

Supporting Information

Ru(II)-Catalyzed C–H Activation/Alkylation of 3-Formylbenzofurans with Conjugated Olefins: Product Divergence

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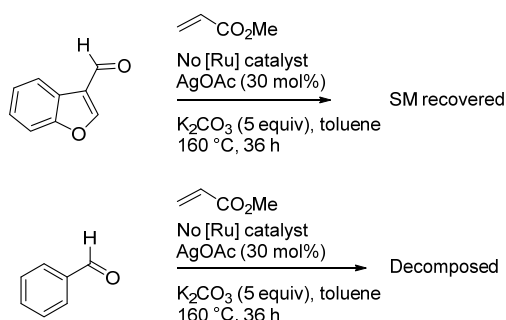
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Scheme S1: Following control experiments have been carried out to understand the course of reaction.

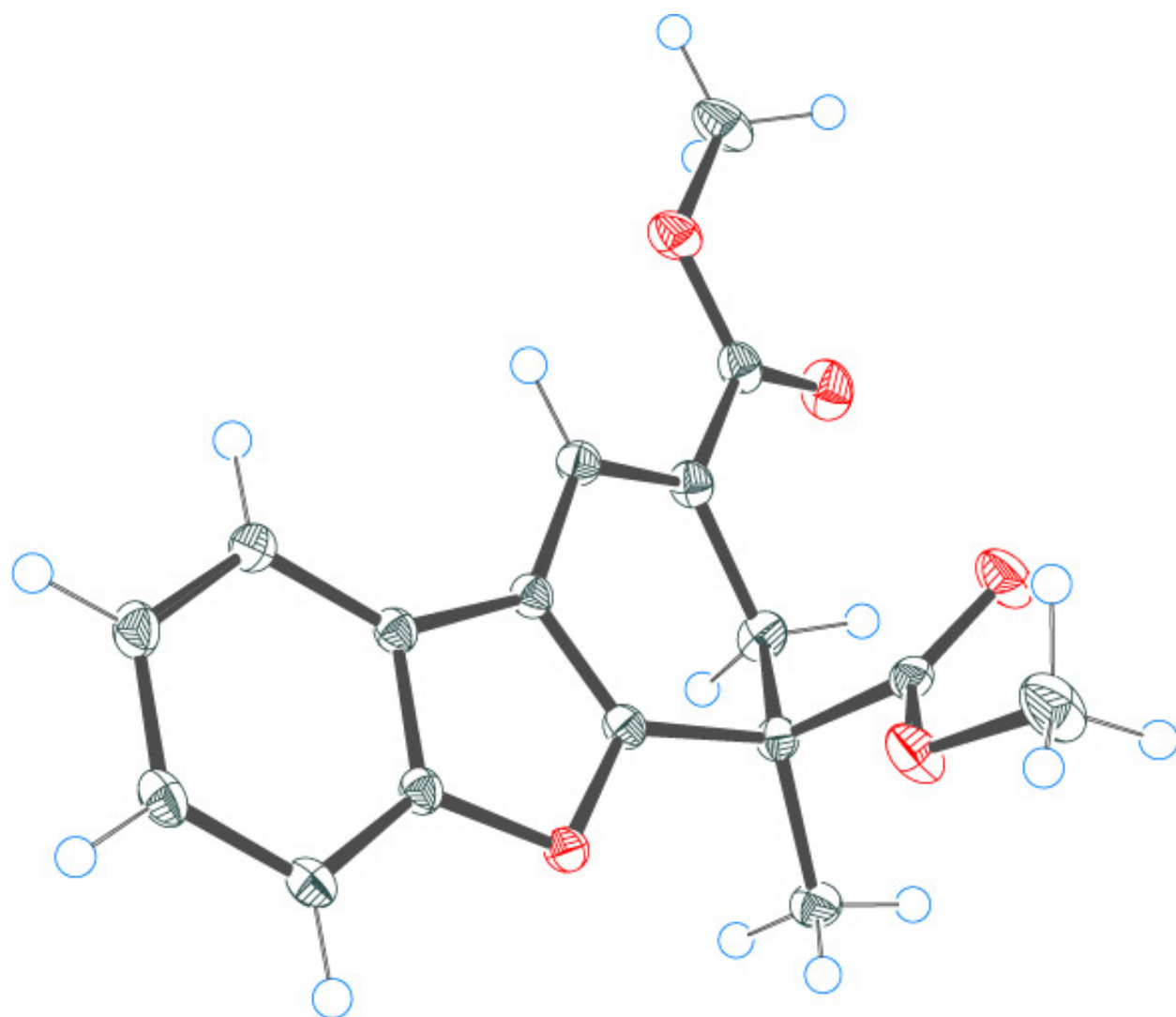


Crystal Structure Determination: X-ray intensity data measurements were carried out on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics. The intensity measurements were carried out with Mo micro-focus sealed tube diffraction source (Mo-K α = 0.72 Å) at 100(2) K temperature. The X-ray generator was operated at 50 kV and 1.4 mA. A preliminary set of cell constants and an orientation matrix were calculated from two sets of 20 frames. Data were collected with ω scan width of 0.5° at different settings of ϕ and 2θ with a frame time of 40 seconds keeping the sample-to-detector distance fixed at 4.00 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2016). All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2016). SHELX-97 was used for structure solution and full matrix least-squares refinement on F^2 . Molecular diagrams were generated using ORTEP-33 and Mercury programs. Geometrical calculations were performed using SHELXTL and PLATON. All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms. An ORTEP III view of both compounds were drawn with 50% probability displacement ellipsoids and H-atoms are shown as small spheres of arbitrary radii.

Crystallographic data for 3aa: Crystallographic data for **3aa** is deposited with the Cambridge Crystallographic Data Centre as supplementary publication no CCDC 186980

Parameters	
Chemical formula	C ₁₇ H ₁₆ O ₅
Formula weight	300.30 g/mol
Crystallization	Dichloromethane (slow evaporation)
Crystal system	Triclinic
Space group	<i>P</i> -1
Unit-cell parameter	a = 7.3739(3) Å, b = 9.7254(3) Å, c = 11.2920(4) Å, α = 108.782(1)° β = 103.782(1)° γ = 98.661(1)°, V = 721.49(5) Å ³
Crystal colour	Colourless needles
Temperature	100(2) K
No. of formula units in unit cell (Z)	2
Density (g cm ⁻³)	1.382
Abs. Coeff. (mm ⁻¹)	0.102
F(000)	316.0
Reflection Data	
No. of reflections measured	13067
No. of unique reflections	4148
No. of obs. reflections	3737
λ (Å)	0.71073
R _{merge}	0.0199
θ _{max}	29.99
θ _{min}	3.004
Refinement Data	
R _{all}	0.0406
R _{obs}	0.0364
wR _{2(all)}	0.0981
wR _{2(obs)}	0.0948
Ext. Coeff.	0.0004
Goodness-of-fit (GOF)	1.052
Largest diff. peak and hole: Delta-rho (eÅ ⁻³) _{max}	0.435
Largest diff. peak and hole: Delta-rho (eÅ ⁻³) _{min}	-0.188

Figure S1. ORTEP diagram of compound **3aa** (with 50% probability displacement ellipsoids and H-atoms)



Crystallographic data for 6al: Crystallographic data for **6al** is deposited with the Cambridge Crystallographic Data Centre as supplementary publication no CCDC 186981

Crystal Structure Information:	
Parameters	
Chemical formula	C ₁₉ H ₁₅ NO ₂
Formula weight	289.3 g/mol
Crystallization	Dichloromethane (slow evaporation)
Crystal system	Trigonal
Space group	R-3
Unit-cell parameter	a = 27.2621(7), b = 27.2621(7), c = 10.2163(3), $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 120^\circ$, V = 6575.7(4) Å ³
Crystal colour	Colourless rod-shaped crystal
Temperature	150(2) K
No. of formula units in unit cell (Z)	18
Density (g cm ⁻³)	1.315
Abs. Coeff. (mm ⁻¹)	0.086
F(000)	2736.0
Reflection Data	
No. of reflections measured	20753
No. of unique reflections	3826
No. of obs. reflections	2920
λ (Å)	0.71073
R _{merge}	0.043
$\theta_{\max}$	28.9
$\theta_{\min}$	1.5
Refinement Data	
R _{all}	0.064
R _{obs}	0.045
wR2 _(all)	0.114
wR2 _(obs)	0.105
Ext. Coeff.	0.0004
Goodness-of-fit (GOF)	1.033
Largest diff. peak and hole: Delta-rho (eÅ ⁻³) _{max}	0.267
Largest diff. peak and hole: Delta-rho (eÅ ⁻³) _{min}	-0.182

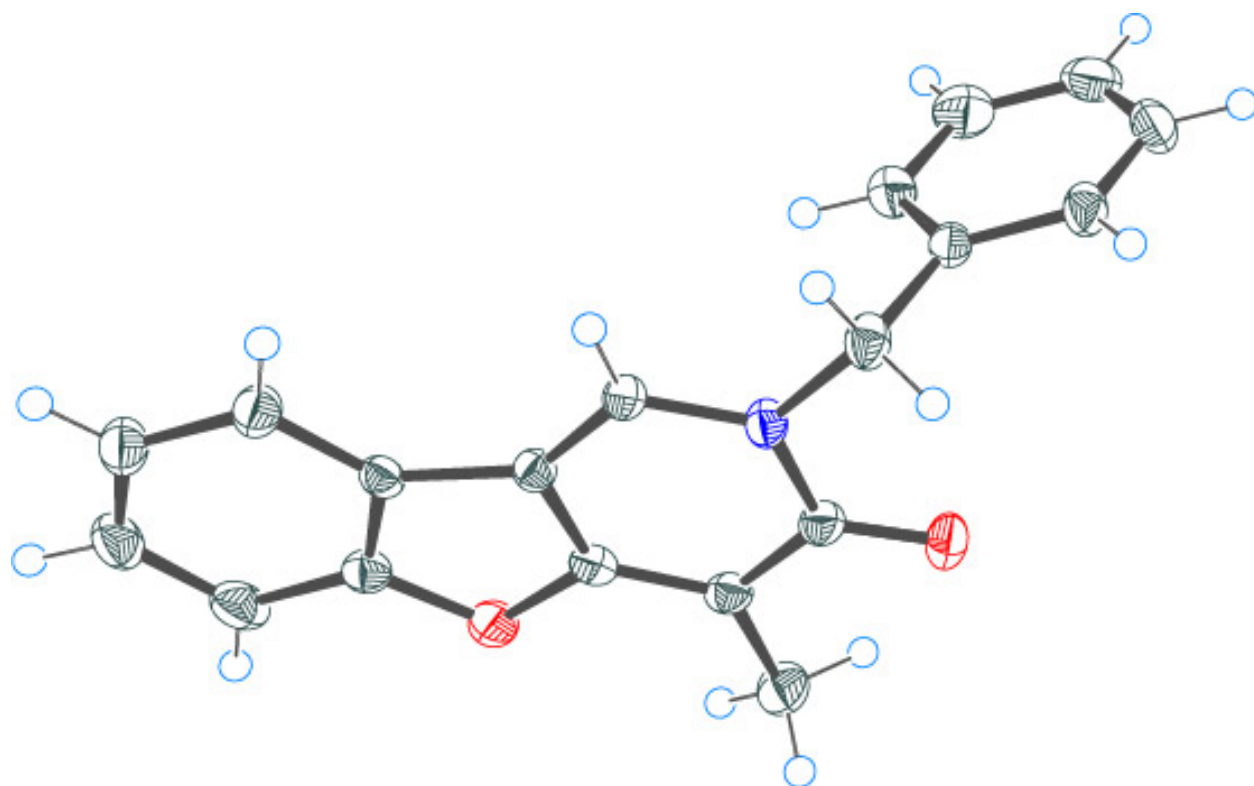
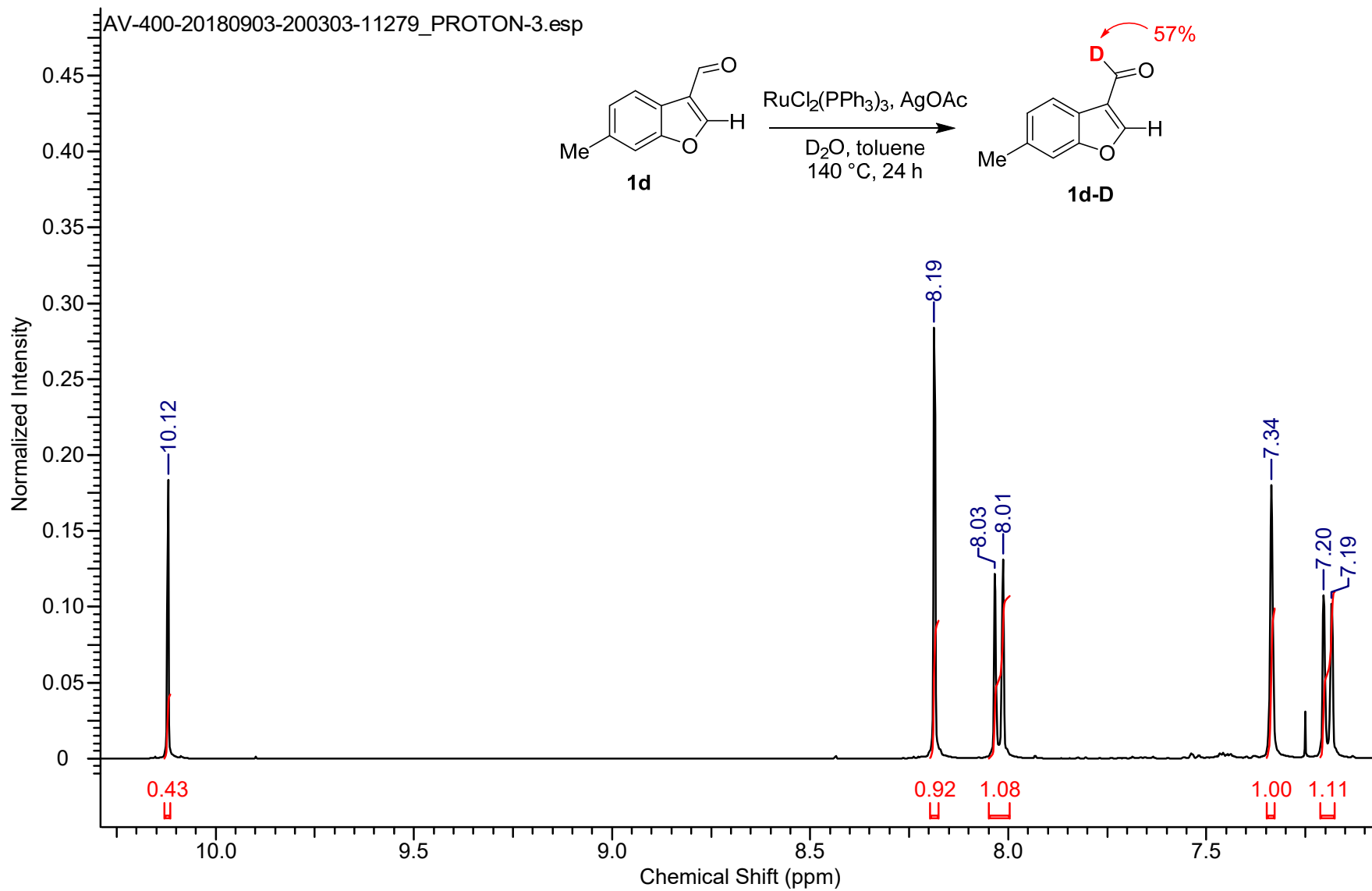
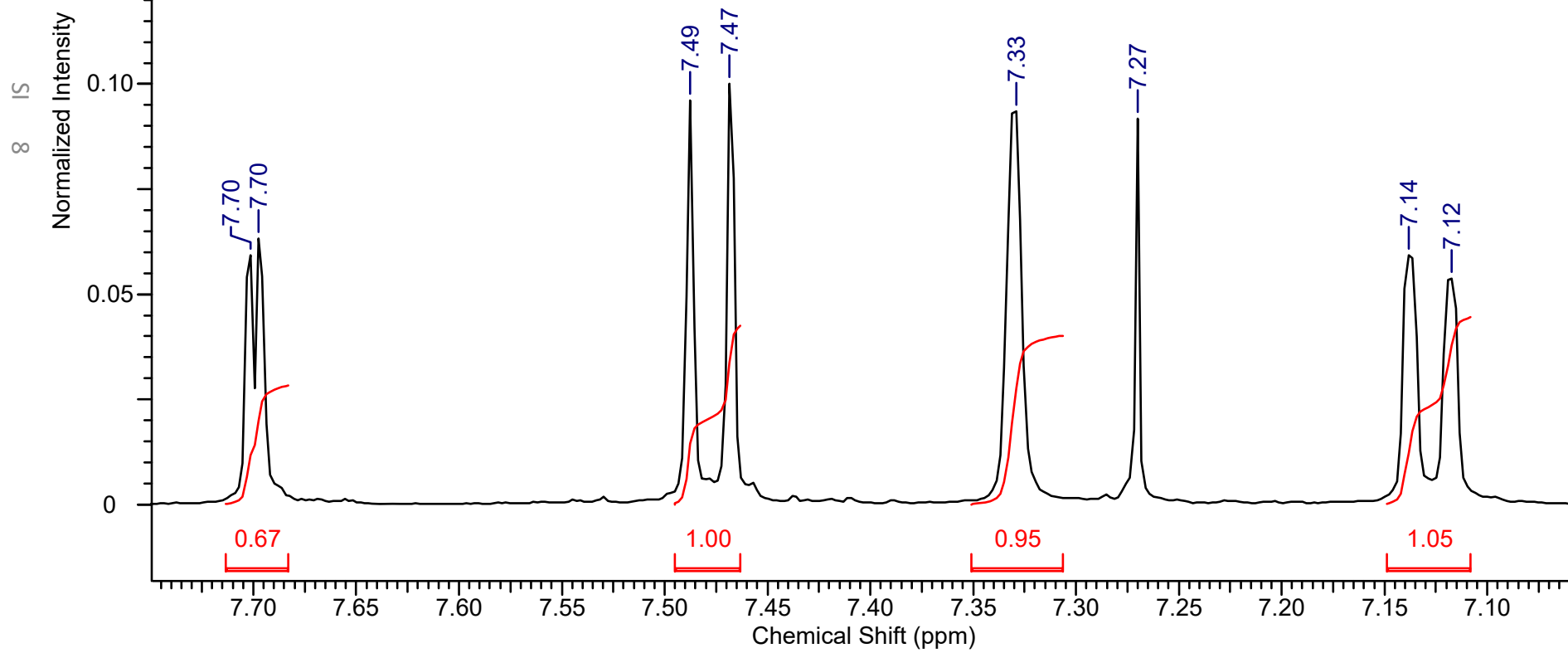
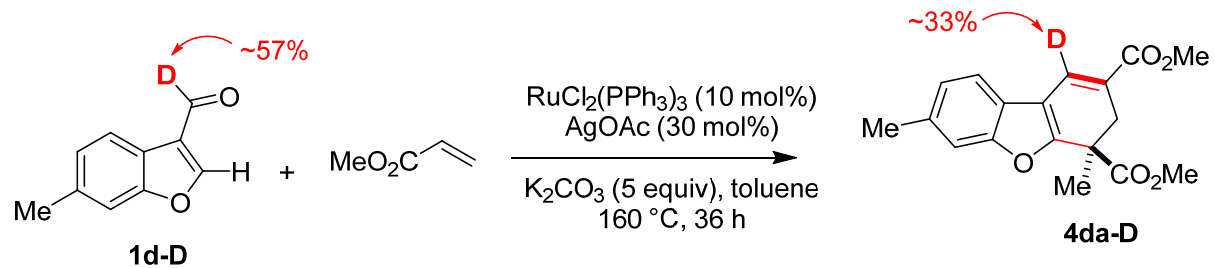
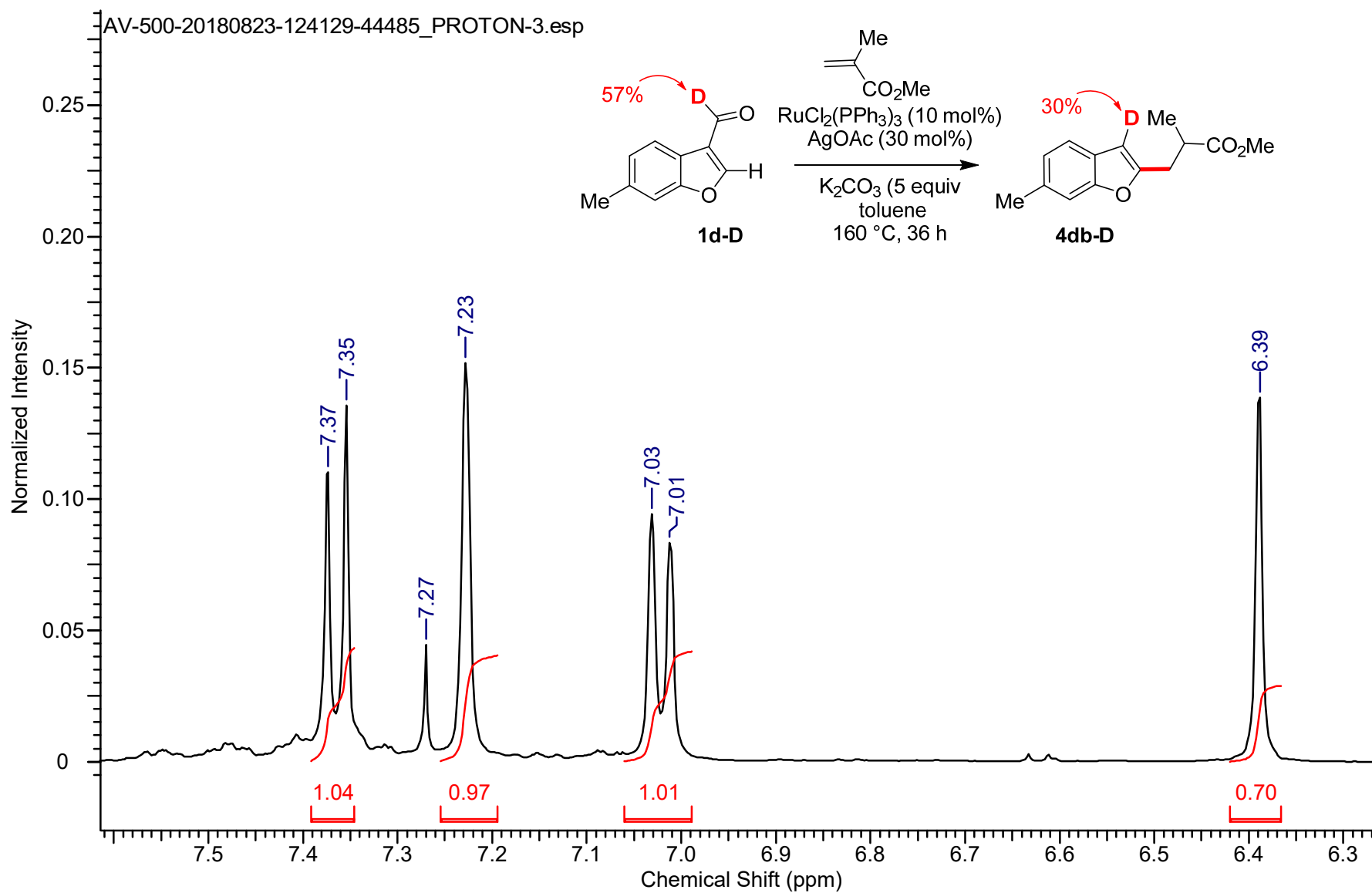


Figure S2. ORTEP diagram of compound **6al** (with 50% probability displacement ellipsoids and H-atoms)

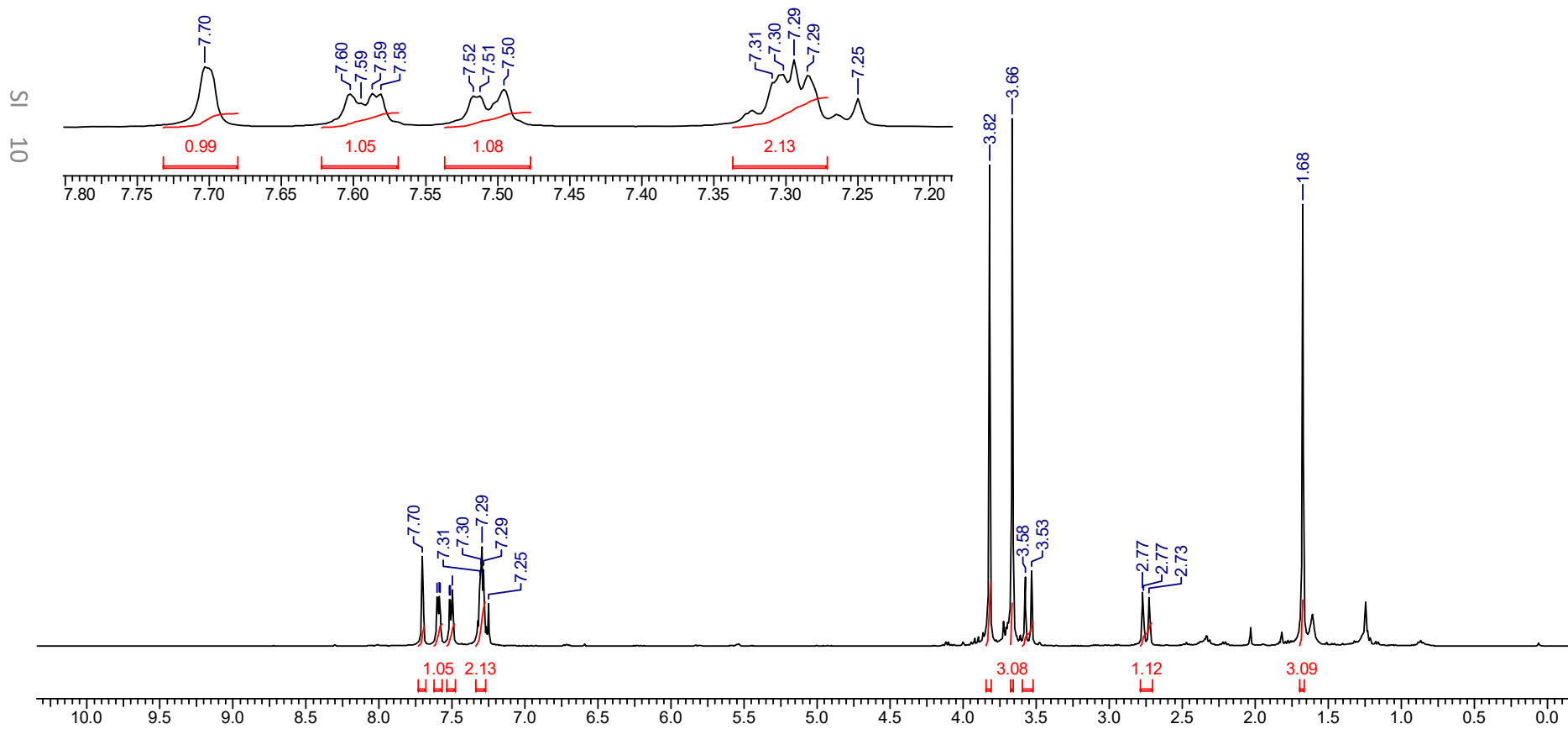
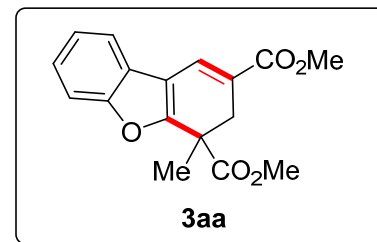


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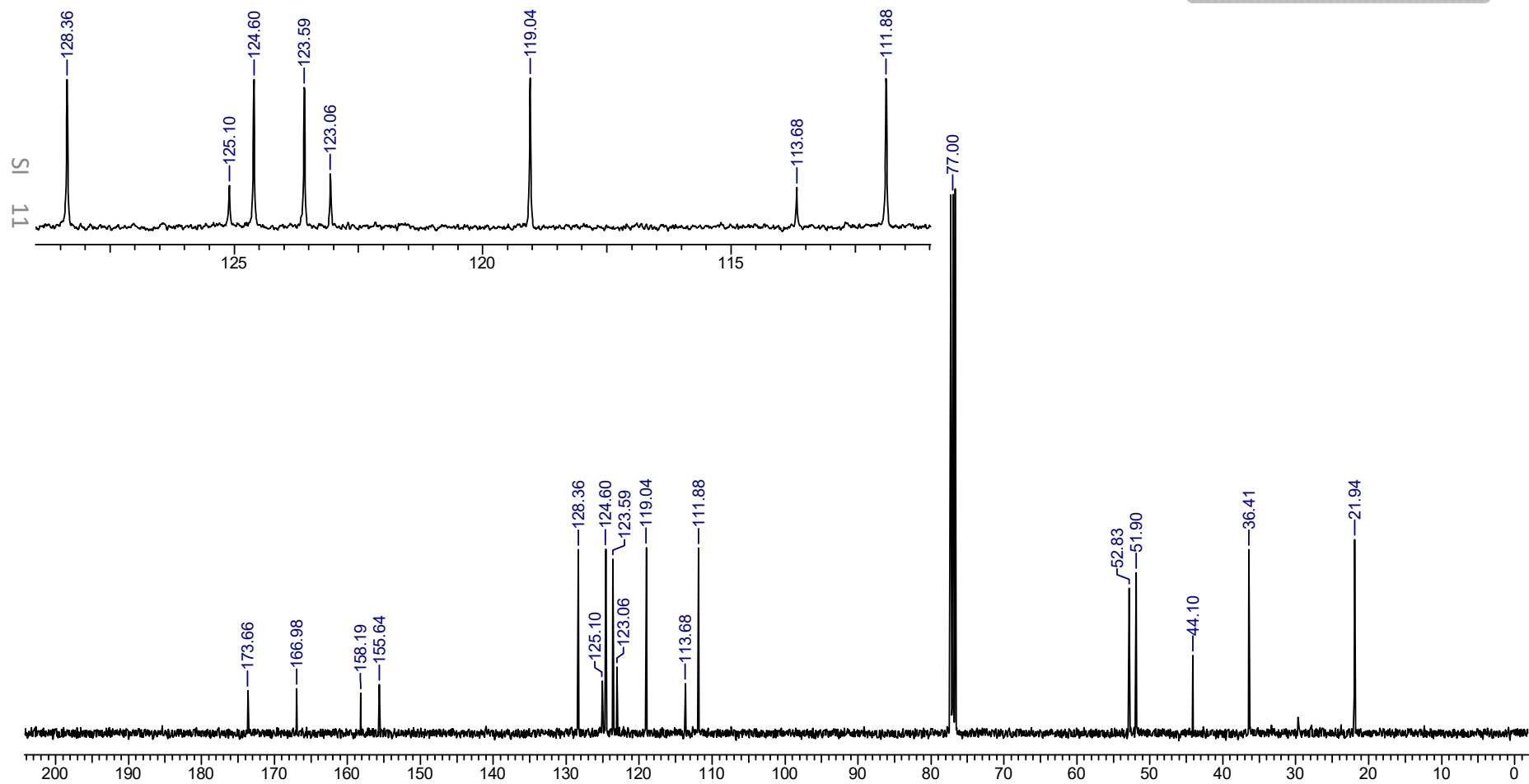
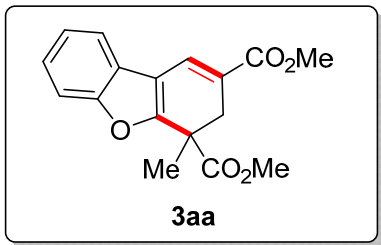




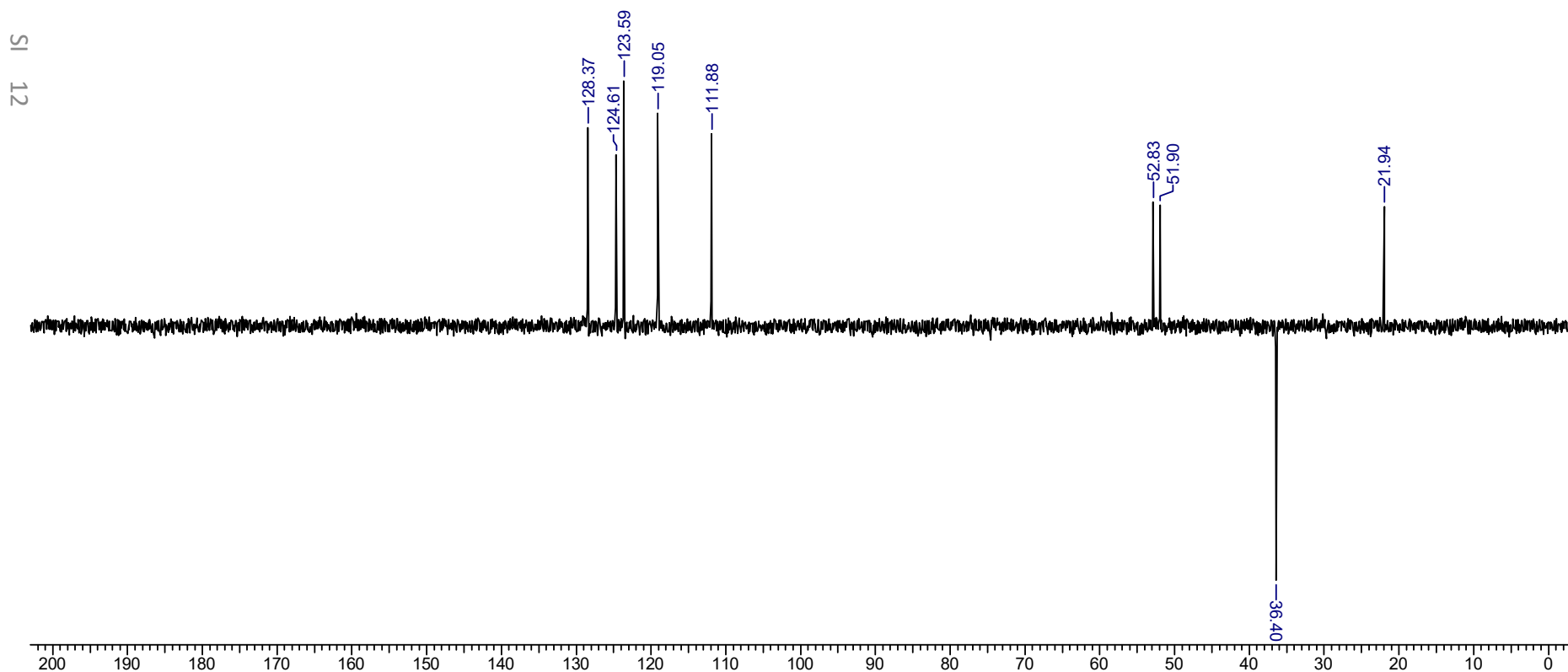
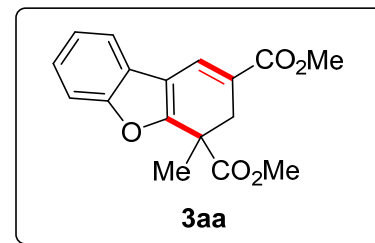
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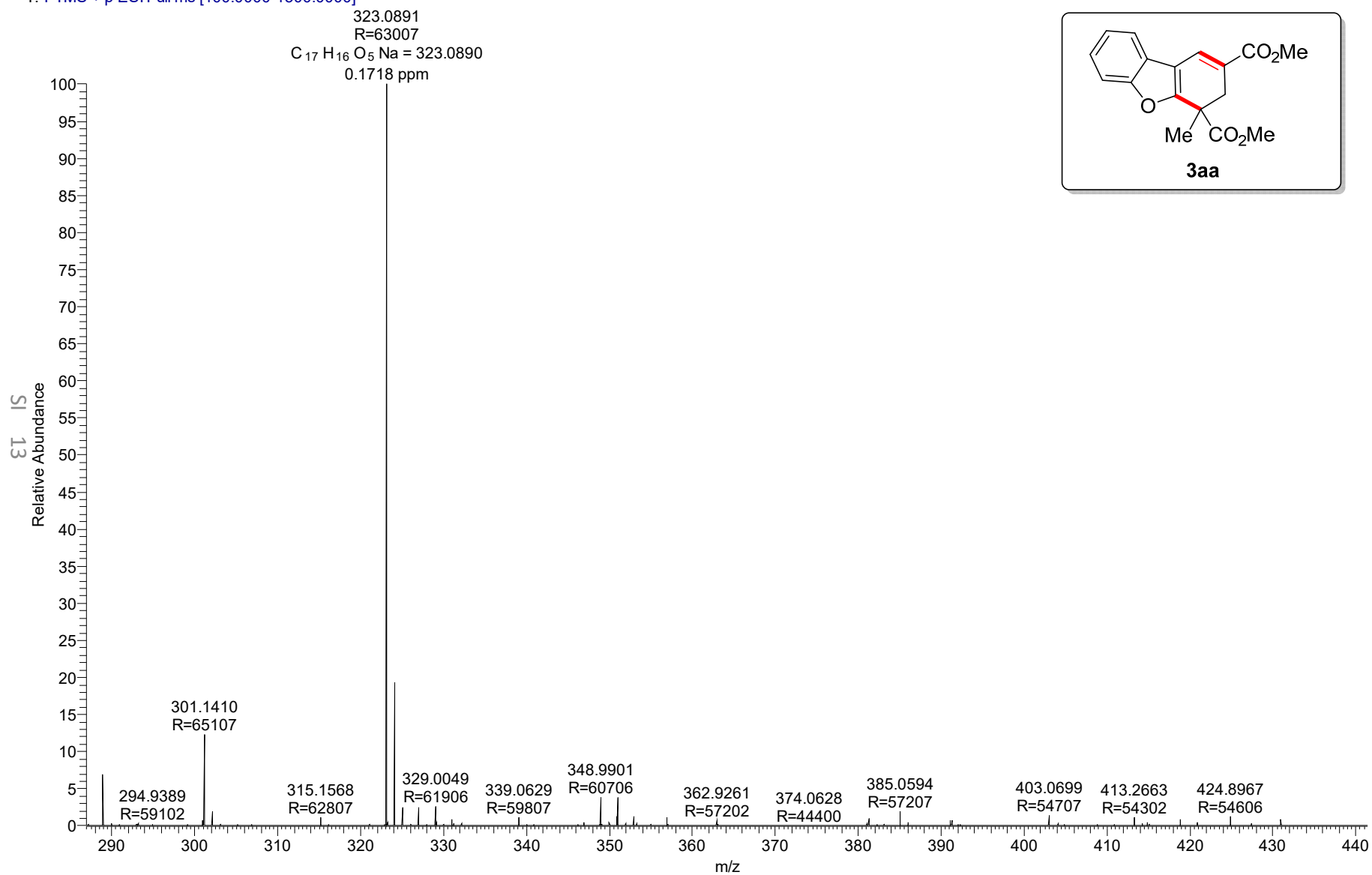
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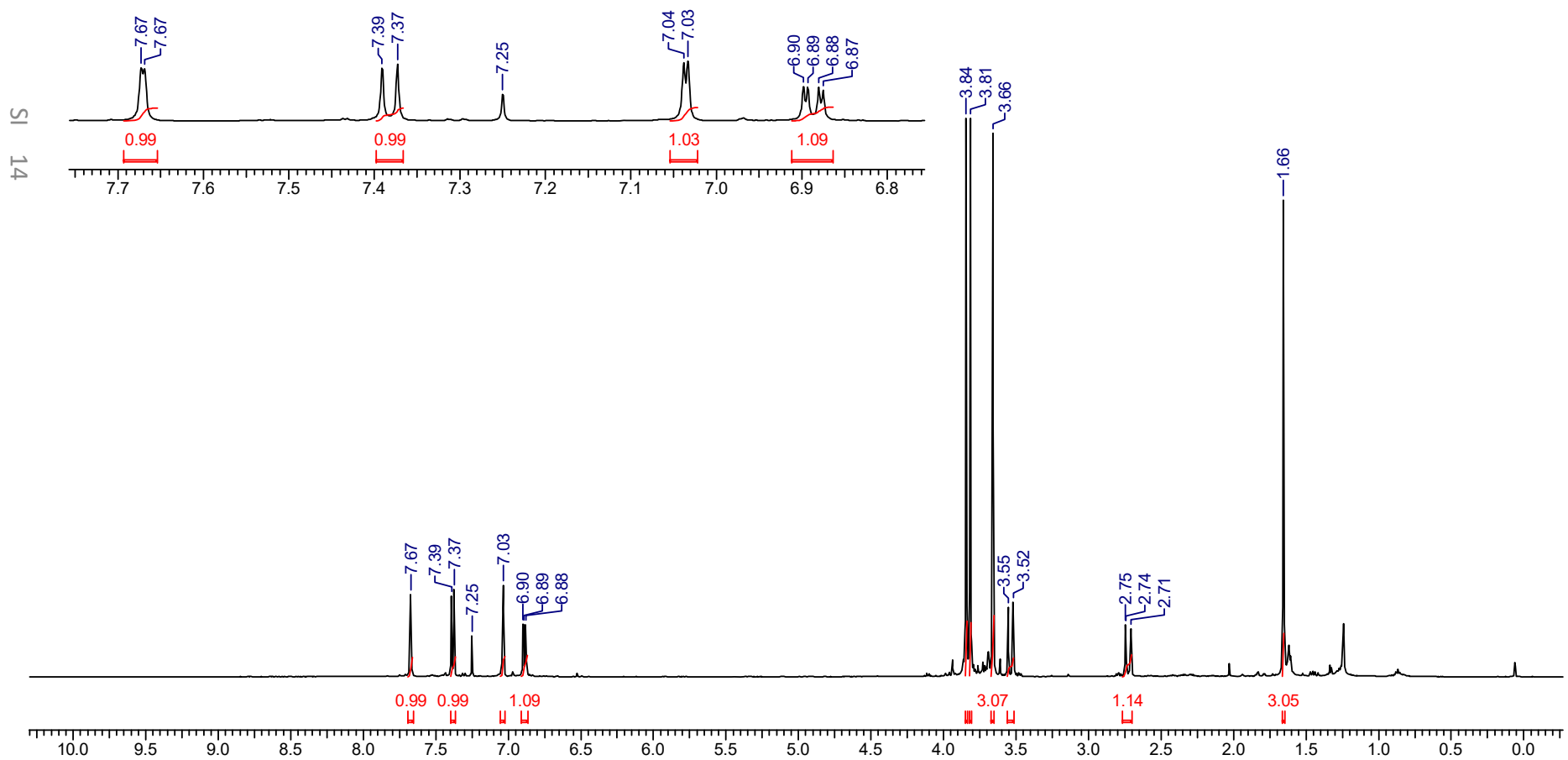
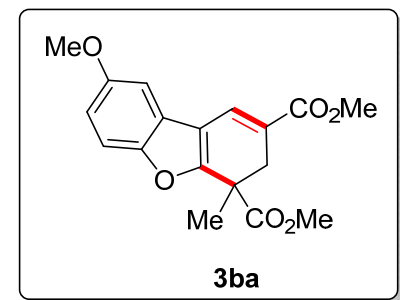
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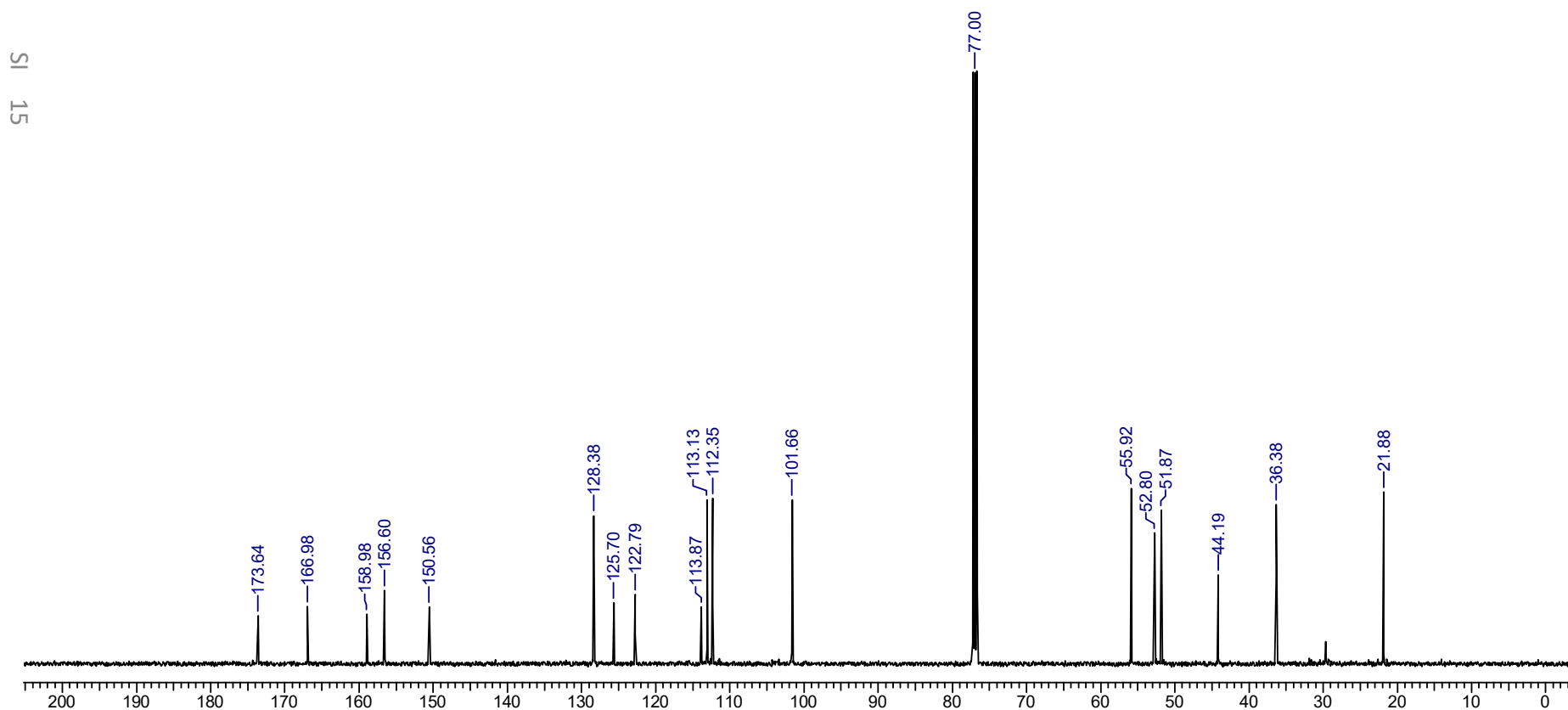
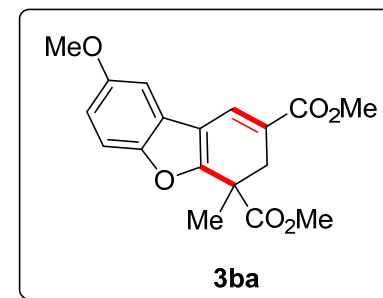
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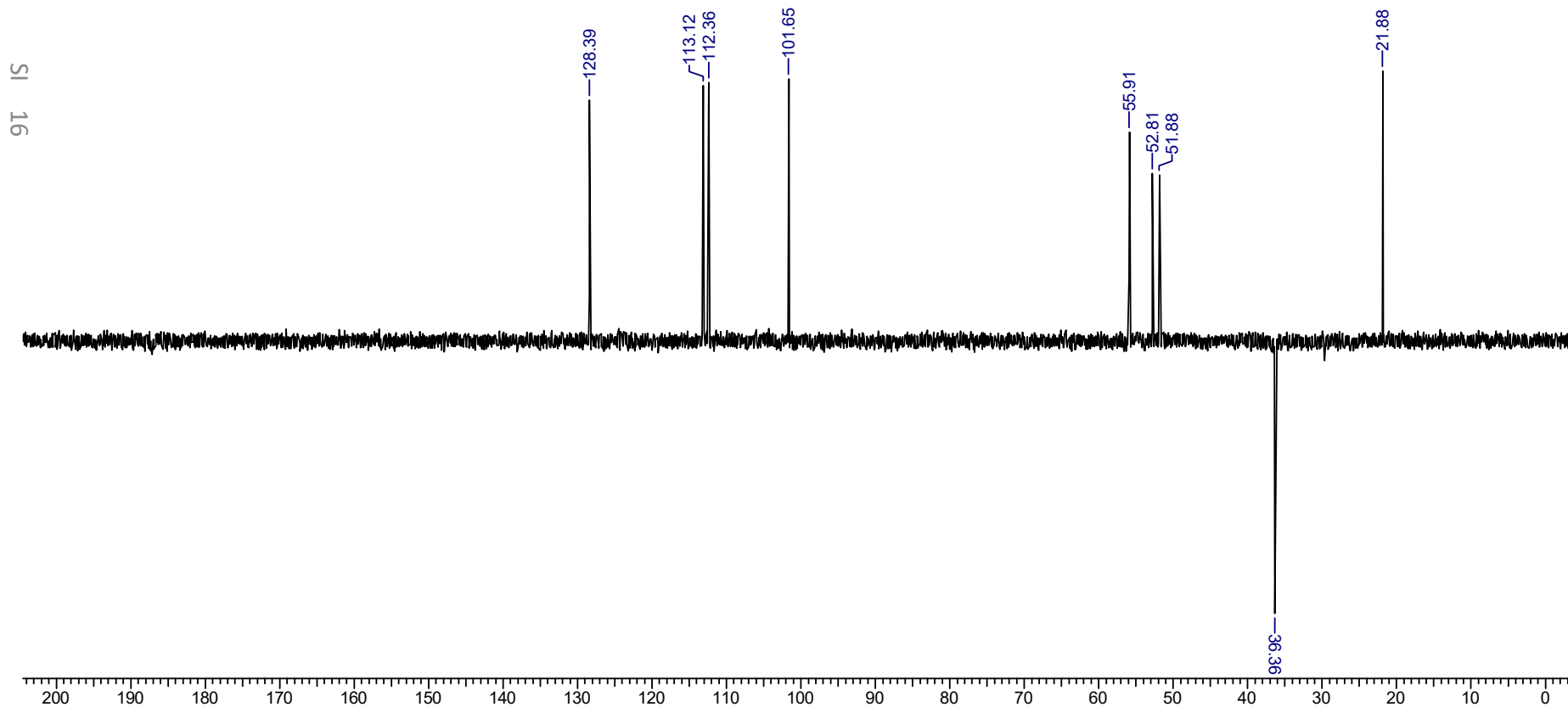
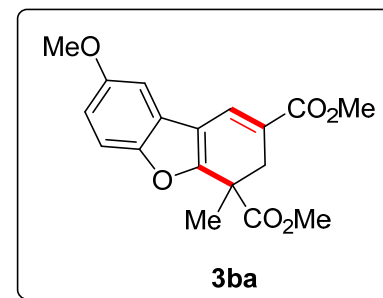
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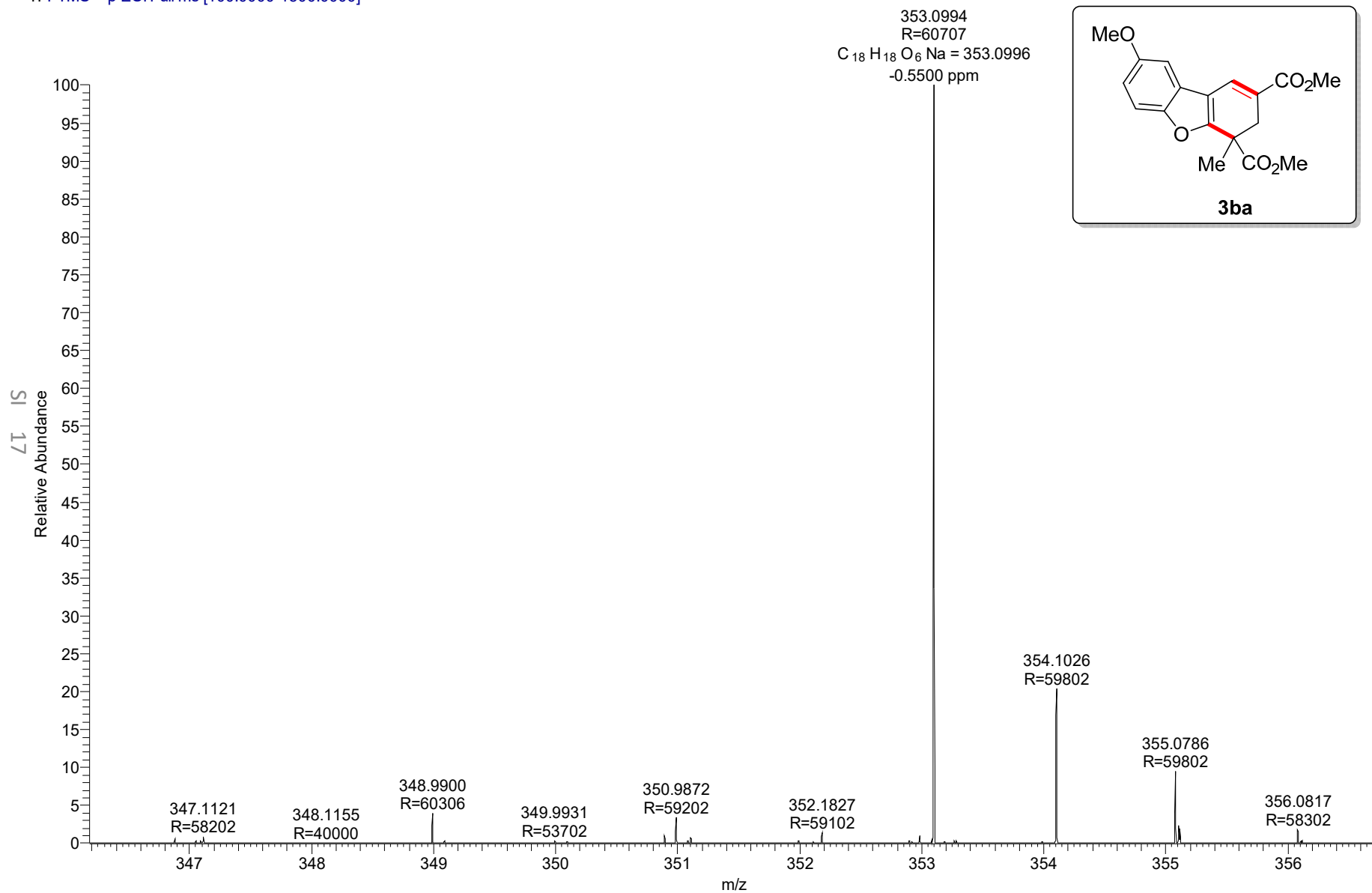
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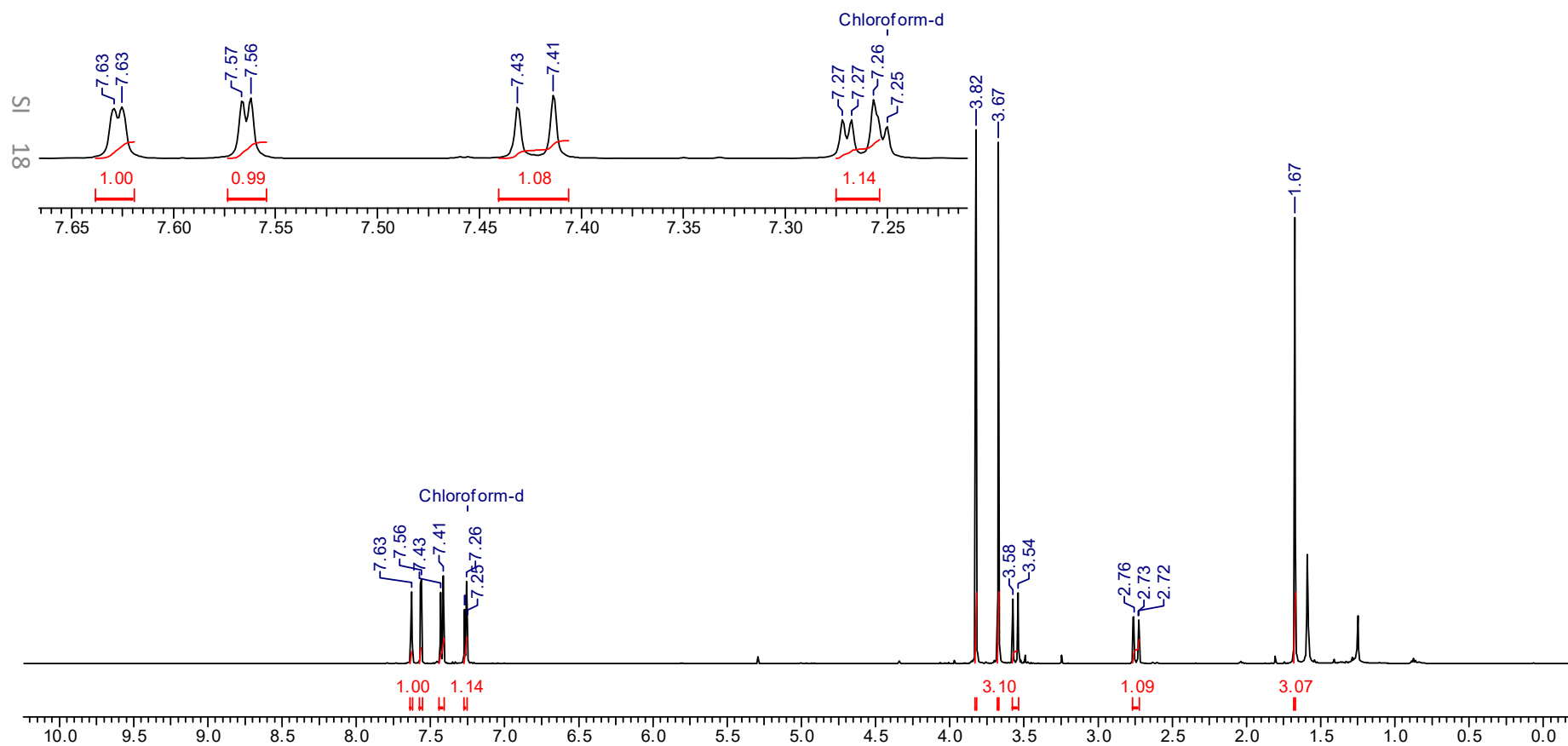
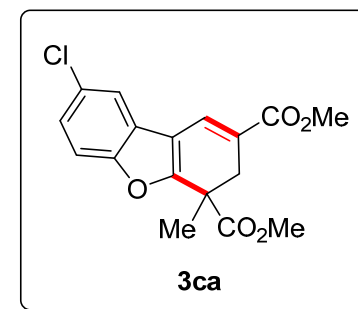
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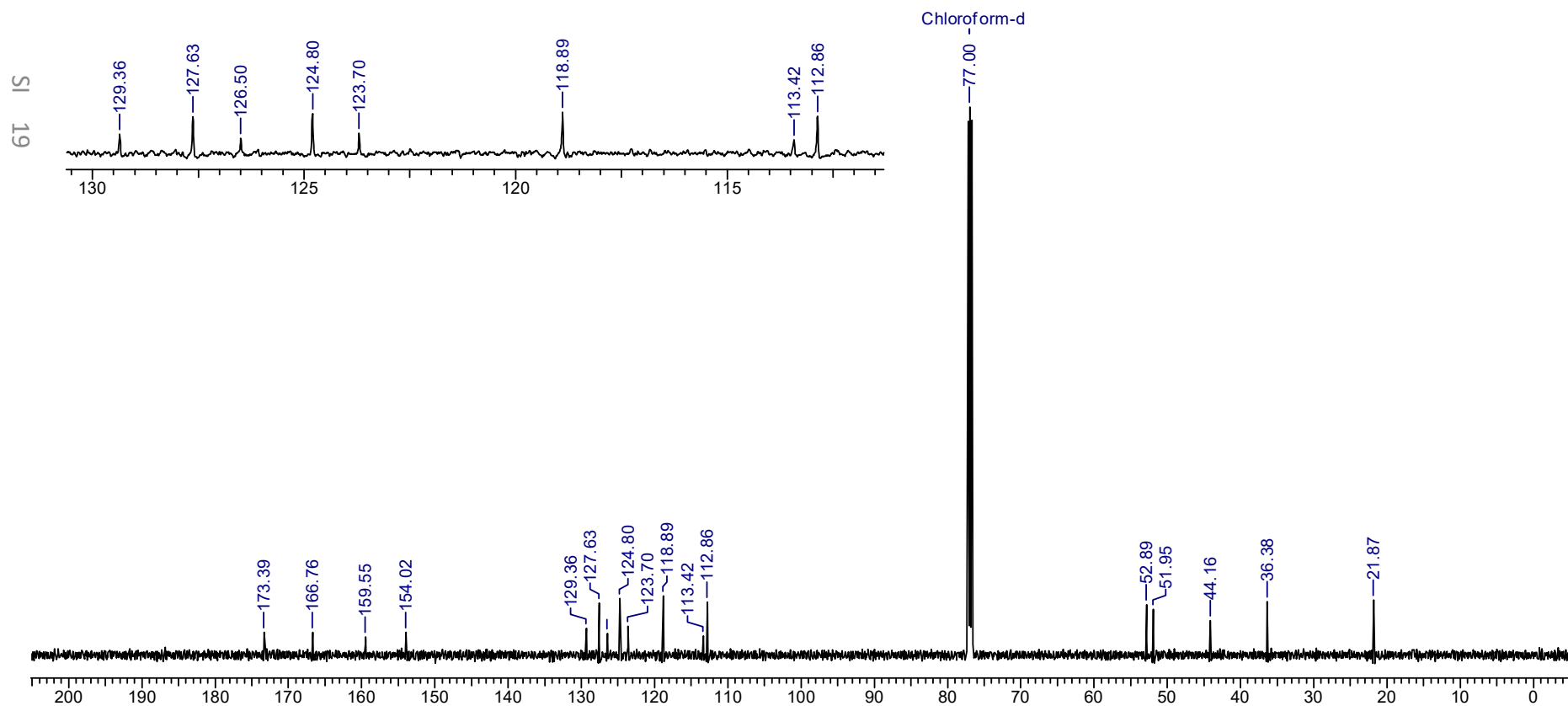
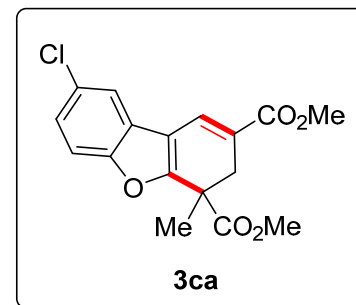
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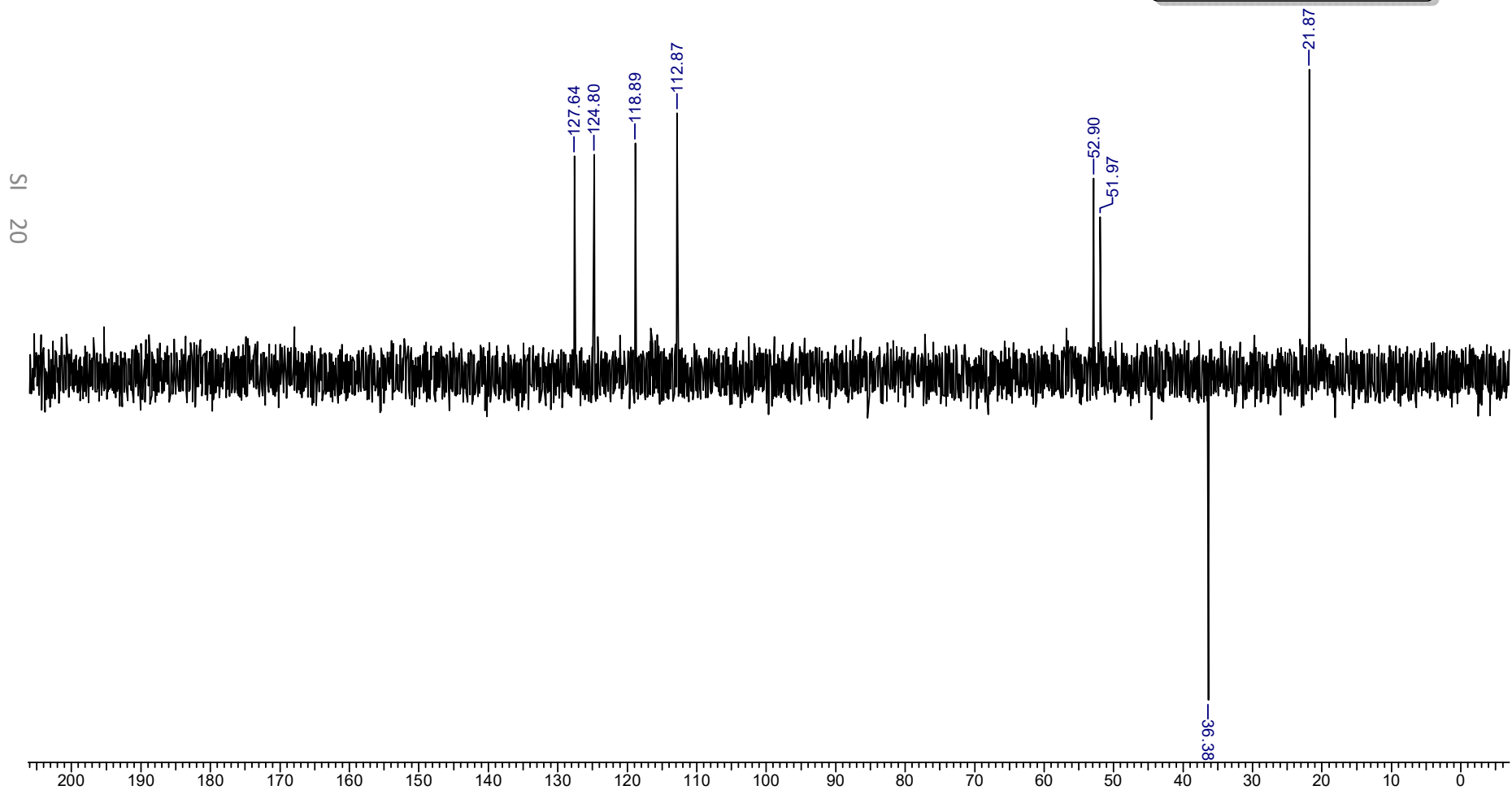
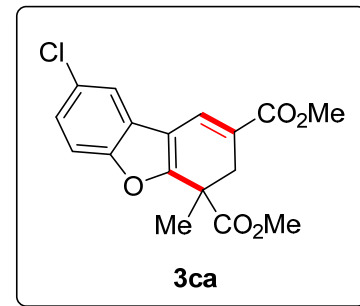
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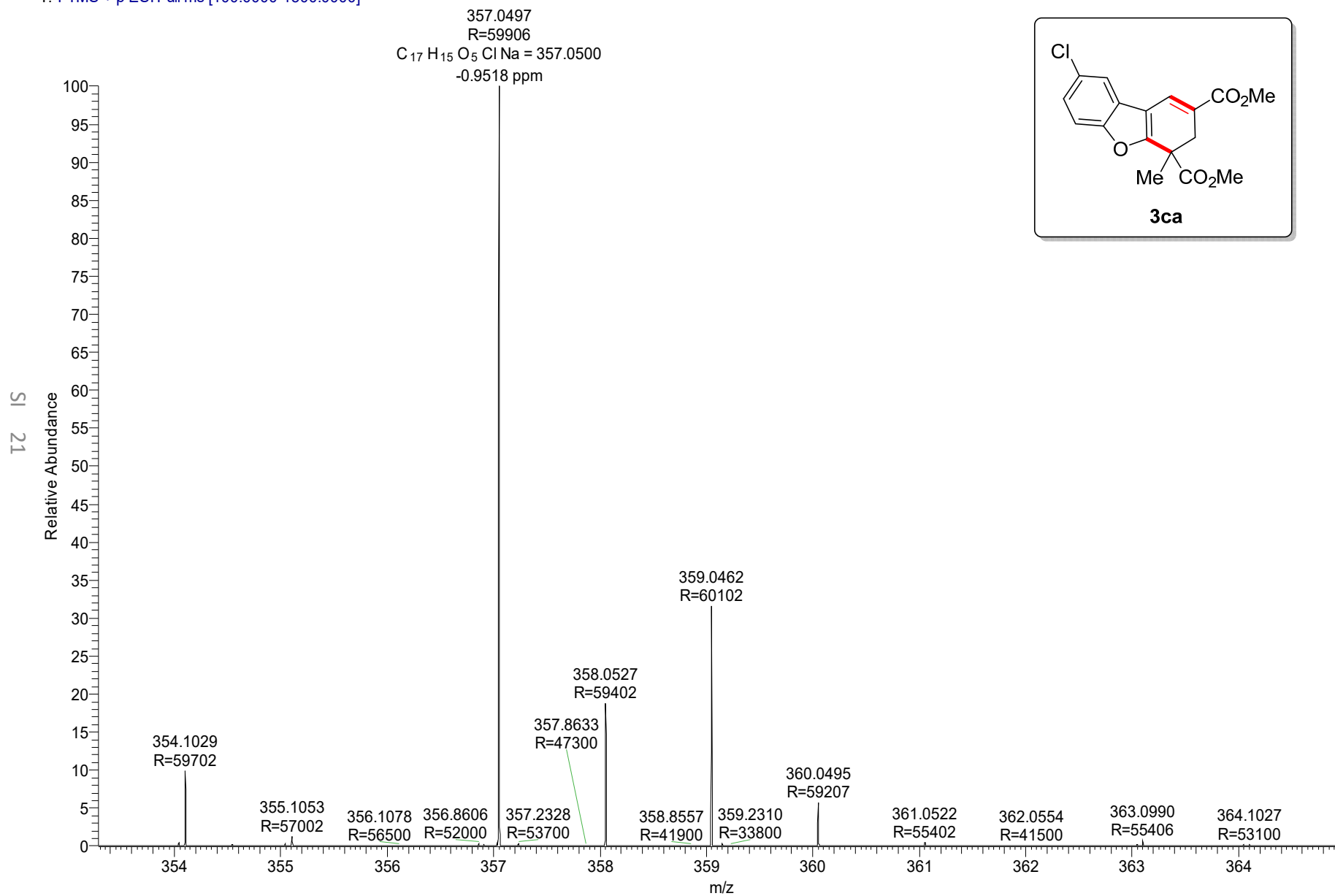
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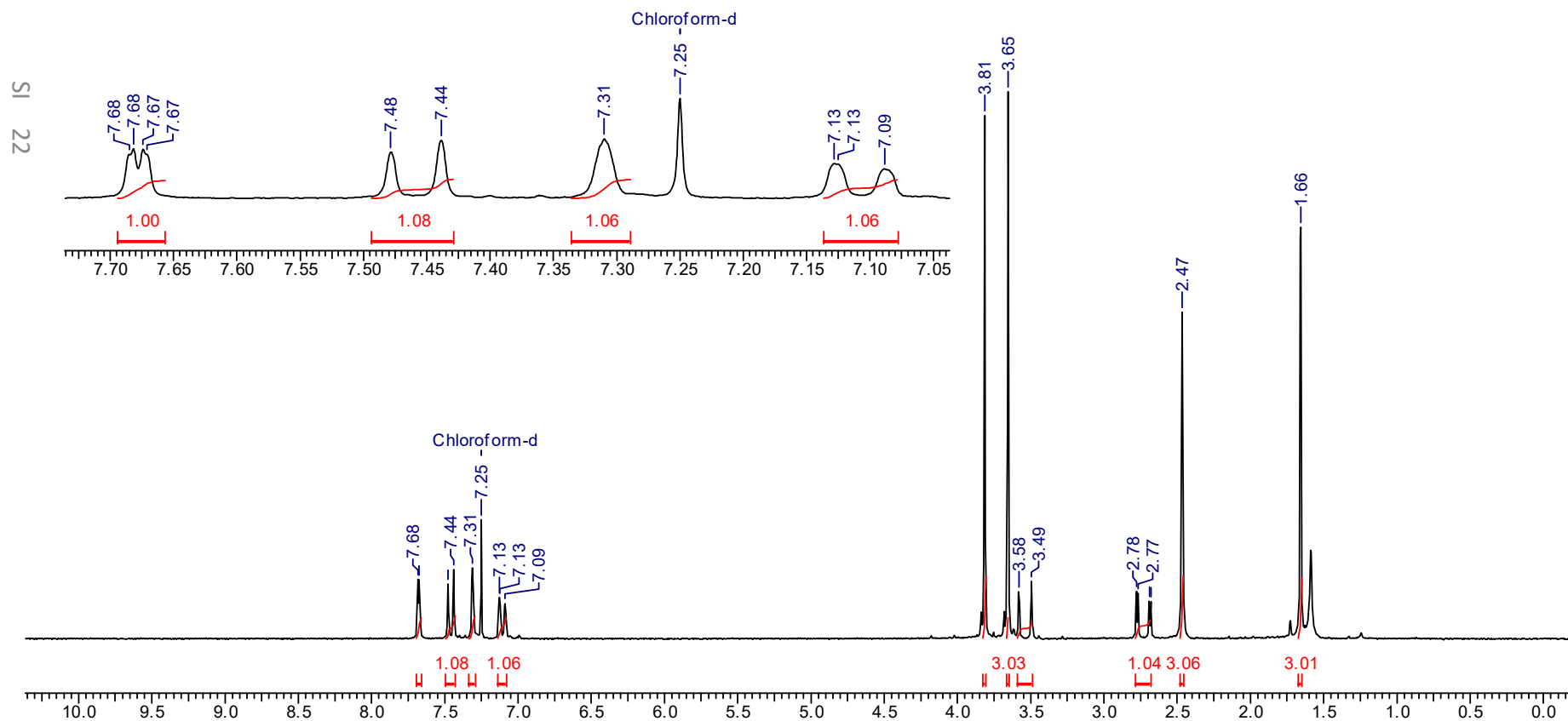
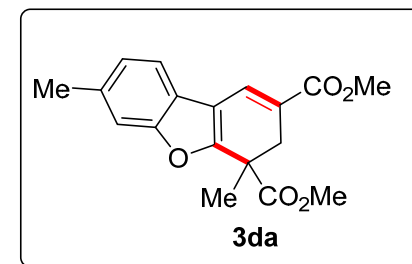
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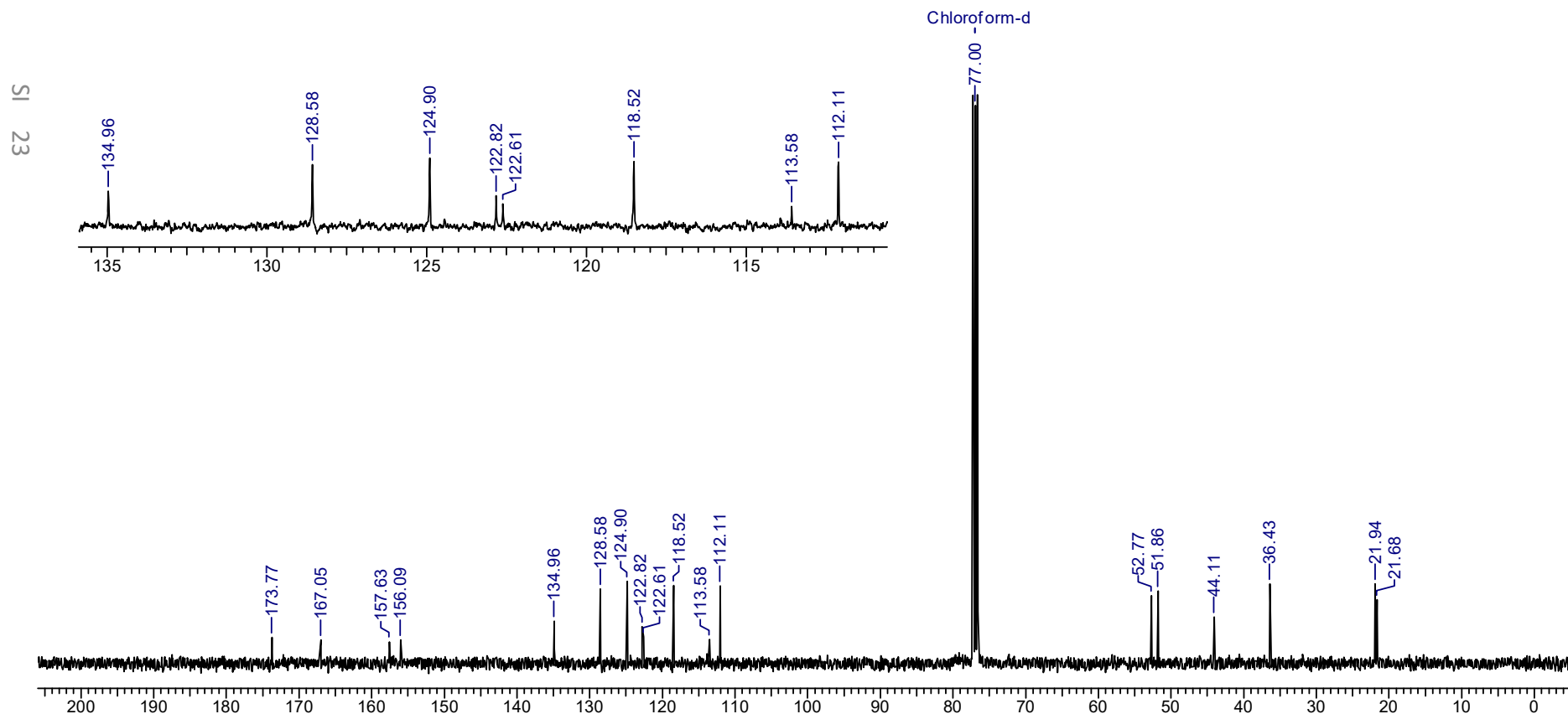
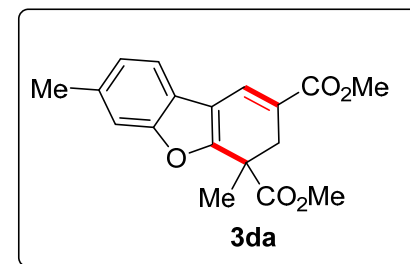
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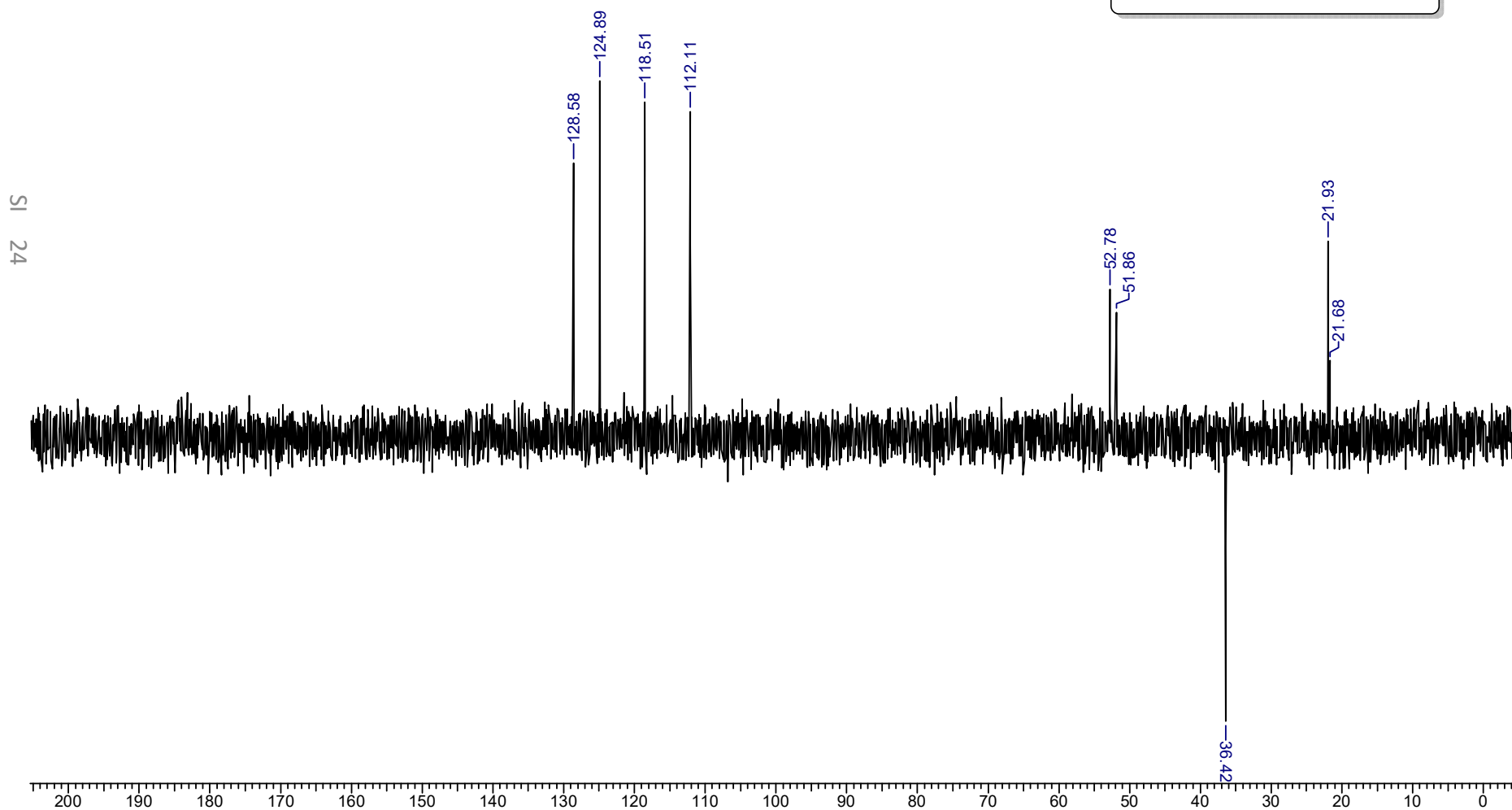
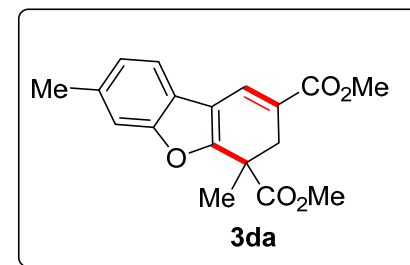
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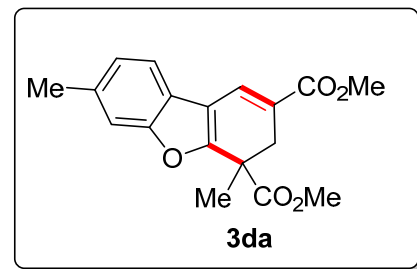
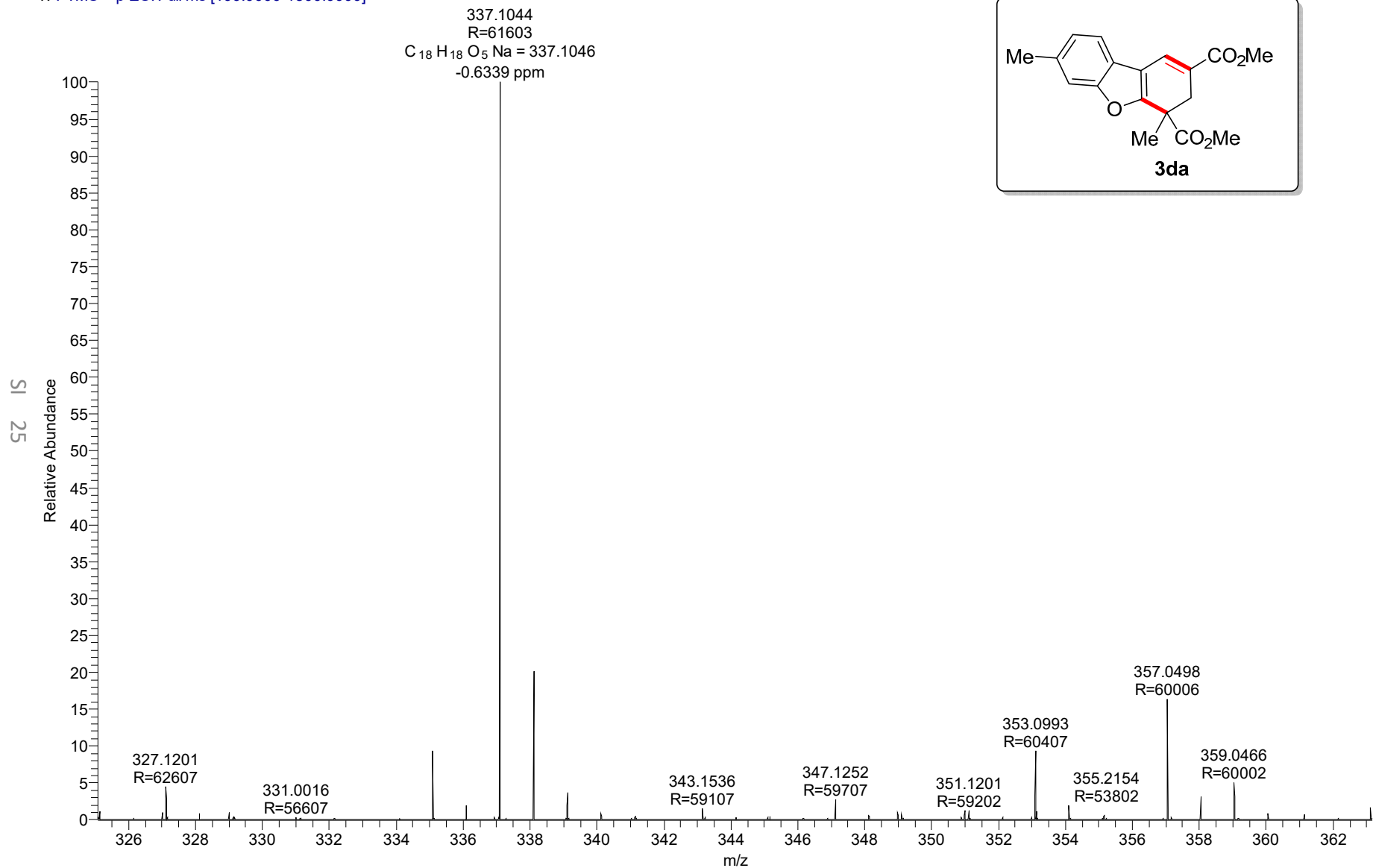
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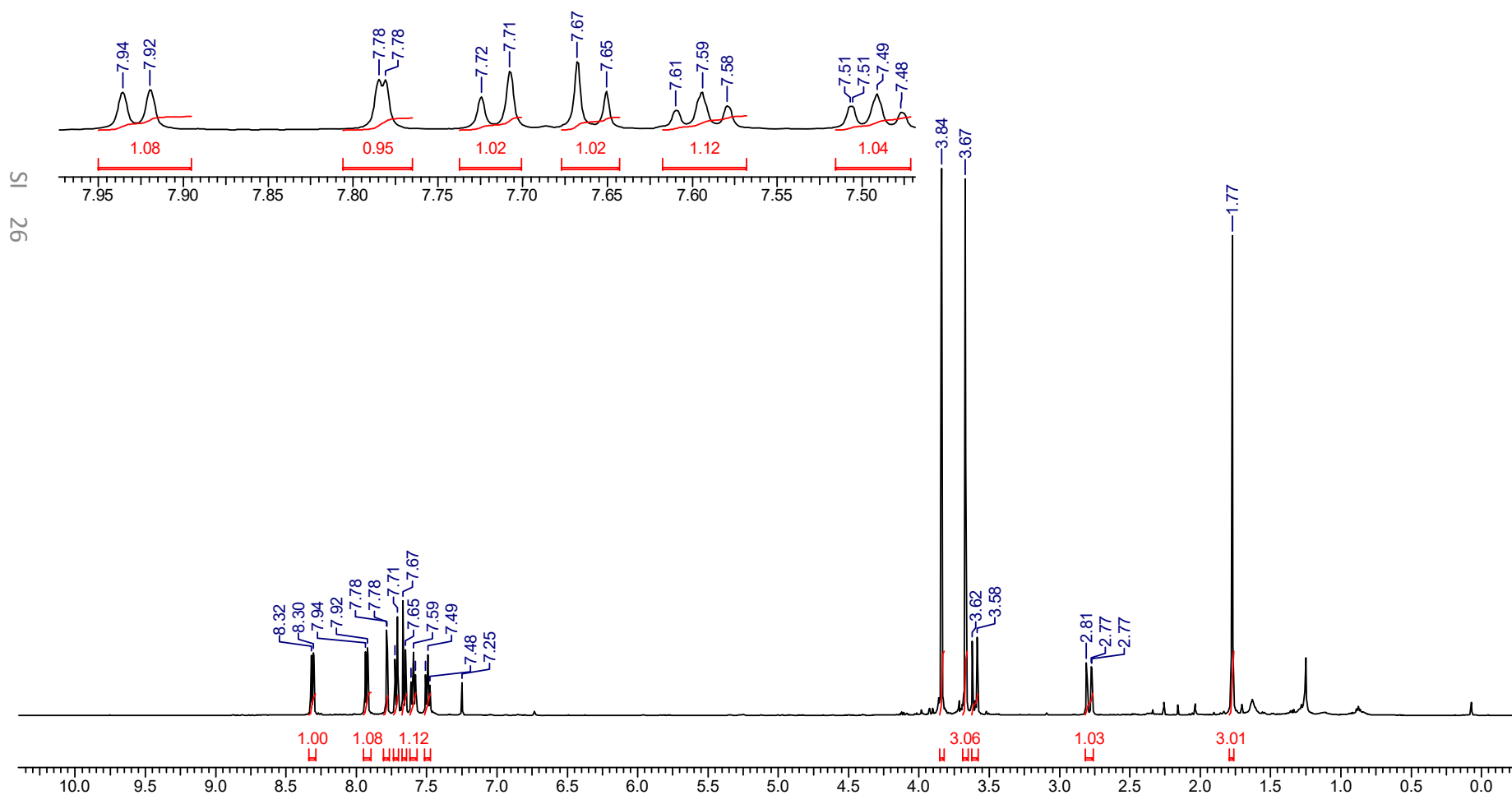
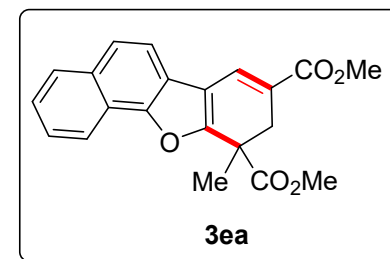
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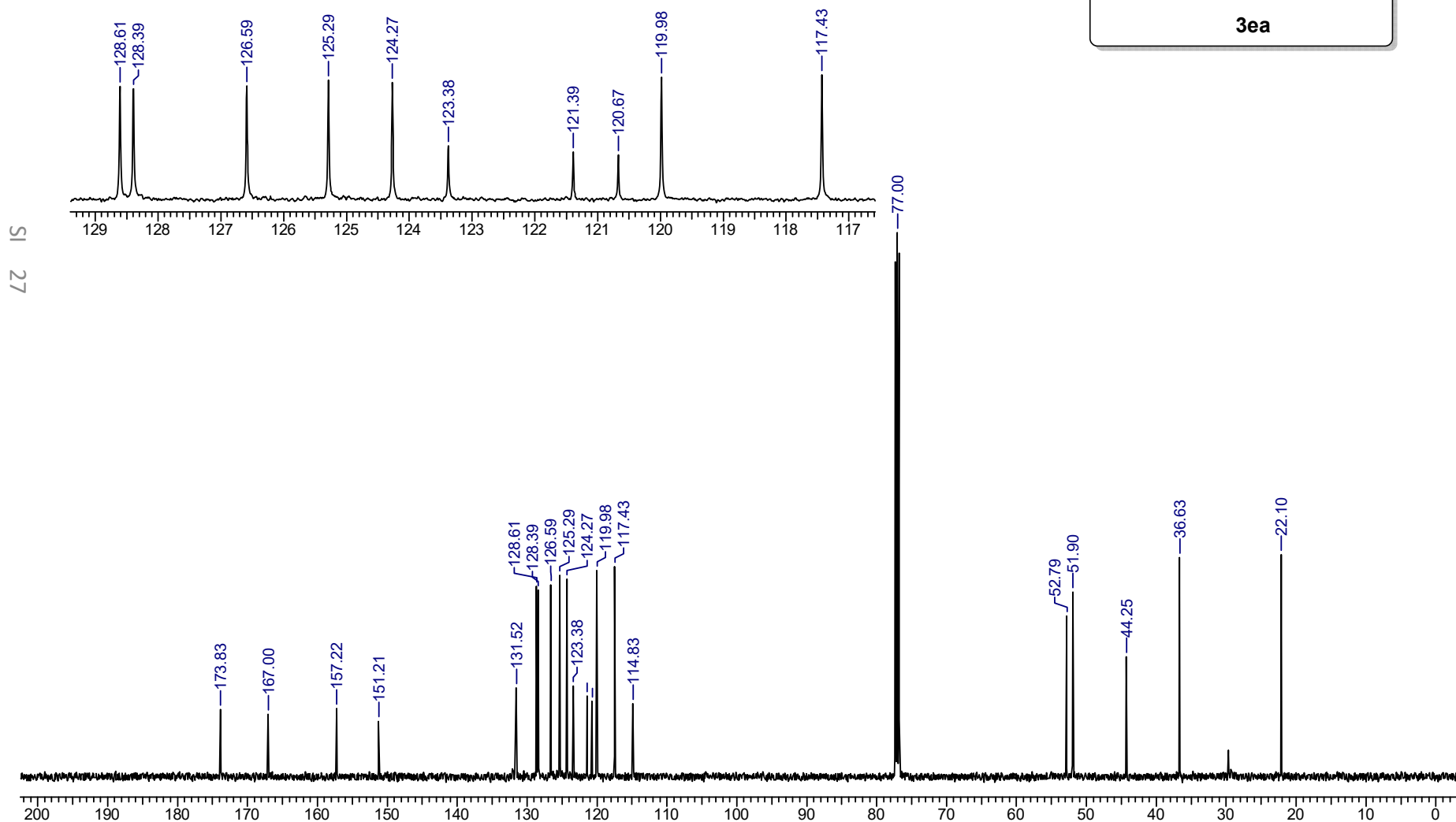
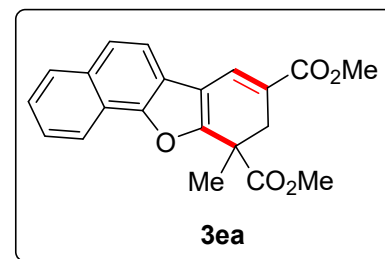
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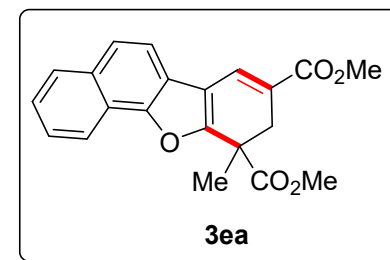
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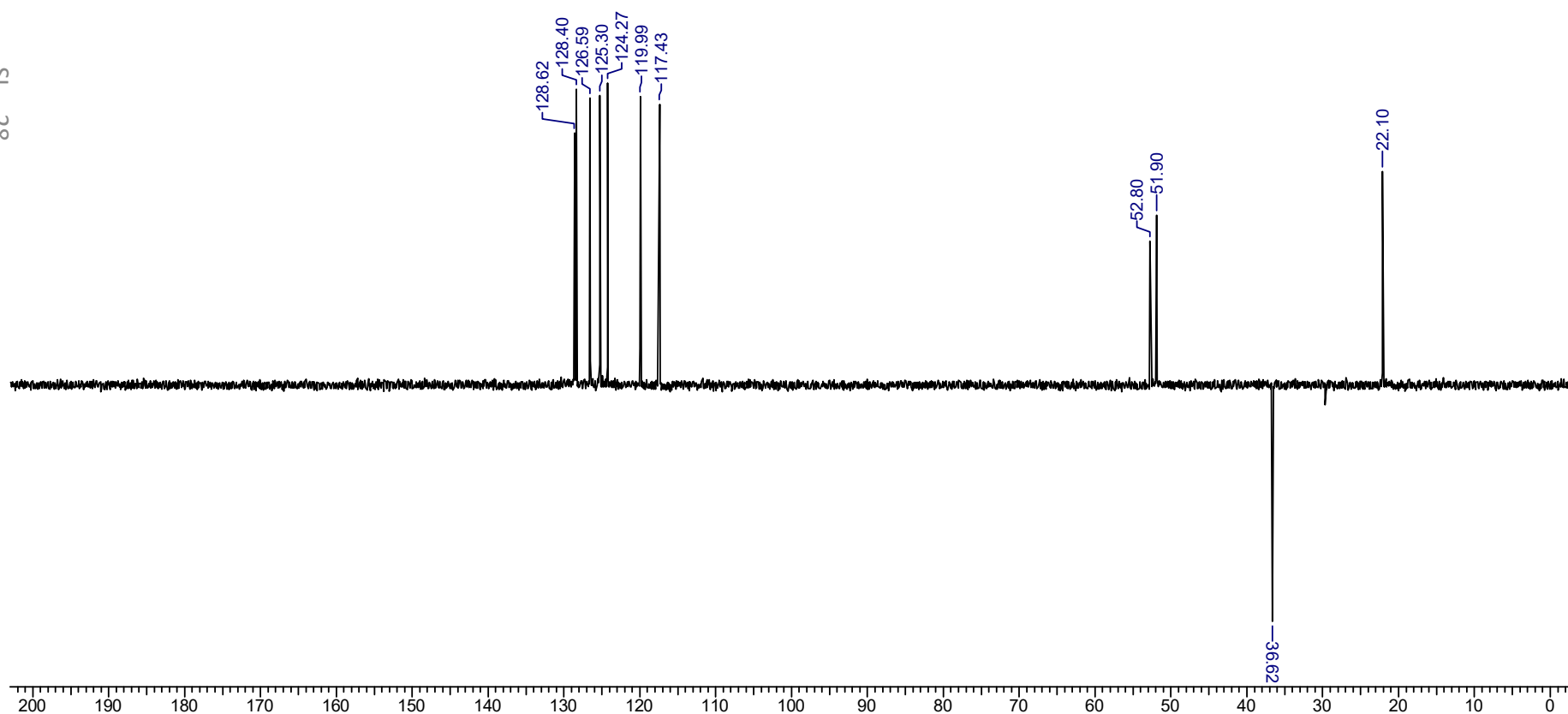
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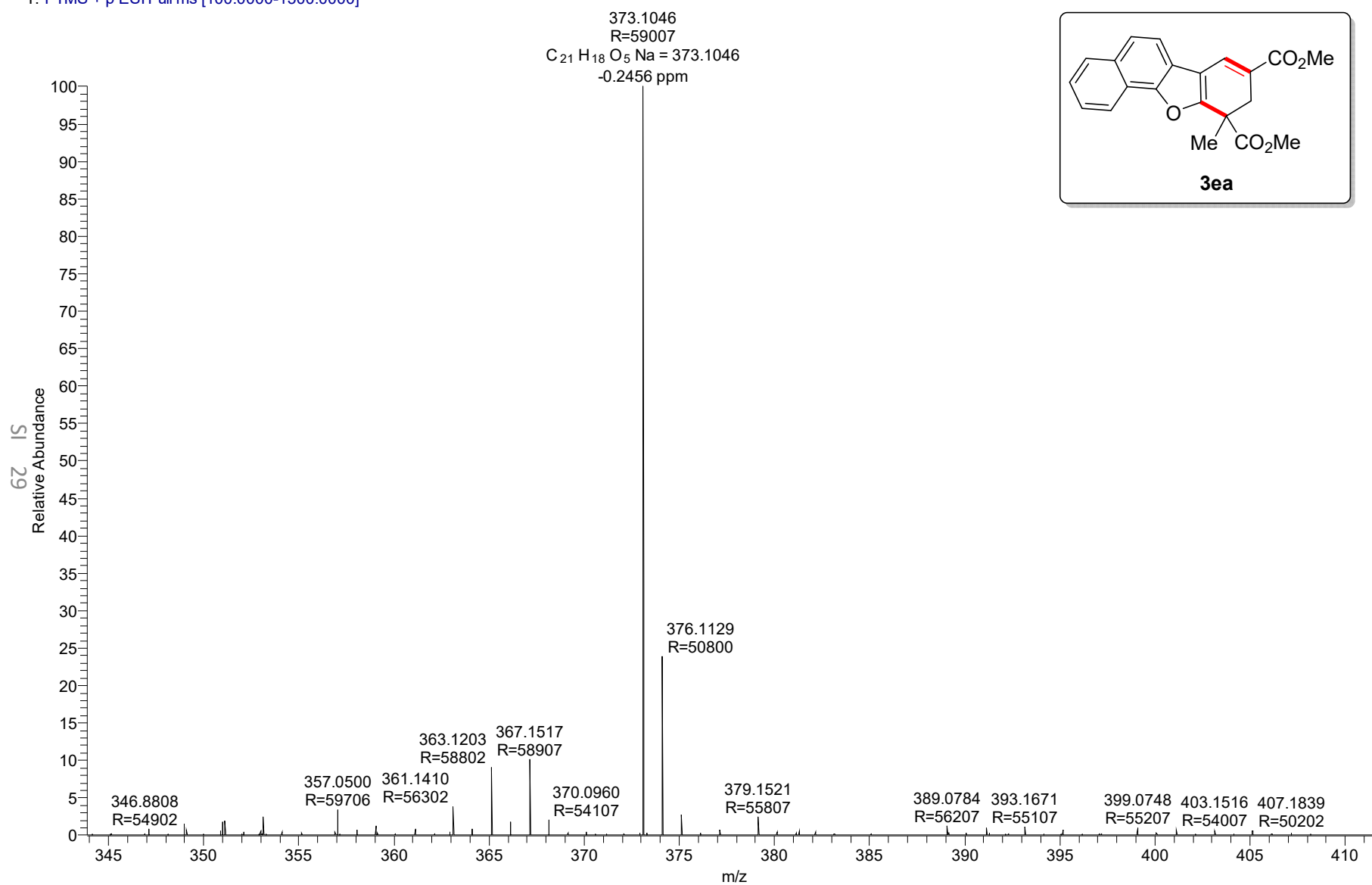
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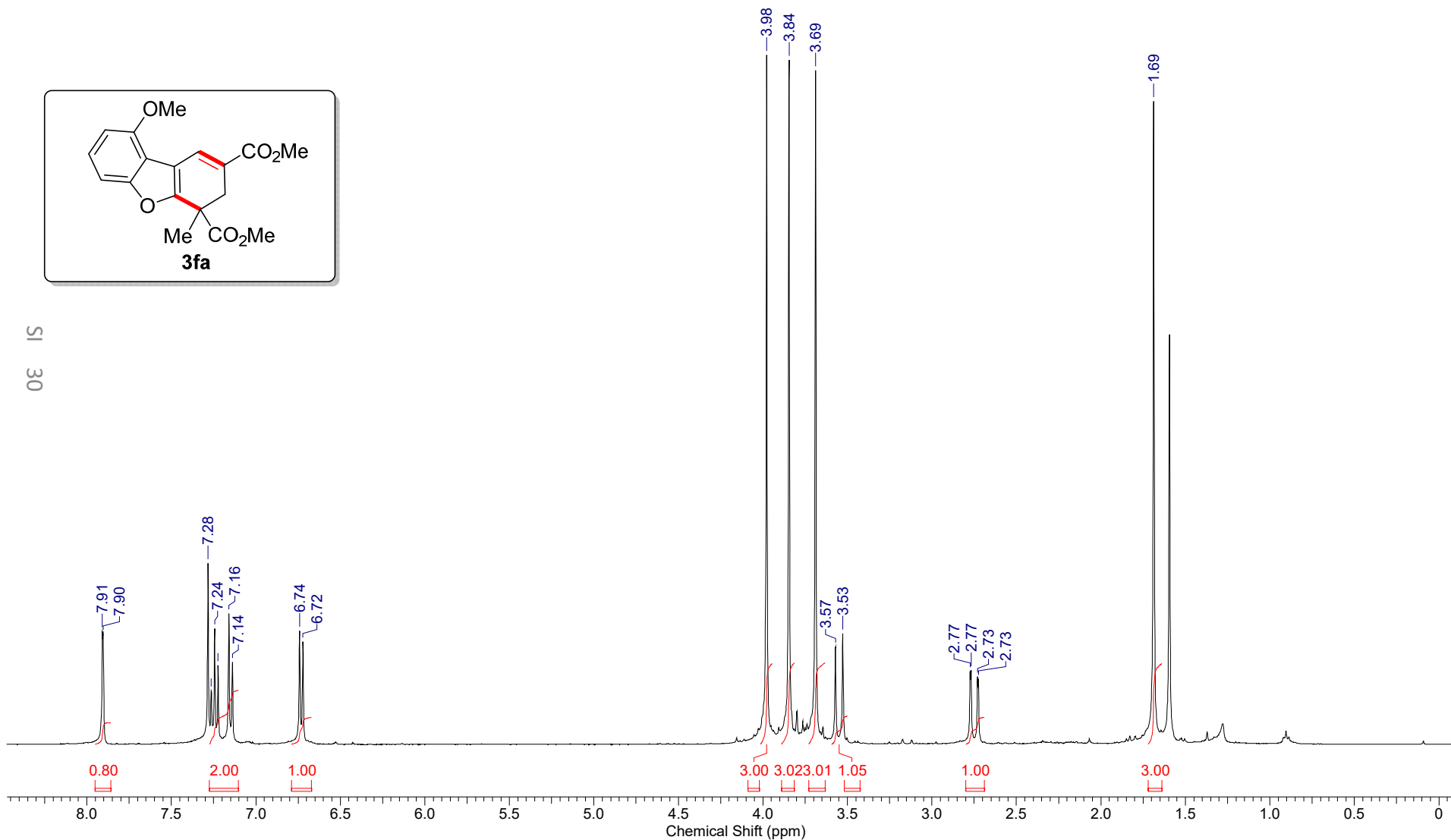
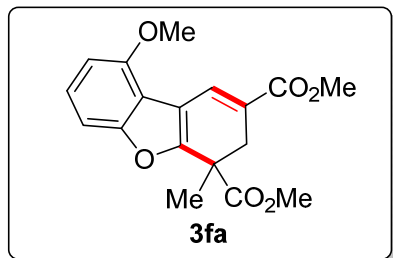
SI 28



