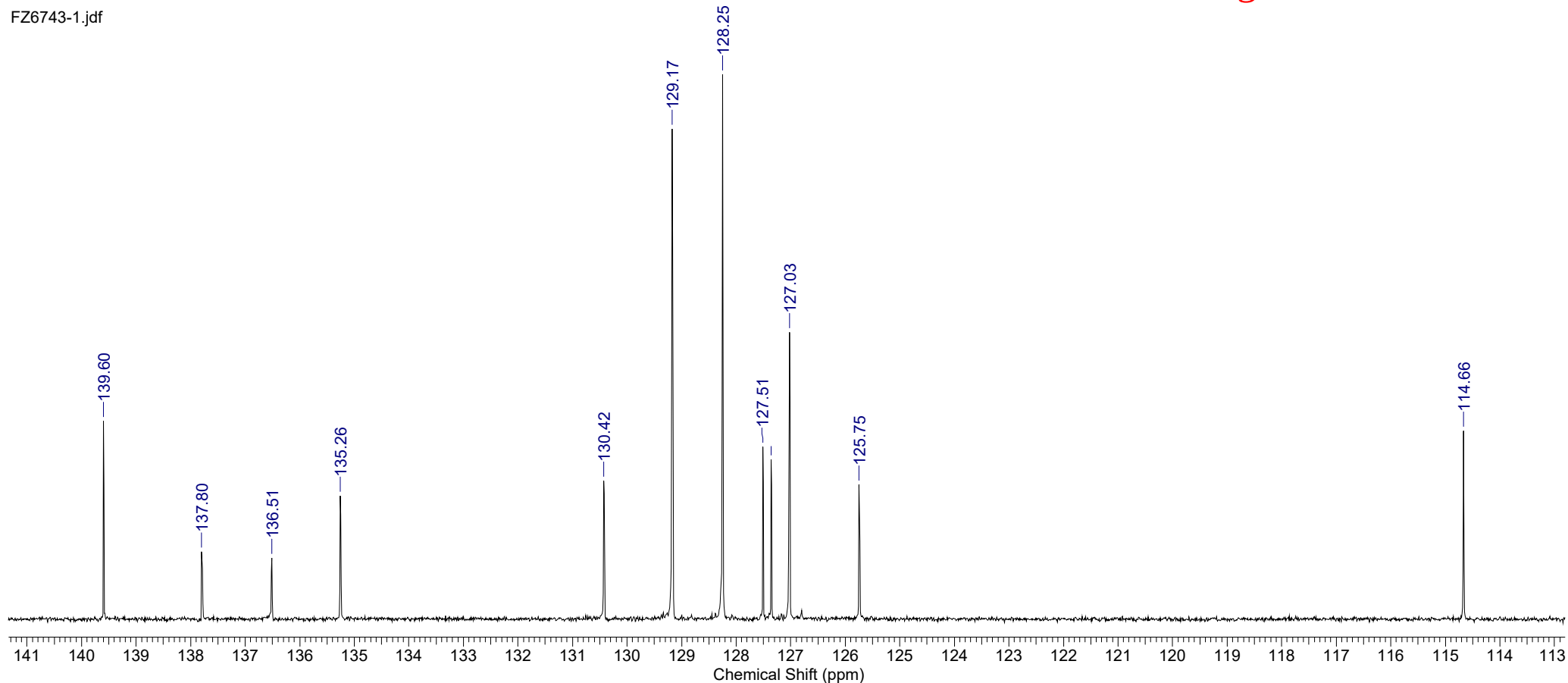
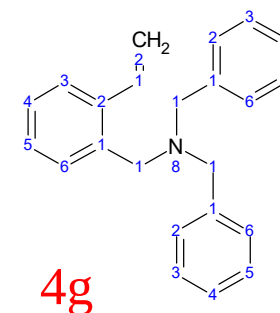
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE			Date	28 May 1990 05:20:52
Date Stamp	24 May 2018 10:07:34		File Name	C:\Users\Fedor\Desktop\22.05.18\FZ6743-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	800	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single_pulse_dec
Receiver Gain	54.00	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	15091.3428
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.000				



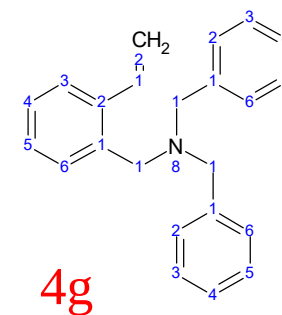
FZ6743-1.jdf



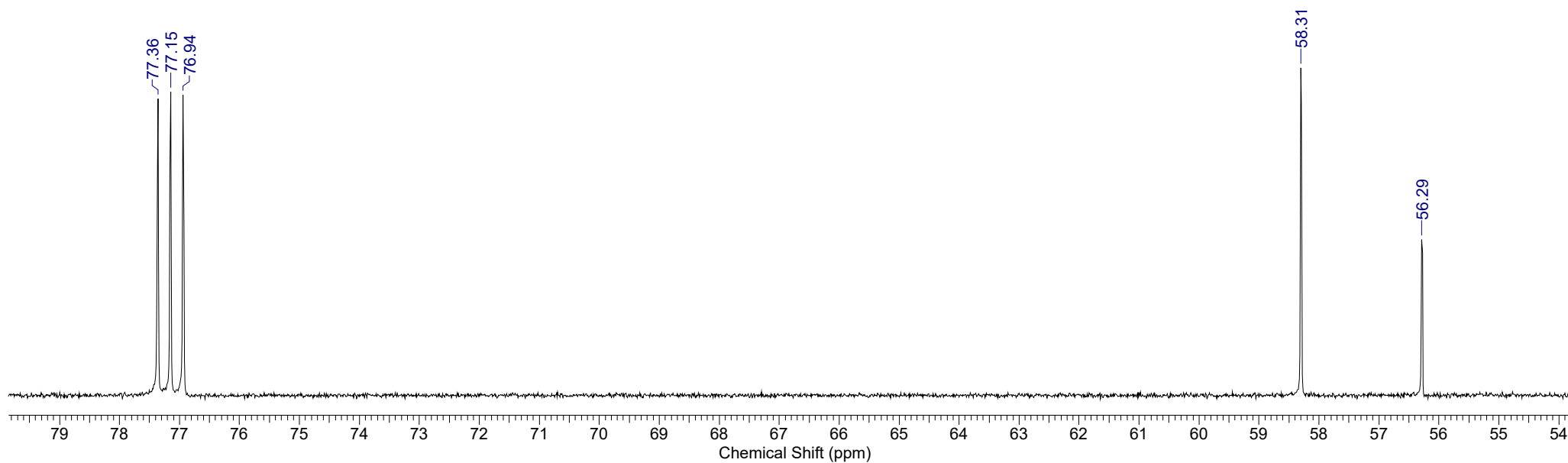
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	28 May 1990 05:20:52	
Date Stamp	24 May 2018 10:07:34		File Name	C:\Users\Fedor\Desktop\22.05.18\FZ6743-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	800	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	54.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.000				



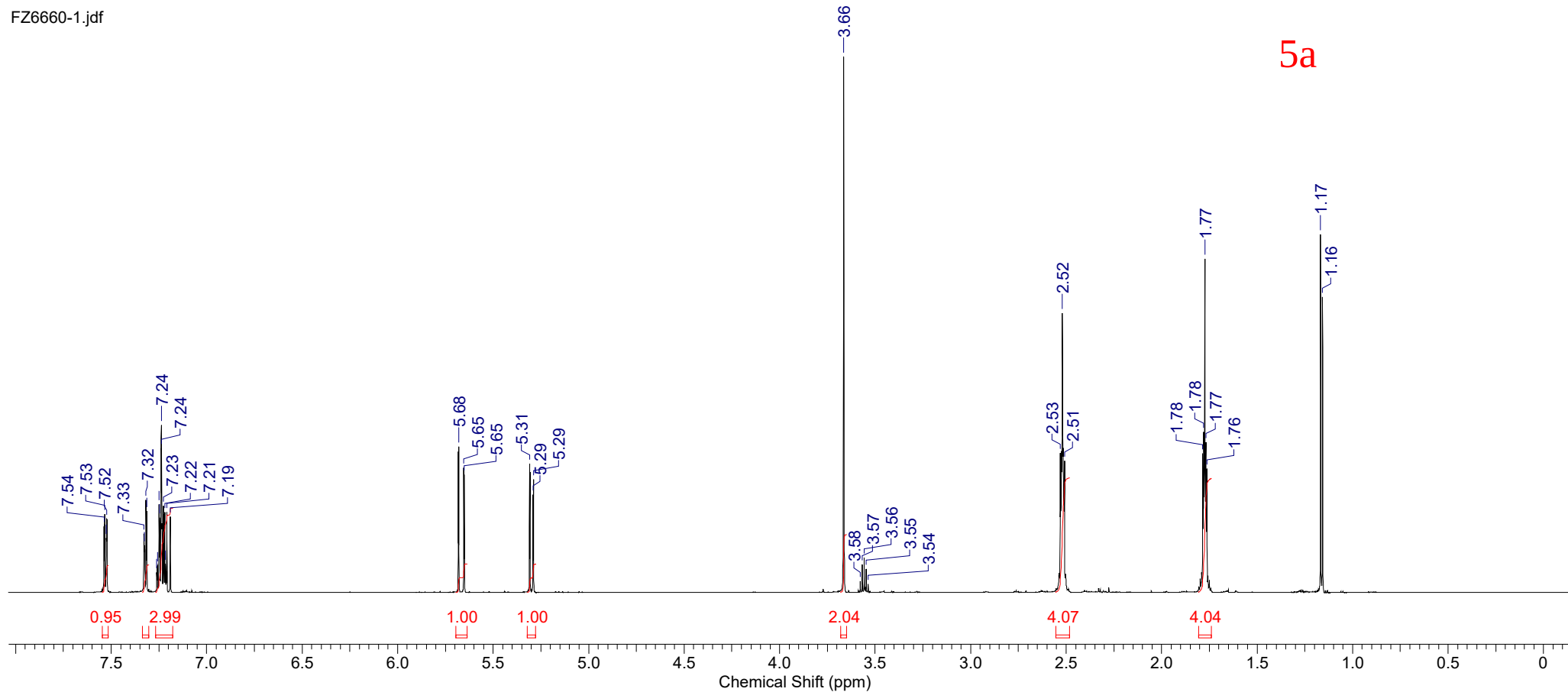
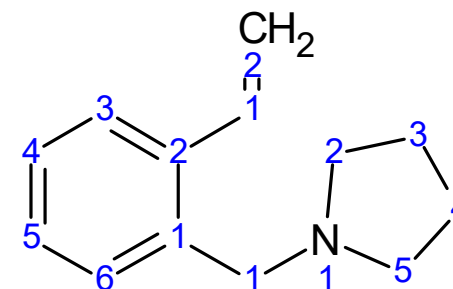
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE			Date	28 May 1990 05:20:52
Date Stamp	24 May 2018 10:07:34		File Name	C:\Users\Fedor\Desktop\22.05.18\FZ6743-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	800	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single_pulse_dec
Receiver Gain	54.00	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	15091.3428
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.000				



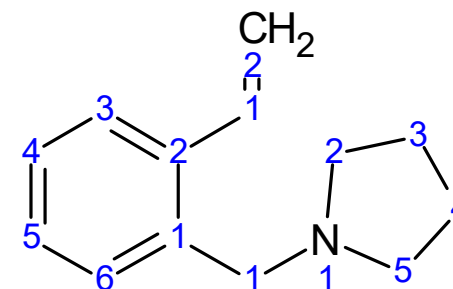
FZ6743-1.jdf



Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	29 Apr 1990 07:51:18	
Date Stamp	25 Apr 2018 12:38:26			File Name	C:\Users\Fedor\Desktop\24.04.18\FZ6660-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 24.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	21.600	

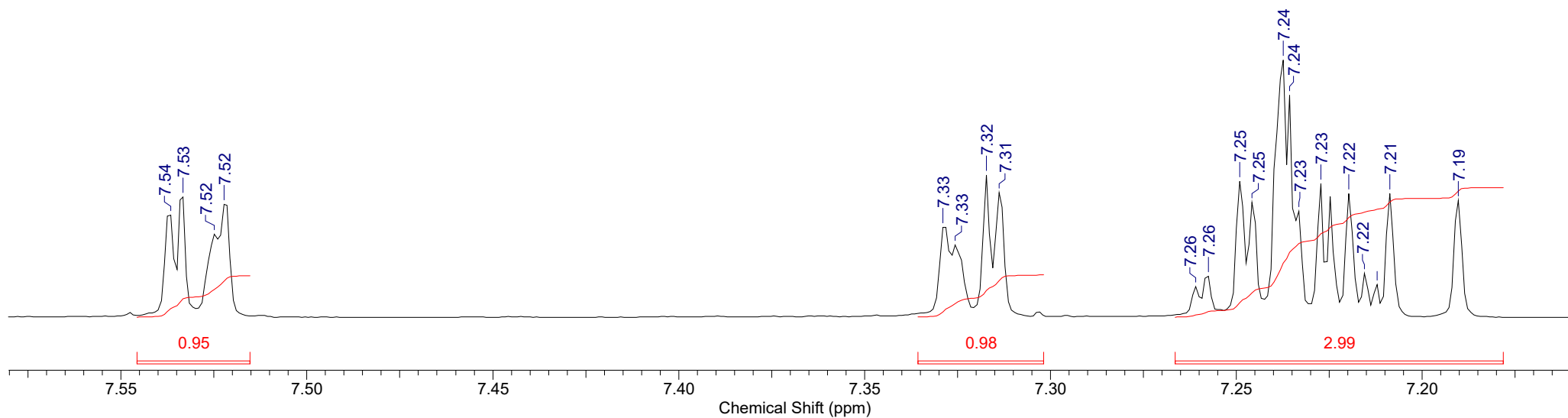


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	29 Apr 1990 07:51:18		
Date Stamp	25 Apr 2018 12:38:26	File Name	C:\Users\Fedor\Desktop\24.04.18\FZ6660-1.jdf			Frequency (MHz)	600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse.ex2			Receiver Gain	24.00
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	21.600		
						Owner	delta
						Solvent	CHLOROFORM-d

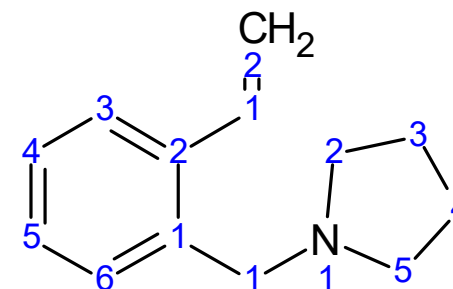


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FZ6660-1.jdf

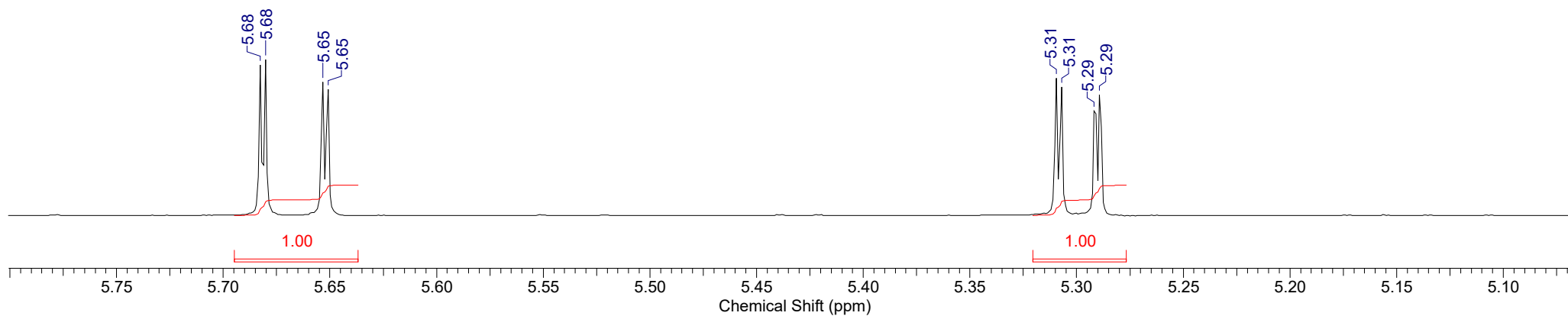


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	29 Apr 1990 07:51:18	
Date Stamp	25 Apr 2018 12:38:26			File Name	C:\Users\Fedor\Desktop\24.04.18\FZ6660-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 24.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	21.600	

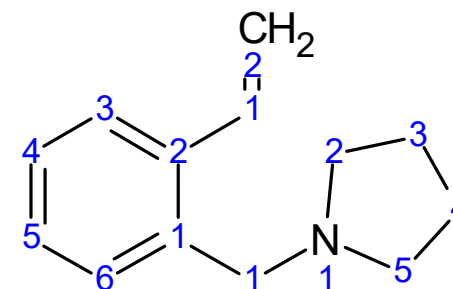


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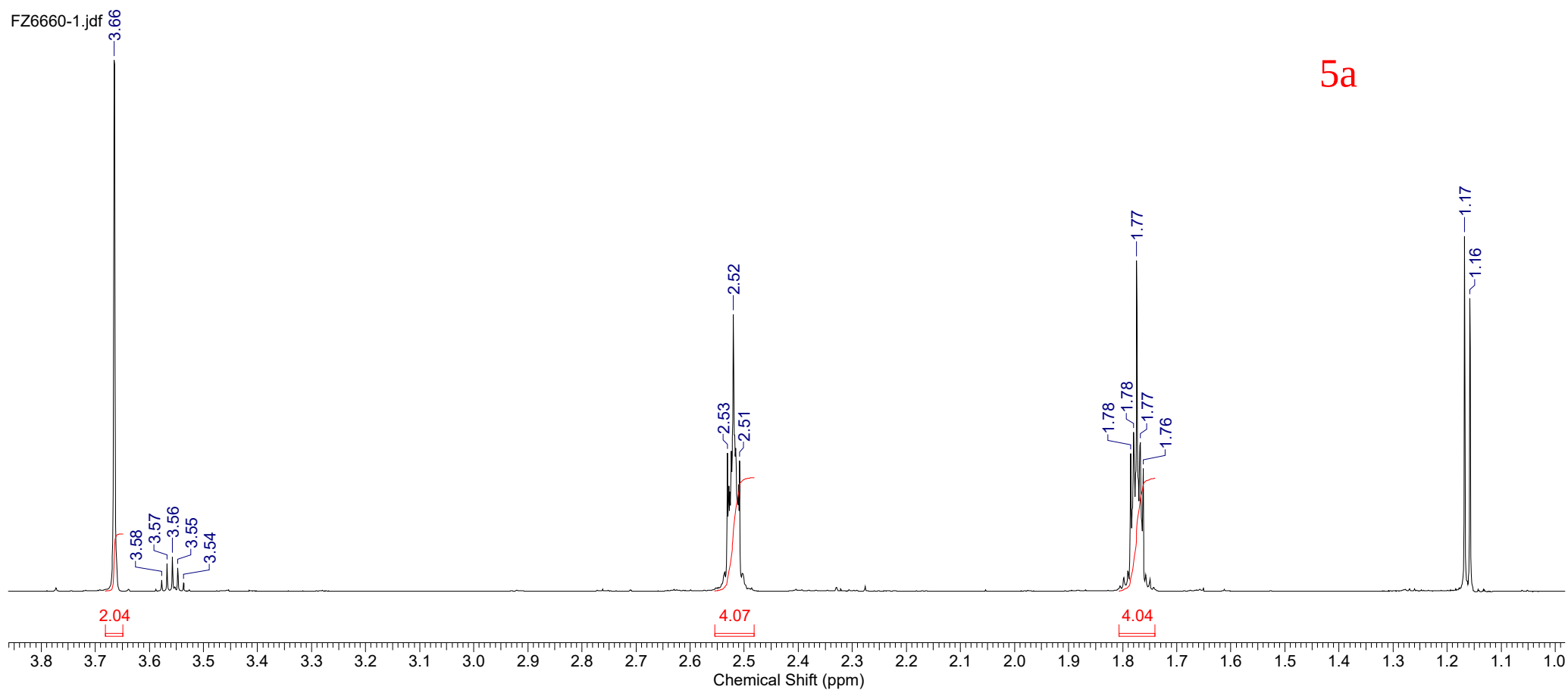
FZ6660-1.jdf



Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	29 Apr 1990 07:51:18	
Date Stamp	25 Apr 2018 12:38:26			File Name	C:\Users\Fedor\Desktop\24.04.18\FZ6660-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 24.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	21.600	

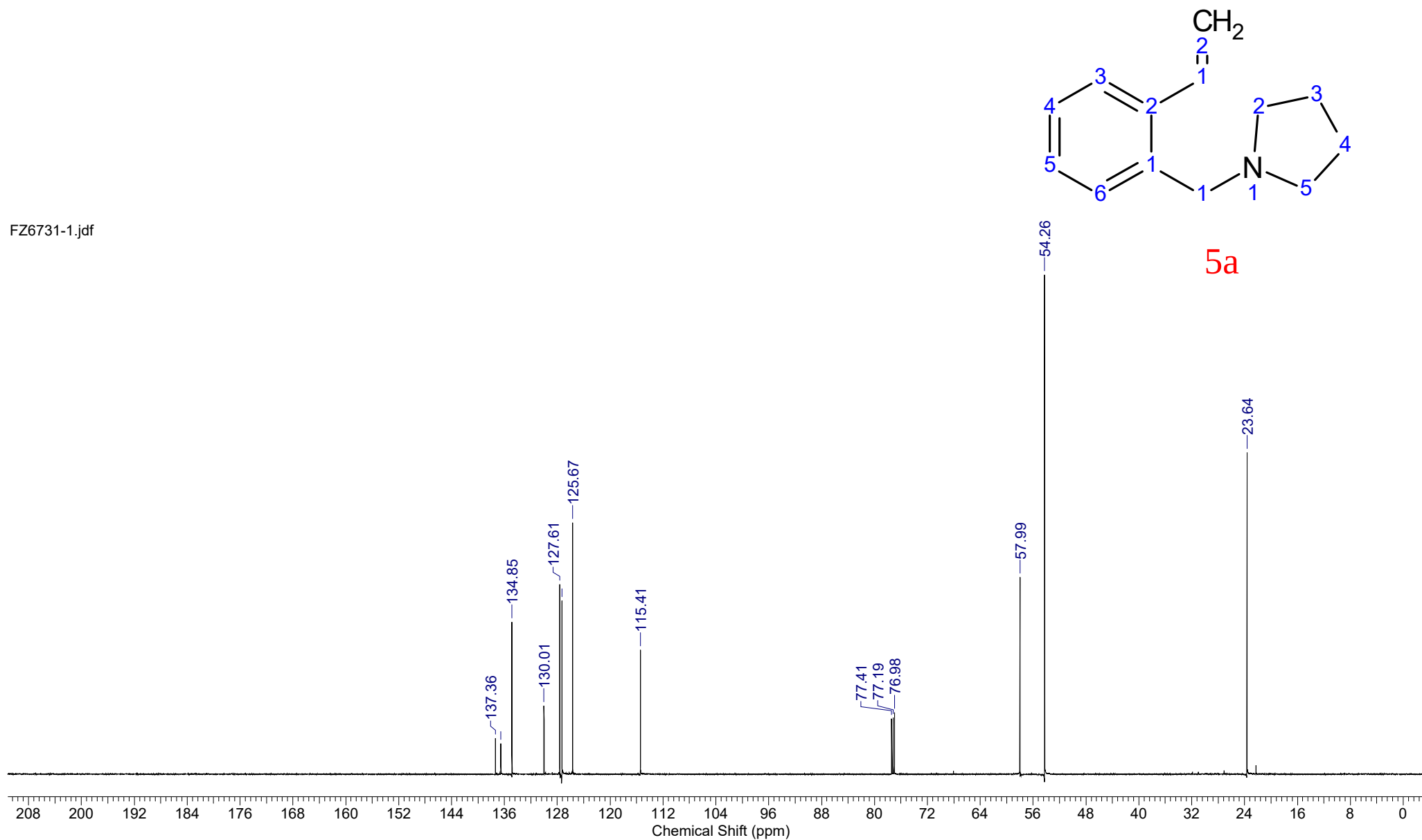


5a

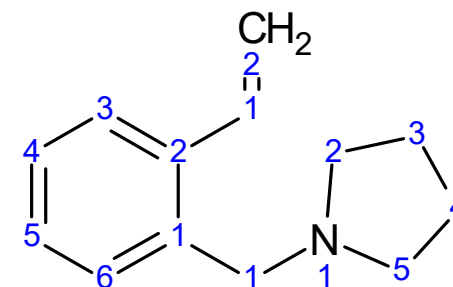


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	27 May 1990 17:44:26	
Date Stamp	24 May 2018 04:18:54		File Name	C:\Users\Fedor\Desktop\22.05.18\FZ6731-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	54.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.200				

FZ6731-1.jdf

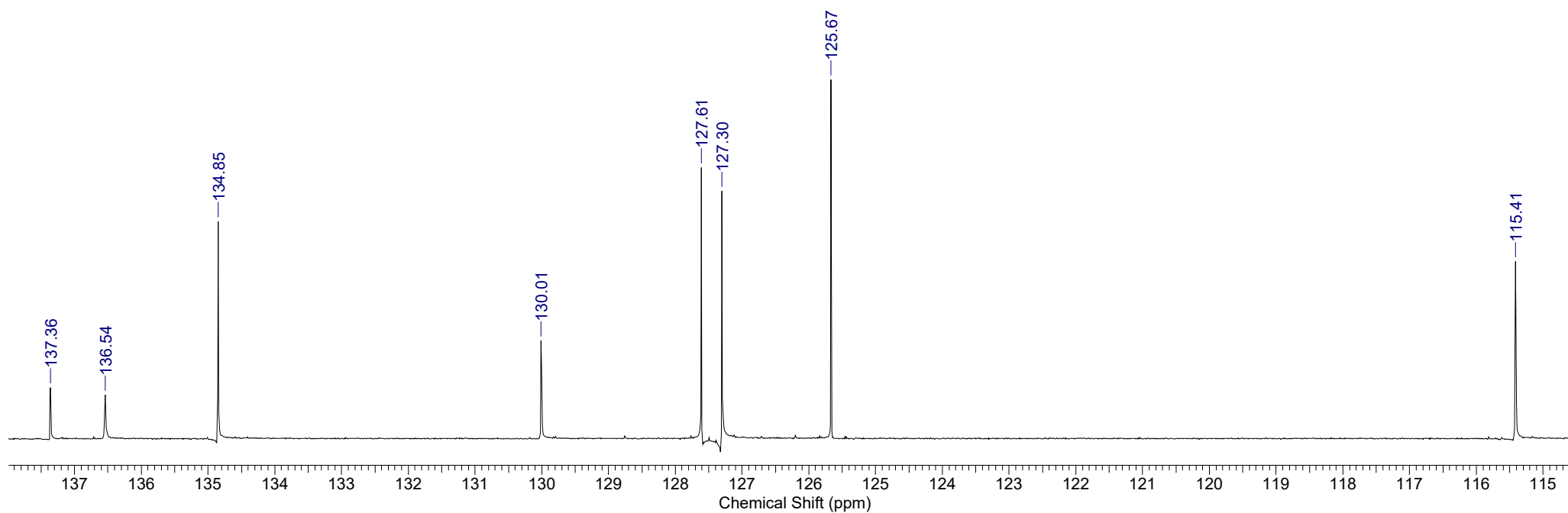


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	27 May 1990 17:44:26	
Date Stamp	24 May 2018 04:18:54		File Name	C:\Users\Fedor\Desktop\22.05.18\FZ6731-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	54.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.200				

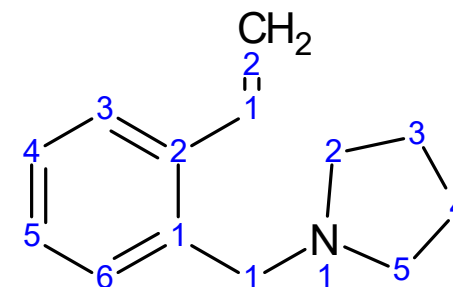


5a

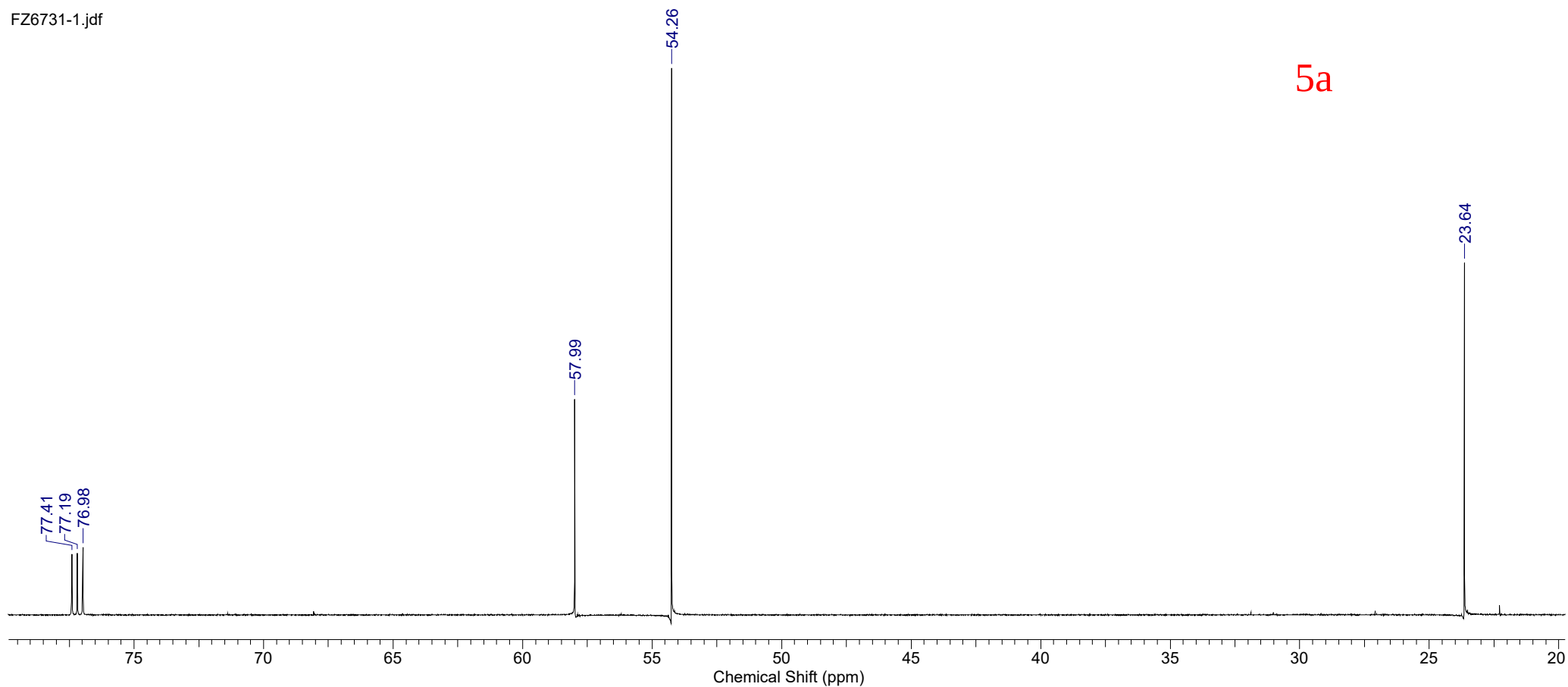
FZ6731-1.jdf



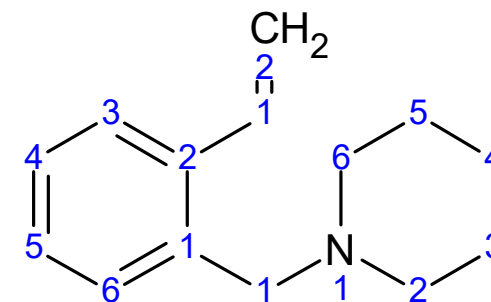
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	27 May 1990 17:44:26	
Date Stamp	24 May 2018 04:18:54		File Name	C:\Users\Fedor\Desktop\22.05.18\FZ6731-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	54.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.200				



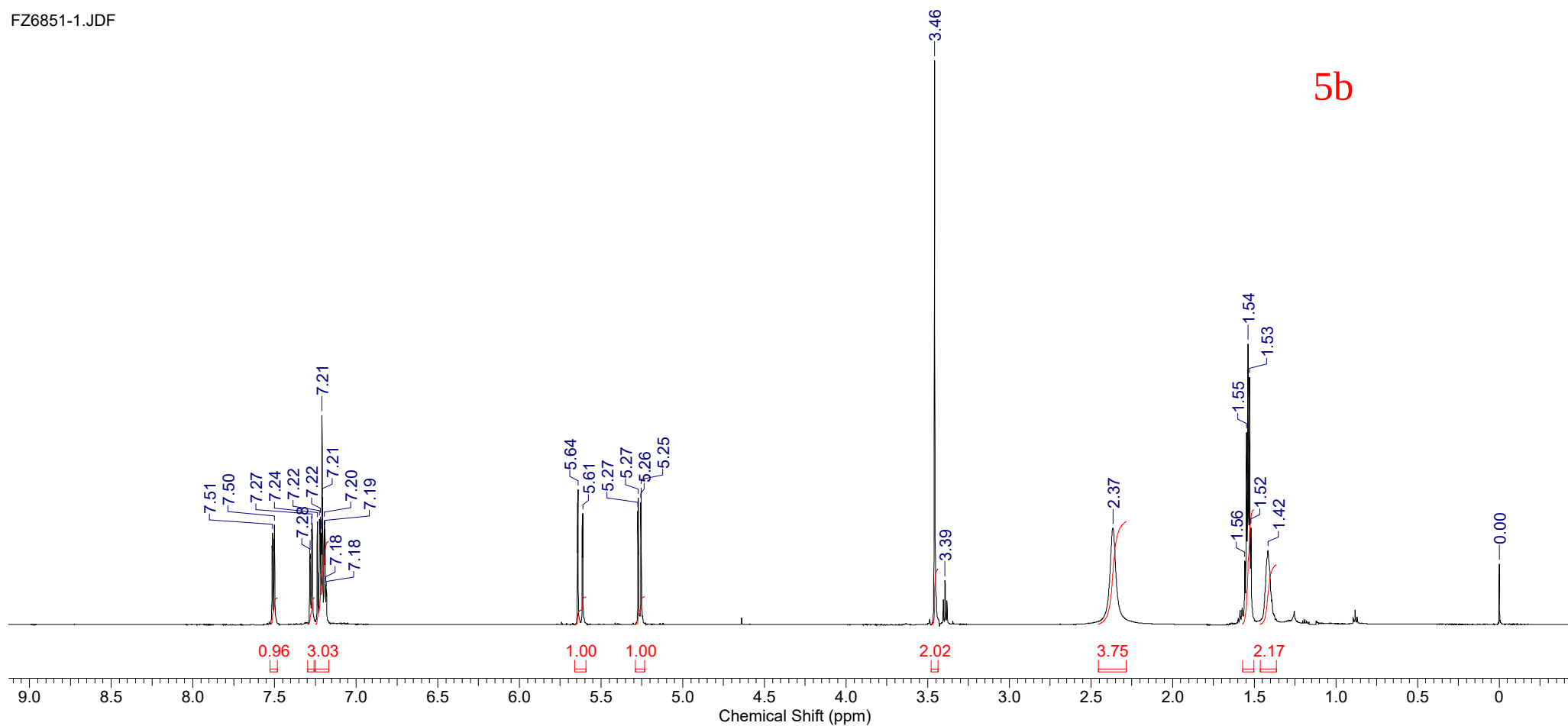
FZ6731-1.jdf



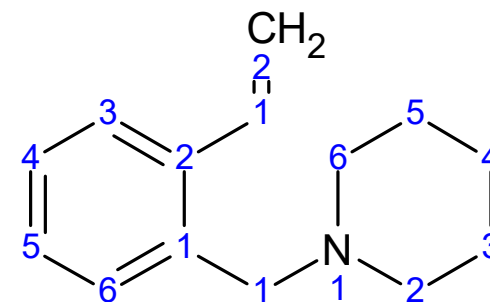
Acquisition Time (sec)	1.9818	Comment	single pulse	Date	09 Feb 1990 03:52:47	Date Stamp	08 Aug 2018 13:22:59
File Name	C:\USERS\FEDOR\DESKTOP\08.08.18\FZ6851-1.JDF	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	24.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5385.9019	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



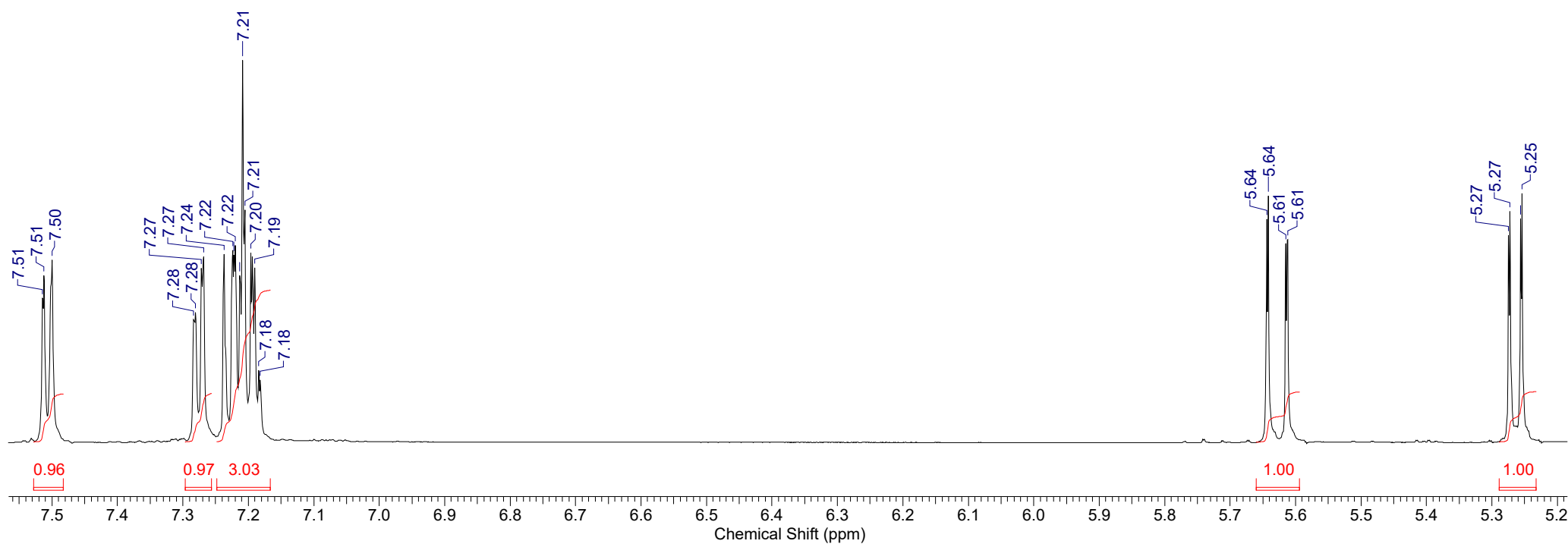
FZ6851-1.JDF



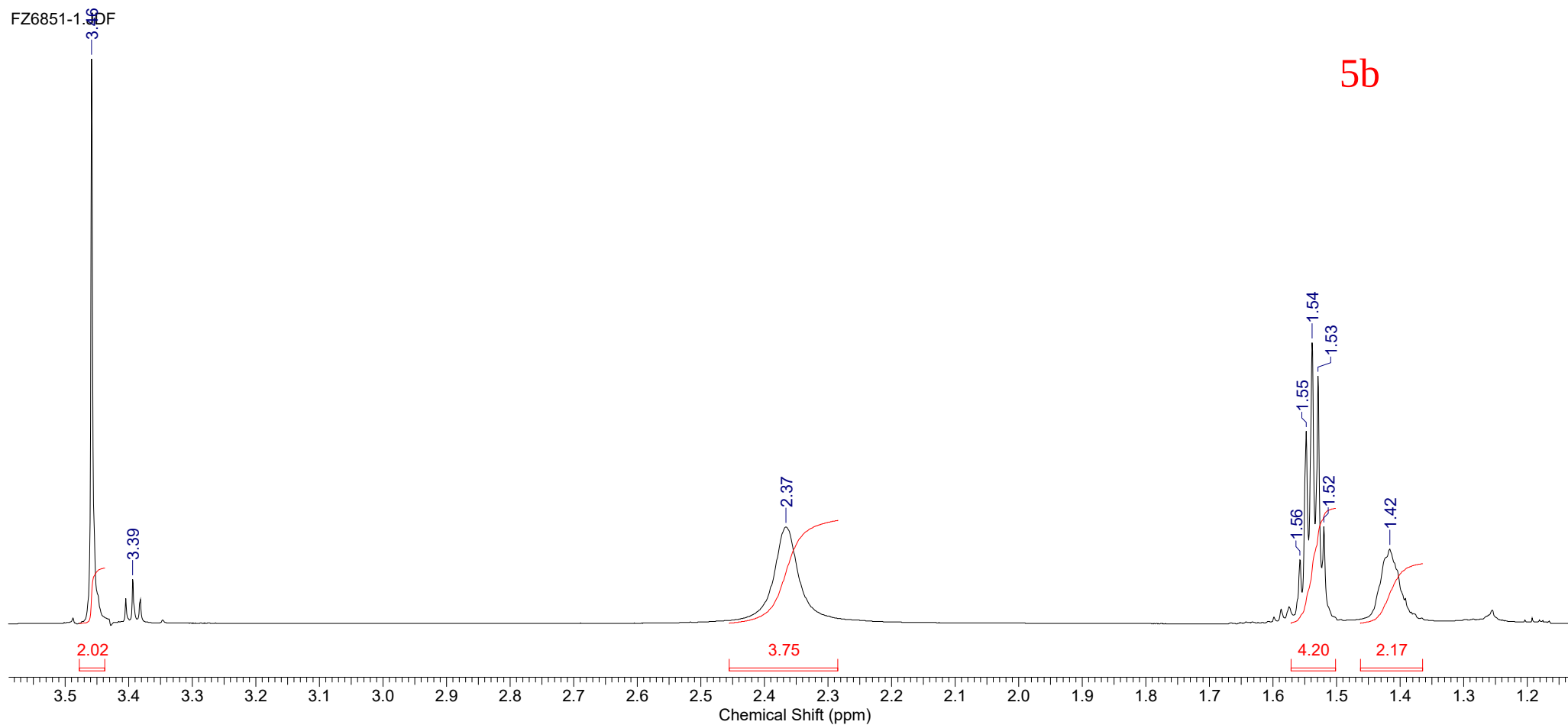
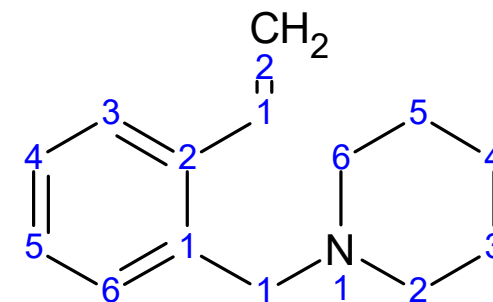
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	09 Feb 1990 03:52:47		Date Stamp	08 Aug 2018 13:22:59	
File Name	C:\USERS\FEDOR\DESKTOP\08.08.18\FZ6851-1.JDF			Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single_pulse.ex2
Receiver Gain	24.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	5385.9019	Sweep Width (Hz)	16534.39	



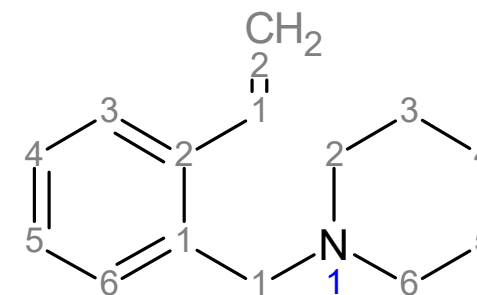
5b



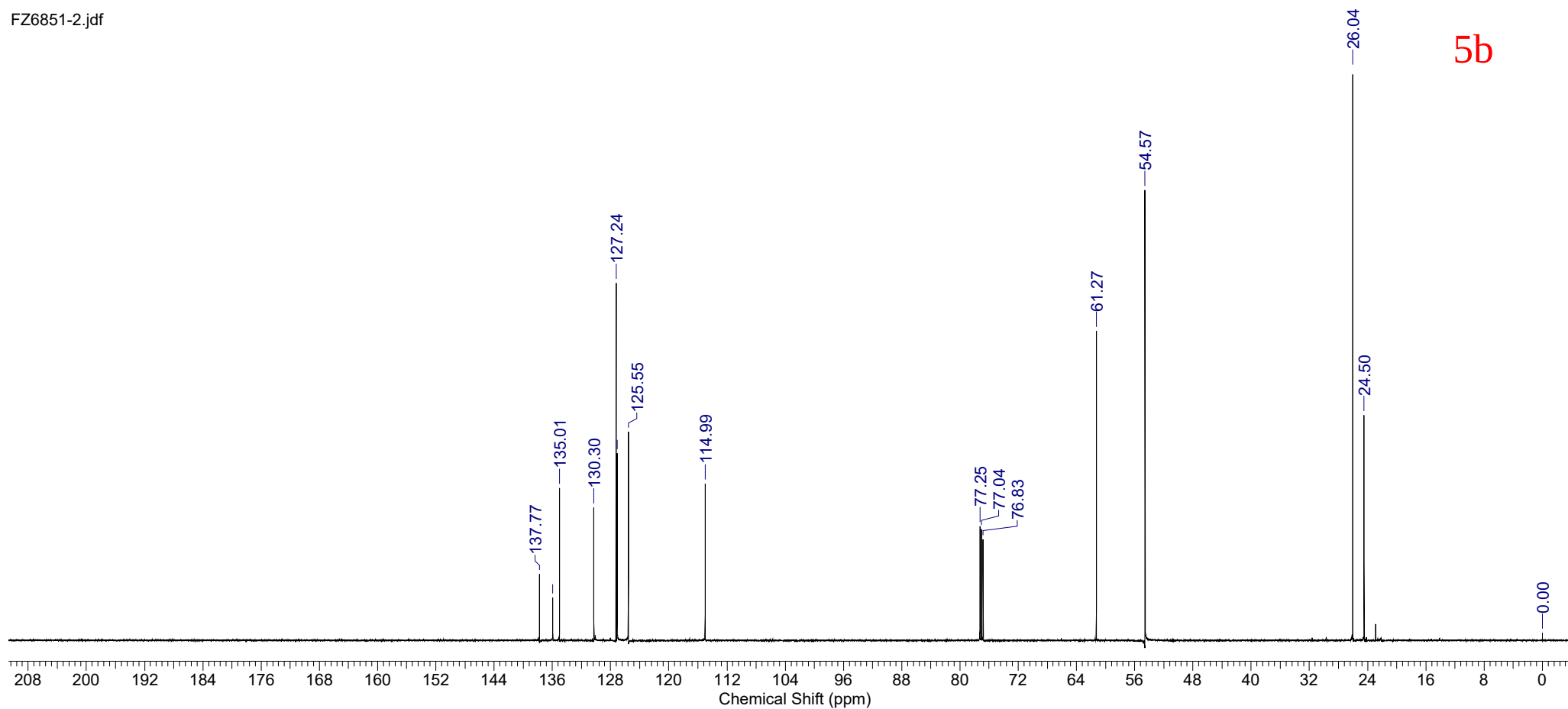
Acquisition Time (sec)	1.9818	Comment	single pulse	Date	09 Feb 1990 03:52:47		Date Stamp	08 Aug 2018 13:22:59	
File Name	C:\USERS\FEDOR\DESKTOP\08.08.18\FZ6851-1.JDF			Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single_pulse.ex2
Receiver Gain	24.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	5385.9019	Sweep Width (Hz)	16534.39	



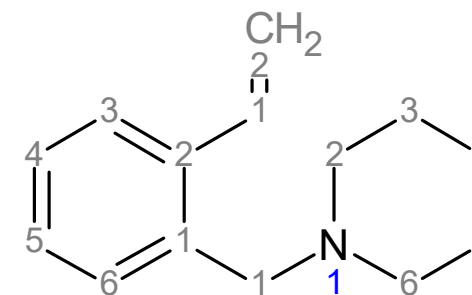
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	14 Feb 1990 01:52:31
Date Stamp	13 Aug 2018 11:22:48	File Name	C:\Users\Fedor\Desktop\08.08.18\FZ6851-2.jdf	Frequency (MHz)	150.91
Nucleus	¹³ C	Number of Transients	969	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15072.1279	Sweep Width (Hz)	47348.49	Receiver Gain	54.00
				Owner	delta
				Solvent	CHLOROFORM-d



FZ6851-2.jdf

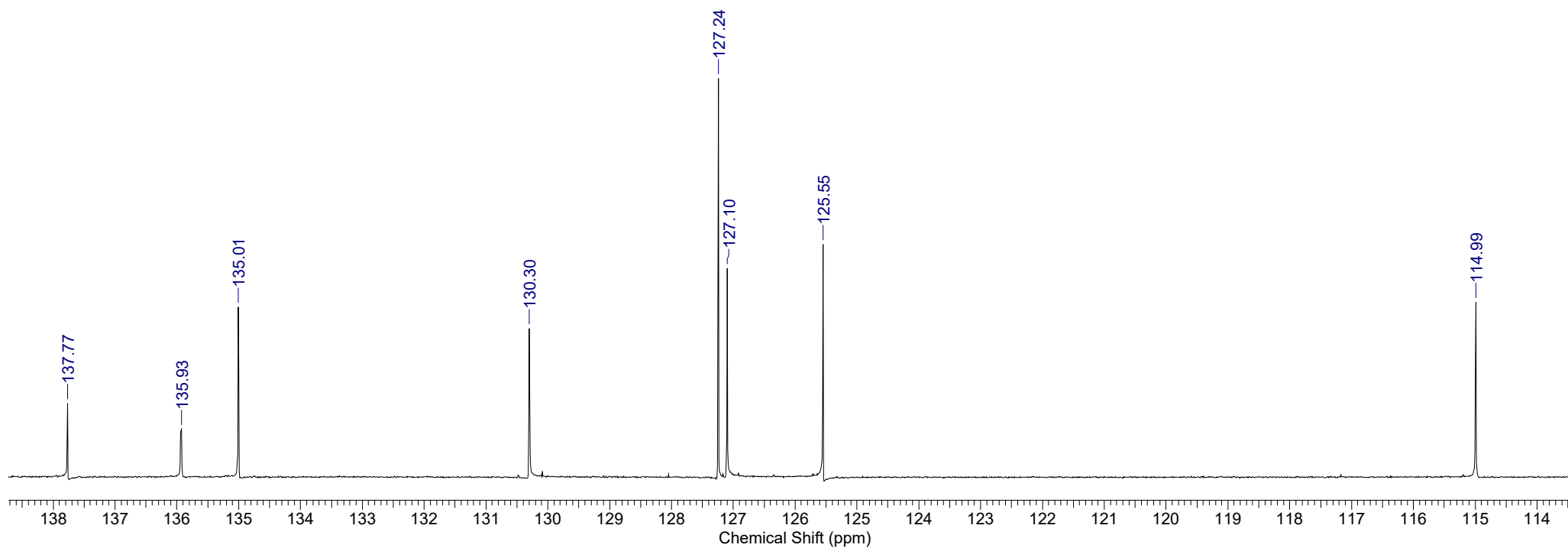


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	14 Feb 1990 01:52:31	
Date Stamp	13 Aug 2018 11:22:48	File Name	C:\Users\Fedor\Desktop\08.08.18\FZ6851-2.jdf			Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	969	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single pulse dec	Receiver Gain	54.00	Owner	delta
Spectrum Offset (Hz)	15072.1279	Sweep Width (Hz)	47348.49	Solvent	CHLOROFORM-d		

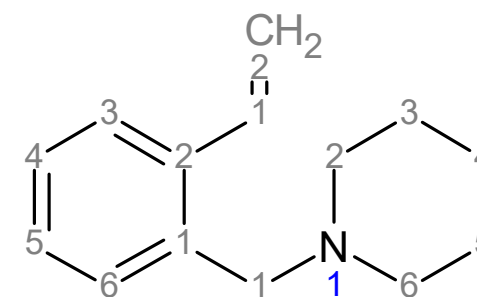


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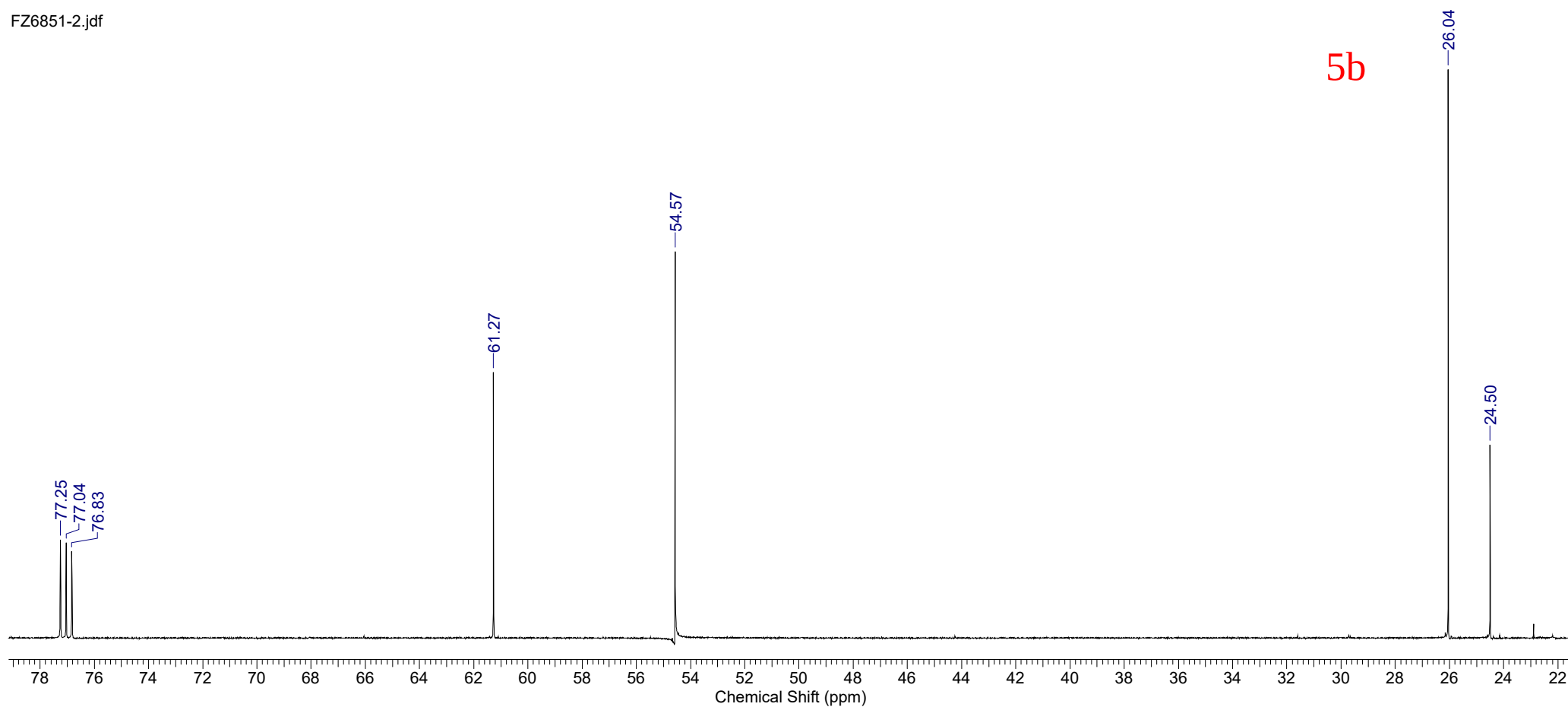
FZ6851-2.jdf



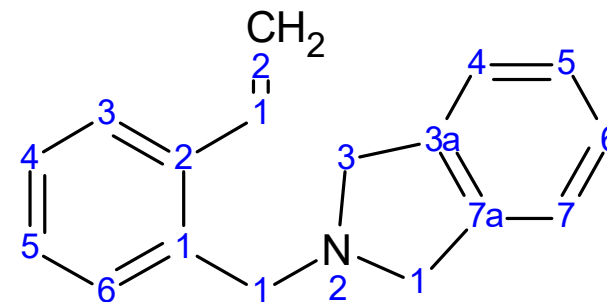
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	14 Feb 1990 01:52:31
Date Stamp	13 Aug 2018 11:22:48	File Name	C:\Users\Fedor\Desktop\08.08.18\FZ6851-2.jdf	Frequency (MHz)	150.91
Nucleus	¹³ C	Number of Transients	969	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15072.1279	Sweep Width (Hz)	47348.49	Receiver Gain	54.00
				Owner	delta
				Solvent	CHLOROFORM-d



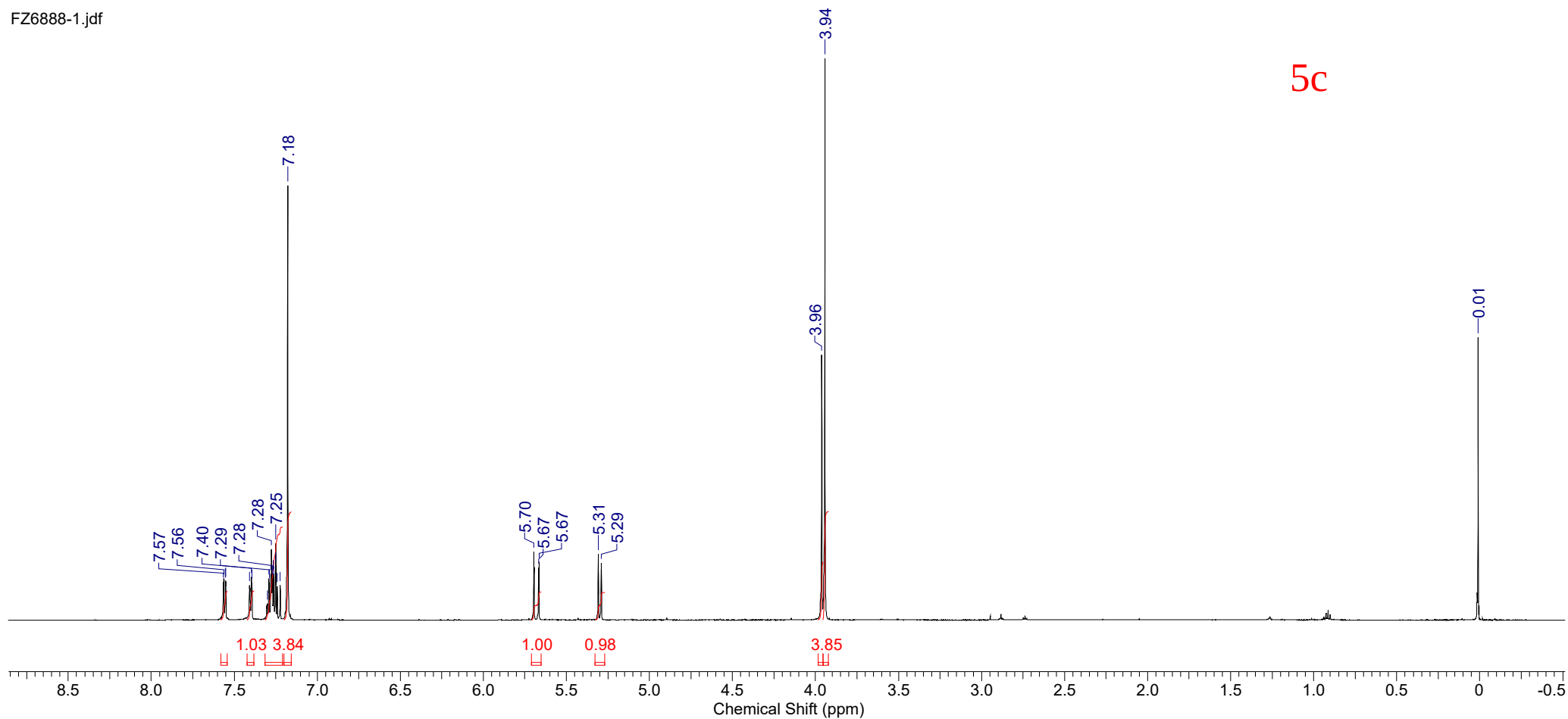
FZ6851-2.jdf



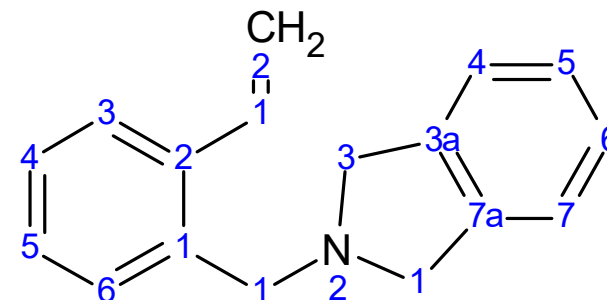
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	29 Mar 1990 02:03:03	Date Stamp	26 Sep 2018 11:32:31
File Name	C:\Users\Fedor\Desktop\26.09.18\FZ6888-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	36.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



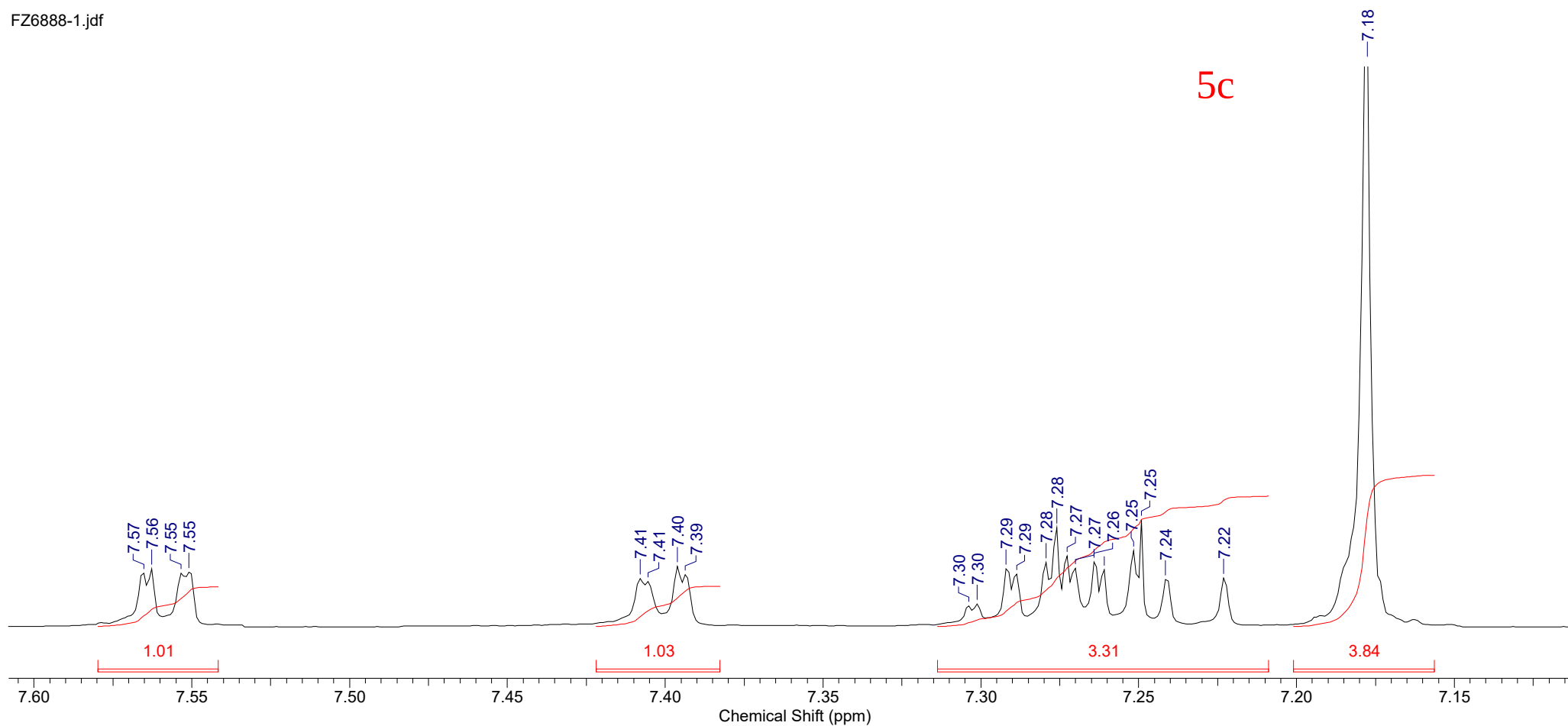
FZ6888-1.jdf



Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	29 Mar 1990 02:03:03	Date Stamp	26 Sep 2018 11:32:31
File Name	C:\Users\Fedor\Desktop\26.09.18\FZ6888-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	36.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39

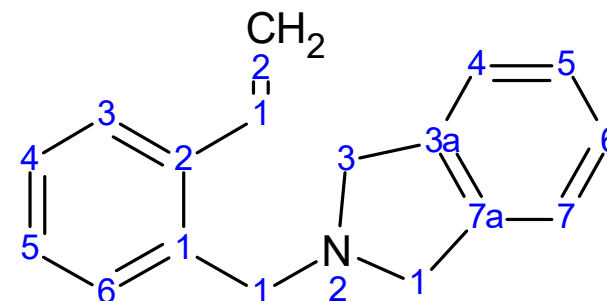


FZ6888-1.jdf

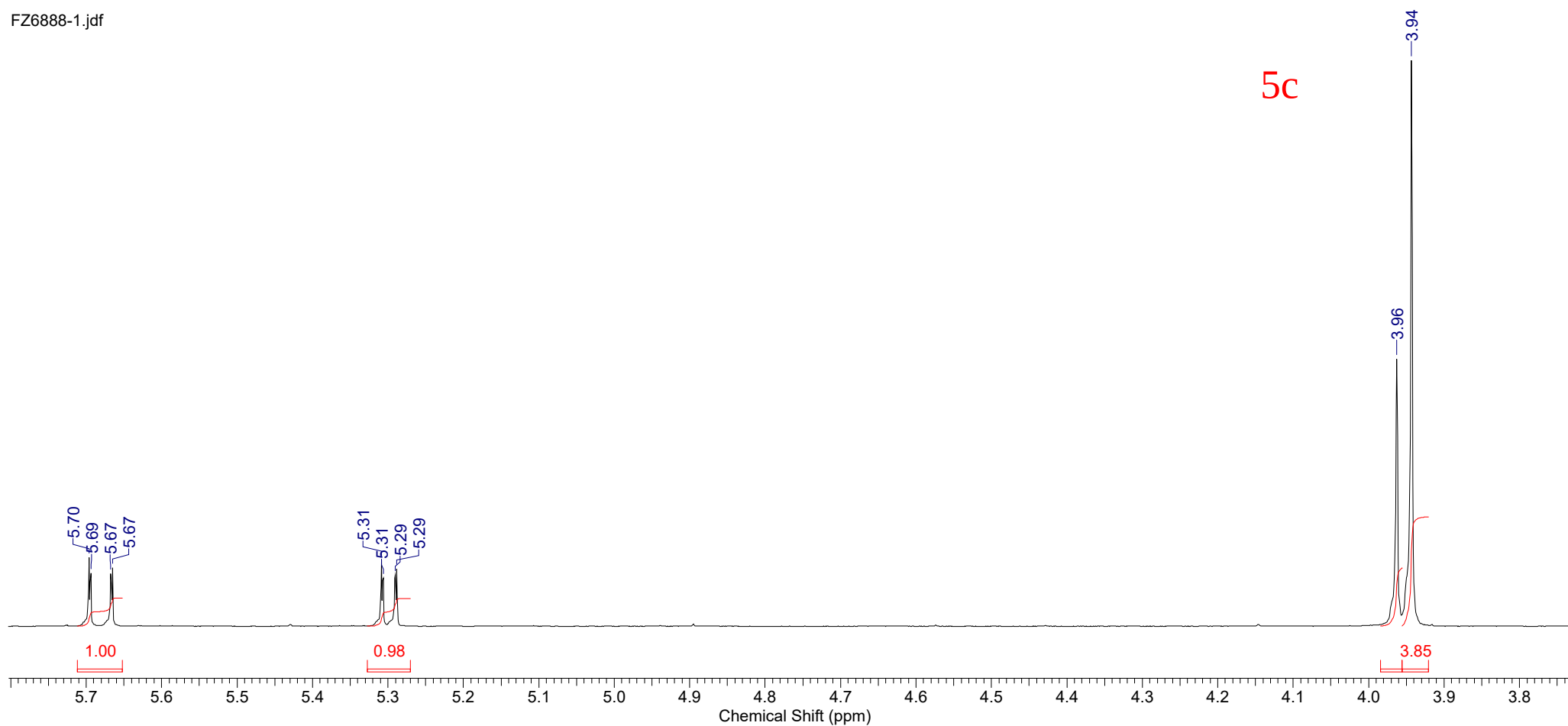


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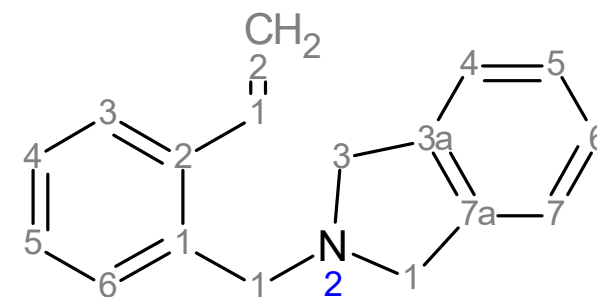
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	29 Mar 1990 02:03:03	Date Stamp	26 Sep 2018 11:32:31
File Name	C:\Users\Fedor\Desktop\26.09.18\FZ6888-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	36.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



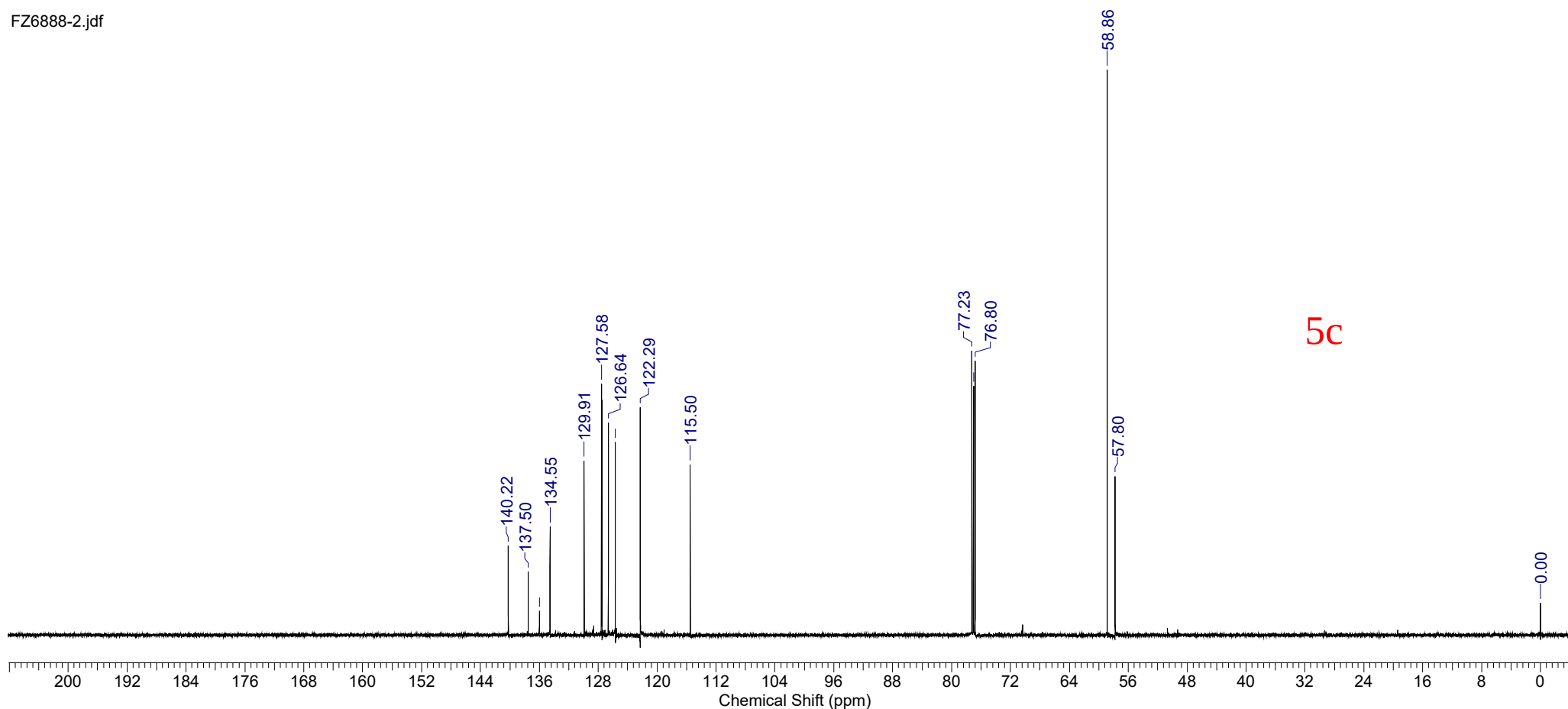
FZ6888-1.jdf



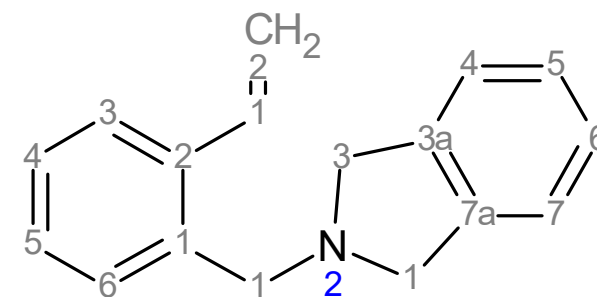
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	30 Mar 1990 17:27:25
Date Stamp	28 Sep 2018 07:59:09	File Name	C:\Users\Fedor\Desktop\26.09.18\FZ6888-2.jdf	Frequency (MHz)	150.91
Nucleus	¹³ C	Number of Transients	1000	Origin	ECA 600
Points Count	32768	Pulse Sequence	single pulse dec	Original Points Count	32768
Spectrum Offset (Hz)	15073.5723	Sweep Width (Hz)	47348.49	Receiver Gain	52.00
				Owner	delta
				Solvent	CHLOROFORM-d



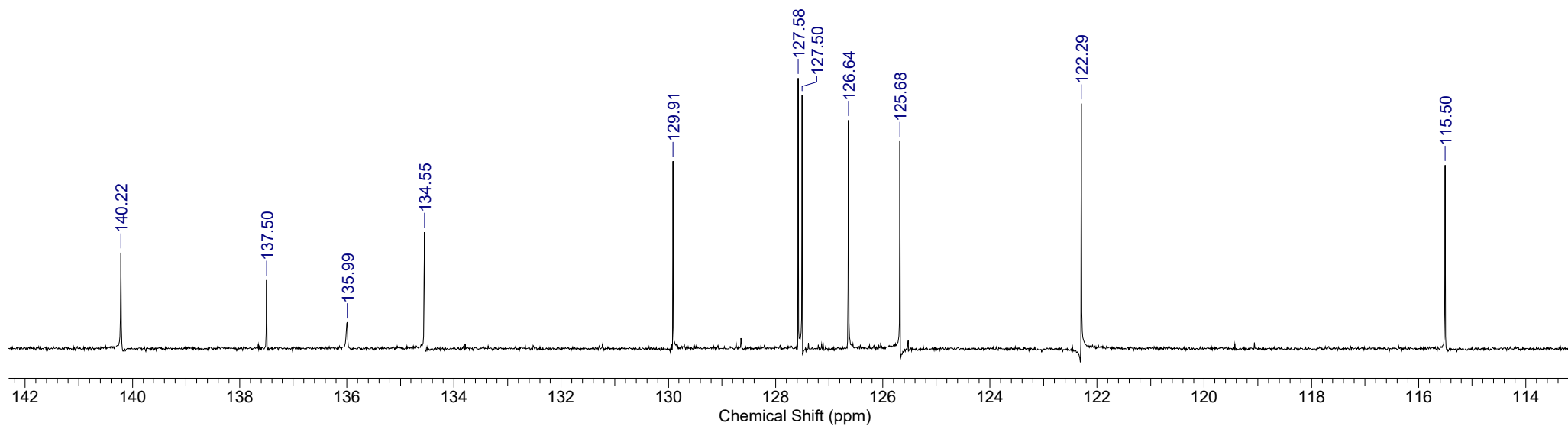
FZ6888-2.jdf



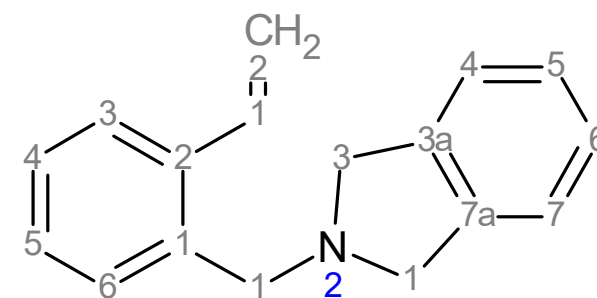
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	30 Mar 1990 17:27:25	
Date Stamp	28 Sep 2018 07:59:09	File Name	C:\Users\Fedor\Desktop\26.09.18\FZ6888-2.jdf			Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	1000	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single pulse dec	Receiver Gain	52.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	15073.5723	Sweep Width (Hz)	47348.49				



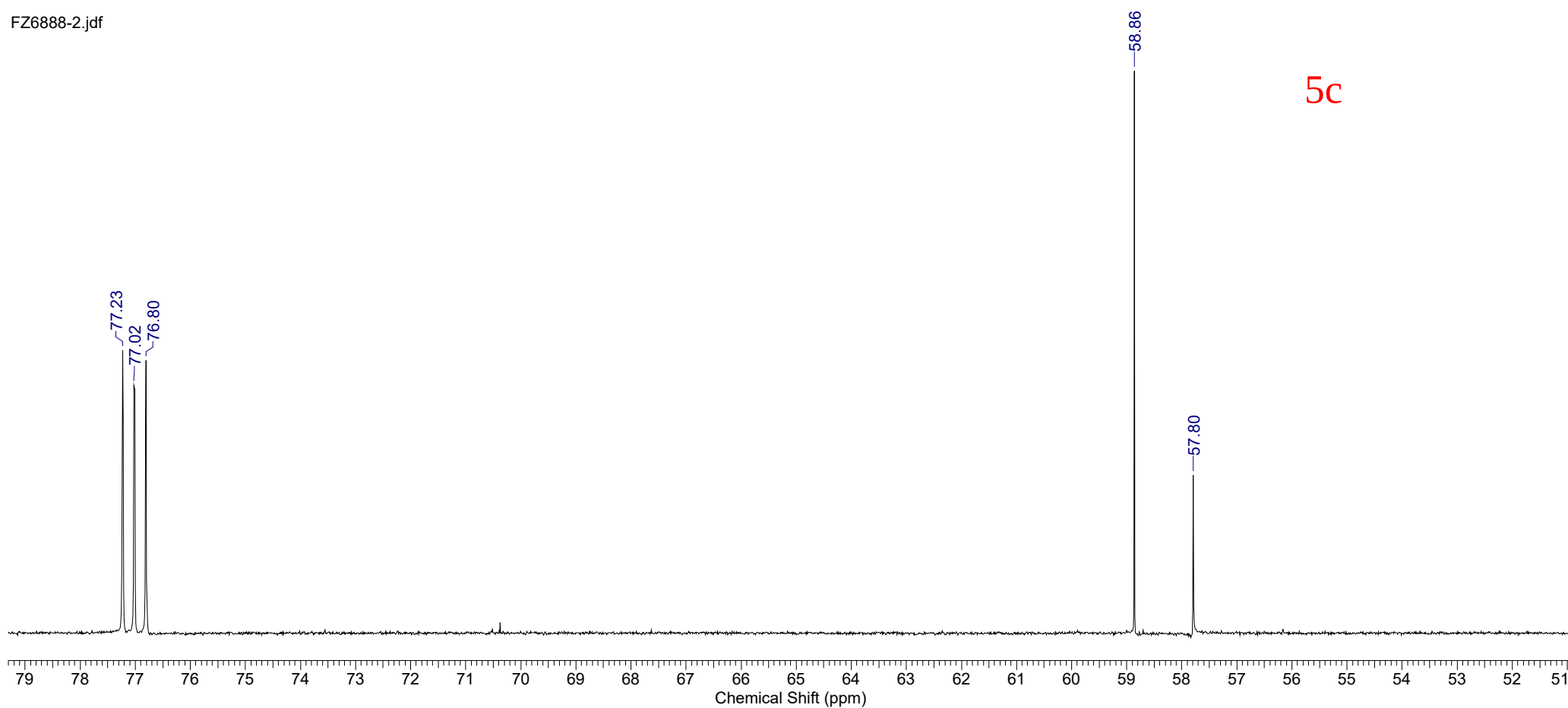
FZ6888-2.jdf



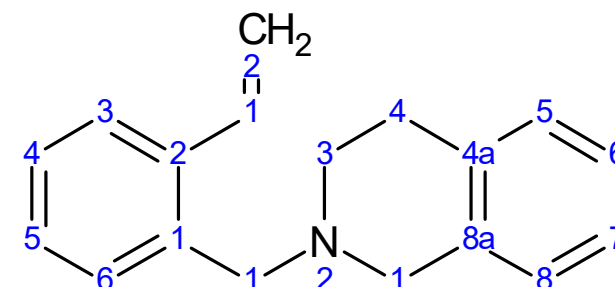
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	30 Mar 1990 17:27:25		
Date Stamp	28 Sep 2018 07:59:09	File Name	C:\Users\Fedor\Desktop\26.09.18\FZ6888-2.jdf			Frequency (MHz)	150.91	
Nucleus	13C	Number of Transients	1000	Origin	ECA 600	Original Points Count	32768	
Points Count	32768	Pulse Sequence	single pulse dec	Receiver Gain	52.00	Owner	delta	
Spectrum Offset (Hz)	15073.5723	Sweep Width (Hz)	47348.49	Solvent				CHLOROFORM-d



FZ6888-2.jdf

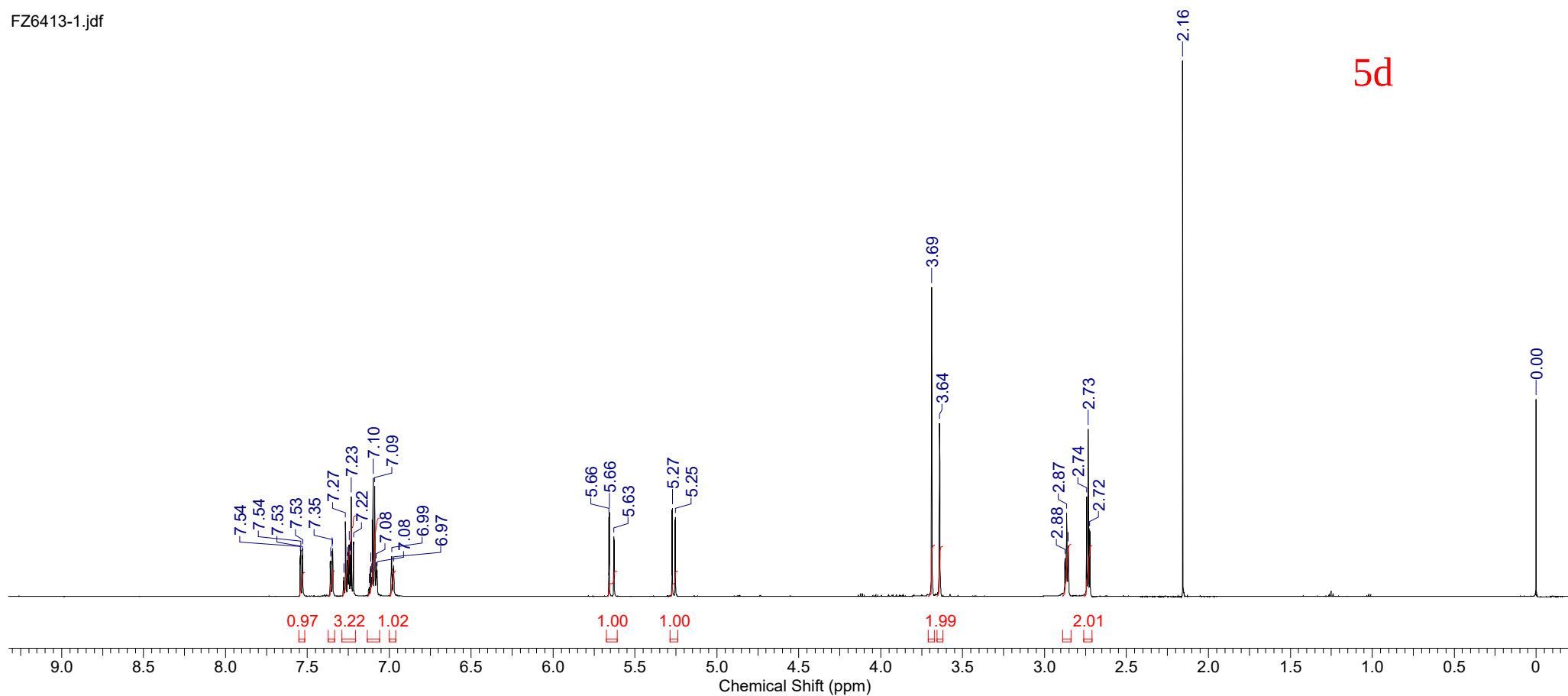


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	19 Feb 1990 07:27:10	
Date Stamp	14 Feb 2018 12:15:19			File Name	C:\Users\Fedor\Desktop\13.02.18\FZ6413-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 36.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5391.4521	Sweep Width (Hz)	16534.39	Temperature (degree C)	25.000	

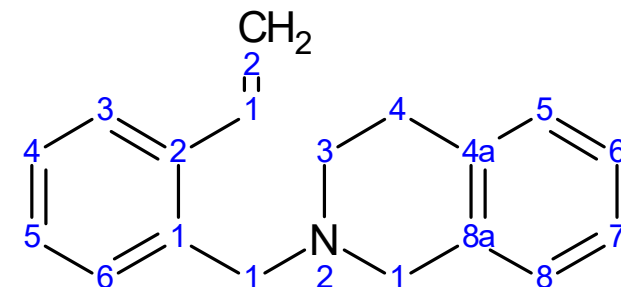


5d

FZ6413-1.jdf

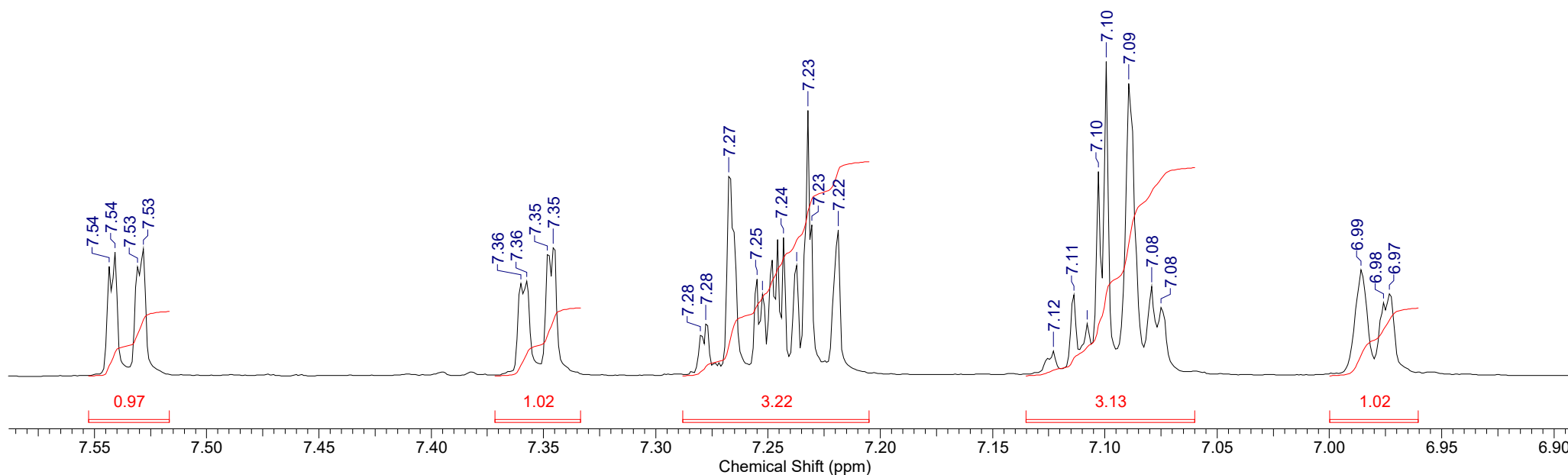


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	19 Feb 1990 07:27:10	
Date Stamp	14 Feb 2018 12:15:19			File Name	C:\Users\Fedor\Desktop\13.02.18\FZ6413-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 36.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5391.4521	Sweep Width (Hz)	16534.39	Temperature (degree C)	25.000	

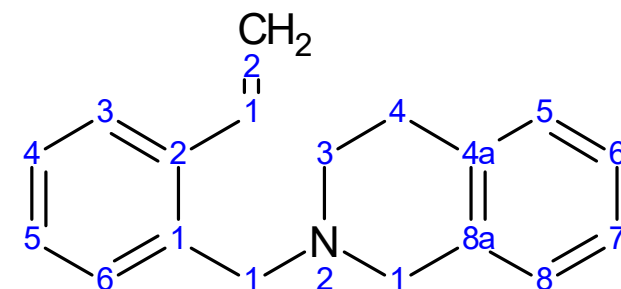


FZ6413-1.jdf

5d

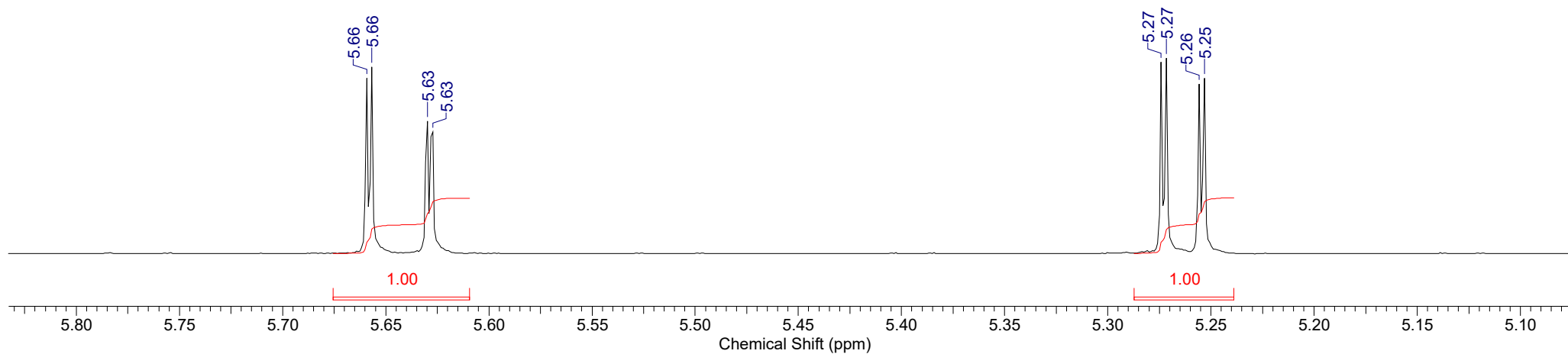


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	19 Feb 1990 07:27:10	
Date Stamp	14 Feb 2018 12:15:19			File Name	C:\Users\Fedor\Desktop\13.02.18\FZ6413-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 36.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5391.4521	Sweep Width (Hz)	16534.39	Temperature (degree C)	25.000	

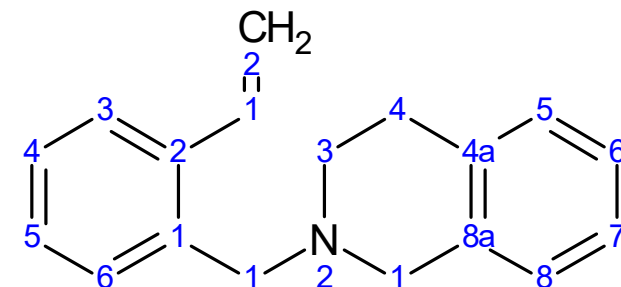


5d

FZ6413-1.jdf

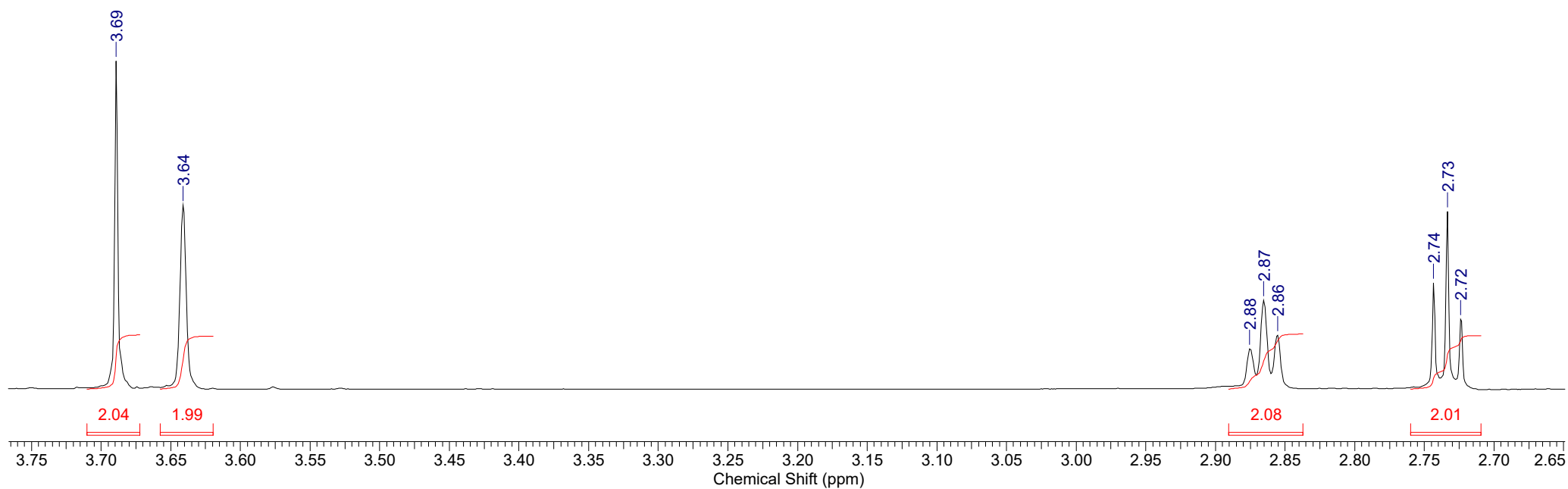


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	19 Feb 1990 07:27:10	
Date Stamp	14 Feb 2018 12:15:19			File Name	C:\Users\Fedor\Desktop\13.02.18\FZ6413-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Original Points Count 32768	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5391.4521	Sweep Width (Hz)	16534.39	Temperature (degree C)	25.000	

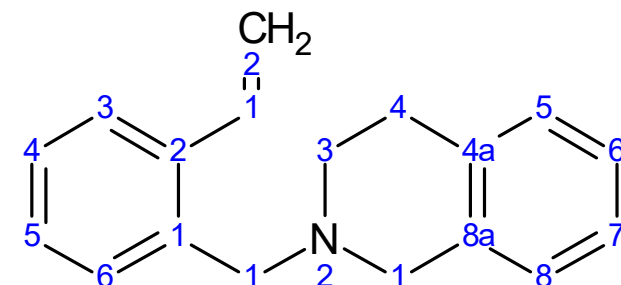


5d

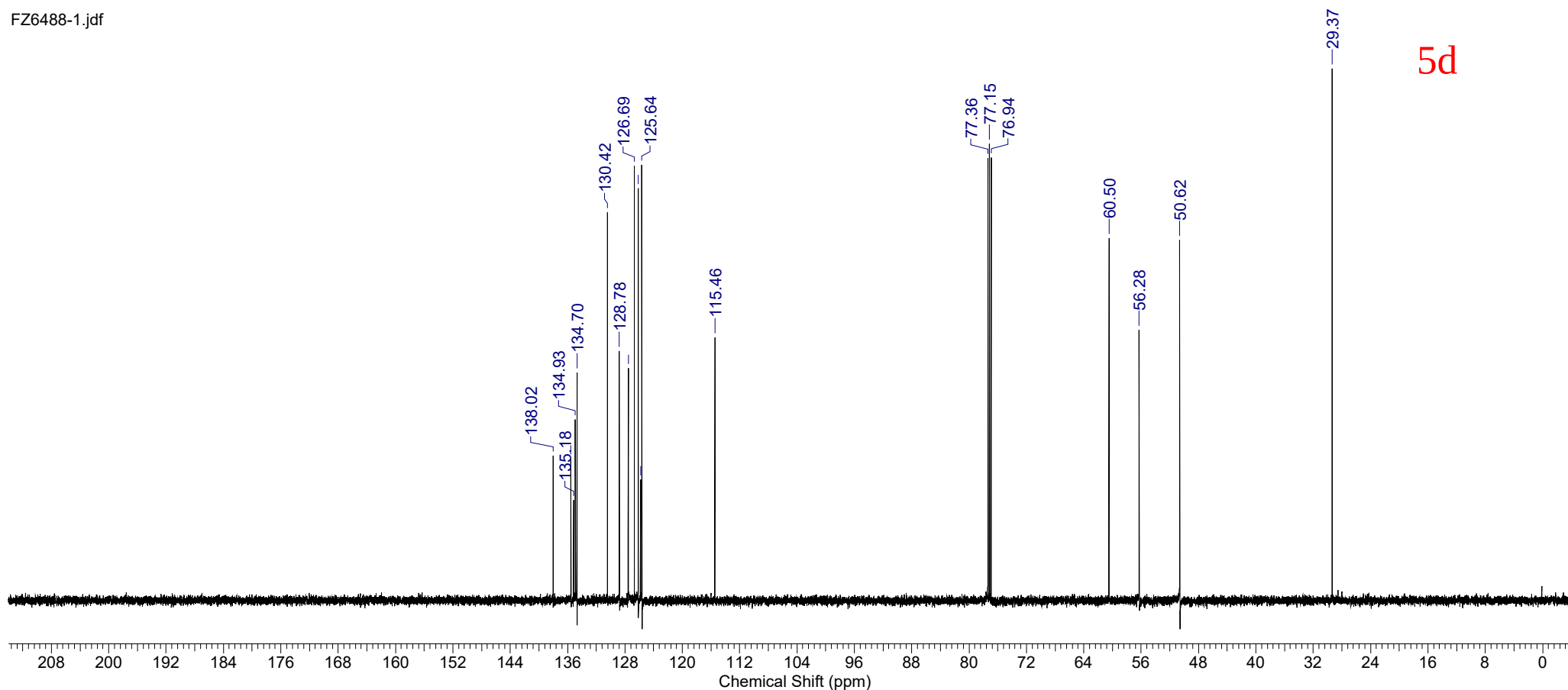
FZ6413-1.jdf



Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	10 Mar 1990 09:44:54	
Date Stamp	06 Mar 2018 14:32:33	File Name	C:\Users\Fedor\Desktop\06.03.18\FZ6488-1.jdf				
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	161	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	23.200				

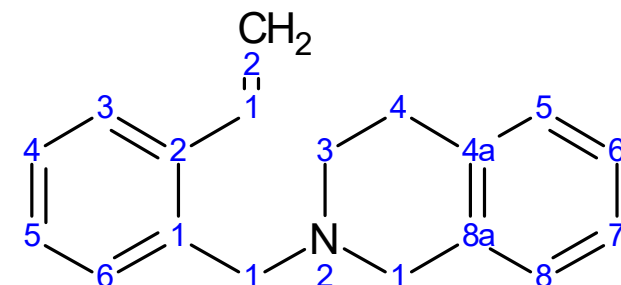


FZ6488-1.jdf

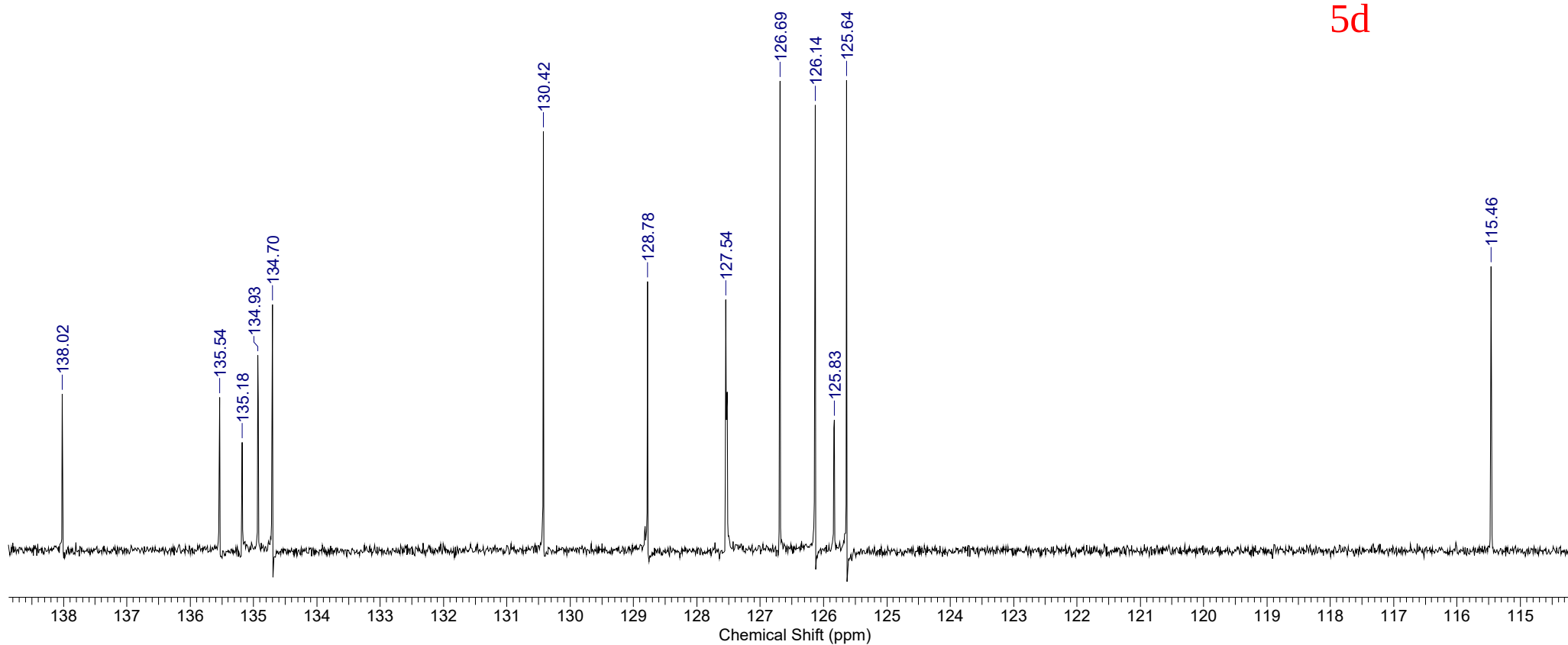


5d

Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	10 Mar 1990 09:44:54	
Date Stamp	06 Mar 2018 14:32:33		File Name	C:\Users\Fedor\Desktop\06.03.18\FZ6488-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	161	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	23.200				

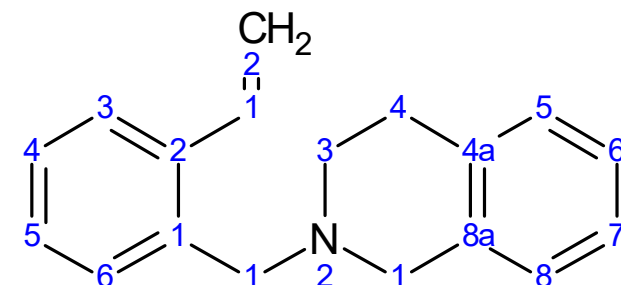


FZ6488-1.jdf

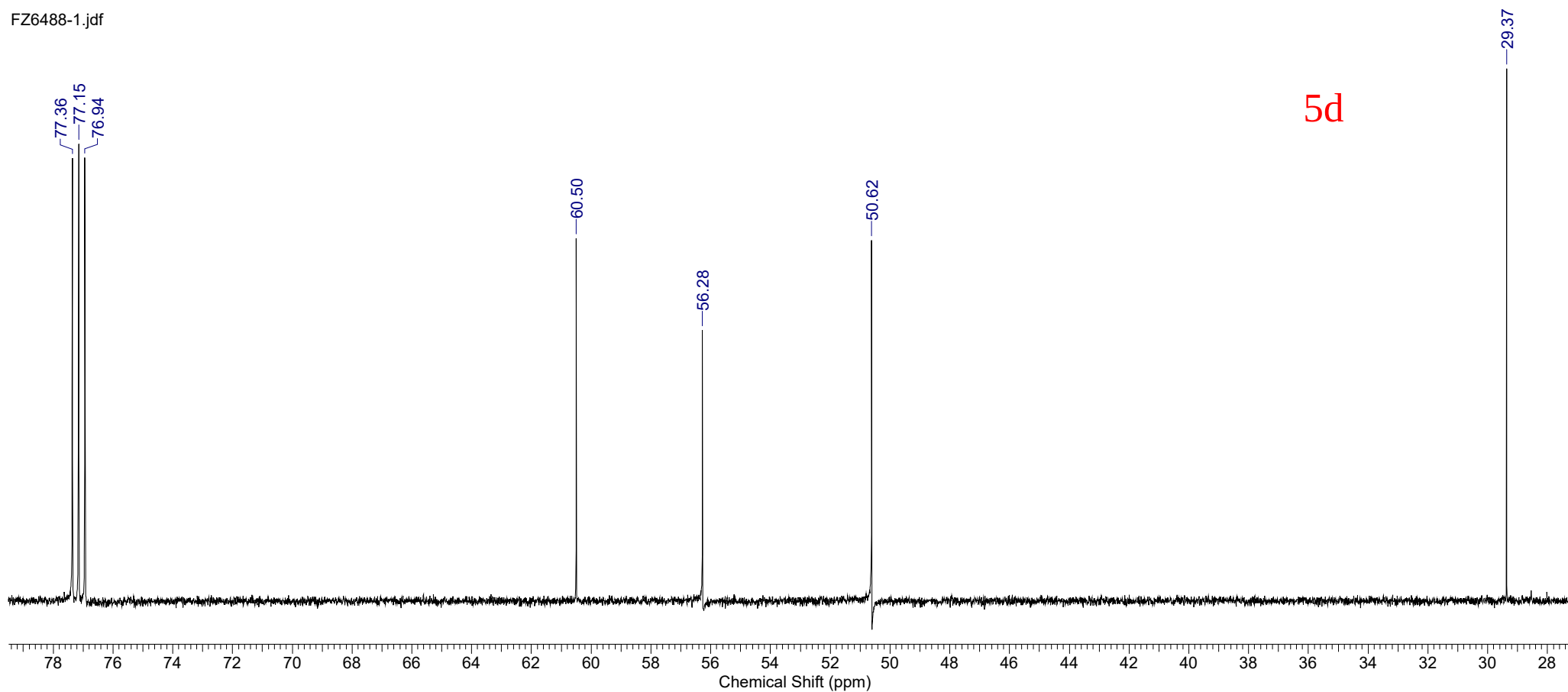


5d

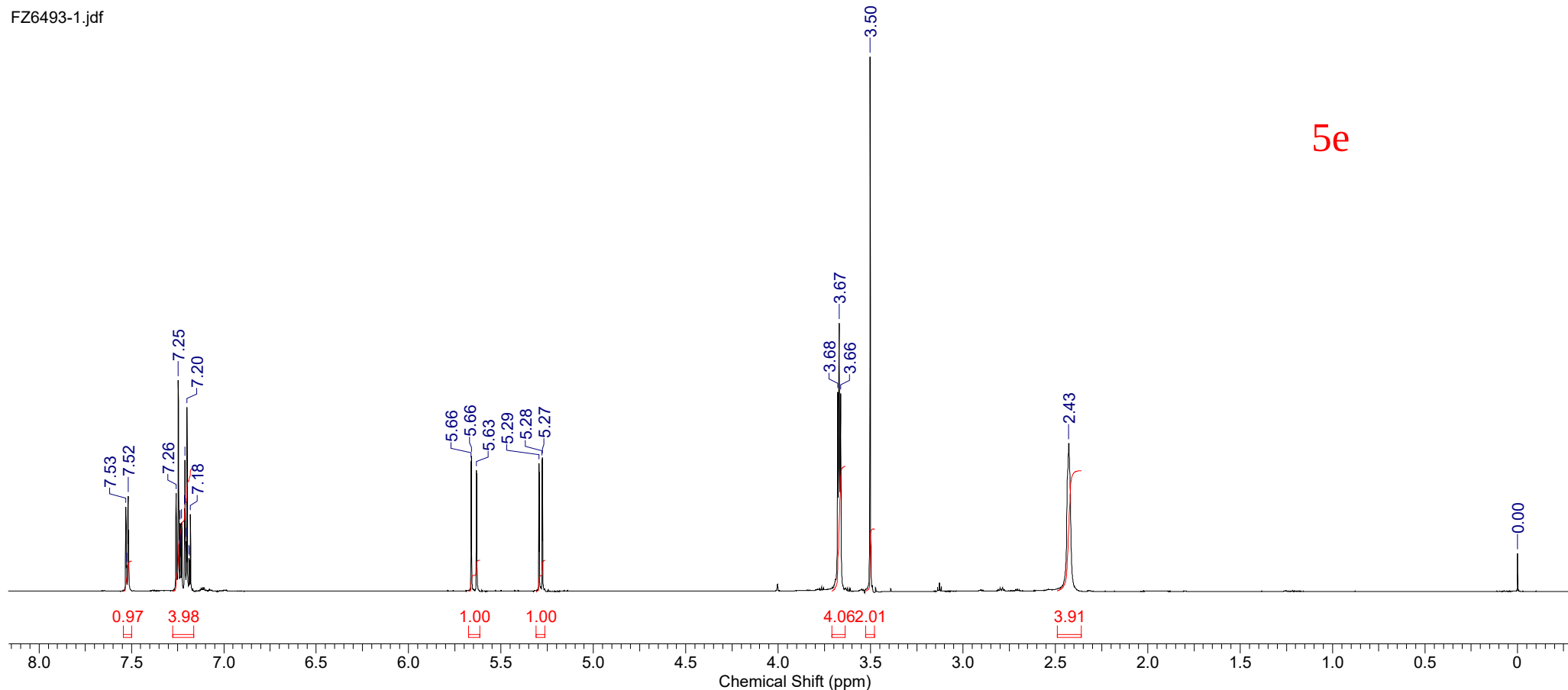
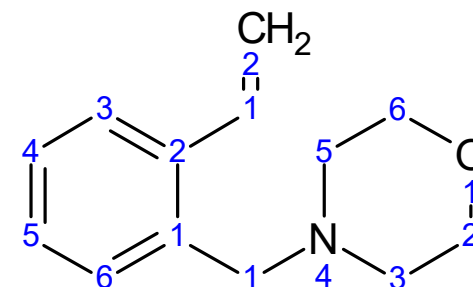
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	10 Mar 1990 09:44:54	
Date Stamp	06 Mar 2018 14:32:33	File Name	C:\Users\Fedor\Desktop\06.03.18\FZ6488-1.jdf				
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	161	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	23.200				



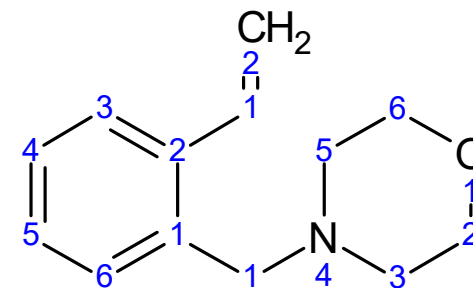
FZ6488-1.jdf



Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	18 Mar 1990 08:34:49	
Date Stamp	14 Mar 2018 13:22:36			File Name	C:\Users\Fedor\Desktop\13.03.18\FZ6493-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 28.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5394.4800	Sweep Width (Hz)	16534.39	Temperature (degree C)	22.200	

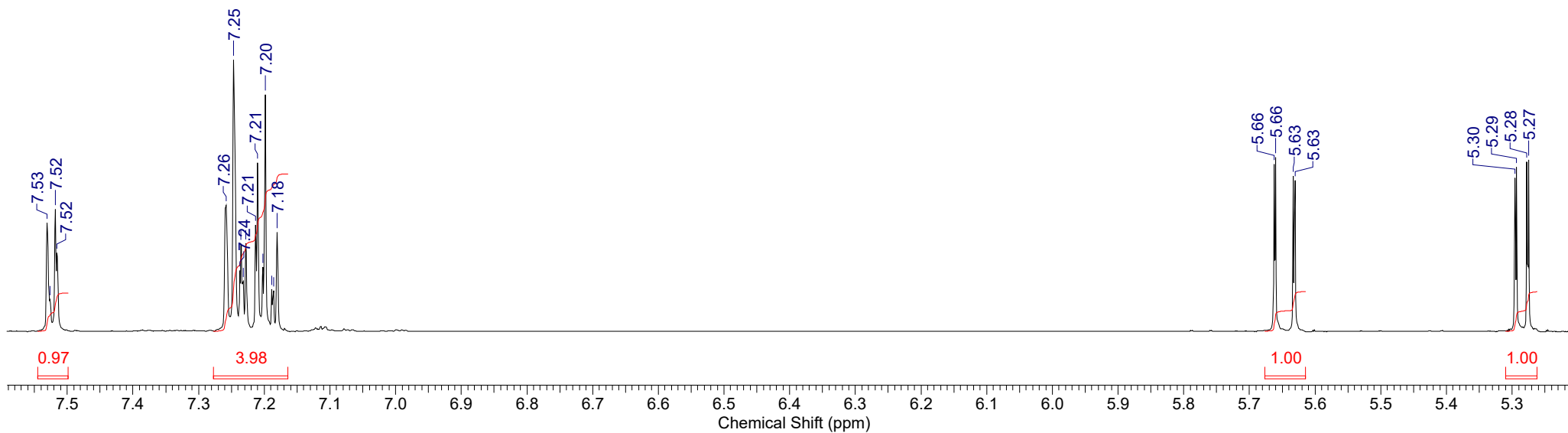


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	18 Mar 1990 08:34:49	
Date Stamp	14 Mar 2018 13:22:36			File Name	C:\Users\Fedor\Desktop\13.03.18\FZ6493-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 28.00	Solvent CHLOROFORM-d
Spectrum Offset (Hz)	5394.4800	Sweep Width (Hz)	16534.39	Temperature (degree C)	22.200	

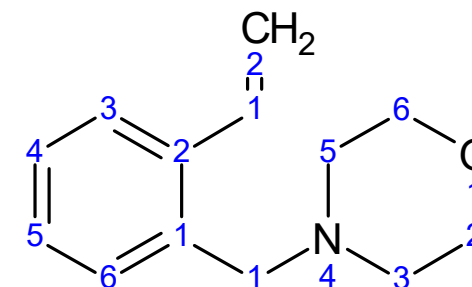


FZ6493-1.jdf

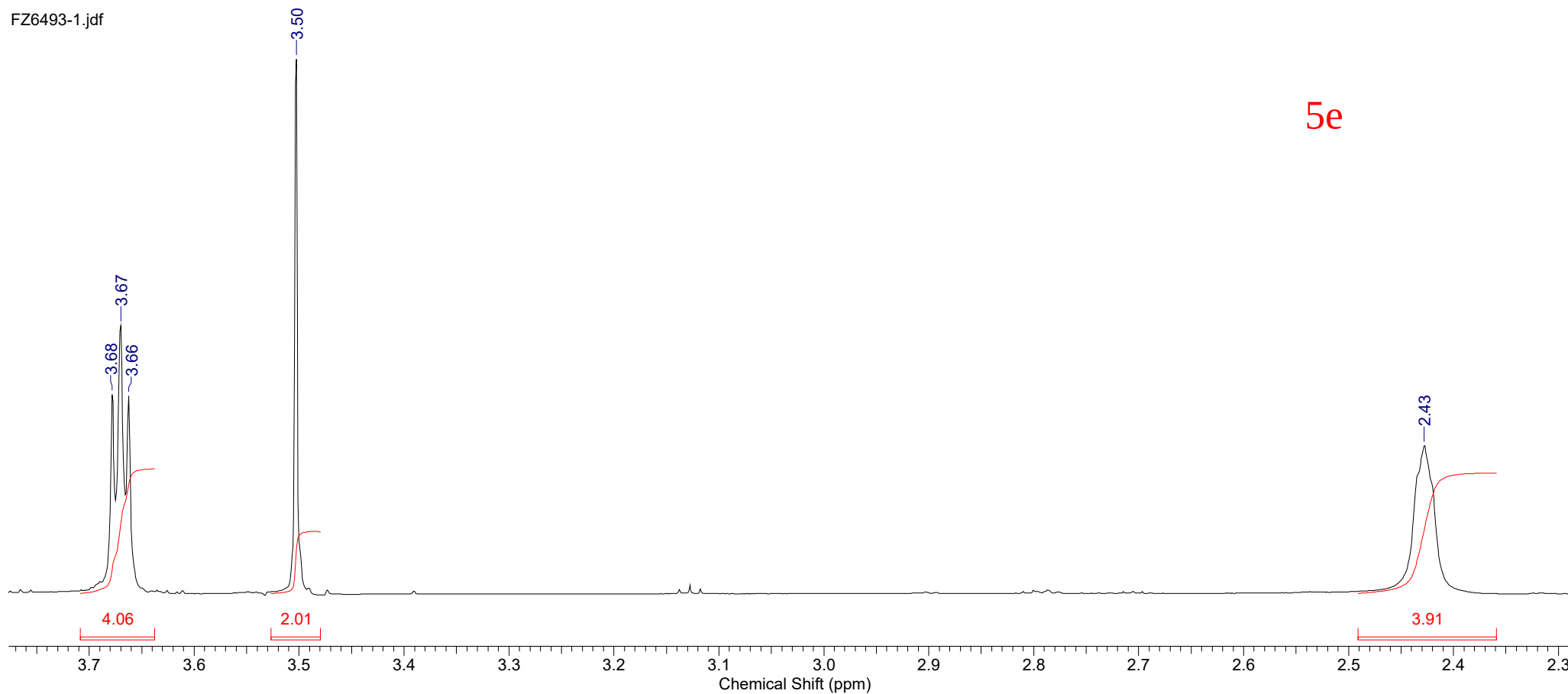
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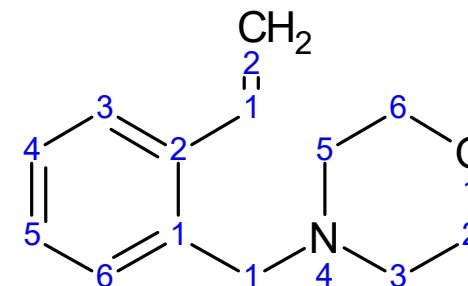
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	18 Mar 1990 08:34:49		
Date Stamp	14 Mar 2018 13:22:36			File Name	C:\Users\Fedor\Desktop\13.03.18\FZ6493-1.jdf	Frequency (MHz)	600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse.ex2			Receiver Gain	28.00
Spectrum Offset (Hz)	5394.4800	Sweep Width (Hz)	16534.39	Temperature (degree C)	22.200	Solvent	CHLOROFORM-d



