Supporting Information

Zn(II), Cd(II) and Cu(II) complexes of 2,5–bis{N–(2,6–diisopropyl phenyl)iminomethyl}pyrrole: synthesis, structures and their high catalytic activity for efficient cyclic carbonate synthesis from epoxides and CO_2 at atmospheric pressure

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Table S1 Crystallographic data for complexes **3a**, **3b**, **5a** and **5b**

Parameters	**3a**	**5a**
Empirical formula	$C_{60}H_{76}N_6Zn$	$C_{61}H_{80}CdN_6O$
Formula weight	946.64	1025.71
Crystal System	Monoclinic	Orthorhombic
Space group	P2(1)/n	Pnma
a (Å)	10.559	19.145
b (Å)	21.306	21.378
c (Å)	24.365	14.170
α (deg)	90	90
β (deg)	97.43	90
γ (deg)	90	90
Volume $(Å)^3$	5435.2	5799.7
Temperature (K)	100(2)	100(2)
Z	4	4
μ mm^{-1}	0.494	0.419
D (calcd.) (g/cm^3)	1.157	1.175
F(000)	2032	2176
Crystal size (mm)	0.16 × 0.12 × 0.10	0.22 × 0.18 × 0.14
θ range (deg)	1.27 to 25.05	1.72 to 25.07
Index ranges	–12<=h<=12 –21<=k<=25 –29<=l<=26	–22<=h<=22 –25<=k<=25 –16<=l<=16
Reflections collected / unique	24621 / 9522 R_{int} = 0.0807	54127 / 5296 R_{int} = 0.0534
Data completeness	98.9 %	99.9 %
Transmission (max/min)	0.9522 / 0.9251	0.9436 / 0.9134
Data / restraints / parameters	9522 / 0 / 652	5296 / 0 / 366
Goodness-of-fit on F^2	1.075	1.161
Final R indices [I>2sigma(I)]	R_1 = 0.0720 wR_2 = 0.1685	R_1 = 0.0440 wR_2 = 0.0984
R indices (all data)	R_1 = 0.0946 wR_2 = 0.1825	R_1 = 0.0472 wR_2 = 0.1003
Largest diff. peak / hole, e $Å^{-3}$	0.749 / –0.399	0.583 / –0.459

Crystal Structure of 3a

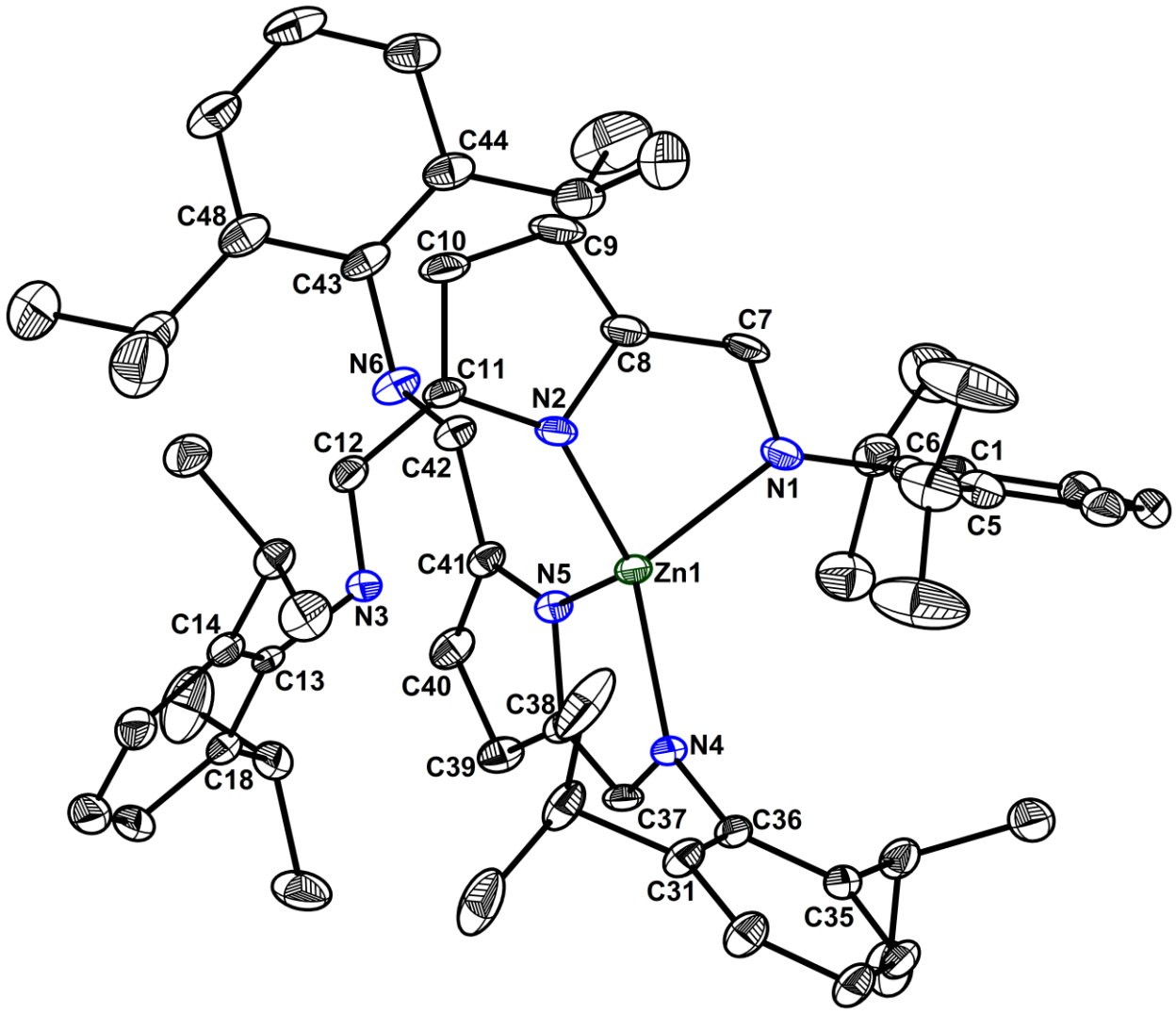


Fig. S1 ORTEP of molecular structure of **3a**. Thermal ellipsoids are shown at 30% probability levels. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Zn1–N2 = 1.971(3), Zn1–N1 = 2.097(3), Zn1–N5 = 1.996(3), Zn1–N4 = 2.054(3), N2–Zn1–N1 = 82.55(12), N4–Zn1–N1 = 116.93(12), N5–Zn1–N4 = 84.00(11), N2–Zn1–N5 = 111.04(12), N5–Zn1–N1 = 117.46(12), N2–Zn1–N4 = 147.48(12), C9–C8–C7 = 133.2(4), C10–C11–C12 = 128.2(4), C7–N1–C6 = 117.7(3), C12–N3–C13 = 119.5(3), C42–N6–C43 = 118.1(3), C40–C41–C42 = 128.6(3), C39–C38–C37 = 132.5(3), C37–N4–C36 = 116.7(3).