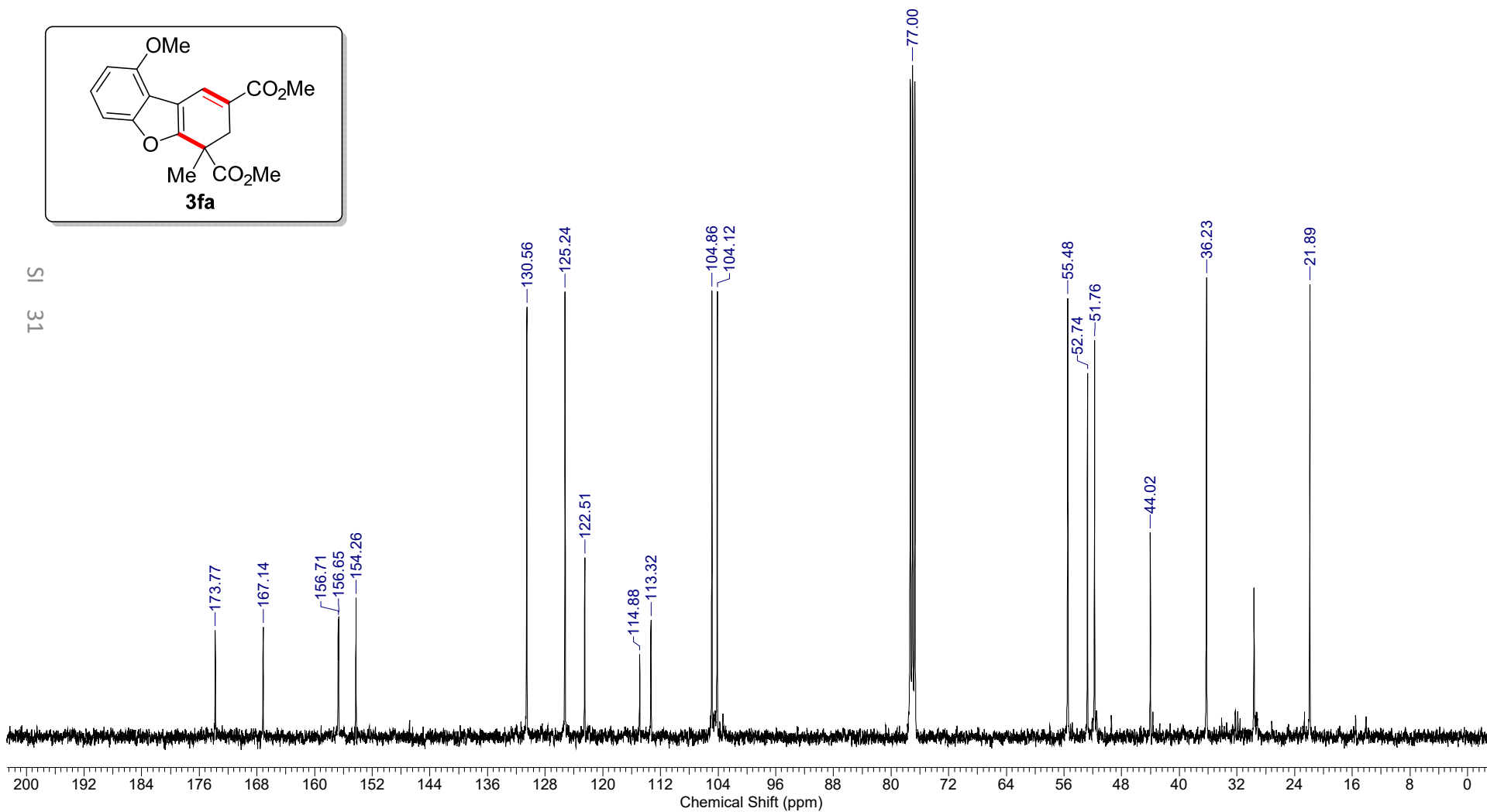
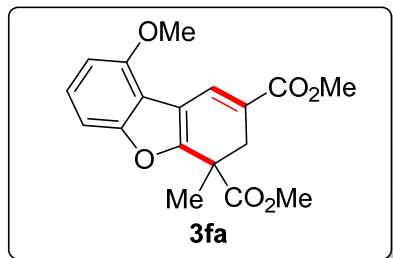
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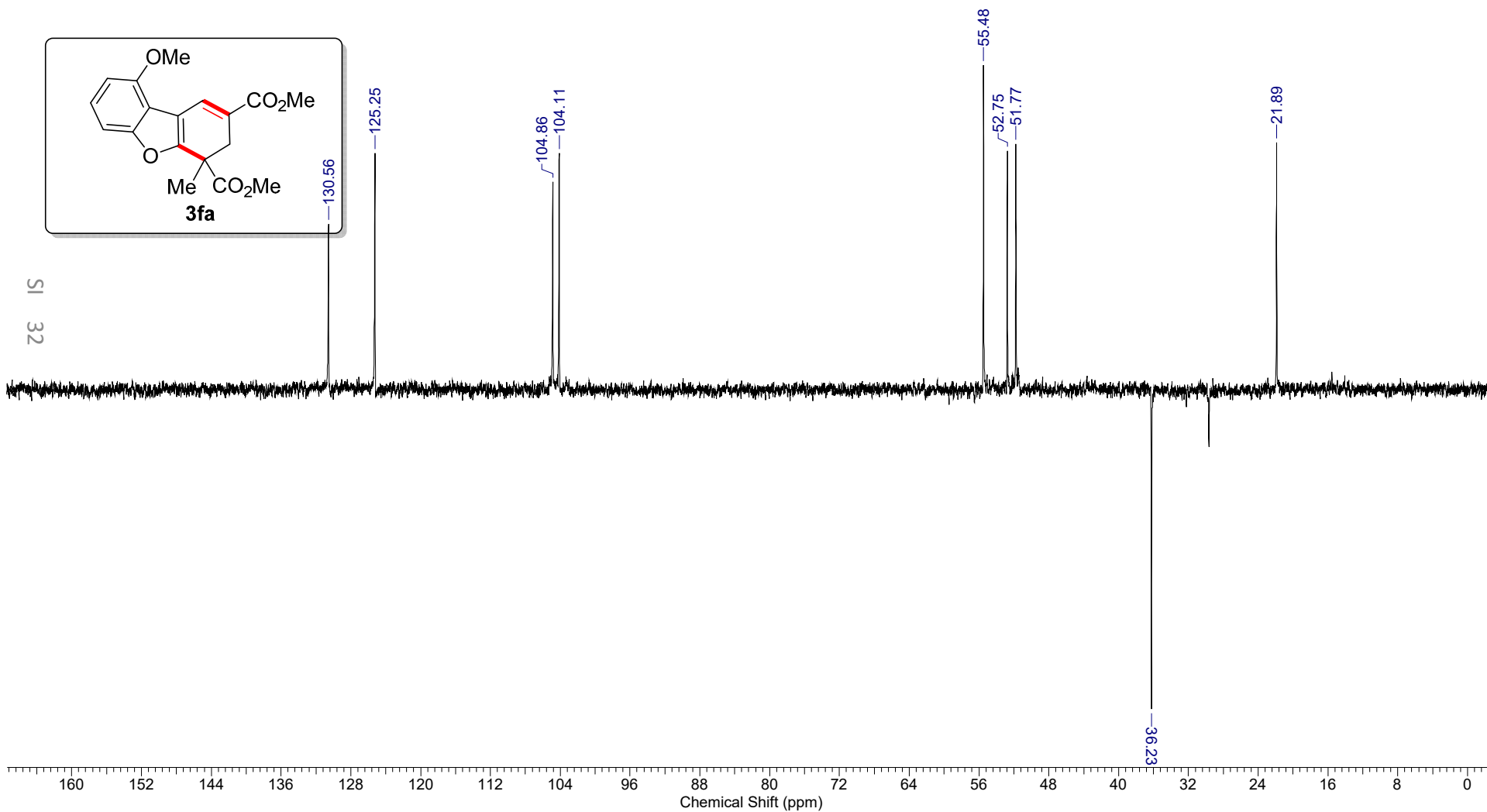
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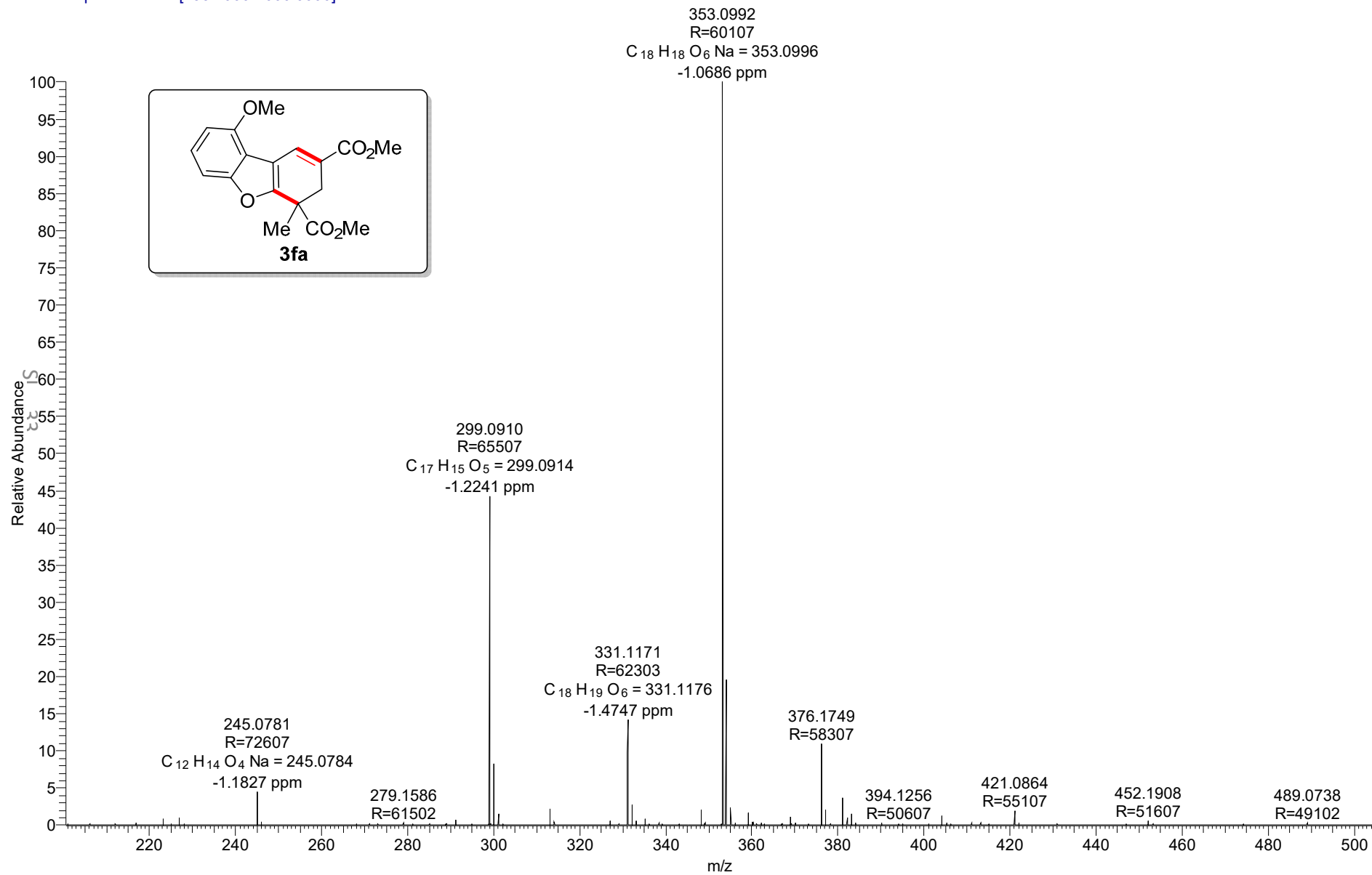
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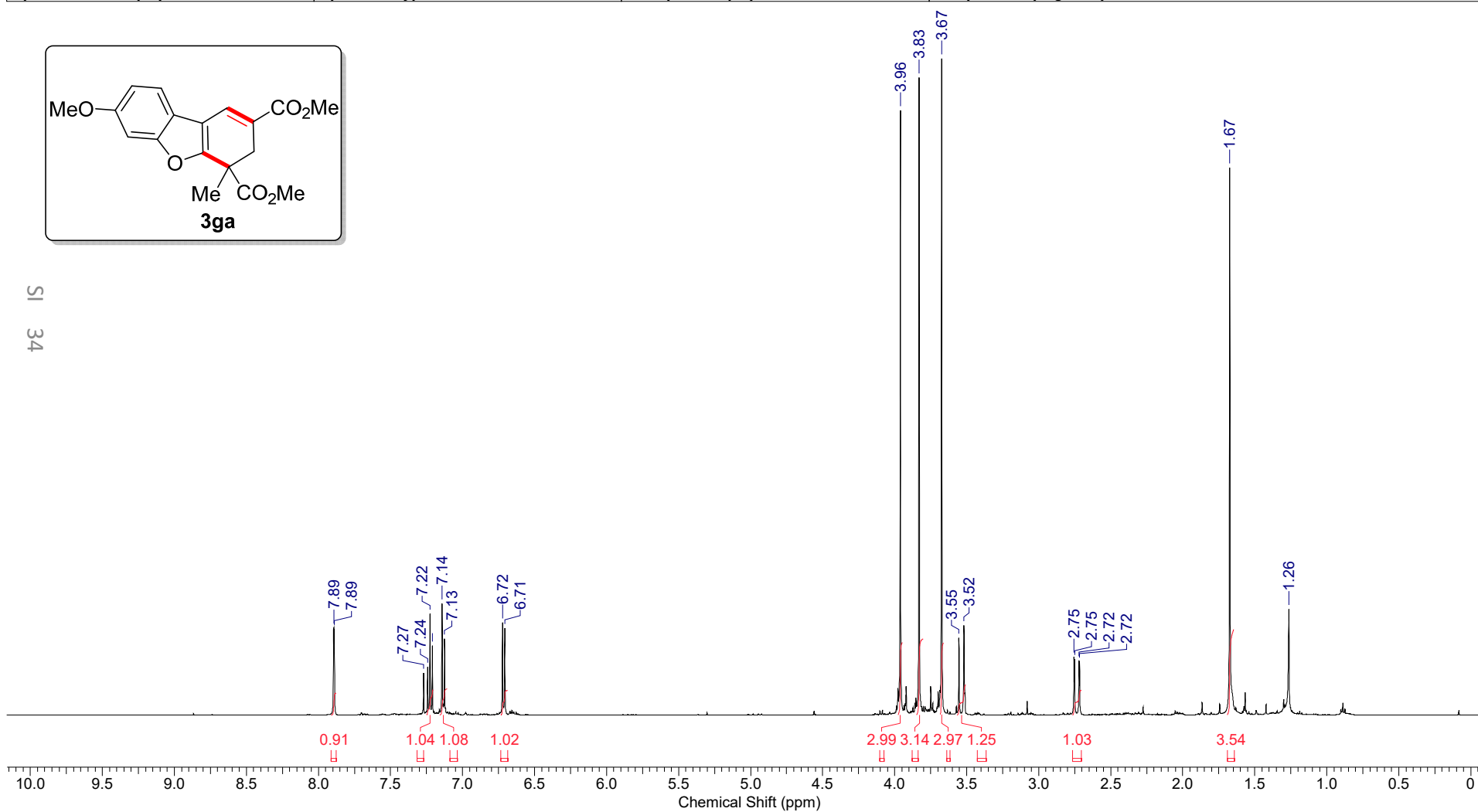
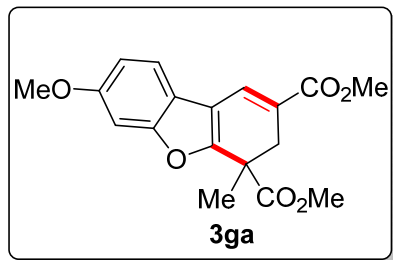
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Date Stamp	08 Aug 2018 15:45:12				
File Name	\\172.16.2.4\nmr_data\AV400\Aug_18_400\data\ep\nmr\AV-400-20180803-114110-44339\2\PDATA\1\1r				Frequency (MHz) 100.61
Nucleus	13C	Number of Transients	519	Origin	spect
Owner	root	Points Count	32768	Pulse Sequence	dept135
SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10056.4512
Spectrum Type	DEPT135	Sweep Width (Hz)	25251.75	Temperature (degree C)	25.200



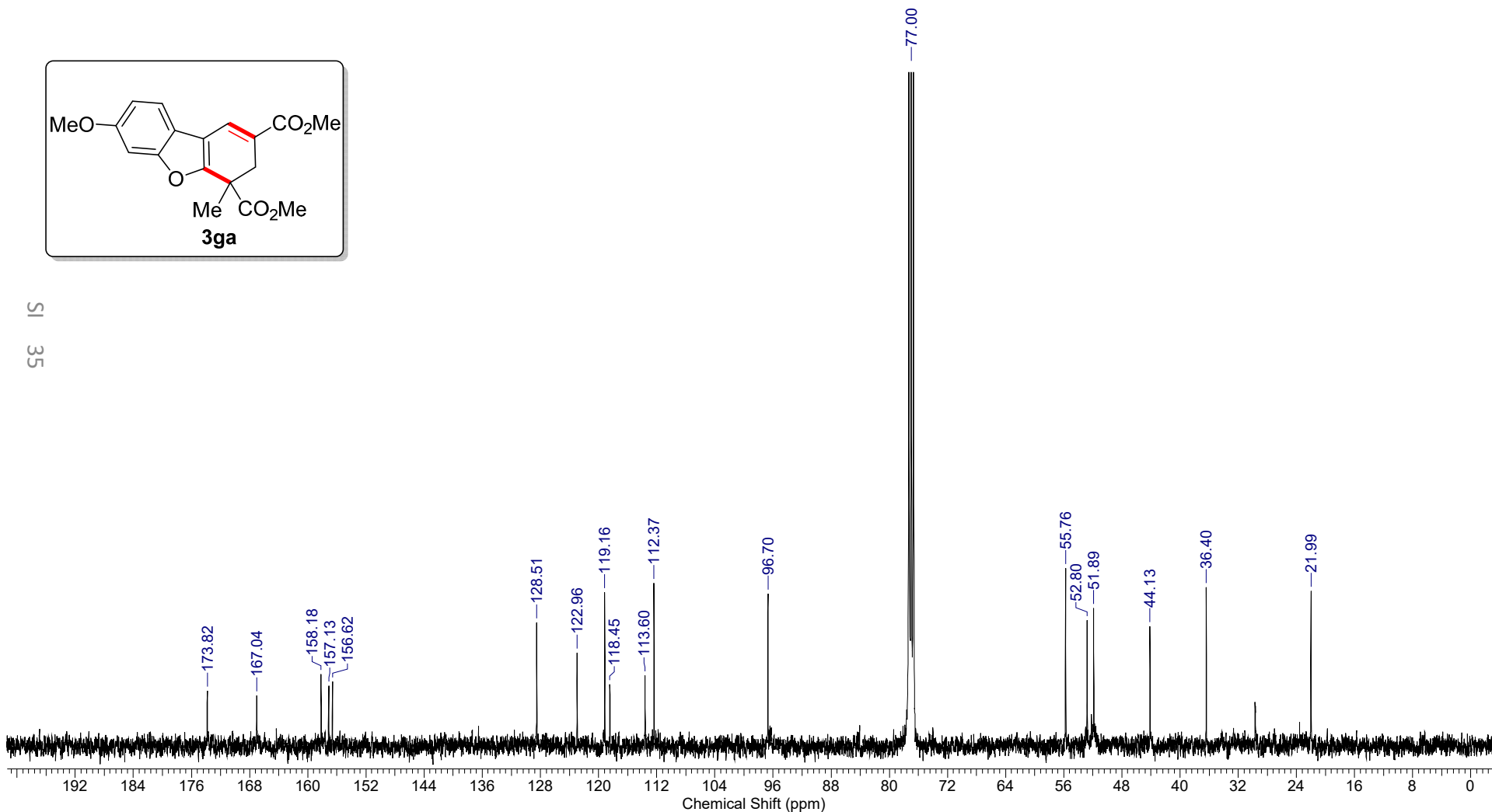
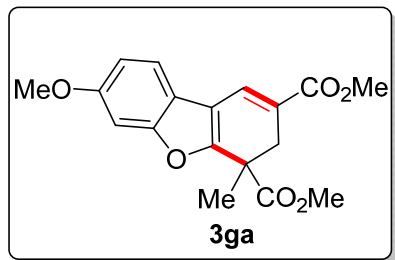
KS-J-31A_190130111804 #284 RT: 1.27 AV: 1 NL: 6.87E8
T: FTMS + p ESI Full ms [133.4000-2000.0000]



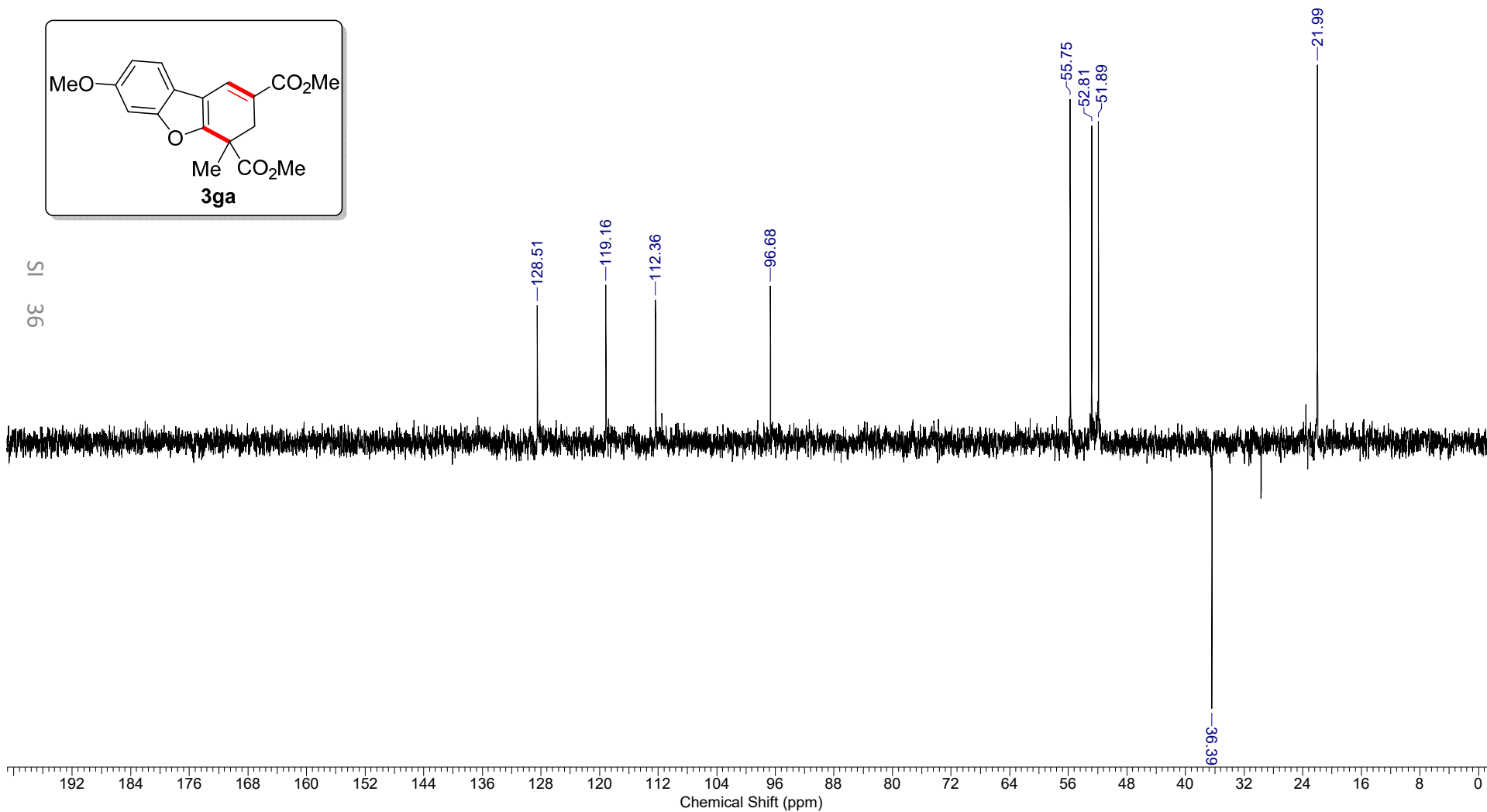
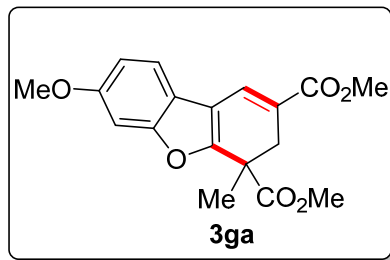
Acquisition Time (sec)	1.3107	Comment	Shaziya 1H	Date	28 Nov 2018 11:27:12		
Date Stamp	28 Nov 2018 11:27:12						
File Name	H:\Srinivas JOC\NMR\paramethoxybenzofuran\Methyl acrylate\AV-500-20181123-104850-11843\1\1r						
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	64	Origin	spect
Original Points Count	16384	Owner	nmr	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	128.00	SW(cyclical) (Hz)	12500.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	3493.0850	Spectrum Type	STANDARD	Sweep Width (Hz)	12499.62	Temperature (degree C)	0.160



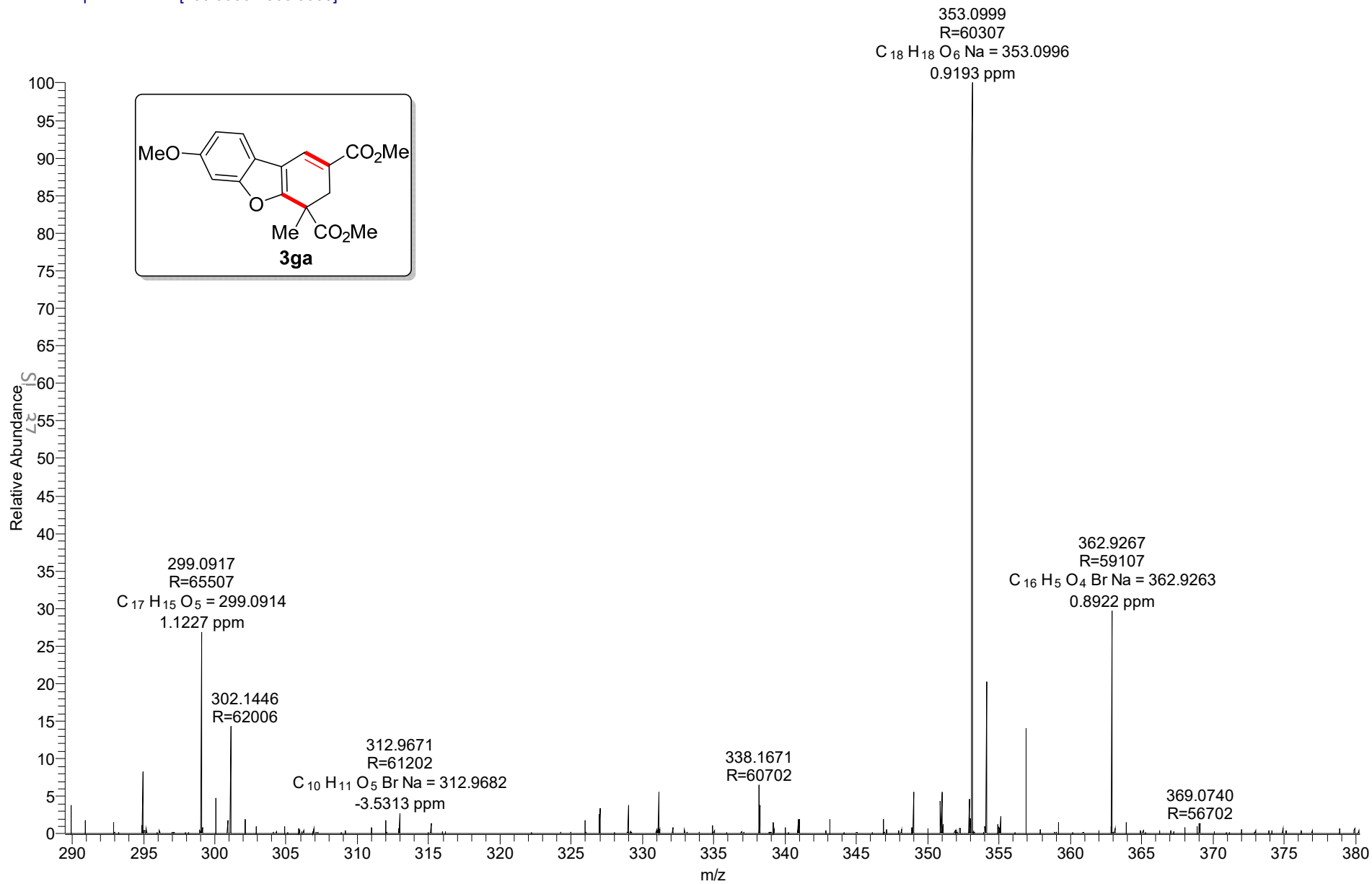
Acquisition Time (sec)	1.0434	Comment	Pawan	Date	03 Sep 2018 13:02:33		
Date Stamp	03 Sep 2018 10:49:29						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State_2018\AV-500-20180820-220232-11839_CARON-3.jdf						
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	2500	Origin	ECX 400
Original Points Count	26214	Owner	delta	Points Count	26214	Pulse Sequence	single_pulse_dec
Receiver Gain	58.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10043.1650	Spectrum Type	STANDARD
Sweep Width (Hz)	25124.29	Temperature (degree C)	21.500				



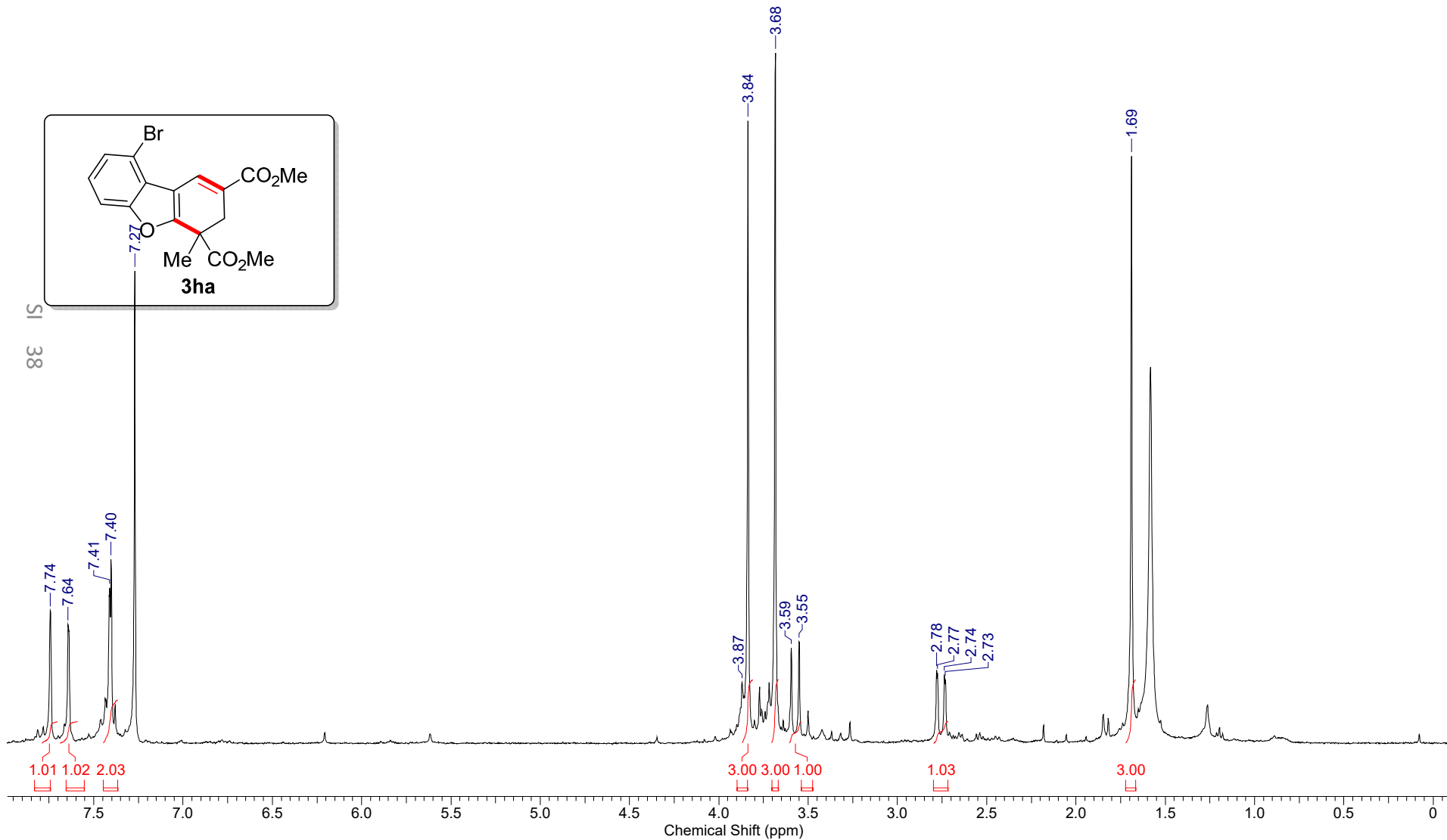
Acquisition Time (sec)	1.0434	Comment	Pawan	Date	03 Sep 2018 13:02:33		
Date Stamp	03 Sep 2018 11:20:55						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State 2018\AV-500-20180820-220232-11839_DEPT135-3.jdf						
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	800	Origin	ECX 400
Original Points Count	26214	Owner	delta	Points Count	26214	Pulse Sequence	dept.ex2 (selection_angle=135)
Receiver Gain	58.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10042.6621	Spectrum Type	DEPT135
Sweep Width (Hz)	25124.29	Temperature (degree C)	21.200				



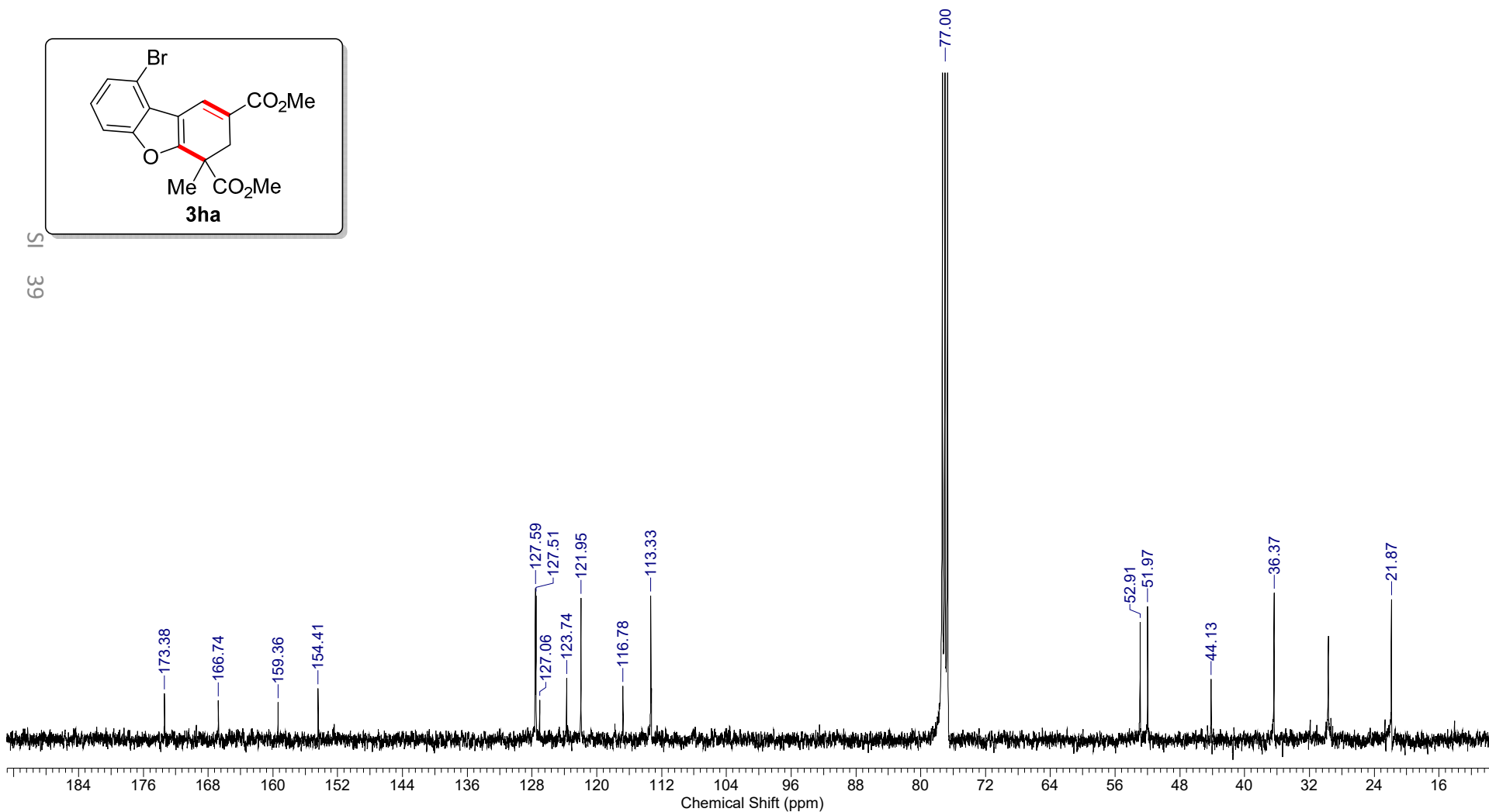
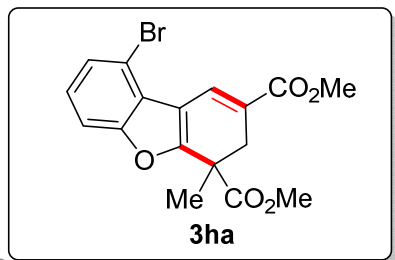
KS-J-36A #506 RT: 2.25 AV: 1 NL: 9.36E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]



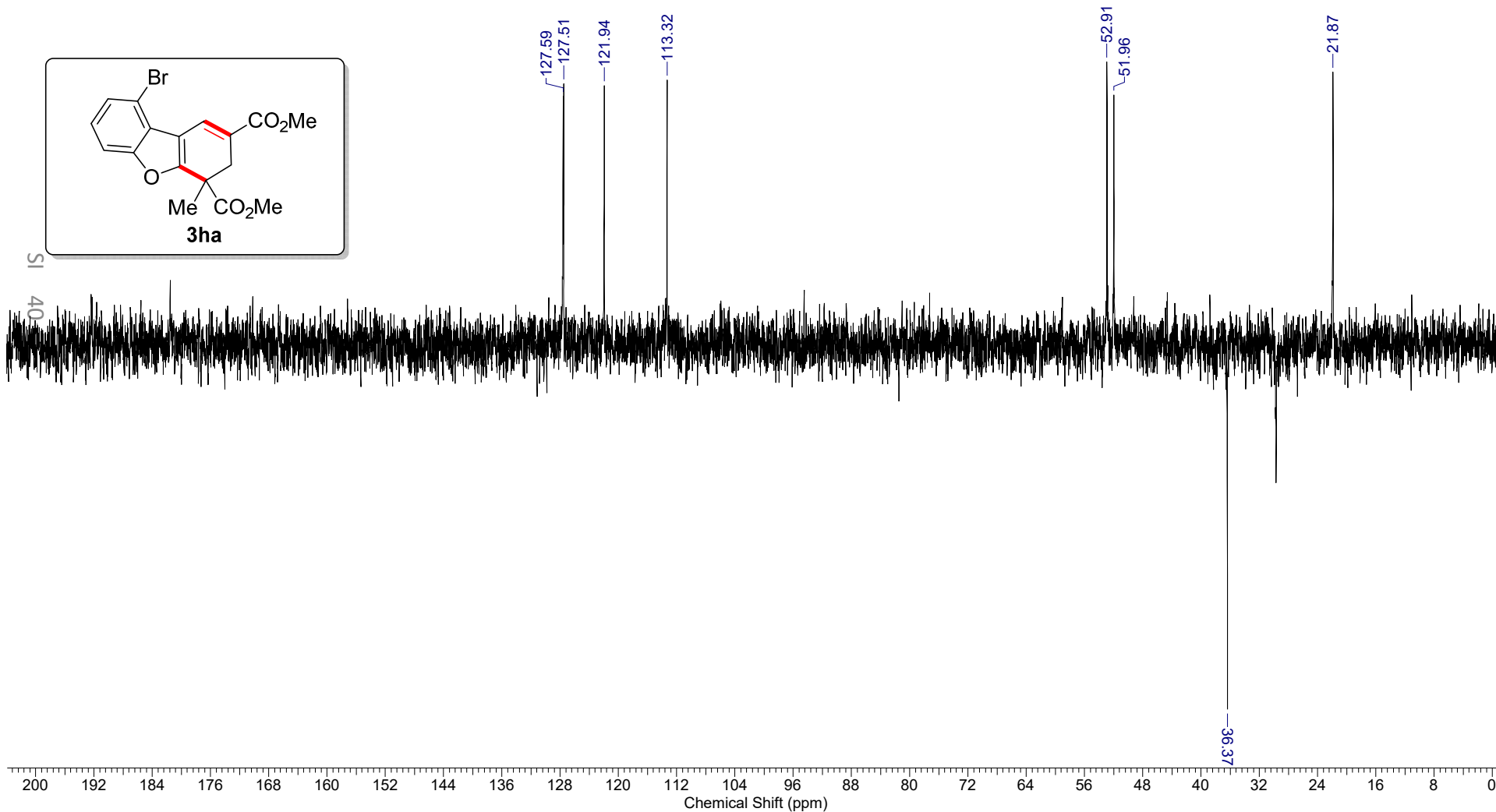
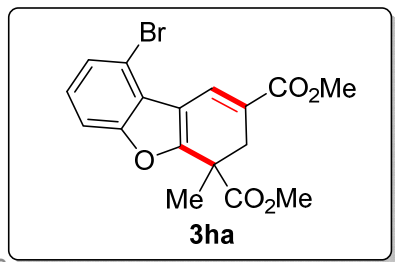
Acquisition Time (sec)	1.6384	Comment	Shaziya 1H	Date	07 Mar 2019 20:33:12		Date Stamp	07 Mar 2019 20:33:12
File Name	F:\AV-400-20190225-125207-11843\1\1r	Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	29	
Origin	spect	Original Points Count	16384	Owner	root	Points Count	16384	Pulse Sequence
Receiver Gain	406.00	SW(cyclical) (Hz)	10000.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2795.7249	zg30
Spectrum Type	STANDARD	Sweep Width (Hz)	9999.39	Temperature (degree C)	22.900			



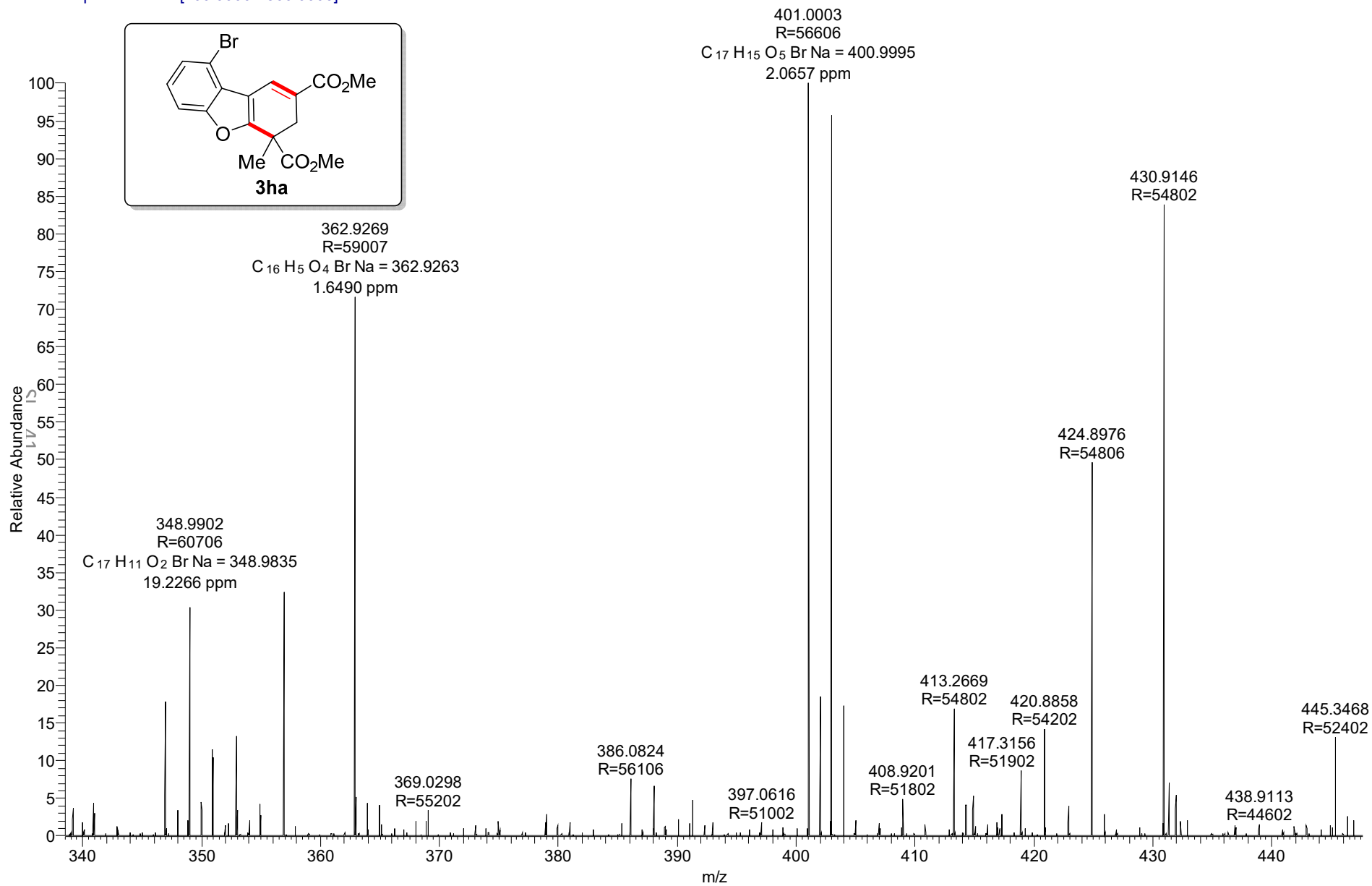
Acquisition Time (sec)	0.6488	Comment	13C	Date	09 Aug 2018 17:44:40
Date Stamp	09 Aug 2018 17:44:40				
File Name	\\172.16.2.4\nmr_data\AV400\Aug_18_400\data\ep\nmr\AV-400-20180803-163326-11843\3\PDATA\1\1r	Frequency (MHz)	100.61		
Nucleus	13C	Number of Transients	2476	Origin	spect
Owner	root	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d	Receiver Gain	2050.00
Spectrum Type	STANDARD	Sweep Width (Hz)	25251.75	Temperature (degree C)	27.000
				Spectrum Offset (Hz)	10060.2773



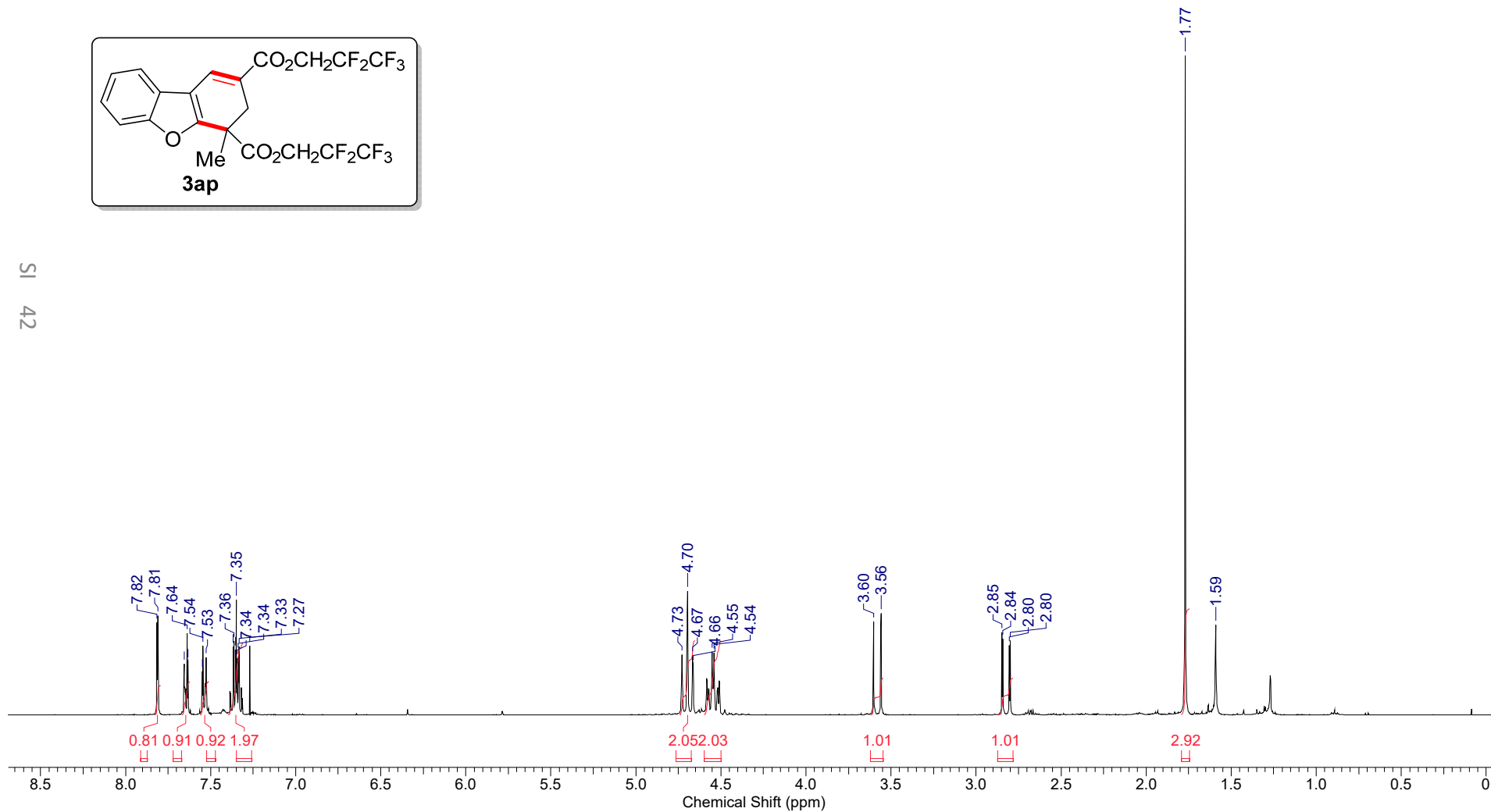
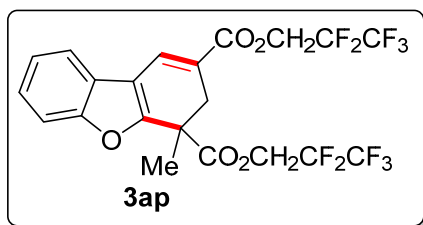
Acquisition Time (sec)	0.6488	Comment	DEPT	Date	09 Aug 2018 17:31:52		
Date Stamp	09 Aug 2018 17:31:52						
File Name	\\172.16.2.4\nmr_data\AV400\Aug_18_400\data\ep\nmr\AV-400-20180803-163326-11843\2\PDATA\1\1r				Frequency (MHz)	100.61	
Nucleus	13C	Number of Transients	800	Origin	spect	Original Points Count	16384
Owner	root	Points Count	32768	Pulse Sequence	dept135	Receiver Gain	16384.00
SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	10059.8340
Spectrum Type	DEPT135	Sweep Width (Hz)	25251.75	Temperature (degree C)	27.000		



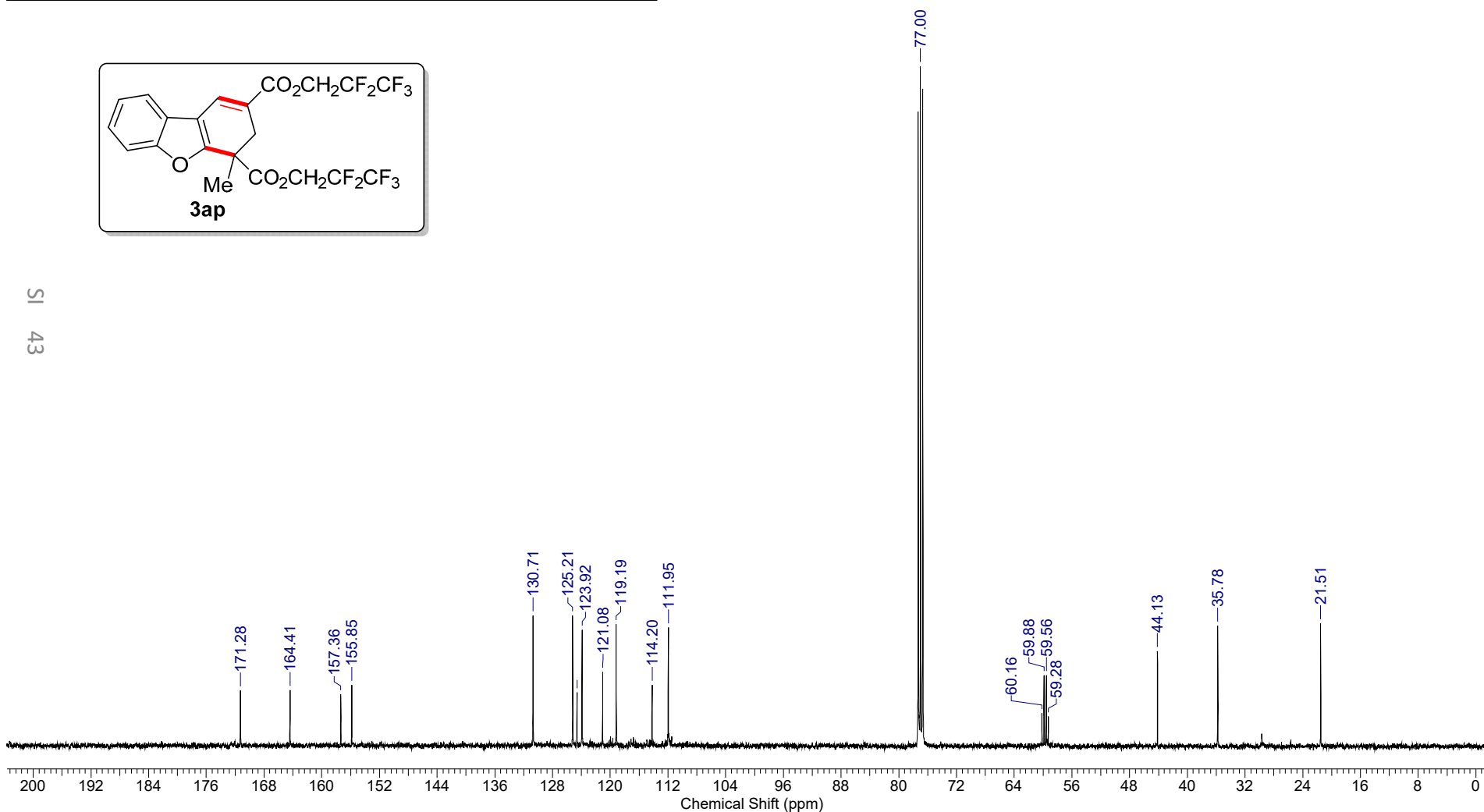
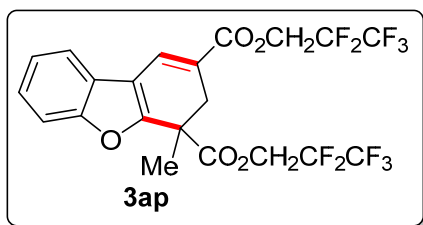
KS-J-27A #530 RT: 2.36 AV: 1 NL: 4.18E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]



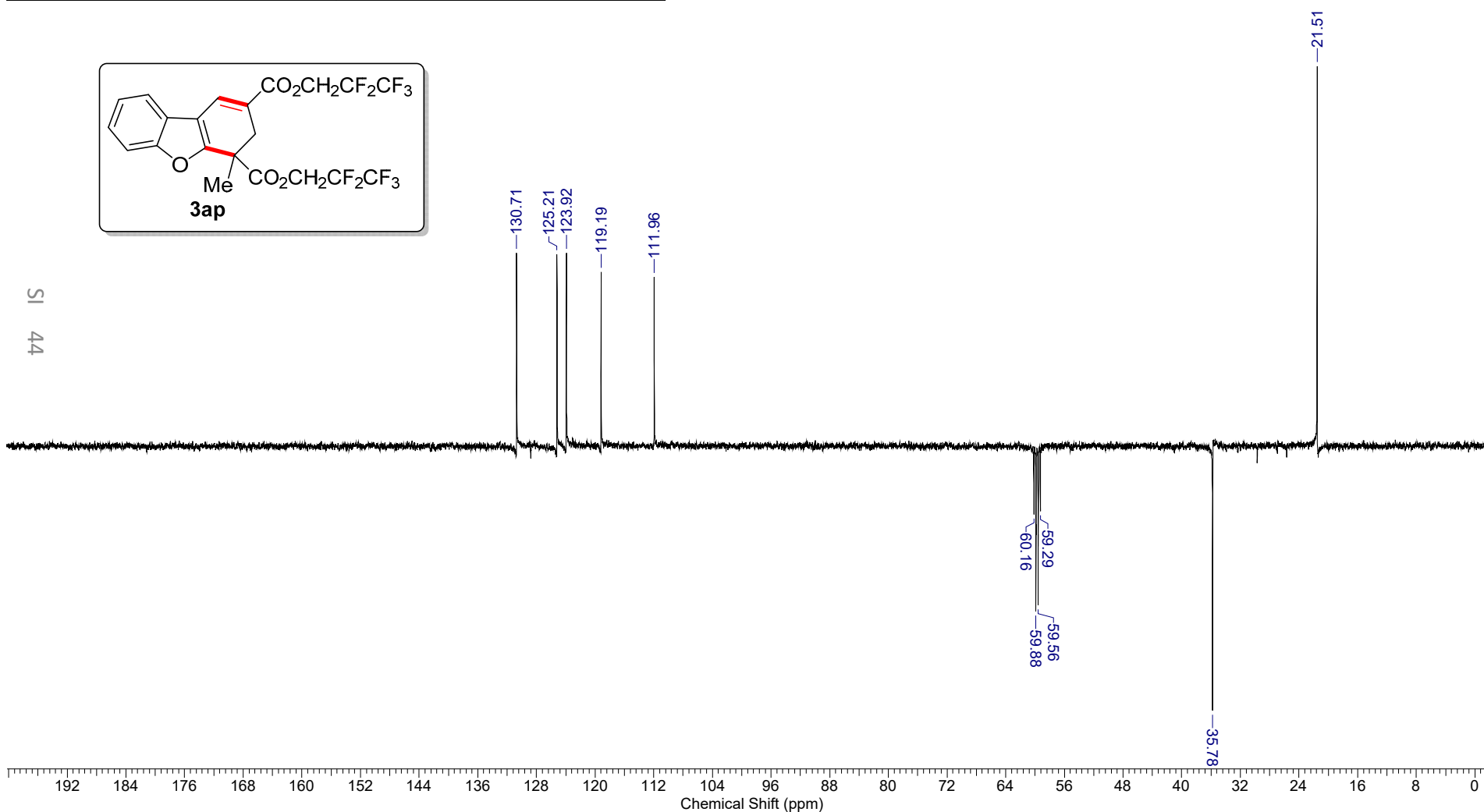
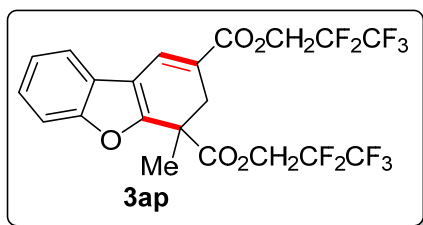
Acquisition Time (sec)	1.3108	Comment	Srinivas	Date	02 Sep 2018 07:26:04		
Date Stamp	02 Sep 2018 05:44:25						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State_2018\AV-400-20180822-113926-11279_PROTON-3.jdf						
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	32	Origin	ECX 400
Original Points Count	13107	Owner	delta	Points Count	13107	Pulse Sequence	single_pulse.ex2
Receiver Gain	38.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2806.4714	Spectrum Type	STANDARD
Sweep Width (Hz)	9999.08	Temperature (degree C)	23.400				



Acquisition Time (sec)	1.0434	Comment	Srinivas	Date	02 Sep 2018 08:44:11		
Date Stamp	02 Sep 2018 06:31:10						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State_2018\AV-400-20180822-113926-11279_CARBON-3.jdf						
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	1200	Origin	ECX 400
Original Points Count	26214	Owner	delta	Points Count	26214	Pulse Sequence	single_pulse_dec
Receiver Gain	58.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10044.1240	Spectrum Type	STANDARD
Sweep Width (Hz)	25124.29	Temperature (degree C)	23.700				

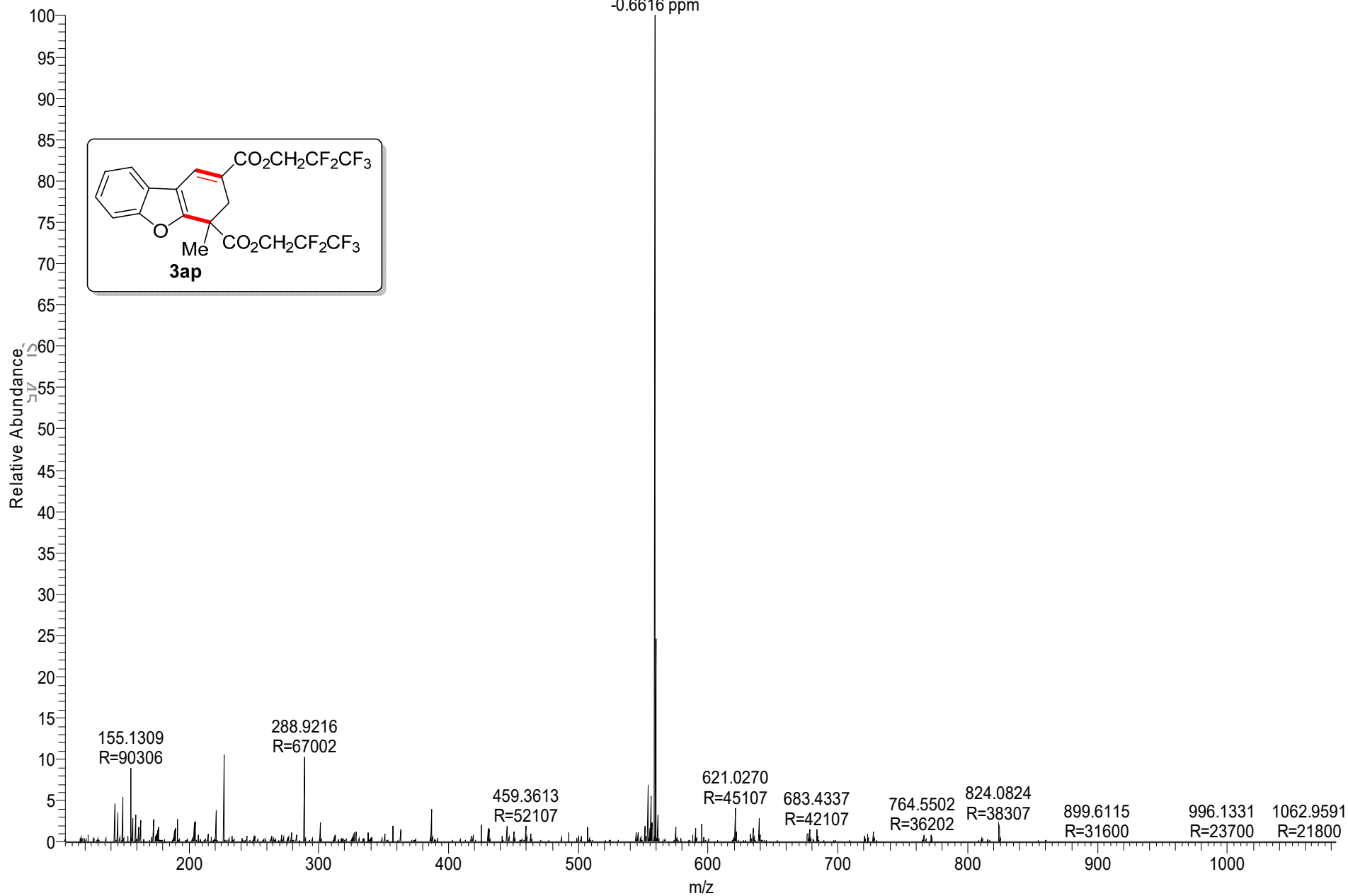


Acquisition Time (sec)	1.0434	Comment	Srinivas	Date	02 Sep 2018 08:44:11		
Date Stamp	02 Sep 2018 07:02:33						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State 2018\AV-400-20180822-113926-11279_DEPT135-3.jdf						
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	800	Origin	ECX 400
Original Points Count	26214	Owner	delta	Points Count	26214	Pulse Sequence	dept.ex2 (selection_angle=135)
Receiver Gain	54.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10044.2500	Spectrum Type	DEPT135
Sweep Width (Hz)	25124.29	Temperature (degree C)	23.500				

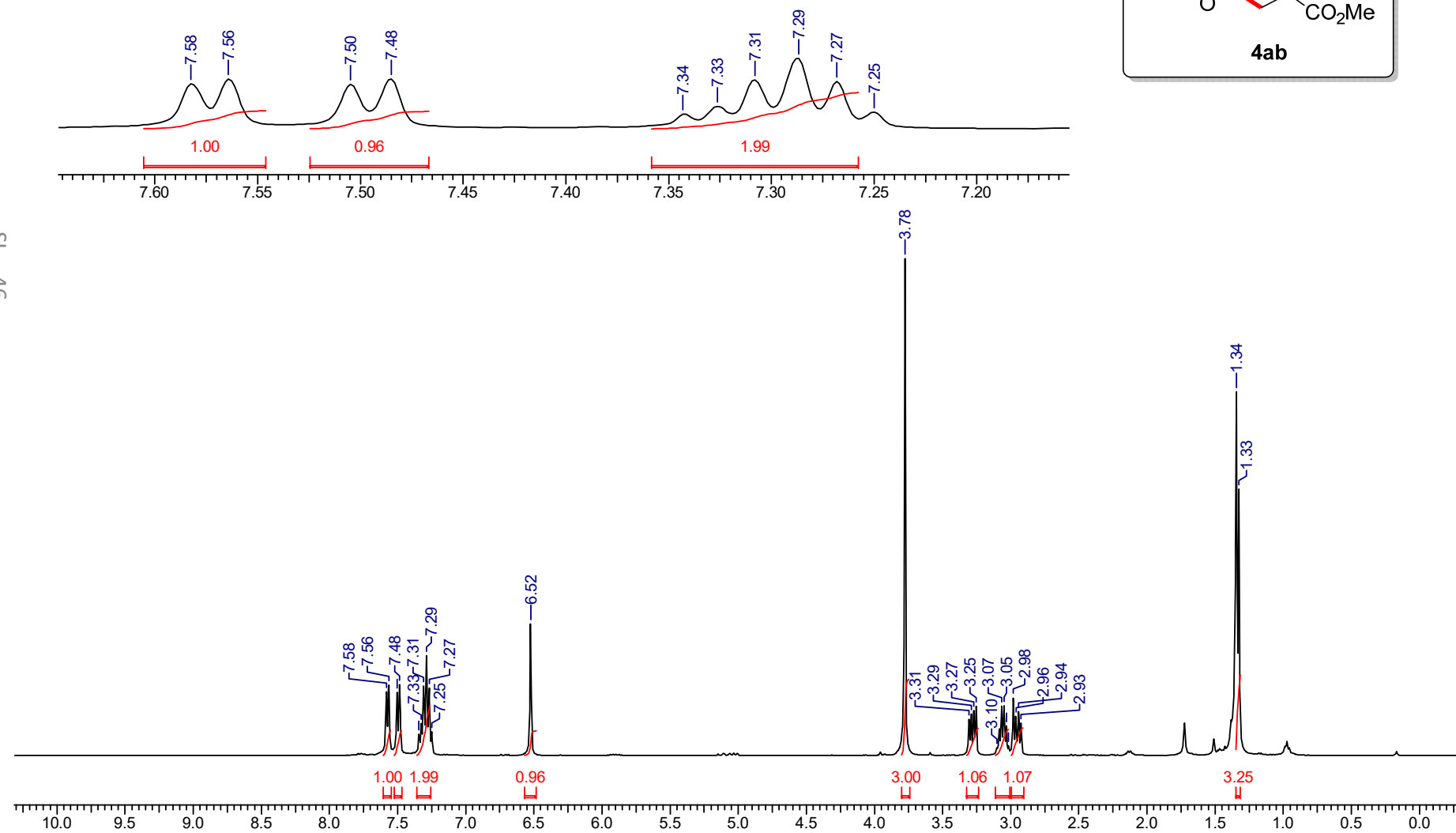
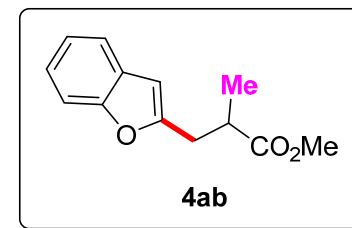


KS-J-40A_180914162729 #683 RT: 3.04 AV: 1 NL: 3.47E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

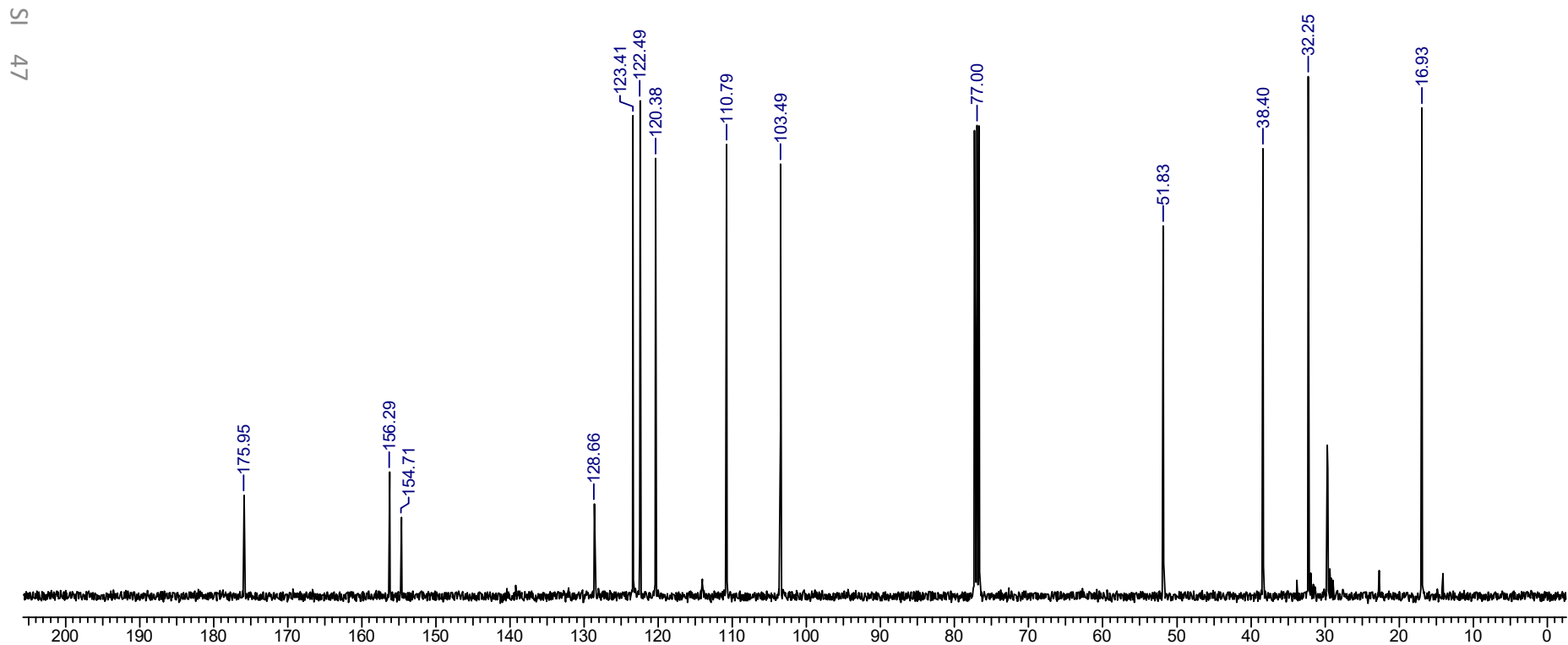
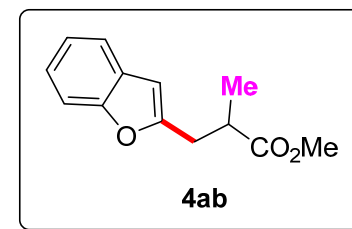
559.0570
R=48107
 $C_{21}H_{14}O_5F_{10}Na = 559.0574$
-0.6616 ppm



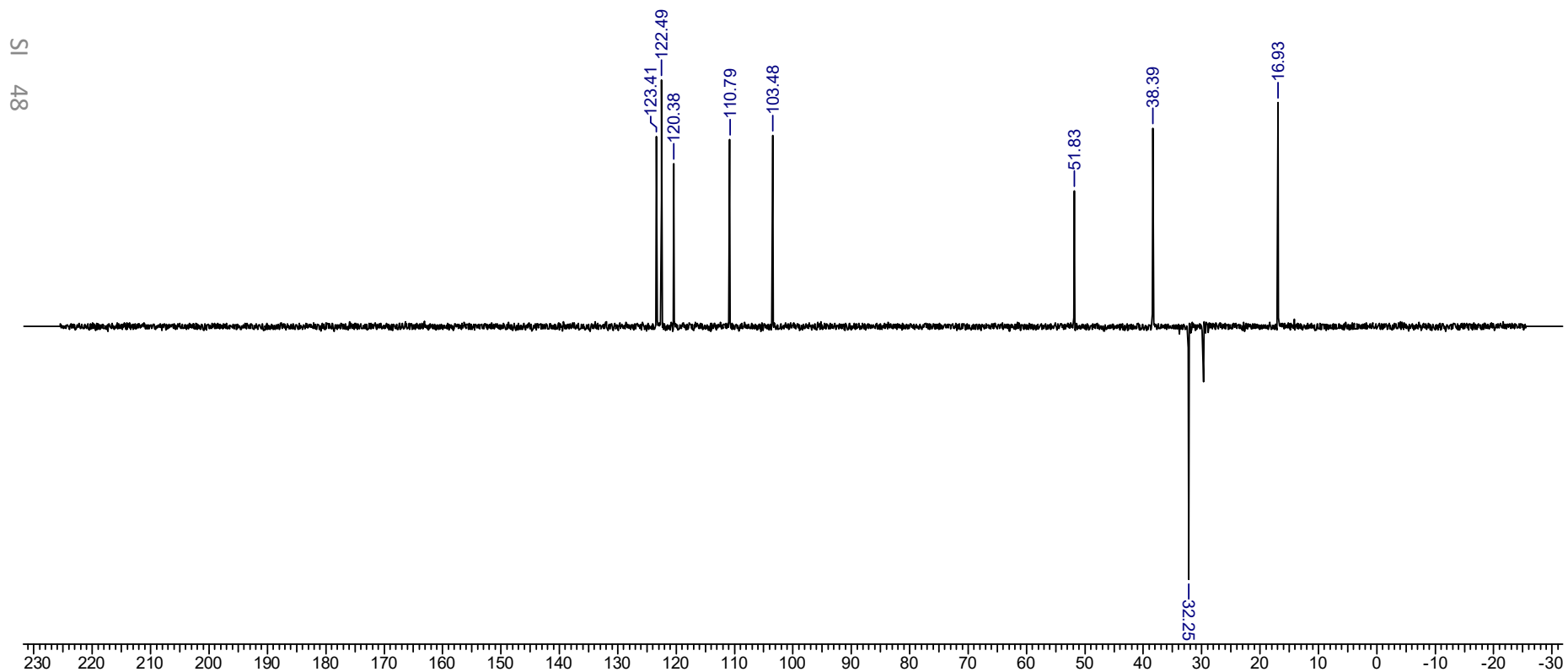
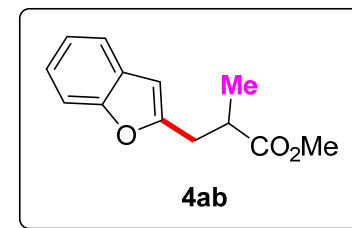
Comment	Mahesh 1H				
Date	02 Jan 2017 18:18:48	Frequency (MHz)	400.13	Nucleus	1H
Number of Transients	64	Original Points Count	16384	Points Count	16384
Solvent	CHLOROFORM-d	Sweep Width (Hz)	9999.39	Temperature (grad C)	20.300