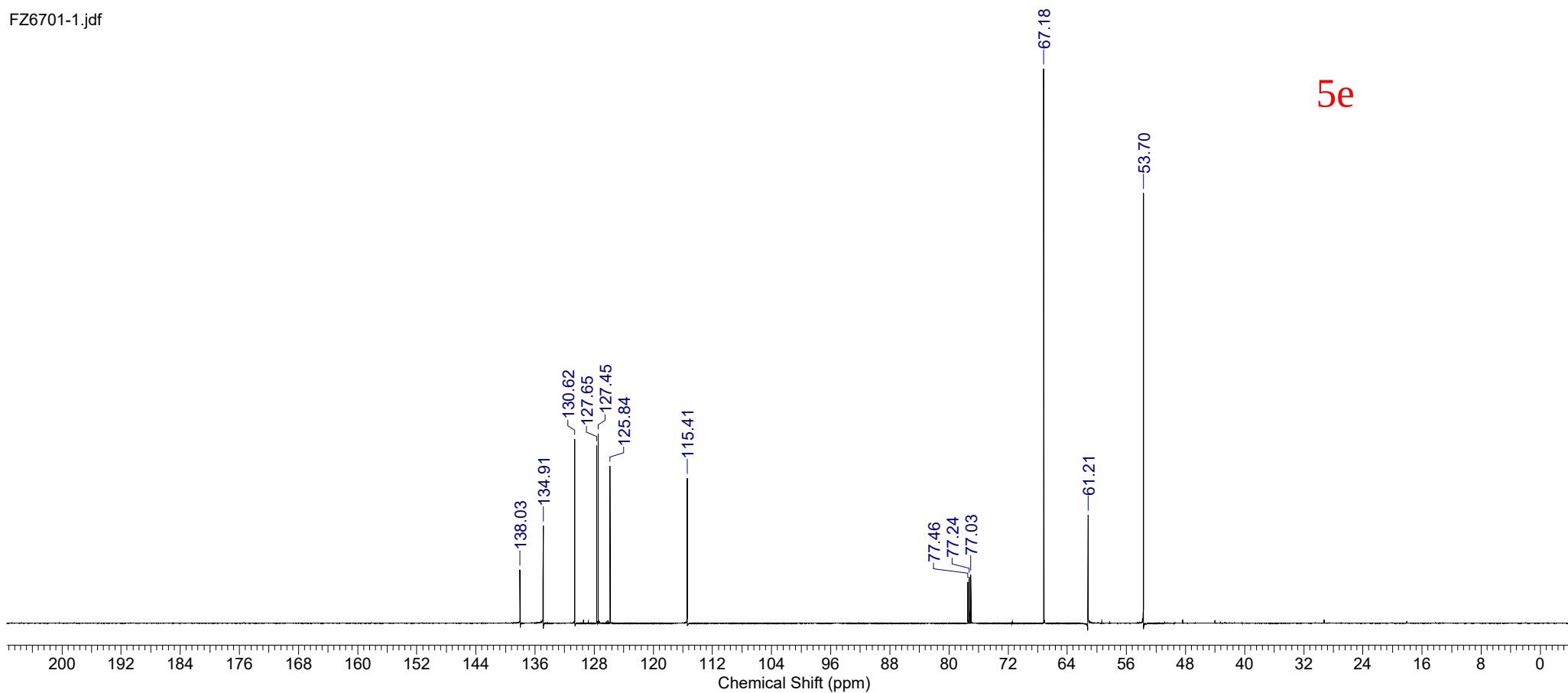
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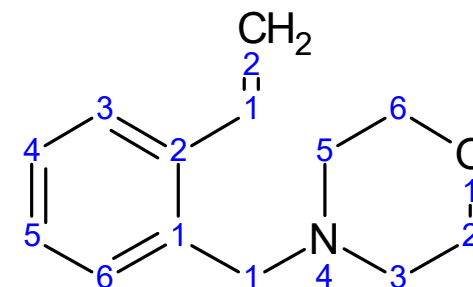
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	14 May 1990 08:53:09	
Date Stamp	10 May 2018 13:40:28	File Name	C:\Users\Fedor\Desktop\08.05.18\FZ6701-1.jdf				
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	15091.3428
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.300				



FZ6701-1.jdf

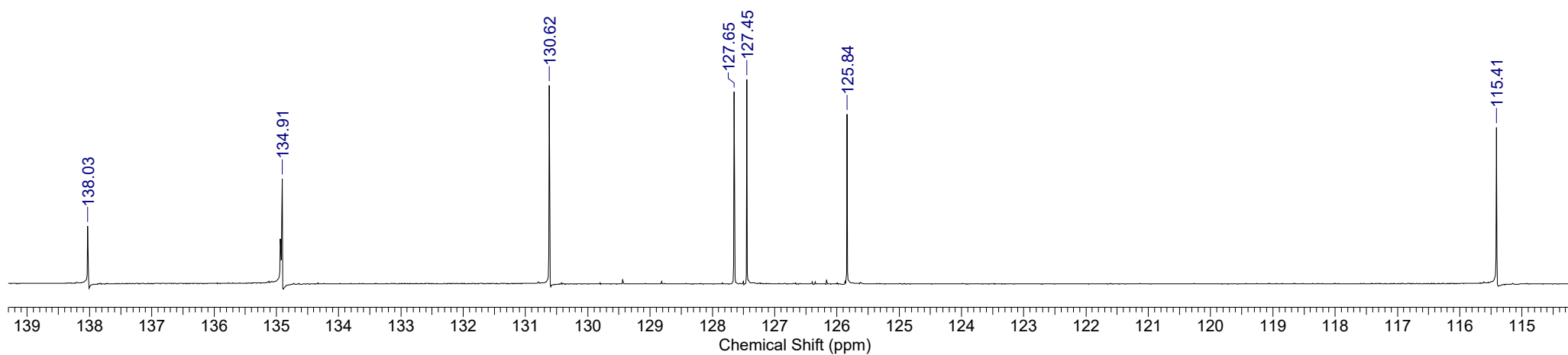


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	14 May 1990 08:53:09	
Date Stamp	10 May 2018 13:40:28		File Name	C:\Users\Fedor\Desktop\08.05.18\FZ6701-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.300				

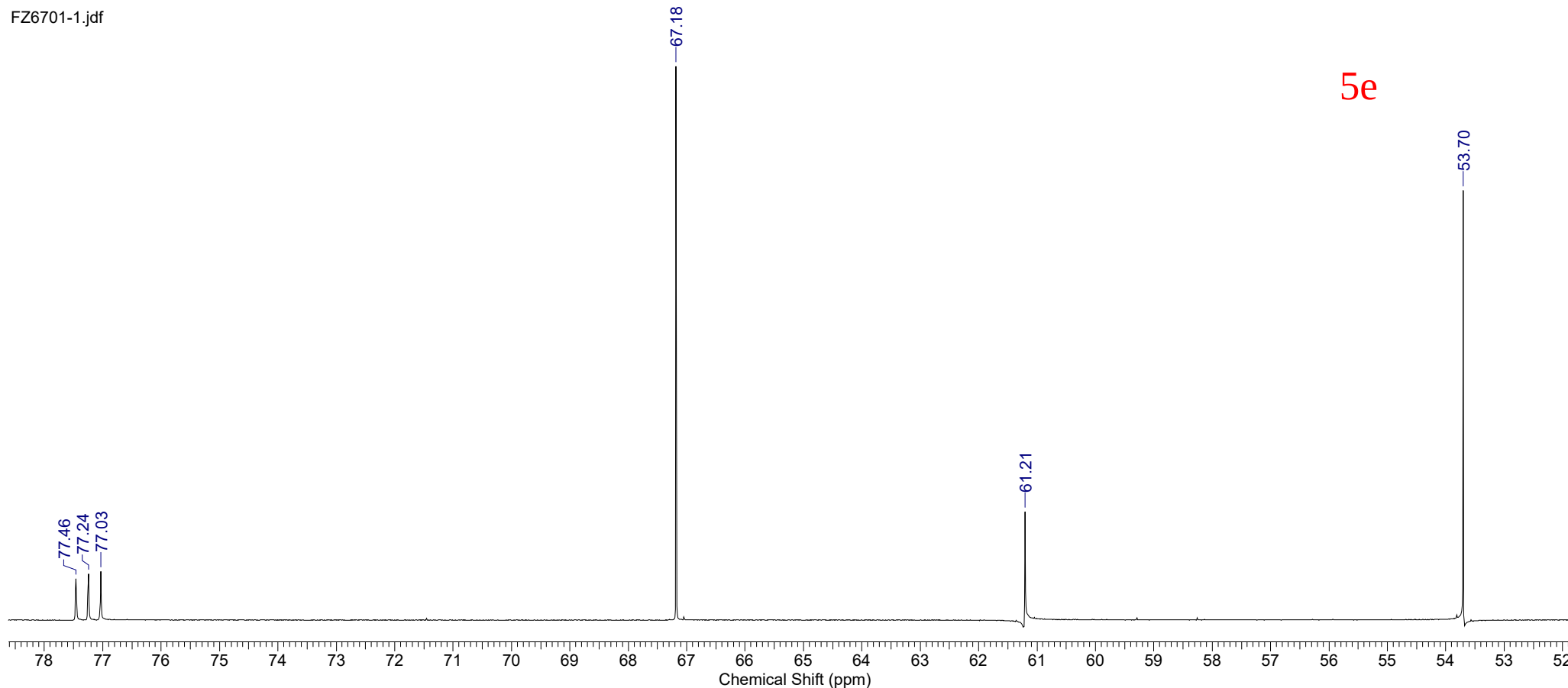
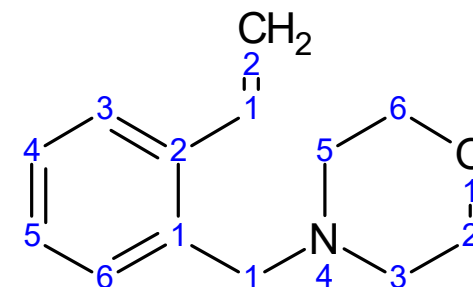


FZ6701-1.jdf

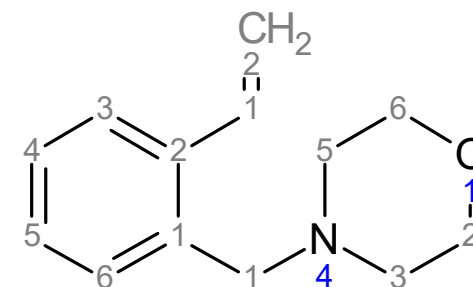
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Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	14 May 1990 08:53:09	
Date Stamp	10 May 2018 13:40:28		File Name	C:\Users\Fedor\Desktop\08.05.18\FZ6701-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.300				

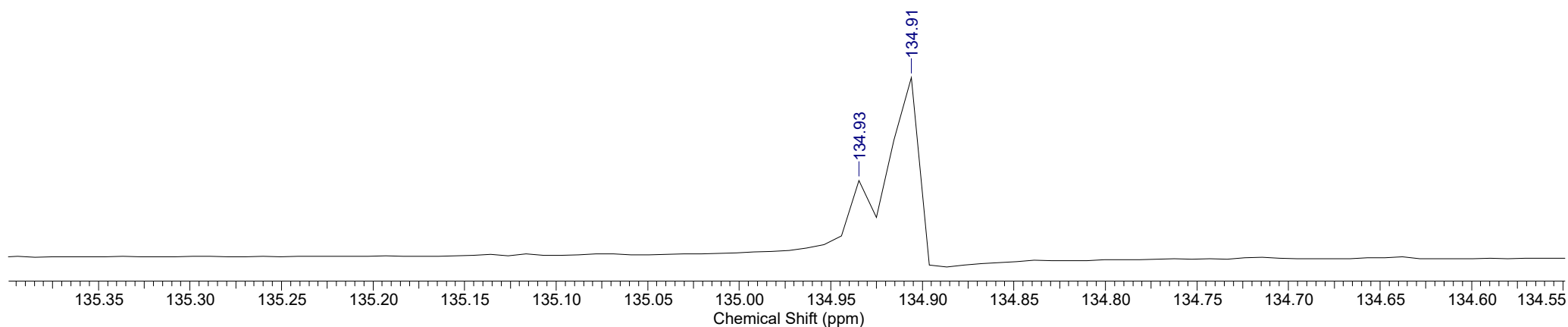


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	14 May 1990 08:53:09	
Date Stamp	10 May 2018 13:40:28		File Name	C:\Users\Fedor\Desktop\08.05.18\FZ6701-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	52.00	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	15091.3428	
Sweep Width (Hz)	47348.49	Temperature (degree C)	22.300				

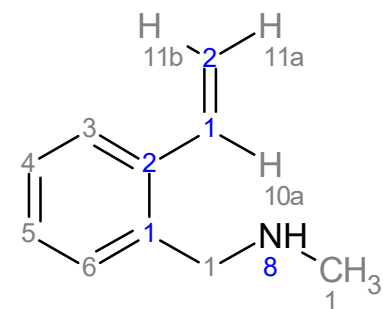


FZ6701-1.jdf

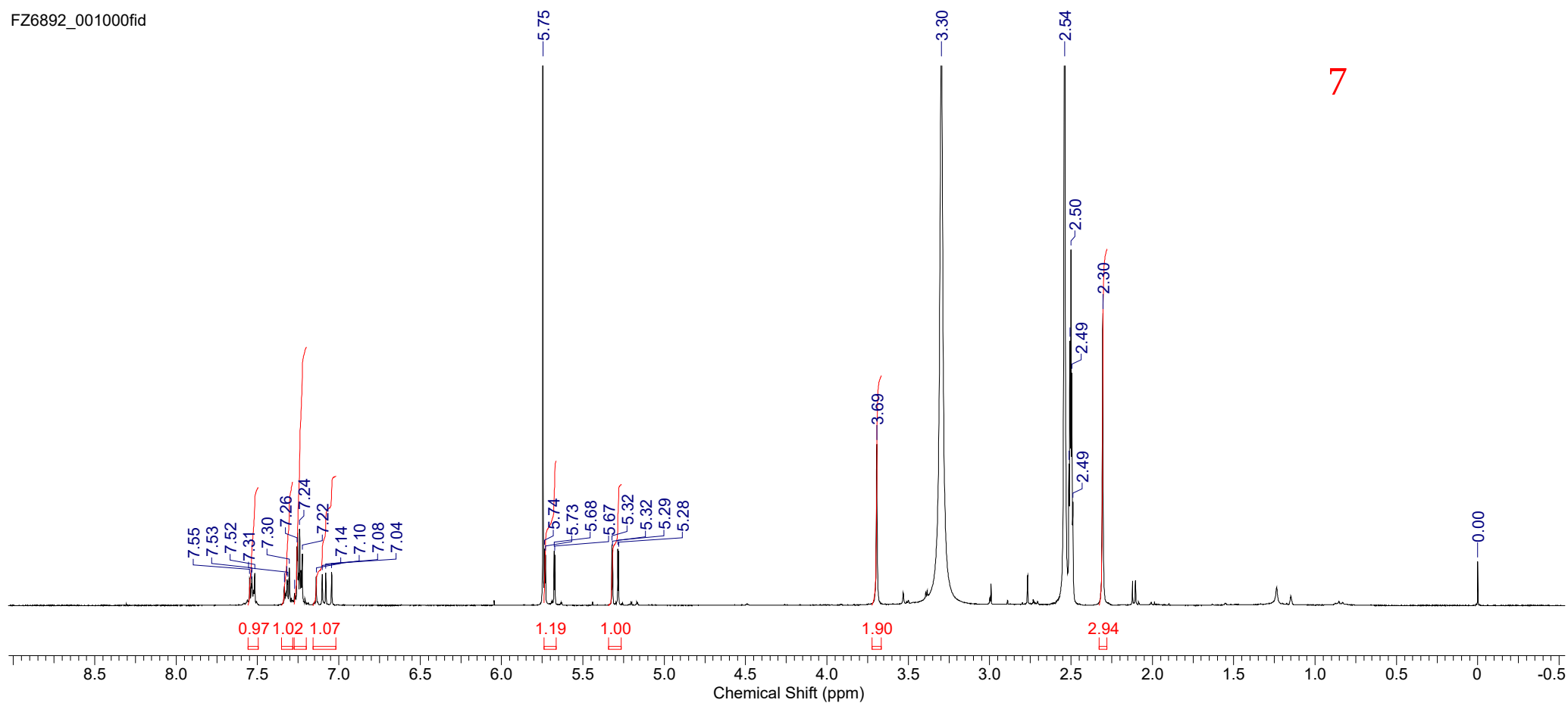
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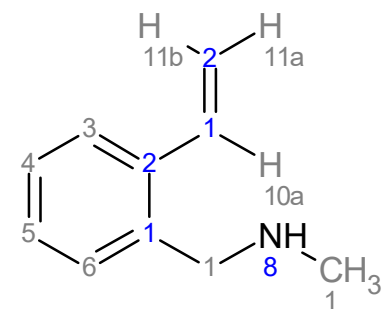
Acquisition Time (sec)	2.7263	Comment	FZ6892	Date	01 Oct 2018 17:46:40	Date Stamp	01 Oct 2018 17:46:40
File Name	C:\Users\Fedor\Desktop\01.10.18\FZ6892\FZ6892_001000fid			Frequency (MHz)	300.13	Nucleus	1H
Number of Transients	64	Origin	spect	Original Points Count	32768	Owner	nmr
Pulse Sequence	zg	Receiver Gain	202.48	SW(cyclical) (Hz)	12019.23	Solvent	DMSO-d6
Sweep Width (Hz)	12018.86	Temperature (degree C)	29.999			Spectrum Offset (Hz)	1348.1652



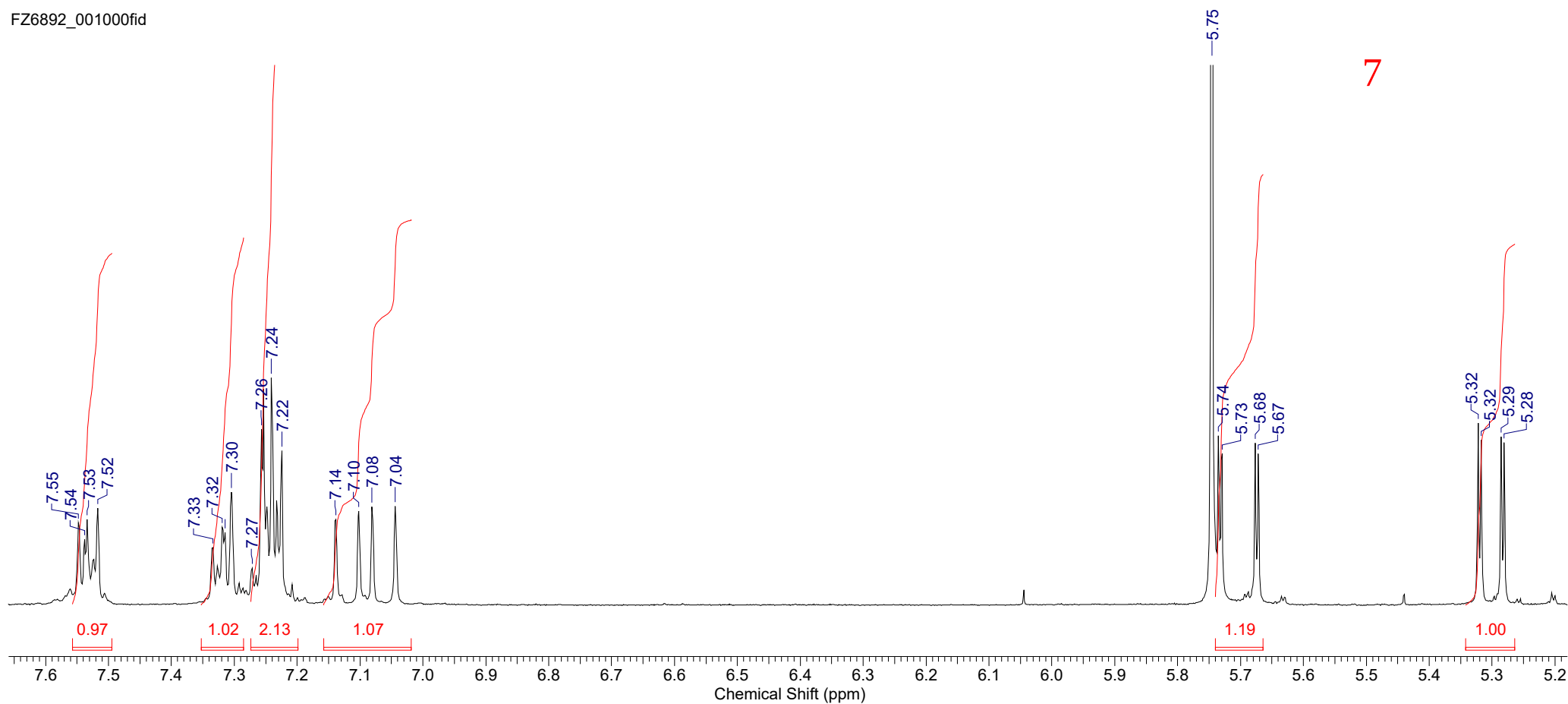
FZ6892_001000fid



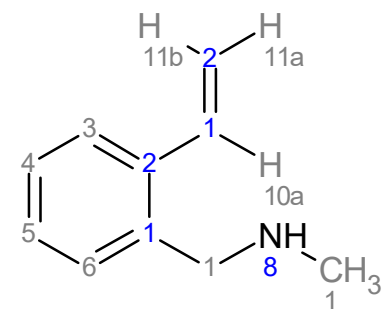
Acquisition Time (sec)	2.7263	Comment	FZ6892	Date	01 Oct 2018 17:46:40	Date Stamp	01 Oct 2018 17:46:40		
File Name	C:\Users\Fedor\Desktop\01.10.18\FZ6892\FZ6892_001000fid				Frequency (MHz)	300.13	Nucleus	1H	
Number of Transients	64	Origin	spect	Original Points Count	32768	Owner	nmr	Points Count	32768
Pulse Sequence	zg	Receiver Gain	202.48	SW(cyclical) (Hz)	12019.23	Solvent	DMSO-d6	Spectrum Offset (Hz)	1348.1652
Sweep Width (Hz)	12018.86	Temperature (degree C)	29.999						



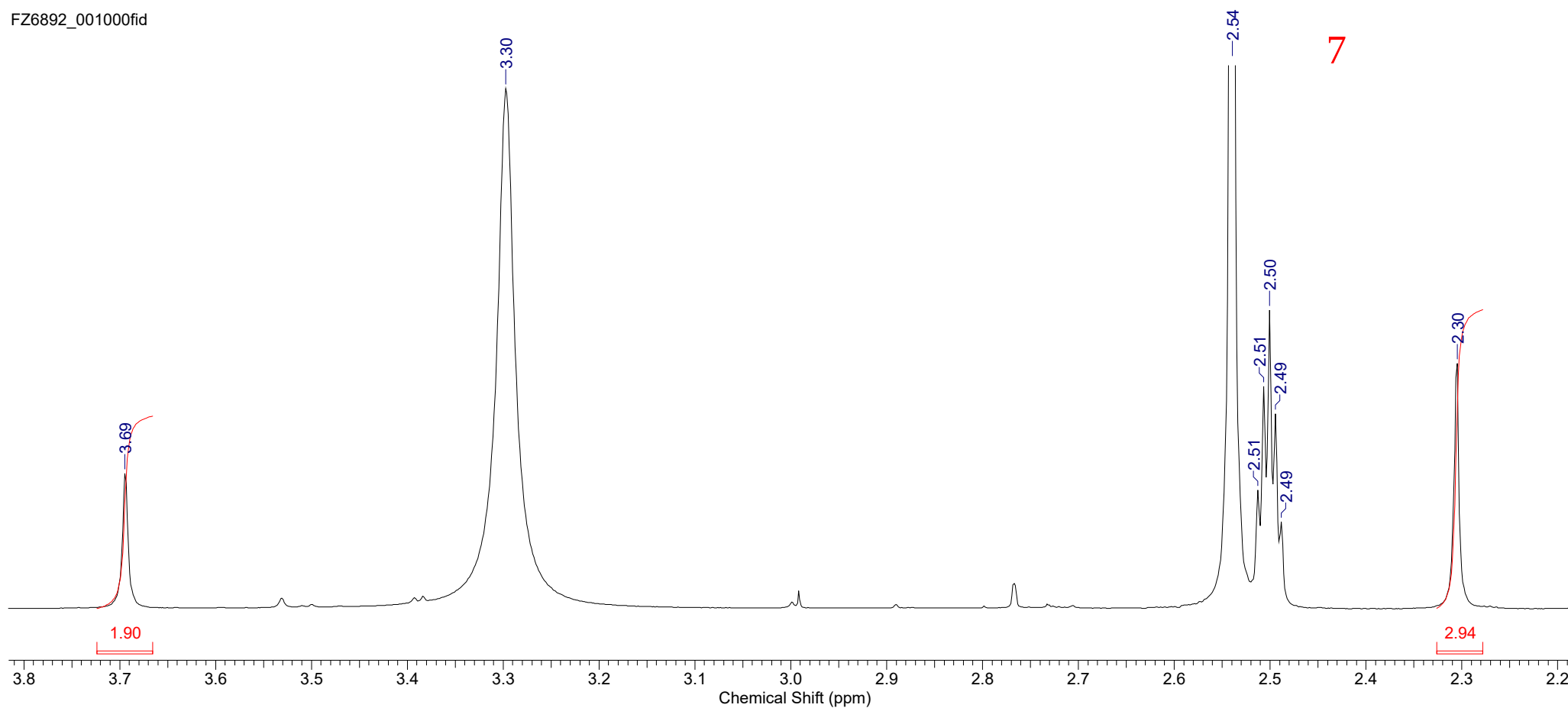
FZ6892_001000fid



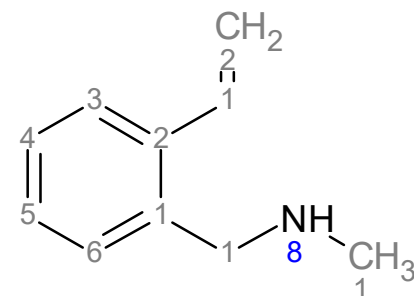
Acquisition Time (sec)	2.7263	Comment	FZ6892	Date	01 Oct 2018 17:46:40	Date Stamp	01 Oct 2018 17:46:40		
File Name	C:\Users\Fedor\Desktop\01.10.18\FZ6892\FZ6892_001000fid				Frequency (MHz)	300.13	Nucleus	1H	
Number of Transients	64	Origin	spect	Original Points Count	32768	Owner	nmr	Points Count	32768
Pulse Sequence	zg	Receiver Gain	202.48	SW(cyclical) (Hz)	12019.23	Solvent	DMSO-d6	Spectrum Offset (Hz)	1348.1652
Sweep Width (Hz)	12018.86	Temperature (degree C)	29.999						



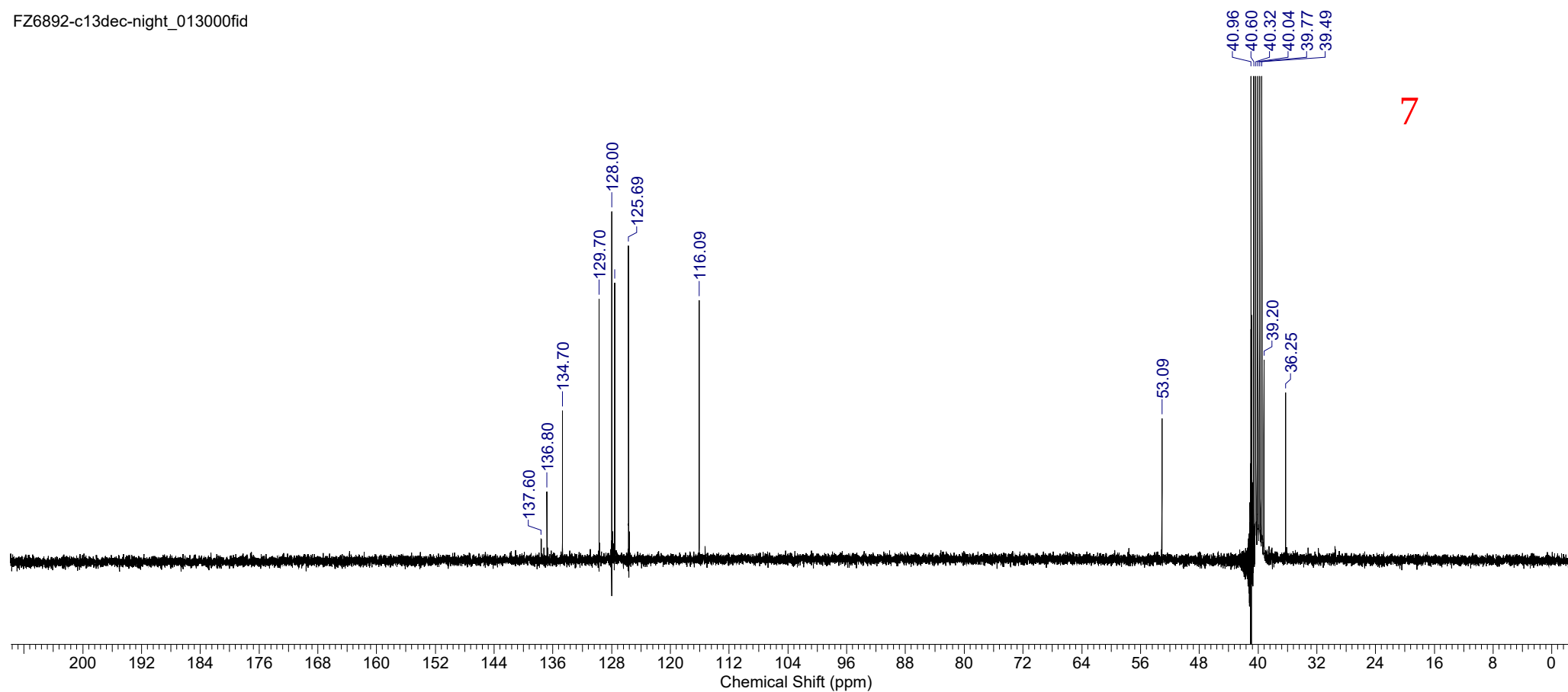
FZ6892_001000fid



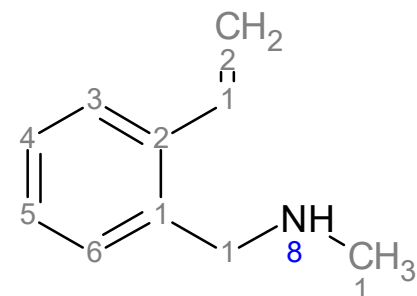
Acquisition Time (sec)	0.8561	Comment	FZ6892-c13dec-night	Date	01 Oct 2018 19:03:28
Date Stamp	01 Oct 2018 19:03:28	File Name	C:\Users\Fedor\Desktop\01.10.18\FZ6892-c13dec-night\FZ6892-c13dec-night_013000fid		
Frequency (MHz)	75.48	Nucleus	¹³ C	Number of Transients	20480
Original Points Count	22528	Owner	nmr	Points Count	32768
Receiver Gain	202.48	SW(cyclical) (Hz)	26315.79	Pulse Sequence	zgpg
Sweep Width (Hz)	26314.99	Temperature (degree C)	29.991	Spectrum Offset (Hz)	7548.8423



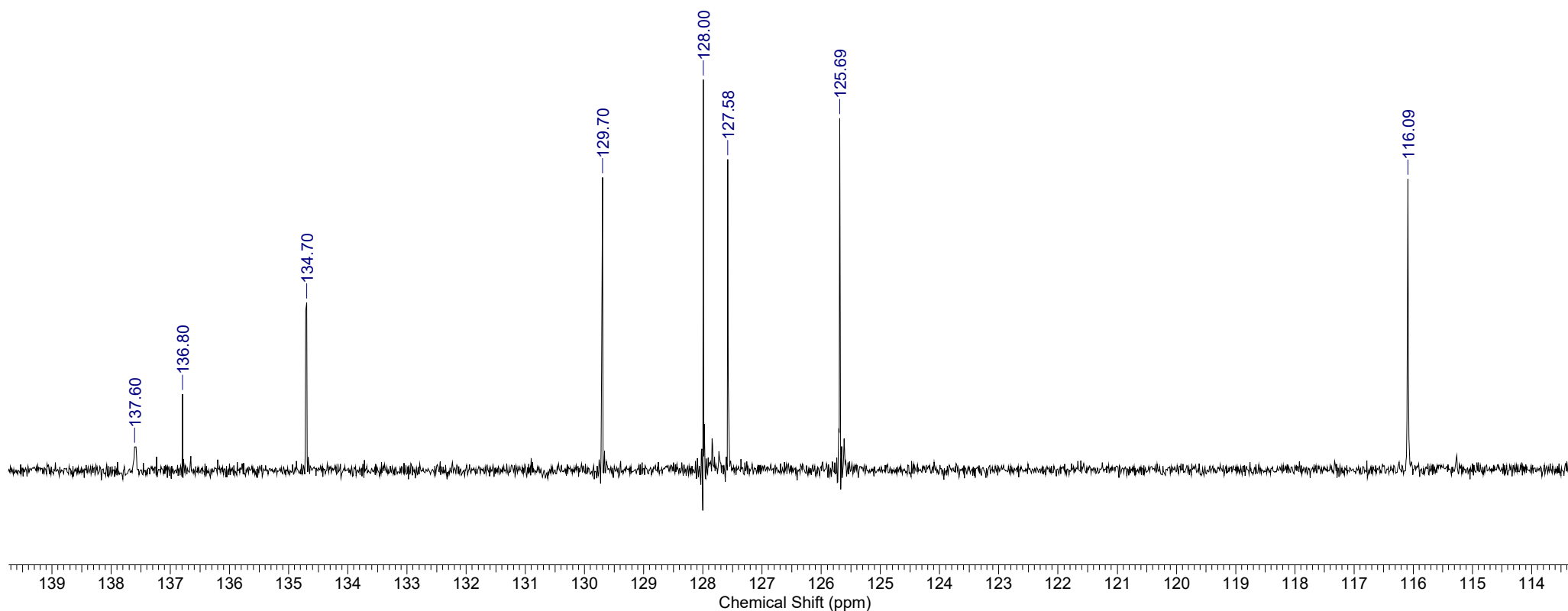
FZ6892-c13dec-night_013000fid



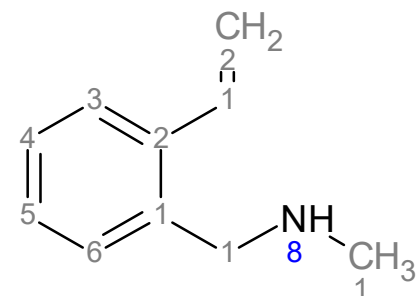
Acquisition Time (sec)	0.8561	Comment	FZ6892-c13dec-night	Date	01 Oct 2018 19:03:28
Date Stamp	01 Oct 2018 19:03:28	File Name	C:\Users\Fedor\Desktop\01.10.18\FZ6892-c13dec-night\FZ6892-c13dec-night_013000fid		
Frequency (MHz)	75.48	Nucleus	¹³ C	Number of Transients	20480
Original Points Count	22528	Owner	nmr	Points Count	32768
Receiver Gain	202.48	SW(cyclical) (Hz)	26315.79	Pulse Sequence	zgpg
Sweep Width (Hz)	26314.99	Temperature (degree C)	29.991	Spectrum Offset (Hz)	7548.8423



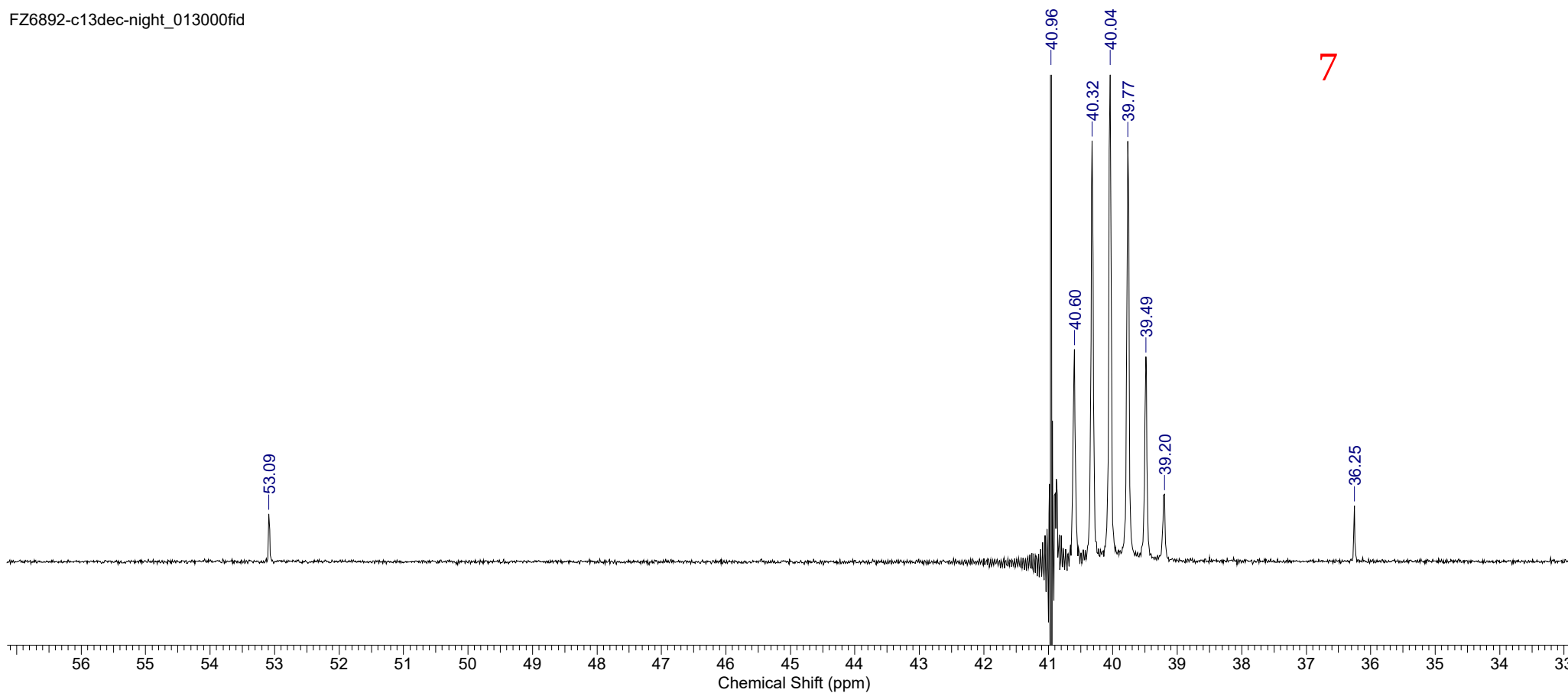
FZ6892-c13dec-night_013000fid



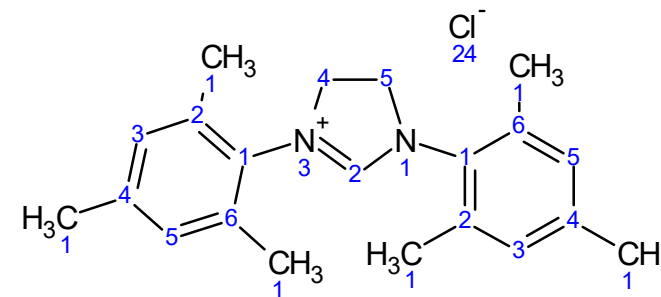
Acquisition Time (sec)	0.8561	Comment	FZ6892-c13dec-night	Date	01 Oct 2018 19:03:28
Date Stamp	01 Oct 2018 19:03:28	File Name	C:\Users\Fedor\Desktop\01.10.18\FZ6892-c13dec-night\FZ6892-c13dec-night_013000fid		
Frequency (MHz)	75.48	Nucleus	¹³ C	Number of Transients	20480
Original Points Count	22528	Owner	nmr	Points Count	32768
Receiver Gain	202.48	SW(cyclical) (Hz)	26315.79	Pulse Sequence	zgpg
Sweep Width (Hz)	26314.99	Temperature (degree C)	29.991	Spectrum Offset (Hz)	7548.8423



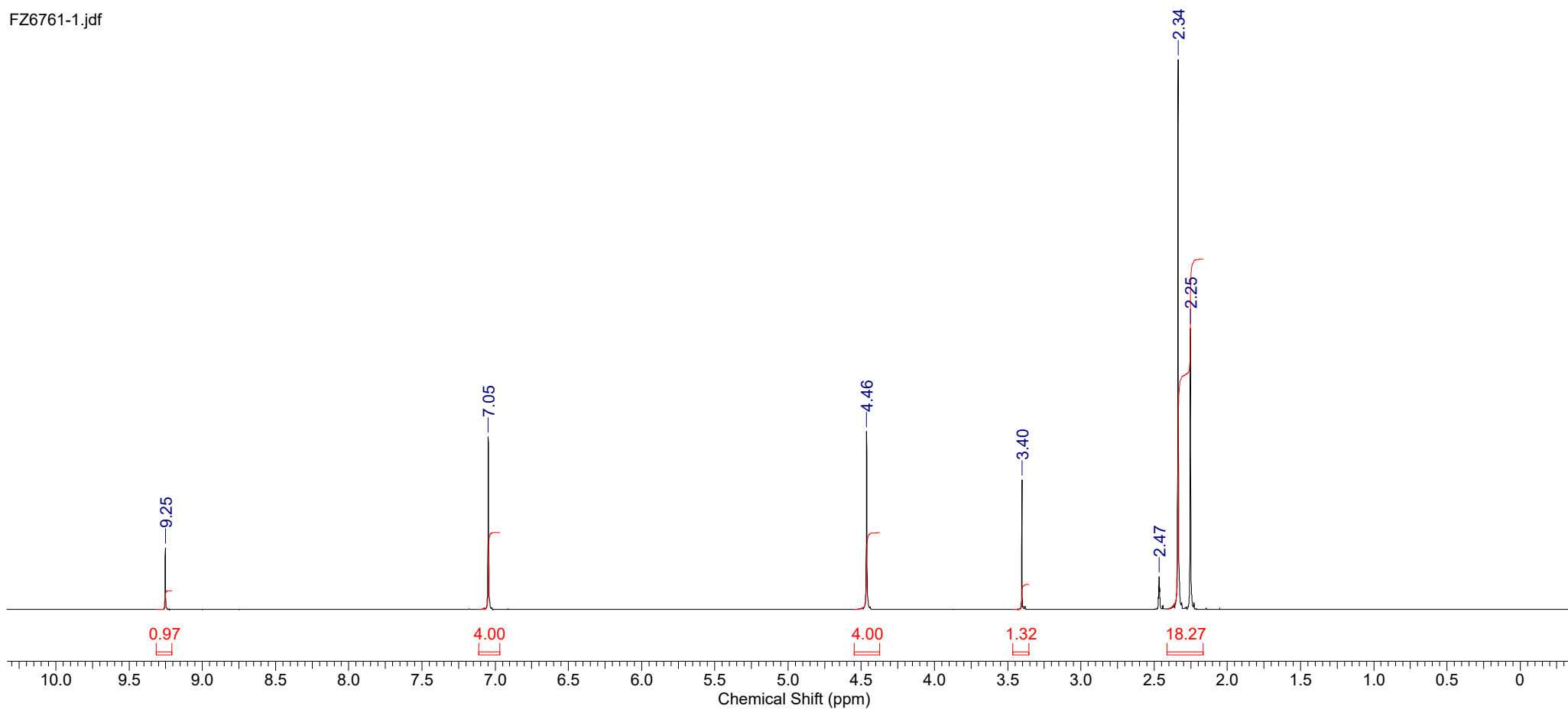
FZ6892-c13dec-night_013000fid



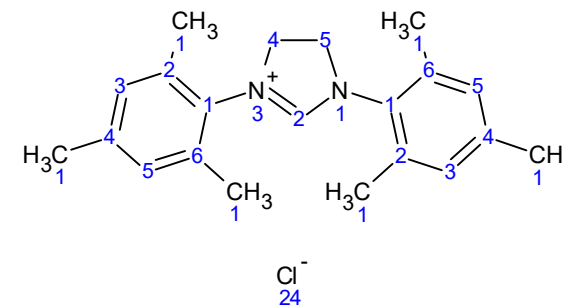
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jun 1990 05:09:58	
Date Stamp	06 Jun 2018 09:56:41			File Name	C:\Users\Fedor\Desktop\05.06.18\FZ6761-1.jdf	Frequency (MHz) 600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Owner delta
Points Count	32768	Pulse Sequence	single_pulse.ex2		Receiver Gain 26.00	Solvent DMSO-d6
Spectrum Offset (Hz)	5401.5503	Sweep Width (Hz)	16534.39	Temperature (degree C)	21.100	



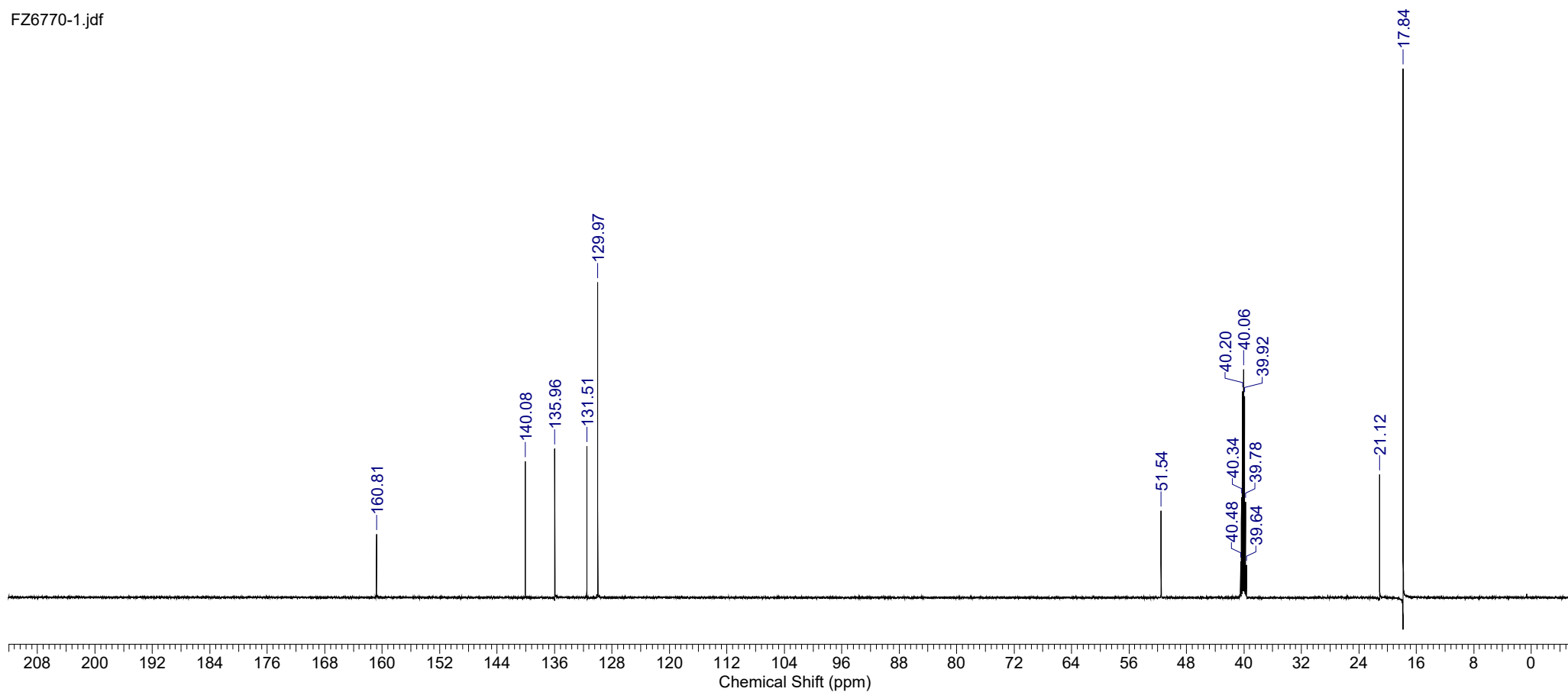
FZ6761-1.jdf



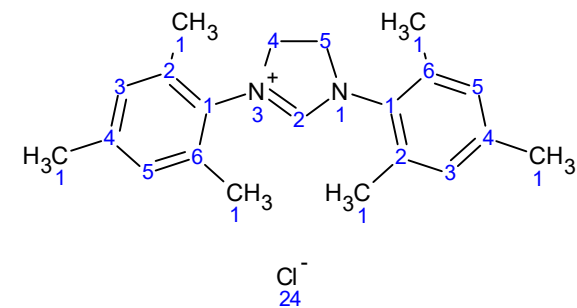
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	17 Jun 1990 13:43:07	
Date Stamp	14 Jun 2018 00:17:21		File Name	C:\Users\Fedor\Desktop\12.06.18\FZ6770-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	54.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49
Temperature (degree C)	21.300						



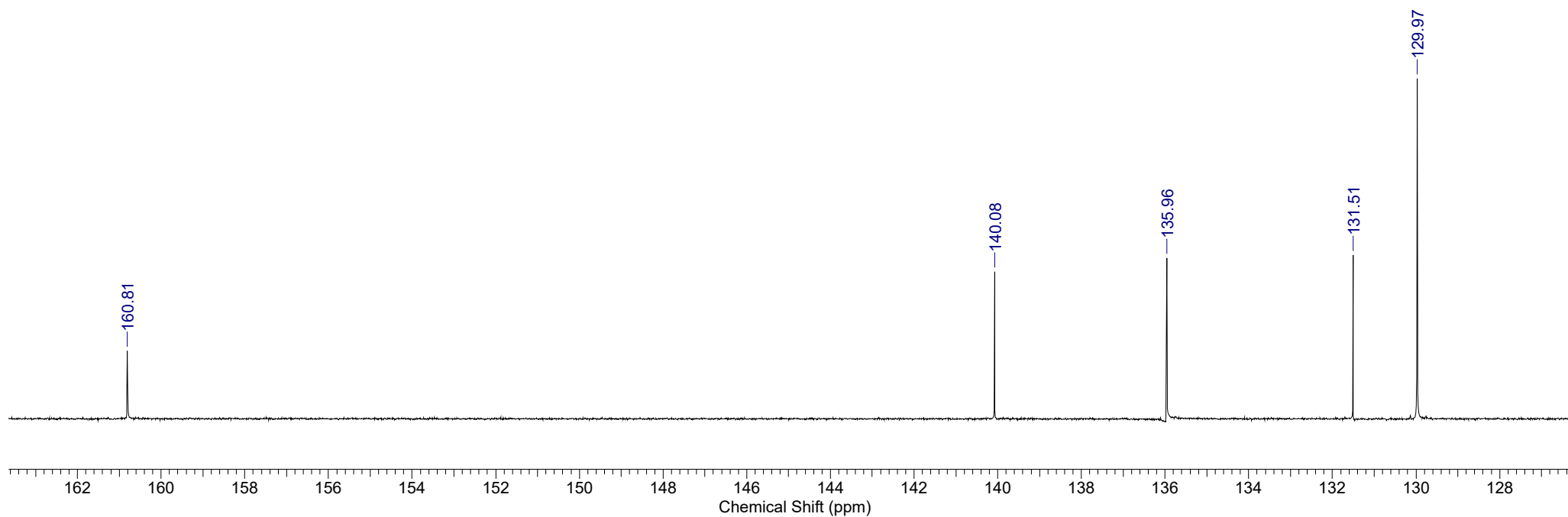
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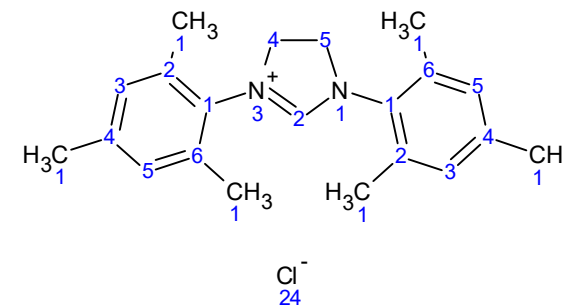
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	17 Jun 1990 13:43:07	
Date Stamp	14 Jun 2018 00:17:21		File Name	C:\Users\Fedor\Desktop\12.06.18\FZ6770-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	54.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49
Temperature (degree C)	21.300						



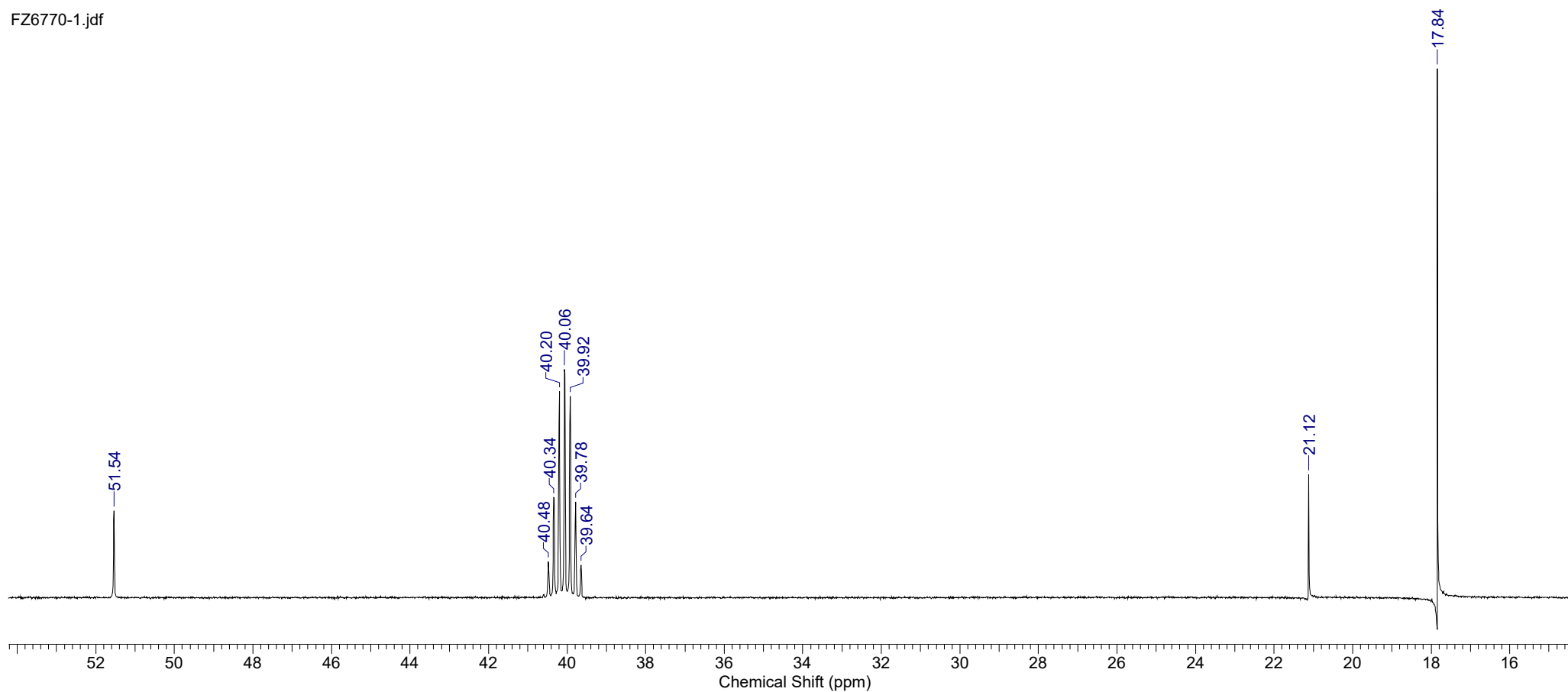
FZ6770-1.jdf



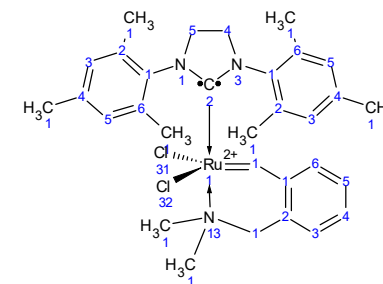
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	17 Jun 1990 13:43:07	
Date Stamp	14 Jun 2018 00:17:21		File Name	C:\Users\Fedor\Desktop\12.06.18\FZ6770-1.jdf			
Frequency (MHz)	150.91	Nucleus	13C	Number of Transients	1000	Origin	ECA 600
Original Points Count	32768	Owner	delta	Points Count	32768	Pulse Sequence	single pulse dec
Receiver Gain	54.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49
Temperature (degree C)	21.300						



FZ6770-1.jdf

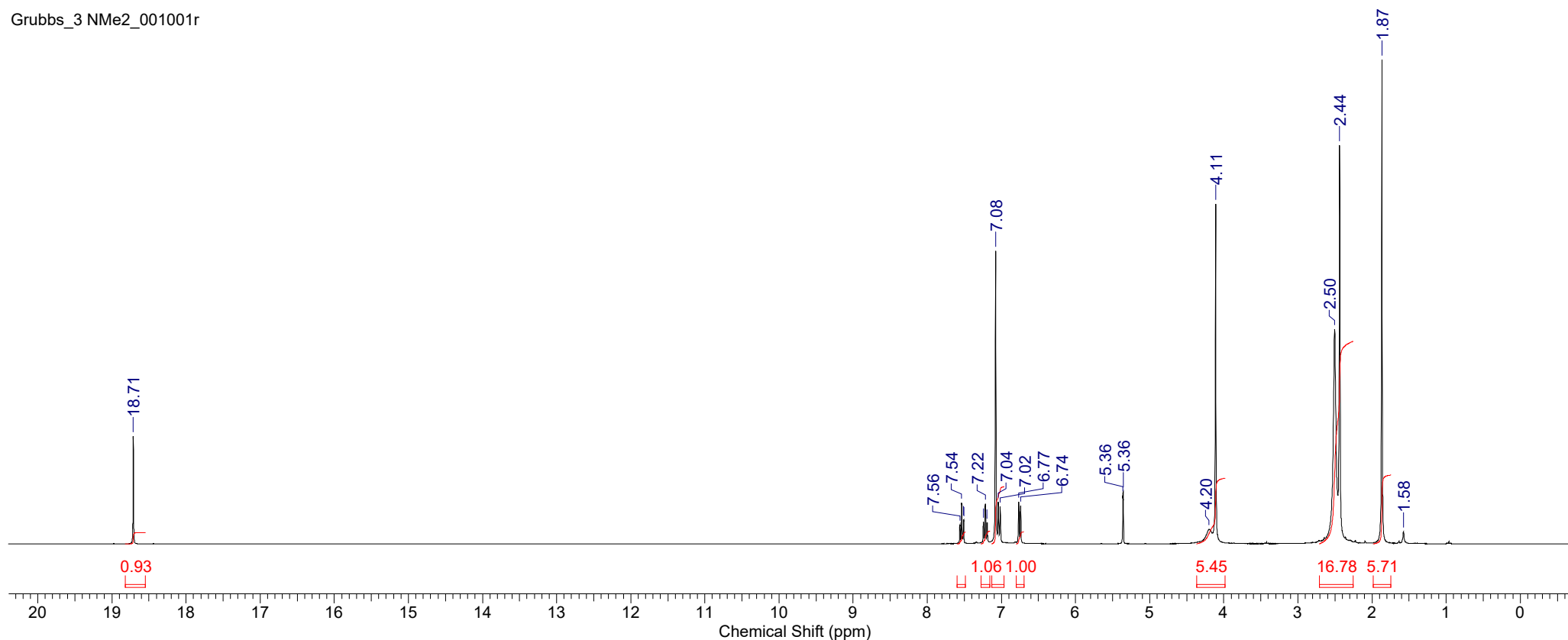


Acquisition Time (sec)	2.5690				
Comment	FZ Grubbs 3 1 Mes2NHC-(cyclo)-RuCl2=CH-C6H4-CH2-NMe2- 26 mg / CD2Cl2 / Jan 12 Spectra - Jan 17, storage at -18C in CD2Cl2 solution				
Date	17 Jan 2018 16:25:36	Date Stamp	17 Jan 2018 16:25:36		
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 3 NMe2_001001r				
Frequency (MHz)	300.13	Nucleus	1H	Number of Transients	32
Origin	spect	Original Points Count	65536	Owner	nmr
Points Count	262144	Pulse Sequence	zg	Receiver Gain	89.51
SW(cyclical) (Hz)	25510.20	Solvent	DICHLOROMETHANE-d2	Spectrum Offset (Hz)	1350.5919
Sweep Width (Hz)	25510.11	Temperature (degree C)	29.998		

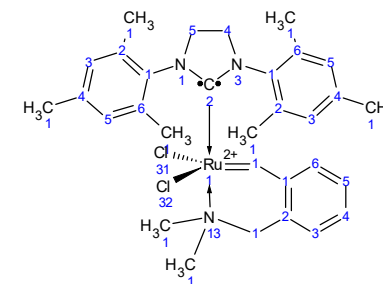


11a

Grubbs_3 NMe2_001001r

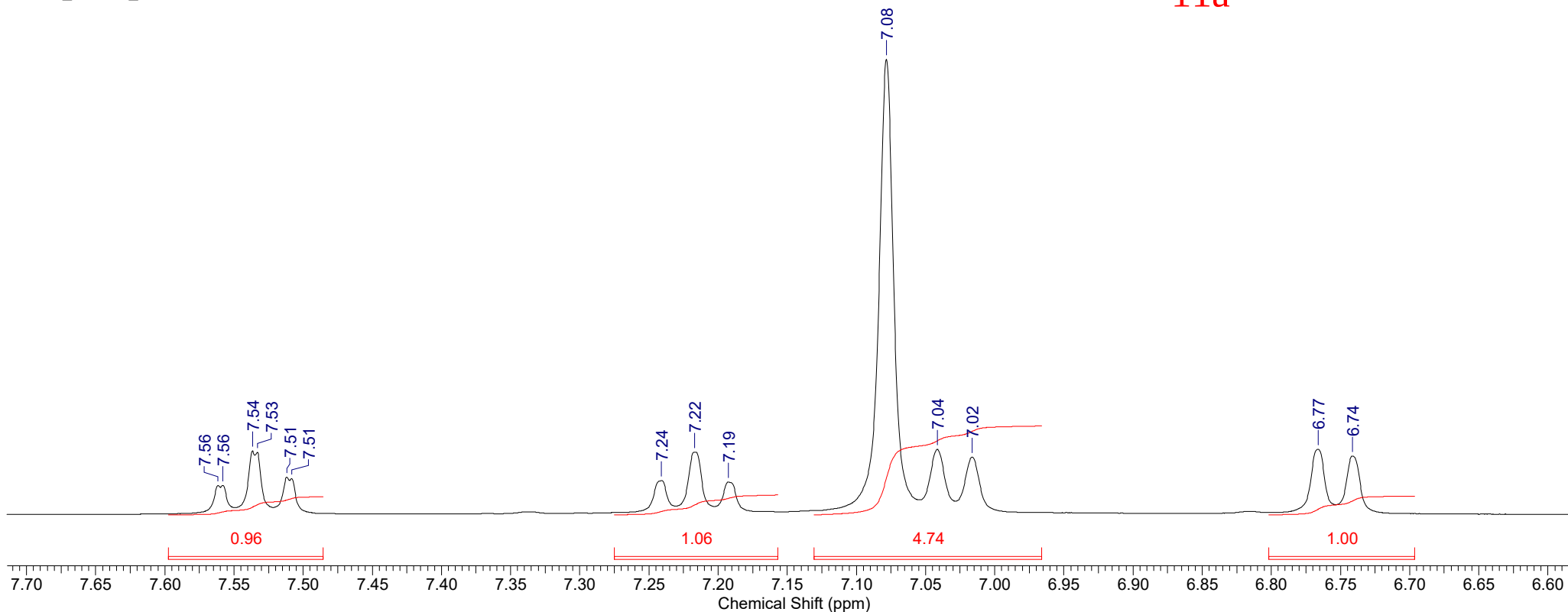


Acquisition Time (sec)	2.5690				
Comment	FZ Grubbs 3 1 Mes2NHC-(cyclo)-RuCl2=CH-C6H4-CH2-NMe2- 26 mg / CD2Cl2 / Jan 12 Spectra - Jan 17, storage at -18C in CD2Cl2 solution				
Date	17 Jan 2018 16:25:36	Date Stamp	17 Jan 2018 16:25:36		
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 3 NMe2_001001r				
Frequency (MHz)	300.13	Nucleus	1H	Number of Transients	32
Origin	spect	Original Points Count	65536	Owner	nmr
Points Count	262144	Pulse Sequence	zg	Receiver Gain	89.51
SW(cyclical) (Hz)	25510.20	Solvent	DICHLOROMETHANE-d2	Spectrum Offset (Hz)	1350.5919
Sweep Width (Hz)	25510.11	Temperature (degree C)	29.998		

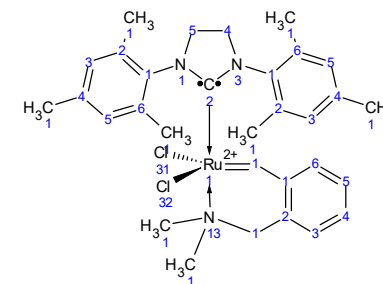


11a

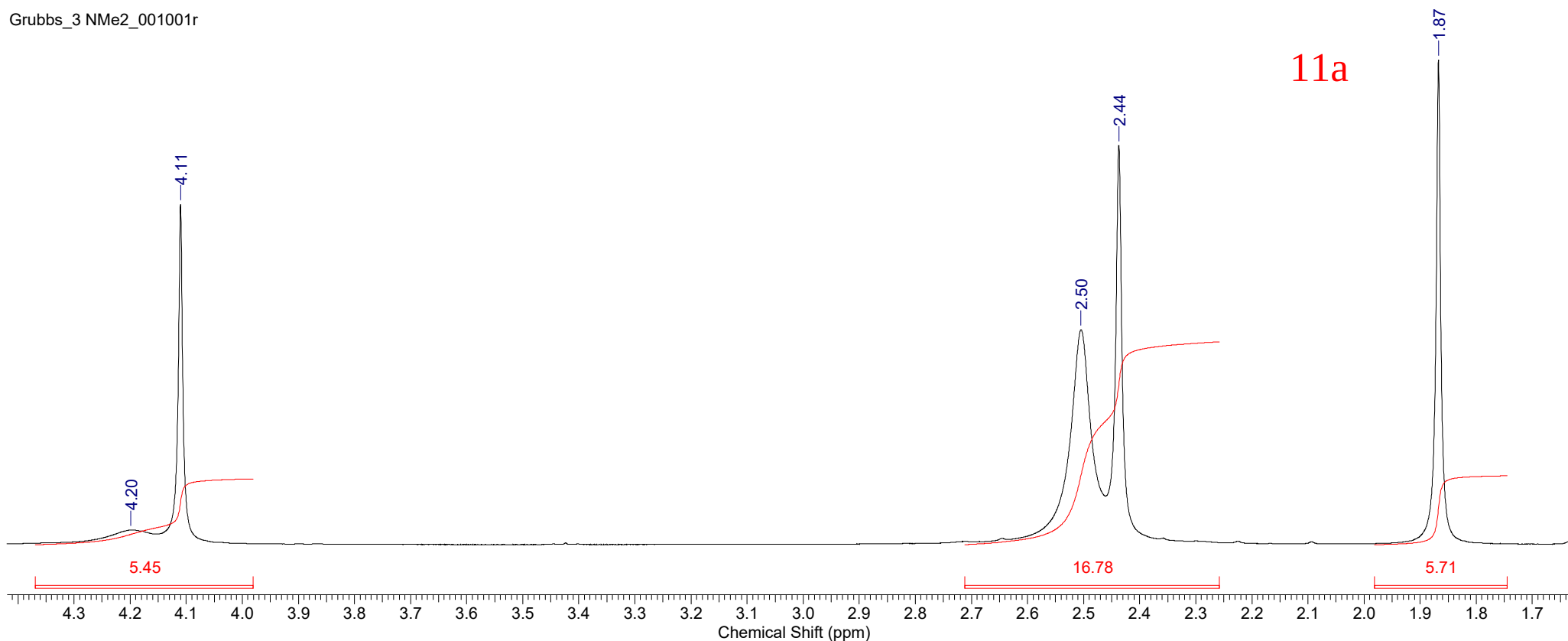
Grubbs_3 NMe2_001001r



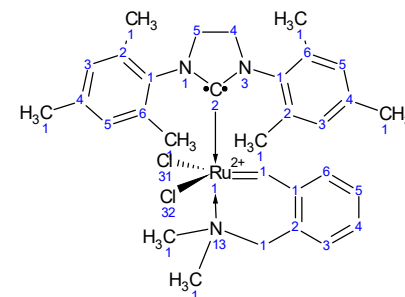
Acquisition Time (sec)	2.5690		
Comment	FZ Grubbs 3 1 Mes2NHC-(cyclo)-RuCl2=CH-C6H4-CH2-NMe2- 26 mg / CD2Cl2 / Jan 12 Spectra - Jan 17, storage at -18C in CD2Cl2 solution		
Date	17 Jan 2018 16:25:36	Date Stamp	17 Jan 2018 16:25:36
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 3 NMe2_001001r		
Frequency (MHz)	300.13	Nucleus	¹ H
Origin	spect	Original Points Count	65536
Points Count	262144	Pulse Sequence	zg
SW(cyclical) (Hz)	25510.20	Solvent	DICHLOROMETHANE-d2
Sweep Width (Hz)	25510.11	Temperature (degree C)	29.998
		Number of Transients	32
		Owner	nmr
		Receiver Gain	89.51
		Spectrum Offset (Hz)	1350.5919



Grubbs_3 NMe2_001001r

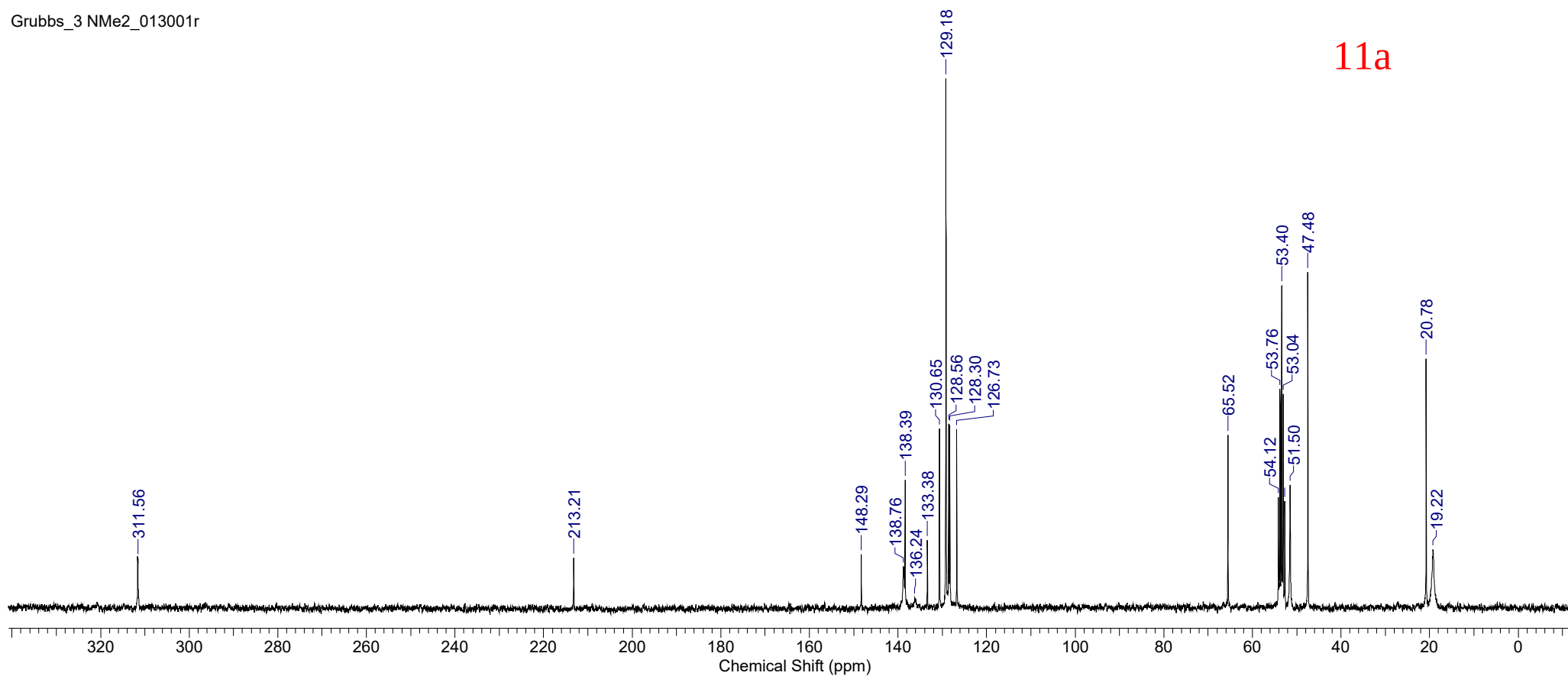


Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 3-C13dc		Date	12 Jan 2018 17:14:40	
Date Stamp	12 Jan 2018 17:14:40						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 3 NMe2 013001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	1208	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zgpg
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.126		

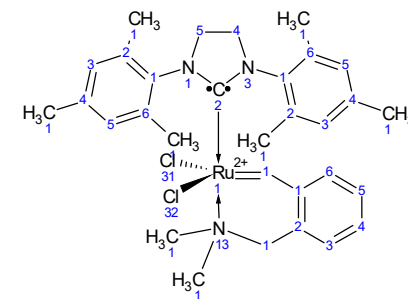


11a

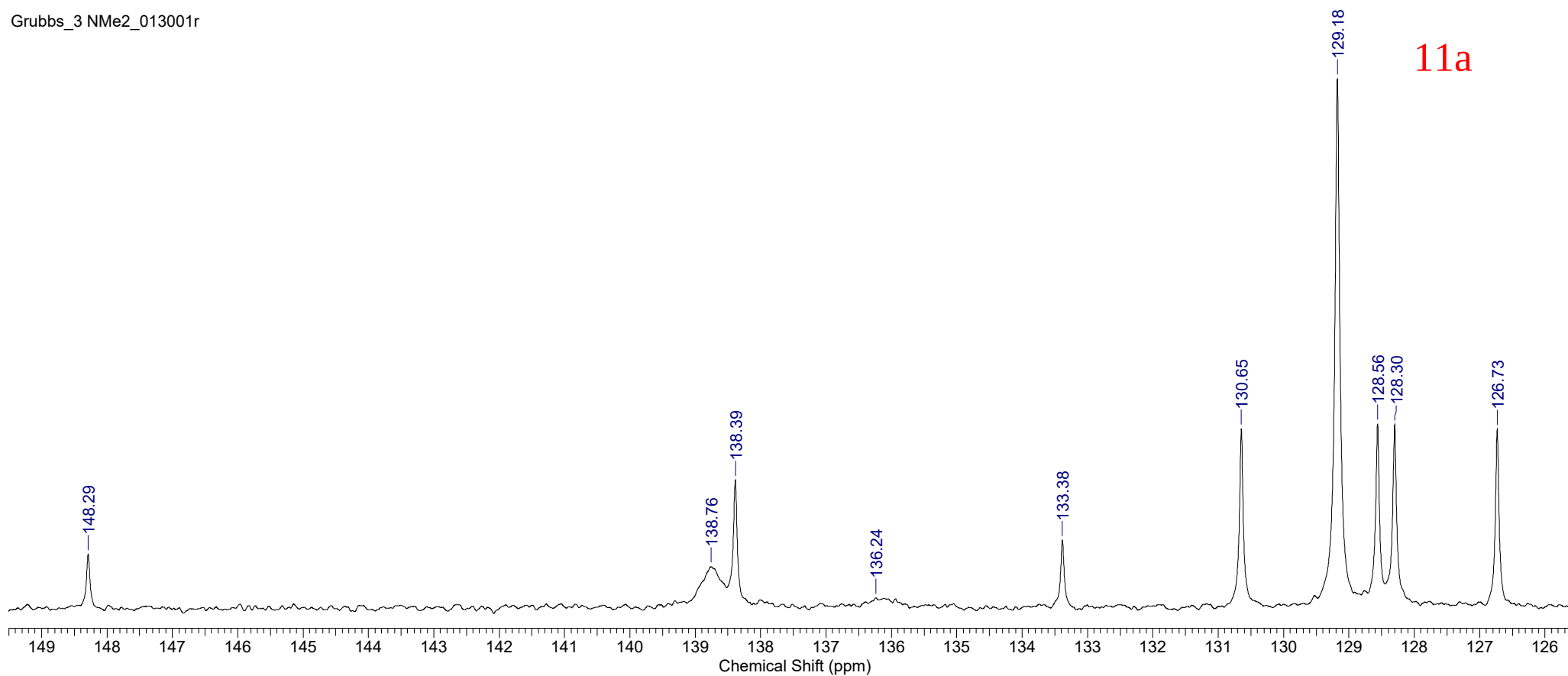
Grubbs_3 NMe2_013001r



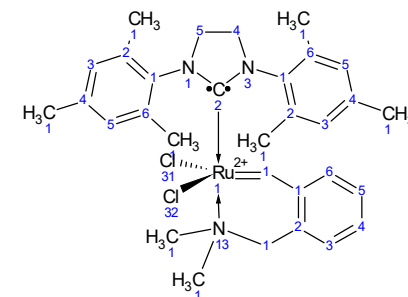
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Date Stamp	12 Jan 2018 17:14:40						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 3 NMe2 013001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	1208	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zgpg
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.126		



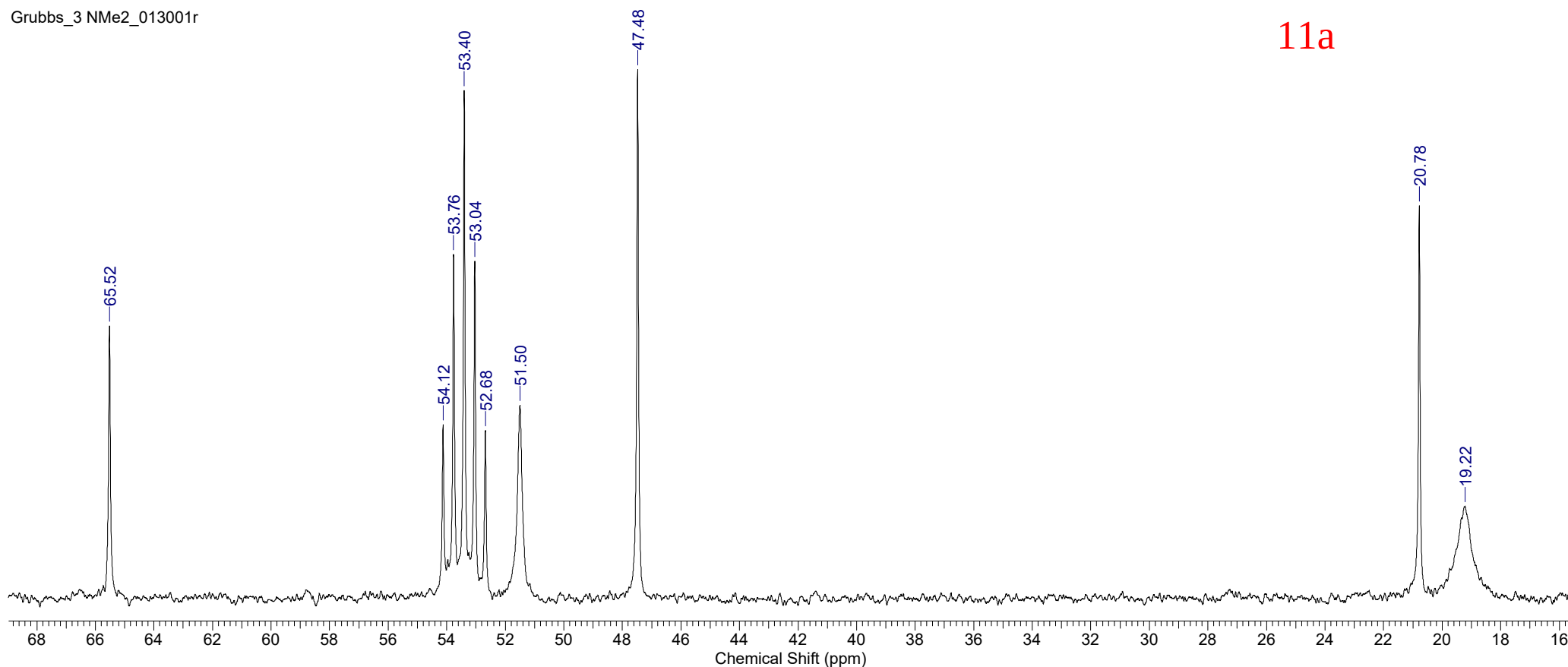
Grubbs_3 NMe2_013001r



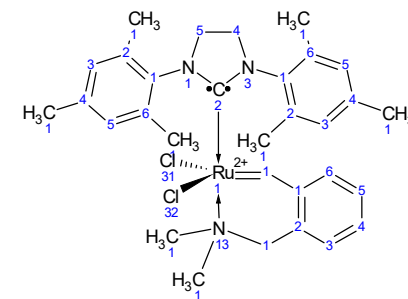
Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 3-C13dc		Date	12 Jan 2018 17:14:40	
Date Stamp	12 Jan 2018 17:14:40						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 3 NMe2 013001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	1208	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zgpg
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.126		



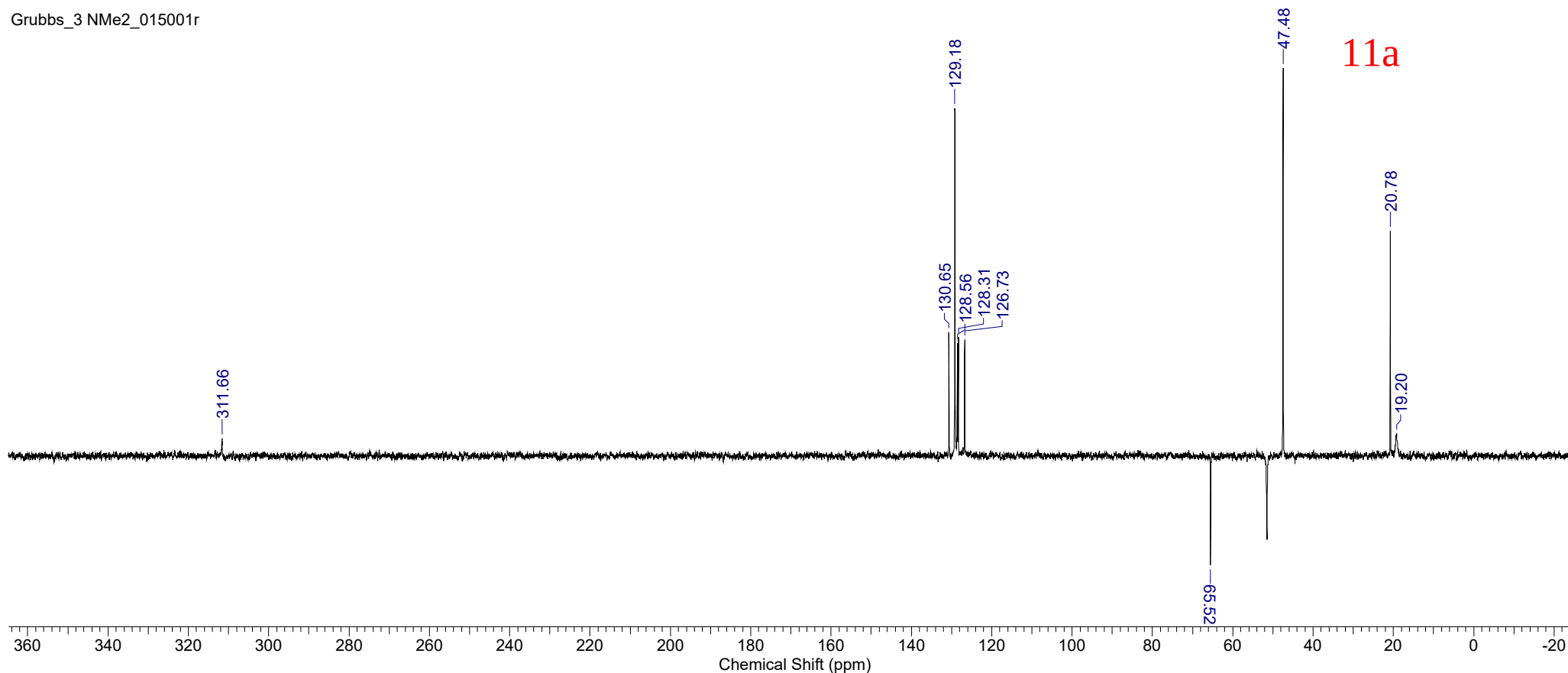
Grubbs_3 NMe2_013001r



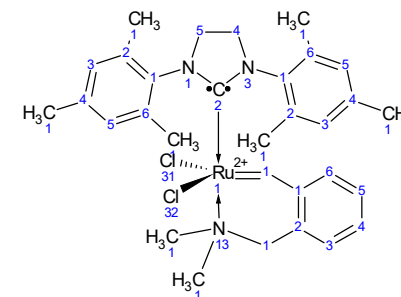
Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 3-dept135		Date	12 Jan 2018 18:03:44	
Date Stamp	12 Jan 2018 18:03:44						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 3 NMe2 015001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	800	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	dept135
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	29.964		



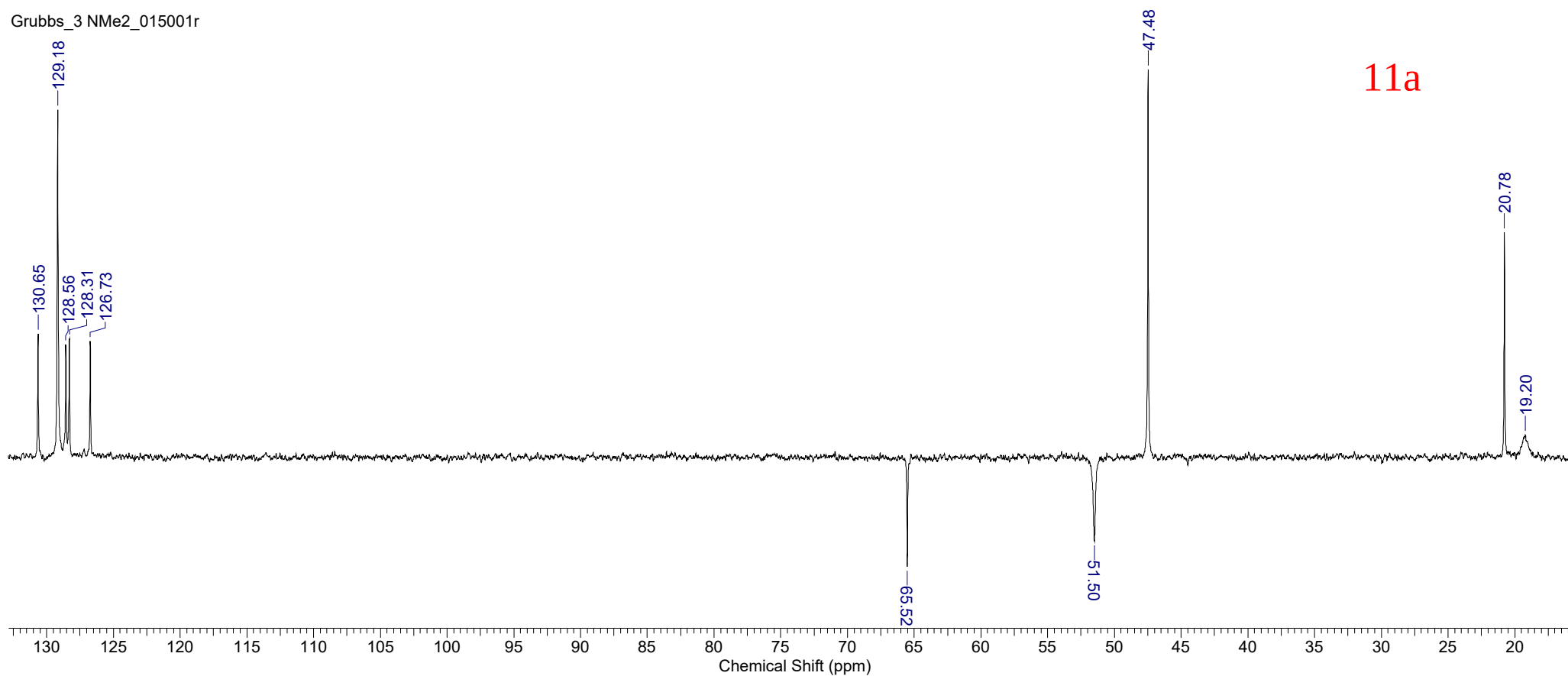
Grubbs_3 NMe2_015001r



Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 3-dept135		Date	12 Jan 2018 18:03:44	
Date Stamp	12 Jan 2018 18:03:44						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 3 NMe2 015001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	800	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	dept135
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	29.964		



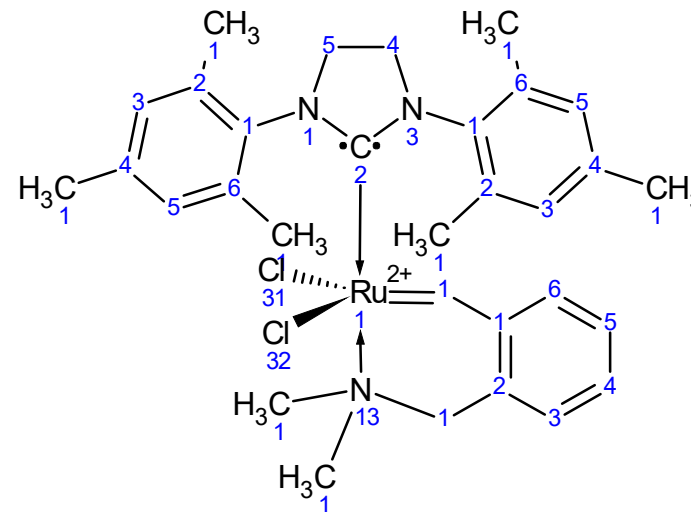
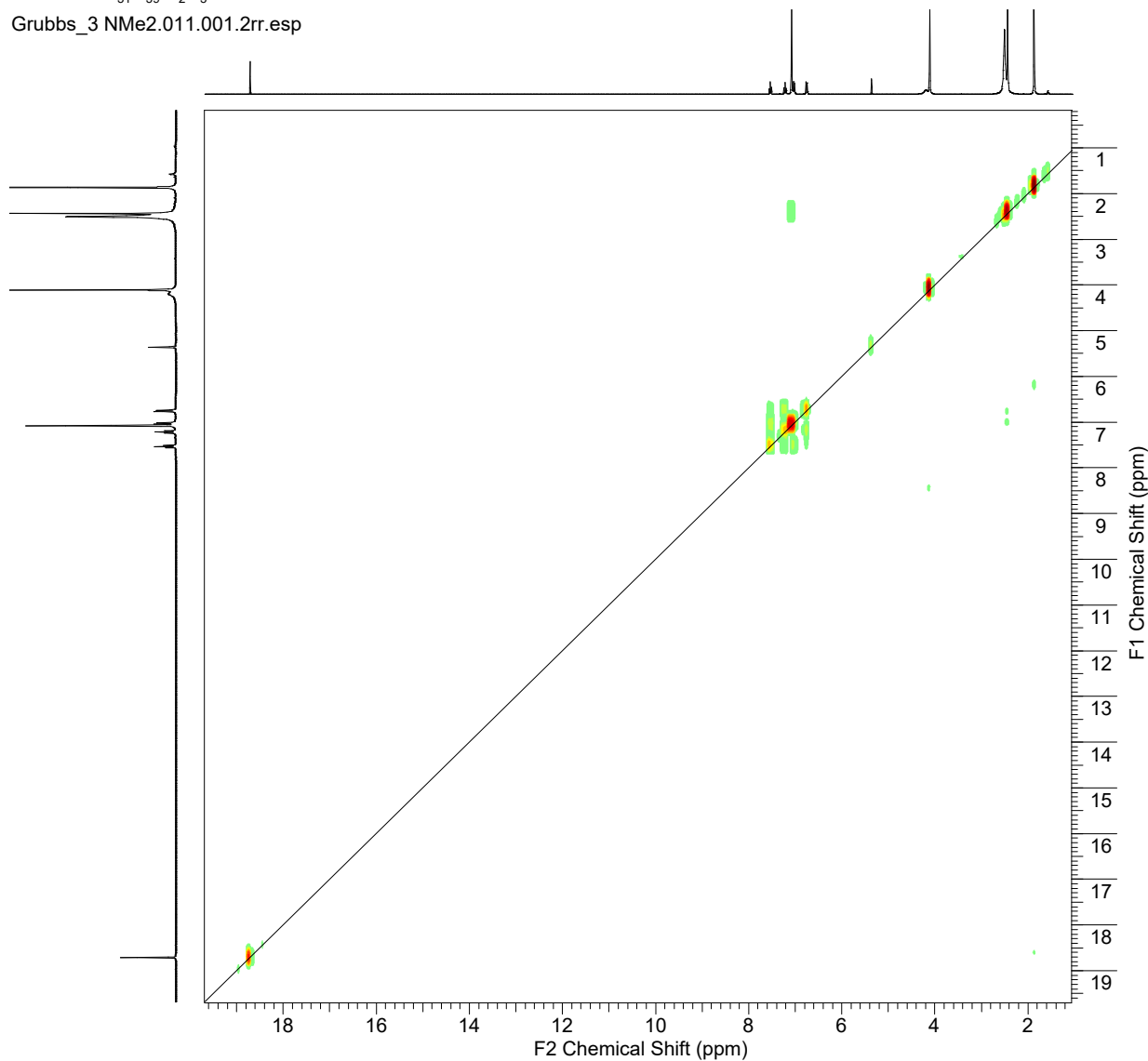
Grubbs_3 NMe2_015001r



Acquisition Time (sec)	(0.3408, 0.0333)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	12 Jan 2018 22:02:36					
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_3 NMe2\11\data\1\2rr					
Frequency (MHz)	(300.13, 300.13)	Nucleus	(1H, 1H)	Number of Transients	1	
Origin	spect	Original Points Count	(3072, 300)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	cosygpqf	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 9009.01)	Temperature (degree C)	29.918	Title	FZ Grubbs 3-COSY	

Formula	C ₃₁ H ₃₉ Cl ₂ N ₂ Ru	FW	625.6364
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Grubbs_3 NMe2.011.001.2rr.esp

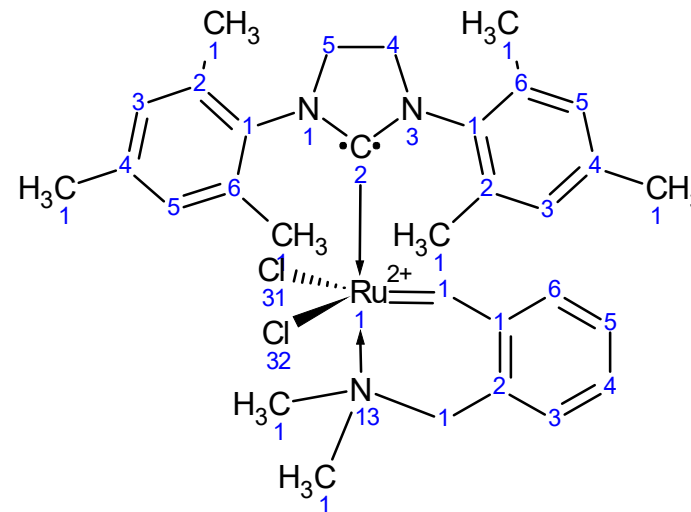
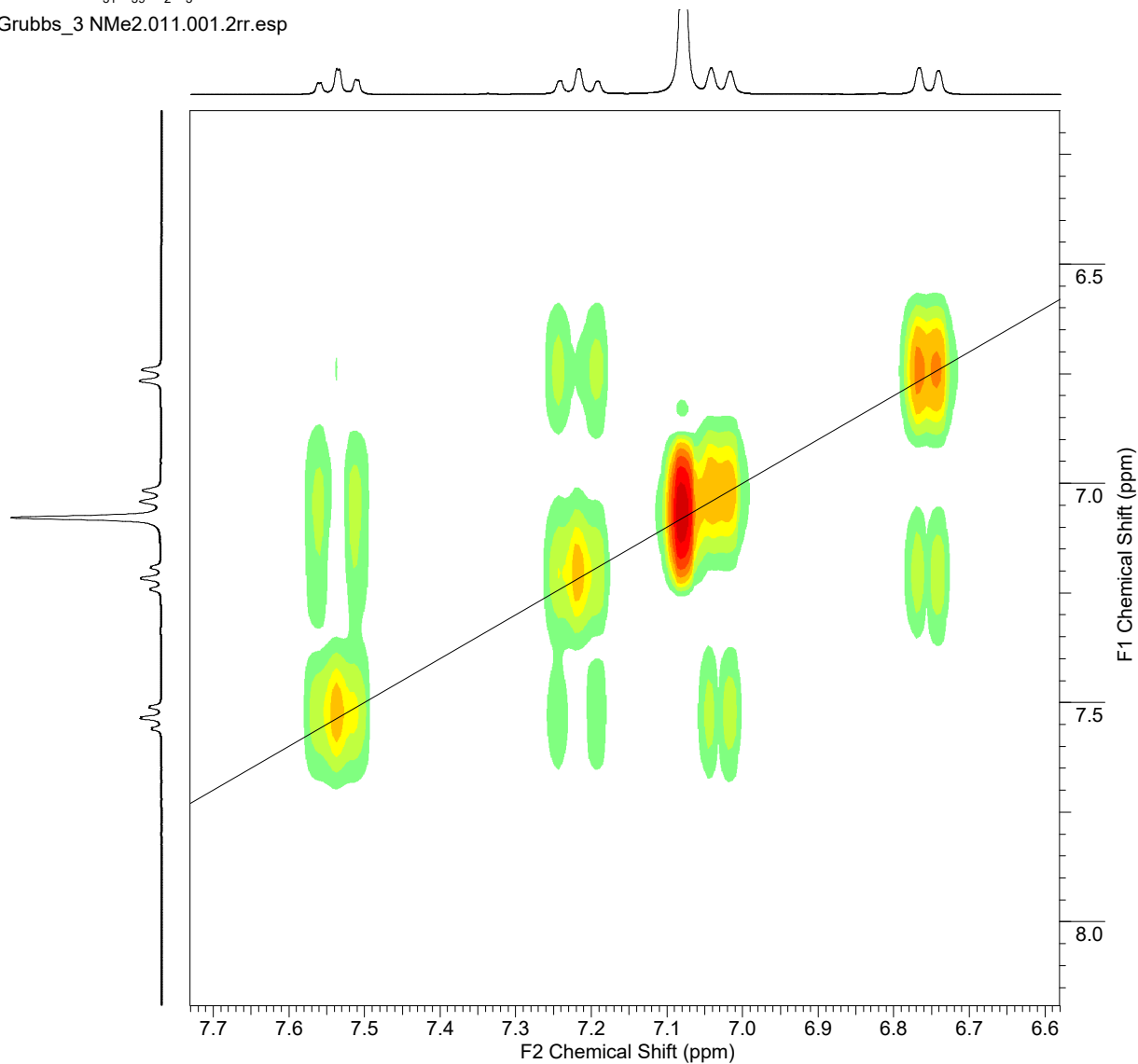


11a

Acquisition Time (sec)	(0.3408, 0.0333)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	12 Jan 2018 22:02:36					
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_3 NMe2\11\data\1\2rr					
Frequency (MHz)	(300.13, 300.13)	Nucleus	(1H, 1H)	Number of Transients	1	
Origin	spect	Original Points Count	(3072, 300)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	cosygpqf	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 9009.01)	Temperature (degree C)	29.918	Title	FZ Grubbs 3-COSY	

Formula C ₃₁ H ₃₉ Cl ₂ N ₂ Ru	FW 625.6364
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Grubbs_3 NMe2.011.001.2rr.esp

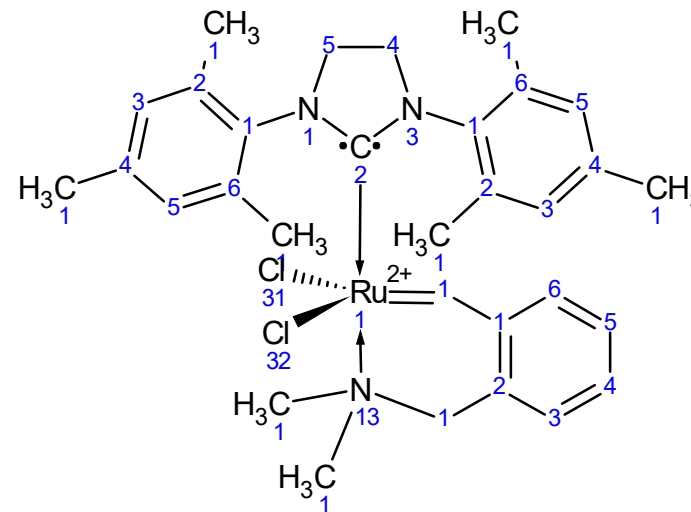
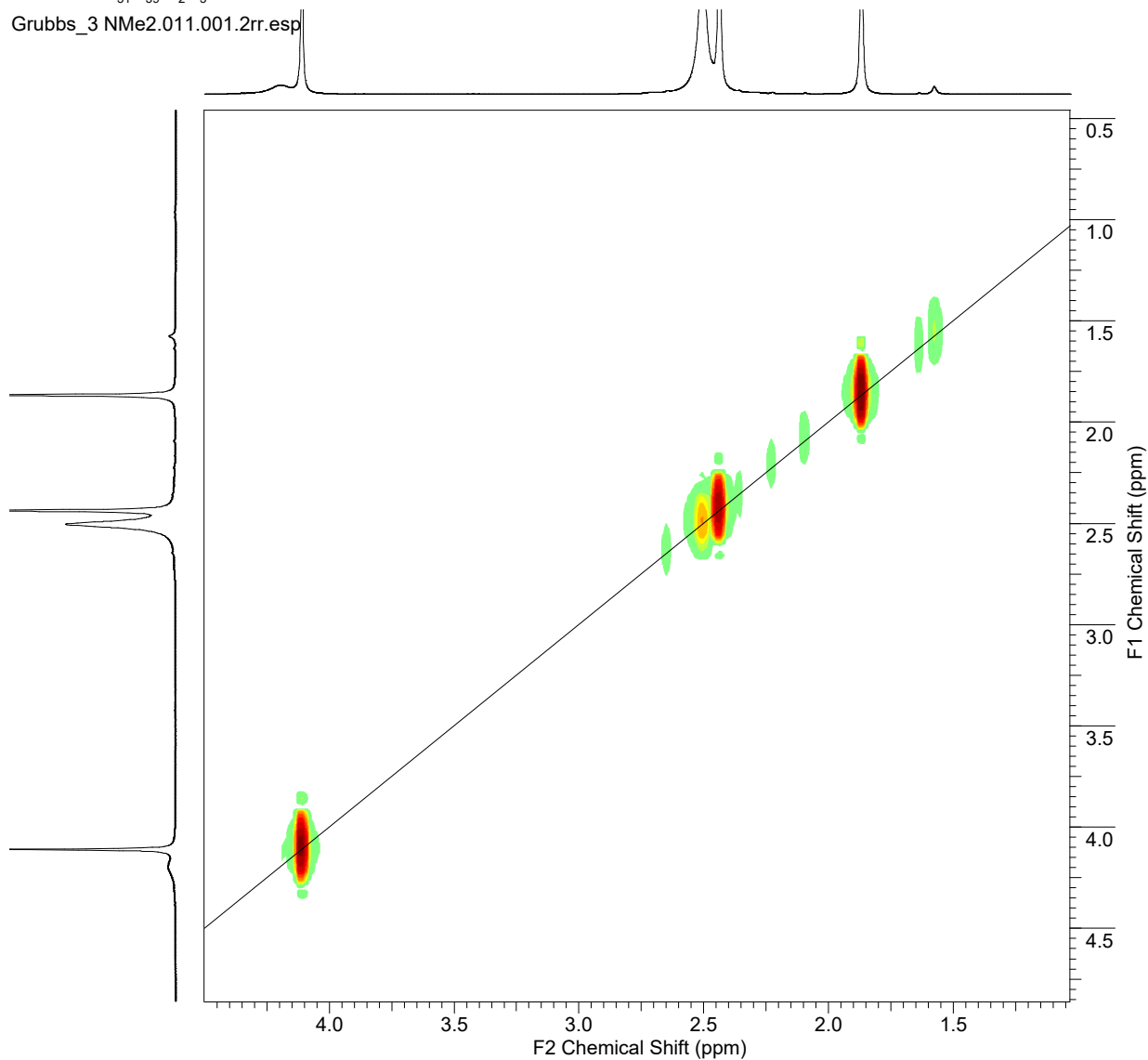


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Acquisition Time (sec)	(0.3408, 0.0333)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	12 Jan 2018 22:02:36					
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_3 NMe2\11\data\1\2rr					
Frequency (MHz)	(300.13, 300.13)	Nucleus	(1H, 1H)	Number of Transients	1	
Origin	spect	Original Points Count	(3072, 300)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	cosygprf	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 9009.01)	Temperature (degree C)	29.918	Title	FZ Grubbs 3-COSY	

Formula	C ₃₁ H ₃₉ Cl ₂ N ₂ Ru	FW	625.6364
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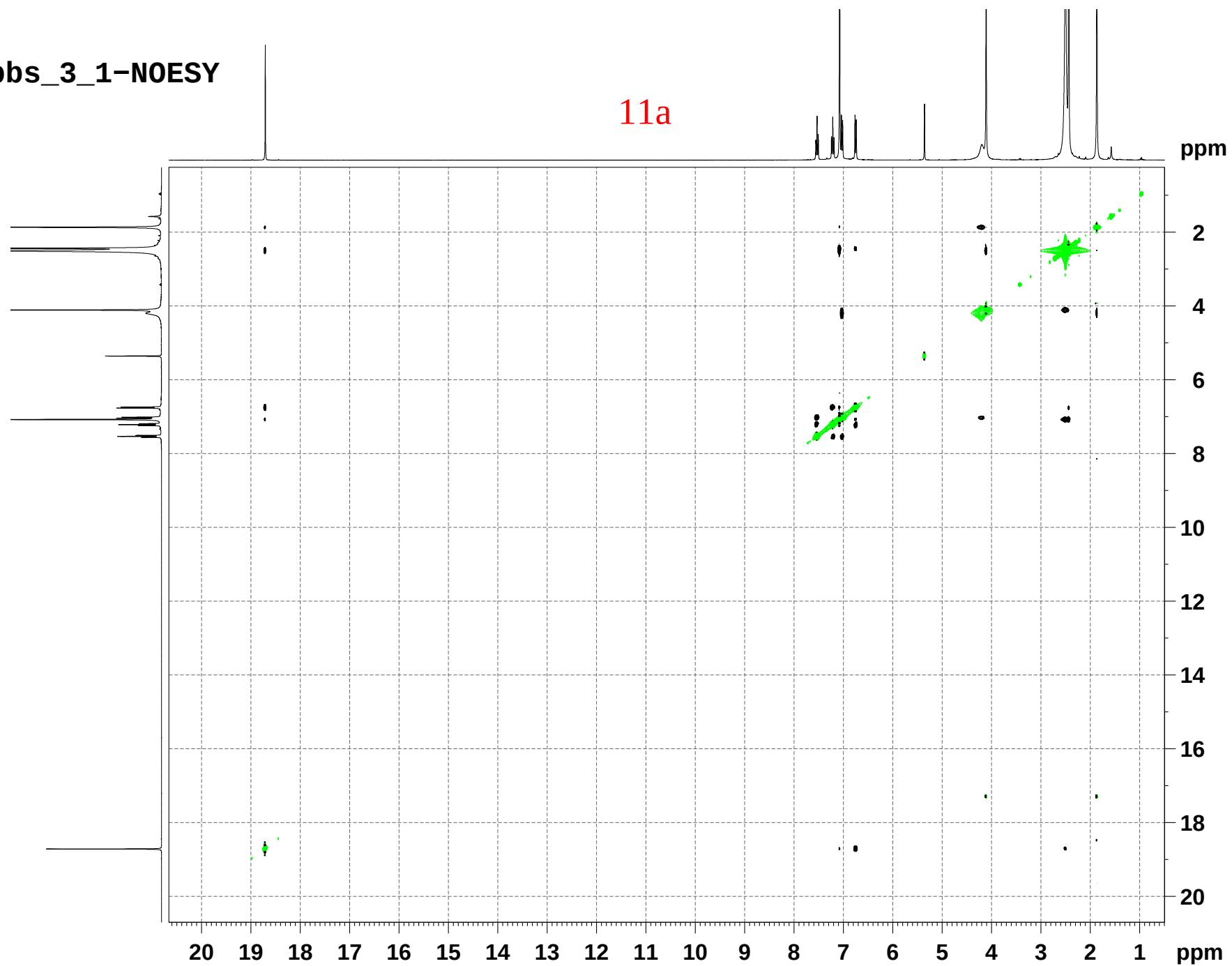
Grubbs_3 NMe2.011.001.2rr.esp



11a

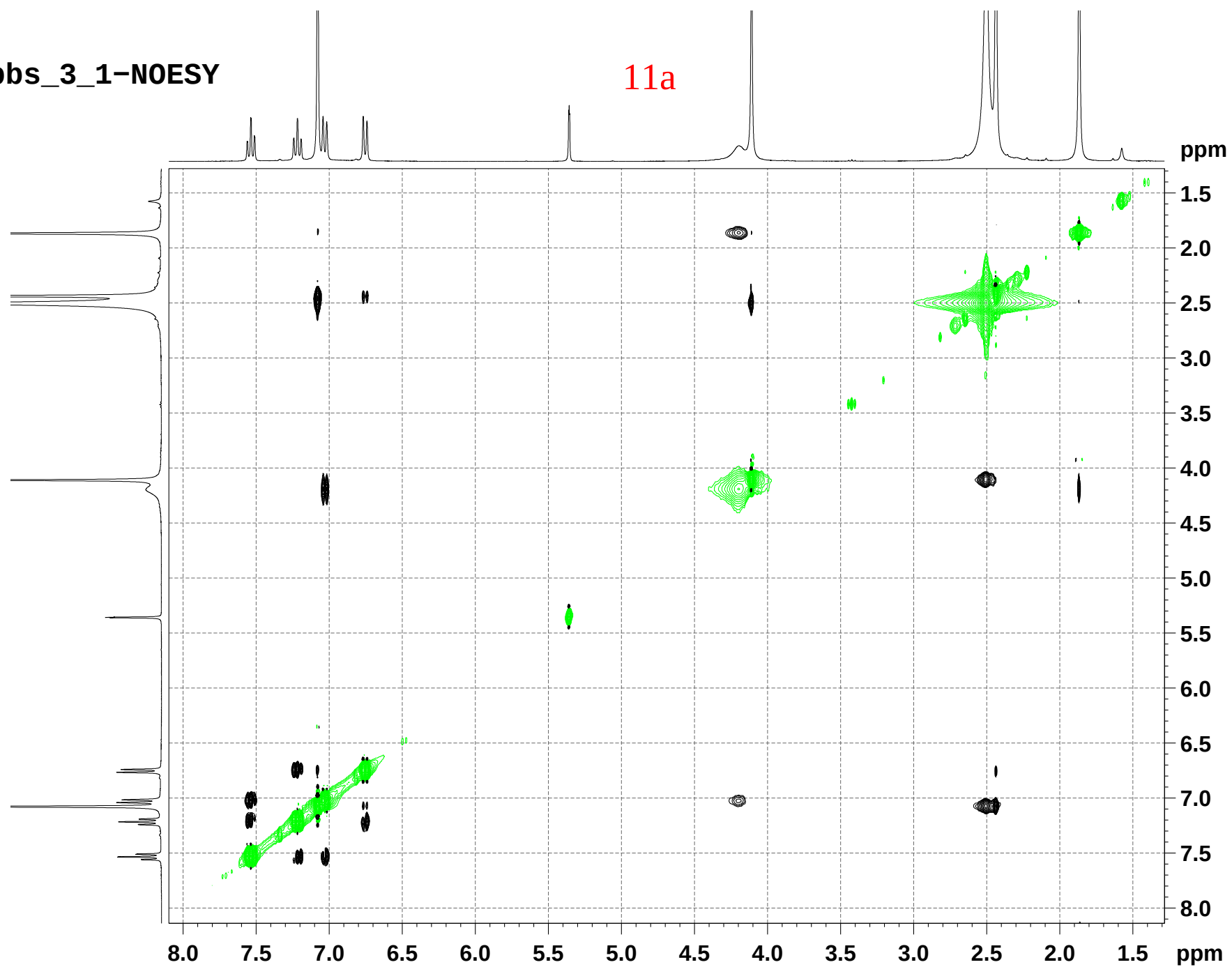
FZ_Grubbs_3_1-NOESY

11a



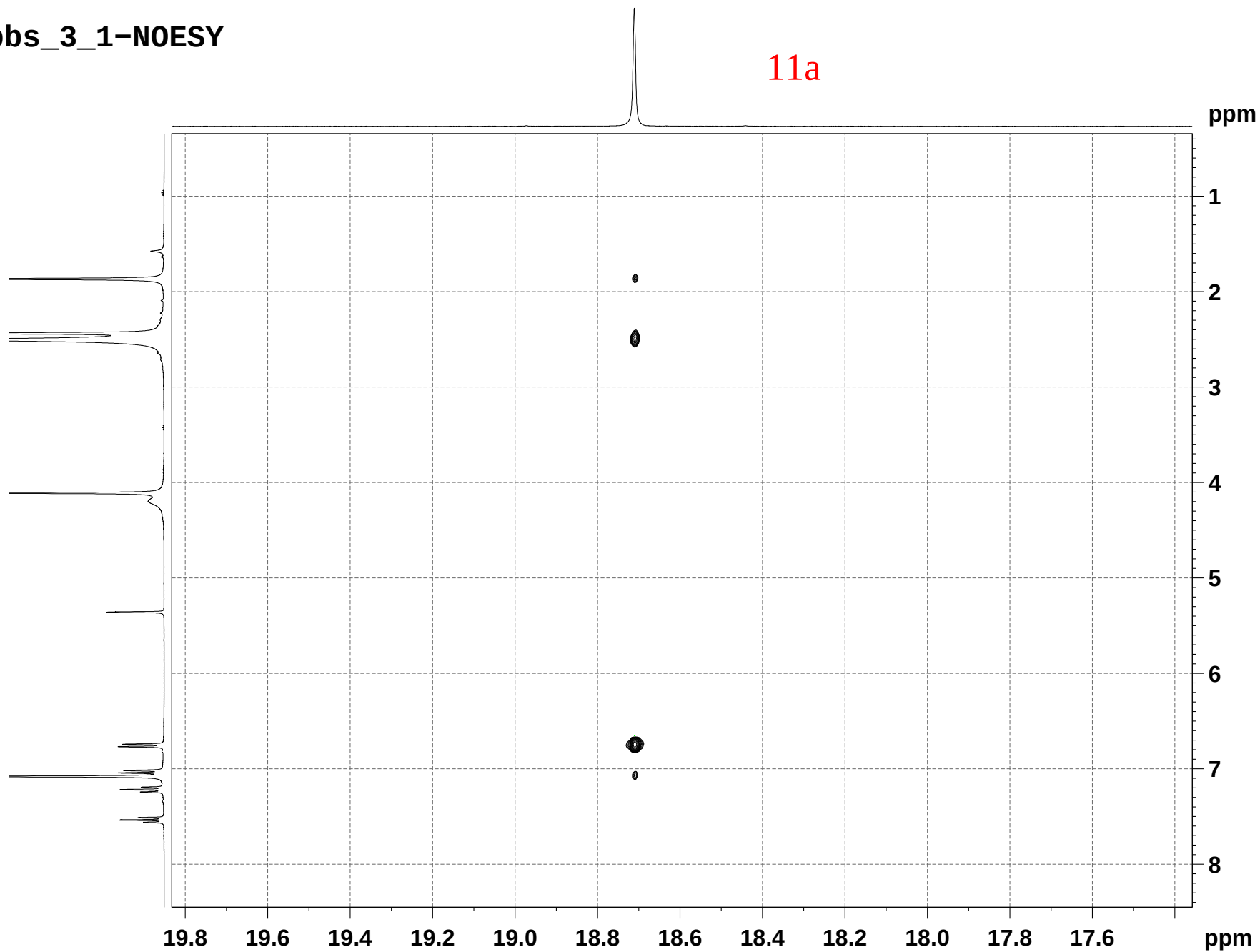
FZ_Grubbs_3_1-NOESY

11a



FZ_Grubbs_3_1-NOESY

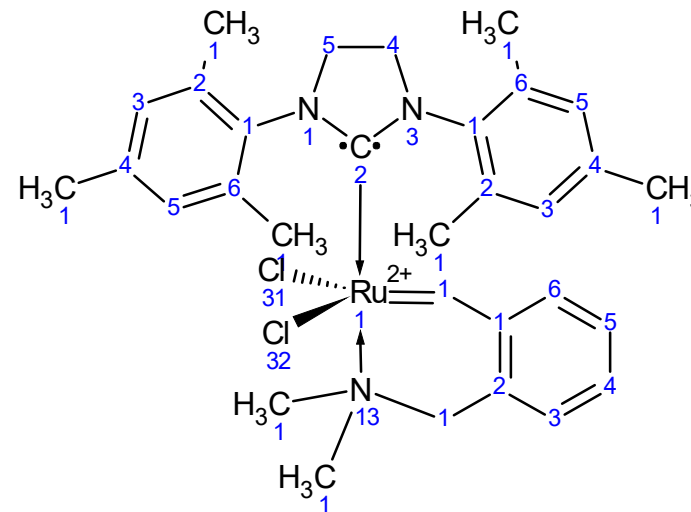
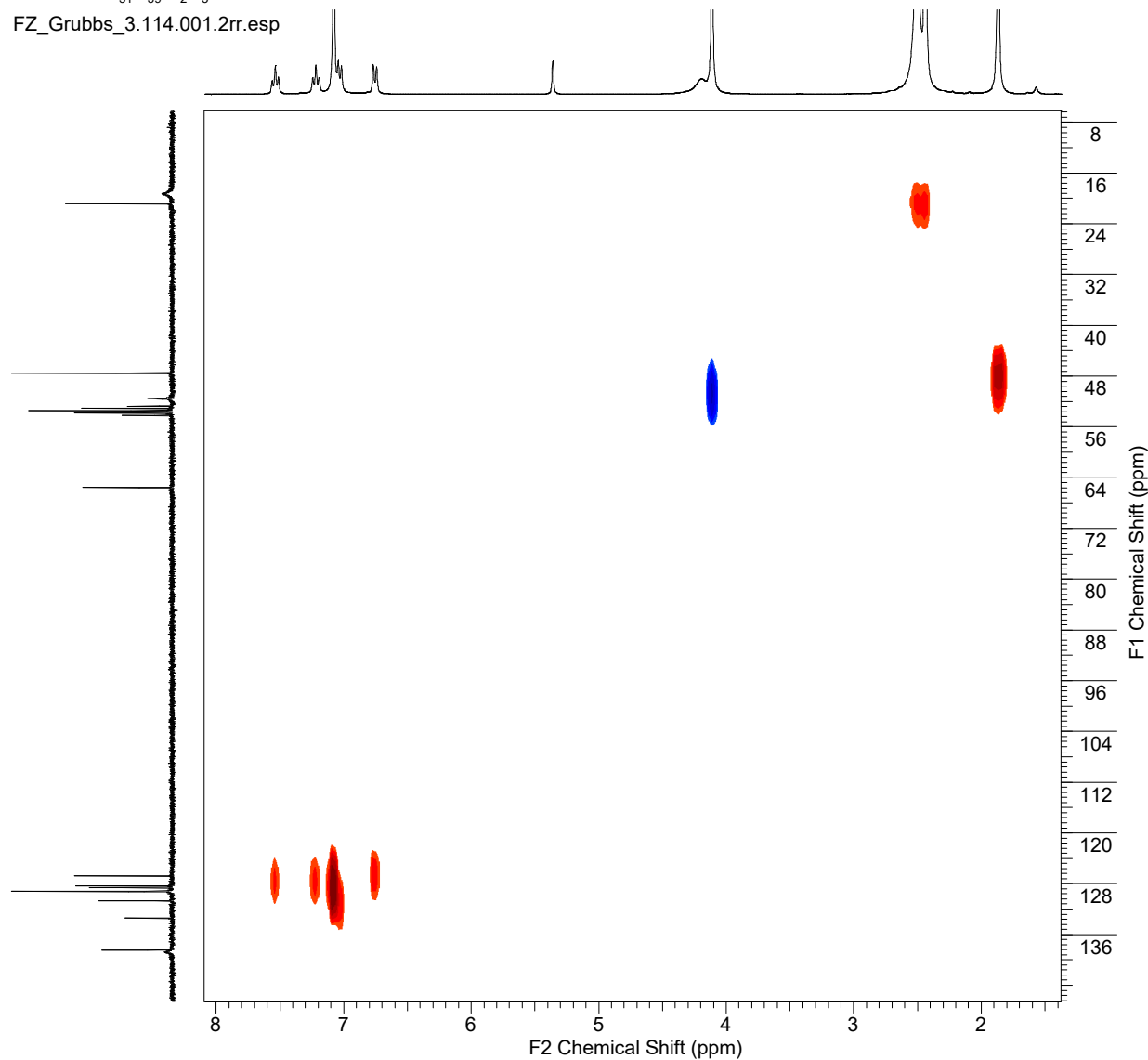
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Acquisition Time (sec)	(0.3408, 0.0037)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	12 Jan 2018 21:44:54					
File Name	C:\Users\Fedor\Desktop\Наброски статей\Кирлл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs_3\114\data\12rr					
Frequency (MHz)	(300.13, 75.48)	Nucleus	(1H, 13C)	Number of Transients	2	
Origin	spect	Original Points Count	(3072, 127)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	hsqcedetgp	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	30.056	Title	FZ_Grubbs_3-edited-HSQC [proc = EM]	