Crystal Structure of 3b

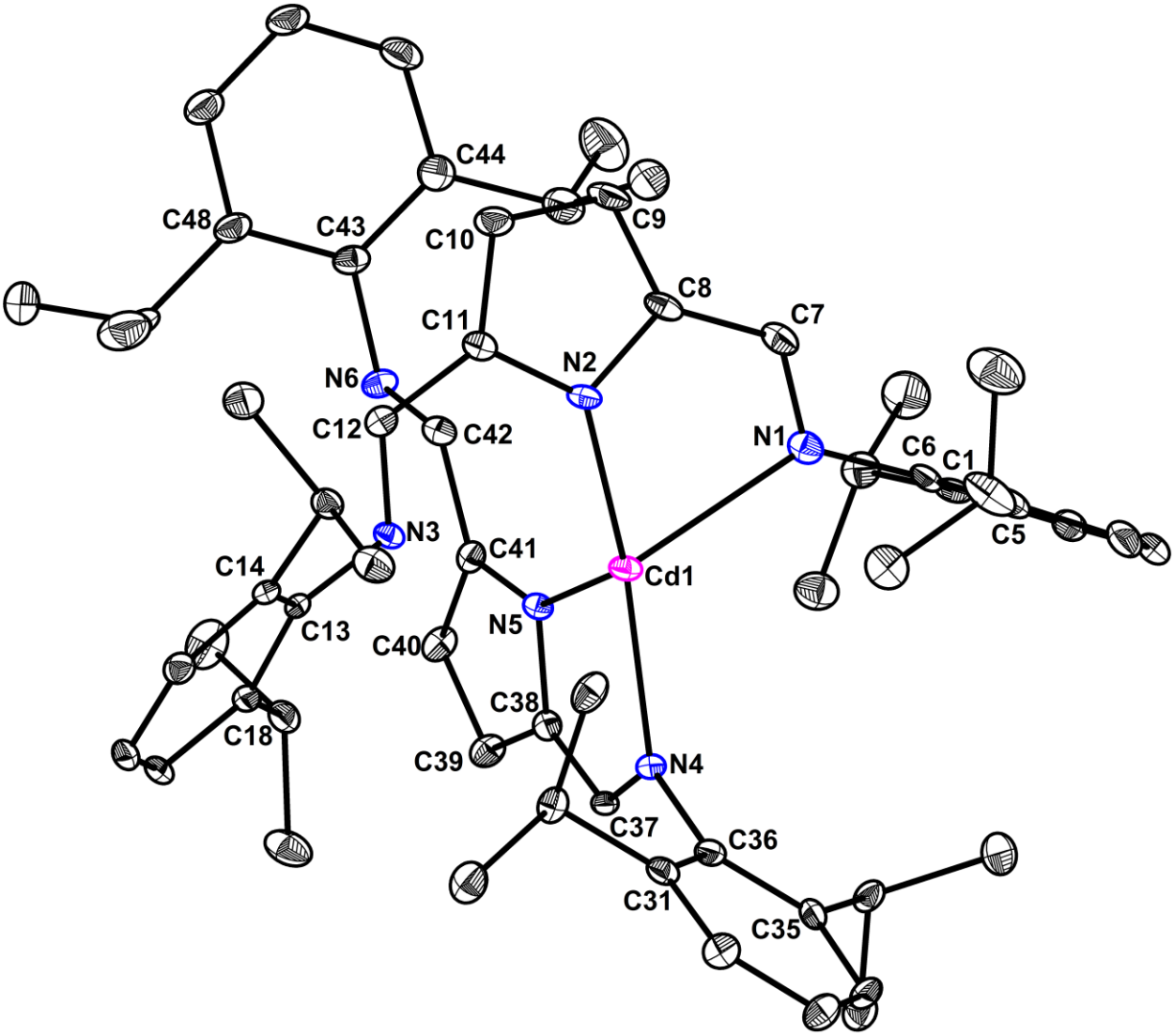


Fig. S2 ORTEP of molecular structure of **3b**. Thermal ellipsoids are shown at 30% probability levels. Hydrogen atoms are omitted for clarity.

Crystal Structure of 5a

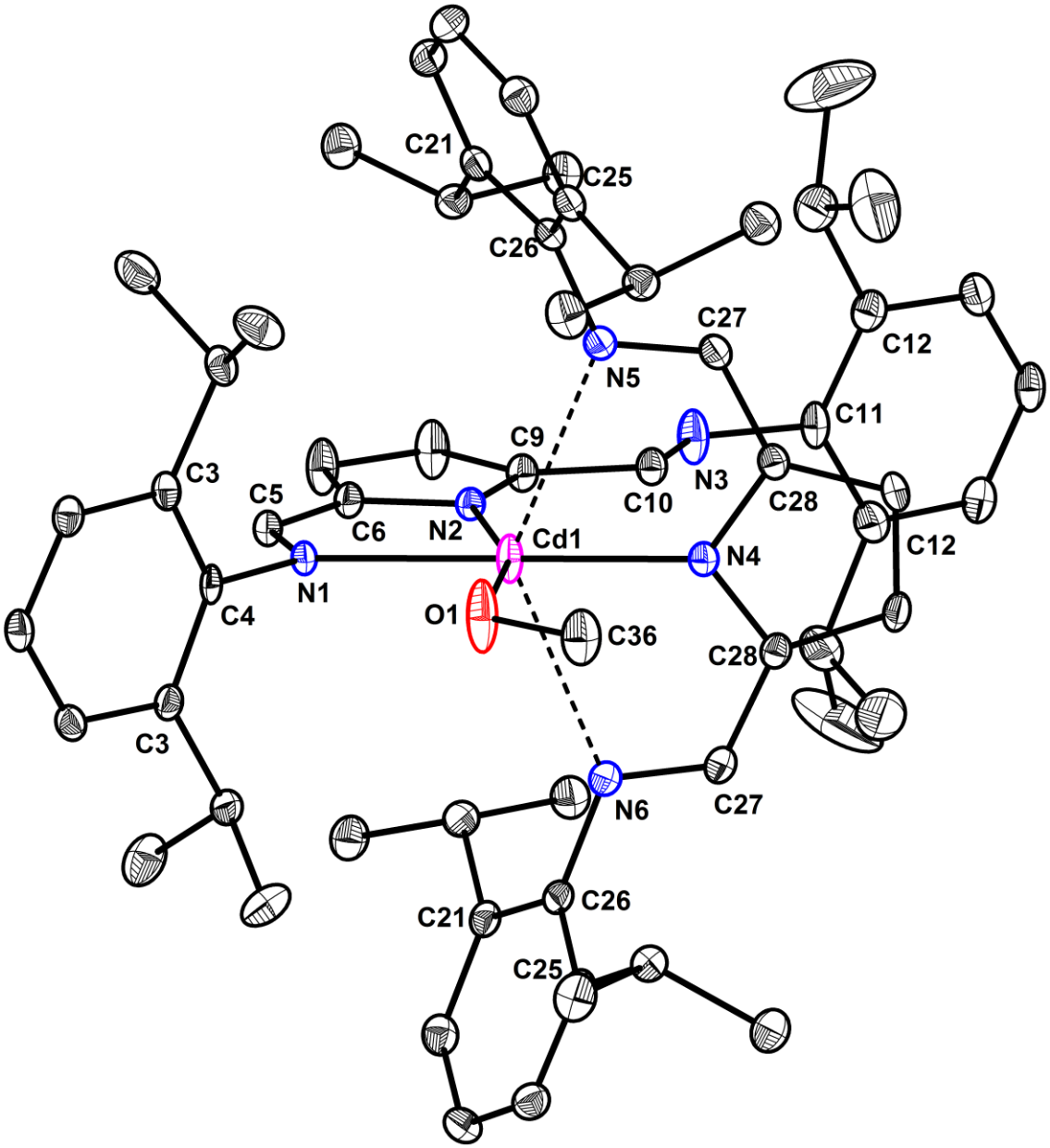


Fig. S3 ORTEP of molecular structure of **5a**. Thermal ellipsoids are shown at 30% probability levels. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Cd1–N2 = 2.271(3), N5–Cd1 = 2.716(3), Cd1–N4 = 2.149(3), N6–Cd1 = 2.716(3), Cd1–N1 = 2.275(3), Cd1–O1 = 2.336(3), N2–Cd1–N1 = 76.37(10), N1–Cd1–O1 = 85.08(11), N4–Cd1–O1 = 94.68(11), N4–Cd1–N2 = 103.87(10), N4–Cd1–N5 = 67.62, N4–Cd1–N6 = 67.62, N5–Cd1–N6 = 135.09, N6–Cd1–O1 = 90.12, N6–Cd1–N1 = 112.38, N6–Cd1–N2 = 96.86, C7–C6–C5 = 128.97, C8–C9–C10 = 127.1(3), C5–N1–C4 = 116.4(3), C10–N3–C11 = 128.5(3), C29–C28–C27 = 132.4(2), C27–N5–C26 = 118.0(2), N4–Cd1–N1 = 179.76(10), N2–Cd1–O1 = 161.45(11).