Comment	13C			
Date	02 Jan 2017 19:18:32	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	1239	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 20.900

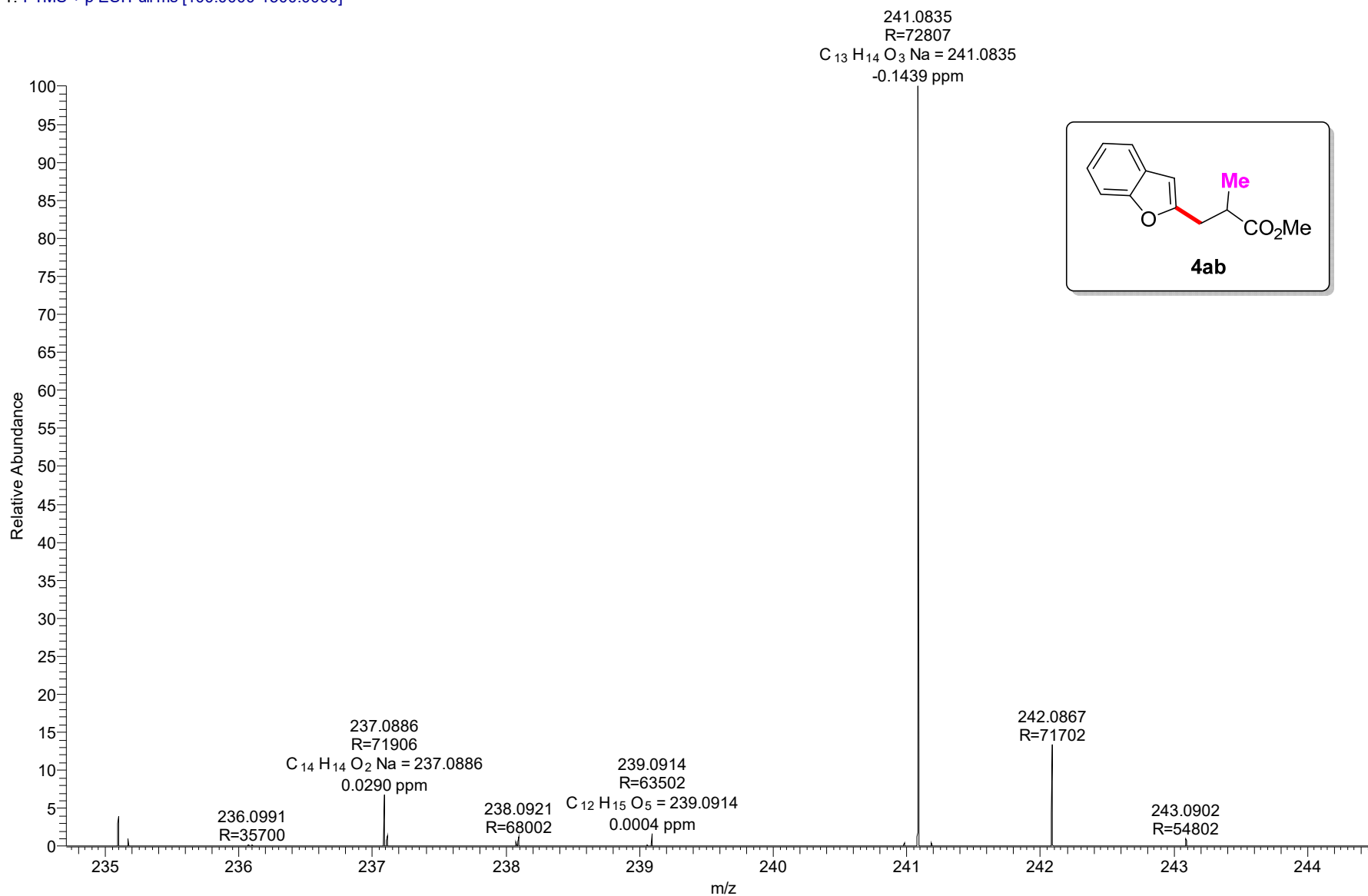


Comment	DEPT				
Date	02 Jan 2017 18:42:16	Frequency (MHz)	100.61	Nucleus	¹³ C
Number of Transients	800	Original Points Count	16384	Points Count	32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C)	20.400

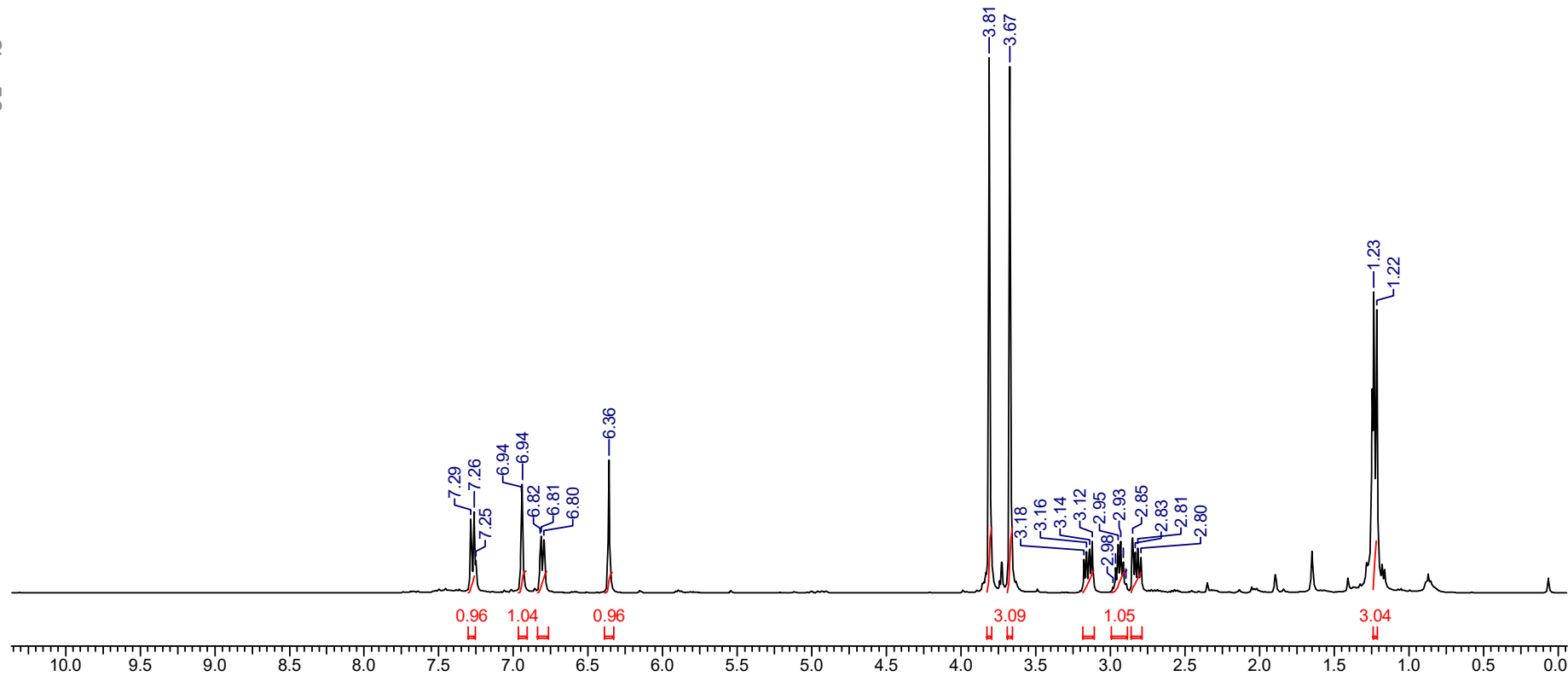
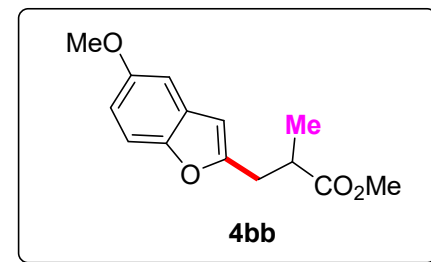
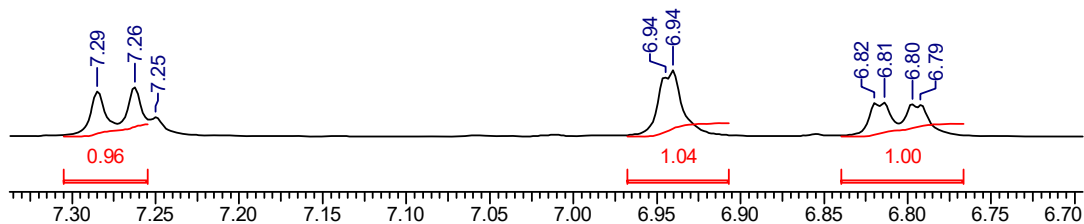


JY-B-3A #129 RT: 0.58 AV: 1 NL: 5.40E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

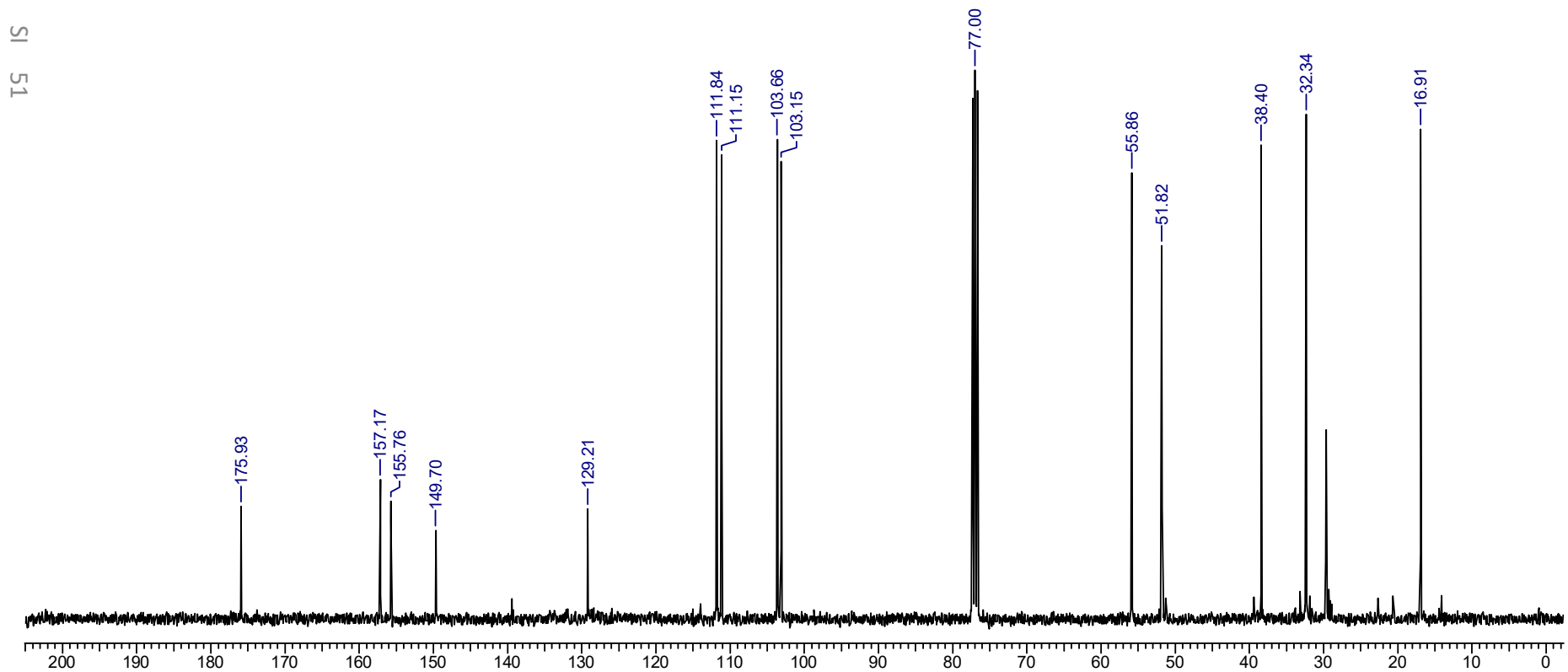
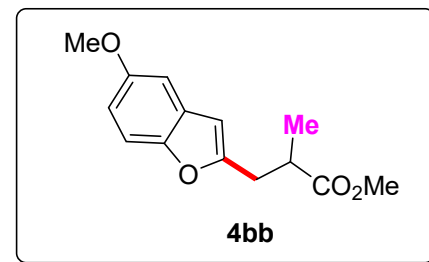
SI 49



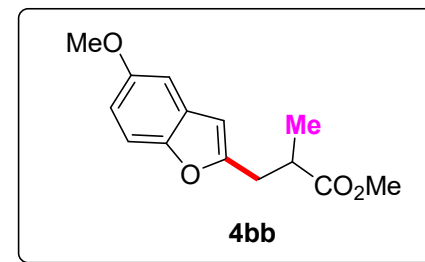
Comment	Srinivas 1H				
Date	15 Jan 2017 11:14:16	Frequency (MHz)	400.13	Nucleus	1H
Number of Transients	64	Original Points Count	16384	Points Count	16384
Solvent	CHLOROFORM-d	Sweep Width (Hz)	9999.39	Temperature (grad C)	21.400



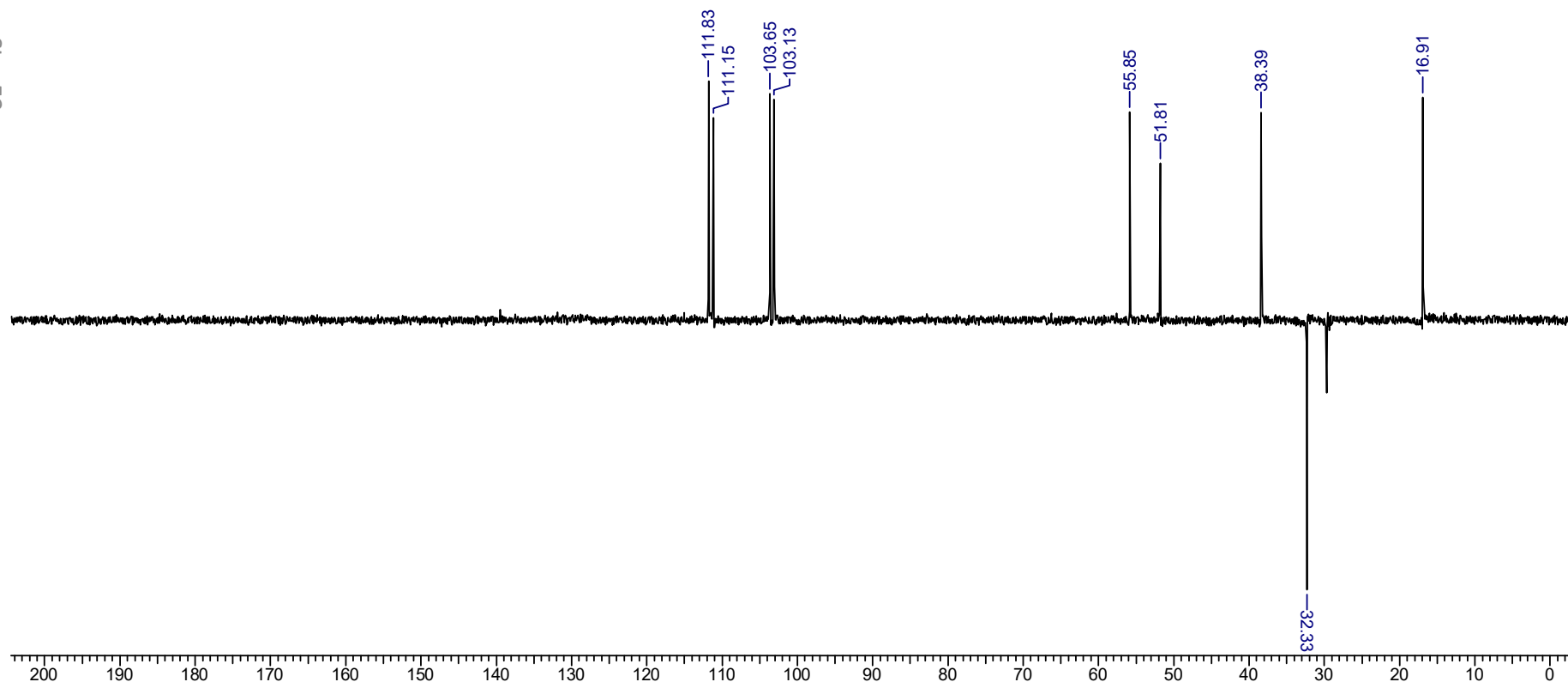
Comment	13C			
Date	15 Jan 2017 12:09:44	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	1104	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 22.100



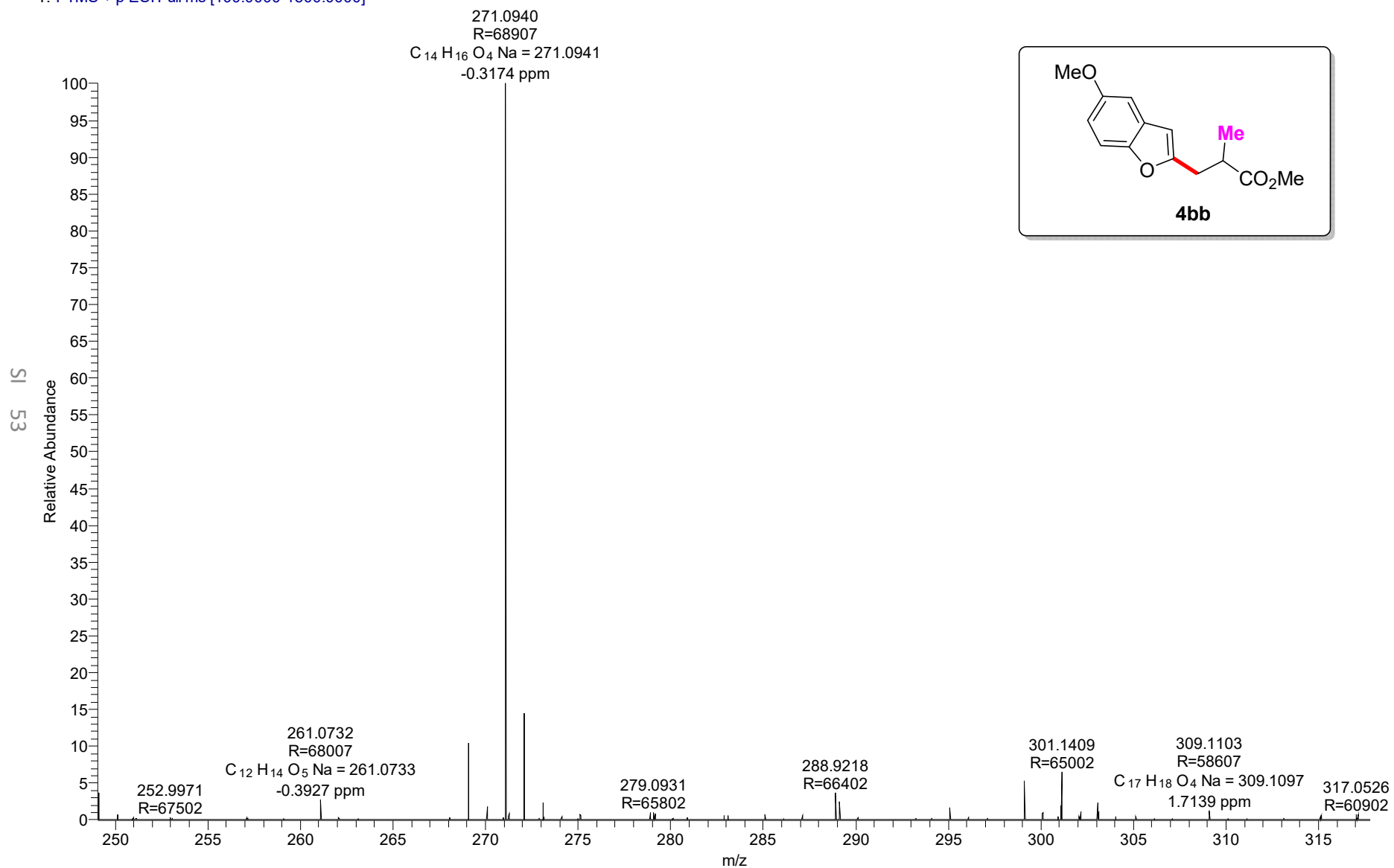
Comment	DEPT			
Date	15 Jan 2017 11:37:44	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	800	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 21.600



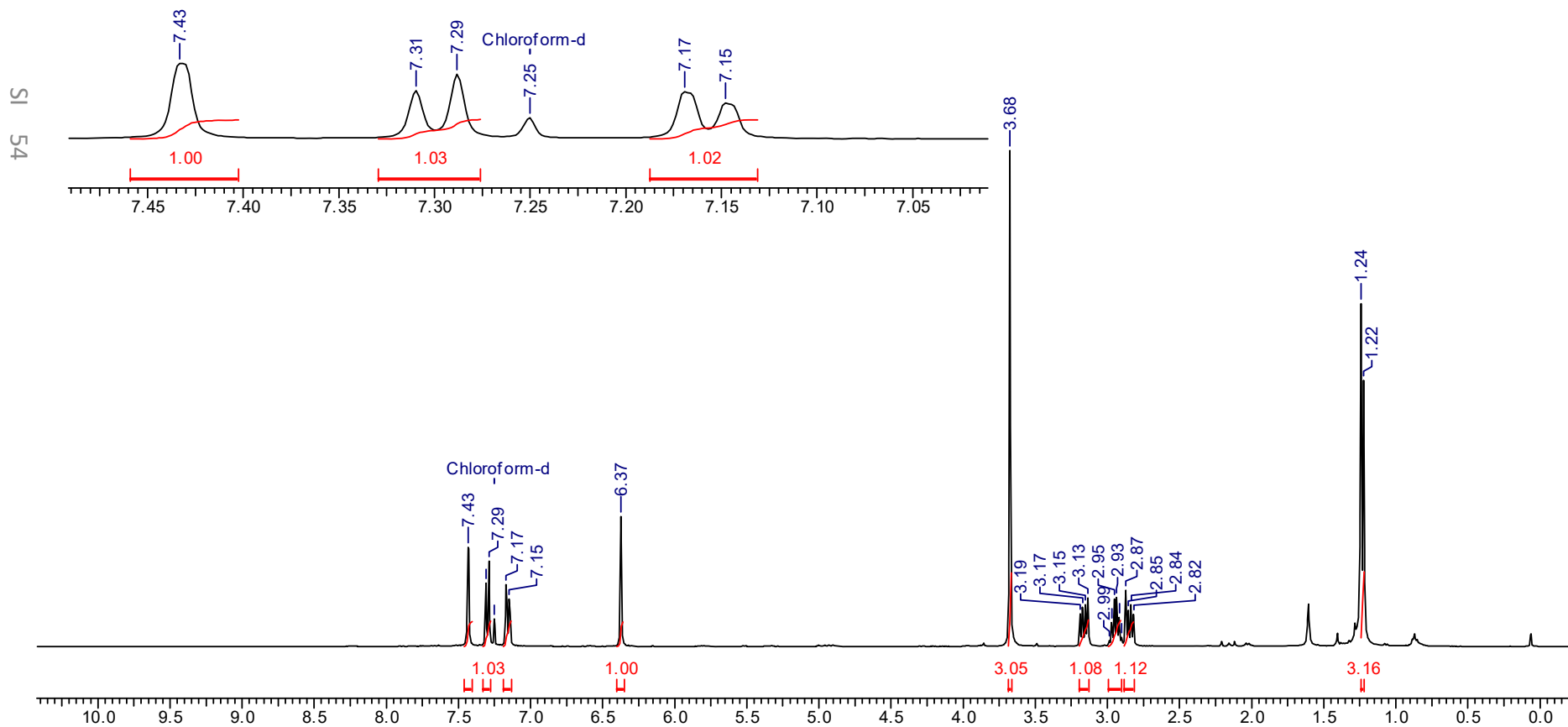
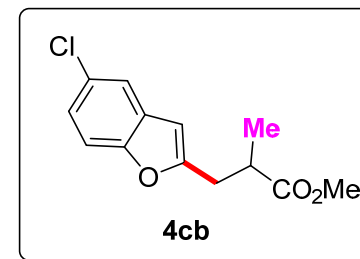
SI 52



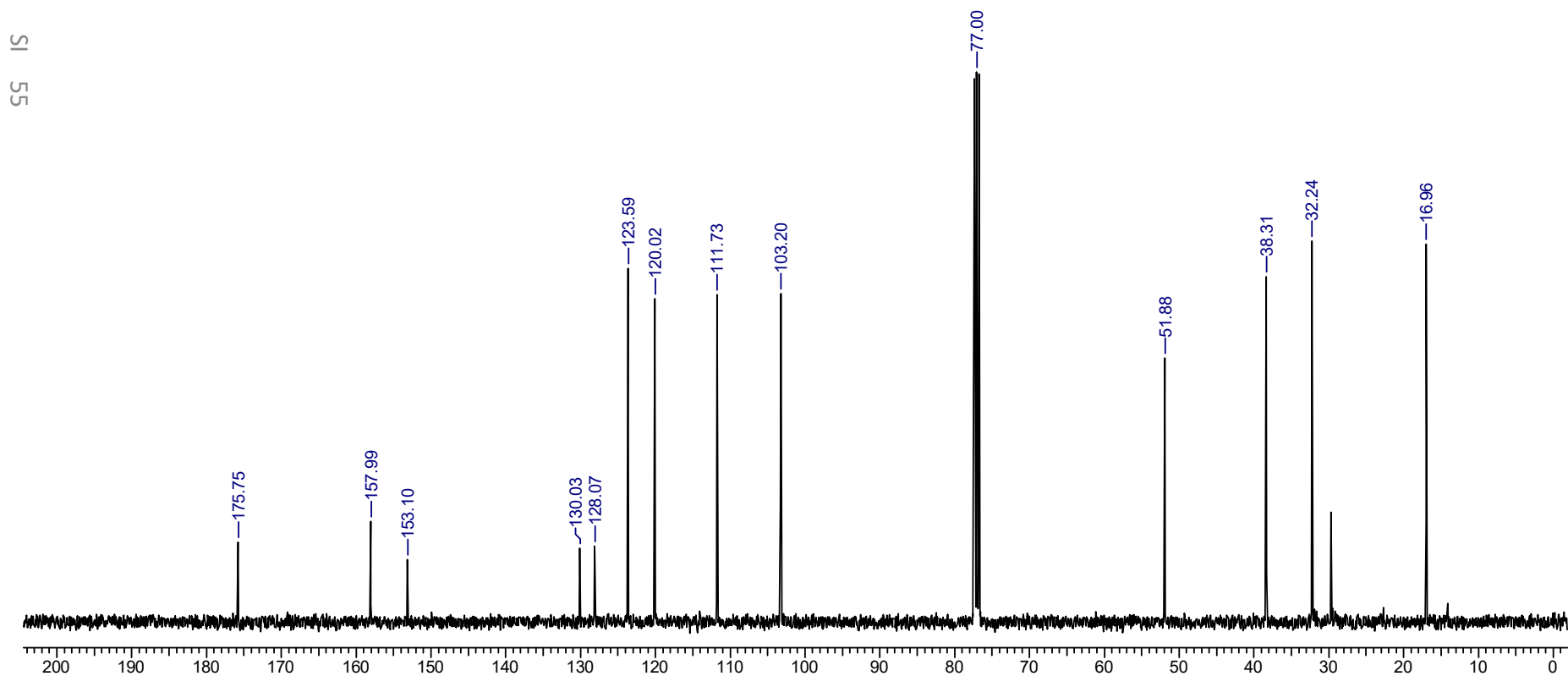
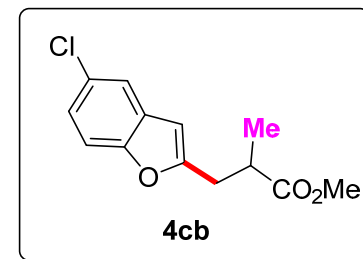
JY-B-1A #130 RT: 0.58 AV: 1 NL: 6.60E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



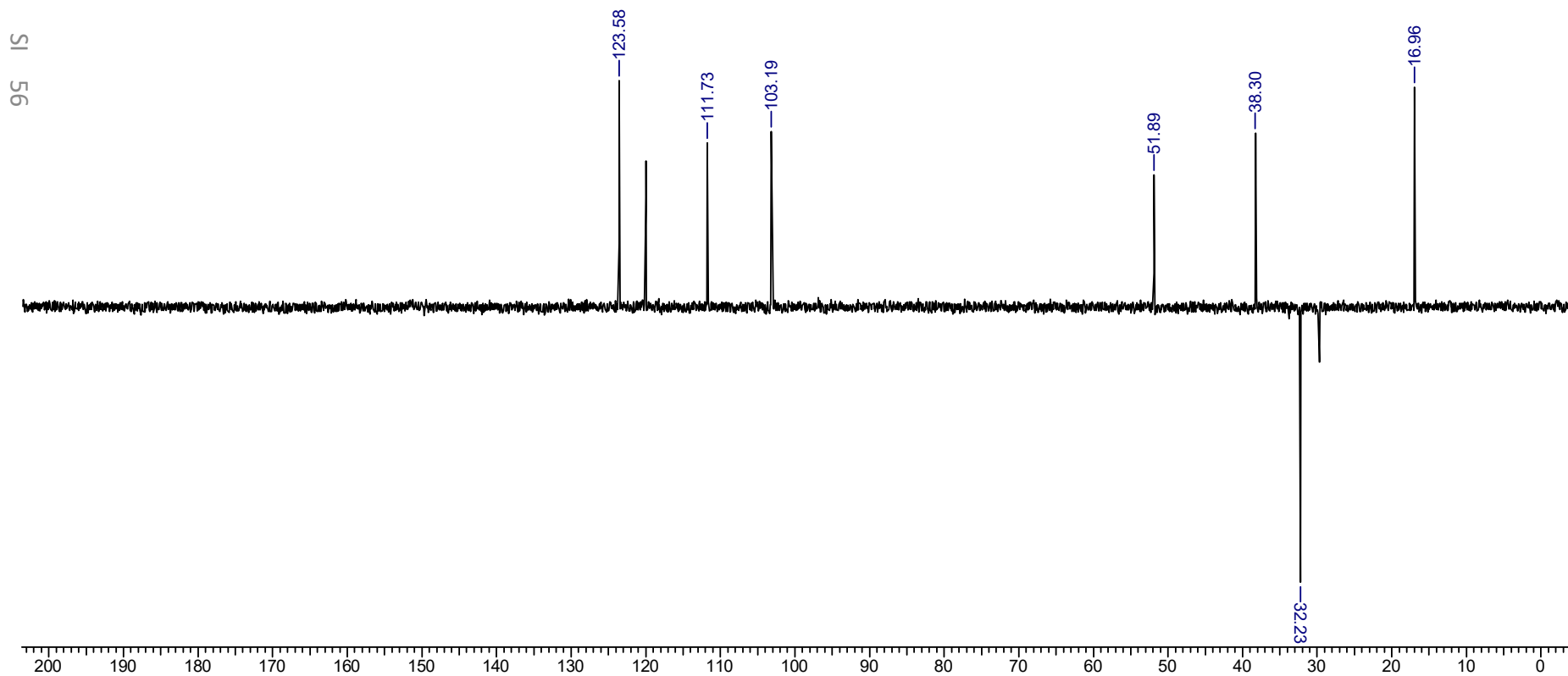
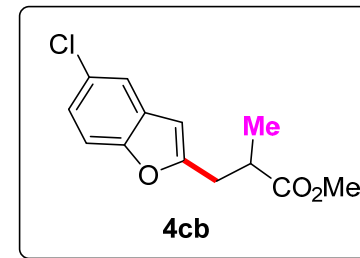
Comment srinivas 1H					
Date 16 Jan 2017 11:35:36		Frequency (MHz) 400.13		Nucleus 1H	
Number of Transients 64		Original Points Count 16384		Points Count 16384	
Solvent CHLOROFORM-d		Sweep Width (Hz) 9999.39		Temperature (grad C) 21.300	



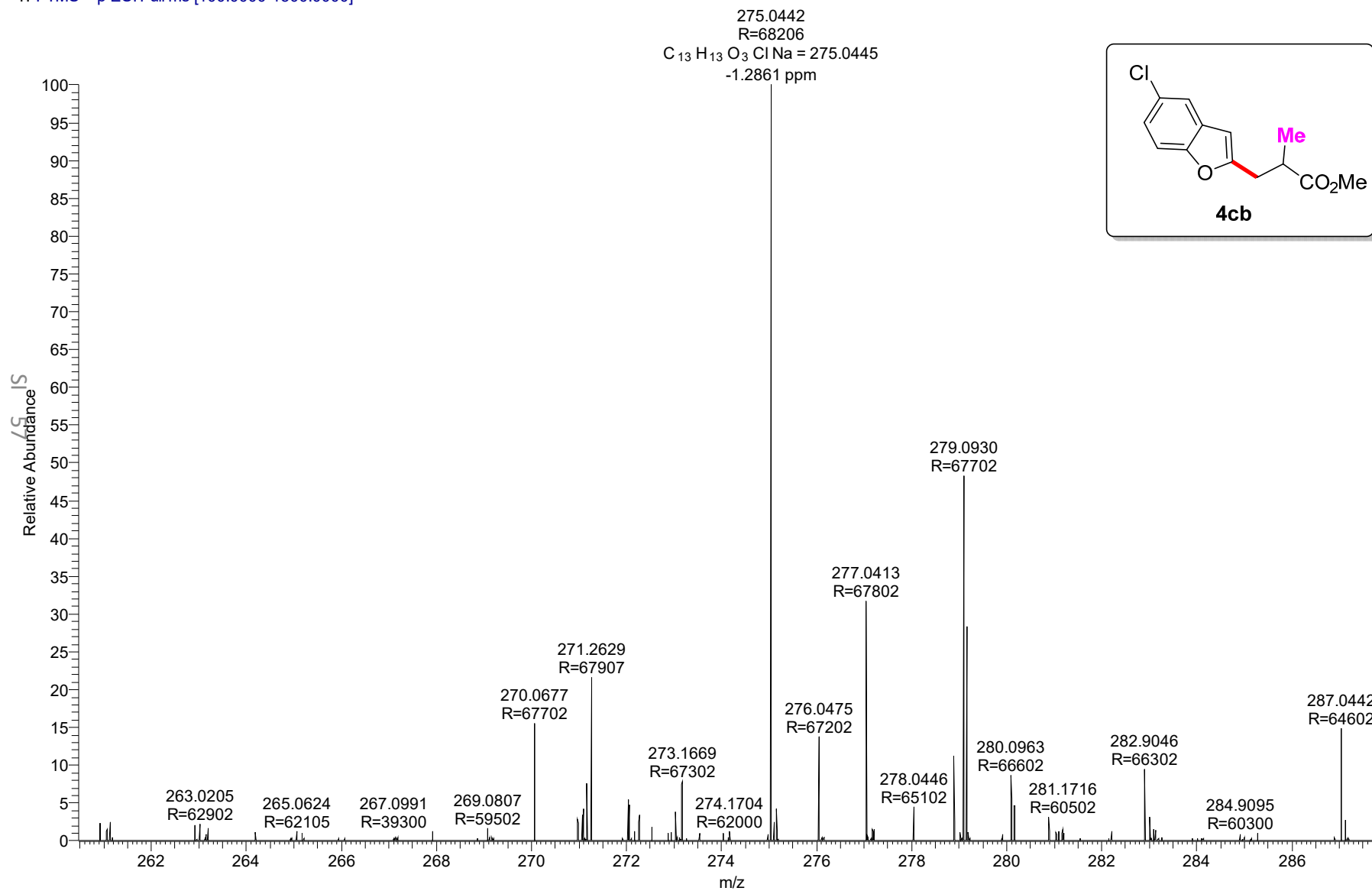
Comment	13C			
Date	16 Jan 2017 12:20:24	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	811	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 22.100



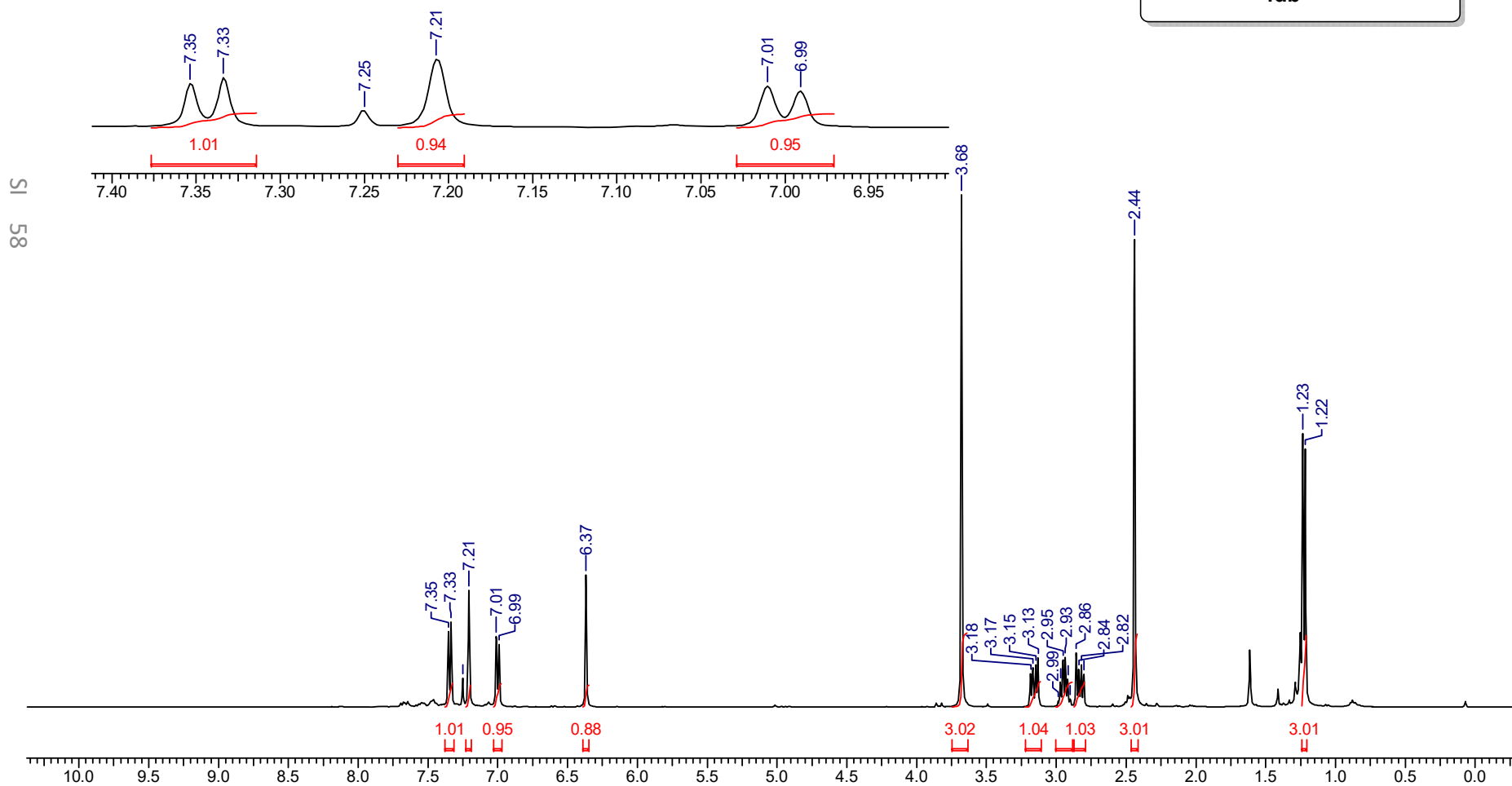
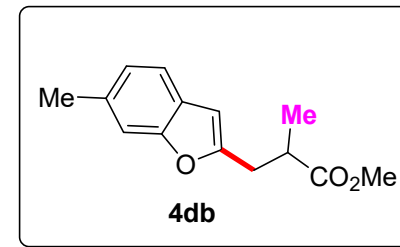
Comment	DEPT				
Date	16 Jan 2017 11:59:04	Frequency (MHz)	100.61	Nucleus	¹³ C
Number of Transients	800	Original Points Count	16384	Points Count	32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C)	21.500



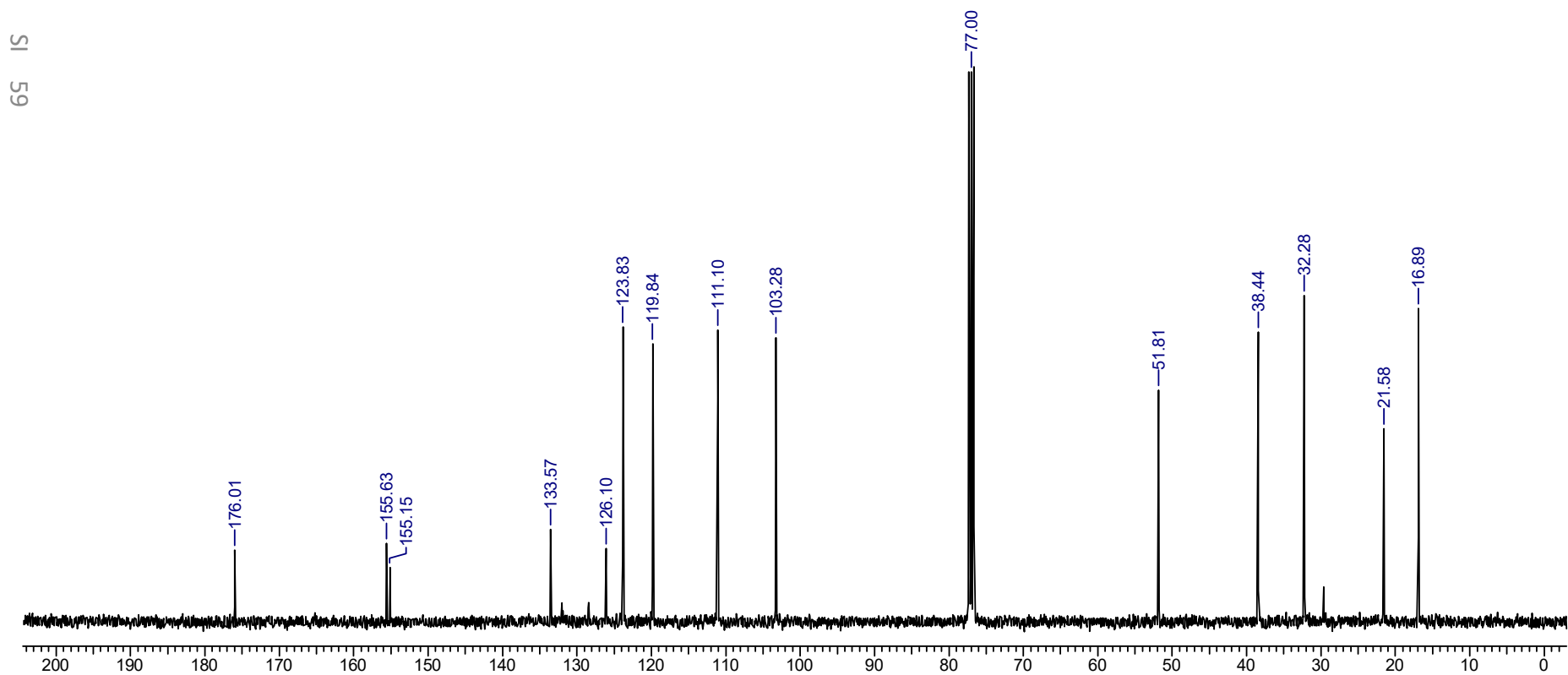
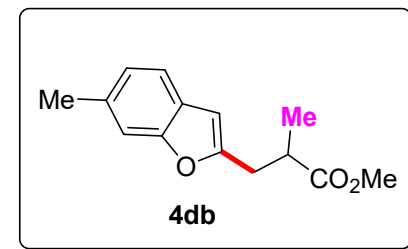
JY-B-FIRST-B_171102145156 #145 RT: 0.65 AV: 1 NL: 3.67E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]



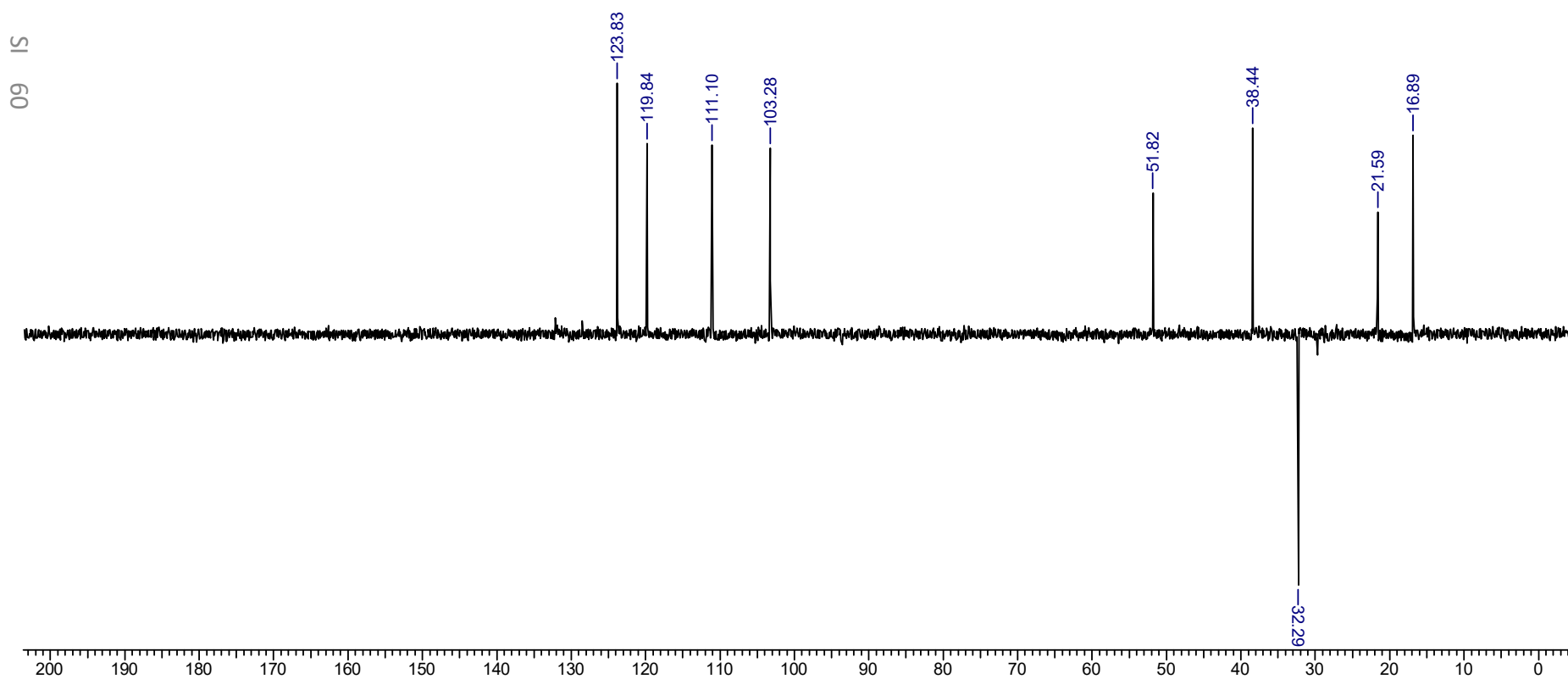
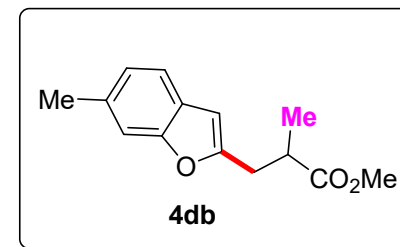
Comment	Srinivas 1H			
Date	16 Jan 2017 16:04:24	Frequency (MHz)	400.13	Nucleus 1H
Number of Transients	64	Original Points Count	16384	Points Count 16384
Solvent	CHLOROFORM-d	Sweep Width (Hz)	9999.39	Temperature (grad C) 21.200



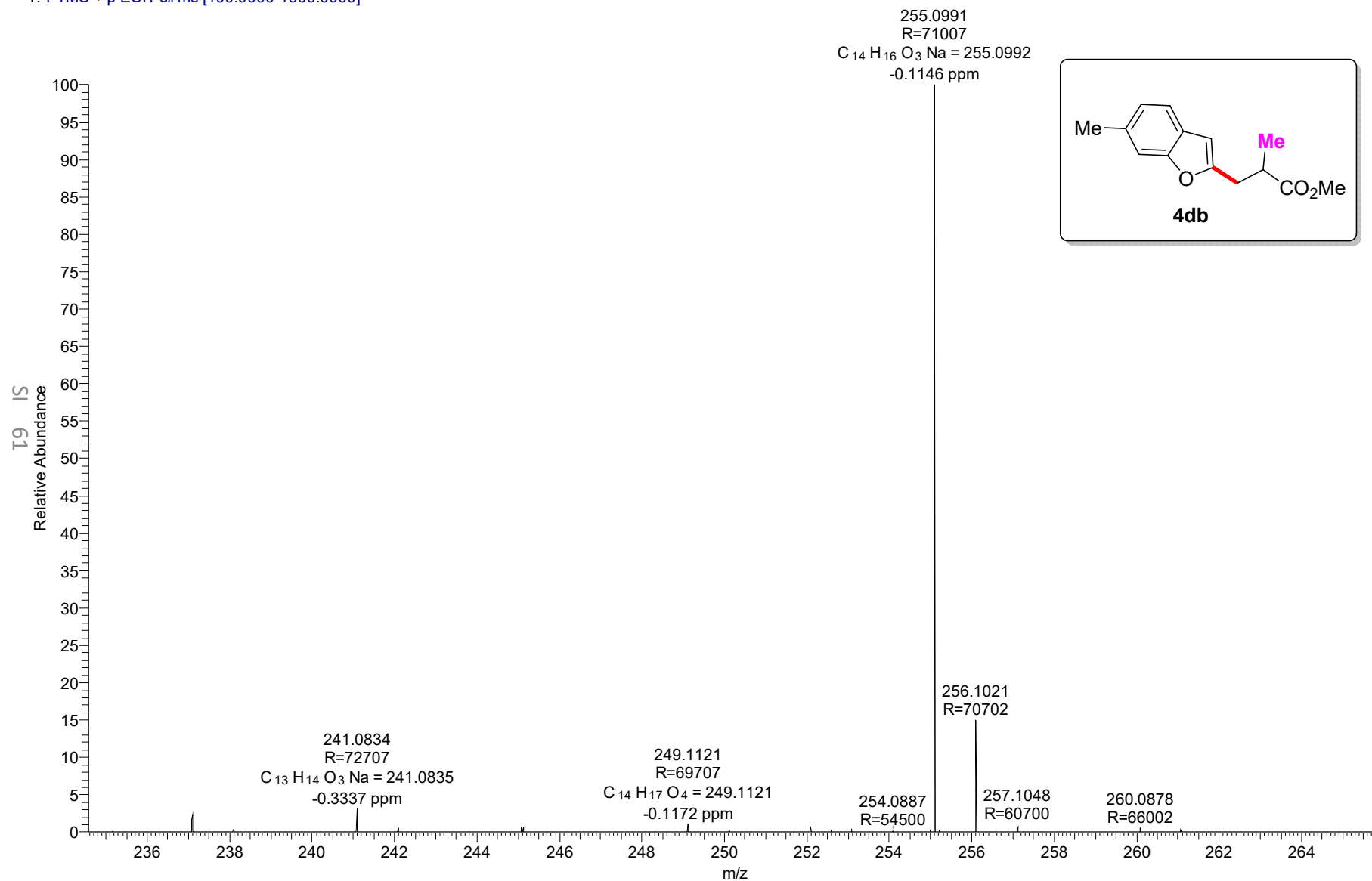
Comment	13C			
Date	16 Jan 2017 16:53:28	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	886	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 22.000



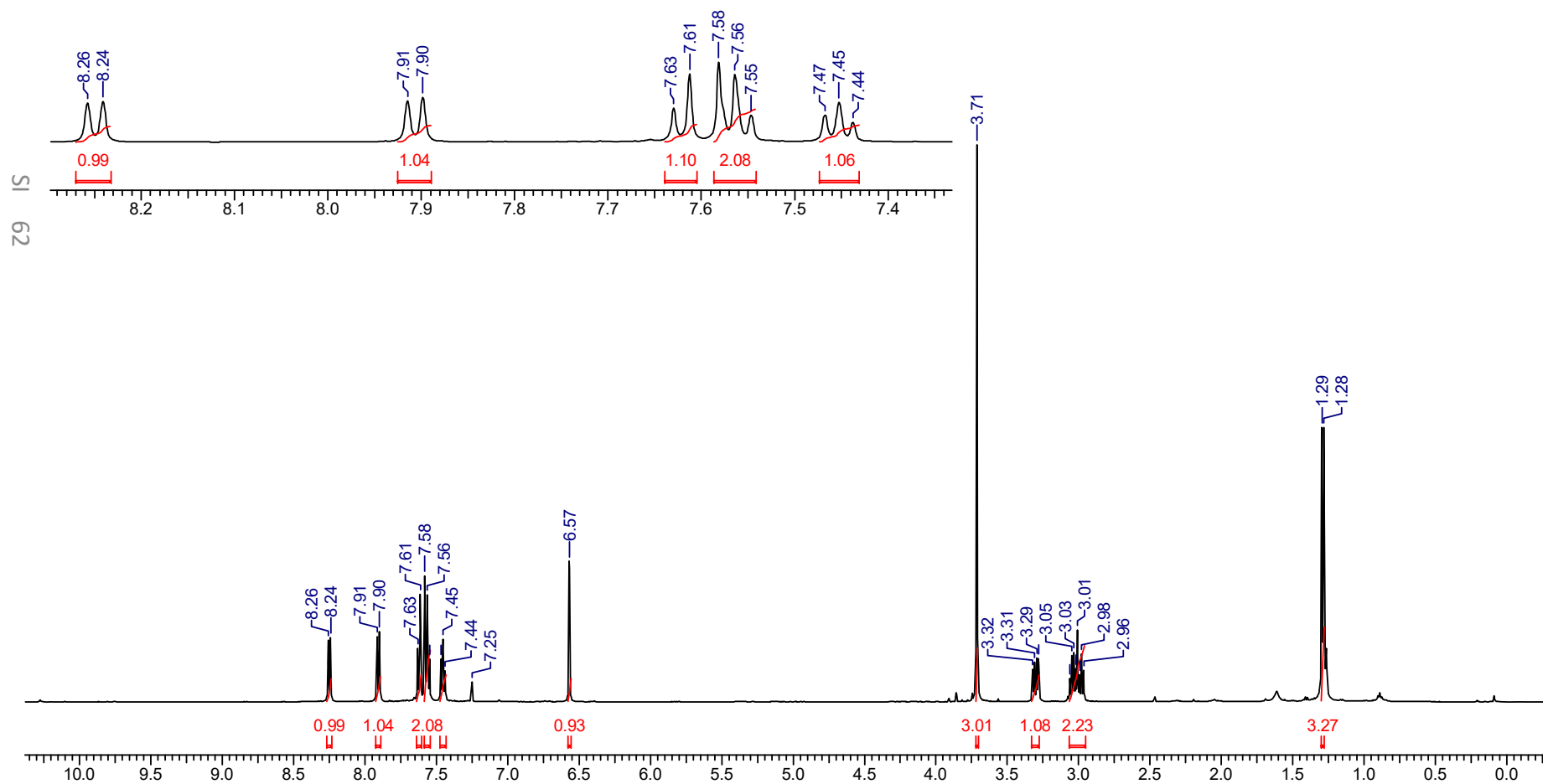
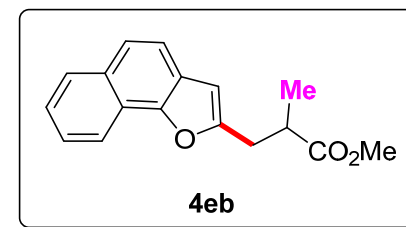
Comment	DEPT			
Date	16 Jan 2017 16:27:52	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	800	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 21.500



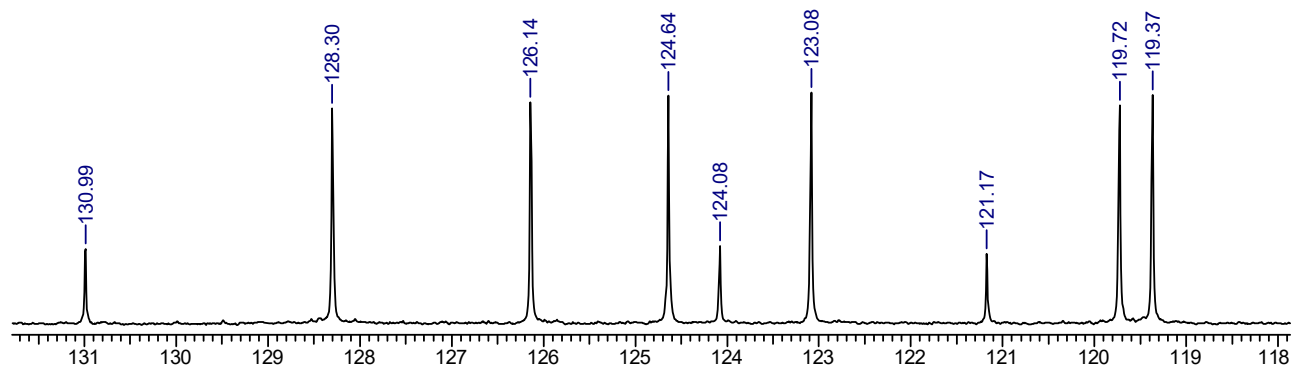
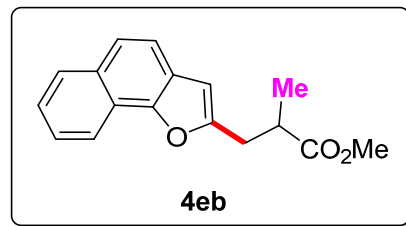
JY-B-FIRST-A #147 RT: 0.66 AV: 1 NL: 2.11E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



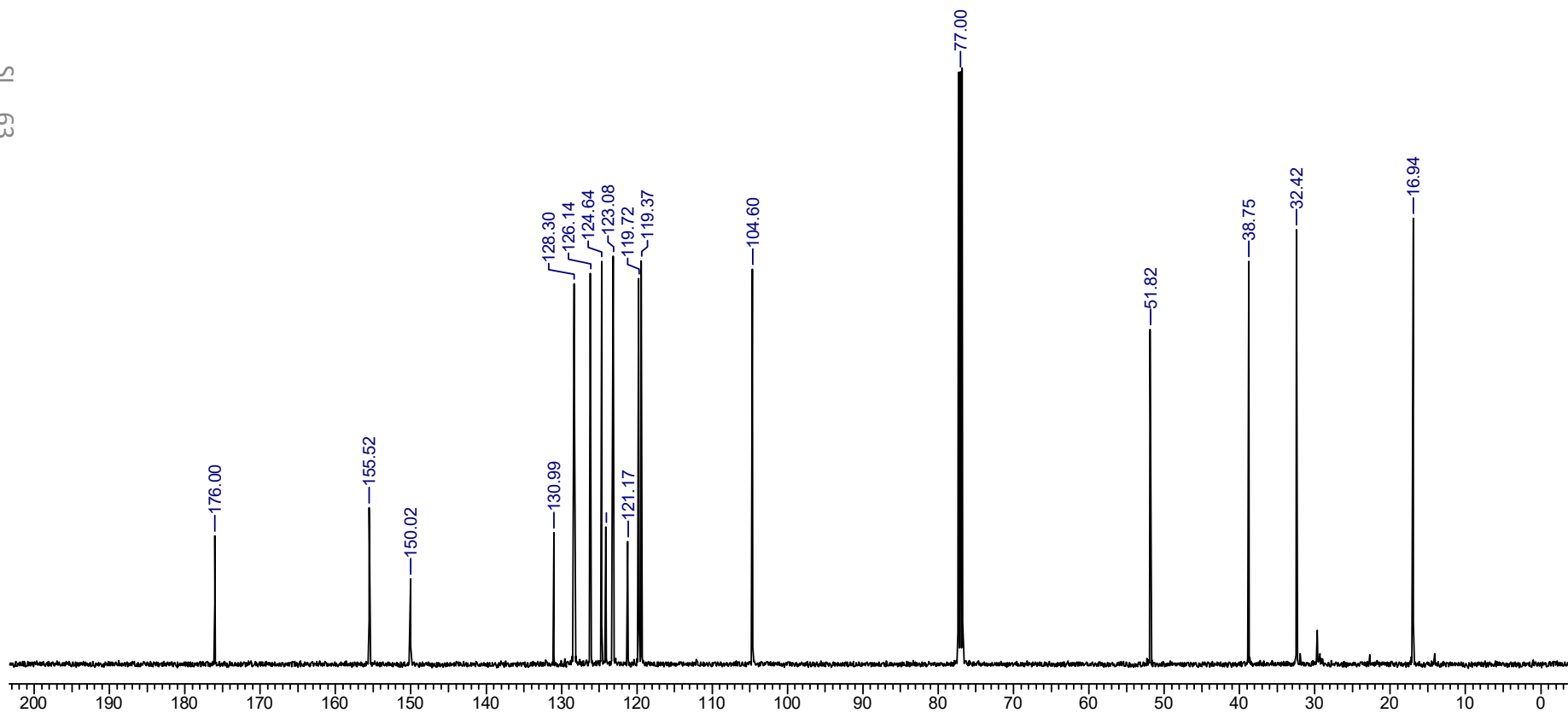
Acquisition Time (sec)	1.2800	Comment	Jyothi 1H	Date	17 Jan 2017 09:51:12
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	64
Solvent	CHLOROFORM-d	Sweep Width (Hz)	12499.62	Original Points Count	16000
				Points Count	32768
				Temperature (grad C)	24.900



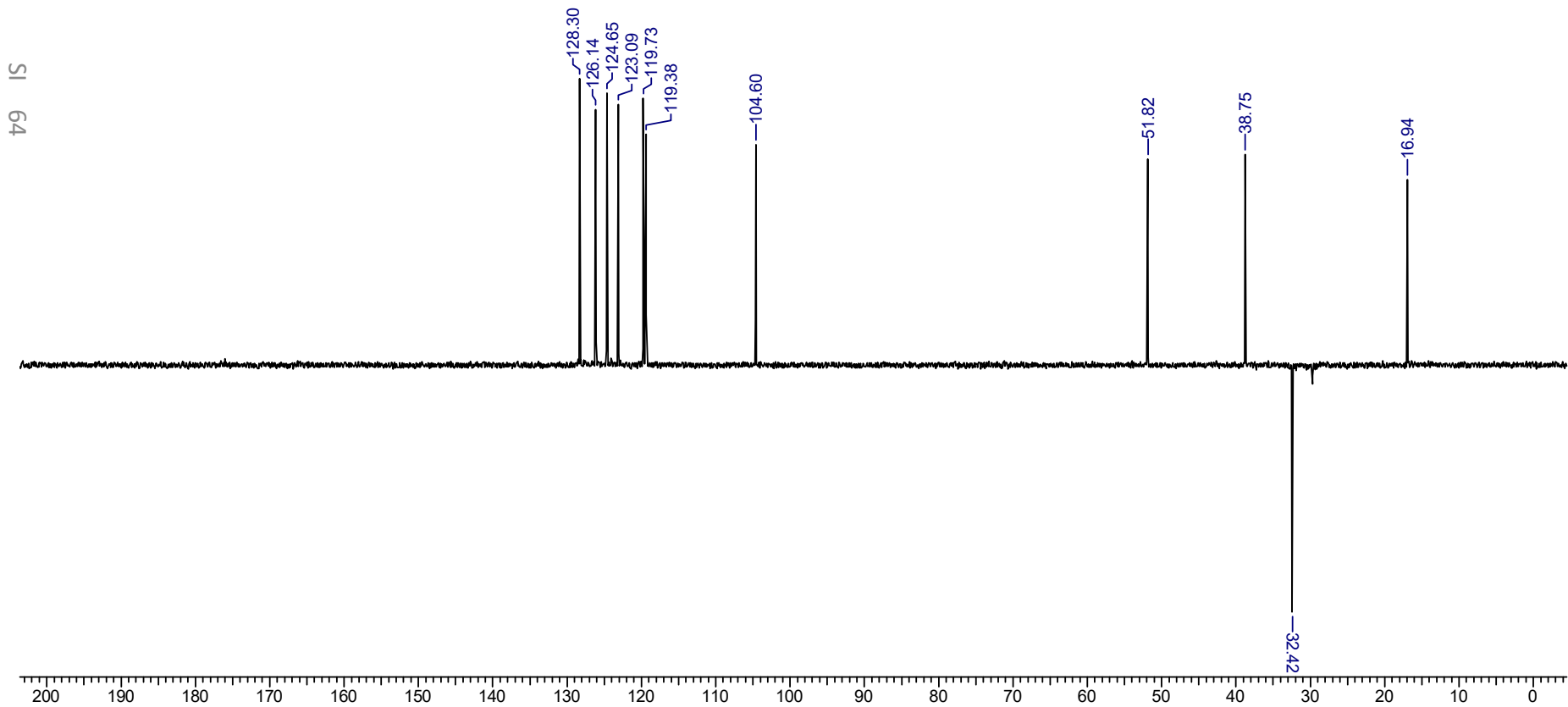
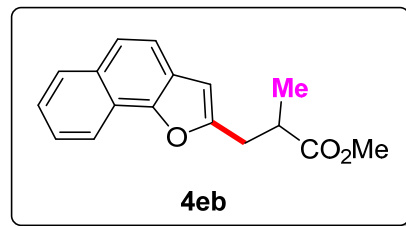
Acquisition Time (sec)	0.6554	Comment	13C	Date	17 Jan 2017 11:10:08	Frequency (MHz)	125.76
Nucleus	13C	Number of Transients	2205	Original Points Count	20480	Points Count	32768
Sweep Width (Hz)	31249.05			Temperature (grad C)	25.500	Solvent	CHLOROFORM-d



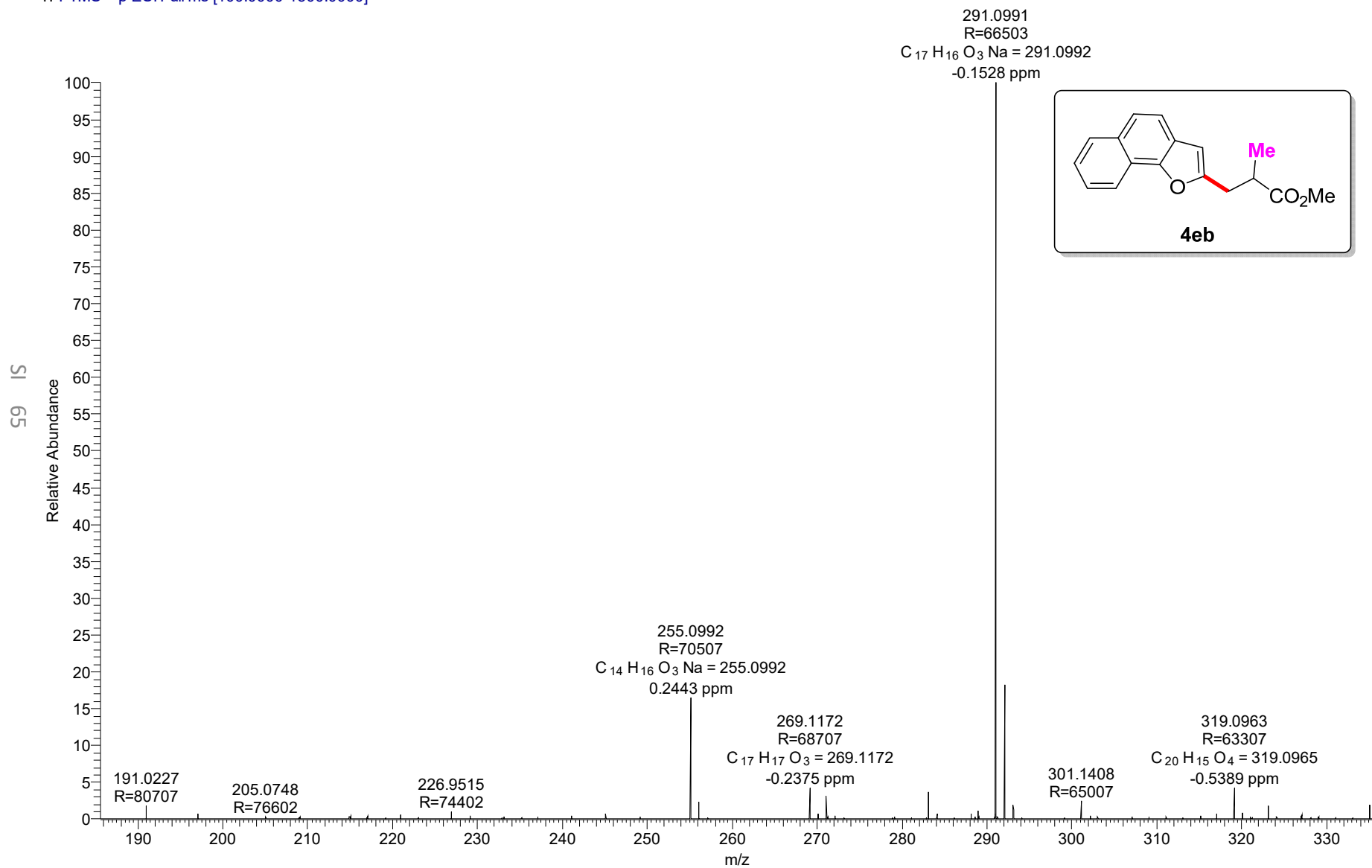
89 IS



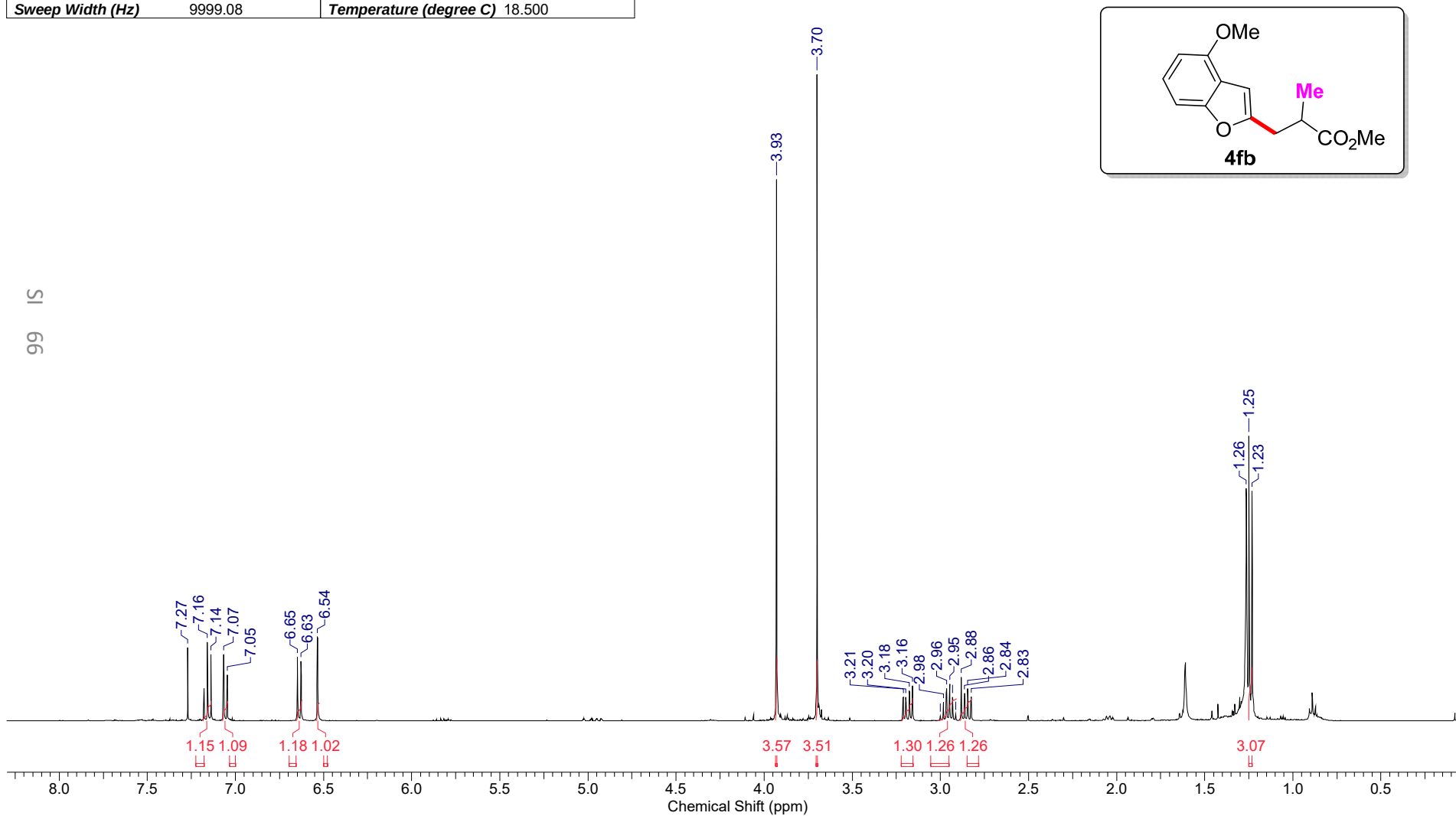
Acquisition Time (sec)	0.6554	Comment	DEPT	Date	17 Jan 2017 10:08:16	Frequency (MHz)	125.76
Nucleus	¹³ C	Number of Transients	600	Original Points Count	20480	Points Count	32768
Sweep Width (Hz)	31249.05	Temperature (grad C)	25.000	Solvent	CHLOROFORM-d		



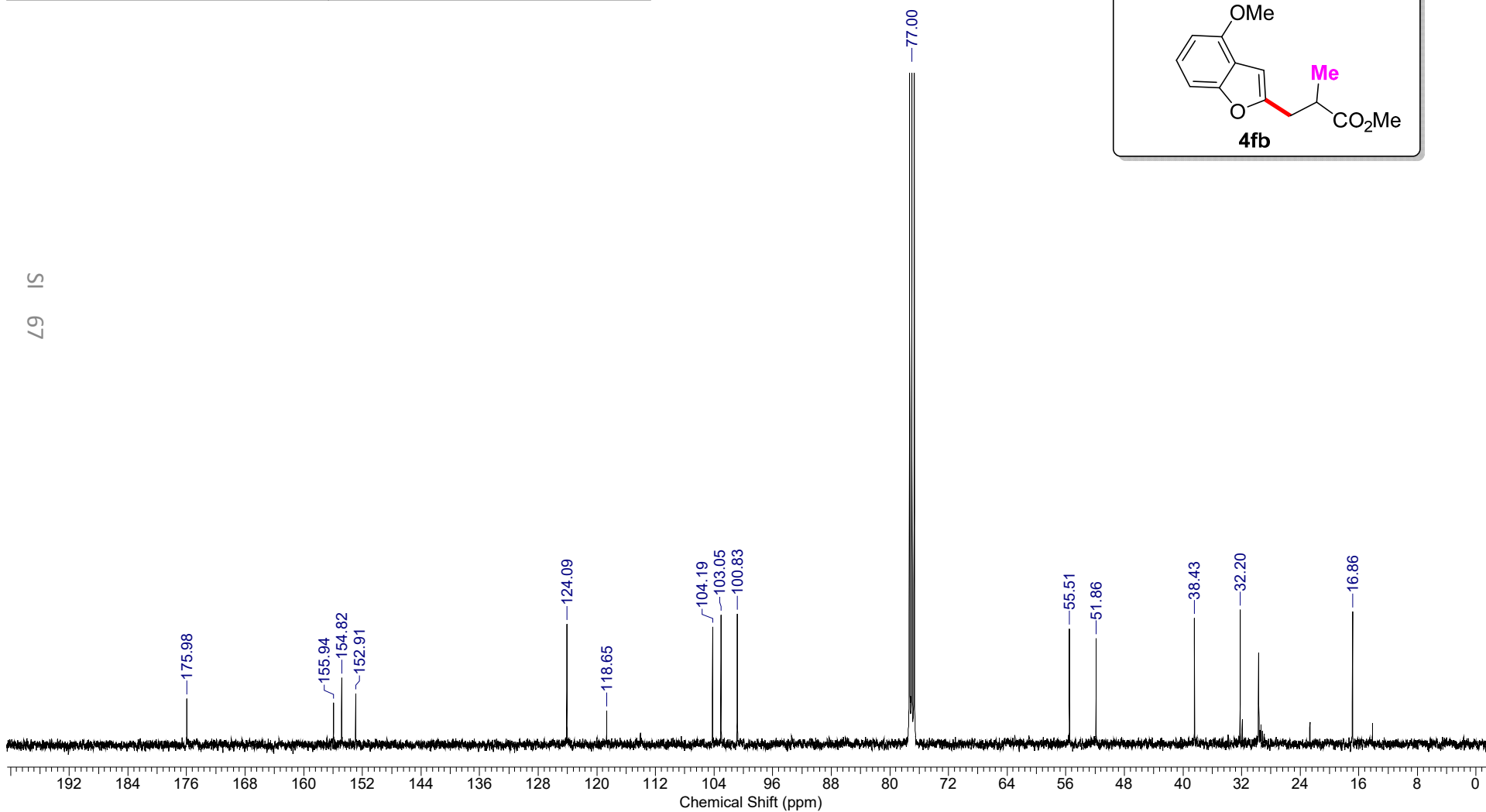
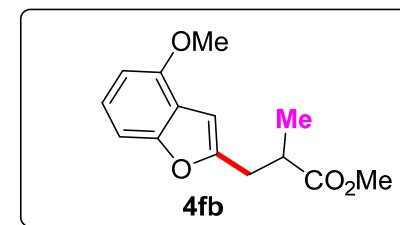
JY-B-2A #154 RT: 0.69 AV: 1 NL: 2.48E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



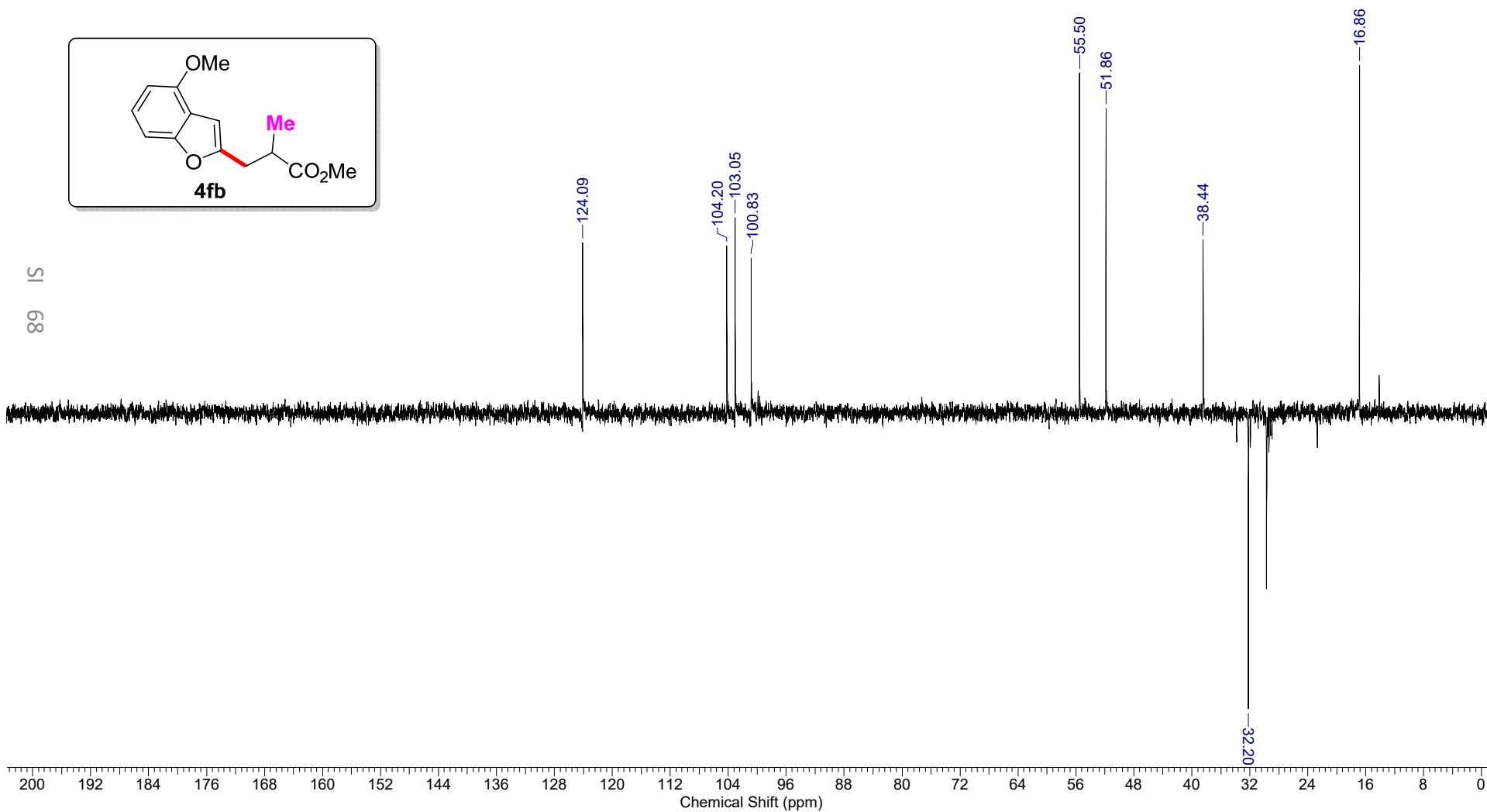
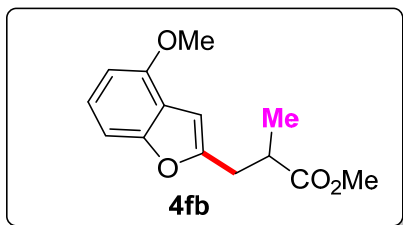
Acquisition Time (sec)	1.3108	Comment	Harish	Date	10 Sep 2018 13:05:49
Date Stamp	10 Sep 2018 11:23:10				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\Sept_Liquid State 2018\AV-500-2018089-202027-44698_PROTON-3.jdf				
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	16
Original Points Count	13107	Owner	delta	Points Count	13107
Receiver Gain	40.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse.ex2
Sweep Width (Hz)	9999.08	Temperature (degree C)	18.500	Spectrum Offset (Hz)	2806.4714
				Spectrum Type	STANDARD



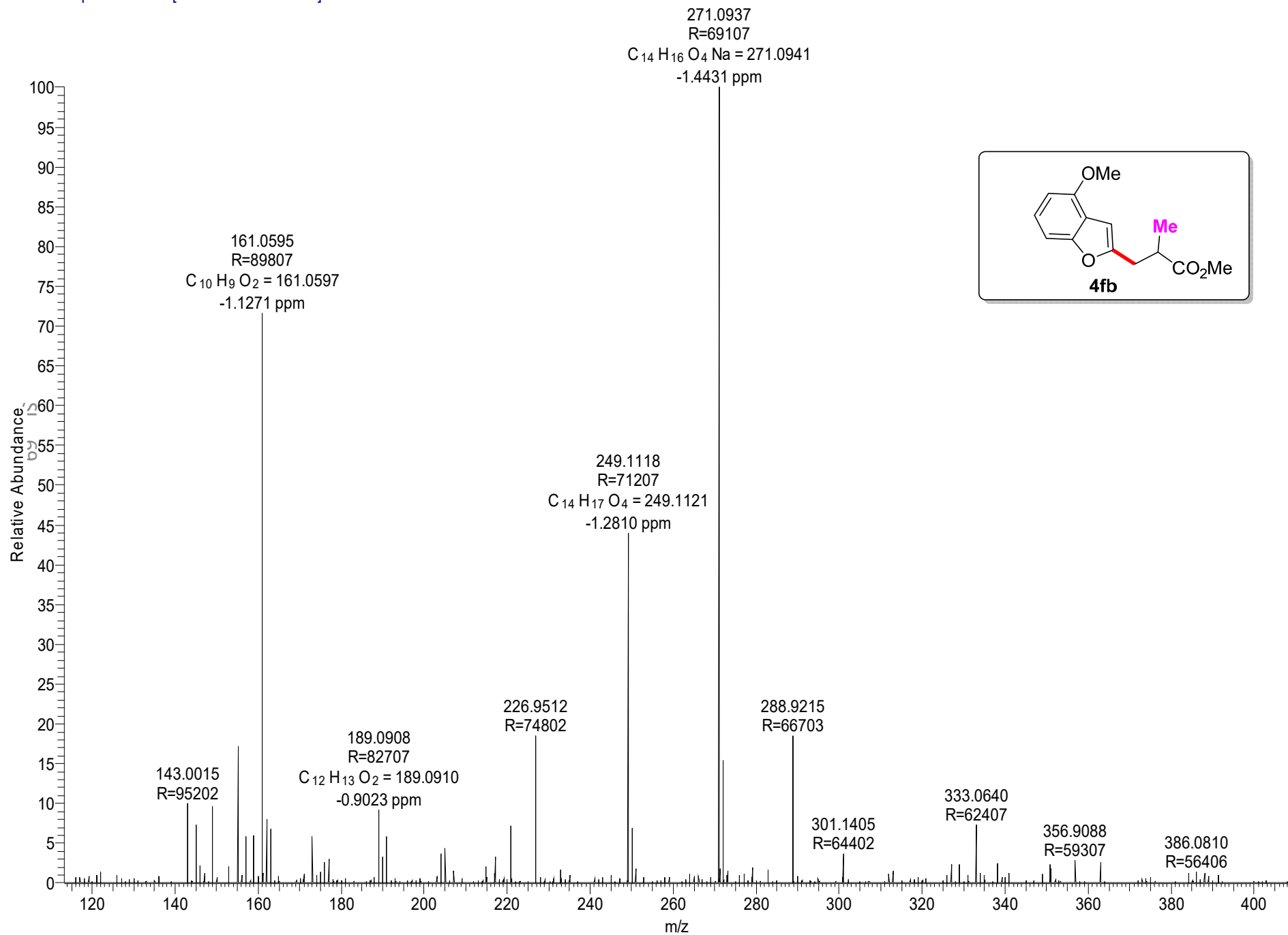
Acquisition Time (sec)	1.0434	Comment	Harish	Date	10 Sep 2018 10:53:43		
Date Stamp	10 Sep 2018 08:55:10						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\Sept_Liquid State 2018\AV-500-2018089-202027-44698 CARBON-3.jdf						
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	800	Origin	ECX 400
Original Points Count	26214	Owner	delta	Points Count	26214	Pulse Sequence	single_pulse_dec
Receiver Gain	54.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10041.2480	Spectrum Type	STANDARD
Sweep Width (Hz)	25124.29	Temperature (degree C)	18.200				



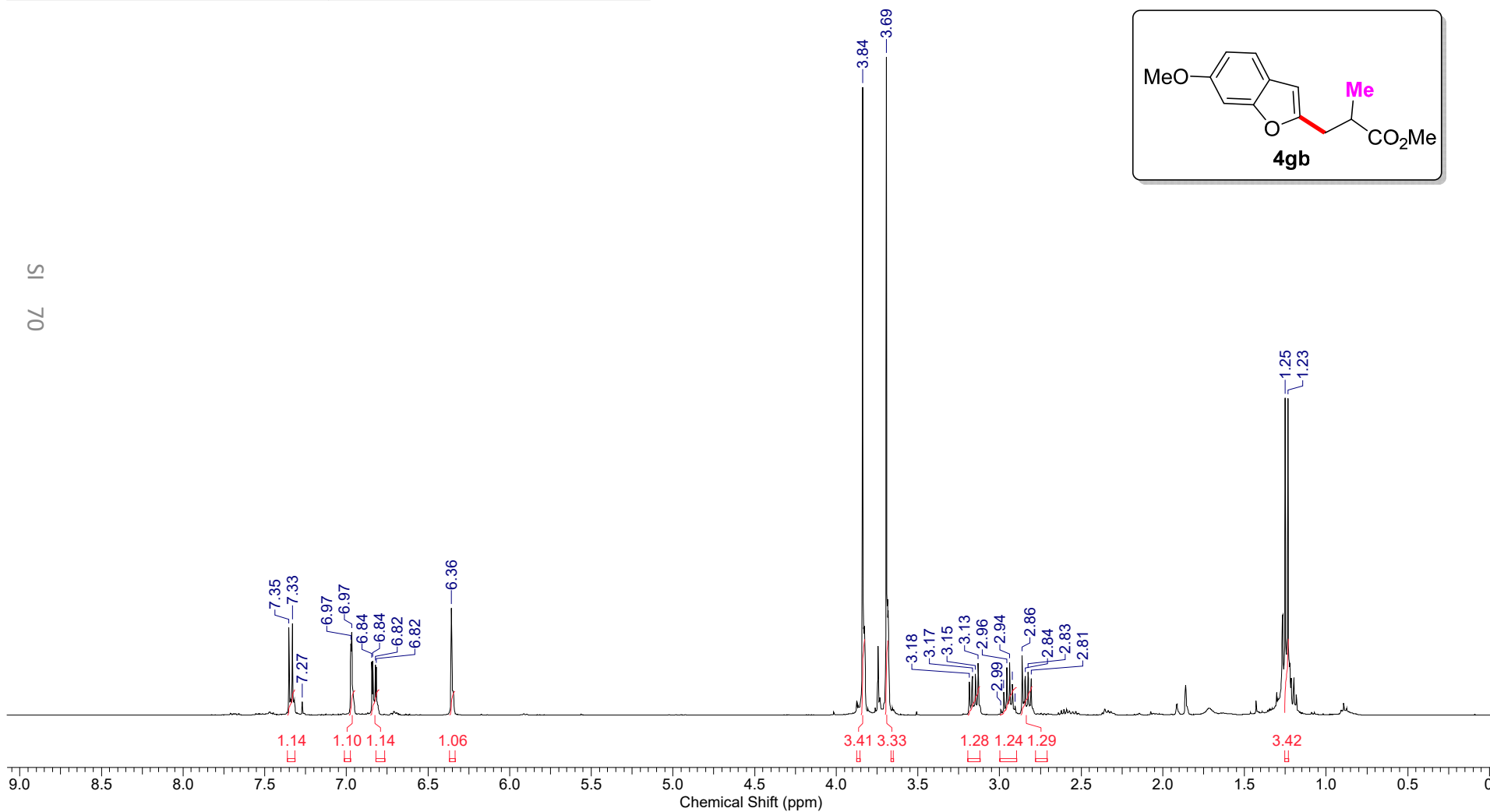
Acquisition Time (sec)	1.0434	Comment	Harish	Date	10 Sep 2018 10:53:43
Date Stamp	10 Sep 2018 09:11:05				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\Sept_Liquid State_2018\AV-500-2018089-202027-44698_DEPT135-3.jdf				
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	400
Original Points Count	26214	Owner	delta	Points Count	26214
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Pulse Sequence	dept.ex2 (selection_angle=135)
Spectrum Offset (Hz)	10041.6641	Spectrum Type	DEPT135		
Sweep Width (Hz)	25124.29	Temperature (degree C)	17.900		