Formula	C ₃₁ H ₃₉ Cl ₂ N ₂ Ru	FW	625.6364
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FZ_Grubbs_3.114.001.2rr.esp

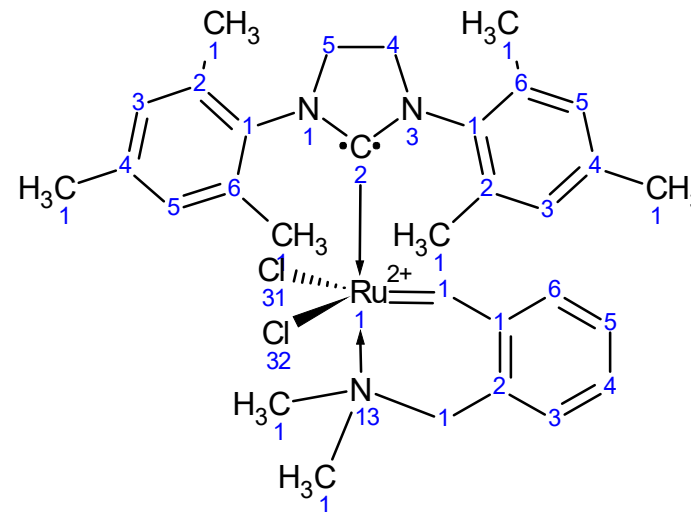
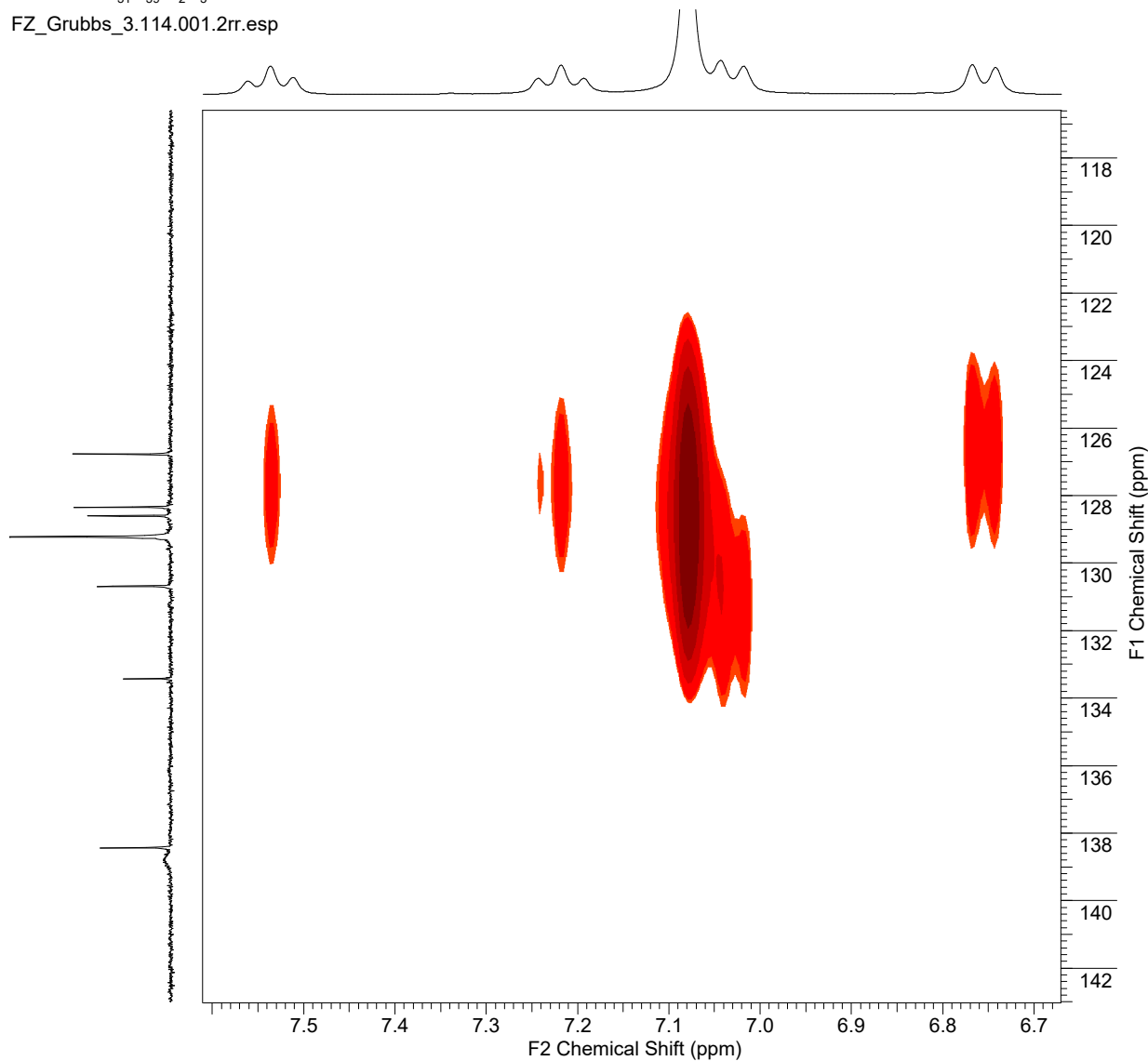


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Acquisition Time (sec)	(0.3408, 0.0037)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	12 Jan 2018 21:44:54					
File Name	C:\Users\Fedor\Desktop\Наброски статей\Кирлл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs_3\114\pdata\1\2rr					
Frequency (MHz)	(300.13, 75.48)	Nucleus	(1H, 13C)	Number of Transients	2	
Origin	spect	Original Points Count	(3072, 127)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	hsqcedetgp	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	30.056	Title	FZ_Grubbs_3-edited-HSQC [proc = EM]	

Formula C ₃₁ H ₃₉ Cl ₂ N ₂ Ru	FW 625.6364
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FZ_Grubbs_3.114.001.2rr.esp

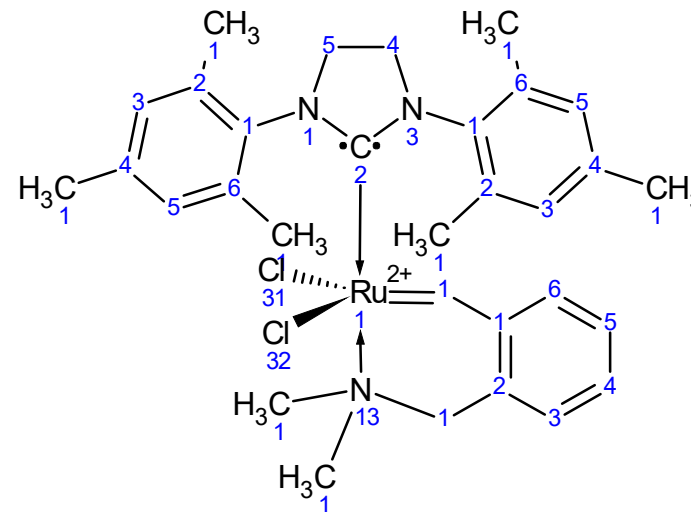
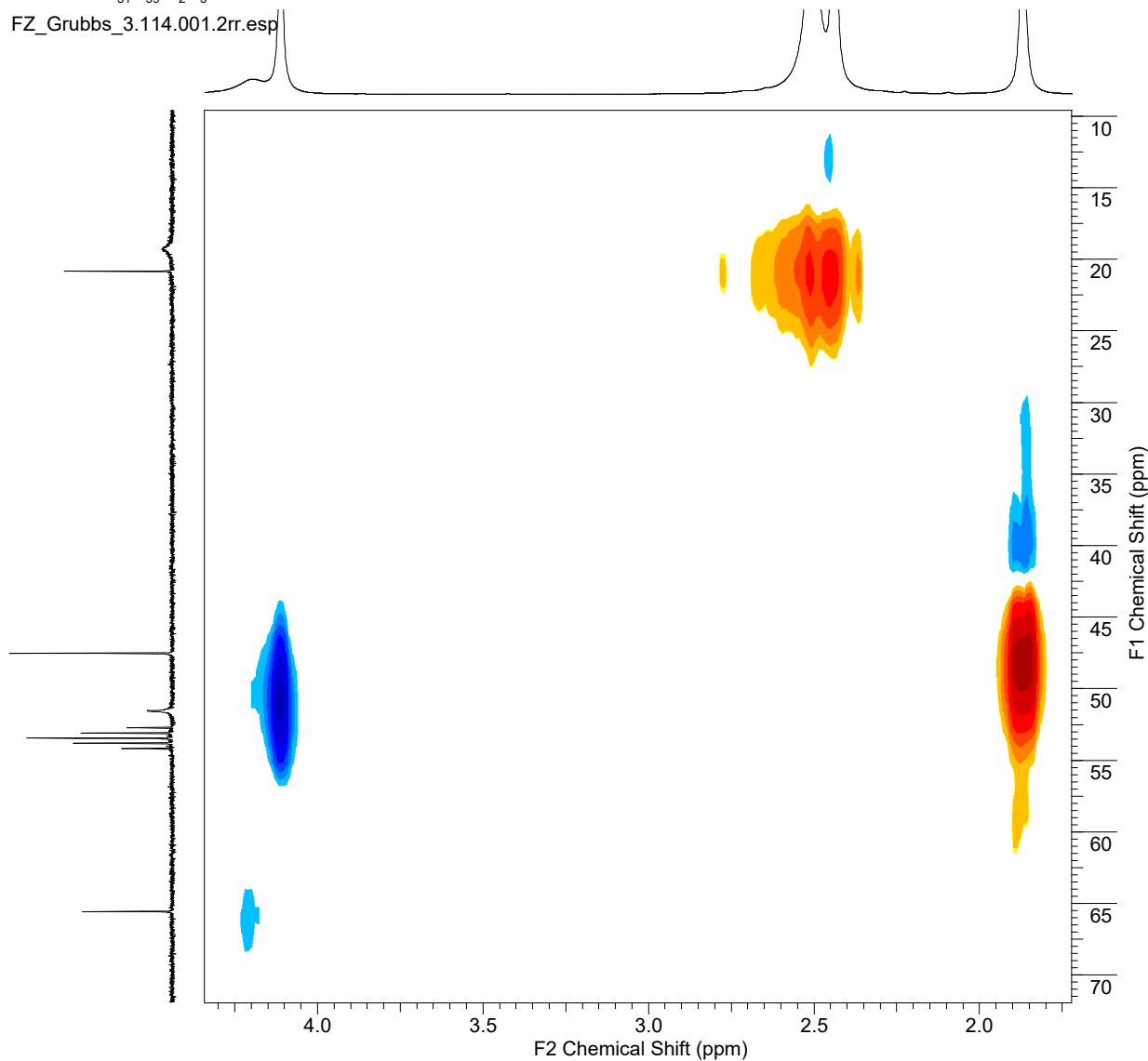


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Acquisition Time (sec)	(0.3408, 0.0037)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	12 Jan 2018 21:44:54					
File Name	C:\Users\Fedor\Desktop\Наброски статей\Кирлл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs_3\114\data\12rr					
Frequency (MHz)	(300.13, 75.48)	Nucleus	(1H, 13C)	Number of Transients	2	
Origin	spect	Original Points Count	(3072, 127)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	hsqcedetgp	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	30.056	Title	FZ_Grubbs_3-edited-HSQC [proc = EM]	

Formula	C ₃₁ H ₃₉ Cl ₂ N ₂ Ru	FW	625.6364
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FZ_Grubbs_3.114.001.2rr.esp

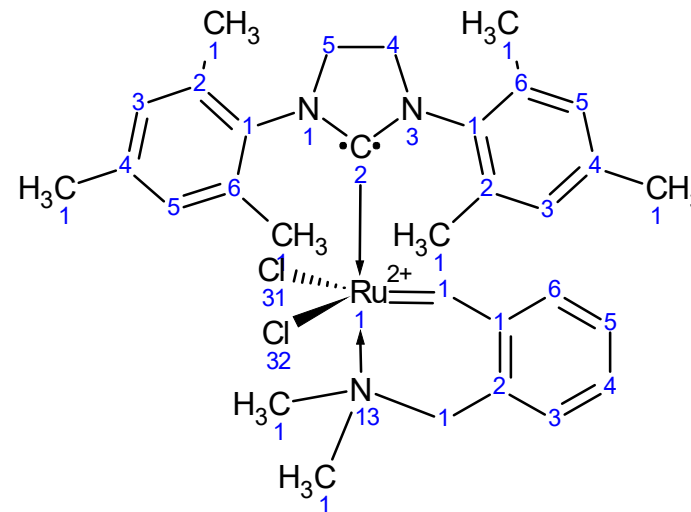
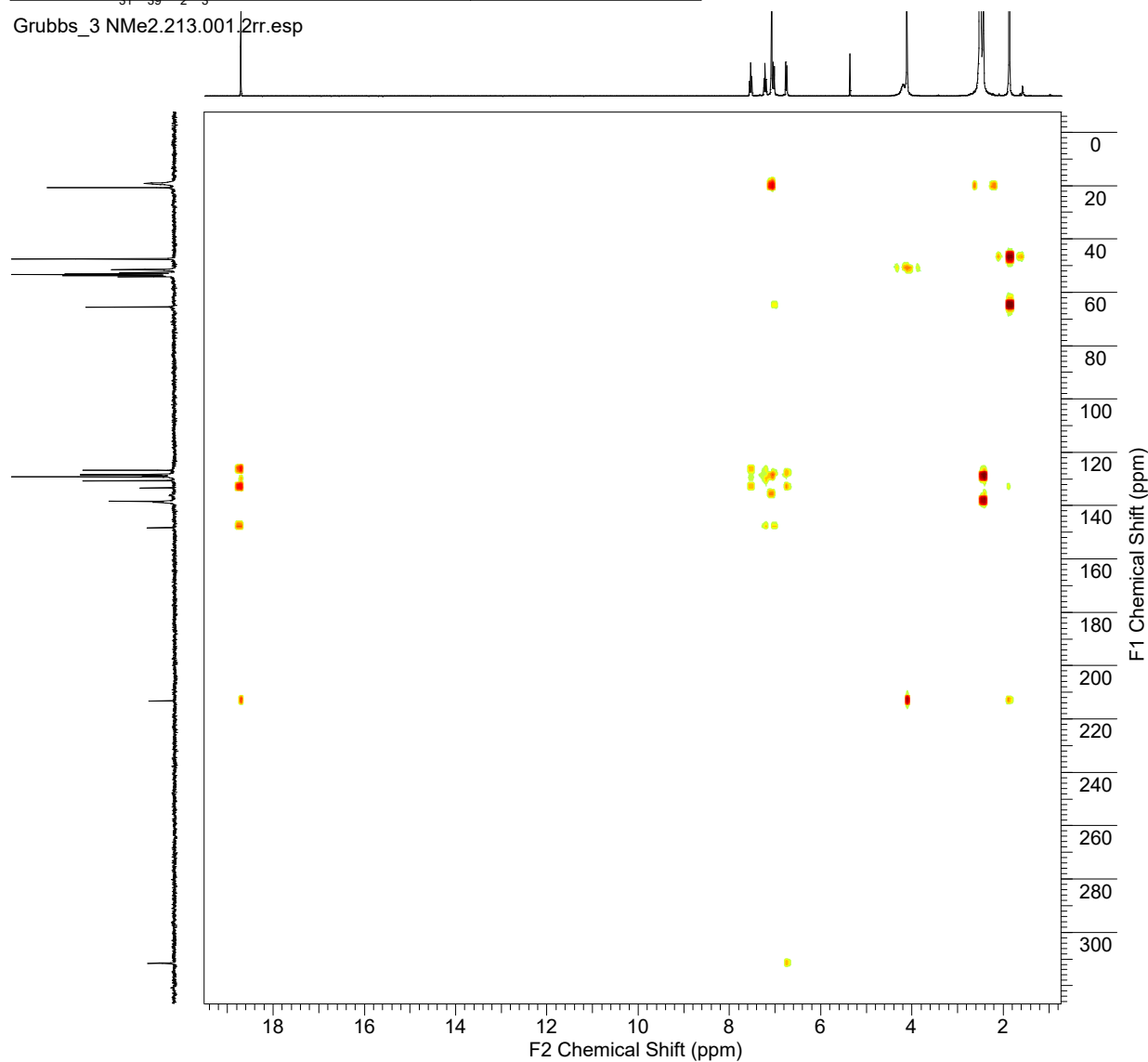


11a

Acquisition Time (sec)	(0.3408, 0.0173)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345		
Date	17 Jan 2018 21:32:24				
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_3 NMe2\213\pdata\1\2rr				
Frequency (MHz)	(300.13, 75.48)	Nucleus	(1H, 13C)	Number of Transients	6
Origin	spect	Original Points Count	(3072, 590)	Owner	nmr
Points Count	(8192, 2048)	Pulse Sequence	hmbcgp1pndqf	Solvent	CD2Cl2
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	30.007	Title	FZ Grubbs 3 1-HMBC

Formula C ₃₁ H ₃₉ Cl ₂ N ₂ Ru	FW 625.6364
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Grubbs_3 NMe2.213.001.2rr.esp

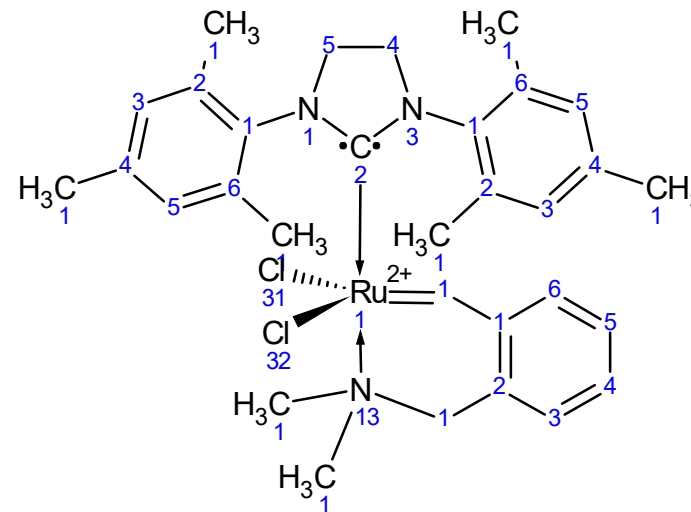
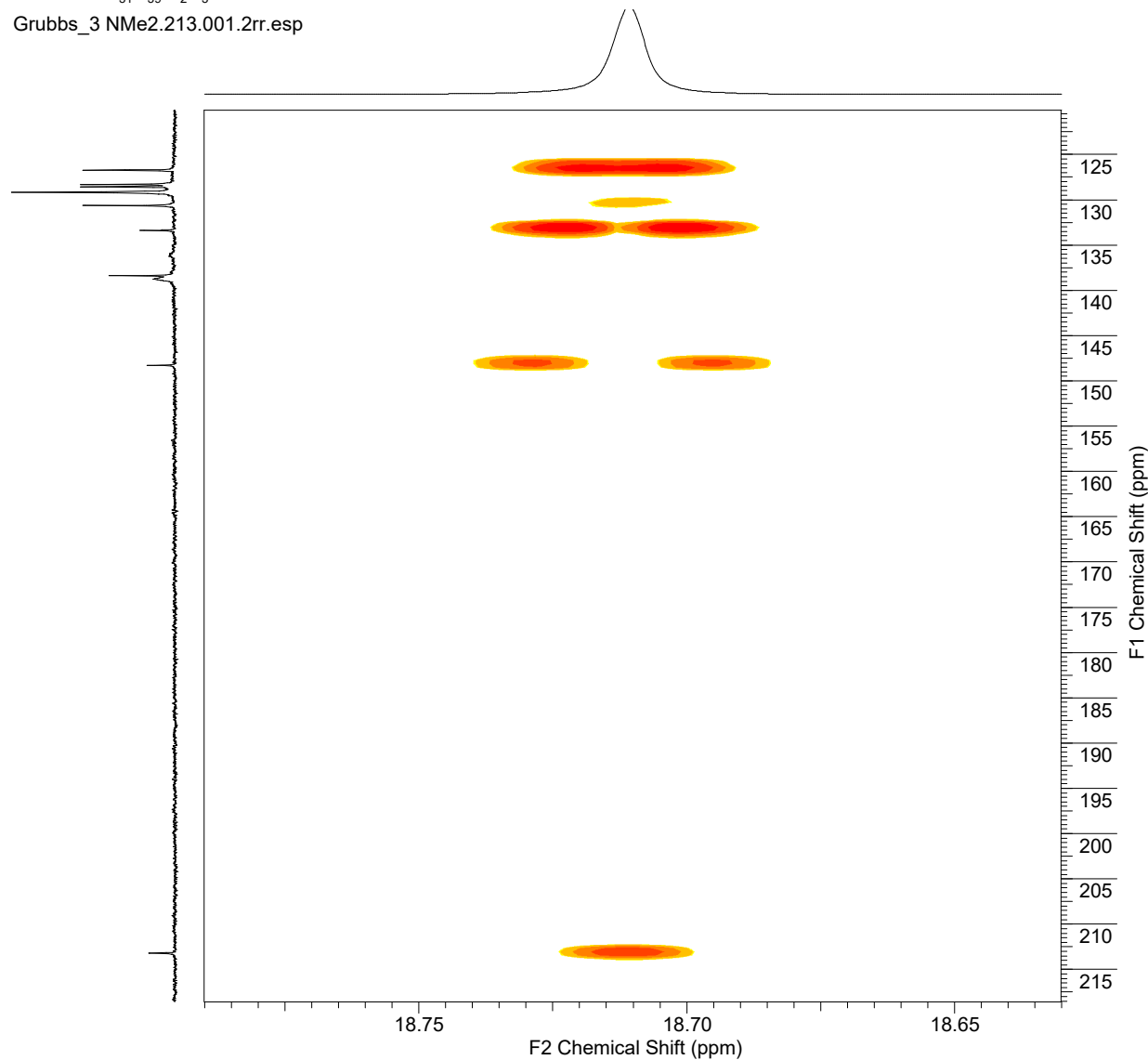


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Acquisition Time (sec)	(0.3408, 0.0173)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345		
Date	17 Jan 2018 21:32:24				
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_3 NMe2\213\data\1\2rr				
Frequency (MHz)	(300.13, 75.48)	Nucleus	(1H, 13C)	Number of Transients	6
Origin	spect	Original Points Count	(3072, 590)	Owner	nmr
Points Count	(8192, 2048)	Pulse Sequence	hmbcgp1pndqf	Solvent	CD2Cl2
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	30.007	Title	FZ Grubbs 3 1-HMBC

Formula C ₃₁ H ₃₉ Cl ₂ N ₂ Ru	FW 625.6364
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Grubbs_3 NMe2.213.001.2rr.esp

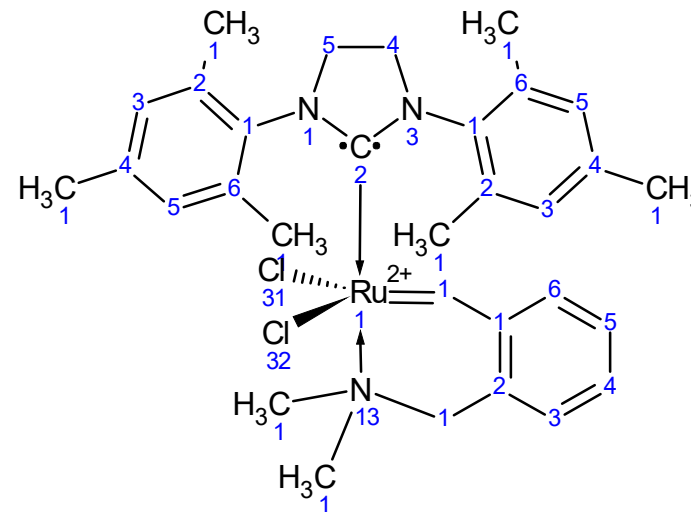
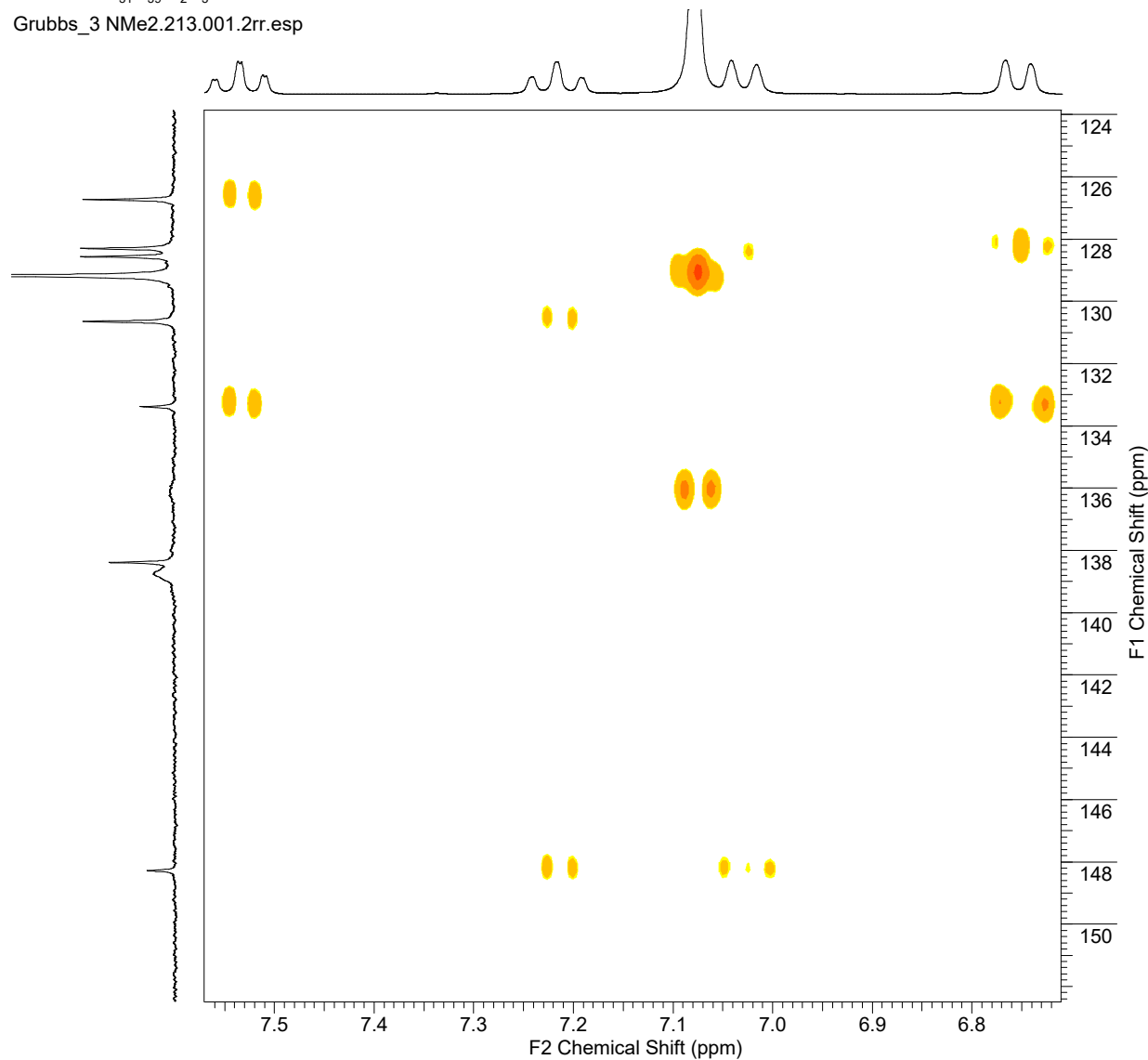


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Acquisition Time (sec)	(0.3408, 0.0173)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345		
Date	17 Jan 2018 21:32:24				
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_3 NMe2\213\data\1\2rr				
Frequency (MHz)	(300.13, 75.48)	Nucleus	(1H, 13C)	Number of Transients	6
Origin	spect	Original Points Count	(3072, 590)	Owner	nmr
Points Count	(8192, 2048)	Pulse Sequence	hmbcgp1pndqf	Solvent	CD2Cl2
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	30.007	Title	FZ Grubbs 3 1-HMBC

Formula	C ₃₁ H ₃₉ Cl ₂ N ₂ Ru	FW	625.6364
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Grubbs_3 NMe2.213.001.2rr.esp

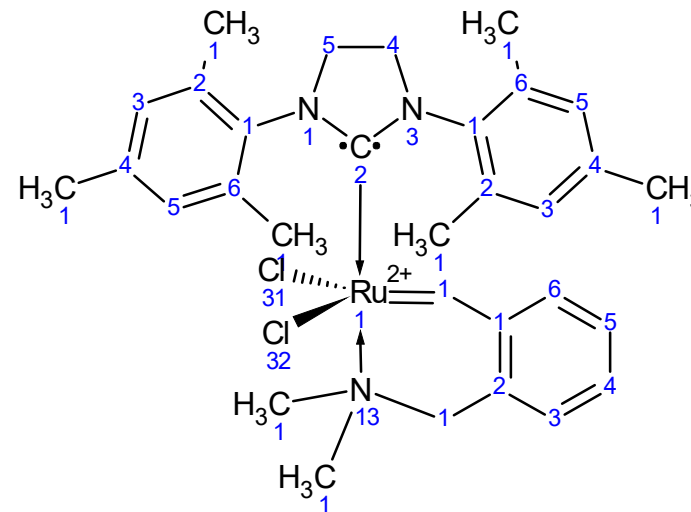
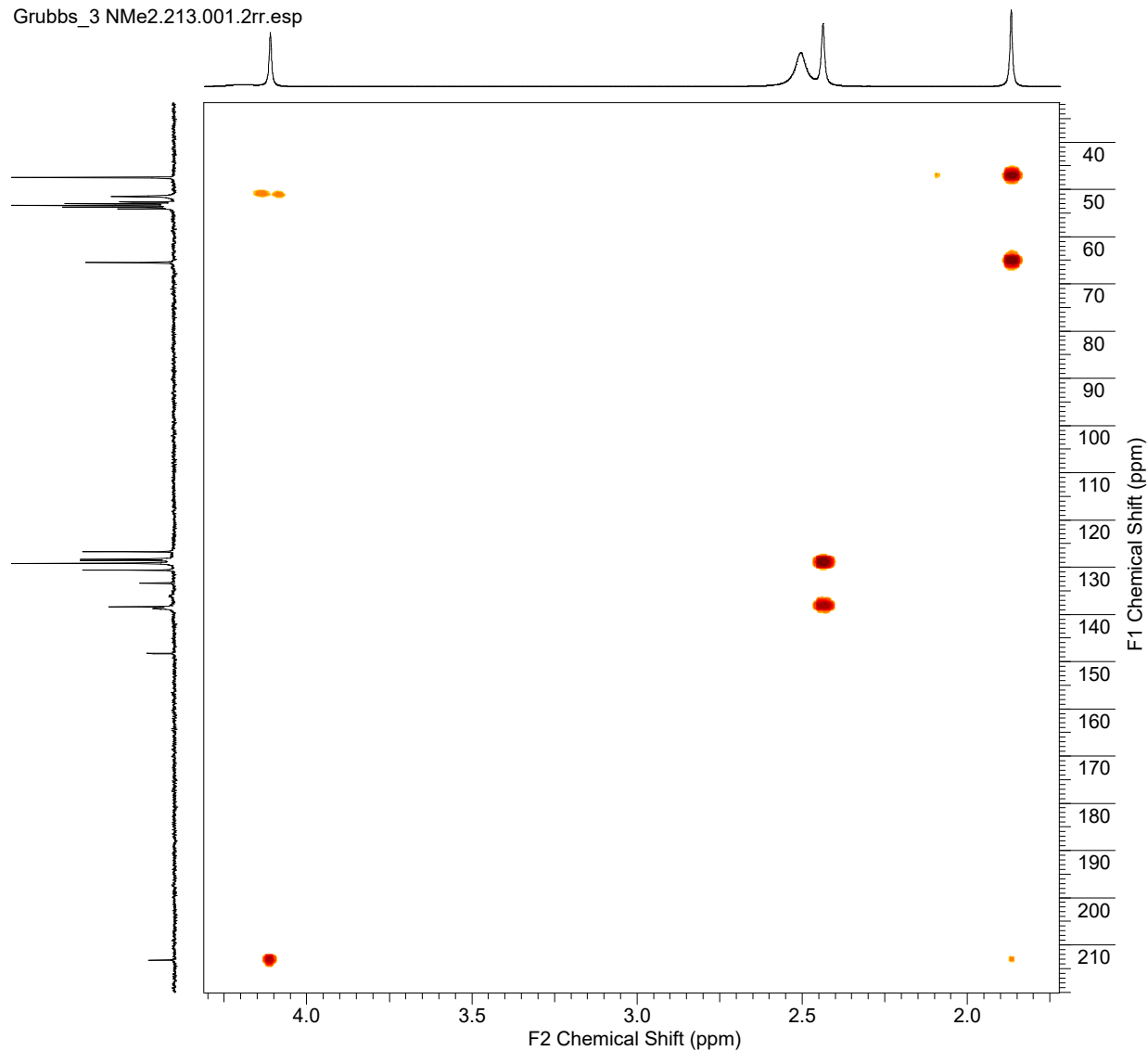


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Acquisition Time (sec)	(0.3408, 0.0173)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345		
Date	17 Jan 2018 21:32:24				
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_3 NMe2\213\data\1\2rr				
Frequency (MHz)	(300.13, 75.48)	Nucleus	(1H, 13C)	Number of Transients	6
Origin	spect	Original Points Count	(3072, 590)	Owner	nmr
Points Count	(8192, 2048)	Pulse Sequence	hmbcgp1pndqf	Solvent	CD2Cl2
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	30.007	Title	FZ Grubbs 3 1-HMBC

Formula C ₃₁ H ₃₉ Cl ₂ N ₂ Ru	FW 625.6364
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Grubbs_3 NMe2.213.001.2rr.esp



11a

FZ_Grubbs_3_1-N15-HMBC

11a

ppm

0

100

200

300

400

500

600

700

800

900

1000

1100

1200

ppm

7.5

7.0

6.5

6.0

5.5

5.0

4.5

4.0

3.5

3.0

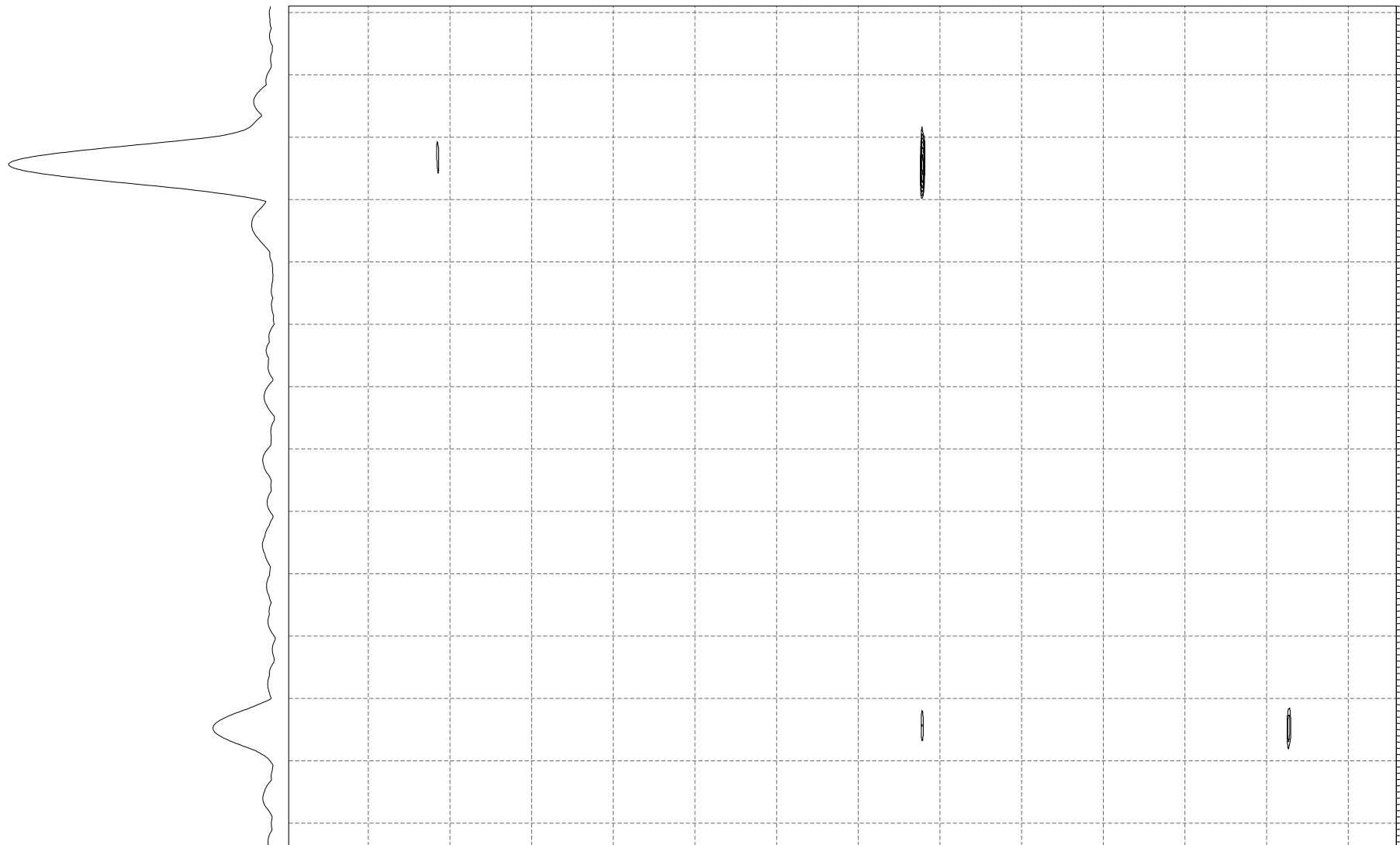
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2.0

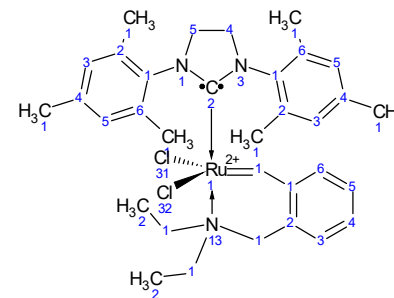
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ppm

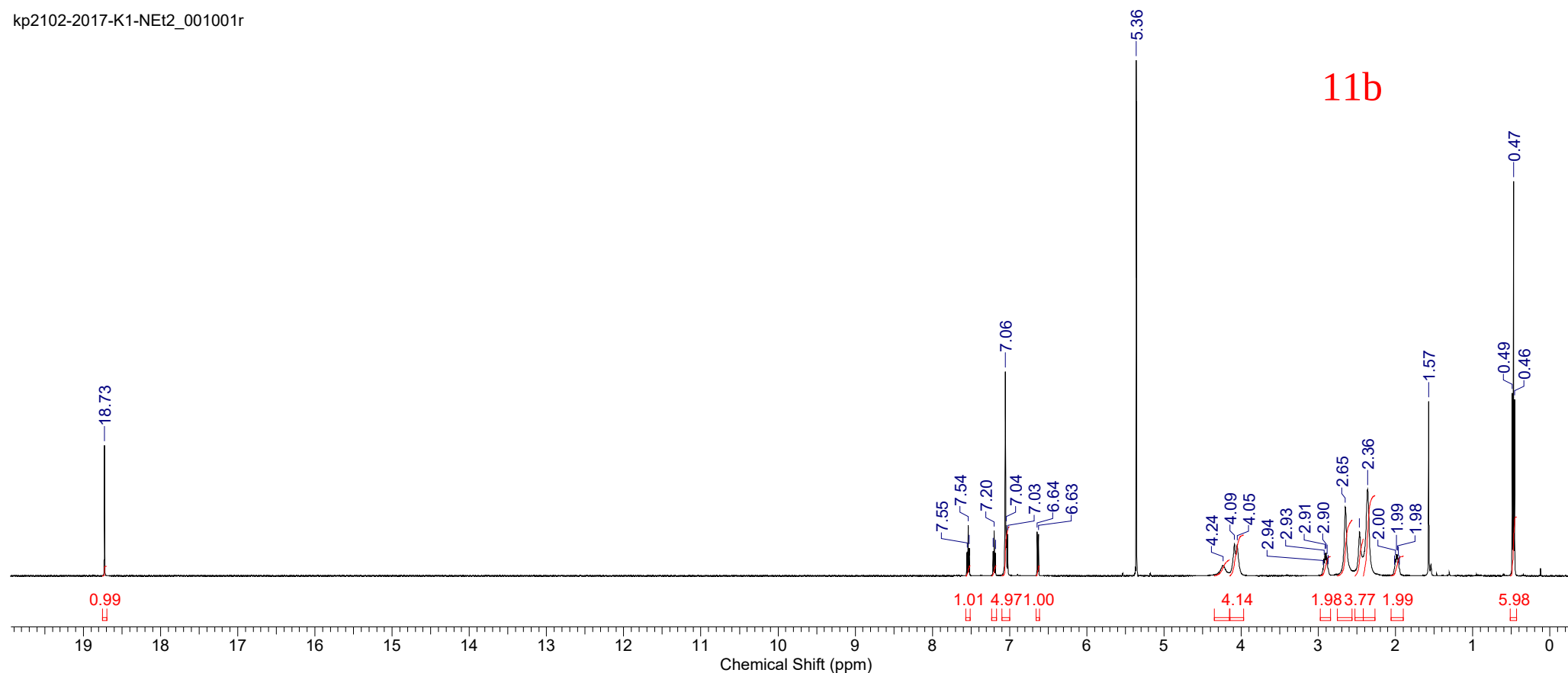
128



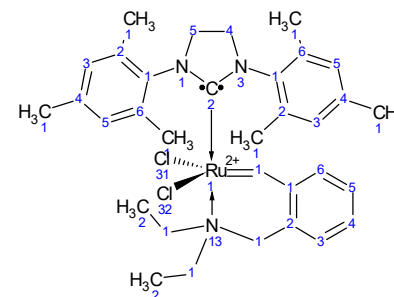
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Date Stamp	21 Feb 2017 05:26:24						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2_001001r						
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	8	Origin	spect
Original Points Count	32768	Owner	nmrsu	Points Count	262144	Pulse Sequence	zg30
Receiver Gain	122.15	SW(cyclical) (Hz)	14097.74	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	4088.6934	Sweep Width (Hz)	14097.69	Temperature (degree C)	25.017		



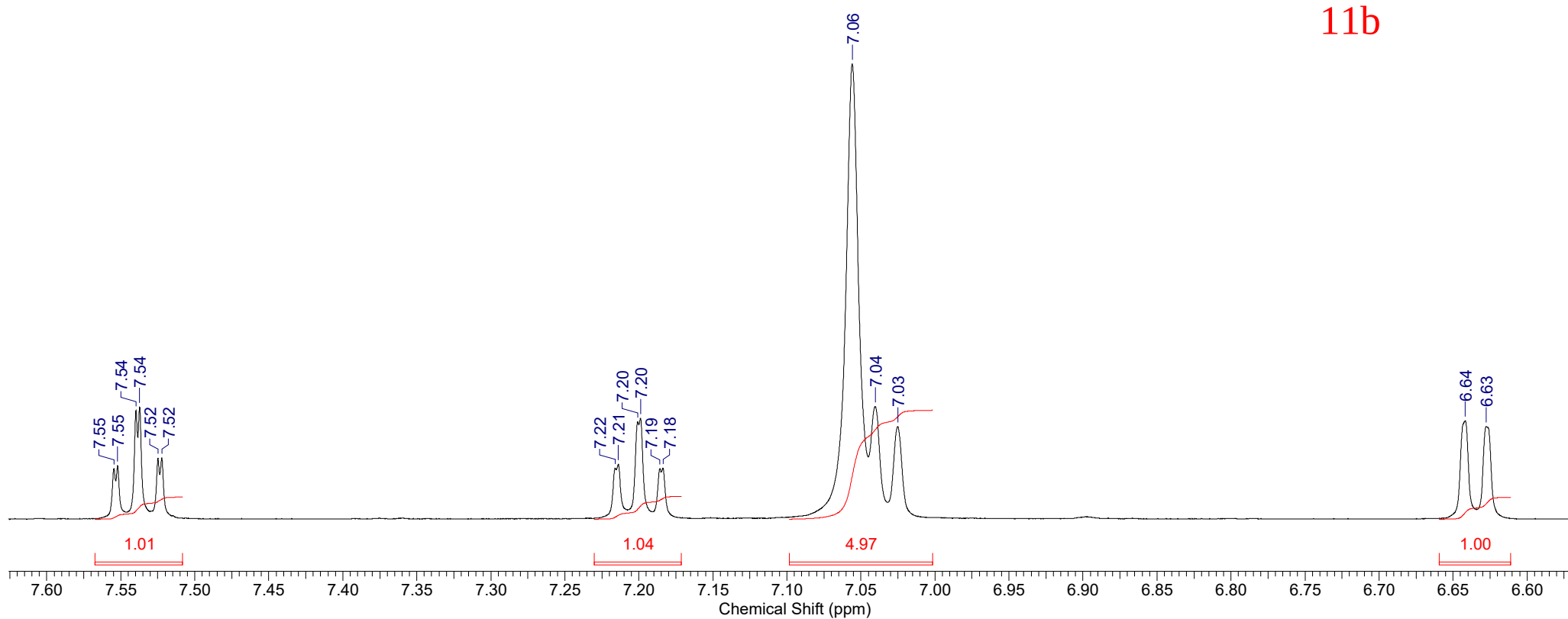
kp2102-2017-K1-NEt2_001001r



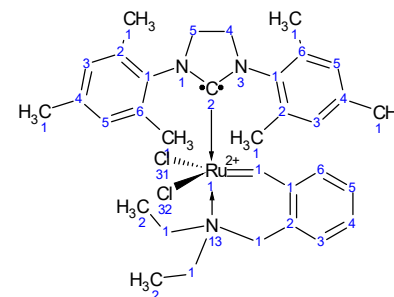
Acquisition Time (sec)	2.3243	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025		Date	21 Feb 2017 05:26:24	
Date Stamp	21 Feb 2017 05:26:24						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2_001001r						
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	8	Origin	spect
Original Points Count	32768	Owner	nmrsu	Points Count	262144	Pulse Sequence	zg30
Receiver Gain	122.15	SW(cyclical) (Hz)	14097.74	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	4088.6934	Sweep Width (Hz)	14097.69	Temperature (degree C)	25.017		



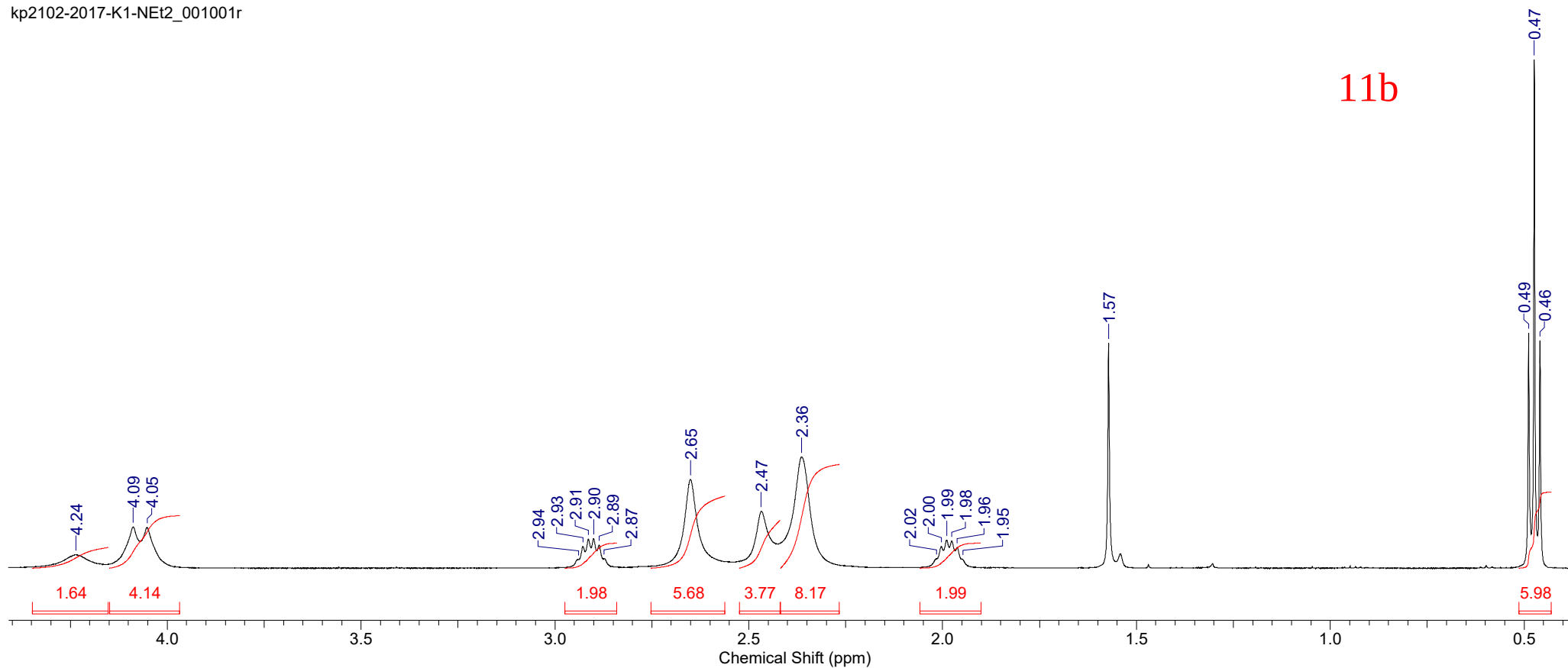
kp2102-2017-K1-NEt2_001001r



Acquisition Time (sec)	2.3243	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025		Date	21 Feb 2017 05:26:24	
Date Stamp	21 Feb 2017 05:26:24						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2_001001r						
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	8	Origin	spect
Original Points Count	32768	Owner	nmr-su	Points Count	262144	Pulse Sequence	zg30
Receiver Gain	122.15	SW(cyclical) (Hz)	14097.74	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	4088.6934	Sweep Width (Hz)	14097.69	Temperature (degree C)	25.017		

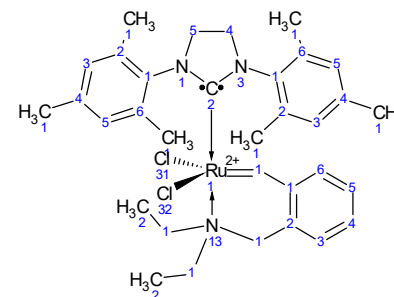


kp2102-2017-K1-NEt2_001001r

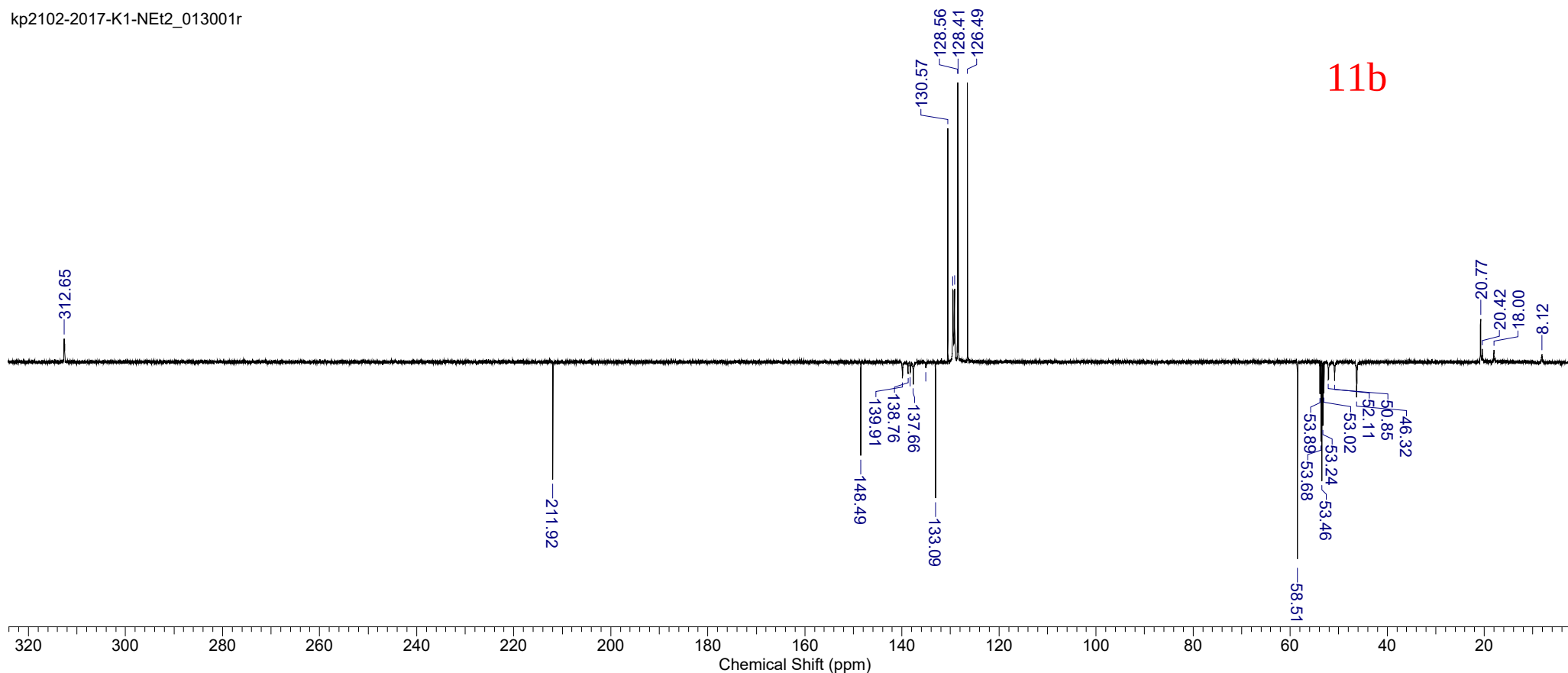


11b

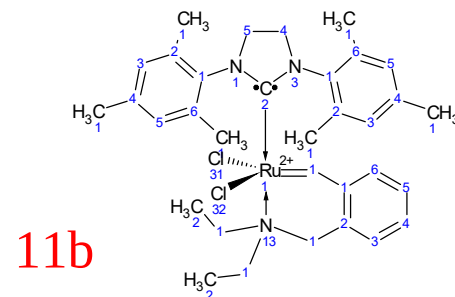
Acquisition Time (sec)	0.6554	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025		Date	21 Feb 2017 06:09:04	
Date Stamp	21 Feb 2017 06:09:04						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2_013001r						
Frequency (MHz)	125.76	Nucleus	¹³ C	Number of Transients	193	Origin	spect
Original Points Count	32768	Owner	nmsu	Points Count	32768	Pulse Sequence	jmod
Receiver Gain	189.77	SW(cyclical) (Hz)	50000.00	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	25151.5527	Sweep Width (Hz)	49998.47	Temperature (degree C)	25.037		



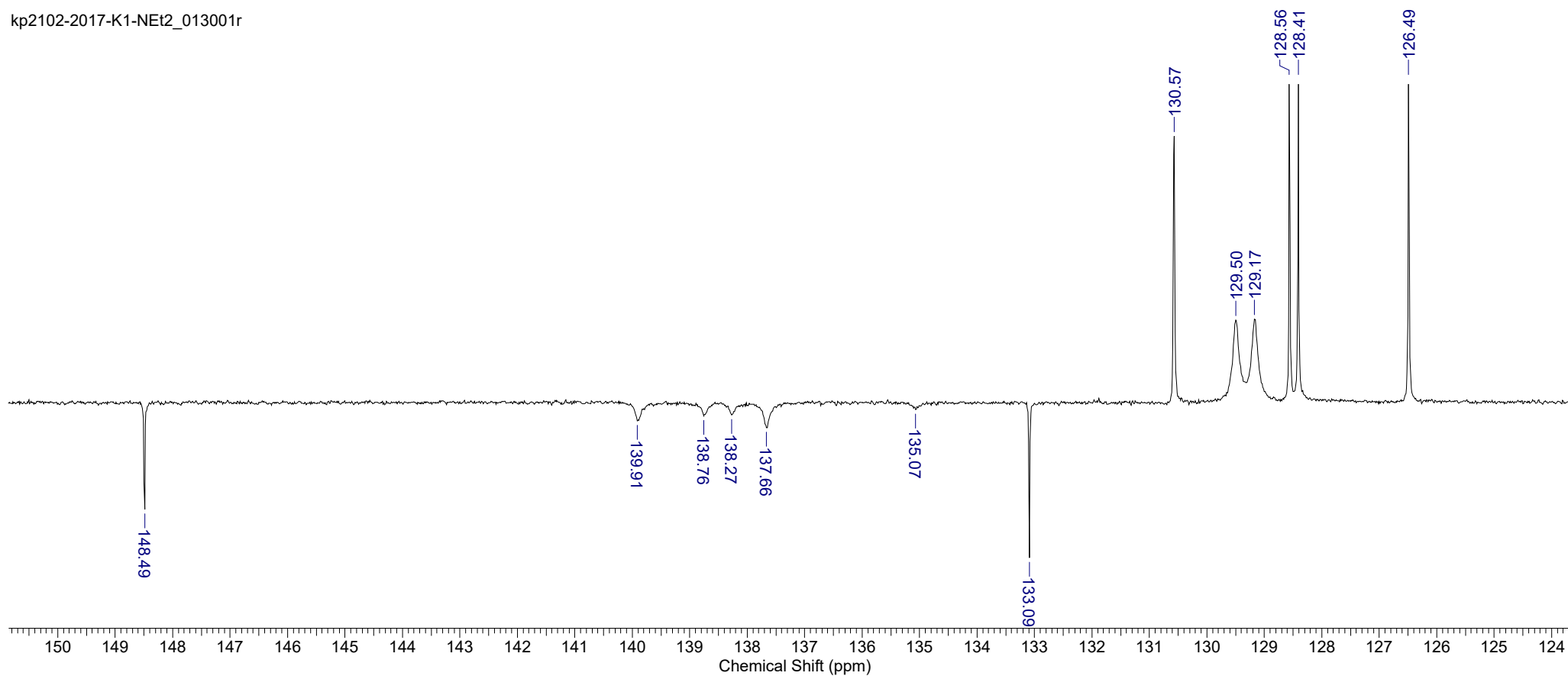
11b



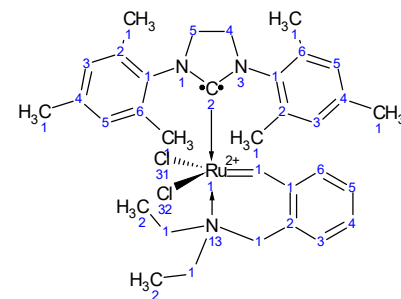
Acquisition Time (sec)	0.6554	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025		Date	21 Feb 2017 06:09:04	
Date Stamp	21 Feb 2017 06:09:04						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2_013001r						
Frequency (MHz)	125.76	Nucleus	¹³ C	Number of Transients	193	Origin	spect
Original Points Count	32768	Owner	nmsu	Points Count	32768	Pulse Sequence	jmod
Receiver Gain	189.77	SW(cyclical) (Hz)	50000.00	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	25151.5527	Sweep Width (Hz)	49998.47	Temperature (degree C)	25.037		



kp2102-2017-K1-NEt2_013001r

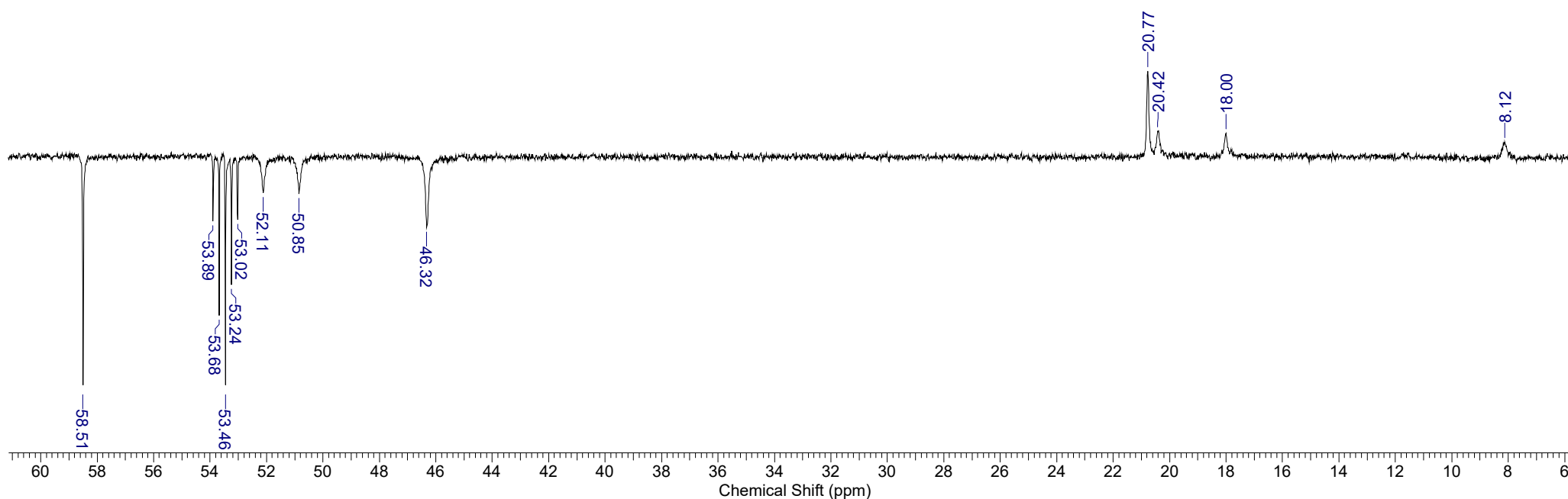


Acquisition Time (sec)	0.6554	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025		Date	21 Feb 2017 06:09:04	
Date Stamp	21 Feb 2017 06:09:04						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2_013001r						
Frequency (MHz)	125.76	Nucleus	¹³ C	Number of Transients	193	Origin	spect
Original Points Count	32768	Owner	nmsu	Points Count	32768	Pulse Sequence	jmod
Receiver Gain	189.77	SW(cyclical) (Hz)	50000.00	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	25151.5527	Sweep Width (Hz)	49998.47	Temperature (degree C)	25.037		



11b

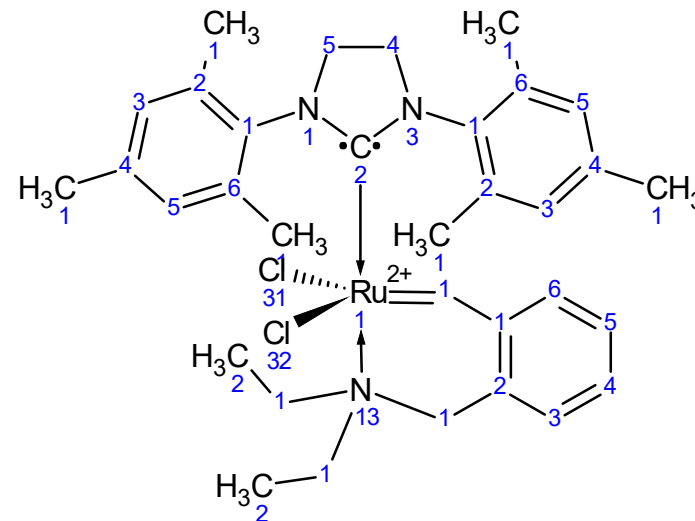
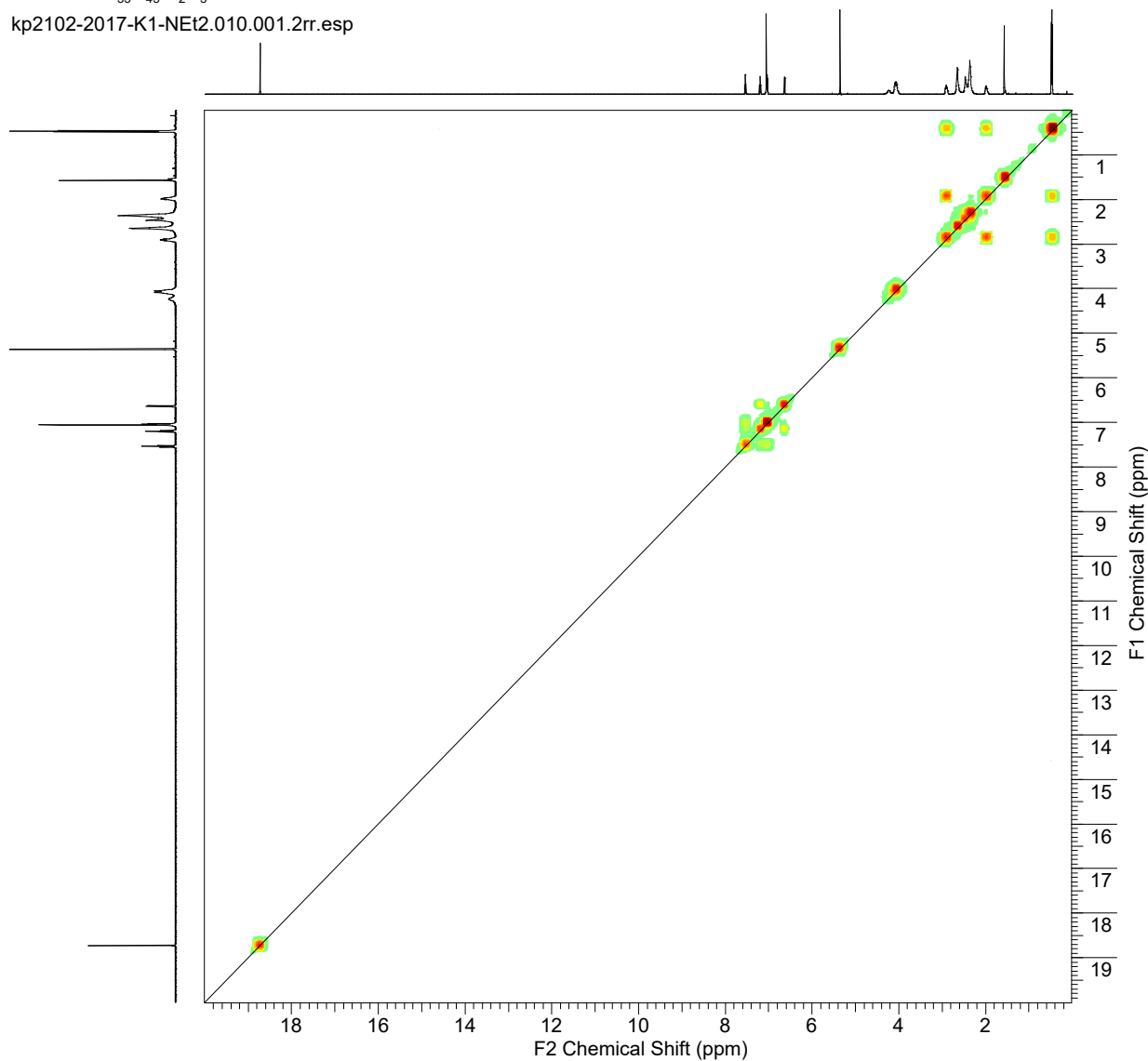
kp2102-2017-K1-NEt2_013001r



Acquisition Time (sec)	(0.0512, 0.0128)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 09:34:24			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2\10\data\1\2rr			
Frequency (MHz)	(500.14, 500.14)	Nucleus	(1H, 1H)	Number of Transients 1
Origin	spect	Original Points Count	(512, 128)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	cosygpgpf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 10000.00)	Temperature (degree C)	25.096	

Formula C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW 653.6895
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kp2102-2017-K1-NEt2.010.001.2rr.esp

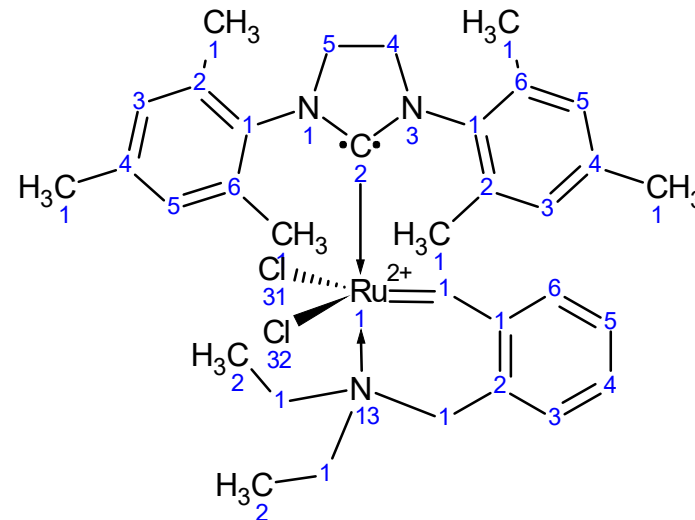
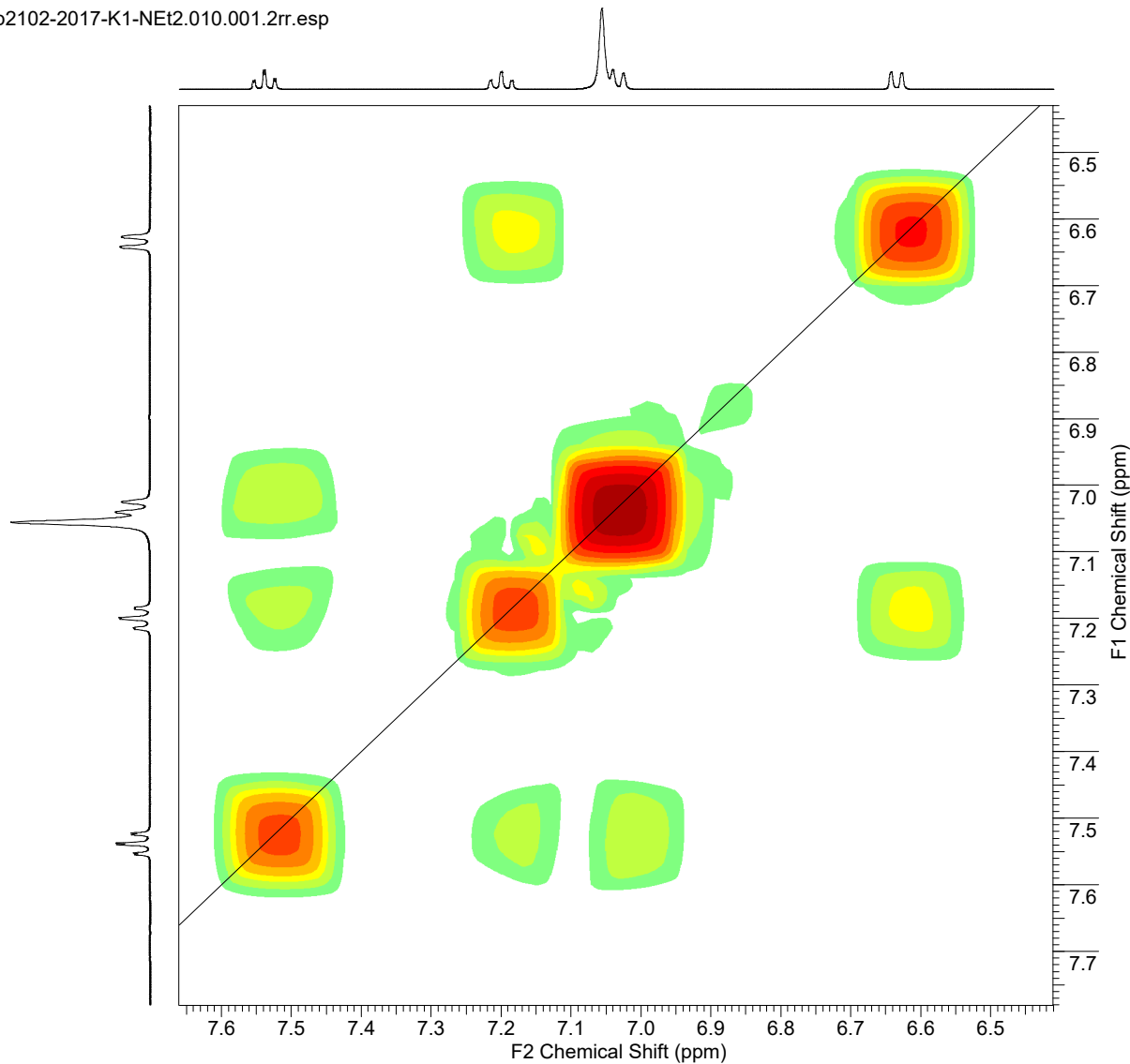


11b

Acquisition Time (sec)	(0.0512, 0.0128)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 09:34:24			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2\10\data\1\2rr			
Frequency (MHz)	(500.14, 500.14)	Nucleus	(1H, 1H)	Number of Transients 1
Origin	spect	Original Points Count	(512, 128)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	cosygppqf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 10000.00)	Temperature (degree C)	25.096	

Formula C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW 653.6895
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kp2102-2017-K1-NEt2.010.001.2rr.esp

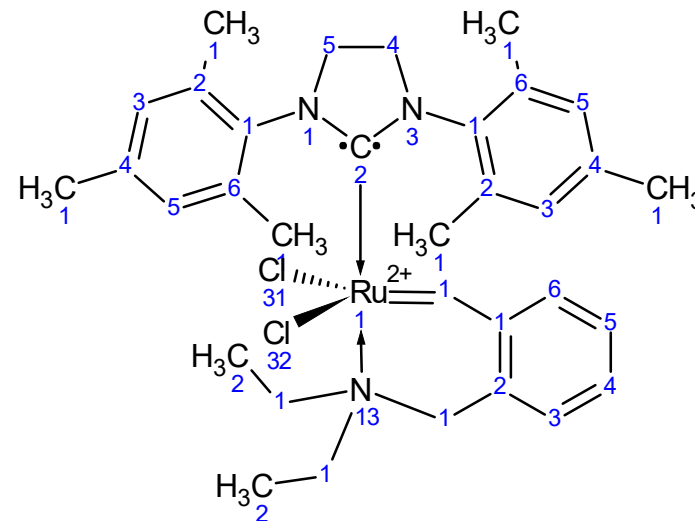
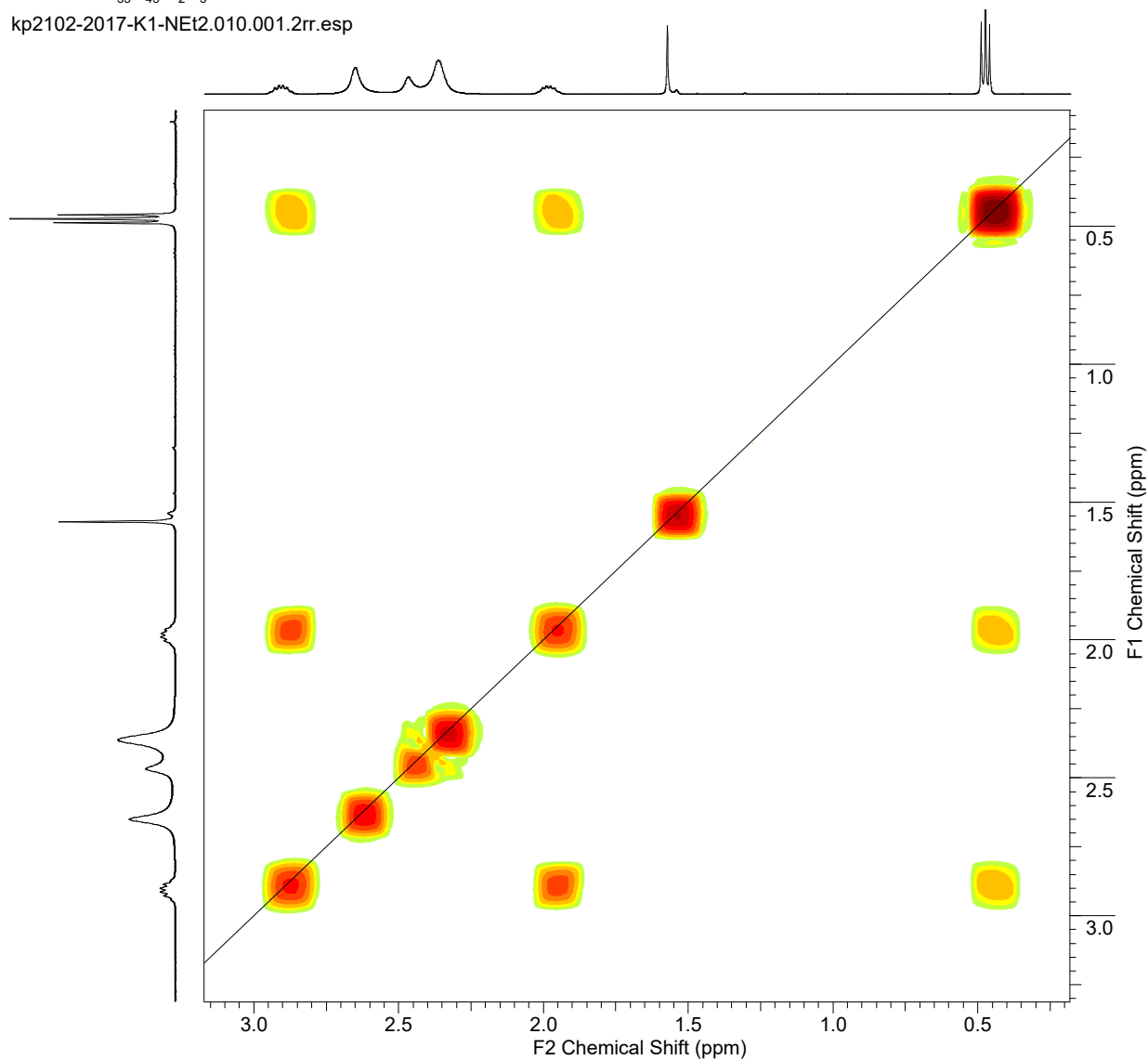


11b

Acquisition Time (sec)	(0.0512, 0.0128)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 09:34:24			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NET2\10\data\1\2rr			
Frequency (MHz)	(500.14, 500.14)	Nucleus	(1H, 1H)	Number of Transients 1
Origin	spect	Original Points Count	(512, 128)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	cosygpcpf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 10000.00)	Temperature (degree C)	25.096	

Formula	C ₃₃ H ₄₃ N ₂ Ru	FW	653.6895
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kp2102-2017-K1-NET2.010.001.2rr.esp

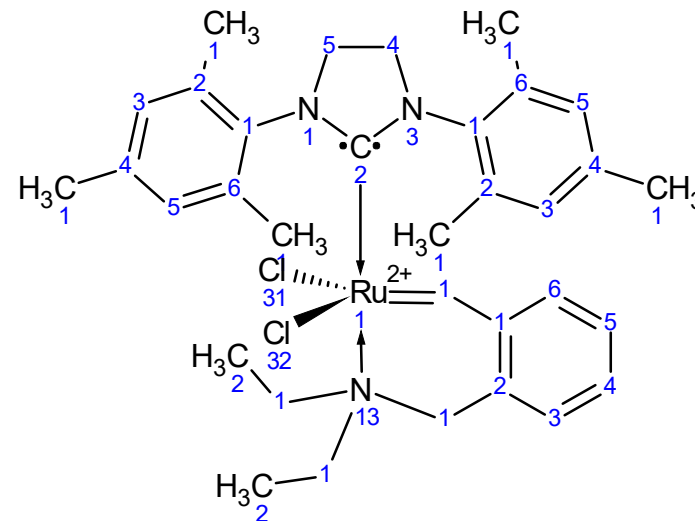
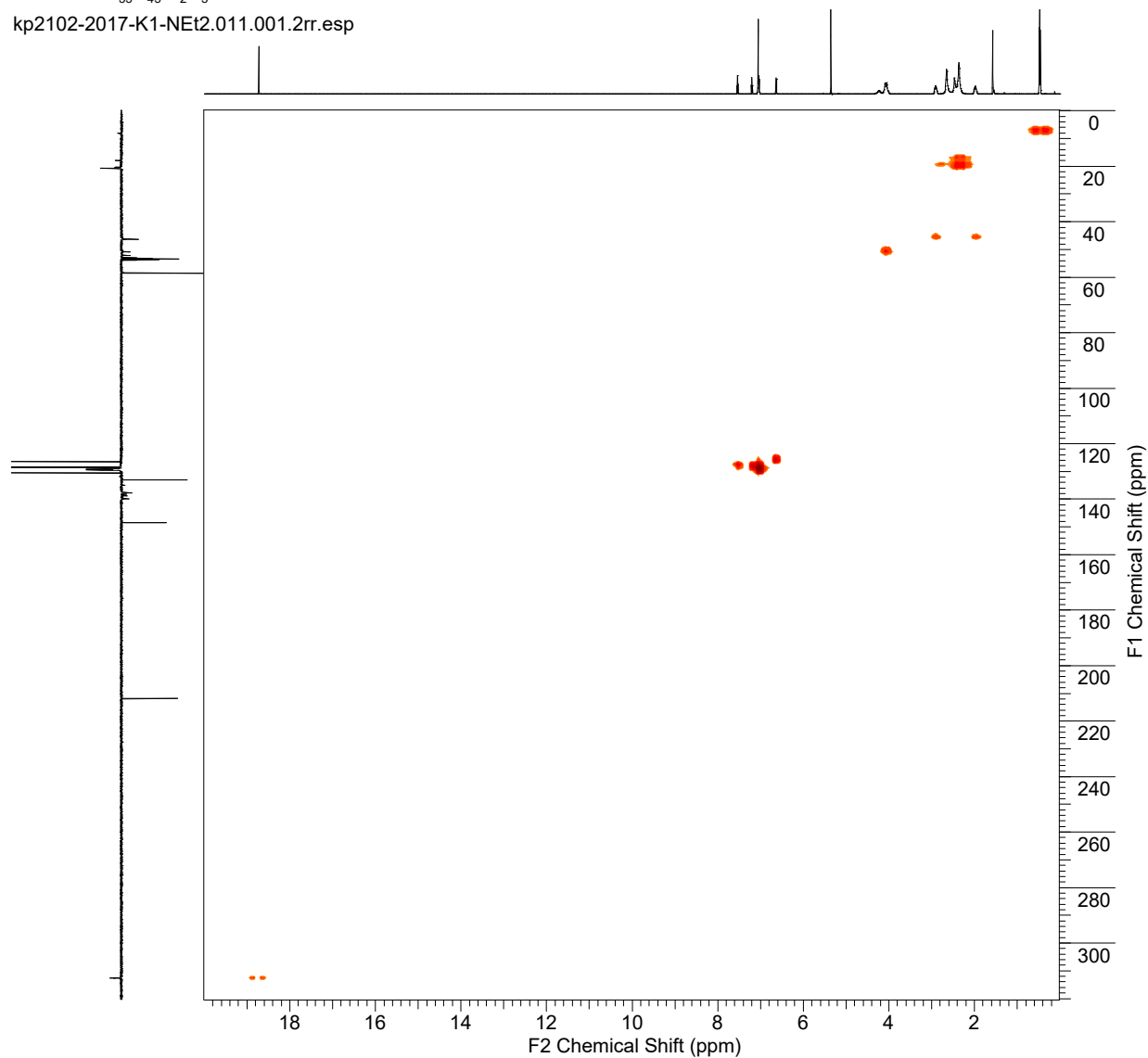


11b

Acquisition Time (sec)	(0.0512, 0.0063)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 10:43:58			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2\11\data\12rr			
Frequency (MHz)	(500.14, 125.78)	Nucleus	(1H, 13C)	Number of Transients 2
Origin	spect	Original Points Count	(512, 256)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	hmqcgpqf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 40322.58)	Temperature (degree C)	25.078	

Formula	C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW	653.6895
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kp2102-2017-K1-NEt2.011.001.2rr.esp

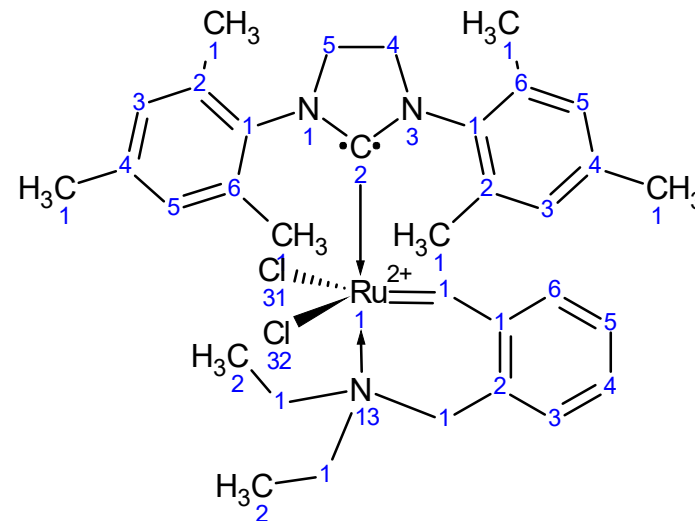
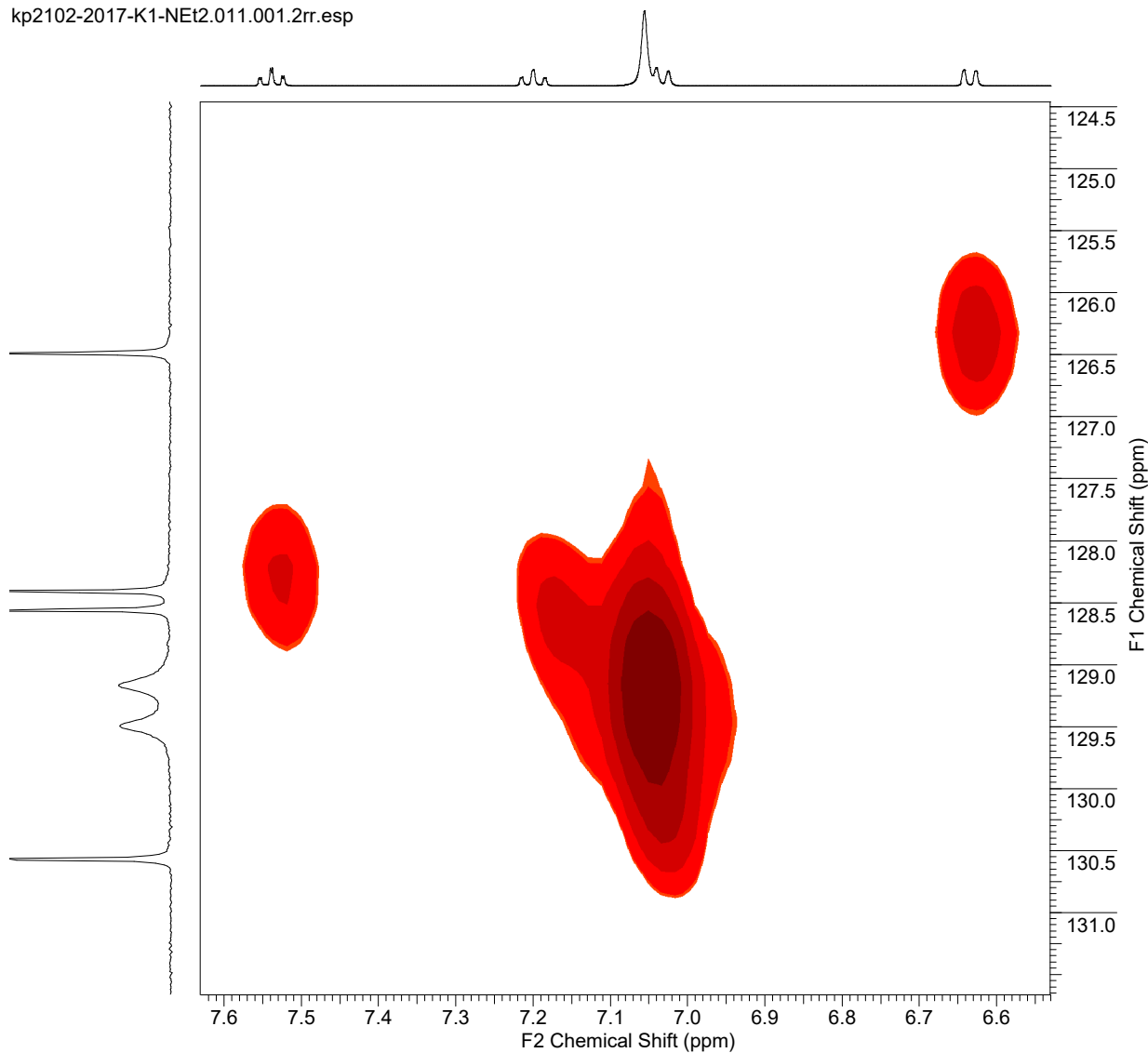


11b

Acquisition Time (sec)	(0.0512, 0.0063)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 10:43:58			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2\11\data\1\2rr			
Frequency (MHz)	(500.14, 125.78)	Nucleus	(1H, 13C)	Number of Transients 2
Origin	spect	Original Points Count	(512, 256)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	hmqcgpqf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 40322.58)	Temperature (degree C)	25.078	

Formula C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW 653.6895
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kp2102-2017-K1-NEt2.011.001.2rr.esp

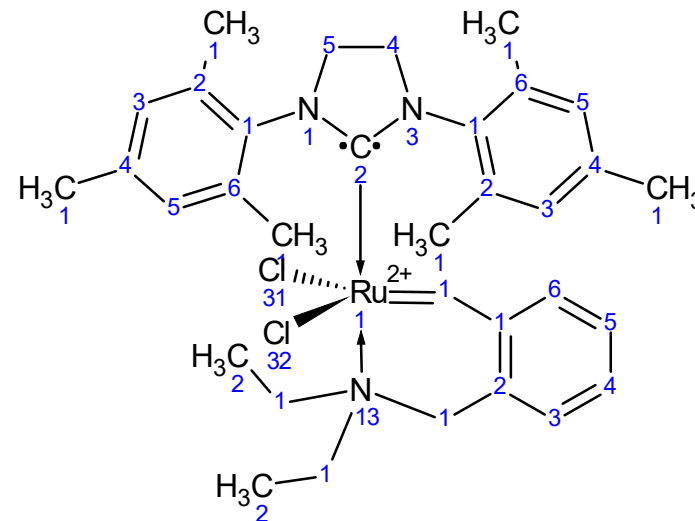
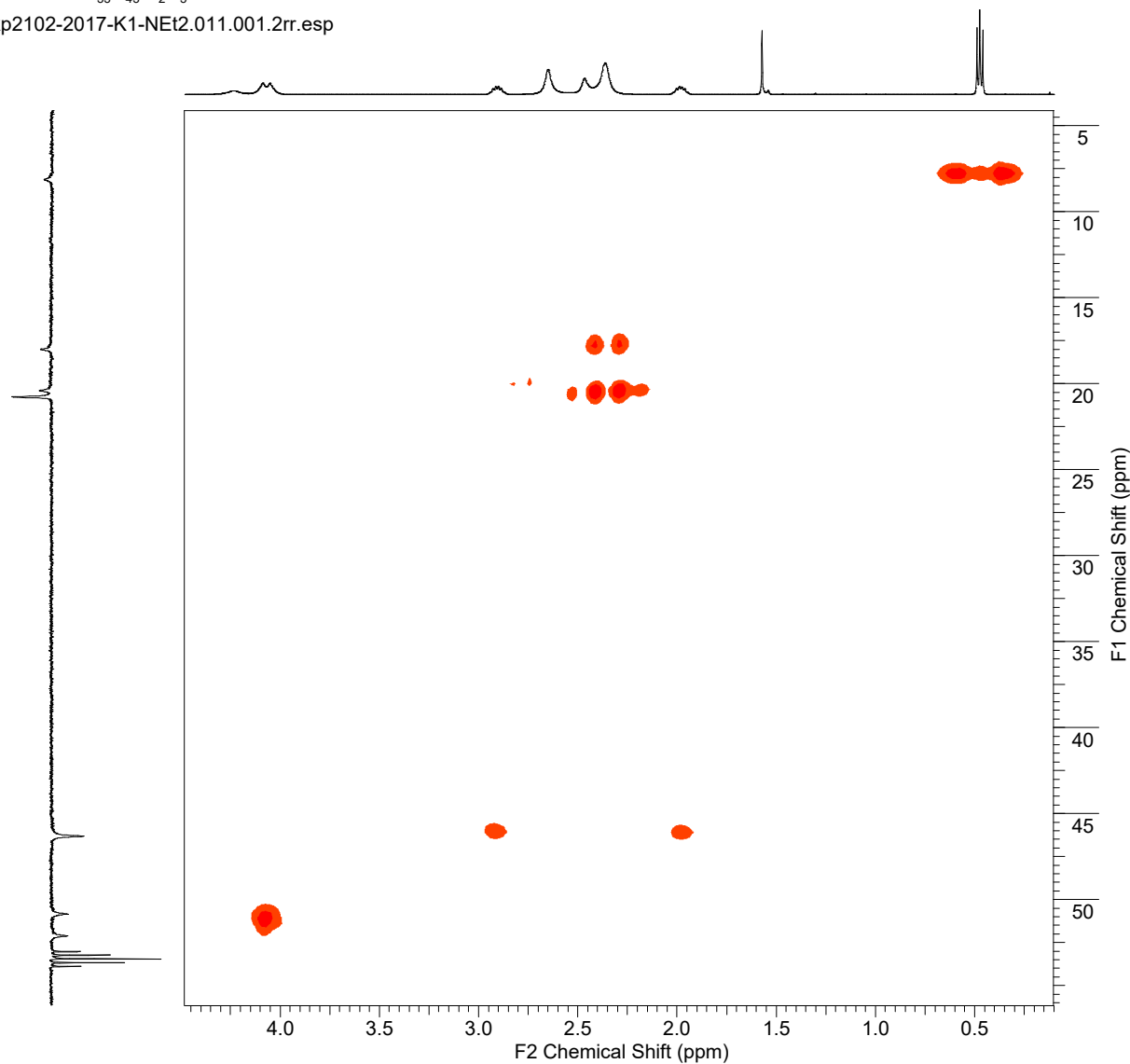


11b

Acquisition Time (sec)	(0.0512, 0.0063)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025		
Date	21 Feb 2017 10:43:58				
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-Net2\11\data\12rr				
Frequency (MHz)	(500.14, 125.78)	Nucleus	(1H, 13C)	Number of Transients	2
Origin	spect	Original Points Count	(512, 256)	Owner	nmrsu
Points Count	(1024, 1024)	Pulse Sequence	hmqcgpqf	Solvent	CD2Cl2
Sweep Width (Hz)	(10000.00, 40322.58)	Temperature (degree C)	25.078		

Formula C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW 653.6895
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kp2102-2017-K1-NET2.011.001.2rr.esp

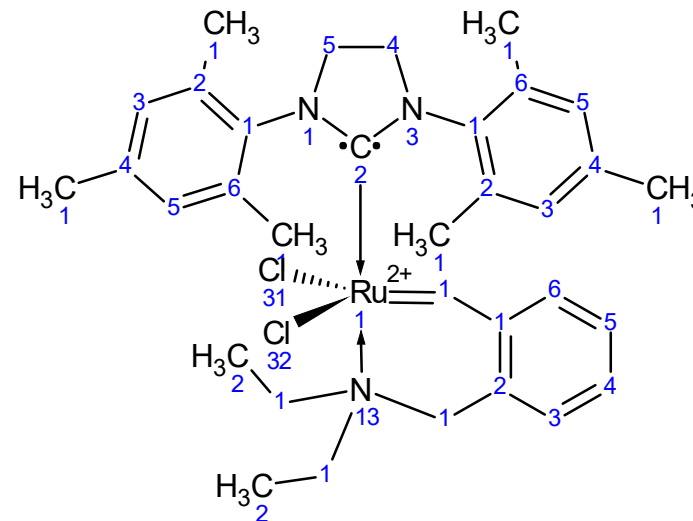
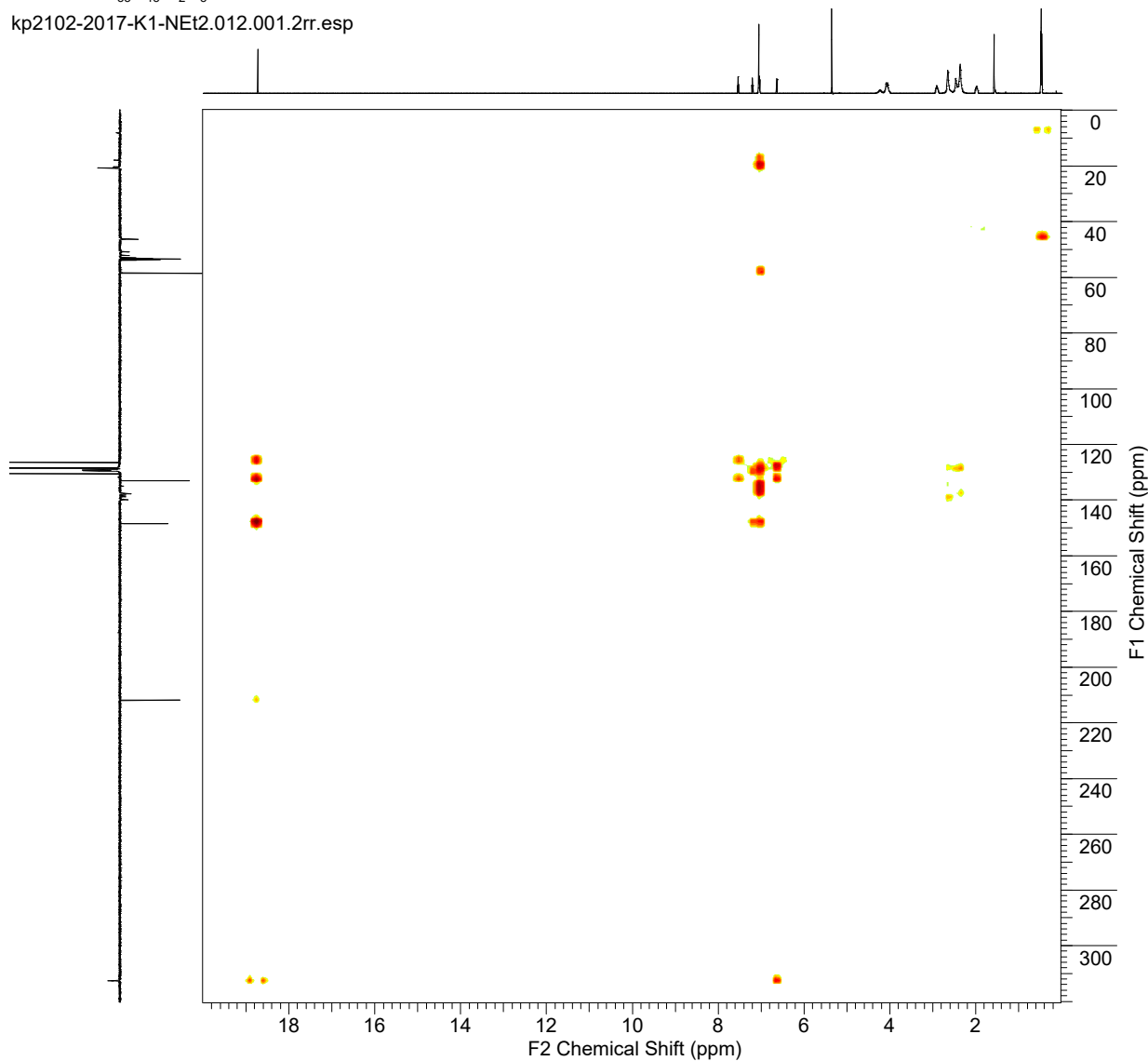


11b

Acquisition Time (sec)	(0.0512, 0.0063)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 11:02:14			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2\12\data\1\2rr			
Frequency (MHz)	(500.14, 125.78)	Nucleus	(1H, 13C)	Number of Transients 4
Origin	spect	Original Points Count	(512, 256)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	hmbcgp1pndqf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 40322.58)	Temperature (degree C)	24.970	

Formula C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW 653.6895
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kp2102-2017-K1-NEt2.012.001.2rr.esp

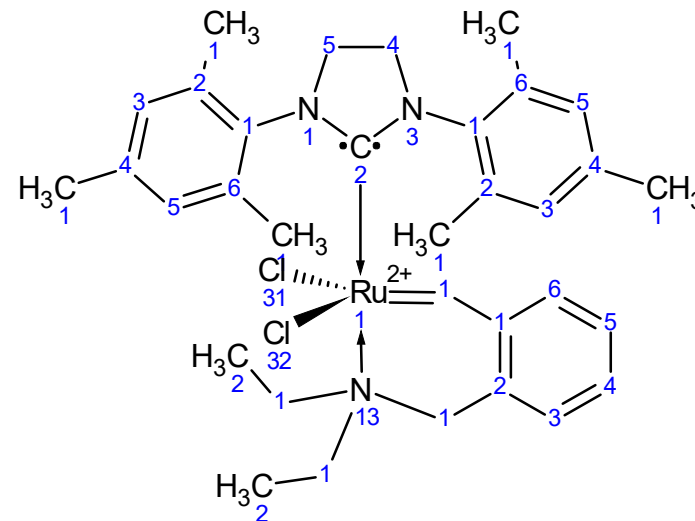
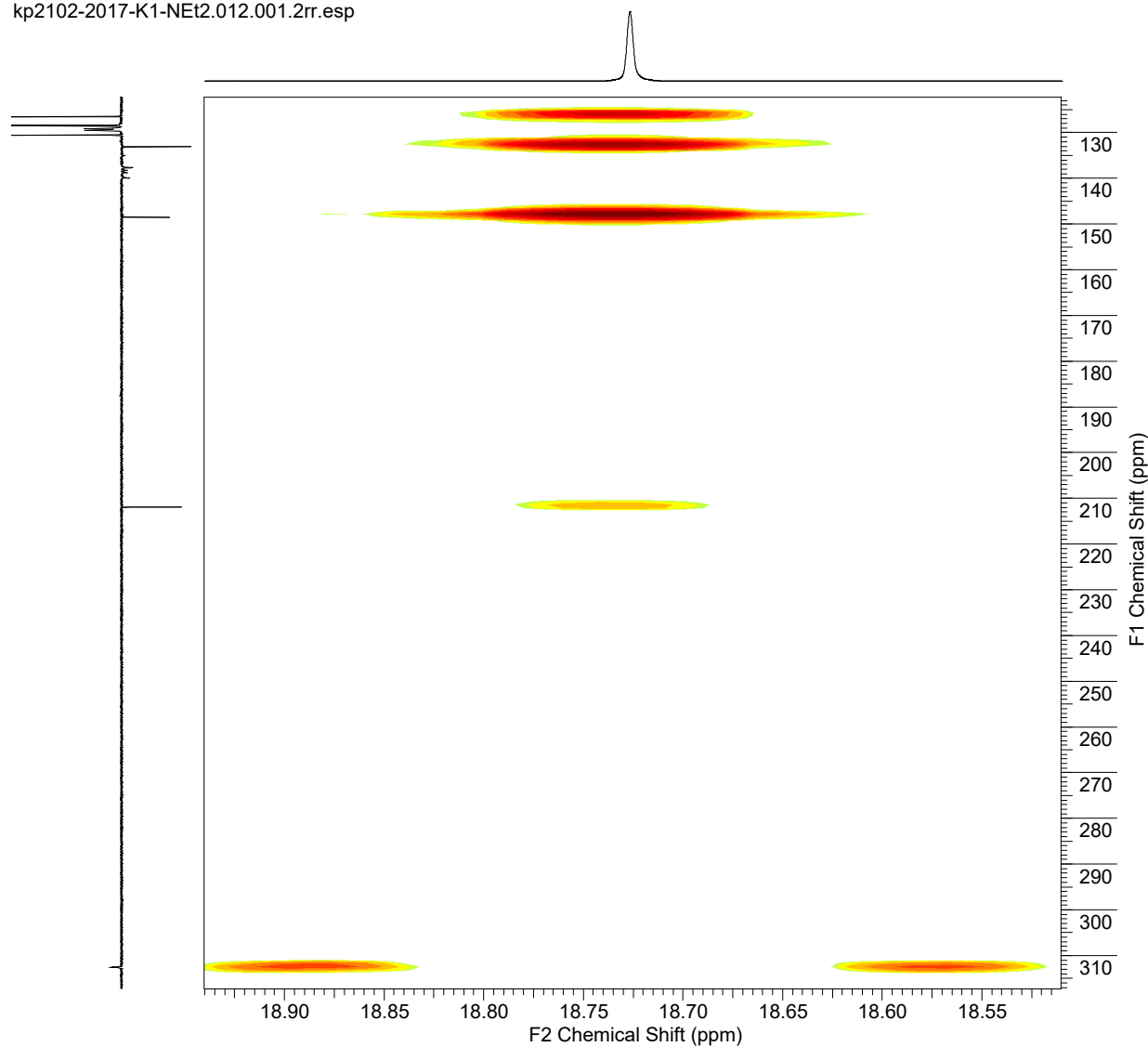


11b

Acquisition Time (sec)	(0.0512, 0.0063)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 11:02:14			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2\12\data\1\2rr			
Frequency (MHz)	(500.14, 125.78)	Nucleus	(1H, 13C)	Number of Transients 4
Origin	spect	Original Points Count	(512, 256)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	hmbcgp1pndqf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 40322.58)	Temperature (degree C)	24.970	

Formula C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW 653.6895
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kp2102-2017-K1-NEt2.012.001.2rr.esp

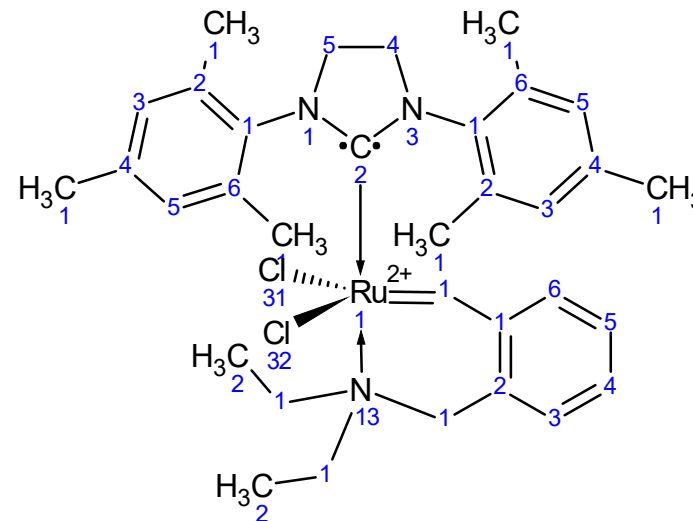
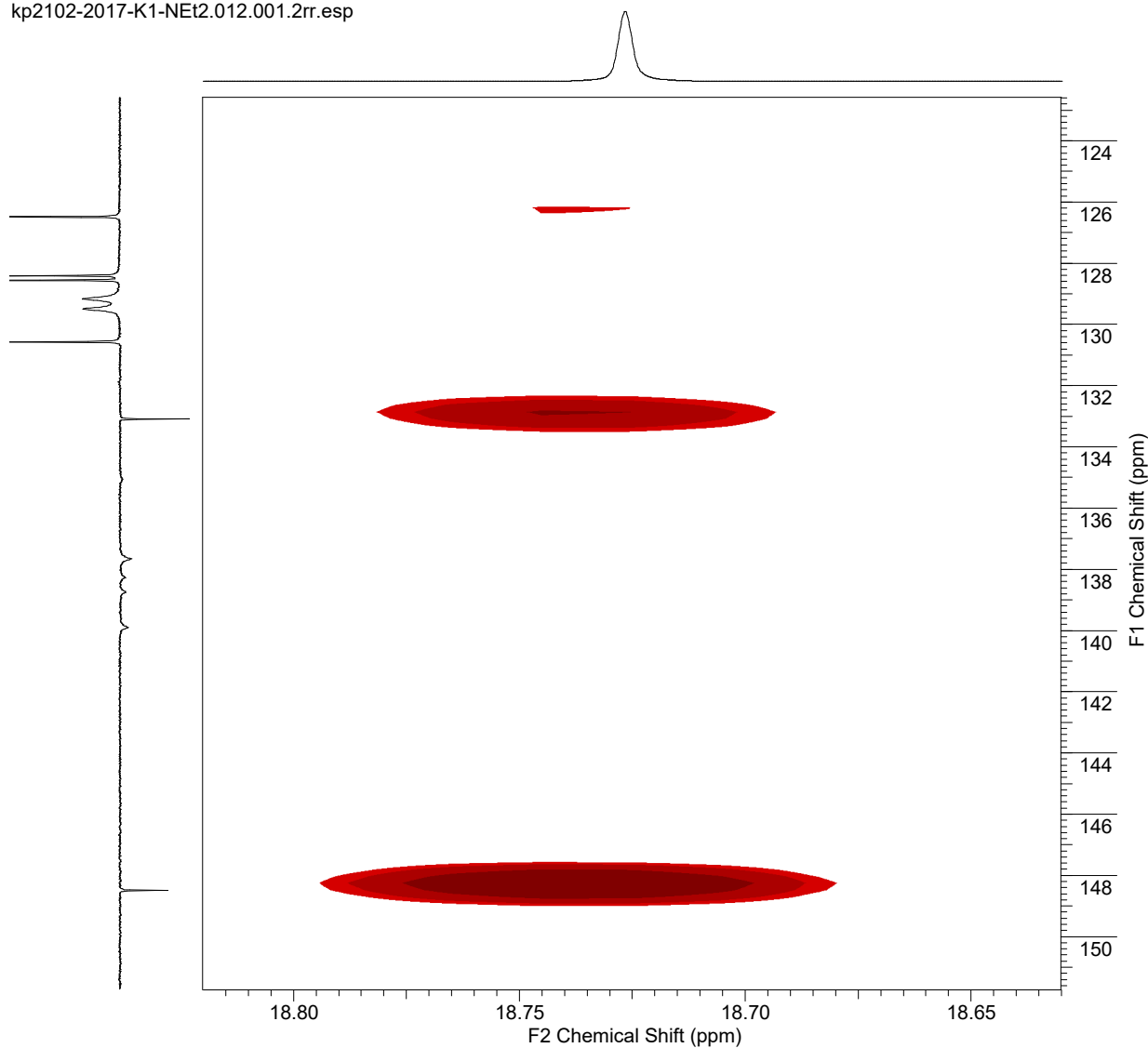


11b

Acquisition Time (sec)	(0.0512, 0.0063)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 11:02:14			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2\12\data\1\2rr			
Frequency (MHz)	(500.14, 125.78)	Nucleus	(1H, 13C)	Number of Transients 4
Origin	spect	Original Points Count	(512, 256)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	hmbcgp1pndqf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 40322.58)	Temperature (degree C)	24.970	

Formula C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW 653.6895
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kp2102-2017-K1-NEt2.012.001.2rr.esp

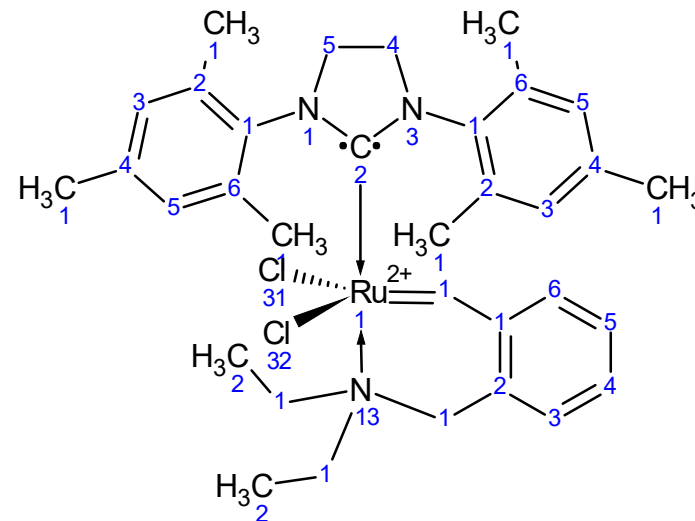
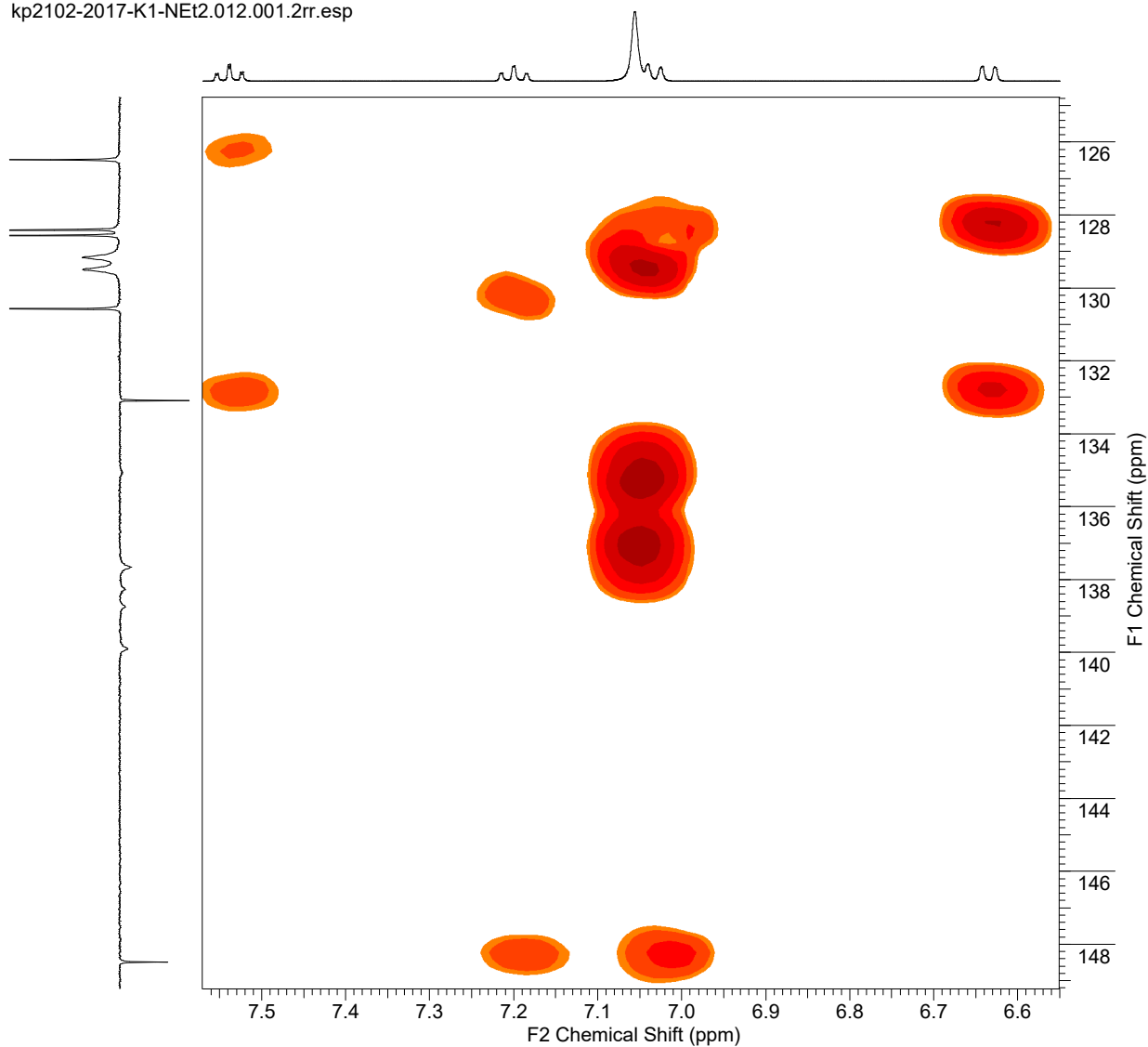