Crystal Structure of 5b

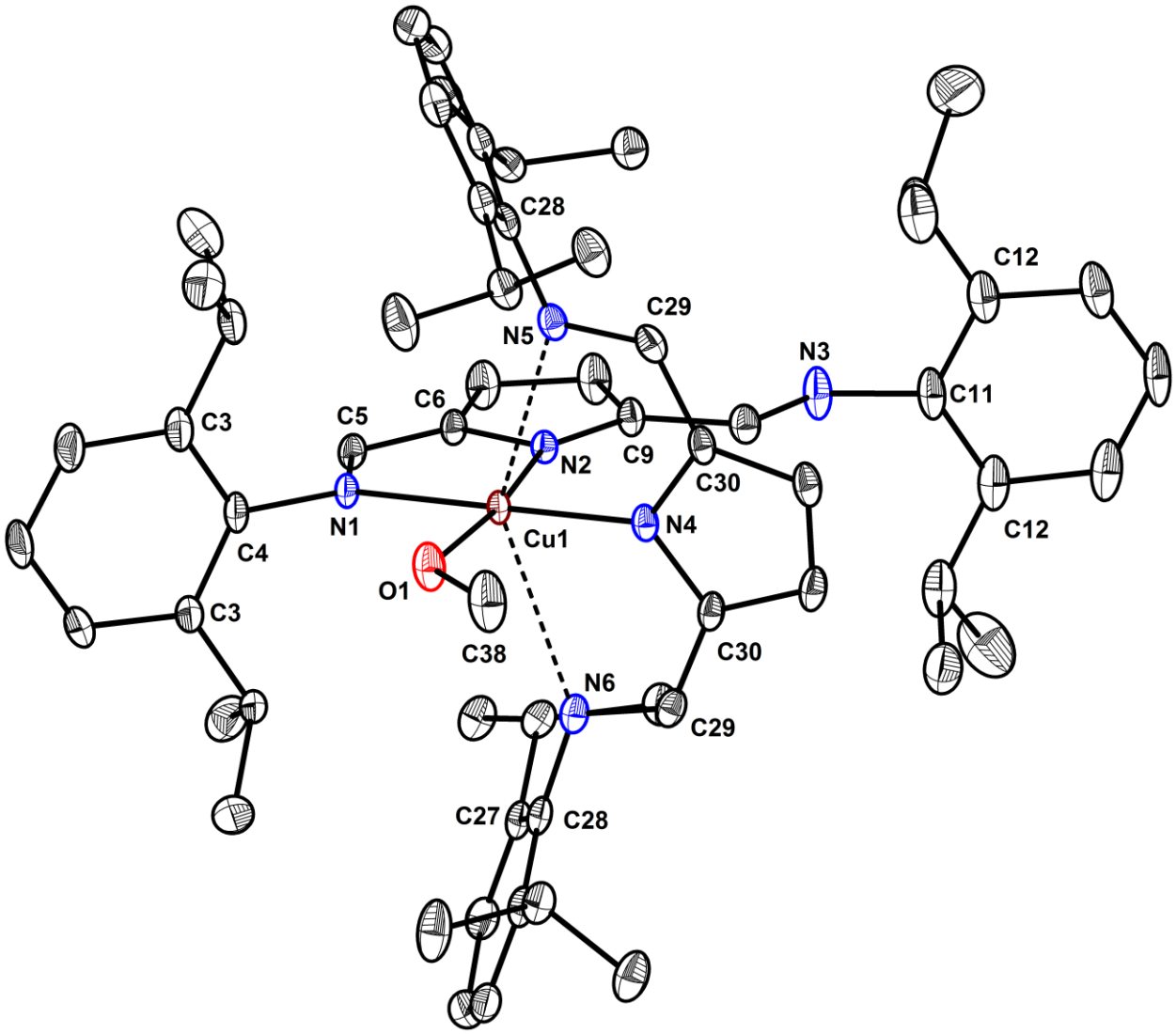
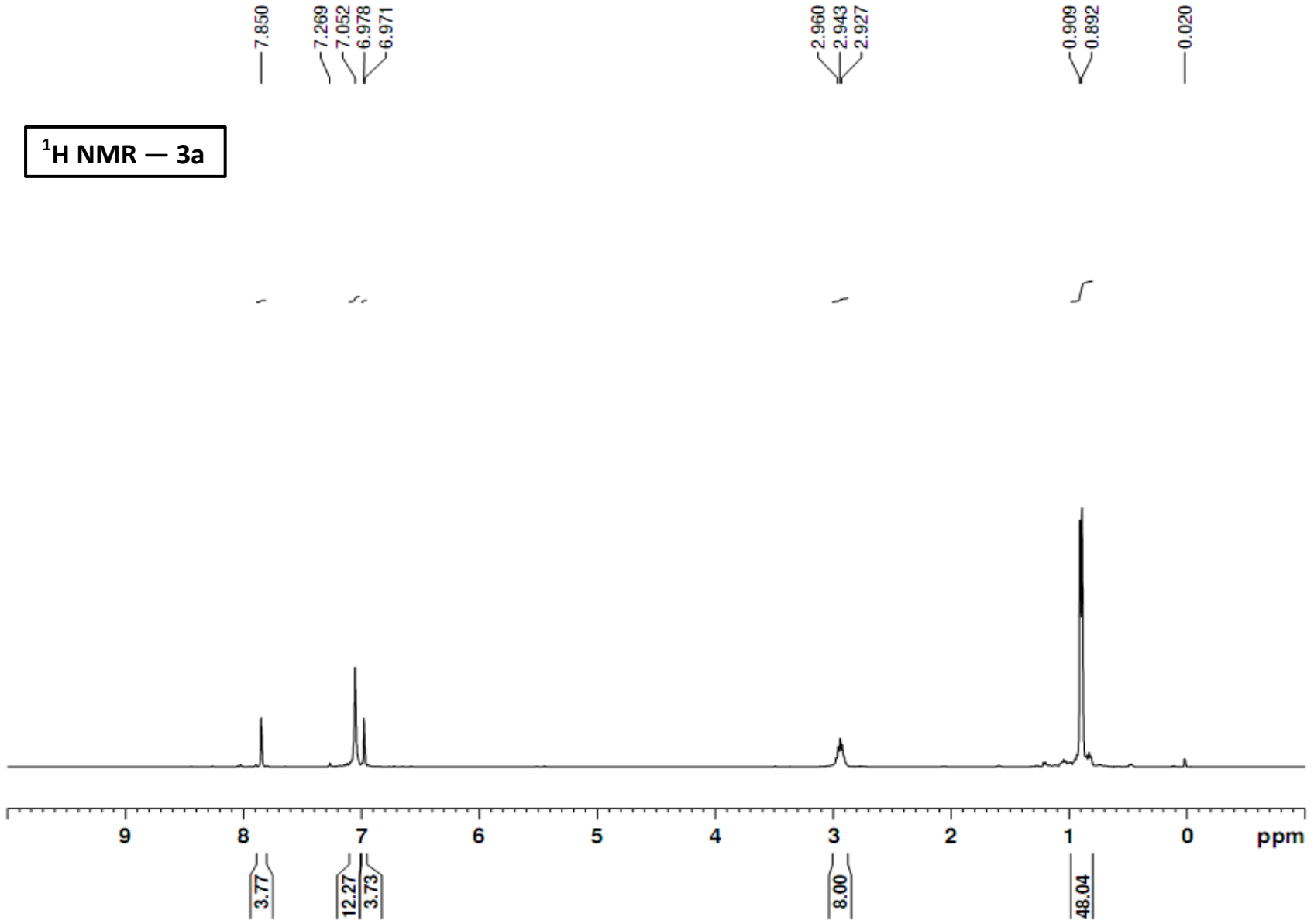
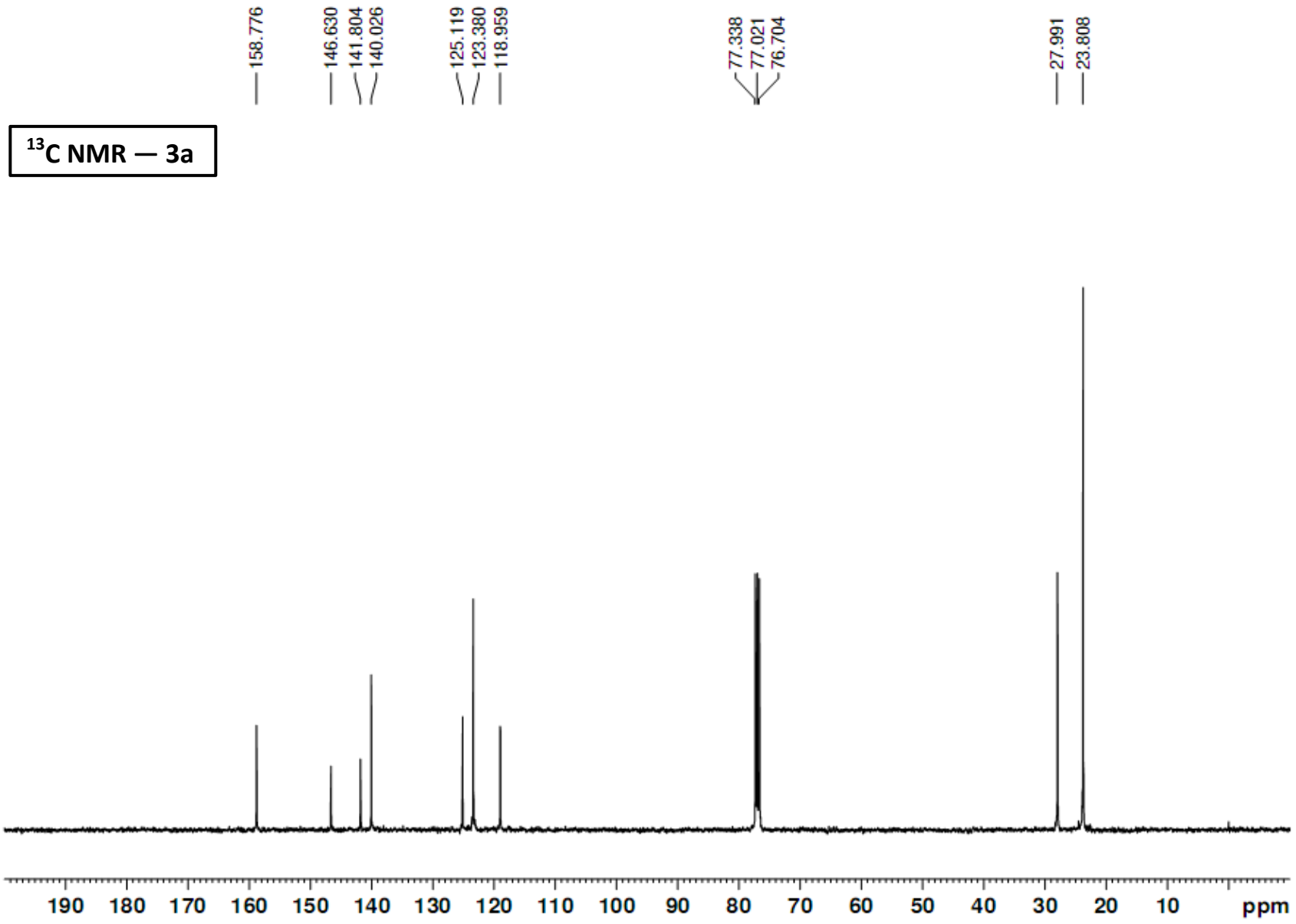