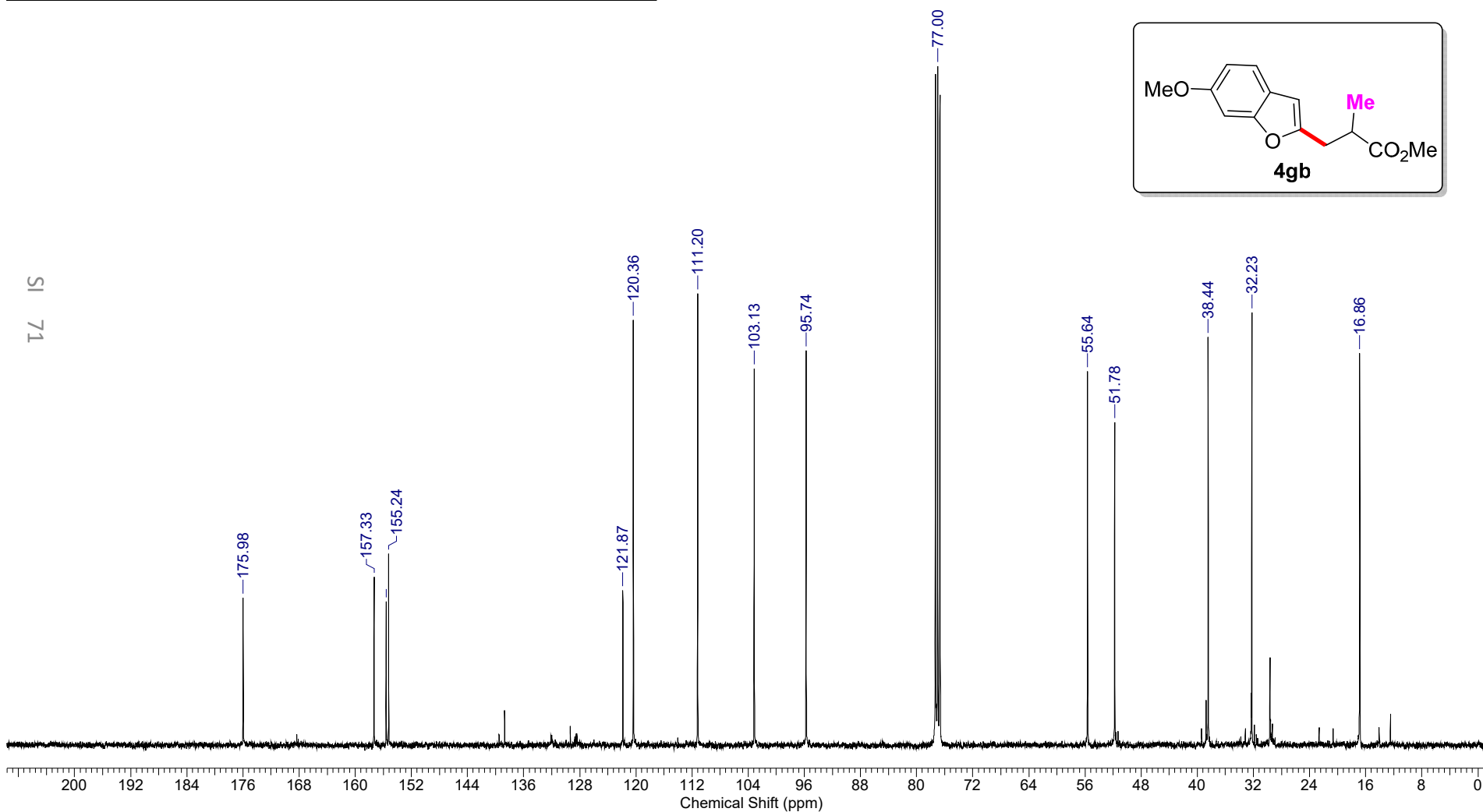
KS-J-30A_180914163239 #578 RT: 2.58 AV: 1 NL: 1.99E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



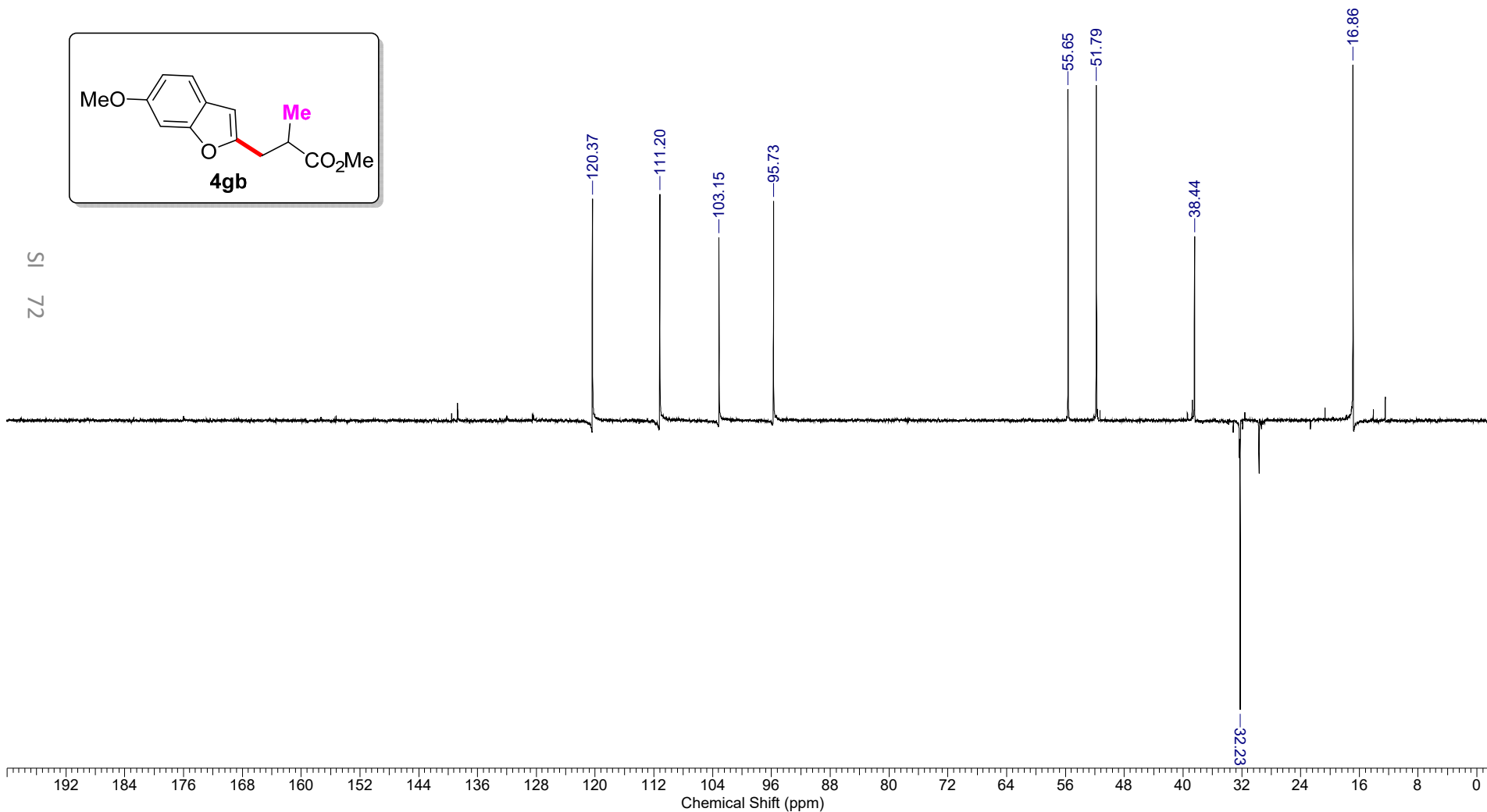
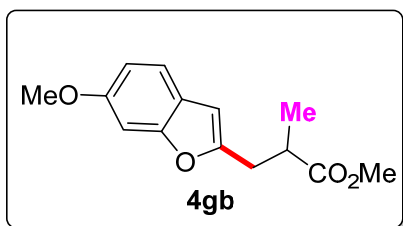
Acquisition Time (sec)	1.3108	Comment	Shaziya	Date	06 Sep 2018 11:57:54		
Date Stamp	06 Sep 2018 10:16:04						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State_2018\AV-400-20180826-173449-11843_PROTON-3.jdf						
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	32	Origin	ECX 400
Original Points Count	13107	Owner	delta	Points Count	13107	Pulse Sequence	single_pulse.ex2
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2806.4717	Spectrum Type	STANDARD
Sweep Width (Hz)	9999.08	Temperature (degree C)	21.000				



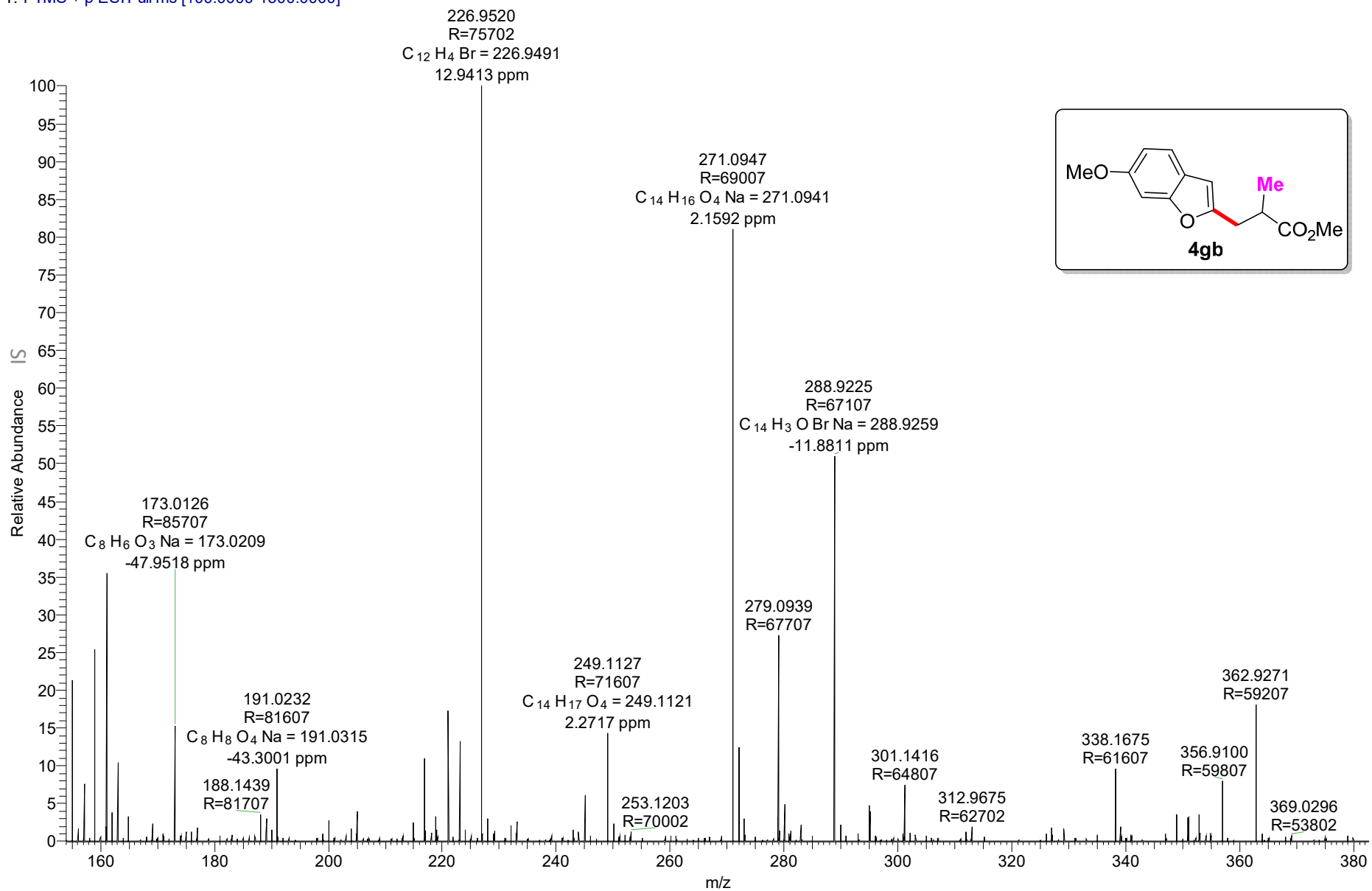
Acquisition Time (sec)	1.0434	Comment	Shaziya	Date	06 Sep 2018 13:21:34		
Date Stamp	06 Sep 2018 11:08:24						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State_2018\AV-400-20180826-173449-11843_CARBON-3.jdf						
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	1347	Origin	ECX 400
Original Points Count	26214	Owner	delta	Points Count	26214	Pulse Sequence	single_pulse_dec
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10038.3721	Spectrum Type	STANDARD
Sweep Width (Hz)	25124.29	Temperature (degree C)	18.500				



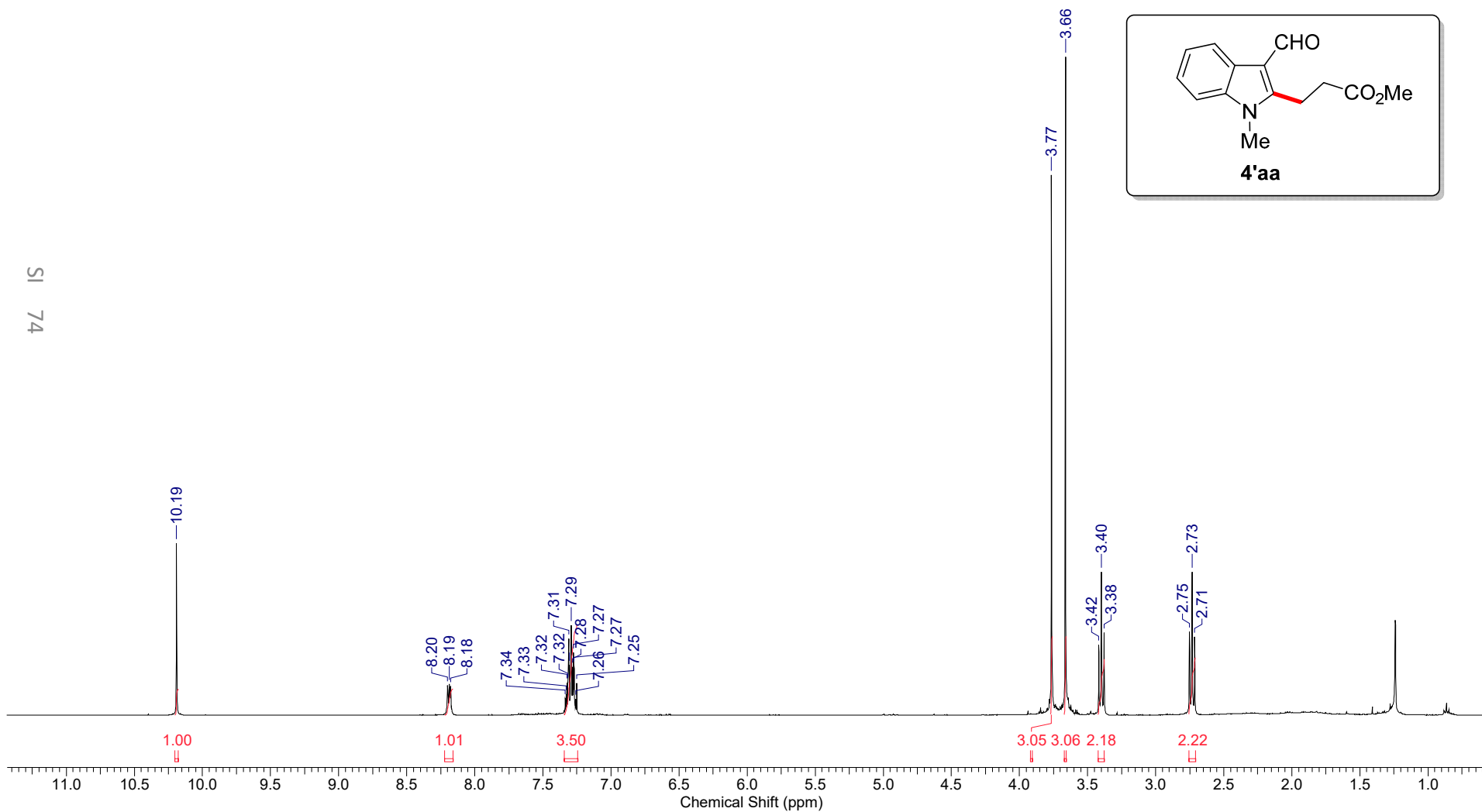
Acquisition Time (sec)	1.0434	Comment	Shaziya	Date	06 Sep 2018 13:21:34
Date Stamp	06 Sep 2018 11:39:42				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State 2018\AV-400-20180826-173449-11843_DEPT135-3.jdf				
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	800
Original Points Count	26214	Owner	delta	Points Count	26214
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Pulse Sequence	dept.ex2 (selection_angle=135)
Sweep Width (Hz)	25124.29	Temperature (degree C)	17.800	Spectrum Offset (Hz)	10038.7881
				Spectrum Type	DEPT135



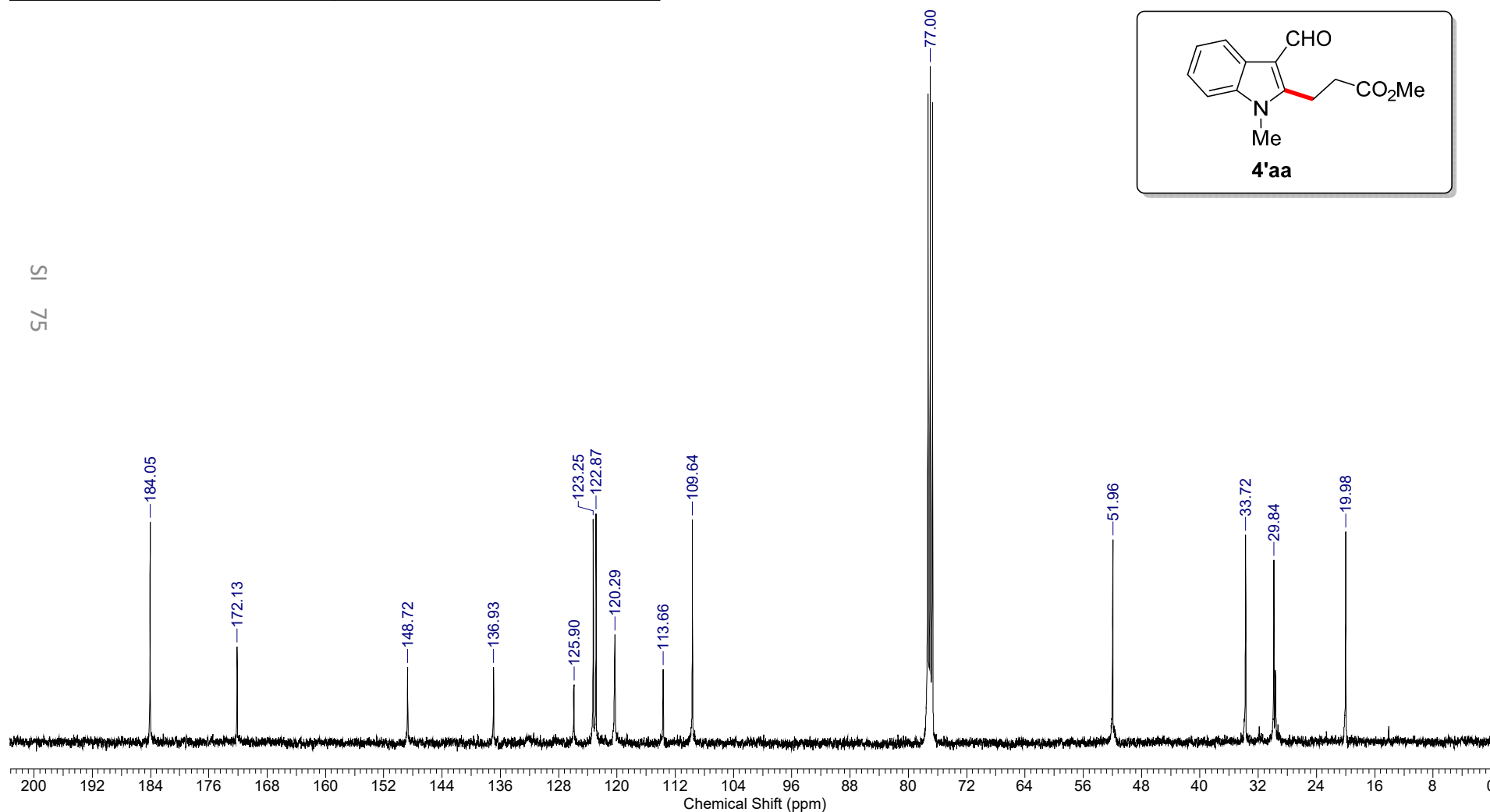
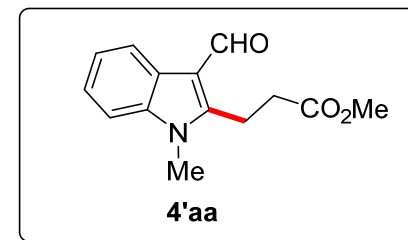
KS-J-37A #511 RT: 2.28 AV: 1 NL: 1.69E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



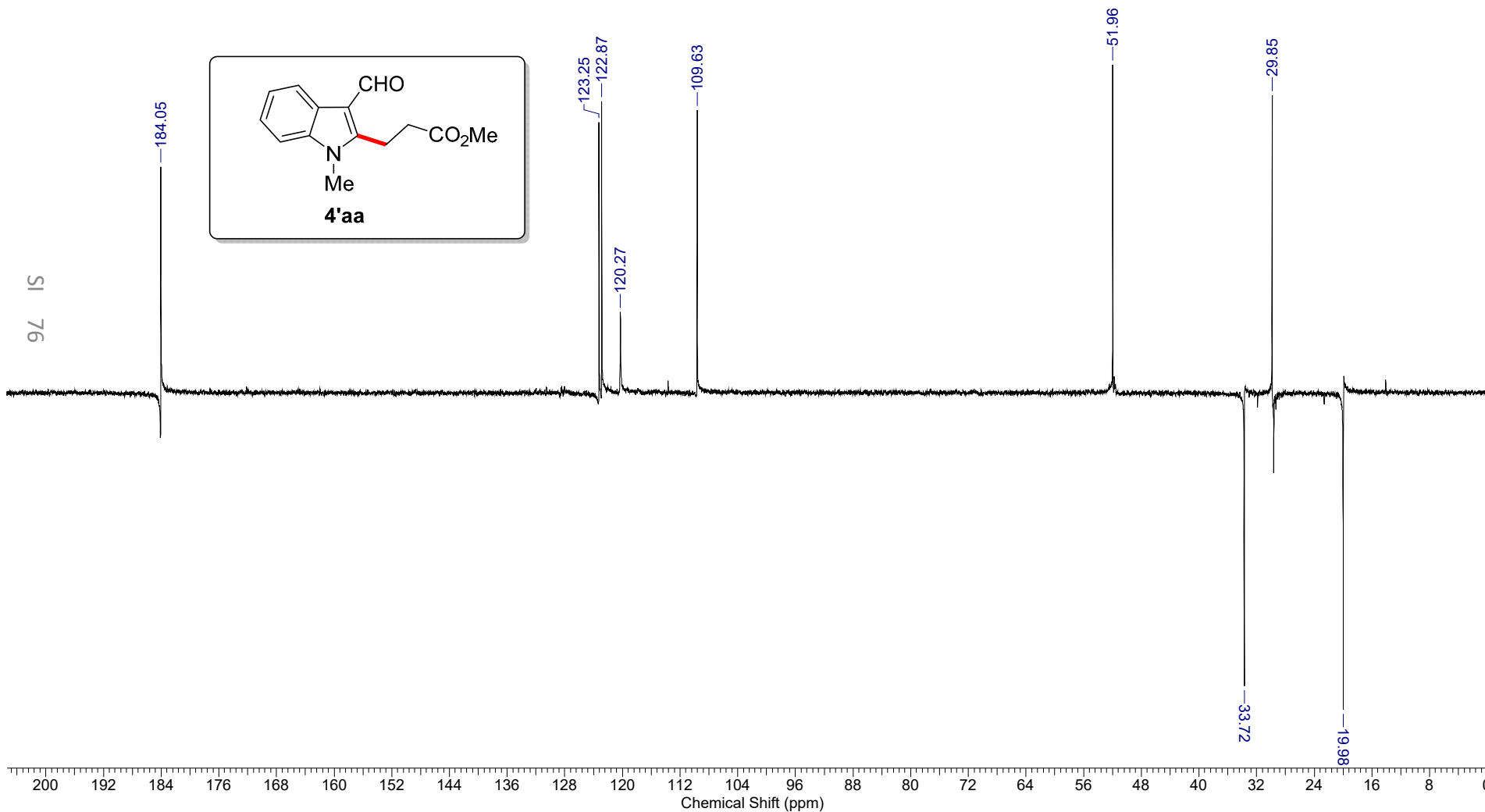
Acquisition Time (sec)	1.3108	Comment	Shaziya	Date	08 Sep 2018 17:31:15
Date Stamp	08 Sep 2018 15:49:25				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State_2018\AV-400-20180903-201014-11843_PROTON-3.jdf				
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	32
Original Points Count	13107	Owner	delta	Points Count	13107
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse.ex2
Sweep Width (Hz)	9999.08	Temperature (degree C)	18.200	Spectrum Offset (Hz)	2798.4753
				Spectrum Type	STANDARD



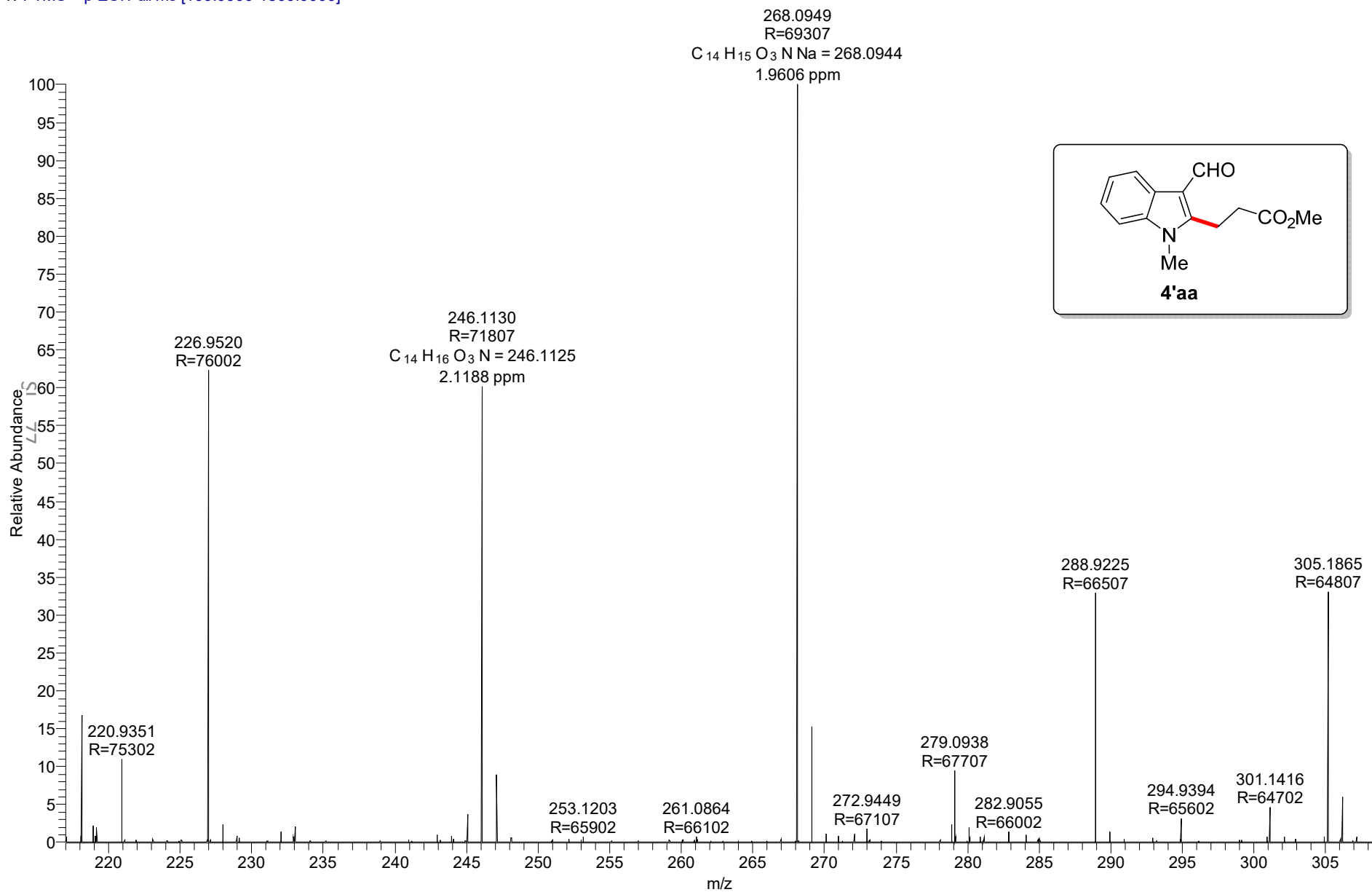
Acquisition Time (sec)	1.0434	Comment	Shaziya	Date	09 Sep 2018 00:38:39		
Date Stamp	08 Sep 2018 16:36:06						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State 2018\AV-400-20180903-201014-11843_CARBON-3.jdf						
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	1200	Origin	ECX 400
Original Points Count	26214	Owner	delta	Points Count	26214	Pulse Sequence	single_pulse_dec
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10036.4551	Spectrum Type	STANDARD
Sweep Width (Hz)	25124.29	Temperature (degree C)	18.500				



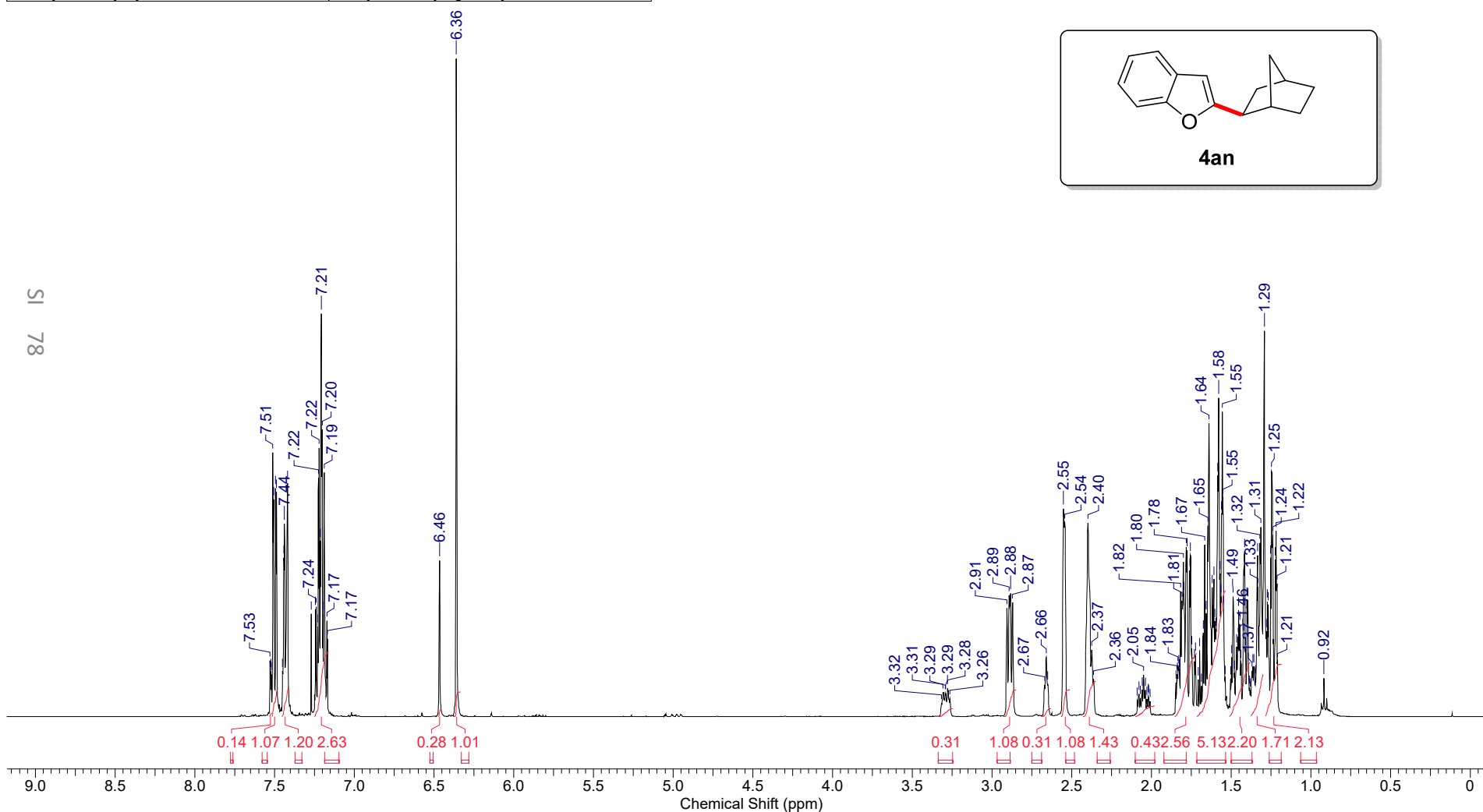
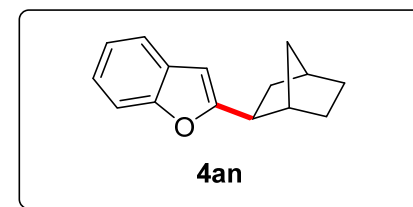
Acquisition Time (sec)	1.0434	Comment	Shaziya	Date	09 Sep 2018 00:38:39
Date Stamp	08 Sep 2018 17:09:04				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State 2018\AV-400-20180903-201014-11843_DEPT135-3.jdf				
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	800
Original Points Count	26214	Owner	delta	Points Count	26214
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Pulse Sequence	dept.ex2 (selection_angle=135)
Sweep Width (Hz)	25124.29	Temperature (degree C)	18.400	Spectrum Offset (Hz)	10014.0889
				Spectrum Type	DEPT135



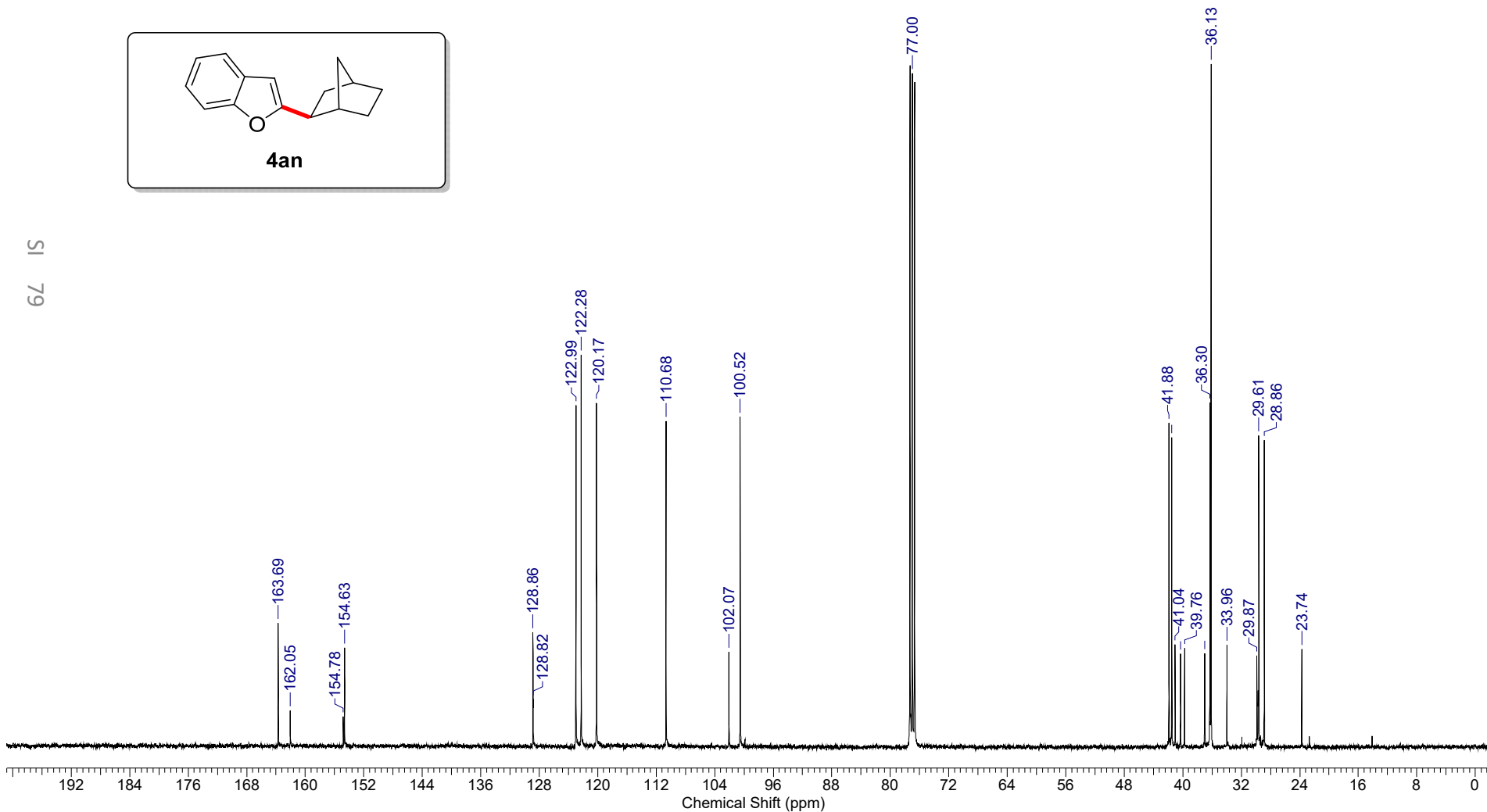
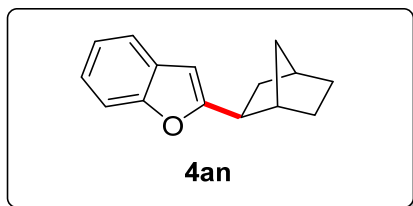
KS-J-27B #475 RT: 2.12 AV: 1 NL: 2.75E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



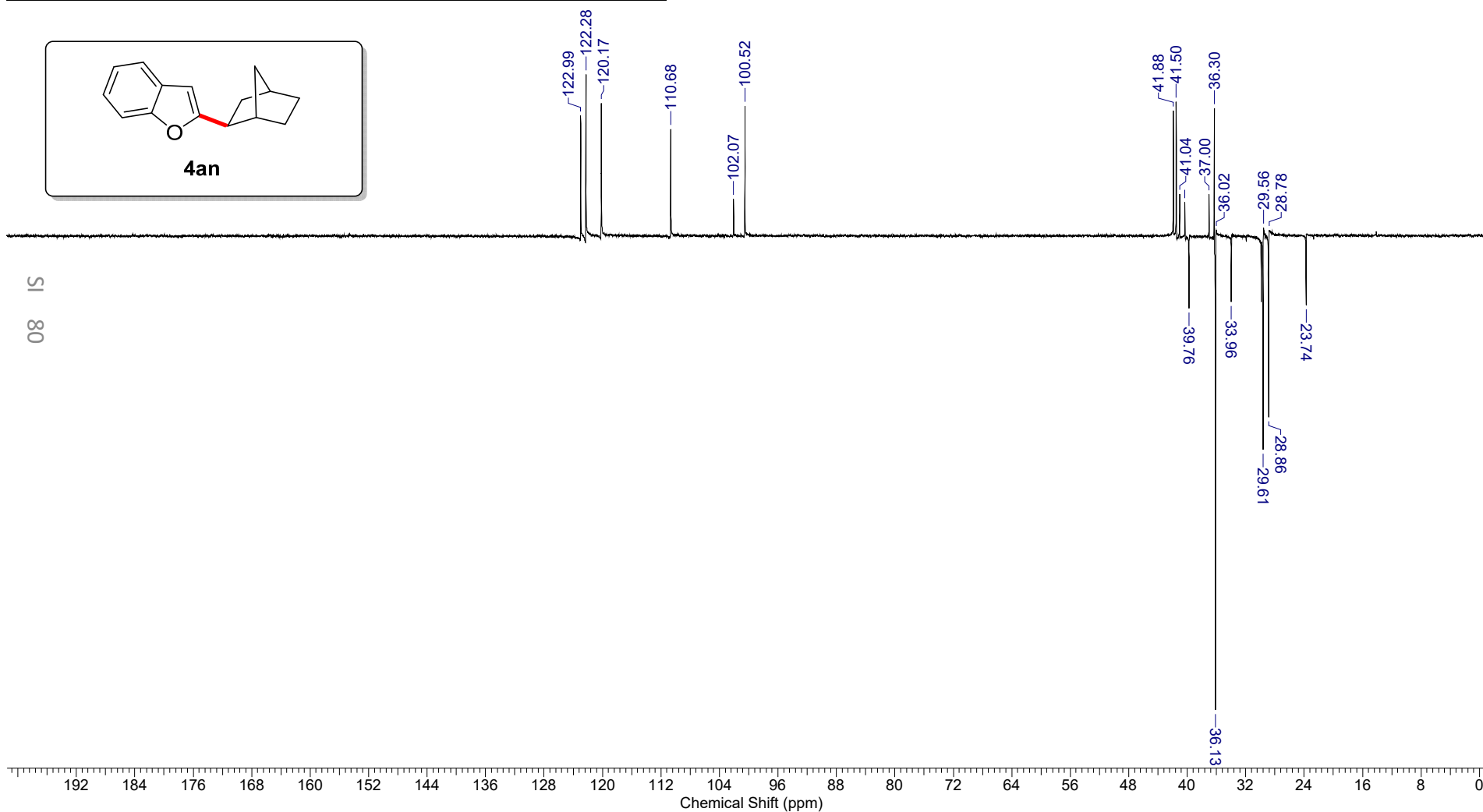
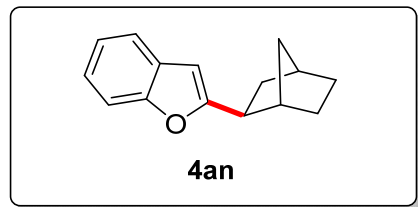
Acquisition Time (sec)	1.3108	Comment	Suparna	Date	31 Aug 2018 12:33:31
Date Stamp	31 Aug 2018 10:51:52				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State_2018\AV-400-20180822-114710-44339_PROTON-3.jdf				
Frequency (MHz)	399.78	Nucleus	¹ H	Number of Transients	32
Original Points Count	13107	Owner	delta	Points Count	13107
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse.ex2
Sweep Width (Hz)	9999.08	Temperature (degree C)	23.100	Spectrum Offset (Hz)	2806.4714
				Spectrum Type	STANDARD



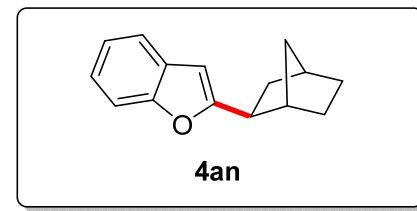
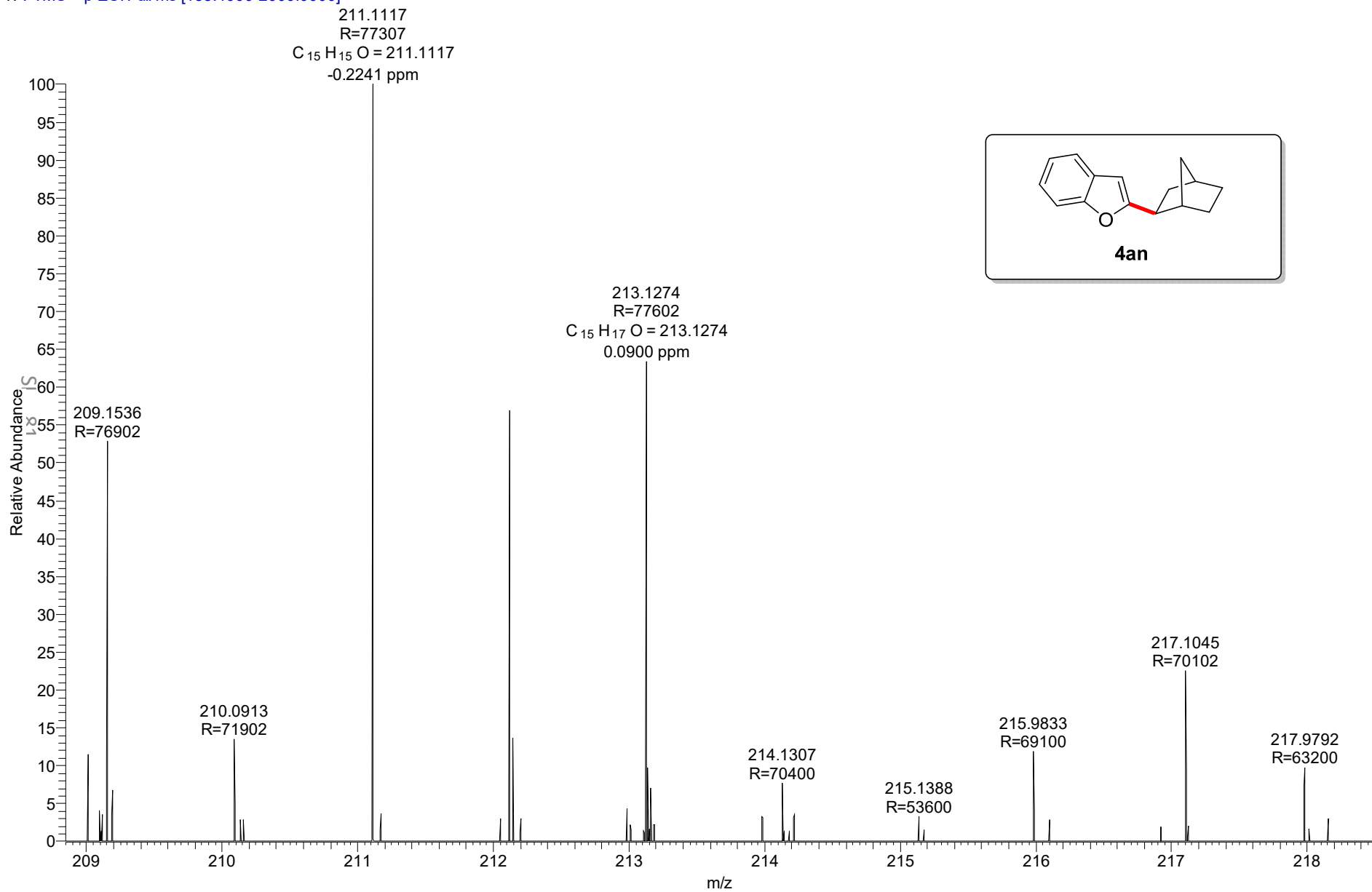
Acquisition Time (sec)	1.0434	Comment	Suparna	Date	31 Aug 2018 14:53:20
Date Stamp	31 Aug 2018 12:24:52				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State_2018\AV-400-20180822-114710-44339_CARBON-3.jdf				
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	2400
Original Points Count	26214	Owner	delta	Points Count	26214
Receiver Gain	58.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse_dec
Sweep Width (Hz)	25124.29	Temperature (degree C)	23.400	Spectrum Offset (Hz)	10040.2900
				Spectrum Type	STANDARD



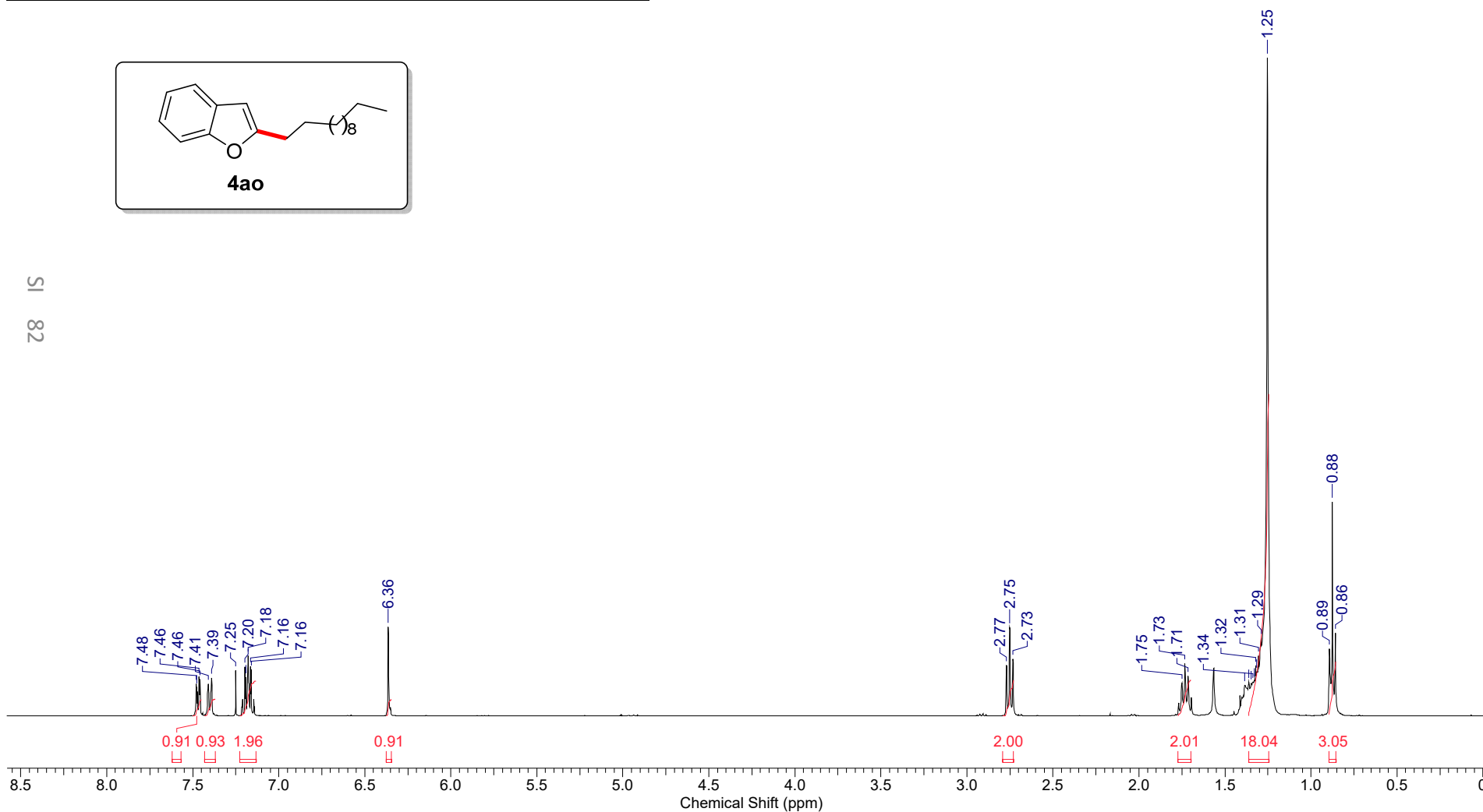
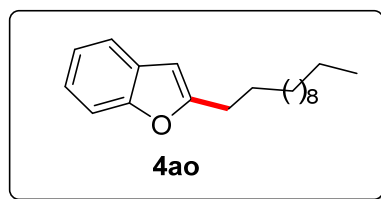
Acquisition Time (sec)	1.0434	Comment	Suparna	Date	31 Aug 2018 14:53:20
Date Stamp	31 Aug 2018 13:11:41				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State 2018\AV-400-20180822-114710-44339_DEPT135-3.jdf				
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	1200
Original Points Count	26214	Owner	delta	Points Count	26214
Receiver Gain	58.00	Solvent	CHLOROFORM-d	Pulse Sequence	dept.ex2 (selection_angle=135)
Sweep Width (Hz)	25124.29	Temperature (degree C)	23.300	Spectrum Offset (Hz)	10040.3066
				Spectrum Type	DEPT135



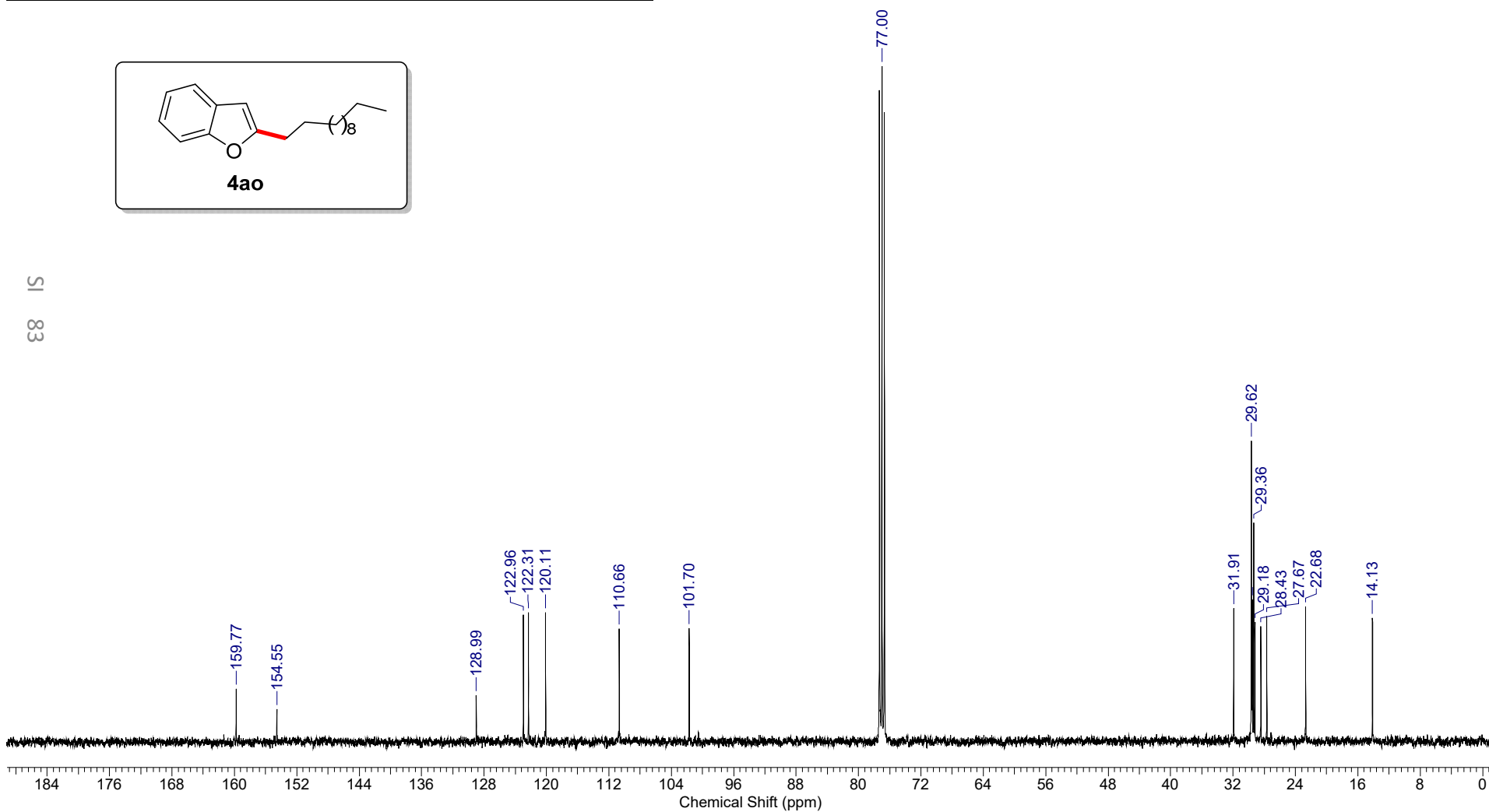
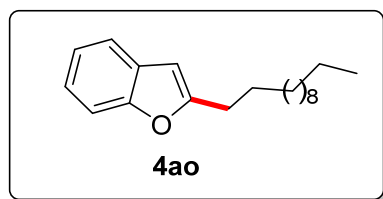
KJS-37A #354 RT: 1.59 AV: 1 NL: 1.45E6
T: FTMS + p ESI Full ms [133.4000-2000.0000]



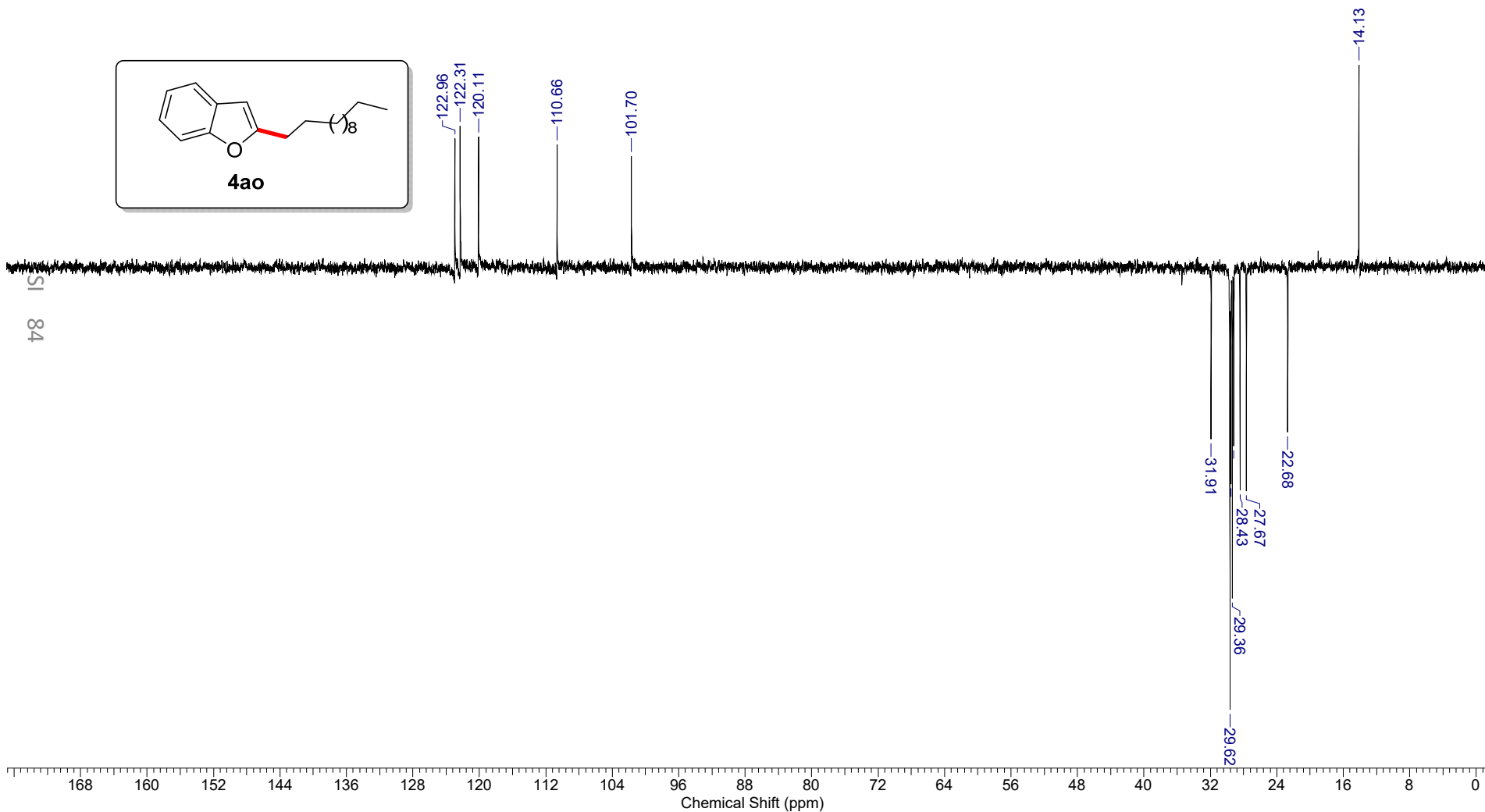
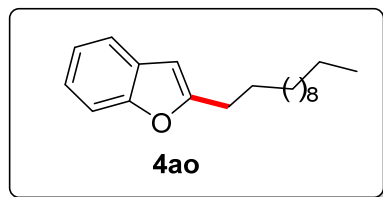
Acquisition Time (sec)	1.3108	Comment	Suparna	Date	10 Sep 2018 08:47:18		
Date Stamp	10 Sep 2018 07:04:39						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\Sept_Liquid State 2018\AV-500-20180822-115410-44339_PROTON-3.jdf						
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	16	Origin	ECX 400
Original Points Count	13107	Owner	delta	Points Count	13107	Pulse Sequence	single_pulse.ex2
Receiver Gain	34.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2798.4753	Spectrum Type	STANDARD
Sweep Width (Hz)	9999.08	Temperature (degree C)	18.400				



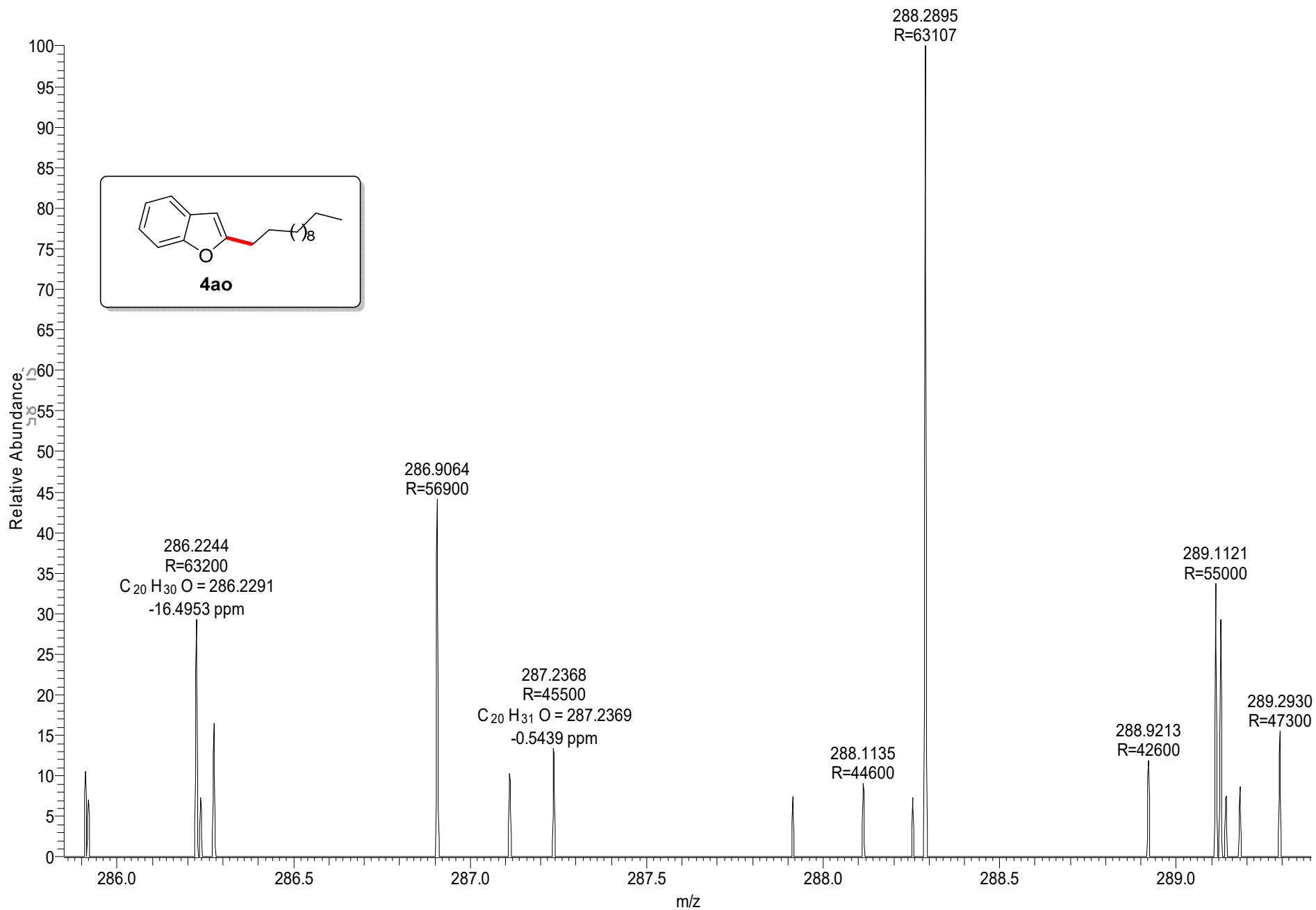
Acquisition Time (sec)	1.0434	Comment	Suparna	Date	10 Sep 2018 09:11:32
Date Stamp	10 Sep 2018 07:19:16				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\Sept_Liquid State 2018\AV-500-20180822-115410-44339_CARBON-3.jdf				
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	347
Original Points Count	26214	Owner	delta	Points Count	26214
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse_dec
Sweep Width (Hz)	25124.29	Temperature (degree C)	18.800	Spectrum Offset (Hz)	10041.2480
				Spectrum Type	STANDARD



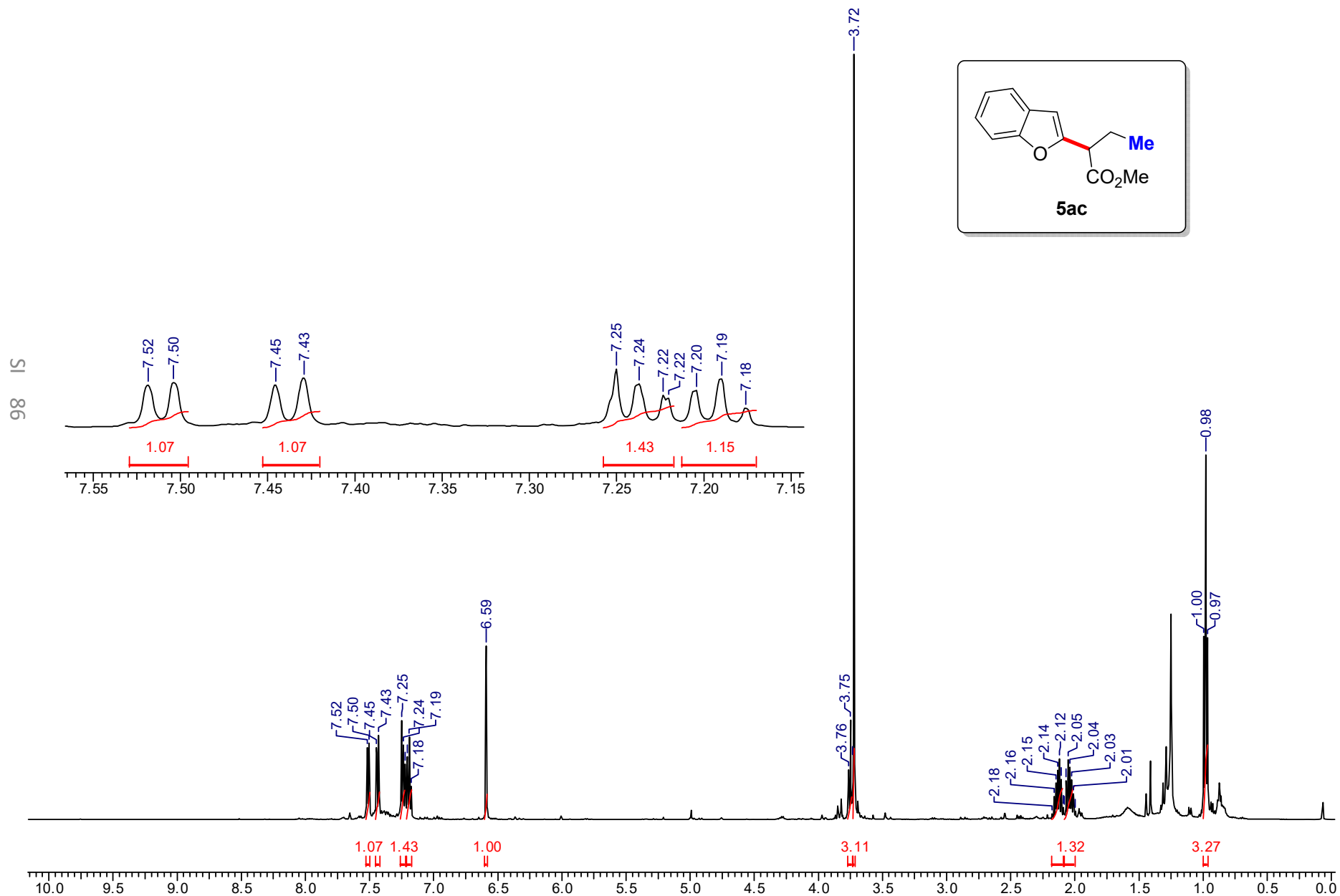
Acquisition Time (sec)	1.0434	Comment	Suparna	Date	10 Sep 2018 09:11:32		
Date Stamp	10 Sep 2018 07:28:53						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\Sept_Liquid State_2018\AV-500-20180822-115410-44339_DEPT135-3.jdf						
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	237	Origin	ECX 400
Original Points Count	26214	Owner	delta	Points Count	26214	Pulse Sequence	dept.ex2 (selection_angle=135)
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10041.3516	Spectrum Type	DEPT135
Sweep Width (Hz)	25124.29	Temperature (degree C)	18.600				



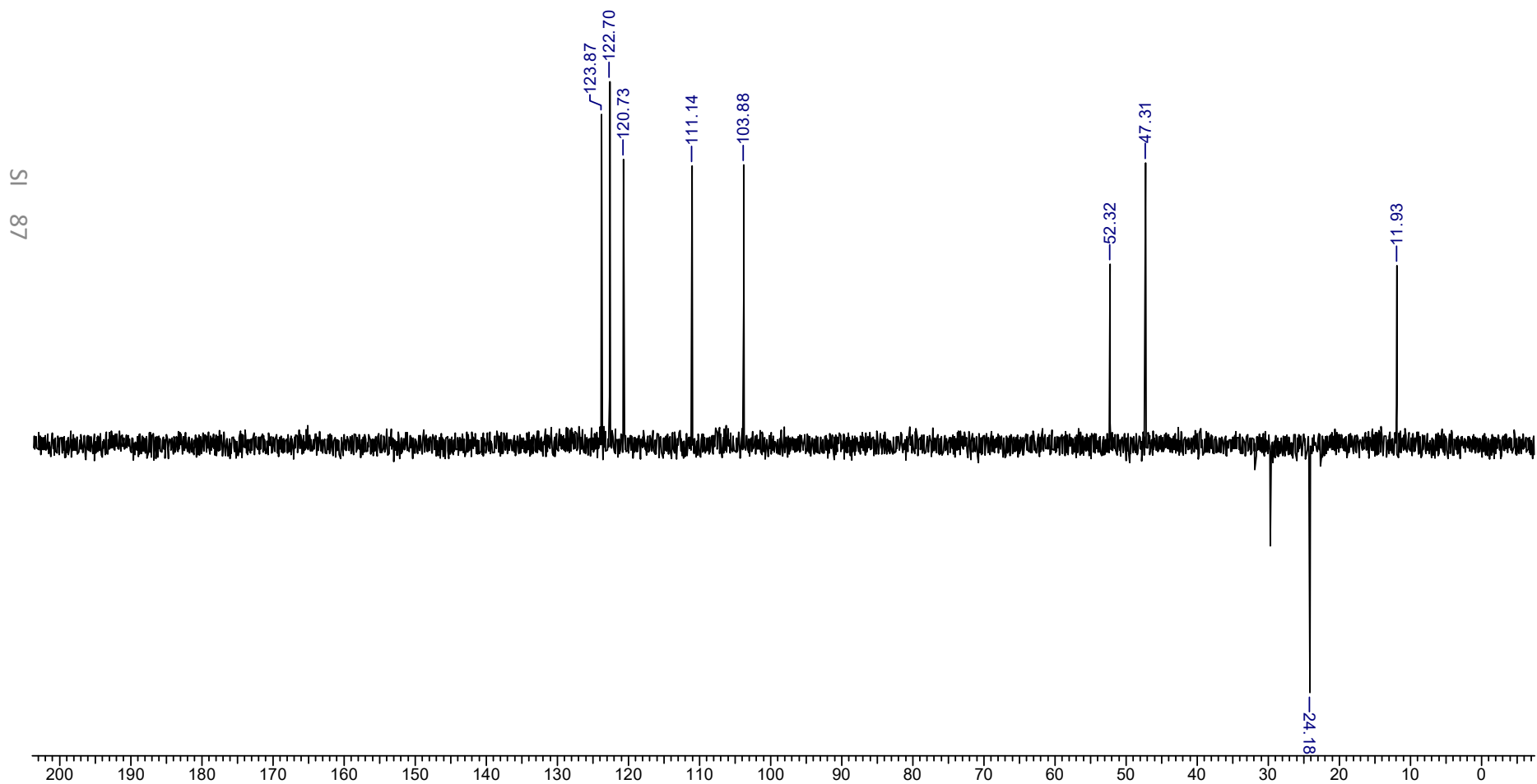
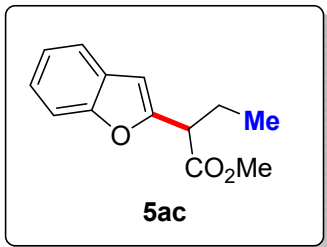
34-B #364 RT: 1.63 AV: 1 NL: 2.28E5
T: FTMS + p ESI Full ms [133.4000-2000.0000]



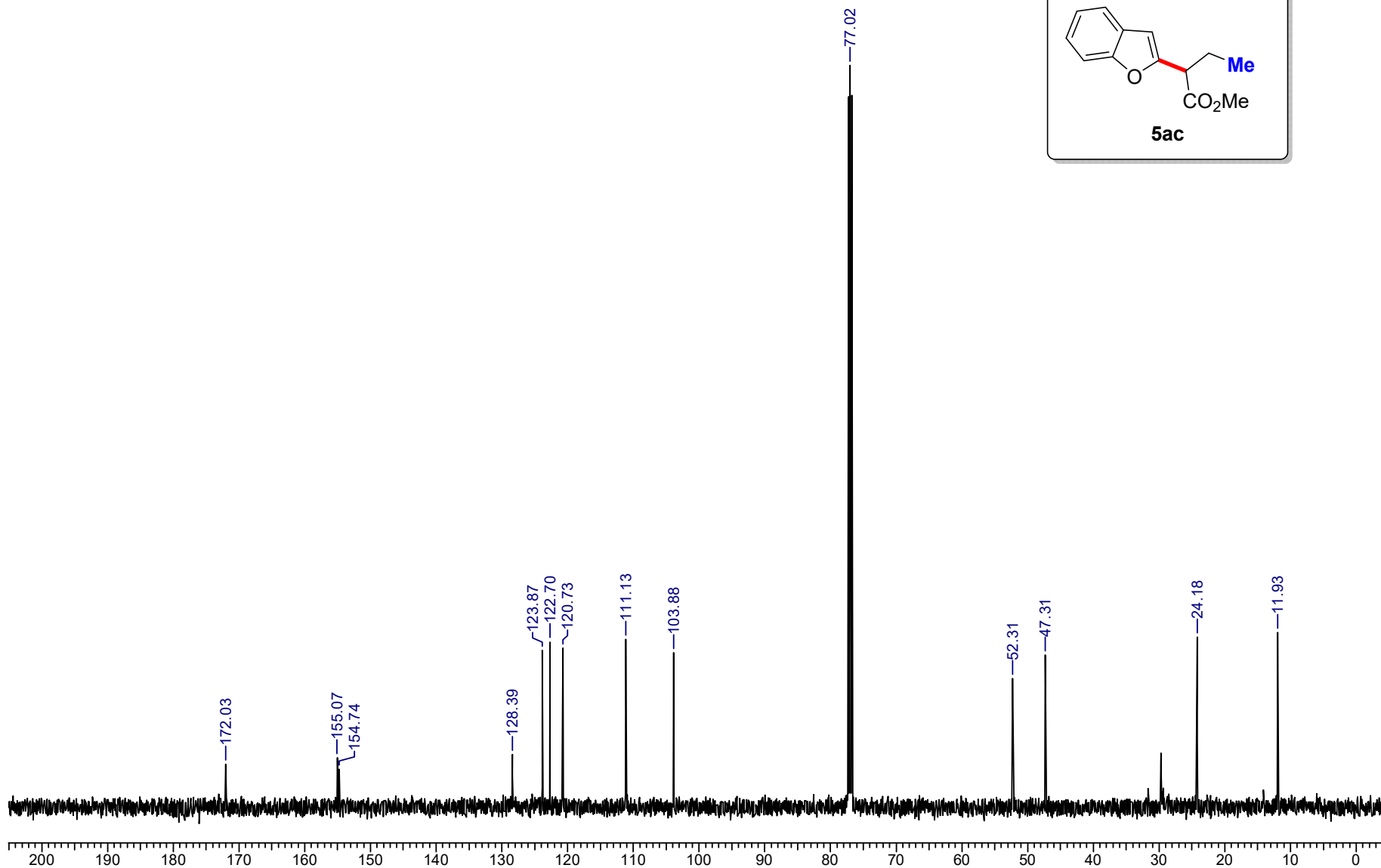
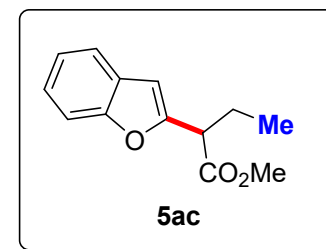
Acquisition Time (sec)	1.2800	Comment	Jyothi 1H	Date	14 Jan 2017 16:36:32
Frequency (MHz)	500.13	Nucleus	¹ H	Number of Transients	64
Solvent	CHLOROFORM-d	Sweep Width (Hz)	12499.62	Original Points Count	16000
				Points Count	32768
				Temperature (grad C)	25.000



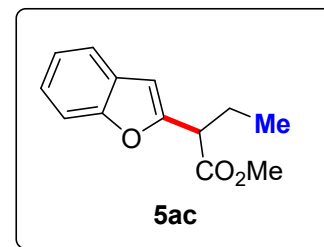
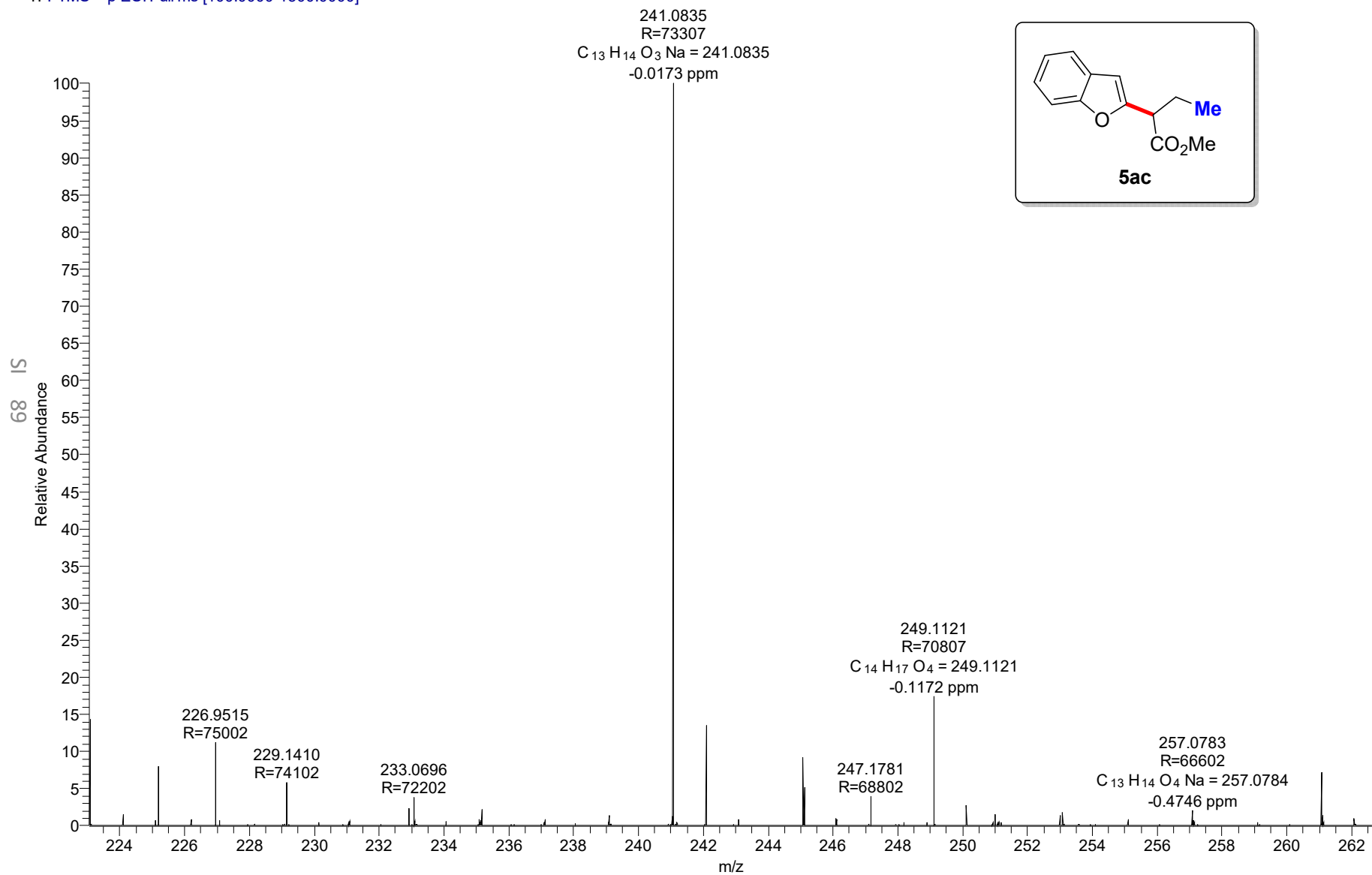
Acquisition Time (sec)	0.6554	Comment	DEPT	Date	14 Jan 2017 16:47:12		Frequency (MHz)	125.76	
Nucleus	13C	Number of Transients	400	Original Points Count	20480	Points Count	32768	Solvent	CHLOROFORM-d
Sweep Width (Hz)	31249.05	Temperature (grad C)	25.300						



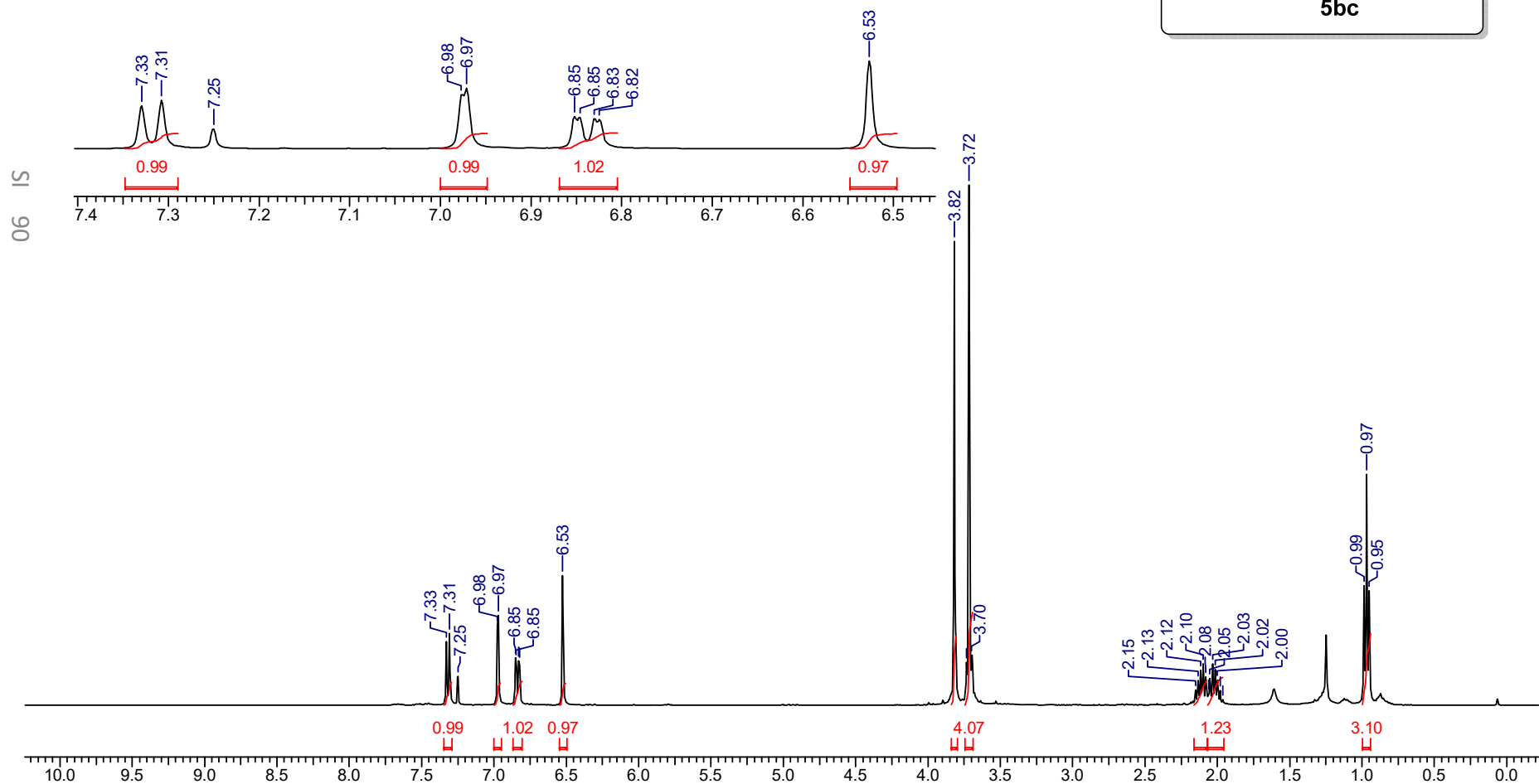
Acquisition Time (sec)	0.6554	Comment	13C	Date	14 Jan 2017 16:49:20	Frequency (MHz)	125.76
Nucleus	13C	Number of Transients	186	Original Points Count	20480	Points Count	32768
Sweep Width (Hz)	31249.05	Temperature (grad C)	25.700	Solvent	CHLOROFORM-d		



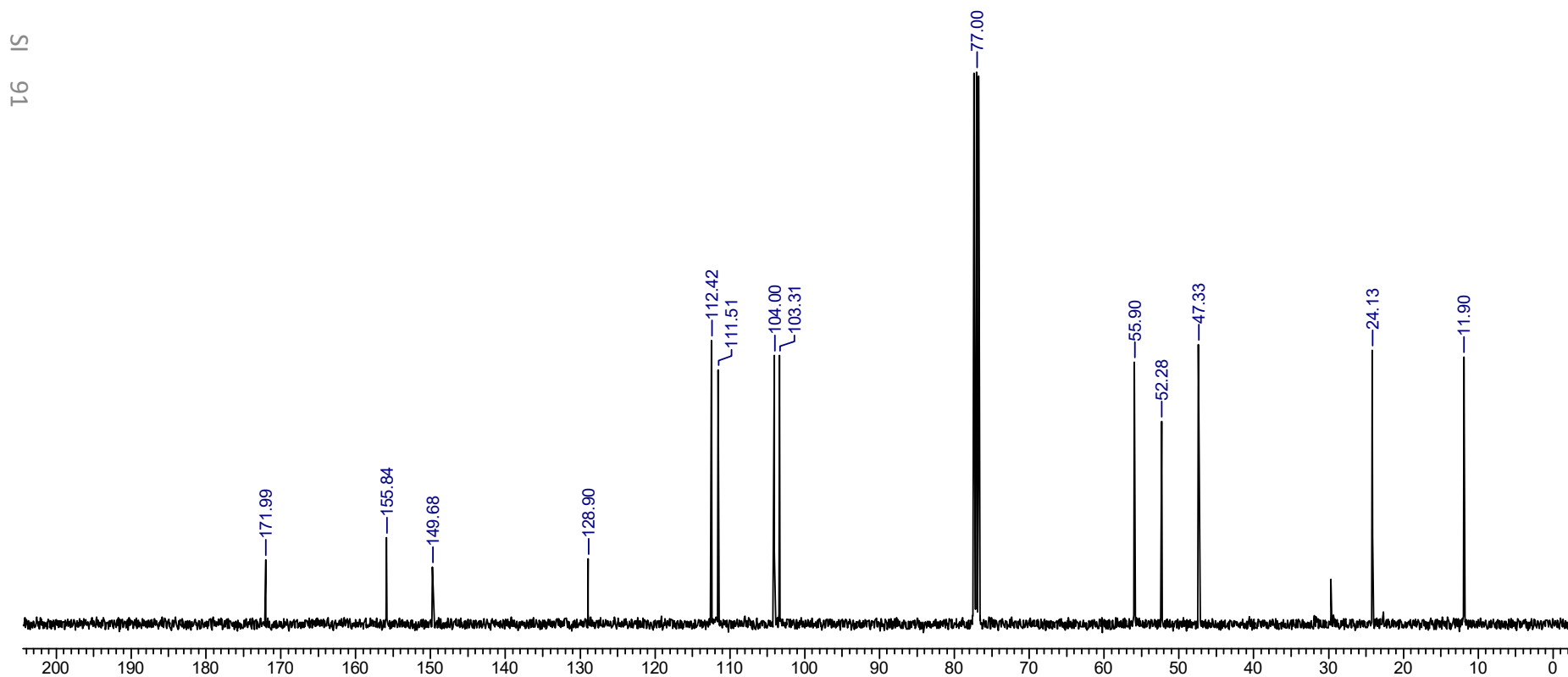
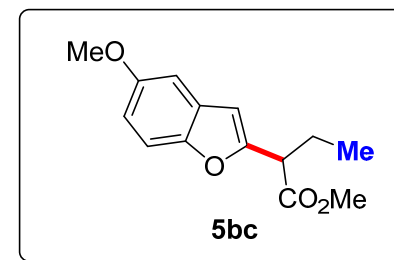
JY-B-1B #126 RT: 0.56 AV: 1 NL: 1.99E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