11b

Acquisition Time (sec)	(0.0512, 0.0063)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 11:02:14			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2\12\data\1\2rr			
Frequency (MHz)	(500.14, 125.78)	Nucleus	(1H, 13C)	Number of Transients 4
Origin	spect	Original Points Count	(512, 256)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	hmbcgp1pndqf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 40322.58)	Temperature (degree C)	24.970	

Formula	C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW	653.6895
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kp2102-2017-K1-NEt2.012.001.2rr.esp

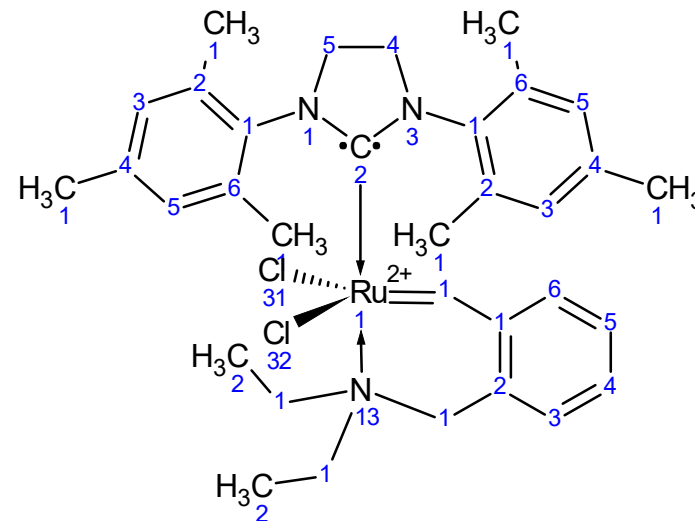
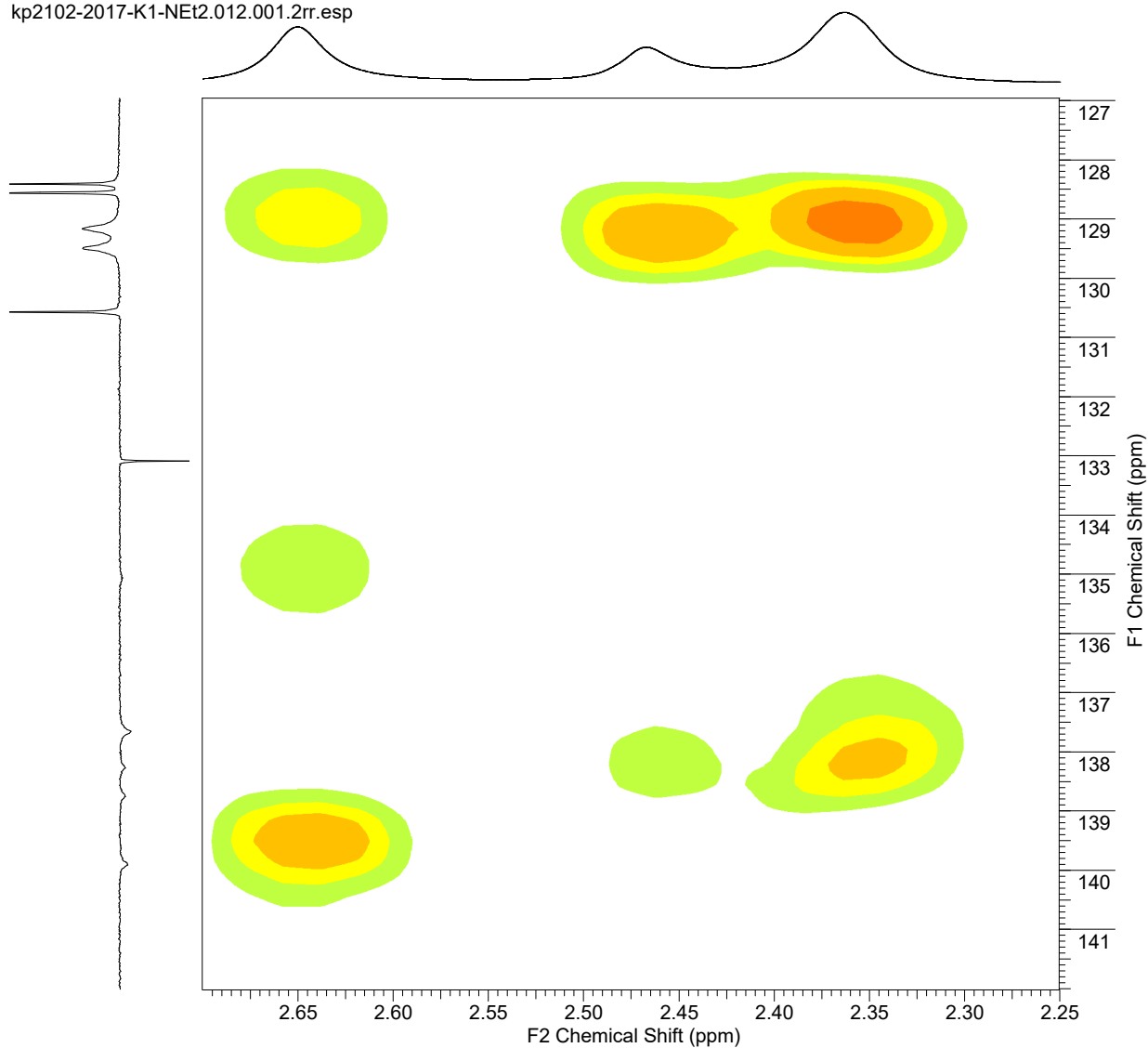


11b

Acquisition Time (sec)	(0.0512, 0.0063)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 11:02:14			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-NEt2\12\data\1\2rr			
Frequency (MHz)	(500.14, 125.78)	Nucleus	(1H, 13C)	Number of Transients 4
Origin	spect	Original Points Count	(512, 256)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	hmbcgp1pndqf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 40322.58)	Temperature (degree C)	24.970	

Formula C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW 653.6895
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kp2102-2017-K1-NEt2.012.001.2rr.esp

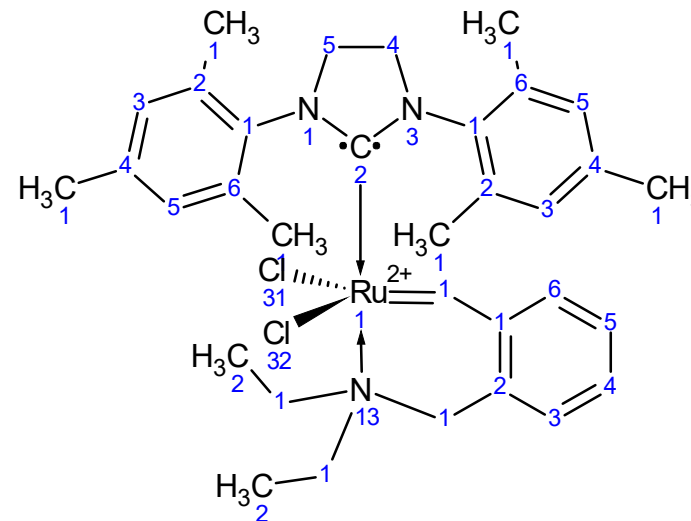
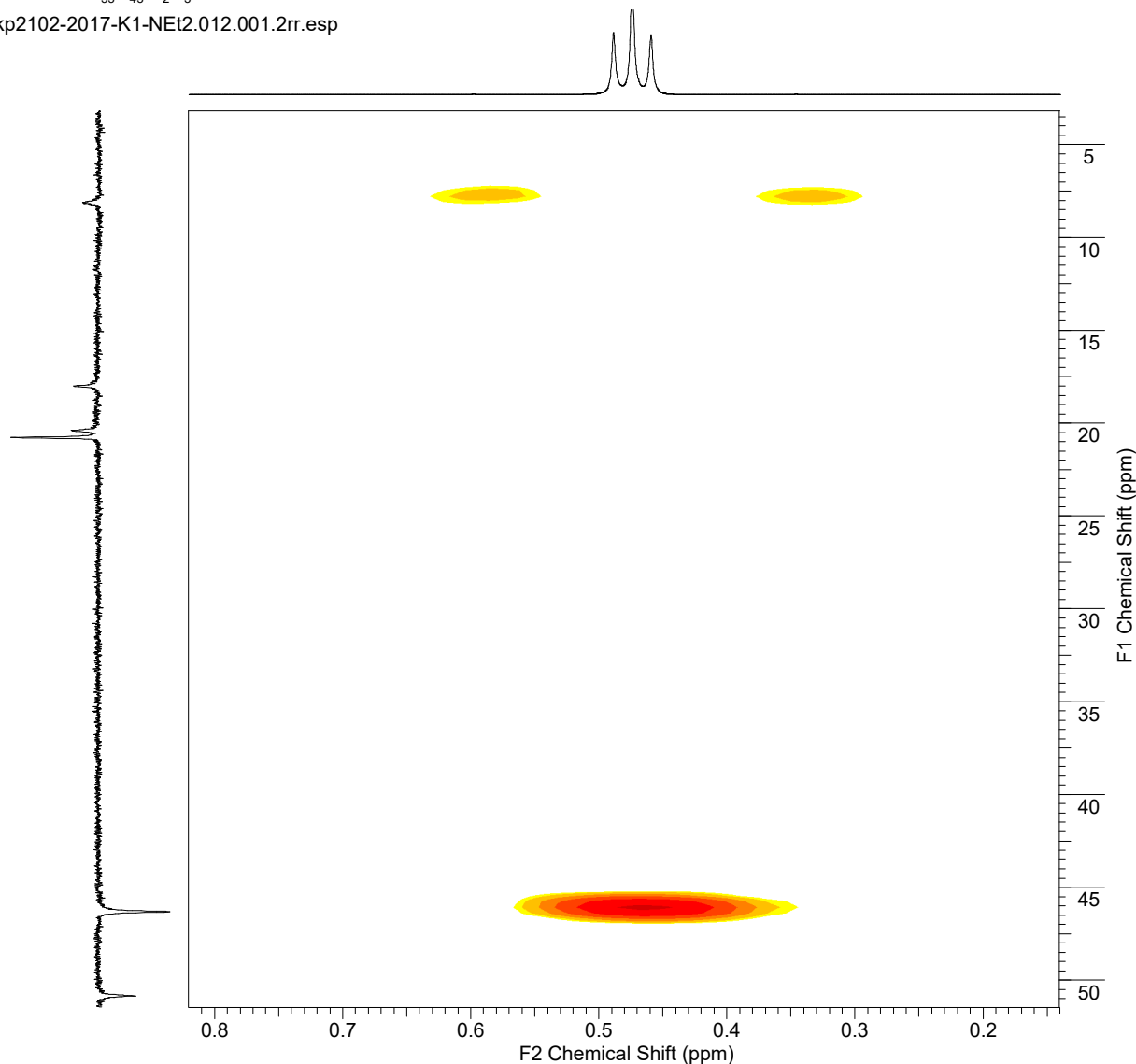


11b

Acquisition Time (sec)	(0.0512, 0.0063)	Comment	5 mm CPPBBO BB-1H/19F/D Z-GRD Z125869/0025	
Date	21 Feb 2017 11:02:14			
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\Kirill-NEW1 Видно слабое поле\kp2102-2017-K1-Net2\12\data\1\2rr			
Frequency (MHz)	(500.14, 125.78)	Nucleus	(1H, 13C)	Number of Transients 4
Origin	spect	Original Points Count	(512, 256)	Owner nmrsu
Points Count	(1024, 1024)	Pulse Sequence	hmbcgp1pndqf	Solvent CD2Cl2
Sweep Width (Hz)	(10000.00, 40322.58)	Temperature (degree C)	24.970	

Formula	C ₃₃ H ₄₃ Cl ₂ N ₂ Ru	FW	653.6895
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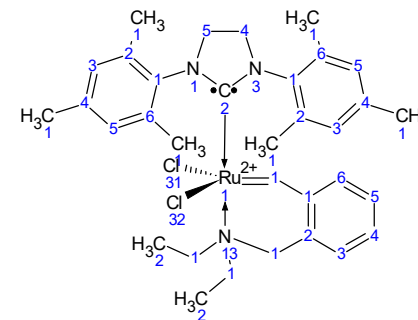
kp2102-2017-K1-NET2.012.001.2rr.esp



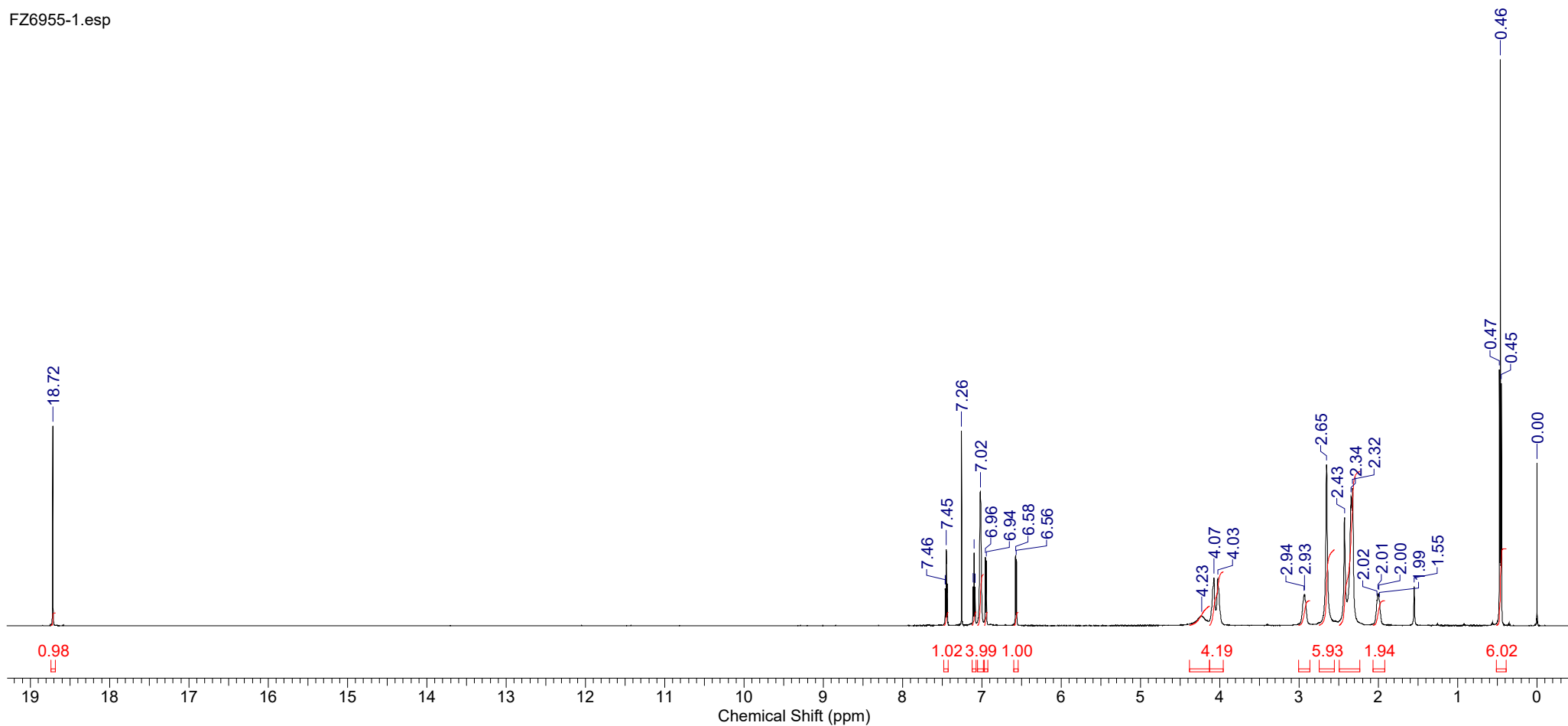
11b

Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	19 Jan 1990 15:19:31	Date Stamp	07 Nov 2018 11:08:25
File Name	C:\Users\Fedor\Desktop\07.11.18\FZ6955-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Pulse Sequence	single_pulse.ex2
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5405.5811	Sweep Width (Hz)	16534.39

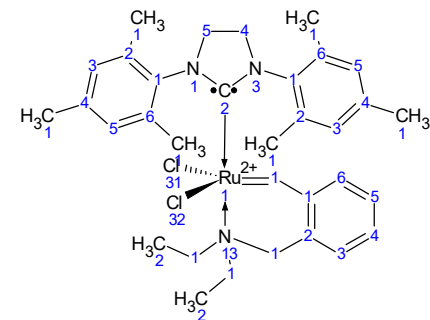
11b in CDCl₃



FZ6955-1.esp

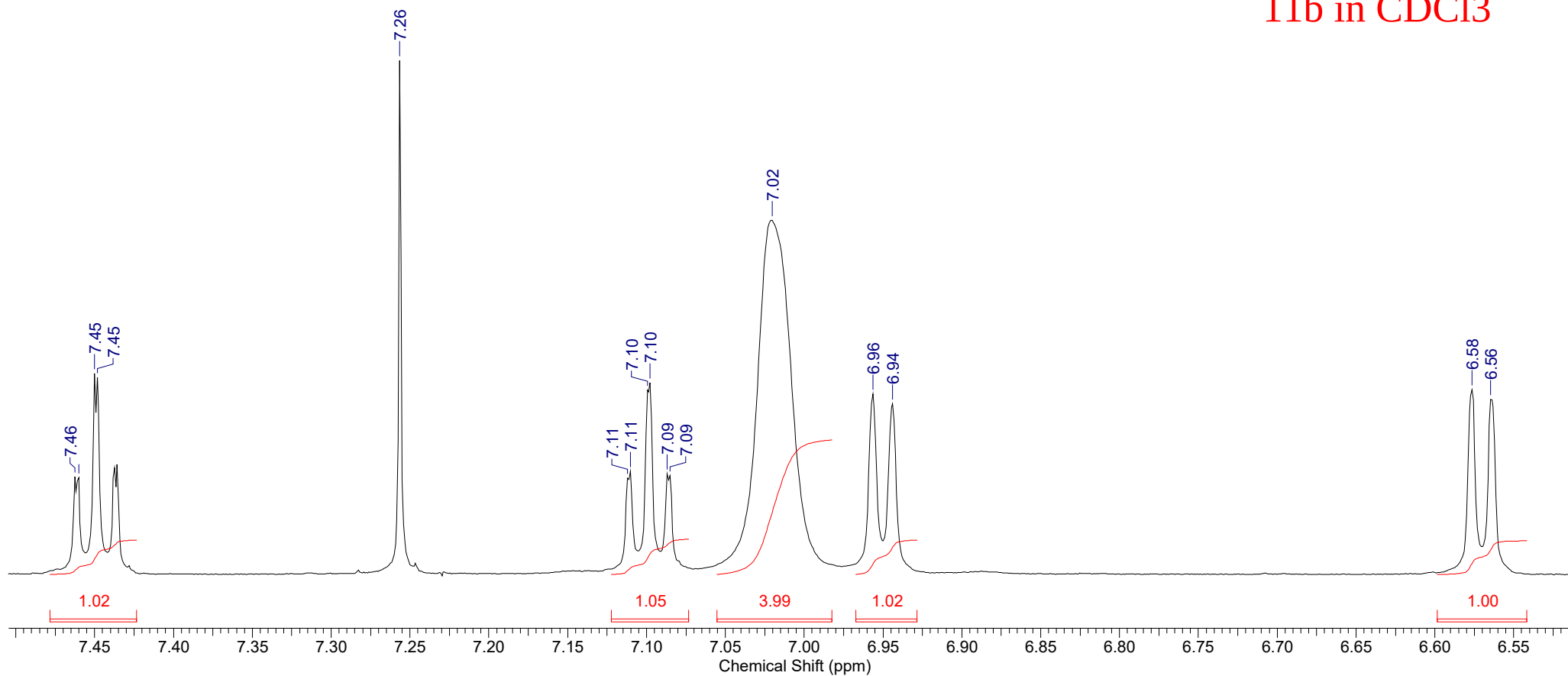


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	19 Jan 1990 15:19:31	Date Stamp	07 Nov 2018 11:08:25
File Name	C:\Users\Fedor\Desktop\07.11.18\FZ6955-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5405.5811	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39

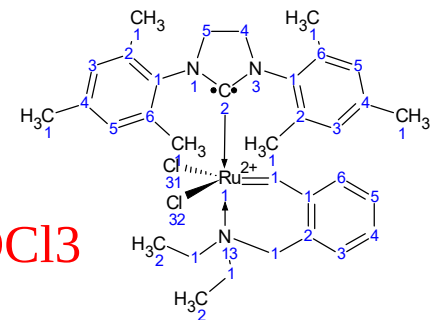


11b in CDCl₃

FZ6955-1.esp

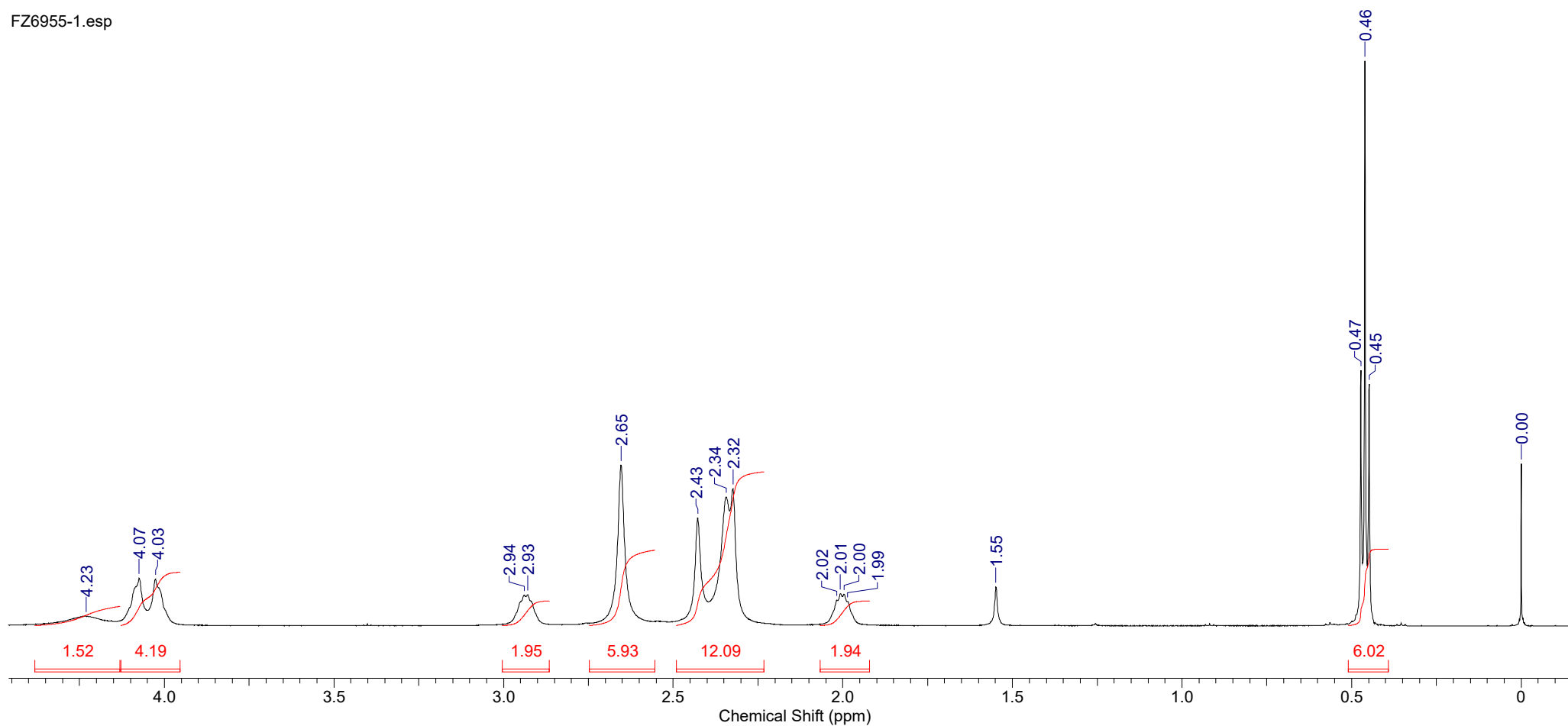


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	19 Jan 1990 15:19:31	Date Stamp	07 Nov 2018 11:08:25
File Name	C:\Users\Fedor\Desktop\07.11.18\FZ6955-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5405.5811	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39

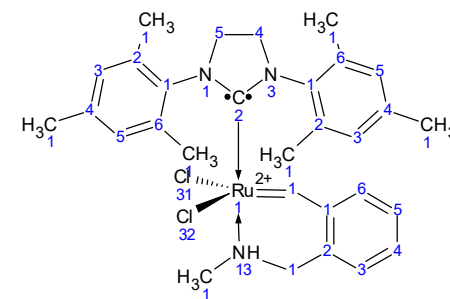


11b in CDCl₃

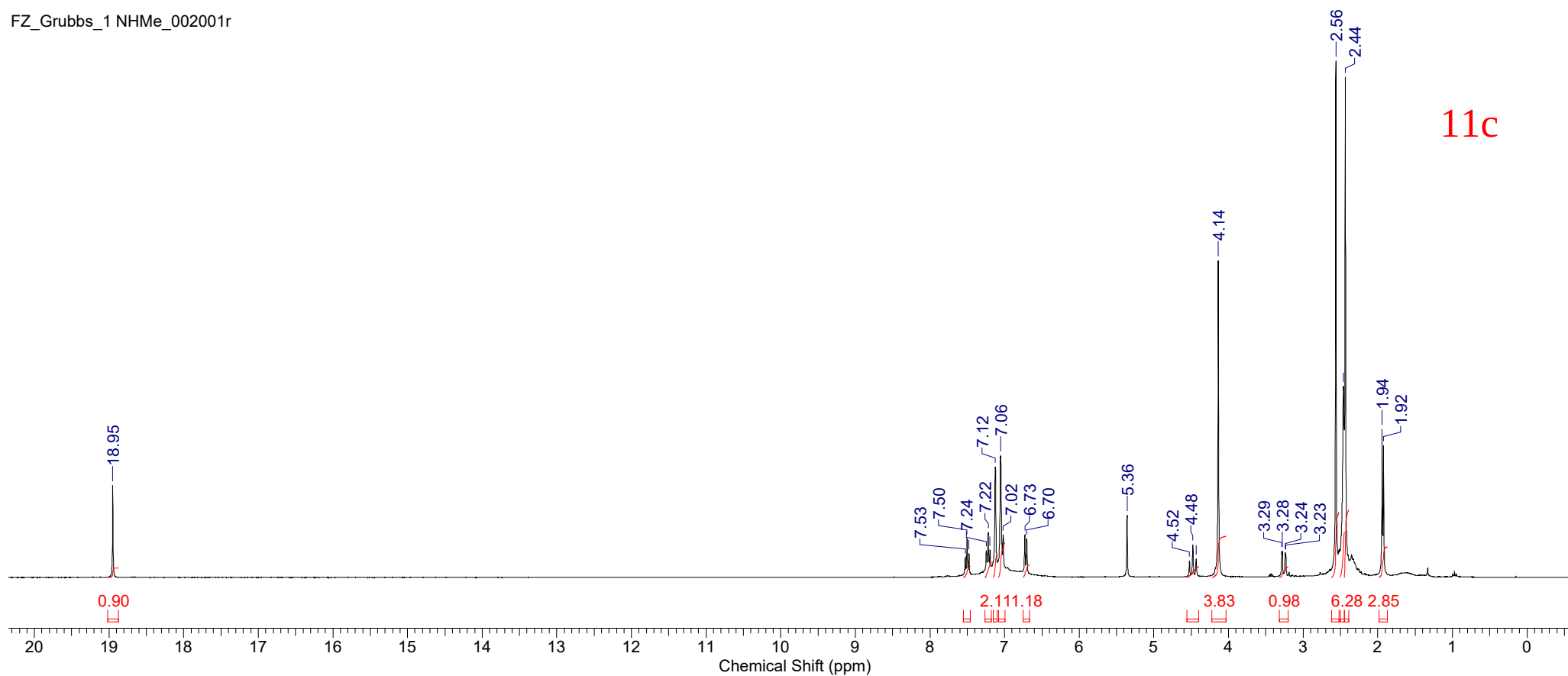
FZ6955-1.esp



Acquisition Time (sec)	2.5690	Comment	H1	Date	02 Oct 2018 18:46:24		
Date Stamp	02 Oct 2018 18:46:24						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ Grubbs 1 NHMe 002001r						
Frequency (MHz)	300.13	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zg
Receiver Gain	72.88	SW(cyclical) (Hz)	25510.20	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	1350.5919	Sweep Width (Hz)	25510.11	Temperature (degree C)	30.010		

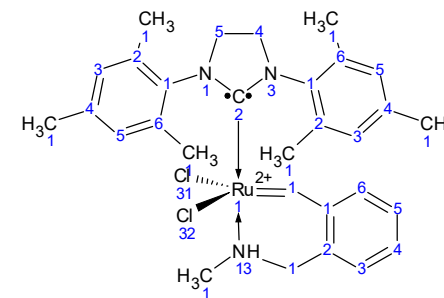


FZ_Grubbs_1 NHMe_002001r



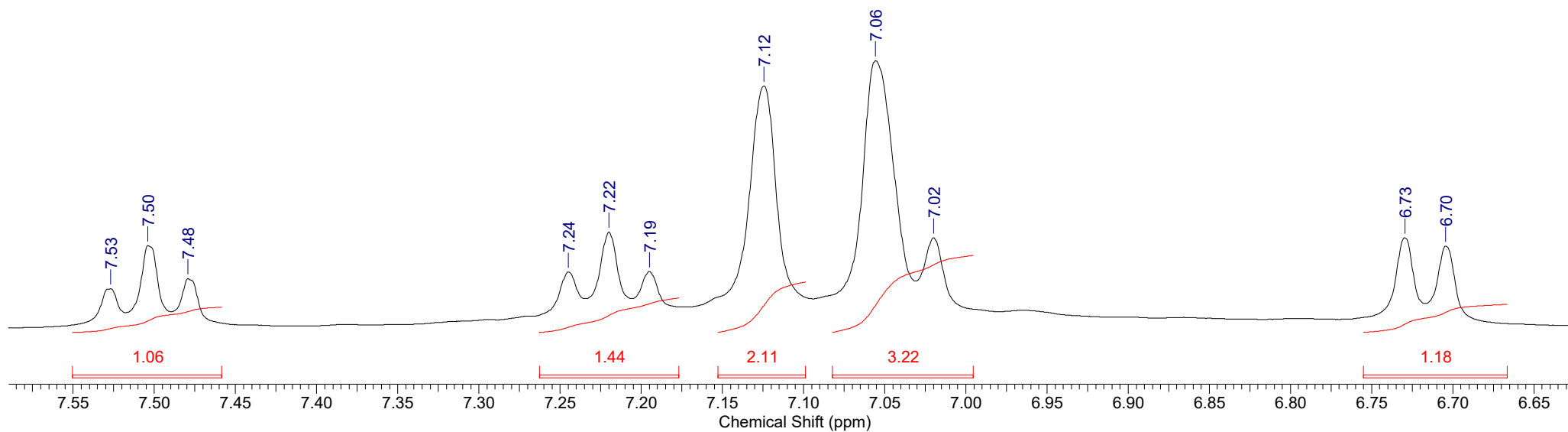
11c

Acquisition Time (sec)	2.5690	Comment	H1	Date	02 Oct 2018 18:46:24		
Date Stamp	02 Oct 2018 18:46:24						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ Grubbs 1 NHMe 002001r						
Frequency (MHz)	300.13	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zg
Receiver Gain	72.88	SW(cyclical) (Hz)	25510.20	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	1350.5919	Sweep Width (Hz)	25510.11	Temperature (degree C)	30.010		

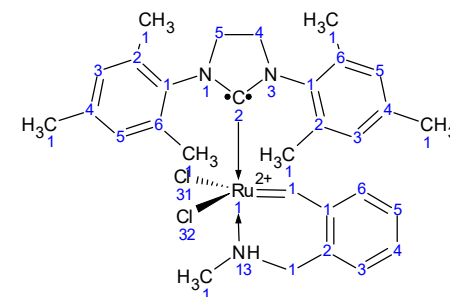


FZ_Grubbs_1 NHMe_002001r

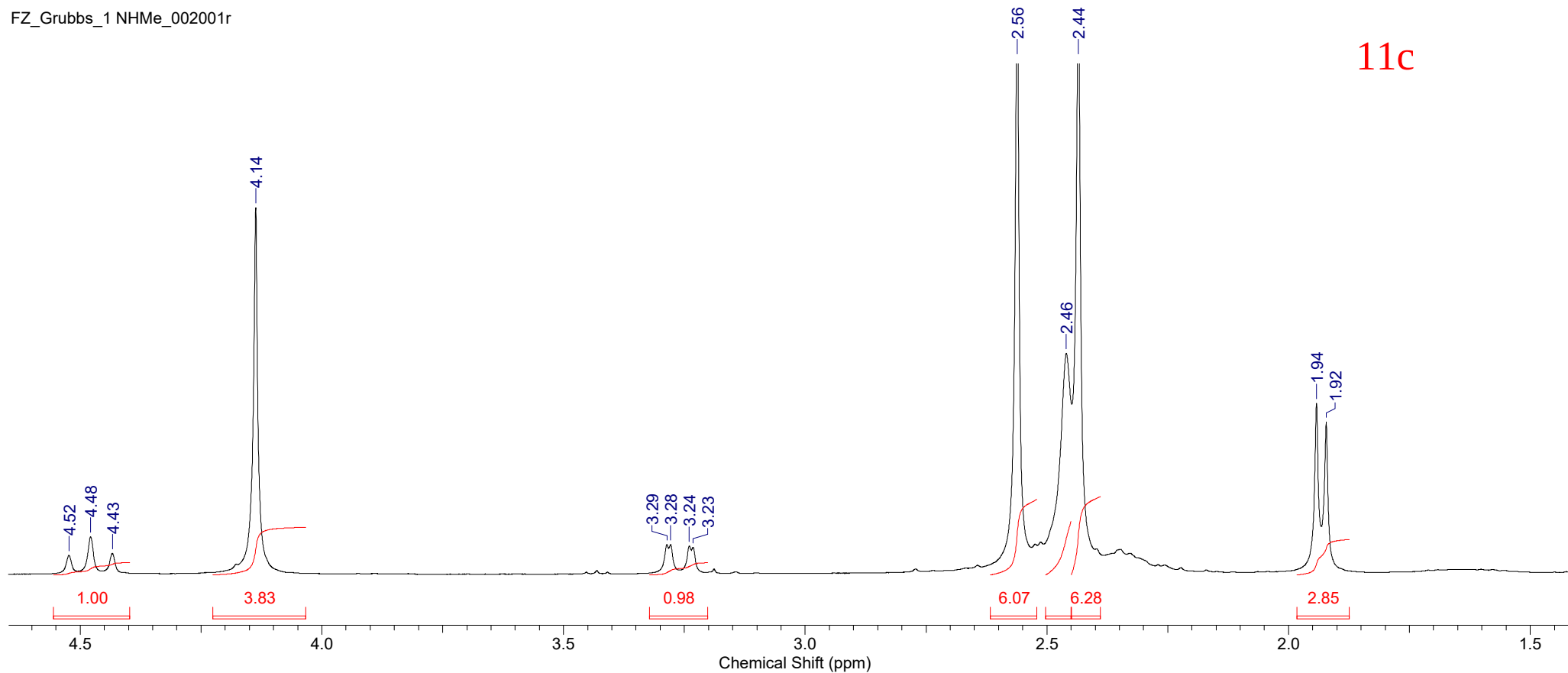
11c



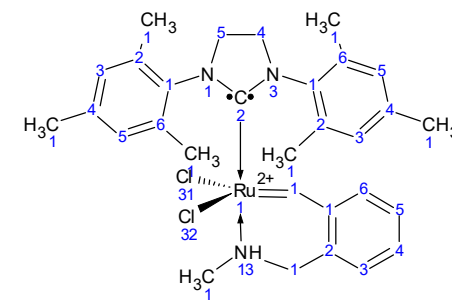
Acquisition Time (sec)	2.5690	Comment	H1	Date	02 Oct 2018 18:46:24
Date Stamp	02 Oct 2018 18:46:24				
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ Grubbs 1 NHMe 002001r				
Frequency (MHz)	300.13	Nucleus	1H	Number of Transients	32
Original Points Count	65536	Owner	nmr	Points Count	262144
Receiver Gain	72.88	SW(cyclical) (Hz)	25510.20	Solvent	DICHLOROMETHANE-d2
Spectrum Offset (Hz)	1350.5919	Sweep Width (Hz)	25510.11	Temperature (degree C)	30.010



11c

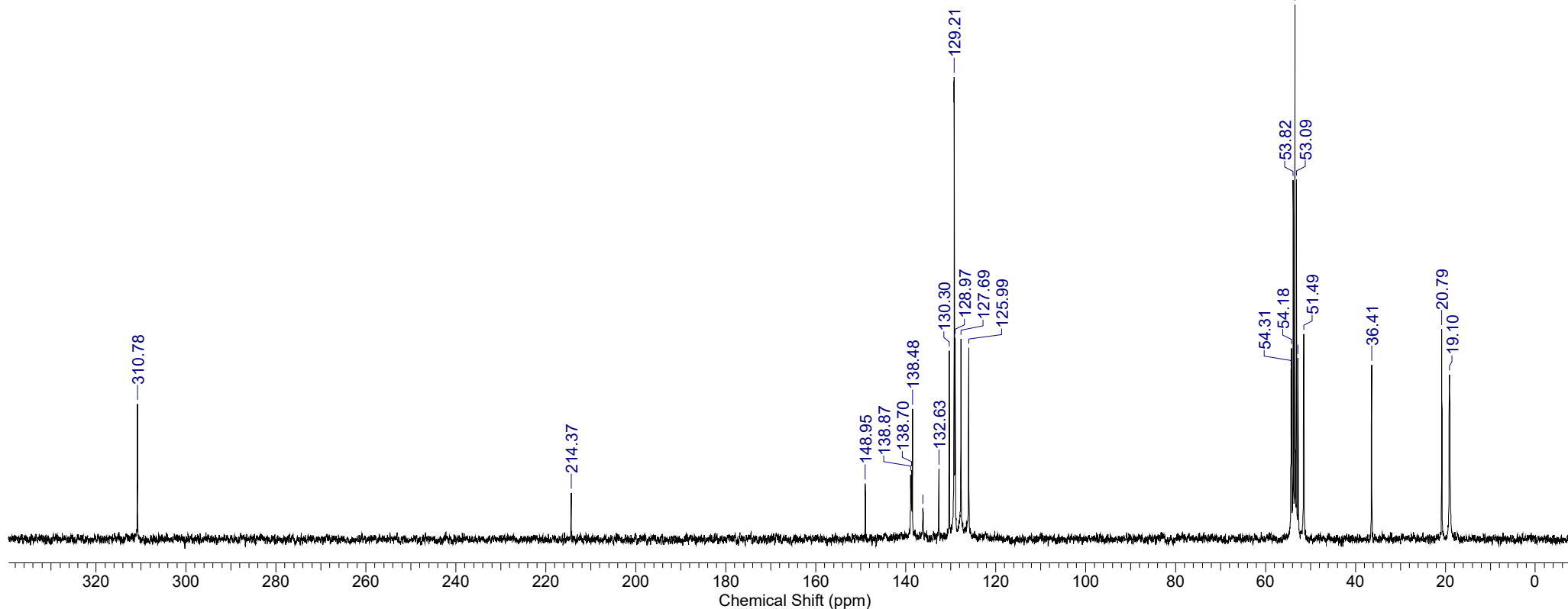


Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 1-K4-C13dec [hp-dec]			Date	02 Oct 2018 17:53:04
Date Stamp	02 Oct 2018 17:53:04						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs 1 NHMe 013001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	584	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zgpg
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.011		

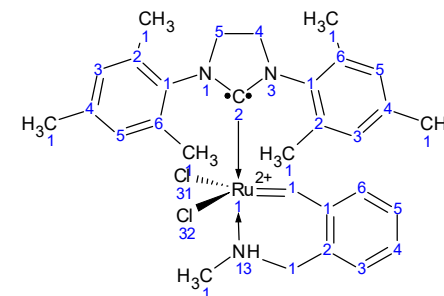


11c

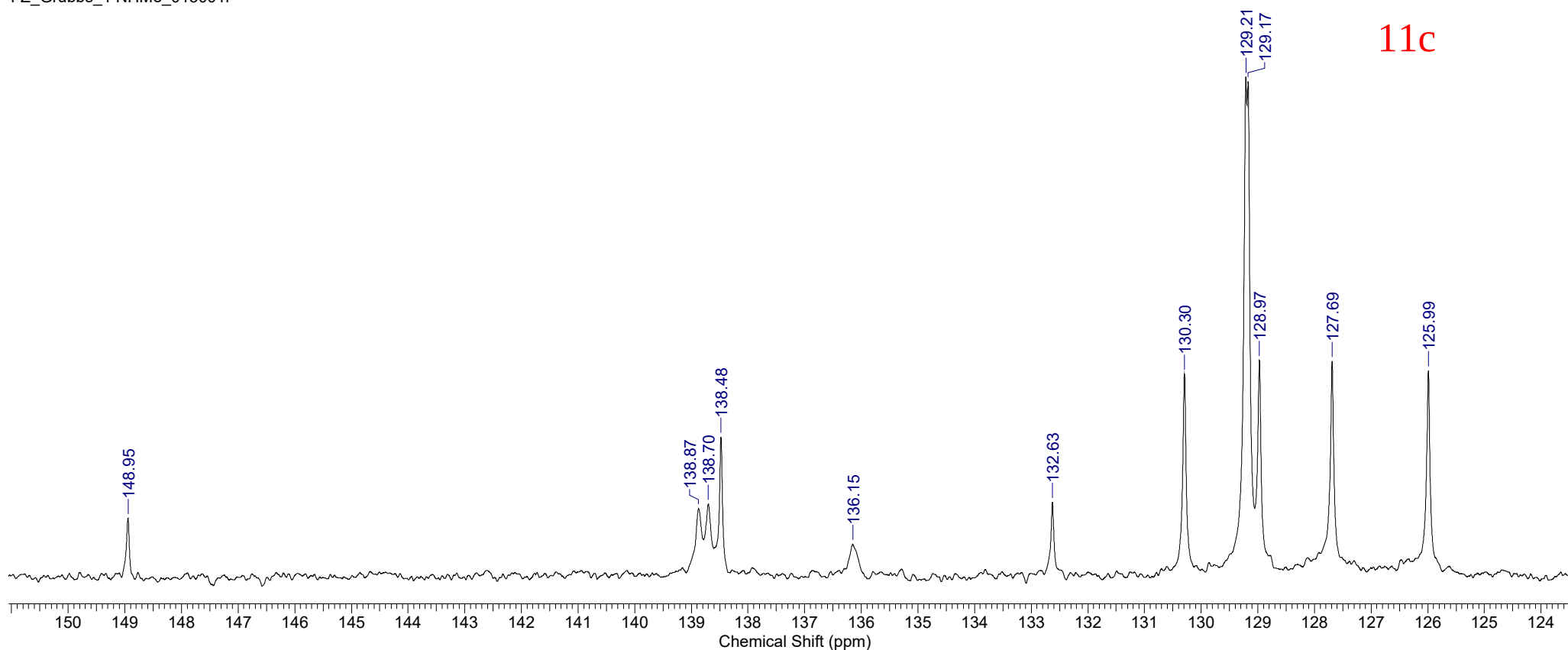
FZ_Grubbs_1 NHMe_013001r



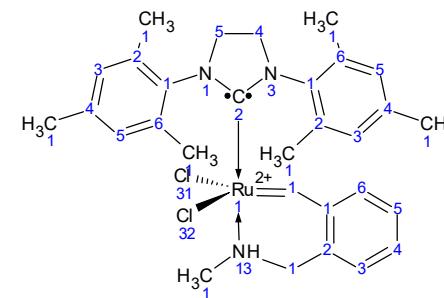
Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 1-K4-C13dec [hp-dec]			Date	02 Oct 2018 17:53:04
Date Stamp	02 Oct 2018 17:53:04						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs 1 NHMe 013001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	584	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zgpg
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.011		



FZ_Grubbs_1 NHMe_013001r

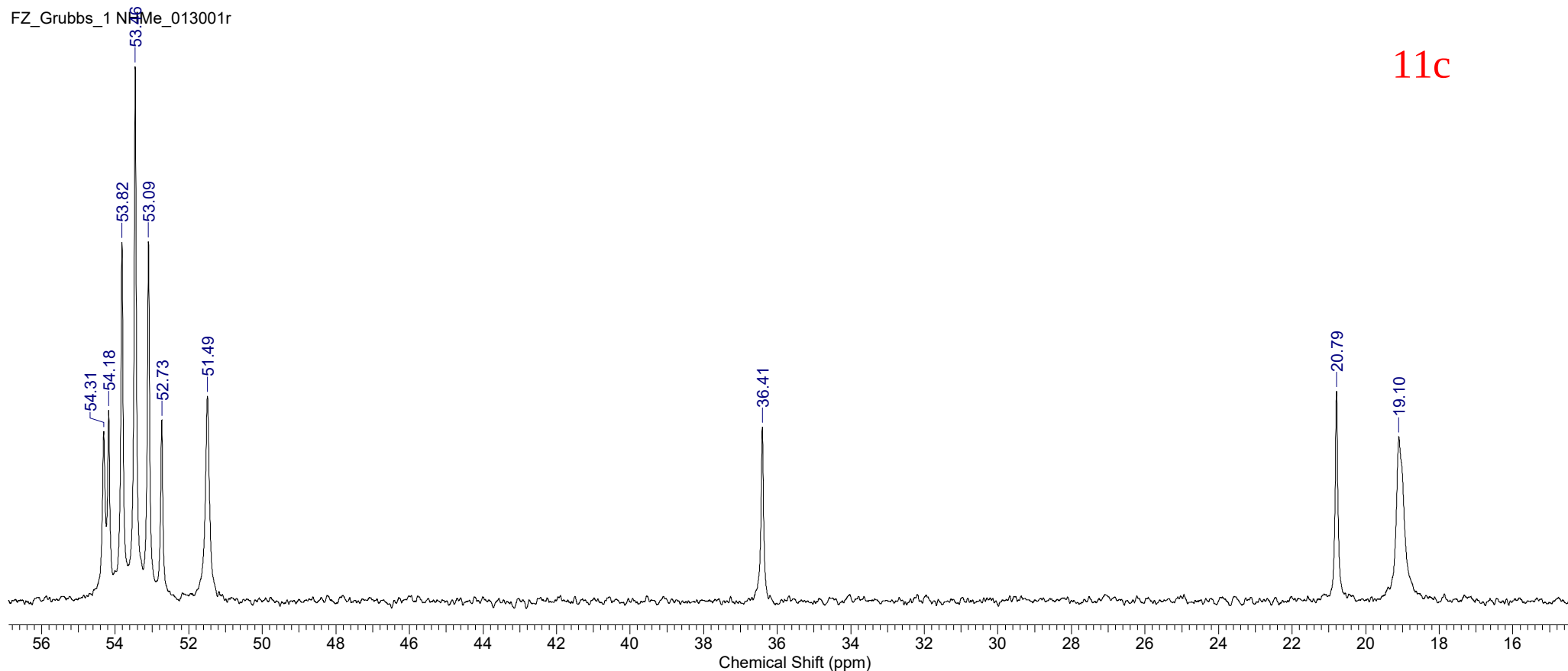


Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 1-K4-C13dec [hp-dec]			Date	02 Oct 2018 17:53:04
Date Stamp	02 Oct 2018 17:53:04						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs 1 NHMe_013001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	584	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zgpg
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.011		

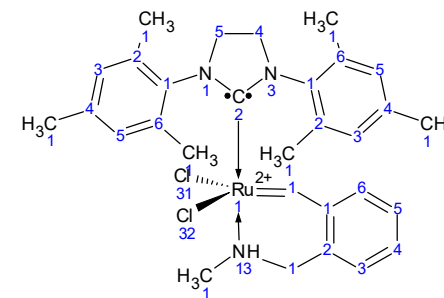


11c

FZ_Grubbs_1 NHMe_013001r

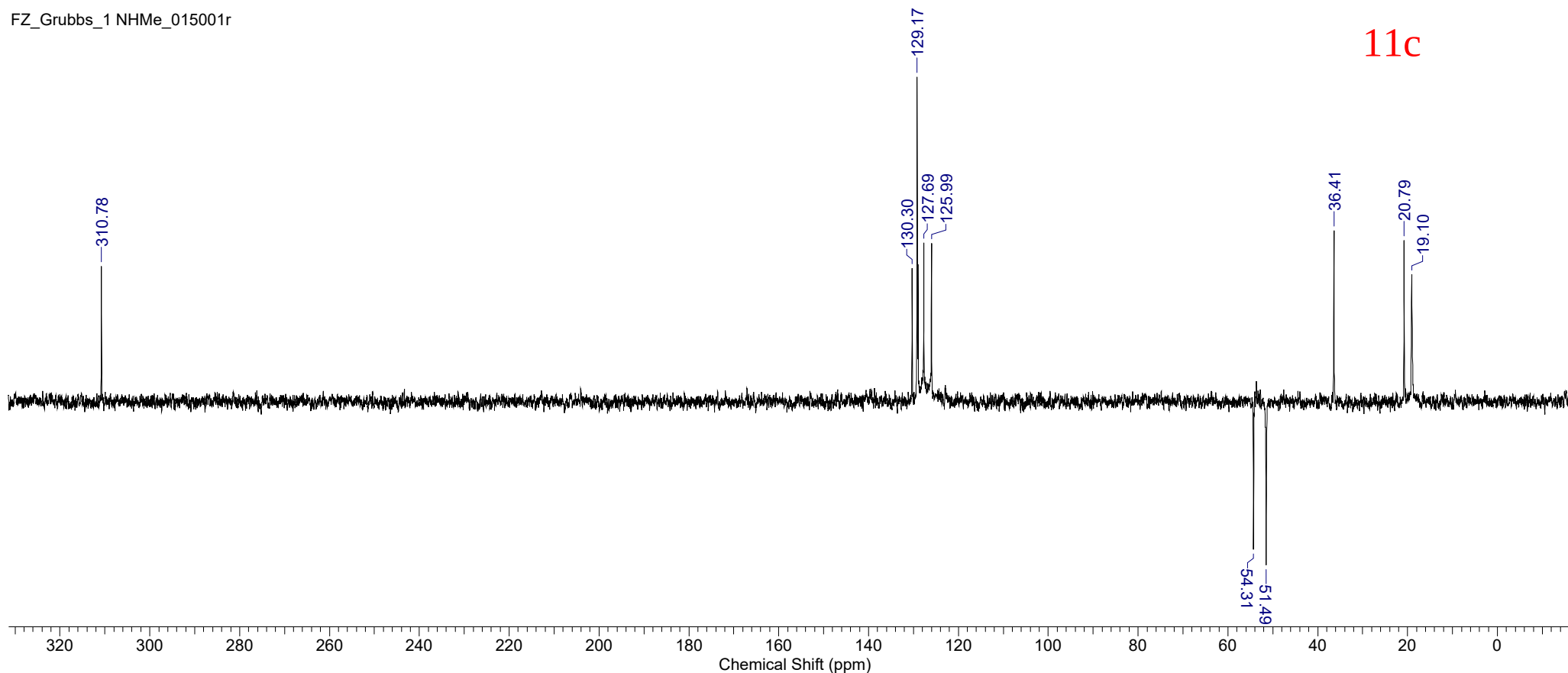


Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 1-K4-dept135 [hp-dec]		Date	02 Oct 2018 18:18:40	
Date Stamp	02 Oct 2018 18:18:40						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs 1 NHMe_015001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	184	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	dept135
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.012		

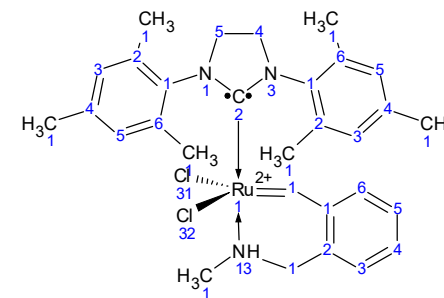


11c

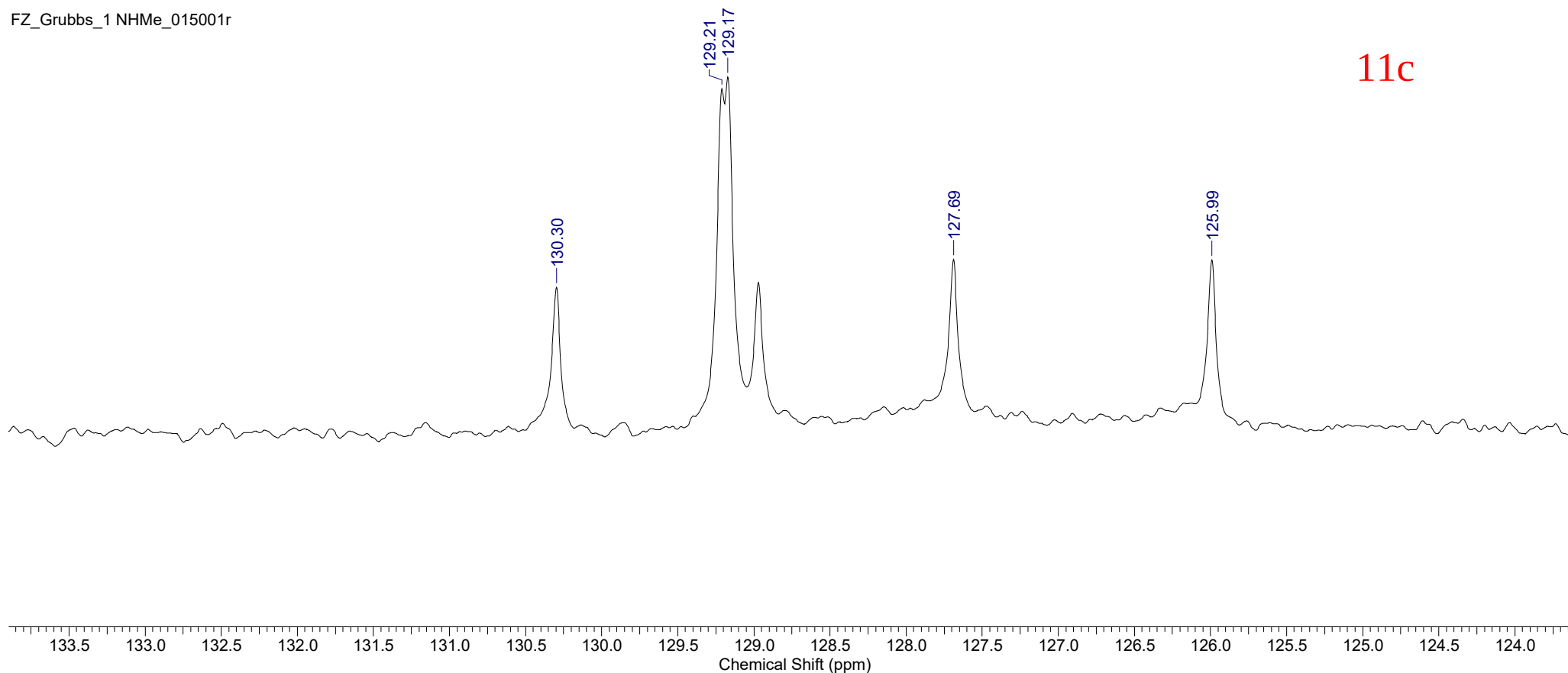
FZ_Grubbs_1 NHMe_015001r



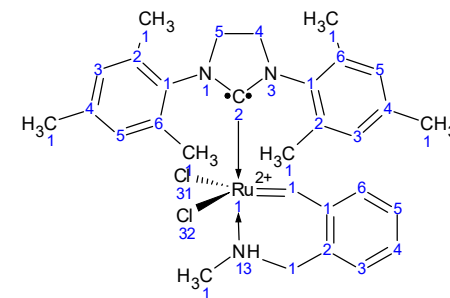
Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 1-K4-dept135 [hp-dec]			Date	02 Oct 2018 18:18:40
Date Stamp	02 Oct 2018 18:18:40						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs 1 NHMe 015001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	184	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	dept135
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.012		



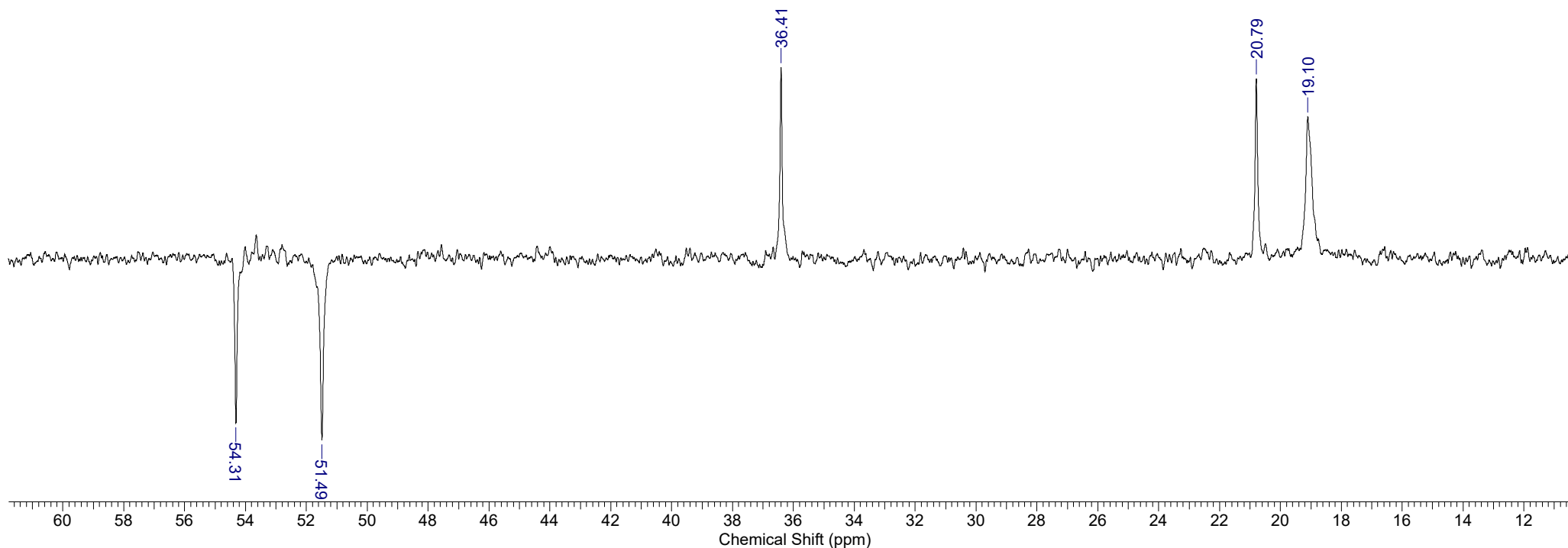
FZ_Grubbs_1 NHMe_015001r



Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 1-K4-dept135 [hp-dec]		Date	02 Oct 2018 18:18:40	
Date Stamp	02 Oct 2018 18:18:40						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs 1 NHMe_015001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	184	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	dept135
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.012		



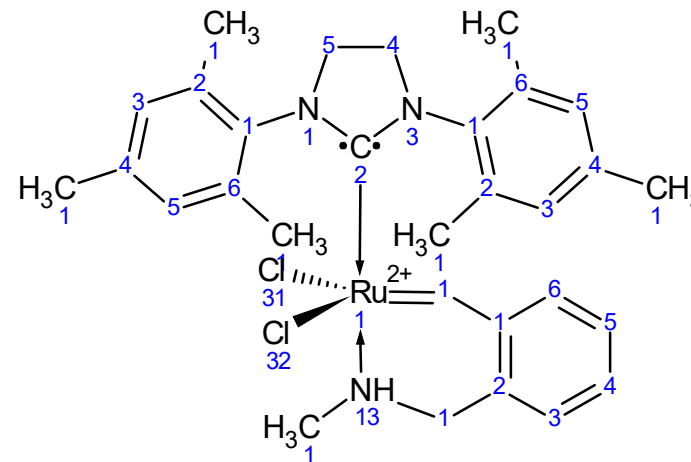
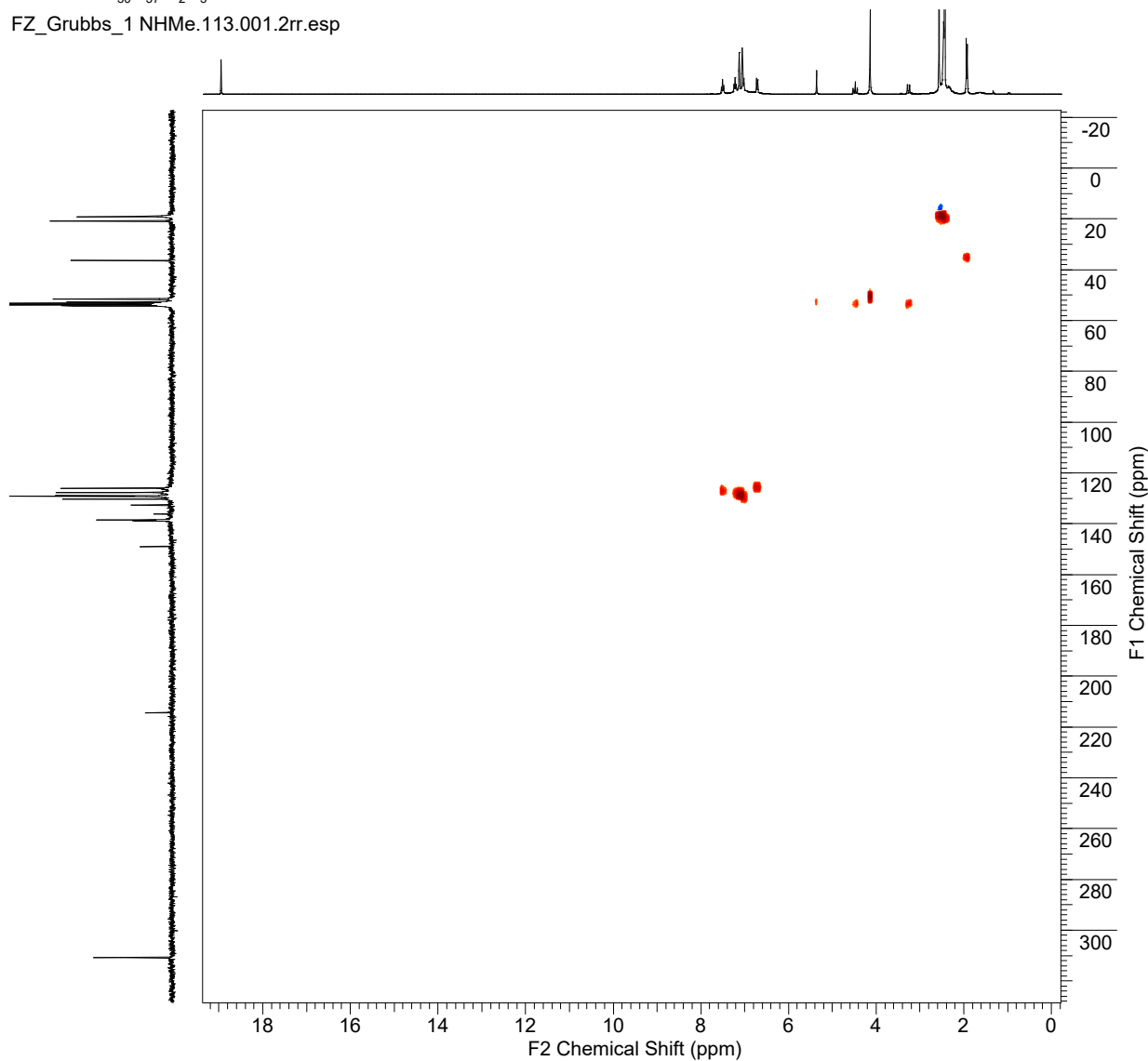
11c



Acquisition Time (sec)	(0.3408, 0.0069)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	02 Oct 2018 21:38:58					
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs_1 NHMe\113\data\1\2rr					
Frequency (MHz)	(300.13, 75.48)	Nucleus	(1H, 13C)	Number of Transients	2	
Origin	spect	Original Points Count	(3072, 233)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	hsqcetgp	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	29.985	Title	FZ_Grubbs_1-K4-HSQC [hp-dec]	

Formula C ₃₀ H ₃₇ Cl ₂ N ₂ Ru	FW 611.6098
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FZ_Grubbs_1 NHMe.113.001.2rr.esp

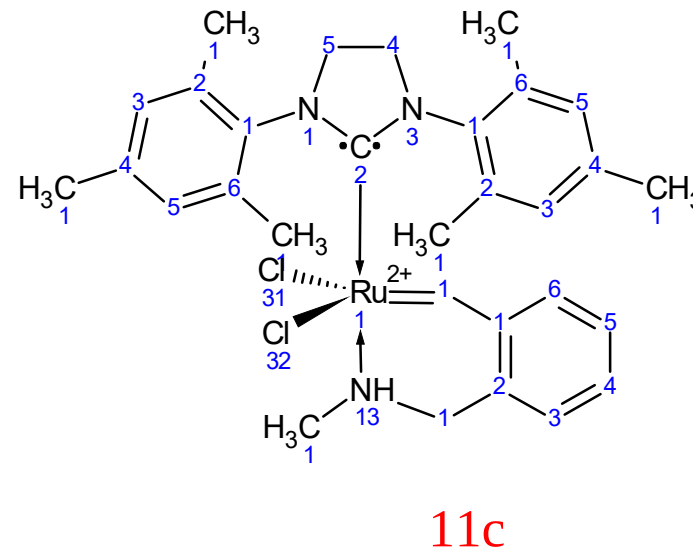
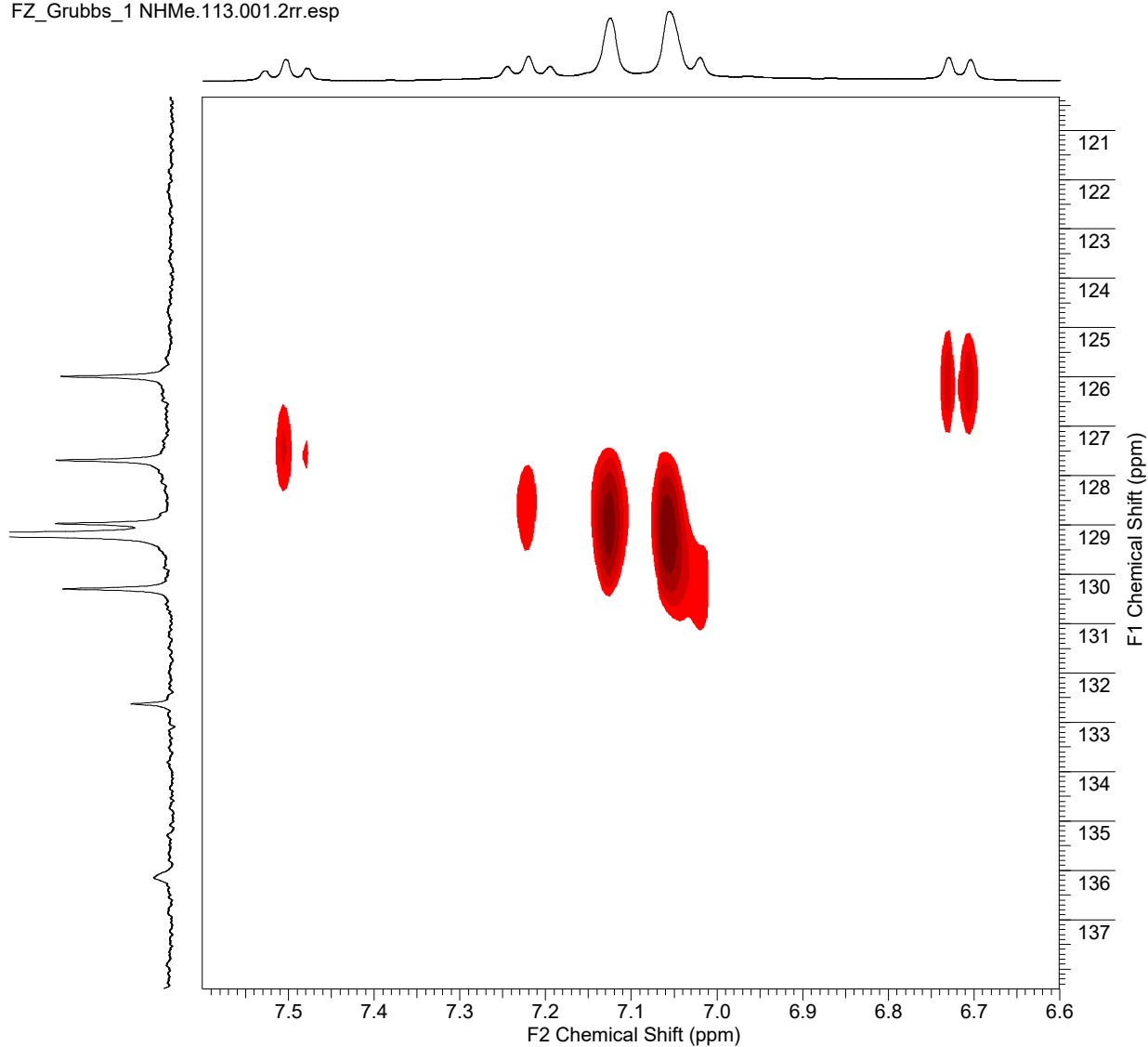


11c

Acquisition Time (sec)	(0.3408, 0.0069)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345		
Date	02 Oct 2018 21:38:58				
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs_1 NHMe\113\data\12rr				
Frequency (MHz)	(300.13, 75.48)	Nucleus	(1H, 13C)	Number of Transients	2
Origin	spect	Original Points Count	(3072, 233)	Owner	nmr
Points Count	(8192, 2048)	Pulse Sequence	hsqcetgp	Solvent	CD2Cl2
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	29.985	Title	FZ_Grubbs_1-K4-HSQC [hp-dec]

Formula C ₃₀ H ₃₇ Cl ₂ N ₂ Ru	FW 611.6098
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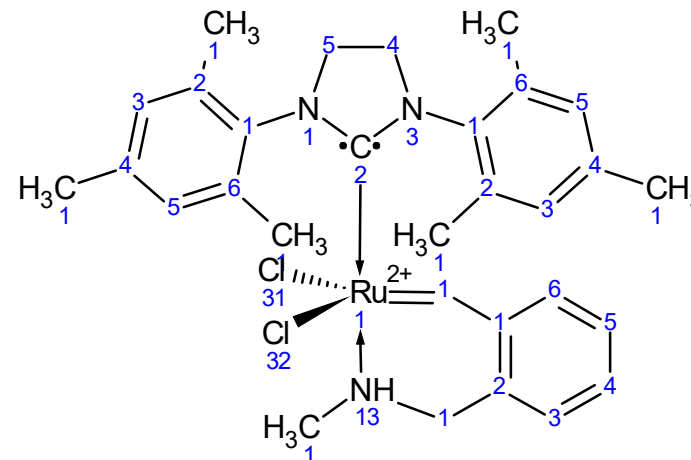
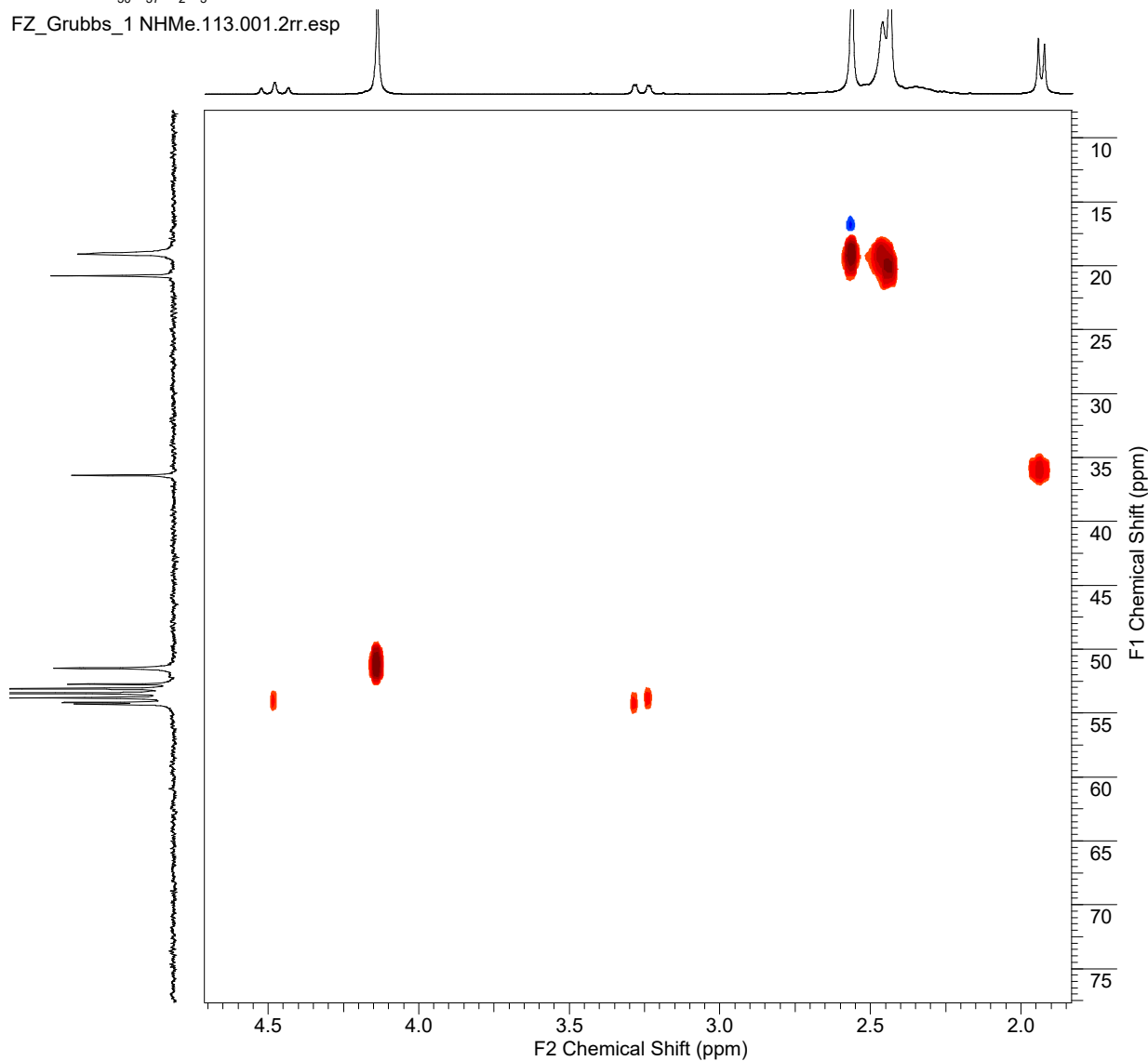
FZ_Grubbs_1 NHMe.113.001.2rr.esp



Acquisition Time (sec)	(0.3408, 0.0069)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	02 Oct 2018 21:38:58					
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\FZ_Grubbs_1 NHMe\113\data\1\2rr					
Frequency (MHz)	(300.13, 75.48)	Nucleus	(1H, 13C)	Number of Transients	2	
Origin	spect	Original Points Count	(3072, 233)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	hsqcetgp	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	29.985	Title	FZ_Grubbs_1-K4-HSQC [hp-dec]	

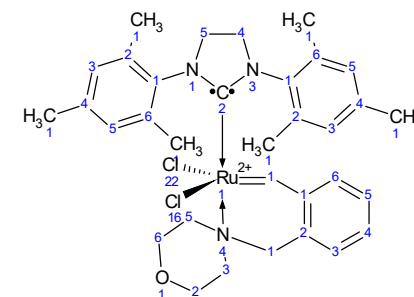
Formula C ₃₀ H ₃₇ Cl ₂ N ₂ Ru	FW 611.6098
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FZ_Grubbs_1 NHMe.113.001.2rr.esp

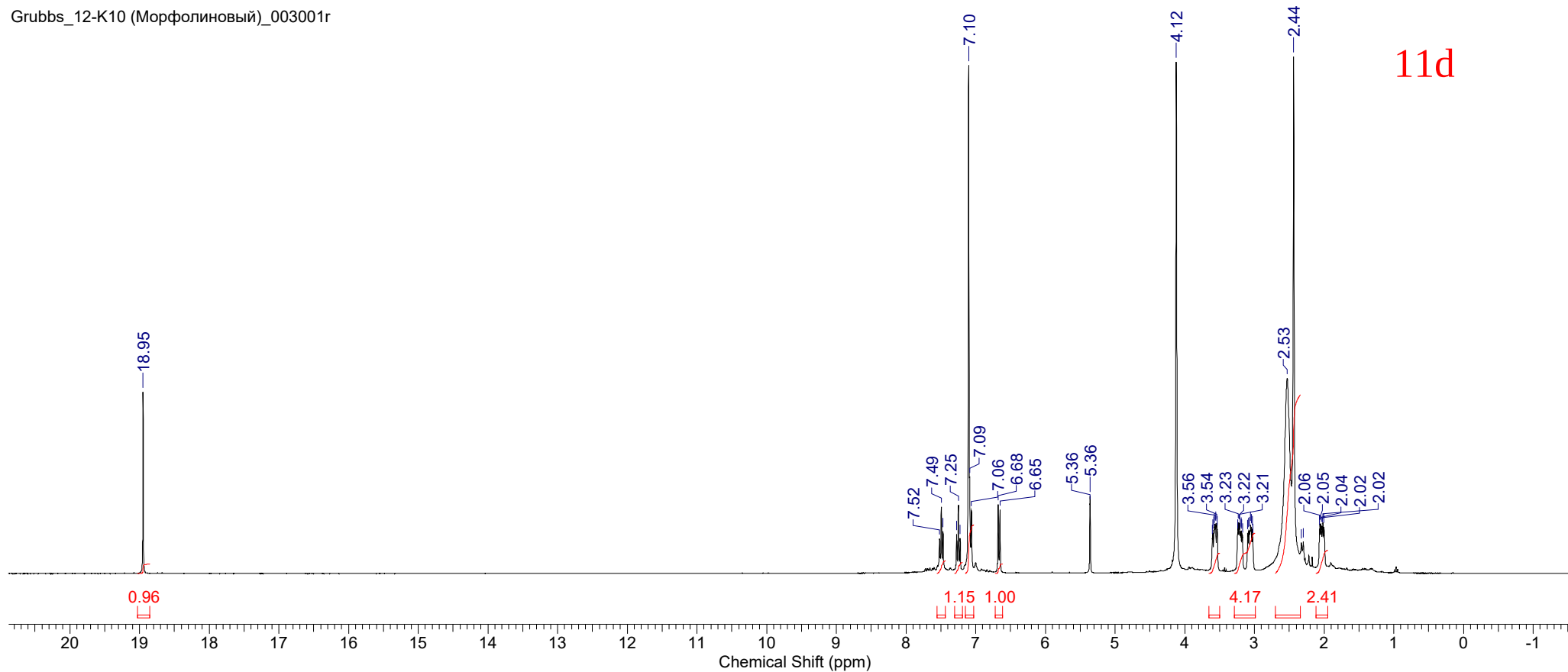


11c

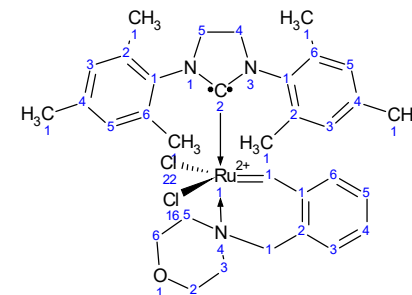
Acquisition Time (sec)	2.5690	Comment	H1	Date	02 Oct 2018 14:56:00		
Date Stamp	02 Oct 2018 14:56:00						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 12-K10 (Морфолиновый) 003001r						
Frequency (MHz)	300.13	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zg
Receiver Gain	36.14	SW(cyclical) (Hz)	25510.20	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	1350.5919	Sweep Width (Hz)	25510.11	Temperature (degree C)	30.008		



Grubbs_12-K10 (Морфолиновый)_003001r

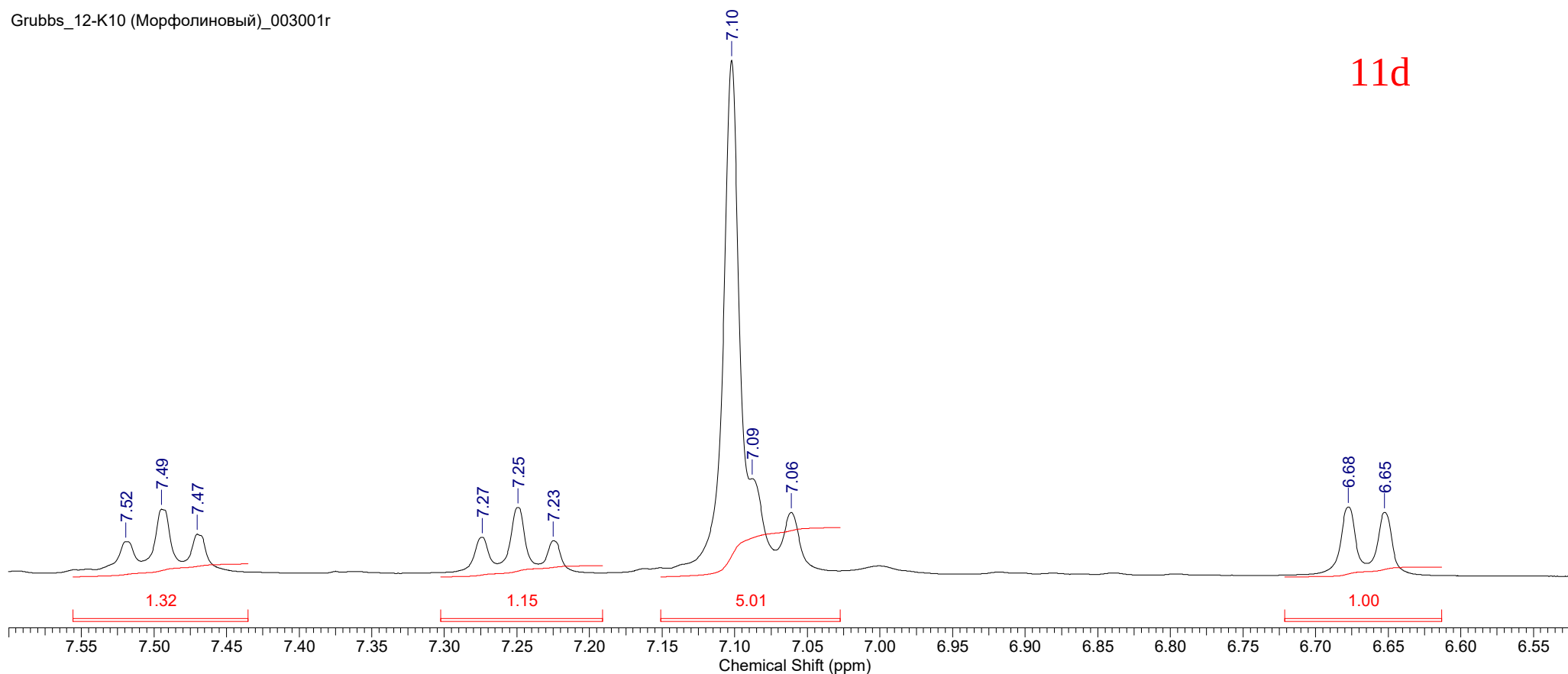


Acquisition Time (sec)	2.5690	Comment	H1	Date	02 Oct 2018 14:56:00		
Date Stamp	02 Oct 2018 14:56:00						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 12-K10 (Морфолиновый) 003001r						
Frequency (MHz)	300.13	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zg
Receiver Gain	36.14	SW(cyclical) (Hz)	25510.20	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	1350.5919	Sweep Width (Hz)	25510.11	Temperature (degree C)	30.008		

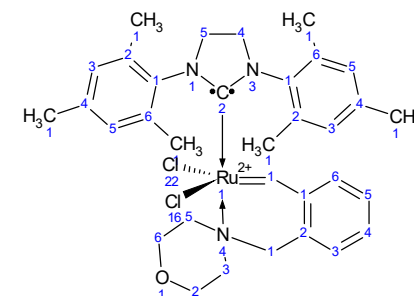


Grubbs_12-K10 (Морфолиновый)_003001r

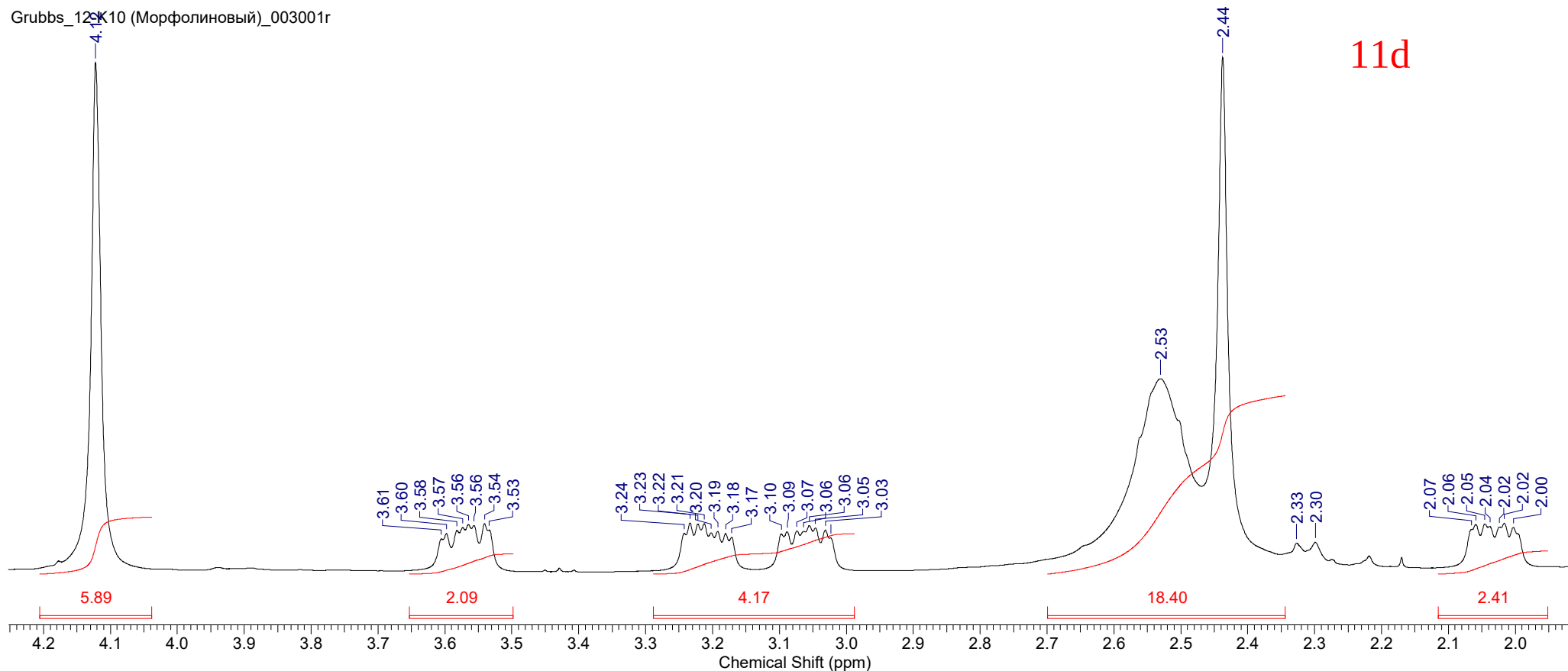
11d



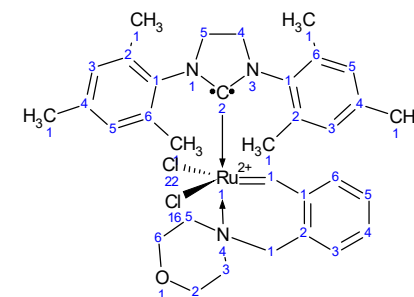
Acquisition Time (sec)	2.5690	Comment	H1	Date	02 Oct 2018 14:56:00		
Date Stamp	02 Oct 2018 14:56:00						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 12-K10 (Морфолиновый) 003001r						
Frequency (MHz)	300.13	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zg
Receiver Gain	36.14	SW(cyclical) (Hz)	25510.20	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	1350.5919	Sweep Width (Hz)	25510.11	Temperature (degree C)	30.008		



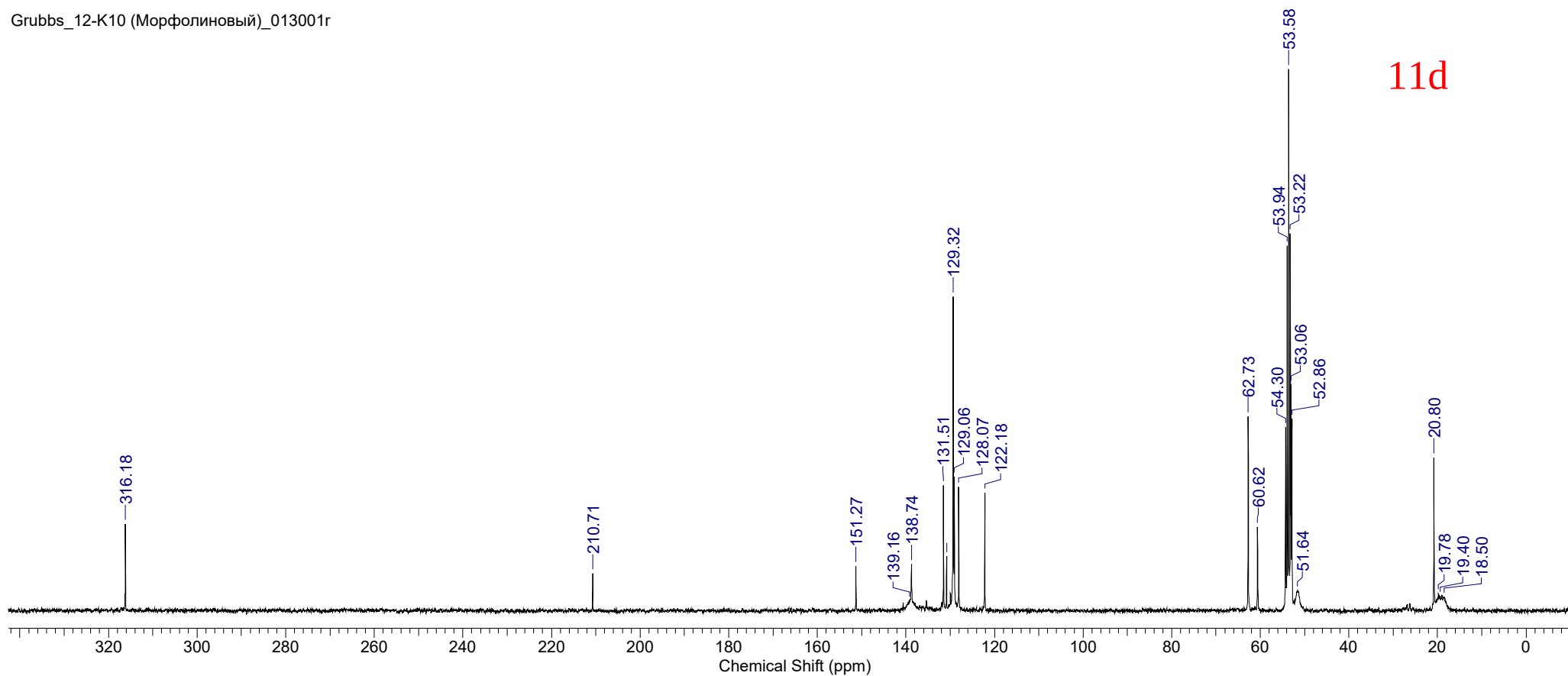
11d



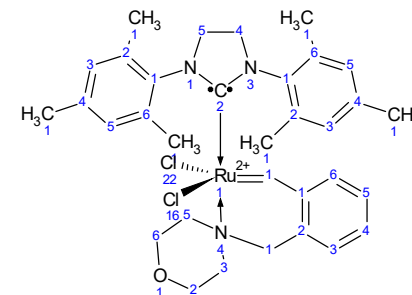
Acquisition Time (sec)	1.1010	Comment	FZ_Grubbs_12-K10-C13dec [hp-dec]	Date	02 Oct 2018 12:50:08
Date Stamp	02 Oct 2018 12:50:08				
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_12-K10 (Морфолиновый)_013001r				
Frequency (MHz)	75.47	Nucleus	¹³ C	Number of Transients	800
Original Points Count	65536	Owner	nmr	Points Count	262144
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.005



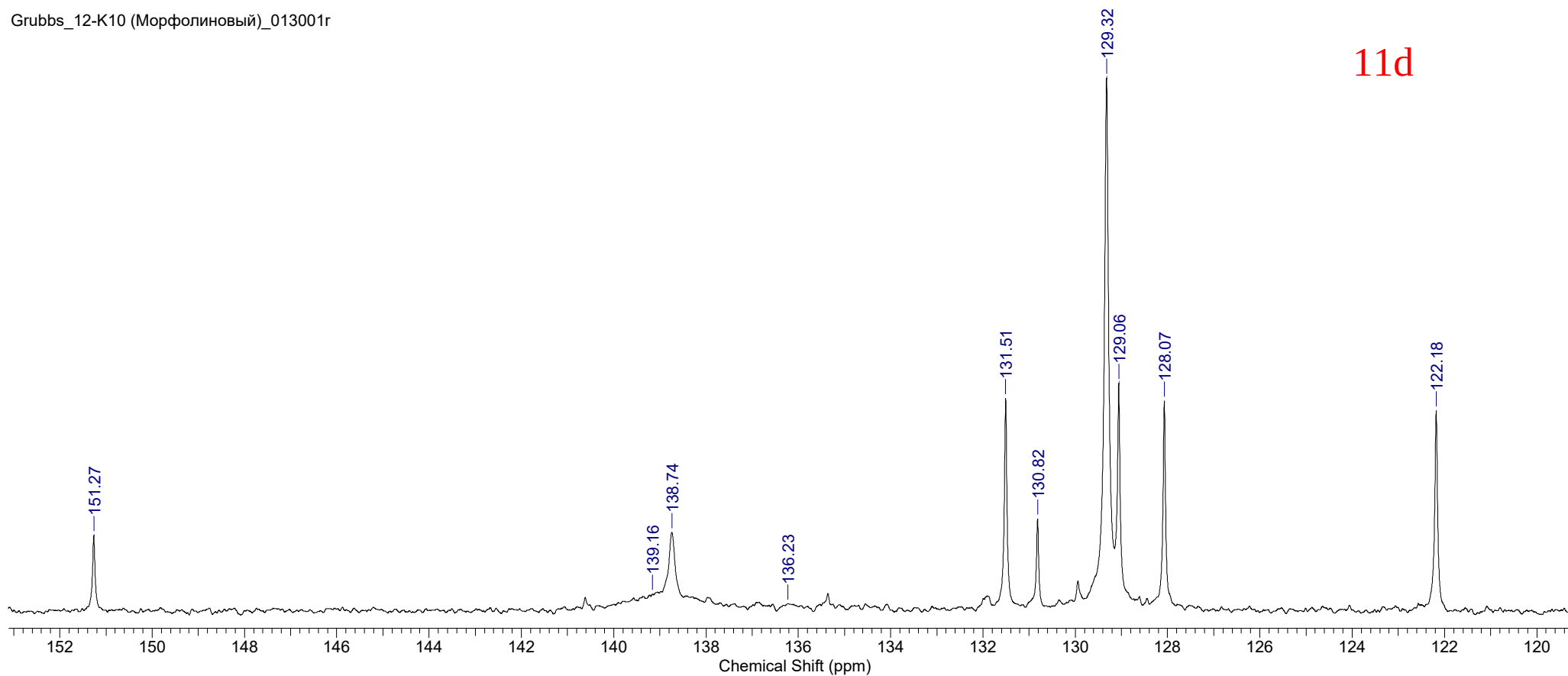
Grubbs_12-K10 (Морфолиновый)_013001r



Acquisition Time (sec)	1.1010	Comment	FZ_Grubbs_12-K10-C13dec [hp-dec]			Date	02 Oct 2018 12:50:08
Date Stamp	02 Oct 2018 12:50:08						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_12-K10 (Морфолиновый)_013001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	800	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zgpg
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.005		

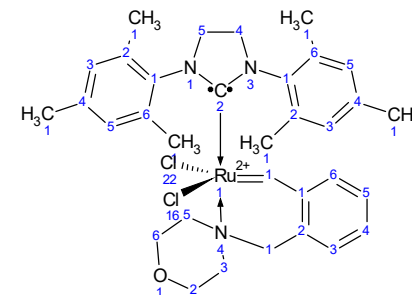


Grubbs_12-K10 (Морфолиновый)_013001r

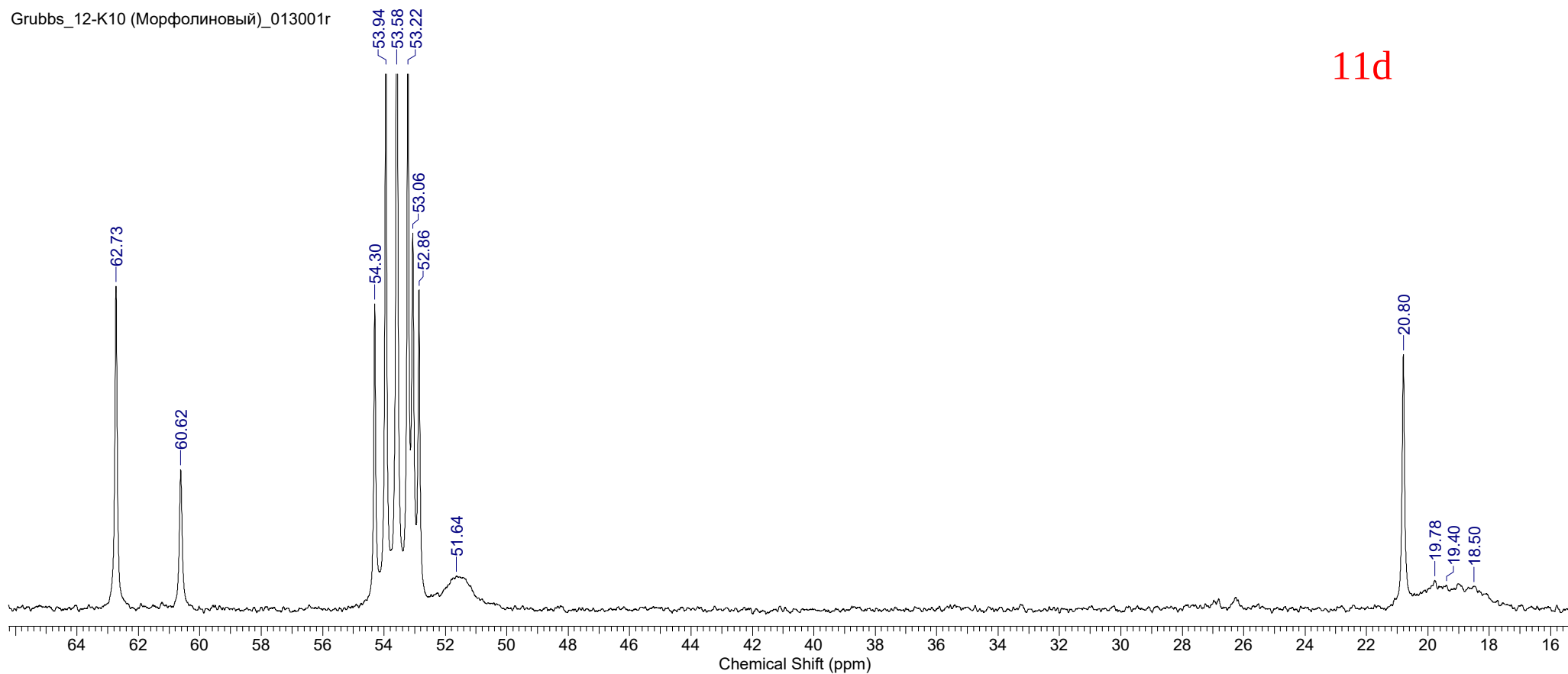


11d

Acquisition Time (sec)	1.1010	Comment	FZ_Grubbs_12-K10-C13dec [hp-dec]		Date	02 Oct 2018 12:50:08	
Date Stamp	02 Oct 2018 12:50:08						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_12-K10 (Морфолиновый)_013001r						
Frequency (MHz)	75.47	Nucleus	¹³ C	Number of Transients	800	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zgpg
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.005		

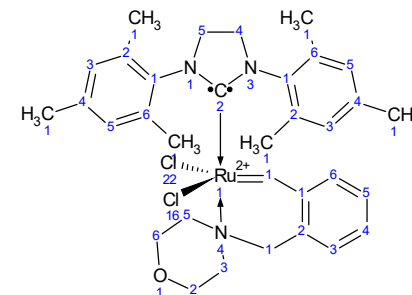


Grubbs_12-K10 (Морфолиновый)_013001r

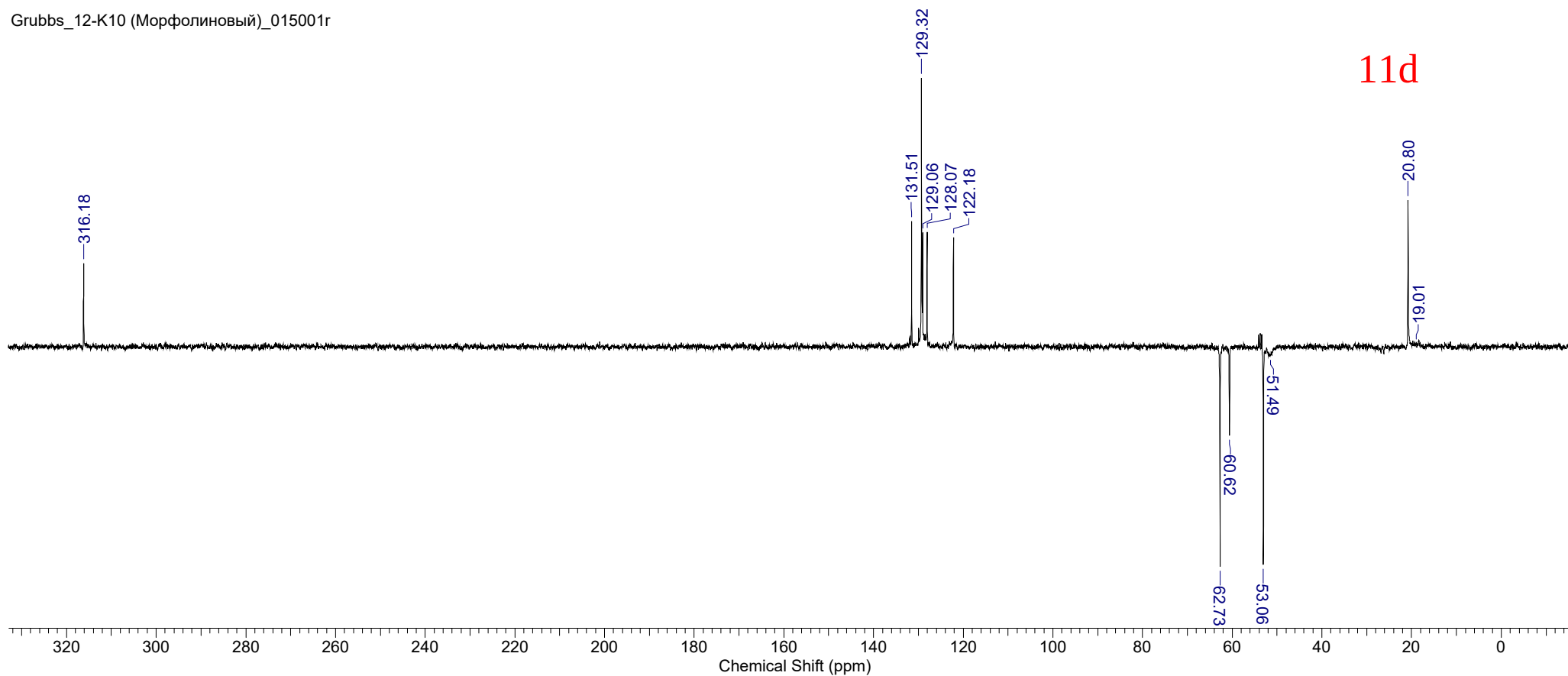


11d

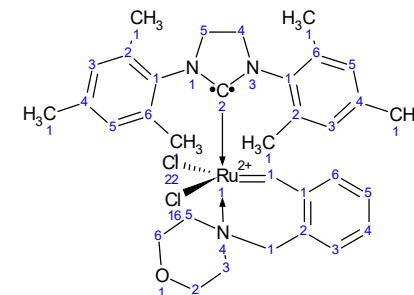
Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 12-K10-dept135 [hp-dec]		Date	02 Oct 2018 15:00:16	
Date Stamp	02 Oct 2018 15:00:16						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 12-K10 (Морфолиновый) 015001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	360	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	dept135
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	29.989		



Grubbs_12-K10 (Морфолиновый)_015001r

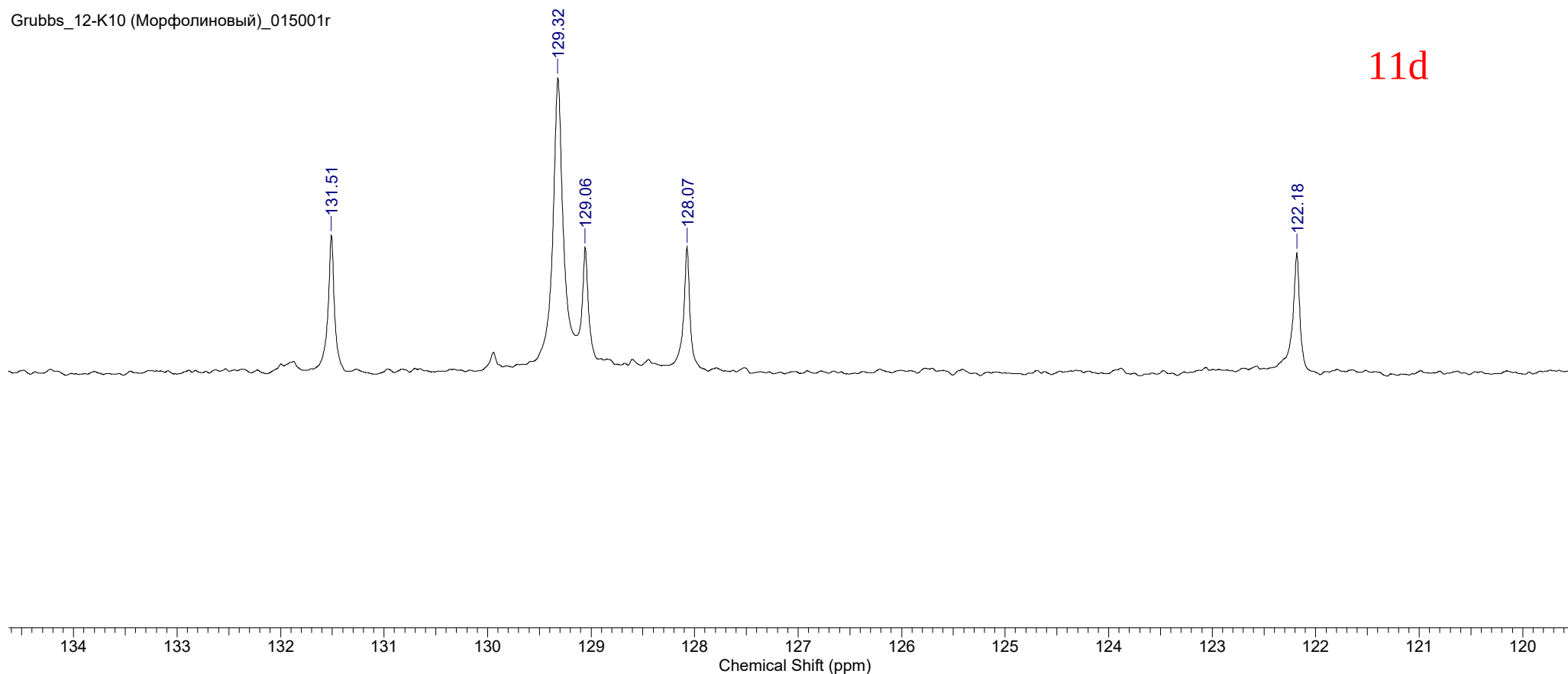


Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 12-K10-dept135 [hp-dec]			Date	02 Oct 2018 15:00:16
Date Stamp	02 Oct 2018 15:00:16						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 12-K10 (Морфолиновый)_015001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	360	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	dept135
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	29.989		

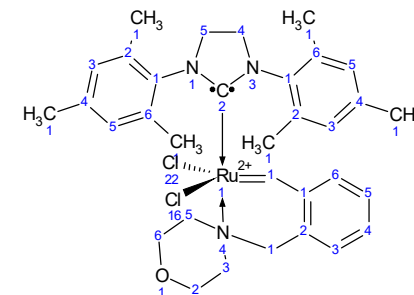


11d

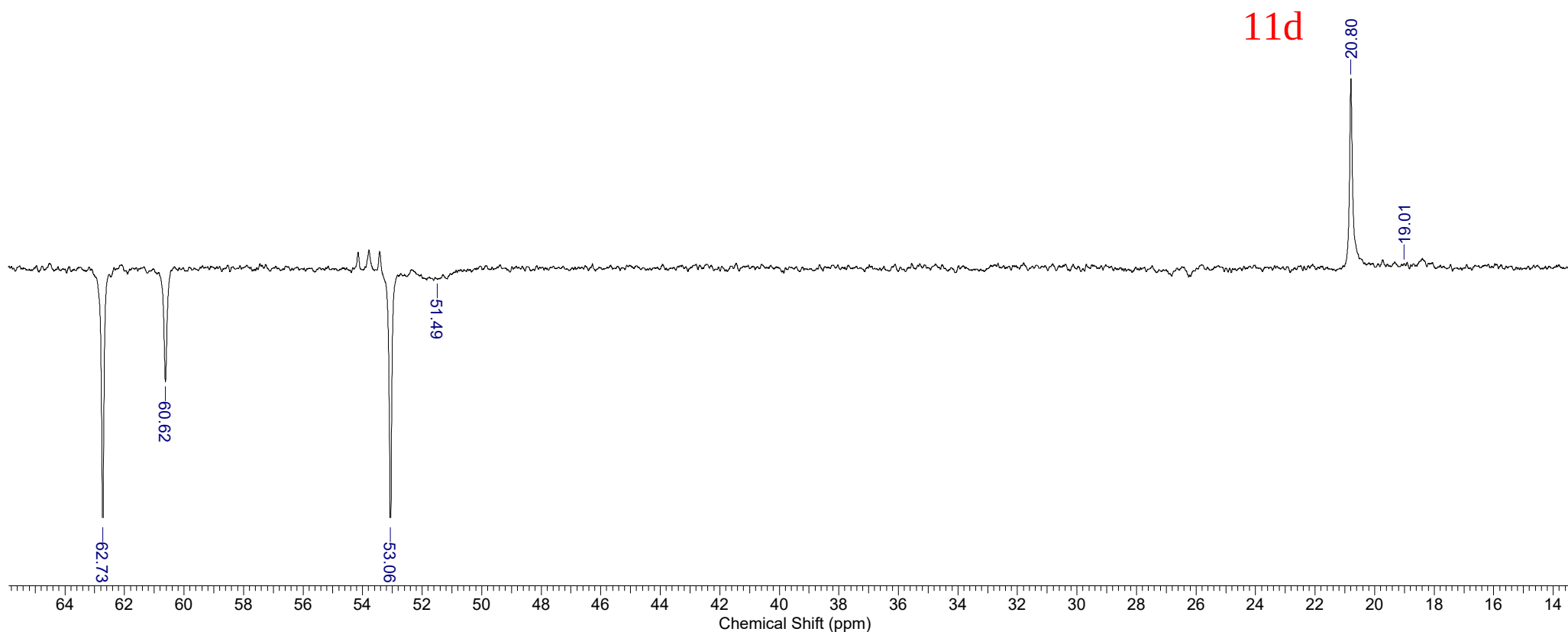
Grubbs_12-K10 (Морфолиновый)_015001r



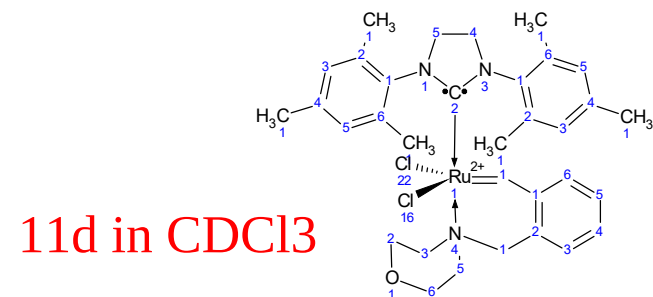
Acquisition Time (sec)	1.1010	Comment	FZ Grubbs 12-K10-dept135 [hp-dec]		Date	02 Oct 2018 15:00:16	
Date Stamp	02 Oct 2018 15:00:16						
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs 12-K10 (Морфолиновый) 015001r						
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	360	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	dept135
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	DICHLOROMETHANE-d2		
Spectrum Offset (Hz)	7546.7783	Sweep Width (Hz)	59523.58	Temperature (degree C)	29.989		



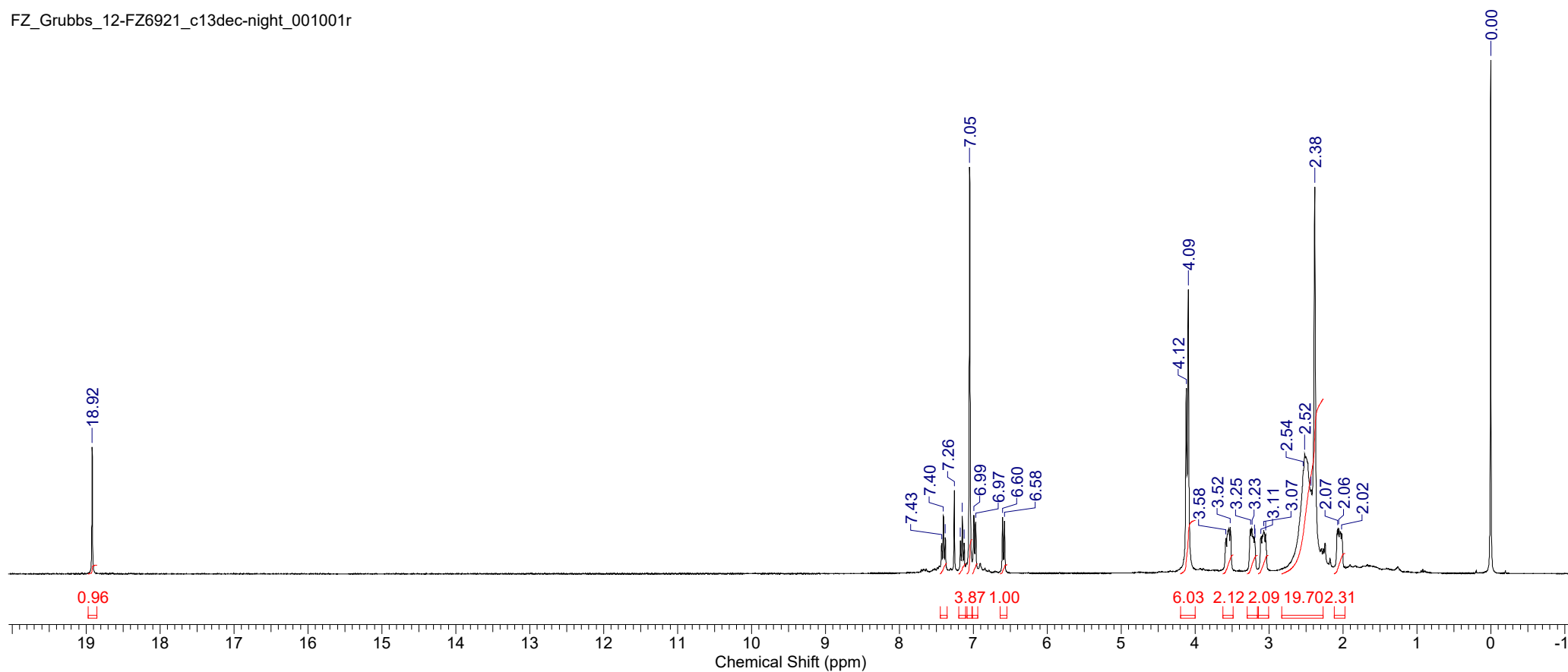
Grubbs_12-K10 (Морфолиновый)_015001r



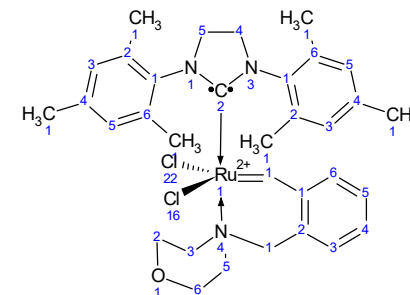
Acquisition Time (sec)	2.5690	Comment	FZ_Grubbs_12-FZ6921 (cyclo){-Ru[SiMes]Cl ₂ =CH-C ₆ H ₄ -CH ₂ -N[-CH ₂ -CH ₂ -O-CH ₂ -CH ₂ -]-}		
Date	02 Nov 2018 19:01:20	Date Stamp	02 Nov 2018 19:01:20		
File Name	C:\Users\Fedor\Desktop\FZ_Grubbs_12-FZ6921_c13dec-night_001001r				Frequency (MHz) 300.13
Nucleus	¹ H	Number of Transients	26	Origin	spect
Owner	nmr	Points Count	262144	Pulse Sequence	zg
SW(cyclical) (Hz)	25510.20	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1342.4913
Temperature (degree C)	29.983			Sweep Width (Hz)	25510.11