Fig. S4 ORTEP of molecular structure of **5b**. Thermal ellipsoids are shown at 30% probability levels. Hydrogen atoms are omitted for clarity.

^{1}H NMR — 3a





^{13}C NMR — 3a

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
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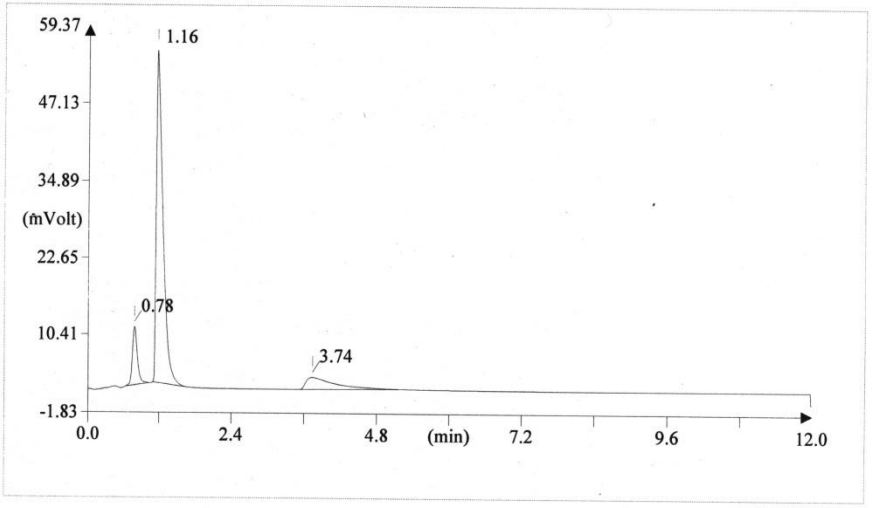
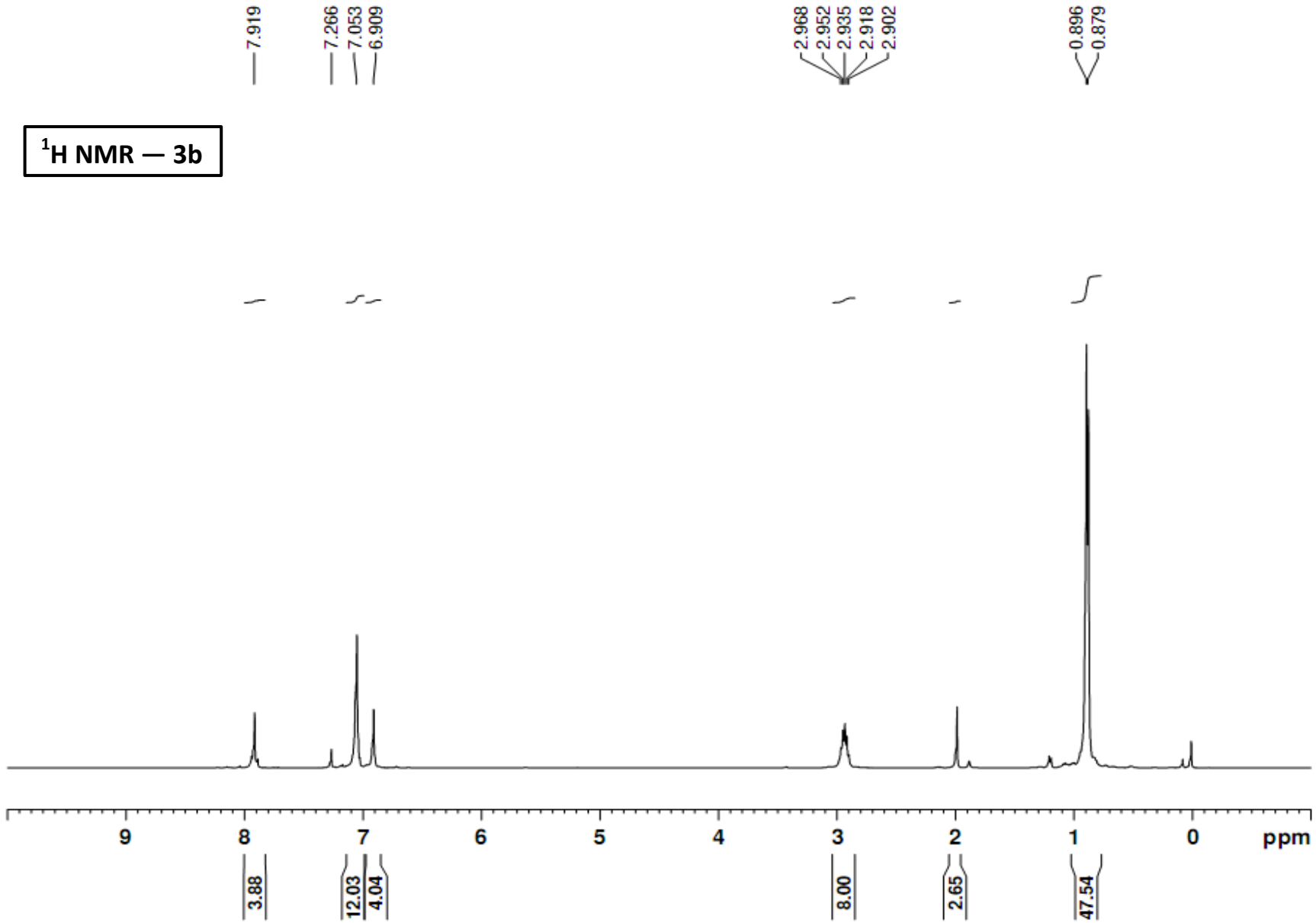
Chromatogram filename:	UNK-31012011-2.dat
Sample weight:	1.221