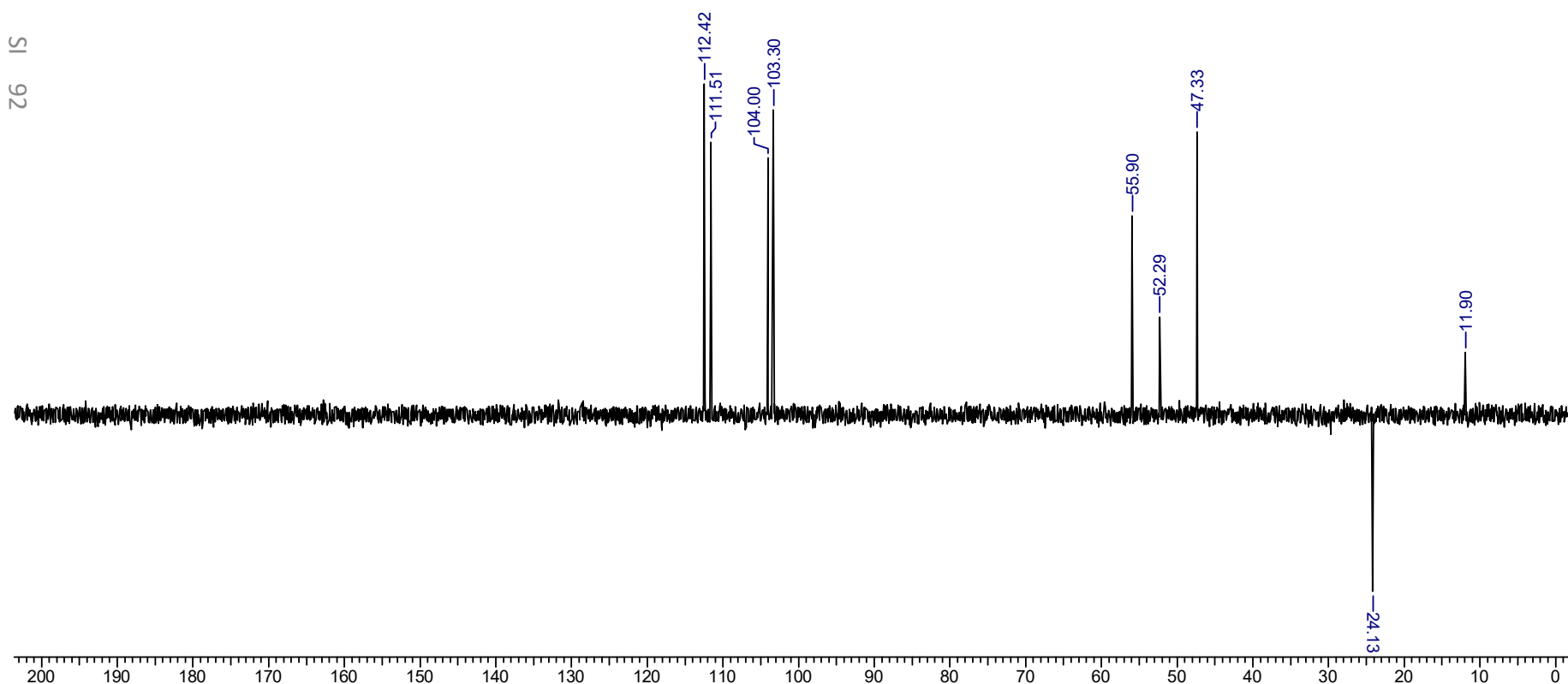
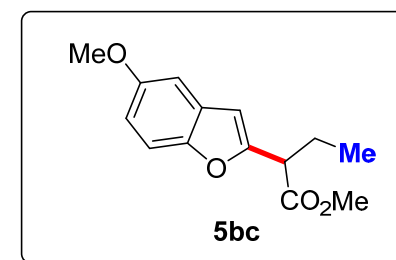
Comment	Srinivas 1H			
Date	31 Jan 2017 18:03:52	Frequency (MHz)	400.13	Nucleus 1H
Number of Transients	64	Original Points Count	16384	Points Count 16384
Solvent	CHLOROFORM-d	Sweep Width (Hz)	9999.39	Temperature (grad C) 21.700



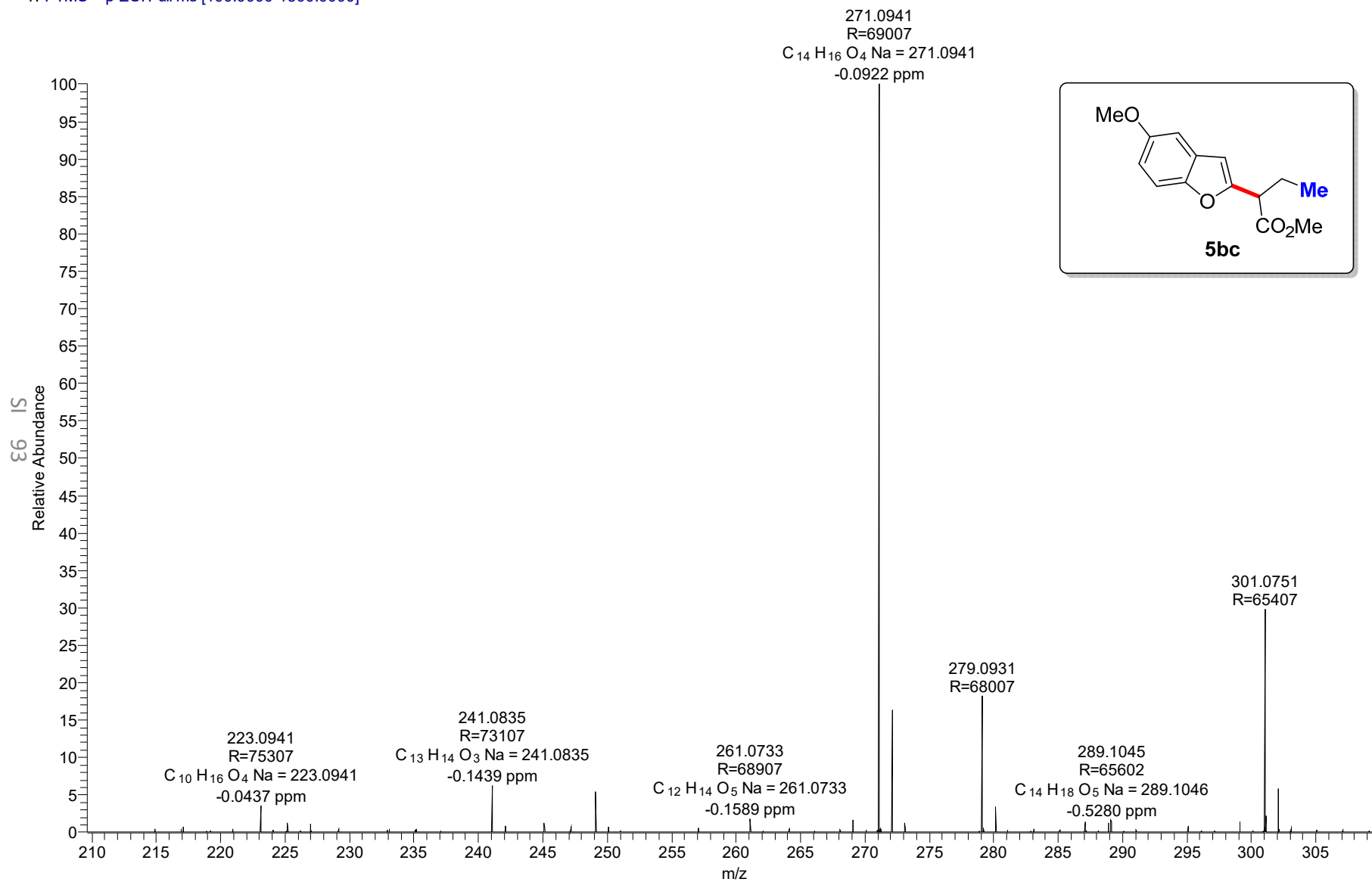
Comment	13C			
Date	31 Jan 2017 18:29:28	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	1184	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 22.600



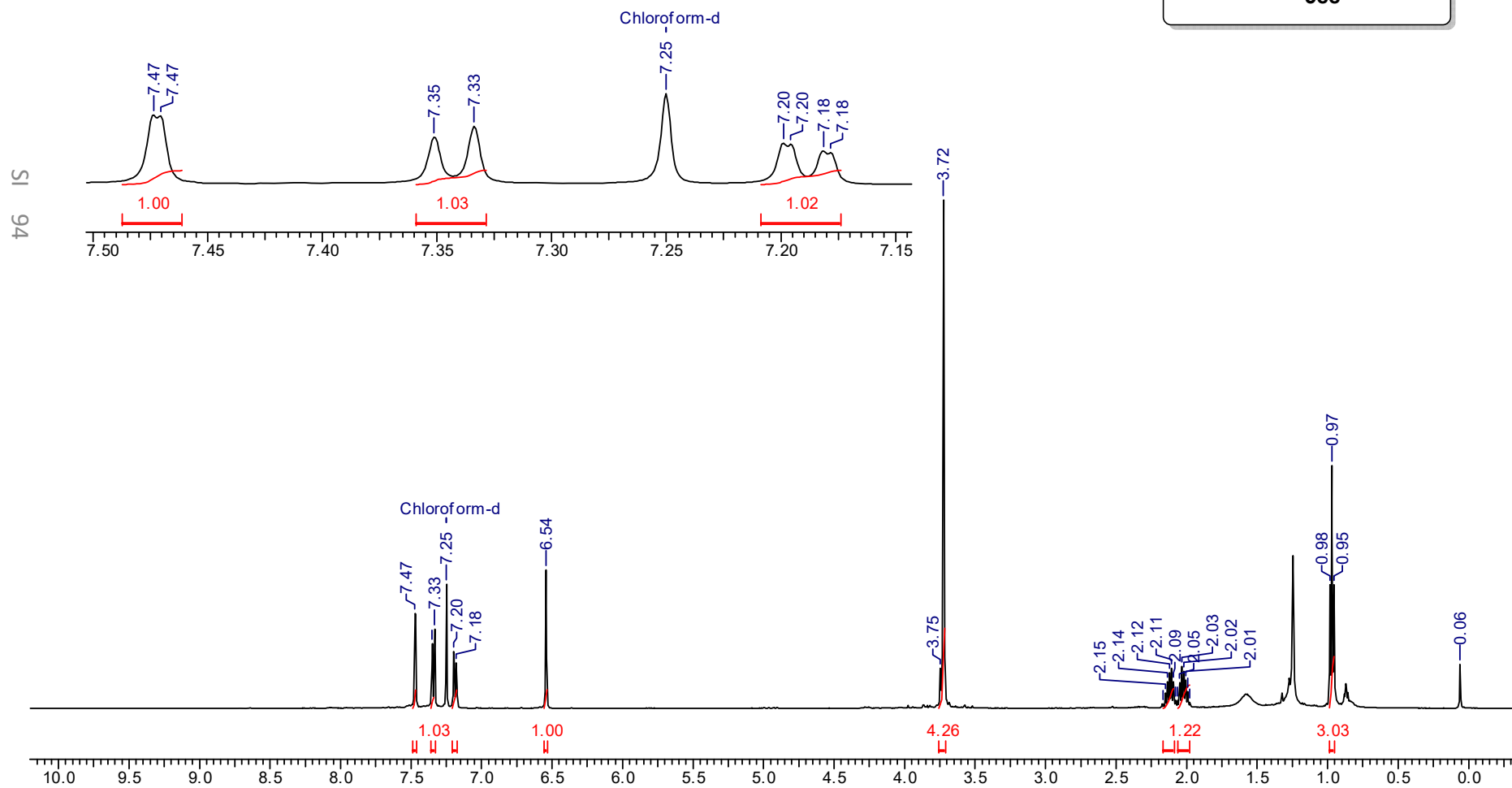
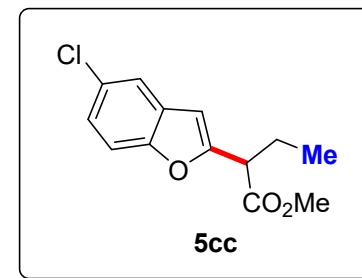
Comment	DEPT				
Date	31 Jan 2017 18:16:40	Frequency (MHz)	100.61	Nucleus	¹³ C
Number of Transients	400	Original Points Count	16384	Points Count	32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C)	21.900



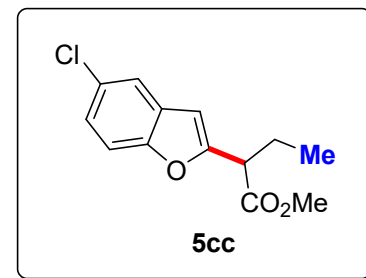
JY-B-5B #121 RT: 0.54 AV: 1 NL: 1.75E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



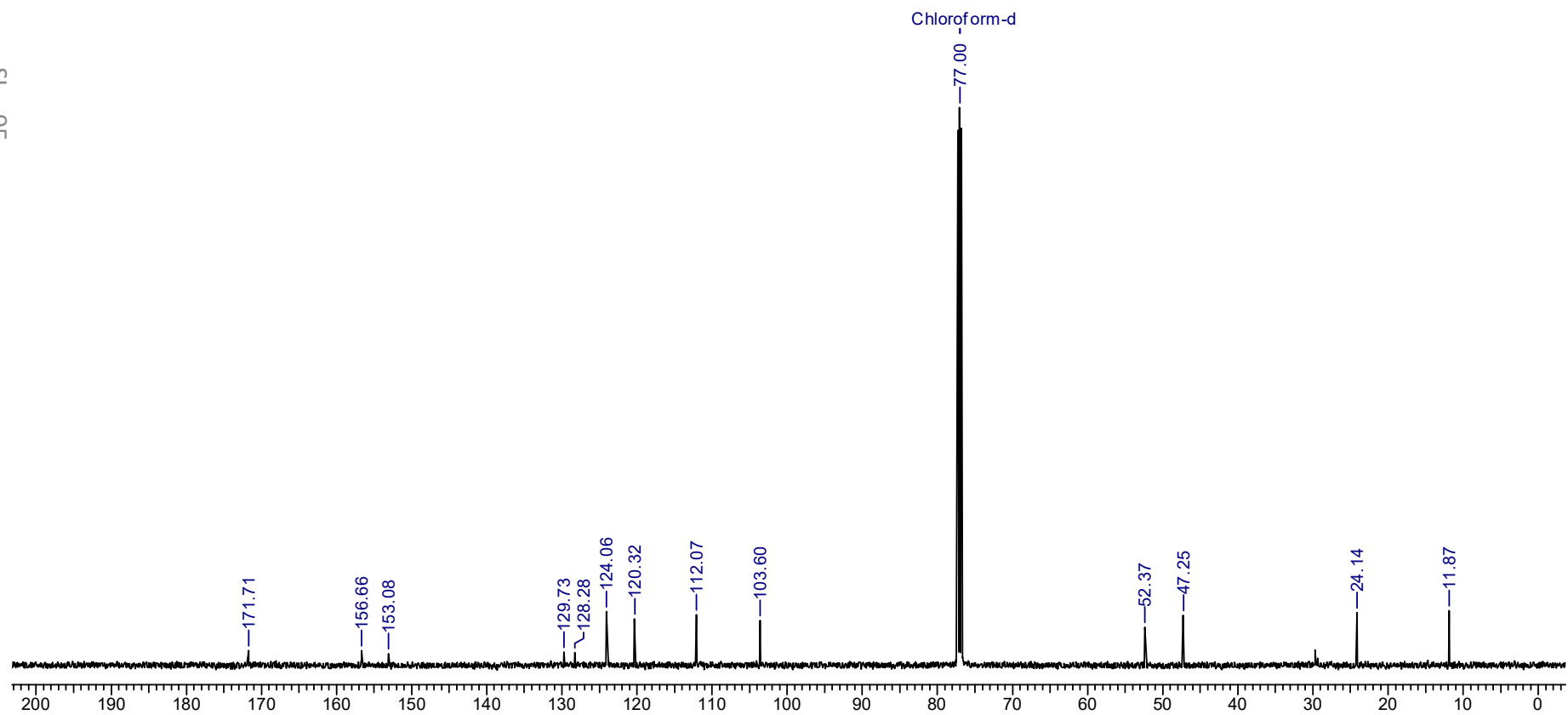
Acquisition Time (sec)	1.2800	Comment	Manmath. B 1H	Date	12 May 2017 12:59:12
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	32
Solvent	CHLOROFORM-d	Sweep Width (Hz)	12499.62	Original Points Count	16000
				Points Count	32768
				Temperature (grad C)	23.600



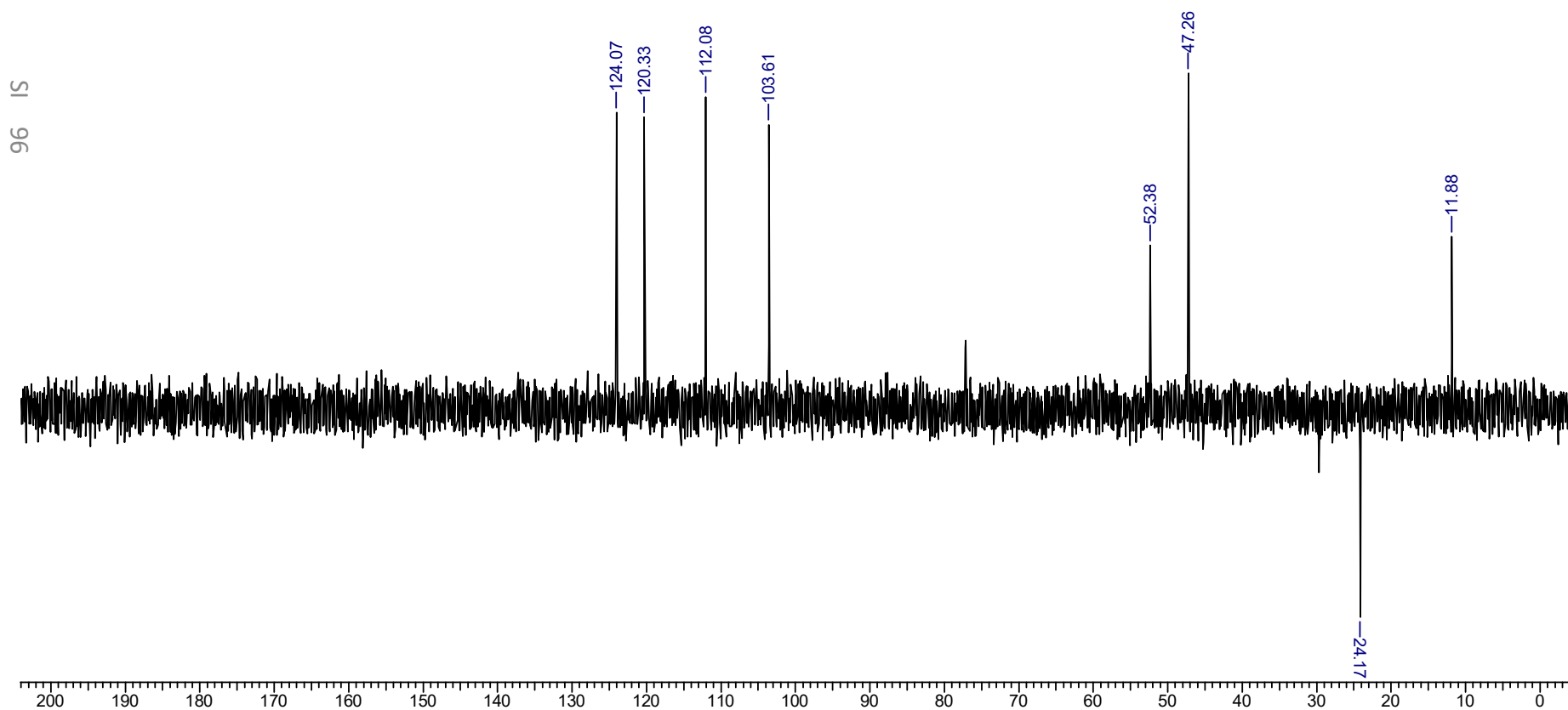
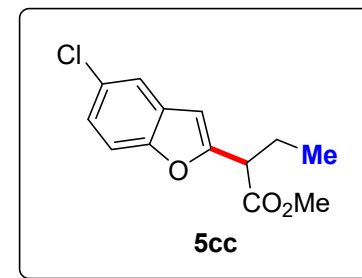
Acquisition Time (sec)	0.6554	Comment	13C	Date	12 May 2017 12:59:12	Frequency (MHz)	125.76
Nucleus	13C	Number of Transients	700	Original Points Count	20480	Points Count	32768
Sweep Width (Hz)	31249.05			Temperature (grad C)	24.100	Solvent	CHLOROFORM-d



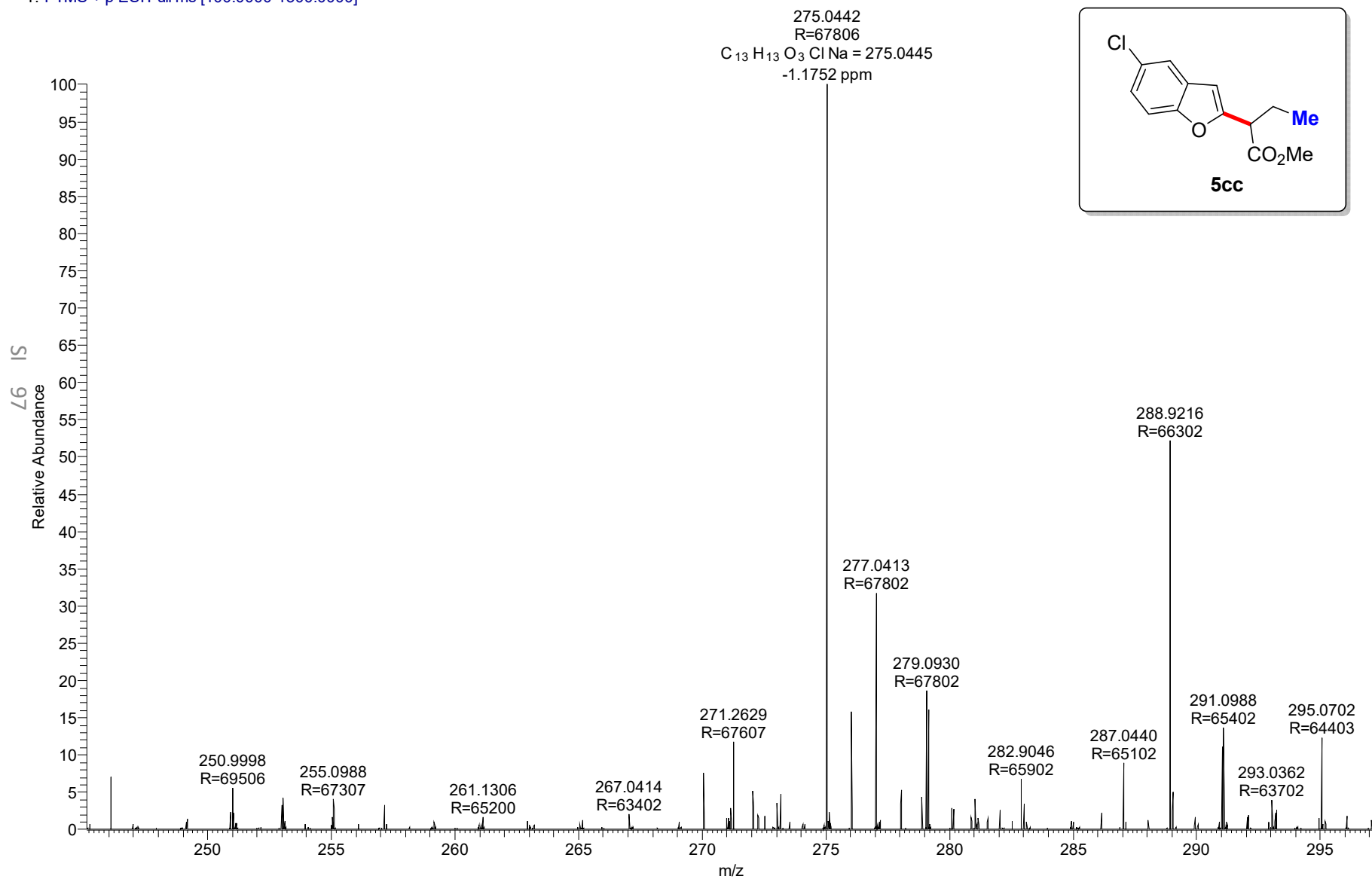
56 IS



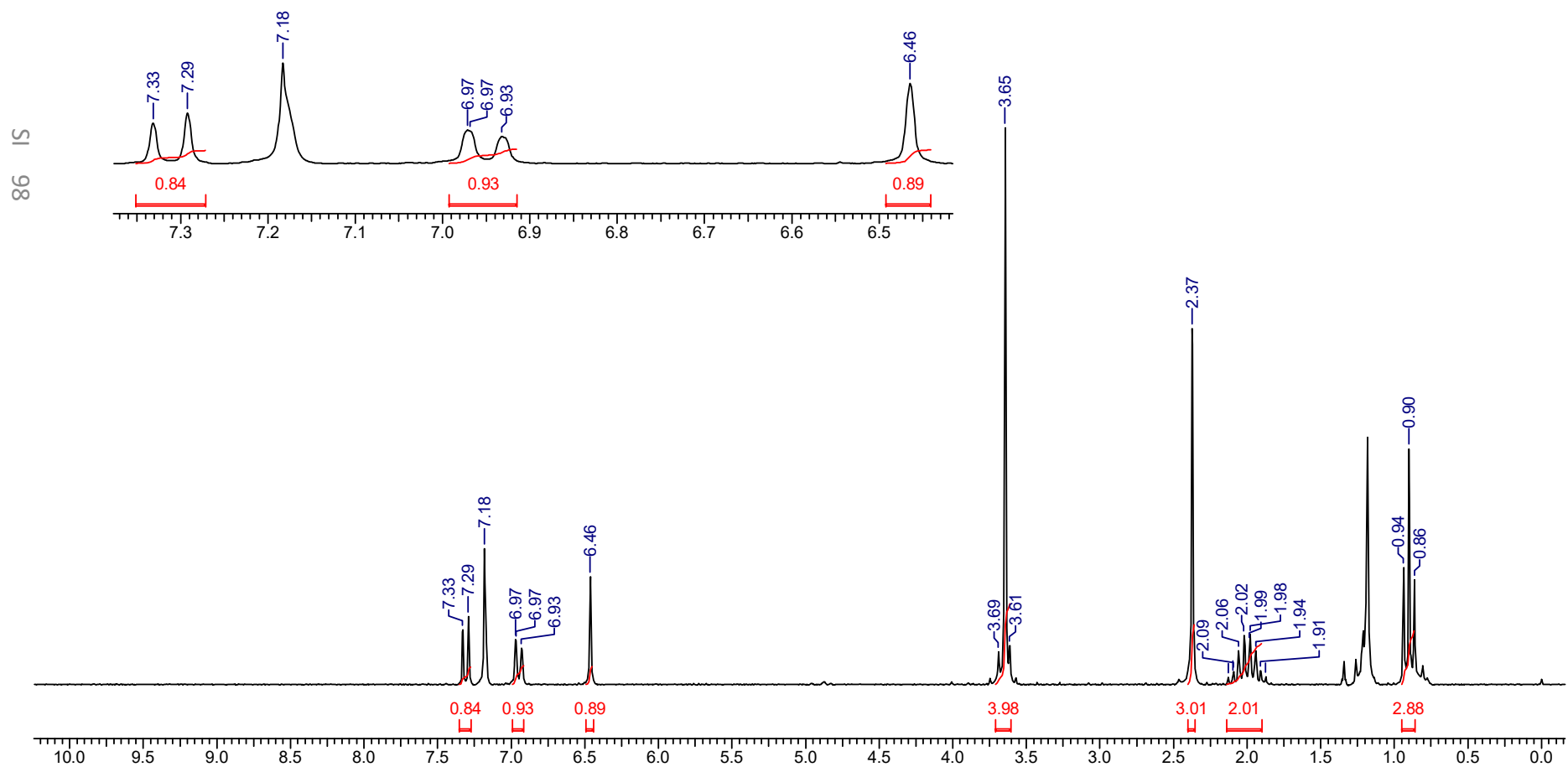
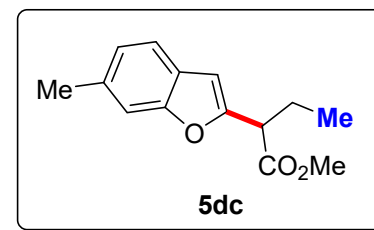
Acquisition Time (sec)	0.6554	Comment	Shrinivas DEPT			Date	27 May 2017 14:33:04		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	400	Original Points Count	20480	Points Count	32768
Solvent	CHLOROFORM-d			Sweep Width (Hz)	31249.05	Temperature (grad C)	25.700		



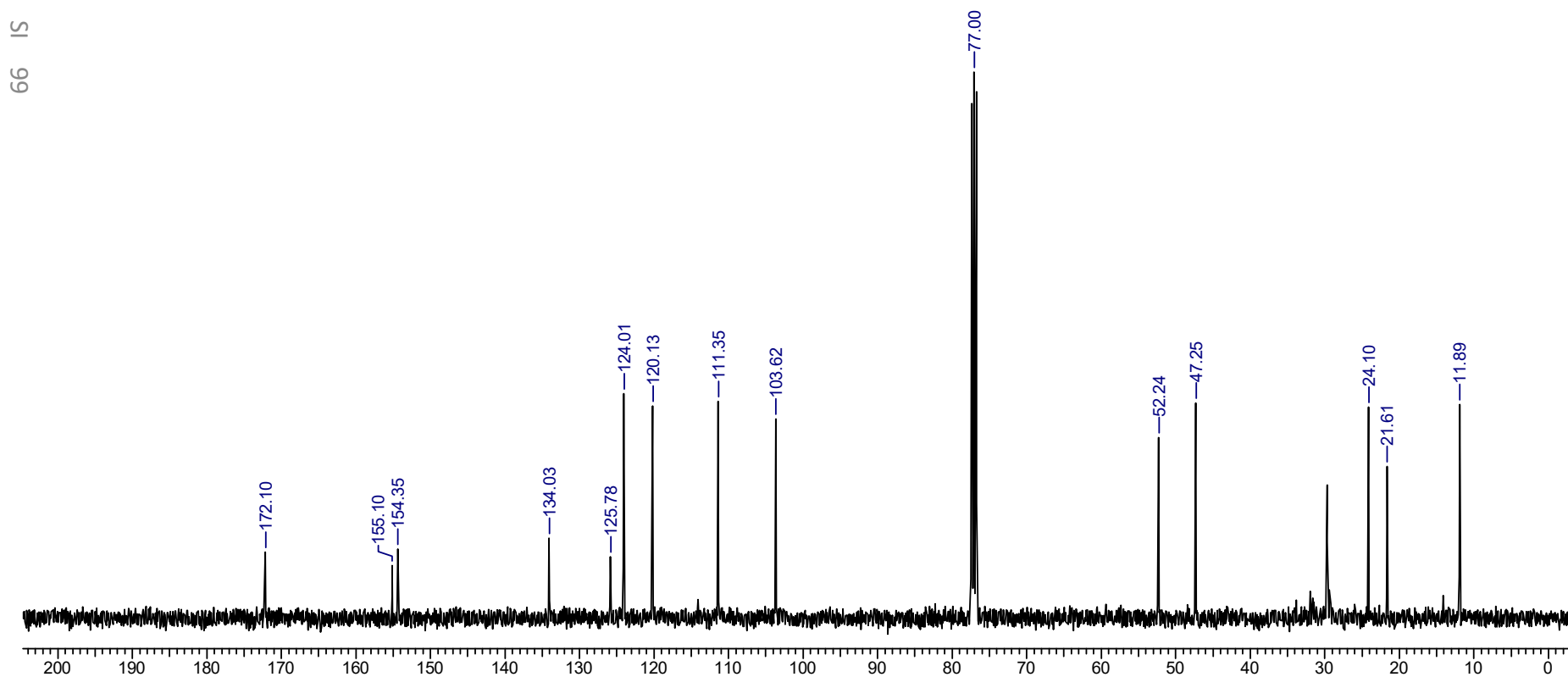
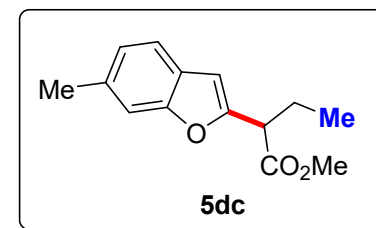
JY-B-6B_171102145506 #151 RT: 0.67 AV: 1 NL: 6.18E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]



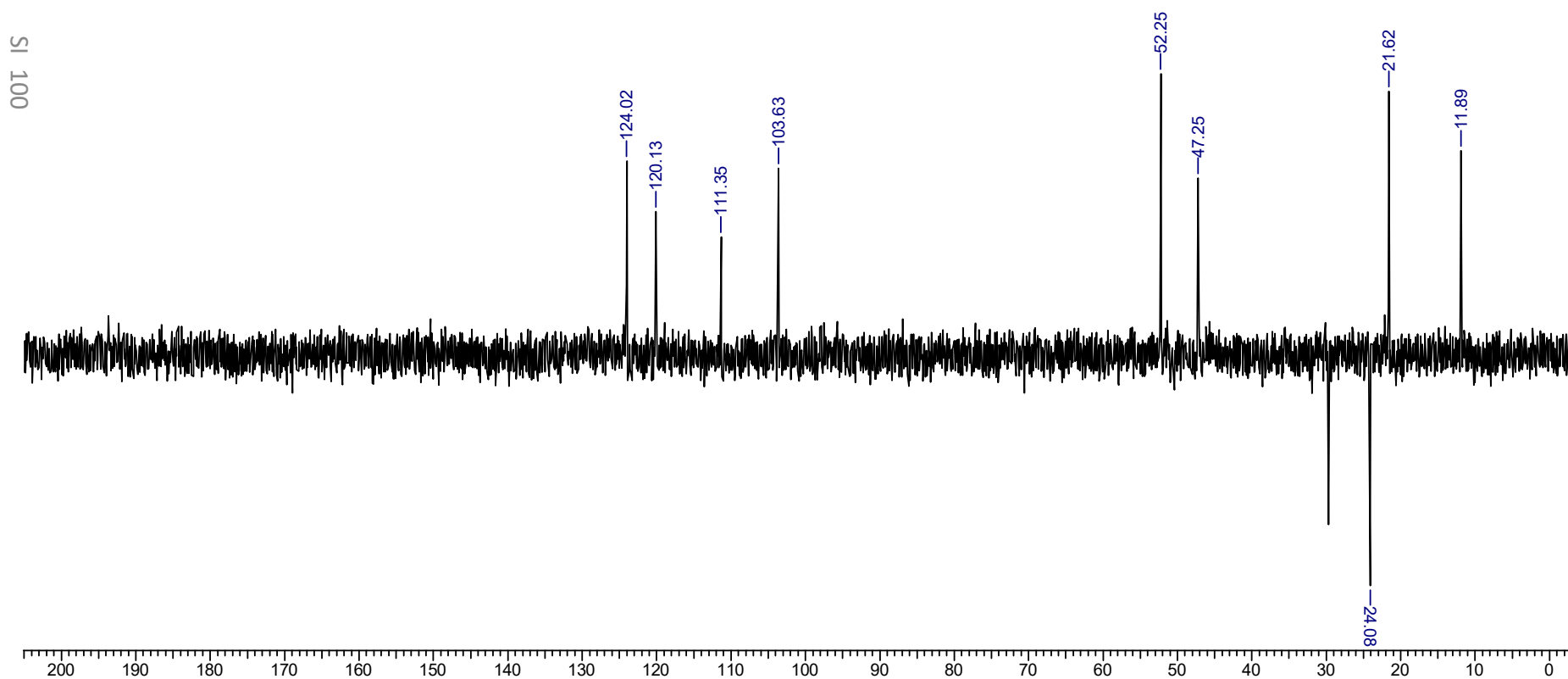
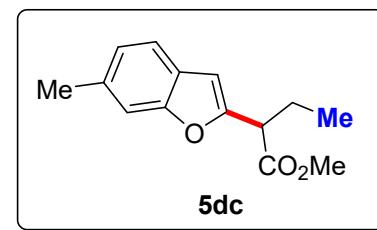
Acquisition Time (sec)	3.9584	Comment	Srinivas	Date	28 Feb 2017 16:08:40		Frequency (MHz)	200.13	
Nucleus	1H	Number of Transients	4	Original Points Count	16384	Points Count	32768	Solvent	CHLOROFORM-d
Sweep Width (Hz)	4138.95	Temperature (grad C)	27.000						



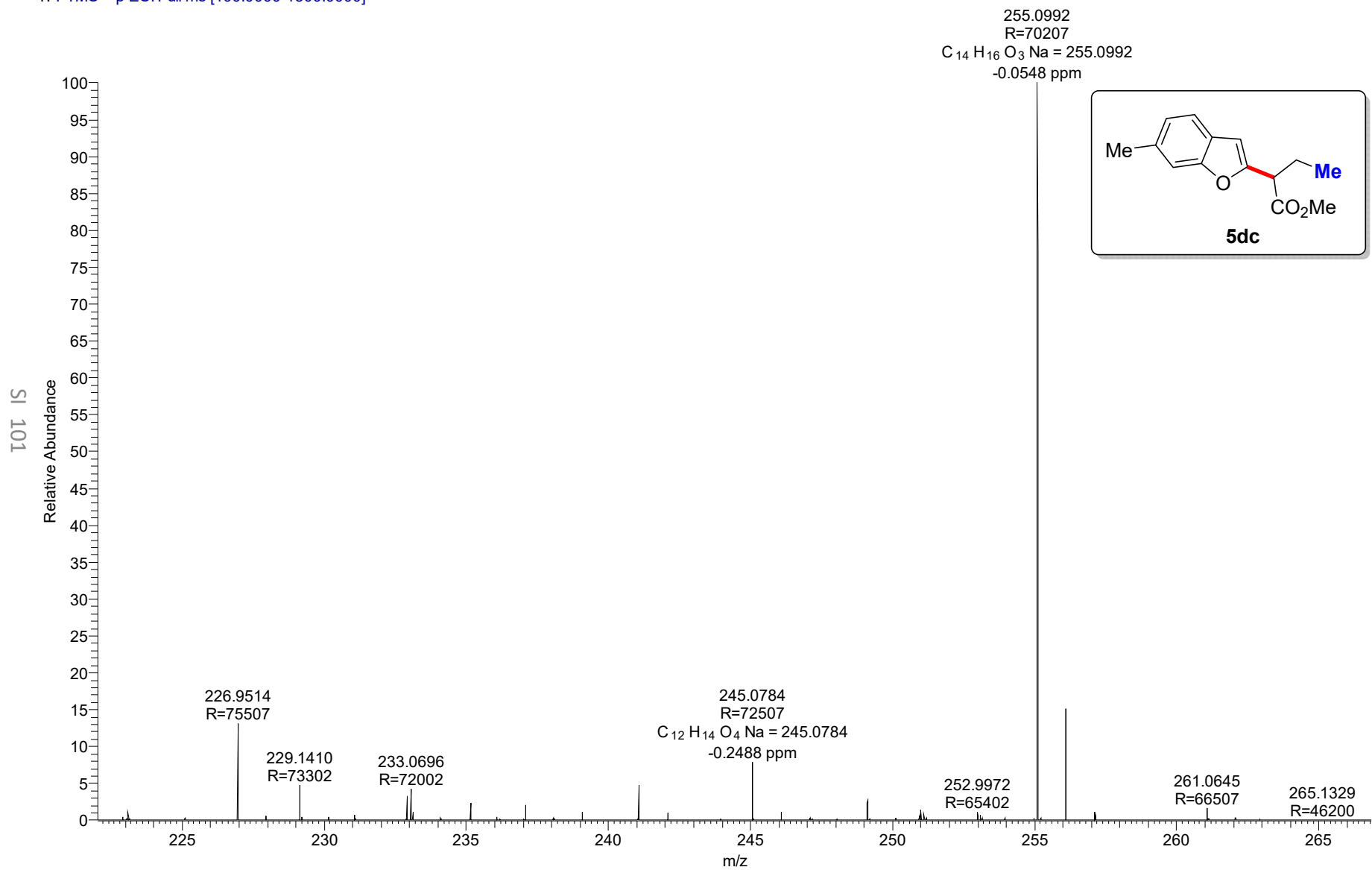
Comment	13C			
Date	09 Mar 2017 12:52:24	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	403	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 22.100



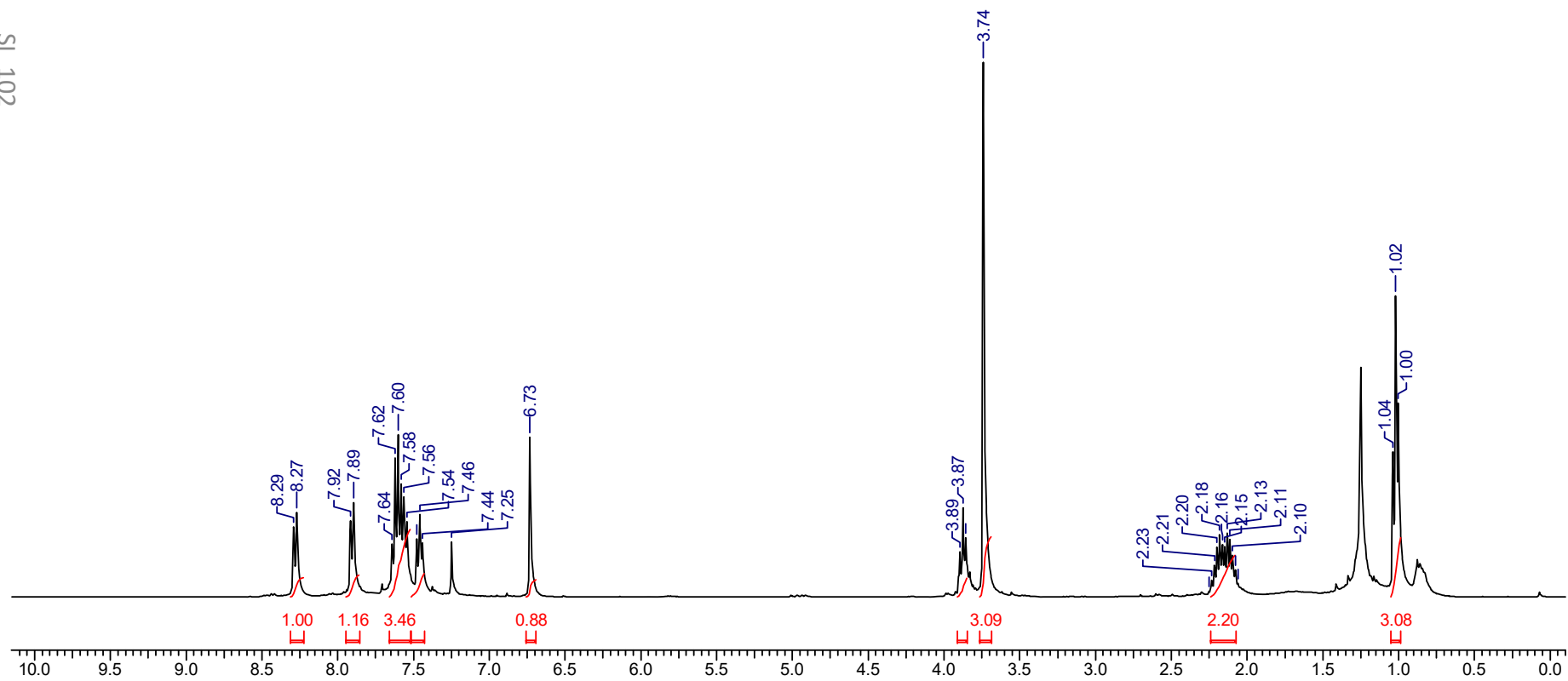
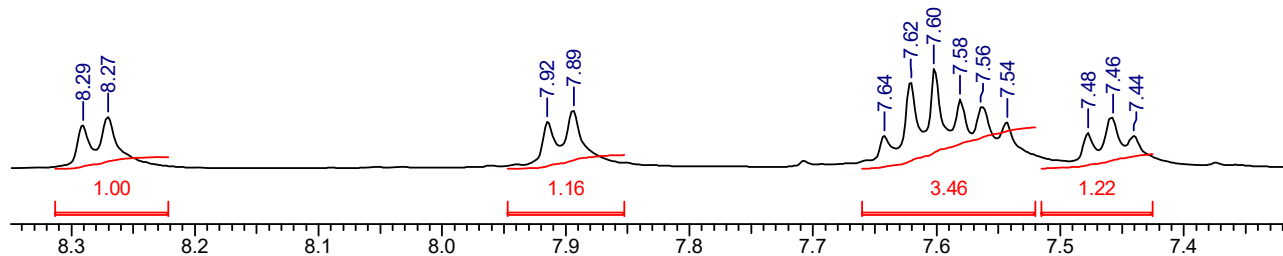
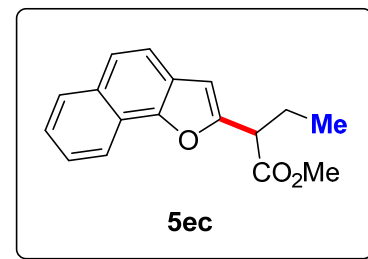
Comment	DEPT			
Date	09 Mar 2017 12:46:00	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	536	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 22.100



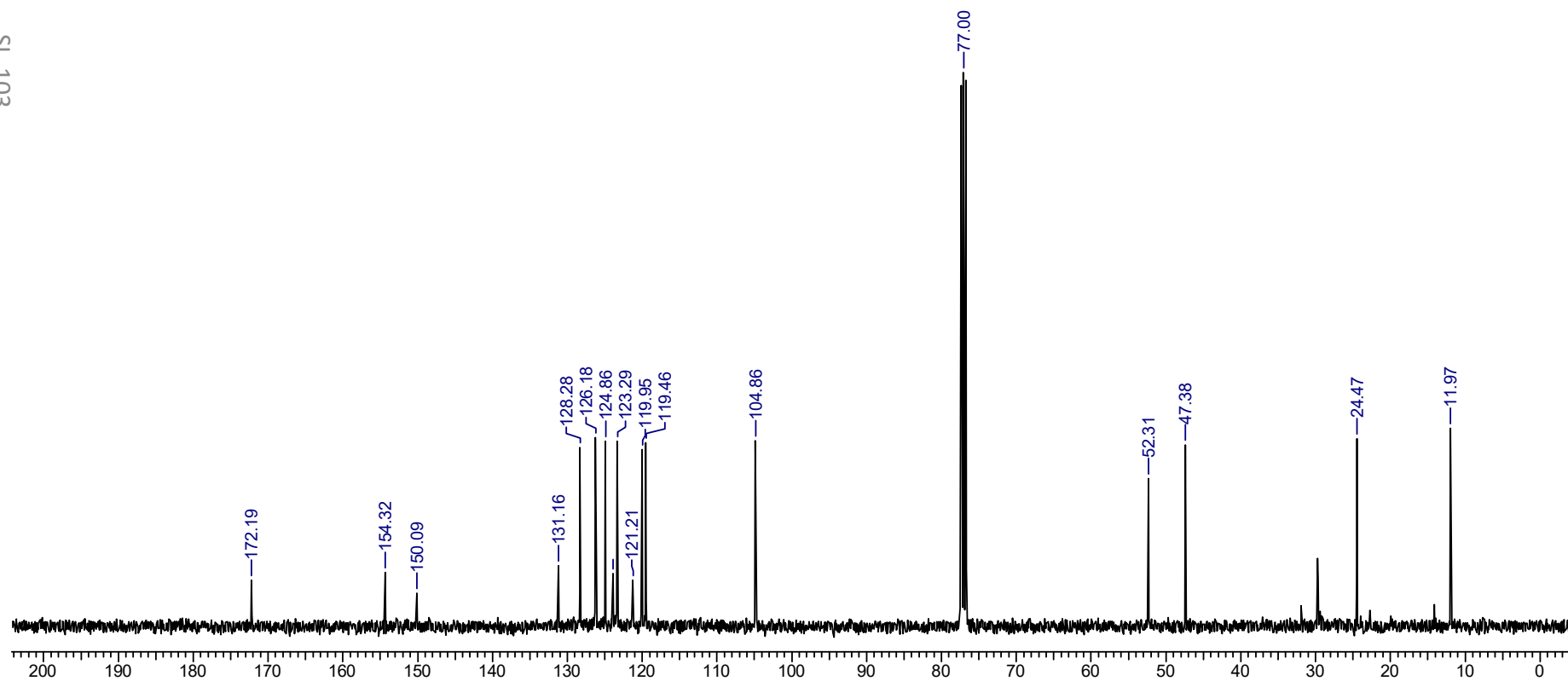
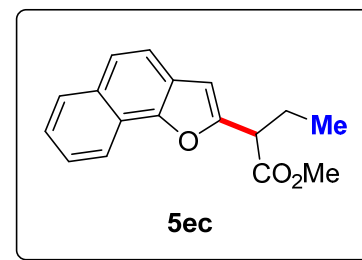
JY-B-6A #150 RT: 0.67 AV: 1 NL: 2.05E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



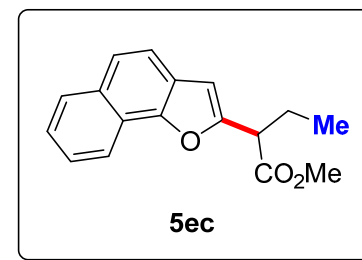
Comment	Jyothi 1H		
Date	11 Apr 2017 12:56:40	Frequency (MHz)	400.13
Number of Transients	64	Original Points Count	16384
Solvent	CHLOROFORM-d	Sweep Width (Hz)	9999.39
		Nucleus	1H
		Points Count	16384
		Temperature (grad C)	21.000



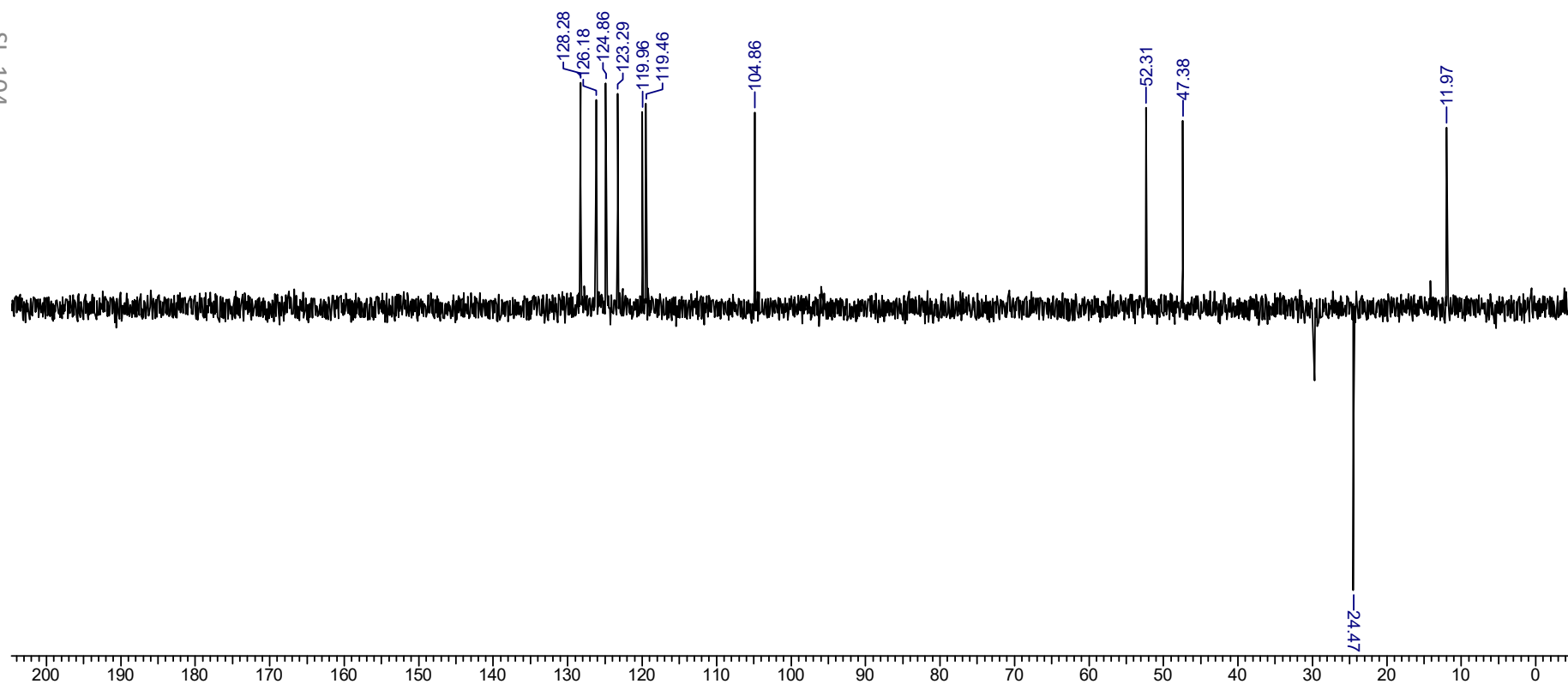
Comment	13C			
Date	11 Apr 2017 14:00:40	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	1603	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 21.900



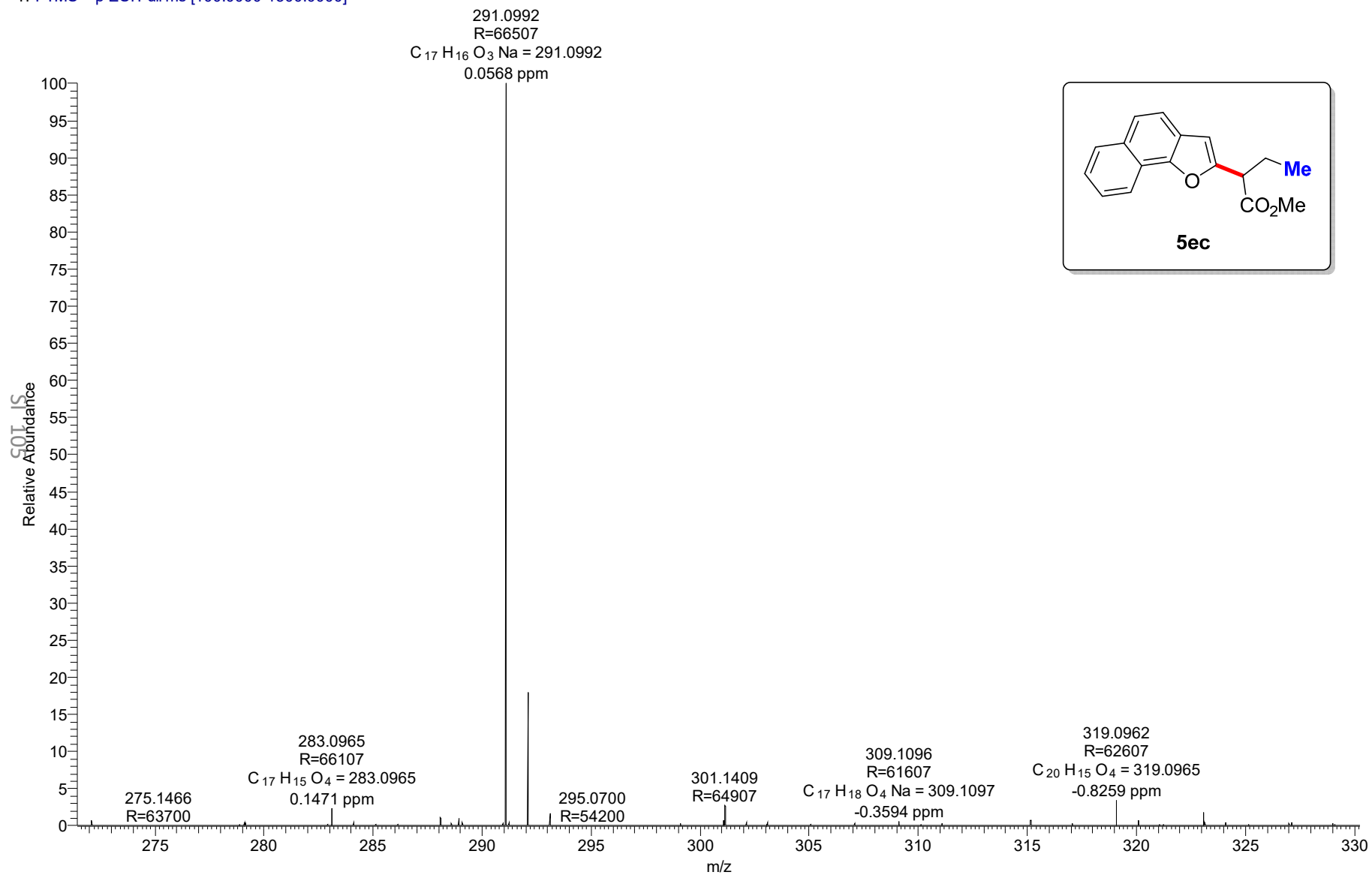
Comment	DEPT			
Date	11 Apr 2017 13:13:44	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	600	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 21.200



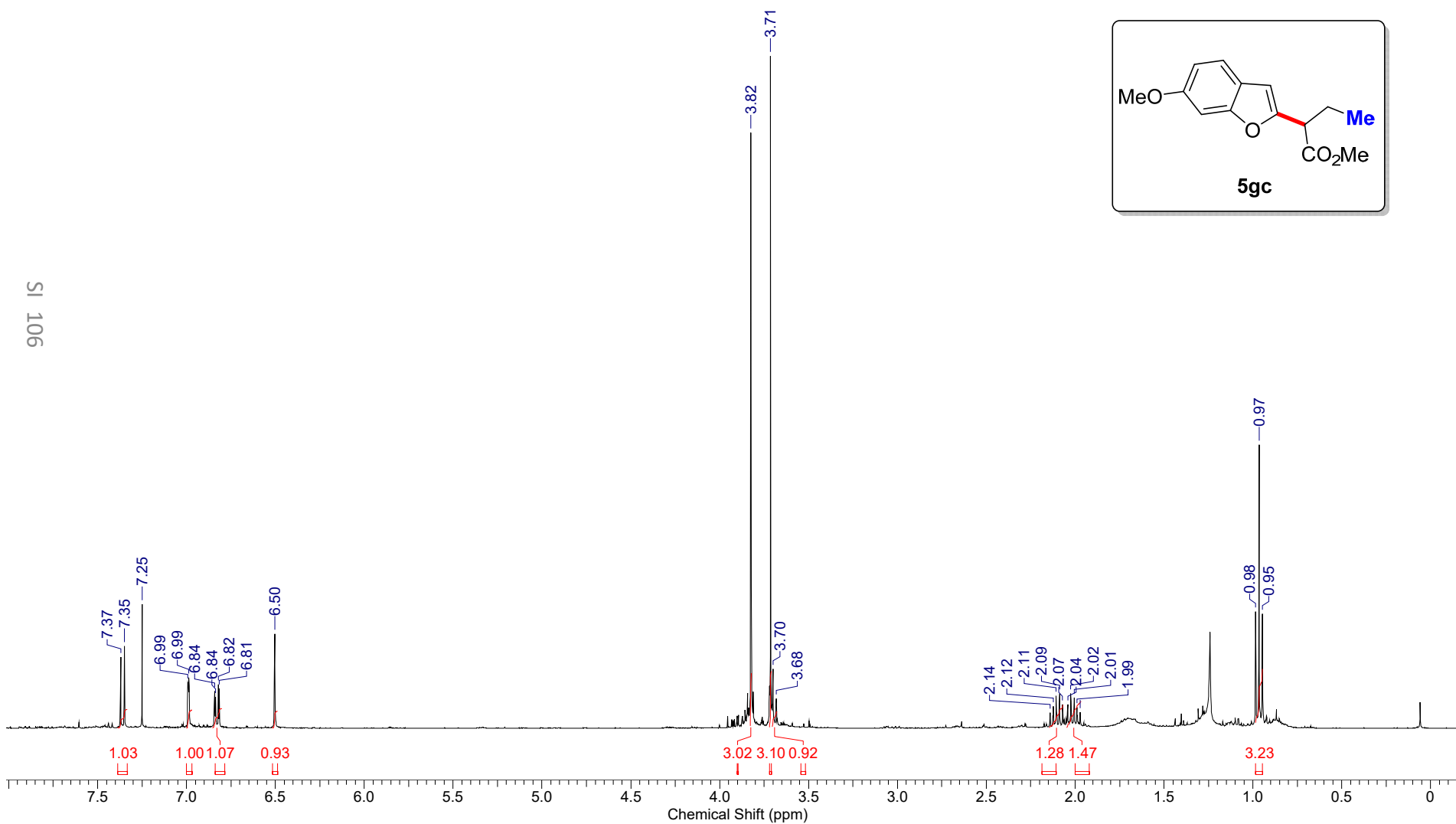
SI 104



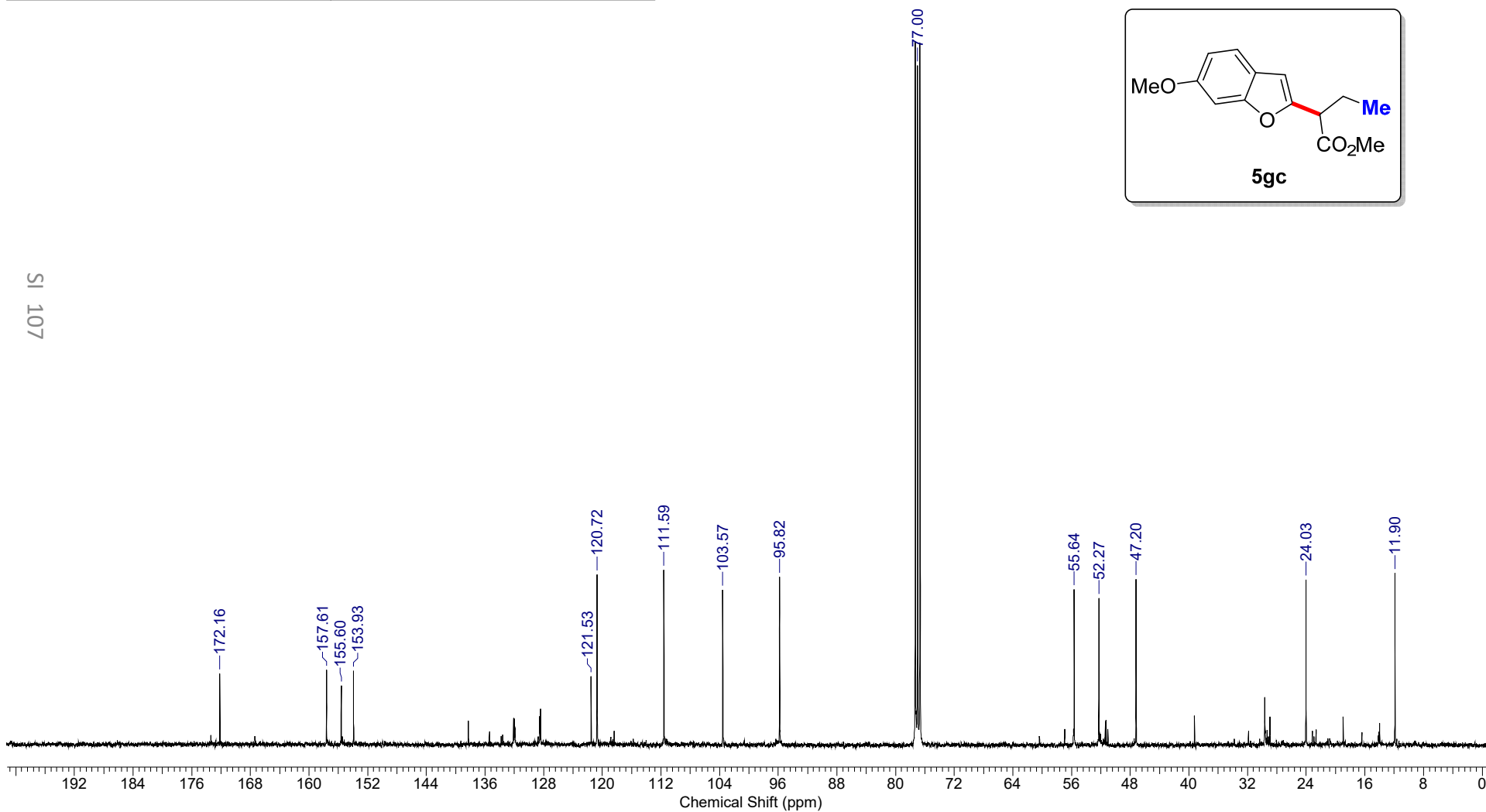
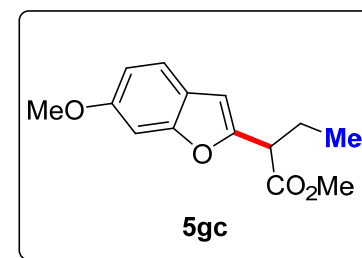
JY-B-11A #157 RT: 0.70 AV: 1 NL: 2.52E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



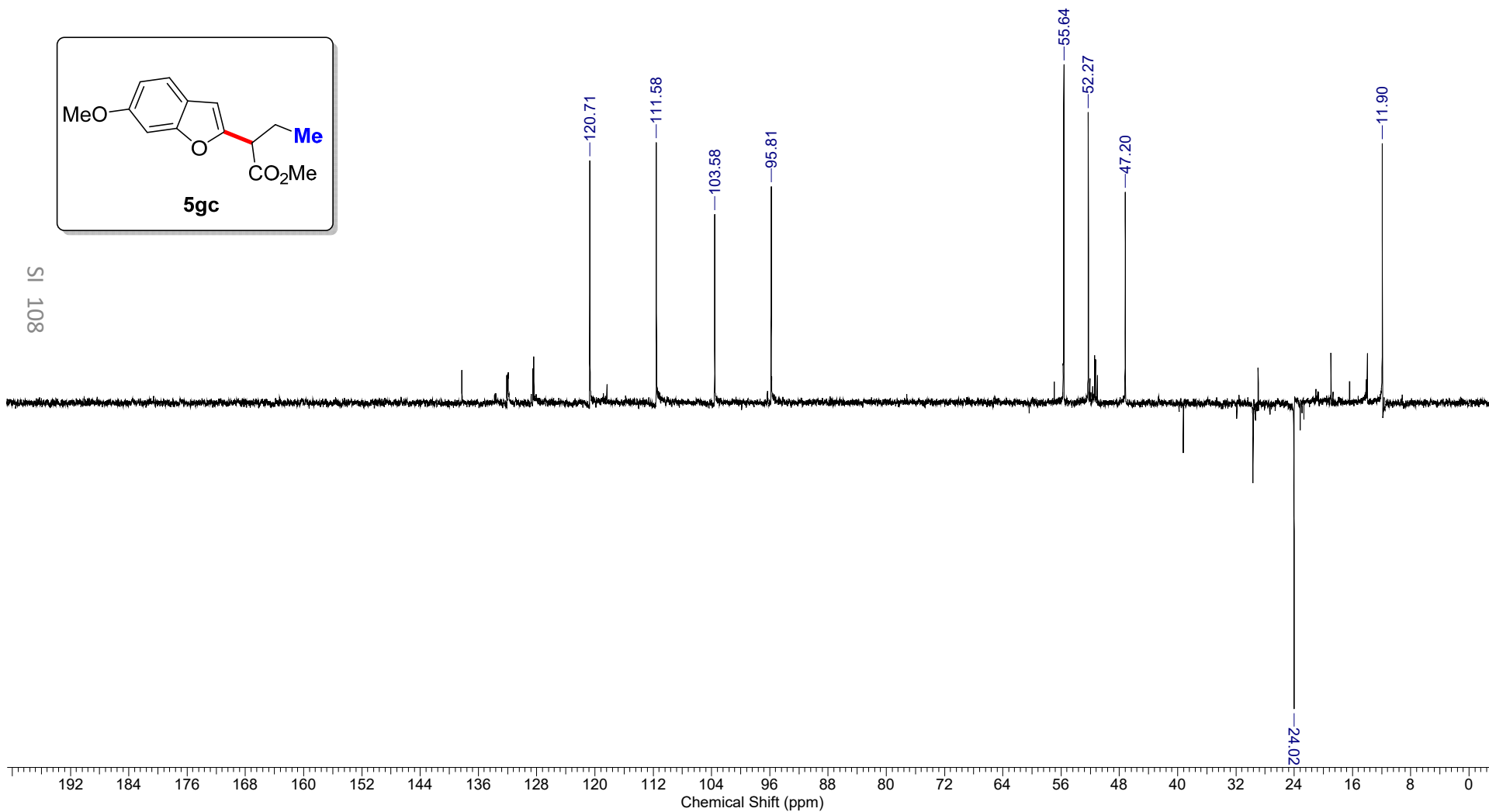
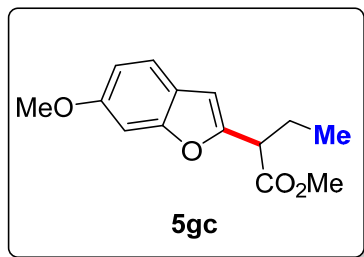
Acquisition Time (sec)	1.3108	Comment	Gaudappagauda	Date	31 Jan 2019 17:28:49
Date Stamp	31 Jan 2019 15:36:53				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2019_JEOL_400\Jan_Liquid state_2019\AV-500-20190123-112115-44698_PROTON-3.jdf				
Frequency (MHz)	399.78	Nucleus	¹ H	Number of Transients	16
Original Points Count	13107	Owner	delta	Points Count	13107
Receiver Gain	42.00	Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse.ex2
Sweep Width (Hz)	9999.08	Temperature (degree C)	18.300	Spectrum Offset (Hz)	2798.4758
				Spectrum Type	STANDARD



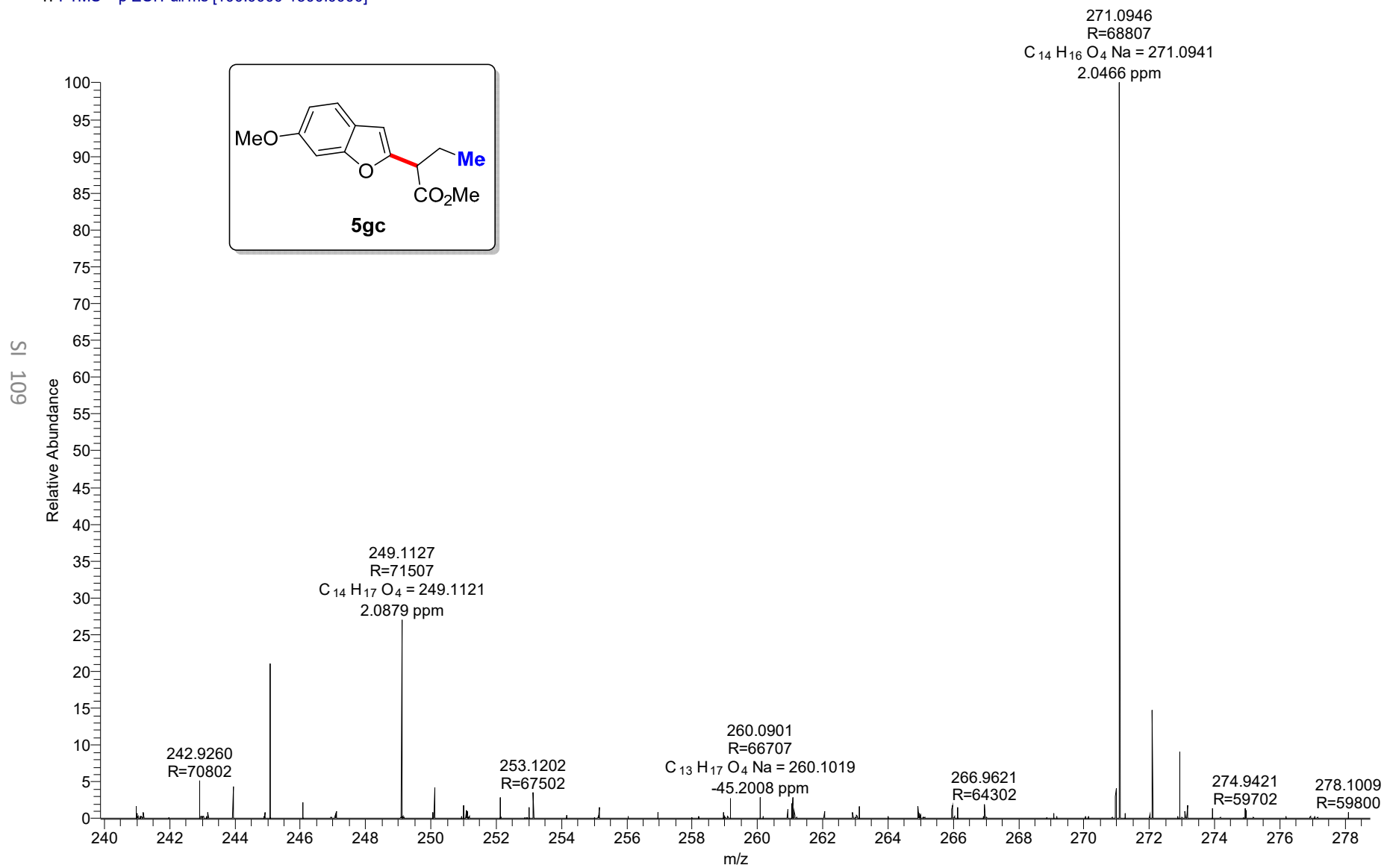
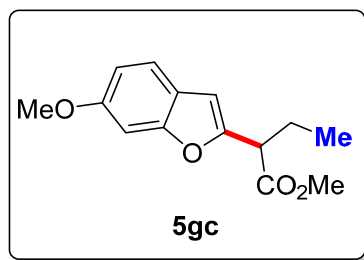
Acquisition Time (sec)	1.0434	Comment	Harish	Date	06 Sep 2018 15:16:50		
Date Stamp	06 Sep 2018 13:03:41						
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State_2018\AV-400-20180829-201935-44698_CARBON-3.jdf						
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	2000	Origin	ECX 400
Original Points Count	26214	Owner	delta	Points Count	26214	Pulse Sequence	single_pulse_dec
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10039.3311	Spectrum Type	STANDARD
Sweep Width (Hz)	25124.29	Temperature (degree C)	16.900				



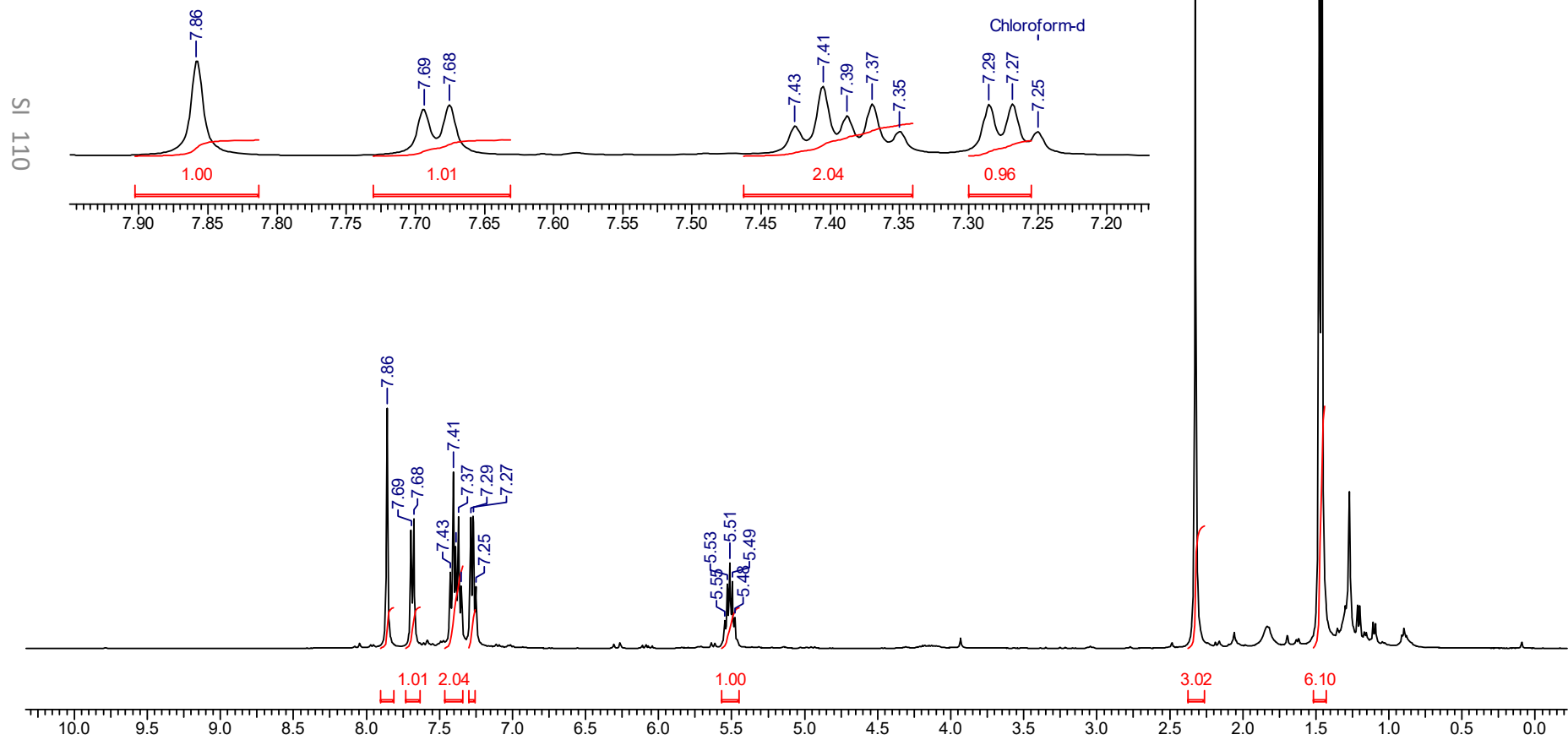
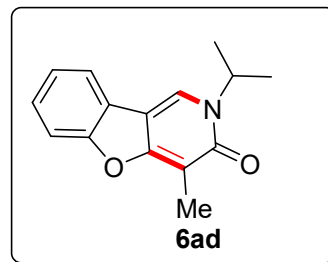
Acquisition Time (sec)	1.0434	Comment	Harish	Date	06 Sep 2018 15:16:50
Date Stamp	06 Sep 2018 13:34:58				
File Name	\\172.16.2.4\nmr_data\Jeol_400\2018_JEOL_400\August_Liquid State 2018\AV-400-20180829-201935-44698_DEPT135-3.jdf				
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	800
Original Points Count	26214	Owner	delta	Points Count	26214
Receiver Gain	60.00	Solvent	CHLOROFORM-d	Pulse Sequence	dept.ex2 (selection_angle=135)
Sweep Width (Hz)	25124.29	Temperature (degree C)	16.800	Spectrum Offset (Hz)	10038.5850
				Spectrum Type	DEPT135



KS-J-36B #506 RT: 2.25 AV: 1 NL: 5.15E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

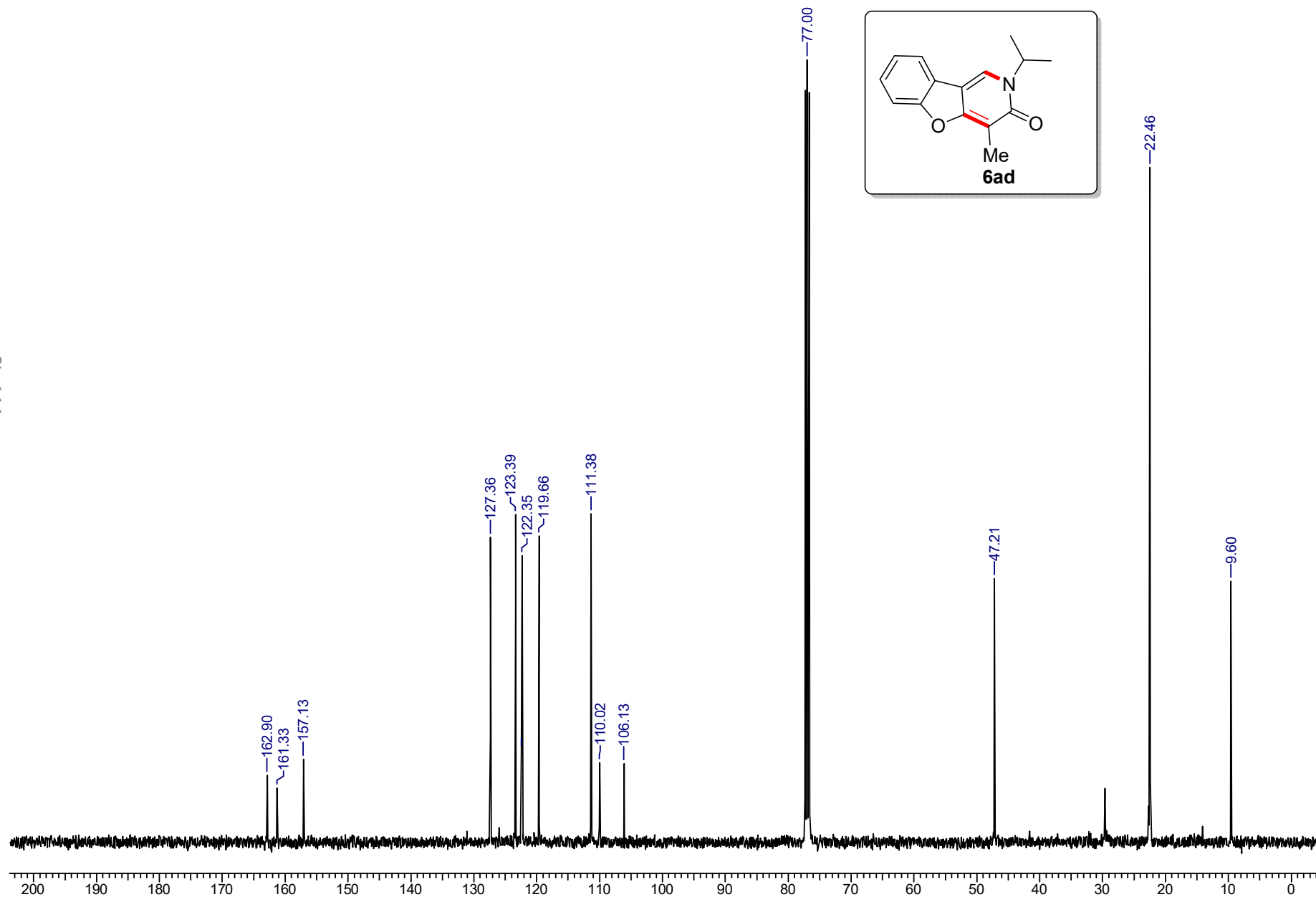


Acquisition Time (sec)	2.0447	Comment	Venkanan	Date	24/01/2016 12:46:26
Frequency (MHz)	400.13	Nucleus	¹ H	Original Points Count	16384
Temperature (grad C)	0.000			Points Count	16384
				Sweep Width (Hz)	8012.82

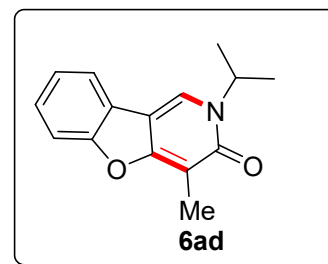


Acquisition Time (sec)	1.2976	Date	24/01/2016 12:45:36	Frequency (MHz)	100.61	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53	Temperature (grad C)	0.000

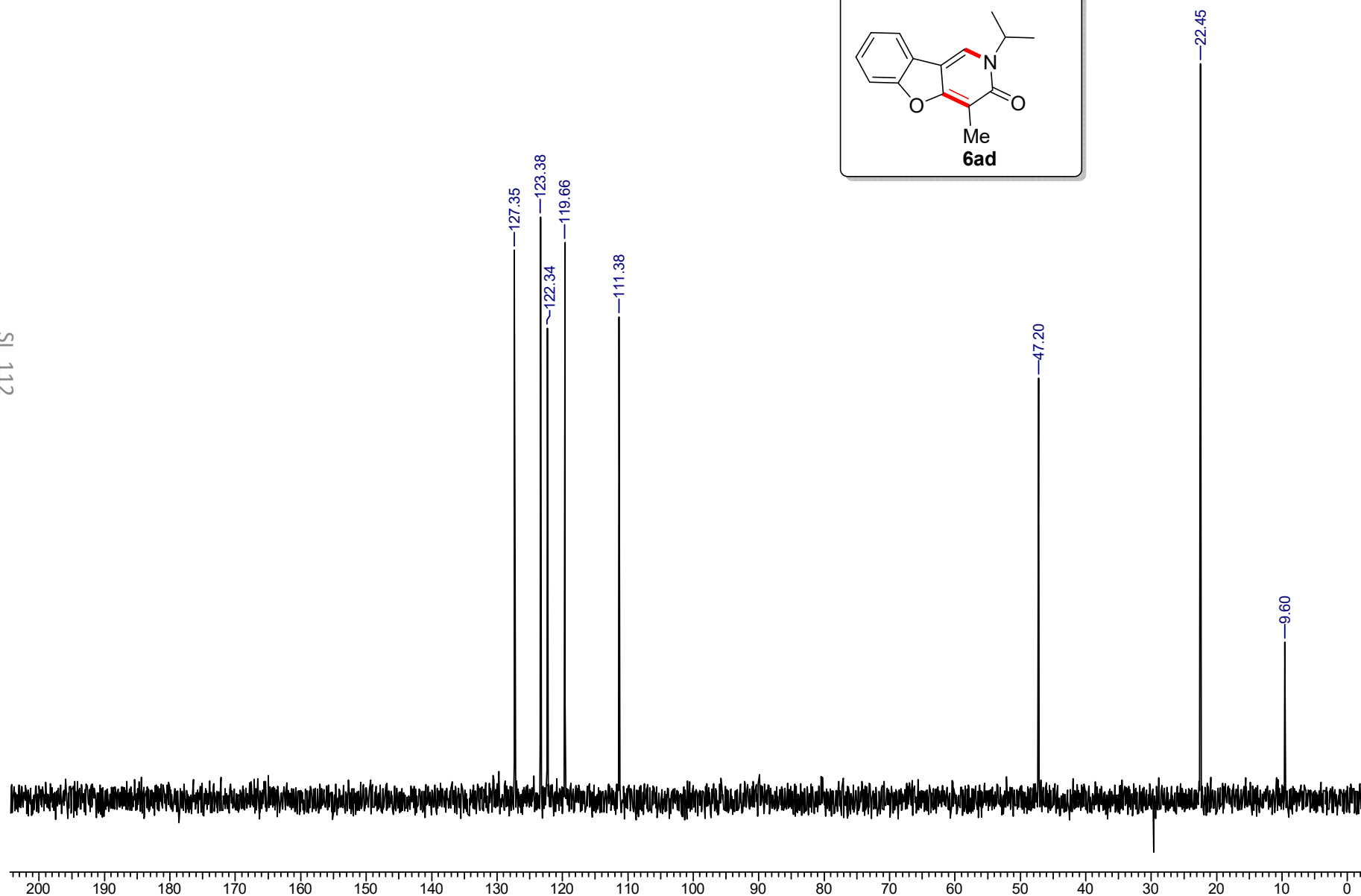
SI 111

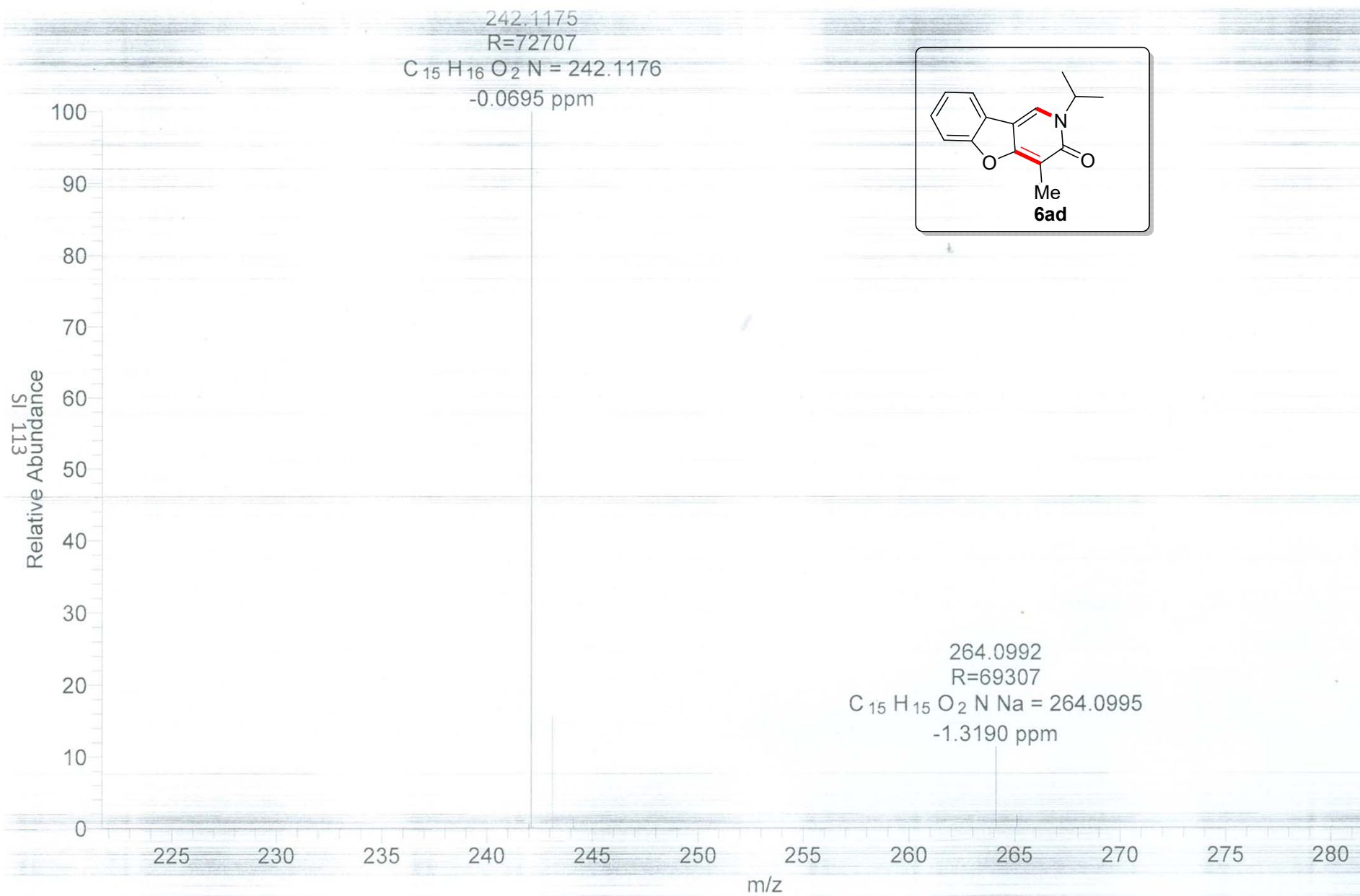


Acquisition Time (sec)	1.2976	Comment	DEPT	Date	31/01/2016 16:33:42	Frequency (MHz)	100.61
Nucleus	13C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53
Temperature (grad C)	0.000						