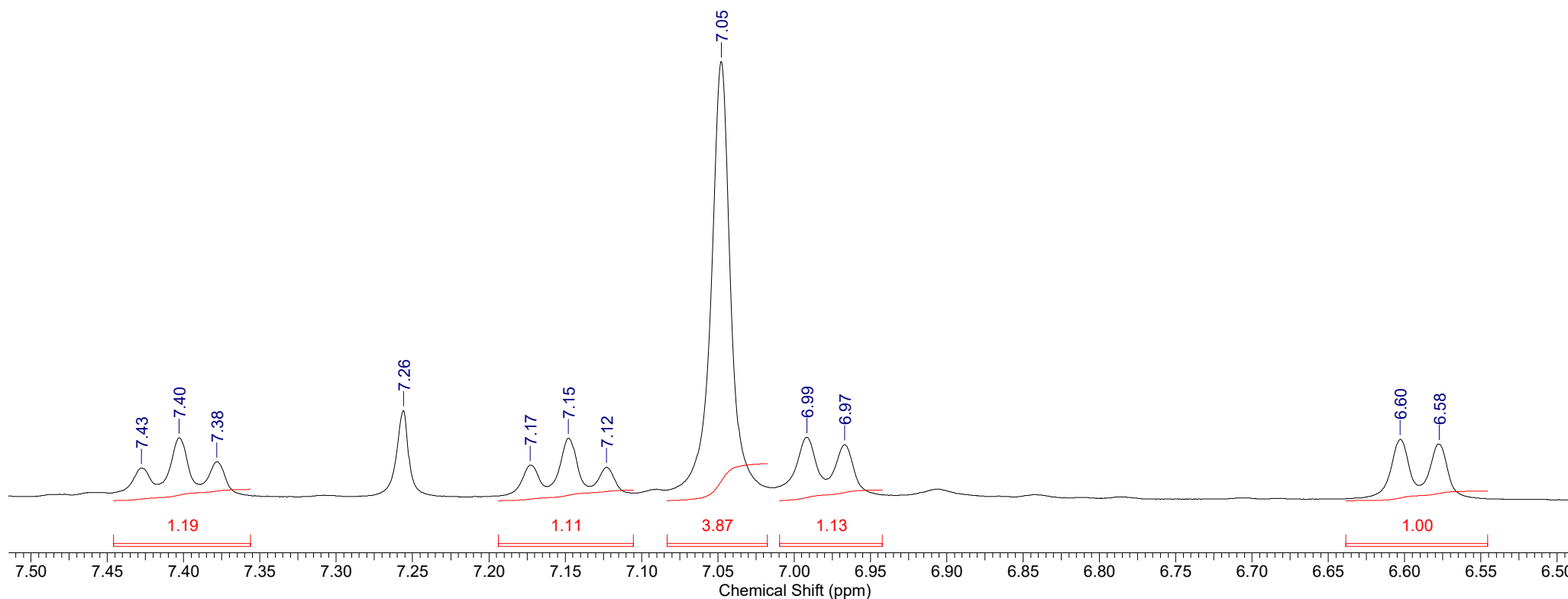
FZ_Grubbs_12-FZ6921_c13dec-night_001001r



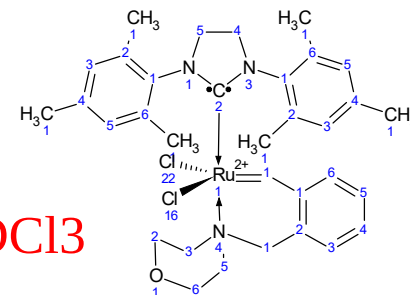
Acquisition Time (sec)	2.5690	Comment	FZ_Grubbs_12-FZ6921 (cyclo){-Ru[SiMes]Cl2=CH-C6H4-CH2-N[-CH2-CH2-O-CH2-CH2-]-}		
Date	02 Nov 2018 19:01:20	Date Stamp	02 Nov 2018 19:01:20		
File Name	C:\Users\Fedor\Desktop\FZ_Grubbs_12-FZ6921_c13dec-night_001001r				Frequency (MHz) 300.13
Nucleus	1H	Number of Transients	26	Origin spect	Original Points Count 65536
Owner	nmr	Points Count	262144	Pulse Sequence zg	Receiver Gain 130.70
SW(cyclical) (Hz)	25510.20	Solvent	CHLOROFORM-d	Spectrum Offset (Hz) 1342.4913	Sweep Width (Hz) 25510.11
Temperature (degree C)	29.983				



11d in CDCl₃

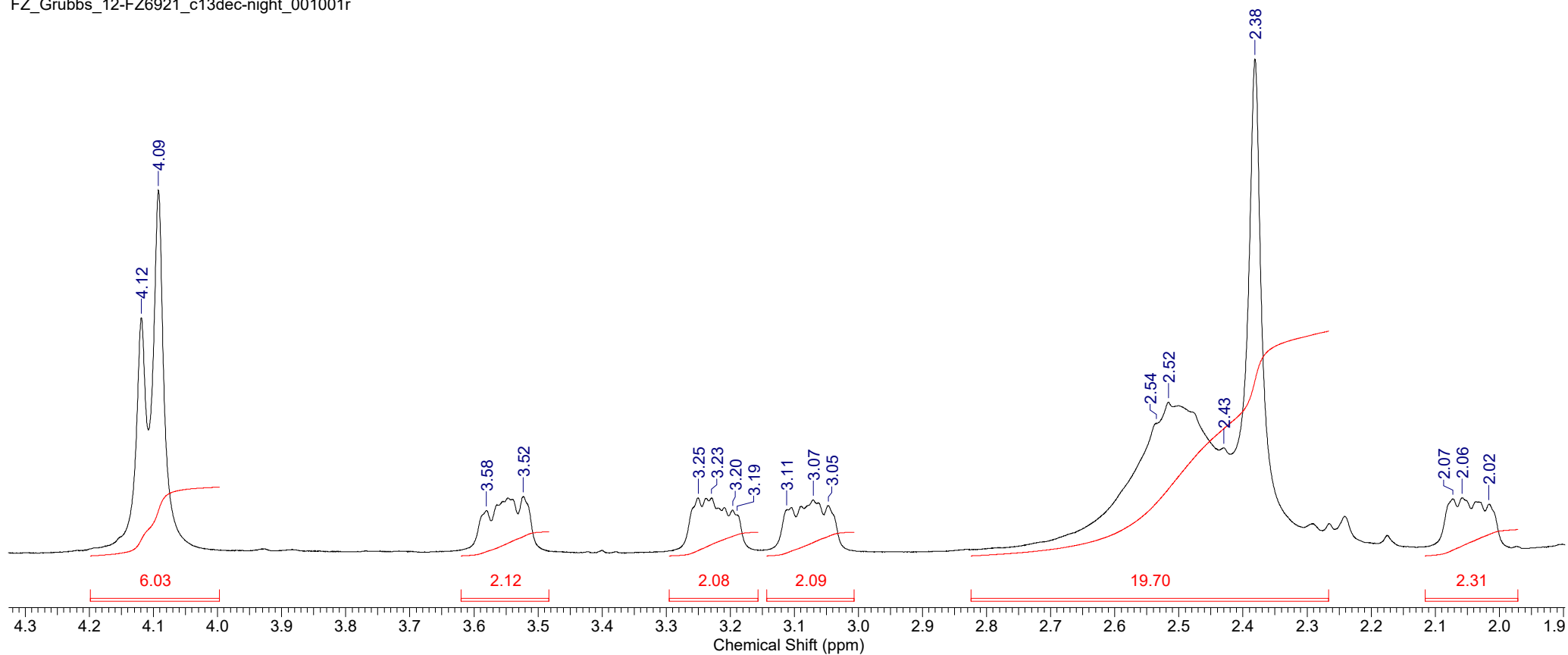


Acquisition Time (sec)	2.5690	Comment FZ_Grubbs_12-FZ6921 (cyclo){-Ru[SiMes]Cl ₂ =CH-C ₆ H ₄ -CH ₂ -N[-CH ₂ -CH ₂ -O-CH ₂ -CH ₂ -]}			
Date	02 Nov 2018 19:01:20	Date Stamp		02 Nov 2018 19:01:20	
File Name	C:\Users\Fedor\Desktop\FZ_Grubbs_12-FZ6921_c13dec-night_001001r	Frequency (MHz)			300.13
Nucleus	¹ H	Number of Transients	26	Origin	spect
Owner	nmr	Points Count	262144	Pulse Sequence	zg
SW(cyclical) (Hz)	25510.20	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	1342.4913
Temperature (degree C)	29.983	Sweep Width (Hz)			25510.11

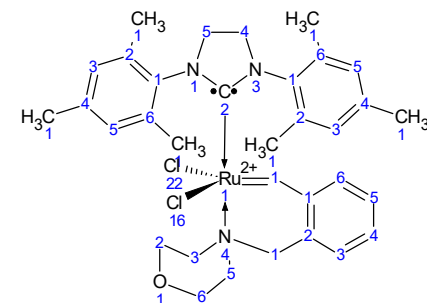


11d in CDCl₃

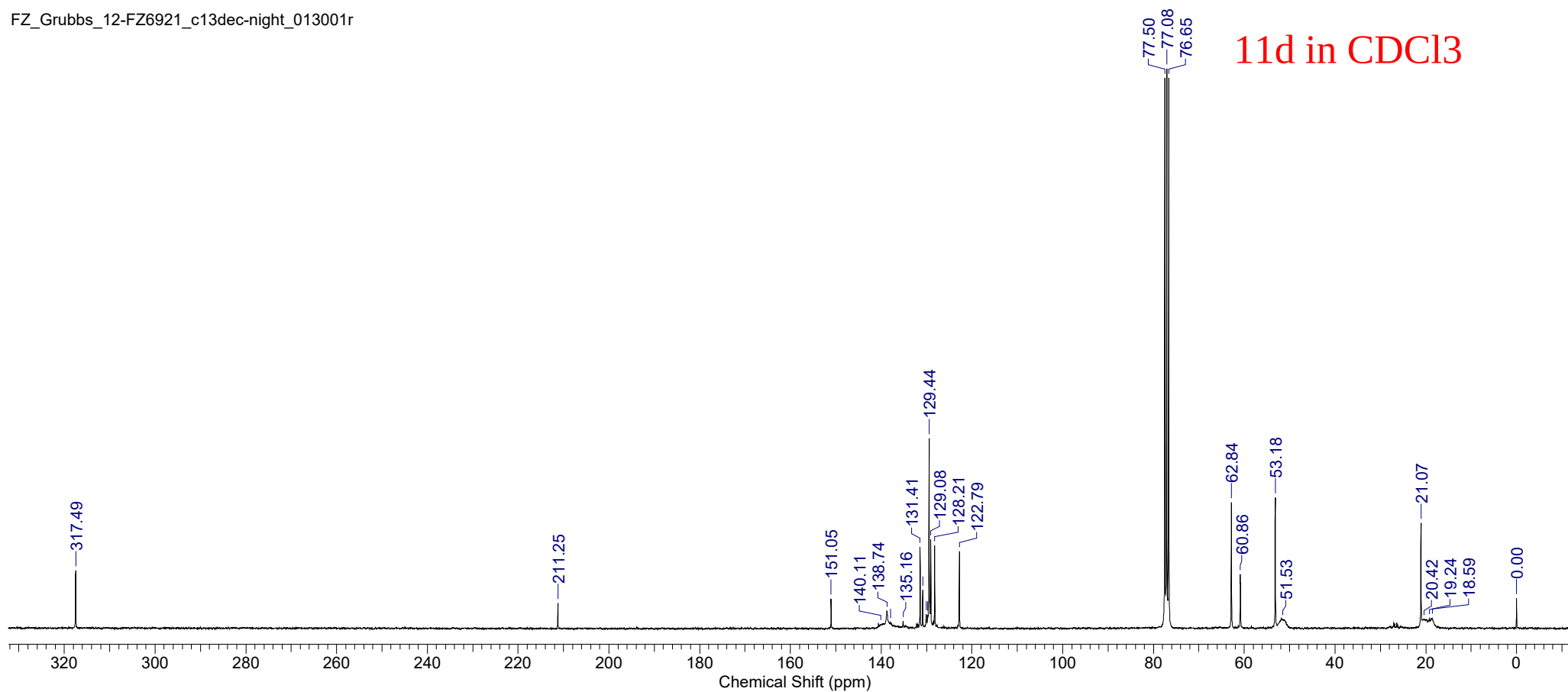
FZ_Grubbs_12-FZ6921_c13dec-night_001001r



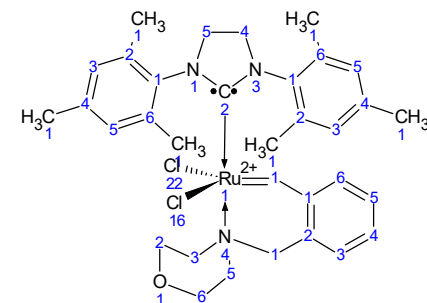
Acquisition Time (sec)	1.1010	Comment	FZ_Grubbs_12-K10-C13dec [hp-dec] [night]	Date	02 Nov 2018 19:07:44
Date Stamp	02 Nov 2018 19:07:44	File Name	C:\Users\Fedor\Desktop\FZ_Grubbs_12-FZ6921_c13dec-night_013001r		
Frequency (MHz)	75.47	Nucleus	¹³ C	Number of Transients	24608
Original Points Count	65536	Owner	nmr	Points Count	262144
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	7547.7637	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.040



FZ_Grubbs_12-FZ6921_c13dec-night_013001r

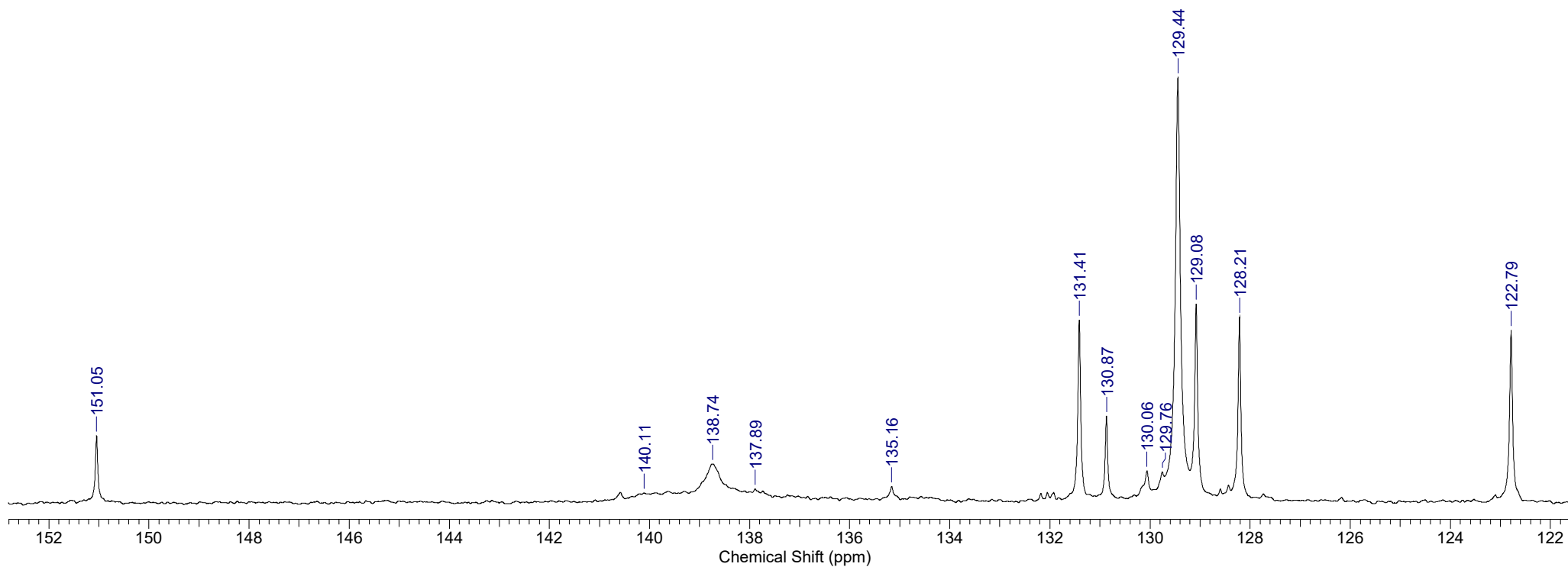


Acquisition Time (sec)	1.1010	Comment	FZ_Grubbs_12-K10-C13dec [hp-dec] [night]			Date	02 Nov 2018 19:07:44
Date Stamp	02 Nov 2018 19:07:44		File Name	C:\Users\Fedor\Desktop\FZ_Grubbs_12-FZ6921_c13dec-night_013001r			
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	24608	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zgpg
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	7547.7637	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.040		

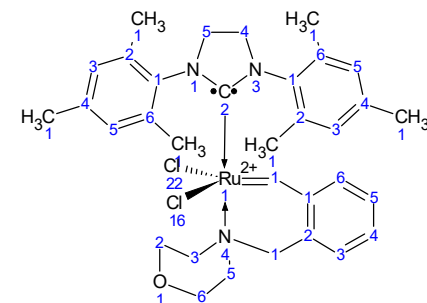


FZ_Grubbs_12-FZ6921_c13dec-night_013001r

11d in CDCl₃

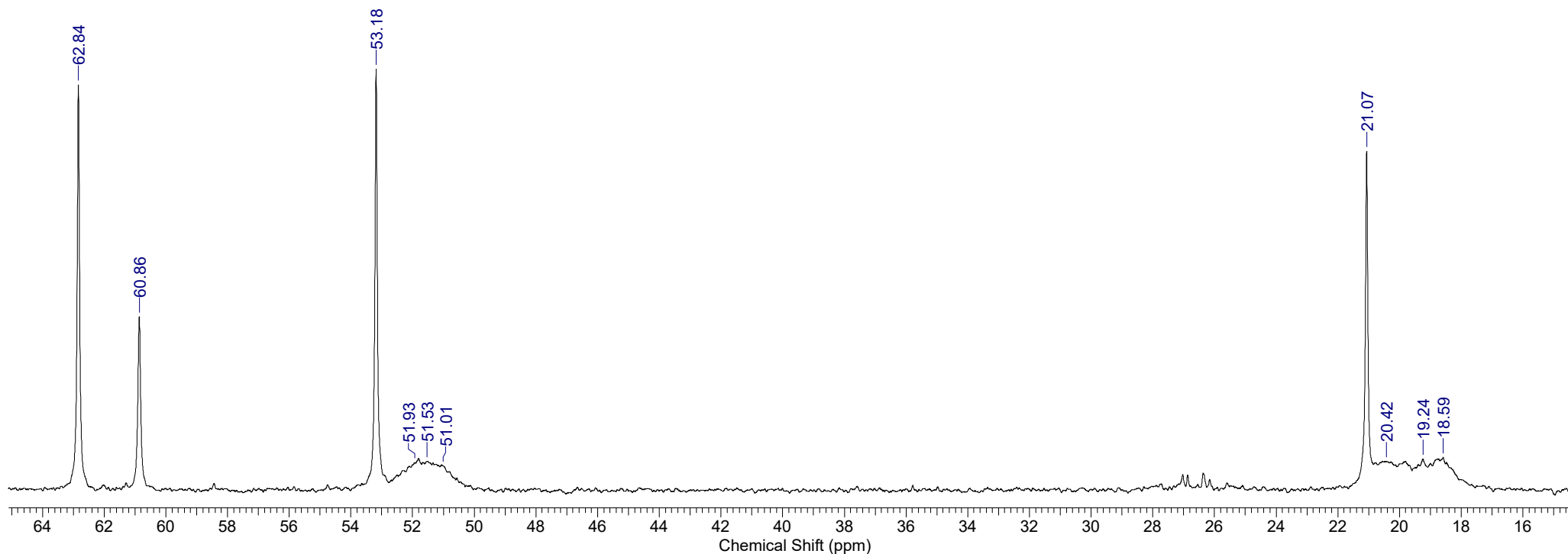


Acquisition Time (sec)	1.1010	Comment	FZ_Grubbs_12-K10-C13dec [hp-dec] [night]			Date	02 Nov 2018 19:07:44
Date Stamp	02 Nov 2018 19:07:44		File Name	C:\Users\Fedor\Desktop\FZ_Grubbs_12-FZ6921_c13dec-night_013001r			
Frequency (MHz)	75.47	Nucleus	13C	Number of Transients	24608	Origin	spect
Original Points Count	65536	Owner	nmr	Points Count	262144	Pulse Sequence	zgpg
Receiver Gain	202.48	SW(cyclical) (Hz)	59523.81	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	7547.7637	Sweep Width (Hz)	59523.58	Temperature (degree C)	30.040		



11d in CDCl₃

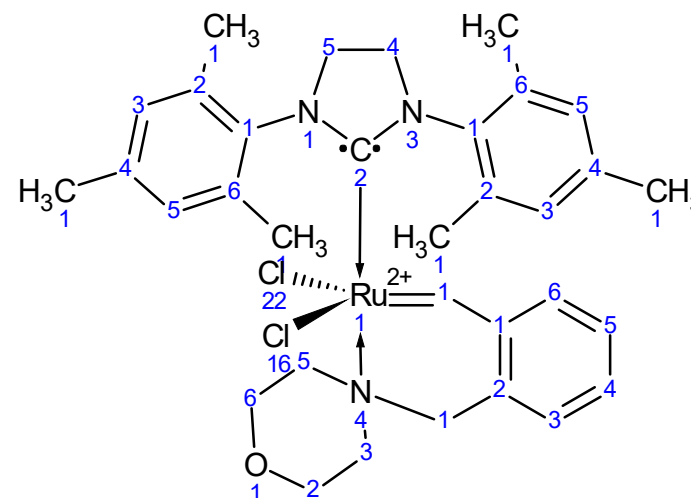
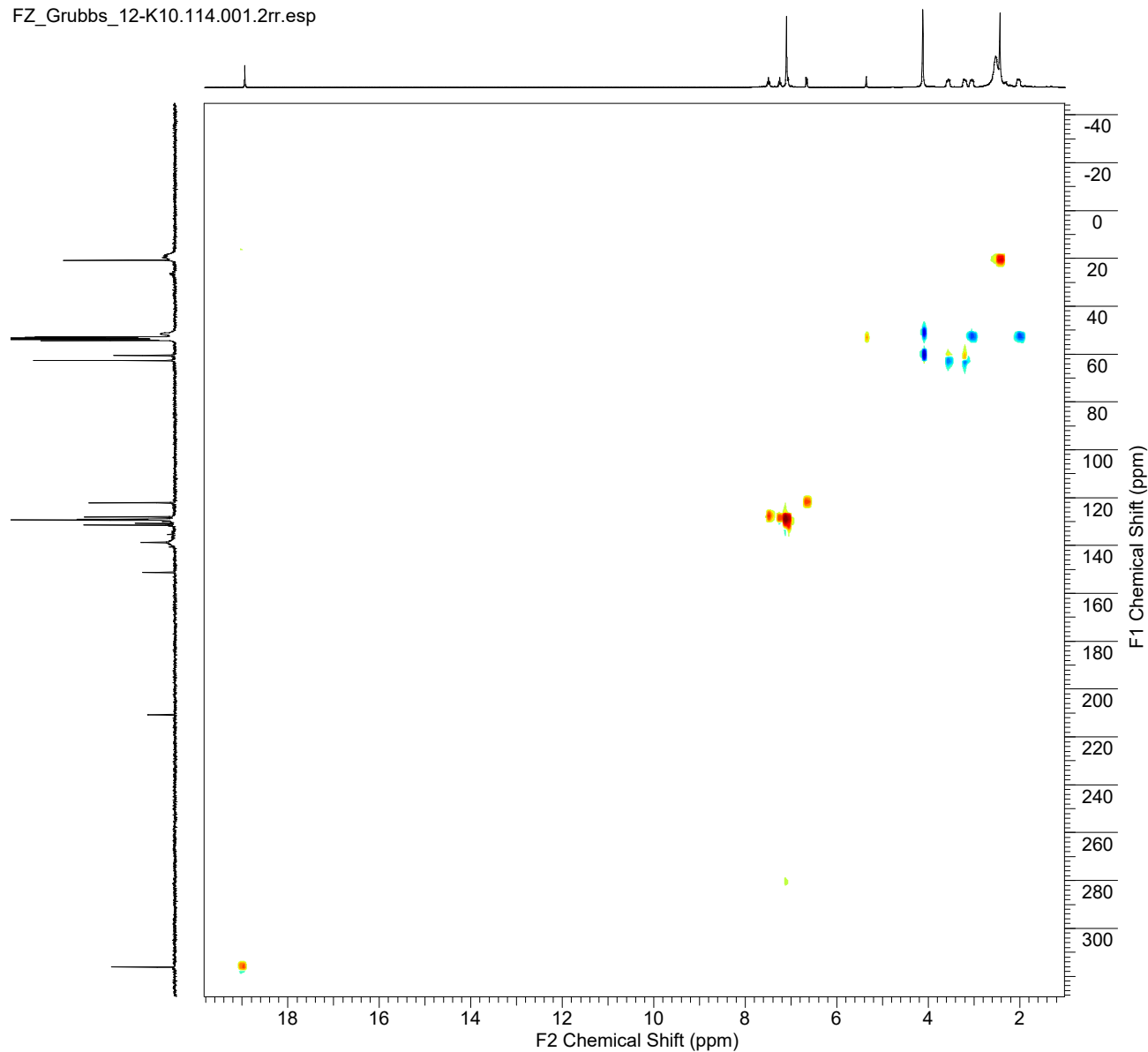
FZ_Grubbs_12-FZ6921_c13dec-night_013001r



Acquisition Time (sec)	(0.3408, 0.0074)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			Date	02 Oct 2018 19:52:12
File Name	C:\Users\Fedor\Desktop\ЯМР Граббс Морфолин\FZ_Grubbs_12-K10\114\pdata\1\2rr					Frequency (MHz)	(300.13, 75.48)
Nucleus	(1H, 13C)	Number of Transients	2	Origin	spect	Original Points Count	(3072, 252)
Owner	nmr	Points Count	(8192, 2048)	Pulse Sequence	hsqcedetgp	Solvent	CD2Cl2
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	30.020	Title	FZ_Grubbs_12-K10-edited-HSQC [hp-dec]		

Formula	C ₃₃ H ₄₁ Cl ₂ N ₂ ORu	FW	667.6730
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FZ_Grubbs_12-K10.114.001.2rr.esp

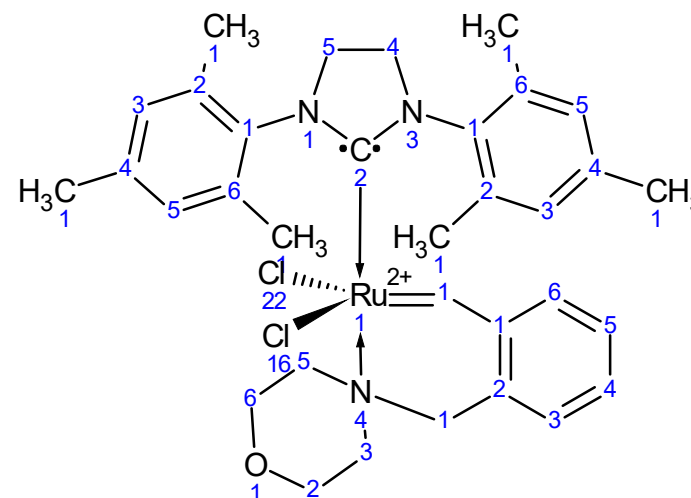
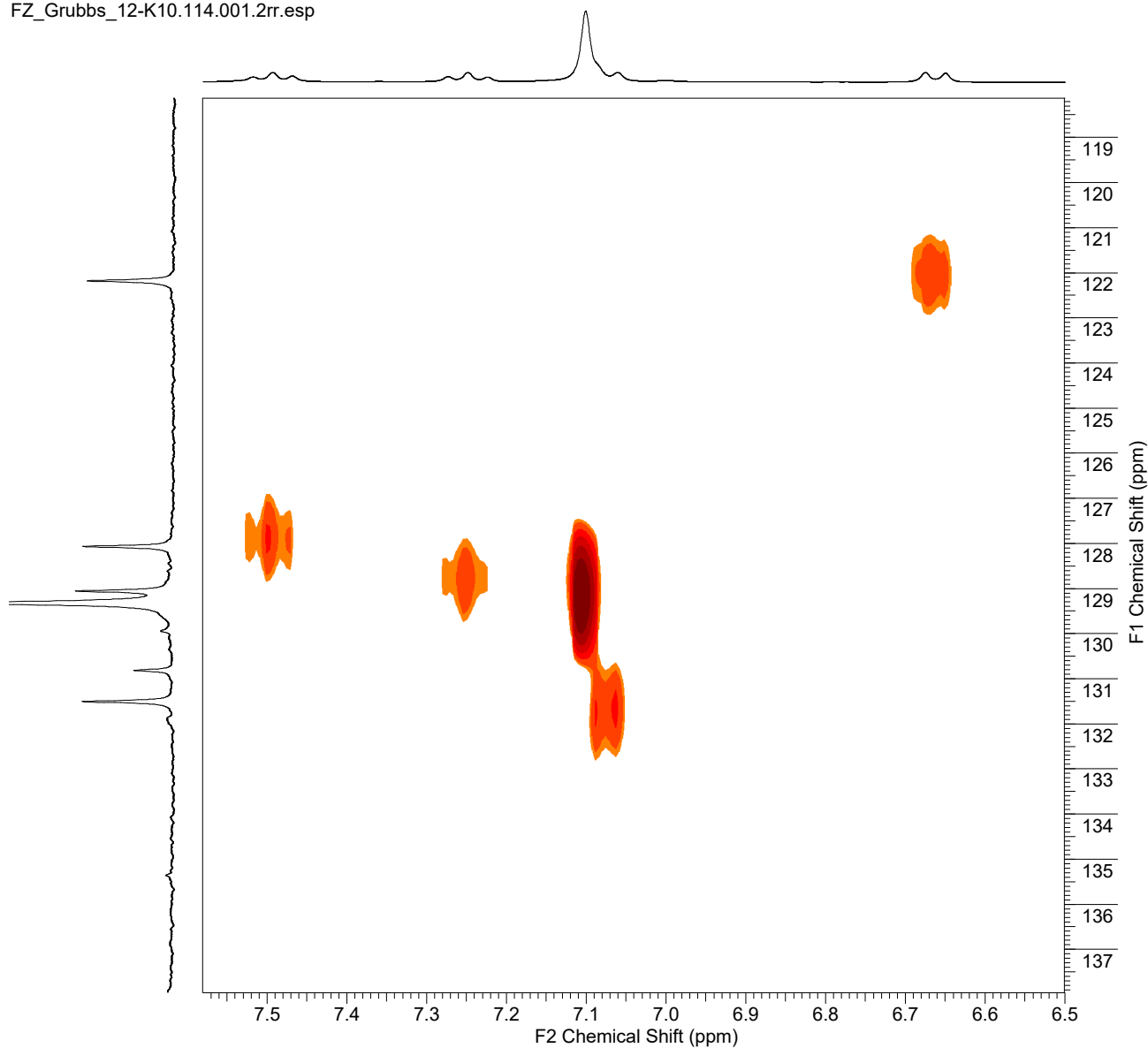


11d

Acquisition Time (sec)	(0.3408, 0.0074)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345	Date	02 Oct 2018 19:52:12
File Name	C:\Users\Fedor\Desktop\ЯМР Граббс Морфолин\FZ_Grubbs_12-K10\114\pdata\1\2rr			Frequency (MHz)	(300.13, 75.48)
Nucleus	(1H, 13C)	Number of Transients	2	Origin	spect
Owner	nmr	Points Count	(8192, 2048)	Pulse Sequence	hsqcedetgp
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	30.020	Solvent	CD2Cl2
				Title	FZ_Grubbs_12-K10-edited-HSQC [hp-dec]

Formula	C ₃₃ H ₄₁ Cl ₂ N ₂ ORu	FW	667.6730
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FZ_Grubbs_12-K10.114.001.2rr.esp

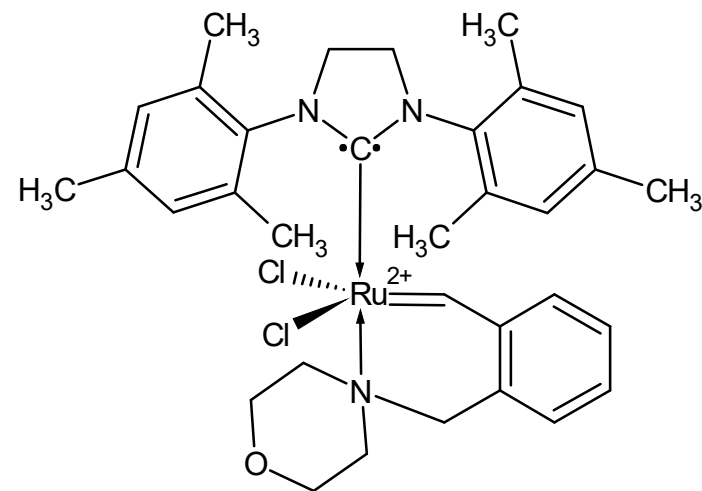
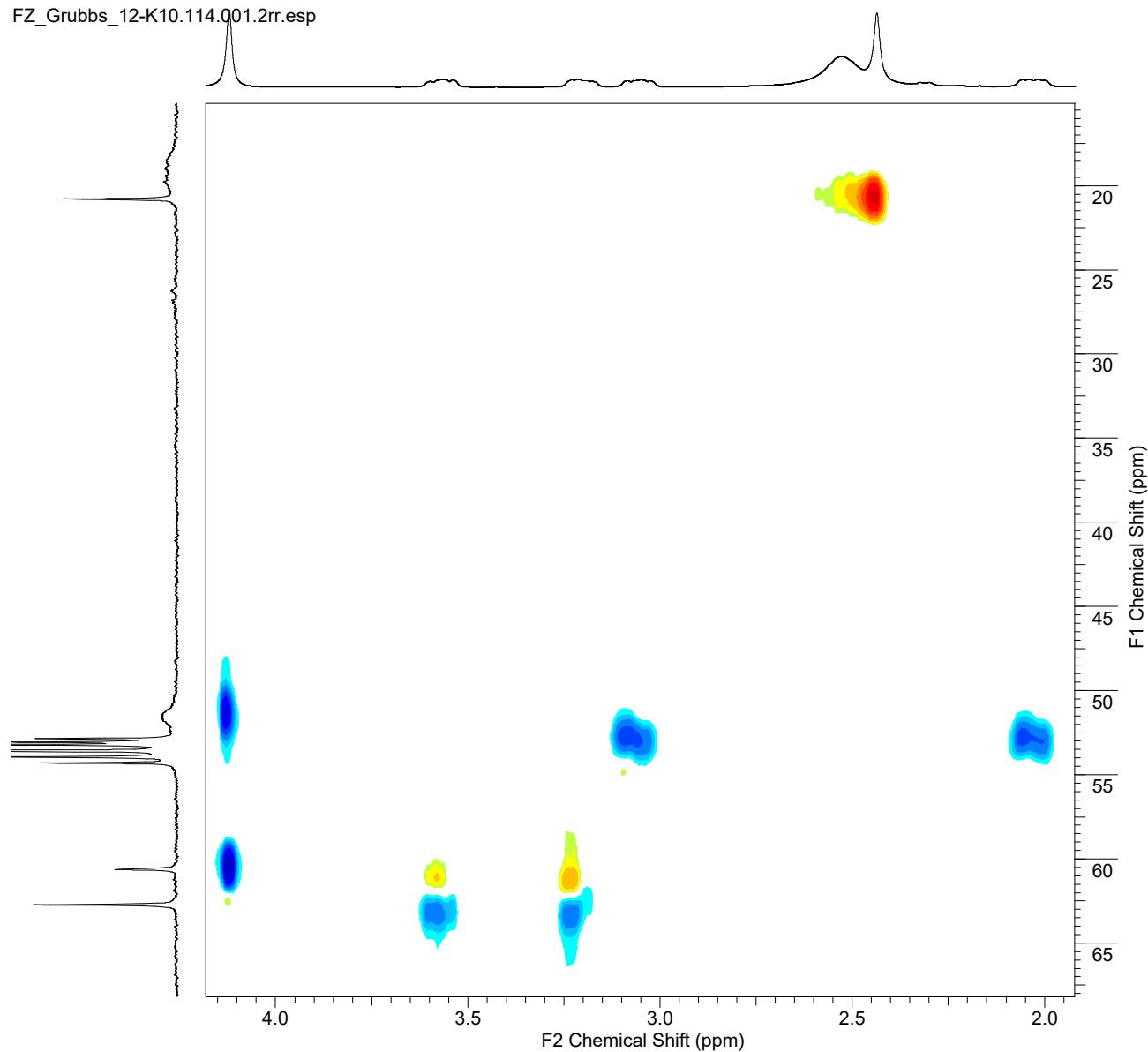


11d

Acquisition Time (sec)	(0.3408, 0.0074)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345	Date	02 Oct 2018 19:52:12
File Name	C:\Users\Fedor\Desktop\ЯМР Граббс Морфолин\FZ_Grubbs_12-K10\114\data\1\2rr			Frequency (MHz)	(300.13, 75.48)
Nucleus	(1H, 13C)	Number of Transients	2	Origin	spect
Owner	nmr	Points Count	(8192, 2048)	Pulse Sequence	hsqcetdgp
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	30.020	Title	FZ_Grubbs_12-K10-edited-HSQC [hp-dec]

Formula	C ₃₃ H ₄₁ Cl ₂ N ₂ ORu	FW	667.6730
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FZ_Grubbs_12-K10.114.001.2rr.esp

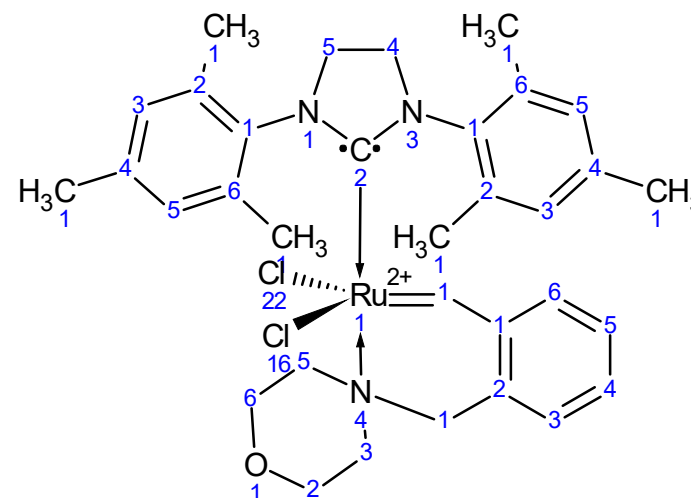
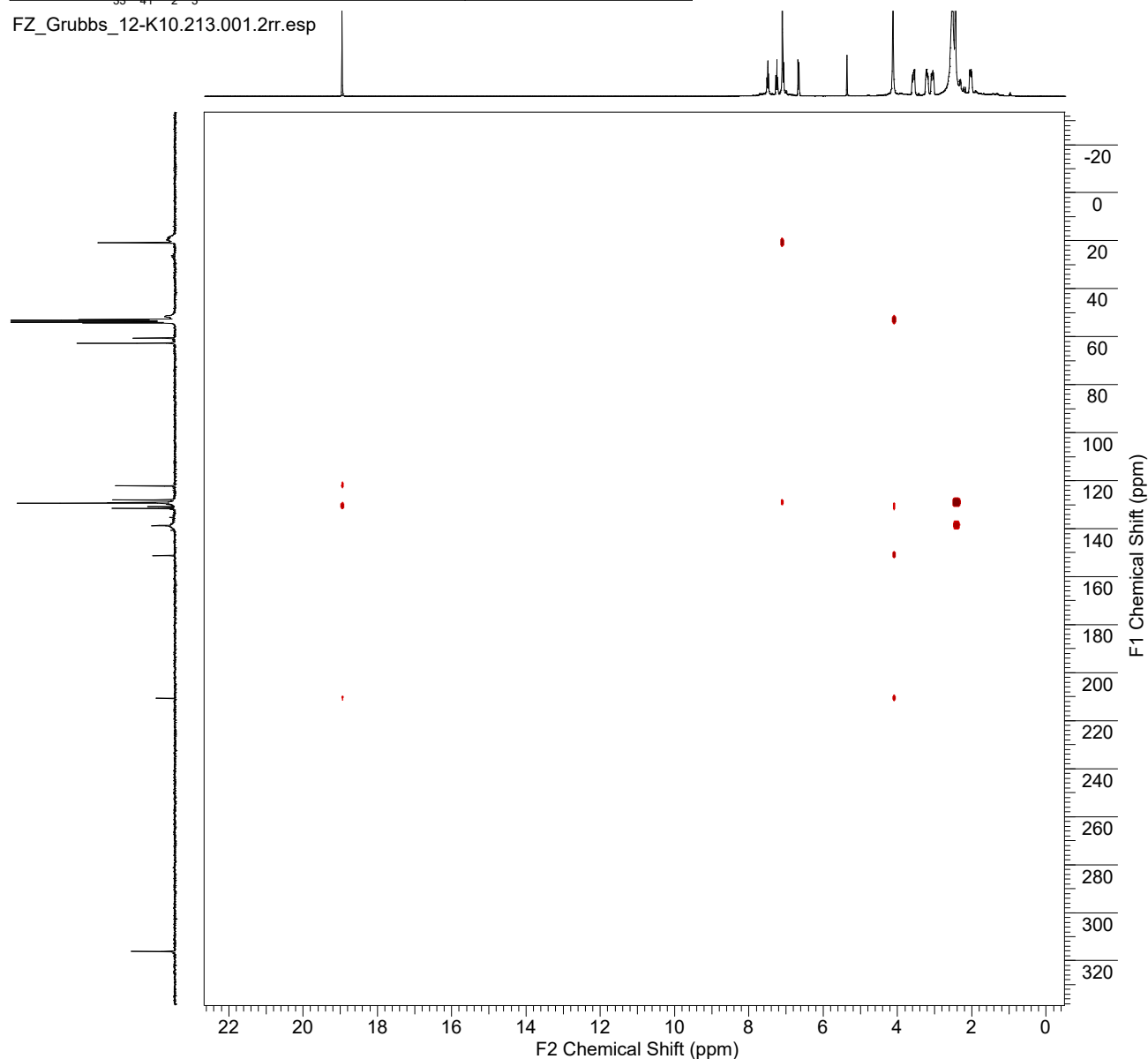


11d

Acquisition Time (sec)	(0.3408, 0.0108)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345	Date	02 Oct 2018 20:28:34
File Name	C:\Users\Fedor\Desktop\ЯМР Граббс Морфолин\FZ_Grubbs_12-K10\213\pdata\1\2rr			Frequency (MHz)	(300.13, 75.48)
Nucleus	(1H, 13C)	Number of Transients	4	Origin	spect
Owner	nmr	Points Count	(8192, 2048)	Pulse Sequence	hmbcgp1pndqf
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	29.873	Title	FZ_Grubbs_12-K10-HMBC

Formula	C ₃₃ H ₄₁ Cl ₂ N ₂ ORu	FW	667.6730
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FZ_Grubbs_12-K10.213.001.2rr.esp

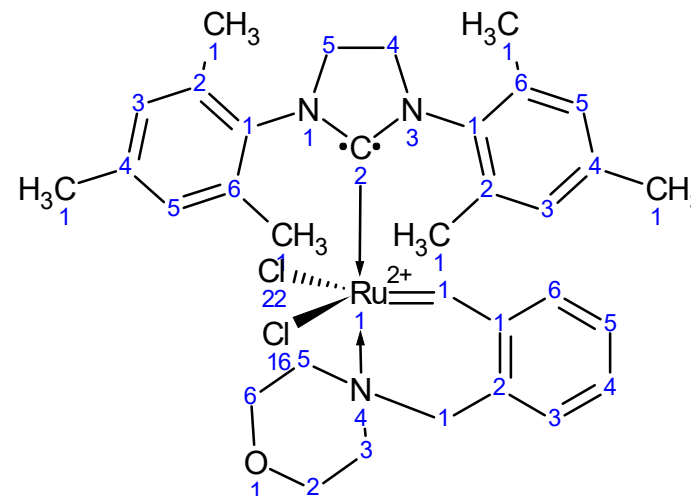
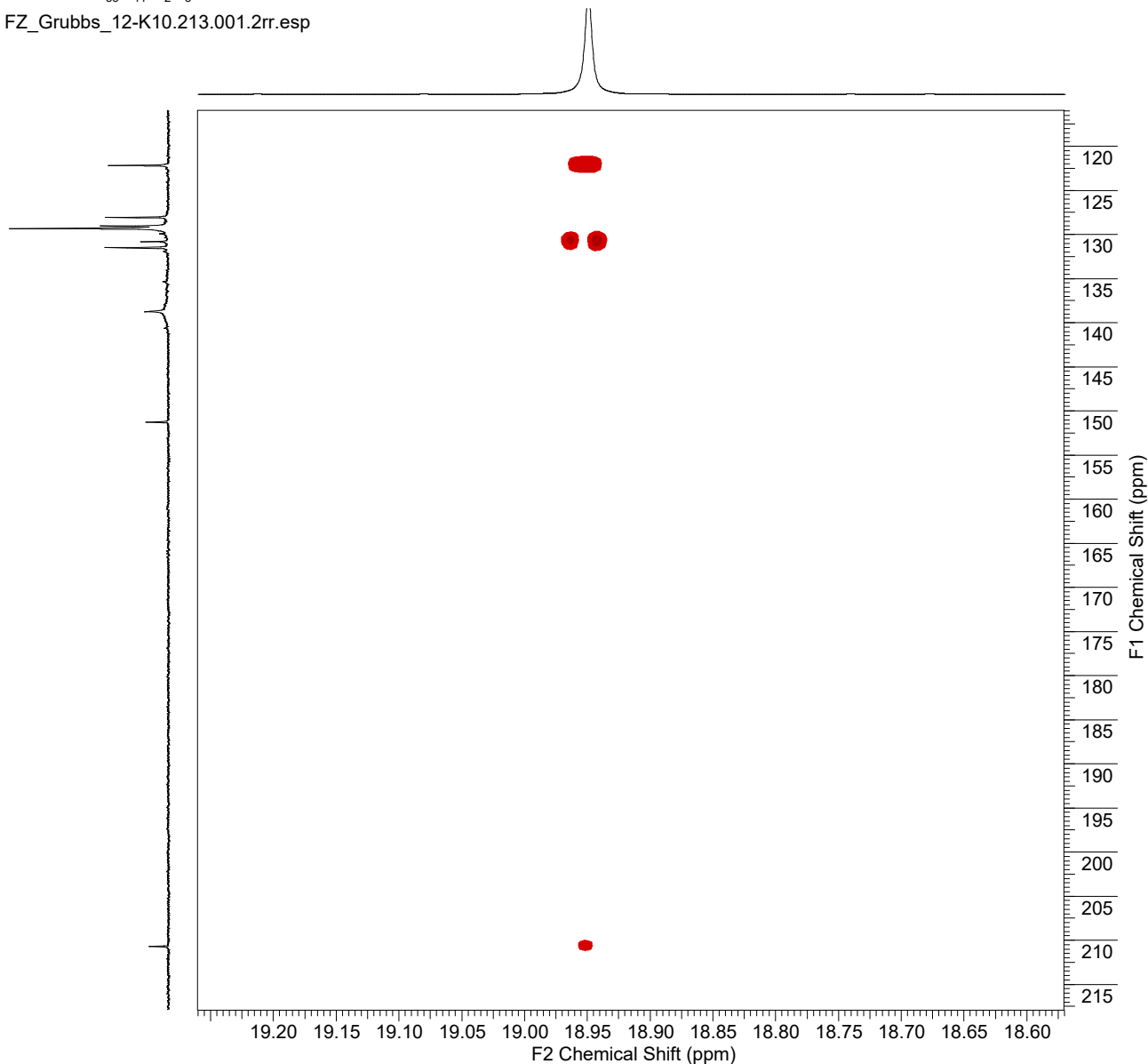


11d

Acquisition Time (sec)	(0.3408, 0.0108)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345	Date	02 Oct 2018 20:28:34
File Name	C:\Users\Fedor\Desktop\ЯМР Граббс Морфолин\FZ_Grubbs_12-K10\213\pdata\1\2rr			Frequency (MHz)	(300.13, 75.48)
Nucleus	(1H, 13C)	Number of Transients	4	Origin	spect
Owner	nmr	Points Count	(8192, 2048)	Pulse Sequence	hmbcgp1pndqf
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	29.873	Solvent	CD2Cl2
		Title	FZ_Grubbs_12-K10-HMBC		

Formula	C ₃₃ H ₄₁ Cl ₂ N ₂ ORu	FW	667.6730
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FZ_Grubbs_12-K10.213.001.2rr.esp

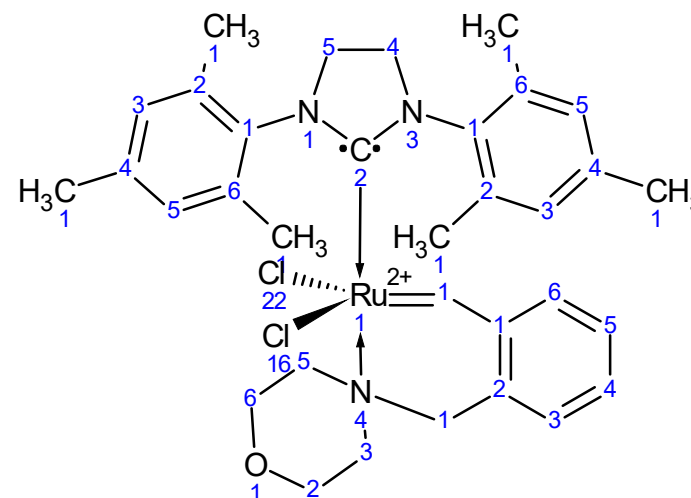
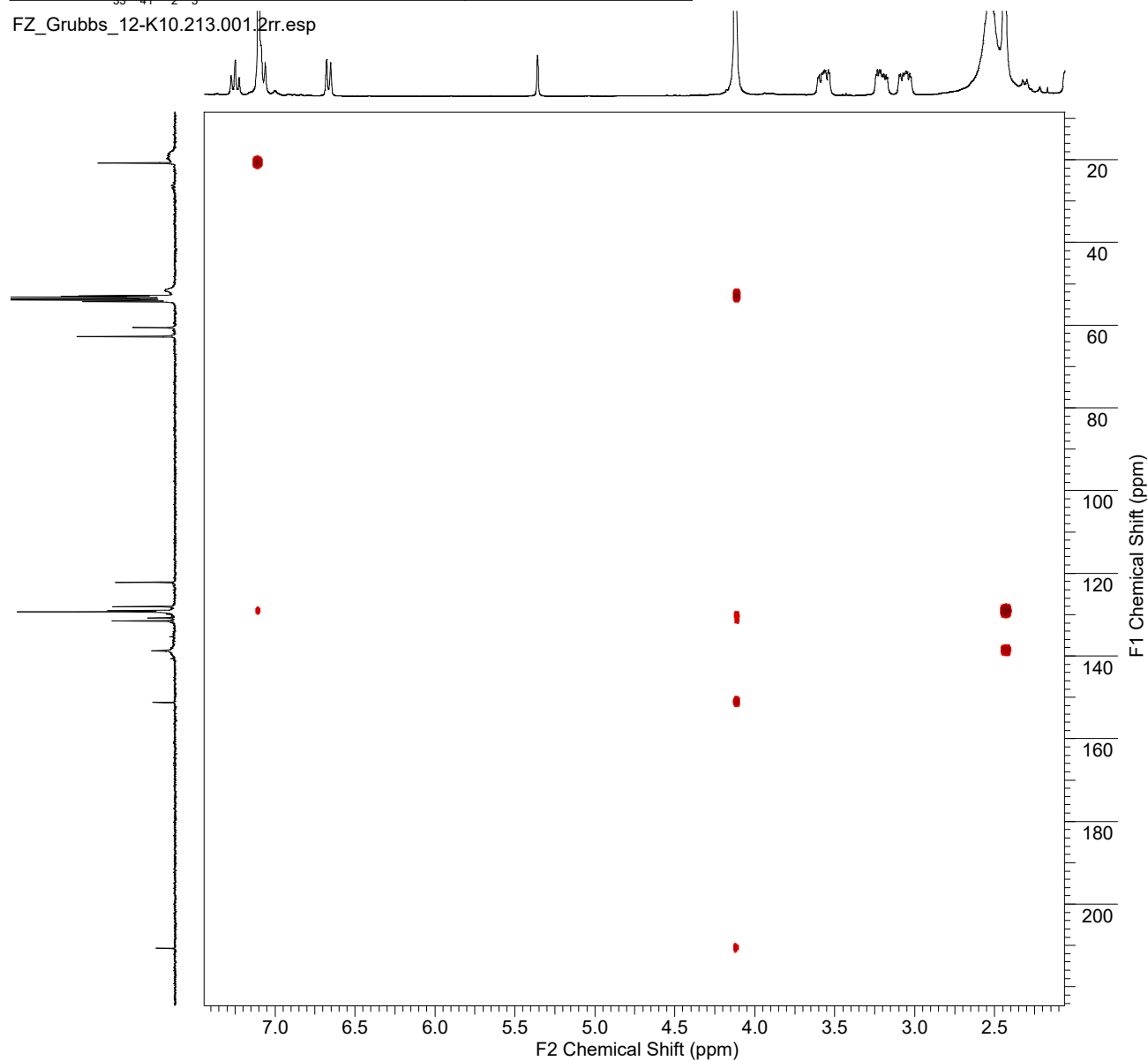


11d

Acquisition Time (sec)	(0.3408, 0.0108)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345	Date	02 Oct 2018 20:28:34
File Name	C:\Users\Fedor\Desktop\ЯМР Граббс Морфолин\FZ_Grubbs_12-K10\213\data\1\2rr			Frequency (MHz)	(300.13, 75.48)
Nucleus	(1H, 13C)	Number of Transients	4	Origin	spect
Owner	nmr	Points Count	(8192, 2048)	Pulse Sequence	hmbcgp1pndqf
Sweep Width (Hz)	(9014.42, 34013.61)	Temperature (degree C)	29.873	Solvent	CD2Cl2
		Title	FZ_Grubbs_12-K10-HMBC		

Formula	C ₃₃ H ₄₁ Cl ₂ N ₂ ORu	FW	667.6730
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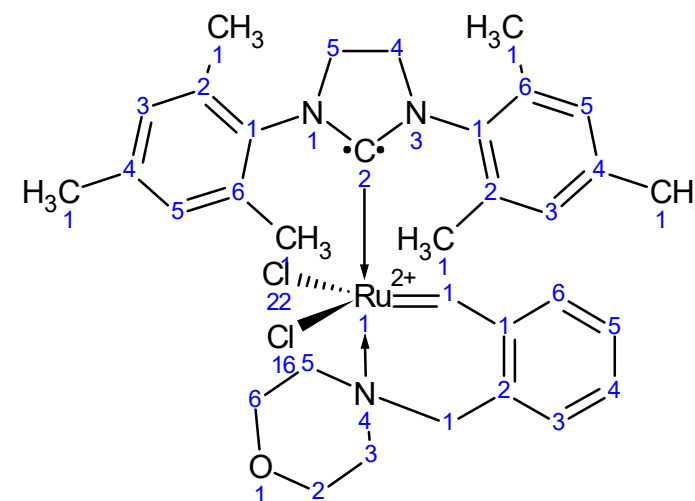
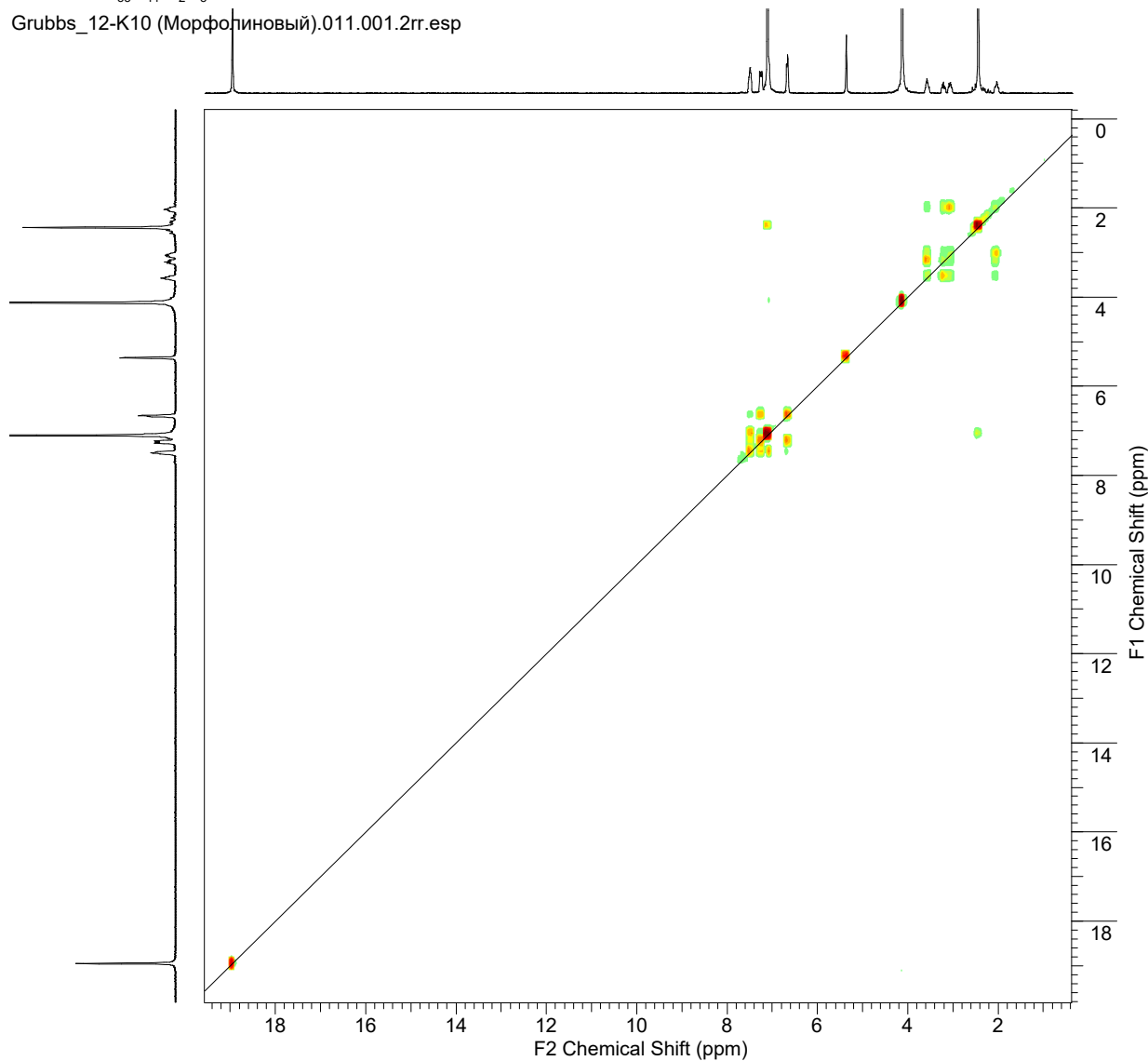
FZ_Grubbs_12-K10.213.001.2rr.esp



11d

Acquisition Time (sec)	(0.3408, 0.0642)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	02 Oct 2018 18:30:04					
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_12-K10 (Морфолиновый)\11\data\1\2rr					
Frequency (MHz)	(300.13, 300.13)	Nucleus	(1H, 1H)	Number of Transients	1	
Origin	spect	Original Points Count	(3072, 578)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	cosygprf	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 9009.01)	Temperature (degree C)	29.656	Title	FZ_Grubbs_12-K10-COSY	
Formula	C ₃₃ H ₄₁ Cl ₂ N ₂ ORu	FW	667.6730			

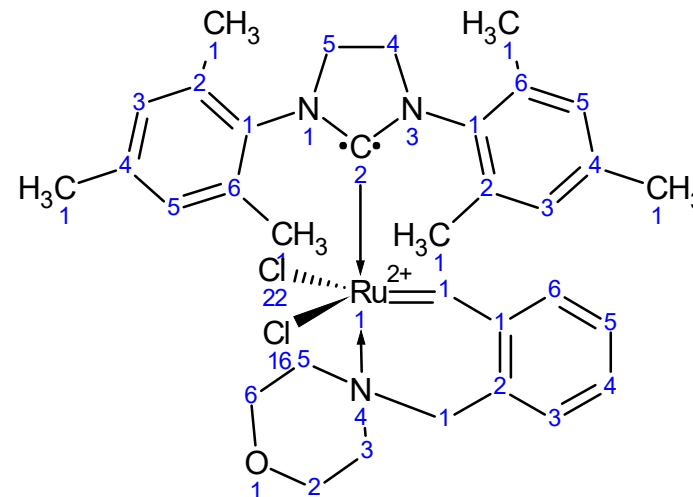
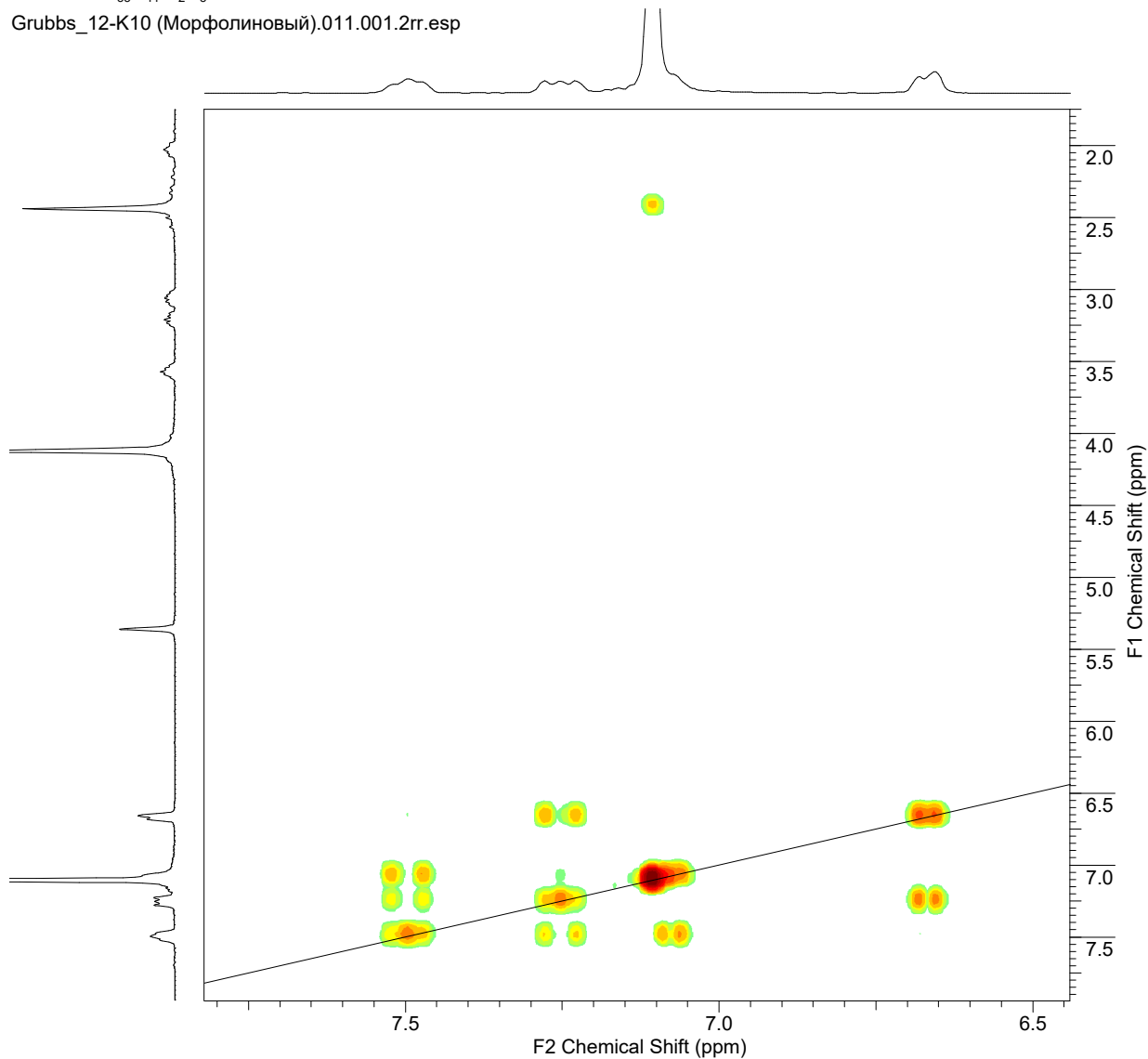
Grubbs_12-K10 (Морфолиновый).011.001.2rr.esp



11d

Acquisition Time (sec)	(0.3408, 0.0642)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	02 Oct 2018 18:30:04					
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_12-K10 (Морфолиновый)\11\data\1\2rr					
Frequency (MHz)	(300.13, 300.13)	Nucleus	(1H, 1H)	Number of Transients	1	
Origin	spect	Original Points Count	(3072, 578)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	cosygprf	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 9009.01)	Temperature (degree C)	29.656	Title	FZ_Grubbs_12-K10-COSY	
Formula	C ₃₃ H ₄₁ Cl ₂ N ₂ ORu	FW	667.6730			

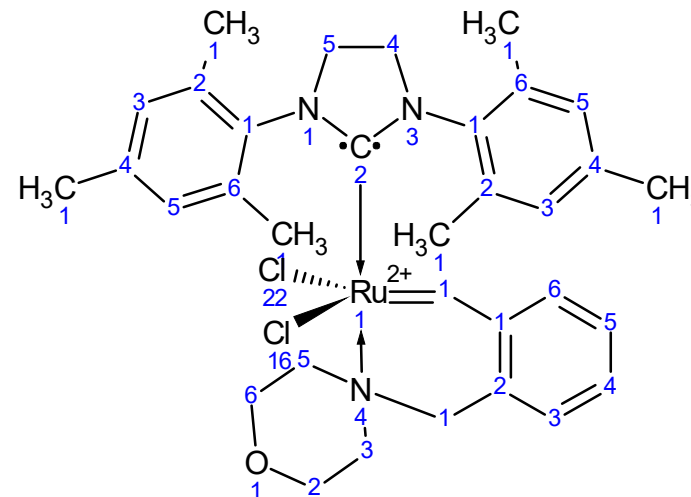
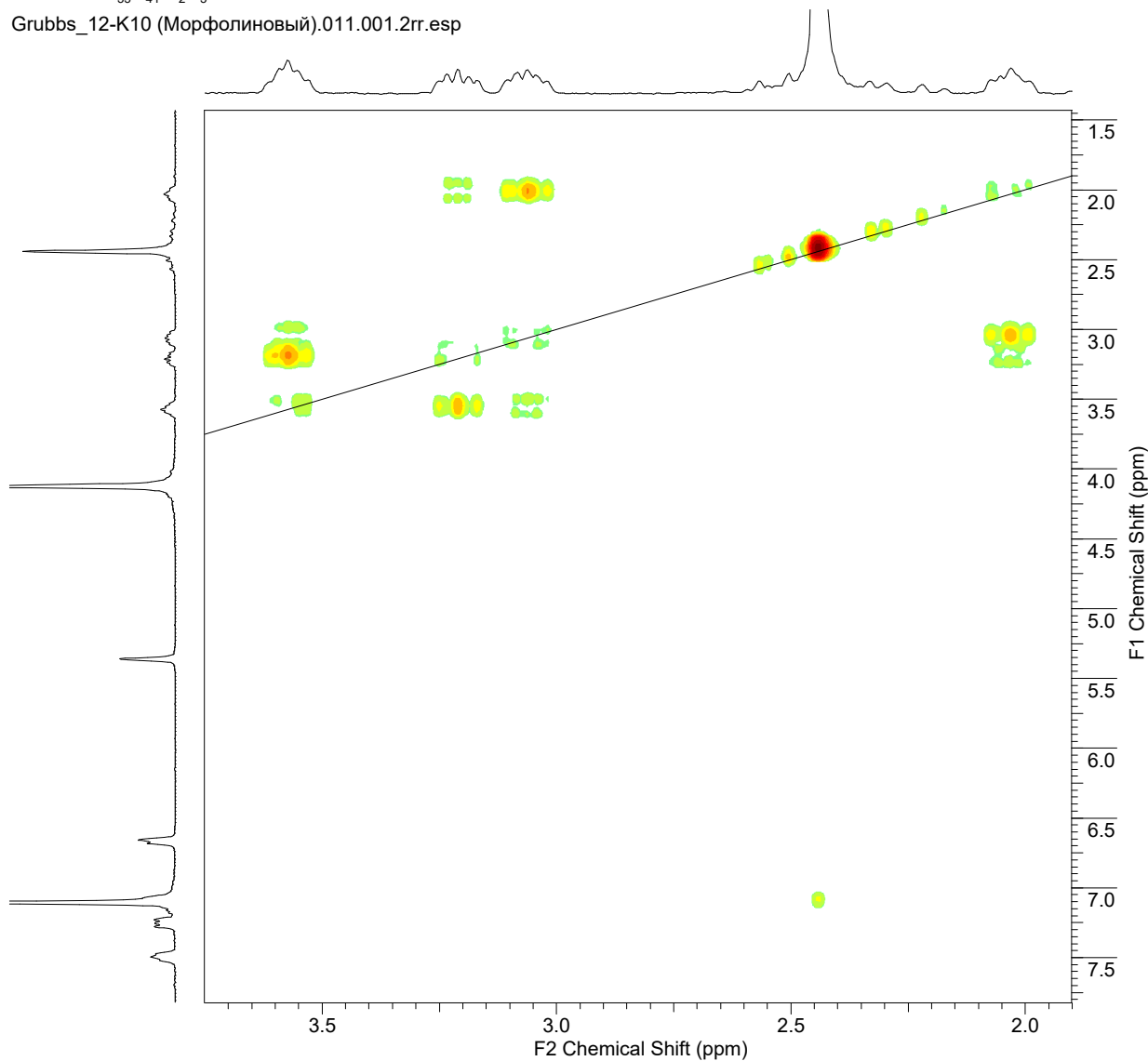
Grubbs_12-K10 (Морфолиновый).011.001.2rr.esp



11d

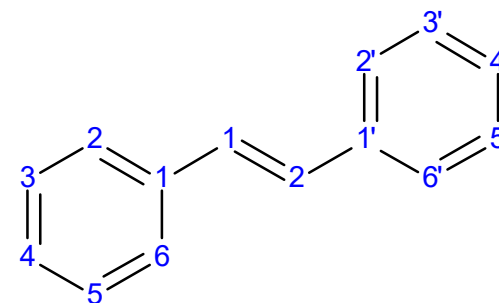
Acquisition Time (sec)	(0.3408, 0.0642)	Comment	5 mm PABBO BB-1H/D Z-GRD Z104275/0345			
Date	02 Oct 2018 18:30:04					
File Name	C:\Users\Fedor\Desktop\Наброски Статей\Кирилл Статья по Катализаторам Граббса\ЯМР Граббс\ЯМР Граббс от Ромы\Grubbs_12-K10 (Морфолиновый)\11\data\1\2rr					
Frequency (MHz)	(300.13, 300.13)	Nucleus	(1H, 1H)	Number of Transients	1	
Origin	spect	Original Points Count	(3072, 578)	Owner	nmr	
Points Count	(8192, 2048)	Pulse Sequence	cosygprf	Solvent	CD2Cl2	
Sweep Width (Hz)	(9014.42, 9009.01)	Temperature (degree C)	29.656	Title	FZ_Grubbs_12-K10-COSY	
Formula	C ₃₃ H ₄₁ Cl ₂ N ₂ ORu	FW	667.6730			

Grubbs_12-K10 (Морфолиновый).011.001.2rr.esp

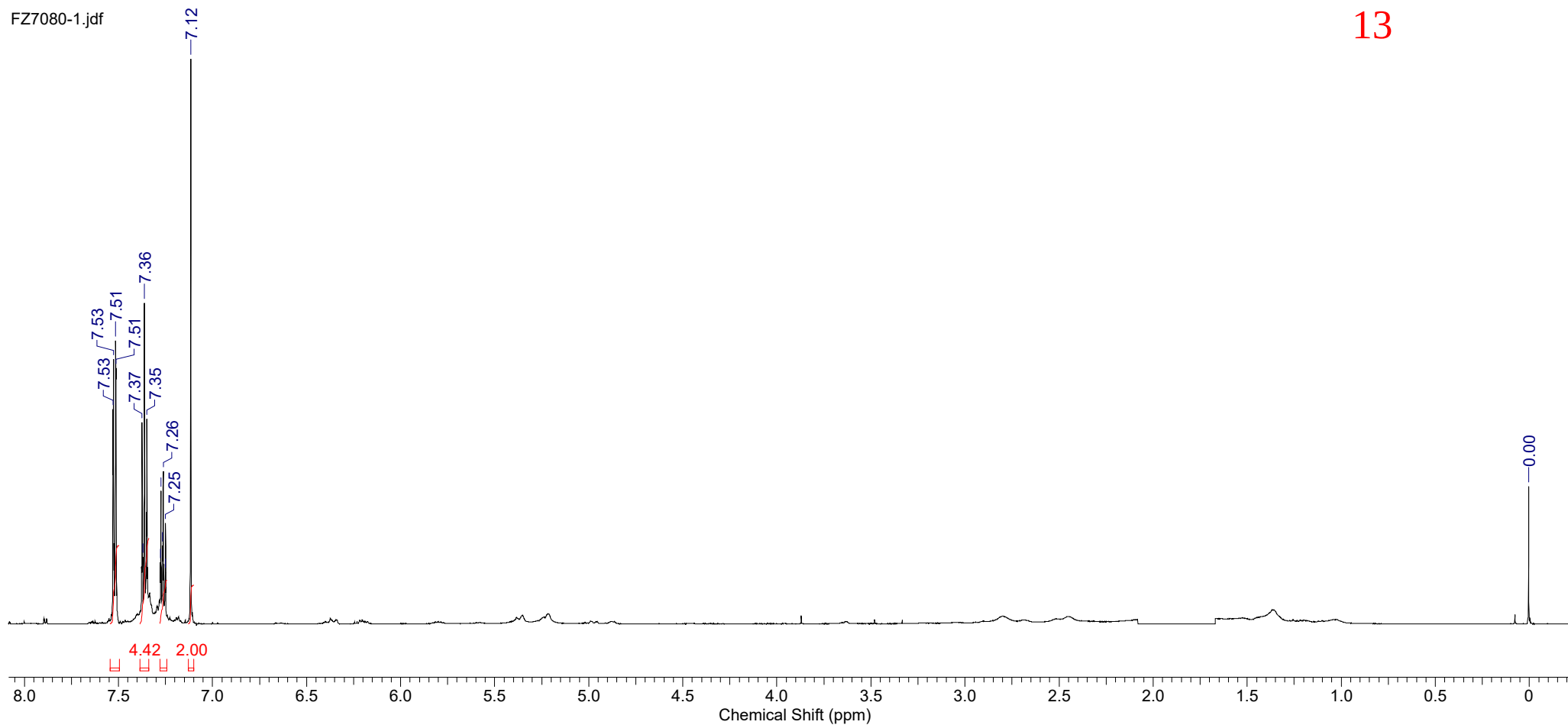


11d

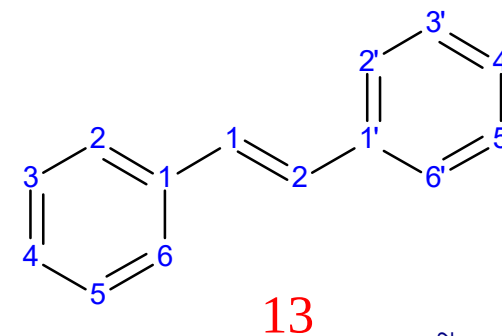
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jan 1990 12:48:43	Date Stamp	13 Dec 2018 08:32:19
File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7080-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



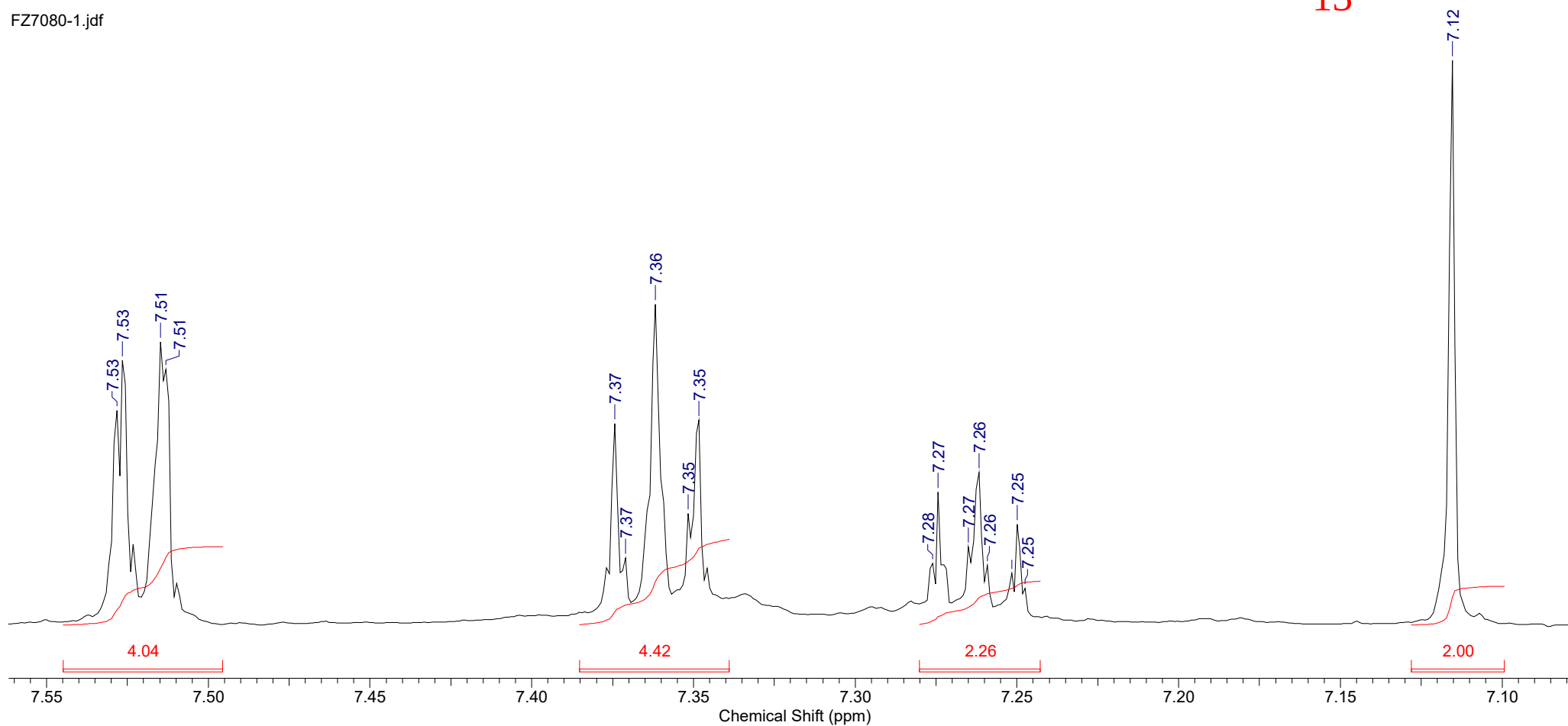
13



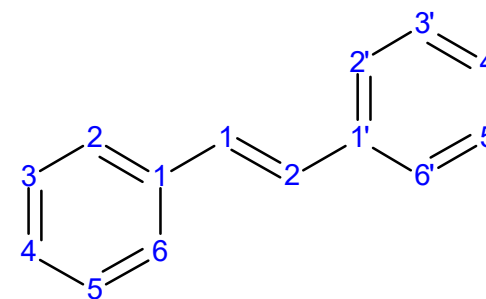
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jan 1990 12:48:43	Date Stamp	13 Dec 2018 08:32:19
File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7080-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



FZ7080-1.jdf

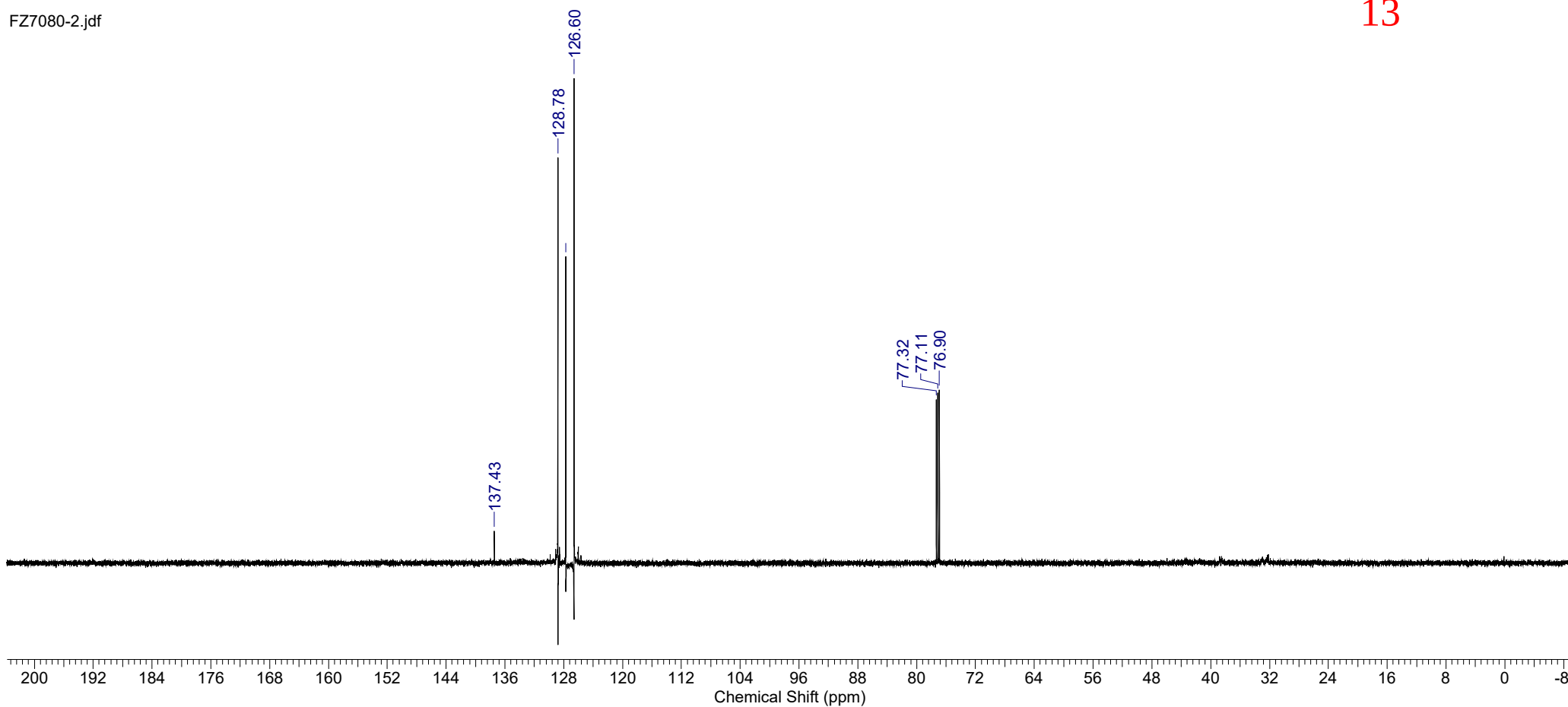


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	10 Jan 1990 12:57:45
Date Stamp	13 Dec 2018 08:41:21	File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7080-2.jdf	Frequency (MHz)	150.91
Nucleus	¹³ C	Number of Transients	400	Origin	ECA 600
Points Count	32768	Pulse Sequence	single pulse dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	56.00
				Owner	delta
				Solvent	CHLOROFORM-d

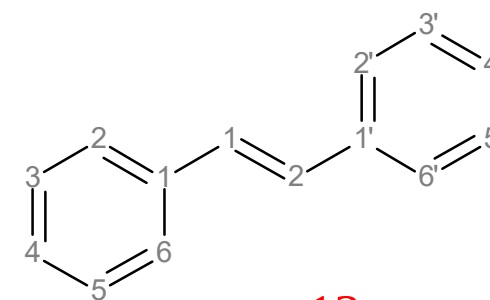


13

FZ7080-2.jdf

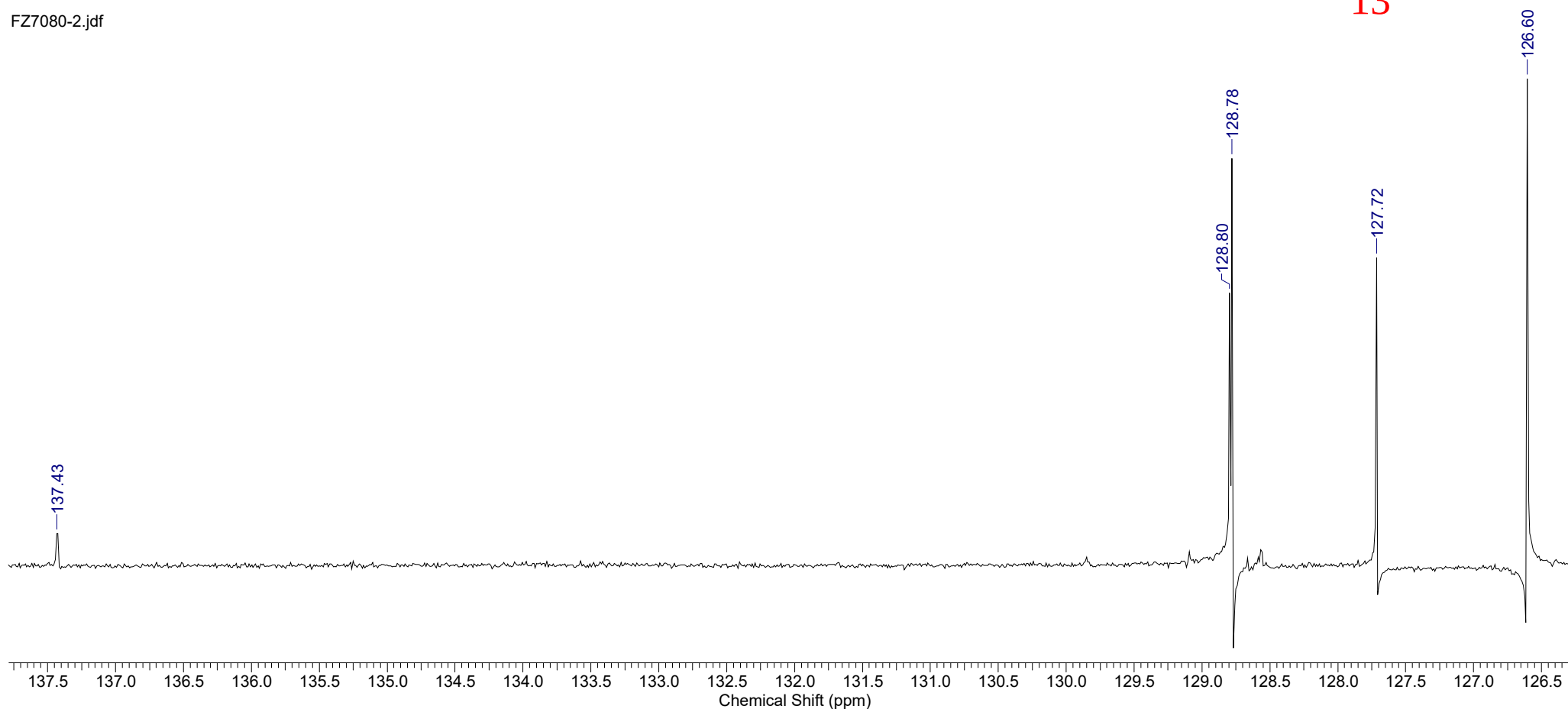


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	10 Jan 1990 12:57:45	
Date Stamp	13 Dec 2018 08:41:21	File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7080-2.jdf			Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	400	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse_dec	Receiver Gain	56.00	Owner	delta
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Solvent	CHLOROFORM-d		

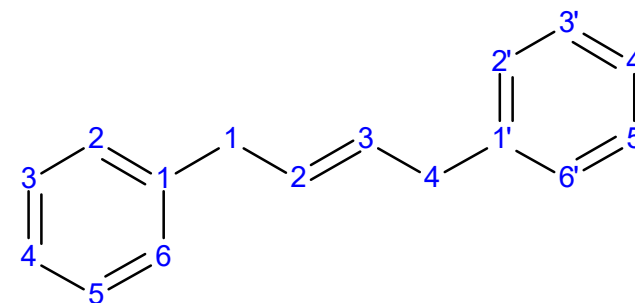


13

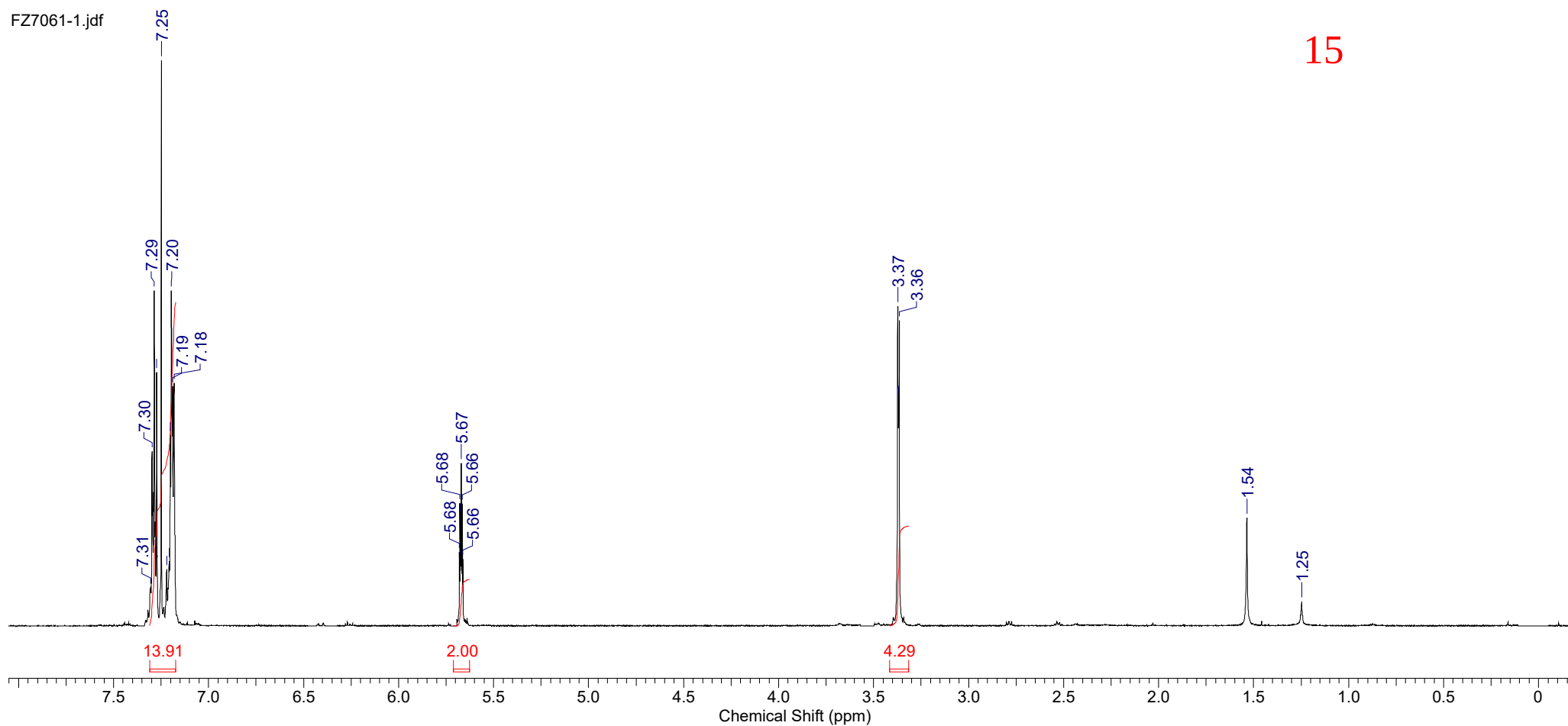
FZ7080-2.jdf



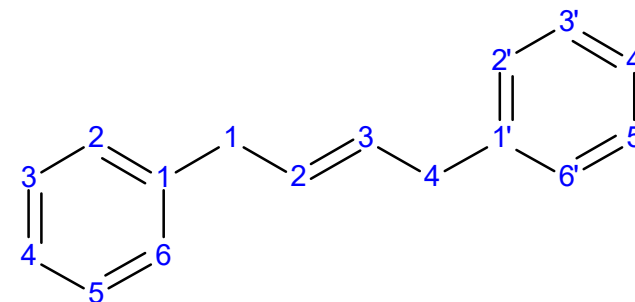
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jan 1990 12:19:53	Date Stamp	13 Dec 2018 08:03:29
File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7061-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	46.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



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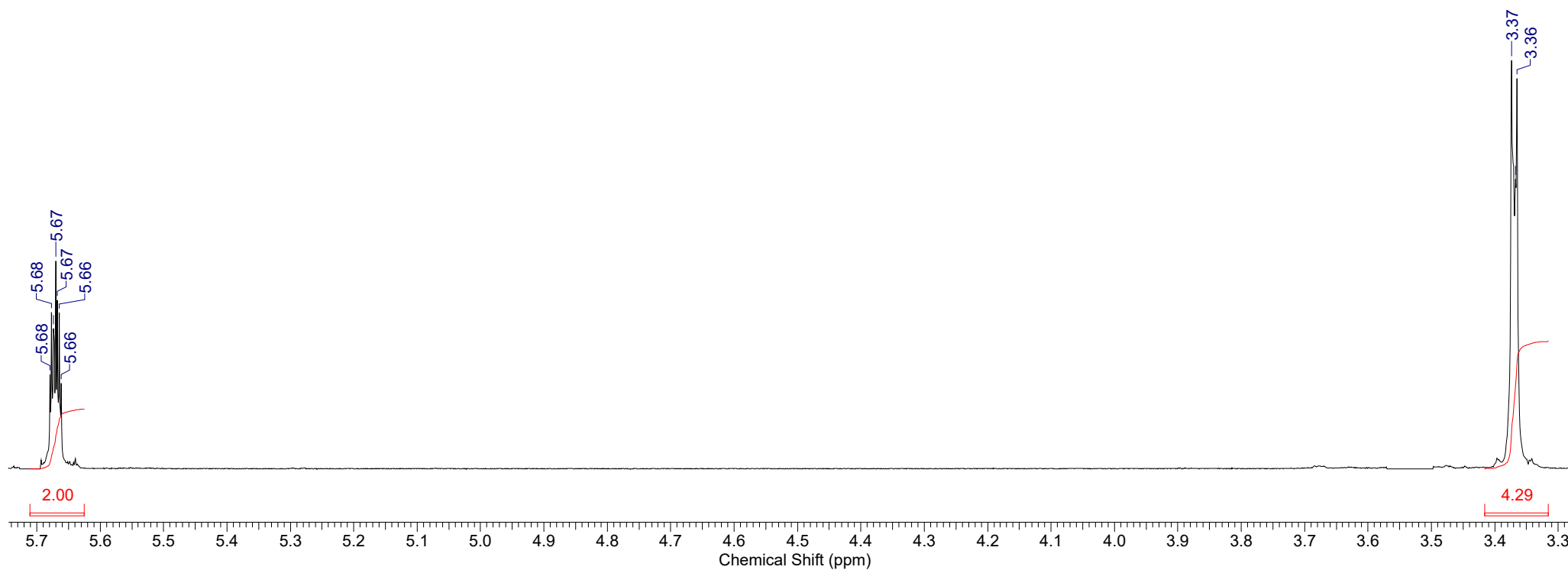


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jan 1990 12:19:53	Date Stamp	13 Dec 2018 08:03:29
File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7061-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	46.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39

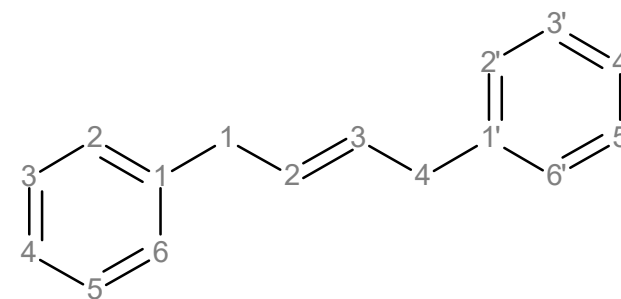


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FZ7061-1.jdf

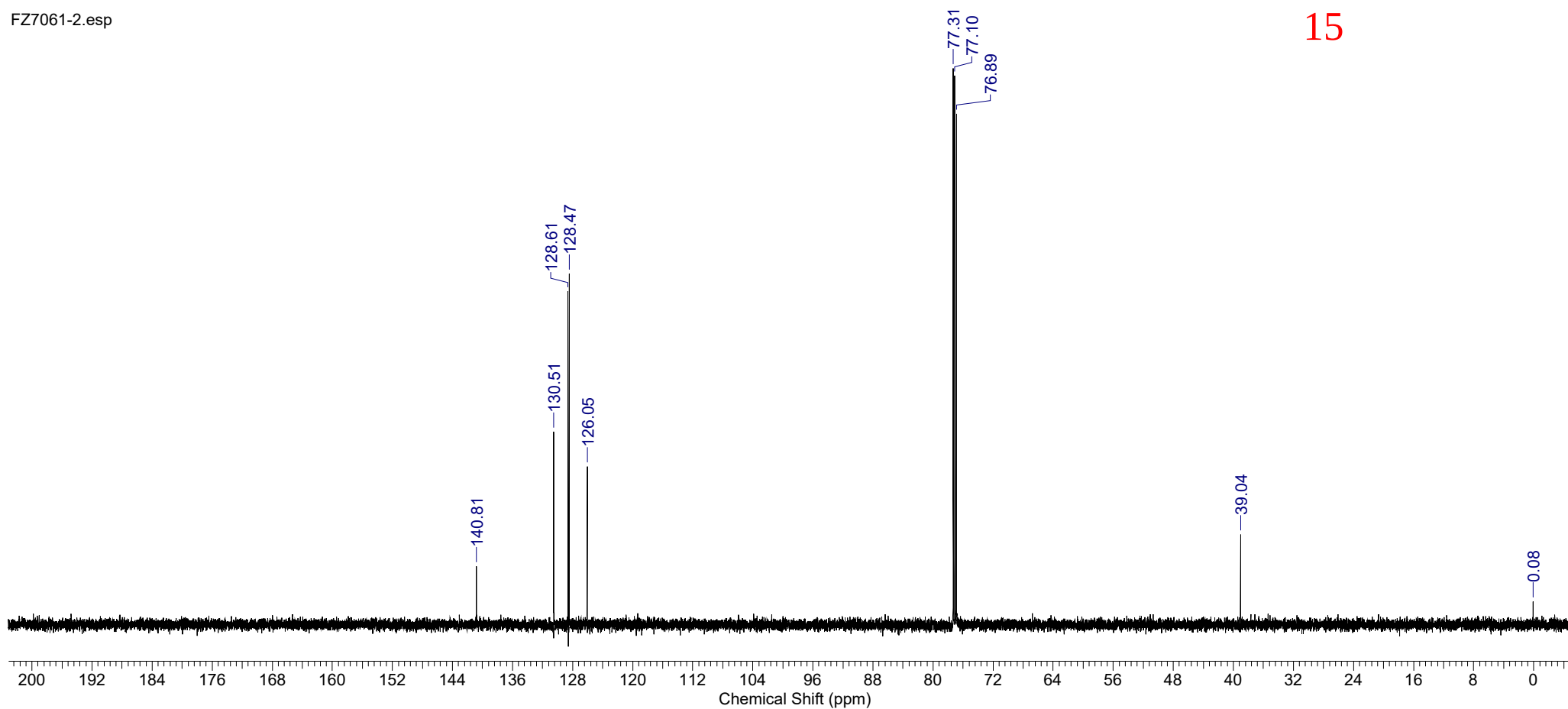


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	10 Jan 1990 12:28:52	
Date Stamp	13 Dec 2018 08:12:28	File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7061-2.jdf			Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	400	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse_dec	Receiver Gain	56.00	Owner	delta
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Solvent	CHLOROFORM-d		

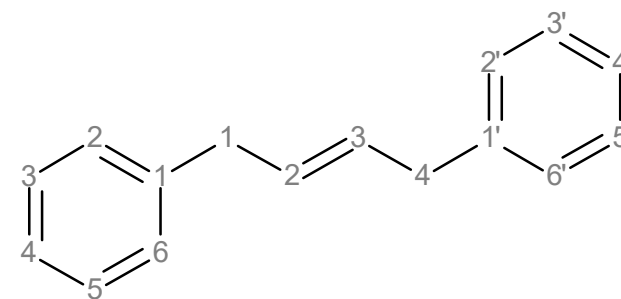


15

FZ7061-2.esp

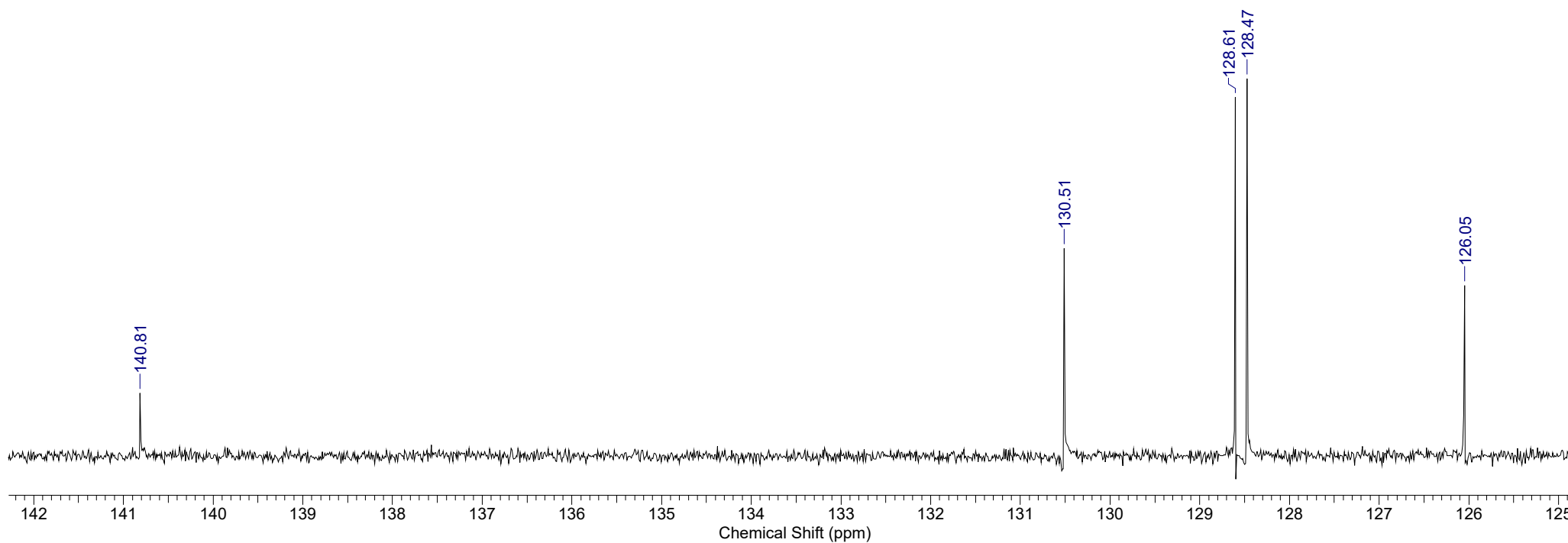


Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	10 Jan 1990 12:28:52	
Date Stamp	13 Dec 2018 08:12:28	File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7061-2.jdf			Frequency (MHz)	150.91
Nucleus	13C	Number of Transients	400	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse_dec	Receiver Gain	56.00	Owner	delta
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Solvent	CHLOROFORM-d		

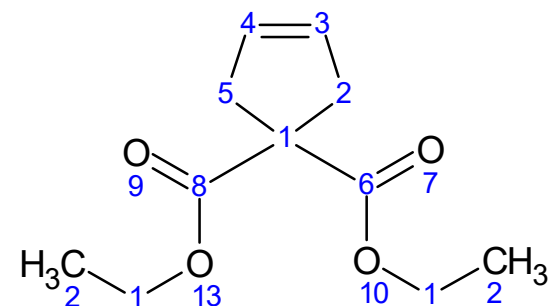


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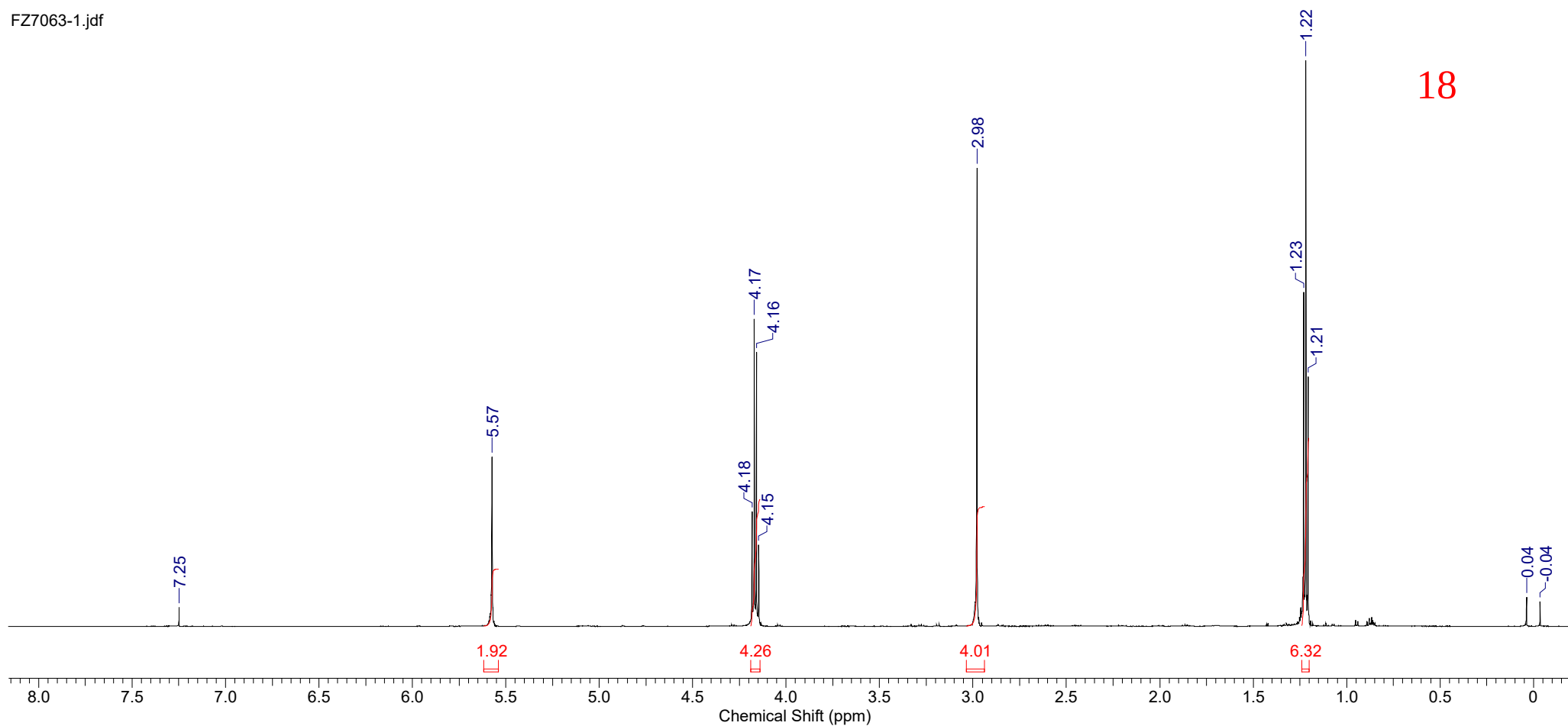
FZ7061-2.esp



Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jan 1990 11:52:50	Date Stamp	13 Dec 2018 07:36:26
File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7063-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	28.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39

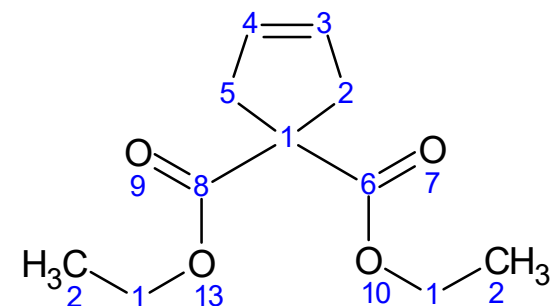


FZ7063-1.jdf

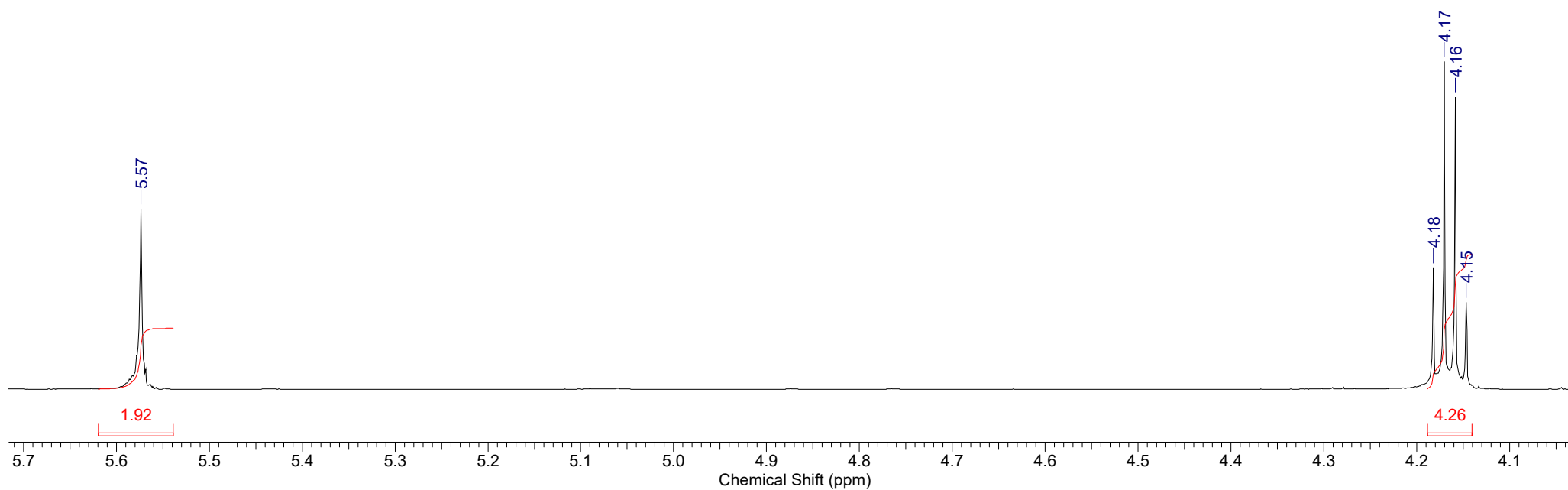


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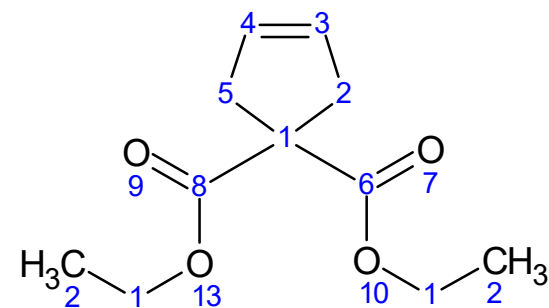
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jan 1990 11:52:50	Date Stamp	13 Dec 2018 07:36:26
File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7063-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	28.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



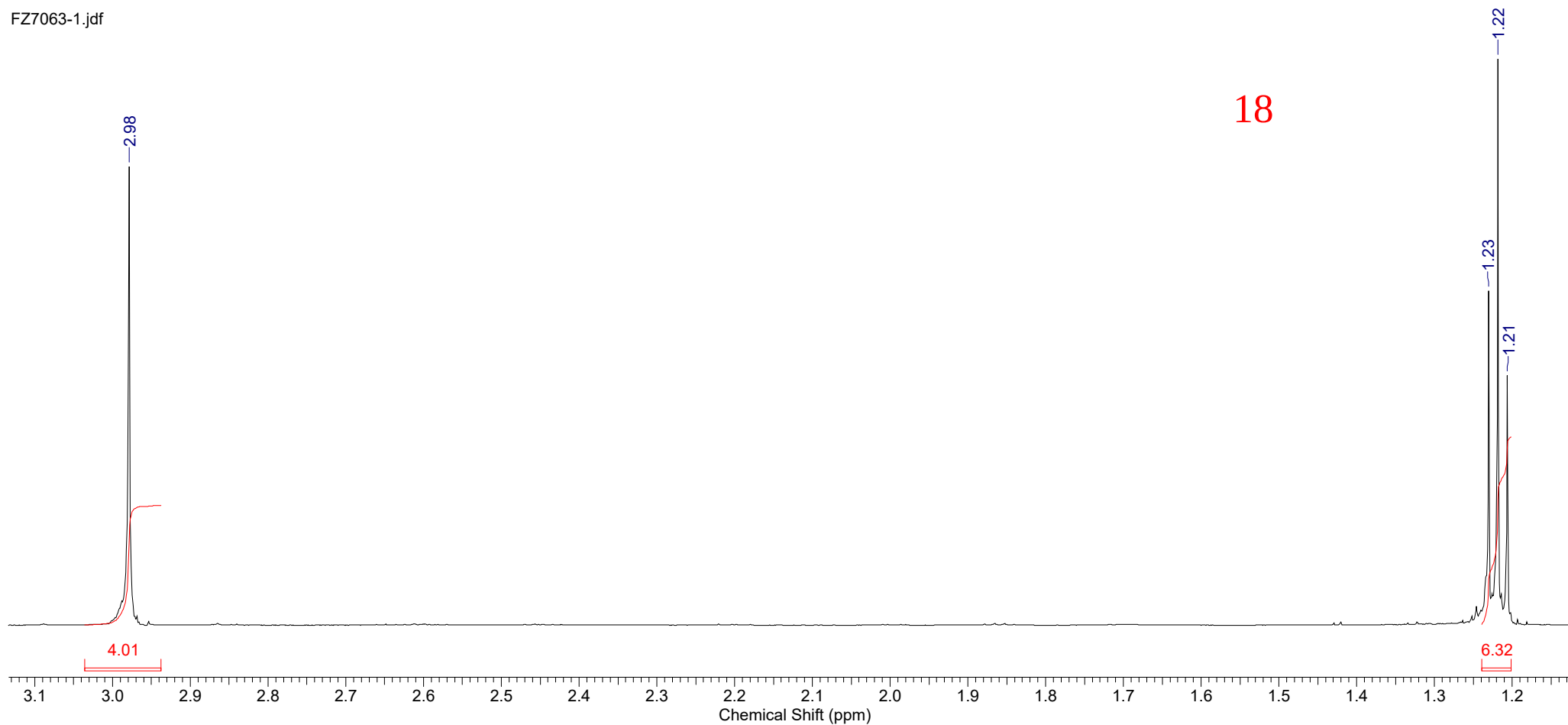
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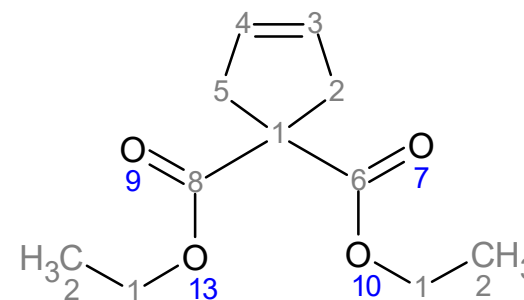
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jan 1990 11:52:50	Date Stamp	13 Dec 2018 07:36:26
File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7063-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	28.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5401.5503	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