CHN — 3a

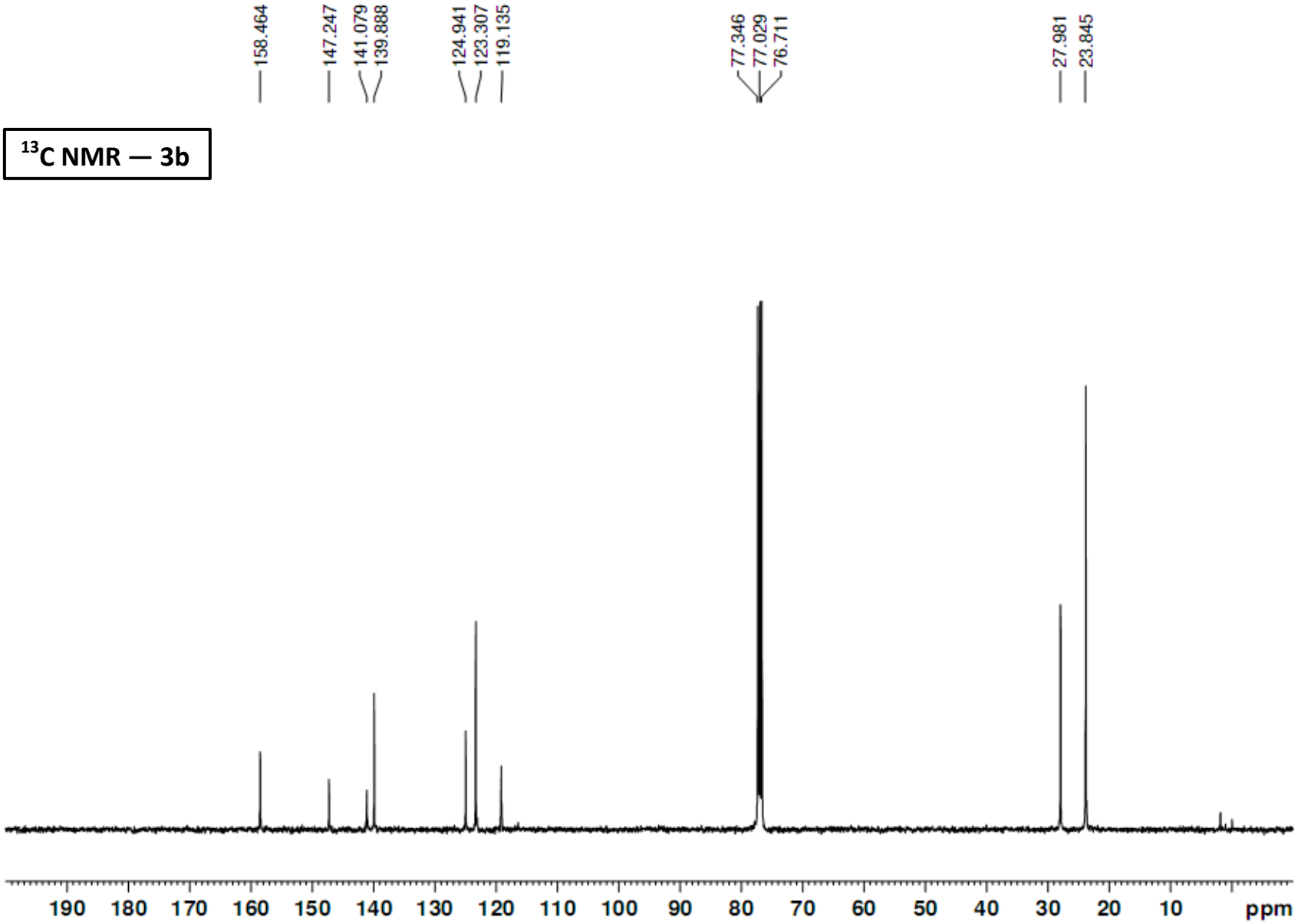


Element Name	Element %	Ret. Time
Nitrogen	8. 75	0. 78
Carbon	76. 32	1. 16
Hydrogen	7. 96	3. 74