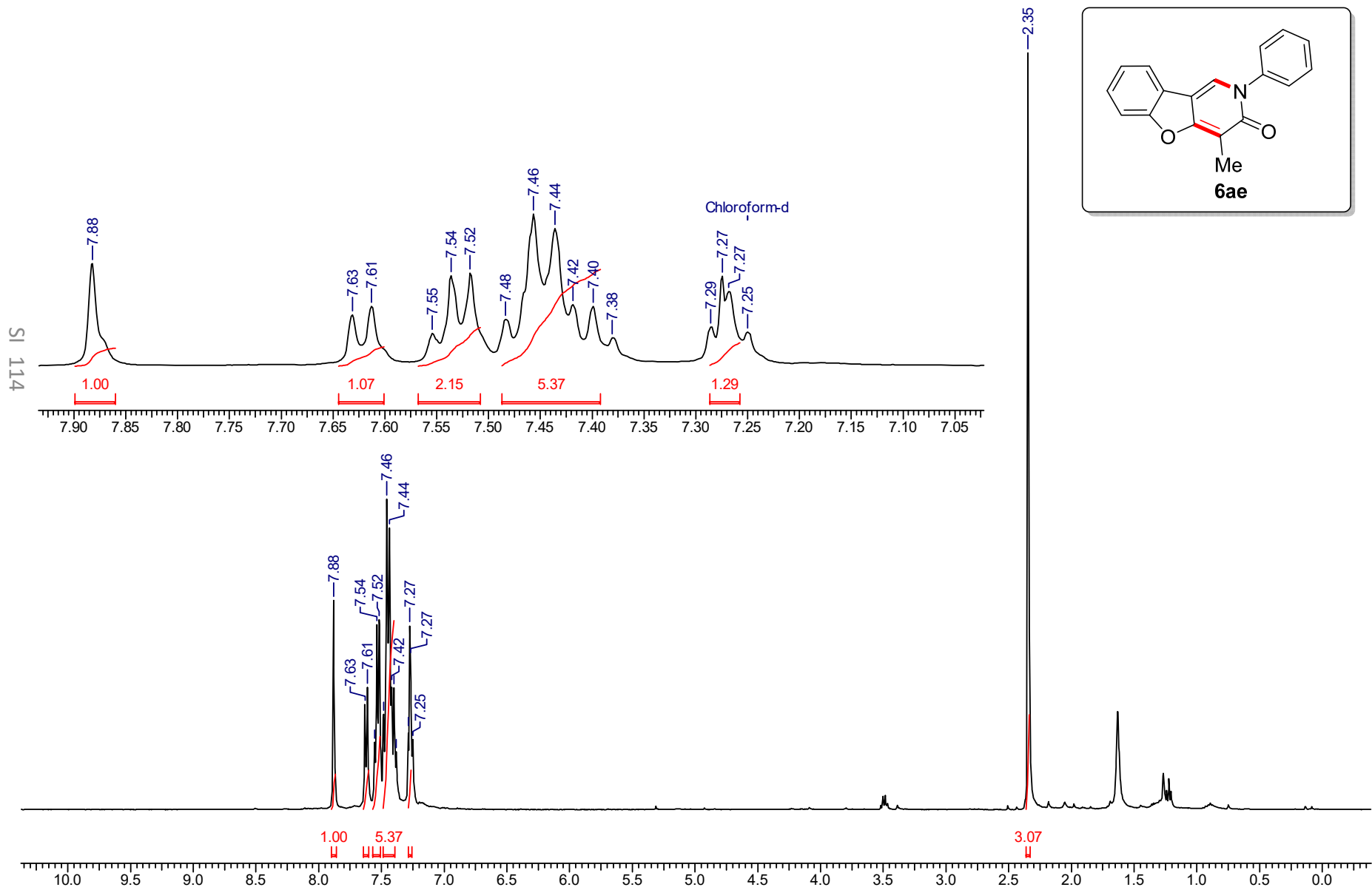


SI 112

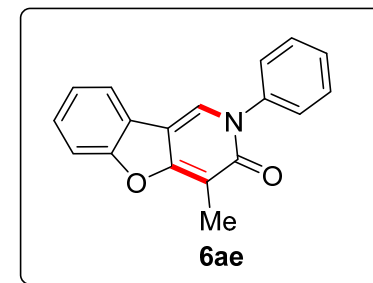
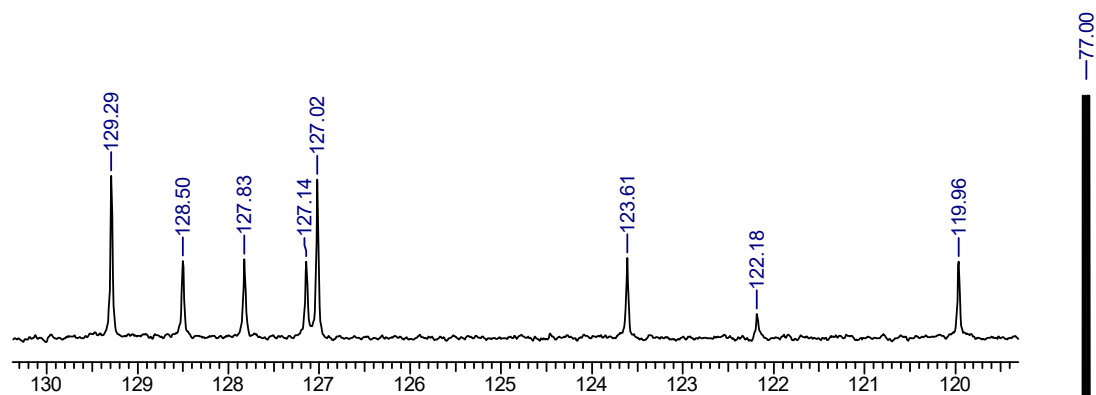




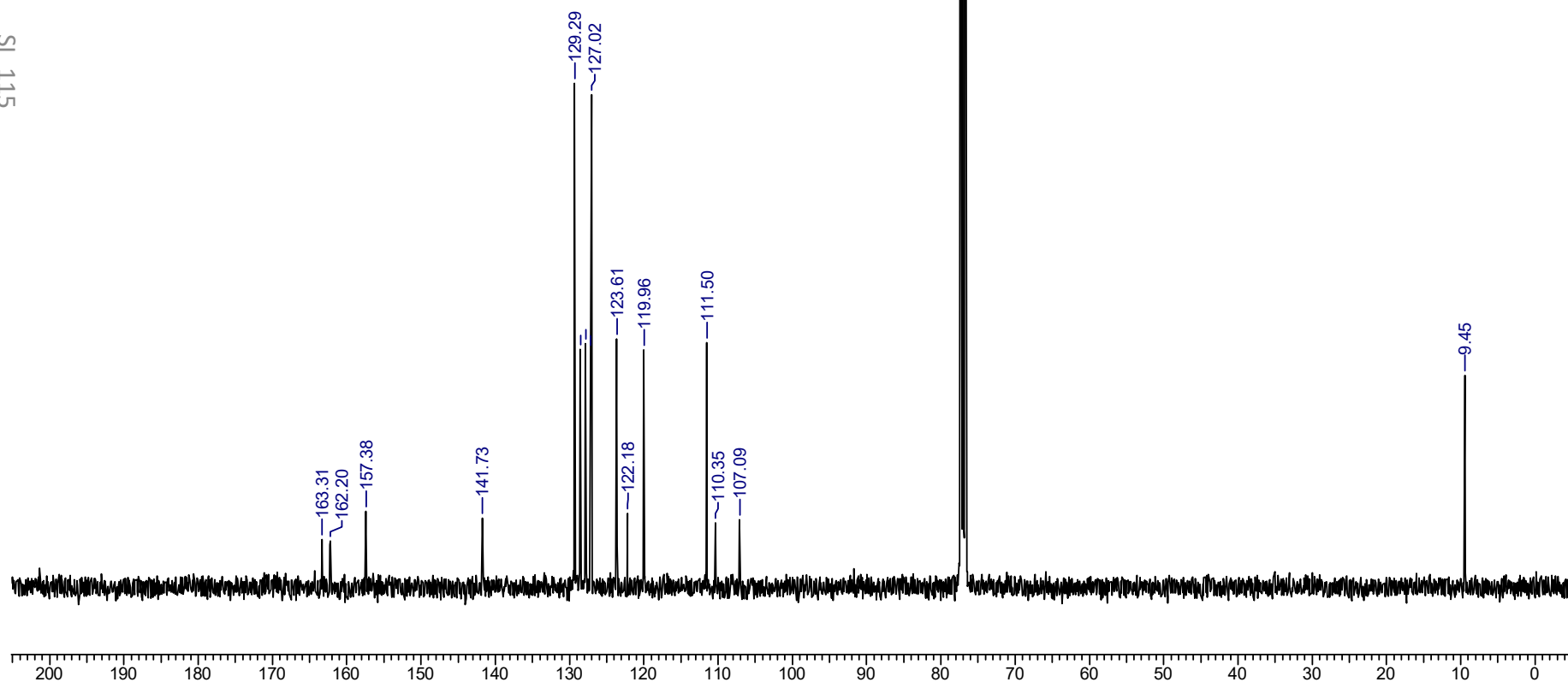
Acquisition Time (sec)	2.0447	Comment	Jyothi	Date	13/05/2016 18:09:06	Frequency (MHz)	400.13
Nucleus	¹ H	Original Points Count	16384	Points Count	16384	Sweep Width (Hz)	8012.82
Temperature (grad C)	0.000						



Acquisition Time (sec)	1.1010	Date	13/05/2016 18:55:22	Frequency (MHz)	100.61	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	29761.90	Temperature (grad C)	0.000

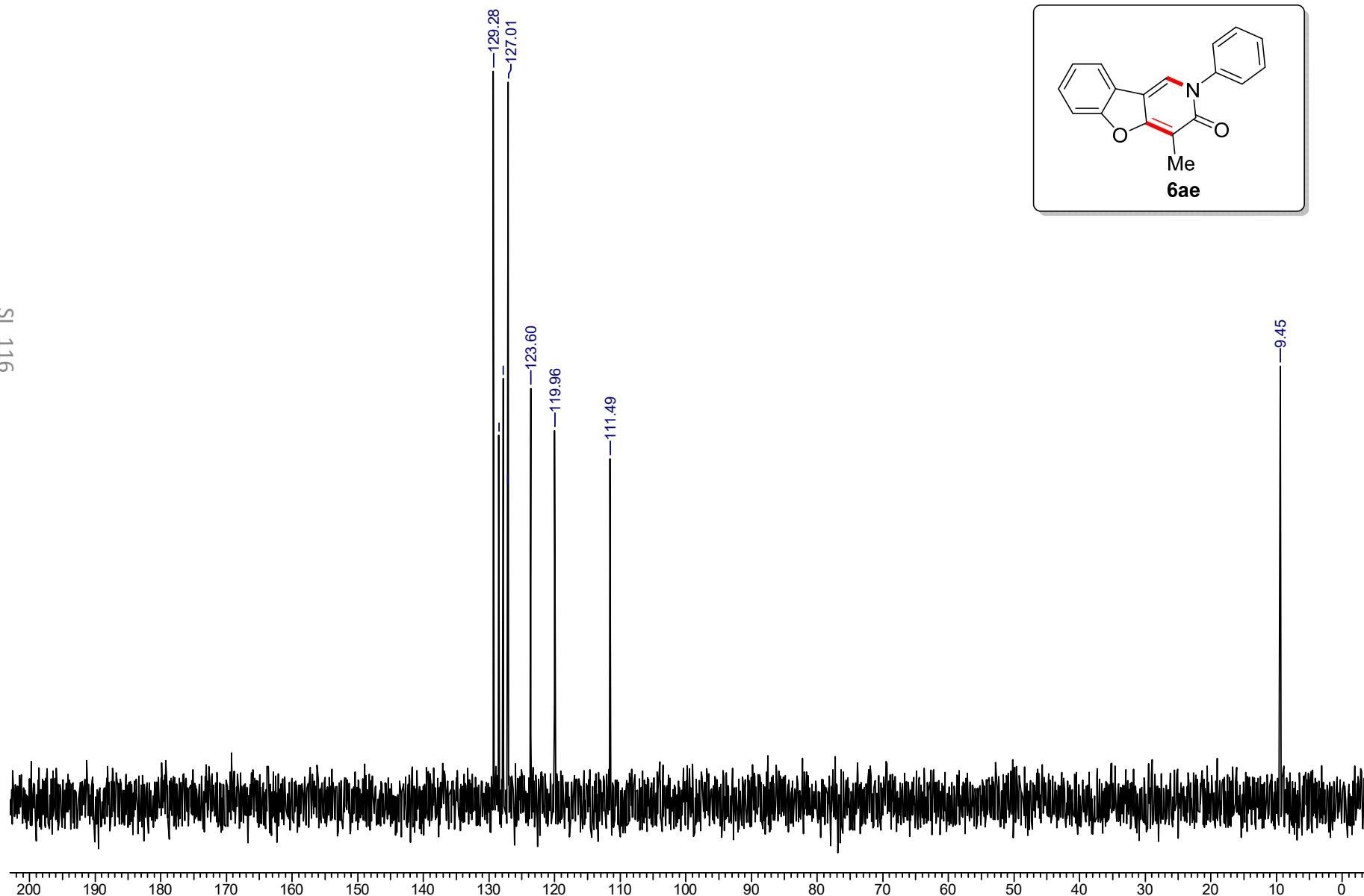


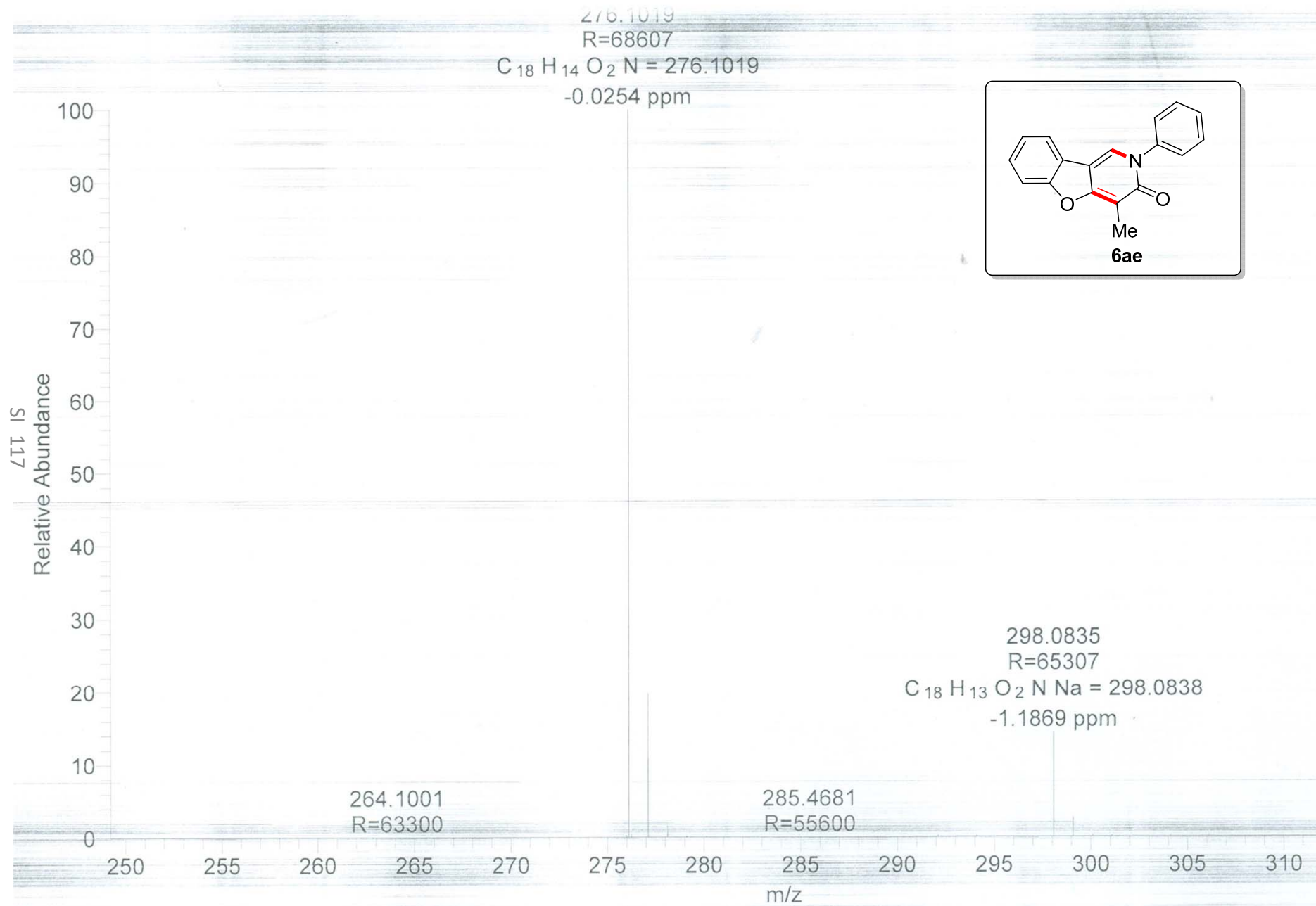
SI 115



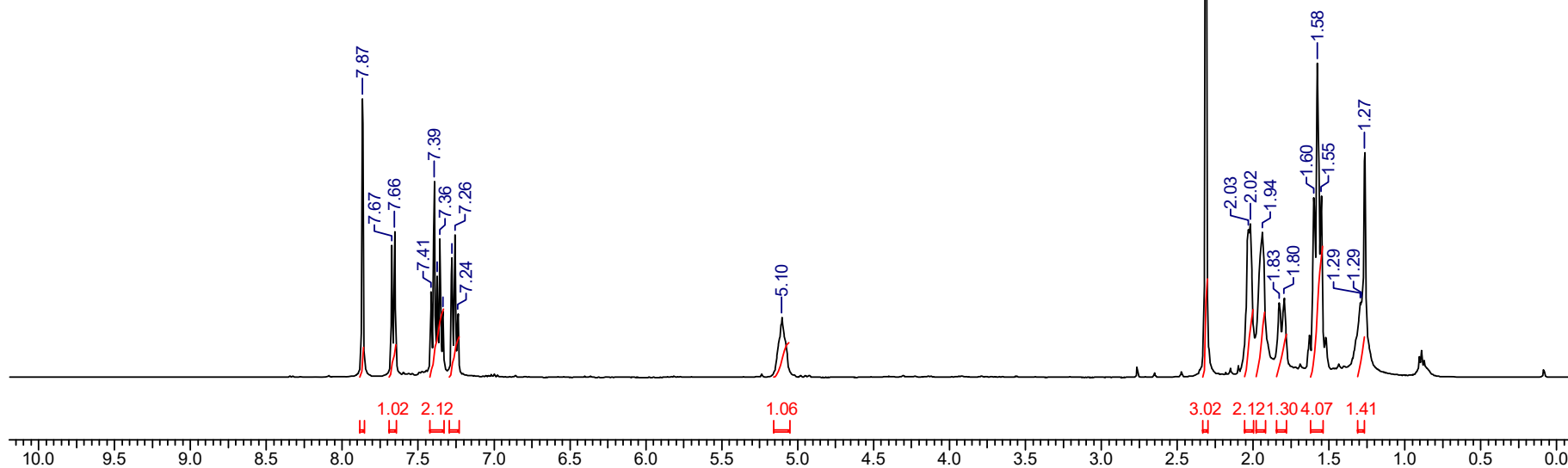
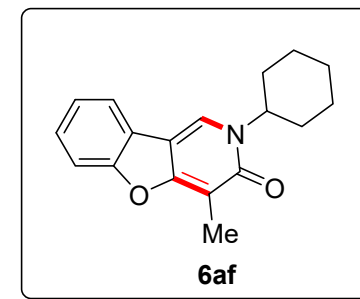
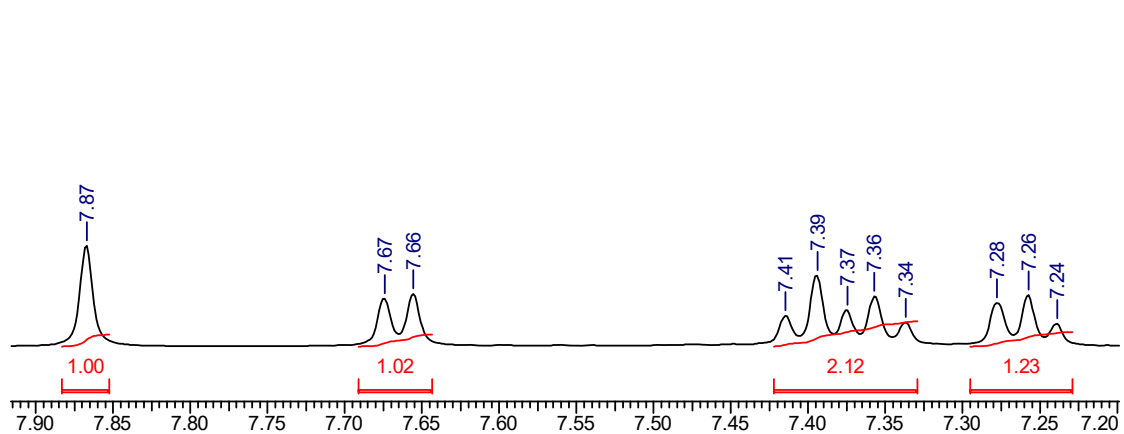
Acquisition Time (sec)	1.2976	Comment	DEPT	Date	13/05/2016 18:09:16	Frequency (MHz)	100.61
Nucleus	¹³ C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53
Temperature (grad C)	0.000						

SI 116



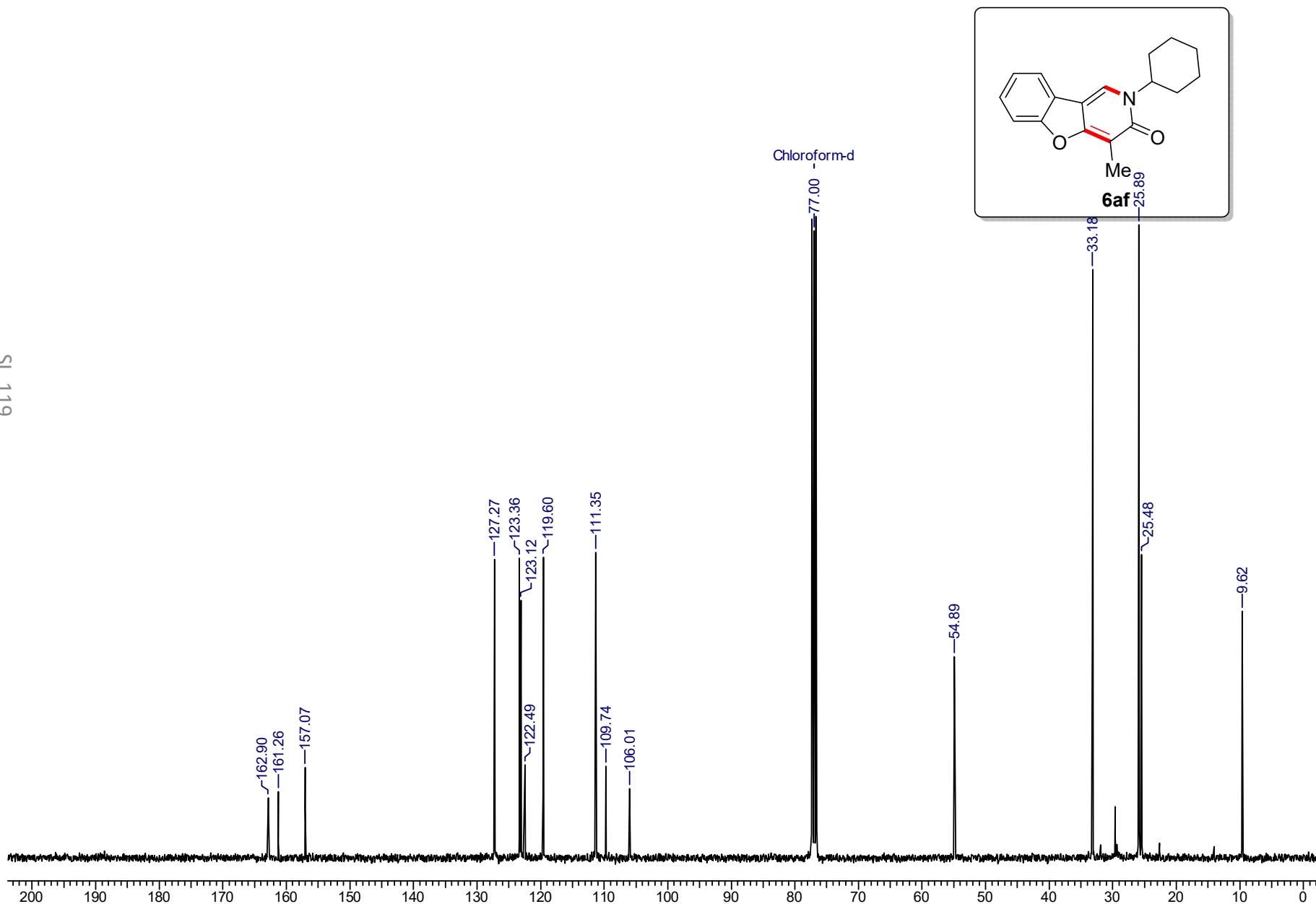


Acquisition Time (sec)	2.0447	Comment	Srinivas	Date	16/02/2016 14:20:02	Frequency (MHz)	400.13
Nucleus	1H	Original Points Count	16384	Points Count	16384	Sweep Width (Hz)	8012.82
						Temperature (grad C)	0.000

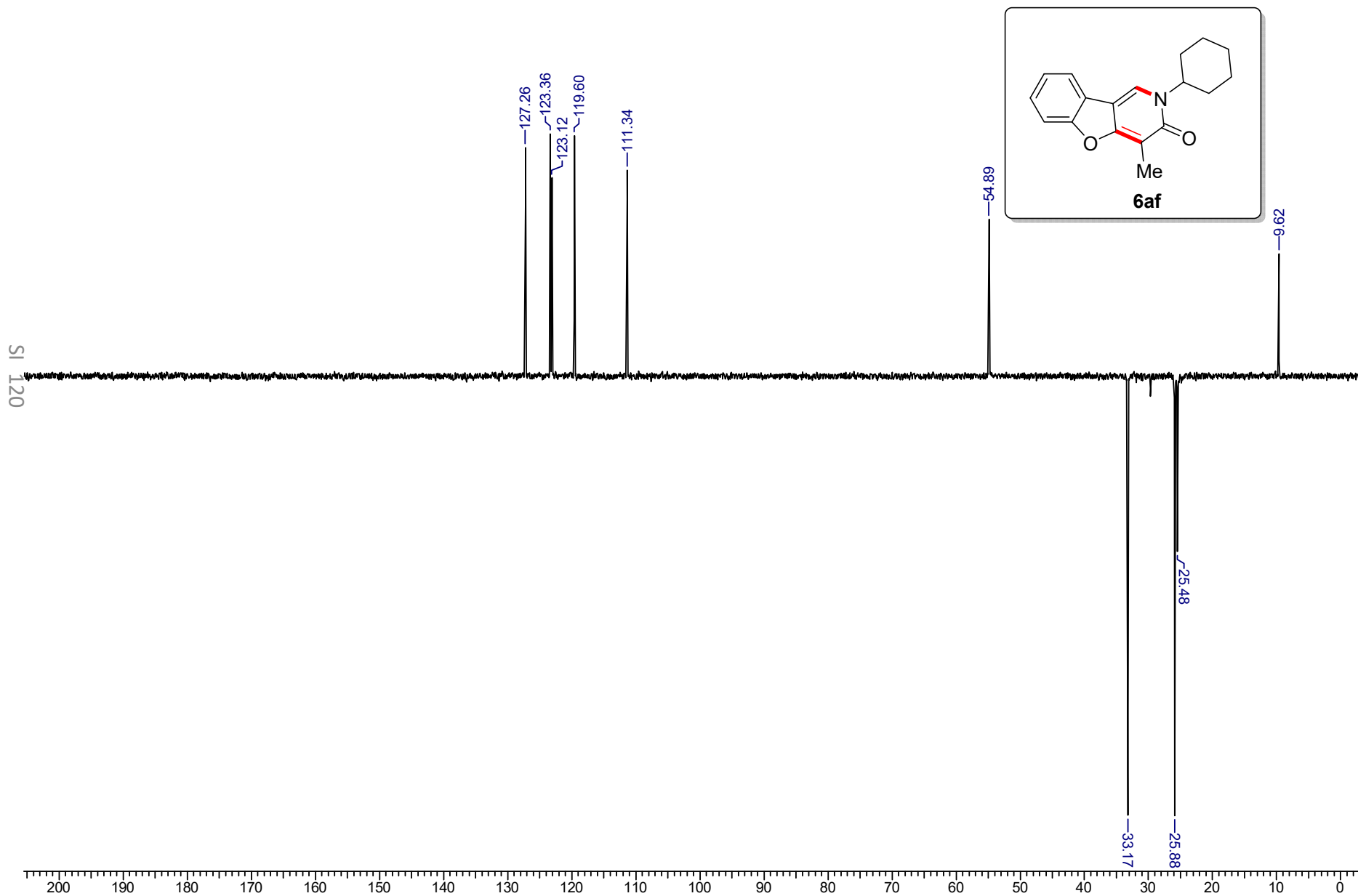


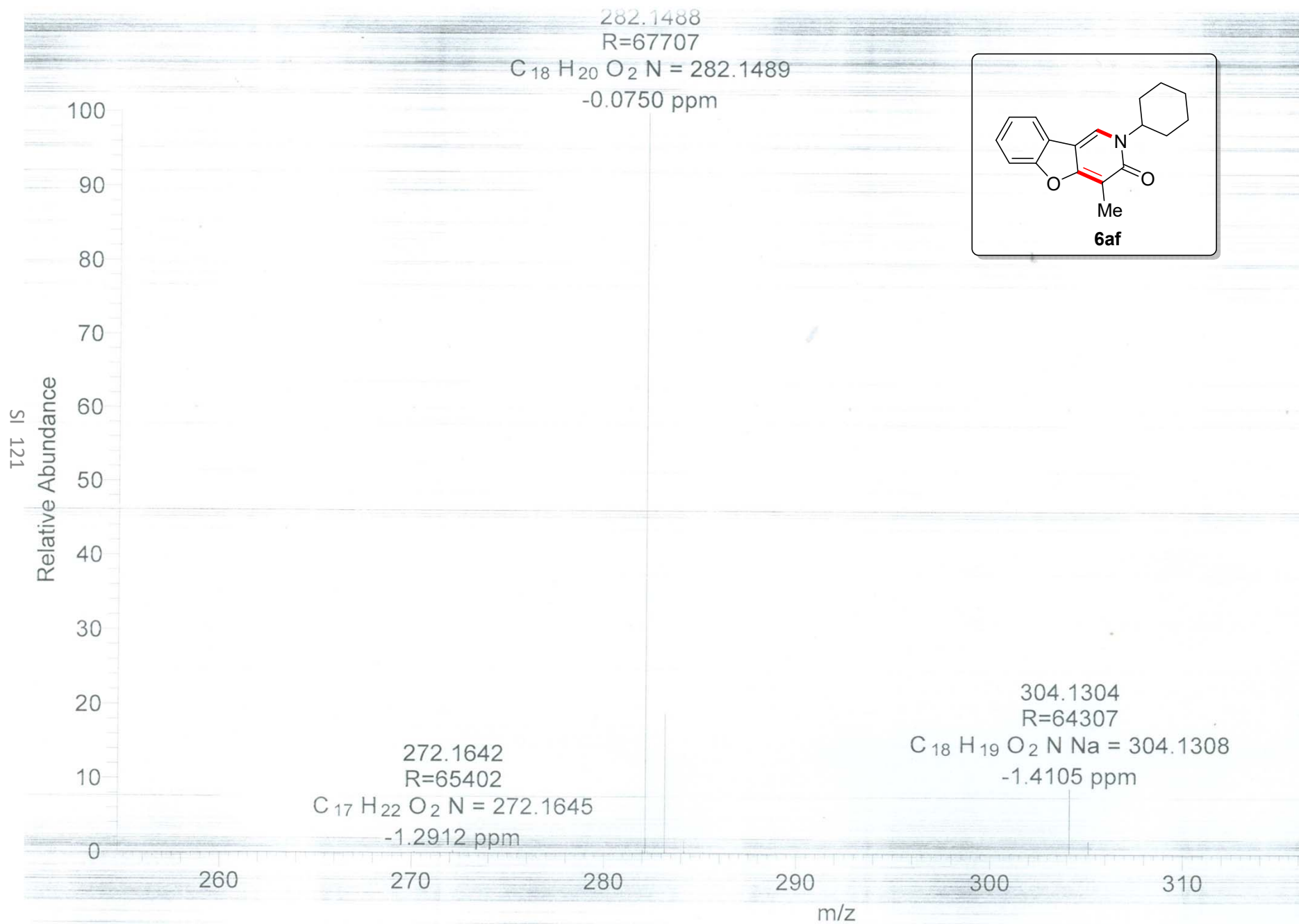
Acquisition Time (sec)	1.2976	Date	16/02/2016 14:20:48	Frequency (MHz)	100.61	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53	Temperature (grad C)	0.000

SI 119

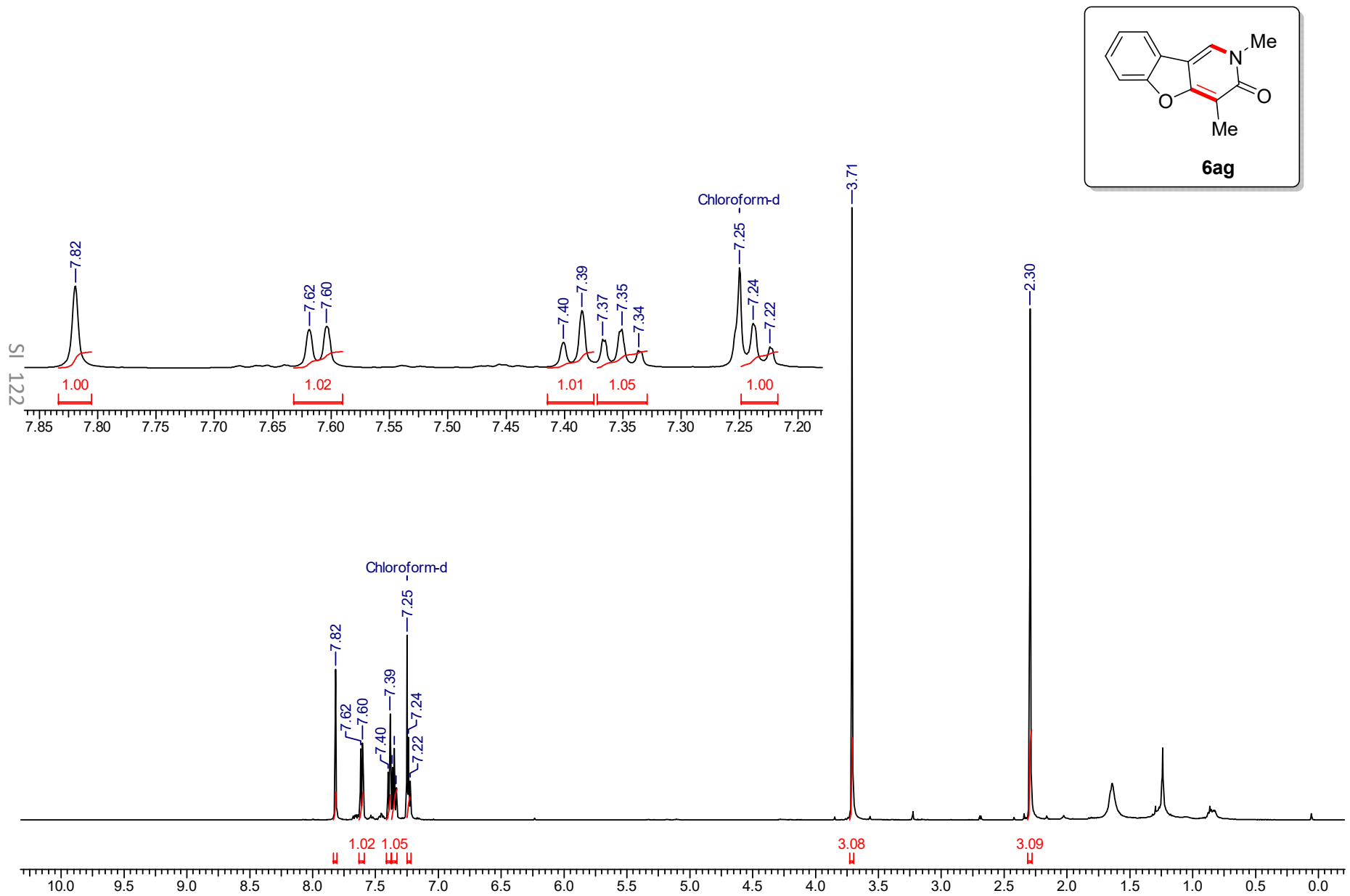


Date	16 Feb 2016 13:13:44	Frequency (MHz)	100.61	Nucleus	¹³ C
Number of Transients	800	Original Points Count	16384	Points Count	32768
Solvent	DMSO-d6	Sweep Width (Hz)	25251.75	Temperature (grad C)	22.500

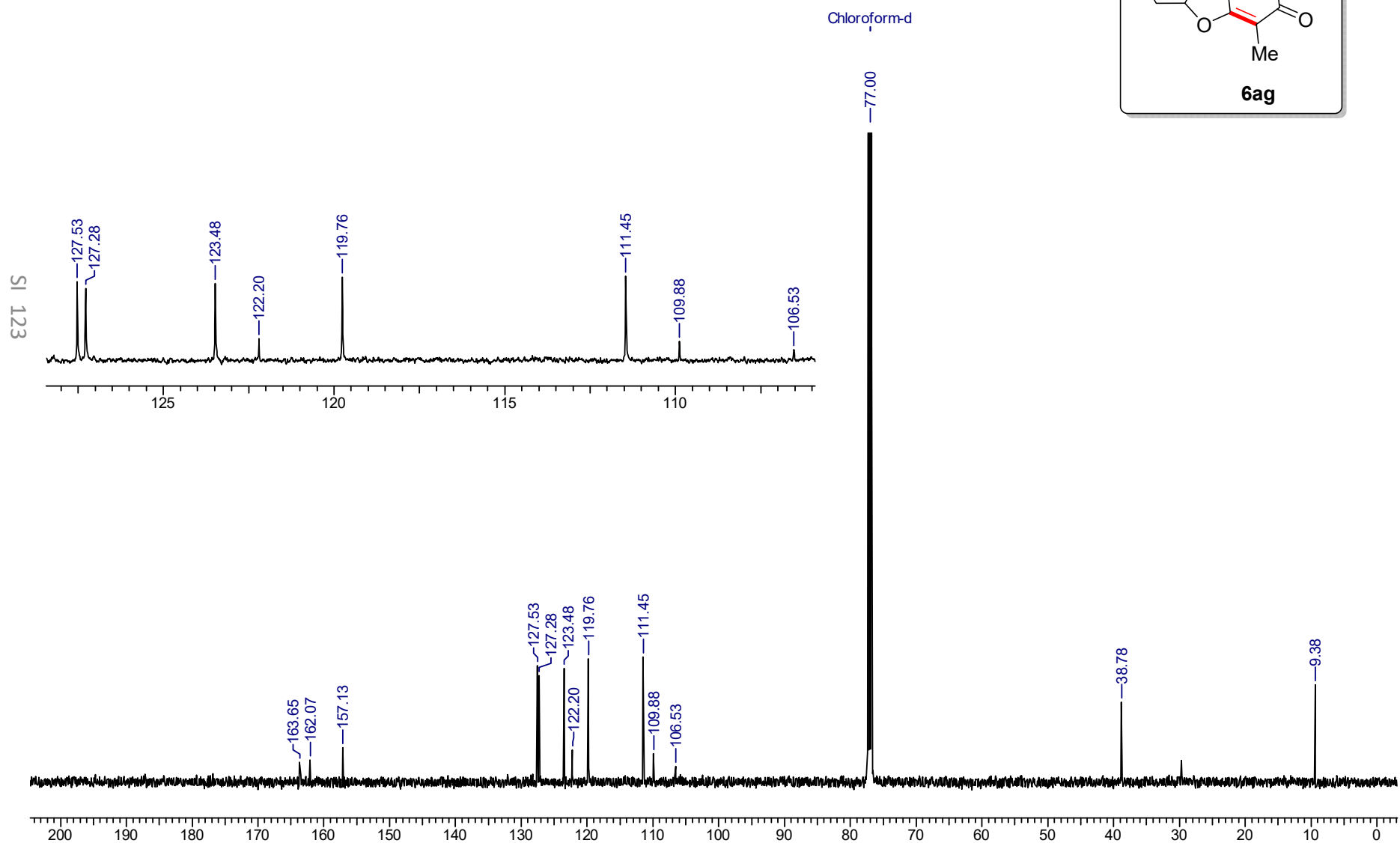




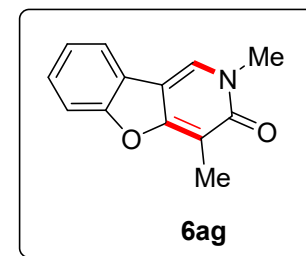
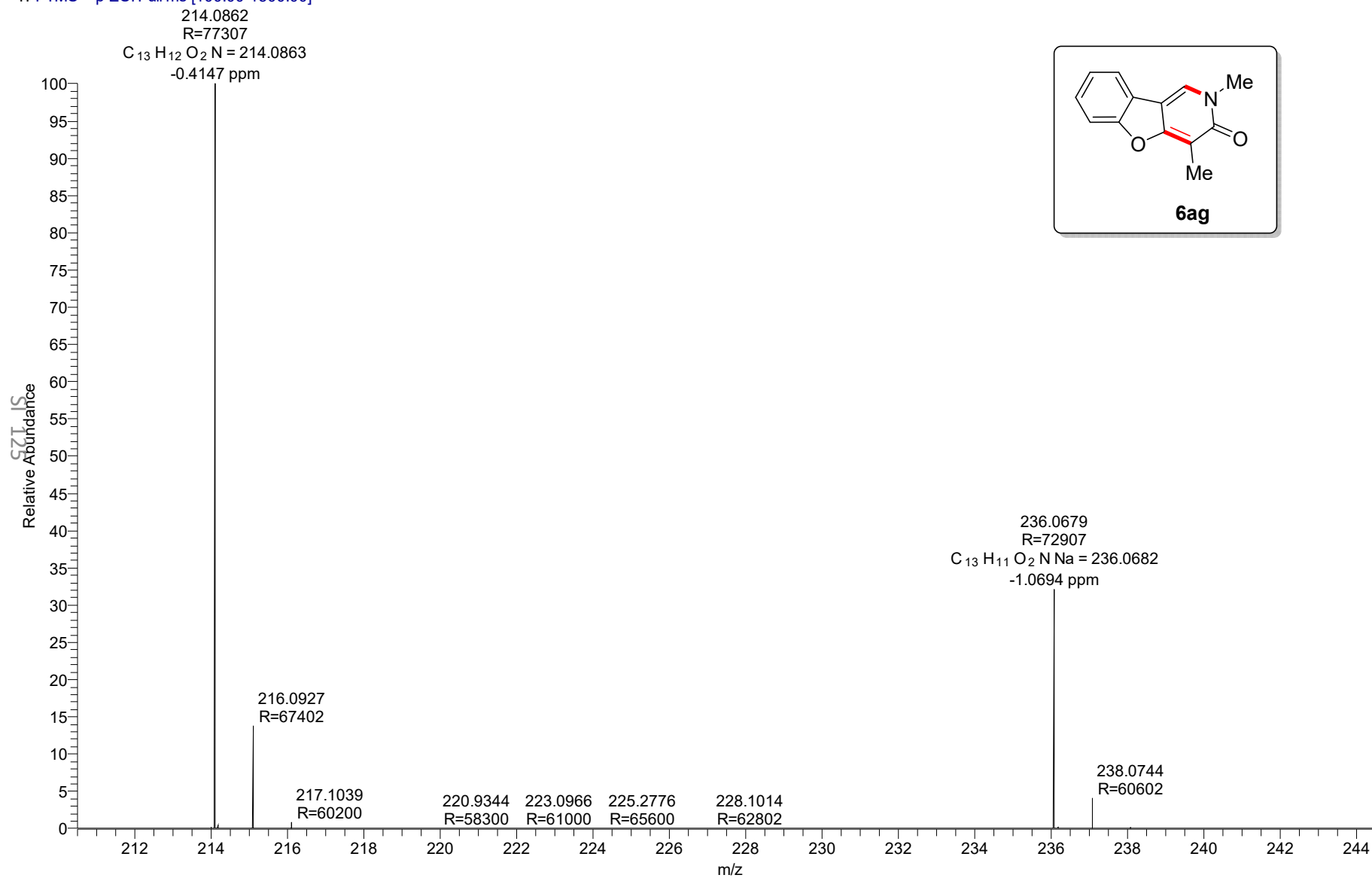
Acquisition Time (sec)	2.6214	Comment	srinivas	Date	04/03/2016 18:34:08	Frequency (MHz)	500.13
Nucleus	¹ H	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	12500.00
Temperature (grad C)	0.000						



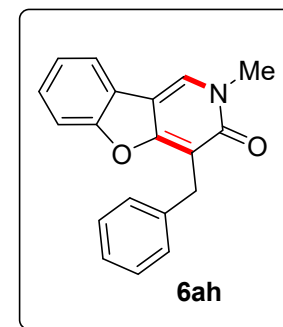
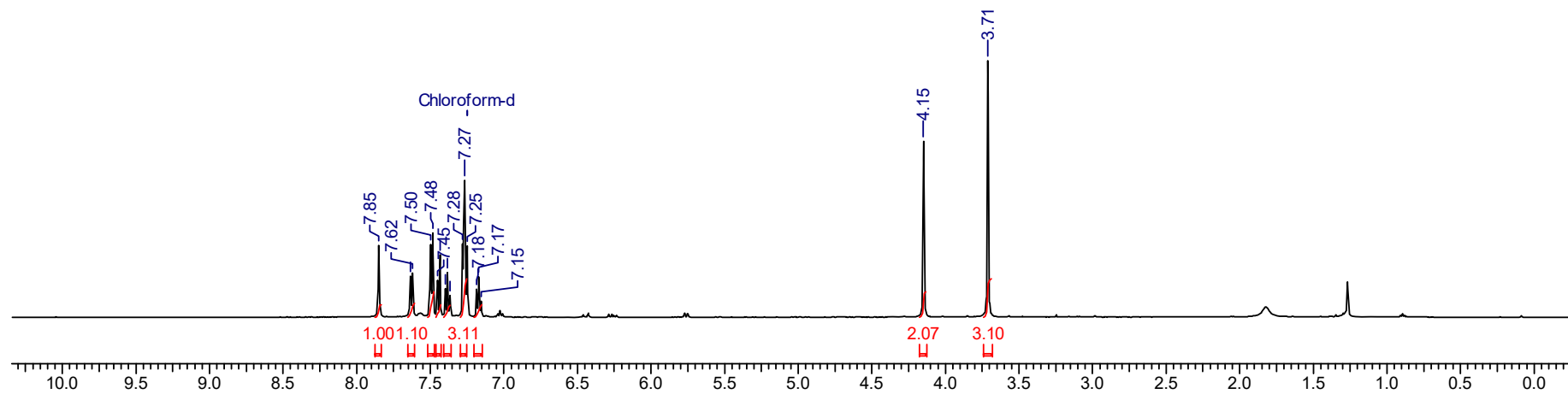
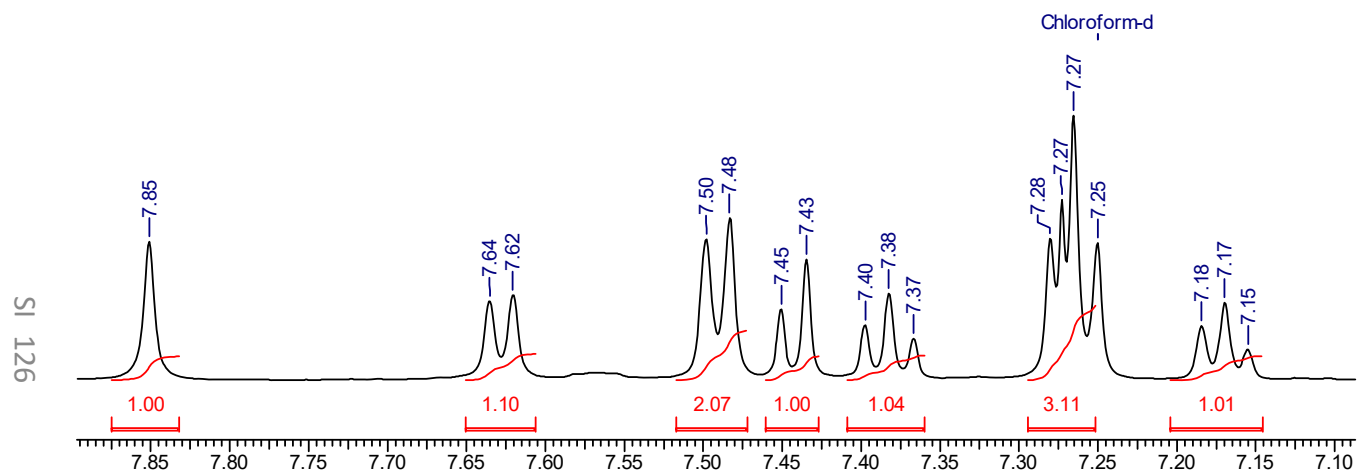
Acquisition Time (sec)	1.0486	Comment	13C	Date	04/03/2016 18:48:14	Frequency (MHz)	125.76
Nucleus	13C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00
Temperature (grad C)	0.000						



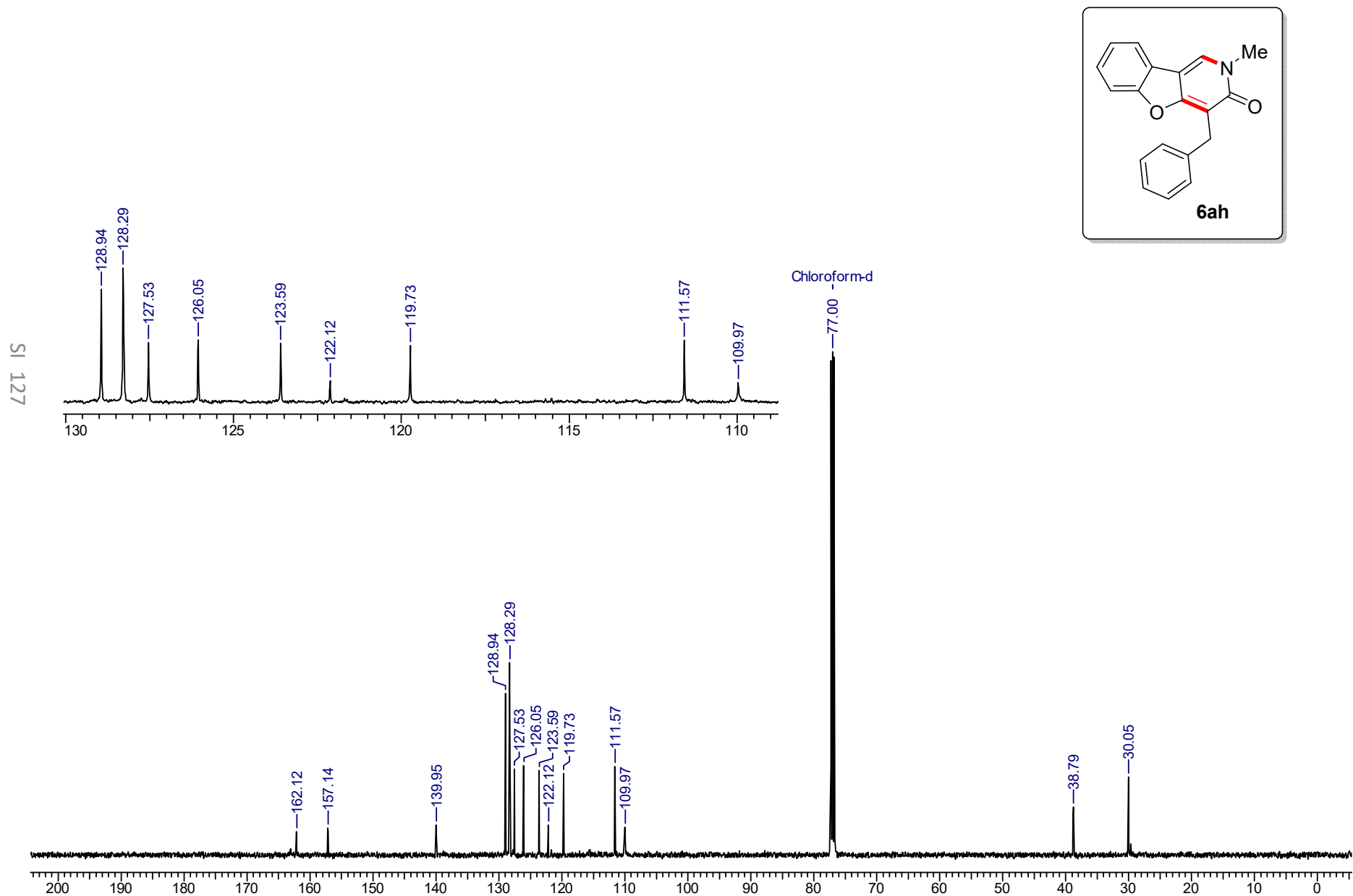
JY-A-15a #108 RT: 0.48 AV: 1 NL: 2.26E9
T: FTMS + p ESI Full ms [100.00-1500.00]



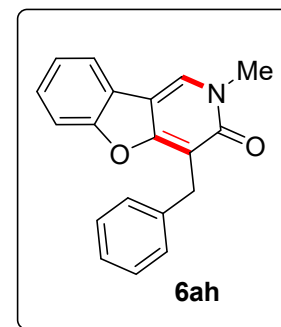
Acquisition Time (sec)	2.6214	Comment	Jyothi	Date	02/01/2017 23:25:22	Frequency (MHz)	500.13
Nucleus	¹ H	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	12500.00
Temperature (grad C)	0.000						



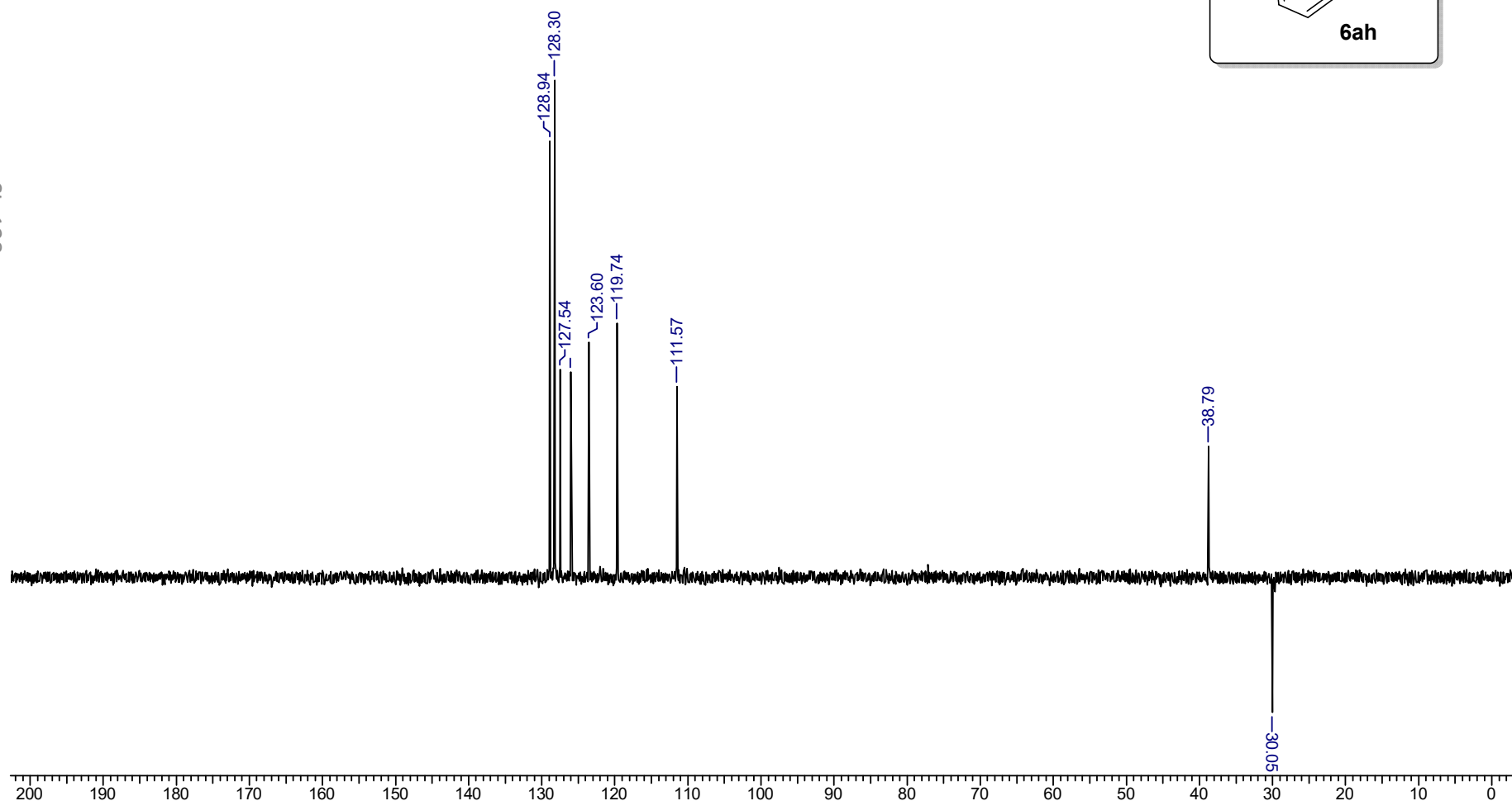
Acquisition Time (sec)	1.0486	Date	20/12/2016 19:37:34	Frequency (MHz)	125.76	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00	Temperature (grad C)	0.000



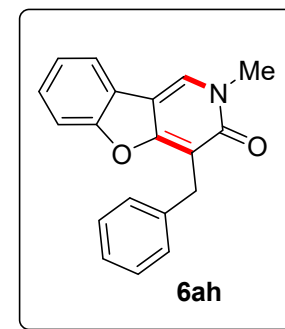
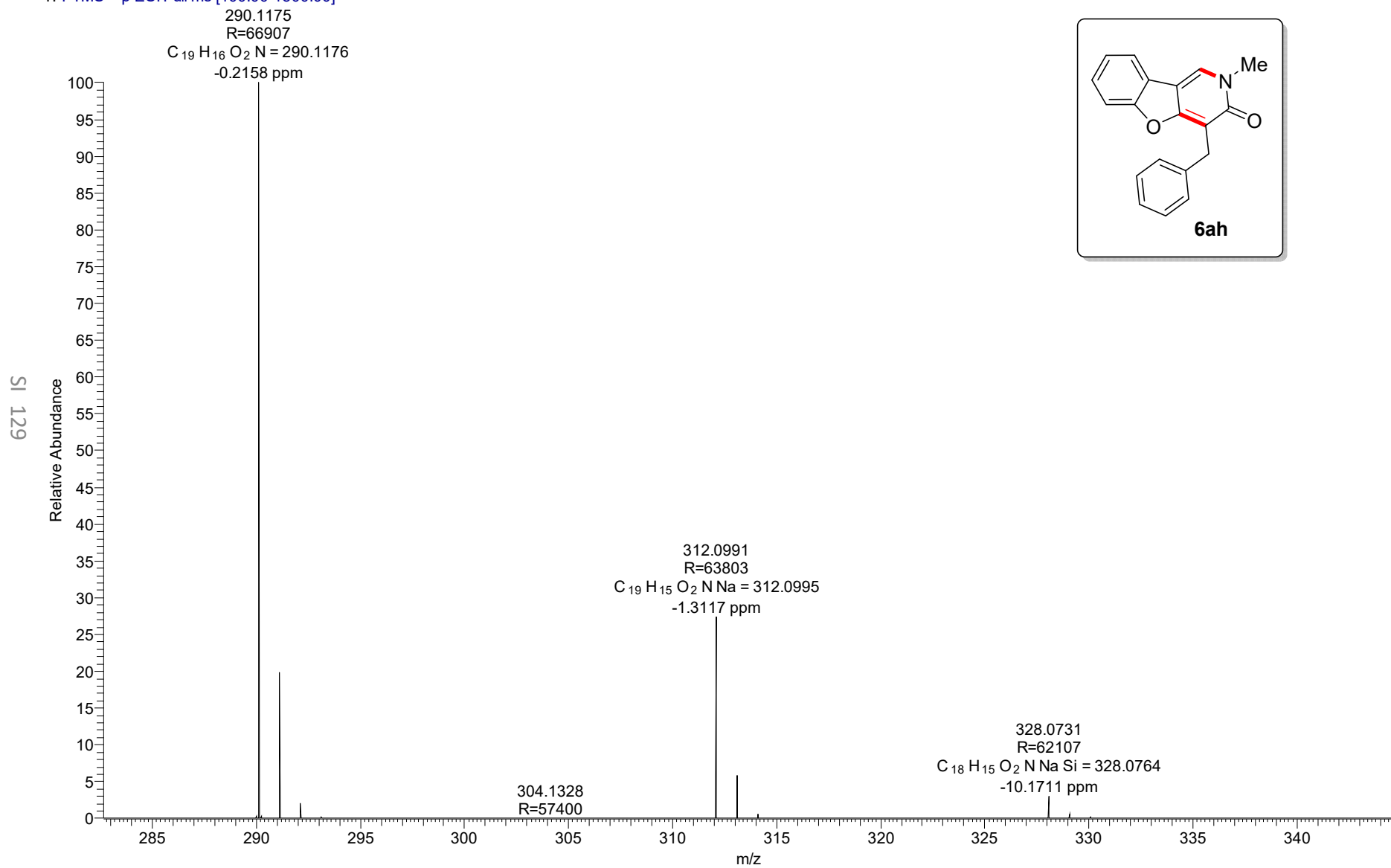
Acquisition Time (sec)	1.0486	Date	20/12/2016 19:34:40	Frequency (MHz)	125.76	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00	Temperature (grad C)	0.000



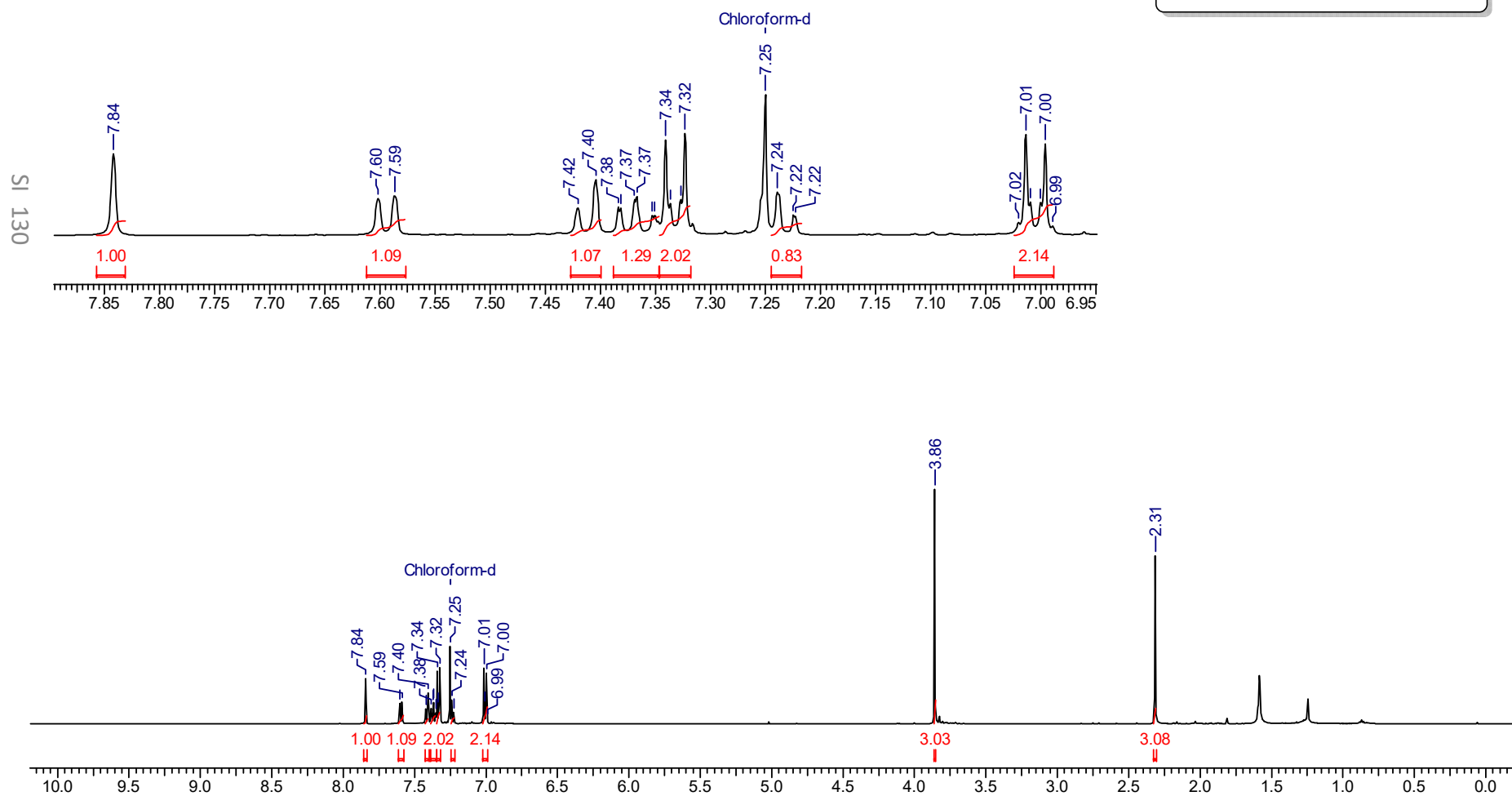
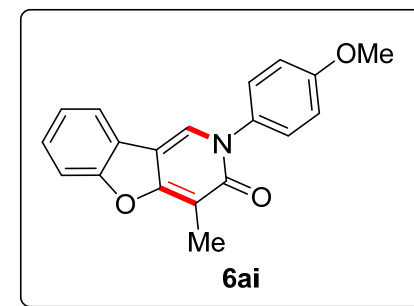
SI 128



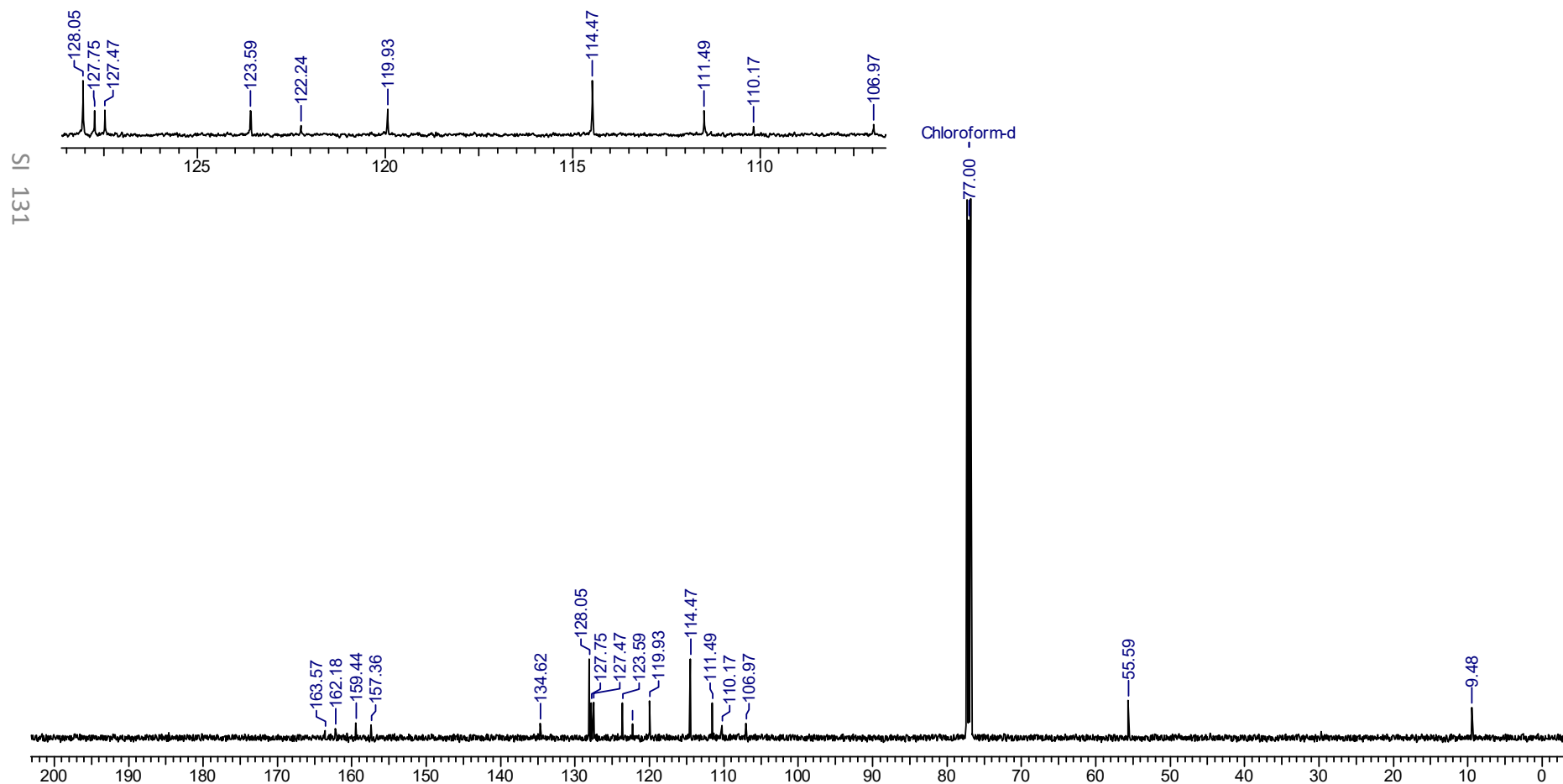
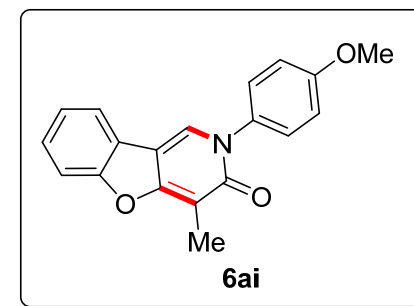
JY-A-13b #123 RT: 0.54 AV: 1 NL: 3.71E9
T: FTMS + p ESI Full ms [100.00-1500.00]



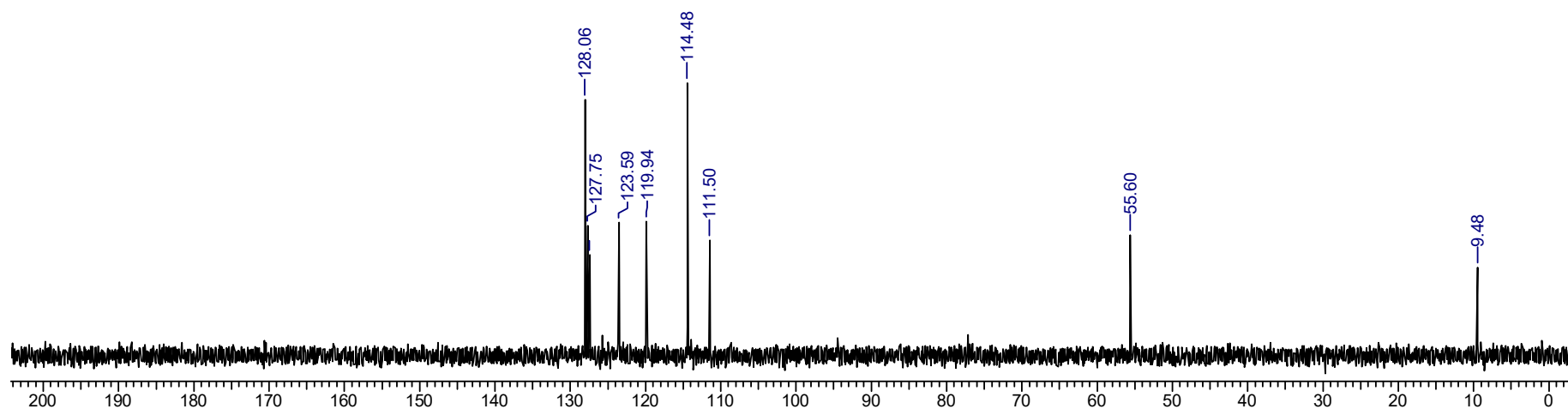
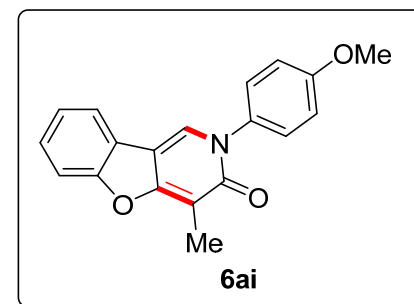
Acquisition Time (sec)	2.6214	Comment	Jyoti	Date	14/05/2016 21:26:50	Frequency (MHz)	500.13
Nucleus	¹ H	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	12500.00
Temperature (grad C)	0.000						

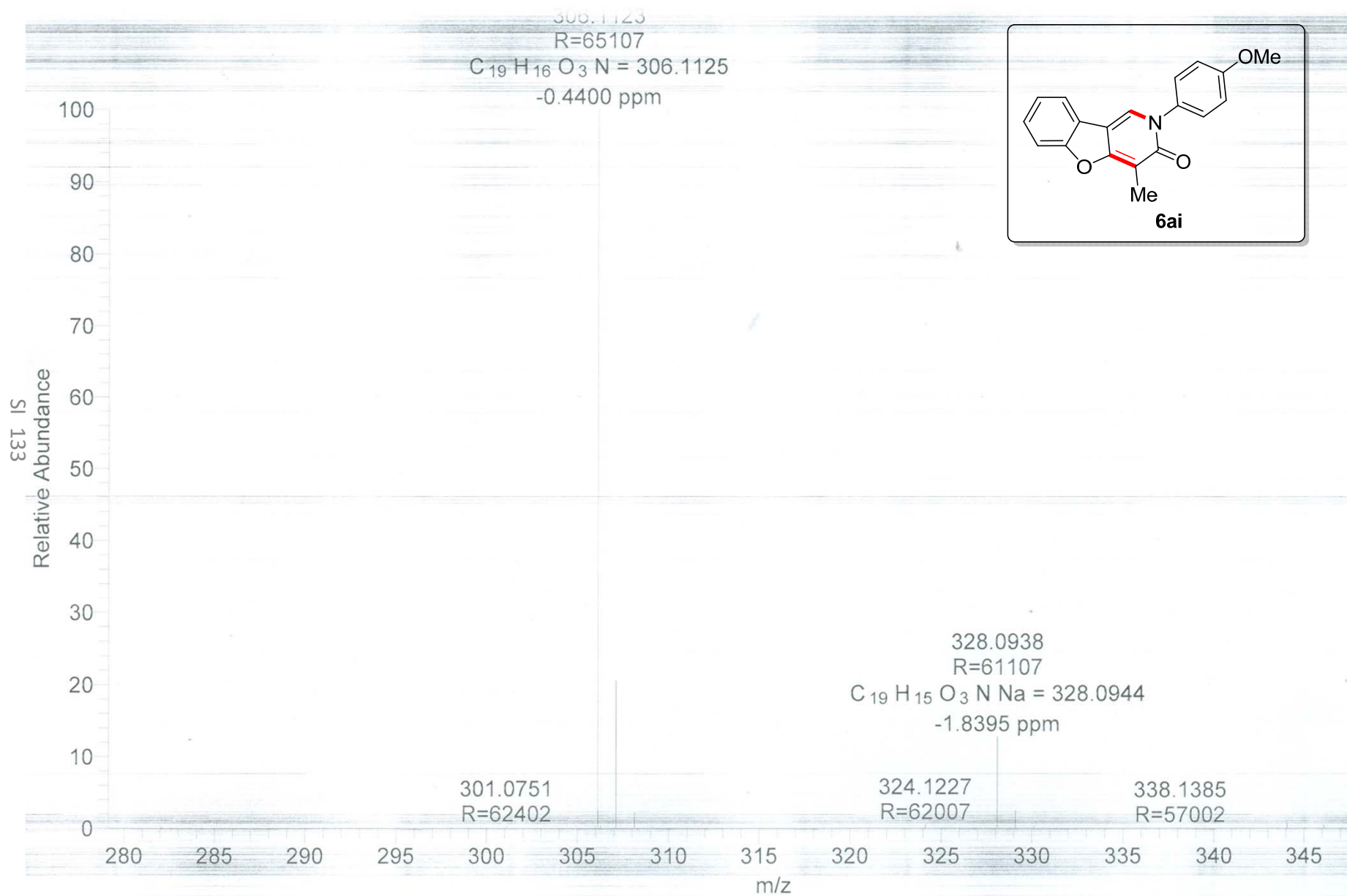


Acquisition Time (sec)	1.0486	Comment	13C	Date	14/05/2016 21:27:48	Frequency (MHz)	125.76
Nucleus	13C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00
Temperature (grad C)	0.000						

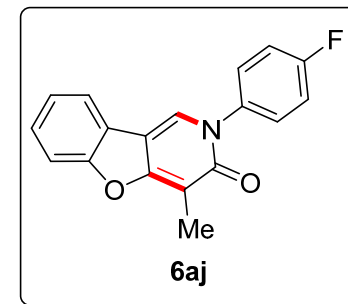


Acquisition Time (sec)	1.0486	Date	14/05/2016 21:27:18	Frequency (MHz)	125.76	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00	Temperature (grad C)	0.000

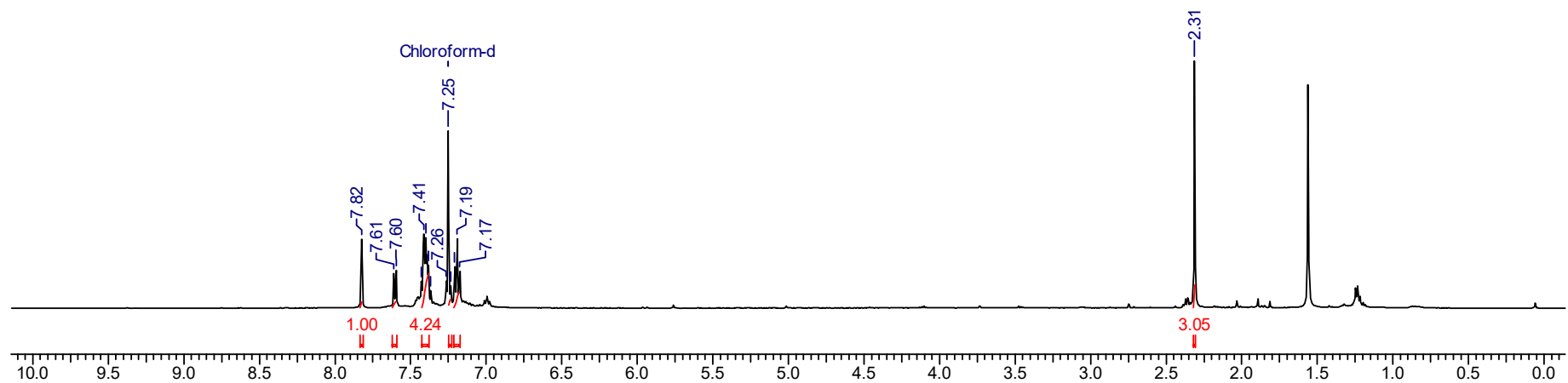
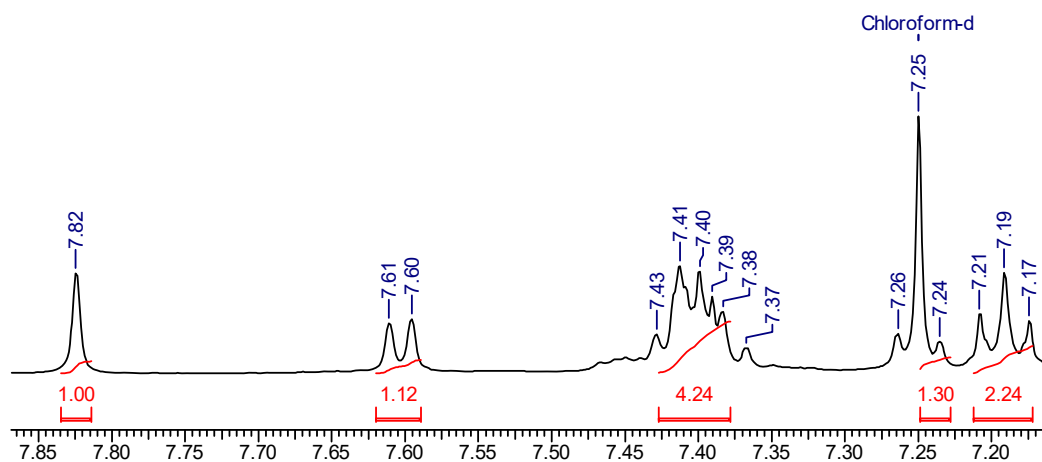




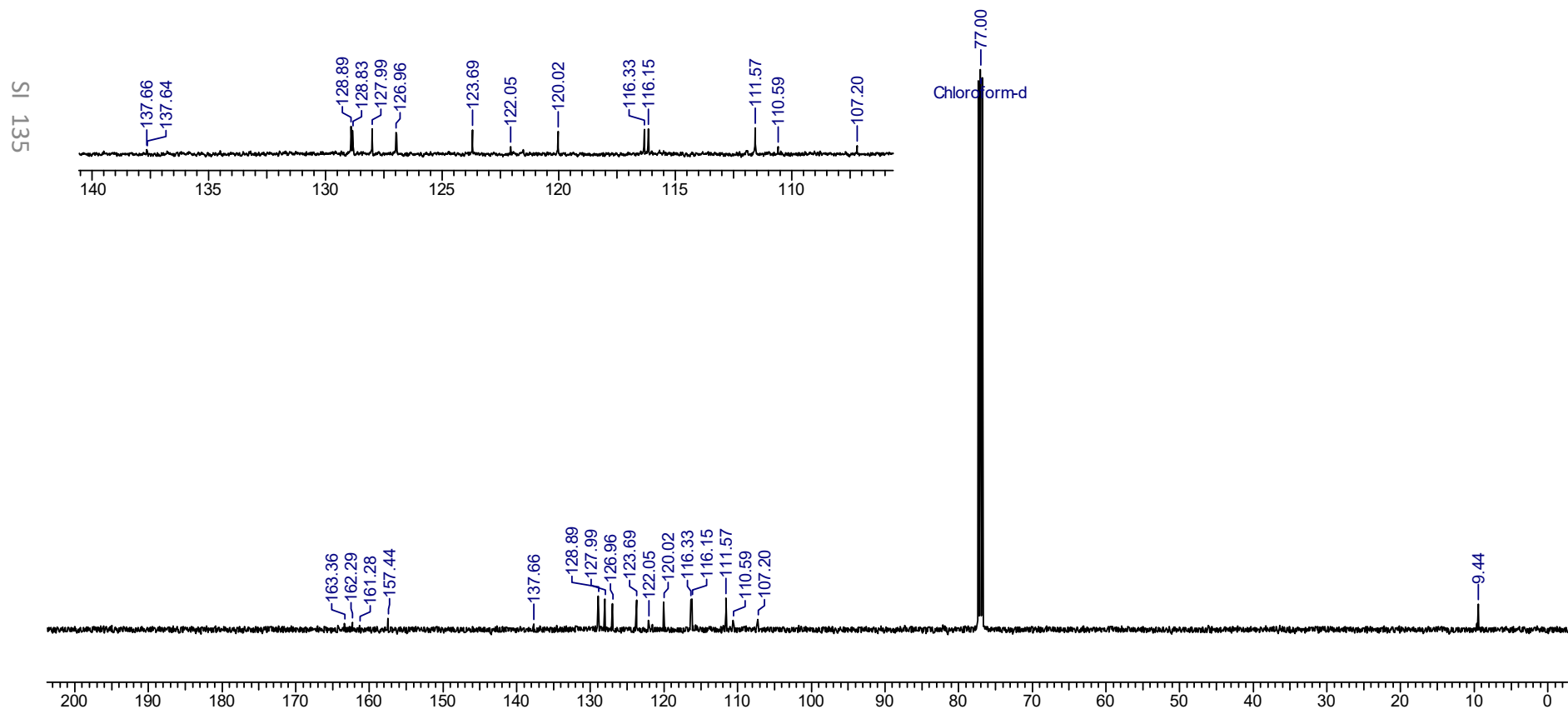
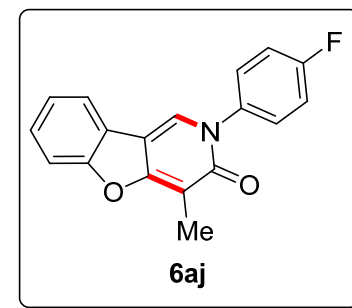
Acquisition Time (sec)	1.6384	Comment	Jyothi	Date	24/12/2016 15:46:46	Frequency (MHz)	500.13
Nucleus	¹ H	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	20000.00
Temperature (grad C)	0.000						



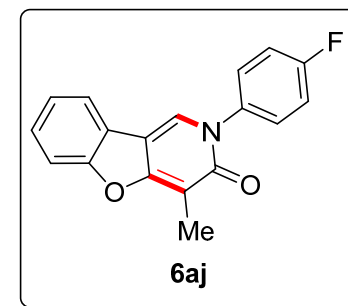
SI 134



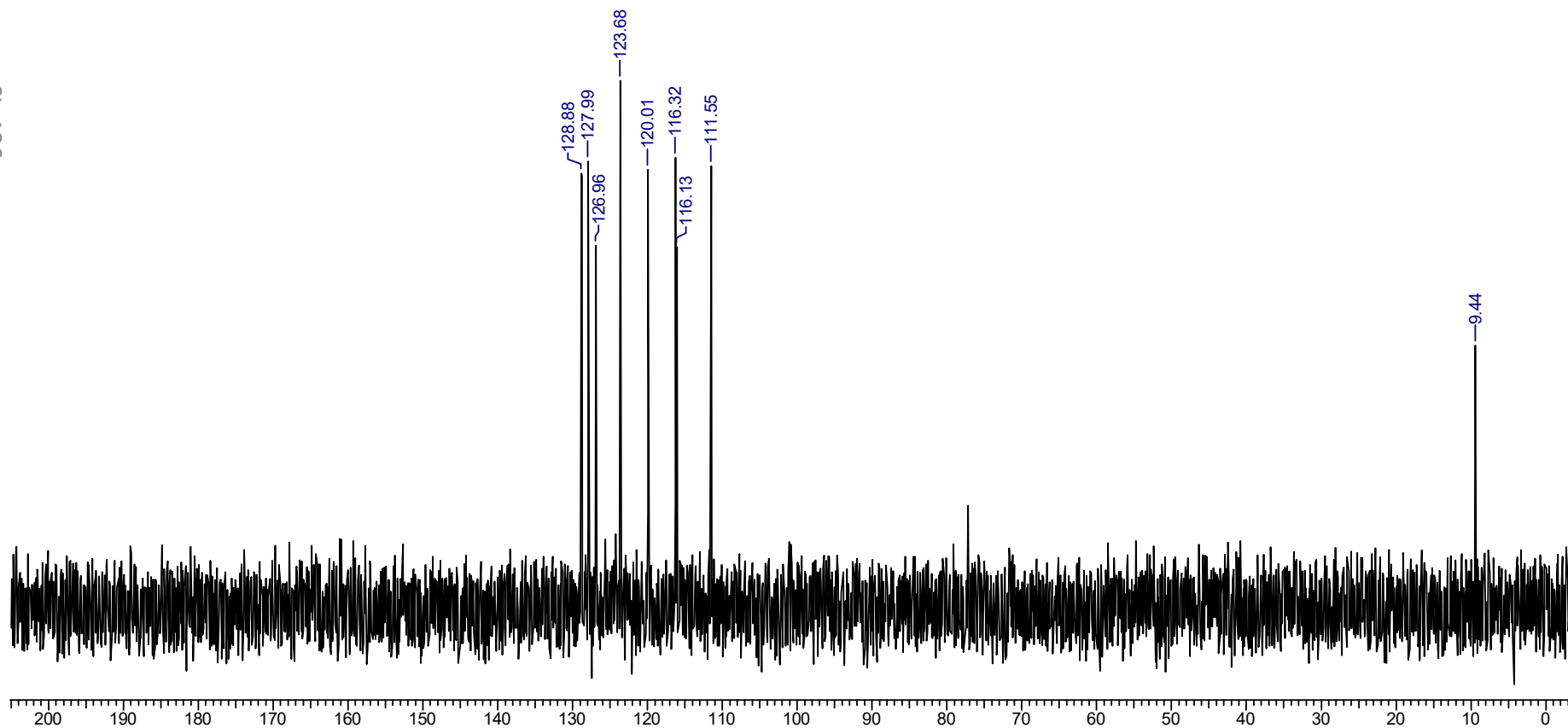
Acquisition Time (sec)	1.0486	Date	24/12/2016 16:46:16	Frequency (MHz)	125.76	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00	Temperature (grad C)	0.000