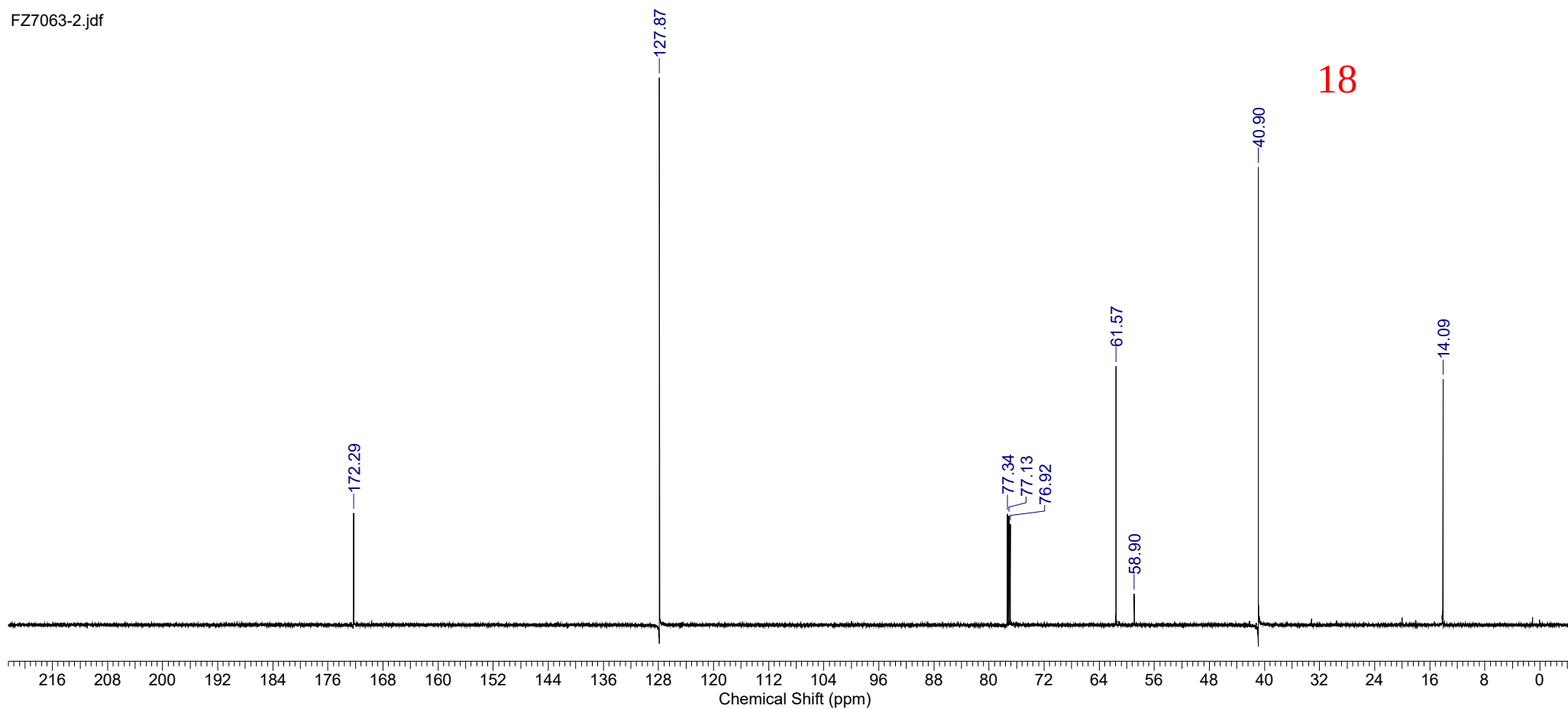
FZ7063-1.jdf



Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	10 Jan 1990 11:59:28
Date Stamp	13 Dec 2018 07:43:04	File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7063-2.jdf	Frequency (MHz)	150.91
Nucleus	¹³ C	Number of Transients	290	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	56.00
				Owner	delta
				Solvent	CHLOROFORM-d

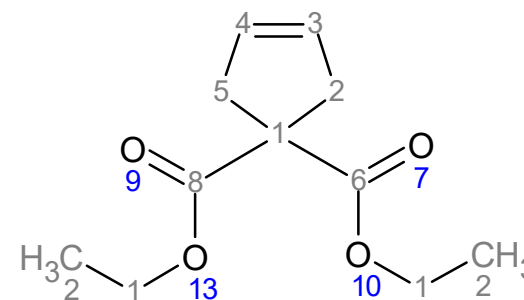


FZ7063-2.jdf

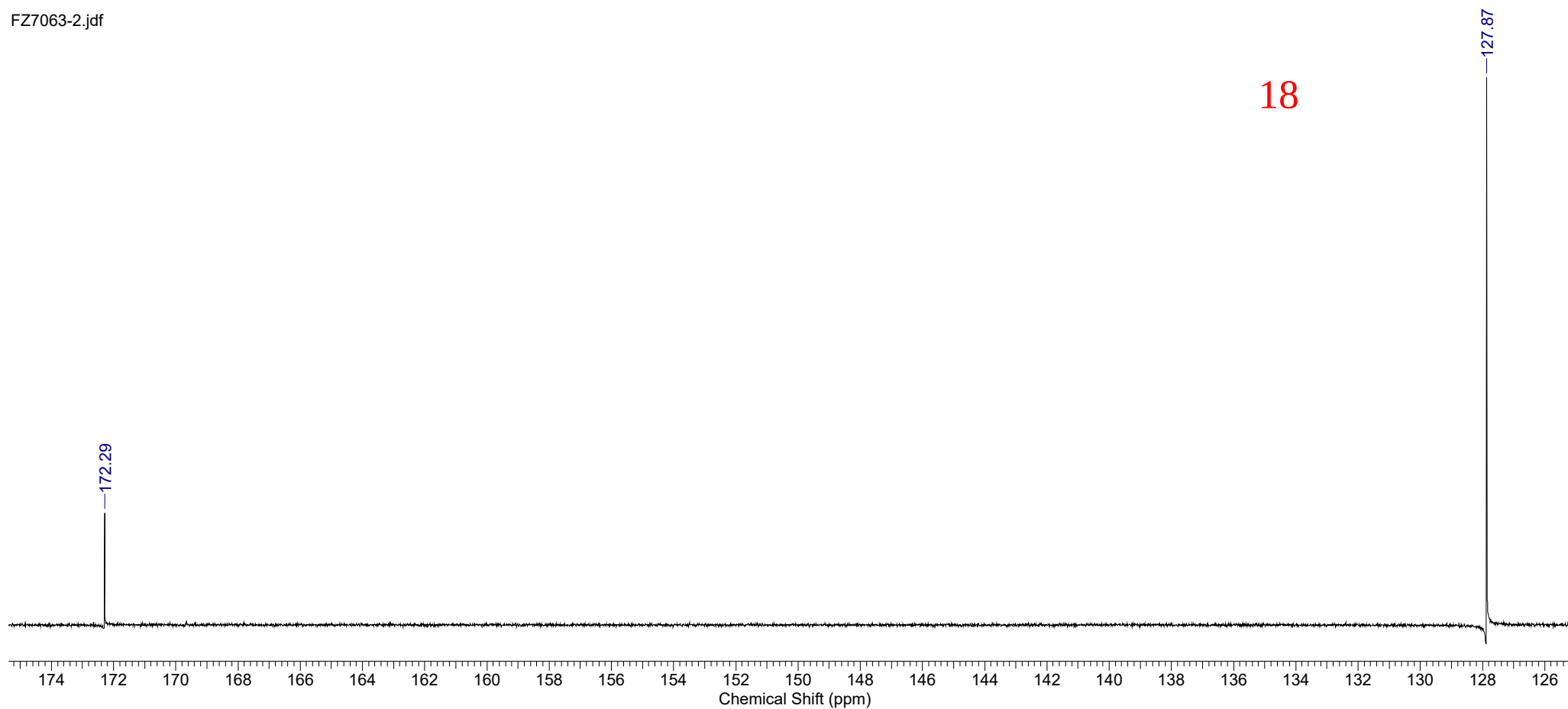


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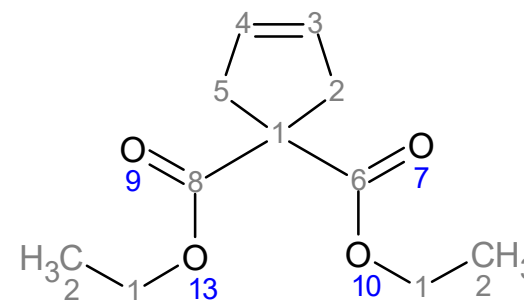
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	10 Jan 1990 11:59:28
Date Stamp	13 Dec 2018 07:43:04	File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7063-2.jdf	Frequency (MHz)	150.91
Nucleus	¹³ C	Number of Transients	290	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49	Receiver Gain	56.00
				Owner	delta
				Solvent	CHLOROFORM-d



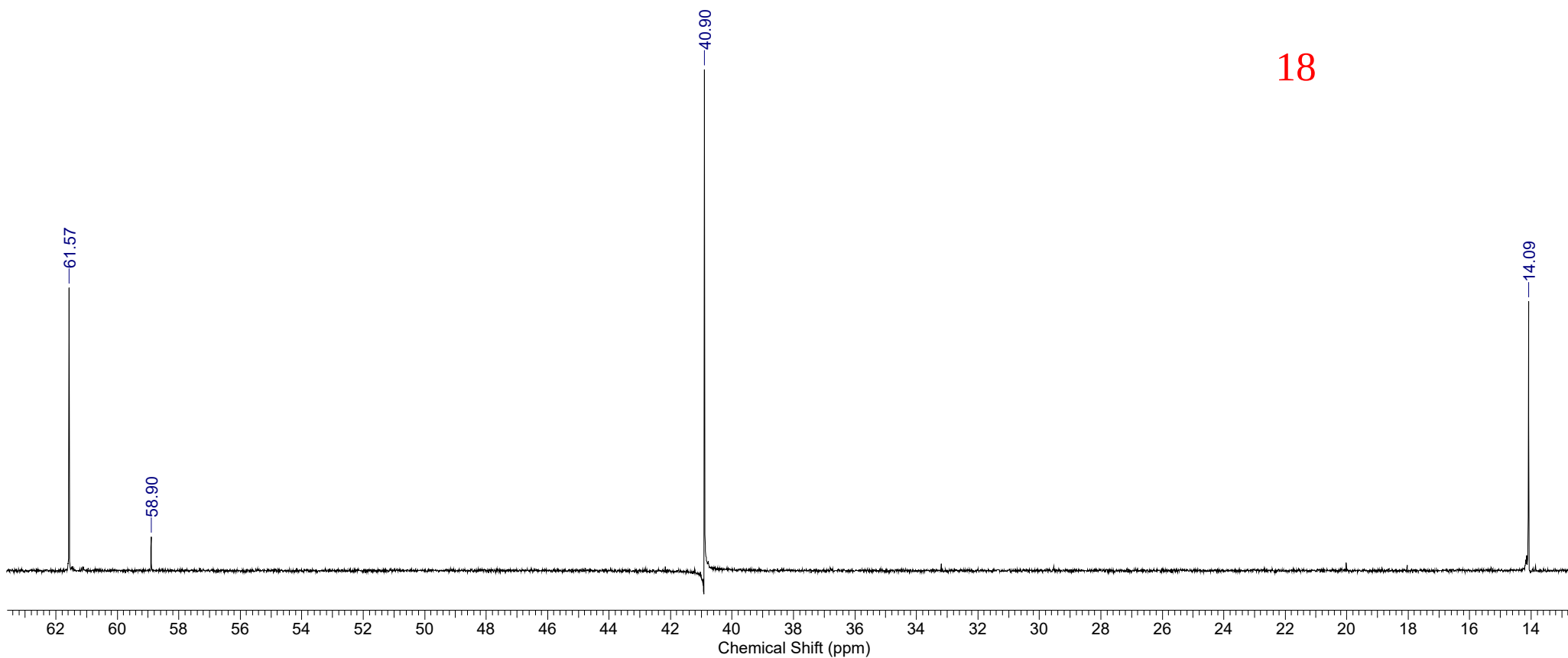
FZ7063-2.jdf



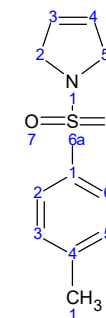
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE		Date	10 Jan 1990 11:59:28		
Date Stamp	13 Dec 2018 07:43:04	File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7063-2.jdf		Frequency (MHz)	150.91		
Nucleus	13C	Number of Transients	290	Origin	ECA 600	Original Points Count	32768	
Points Count	32768	Pulse Sequence	single pulse dec		Receiver Gain	56.00	Owner	delta
Spectrum Offset (Hz)	15091.3428	Sweep Width (Hz)	47348.49		Solvent			CHLOROFORM-d



FZ7063-2.jdf

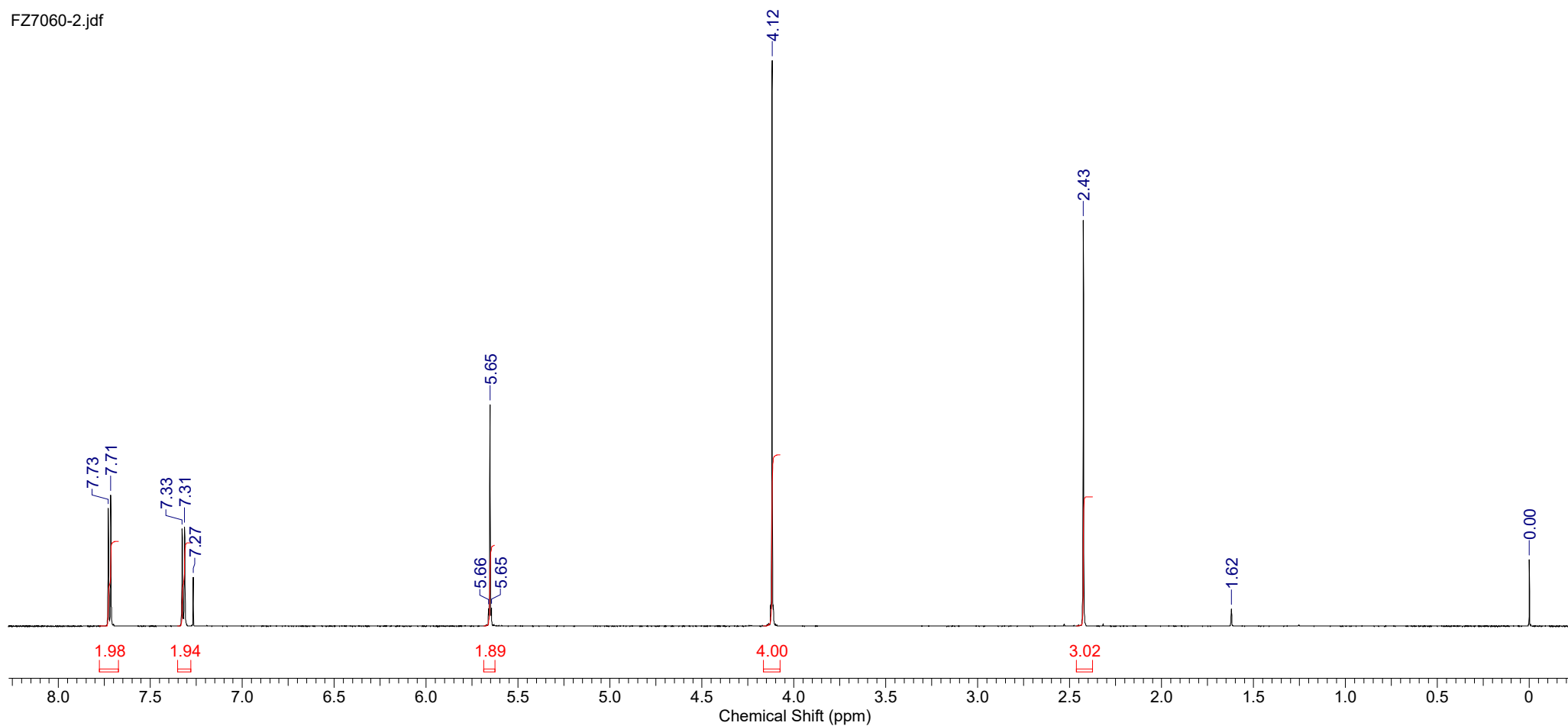


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jan 1990 12:13:38	Date Stamp	13 Dec 2018 07:57:14
File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7060-2.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	40.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5412.1411	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39

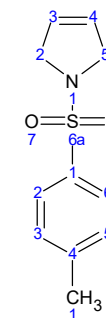


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FZ7060-2.jdf

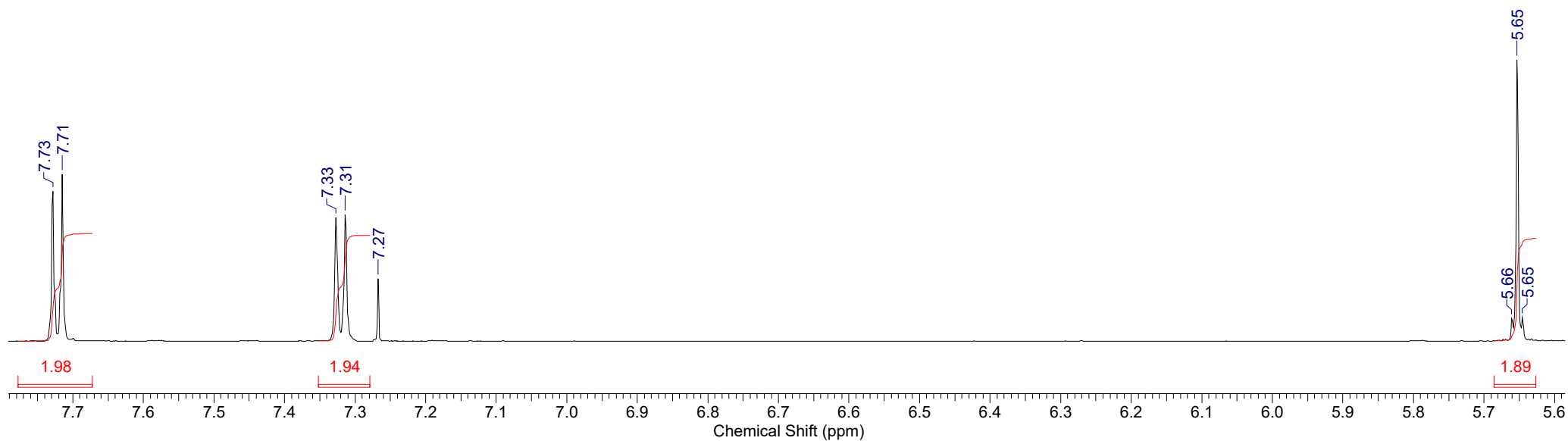


Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jan 1990 12:13:38	Date Stamp	13 Dec 2018 07:57:14
File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7060-2.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	40.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5412.1411	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39

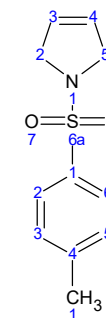


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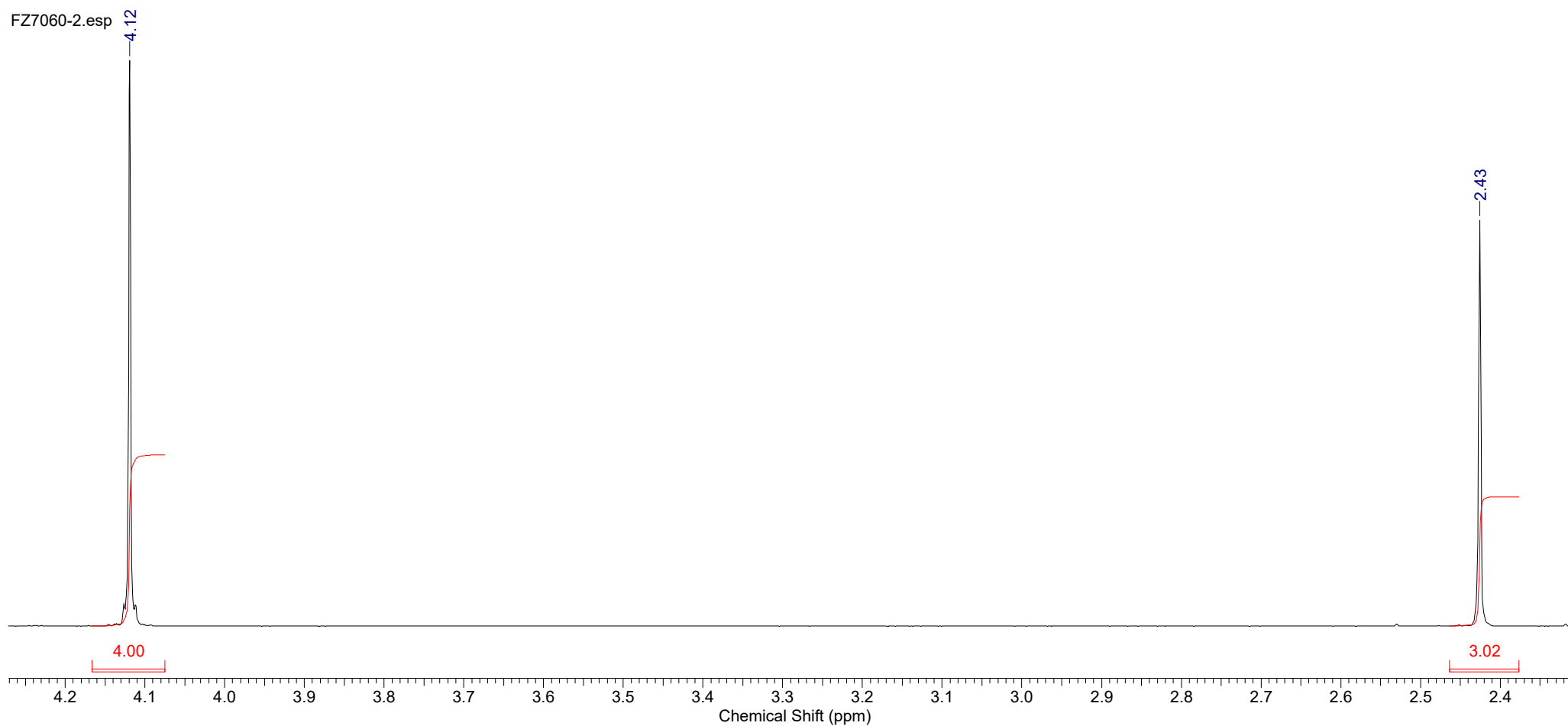
FZ7060-2.esp



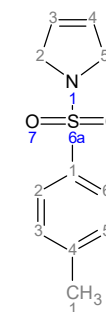
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	10 Jan 1990 12:13:38	Date Stamp	13 Dec 2018 07:57:14
File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7060-2.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	40.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5412.1411	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



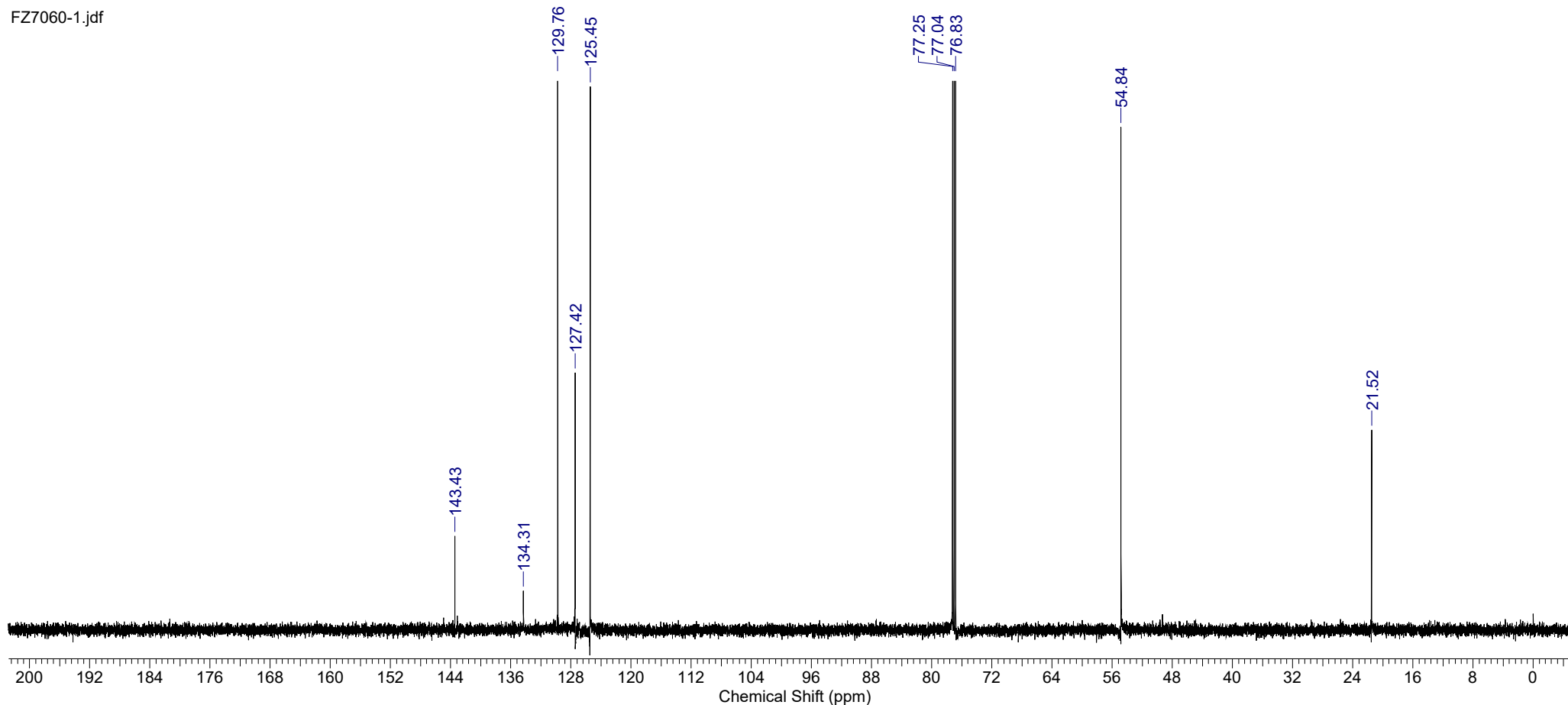
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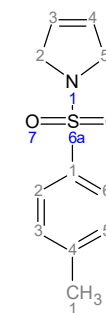
Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	10 Jan 1990 12:12:28
Date Stamp	13 Dec 2018 07:56:04	File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7060-1.jdf	Frequency (MHz)	150.91
Nucleus	¹³ C	Number of Transients	400	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15079.3525	Sweep Width (Hz)	47348.49	Receiver Gain	56.00
				Owner	delta
				Solvent	CHLOROFORM-d



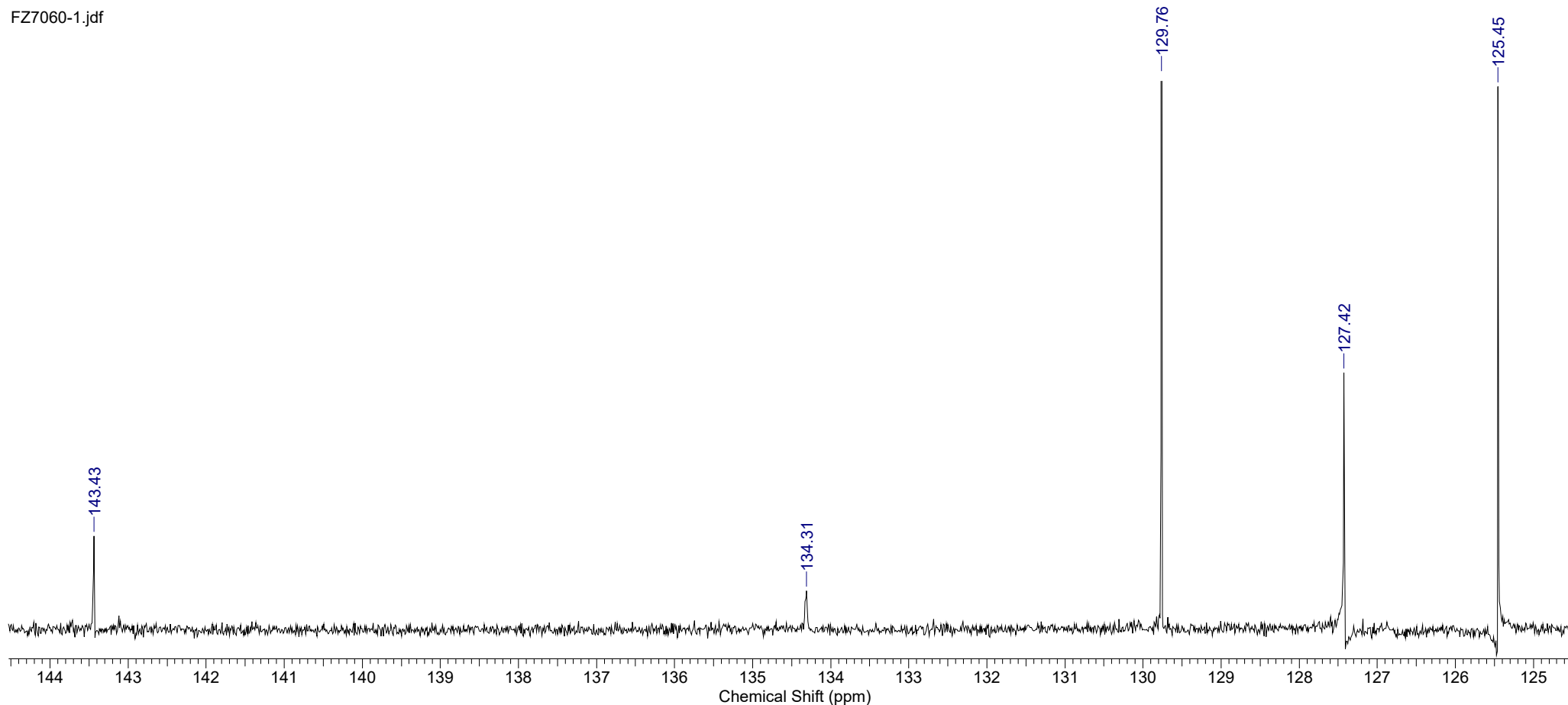
20



Acquisition Time (sec)	0.6921	Comment	single pulse decoupled gated NOE	Date	10 Jan 1990 12:12:28
Date Stamp	13 Dec 2018 07:56:04	File Name	C:\Users\Fedor\Desktop\11.12.18\FZ7060-1.jdf	Frequency (MHz)	150.91
Nucleus	¹³ C	Number of Transients	400	Origin	ECA 600
Points Count	32768	Pulse Sequence	single_pulse_dec	Original Points Count	32768
Spectrum Offset (Hz)	15079.3525	Sweep Width (Hz)	47348.49	Receiver Gain	56.00
				Owner	delta
				Solvent	CHLOROFORM-d



20



2. Selected GC-MS data for metathesis products (**13-27**)

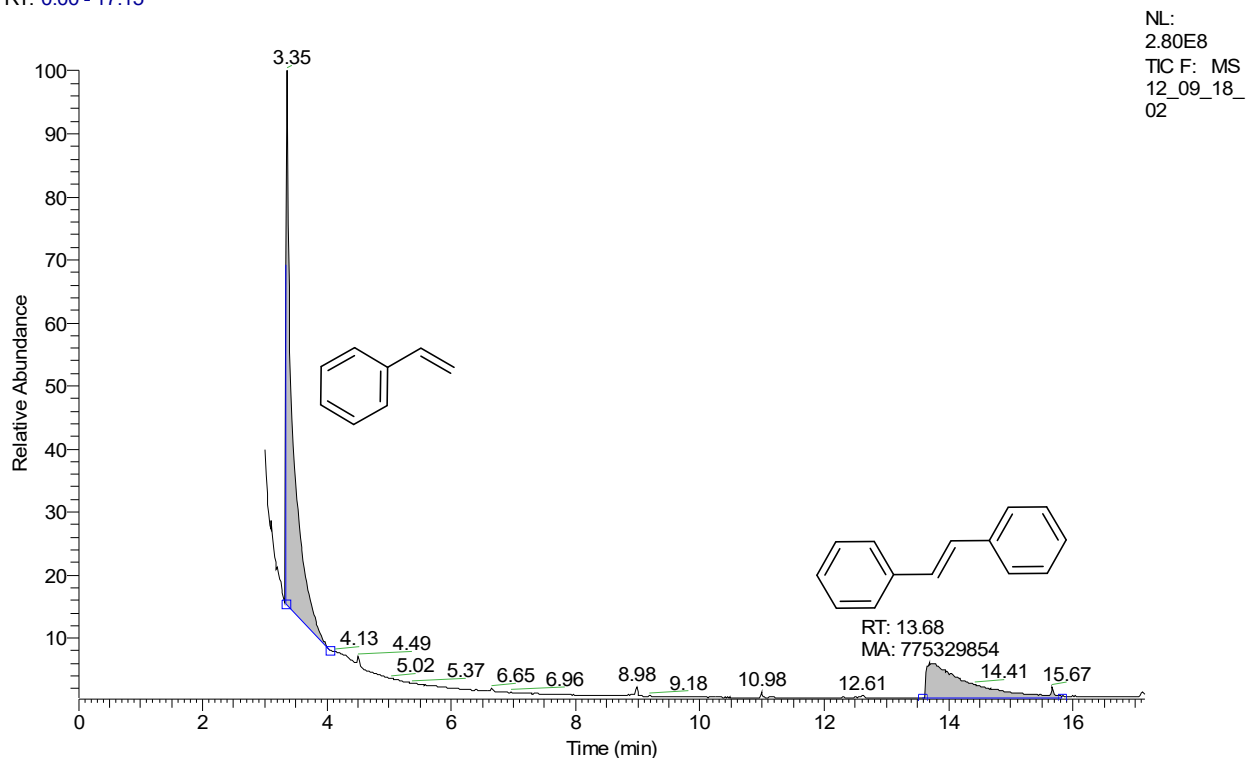
Table 3: Reaction conditions and yields of the metathesis products

Entry	Starting compound	Catalyst	Catalyst concentration (mol %)	Solvent ^a (conditions)	Yield (%), ratio ^b of the products
1	12	11a	1	PhMe (Ar)	13 (traces) ^c
2	12	11b	1	PhMe (Ar)	12/13 (43%), 51/49
3	12	11a	1	PhH (Ar)	13 (traces) ^c
4	12	11b	1	PhH (Ar)	12/13 (52%), 40/60
5	12	11a	1	MeCN (Ar)	no product ^c
6	12	11a	1	THF (Ar)	no product ^c
7	12	11a	1	CH ₂ Cl ₂ (Ar)	13 (17%) ^d
8	12	11a	0.1	CH ₂ Cl ₂ (Ar)	13 (traces) ^c
9	12	11b	1	CH ₂ Cl ₂ (Ar)	13 (49%) ^d
10	12	11b	0.1	CH ₂ Cl ₂ (Ar)	13 (79%) ^d
11	12	11c	1	CH ₂ Cl ₂ (Ar)	12/13 (51%), 44/56
12	12	11d	1	CH ₂ Cl ₂ (Ar)	13 (91%) ^d
13	12	11d	0.1	CH ₂ Cl ₂ (Ar)	13 (97%) ^d
14	12	11d	0.01	CH ₂ Cl ₂ (Ar)	12/13 (93%), 69/31
15	12	11a	1	CHCl ₃ (Ar)	13 (86%) ^d
16	12	11a	0.1	CHCl ₃ (Ar)	13 (95%) ^d
17	12	11b	1	CHCl ₃ (Ar)	13 (96%) ^d
18	12	11b	0.1	CHCl ₃ (Ar)	13 (97%) ^d
19	12	11b	0.01	CHCl ₃ (Ar)	13 (81%) ^d
20	12	11b	0.1	CHCl ₃ (air)	13 (89%) ^d
21	12	11d	1	CHCl ₃ (Ar)	13 (95%) ^d
22	12	11d	0.1	CHCl ₃ (Ar)	13 (99%) ^d
23	12	11d	0.01	CHCl ₃ (Ar)	12/13 (98%), 64/36
24	14	11b	0.1	CHCl ₃ (Ar)	15/16 (93%), 64/36
25	17	11a	0.1	CHCl ₃ (air)	17/18 (46%), 44/56
26	17	11b	0.1	CHCl ₃ (air)	17/18 (58%), 42/58
27	17	11b	0.01	CHCl ₃ (Ar)	18 (traces) ^c
28	17	11b	0.1	CHCl ₃ (Ar)	17/18 (98%), 2/98
29	17	11d	0.1	CHCl ₃ (air)	17/18 (63%), 42/58
30	17	11d	0.1	CHCl ₃ (Ar)	17/18 (96%), 4/96
31	17	11d	0.01	CHCl ₃ (air)	18 (traces)
32	19	11d	0.1	CHCl ₃ (Ar)	19/20 (99%), 5/95
33	19	11d	0.01	CHCl ₃ (Ar)	19/20 (75%), 23/77
34	21 + 2 eq 12	11a	0.1	CHCl ₃ (Ar)	13/22/23 (71%), ~77/20/3 ^f
35	21 + 2 eq 12	11d	0.1	CHCl ₃ (Ar)	13/22/23 (78%), ~81/18/1 ^f
36	21 + 2 eq 24	11a	0.1	CHCl ₃ (Ar)	25/26/27 (40%), ~3/76/21 ^f
37	21 + 2 eq 24	11b	0.1	CHCl ₃ (Ar)	25/26/27 (52%), ~2/72/26 ^f

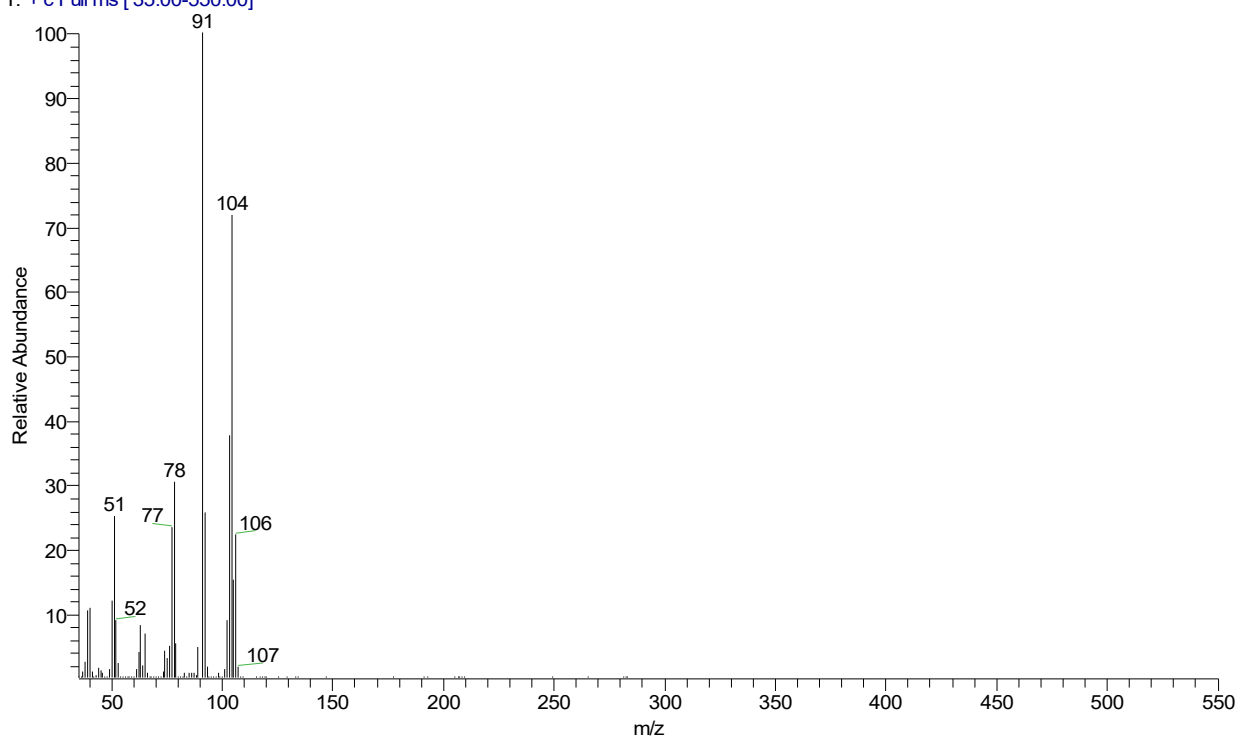
Entry 2.

Starting compound – **12**. Catalyst – **11a** (1 mol %). The reaction mixture was heated at reflux in PhH for 4 h under an argon atmosphere.

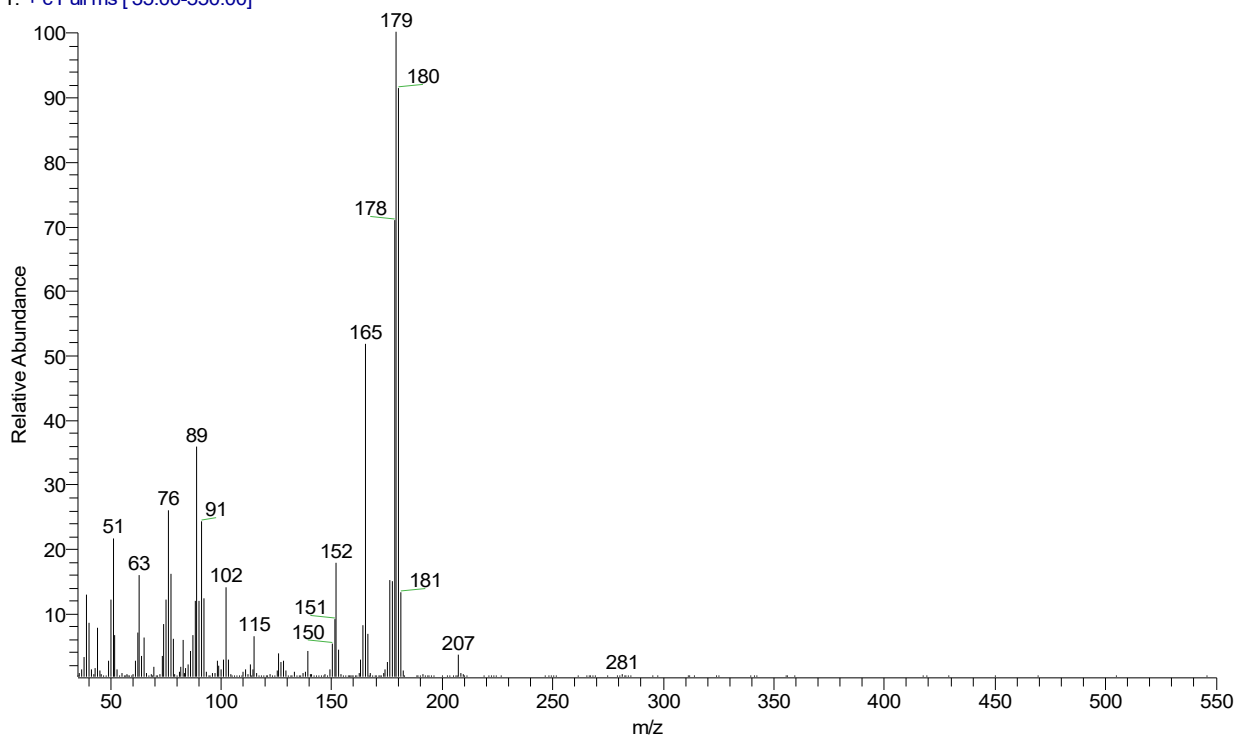
RT: 0.00 - 17.15



12_09_18_02 #23 RT: 3.35 AV: 1 NL: 5.85E7
T: + c Full ms [35.00-550.00]



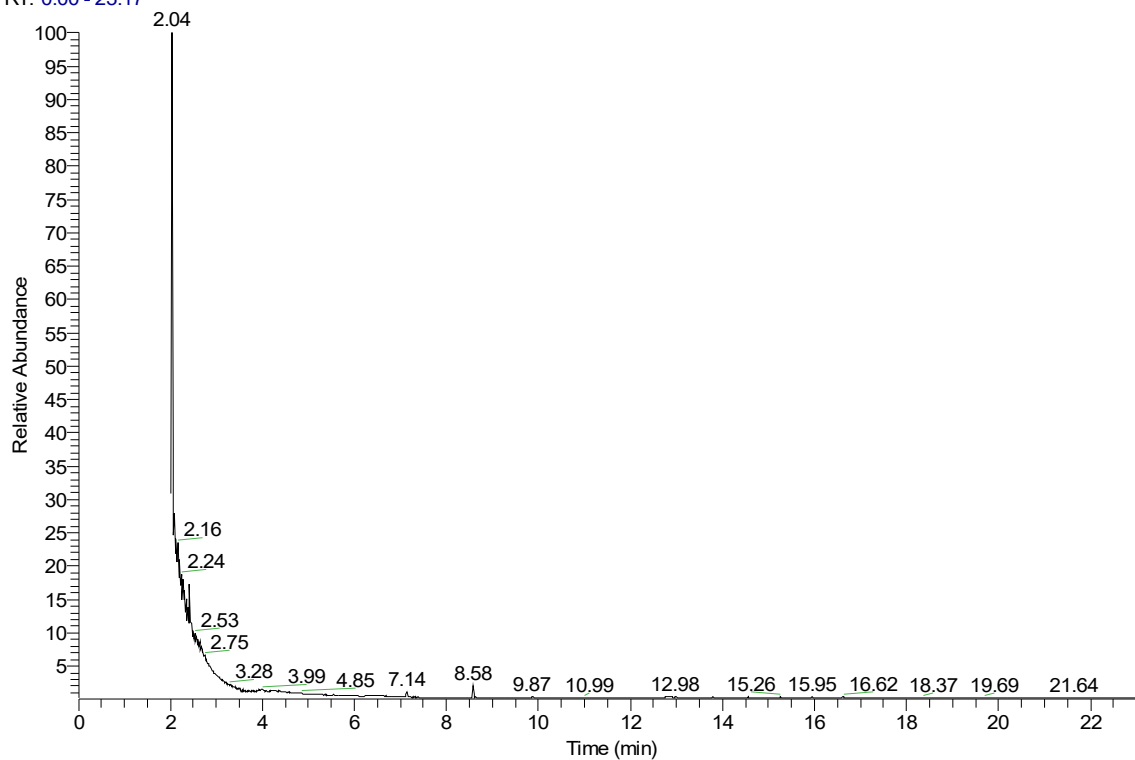
12_09_18_02 #590 RT: 13.68 AV: 1 NL: 2.10E6
T: + c Full ms [35.00-550.00]



Entry 3.

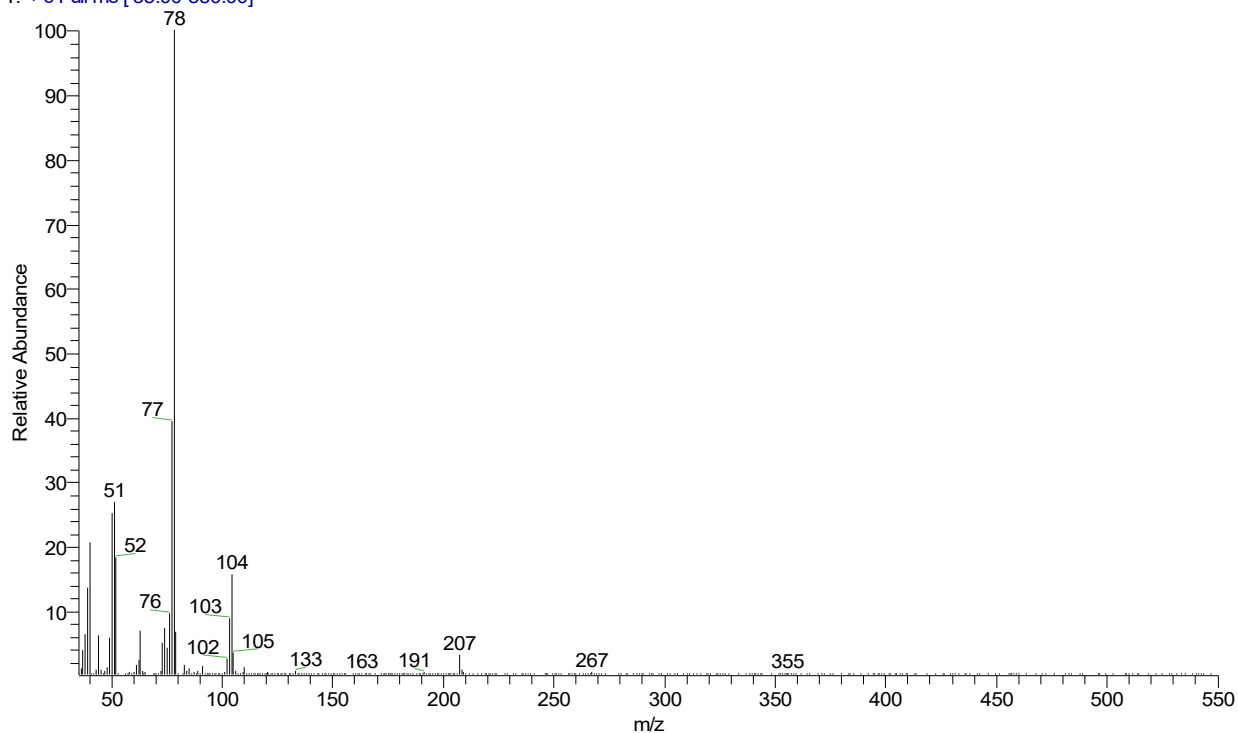
Starting compound – **12**. Catalyst – **11a** (1 mol %). The reaction mixture was heated at reflux in PhH for 4 h under an argon atmosphere.

RT: 0.00 - 23.17



NL:
4.48E9
TIC F: MS
21_09_18_
04

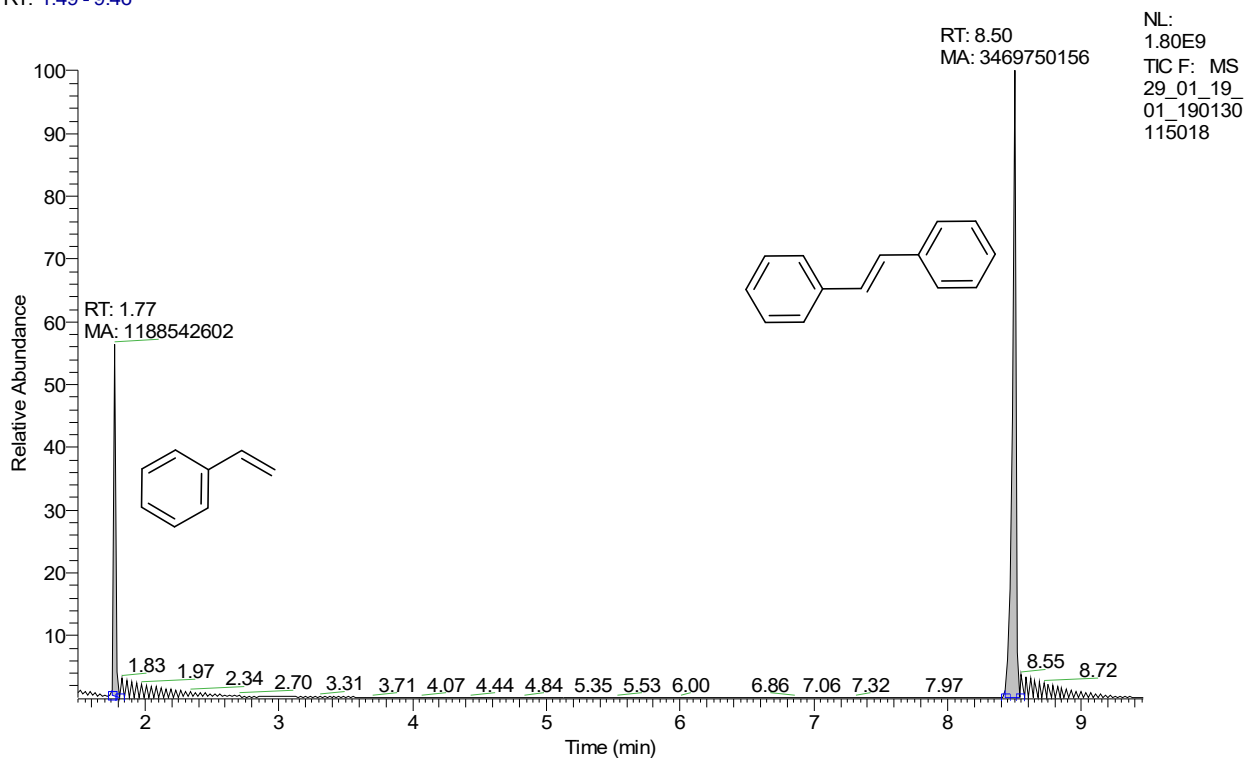
21_09_18_04 #124 RT: 4.25 AV: 1 NL: 1.51E7
T: + c Full ms [35.00-550.00]



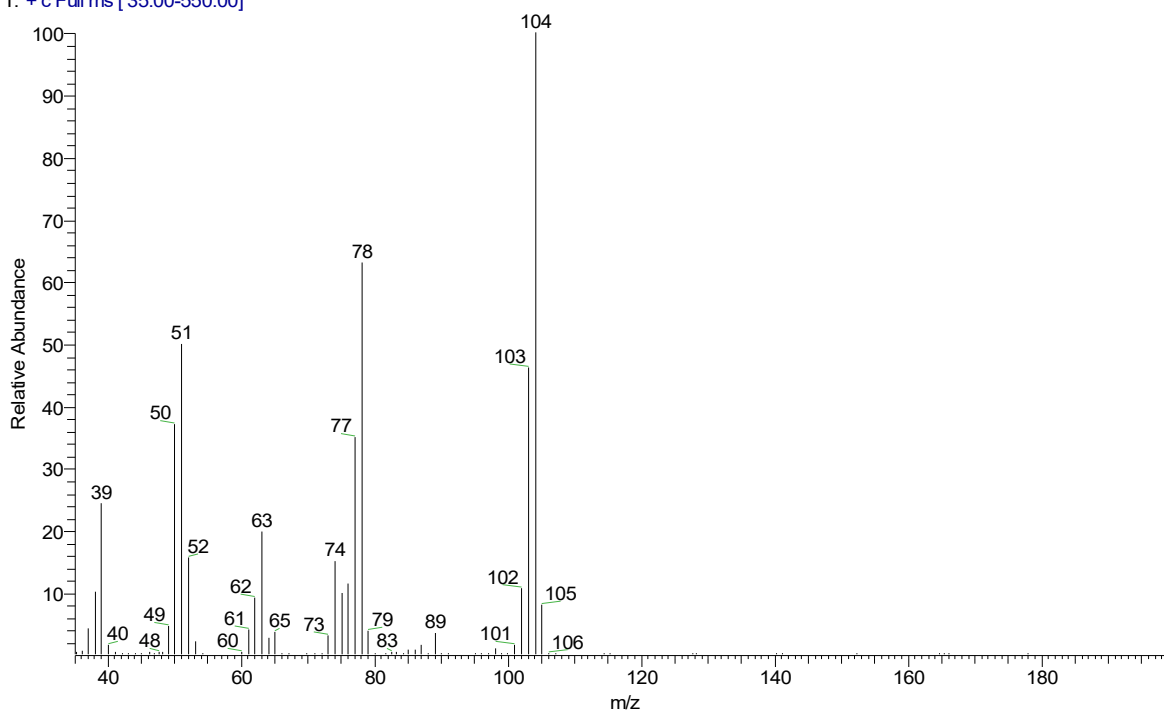
Entry 4.

Starting compound – **12**. Catalyst – **11d** (1 mol %). The reaction mixture was heated at reflux in PhMe for 4 h.

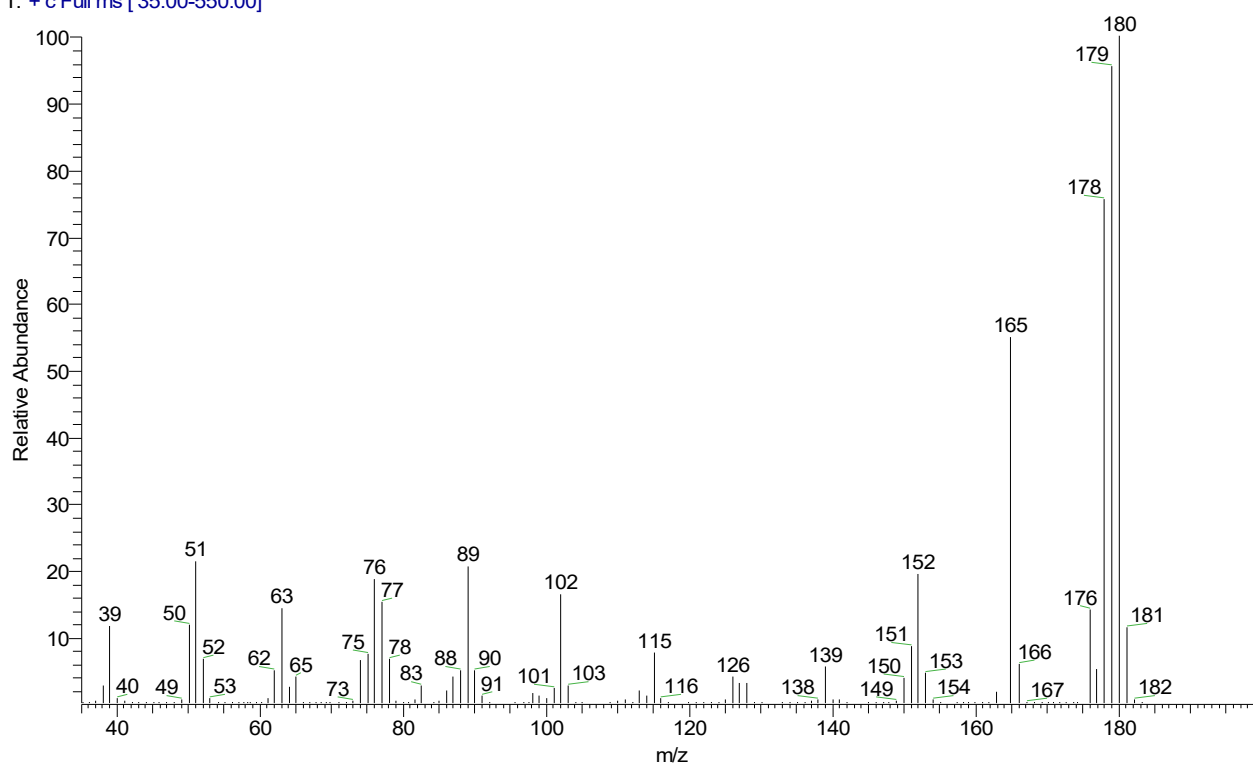
RT: 1.49 - 9.46



29_01_19_01_190130115018 #96 RT: 1.77 AV: 1 NL: 1.97E8
T: + c Full ms [35.00-550.00]



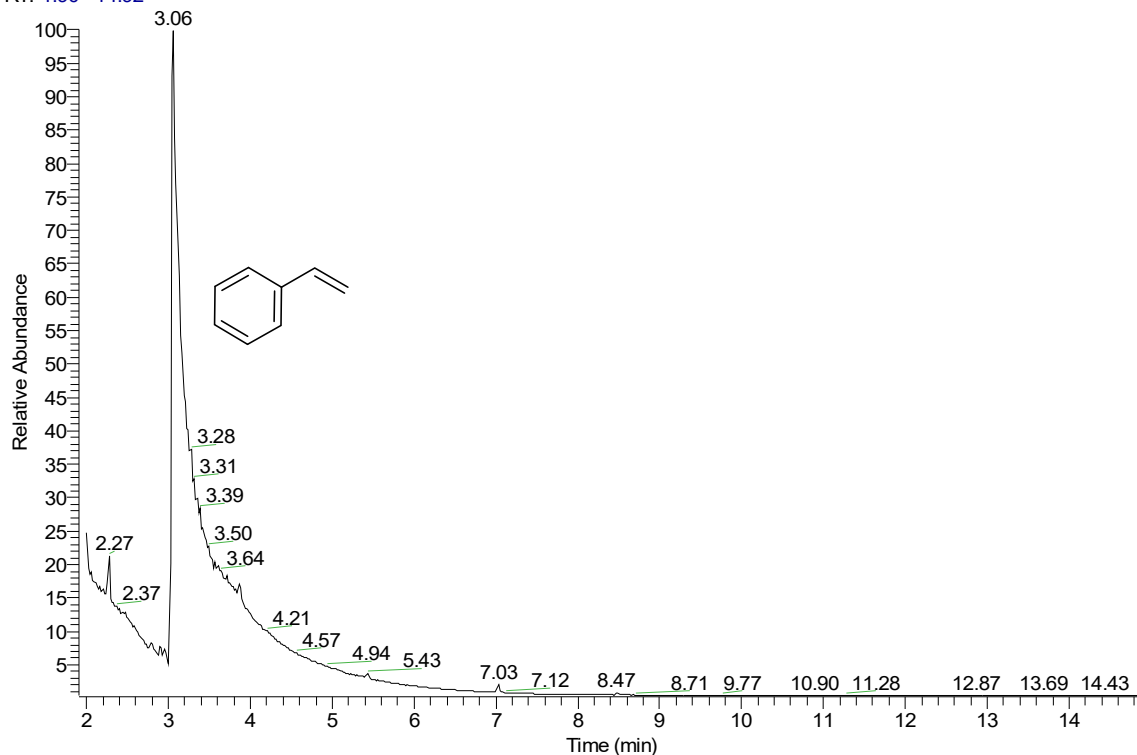
29_01_19_01_190130115018 #465 RT: 8.50 AV: 1 NL: 2.77E8
T: + c Full ms [35.00-550.00]



Entry 5.

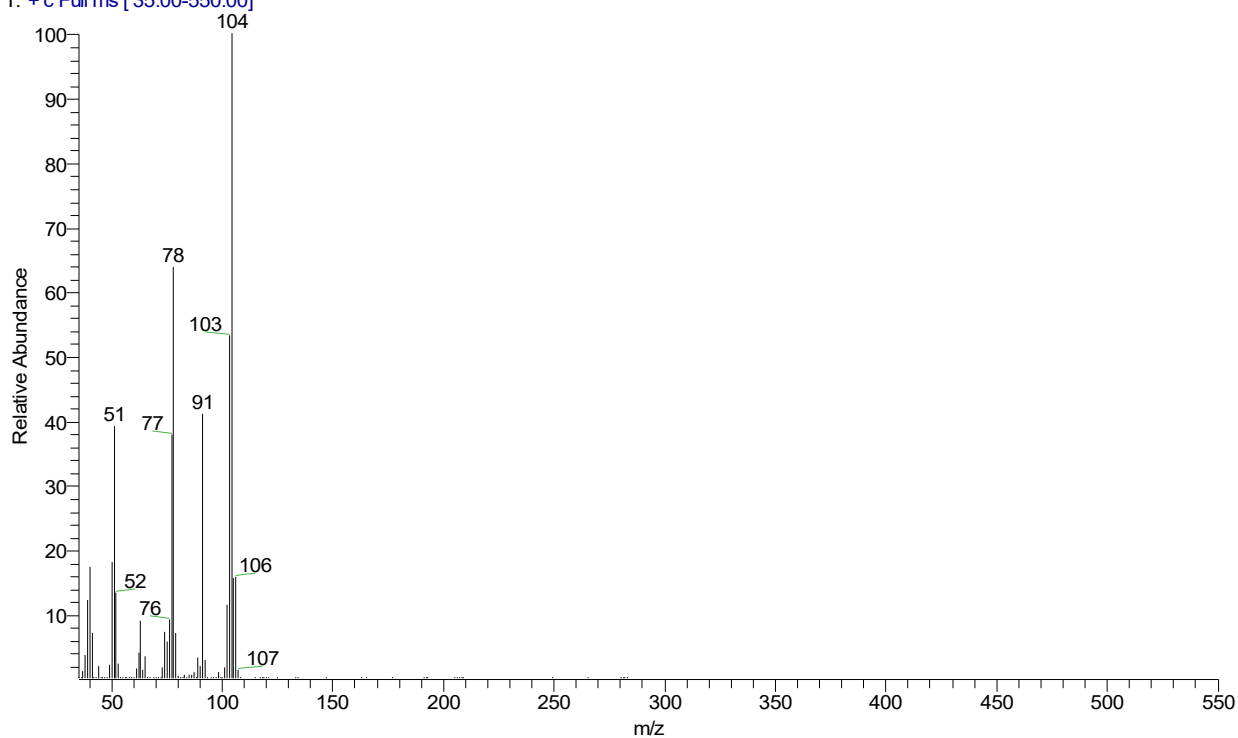
Starting compound – **12**. Catalyst – **11a** (1 mol %). The reaction mixture was heated at reflux in MeCN for 4 h under an argon atmosphere.

RT: 1.90 - 14.92



NL:
2.08E9
TIC F: MS
15_10_18_
02

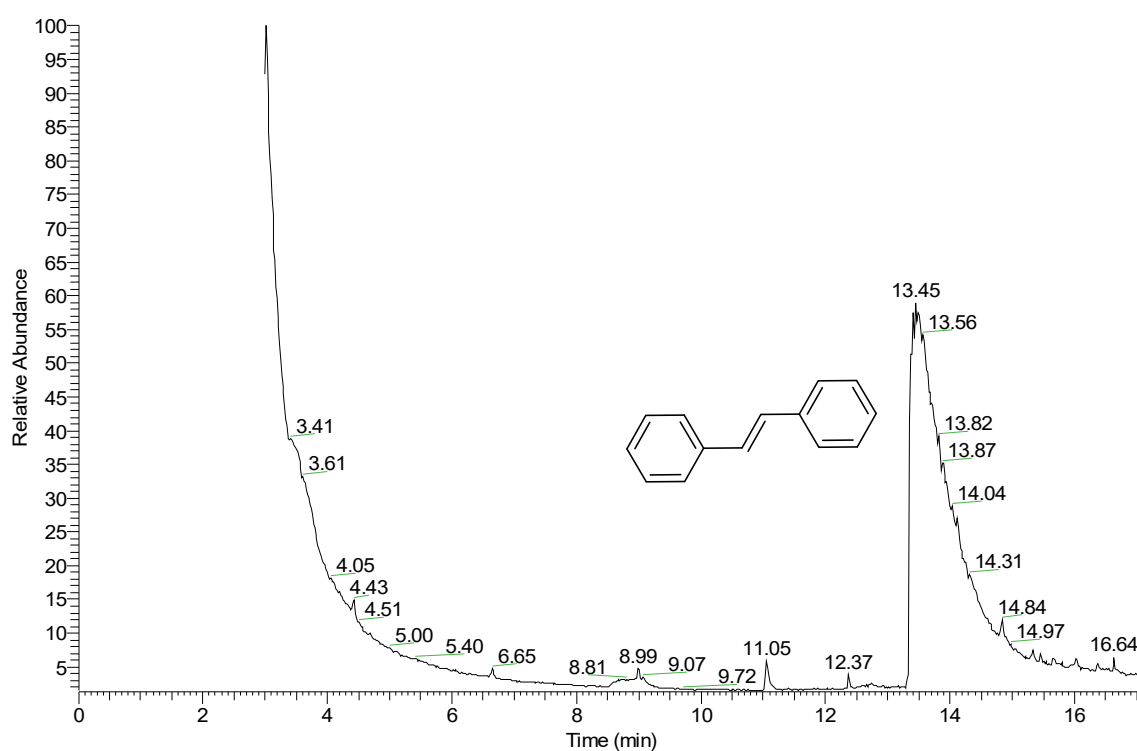
15_10_18_02 #59 RT: 3.06 AV: 1 NL: 3.92E8
T: + c Full ms [35.00-550.00]



Entry 9.

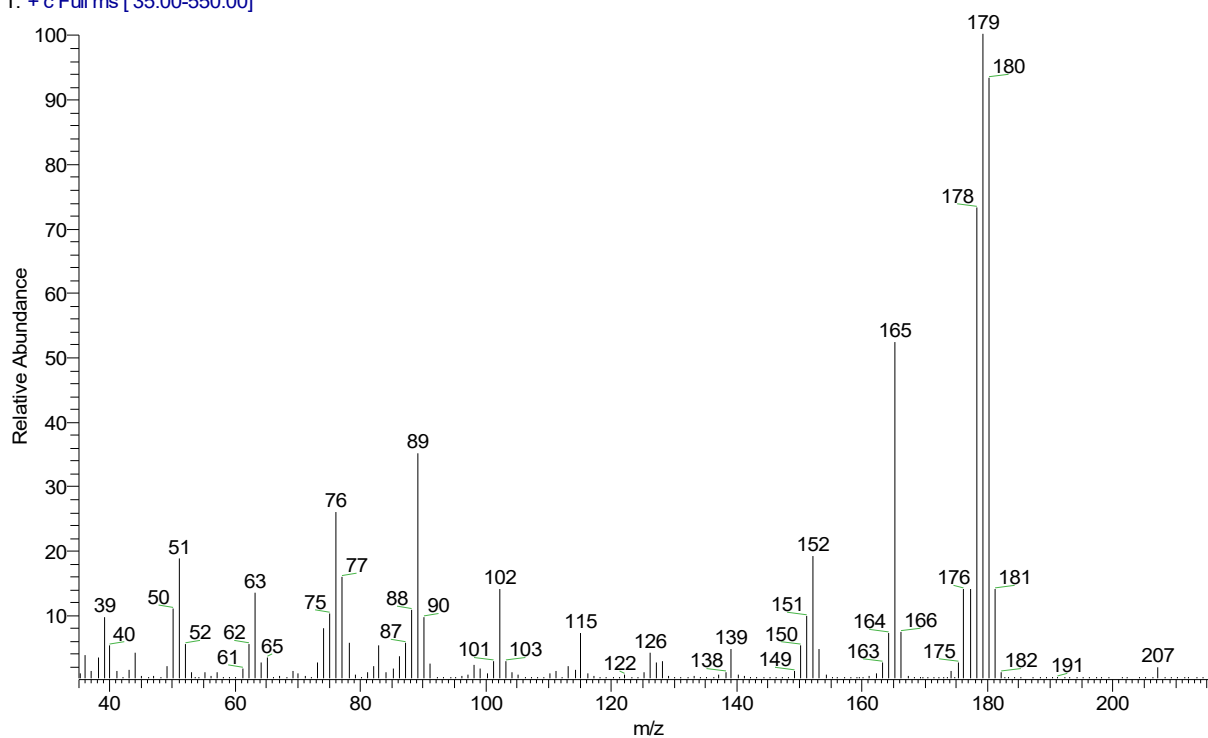
Starting compound – **12**. Catalyst – **11b** (1 mol %). The reaction mixture was heated at reflux in CH₂Cl₂ for 4 h under an argon atmosphere.

RT: 0.00 - 17.11



NL:
3.91E7
TIC F: MS
20_09_18_
03

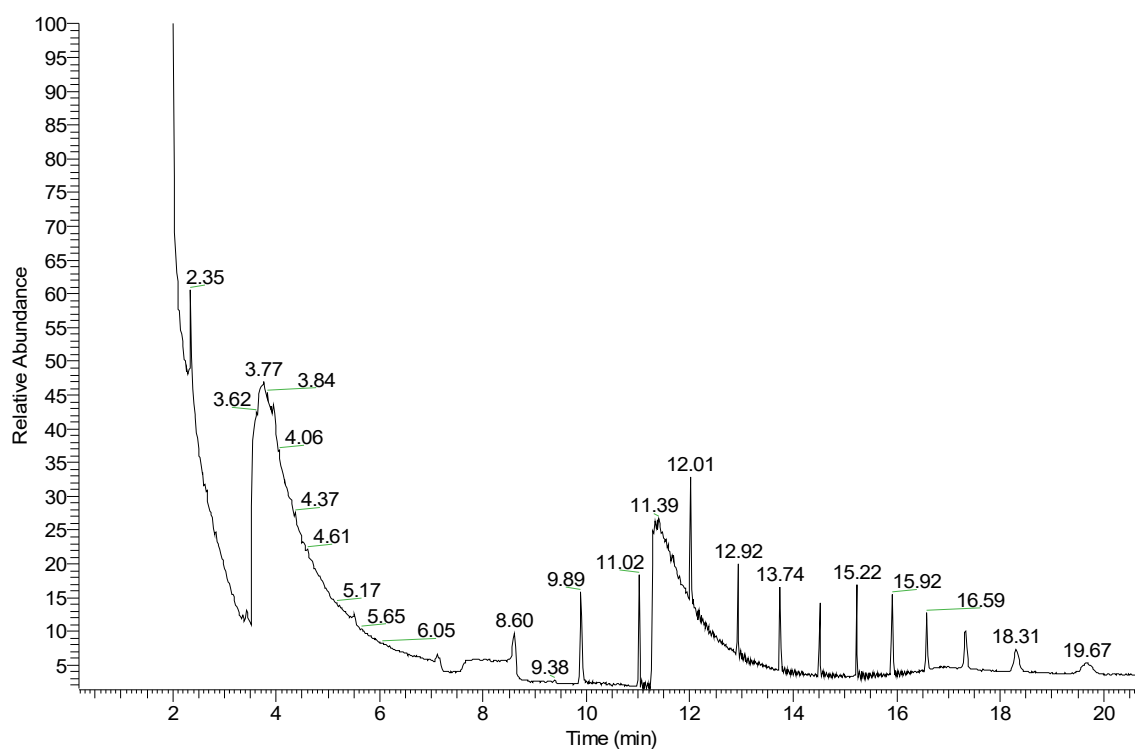
20_09_18_03 #573 RT: 13.45 AV: 1 NL: 3.07E6
T: + c Full ms [35.00-550.00]



Entry 11.

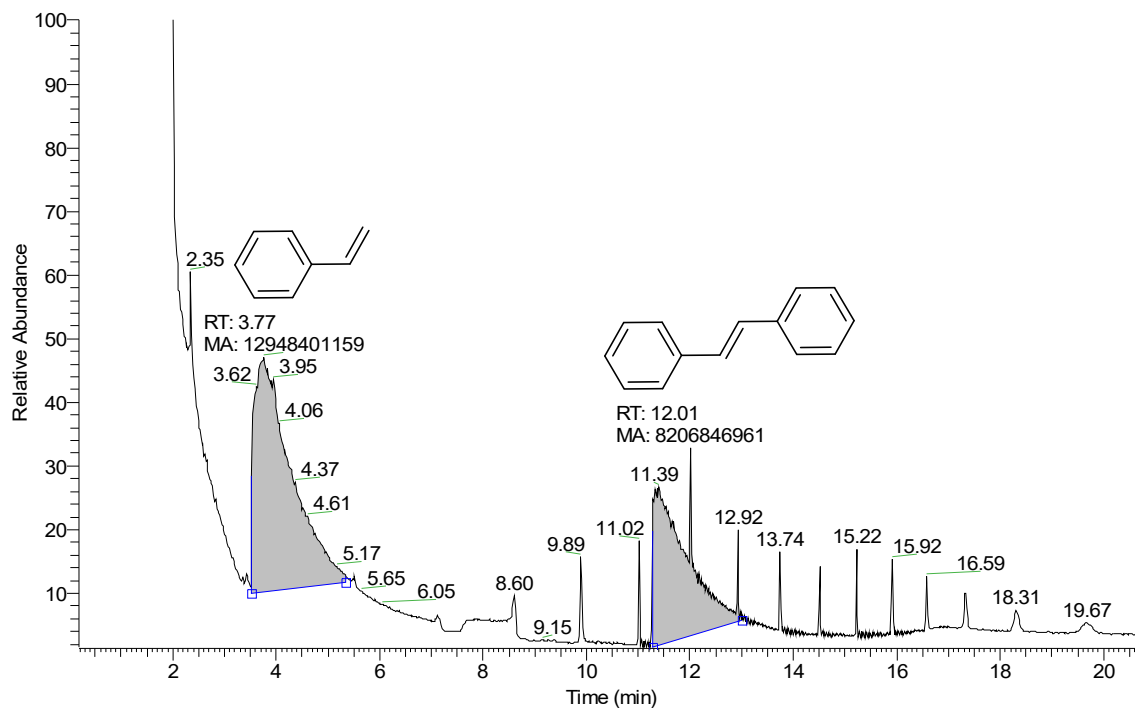
Starting compound – **12**. Catalyst – **11c** (1 mol %). The reaction mixture was heated at reflux in CH₂Cl₂ for 4 h under an argon atmosphere.

RT: 0.17 - 20.78



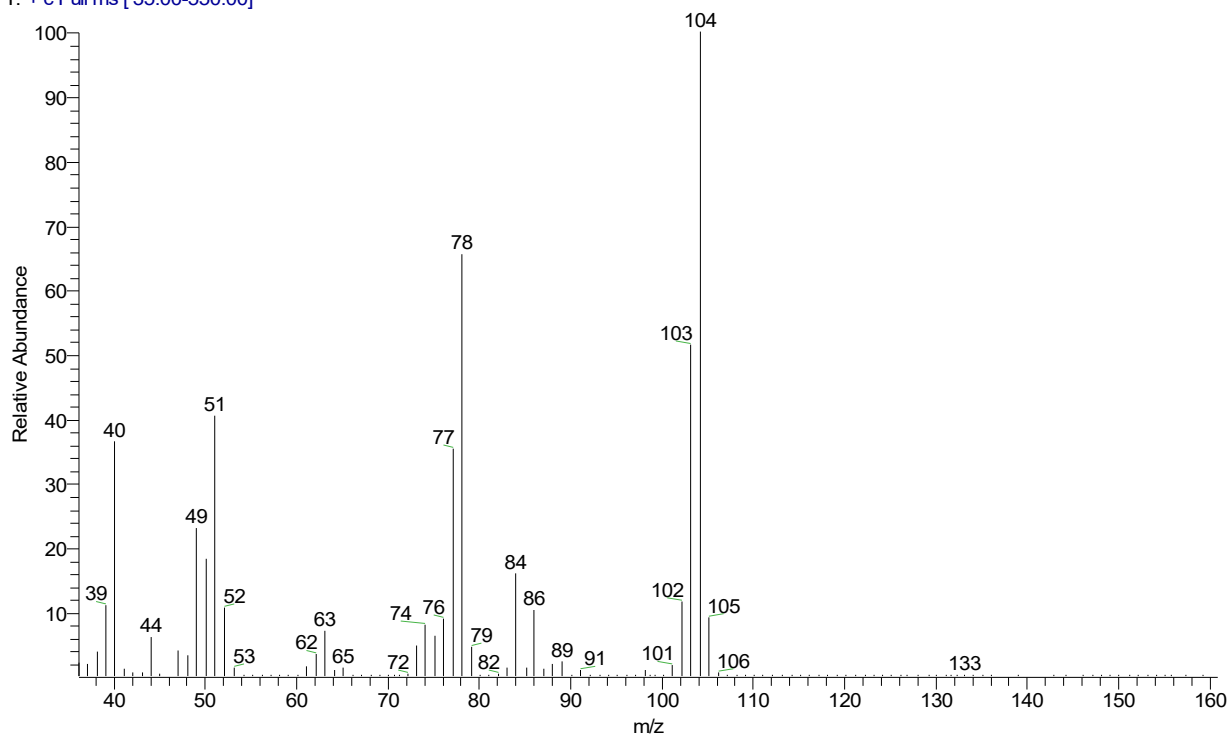
NL:
7.07E8
TIC F: MS
16_10_18_
01

RT: 0.17 - 20.78

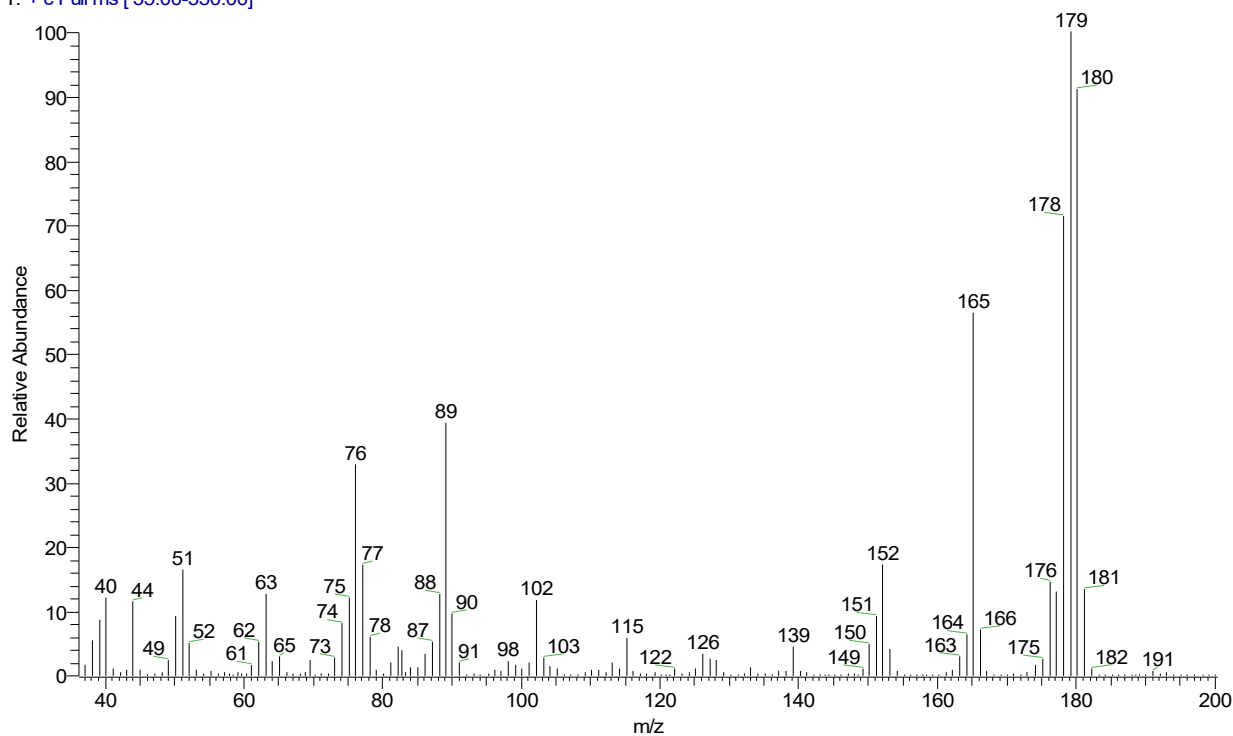


NL:
7.07E8
TIC F: MS
16_10_18_
01

16_10_18_01 #96 RT: 3.73 AV: 1 NL: 6.01E7
T: + c Full ms [35.00-550.00]



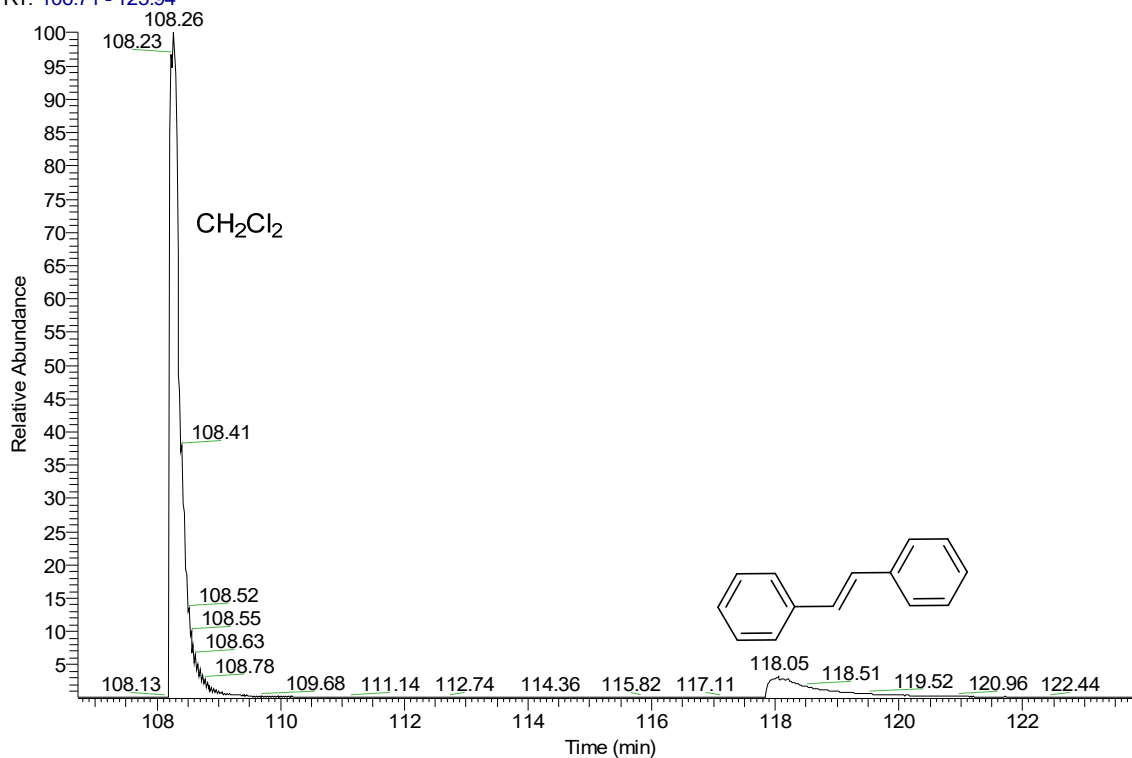
16_10_18_01 #520 RT: 11.45 AV: 1 NL: 2.21E7
T: + c Full ms [35.00-550.00]



Entry 12.

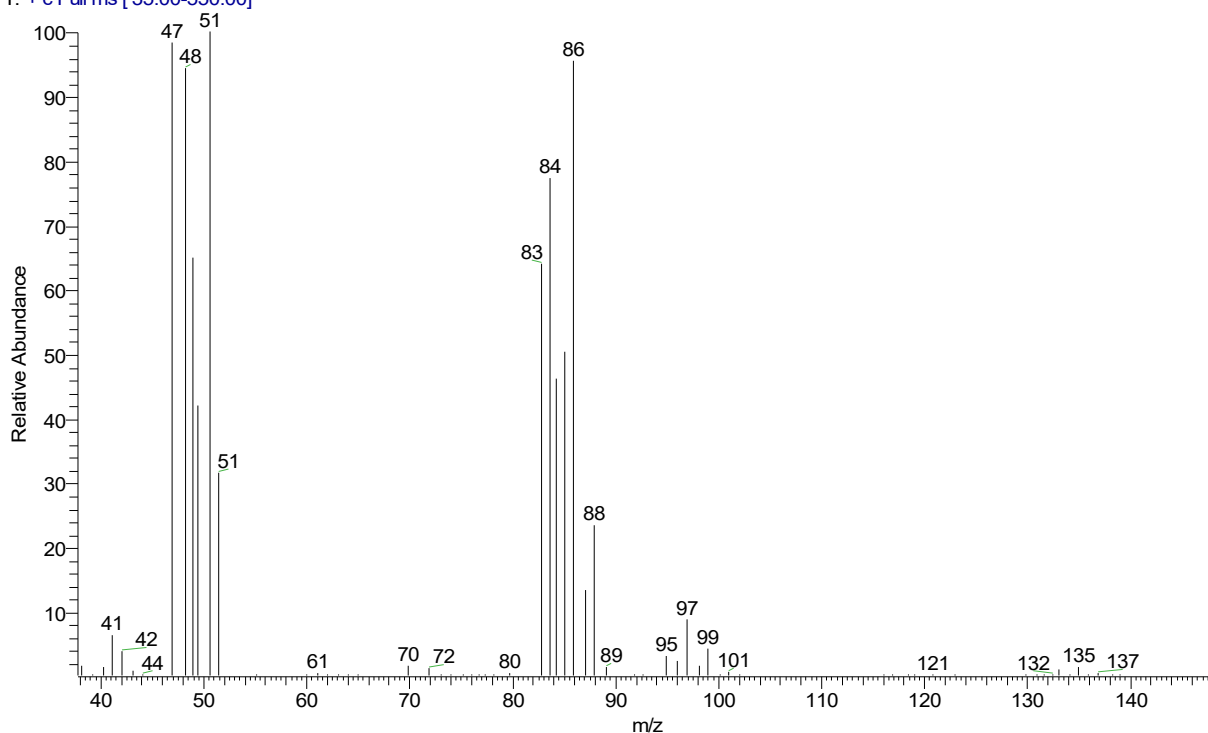
Starting compound – **12**. Catalyst – **11d** (1 mol %). The reaction mixture was heated at reflux in CH₂Cl₂ for 4 h under an argon atmosphere.

RT: 106.71 - 123.94

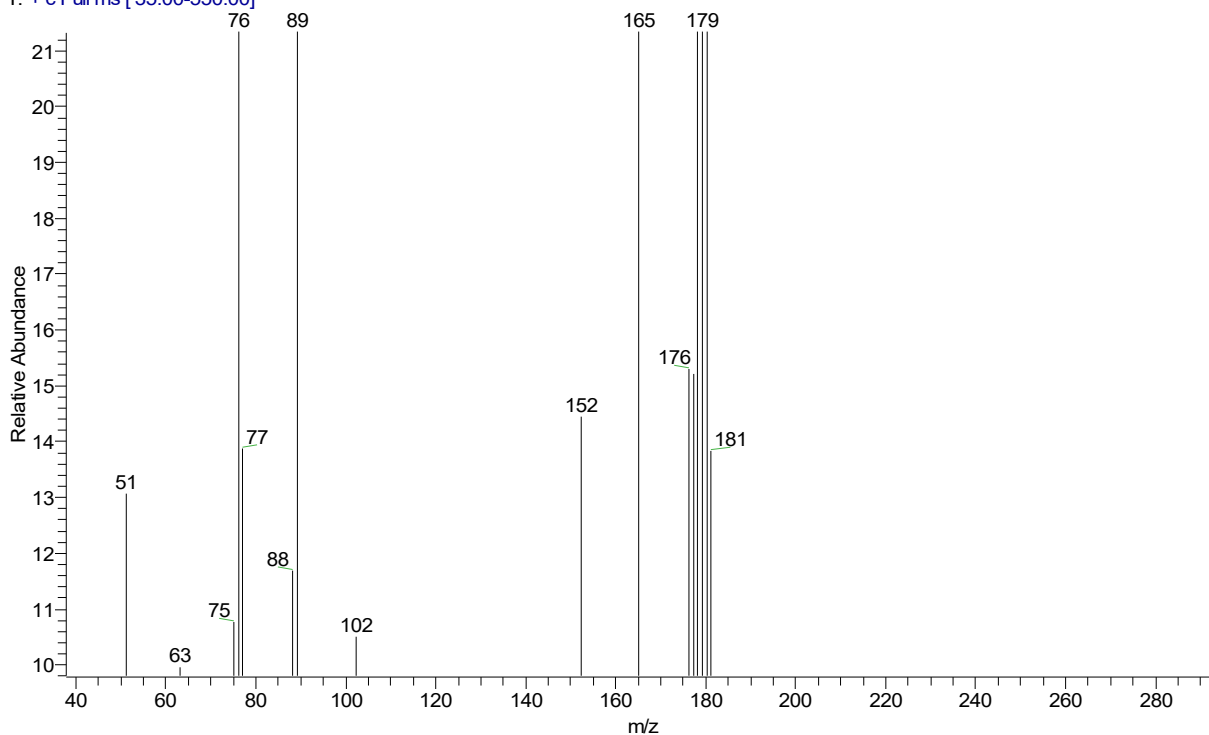


NL:
1.15E10
TIC F: MS
21_09_18_
12_180926
142135

21_09_18_12_180926142135 #5961 RT: 108.25 AV: 1 NL: 1.22E9
T: + c Full ms [35.00-550.00]



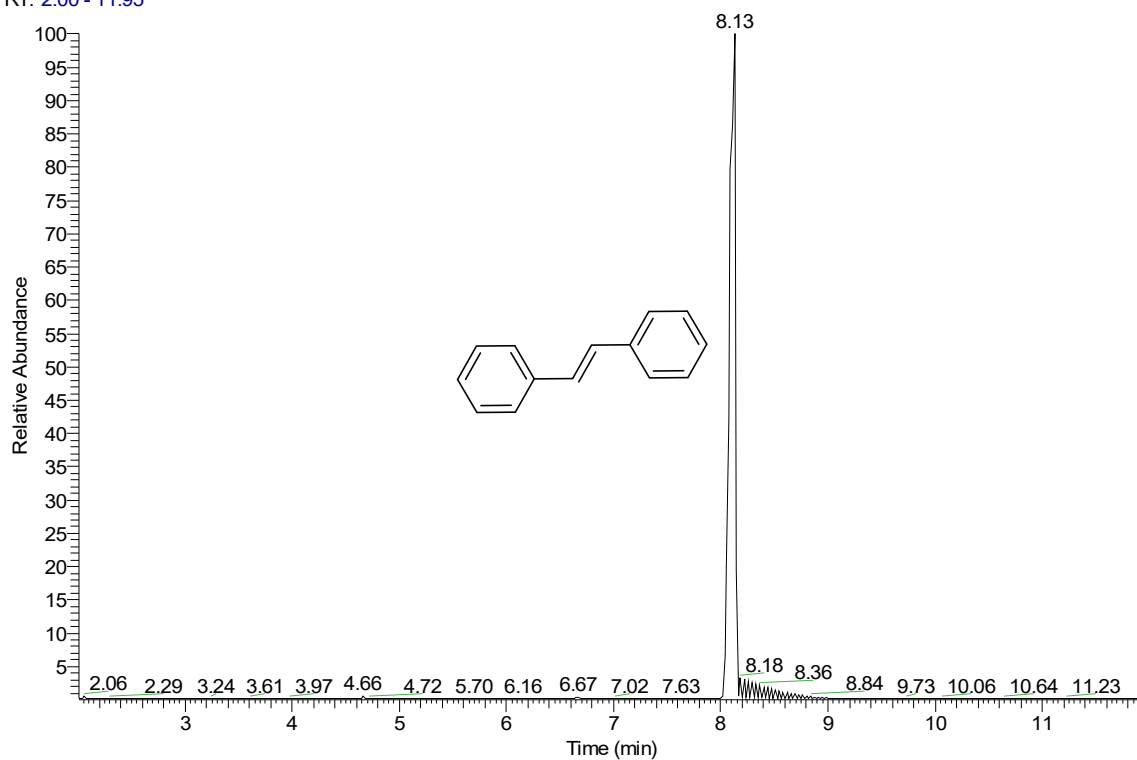
21_09_18_12_180926142135 #6504 RT: 118.18 AV: 1 NL: 4.62E7
T: + c Full ms [35.00-550.00]



Entry 13.

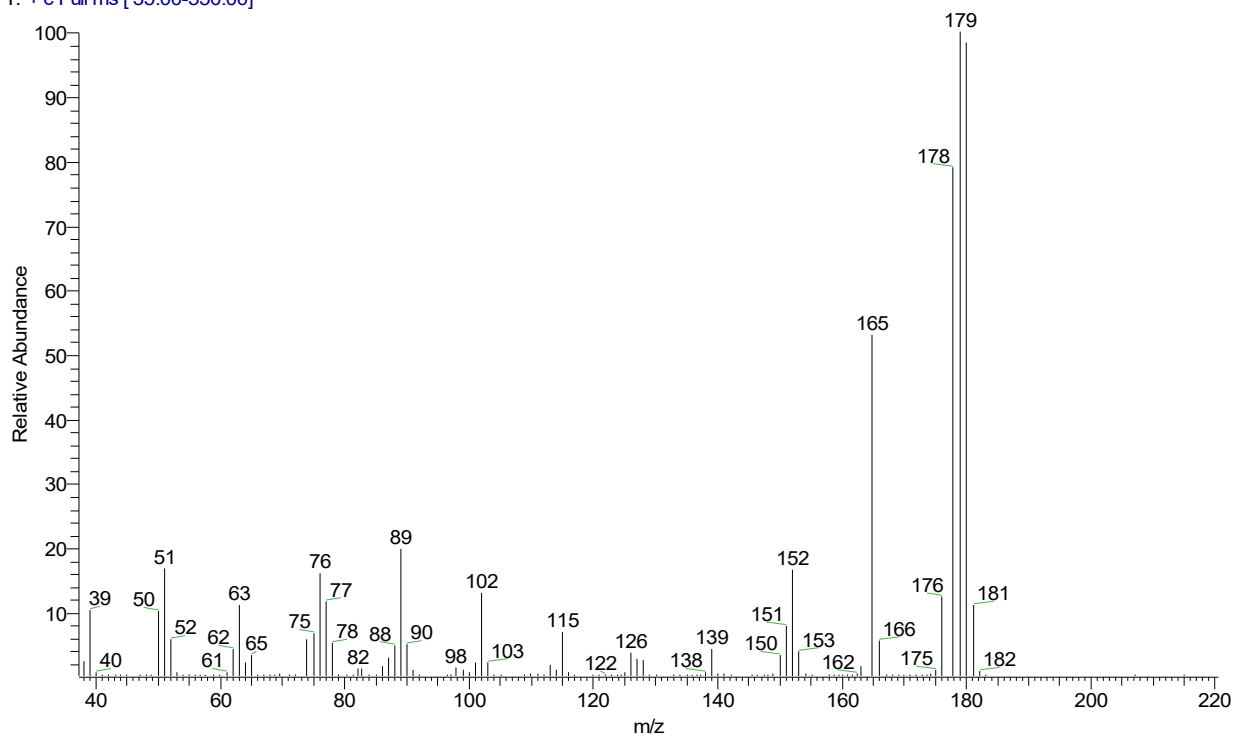
Starting compound – **12**. Catalyst – **11d** (0.1 mol %). The reaction mixture was heated at reflux in CH₂Cl₂ for 4 h under an argon atmosphere.

RT: 2.00 - 11.95



NL:
2.02E9
TIC F: MS
25_01_19_
10

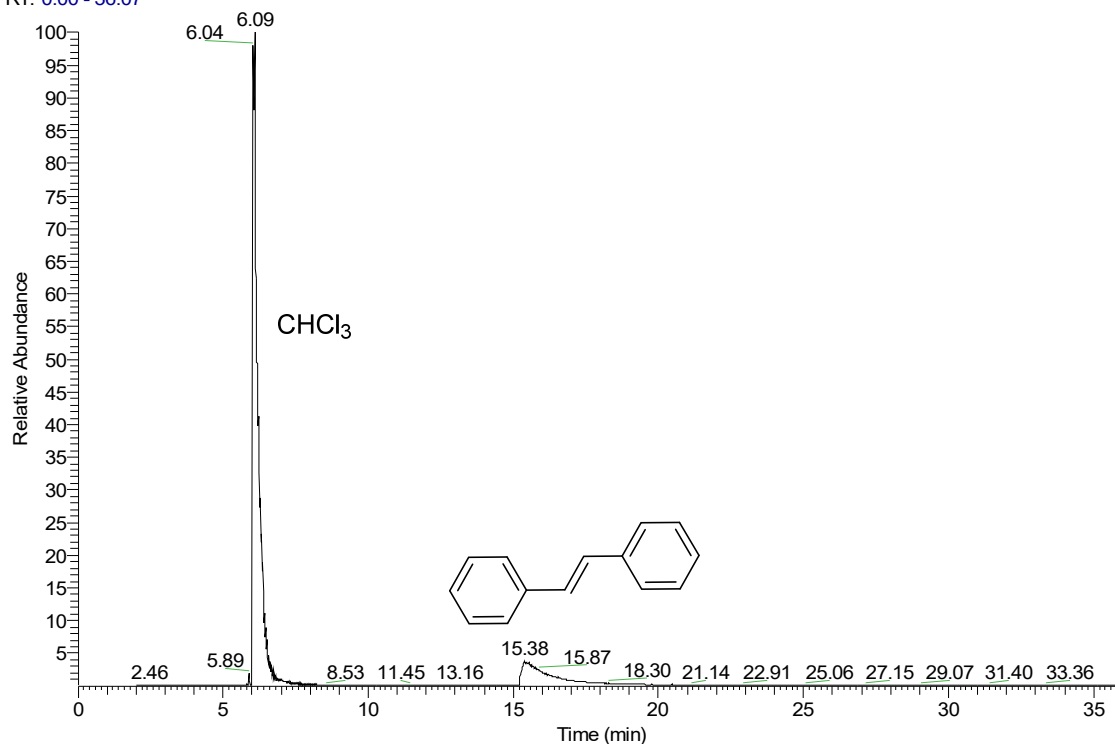
25_01_19_10 #337 RT: 8.13 AV: 1 NL: 3.34E8
T: + c Full ms [35.00-550.00]



Entry 17.

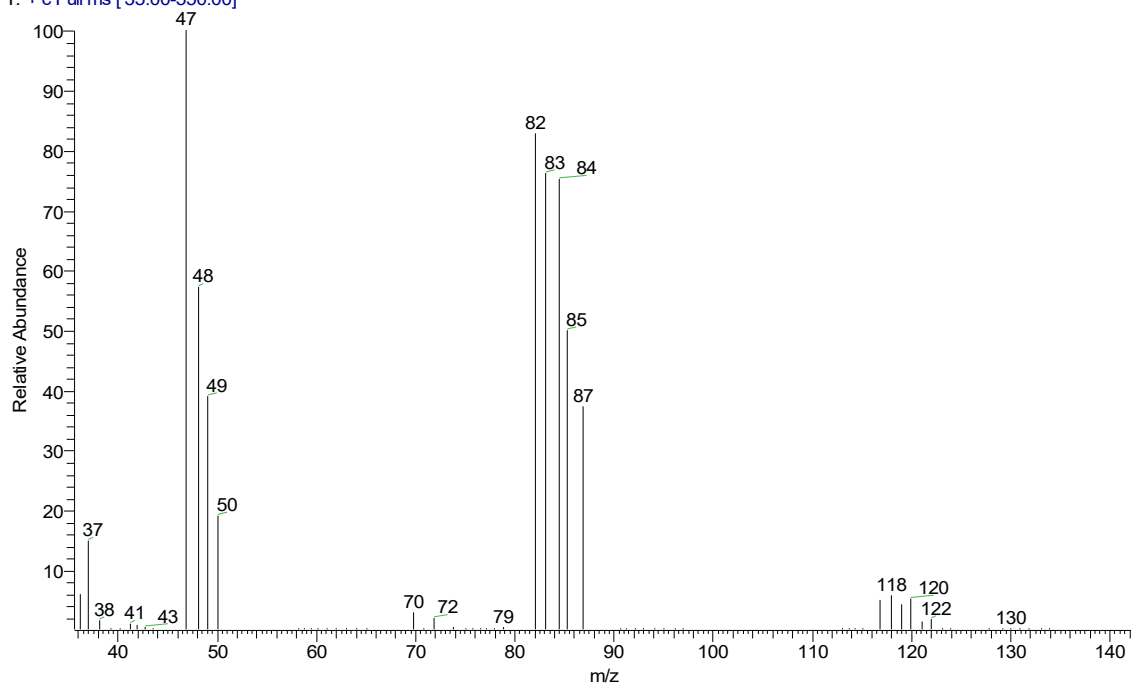
Starting compound – **12**. Catalyst – **11b** (1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h under an argon atmosphere.

RT: 0.00 - 36.07

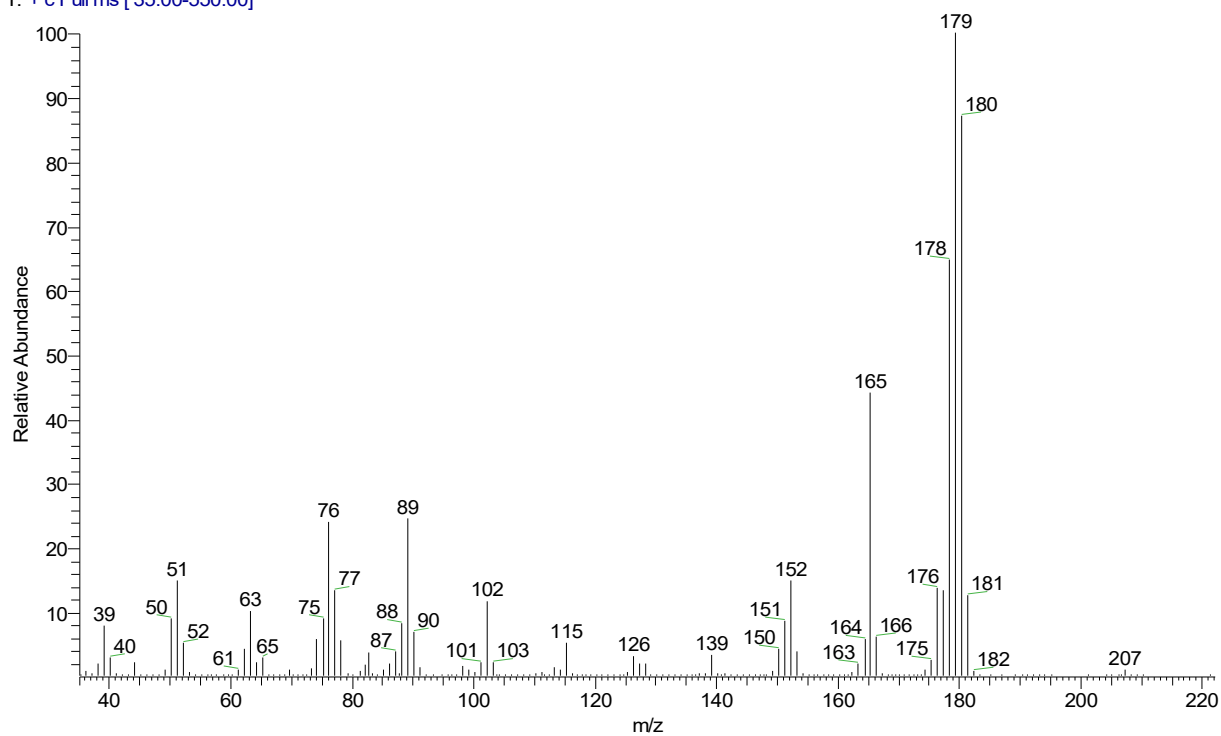


NL:
9.32E9
TIC F: MS
21_09_18_
13

21_09_18_13 #224 RT: 6.09 AV: 1 NL: 1.52E9
T: + c Full ms [35.00-550.00]



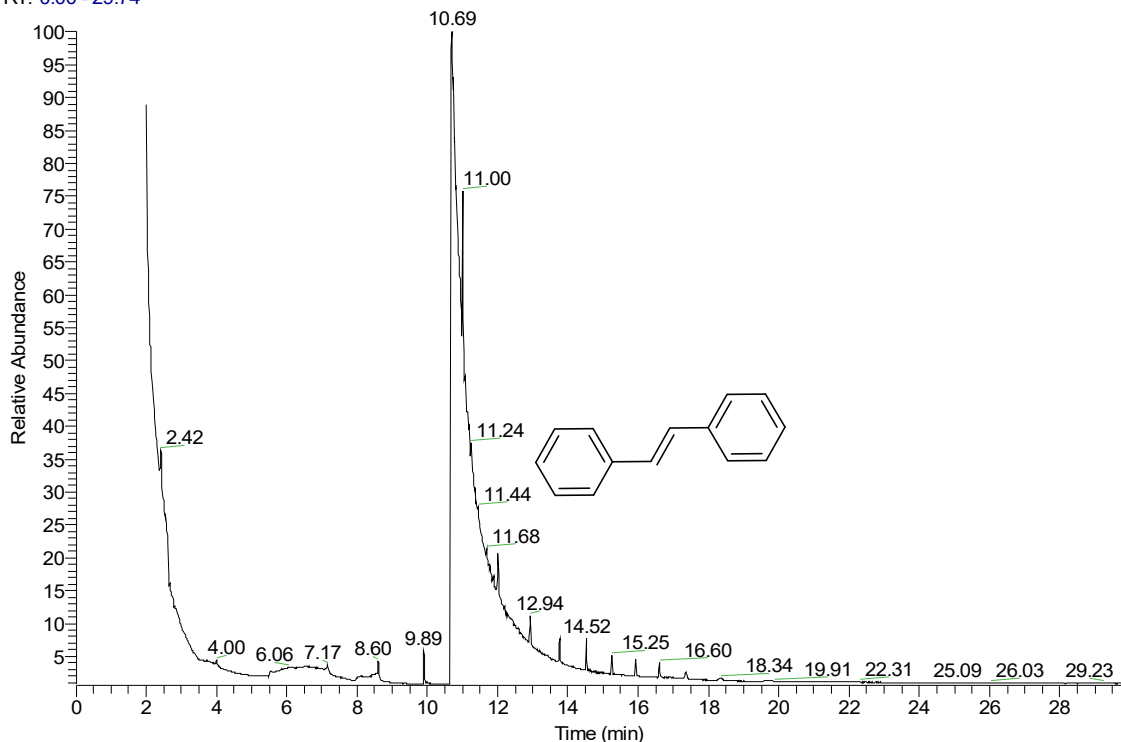
21_09_18_13 #735 RT: 15.38 AV: 1 NL: 5.52E7
T: + c Full ms [35.00-550.00]



Entry 19.

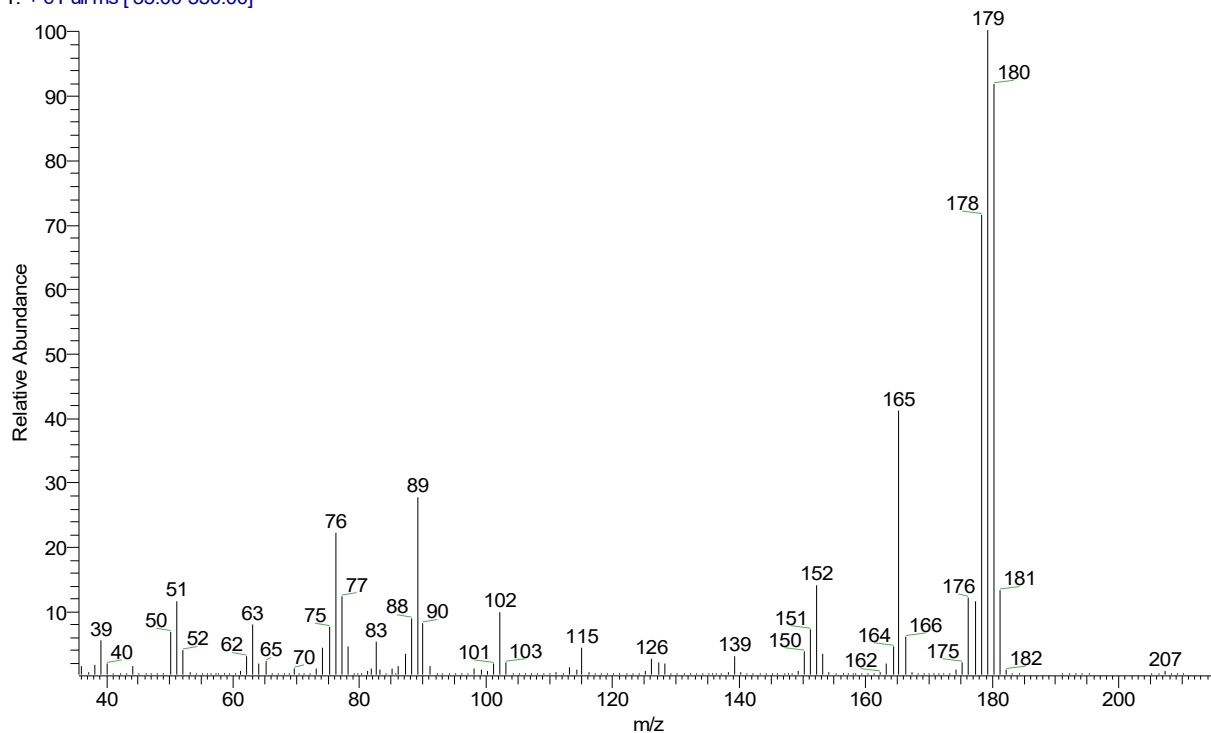
Starting compound – **12**. Catalyst – **11b** (0.01 mol %). The reaction mixture was heated at reflux in CHCl₃ for 4 h under an argon atmosphere.

RT: 0.00 - 29.74



NL:
8.88E8
TIC F: MS
28_09_18_
02

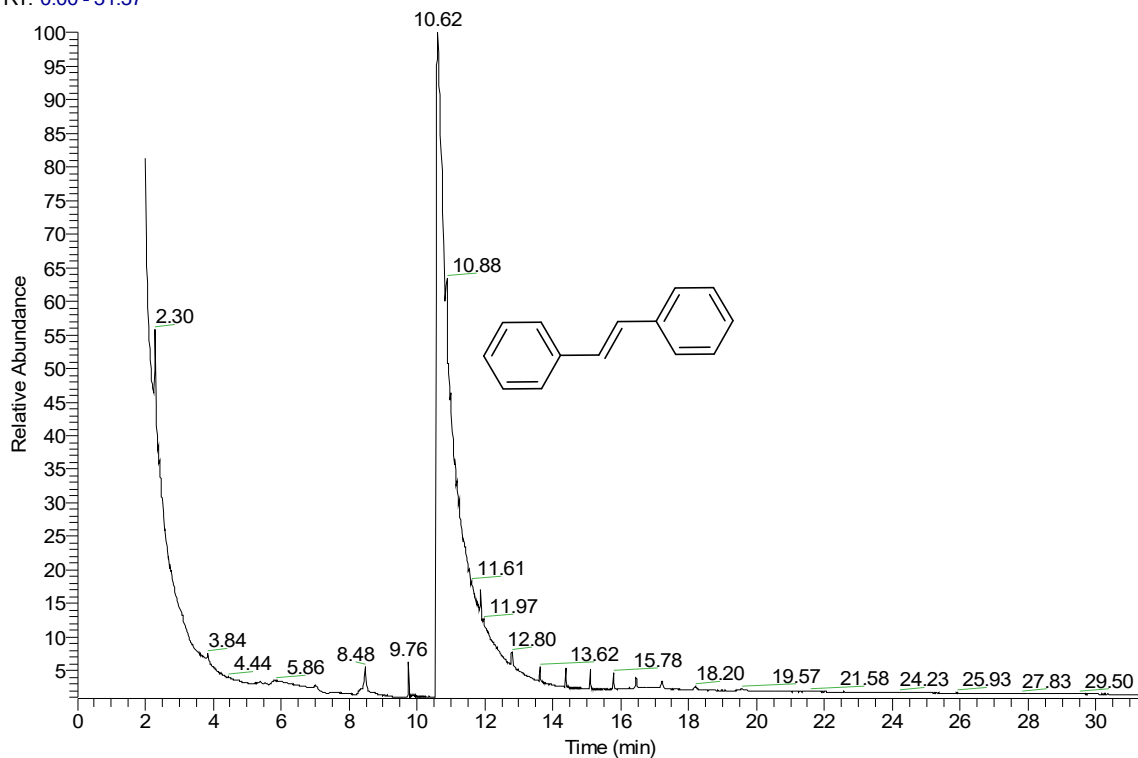
28_09_18_02 #476 RT: 10.69 AV: 1 NL: 1.49E8
T: + c Full ms [35.00-550.00]



Entry 20.

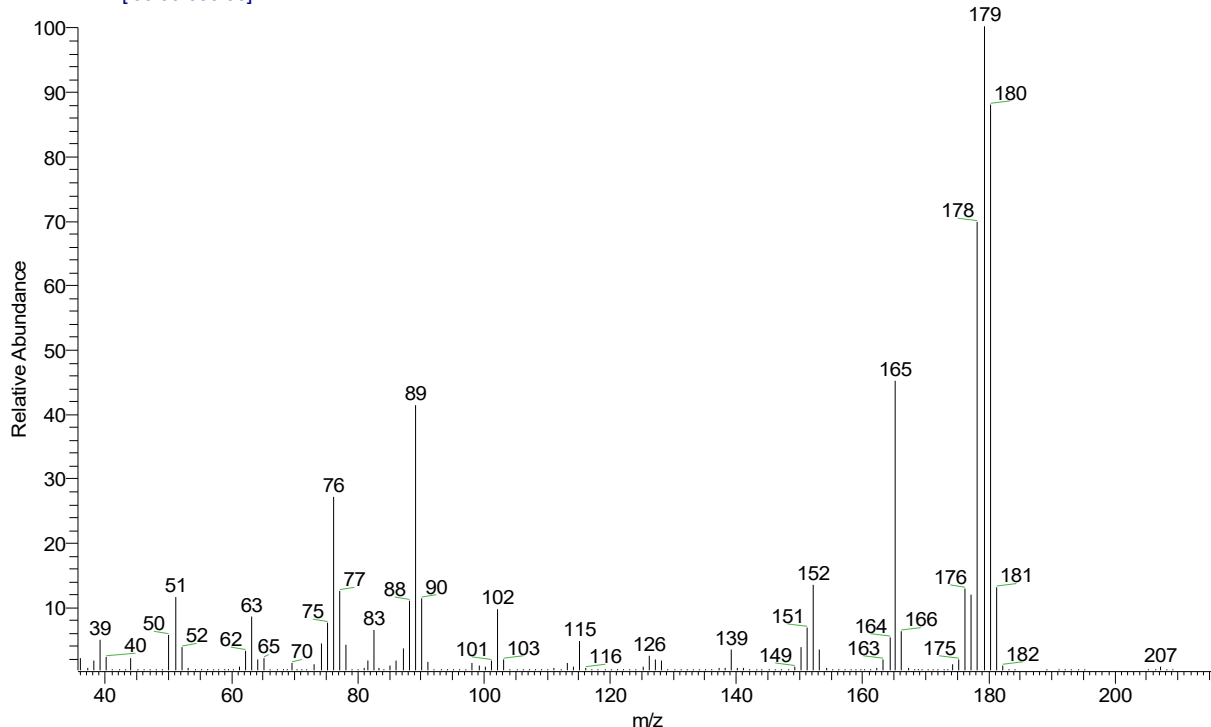
Starting compound – **12**. Catalyst – **11b** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h.