^{1}H NMR — 3b



^{13}C NMR — 3b



FLASH EA 1112 SERIES CHN REPORT
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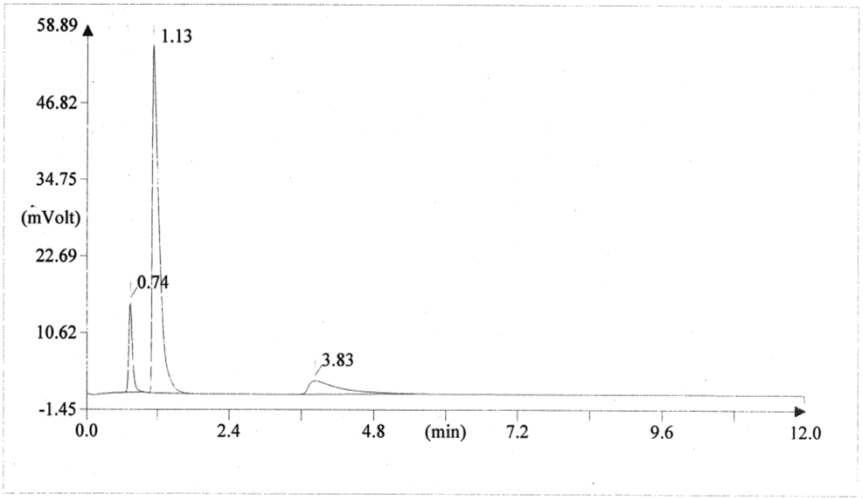
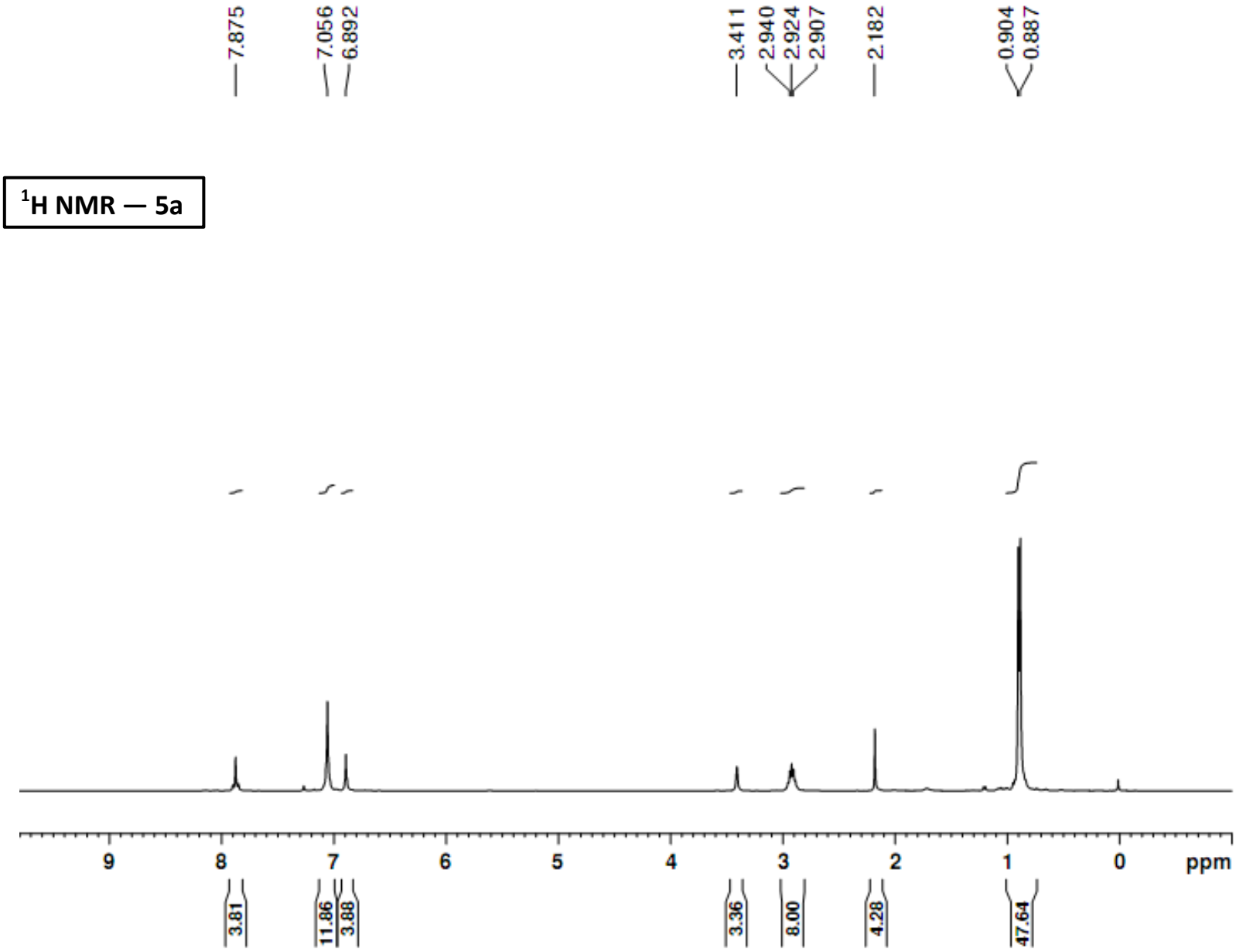
Analysis type:	UnkNown
Chromatogram filename:	UNK-28022011-7.dat
Sample weight:	1.135

CHN — 3b

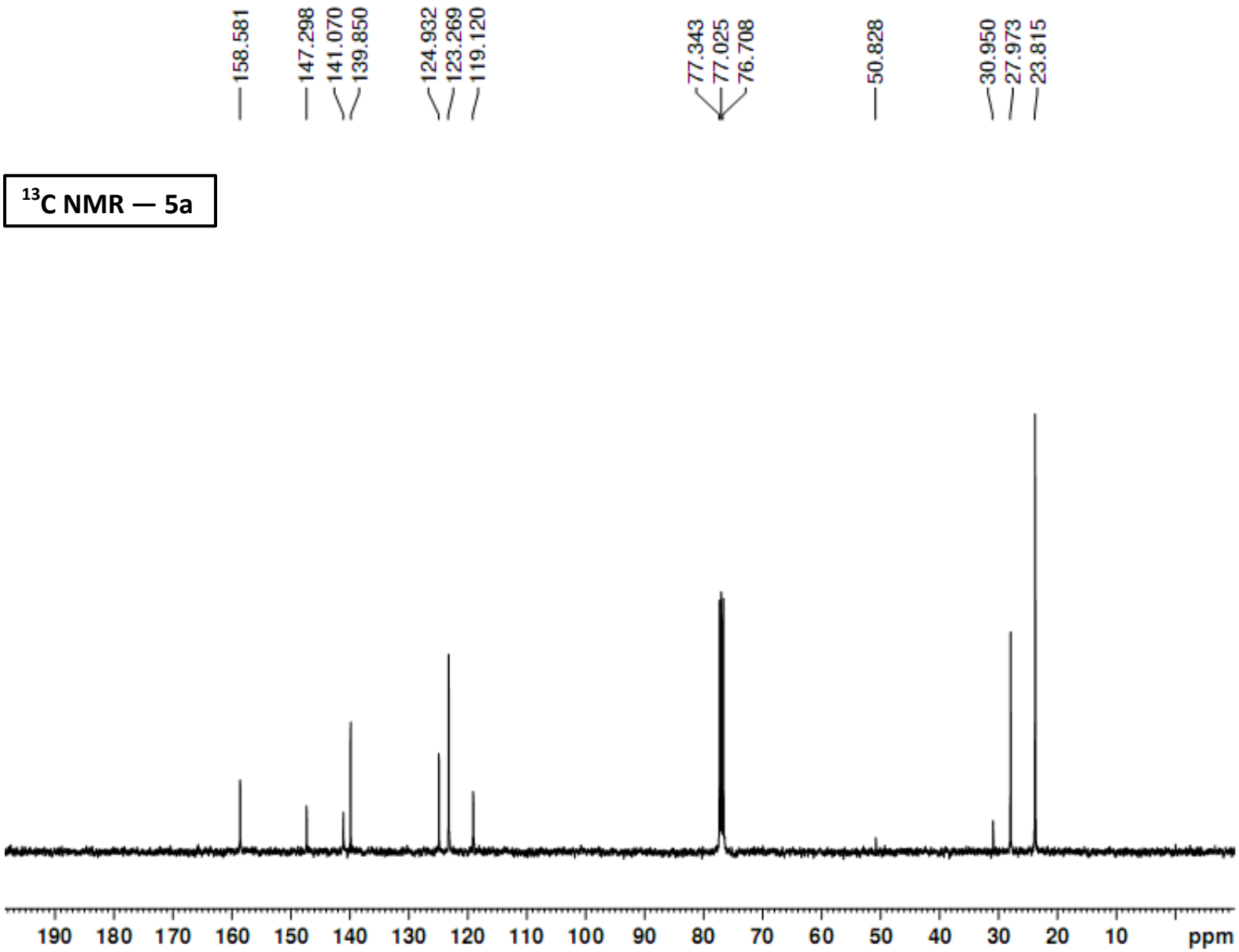


Element Name	Element %	Ret. Time
Nitrogen	8. 36	0. 74
Carbon	72. 45	1. 13
Hydrogen	7. 78	3. 83

^{1}H NMR — 5a



^{13}C NMR — 5a



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Method filename:	I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exa
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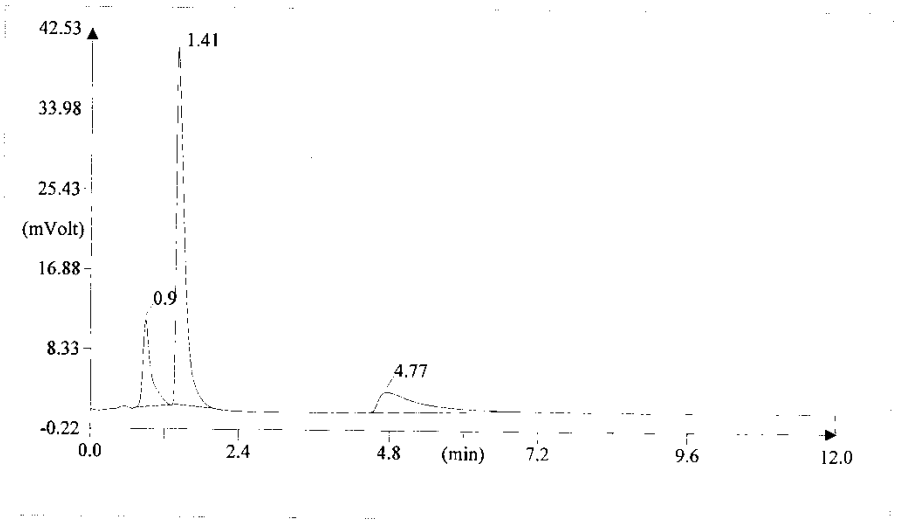
Analysis type:	UnkNown
Chromatogram filename:	UNK-28022011-9.dat
Sample weight:	1.106