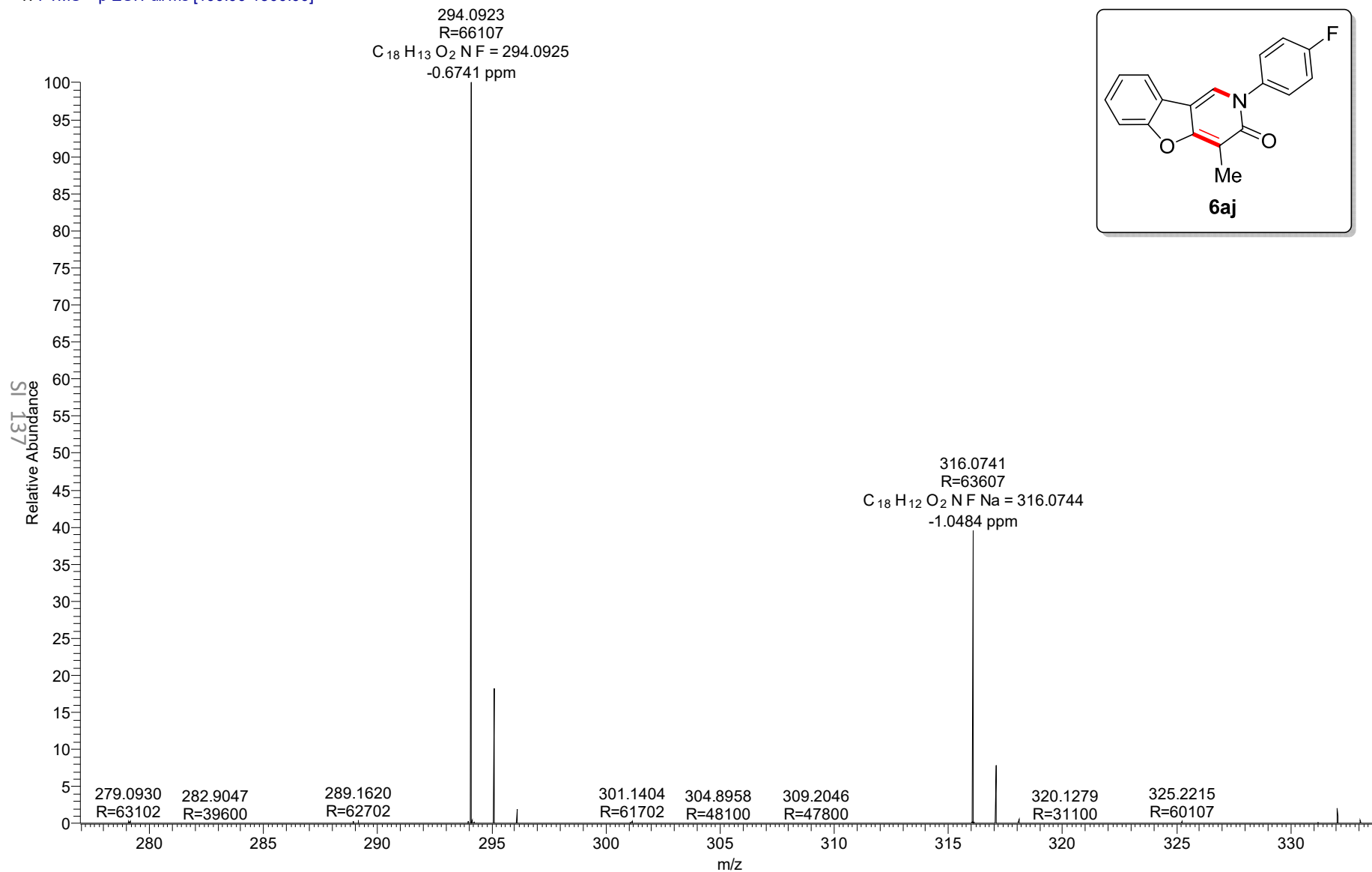
Acquisition Time (sec)	1.0486	Date	24/12/2016 16:11:22	Frequency (MHz)	125.76	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00	Temperature (grad C)	0.000



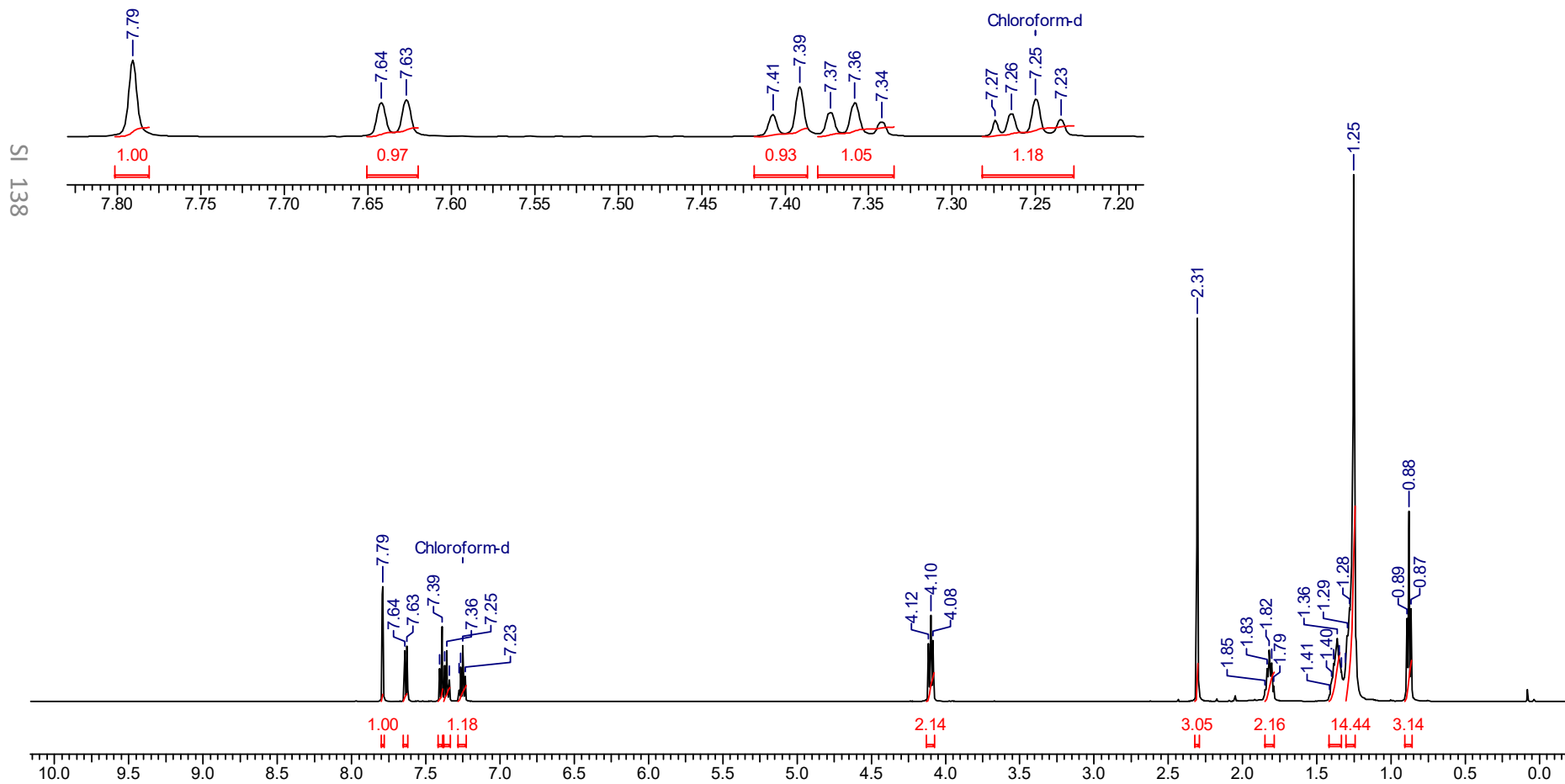
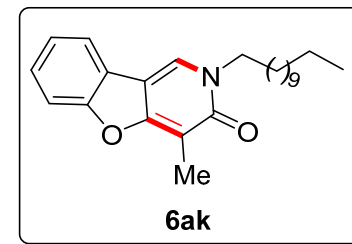
SI 136



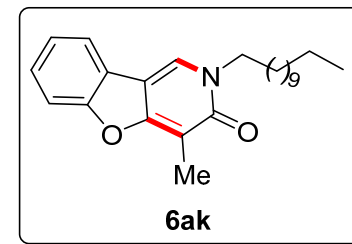
JY-A-22B #111 RT: 0.49 AV: 1 NL: 1.13E9
T: FTMS + p ESI Full ms [100.00-1500.00]



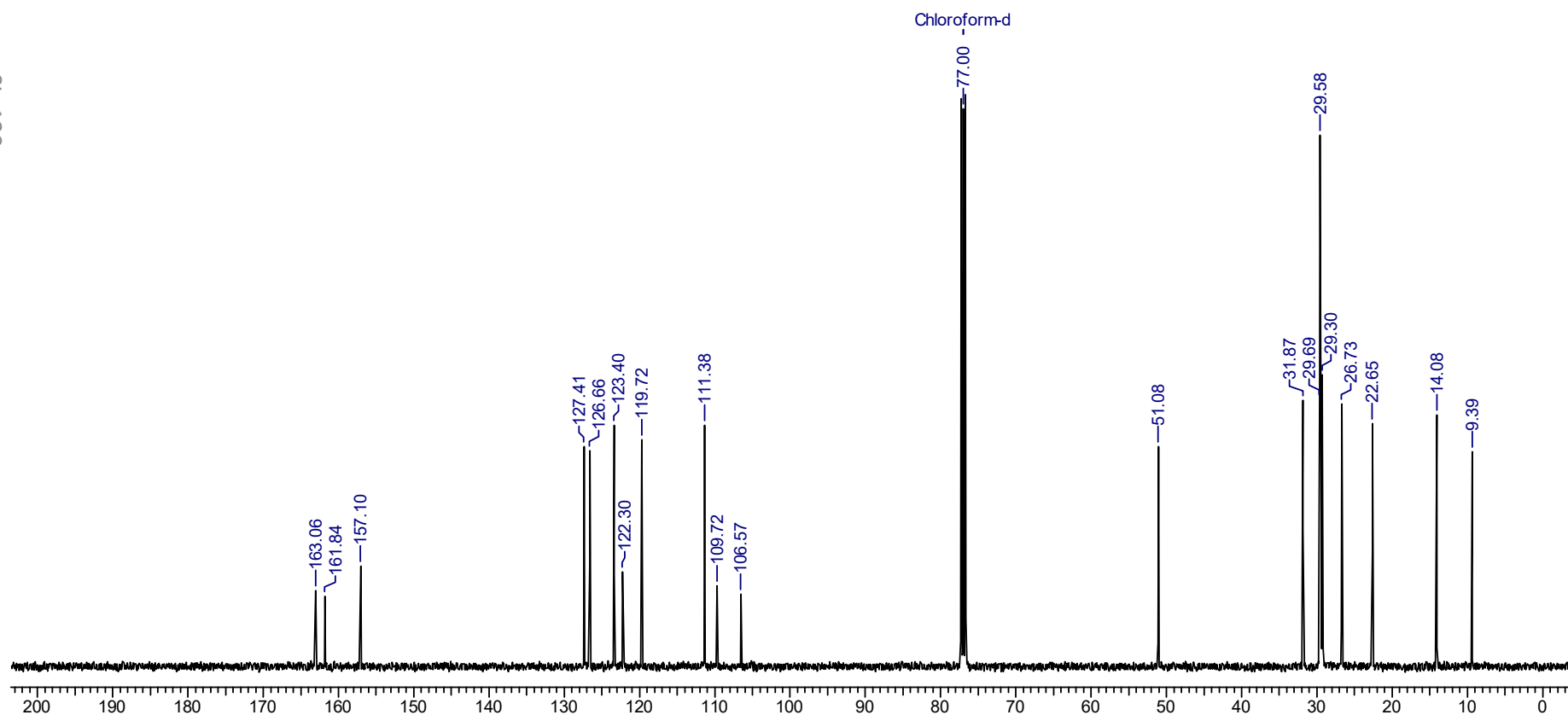
Acquisition Time (sec)	2.6214	Comment	Srinivas	Date	26/03/2016 15:17:48	Frequency (MHz)	500.13
Nucleus	¹ H	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	12500.00
Temperature (grad C)	0.000						



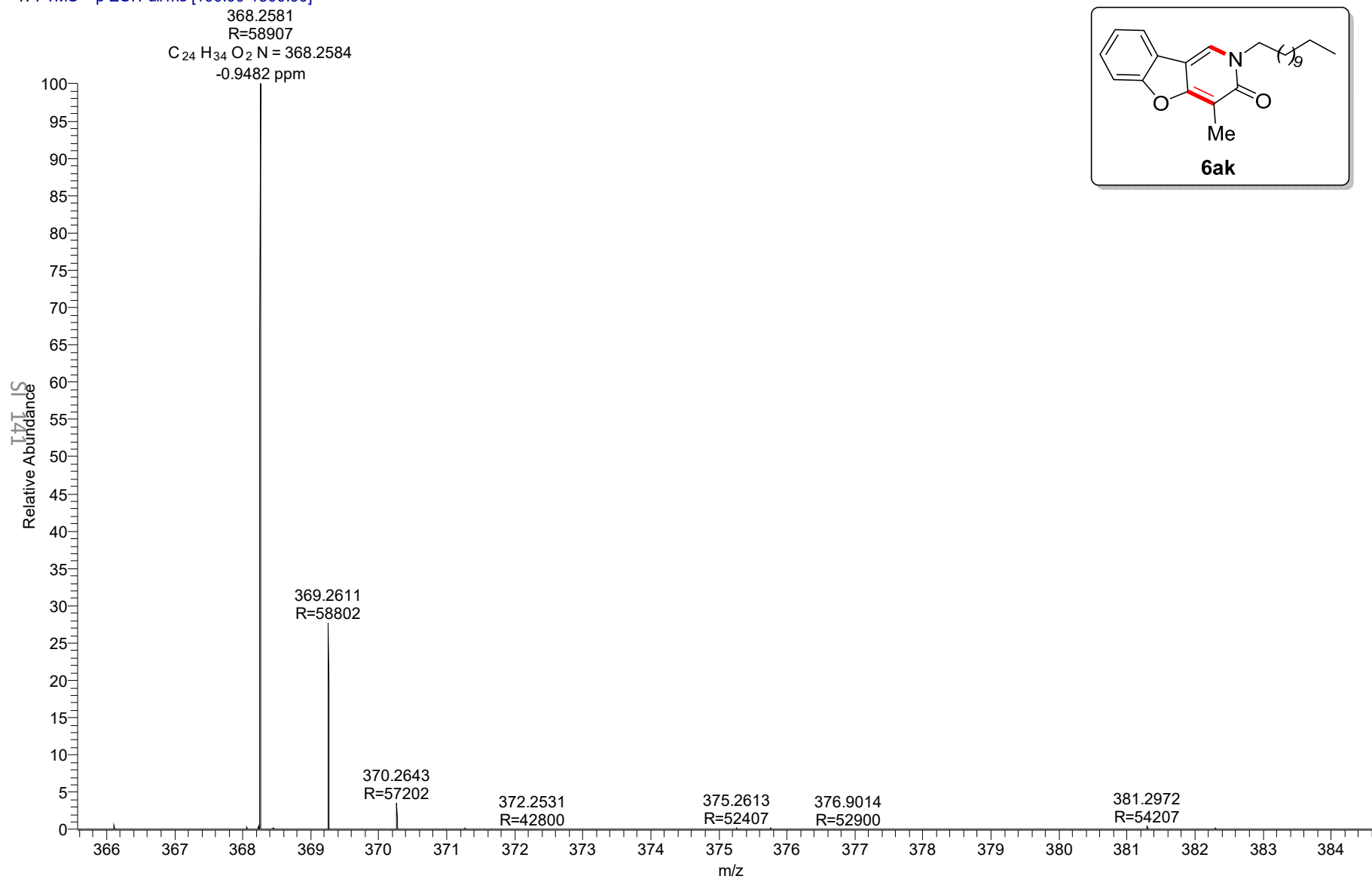
Acquisition Time (sec)	1.0486	Comment	13C	Date	26/03/2016 15:19:16	Frequency (MHz)	125.76
Nucleus	13C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00
Temperature (grad C)	0.000						



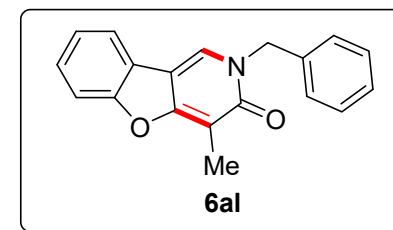
SI 139



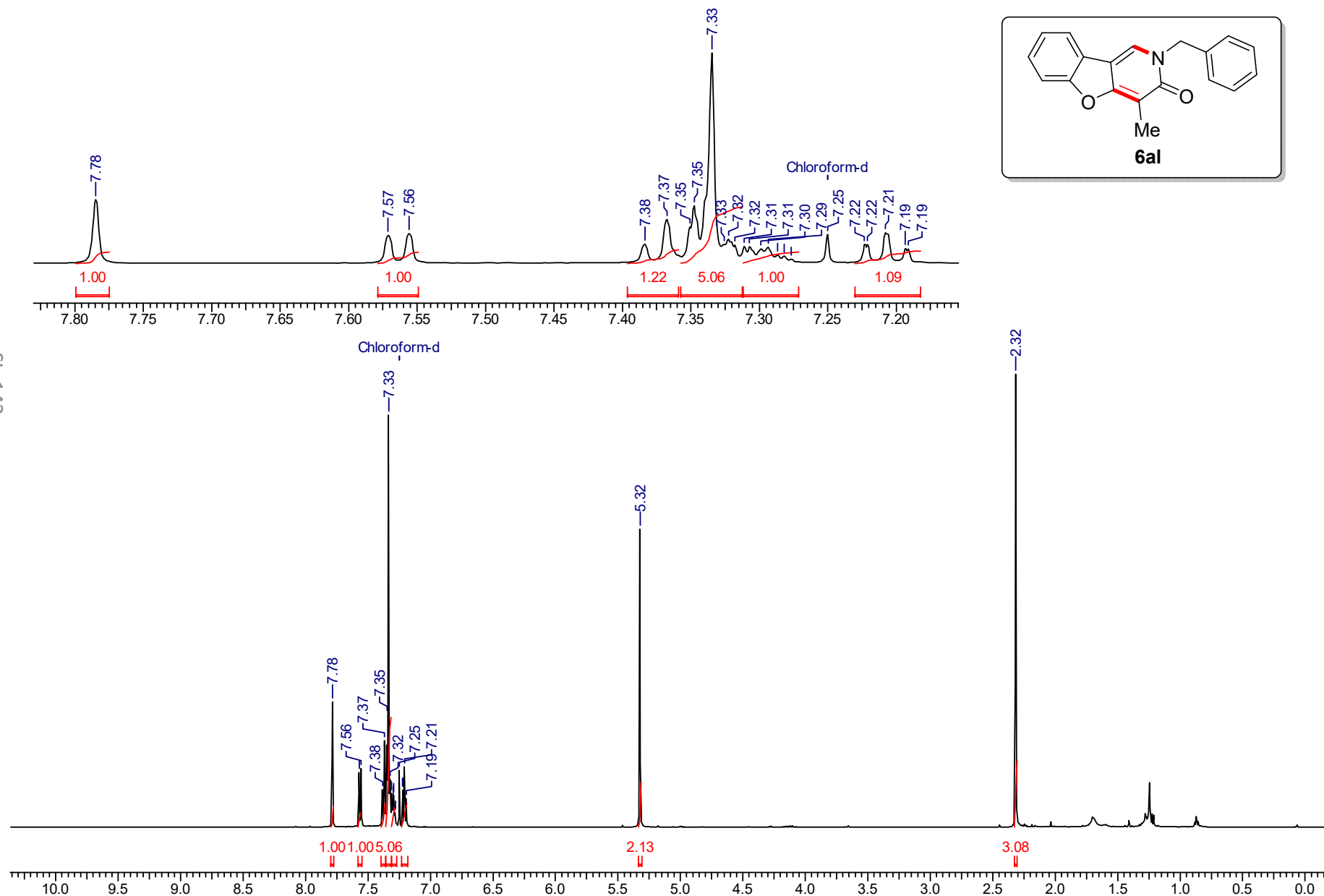
JY-A-25B #397 RT: 1.77 AV: 1 NL: 1.87E8
T: FTMS + p ESI Full ms [100.00-1500.00]



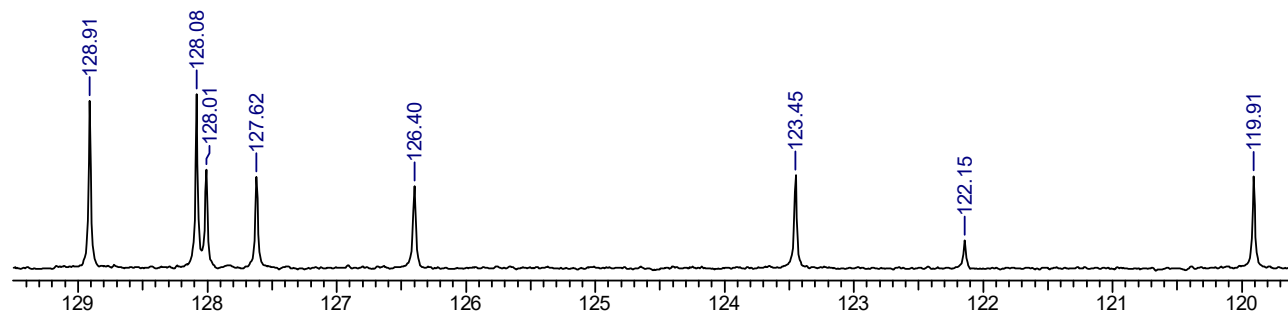
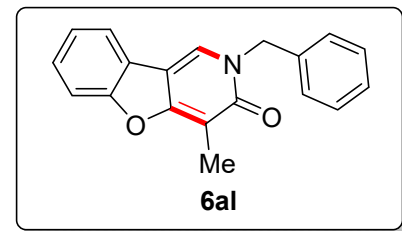
Acquisition Time (sec)	2.6214	Comment	Jyothi	Date	29/03/2016 19:31:22	Frequency (MHz)	500.13
Nucleus	¹ H	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	12500.00
Temperature (grad C)	0.000						



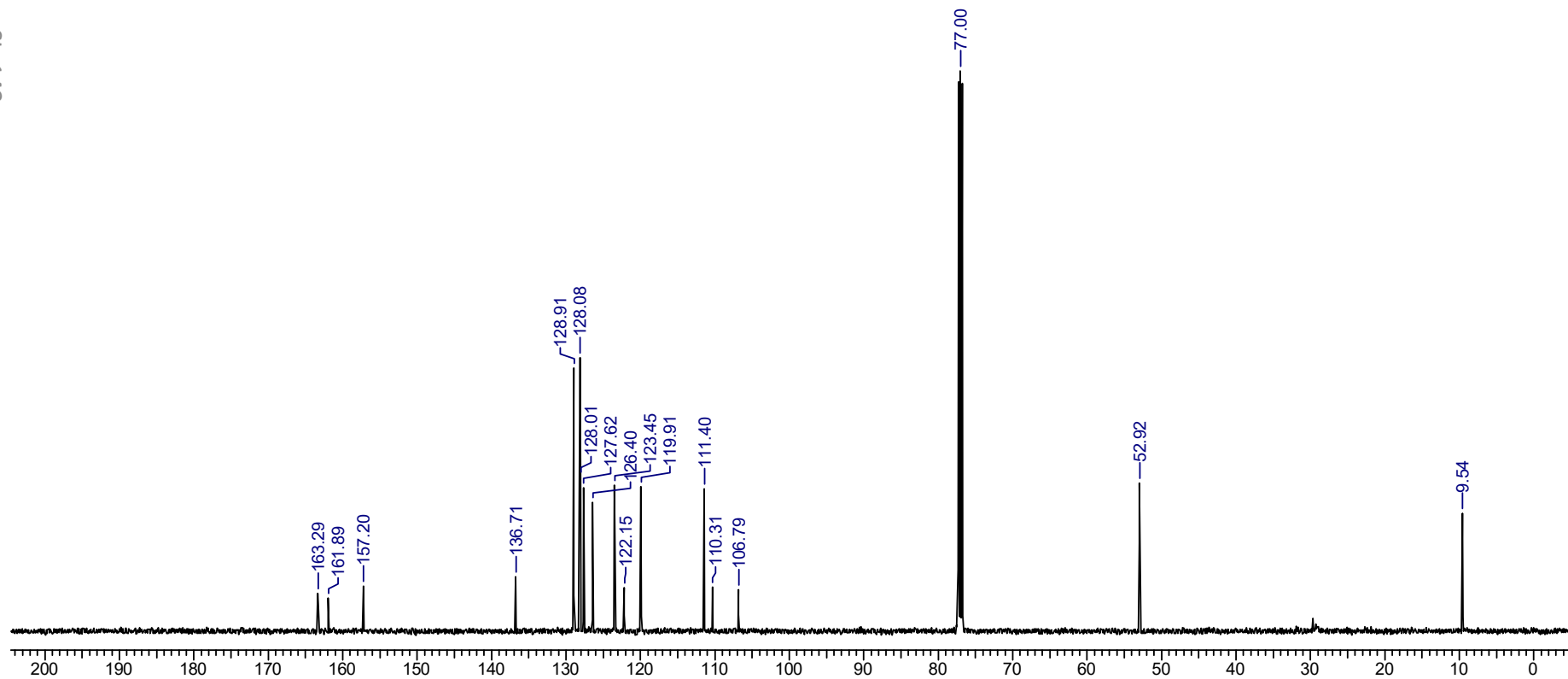
SI 142



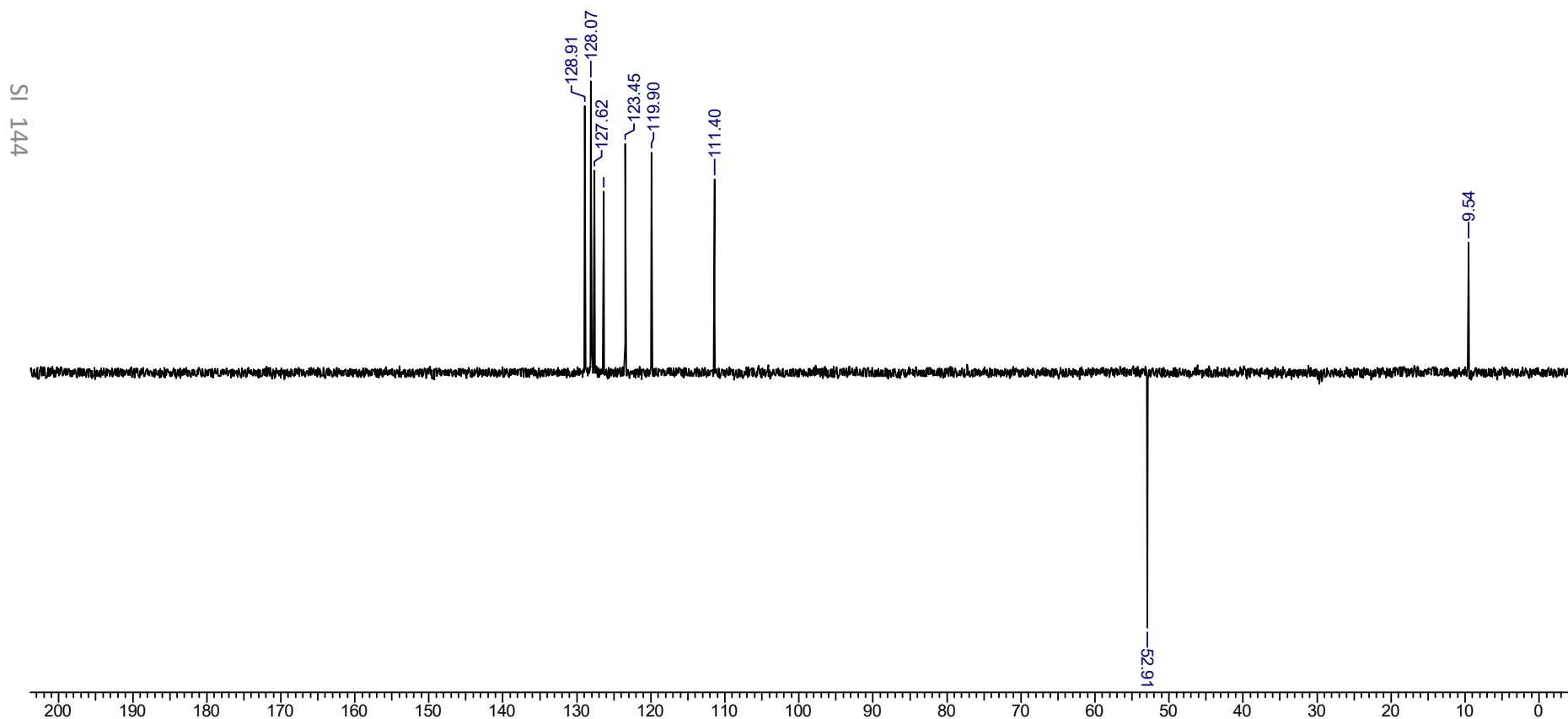
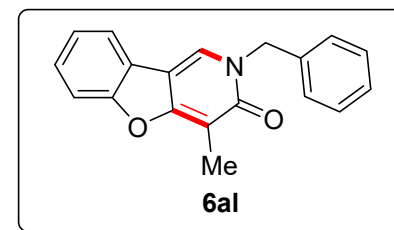
Acquisition Time (sec)	1.0486	Comment	13C	Date	29/03/2016 19:32:32	Frequency (MHz)	125.76
Nucleus	13C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00
Temperature (grad C)	0.000						



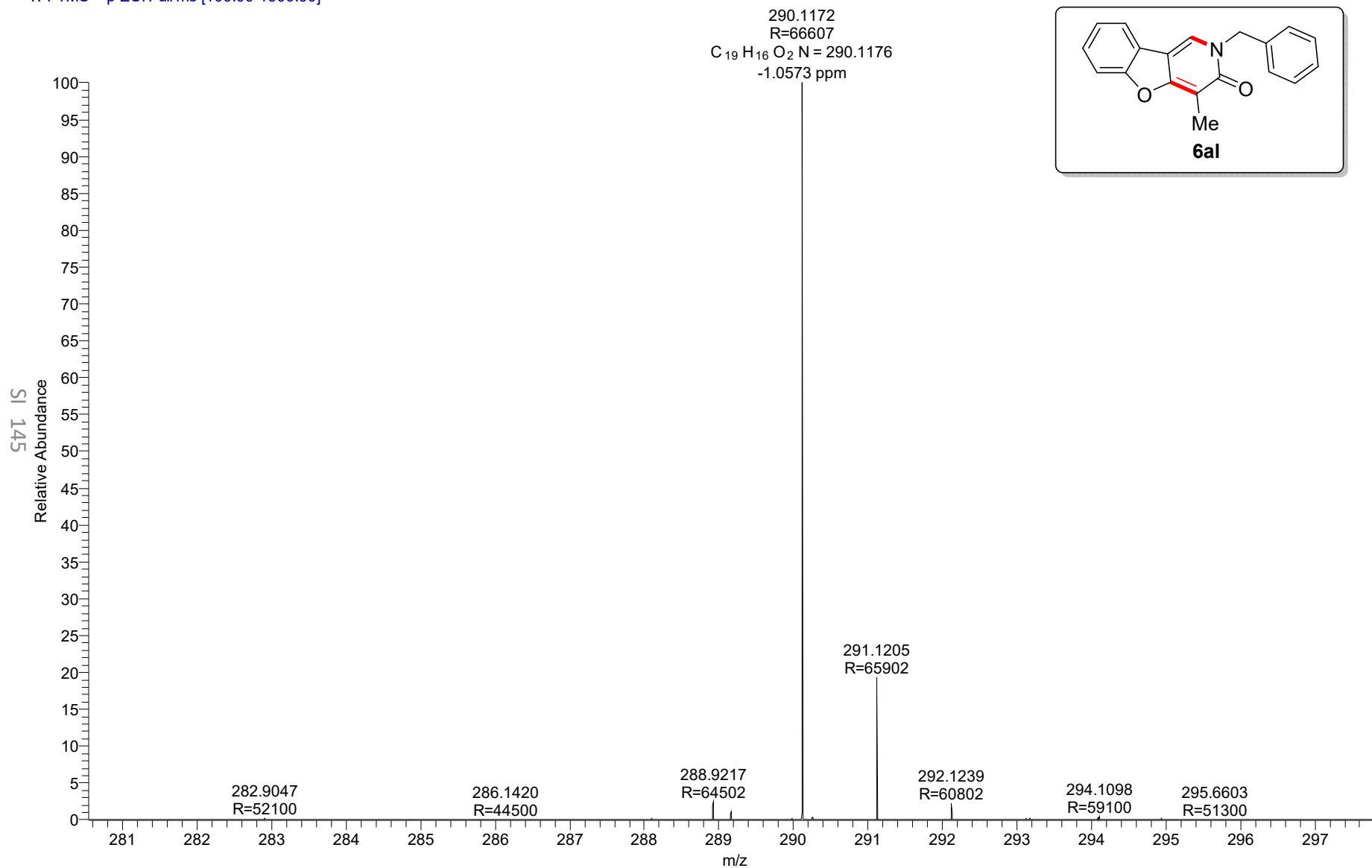
Chloroform-d



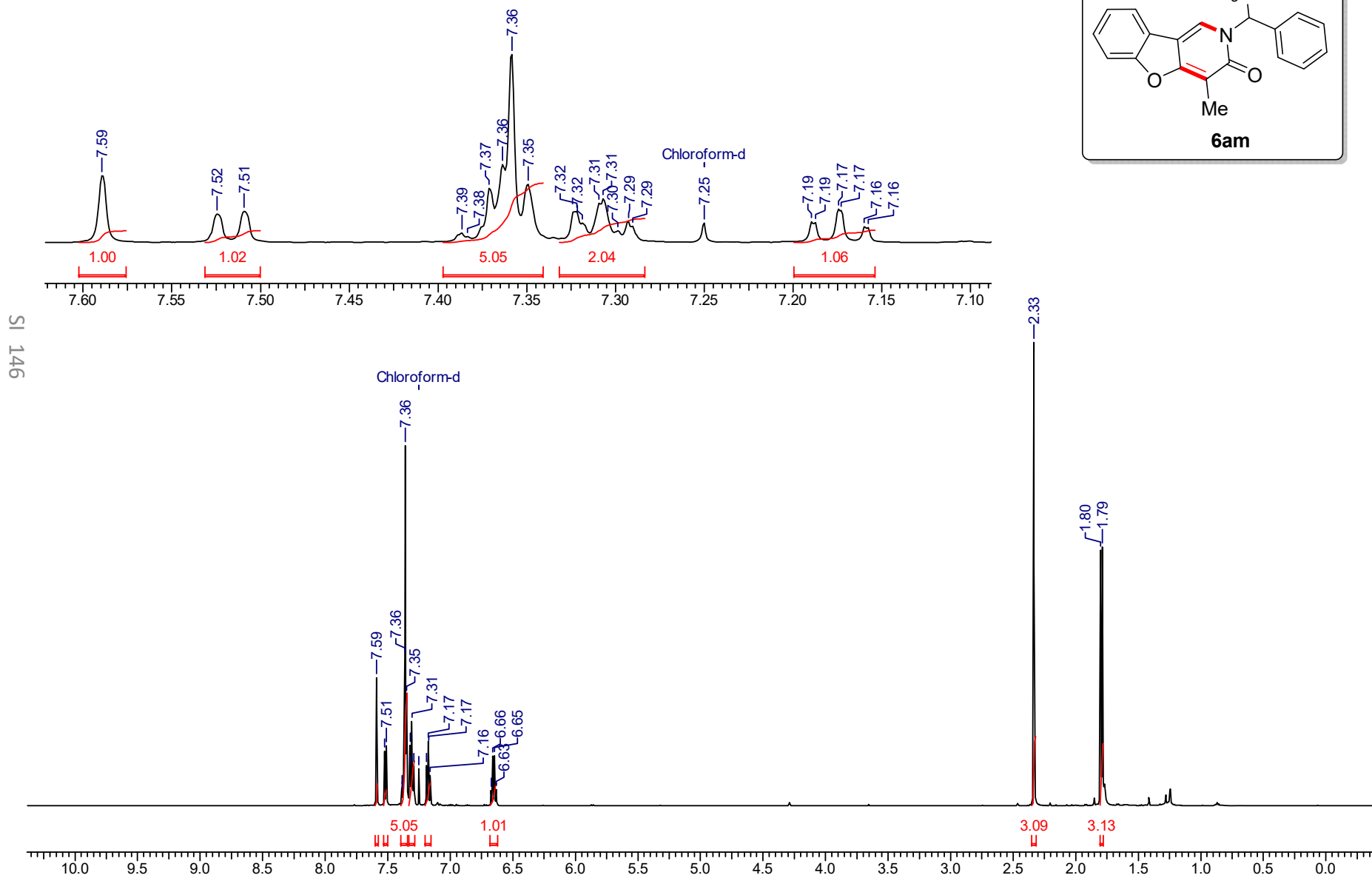
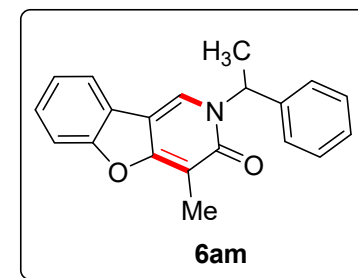
Acquisition Time (sec)	1.0486	Date	29/03/2016 19:31:52	Frequency (MHz)	125.76	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00	Temperature (grad C)	0.000



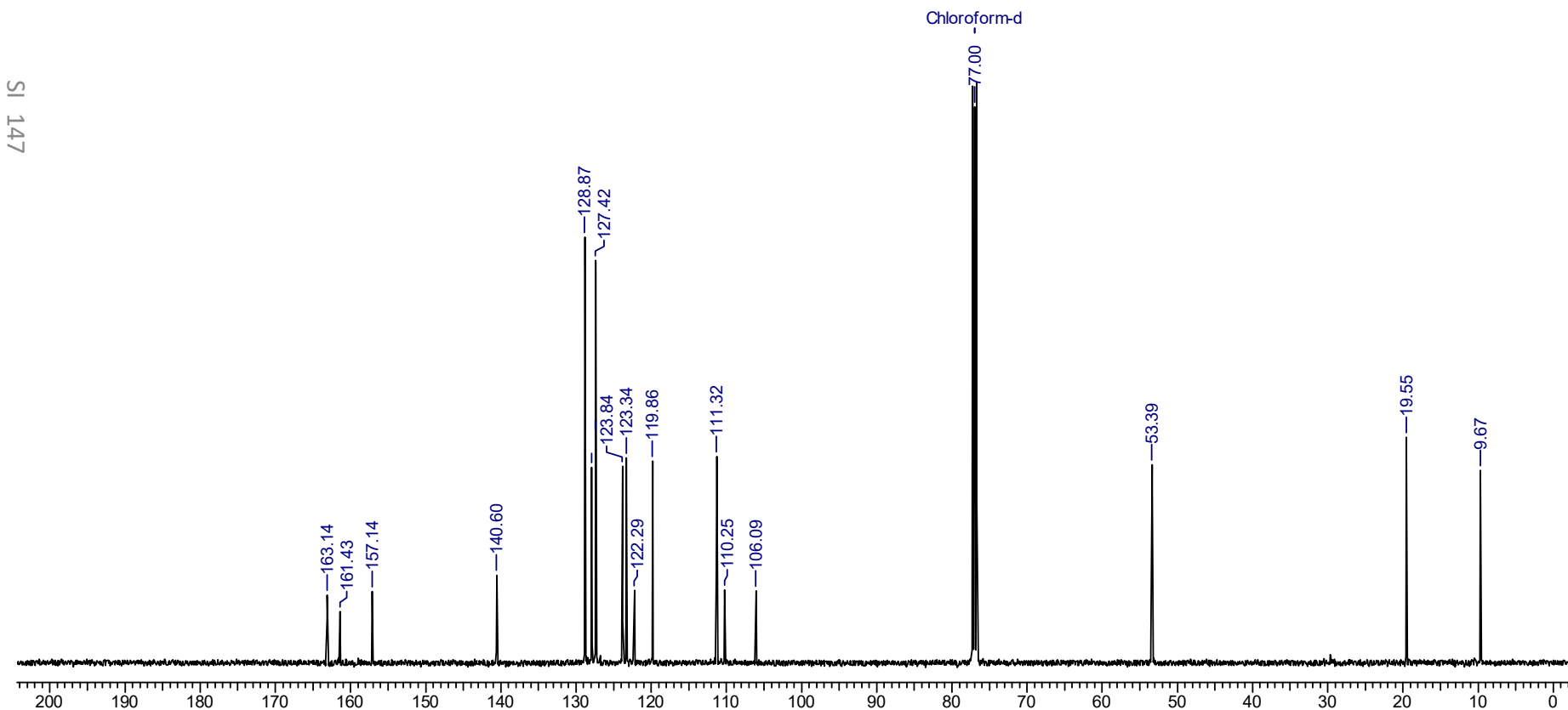
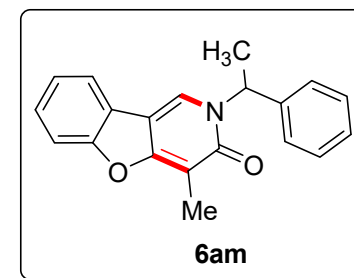
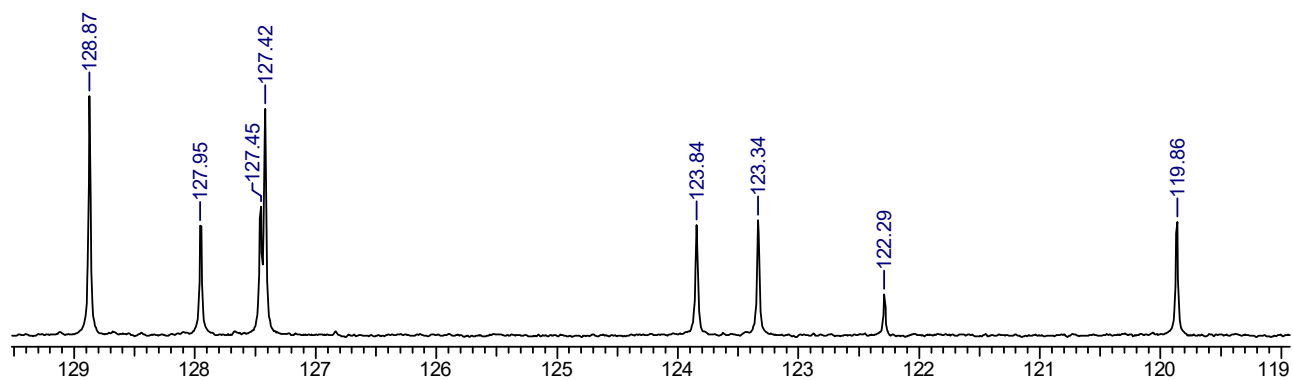
JY-A-26A #127 RT: 0.57 AV: 1 NL: 1.79E8
T: FTMS + p ESI Full ms [100.00-1500.00]



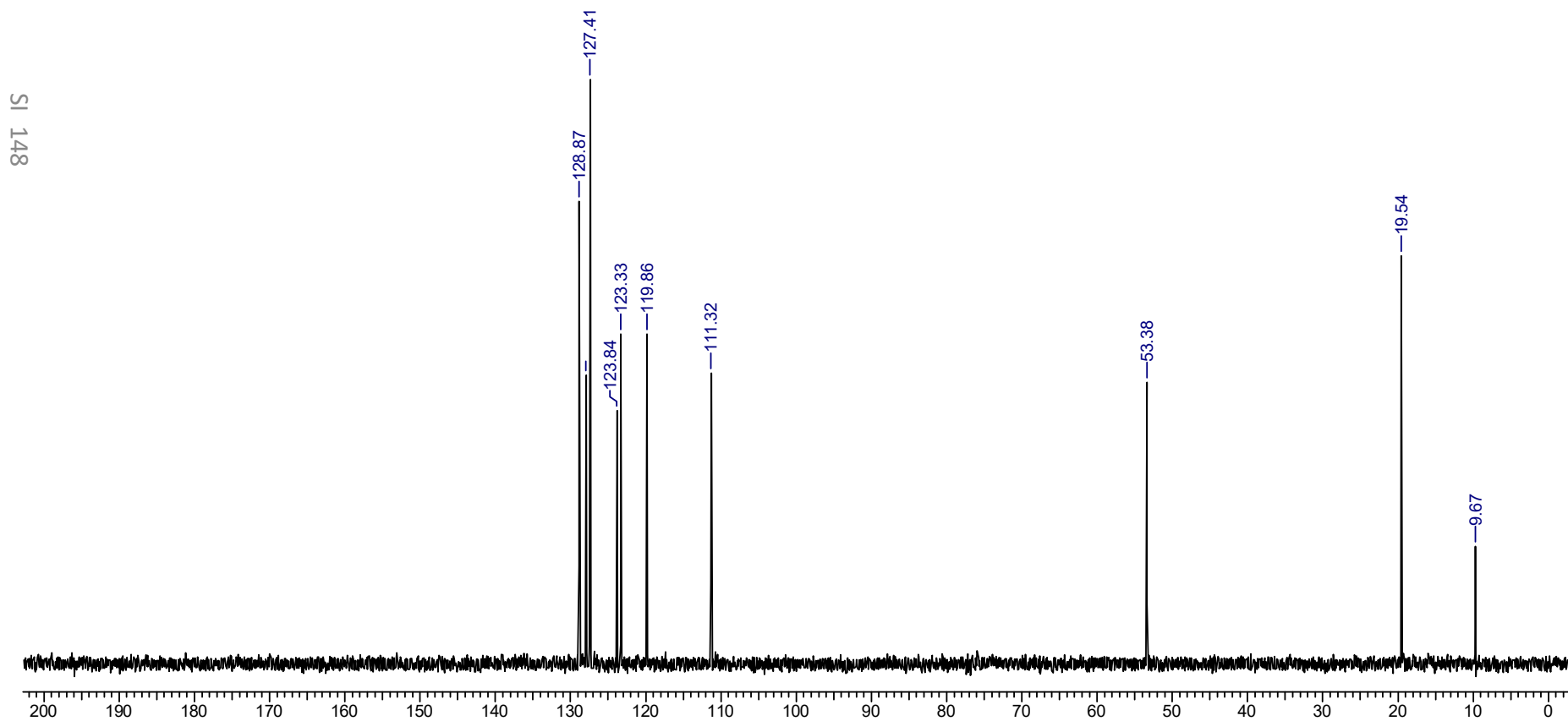
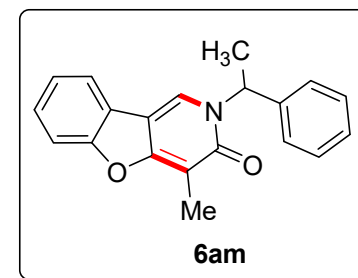
Acquisition Time (sec)	2.6214	Comment	jyothi	Date	30/03/2016 22:44:08	Frequency (MHz)	500.13
Nucleus	¹ H	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	12500.00
Temperature (grad C)	0.000						



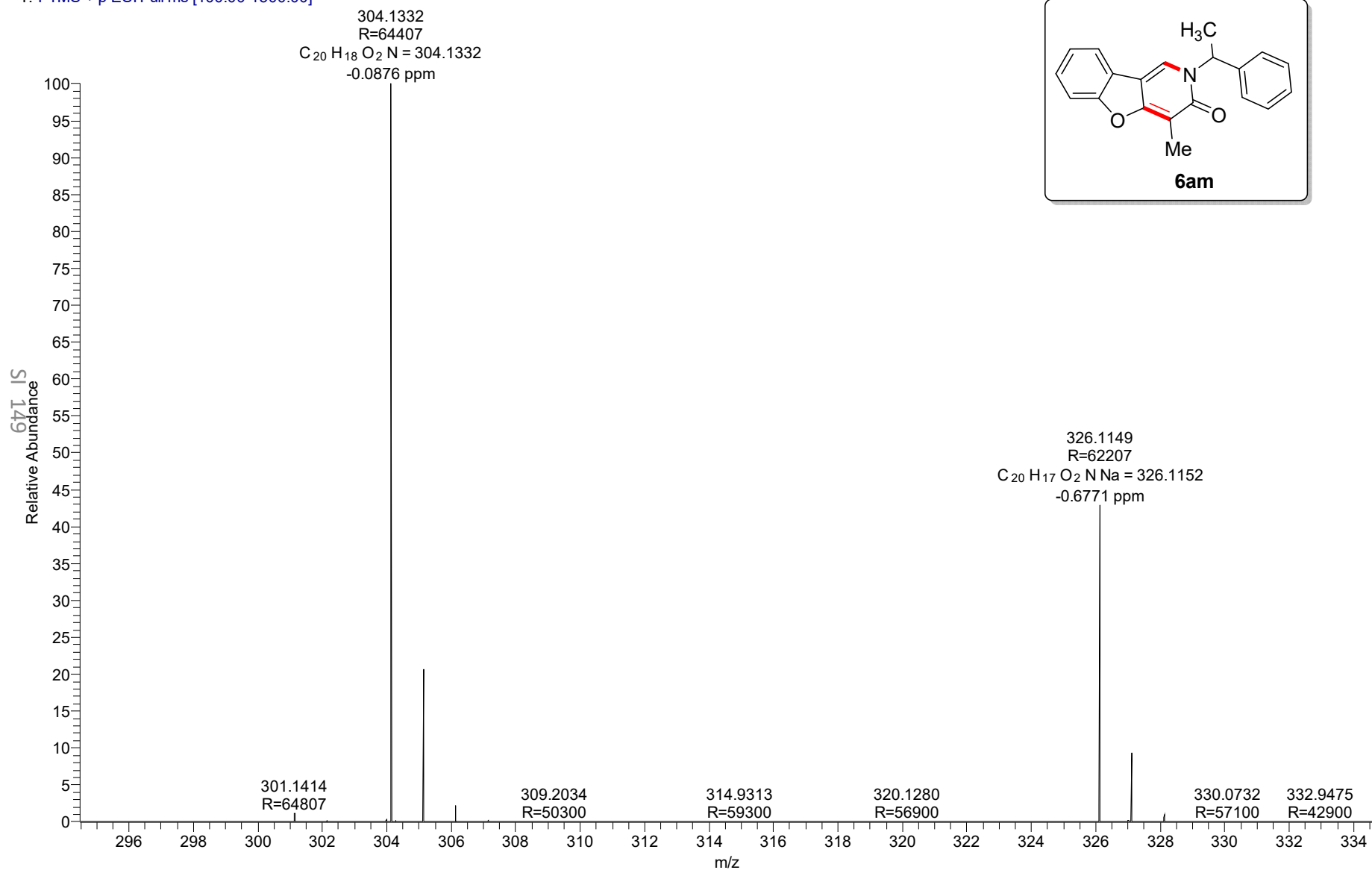
Acquisition Time (sec)	1.0486	Comment	13C	Date	30/03/2016 23:22:18	Frequency (MHz)	125.76
Nucleus	13C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00
Temperature (grad C)	0.000						



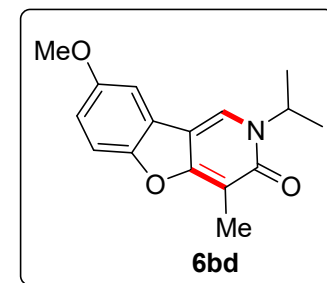
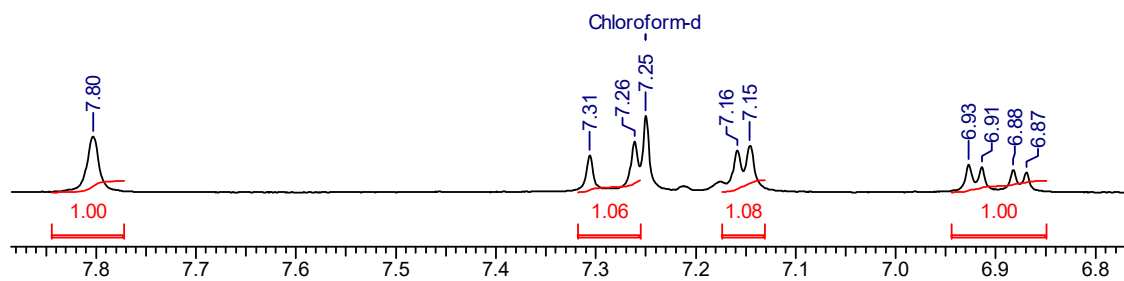
Acquisition Time (sec)	1.0486	Date	30/03/2016 23:21:56	Frequency (MHz)	125.76	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00	Temperature (grad C)	0.000



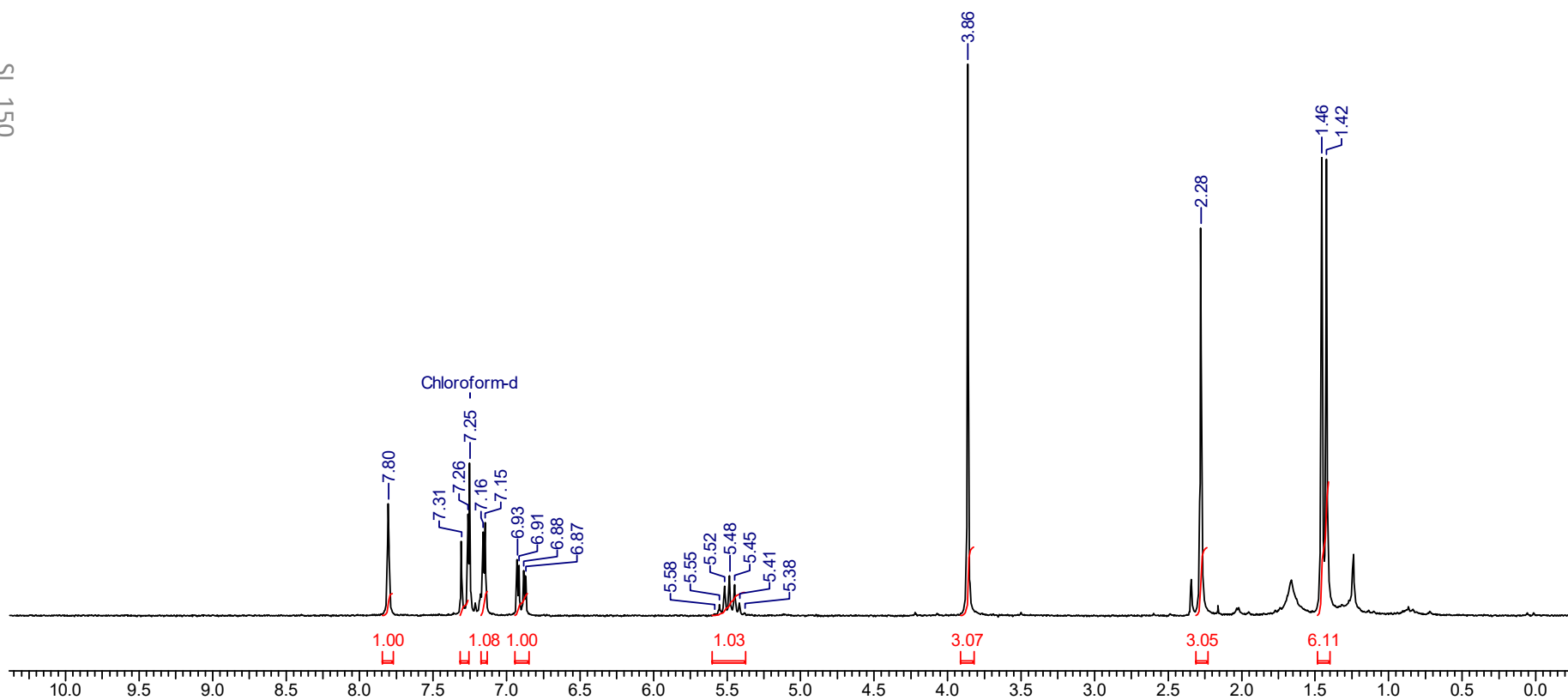
JY-A-24A #153 RT: 0.68 AV: 1 NL: 6.58E8
T: FTMS + p ESI Full ms [100.00-1500.00]



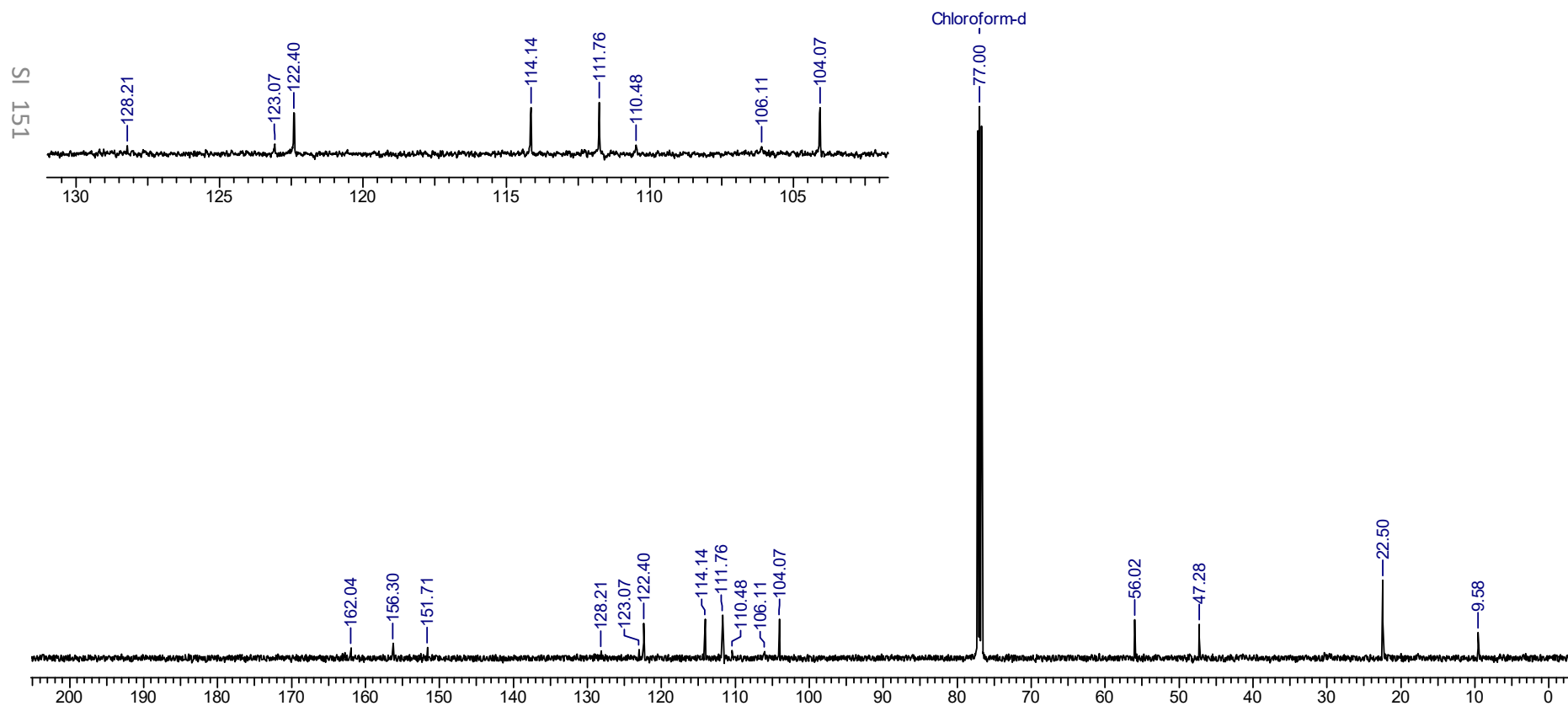
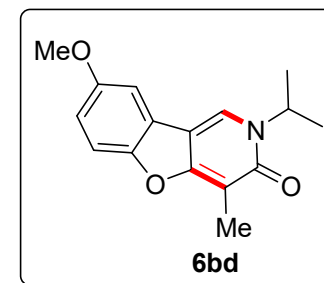
Acquisition Time (sec)	7.9167	Comment	Srinivas	Date	27/02/2016 15:39:24	Frequency (MHz)	200.13
Nucleus	¹ H	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	4139.07
						Temperature (grad C)	0.000



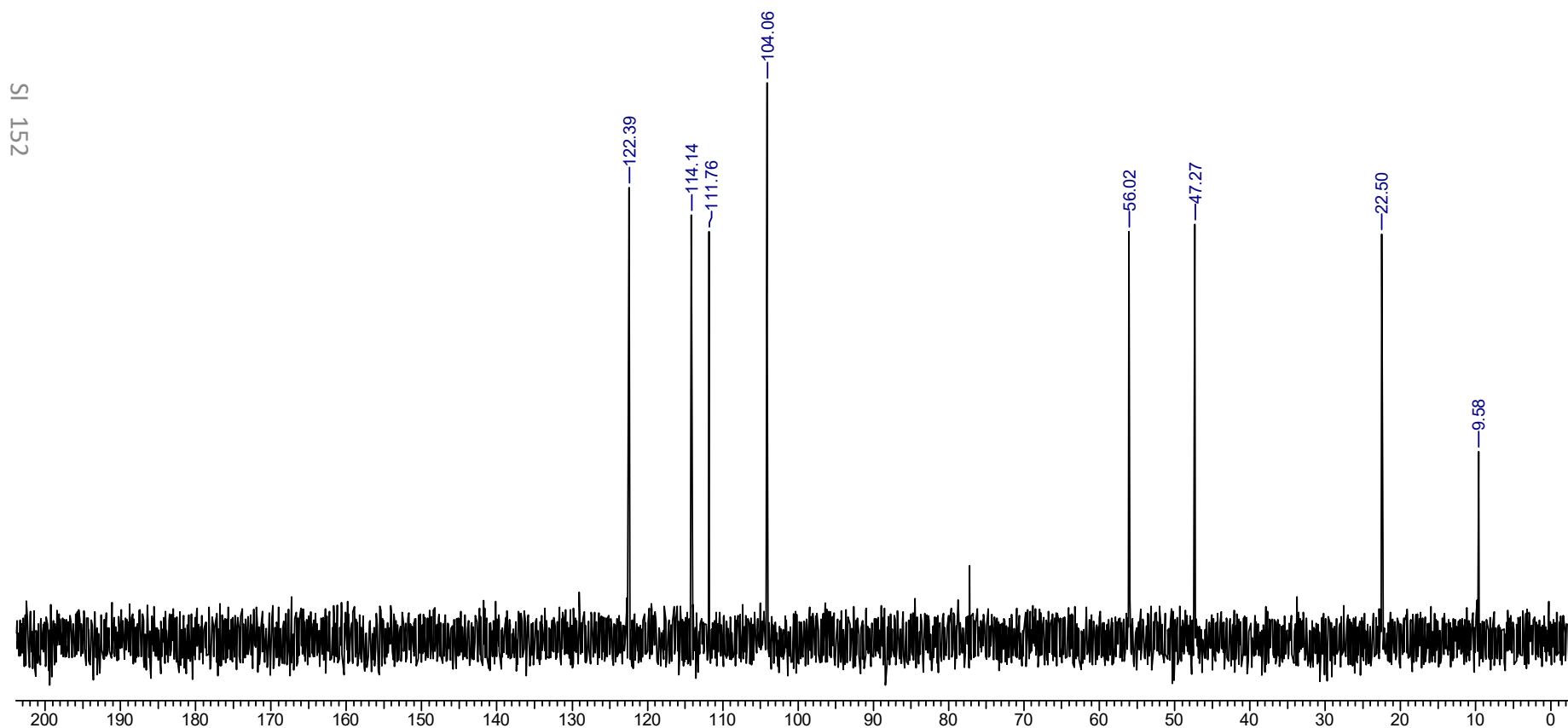
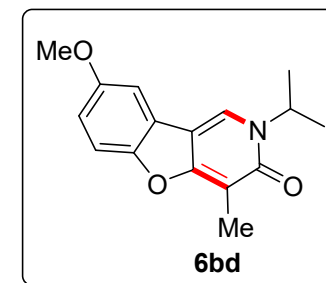
SI 150



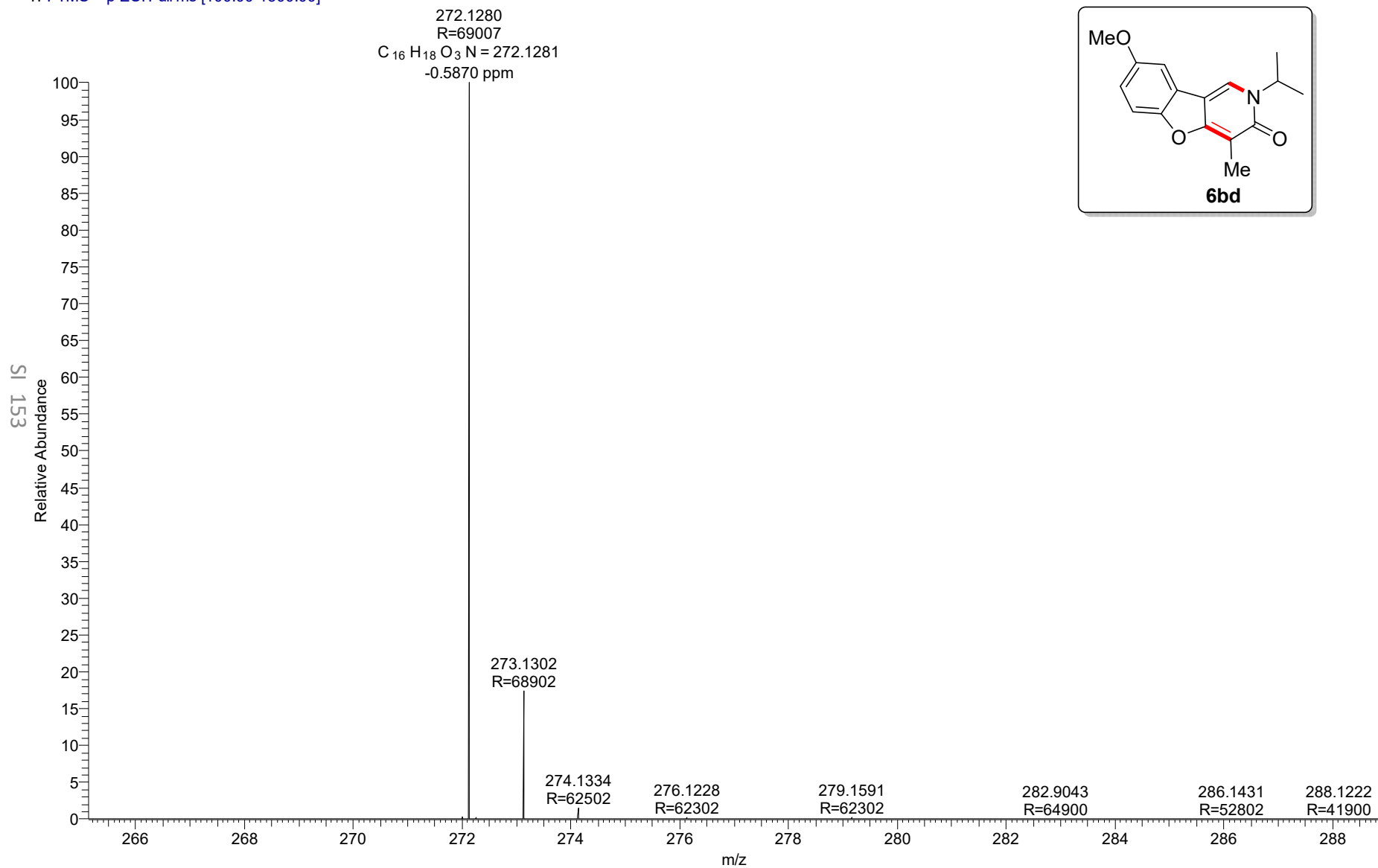
Acquisition Time (sec)	1.0486	Comment	13C	Date	07/03/2016 22:43:12	Frequency (MHz)	125.76
Nucleus	13C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00
Temperature (grad C)	0.000						



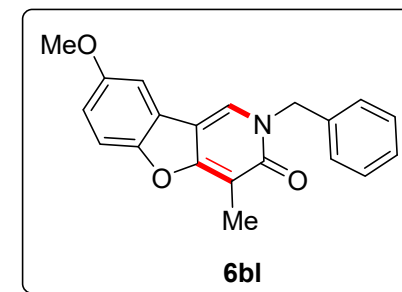
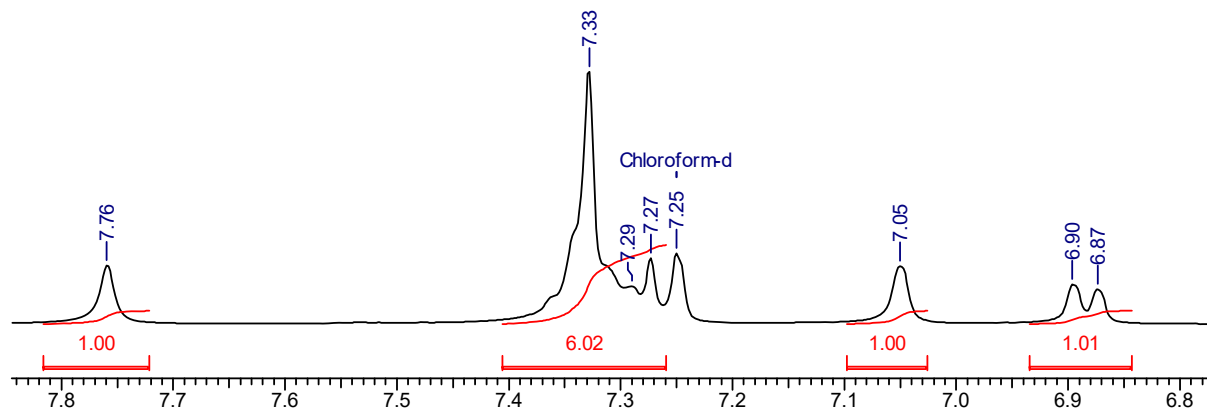
Acquisition Time (sec)	1.0486	Date	07/03/2016 22:29:30	Frequency (MHz)	125.76	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	31250.00	Temperature (grad C)	0.000



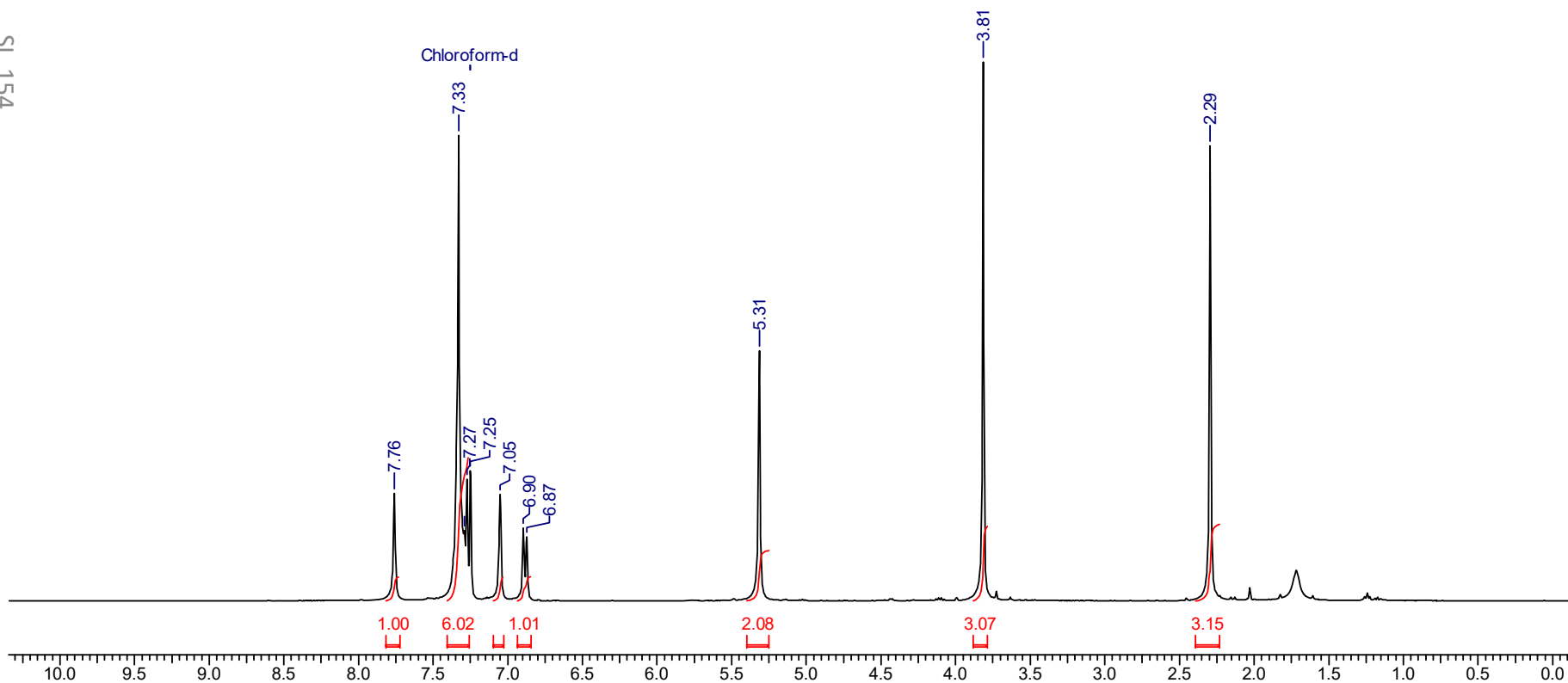
JY-A-18A #119 RT: 0.53 AV: 1 NL: 1.43E9
T: FTMS + p ESI Full ms [100.00-1500.00]



Acquisition Time (sec)	1.6384	Comment	Jyoti	Date	20/12/2016 12:04:48	Frequency (MHz)	400.13
Nucleus	¹ H	Original Points Count	16384	Points Count	16384	Sweep Width (Hz)	10000.00
Temperature (grad C)	0.000						

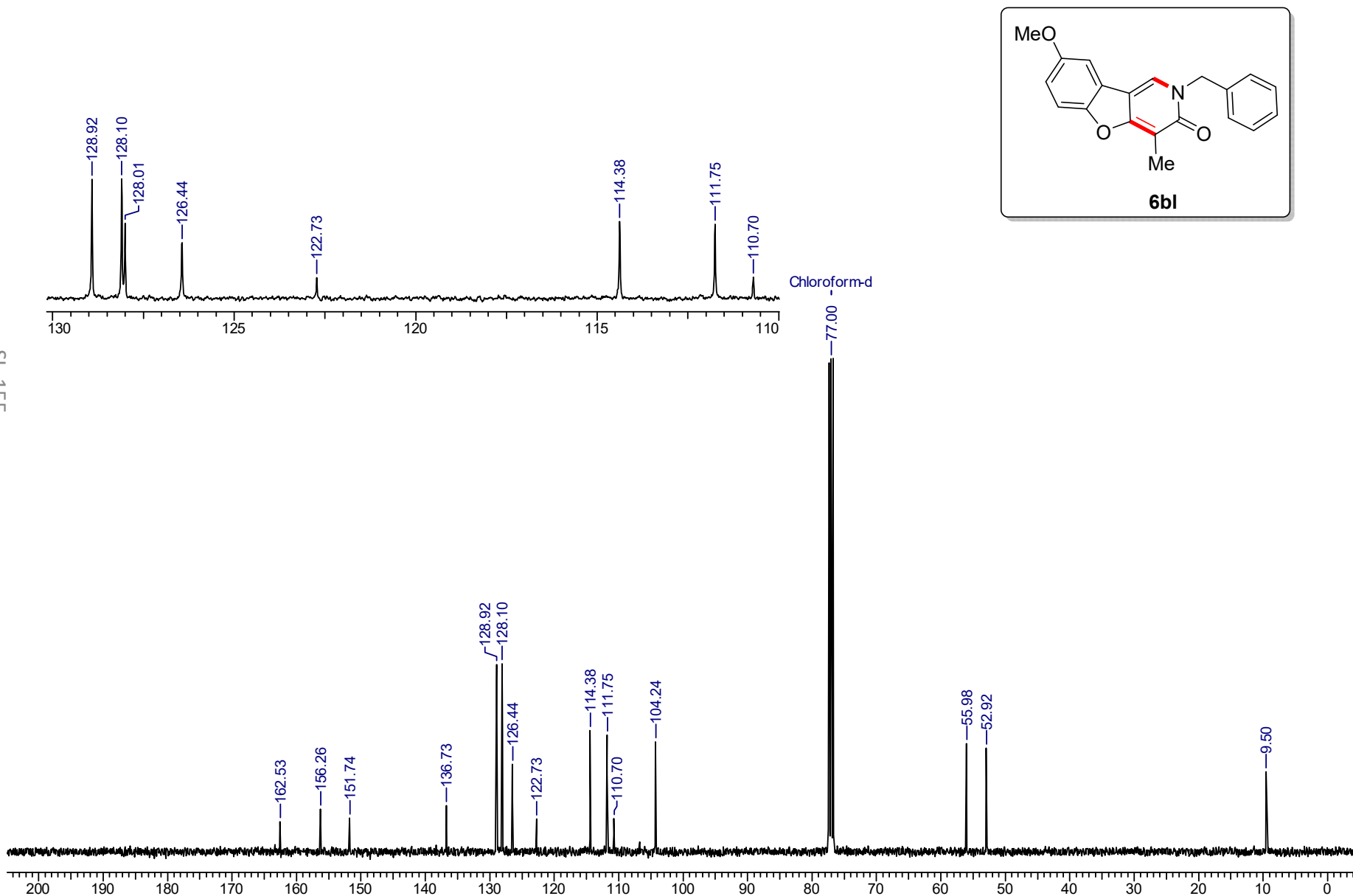


SI 154

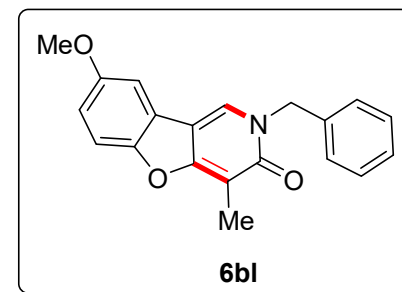


Acquisition Time (sec)	1.2976	Date	20/12/2016 12:19:32	Frequency (MHz)	100.61	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53	Temperature (grad C)	0.000

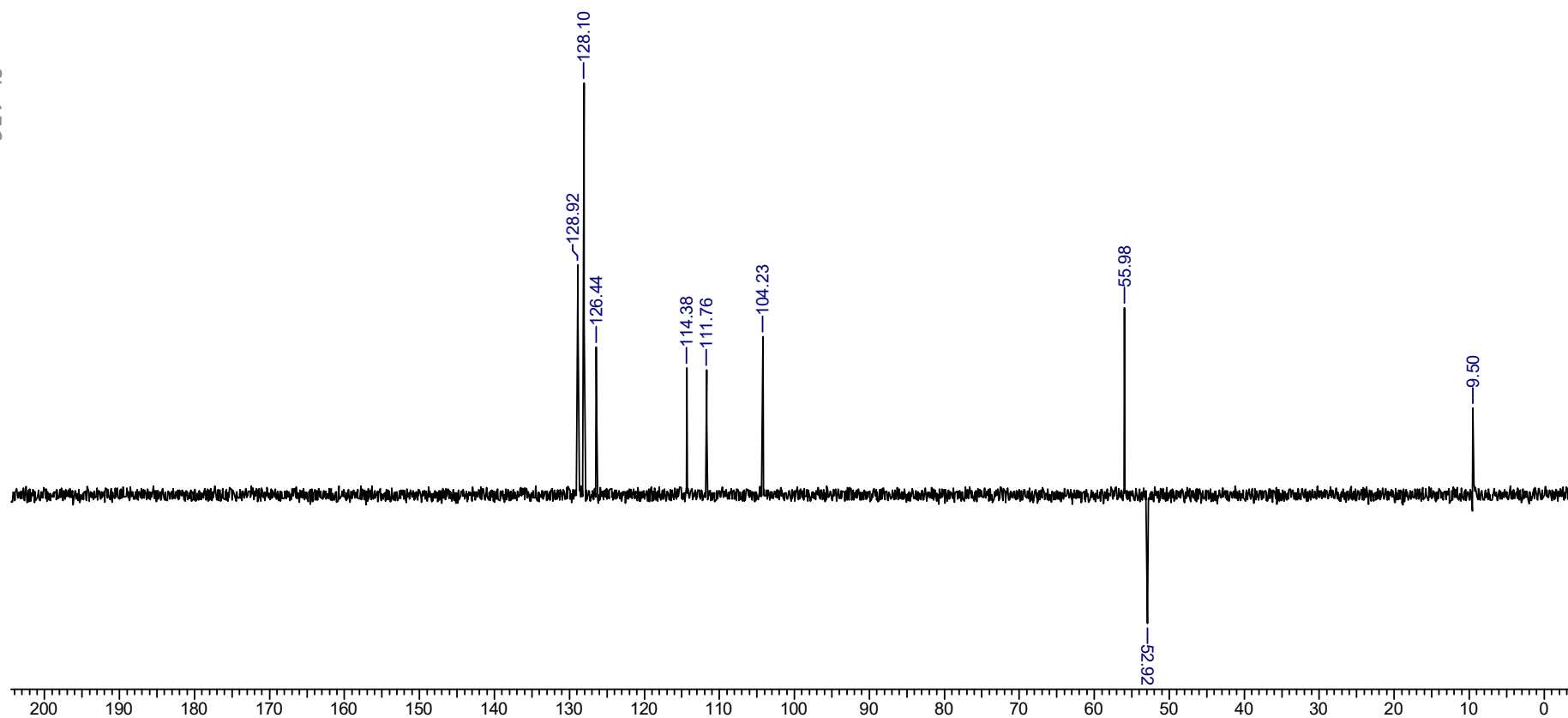
SI 155



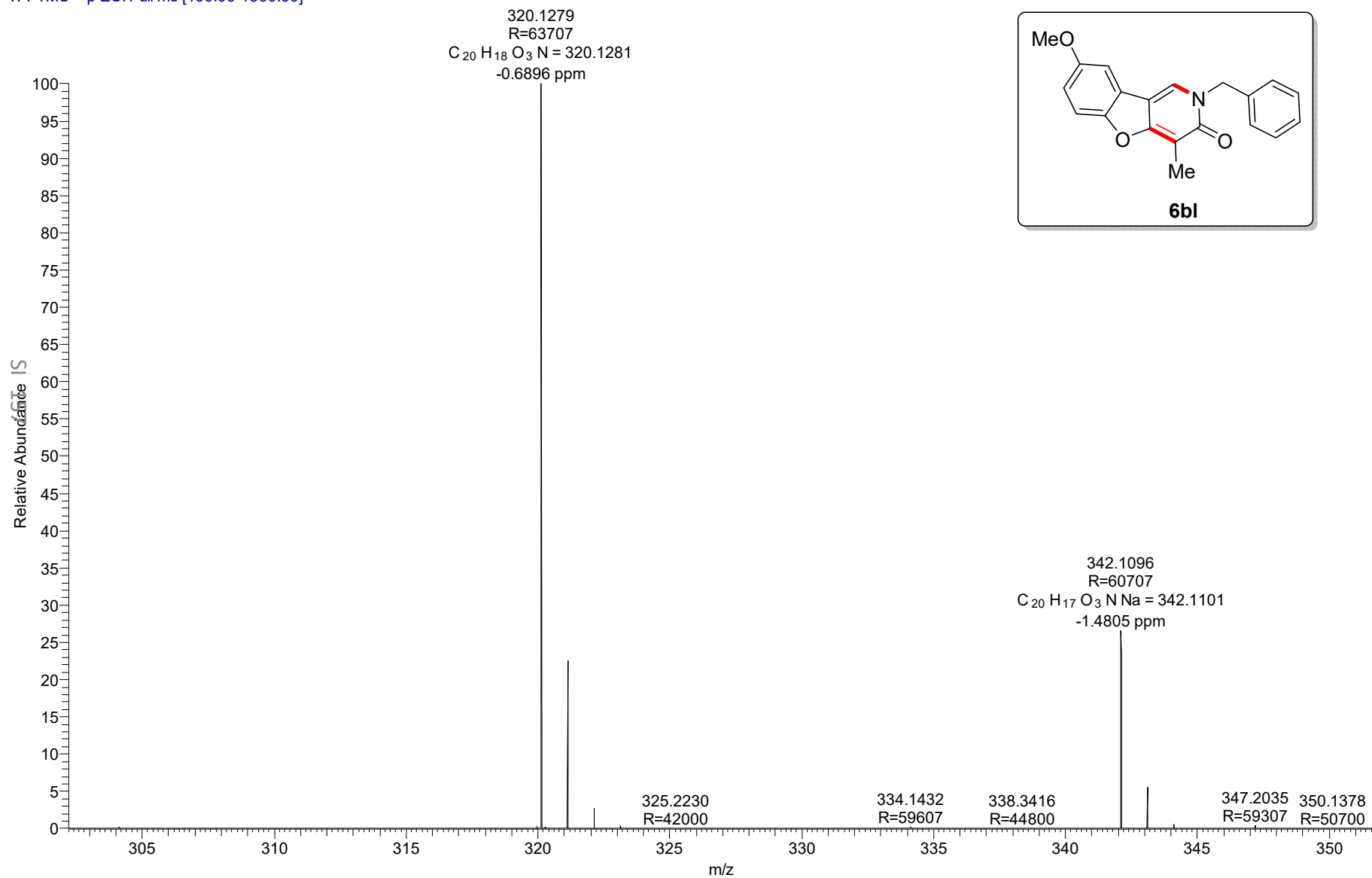
Acquisition Time (sec)	1.2976	Comment	DEPT	Date	20/12/2016 12:05:02	Frequency (MHz)	100.61
Nucleus	¹³ C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53
Temperature (grad C)	0.000						



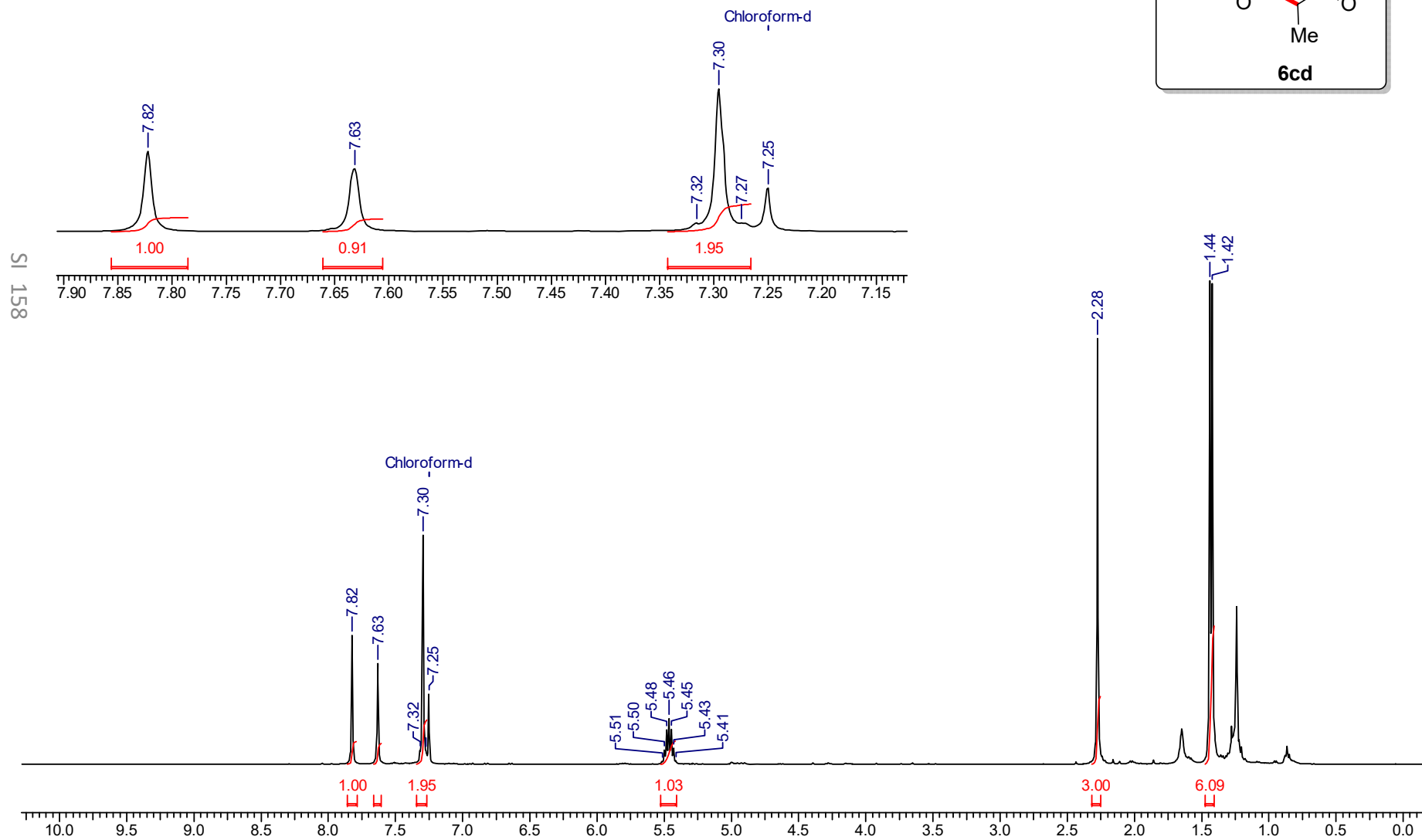
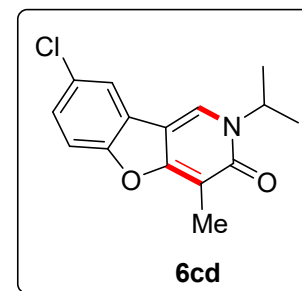
SI 156



JY-A-34B #134 RT: 0.59 AV: 1 NL: 1.58E9
T: FTMS + p ESI Full ms [100.00-1500.00]