RT: 0.00 - 31.37



NL:
1.08E9
TIC F: MS
03_10_18_
06

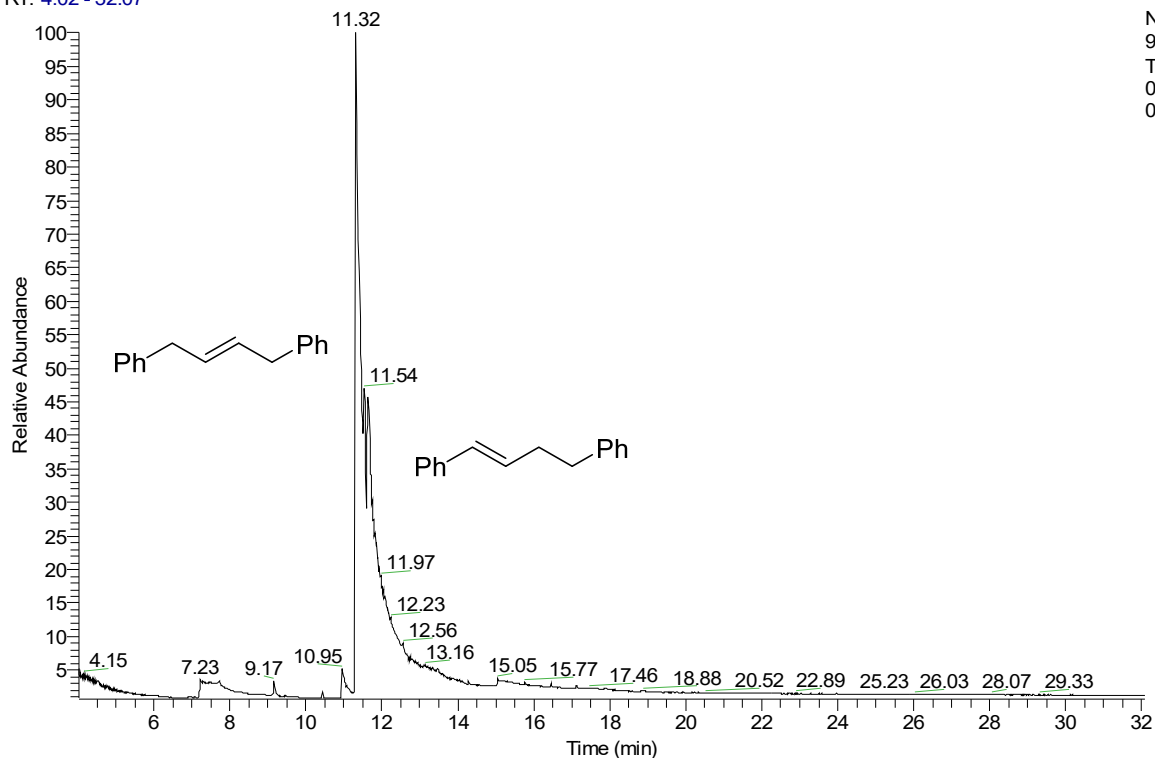
03_10_18_06 #473 RT: 10.64 AV: 1 NL: 1.69E8
T: + c Full ms [35.00-550.00]



Entry 24.

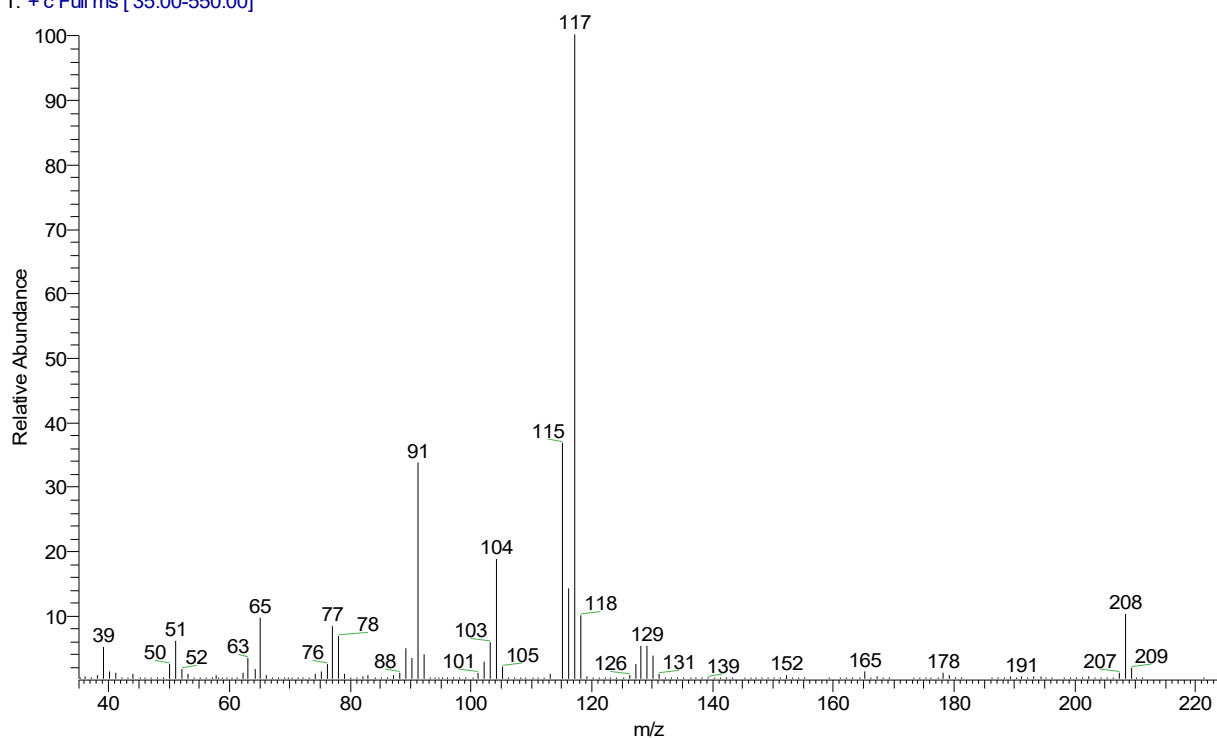
Starting compound – **14**. Catalyst – **11b** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h under an argon atmosphere.

RT: 4.02 - 32.07

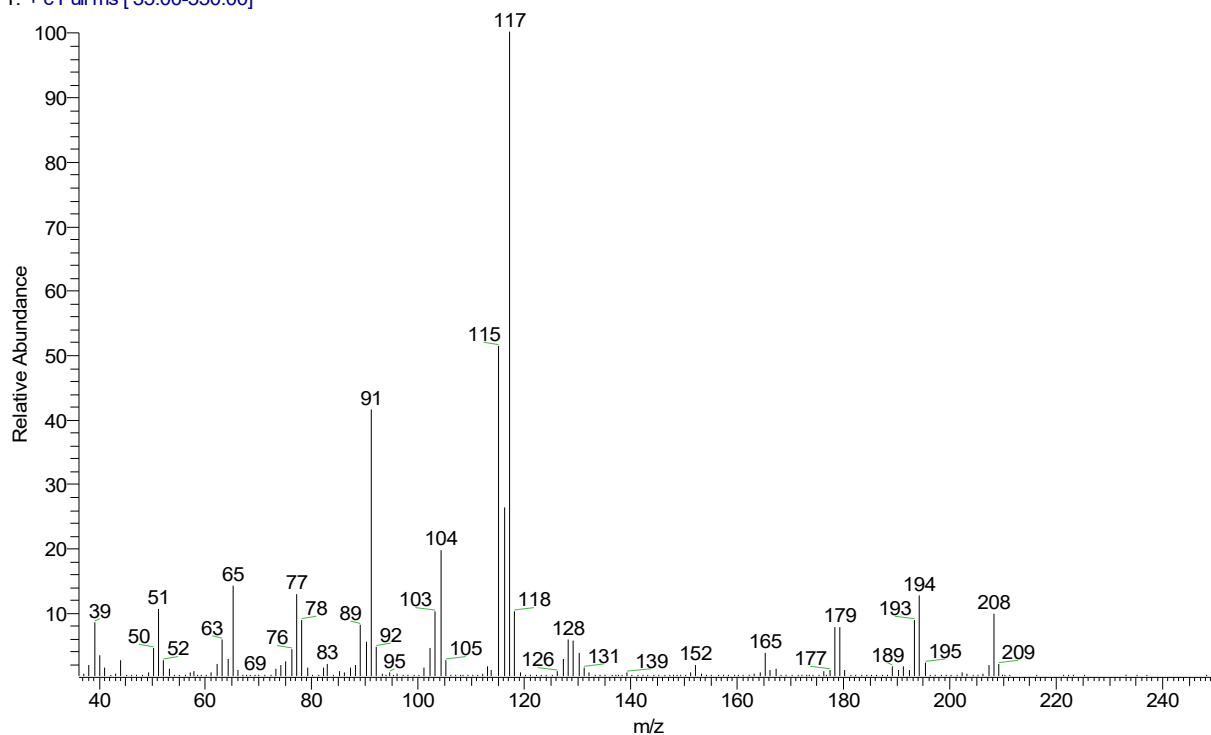


NL:
9.69E8
TIC F: MS
01_10_18_
03

01_10_18_03 #512 RT: 11.32 AV: 1 NL: 2.77E8
T: + c Full ms [35.00-550.00]



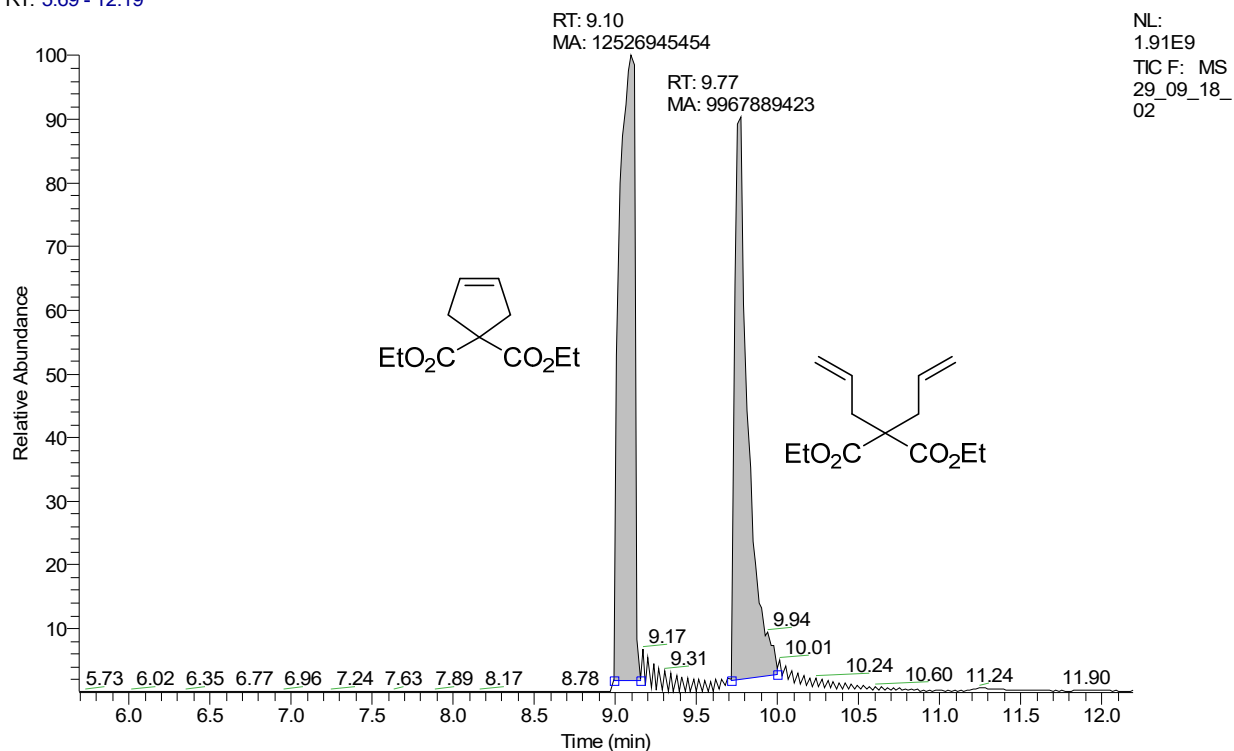
01_10_18_03 #526 RT: 11.57 AV: 1 NL: 6.56E7
T: + c Full ms [35.00-550.00]



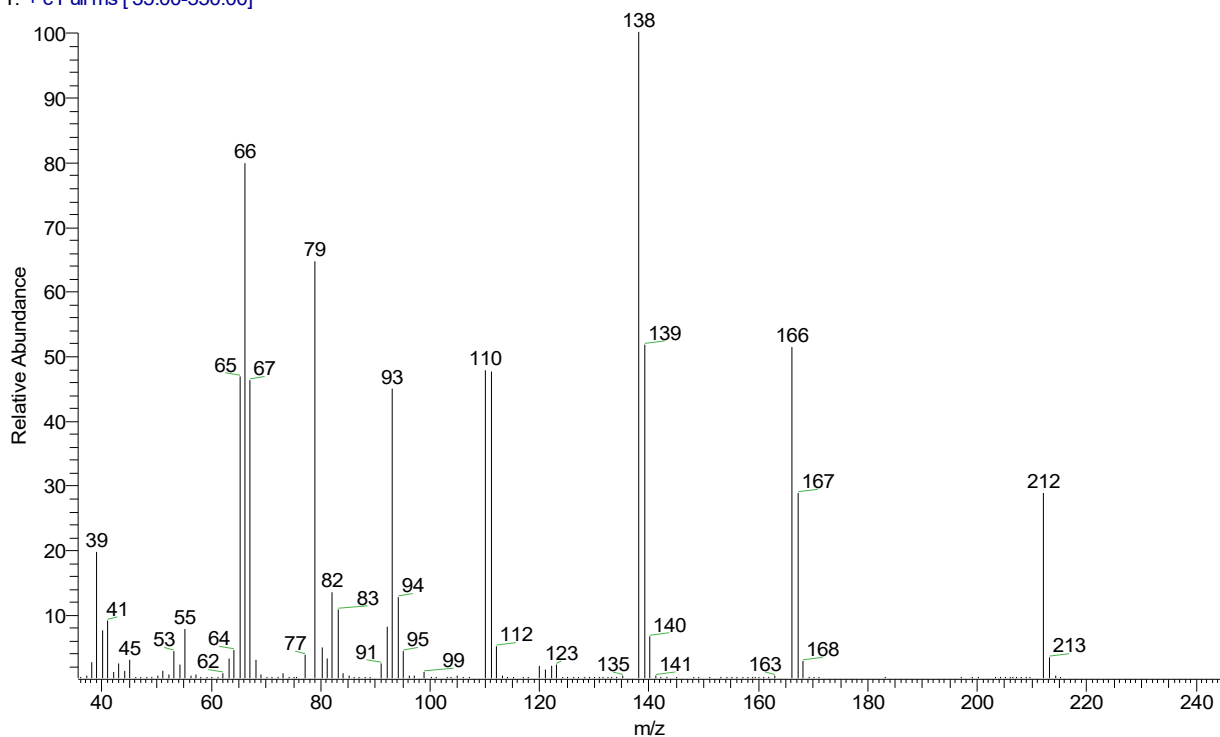
Entry 25.

Starting compound – **17**. Catalyst – **11a** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h.

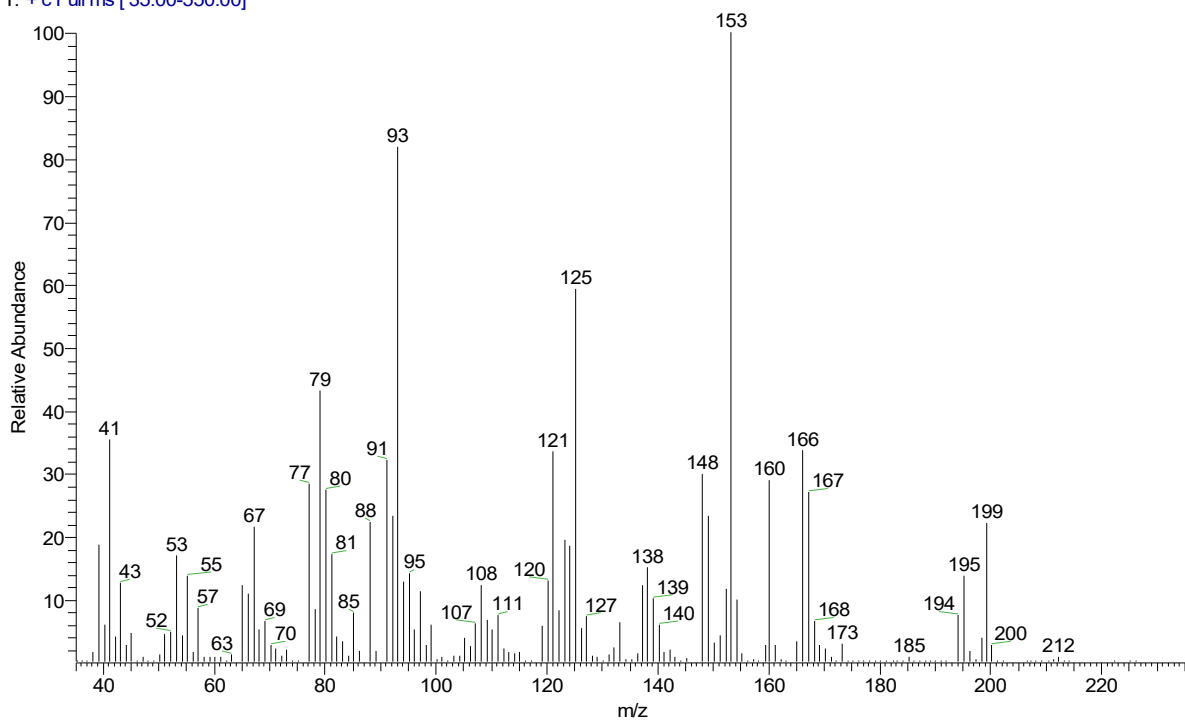
RT: 5.69 - 12.19



29_09_18_02 #328 RT: 9.10 AV: 1 NL: 2.34E8
T: + c Full ms [35.00-550.00]



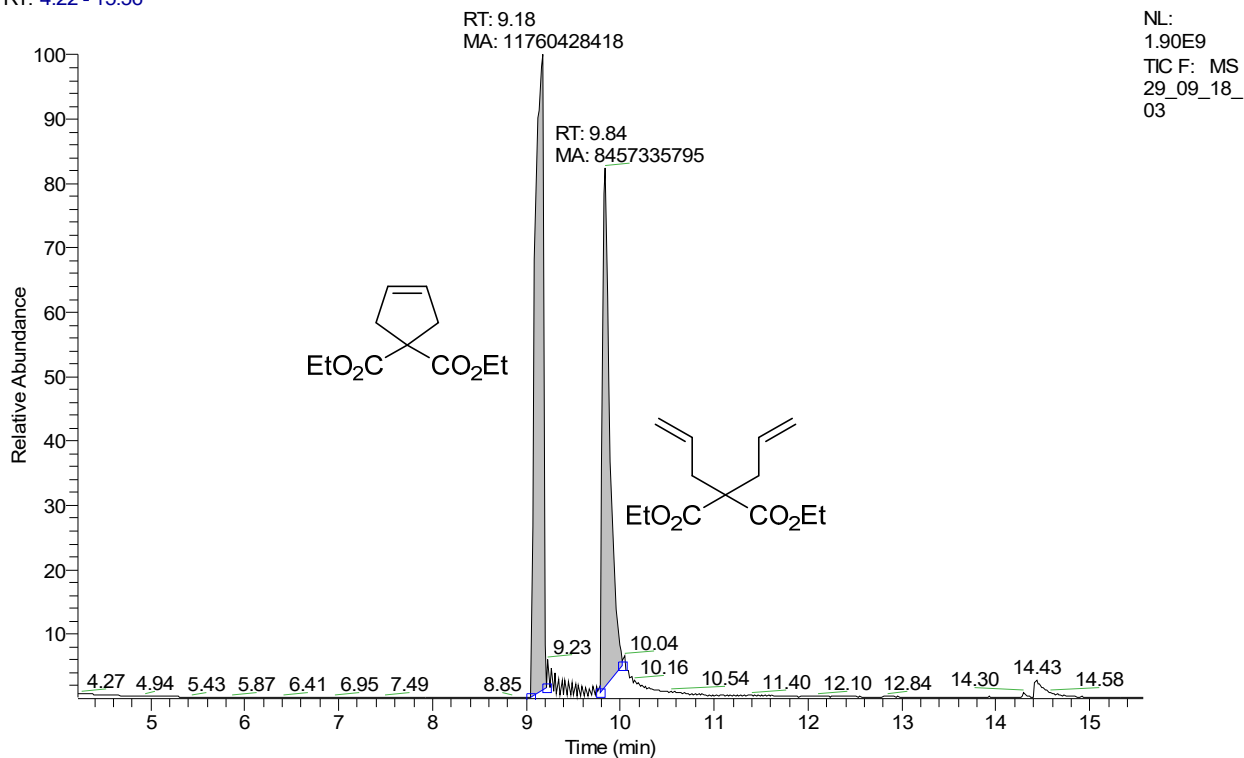
29_09_18_02 #366 RT: 9.77 AV: 1 NL: 1.42E8
T: + c Full ms [35.00-550.00]



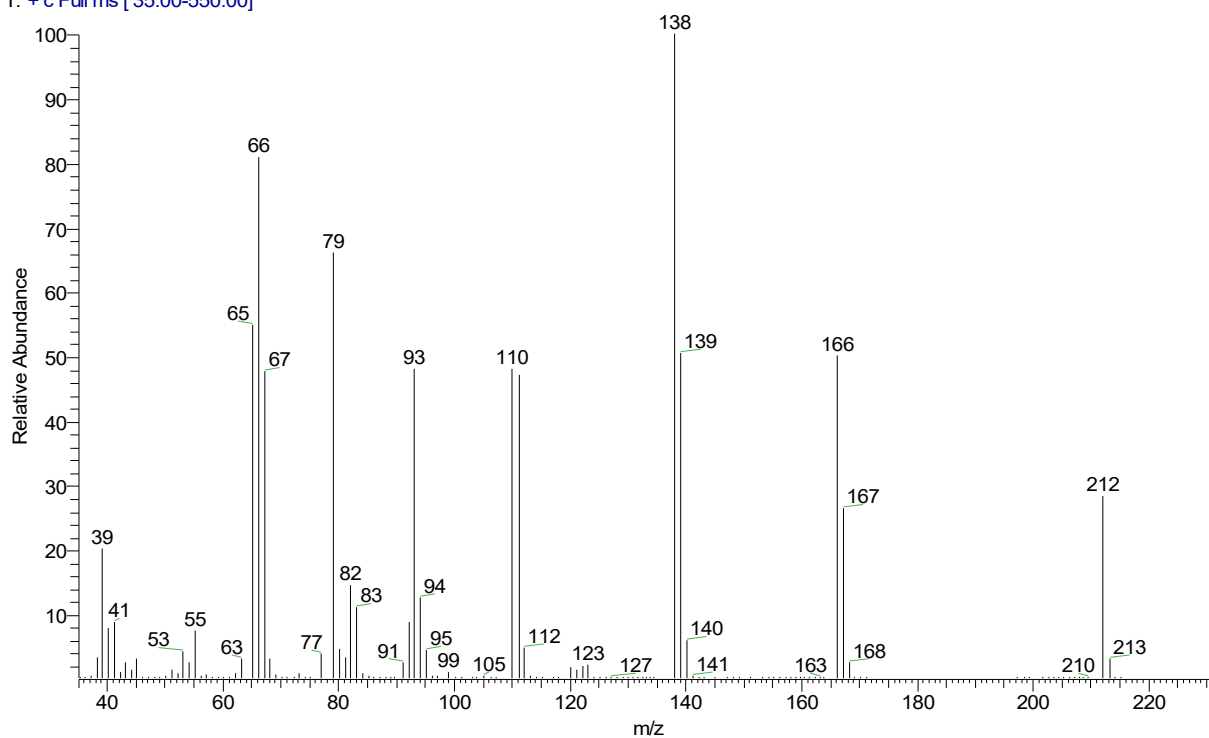
Entry 26.

Starting compound – **17**. Catalyst – **11b** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h.

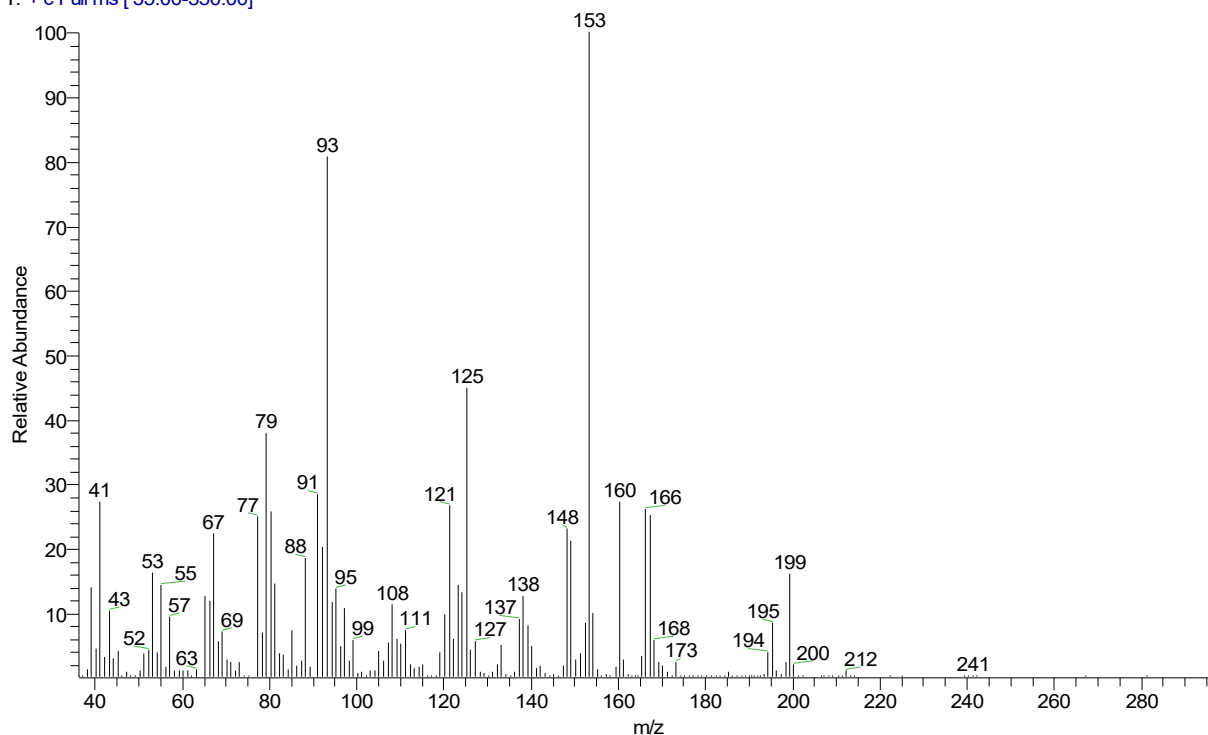
RT: 4.22 - 15.56



29_09_18_03 #338 RT: 9.18 AV: 1 NL: 2.30E8
T: + c Full ms [35.00-550.00]



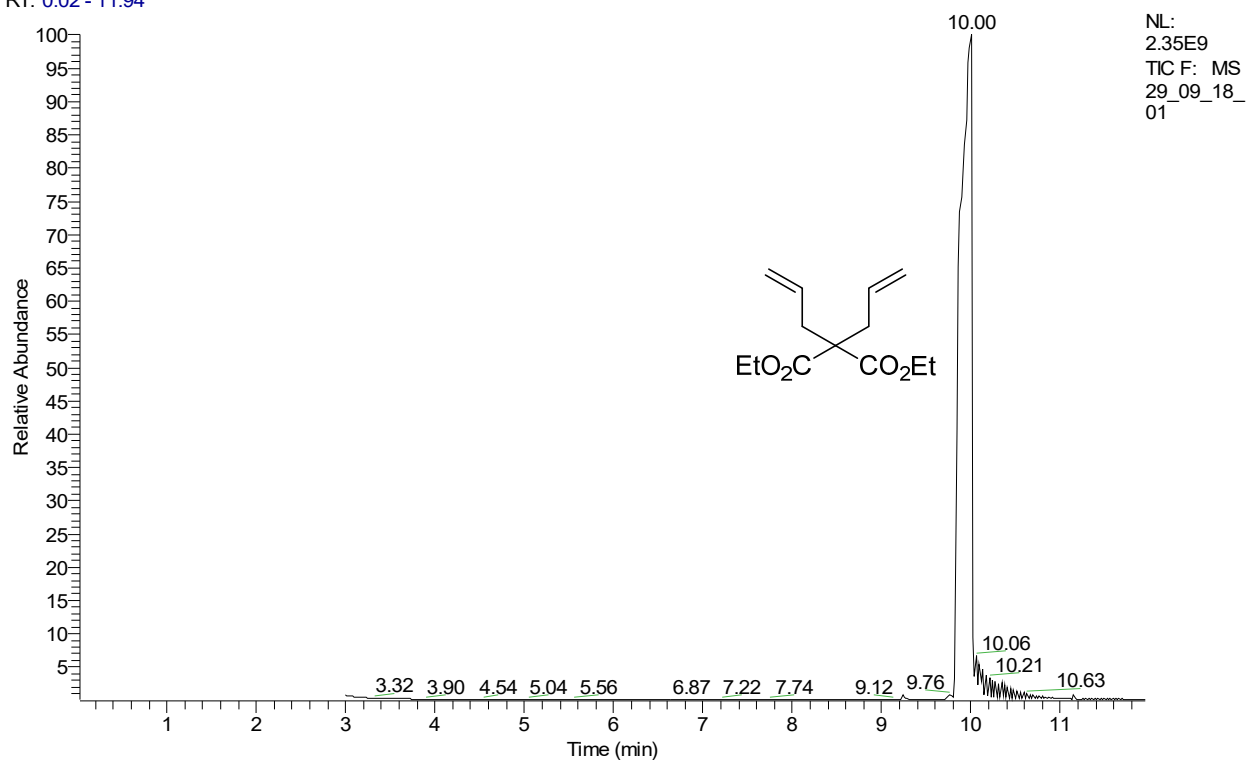
29_09_18_03 #373 RT: 9.82 AV: 1 NL: 1.39E8
T: + c Full ms [35.00-550.00]



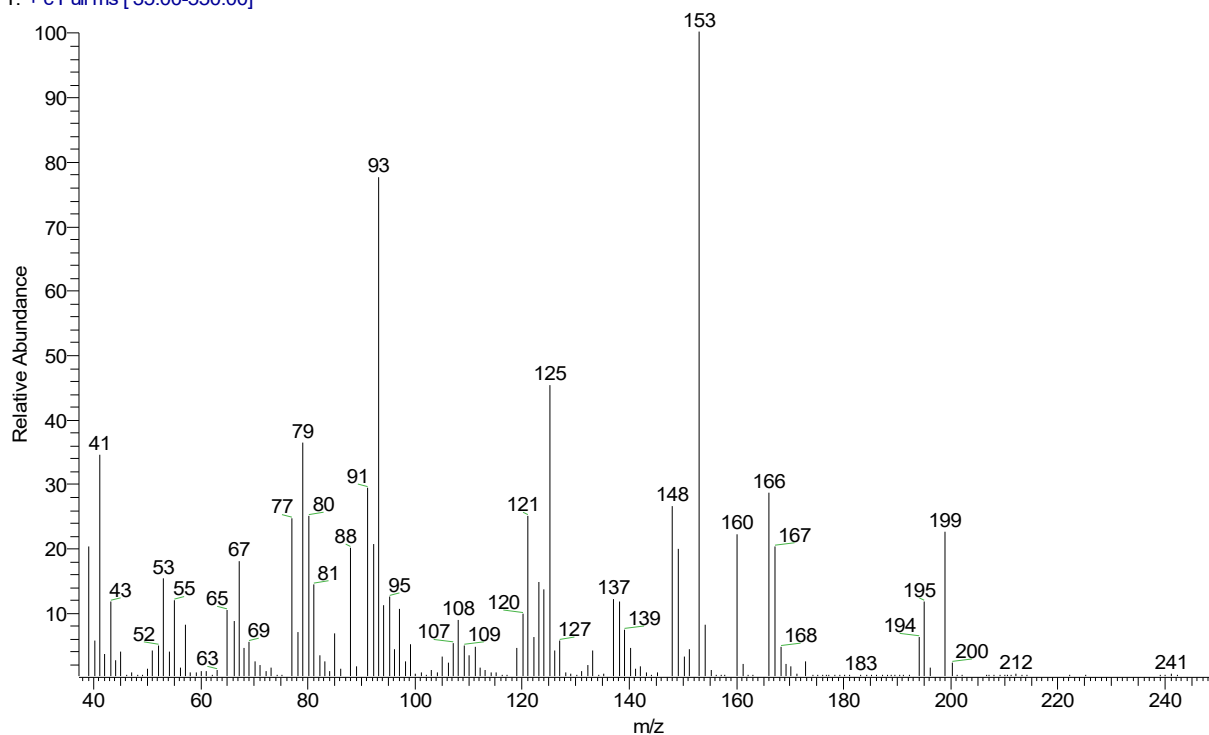
Entry 27.

Starting compound – **17**. Catalyst – **11b** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h.

RT: 0.02 - 11.94



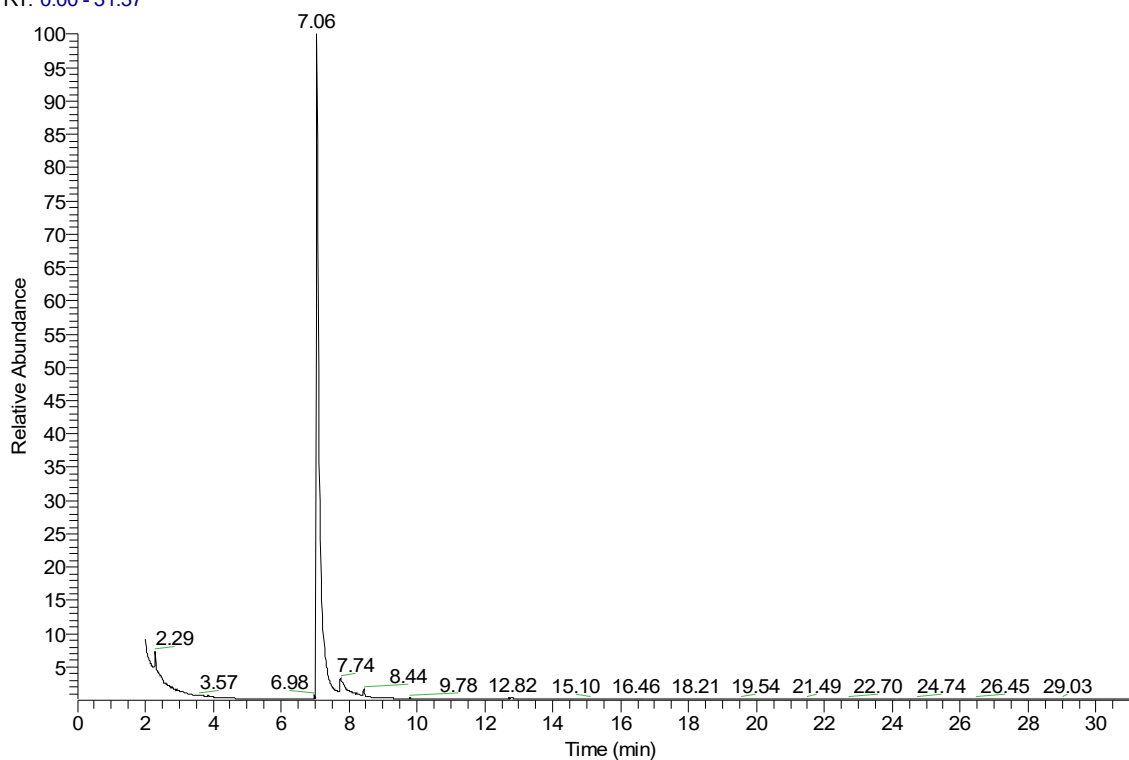
29_09_18_01 #383 RT: 9.95 AV: 1 NL: 2.00E8
T: + c Full ms [35.00-550.00]



Entry 28.

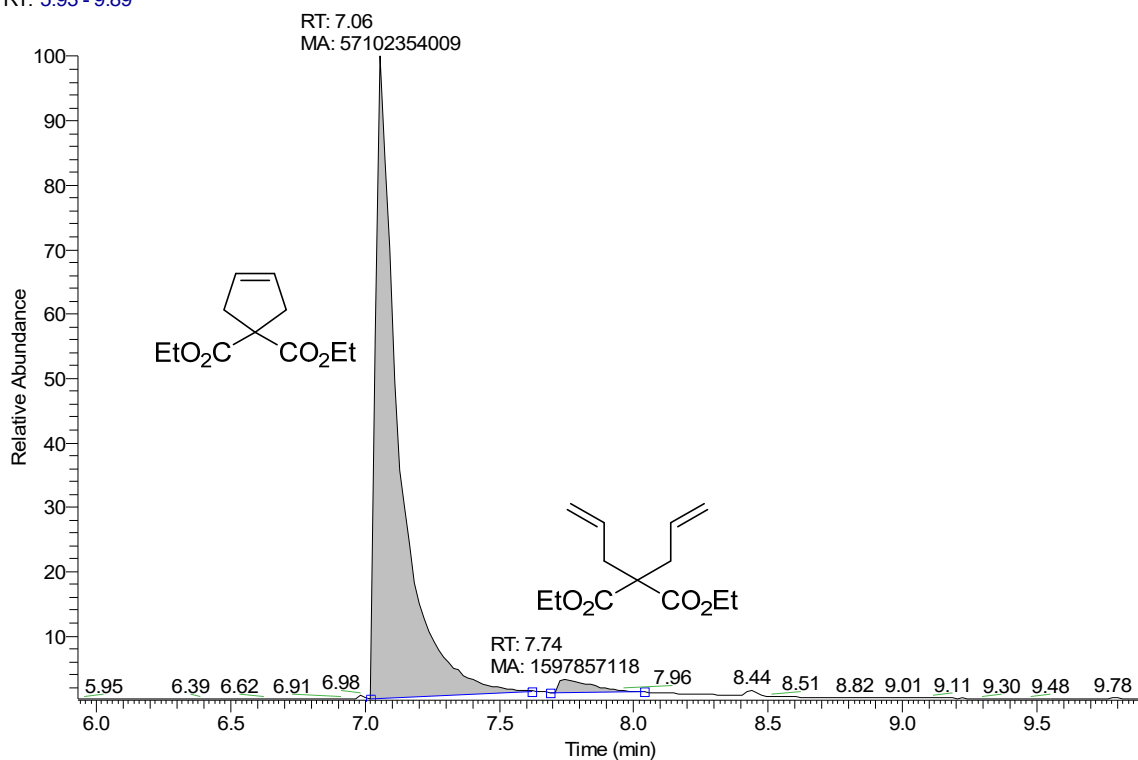
Starting compound – **17**. Catalyst – **11b** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h.

RT: 0.00 - 31.37



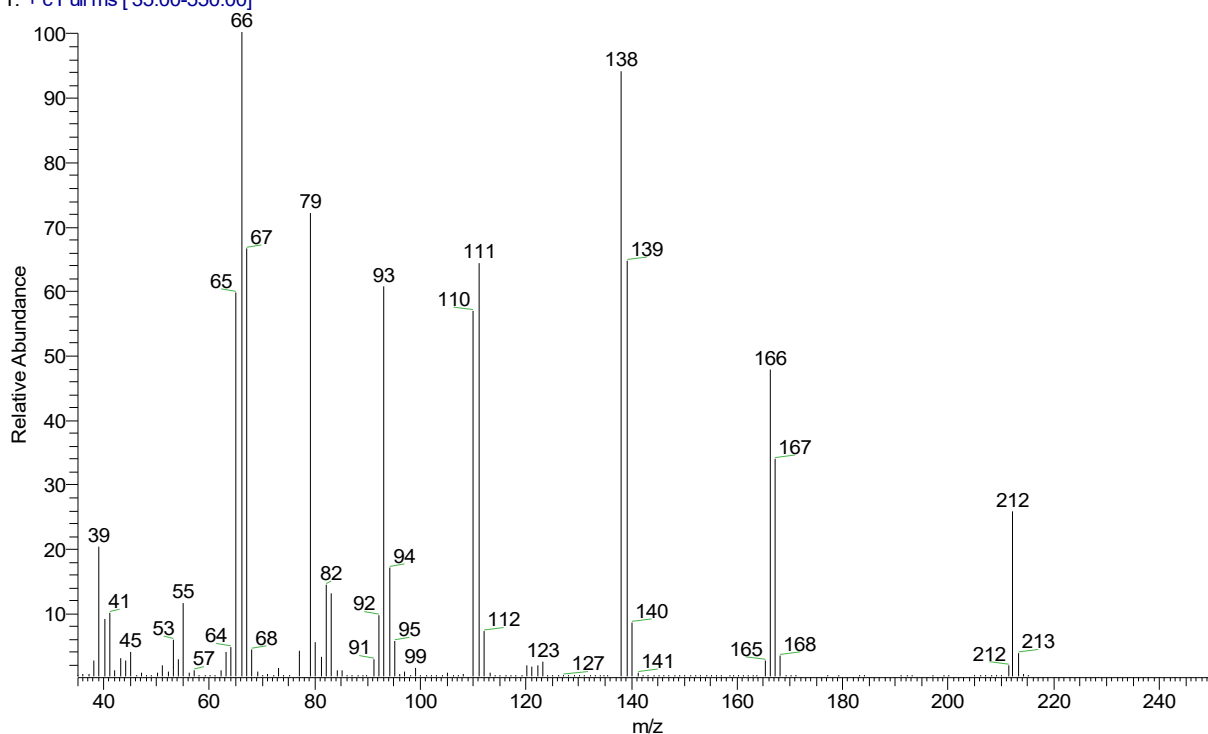
NL:
9.49E9
TIC F: MS
03_10_18_
07

RT: 5.93 - 9.89

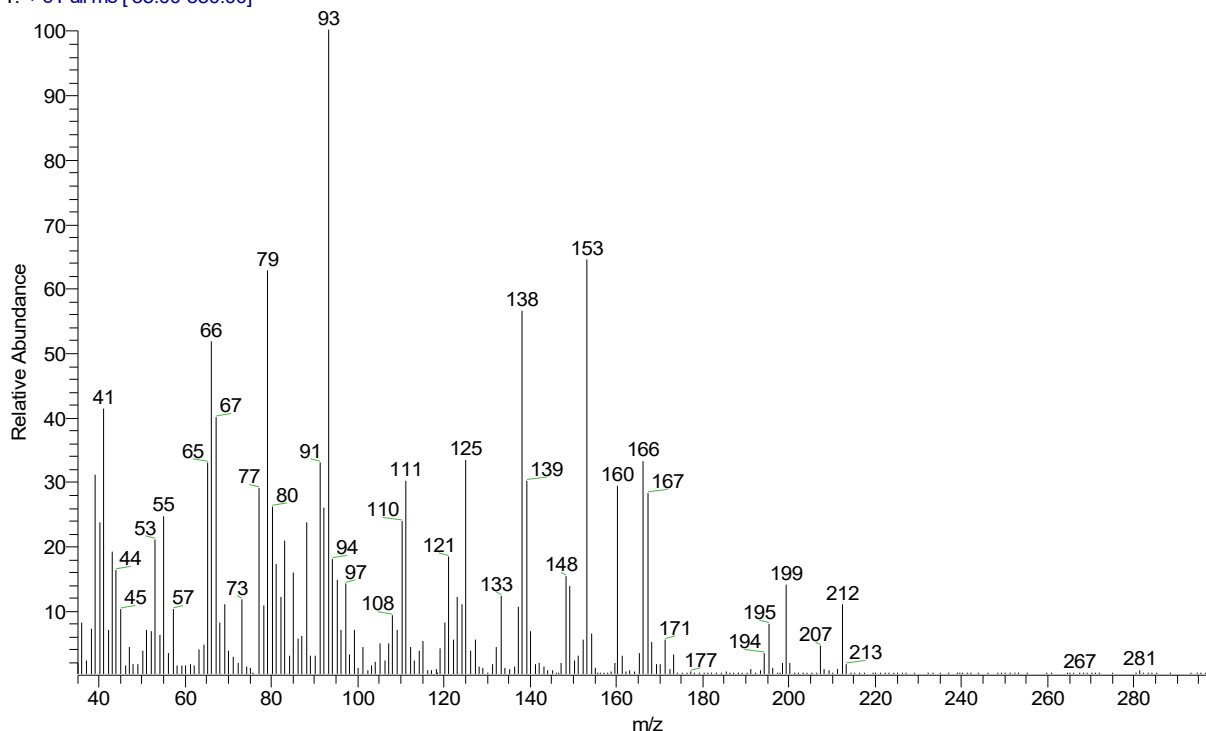


NL:
9.49E9
TIC F: MS
03_10_18_
07

03_10_18_07 #280 RT: 7.08 AV: 1 NL: 8.24E8
T: + c Full ms [35.00-550.00]



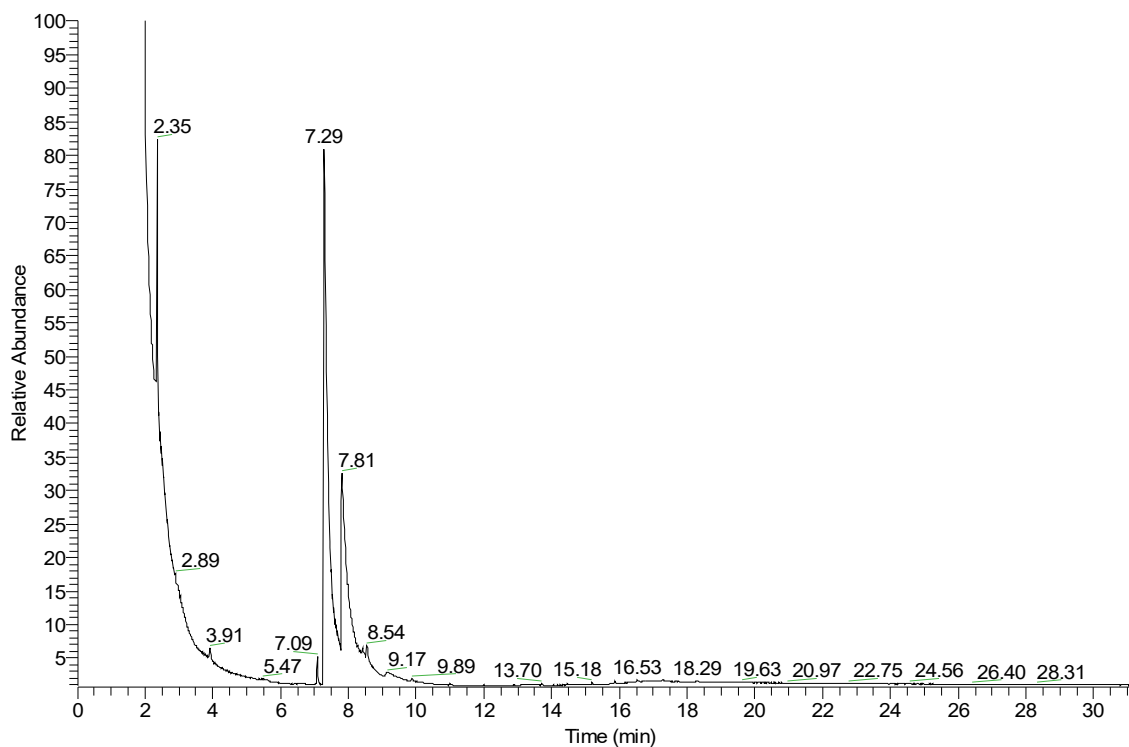
03_10_18_07 #317 RT: 7.74 AV: 1 NL: 2.02E7
T: + c Full ms [35.00-550.00]



Entry 29.

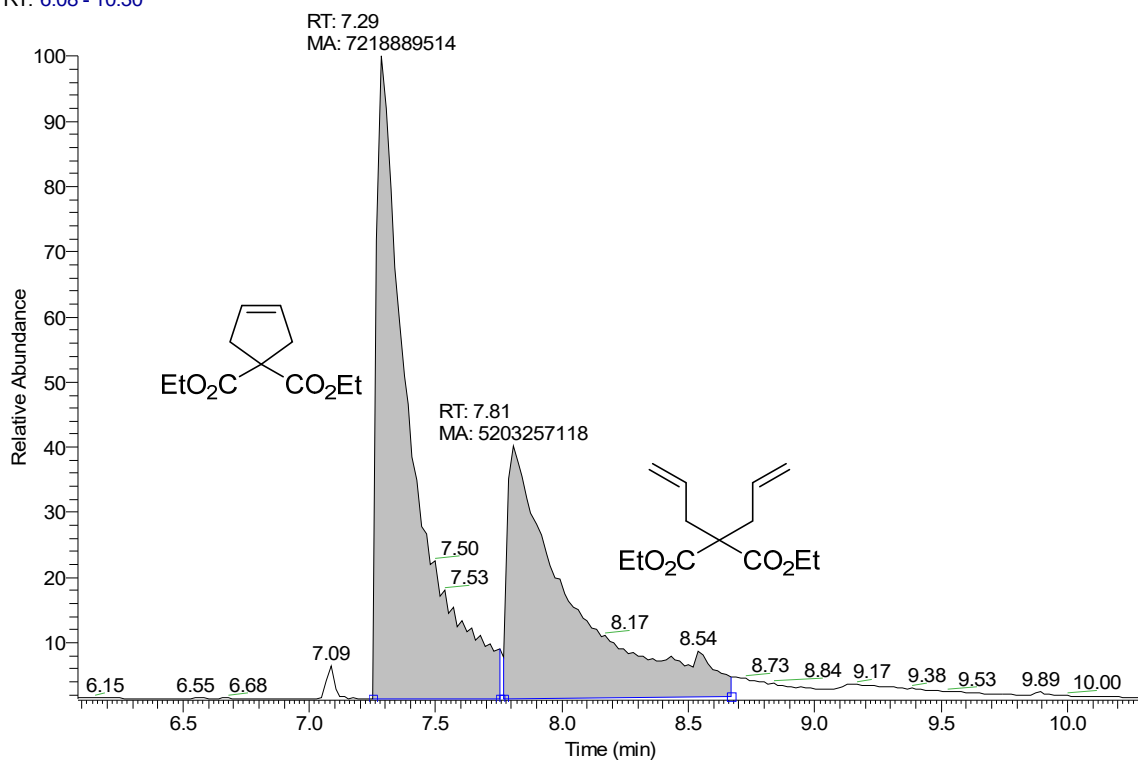
Starting compound – **17**. Catalyst – **11d** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 6 h under an argon atmosphere.

RT: 0.00 - 31.45



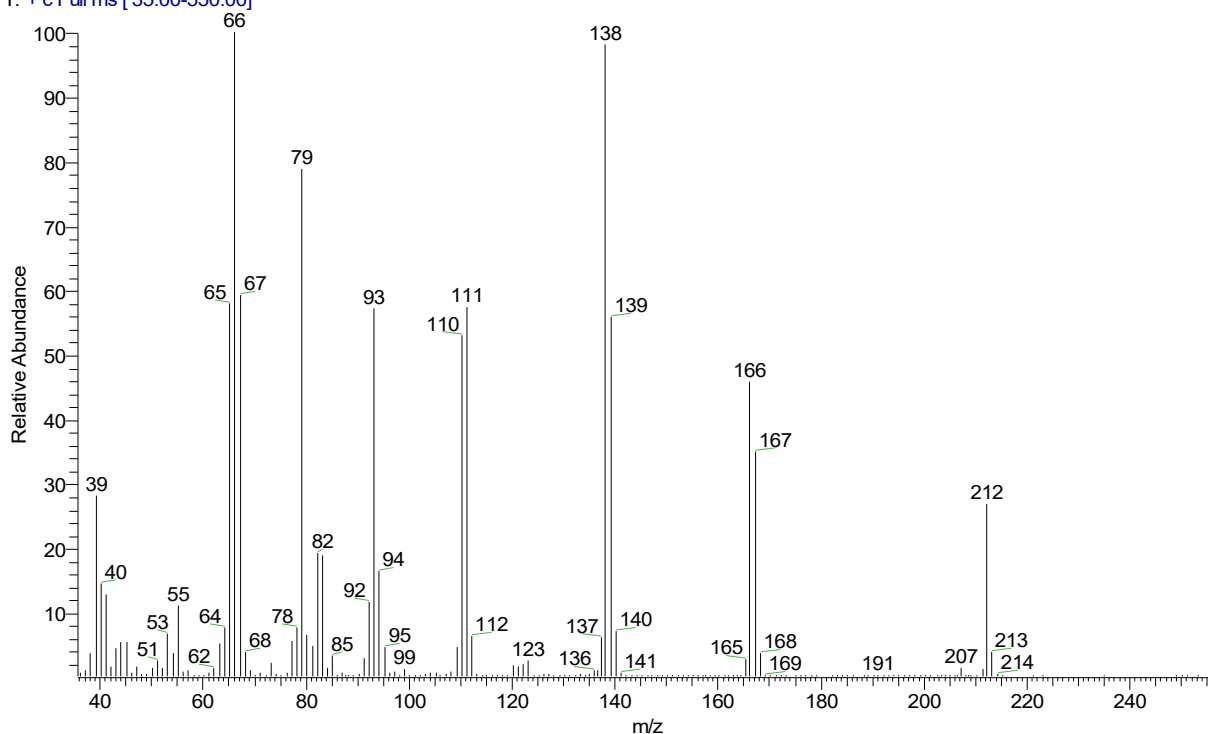
NL:
9.50E8
TIC F: MS
04_10_18_
05

RT: 6.08 - 10.30

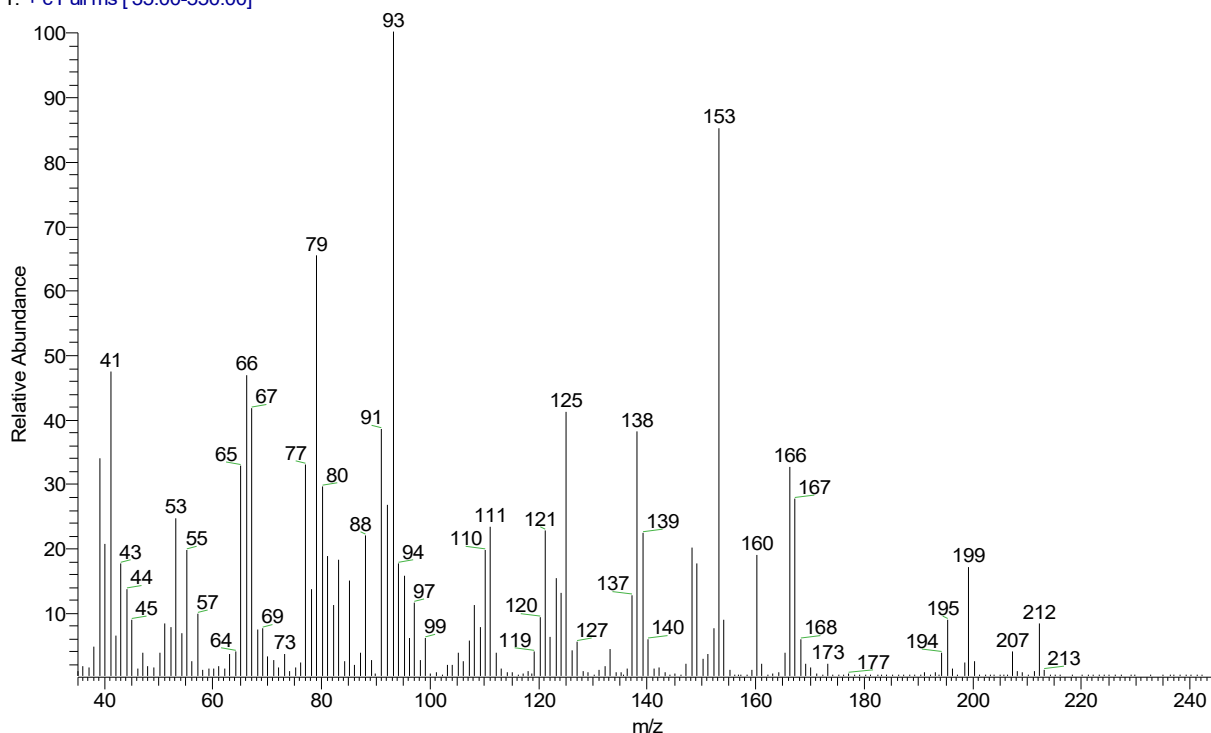


NL:
7.68E8
TIC F: MS
04_10_18_
05

04_10_18_05 #288 RT: 7.29 AV: 1 NL: 7.43E7
T: + c Full ms [35.00-550.00]



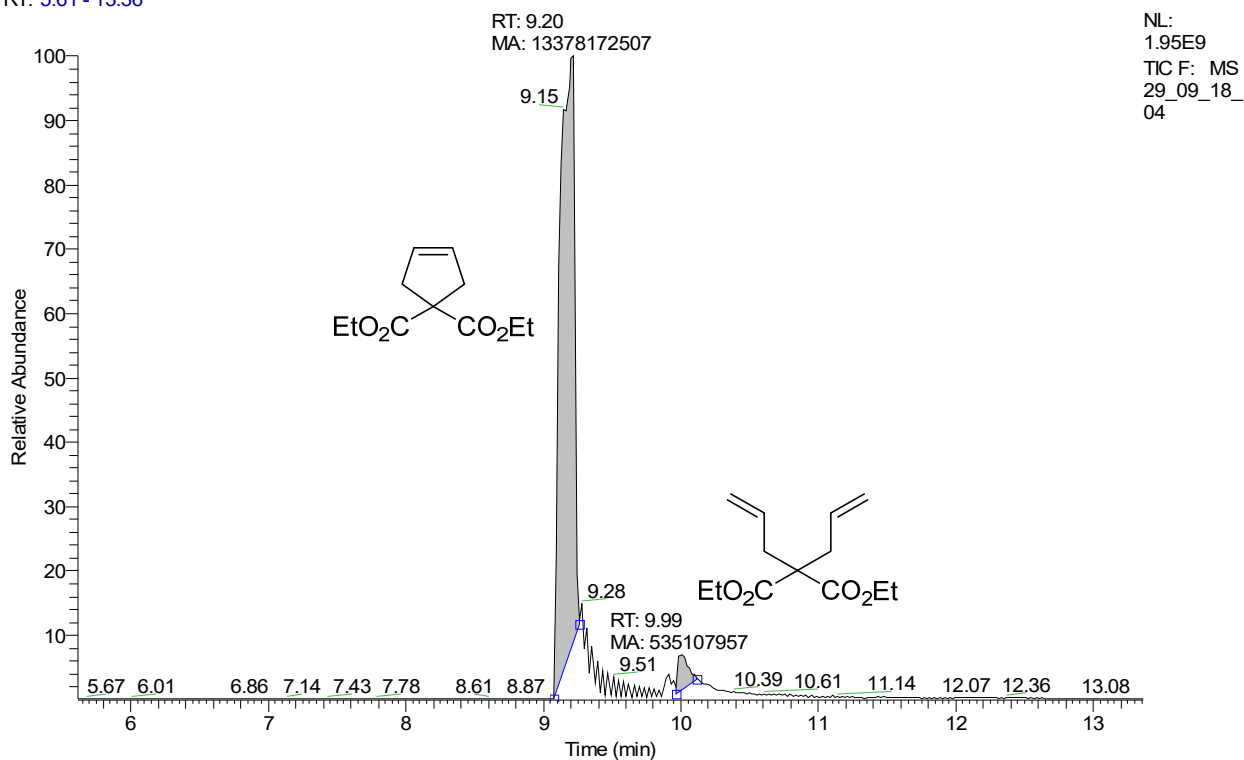
04_10_18_05 #317 RT: 7.81 AV: 1 NL: 2.08E7
T: + c Full ms [35.00-550.00]



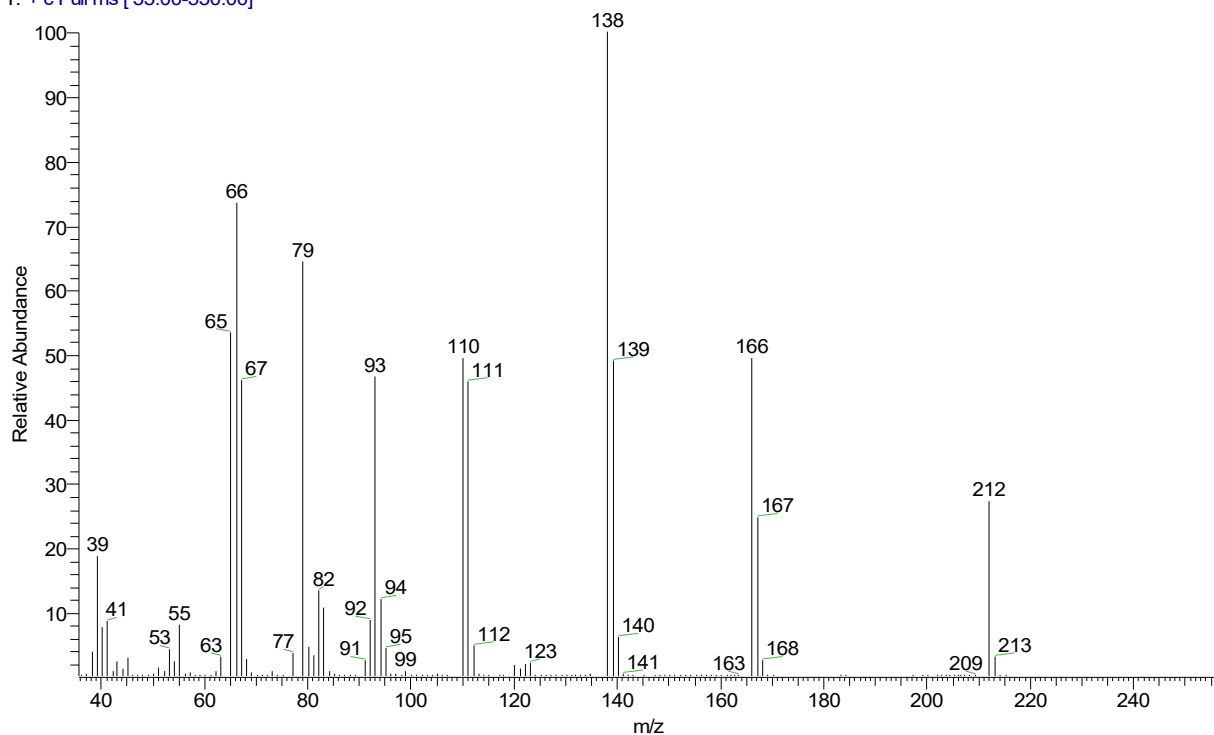
Entry 30.

Starting compound – **17**. Catalyst – **11d** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h under an argon atmosphere.

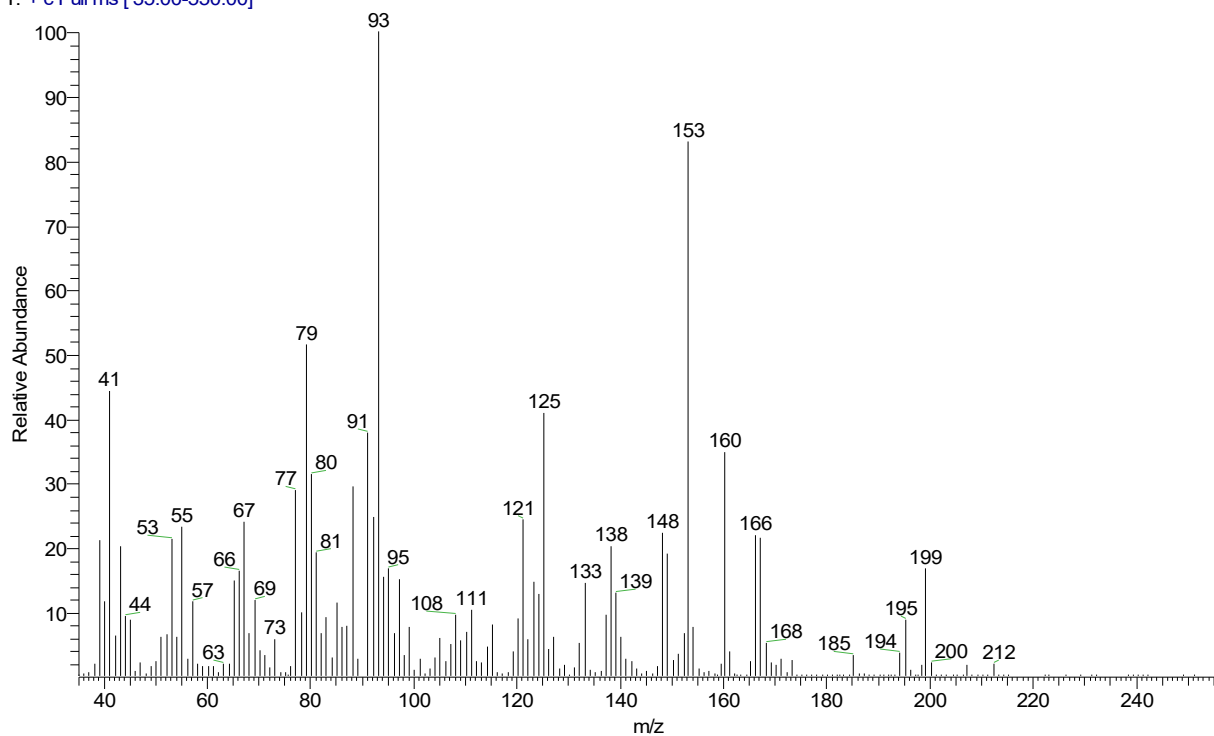
RT: 5.61 - 13.36



29_09_18_04 #338 RT: 9.22 AV: 1 NL: 2.43E8
T: + c Full ms [35.00-550.00]



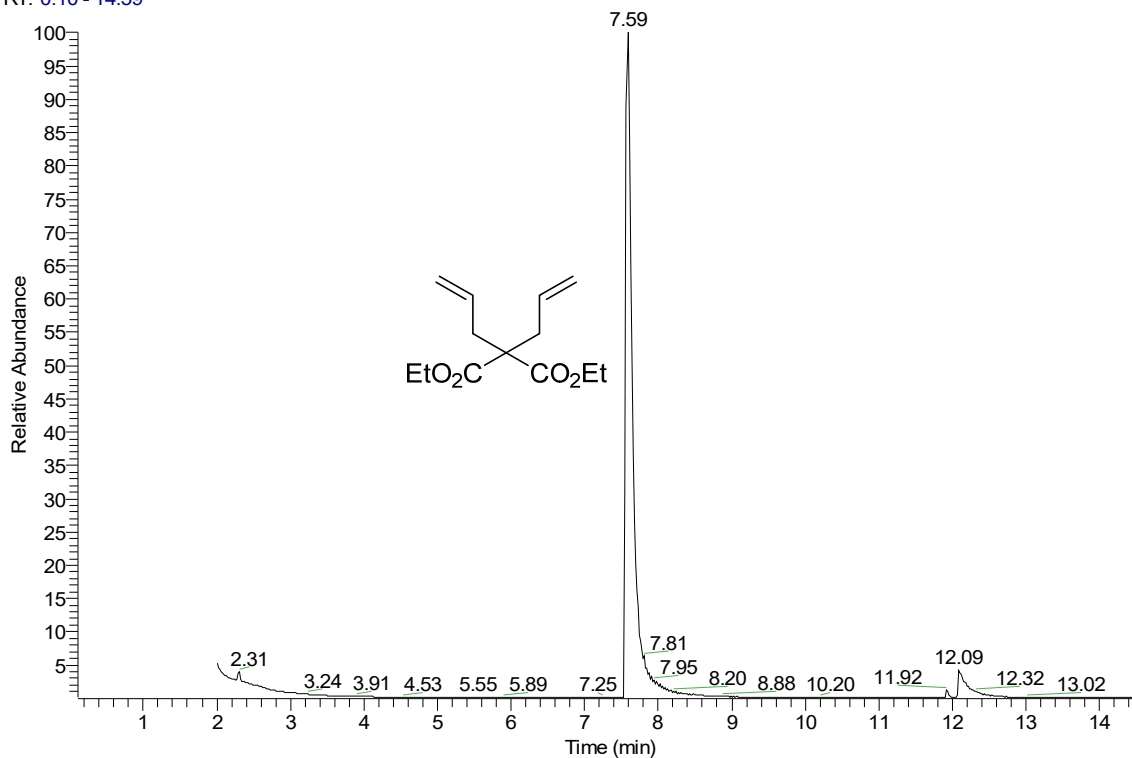
29_09_18_04 #380 RT: 10.01 AV: 1 NL: 1.01E7
T: + c Full ms [35.00-550.00]



Entry 31.

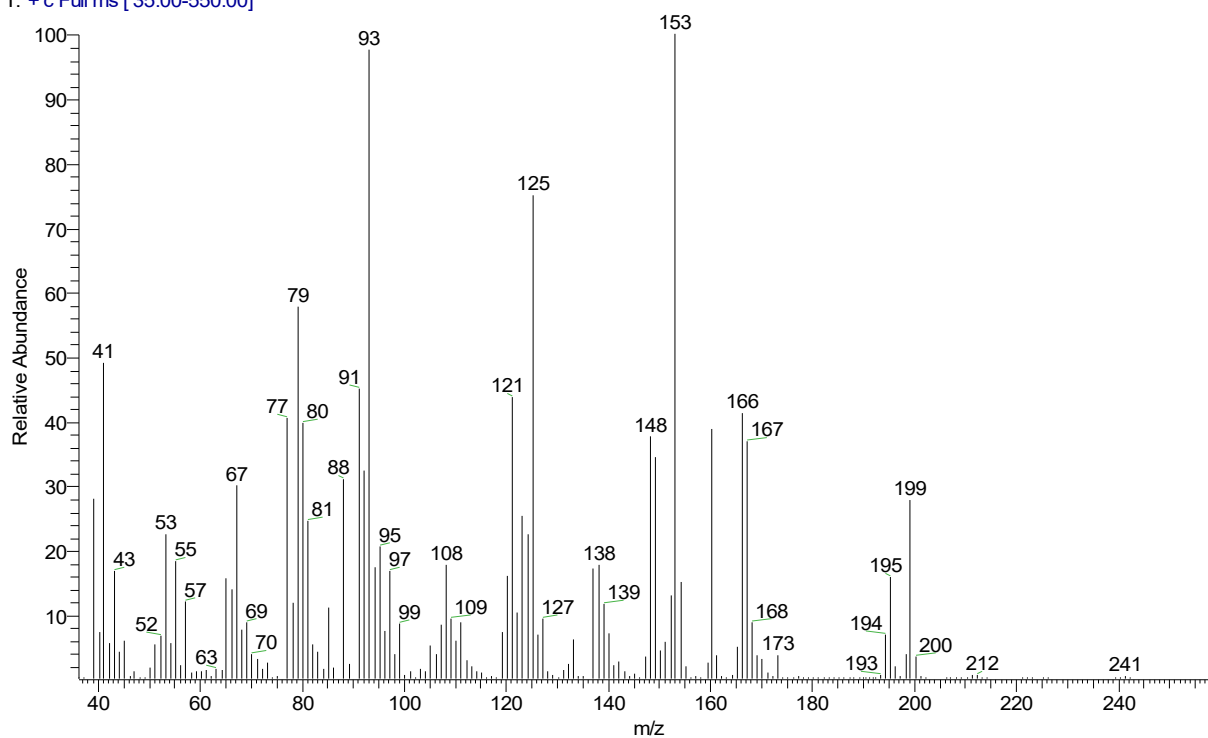
Starting compound – **17**. Catalyst – **11d** (0.01 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h under an argon atmosphere.

RT: 0.10 - 14.59

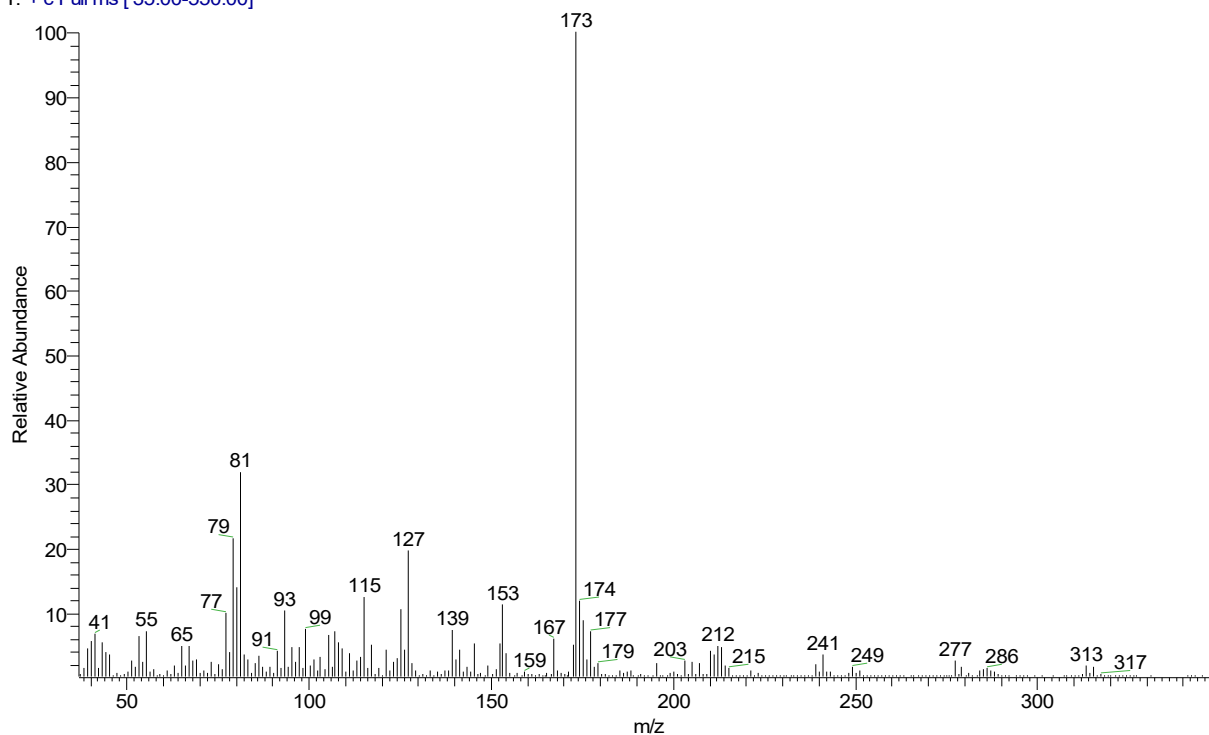


NL:
1.54E10
TIC F: MS
03_10_18_
04

03_10_18_04 #308 RT: 7.60 AV: 1 NL: 8.22E8
T: + c Full ms [35.00-550.00]



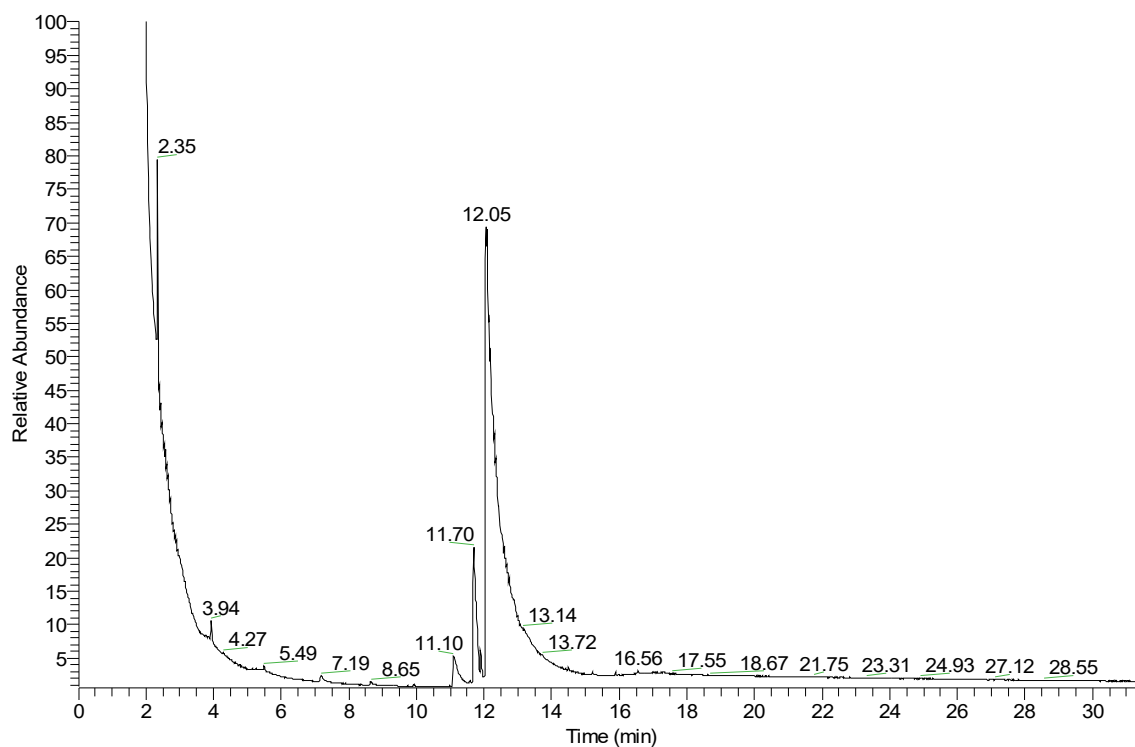
03_10_18_04 #553 RT: 12.09 AV: 1 NL: 1.00E8
T: + c Full ms [35.00-550.00]



Entry 32.

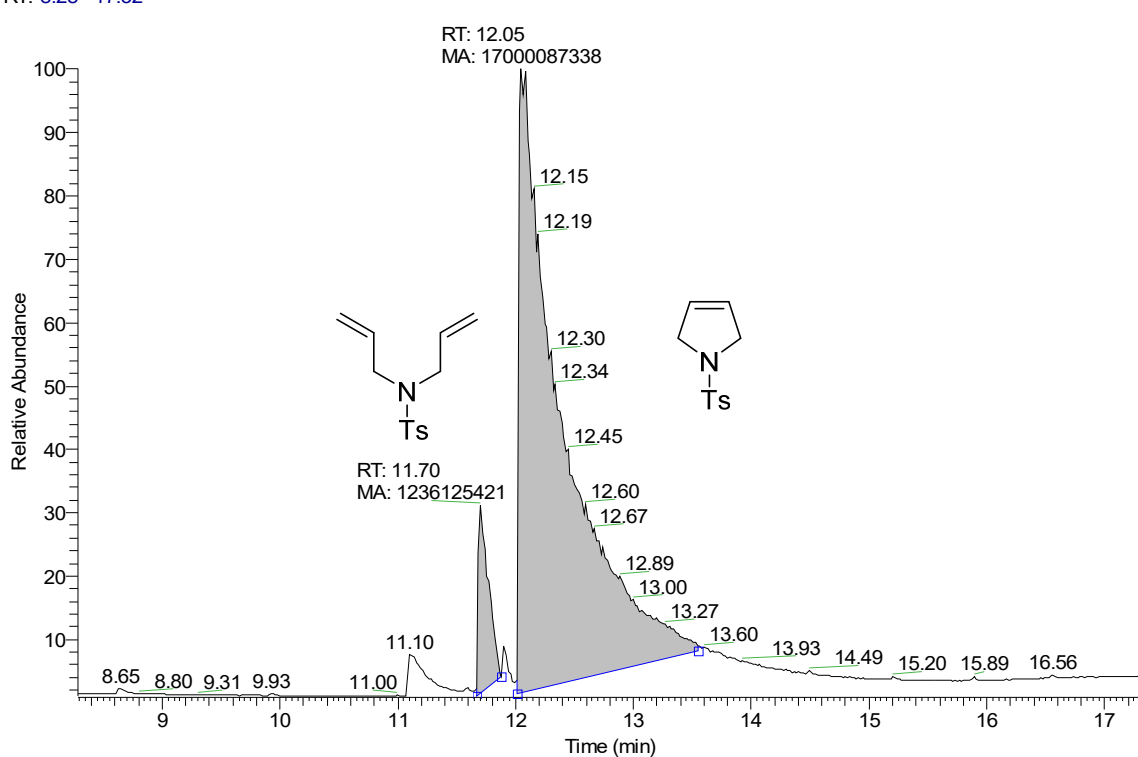
Starting compound – **19**. Catalyst – **11d** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h under an argon atmosphere.

RT: 0.00 - 31.51



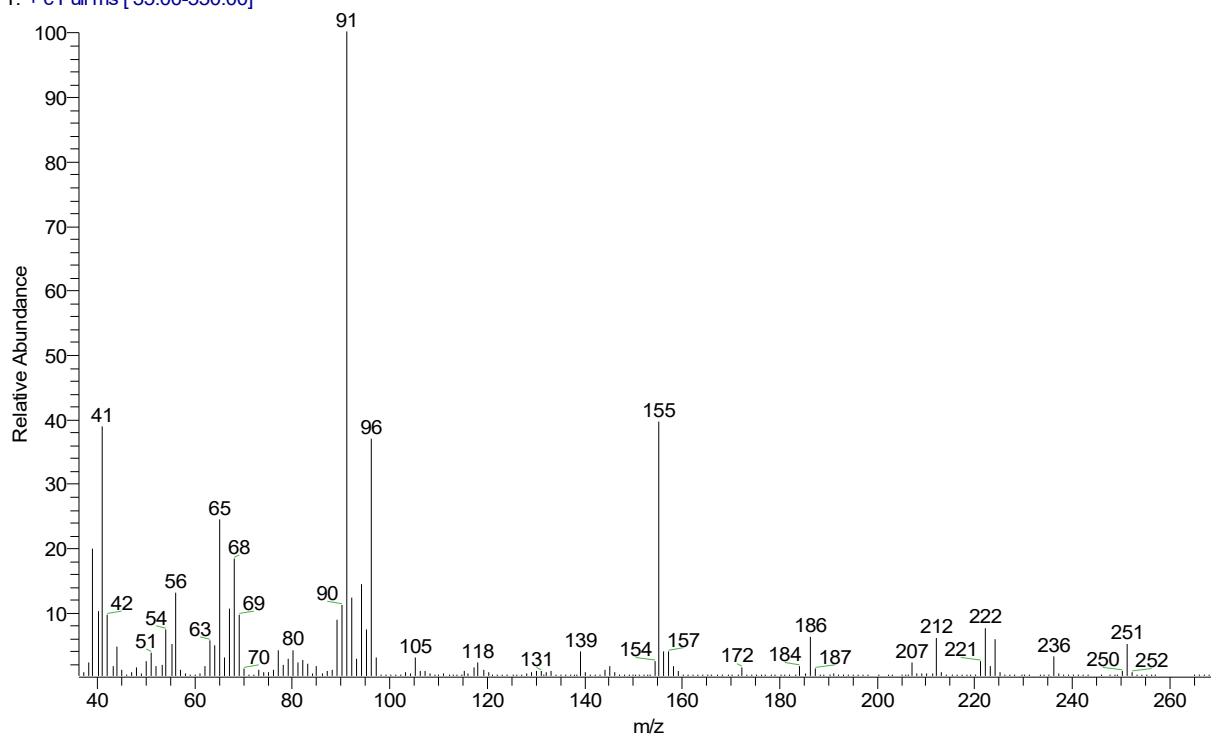
NL:
9.77E8
TIC F: MS
16_10_18_
04

RT: 8.28 - 17.32

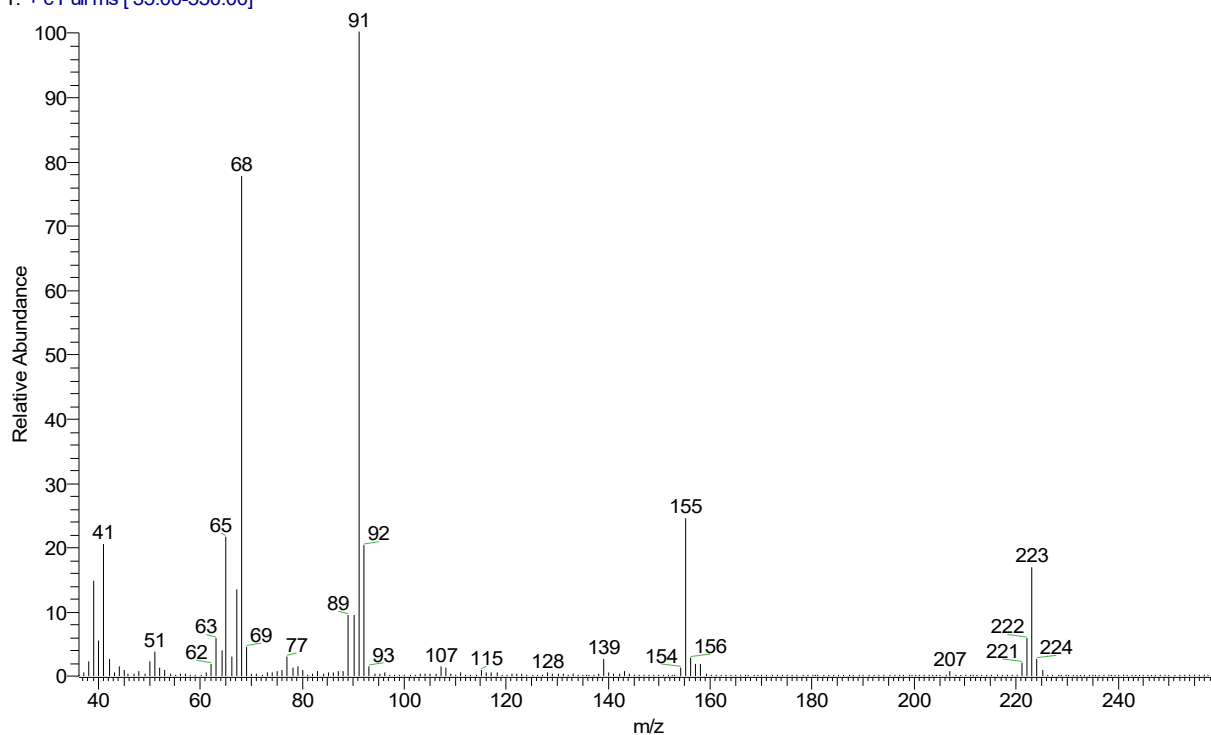


NL:
6.77E8
TIC F: MS
16_10_18_
04

16_10_18_04 #534 RT: 11.70 AV: 1 NL: 3.67E7
T: + c Full ms [35.00-550.00]



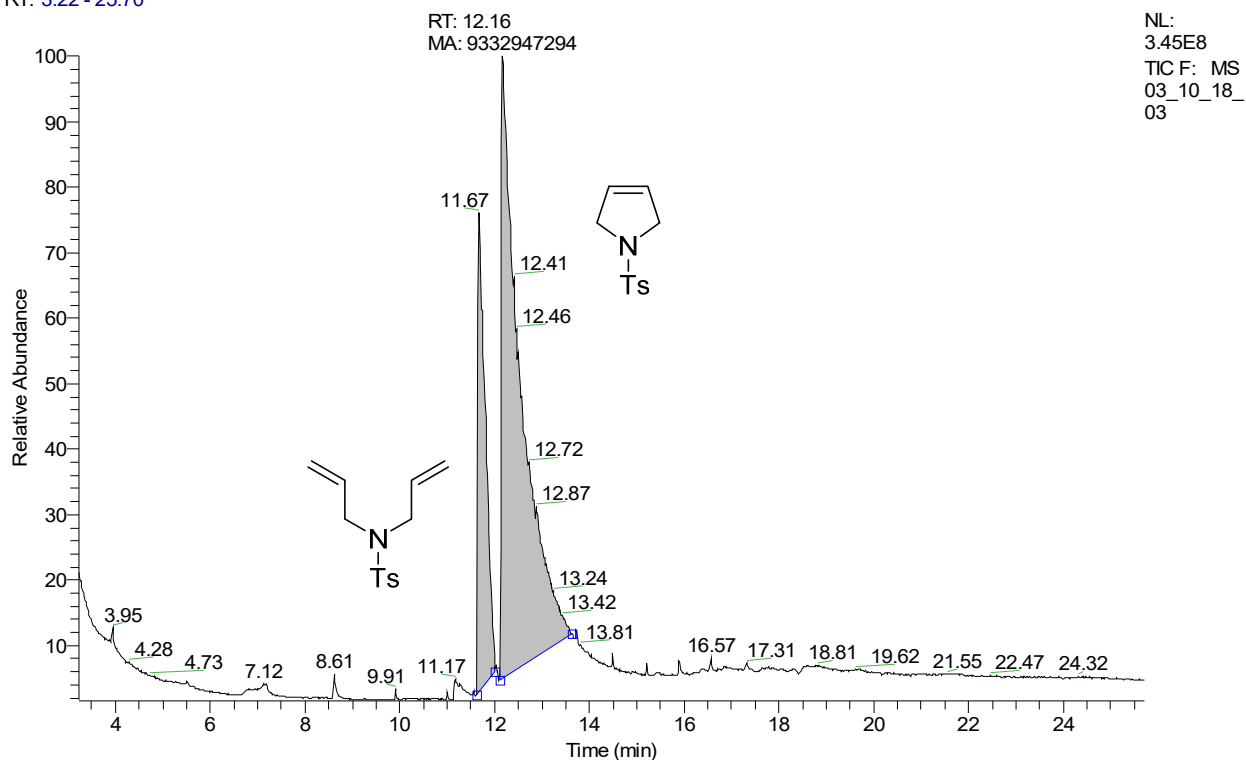
16_10_18_04 #553 RT: 12.05 AV: 1 NL: 1.59E8
T: + c Full ms [35.00-550.00]



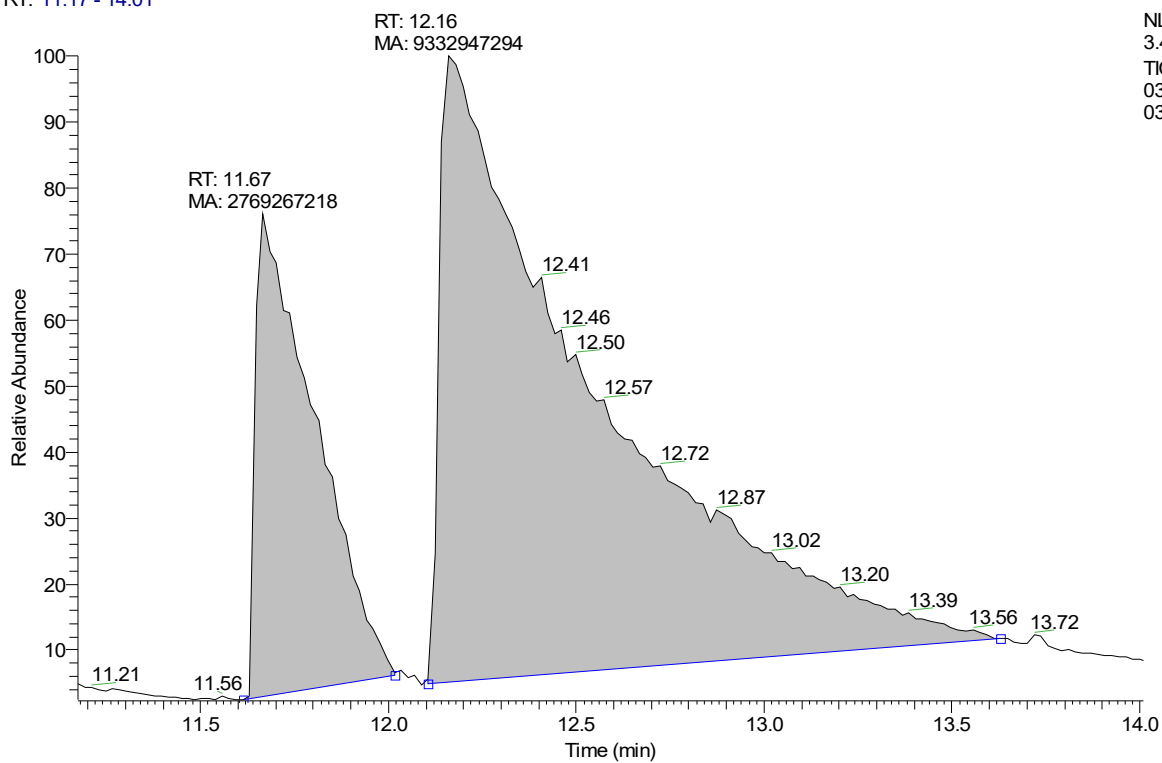
Entry 33.

Starting compound – **19**. Catalyst – **11d** (0.01 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h under an argon atmosphere.

RT: 3.22 - 25.70

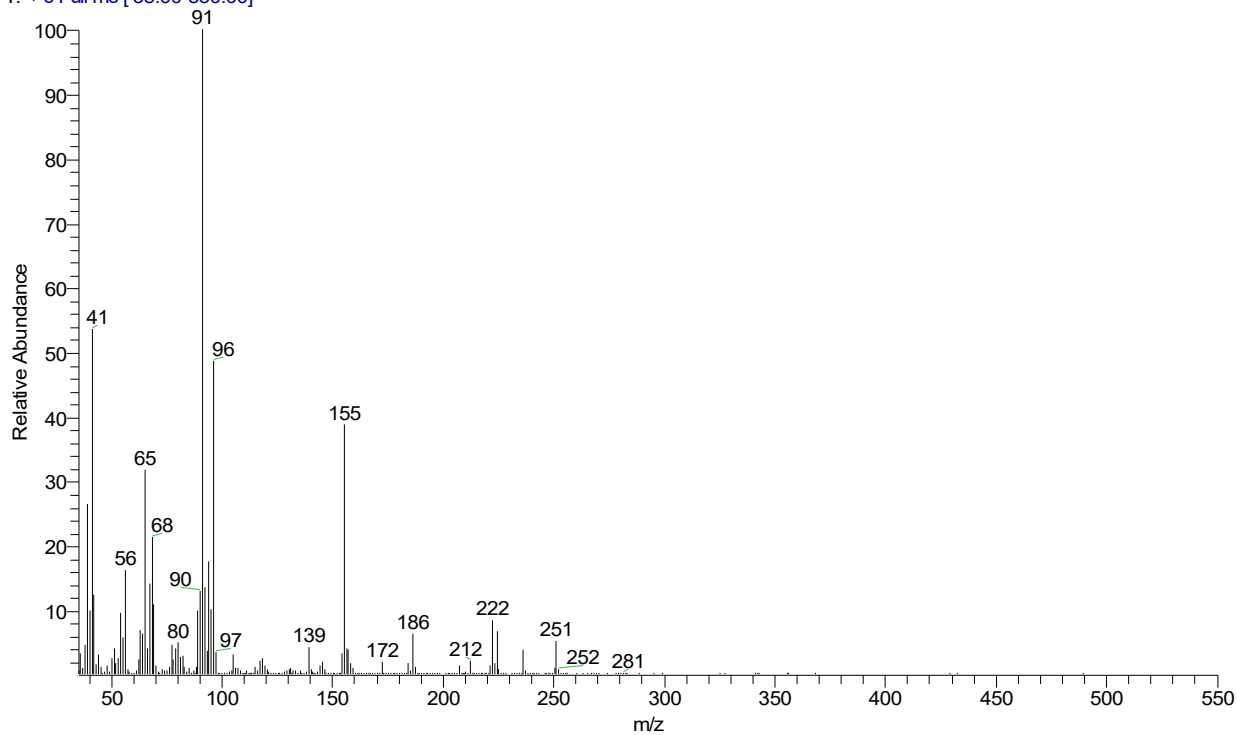


RT: 11.17 - 14.01

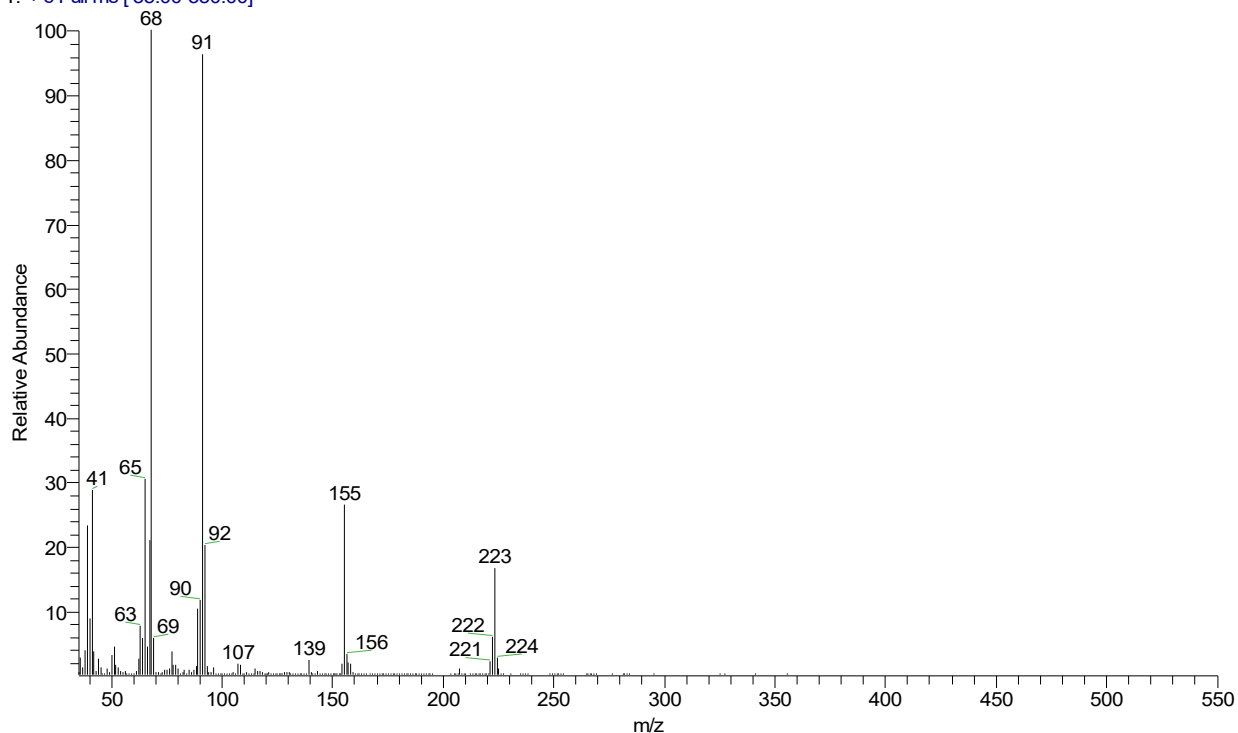


NL:
3.45E8
TIC F: MS
03_10_18_
03

03_10_18_03 #530 RT: 11.67 AV: 1 NL: 3.95E7
T: + c Full ms [35.00-550.00]



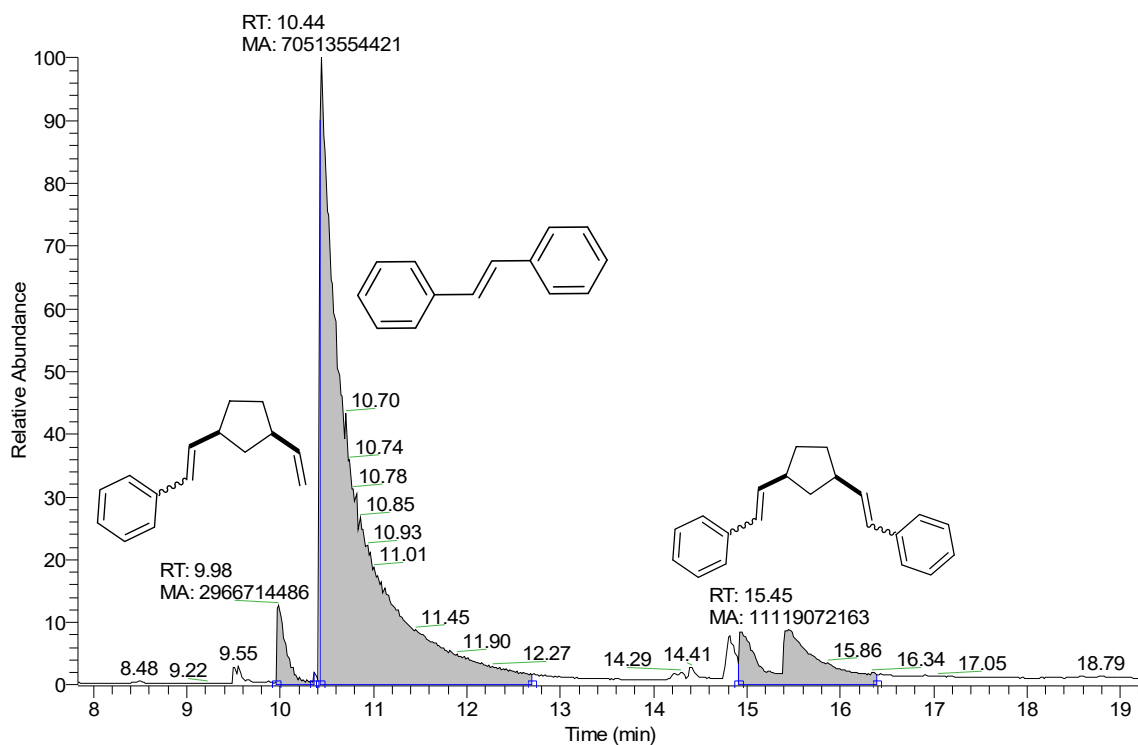
03_10_18_03 #557 RT: 12.16 AV: 1 NL: 6.62E7
T: + c Full ms [35.00-550.00]



Entry 34.

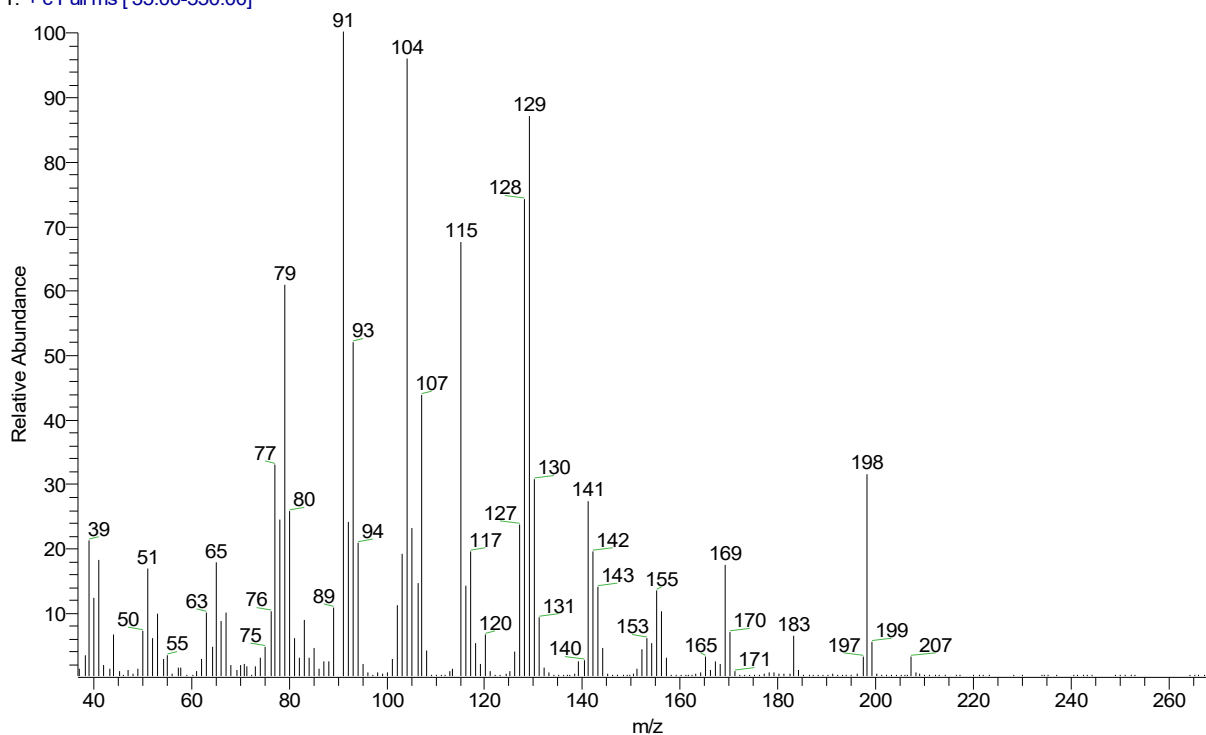
Starting compounds are **21** + 2 eq. **12**. Catalyst is **11a** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h under an argon atmosphere.

RT: 7.83 - 19.24

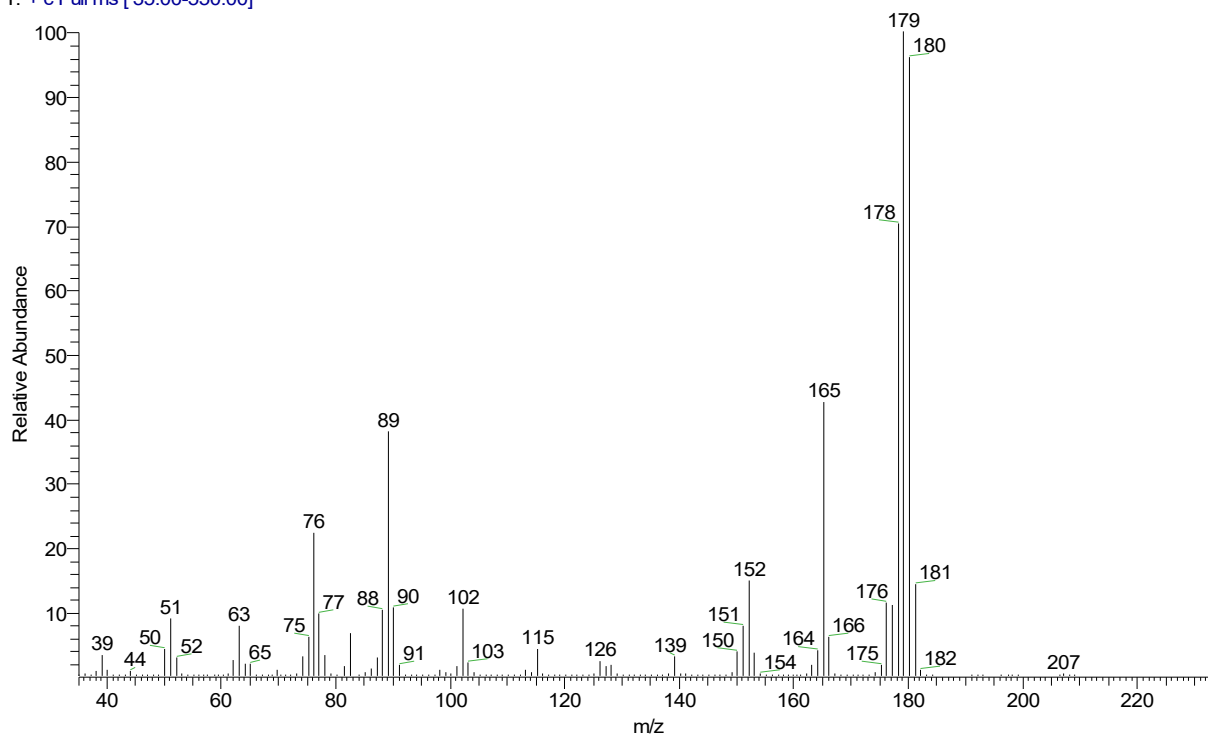


NL:
3.13E9
TIC F: MS
03_10_18_05

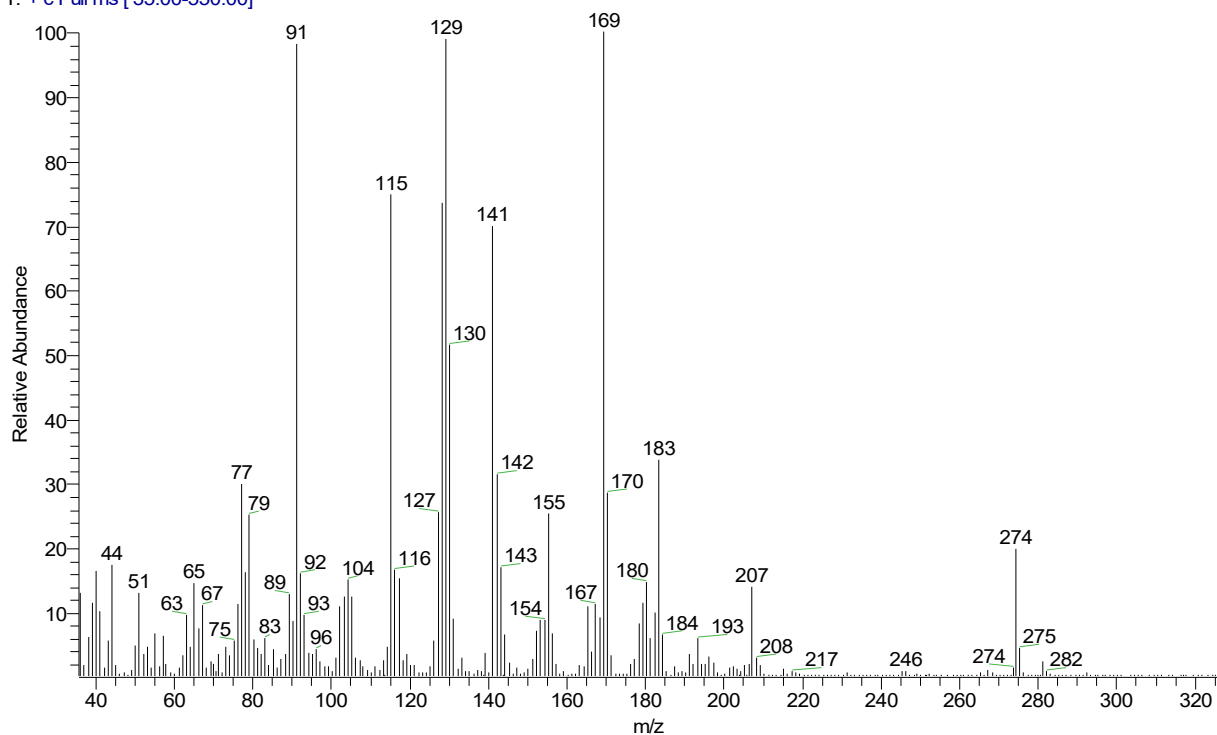
03_10_18_05 #435 RT: 10.00 AV: 1 NL: 2.52E7
T: + c Full ms [35.00-550.00]



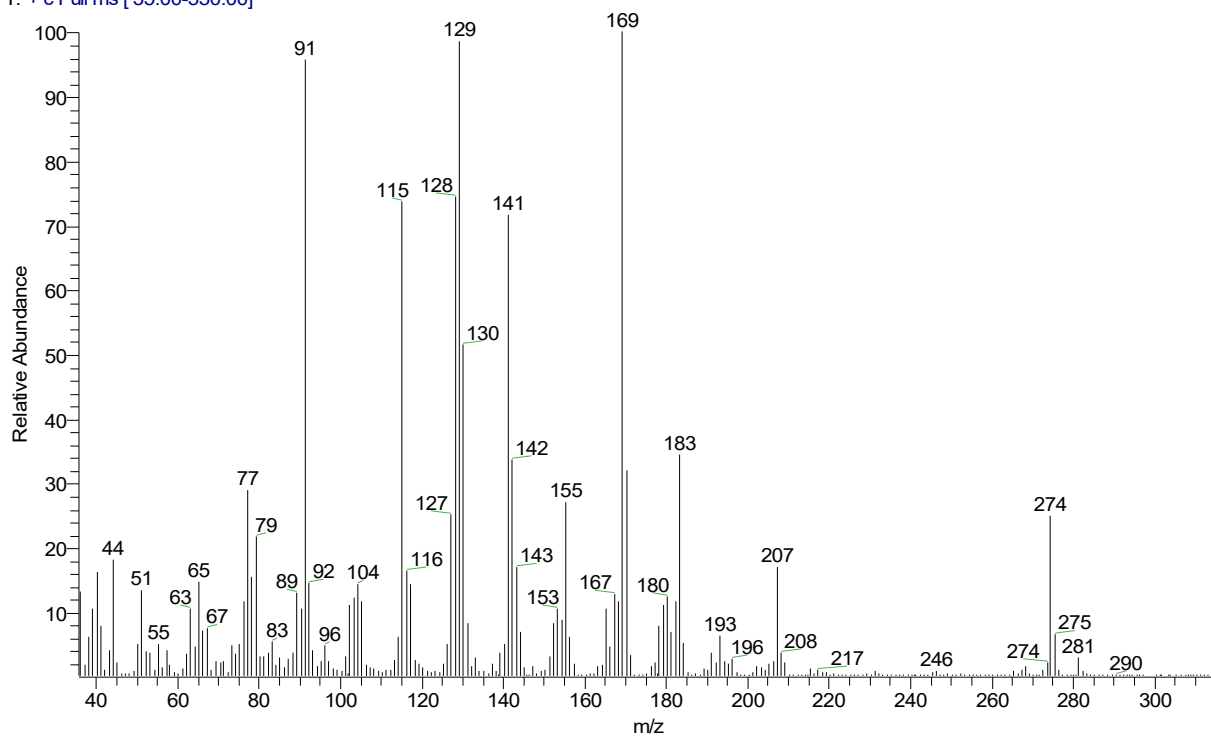
03_10_18_05 #458 RT: 10.44 AV: 1 NL: 5.24E8
T: + c Full ms [35.00-550.00]



03_10_18_05 #698 RT: 14.95 AV: 1 NL: 1.74E7
T: + c Full ms [35.00-550.00]



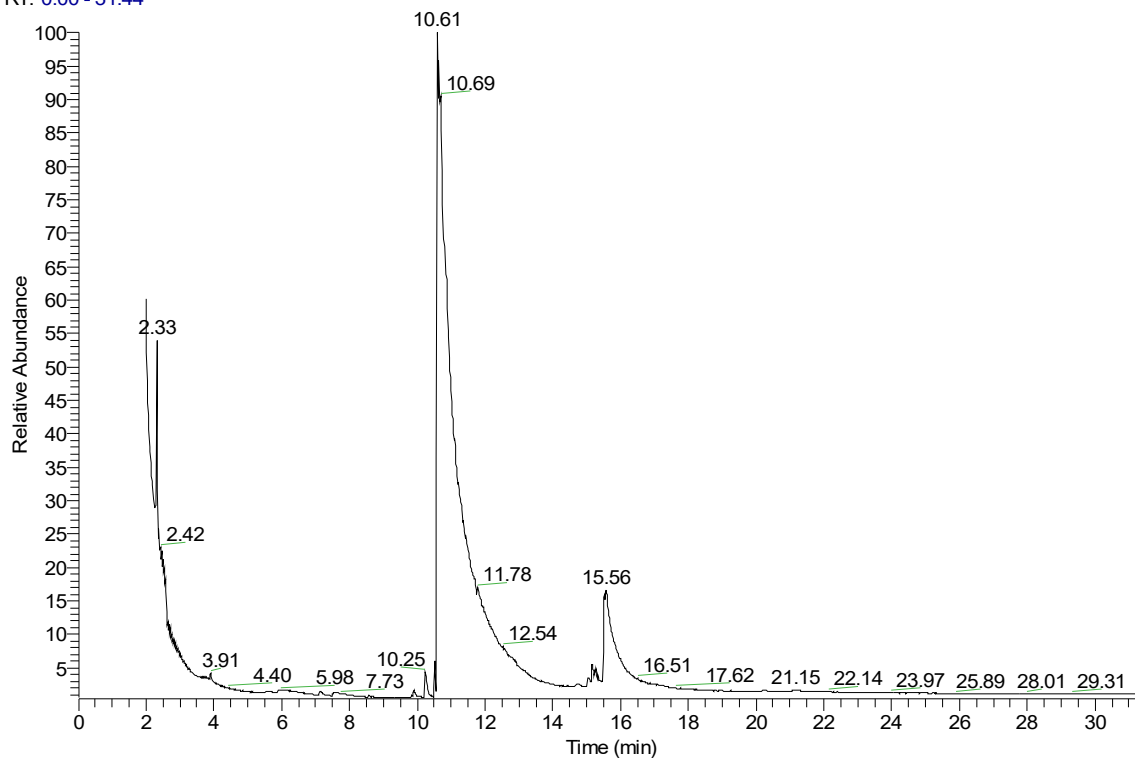
03_10_18_05 #725 RT: 15.45 AV: 1 NL: 1.81E7
T: + c Full ms [35.00-550.00]



Entry 35.

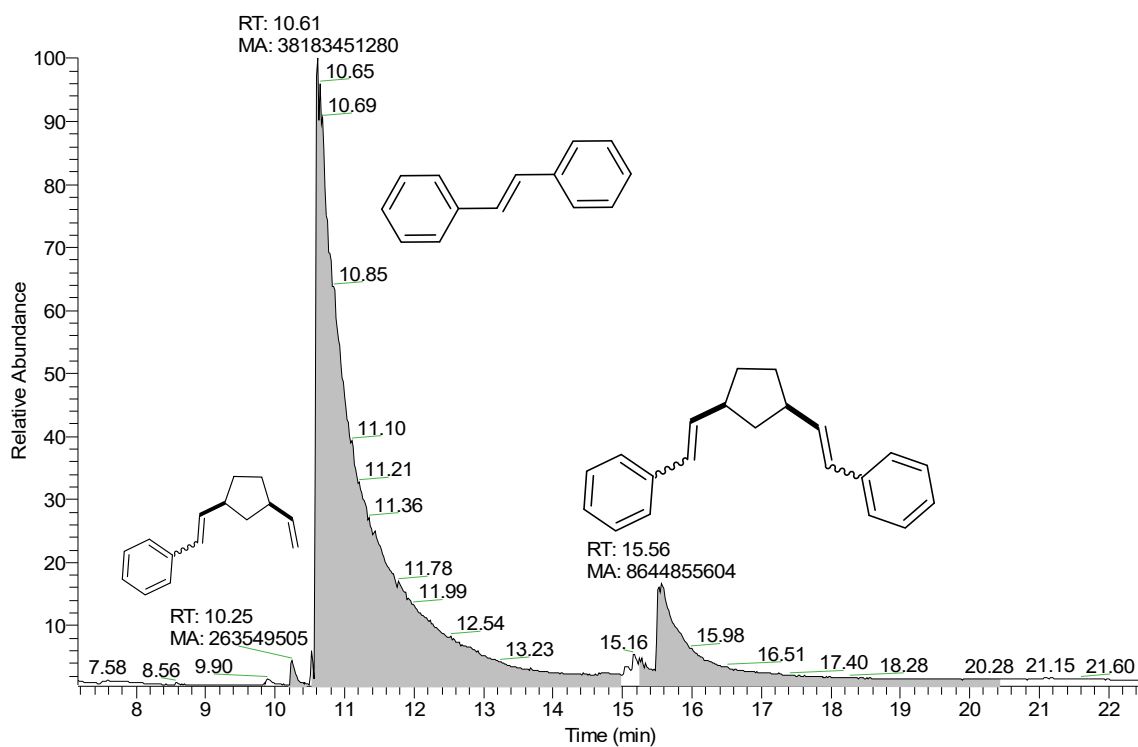
Starting compounds are **21** + 2 eq. **12**. Catalyst is **11d** (0.1 mol %). The reaction mixture was heated at reflux in CHCl₃ for 4 h under an argon atmosphere.