CHN — 5a



Element Name	Element %	Ret. Time
Nitrogen	8. 15	0. 90
Carbon	71. 55	1. 41
Hydrogen	7. 81	4. 77

FLASH EA 1112 SERIES CHN REPORT
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Method filename:	C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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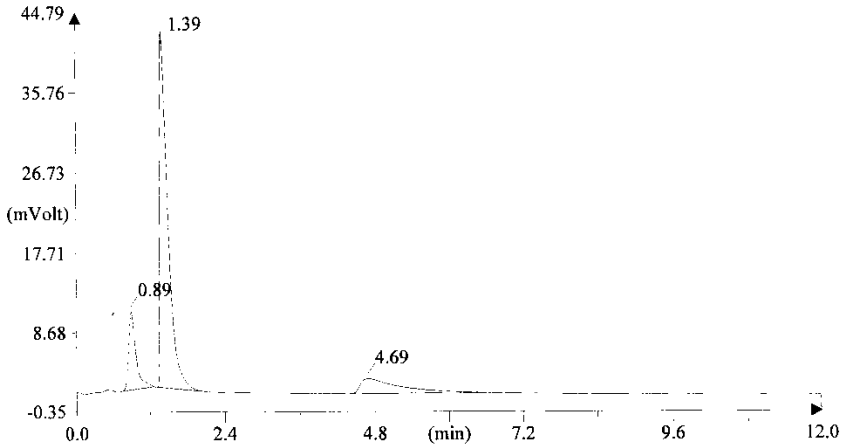
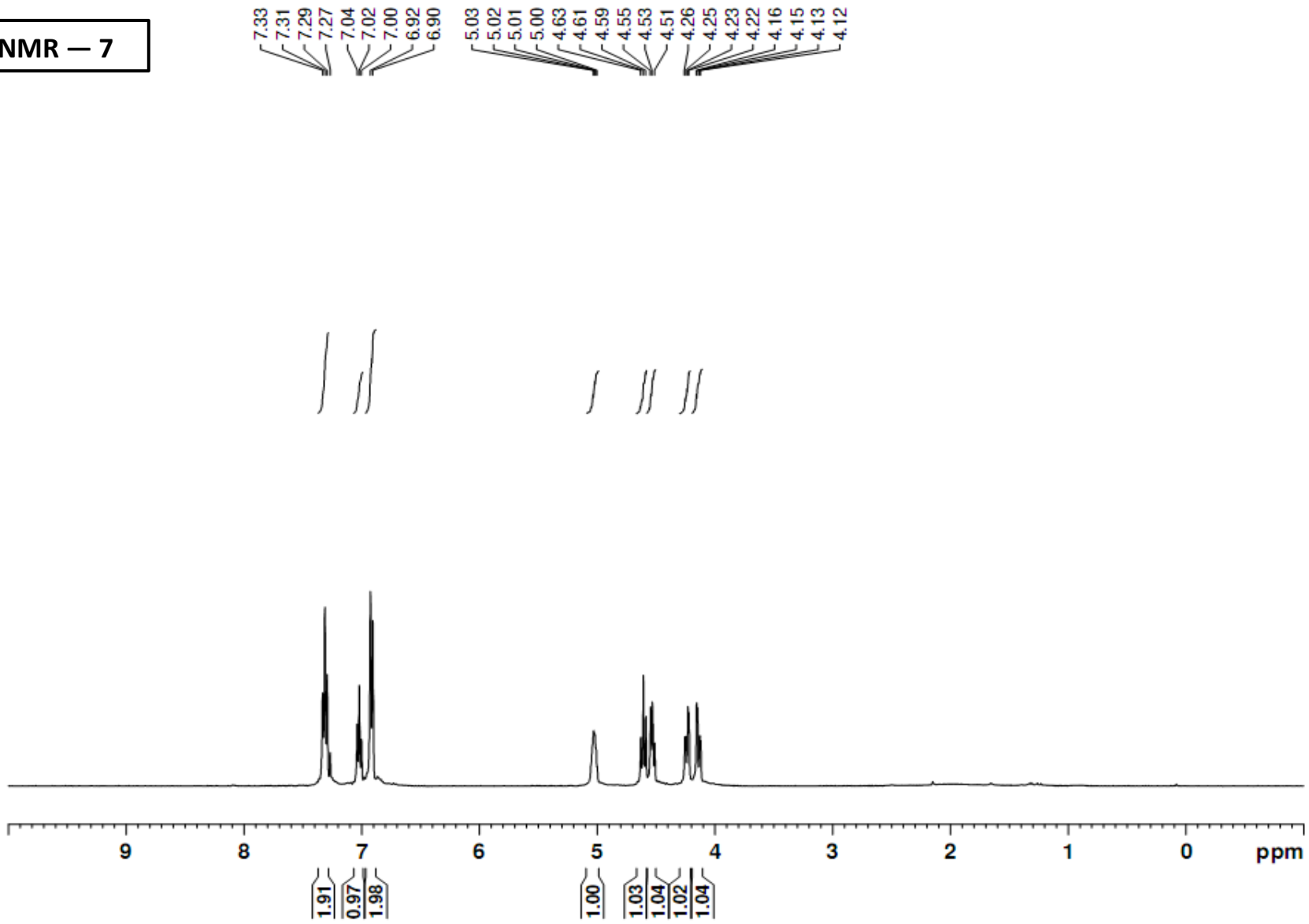
Analysis type:	UnkNown
Chromatogram filename:	UNK-31012011-4.dat
Sample weight:	1.108