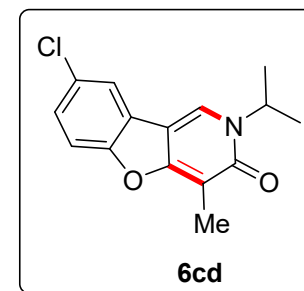
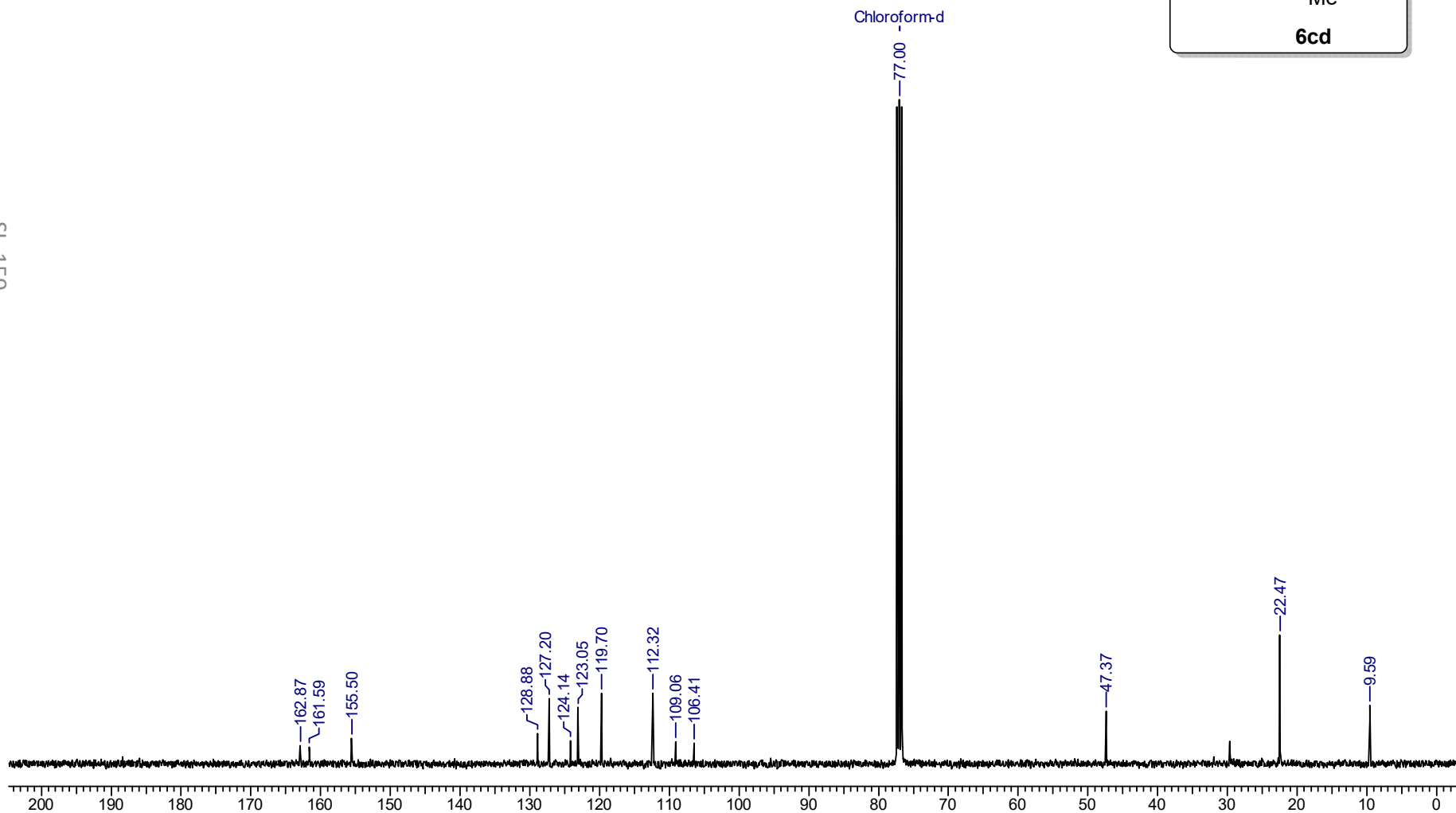


Acquisition Time (sec)	2.0447	Comment	Jyothi	Date	31/03/2016 18:46:34	Frequency (MHz)	400.13
Nucleus	¹ H	Original Points Count	16384	Points Count	16384	Sweep Width (Hz)	8012.82
Temperature (grad C)	0.000						

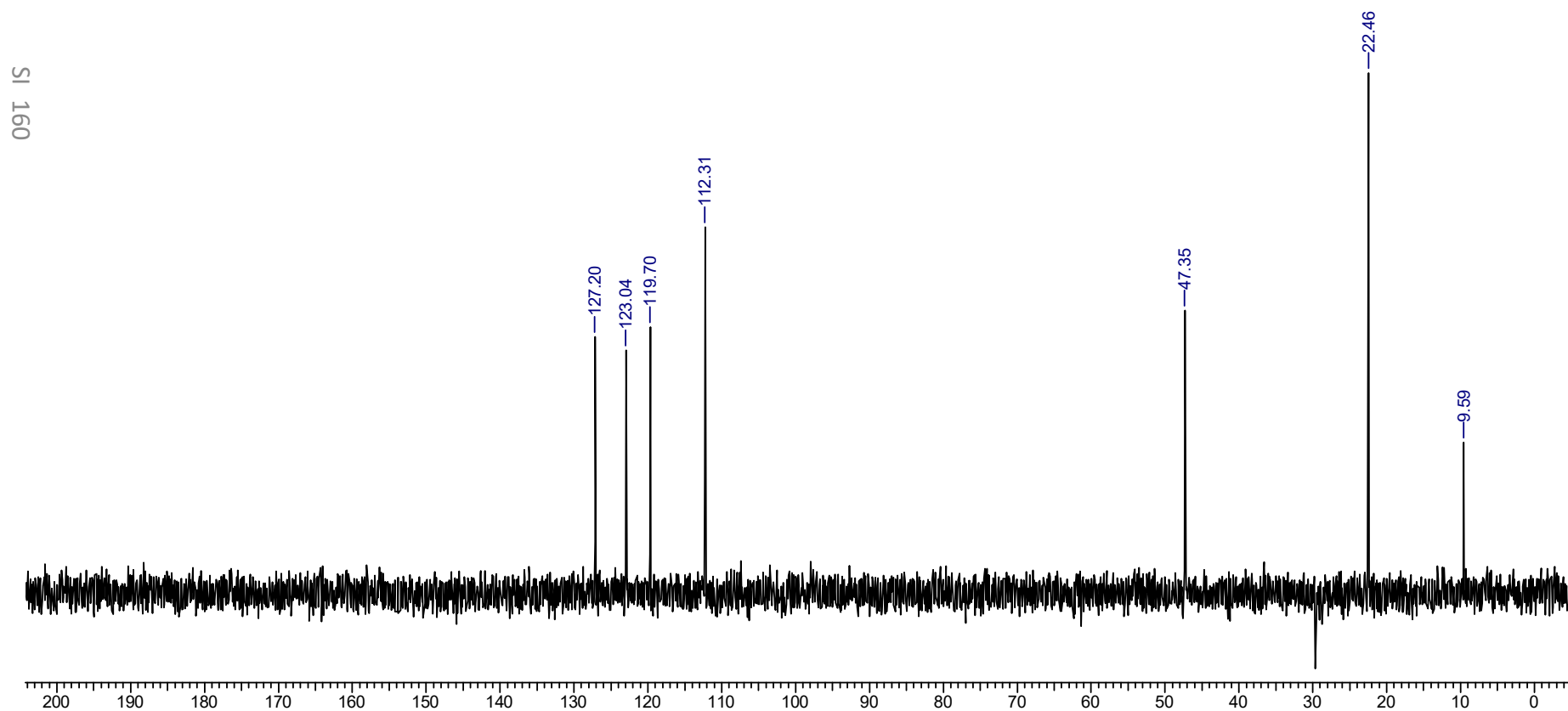
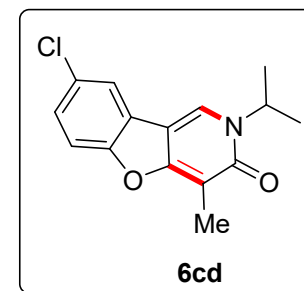


Acquisition Time (sec)	1.2976	Date	31/03/2016 19:06:14	Frequency (MHz)	100.61	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53	Temperature (grad C)	0.000

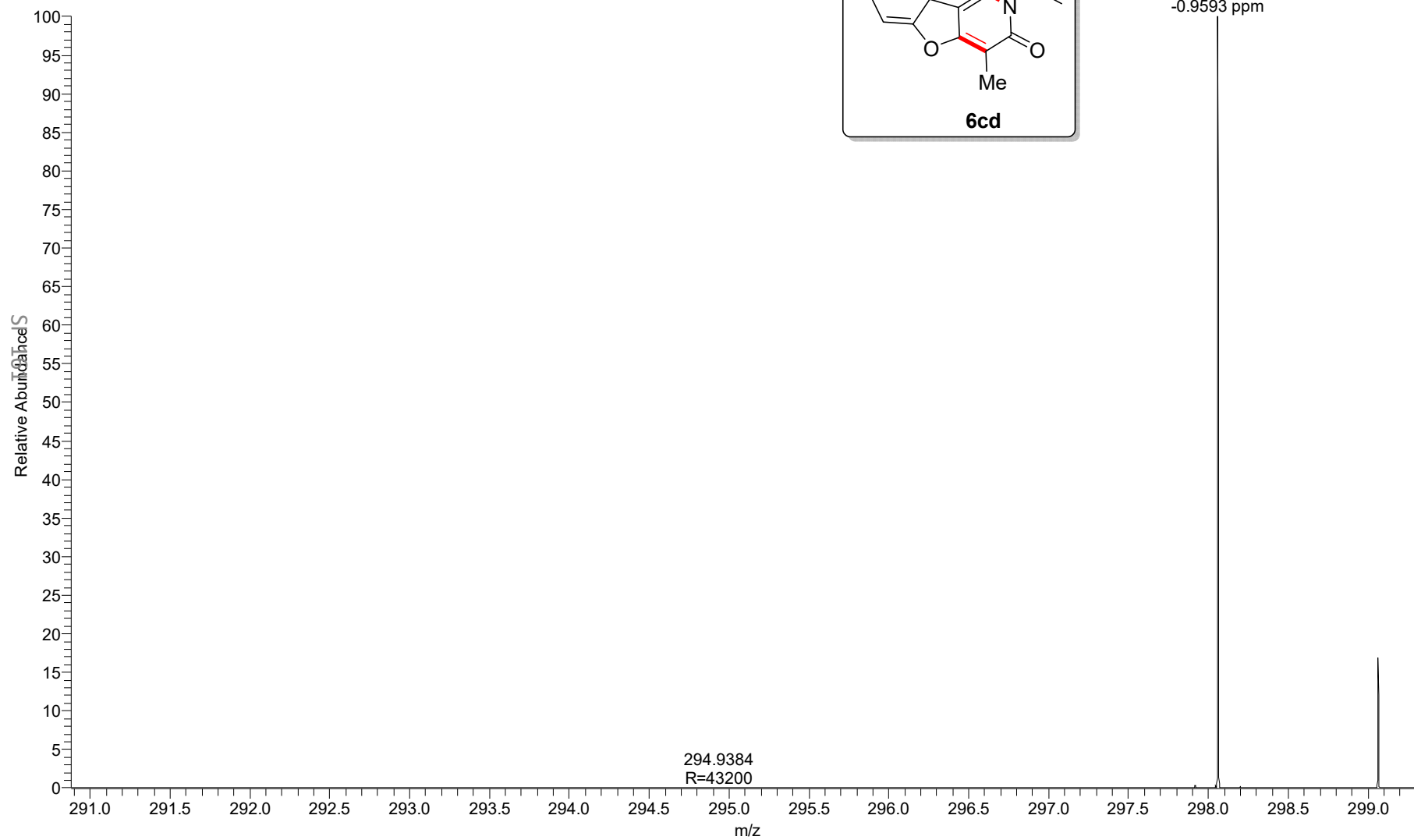
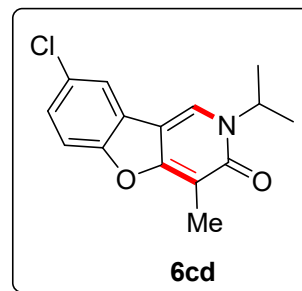
SI 159



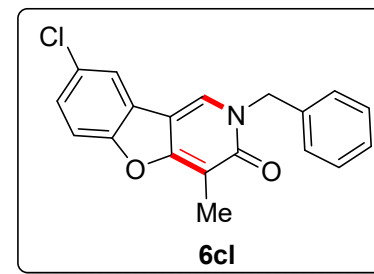
Acquisition Time (sec)	1.2976	Comment	DEPT	Date	31/03/2016 18:47:00	Frequency (MHz)	100.61
Nucleus	¹³ C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53
Temperature (grad C)	0.000						



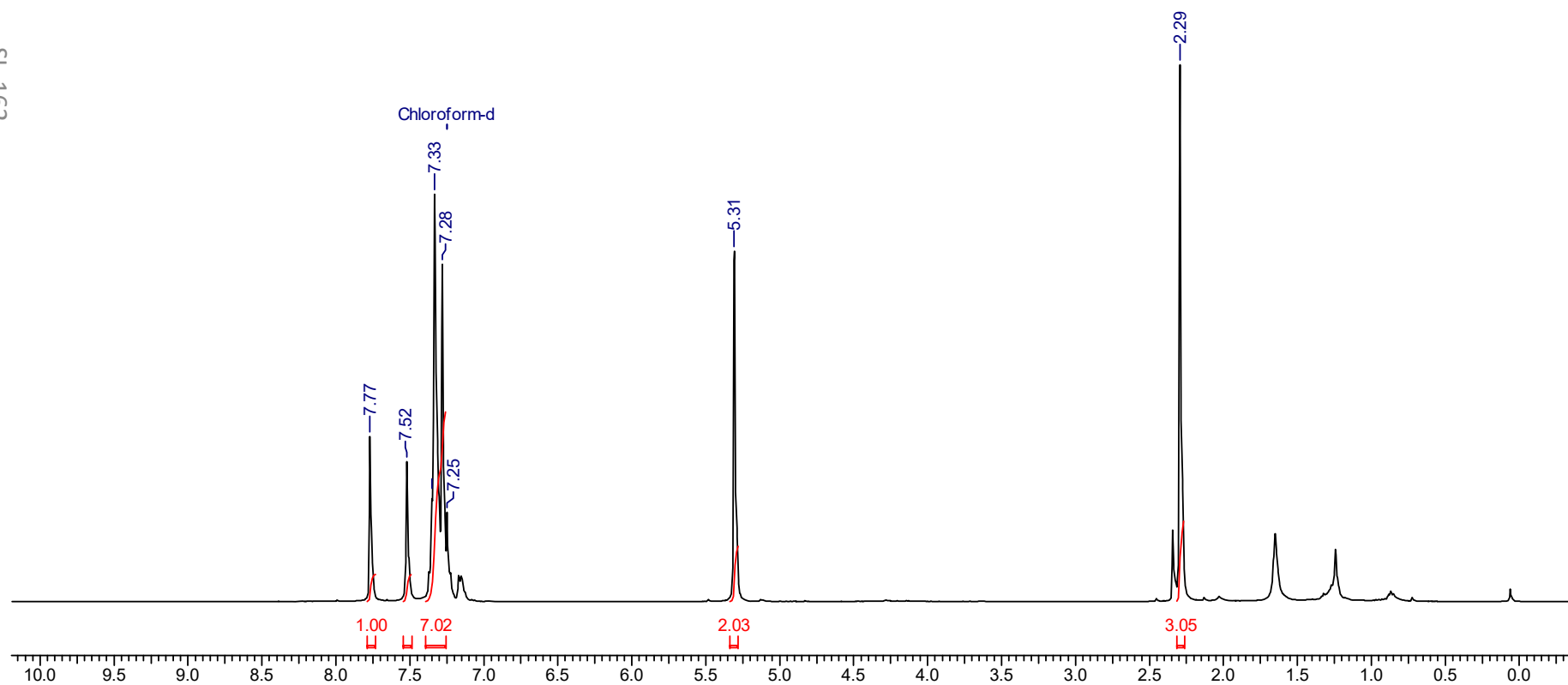
JY-A-26B #130 RT: 0.58 AV: 1 NL: 1.26E9
T: FTMS + p ESI Full ms [100.00-1500.00]



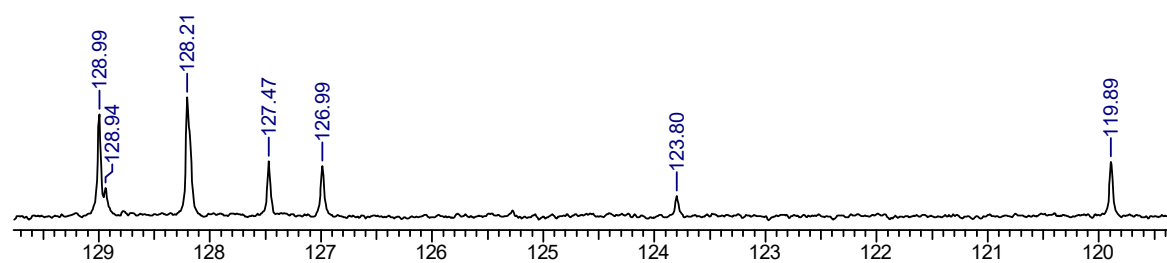
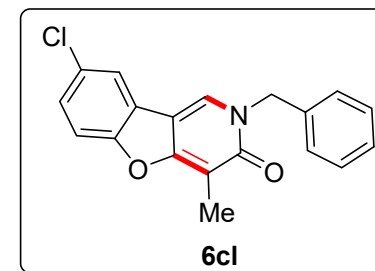
Acquisition Time (sec)	2.0447	Comment	Jyothi	Date	18/04/2016 10:59:06	Frequency (MHz)	400.13
Nucleus	¹ H	Original Points Count	16384	Points Count	16384	Sweep Width (Hz)	8012.82
Temperature (grad C)	0.000						



SI 162



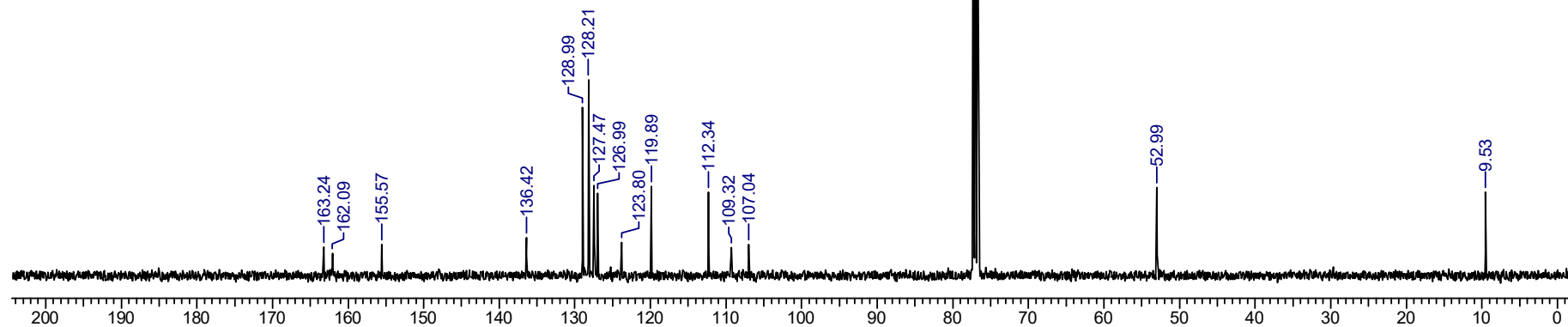
Acquisition Time (sec)	1.2976	Date	18/04/2016 11:00:36	Frequency (MHz)	100.61	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53	Temperature (grad C)	0.000



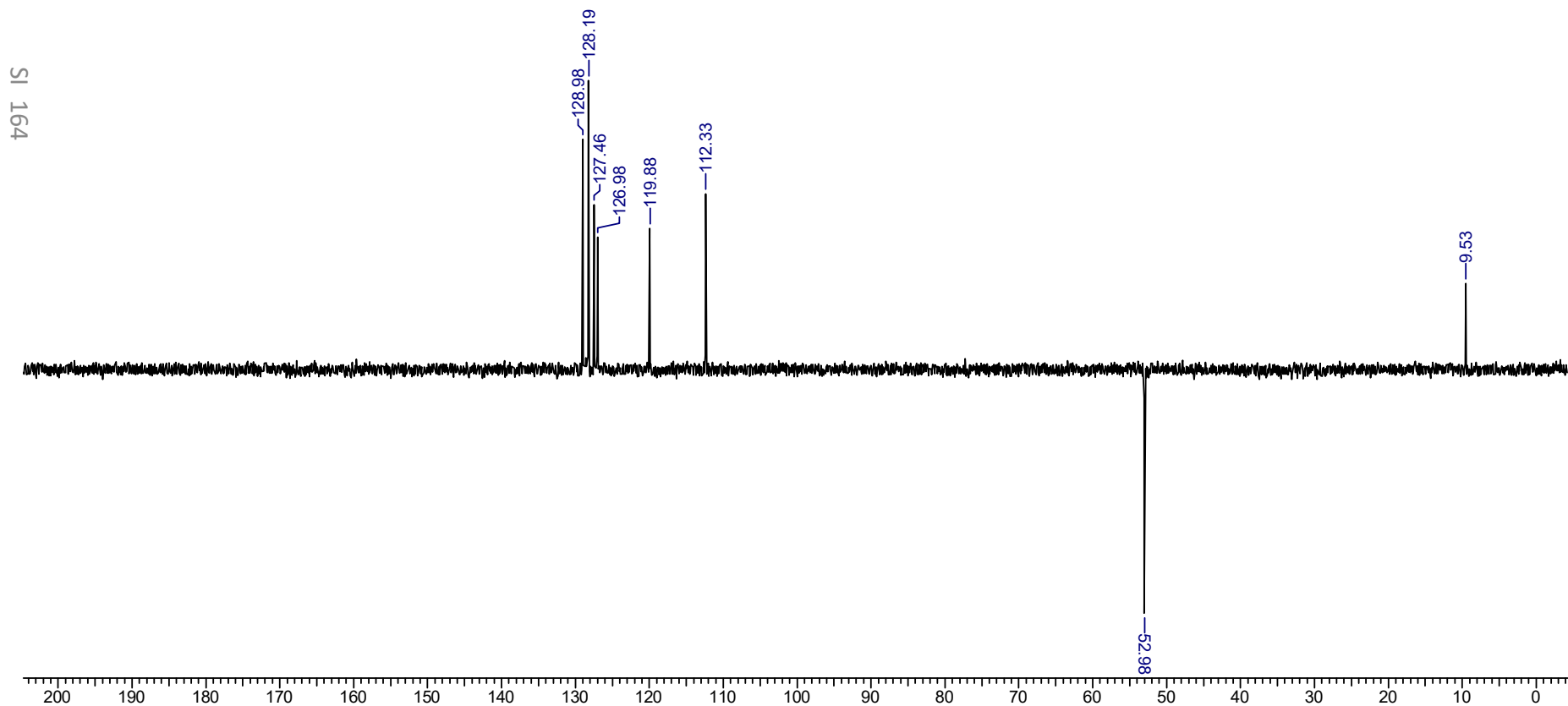
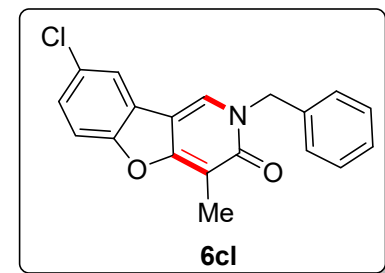
Chloroform-d

77.00

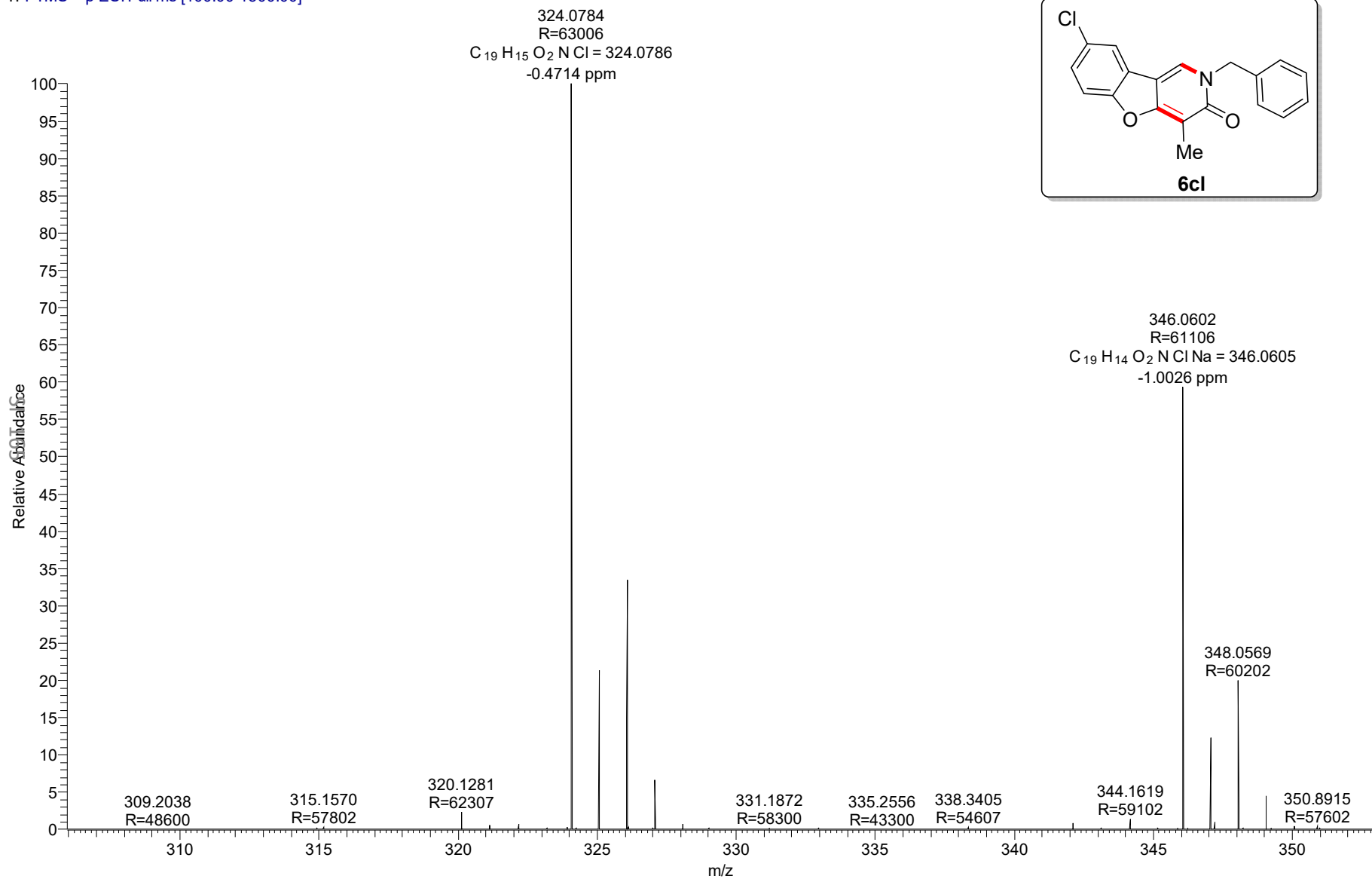
SI 163



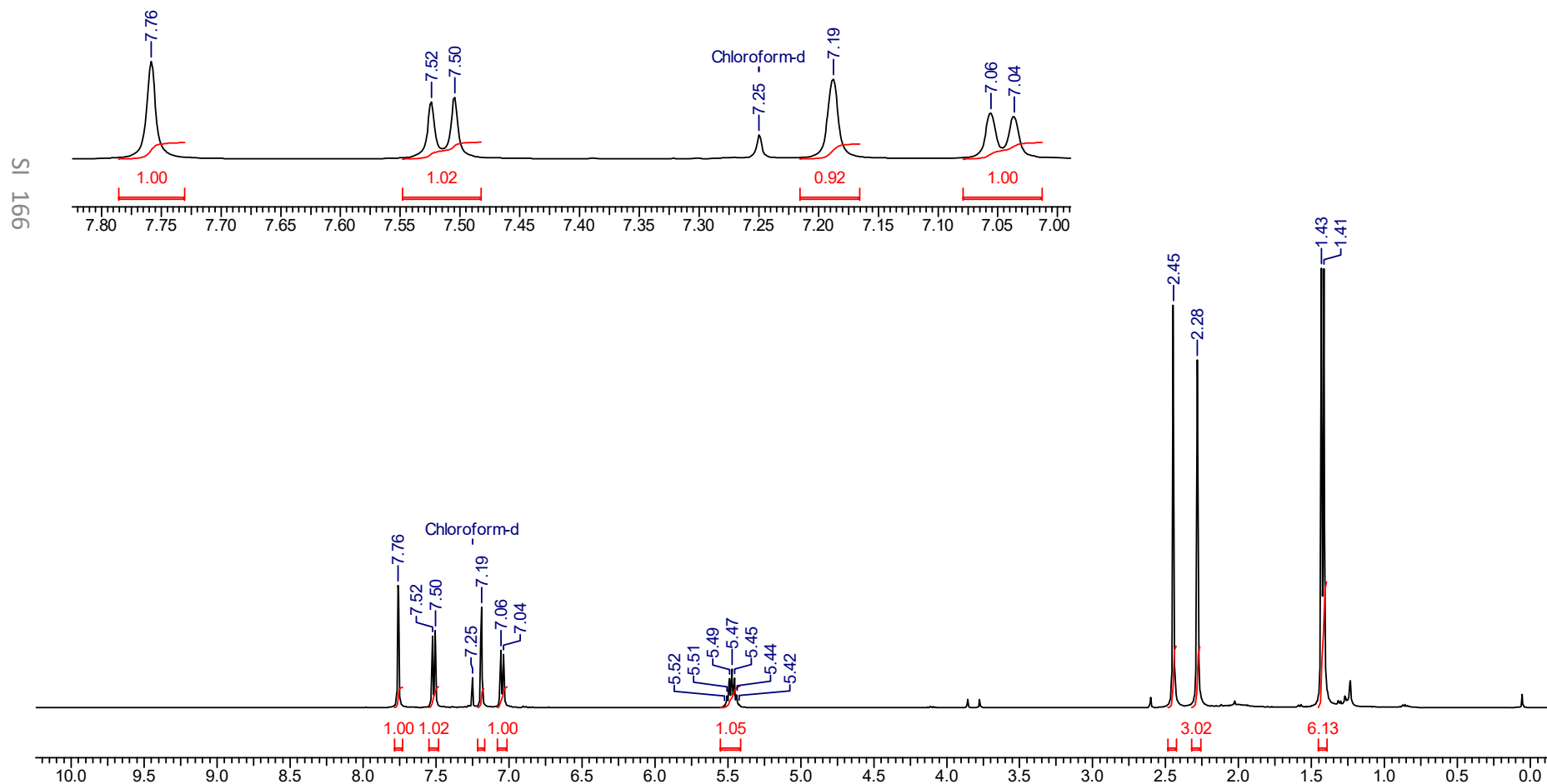
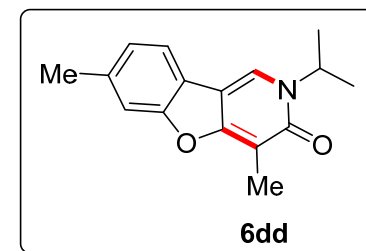
Acquisition Time (sec)	1.2976	Comment	DEPT	Date	18/04/2016 10:59:12	Frequency (MHz)	100.61
Nucleus	¹³ C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53
Temperature (grad C)	0.000						



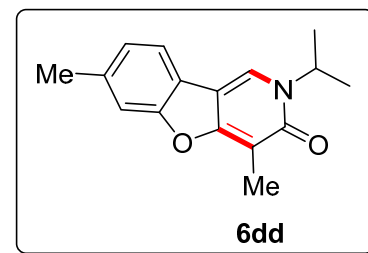
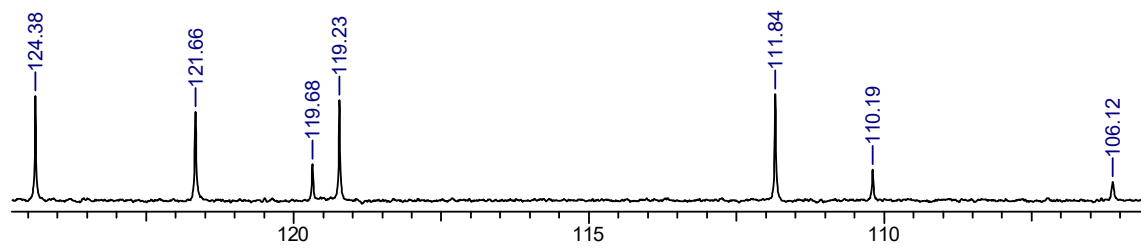
JY-A-35B #142 RT: 0.63 AV: 1 NL: 4.05E8
T: FTMS + p ESI Full ms [100.00-1500.00]



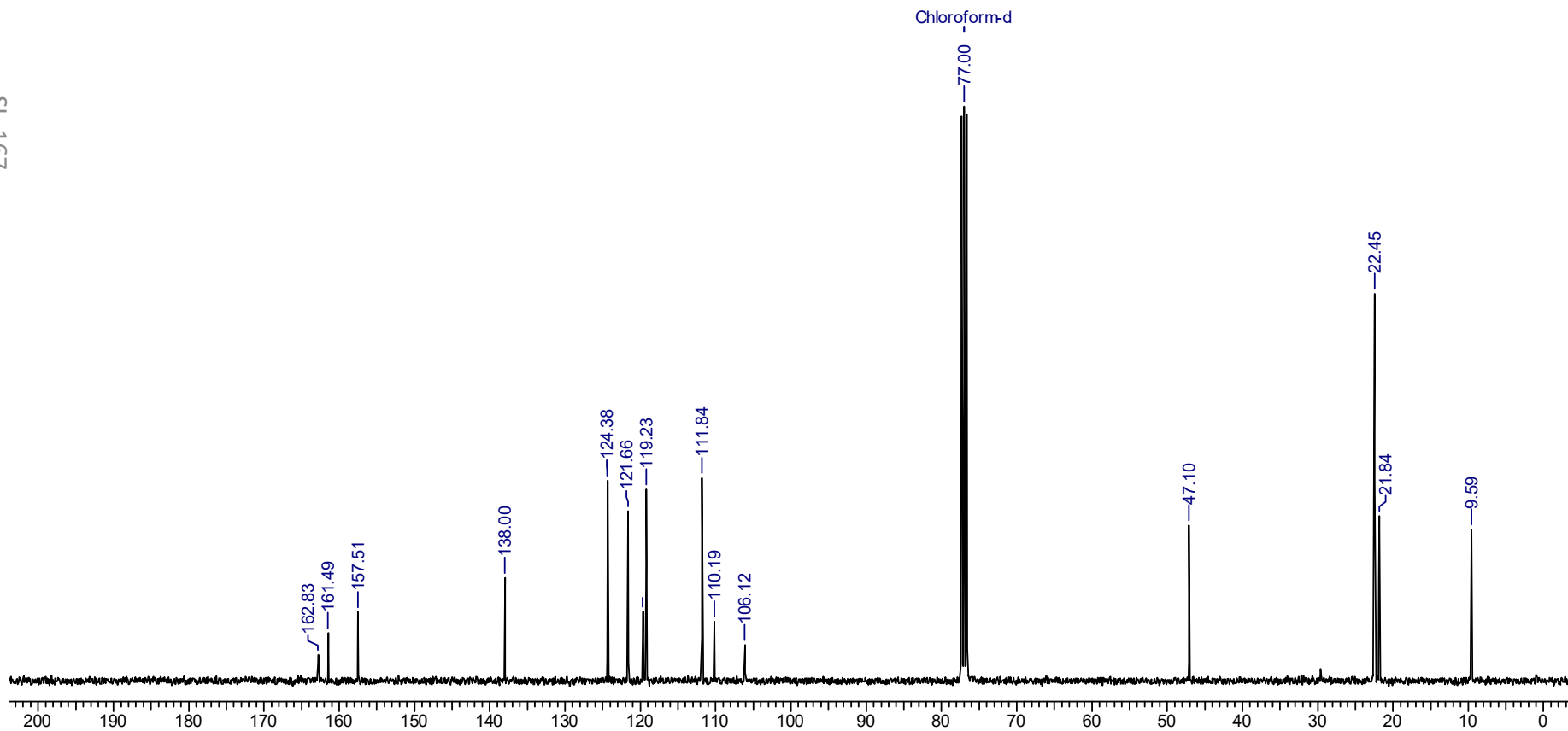
Acquisition Time (sec)	2.0447	Comment	Jyothi	Date	14/04/2016 10:42:30	Frequency (MHz)	400.13
Nucleus	¹ H	Original Points Count	16384	Points Count	16384	Sweep Width (Hz)	8012.82
Temperature (grad C)	0.000						



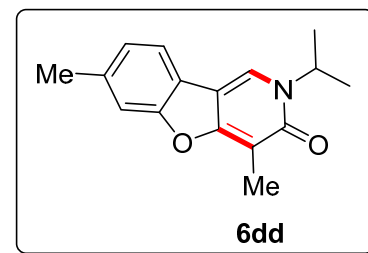
Acquisition Time (sec)	1.2976	Date	14/04/2016 11:50:52	Frequency (MHz)	100.61	Nucleus	13C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53	Temperature (grad C)	0.000



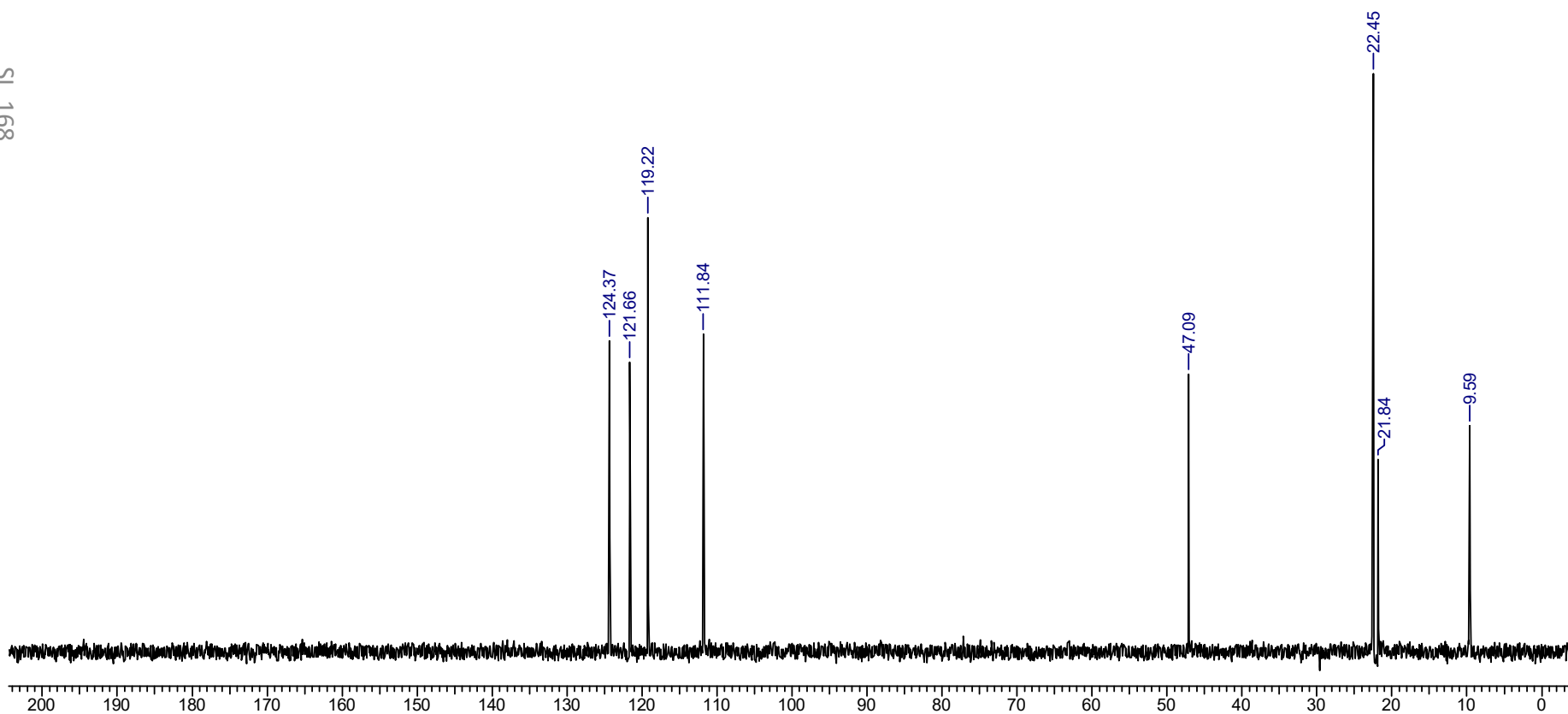
SI 167



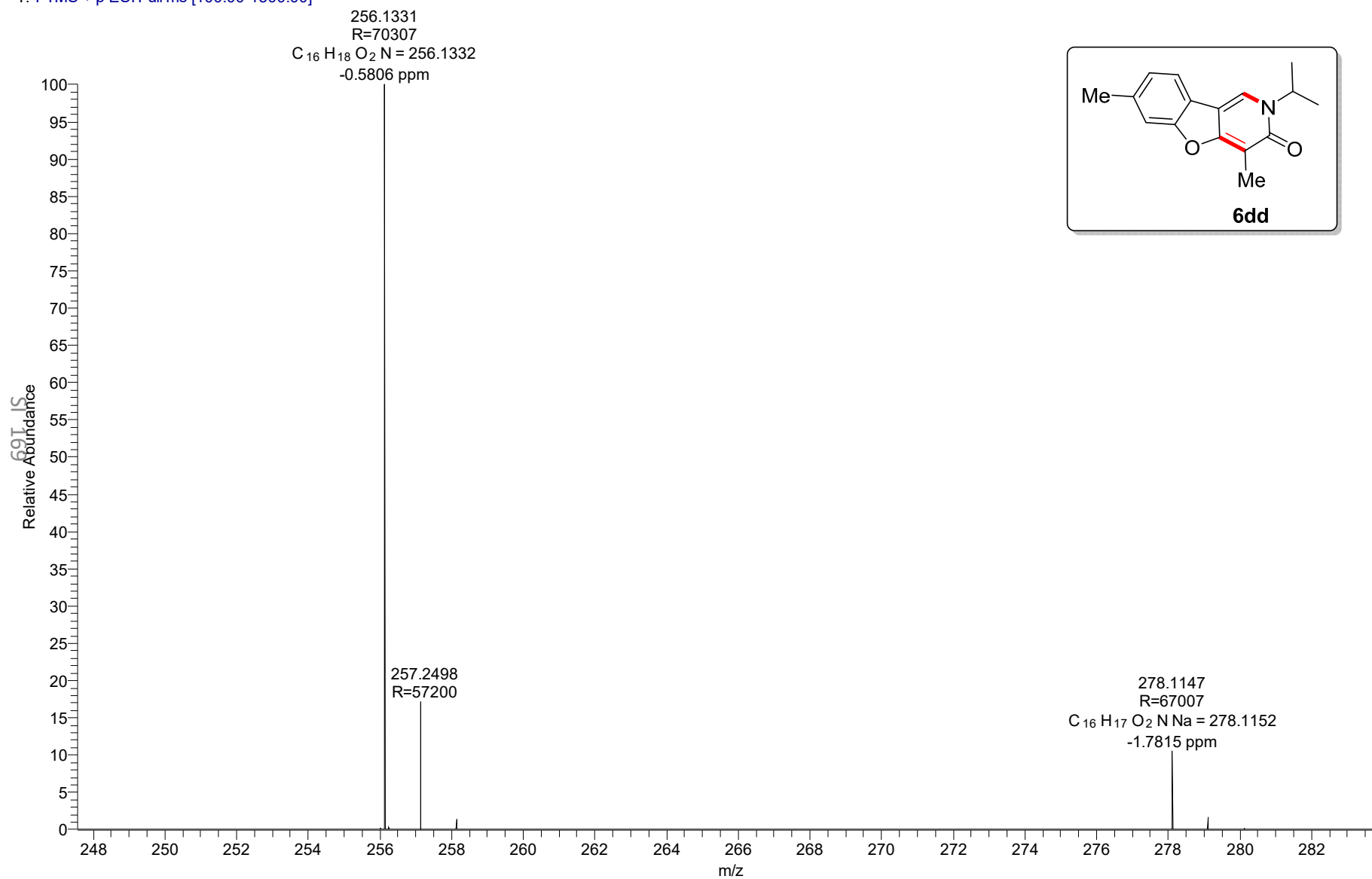
Acquisition Time (sec)	1.2976	Comment	DEPT	Date	14/04/2016 11:50:14	Frequency (MHz)	100.61
Nucleus	¹³ C	Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	25252.53
Temperature (grad C)	0.000						



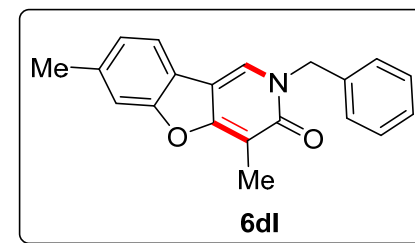
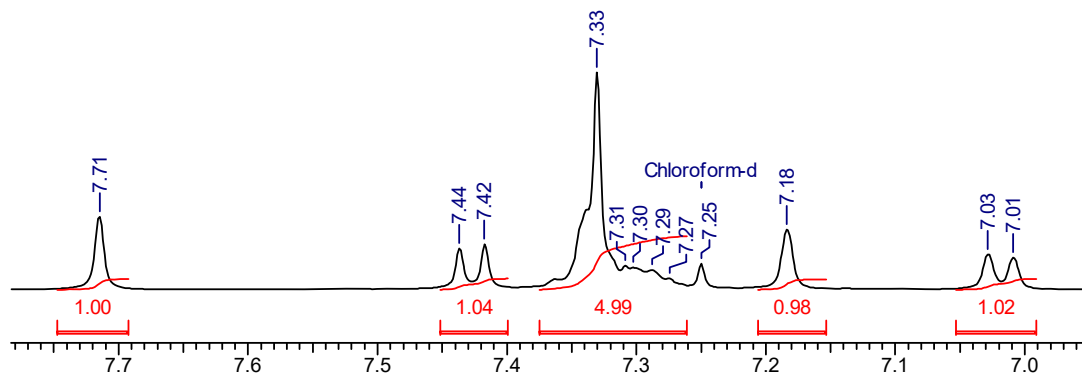
SI 168



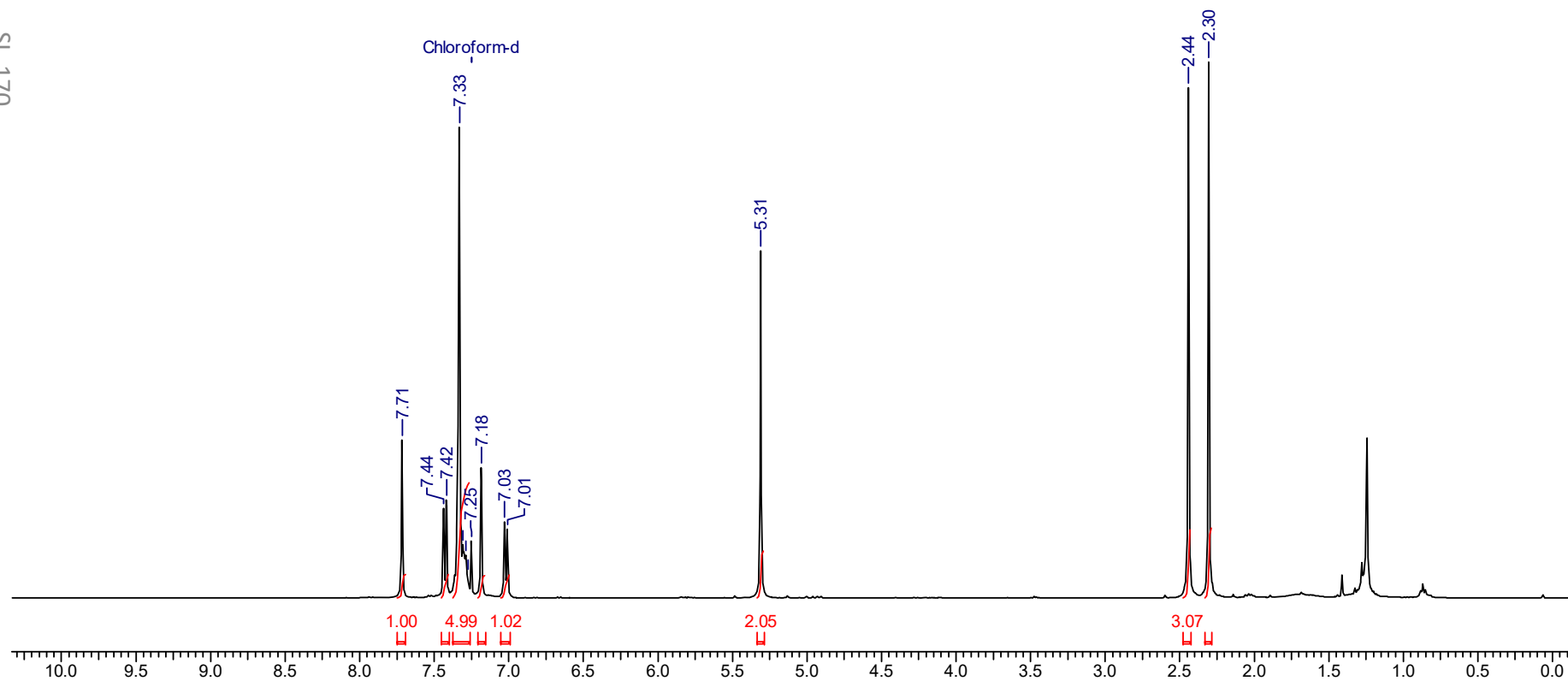
JY-A-37A #129 RT: 0.57 AV: 1 NL: 9.91E9
T: FTMS + p ESI Full ms [100.00-1500.00]



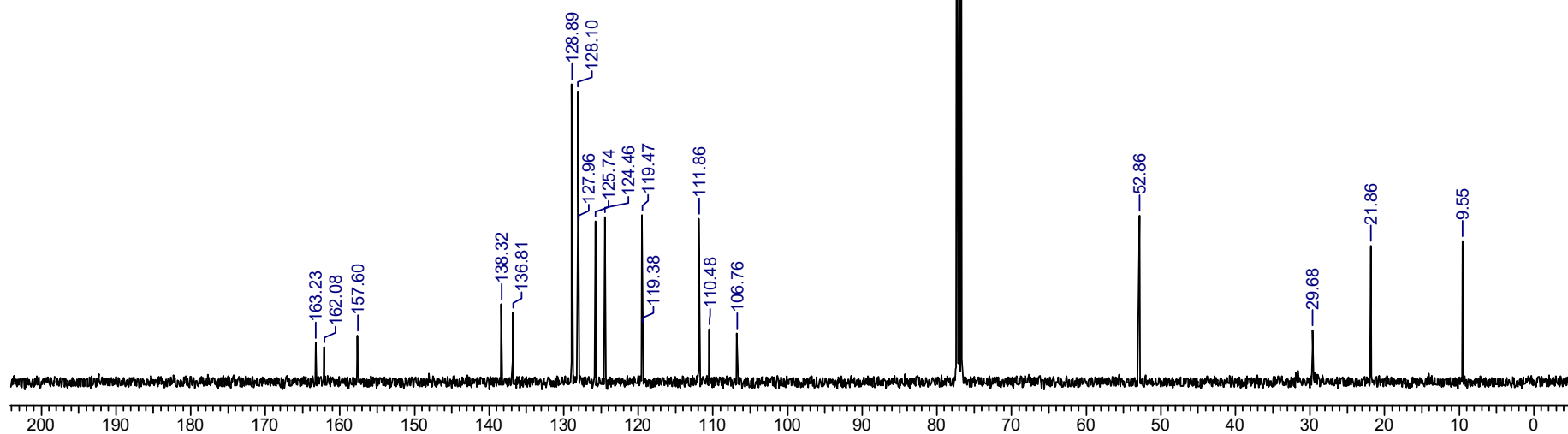
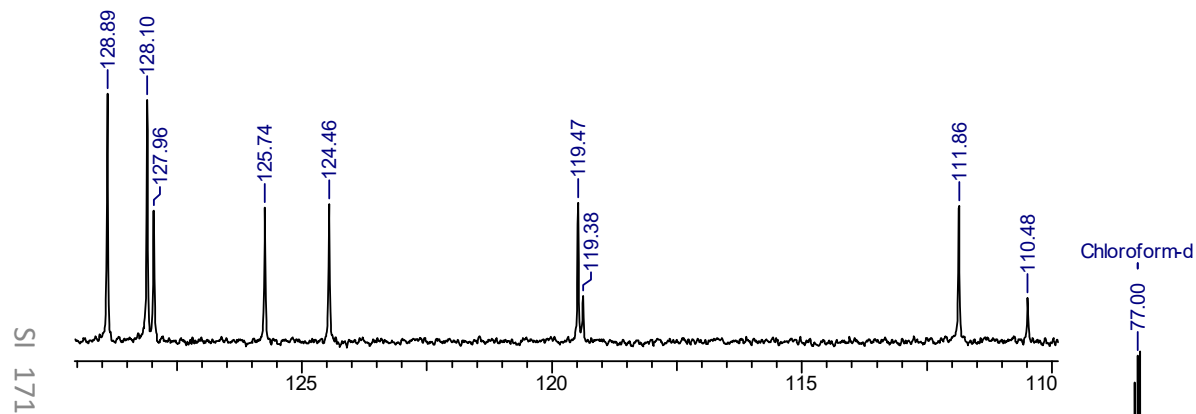
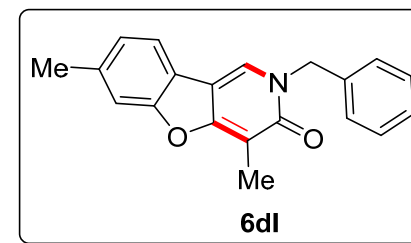
Acquisition Time (sec)	2.0447	Comment	Jyothi	Date	13/05/2016 17:14:38	Frequency (MHz)	400.13
Nucleus	¹ H	Original Points Count	16384	Points Count	16384	Sweep Width (Hz)	8012.82
Temperature (grad C)	0.000						



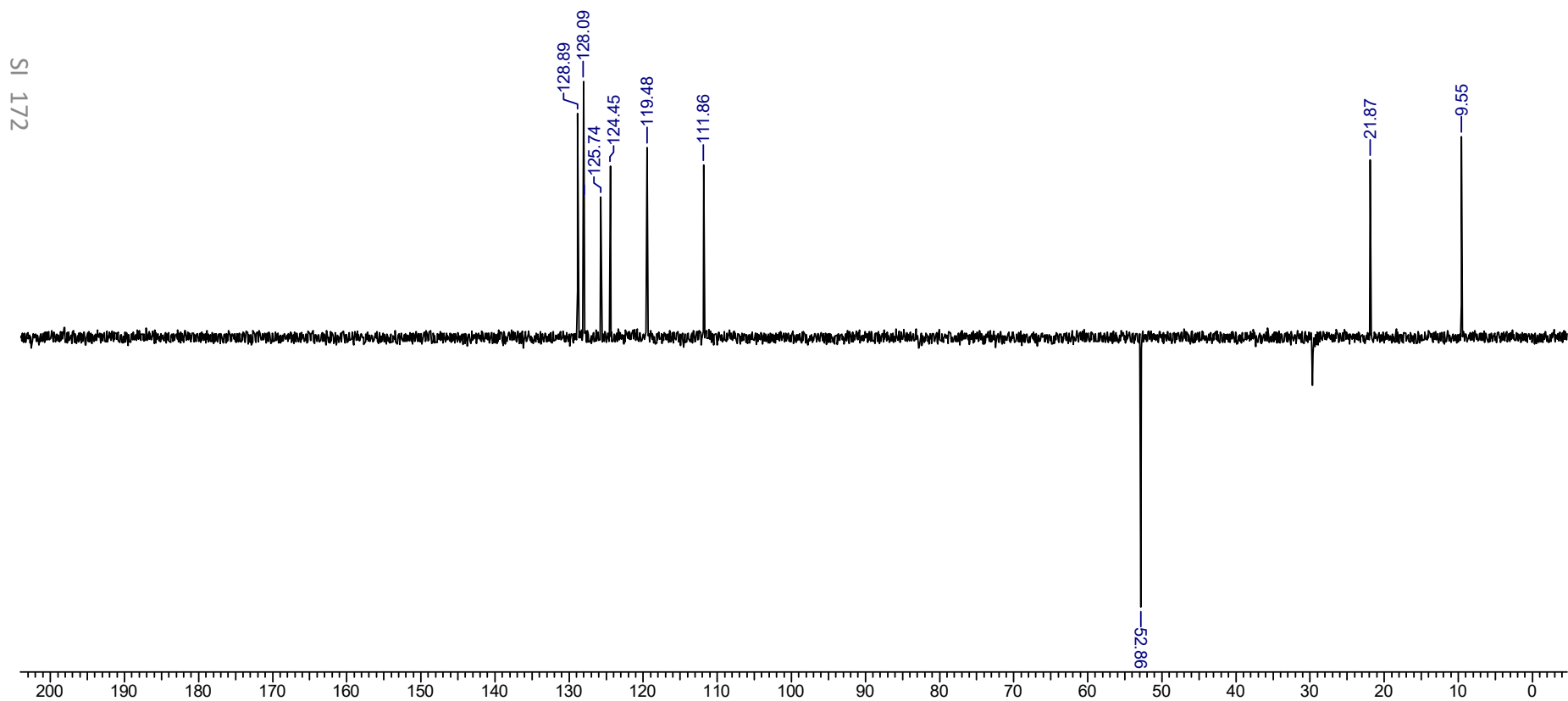
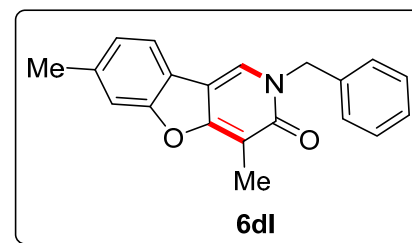
SI 170



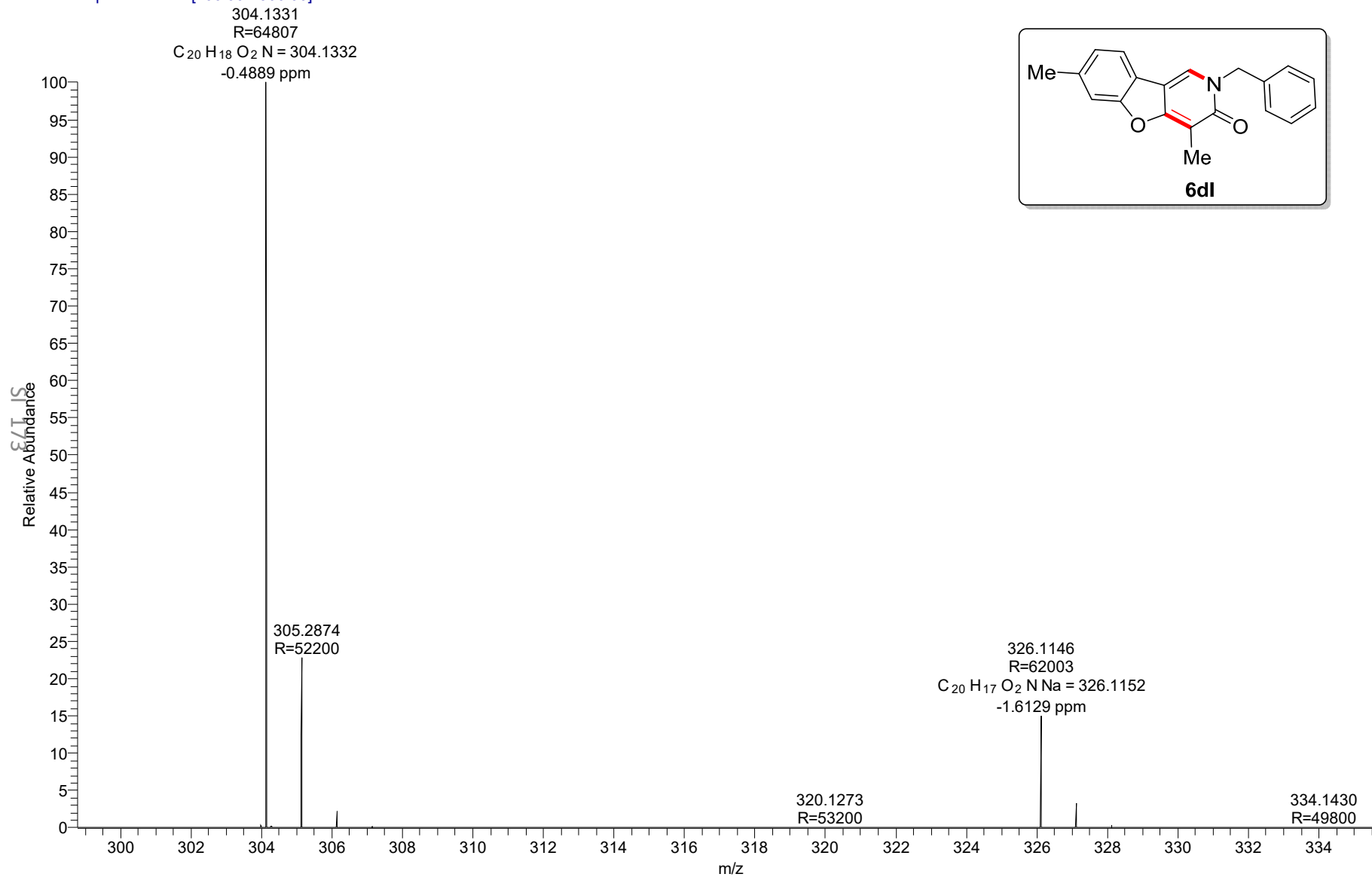
Acquisition Time (sec)	1.1010	Date	13/05/2016 17:35:16	Frequency (MHz)	100.61	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768	Sweep Width (Hz)	29761.90	Temperature (grad C)	0.000



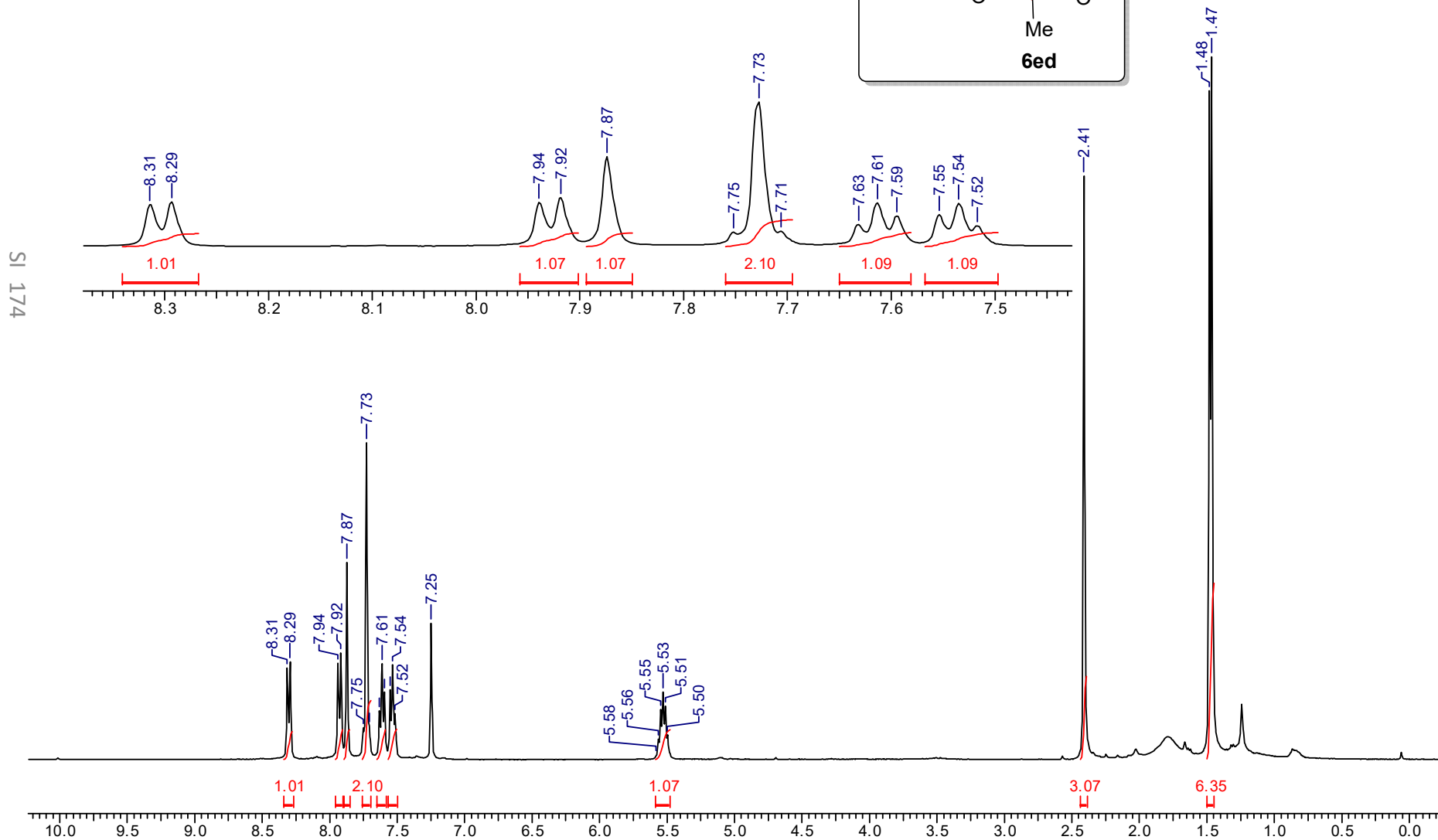
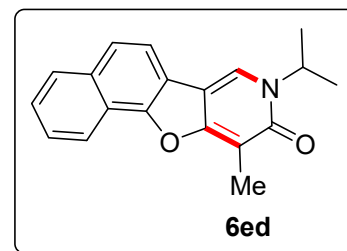
Comment	DEPT			
Date	13 May 2016 16:57:44	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	600	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 22.700



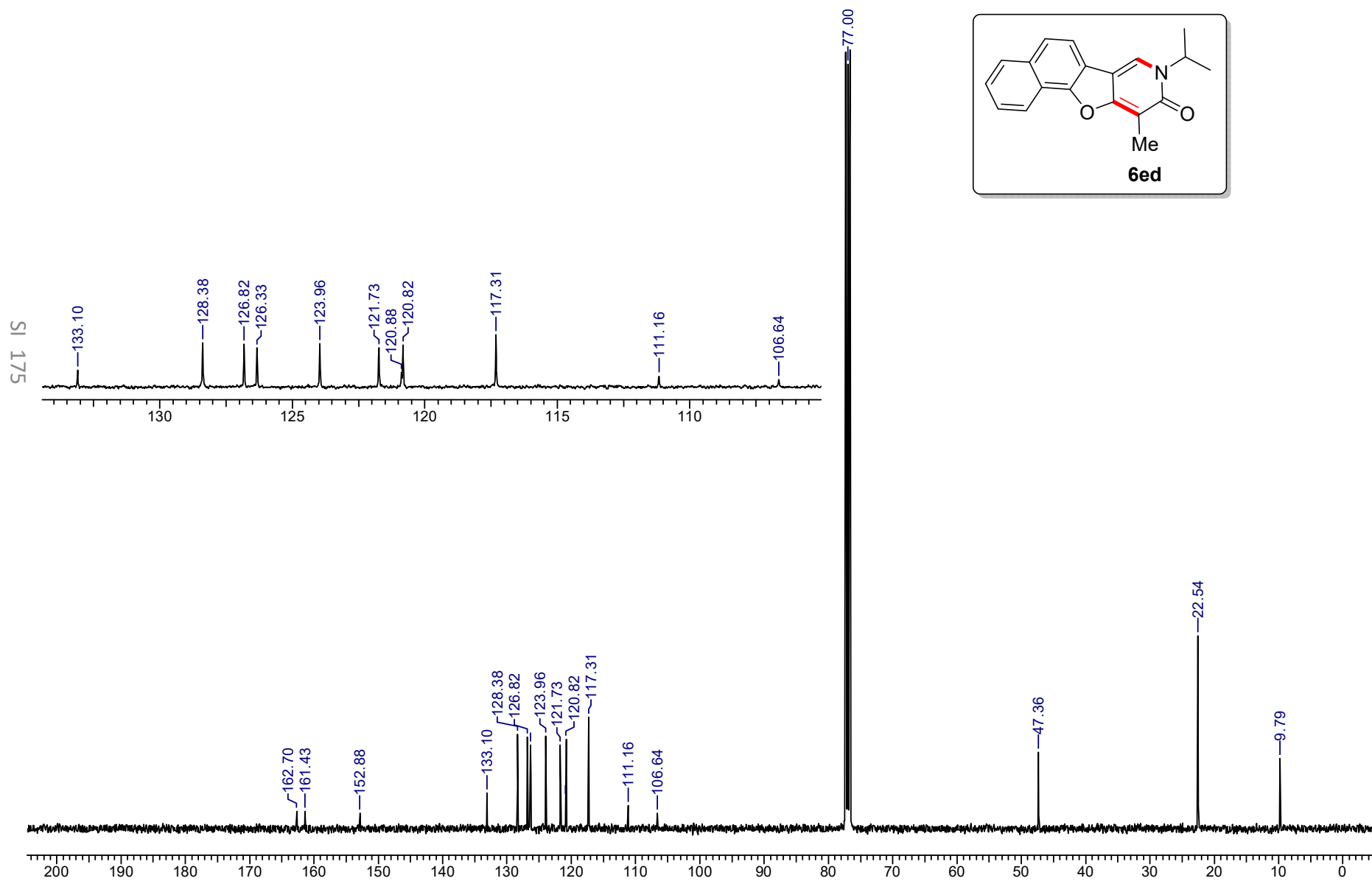
JY-A-41B #134 RT: 0.59 AV: 1 NL: 4.08E9
T: FTMS + p ESI Full ms [100.00-1500.00]



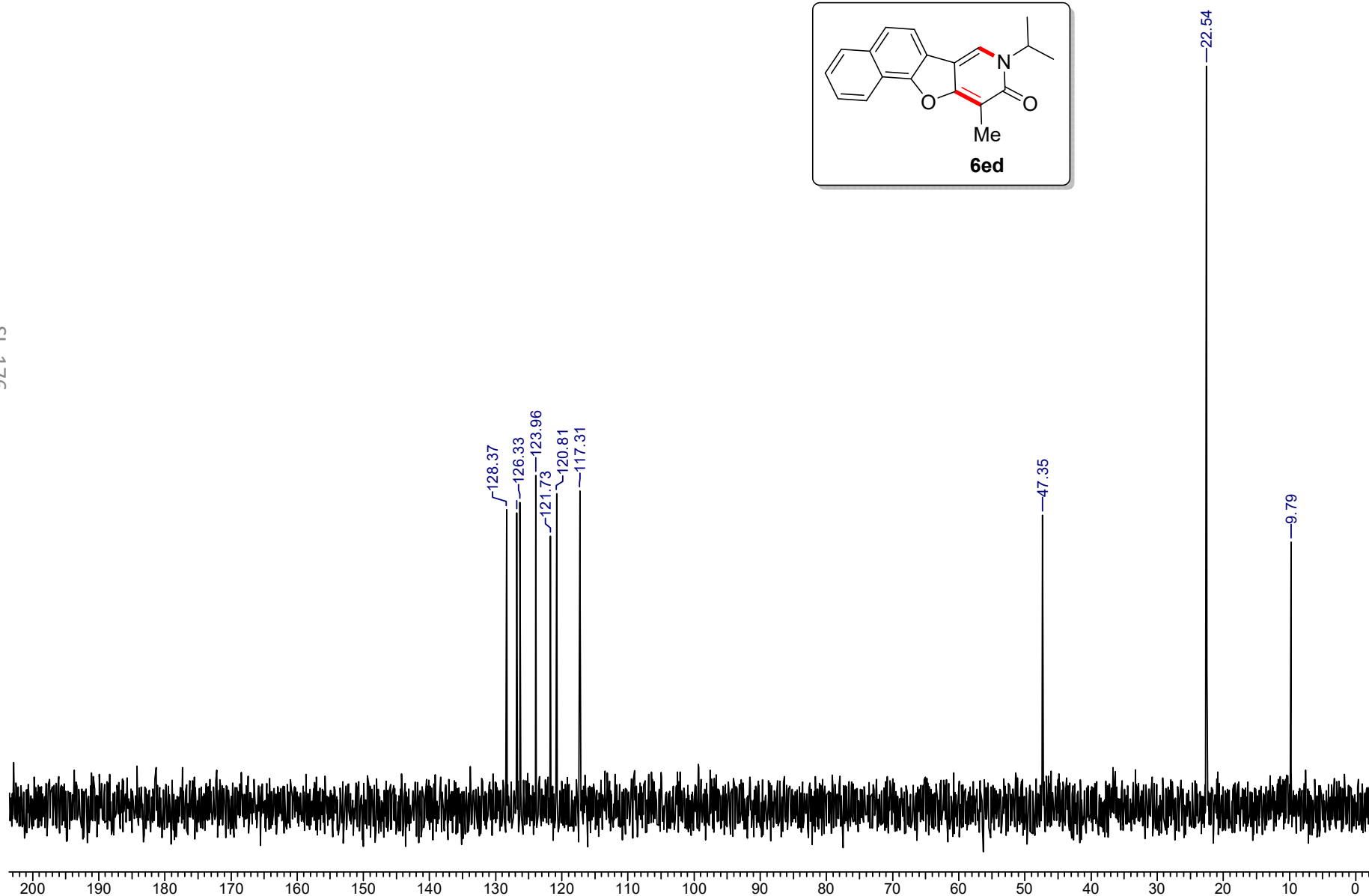
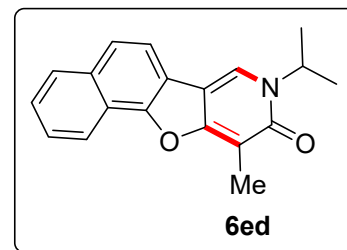
Comment srinivas 1H					
Date 22 Apr 2017 12:16:08		Frequency (MHz) 400.13		Nucleus 1H	
Number of Transients 32		Original Points Count 16384		Points Count 16384	
Solvent CHLOROFORM-d		Sweep Width (Hz) 9999.39		Temperature (grad C) 23.800	



Comment 13C					
Date	22 Apr 2017 12:35:20	Frequency (MHz)	100.61	Nucleus	13C
Number of Transients	3282	Original Points Count	16384	Points Count	32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C)	24.800

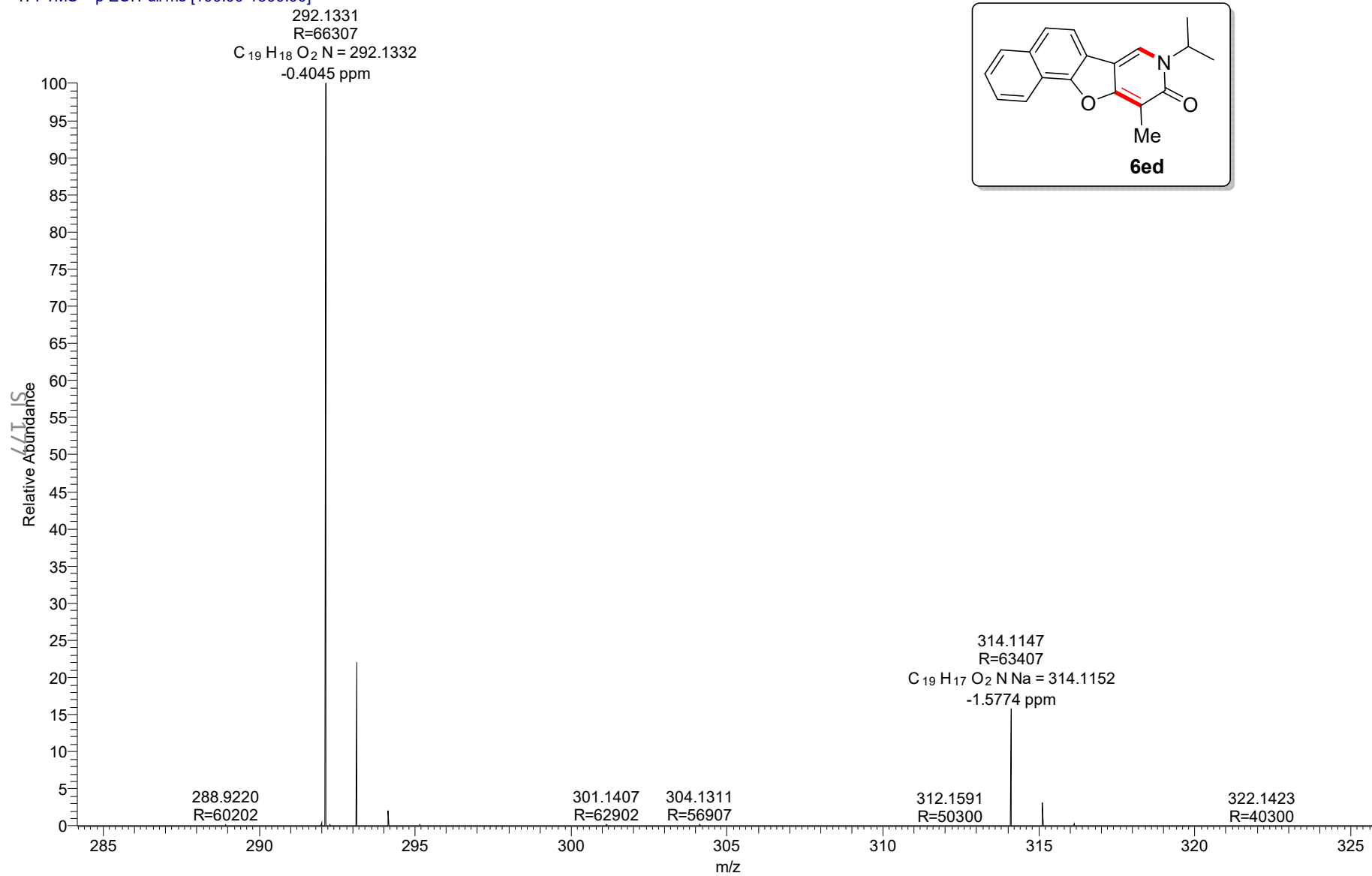


Comment	DEPT			
Date	22 Apr 2017 12:18:16	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	500	Original Points Count	16384	Points Count 32768
Solvent	CHLOROFORM-d	Sweep Width (Hz)	25251.75	Temperature (grad C) 24.100

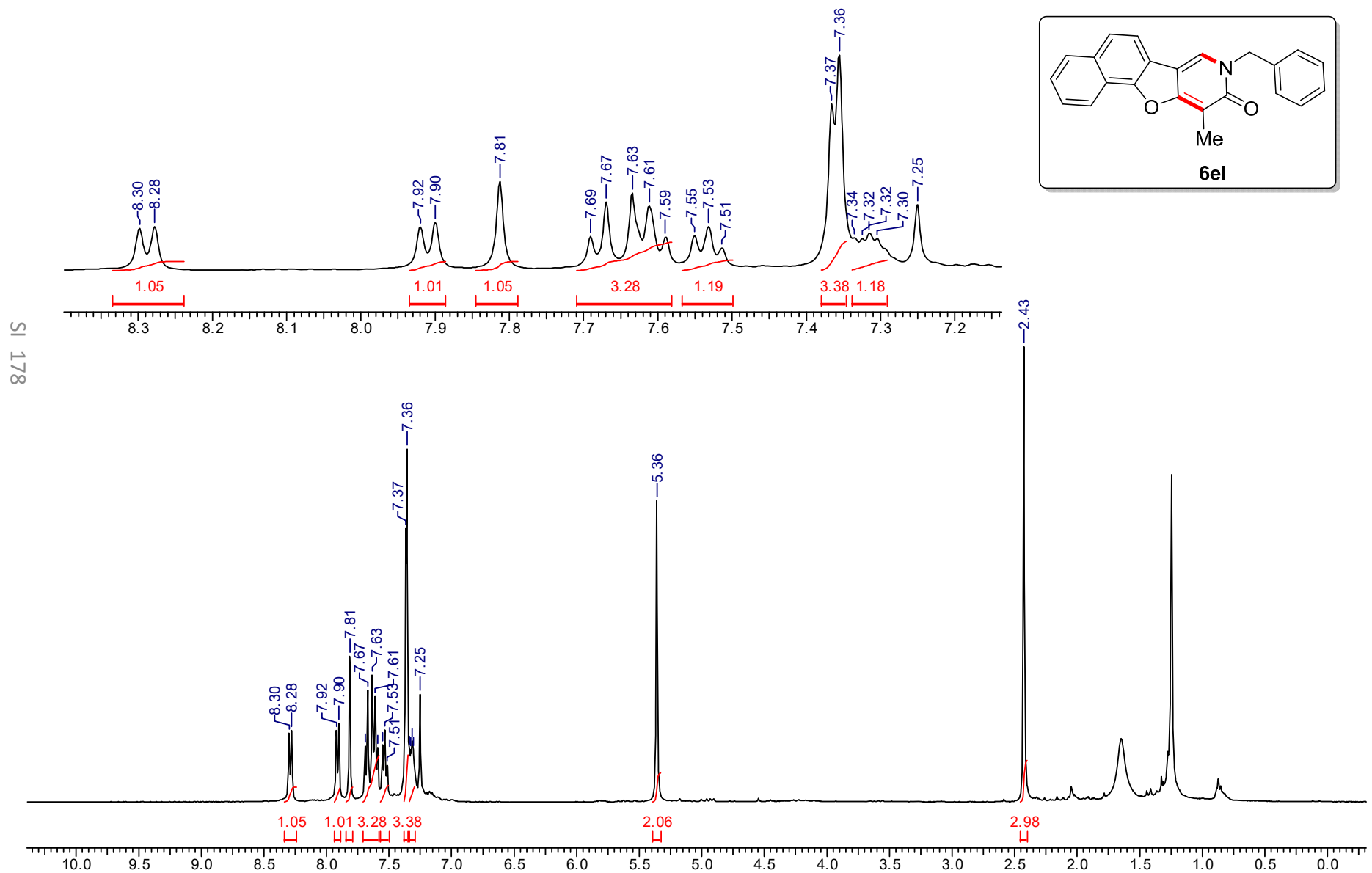


JY-A-3ab #146 RT: 0.65 AV: 1 NL: 3.21E9

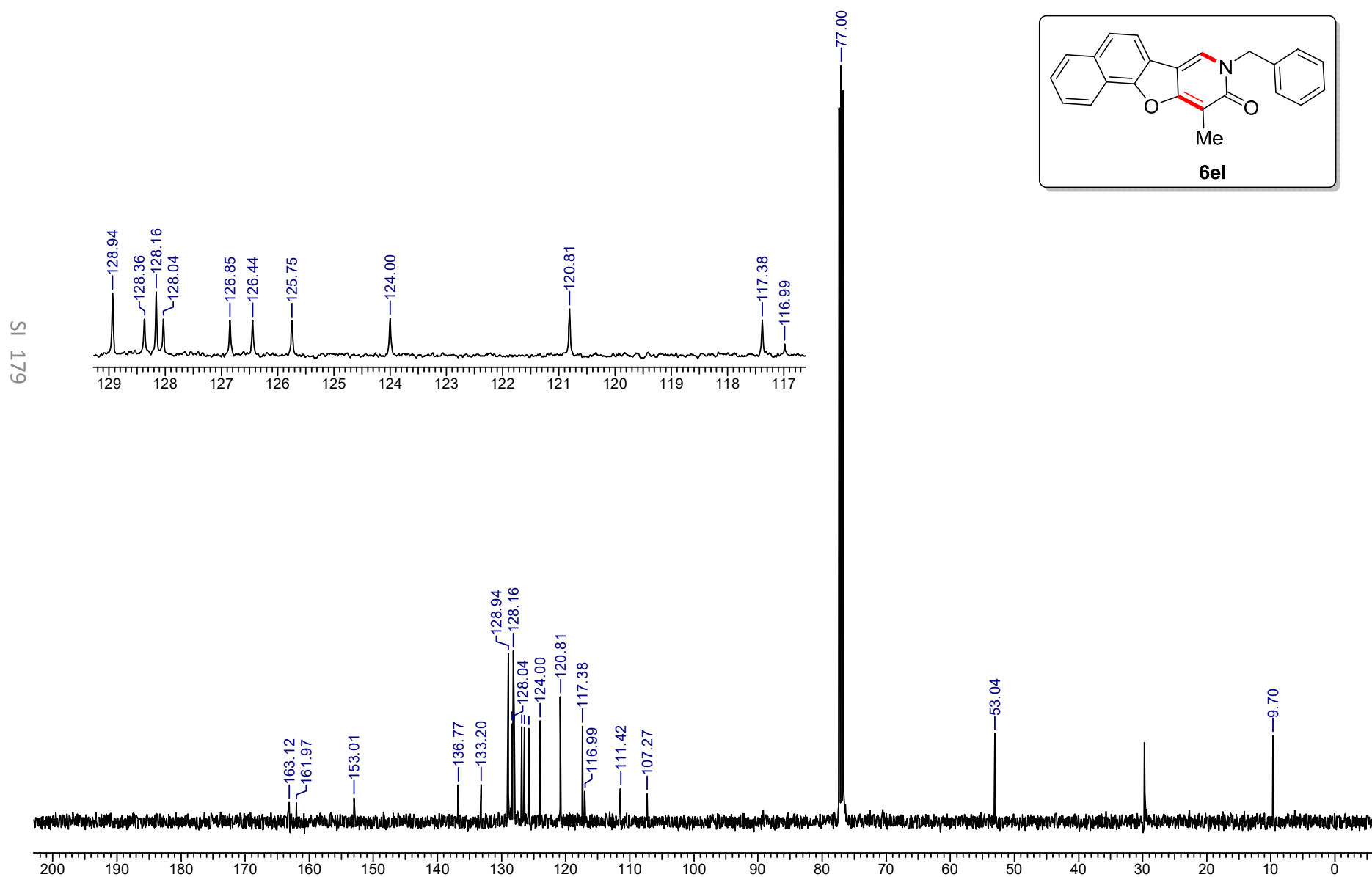
T: FTMS + p ESI Full ms [100.00-1500.00]



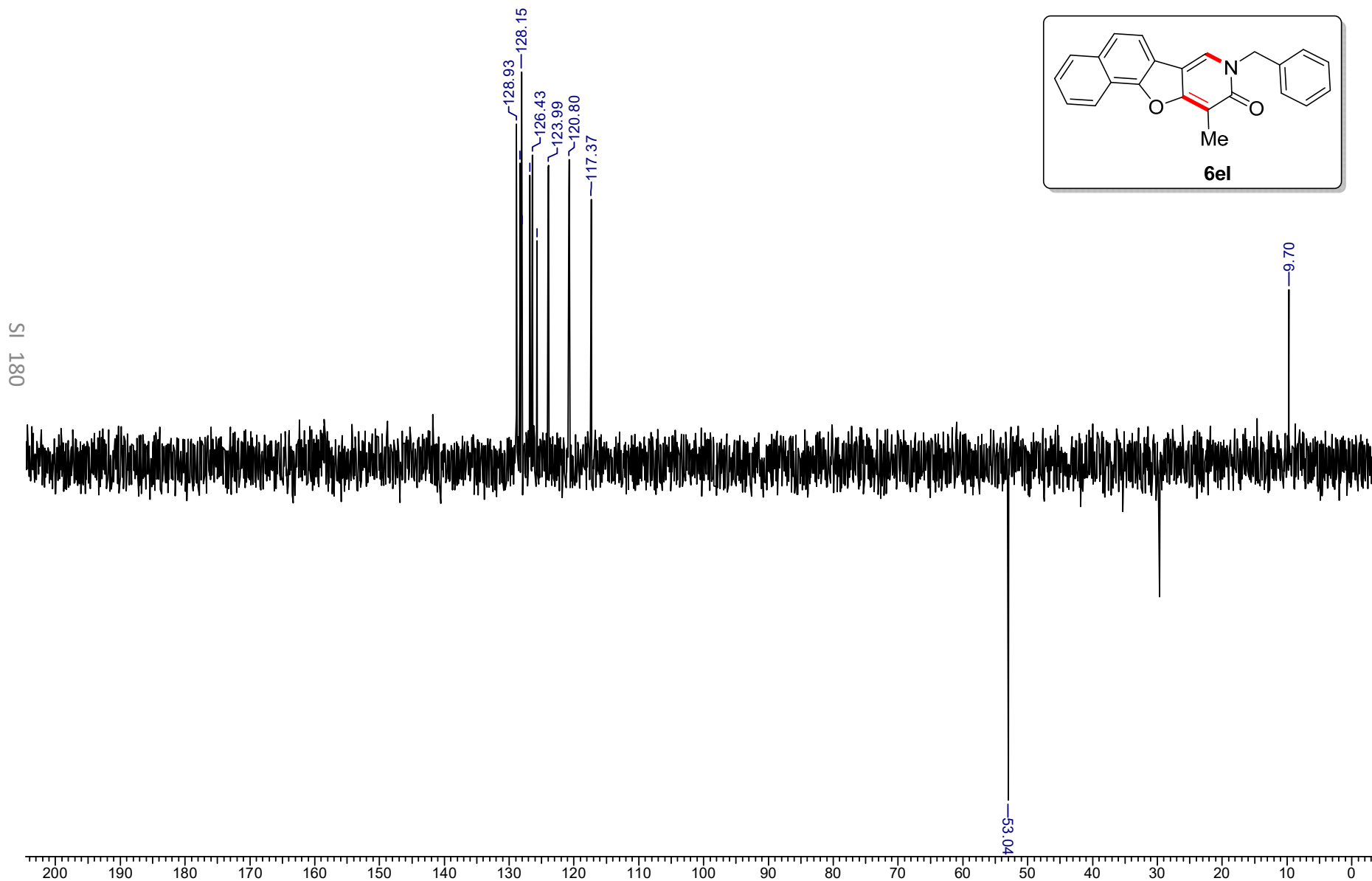
Comment	Srinivas 1H			
Date	25 Sep 2017 12:07:36	Frequency (MHz)	400.13	Nucleus 1H
Number of Transients	64	Original Points Count	16384	Points Count 16384
Solvent	CHLOROFORM-d	Sweep Width (Hz)	9999.39	Temperature (grad C) 25.000



Comment	13C			
Date	25 Sep 2017 13:39:20	Frequency (MHz)	100.61	Nucleus 13C
Number of Transients	2571	Original Points Count	16384	Points Count 32768
Solvent	DMSO-d6	Sweep Width (Hz)	25251.75	Temperature (grad C) 25.400



Comment	DEPT		
Date	25 Sep 2017 12:09:44	Frequency (MHz)	100.61
Number of Transients	800	Original Points Count	16384
Solvent	DMSO-d6	Sweep Width (Hz)	25251.75
		Nucleus	¹³ C
		Points Count	32768
		Temperature (grad C)	25.000



JY-A-36a #151 RT: 0.67 AV: 1 NL: 2.81E9
T: FTMS + p ESI Full ms [100.00-1500.00]