RT: 0.00 - 31.44



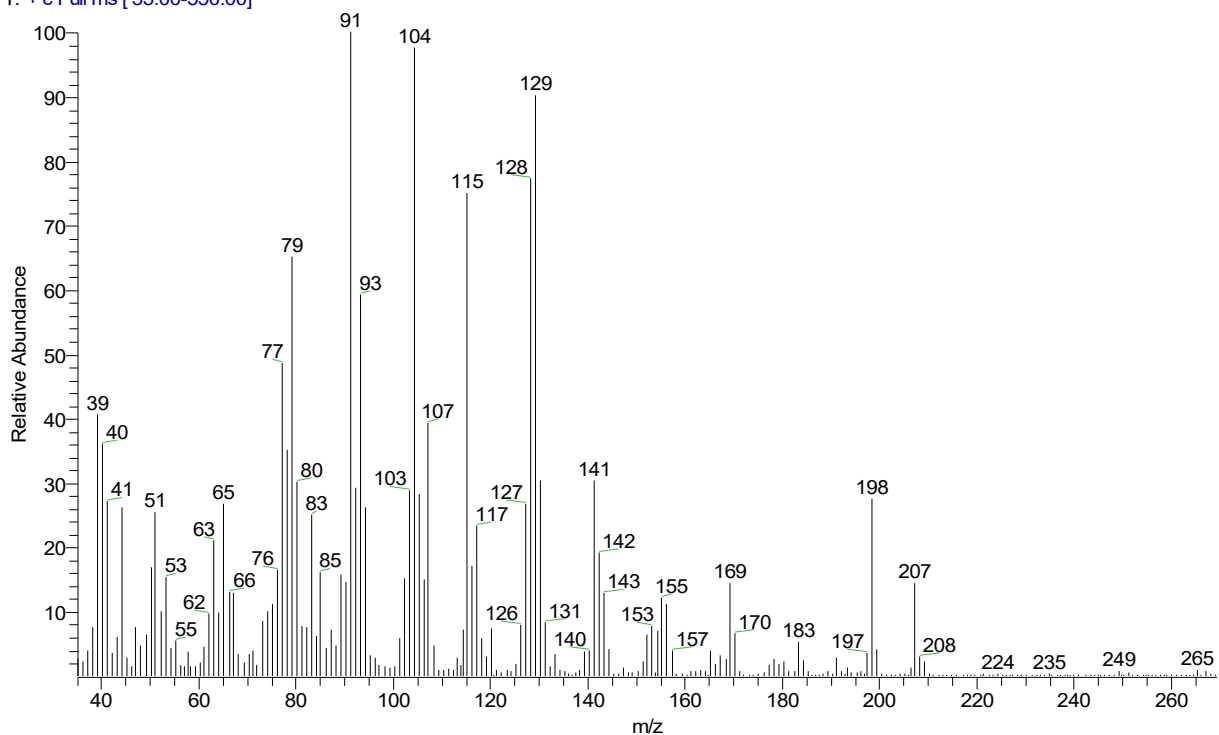
NL:
9.15E8
TIC F: MS
28_09_18_
04

RT: 7.15 - 22.49

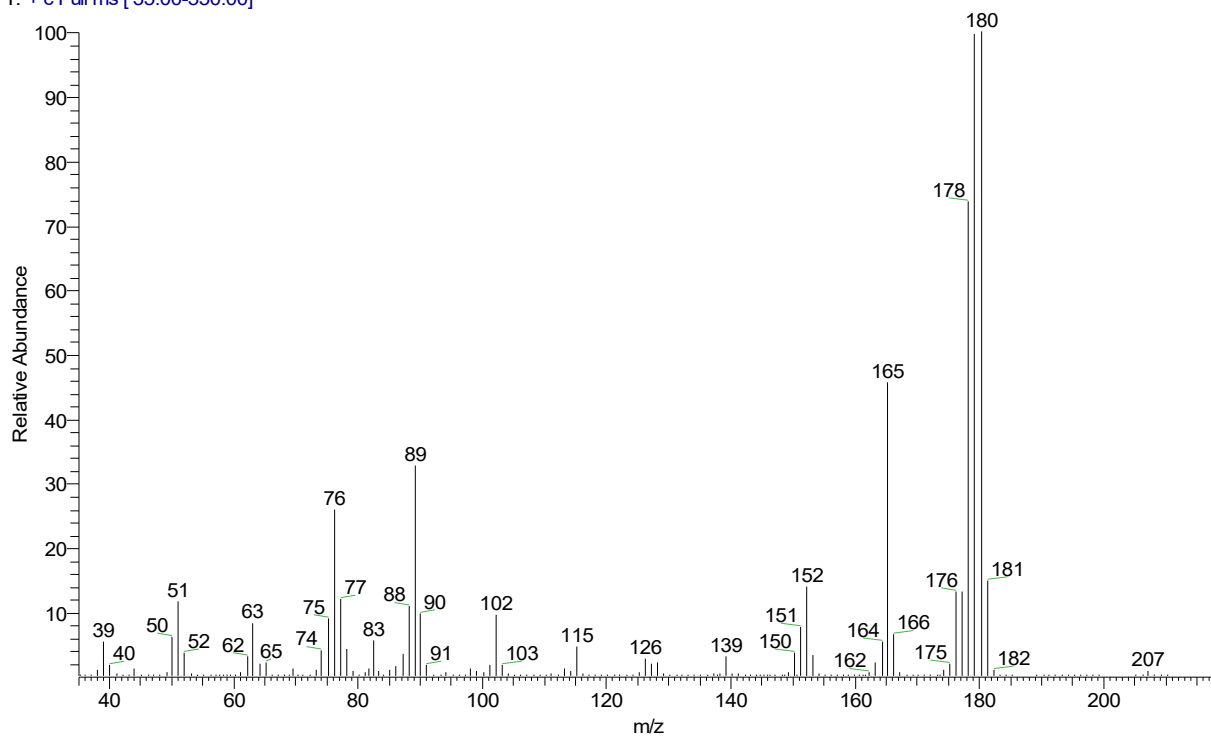


NL:
9.15E8
TIC F: MS
28_09_18_
04

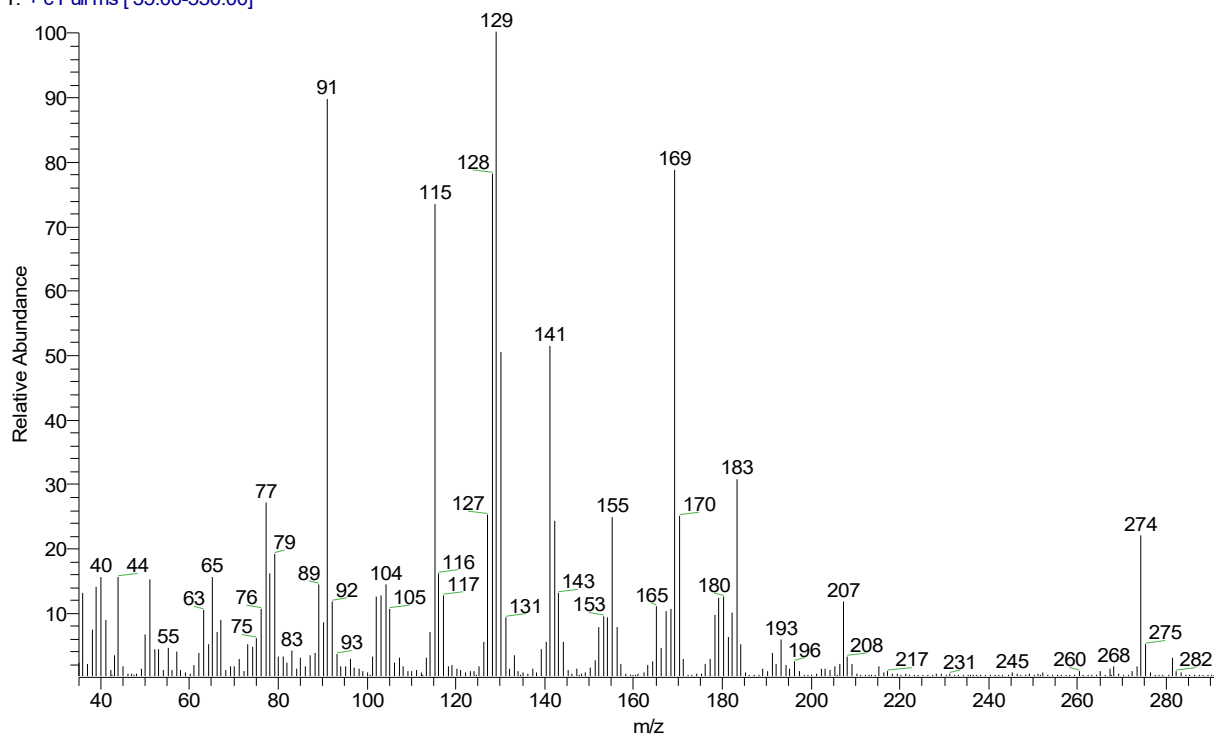
28_09_18_04 #454 RT: 10.25 AV: 1 NL: 2.15E6
T: + c Full ms [35.00-550.00]



28_09_18_04 #476 RT: 10.65 AV: 1 NL: 1.37E8
T: + c Full ms [35.00-550.00]



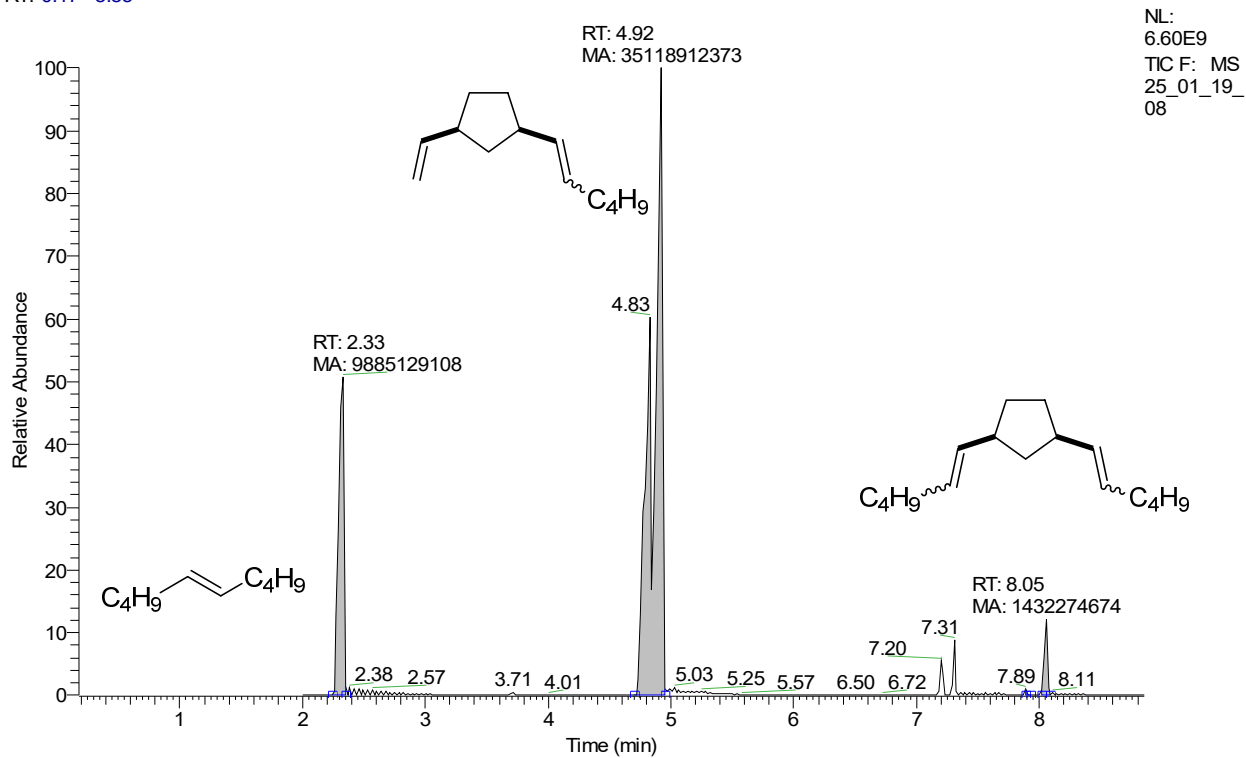
28_09_18_04 #743 RT: 15.54 AV: 1 NL: 9.77E6
T: + c Full ms [35.00-550.00]



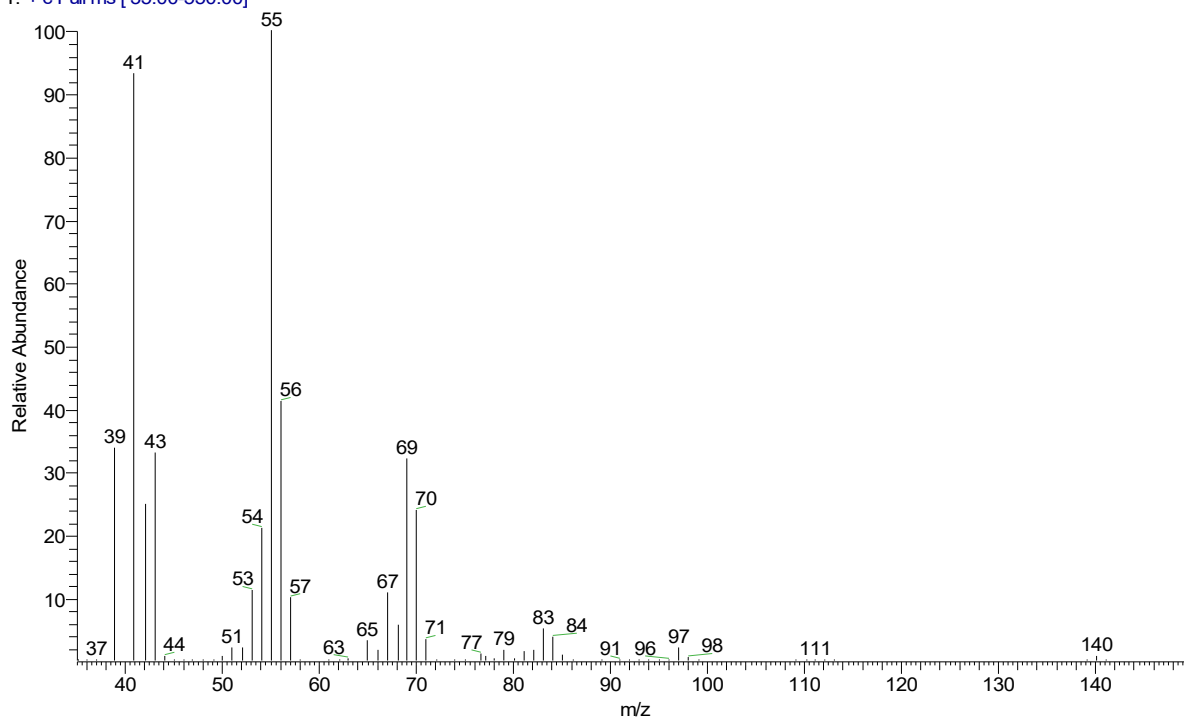
Entry 36.

Starting compounds are **21** + 2 eq. **24**. Catalyst is **11a** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h under an argon atmosphere.

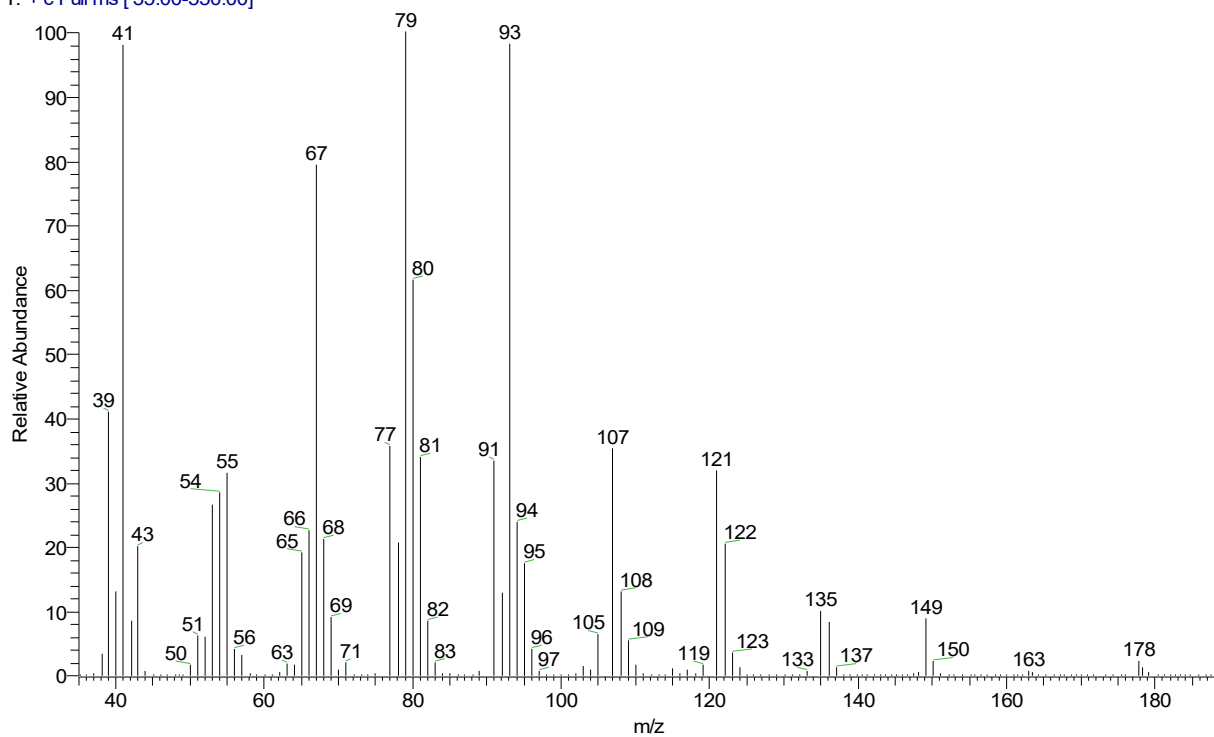
RT: 0.17 - 8.85



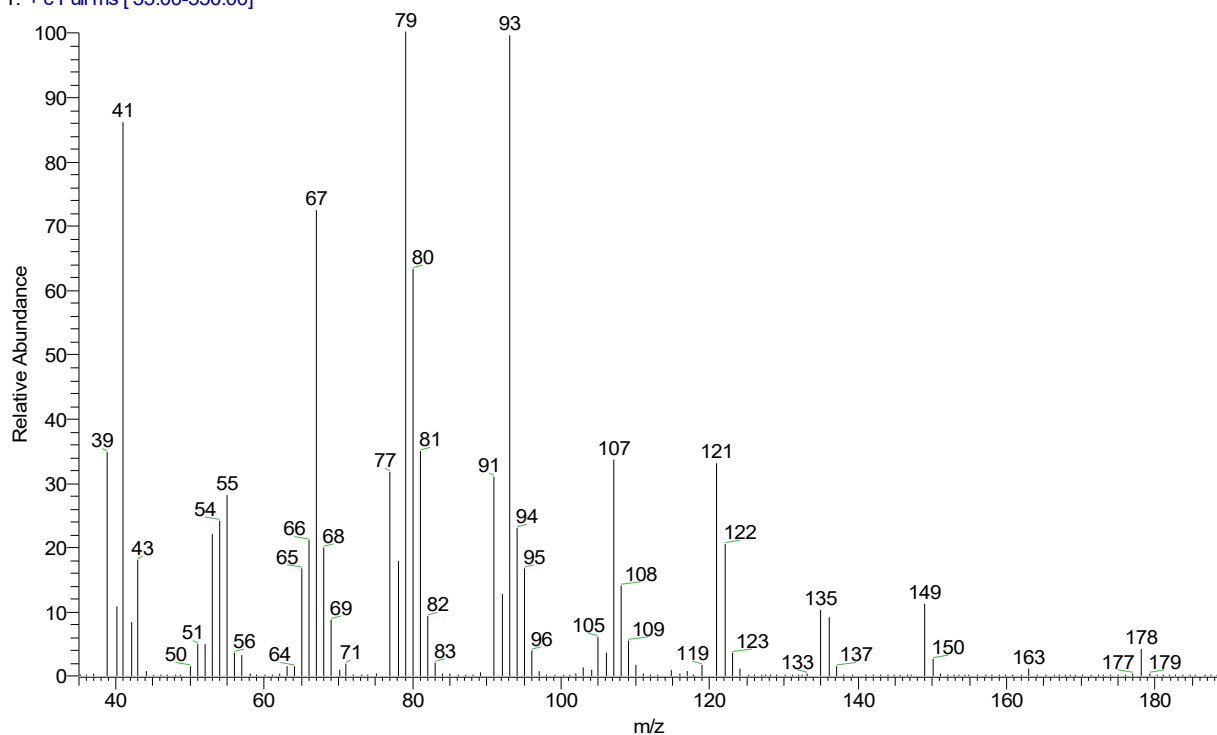
25_01_19_08 #19 RT: 2.33 AV: 1 NL: 6.95E8
T: + c Full ms [35.00-550.00]



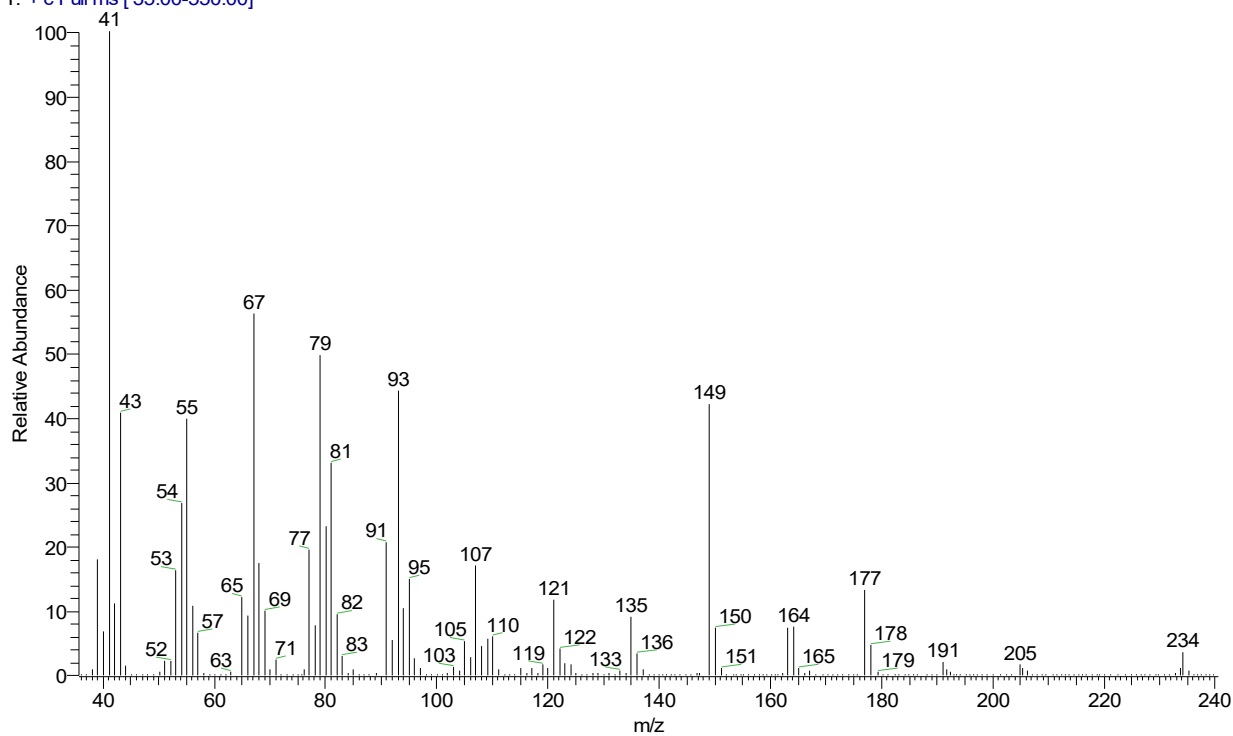
25_01_19_08 #156 RT: 4.83 AV: 1 NL: 3.73E8
T: + c Full ms [35.00-550.00]



25_01_19_08 #161 RT: 4.92 AV: 1 NL: 6.51E8
T: + c Full ms [35.00-550.00]



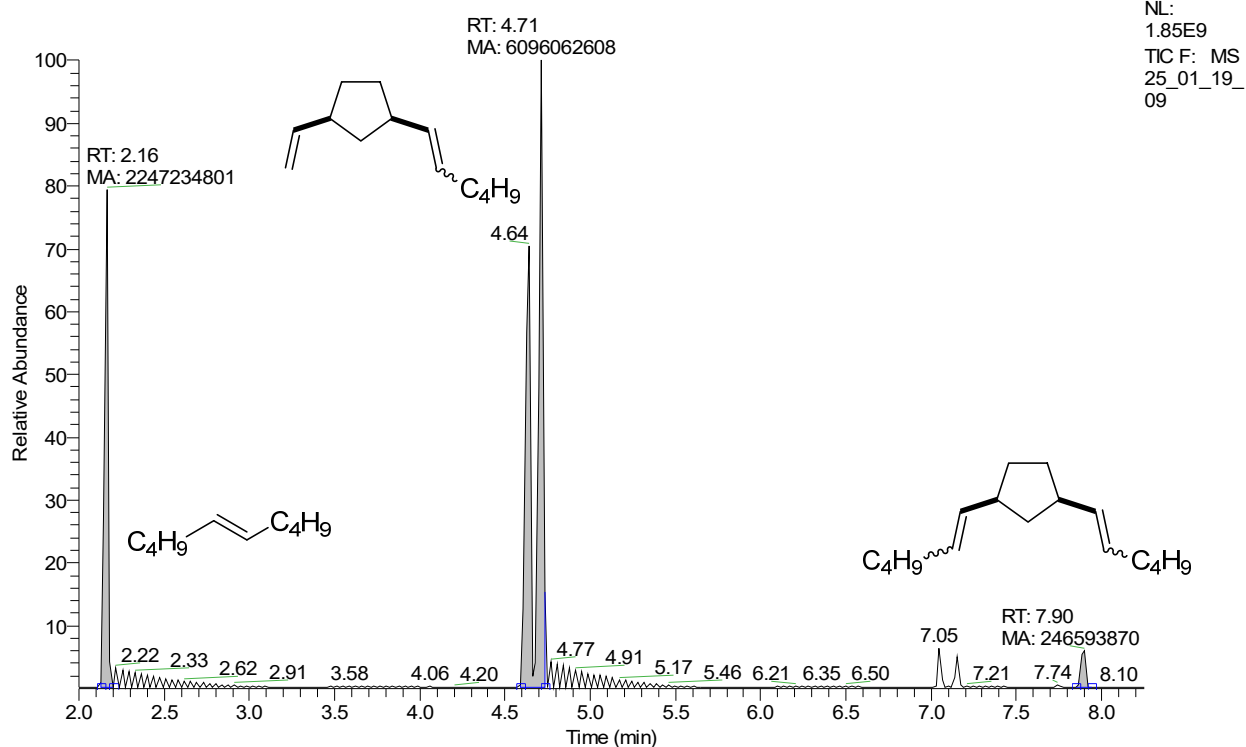
25_01_19_08 #334 RT: 8.05 AV: 1 NL: 9.68E7
T: + c Full ms [35.00-550.00]



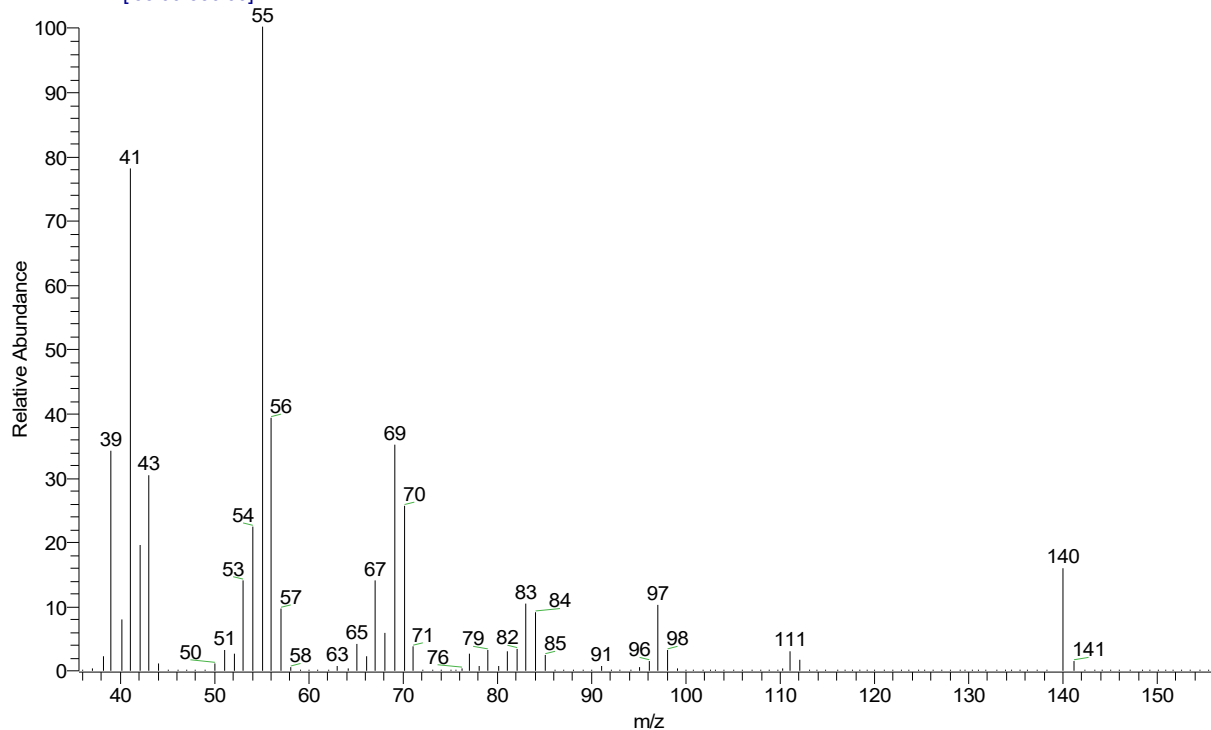
Entry 37.

Starting compounds are **21** + 2 eq. **24**. Catalyst is **11b** (0.1 mol %). The reaction mixture was heated at reflux in CHCl_3 for 4 h under an argon atmosphere.

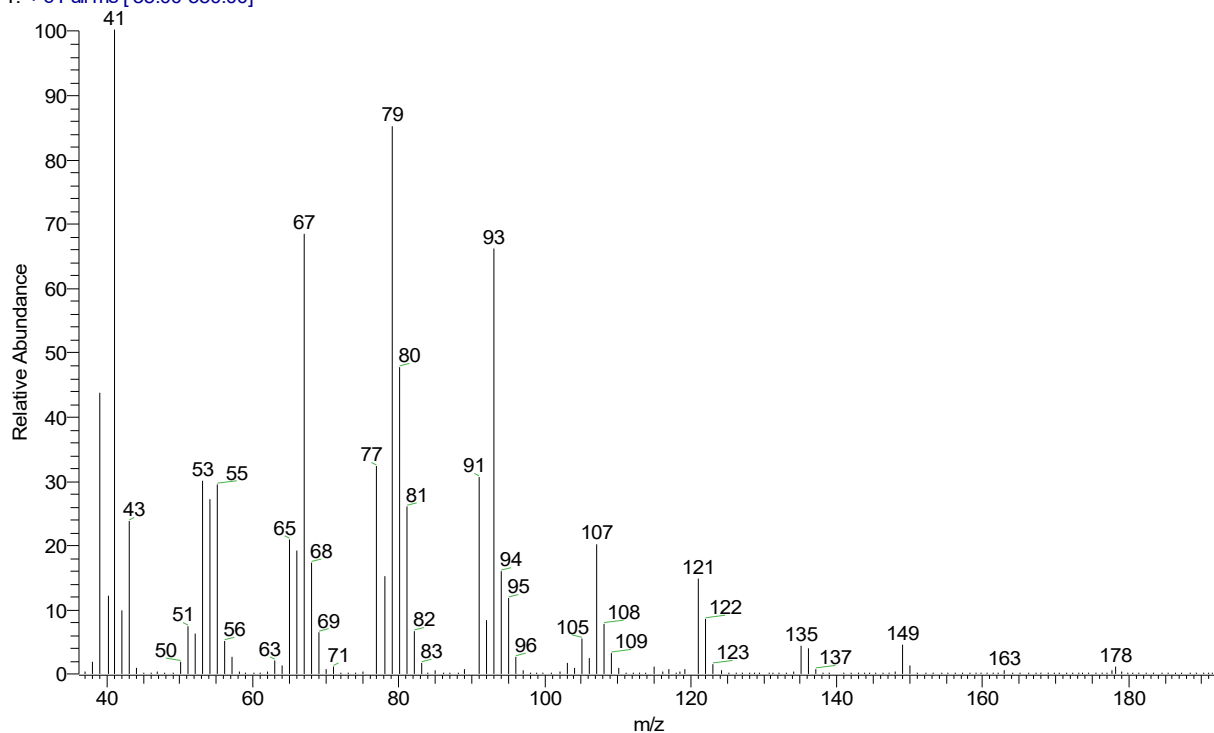
RT: 2.00 - 8.25



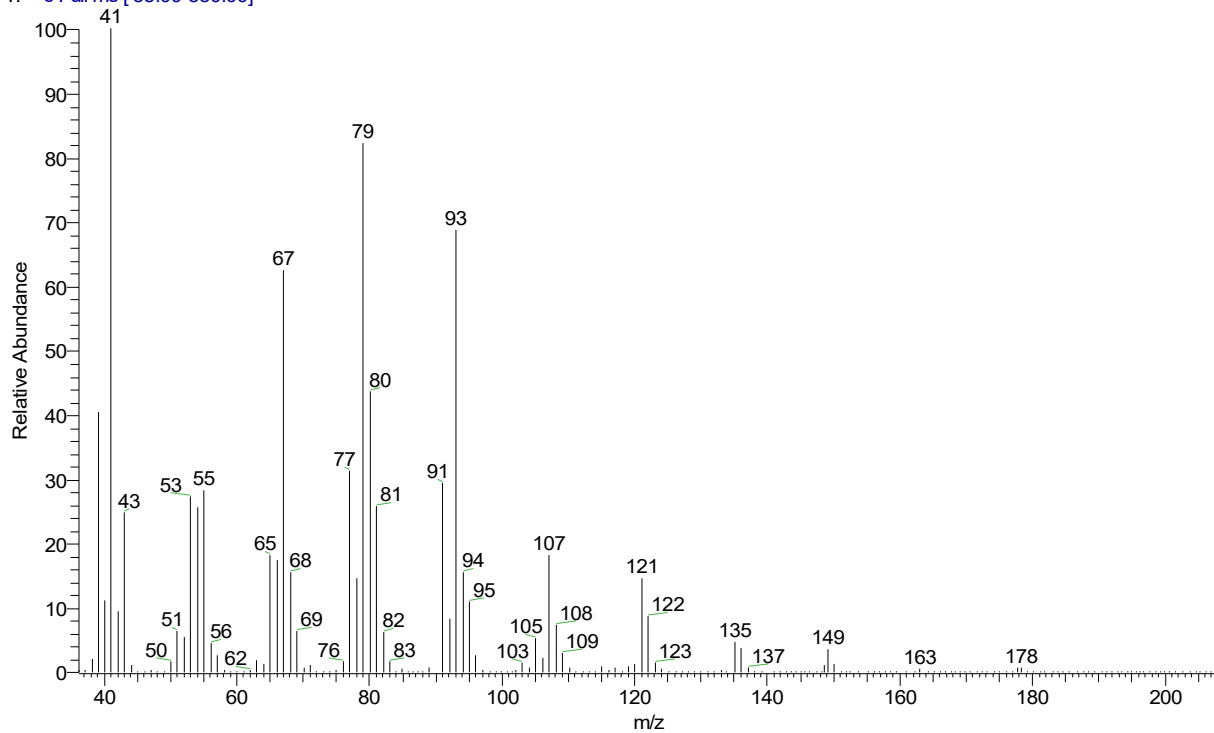
25_01_19_09#10 RT: 2.16 AV: 1 NL: 2.76E8
T: + c Full ms [35.00-550.00]



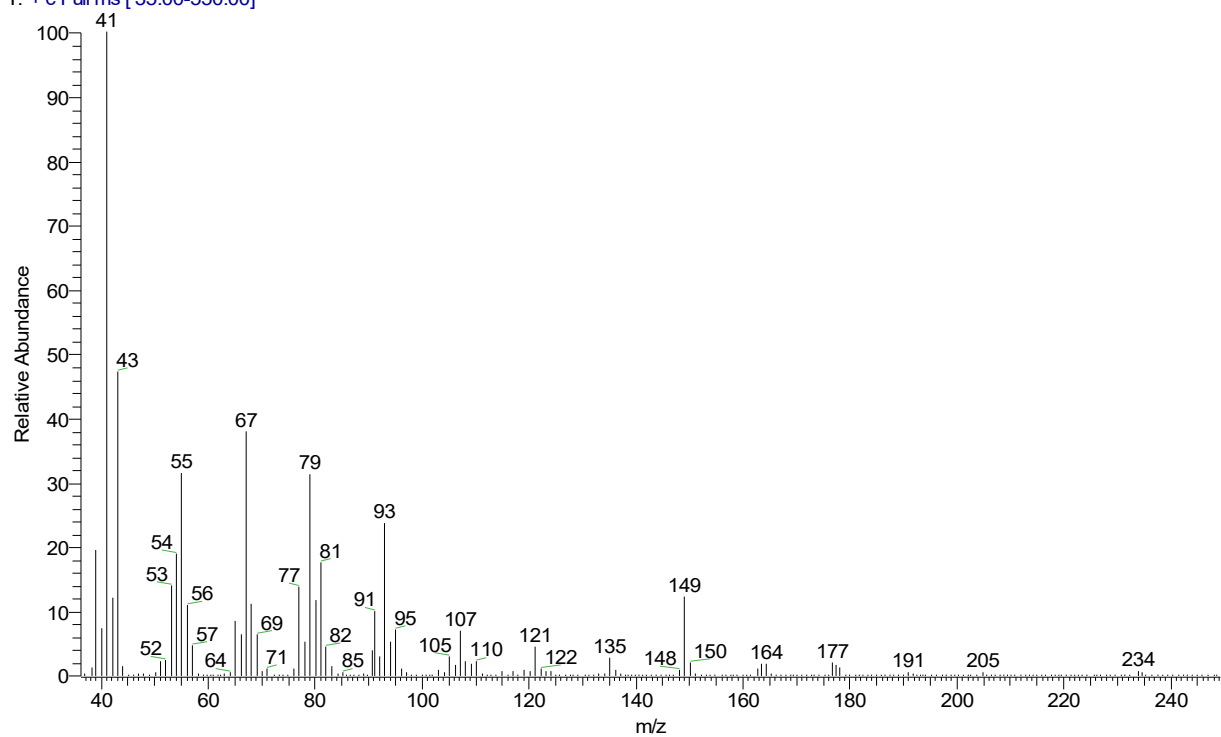
25_01_19_09 #145 RT: 4.62 AV: 1 NL: 1.19E8
T: + c Full ms [35.00-550.00]



25_01_19_09 #149 RT: 4.70 AV: 1 NL: 1.04E8
T: + c Full ms [35.00-550.00]



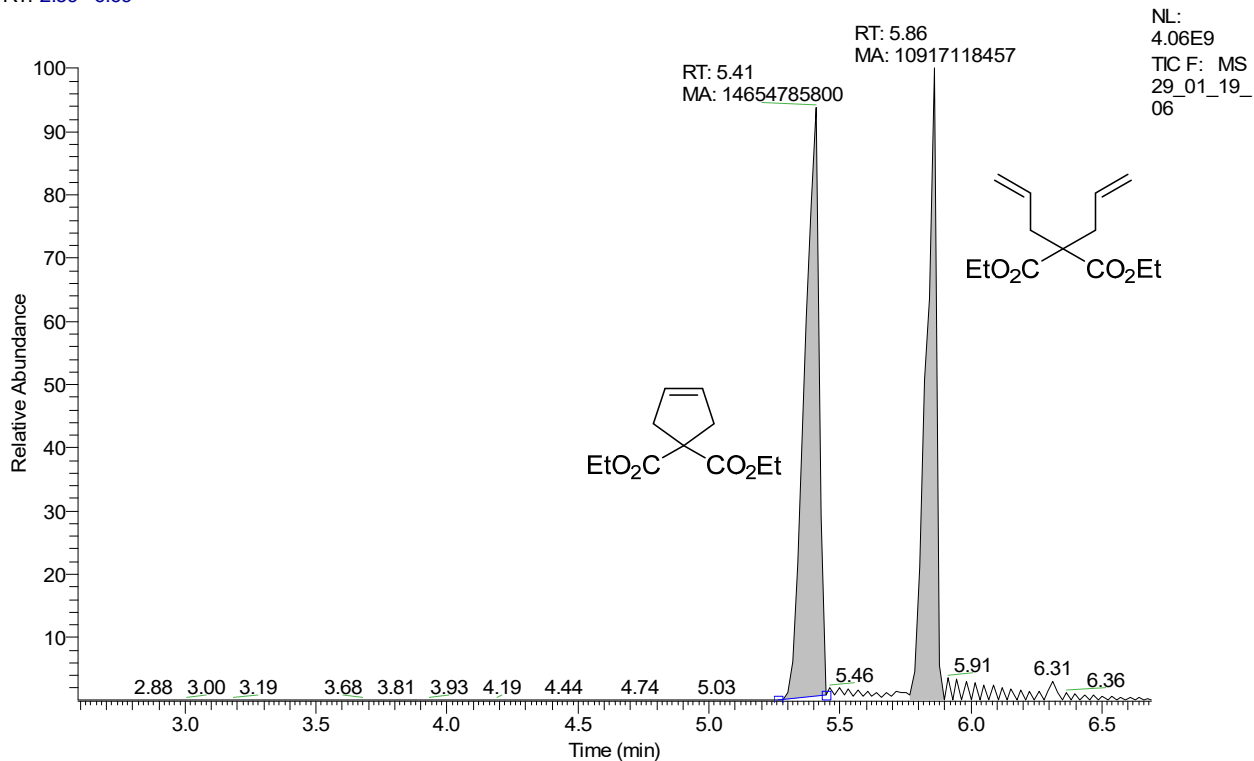
25_01_19_09 #325 RT: 7.90 AV: 1 NL: 2.00E7
T: + c Full ms [35.00-550.00]



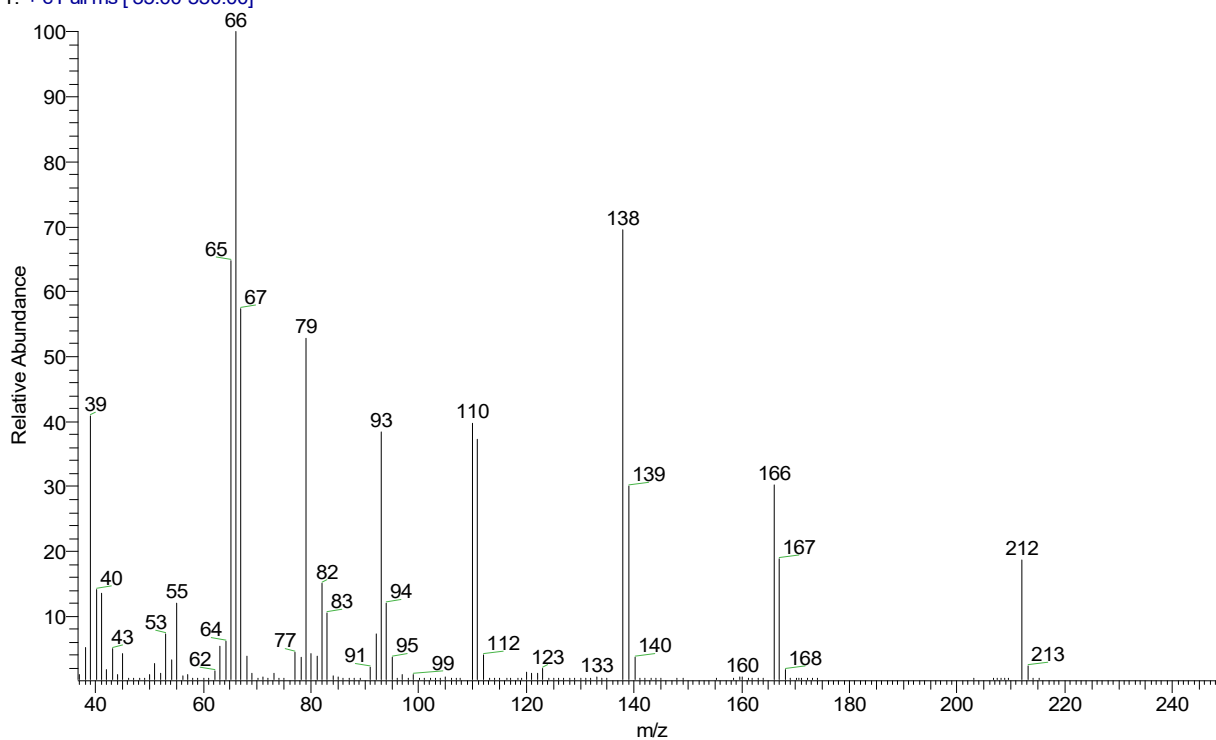
3. Comparison of ^1H NMR and GC/MS methods for quantitative analysis of mixtures *diallylmalonate (17)/ diethyl cyclopent-3-ene-1,1-dicarboxylate (18)*, and *diallyltosylamide (19)/ 1-tosyl-2,5-dihydro-1H-pyrrole (20)* obtained in the course of metathesis reactions.

GC-MS analysis of a mixture of *diethyl diallylmalonate* (**17**)/ *diethyl cyclopent-3-ene-1,1-dicarboxylate* (**18**), the observed ratio is 44/56.

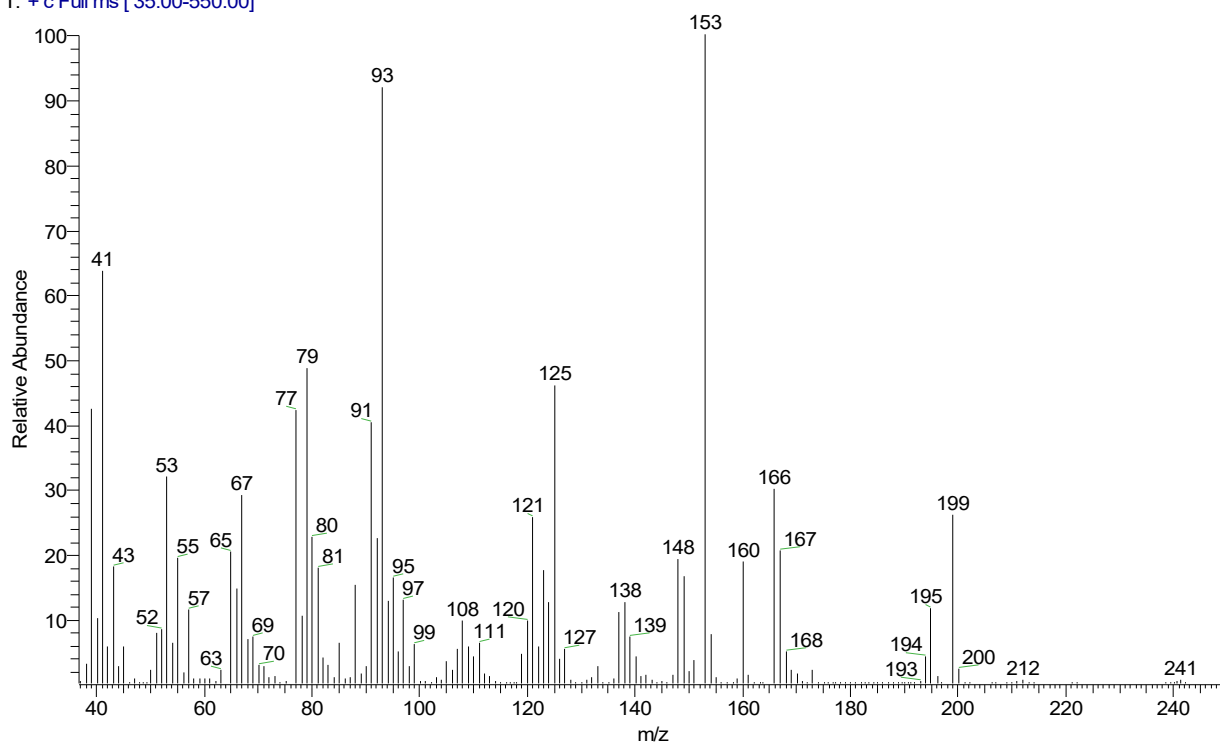
RT: 2.59 - 6.69



29_01_19_06 #188 RT: 5.41 AV: 1 NL: 4.86E8
T: +c Full ms [35.00-550.00]

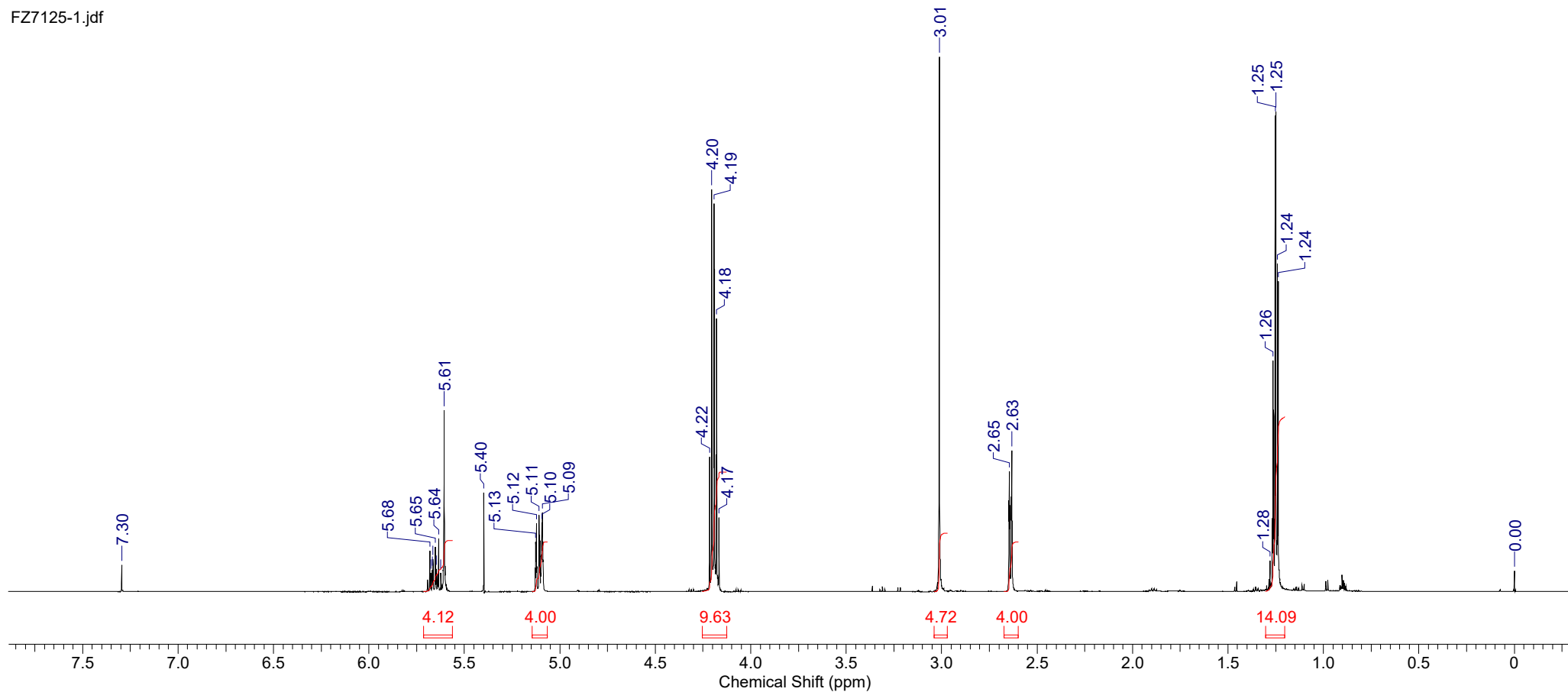
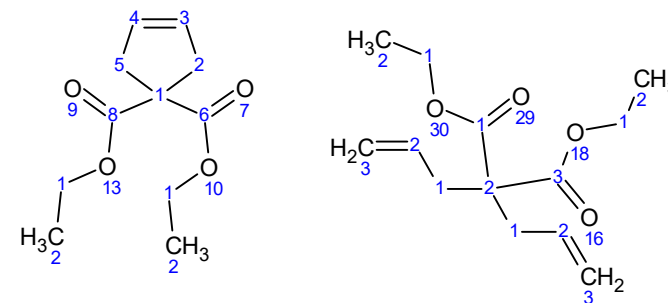


29_01_19_06 #213 RT: 5.86 AV: 1 NL: 3.28E8
T: + c Full ms [35.00-550.00]

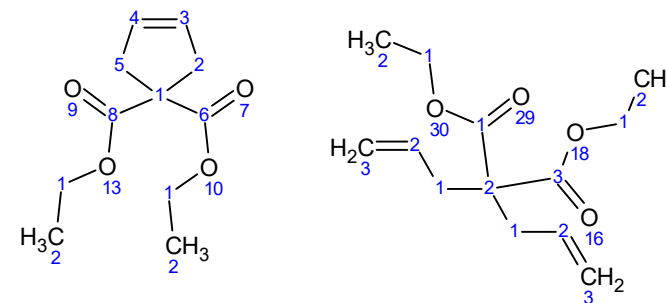


^1H NMR analysis of the same mixture of diethyl diallylmalonate (**17**)/ diethyl cyclopent-3-ene-1,1-dicarboxylate (**18**), the observed ratio is 47/53.

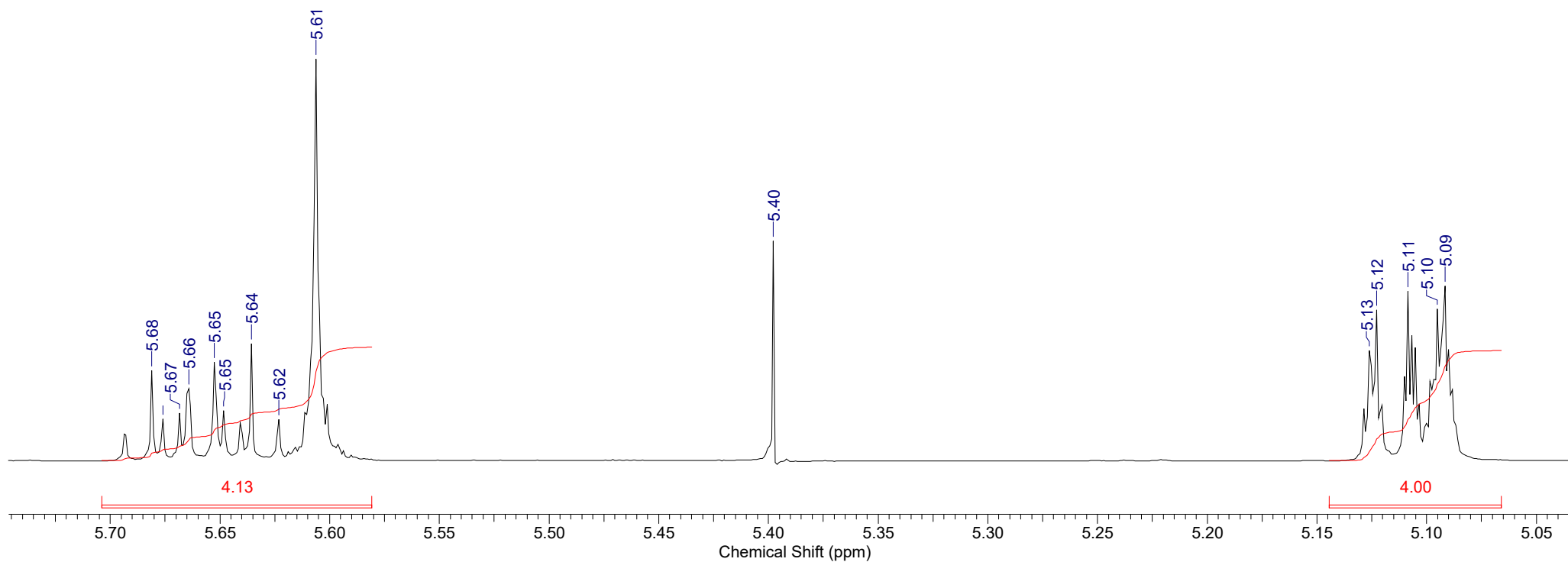
Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	26 Feb 1990 12:08:37		
Date Stamp	29 Jan 2019 07:51:37			File Name	C:\Users\Fedor\Desktop\28.01.19\FZ7125-1.jdf	Frequency (MHz)	600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse.ex2			Receiver Gain	26.00
Spectrum Offset (Hz)	5429.8022	Sweep Width (Hz)	16534.39	Temperature (degree C)	32.300	Solvent	CHLOROFORM-d



Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	26 Feb 1990 12:08:37		
Date Stamp	29 Jan 2019 07:51:37			File Name	C:\Users\Fedor\Desktop\28.01.19\FZ7125-1.jdf	Frequency (MHz)	600.17
Nucleus	1H	Number of Transients	8	Origin	ECA 600	Original Points Count	32768
Points Count	32768	Pulse Sequence	single_pulse.ex2			Receiver Gain	26.00
Spectrum Offset (Hz)	5429.8022	Sweep Width (Hz)	16534.39	Temperature (degree C)	32.300	Solvent	CHLOROFORM-d

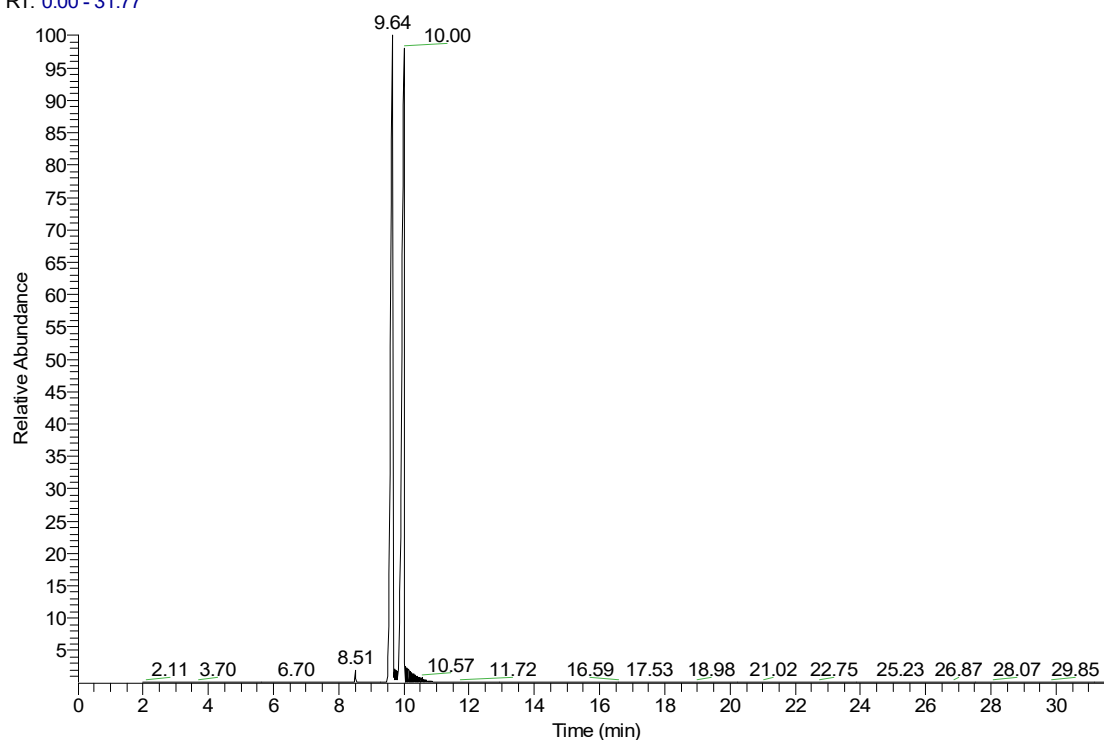


FZ7125-1.jdf



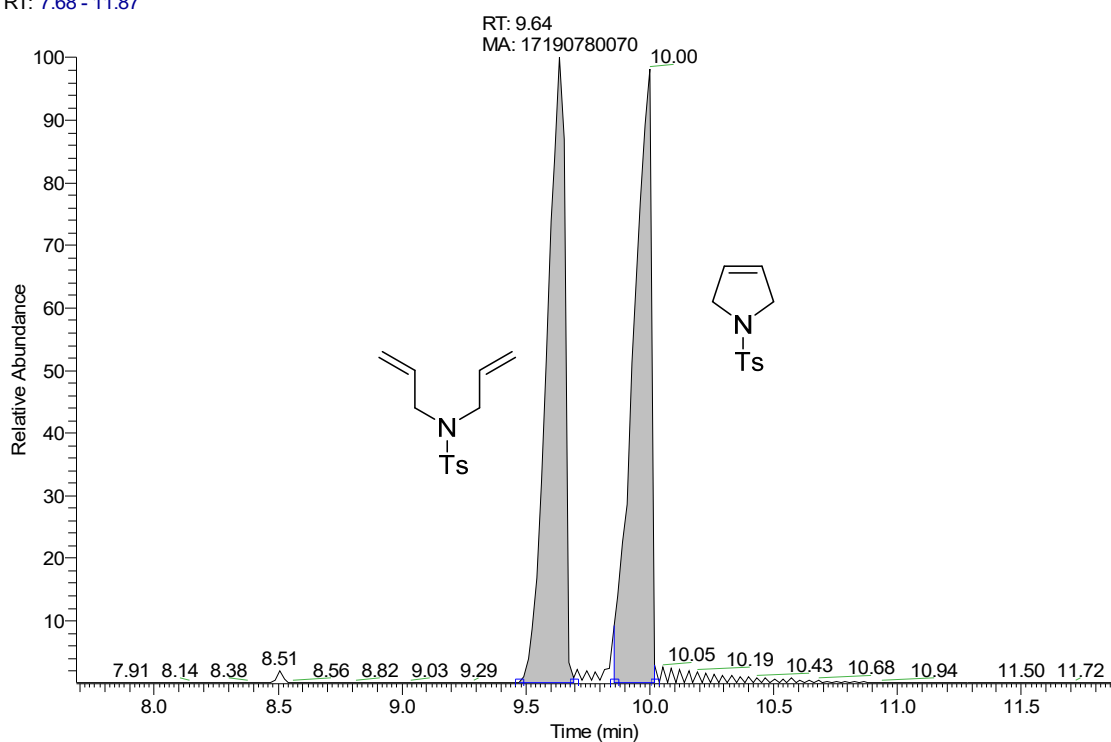
GC-MS analysis of a mixture of *diallyltosylamide* (**19**)/ *1-tosyl-2,5-dihydro-1H-pyrrole* (**20**), the established ratio is 49/51.

RT: 0.00 - 31.77



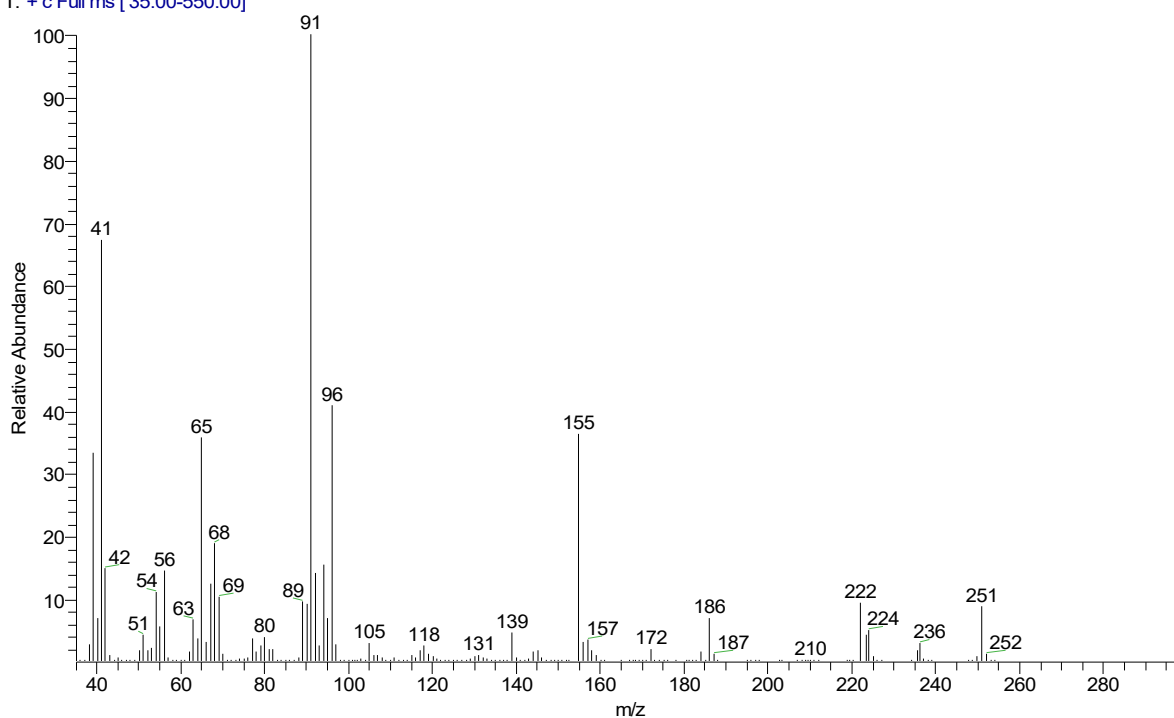
NL:
3.39E9
TIC F: MS
25_01_19_
12_190125
181501

RT: 7.68 - 11.87

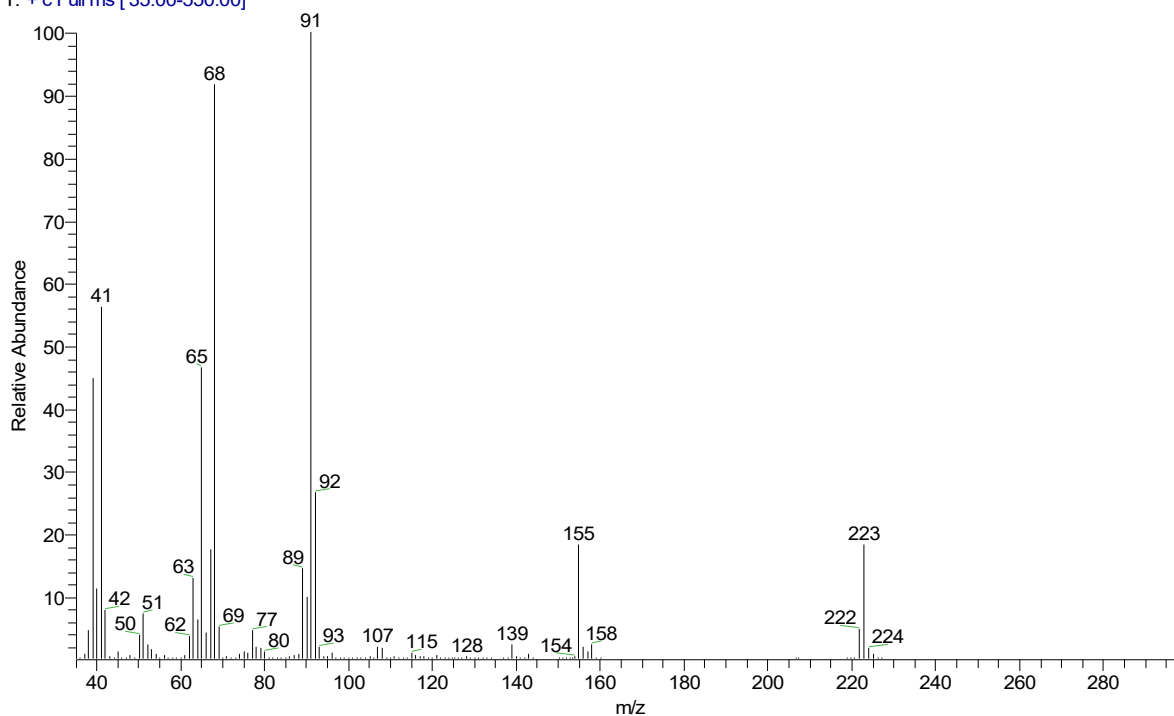


NL:
3.39E9
TIC F: MS
25_01_19
12_190125
181501

25_01_19_12_190125181501 #420 RT: 9.64 AV: 1 NL: 5.52E8
T: + c Full ms [35.00-550.00]

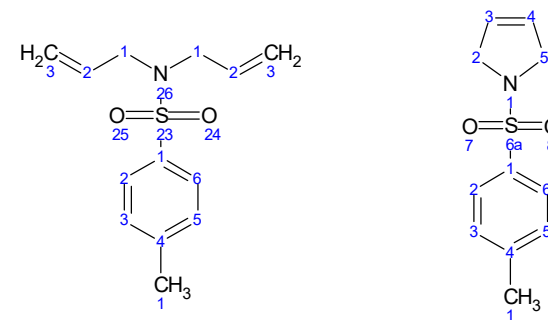


25_01_19_12_190125181501 #436 RT: 9.93 AV: 1 NL: 3.01E8
T: + c Full ms [35.00-550.00]

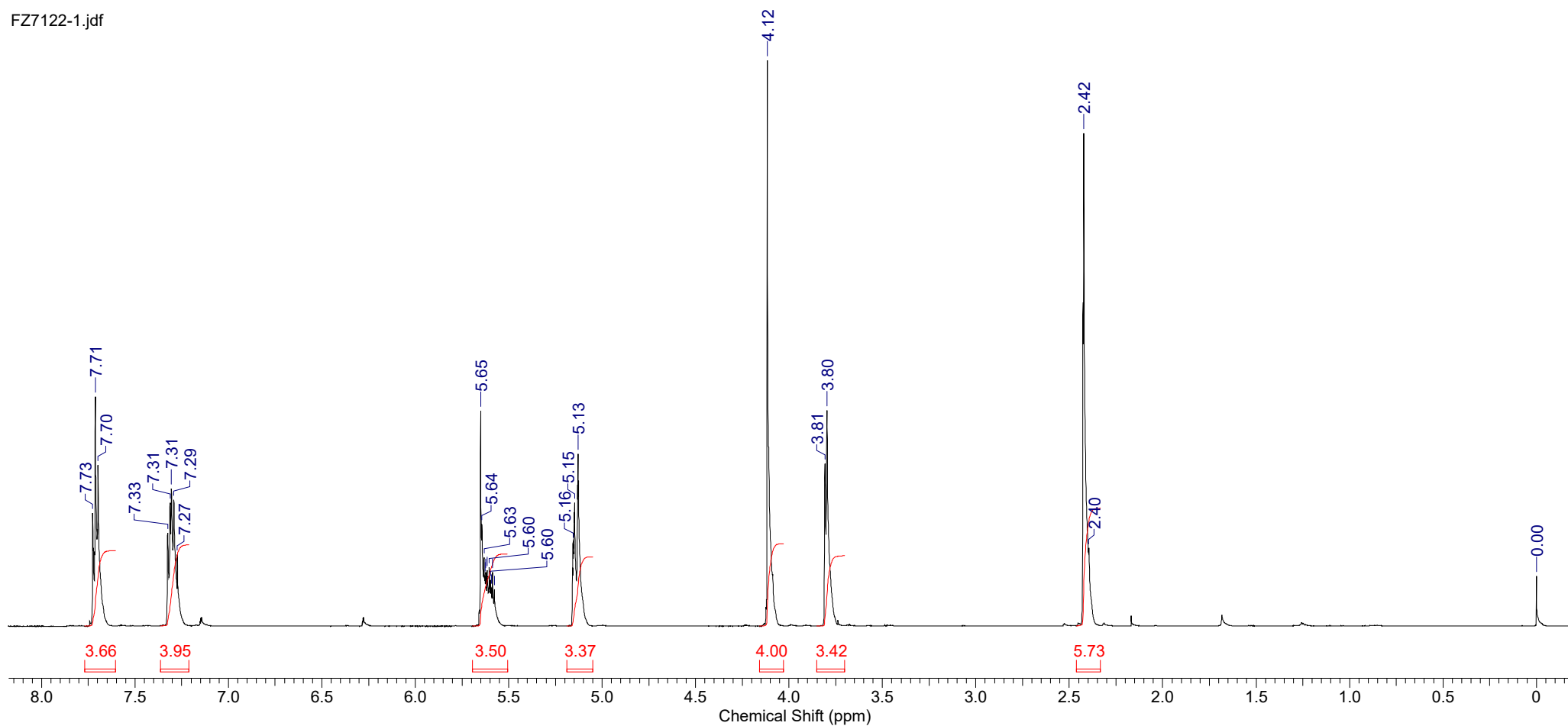


^1H NMR analysis of a mixture of of *diallyltosylamide* (**19**)/ *1-tosyl-2,5-dihydro-1H-pyrrole* (**20**), the established ratio is 47/53.

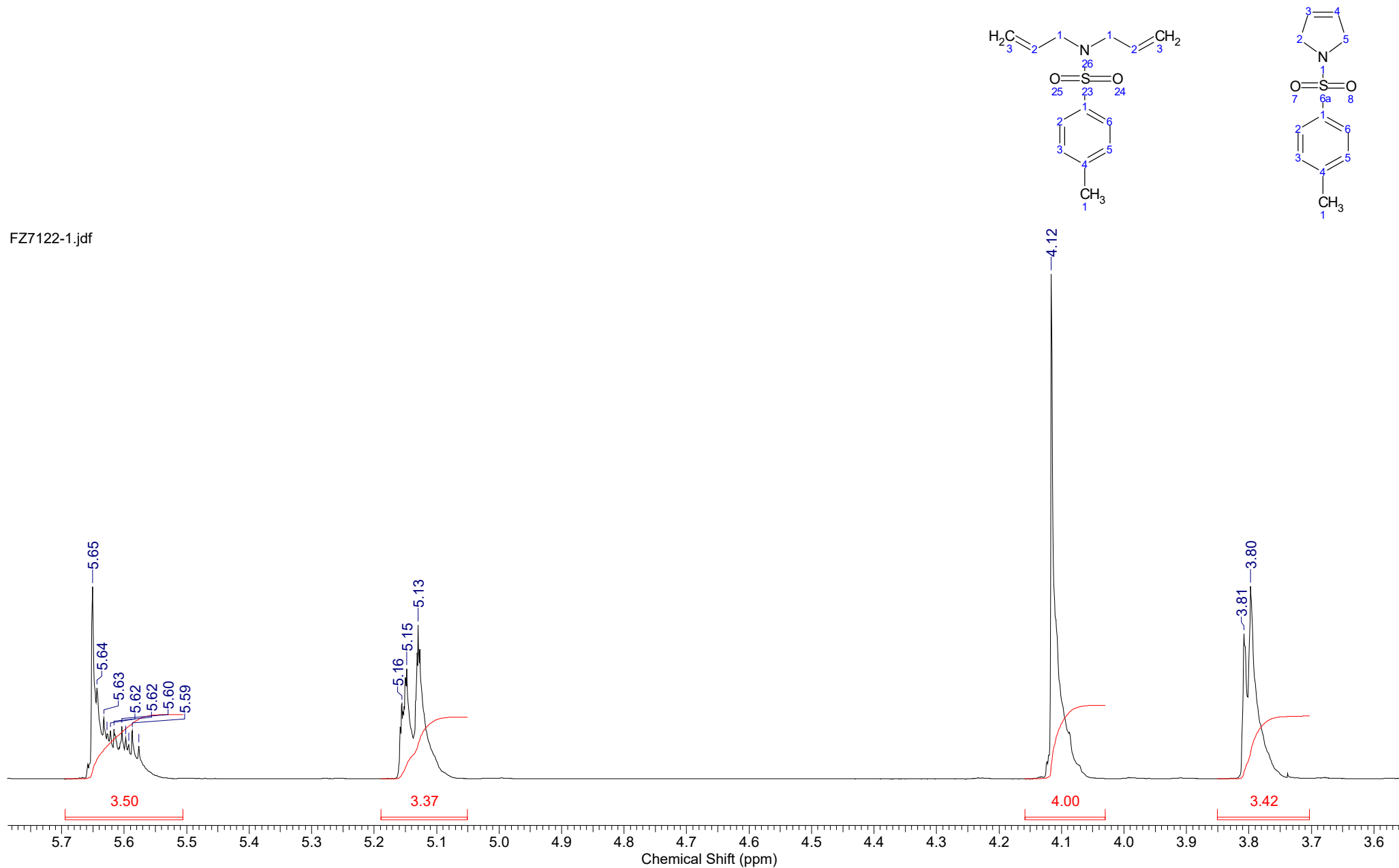
Acquisition Time (sec)	1.9818	Comment	single pulse	Date	22 Feb 1990 16:28:00	Date Stamp	25 Jan 2019 12:10:57
File Name	C:\Users\Fedor\Desktop\25.01.19\FZ7122-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	34.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5414.6641	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



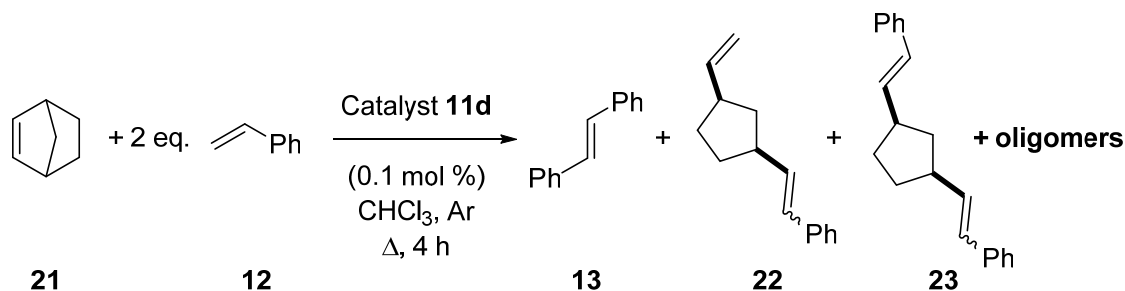
FZ7122-1.jdf



Acquisition Time (sec)	1.9818	Comment	single_pulse	Date	22 Feb 1990 16:28:00	Date Stamp	25 Jan 2019 12:10:57
File Name	C:\Users\Fedor\Desktop\25.01.19\FZ7122-1.jdf	Frequency (MHz)	600.17	Nucleus	1H	Number of Transients	8
Origin	ECA 600	Original Points Count	32768	Owner	delta	Points Count	32768
Receiver Gain	34.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	5414.6641	Pulse Sequence	single_pulse.ex2
						Sweep Width (Hz)	16534.39



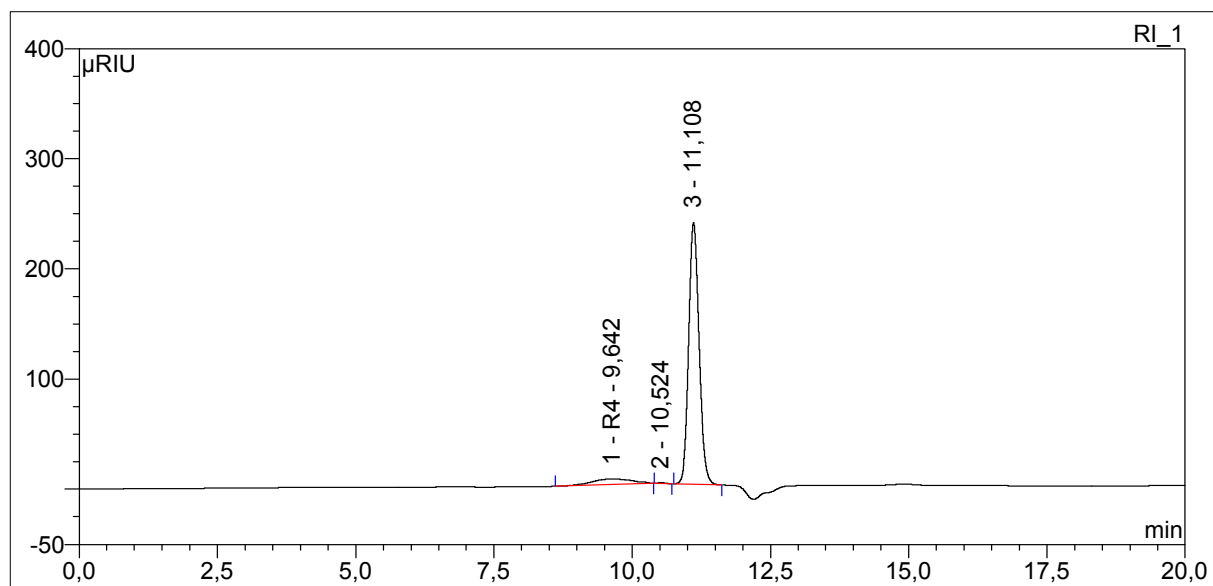
4. Experimental details and GPC analysis of polymer materials obtained in the metathesis reaction between norbornene **21** and styrene **12** (see Entry 35, Table 3).



A mixture of norbornene **21** (0.19 g, 2.0 mmol) and styrene **12** (0.46 mL, 4.0 mmol) was added to a solution of catalyst (**11d**) 0.1 mol % (1.34 mg, 0.002 mmol) in dry chloroform (10 mL) in a Schlenk flask purged with argon. The resulting mixture was heated at reflux for 4 h under continuous stirring and in an argon atmosphere (after this time the green color of the reaction mixture changes to yellow). Inorganic products were separated by filtration through a layer of Al₂O₃ (2×2 cm, neutral, using CHCl₃ as eluent). The solvent was evaporated under reduced pressure. High-molecular products were separated by addition of MeOH (20 mL) and following filtration of a precipitate. The solution was concentrated under reduced pressure yield the mixture of non-polymeric compounds **13**, **22**, **23** as colourless oil (0.51 g, 78%). The composition of the mixture was determined by GC-MS analysis as **13/22/23**, ~ 81/18/1. Molecular weight of the obtained solid (0.06 g) was evaluated by gel permeation chromatography (GPC) relative to a polystyrene standard reference material. GPC analysis was performed on a Dionex Ultimate 3000 device with a refractometric detector for 1% solution of the polymer in PhMe. The column Agilent PLgel 5 μm MIXED-C, 7.5 × 300 mm and PhMe as a solvent have been used for separation of the components in GPC analysis. Total peak area (%), weight-average molecular weight (Da), polydispersity: peak 1, a norbornene oligomer (7.9 %, 923 Da, 1.55), peak 2, an impurity or a noise (0.2 %, 109 Da, 1.02), peak 3, a solvent (91.9 %, 33 Da, 1.04) (see Pictures below).

Sample Report

Sample Name	PK-1210	Quantif. Method	GPC
Sequence	GPC test-04.2018	Start Time	2018-12-11 14:48
Directory	ROSNEFT\2 Data	Injection Volume	50,0
Sample Type	unknown	Channel	RI_1
Control Program	GPC	Number of Peak Slices	25



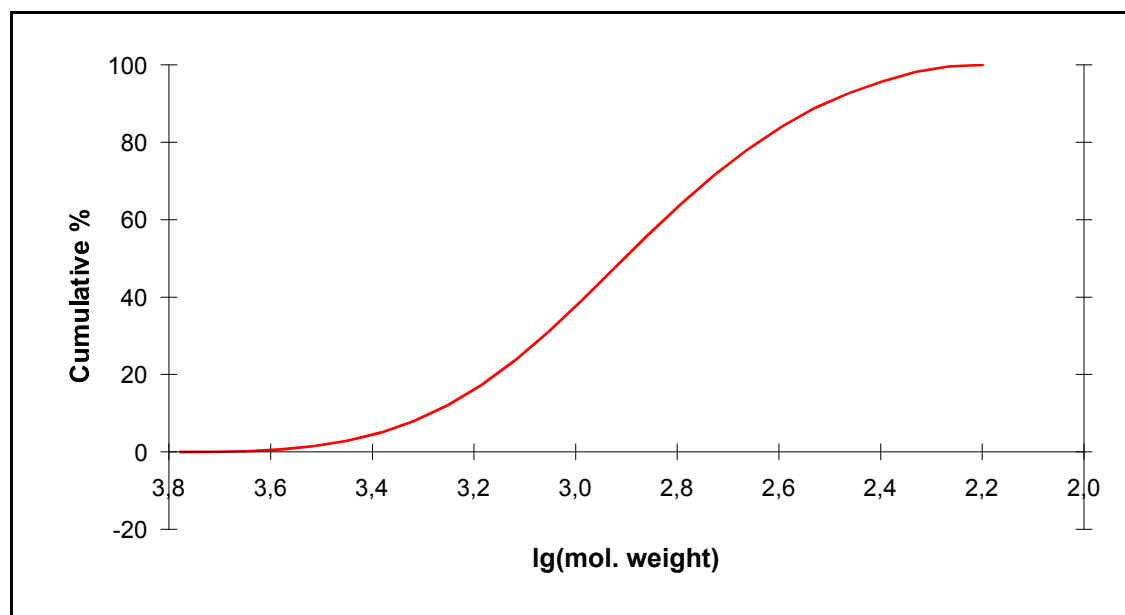
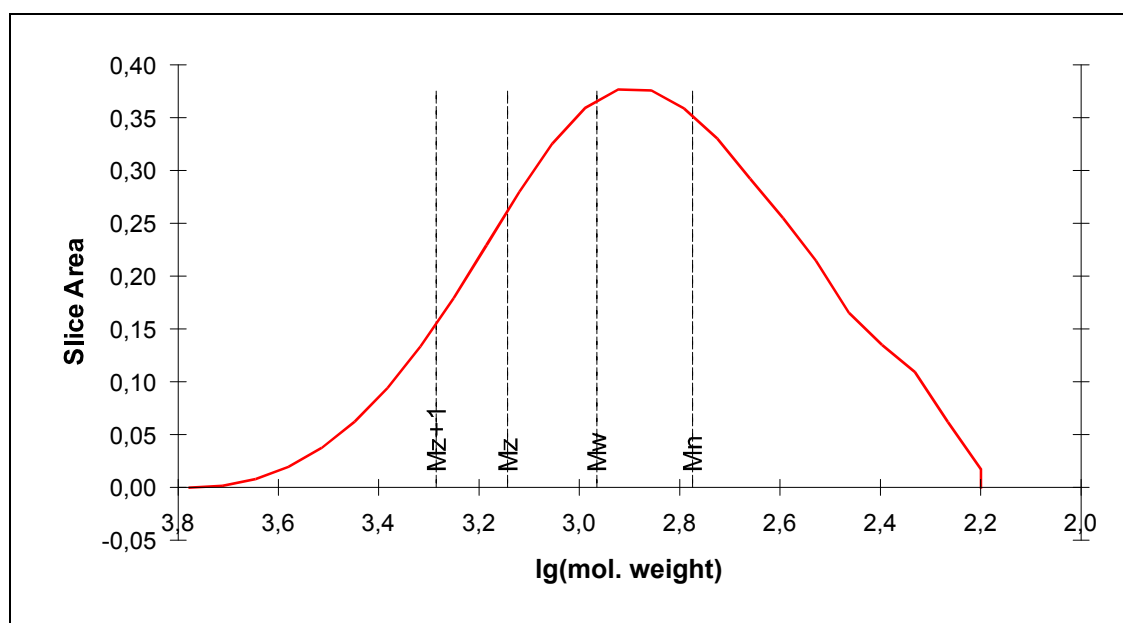
Peaks			
Peak number	1	2	3
Peak name	R4	n.a.	n.a.
Peak Parameters			
Ret. Time Peak Start [min]	8,61	10,39	10,75
Mw (Peak Start) [Da]	6450	146	68
Ret. Time Peak Maximum [min]	9,64	10,52	11,11
Mw (Peak Maximum) [Da]	724	111	32
Ret. Time Peak End [min]	10,39	10,72	11,62
Mw (Peak End) [Da]	147	73	11
Peak Area [rel. units]	4,42	0,12	51,43
% Total Peak Area	7,90	0,22	91,88
Averages			
Number Average Mn	595	107	30
Weight Average Mw	923	109	32
Z Average Mz	1390	110	33
(Z+1) Average Mz+1	1930	112	34
Polydispersity			
Polydispersity PD	1,55	1,02	1,04

Molecular Weight Distribution Report: R4

Sample		Peak Parameters	
Sample Name	PK-1210	Peak number	1
Sequence	GPC_test-04.2018	Peak name	R4
Directory	ROSNEFT\2_Data	Ret. Time Peak Start [min]	8,61
Sample Type	unknown	Mw (Peak Start) [Da]	6450
Control Program	GPC	Ret. Time Peak Maximum [min]	9,64
Quantif. Method	GPC	Mw (Peak Maximum) [Da]	724
Start Time	2018-12-11 14:48	Ret. Time Peak End [min]	10,39
Injection Volume	50,0	Mw (Peak End) [Da]	147
Channel	RI_1	Peak Area [rel. units]	4,42
Number of Peak Slices	25	% Total Peak Area	7,90

Averages and Polydispersity

Number Average Mn	595
Weight Average Mw	923
Z Average Mz	1390
(Z+1) Average Mz+1	1930
Polydispersity PD	1,55



Slice Detail Report: R4

Sample		Peak Parameters	
Sample Name	PK-1210	Peak number	1
Sequence	GPC_test-04.2018	Peak name	R4
Directory	ROSNEFT2_Data	Ret. Time Peak Start [min]	8,61
Sample Type	unknown	Mw (Peak Start) [Da]	6450
Control Program	GPC	Ret. Time Peak Maximum [min]	9,64
Quantif. Method	GPC	Mw (Peak Maximum) [Da]	724
Start Time	2018-12-11 14:48	Ret. Time Peak End [min]	10,39
Injection Volume	50,0	Mw (Peak End) [Da]	147
Channel	RI_1	Peak Area [rel. units]	4,4
Number of Peak Slices	25	% Total Peak Area	7,90

Averages and Polydispersity

Number Average Mn	595
Weight Average Mw	923
Z Average Mz	1390
(Z+1) Average Mz+1	1930
Polydispersity PD	1,55

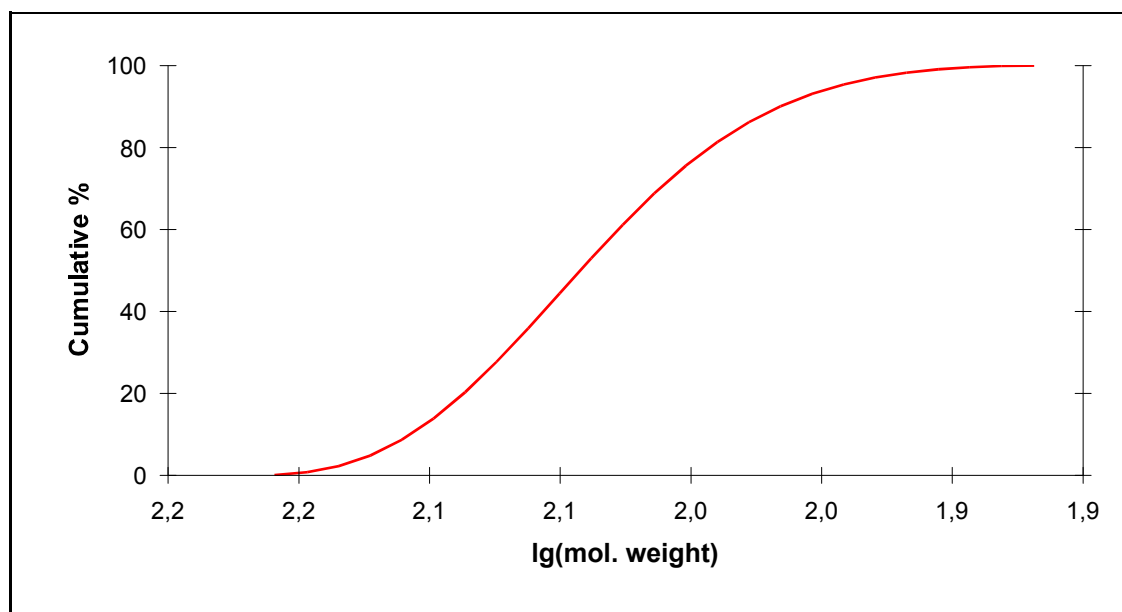
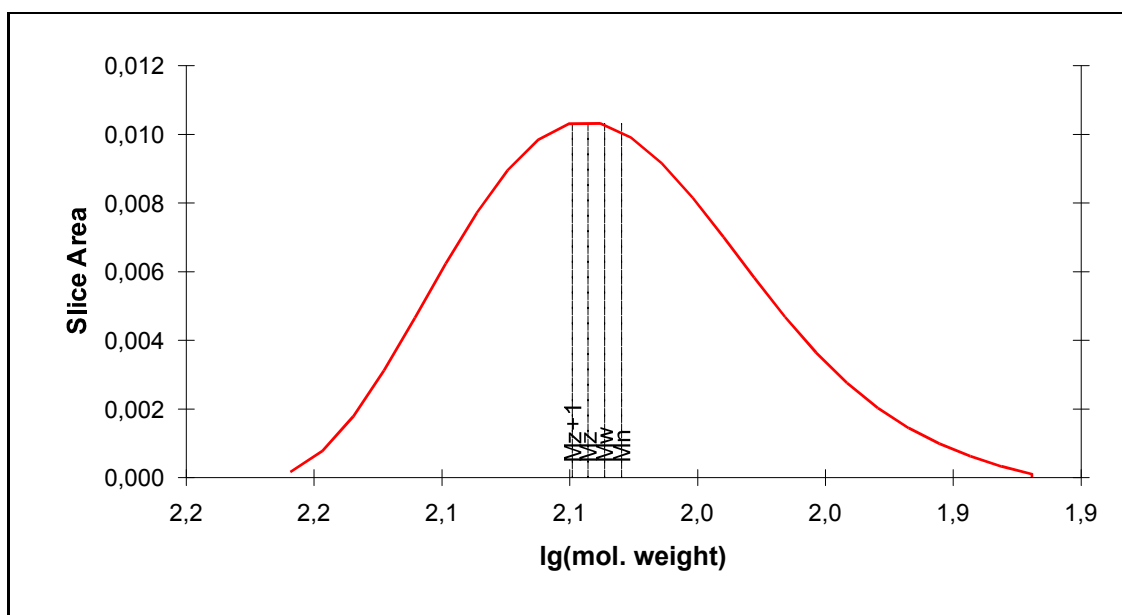
Slice No.	Slice Start [min]	Slice End [min]	lg(Mw)	Mw [Da]	Slice Area [rel. units]	Percentage [%]	Cumulative [%]
1	8,614	8,685	3,777	5980	-0,00016	-0,004	-0,004
2	8,685	8,756	3,711	5140	0,00160	0,036	0,033
3	8,756	8,827	3,645	4418	0,00790	0,179	0,211
4	8,827	8,898	3,580	3798	0,01953	0,442	0,653
5	8,898	8,969	3,514	3265	0,03732	0,844	1,497
6	8,969	9,040	3,448	2806	0,06205	1,403	2,901
7	9,040	9,111	3,382	2412	0,09414	2,129	5,030
8	9,111	9,182	3,317	2073	0,13349	3,019	8,049
9	9,182	9,254	3,251	1782	0,17922	4,054	12,103
10	9,254	9,325	3,185	1532	0,22928	5,186	17,289
11	9,325	9,396	3,120	1317	0,27999	6,333	23,622
12	9,396	9,467	3,054	1132	0,32555	7,363	30,985
13	9,467	9,538	2,988	973	0,35950	8,131	39,116
14	9,538	9,609	2,922	836	0,37679	8,522	47,639
15	9,609	9,680	2,857	719	0,37588	8,502	56,140
16	9,680	9,751	2,791	618	0,35864	8,112	64,252
17	9,751	9,822	2,725	531	0,33040	7,473	71,725
18	9,822	9,894	2,660	457	0,29215	6,608	78,333
19	9,894	9,965	2,594	393	0,25492	5,766	84,099
20	9,965	10,036	2,528	337	0,21458	4,853	88,953
21	10,036	10,107	2,462	290	0,16512	3,735	92,687
22	10,107	10,178	2,397	249	0,13491	3,051	95,739
23	10,178	10,249	2,331	214	0,10910	2,468	98,206
24	10,249	10,320	2,265	184	0,06203	1,403	99,609
25	10,320	10,391	2,200	158	0,01727	0,391	100,000

Molecular Weight Distribution Report: Peak No. 2

Sample		Peak Parameters	
Sample Name	PK-1210	Peak number	2
Sequence	GPC_test-04.2018	Peak name	n.a.
Directory	ROSNEFT\2_Data	Ret. Time Peak Start [min]	10,39
Sample Type	unknown	Mw (Peak Start) [Da]	146
Control Program	GPC	Ret. Time Peak Maximum [min]	10,52
Quantif. Method	GPC	Mw (Peak Maximum) [Da]	111
Start Time	2018-12-11 14:48	Ret. Time Peak End [min]	10,72
Injection Volume	50,0	Mw (Peak End) [Da]	73
Channel	RI_1	Peak Area [rel. units]	0,12
Number of Peak Slices	25	% Total Peak Area	0,22

Averages and Polydispersity

Number Average Mn	107
Weight Average Mw	109
Z Average Mz	110
(Z+1) Average Mz+1	112
Polydispersity PD	1,02



Slice Detail Report: Peak No. 2

Sample		Peak Parameters	
Sample Name	PK-1210	Peak number	2
Sequence	GPC_test-04.2018	Peak name	n.a.
Directory	ROSNEFT\2_Data	Ret. Time Peak Start [min]	10,39
Sample Type	unknown	Mw (Peak Start) [Da]	146
Control Program	GPC	Ret. Time Peak Maximum [min]	10,52
Quantif. Method	GPC	Mw (Peak Maximum) [Da]	111
Start Time	2018-12-11 14:48	Ret. Time Peak End [min]	10,72
Injection Volume	50	Mw (Peak End) [Da]	73
Channel	RI_1	Peak Area [rel. units]	0,1
Number of Peak Slices	25	% Total Peak Area	0,22

Averages and Polydispersity

Number Average Mn	107
Weight Average Mw	109
Z Average Mz	110
(Z+1) Average Mz+1	112
Polydispersity PD	1,02

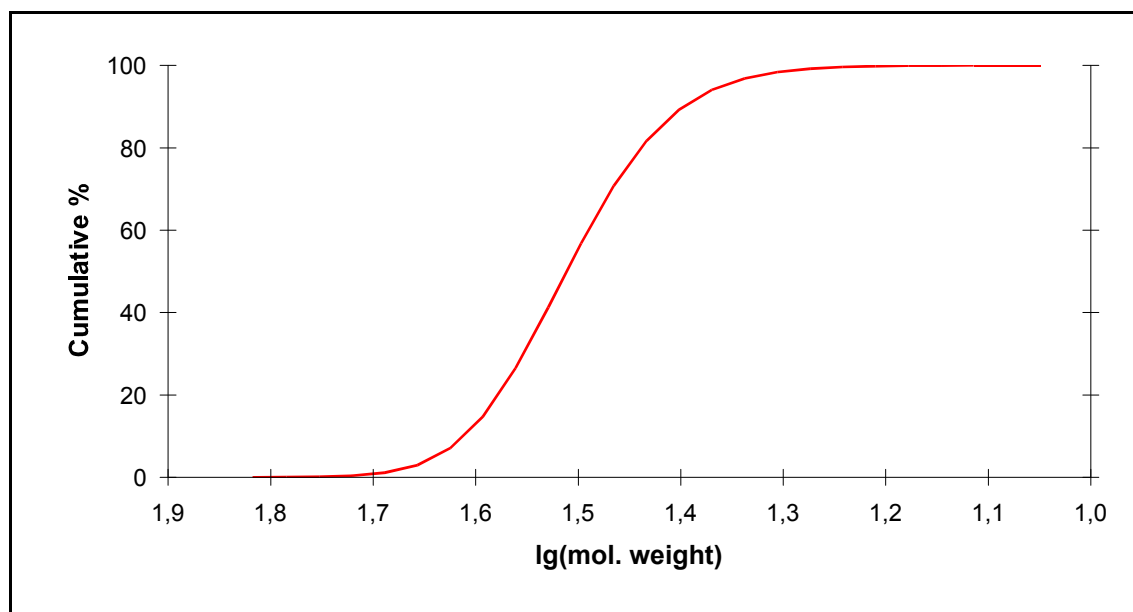
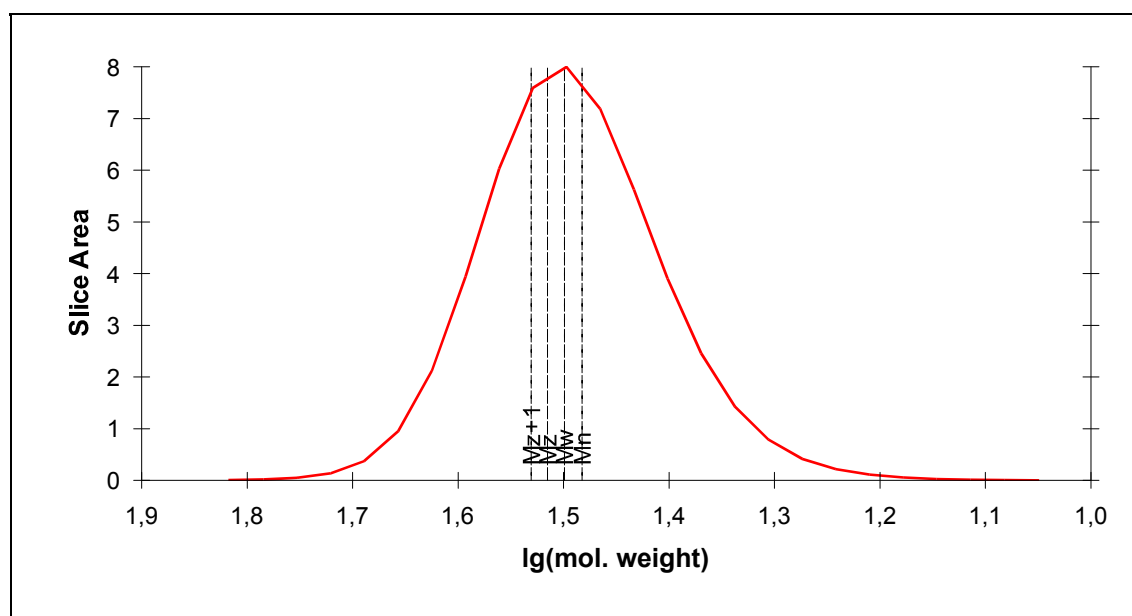
Slice No.	Slice Start [min]	Slice End [min]	lg(Mw)	Mw [Da]	Slice Area [rel. units]	Percentage [%]	Cumulative [%]
1	10,393	10,406	2,159	144	0,00019	0,156	0,156
2	10,406	10,419	2,147	140	0,00078	0,646	0,802
3	10,419	10,433	2,135	136	0,00178	1,476	2,278
4	10,433	10,446	2,123	133	0,00312	2,588	4,866
5	10,446	10,459	2,111	129	0,00466	3,864	8,731
6	10,459	10,472	2,099	125	0,00623	5,172	13,903
7	10,472	10,485	2,086	122	0,00771	6,394	20,297
8	10,485	10,498	2,074	119	0,00895	7,425	27,722
9	10,498	10,511	2,062	115	0,00984	8,166	35,888
10	10,511	10,524	2,050	112	0,01031	8,552	44,441
11	10,524	10,537	2,038	109	0,01032	8,559	53,000
12	10,537	10,550	2,026	106	0,00991	8,223	61,223
13	10,550	10,563	2,014	103	0,00916	7,600	68,823
14	10,563	10,576	2,002	100	0,00815	6,763	75,586
15	10,576	10,589	1,990	98	0,00701	5,813	81,400
16	10,589	10,602	1,978	95	0,00582	4,829	86,228
17	10,602	10,615	1,966	92	0,00467	3,878	90,106
18	10,615	10,628	1,954	90	0,00365	3,024	93,131
19	10,628	10,641	1,942	87	0,00276	2,291	95,422
20	10,641	10,655	1,930	85	0,00203	1,683	97,106
21	10,655	10,668	1,917	83	0,00144	1,198	98,304
22	10,668	10,681	1,905	80	0,00099	0,819	99,123
23	10,681	10,694	1,893	78	0,00062	0,518	99,641
24	10,694	10,707	1,881	76	0,00033	0,274	99,915
25	10,707	10,720	1,869	74	0,00010	0,085	100,000

Molecular Weight Distribution Report: Peak No. 3

Sample		Peak Parameters	
Sample Name	PK-1210	Peak number	3
Sequence	GPC_test-04.2018	Peak name	n.a.
Directory	ROSNEFT\2_Data	Ret. Time Peak Start [min]	10,75
Sample Type	unknown	Mw (Peak Start) [Da]	68
Control Program	GPC	Ret. Time Peak Maximum [min]	11,11
Quantif. Method	GPC	Mw (Peak Maximum) [Da]	32
Start Time	2018-12-11 14:48	Ret. Time Peak End [min]	11,62
Injection Volume	50,0	Mw (Peak End) [Da]	11
Channel	RI_1	Peak Area [rel. units]	51,43
Number of Peak Slices	25	% Total Peak Area	91,88

Averages and Polydispersity

Number Average Mn	30
Weight Average Mw	32
Z Average Mz	33
(Z+1) Average Mz+1	34
Polydispersity PD	1,04



Slice Detail Report: Peak No. 3

Sample		Peak Parameters	
Sample Name	PK-1210	Peak number	3
Sequence	GPC_test-04.2018	Peak name	n.a.
Directory	ROSNEFT\2_Data	Ret. Time Peak Start [min]	10,75
Sample Type	unknown	Mw (Peak Start) [Da]	68
Control Program	GPC	Ret. Time Peak Maximum [min]	11,11
Quantif. Method	GPC	Mw (Peak Maximum) [Da]	32
Start Time	2018-12-11 14:48	Ret. Time Peak End [min]	11,62
Injection Volume	50	Mw (Peak End) [Da]	11
Channel	RI_1	Peak Area [rel. units]	51,4
Number of Peak Slices	25	% Total Peak Area	91,88

Averages and Polydispersity

Number Average Mn	30
Weight Average Mw	32
Z Average Mz	33
(Z+1) Average Mz+1	34
Polydispersity PD	1,04

Slice No.	Slice Start [min]	Slice End [min]	lg(Mw)	Mw [Da]	Slice Area [rel. units]	Percentage [%]	Cumulative [%]
1	10,753	10,788	1,816	66	0,00306	0,006	0,006
2	10,788	10,822	1,784	61	0,01538	0,030	0,036
3	10,822	10,857	1,753	57	0,04908	0,095	0,131
4	10,857	10,891	1,721	53	0,13820	0,269	0,400
5	10,891	10,926	1,689	49	0,37508	0,729	1,129
6	10,926	10,960	1,657	45	0,95165	1,850	2,979
7	10,960	10,995	1,625	42	2,11819	4,118	7,097
8	10,995	11,029	1,593	39	3,94277	7,665	14,762
9	11,029	11,064	1,561	36	6,02650	11,716	26,477
10	11,064	11,099	1,529	34	7,59118	14,757	41,234
11	11,099	11,133	1,497	31	7,99992	15,552	56,786
12	11,133	11,168	1,465	29	7,18934	13,976	70,762
13	11,168	11,202	1,433	27	5,62312	10,931	81,694
14	11,202	11,237	1,401	25	3,90571	7,593	89,286
15	11,237	11,271	1,370	23	2,45754	4,777	94,064
16	11,271	11,306	1,338	22	1,43084	2,782	96,845
17	11,306	11,340	1,306	20	0,78610	1,528	98,373
18	11,340	11,375	1,274	19	0,41561	0,808	99,181
19	11,375	11,409	1,242	17	0,21479	0,418	99,599
20	11,409	11,444	1,210	16	0,10939	0,213	99,812
21	11,444	11,479	1,178	15	0,05463	0,106	99,918
22	11,479	11,513	1,146	14	0,02611	0,051	99,969
23	11,513	11,548	1,114	13	0,01136	0,022	99,991
24	11,548	11,582	1,082	12	0,00400	0,008	99,998
25	11,582	11,617	1,050	11	0,00080	0,002	100,000

5. Check-cif reports (CCDC) for compounds **11a**, **11b**, **11c**.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 11a

Bond precision:	C-C = 0.0046 Å	Wavelength=0.71073
Cell:	a=10.208(6)	b=10.837(7) c=14.745(6)
	alpha=76.76(2)	beta=85.41(2) gamma=70.66(2)
Temperature:	295 K	
	Calculated	Reported
Volume	1498.2(15)	1498.2(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C31 H39 Cl2 N3 Ru	C31 H39 Cl2 N3 Ru
Sum formula	C31 H39 Cl2 N3 Ru	C31 H39 Cl2 N3 Ru
Mr	625.62	625.62
Dx, g cm-3	1.387	1.389
Z	2	2
Mu (mm-1)	0.726	0.726
F000	648.0	648.0
F000'	646.23	
h, k, lmax	12, 13, 18	12, 13, 18
Nref	5858	5856
Tmin, Tmax	0.865, 0.865	0.792, 0.864
Tmin'	0.865	

Correction method= # Reported T Limits: Tmin=0.792 Tmax=0.864
AbsCorr = PSI-SCAN

Data completeness= 1.000 Theta(max)= 25.970

R(reflections)= 0.0368(4768) wR2(reflections)= 0.0762(5856)

S = 0.992 Npar= 342

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

● Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.02 Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru -- Cl2 ..	5.8 s.u.
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2016 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 0 **ALERT level B** = A potentially serious problem, consider carefully
 - 0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 4 **ALERT level G** = General information/check it is not something unexpected
-
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 1 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 0 ALERT type 3 Indicator that the structure quality may be low
 - 1 ALERT type 4 Improvement, methodology, query or suggestion
 - 1 ALERT type 5 Informative message, check
-

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

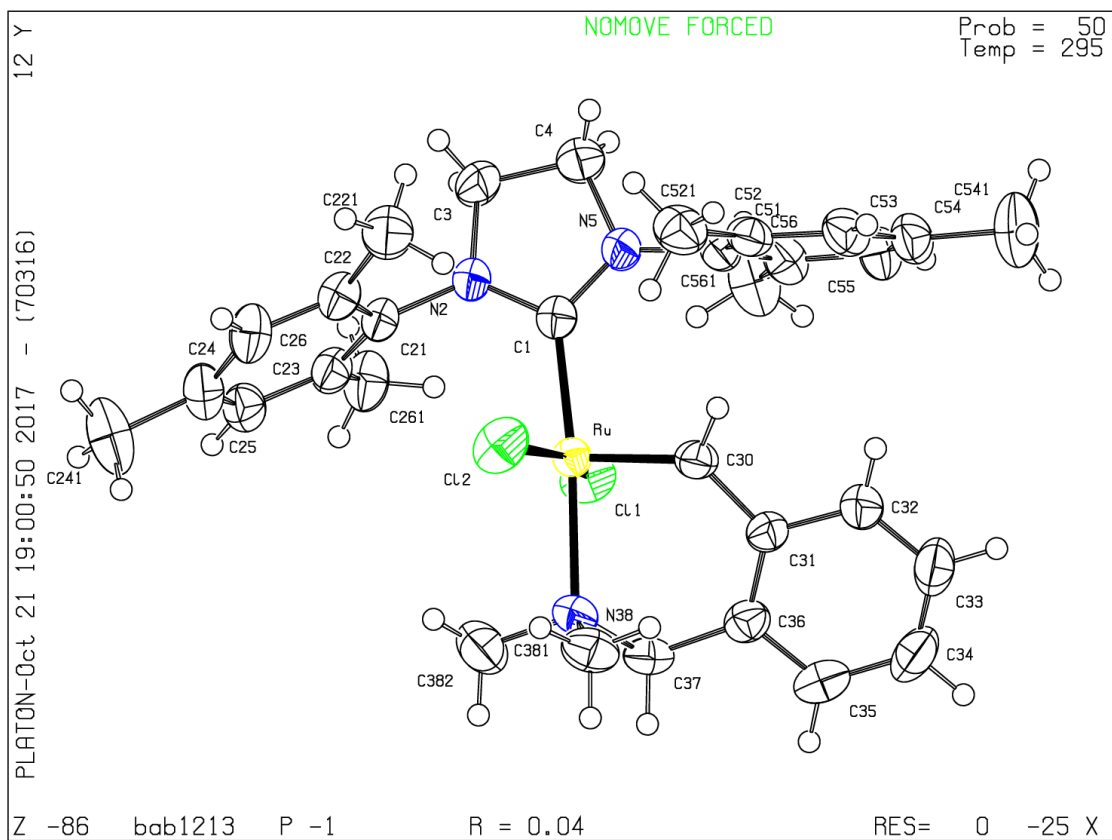
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2017; check.def file version of 27/07/2017



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) K1

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 11b

Bond precision: C-C = 0.0074 Å Wavelength=0.71073

Cell: a=21.218(3) b=19.218(2) c=15.3386(19)
 alpha=90 beta=95.830(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	6222.2(13)	6222.4(13)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C33 H43 Cl2 N3 Ru	C33 H43 Cl2 N3 Ru
Sum formula	C33 H43 Cl2 N3 Ru	C33 H43 Cl2 N3 Ru
Mr	653.67	653.67
Dx, g cm-3	1.396	1.396
Z	8	8
Mu (mm-1)	0.702	0.702
F000	2720.0	2720.0
F000'	2712.95	
h, k, lmax	26, 23, 18	26, 23, 18
Nref	12238	12236
Tmin, Tmax	0.838, 0.932	0.834, 0.921
Tmin'	0.822	

Correction method= # Reported T Limits: Tmin=0.834 Tmax=0.921
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.999

R(reflections)= 0.0612(9638) wR2(reflections)= 0.1547(12236)

S = 1.203 Npar= 719

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT971_ALERT_2_B	Check Calcd Resid. Dens.	0.94A	From Ru1	2.83 eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens.	0.97A	From Ru1	2.66 eA-3

Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.02	Report	
PLAT220_ALERT_2_C	Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range	3.9	Ratio	
PLAT222_ALERT_3_C	Non-Solv. Resd 2 H Uiso(max)/Uiso(min) Range	4.9	Ratio	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	6.479	Check	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2	Report	
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.90A	From Ru2	2.50 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.98A	From Ru2	2.22 eA-3

Alert level G

PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	4	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	3	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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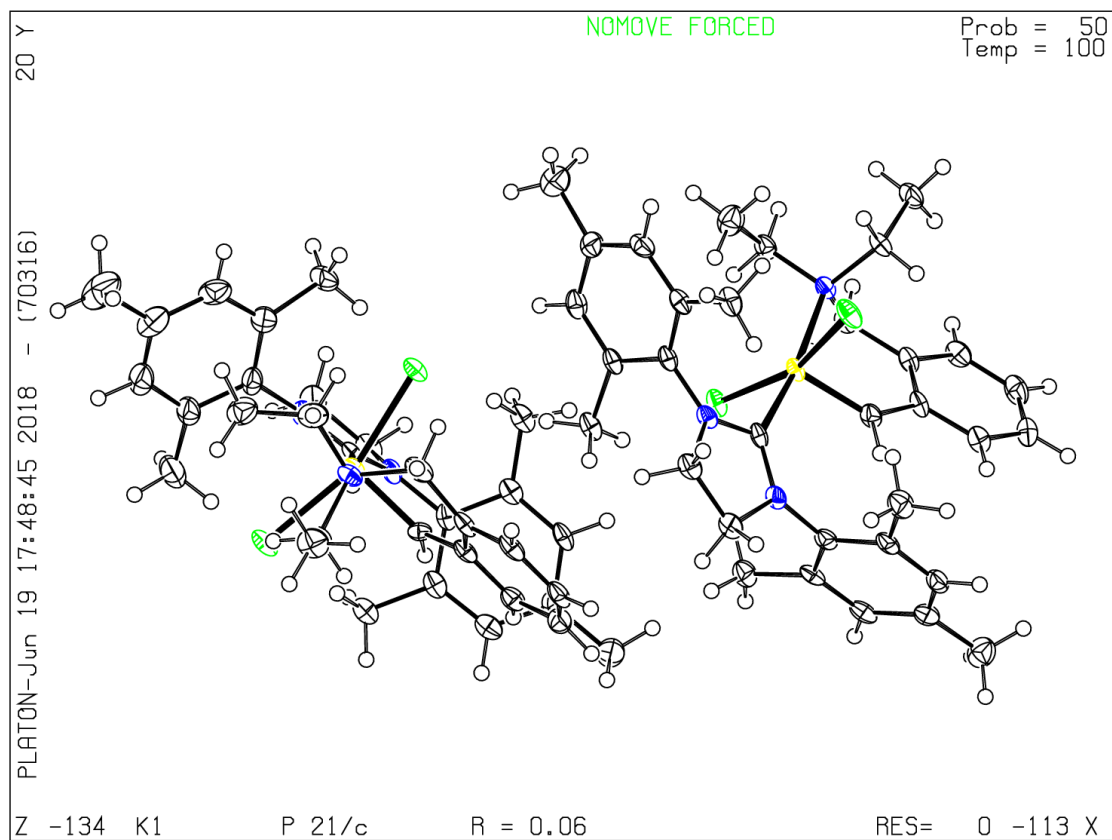
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 23/04/2018; check.def file version of 23/04/2018



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FZ1

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 11c

Bond precision:	C-C = 0.0090 Å	Wavelength=0.71073	
Cell:	a=12.9054(12)	b=10.8240(11)	c=21.684(2)
	alpha=90	beta=104.828(6)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	2928.1(5)	2928.1(5)	
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C30 H37 Cl2 N3 Ru	C30 H37 Cl2 N3 Ru	
Sum formula	C30 H37 Cl2 N3 Ru	C30 H37 Cl2 N3 Ru	
Mr	611.60	611.59	
Dx, g cm-3	1.387	1.387	
Z	4	4	
Mu (mm-1)	0.741	0.741	
F000	1264.0	1264.0	
F000'	1260.45		
h, k, lmax	15, 13, 26	15, 13, 26	
Nref	5796	5778	
Tmin, Tmax	0.899, 0.949	0.885, 0.941	
Tmin'	0.875		

Correction method= # Reported T Limits: Tmin=0.885 Tmax=0.941
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 26.074

R(reflections)= 0.0581(3076) wR2(reflections)= 0.1173(5778)

S = 0.985 Npar= 332

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

● Alert level C

PLAT234_ALERT_4_C	Large Hirshfeld Difference N3' --C4'	0.17	Ang.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00904	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.077	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	6	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2	Report
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Info

● Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3	Note
PLAT793_ALERT_4_G	Model has Chirality at N3' (Centro SPGR)	R	Verify
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	10	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	6	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

Datablock FZ1 - ellipsoid plot