CHN — 5b

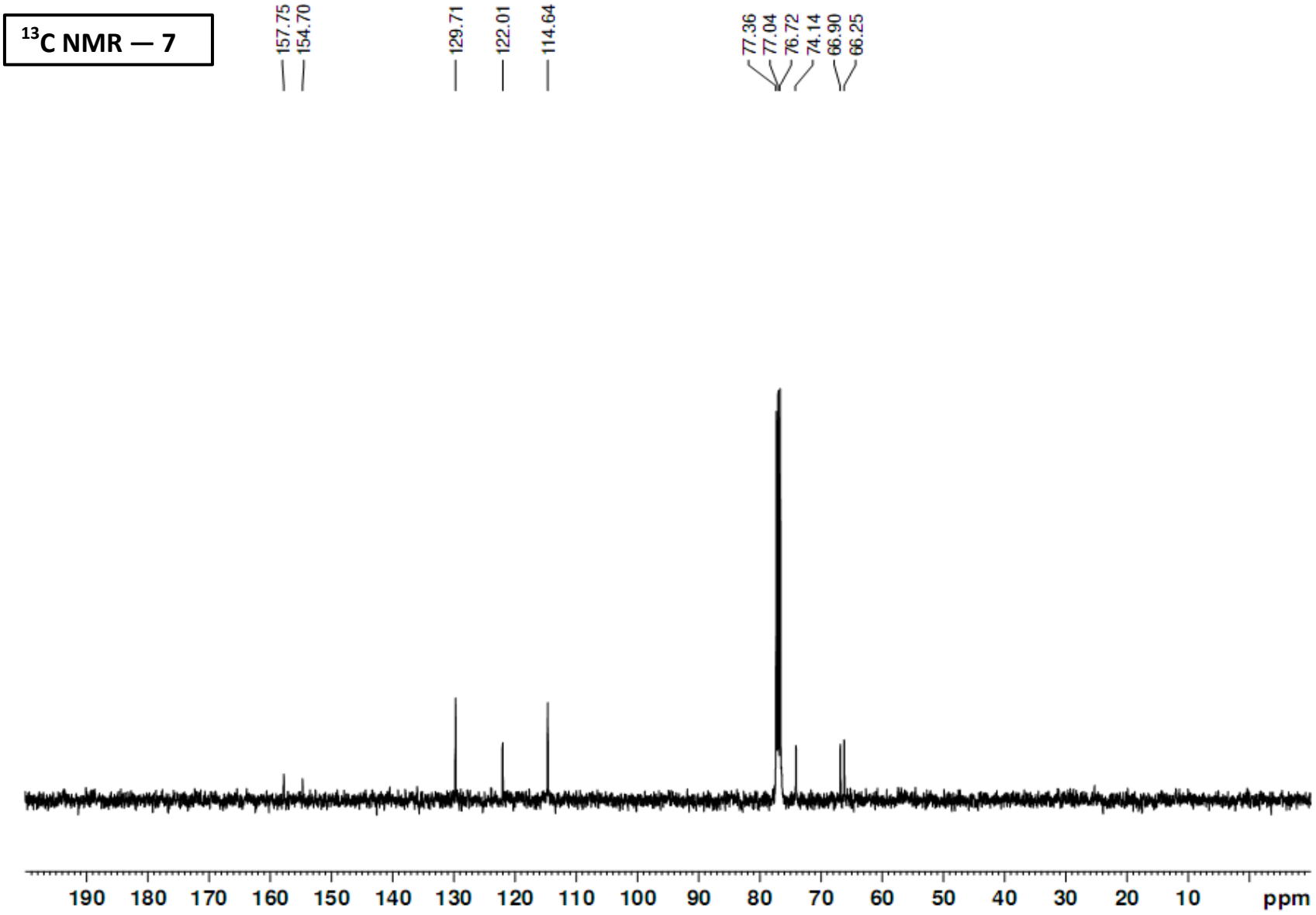


Element Name	Element %	Ret. Time
Nitrogen	8. 53	0. 89
Carbon	75. 22	1. 39
Hydrogen	8. 09	4. 69

^{1}H NMR — 7



^{13}C NMR — 7



LCMS-2010A DATA REPORT
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Mass Spectra— 7

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Sample	: HVB219
Inj. Volume	: 5.000
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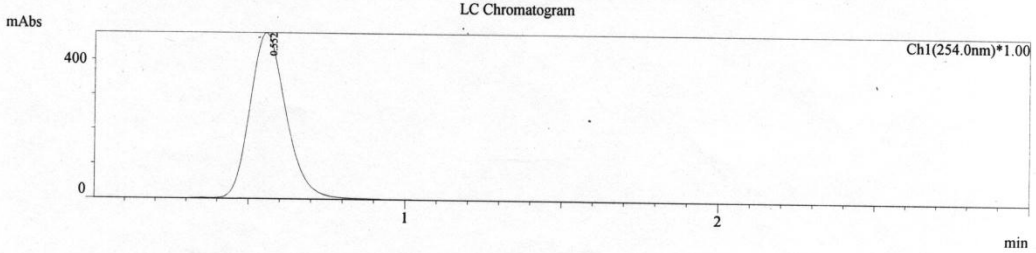
Method Name	: C:\LCMSsolution\User\Method\esi.qlm

LC Chromatogram



MS Spectrum

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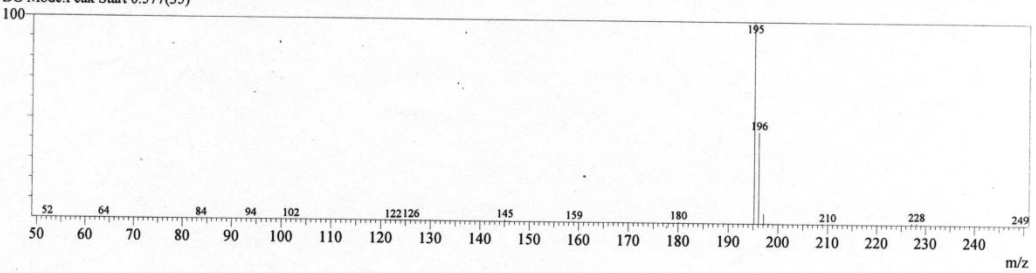
RawMode:Single 0.791(48)
BG Mode:Peak Start 0.577(35)



MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
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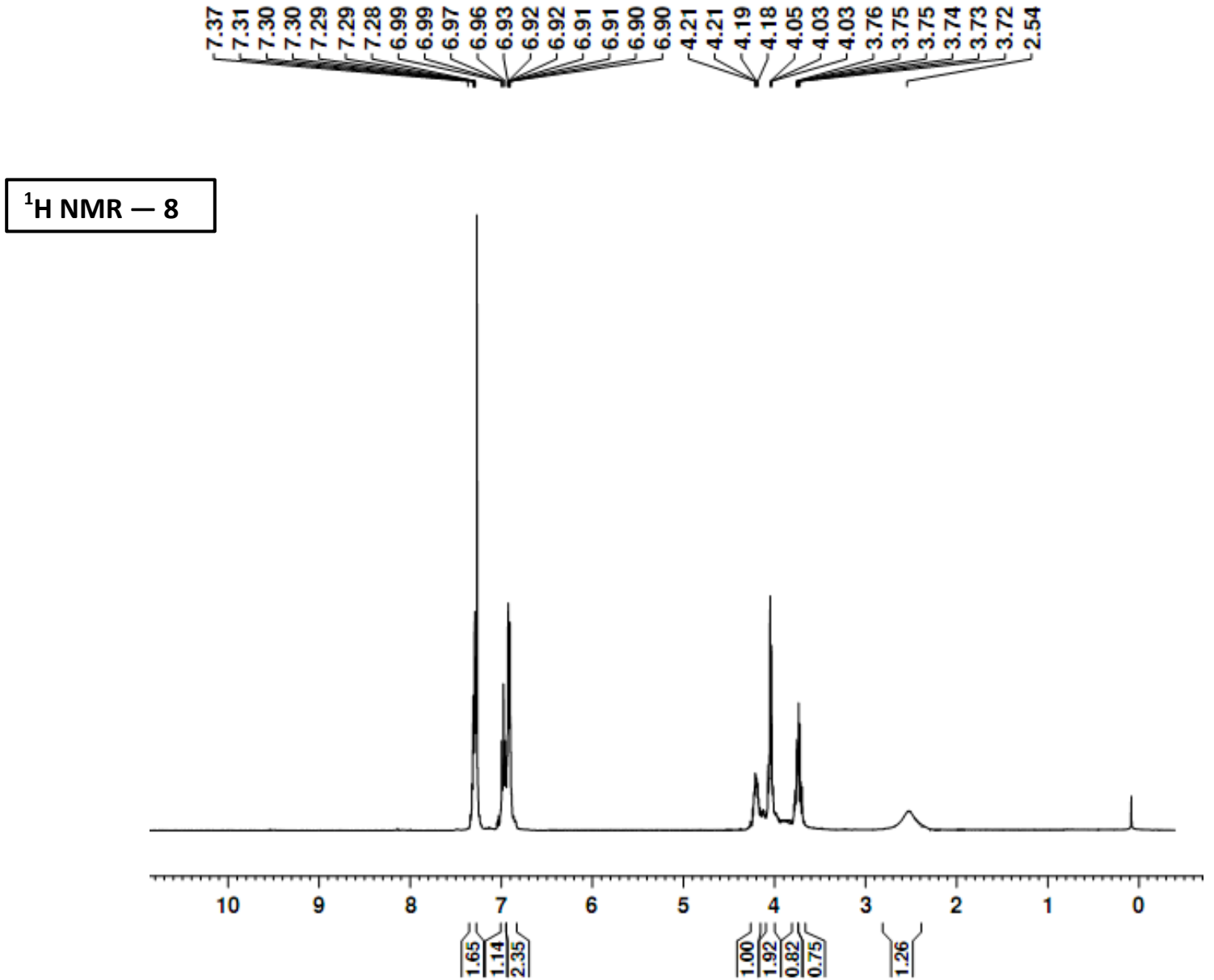
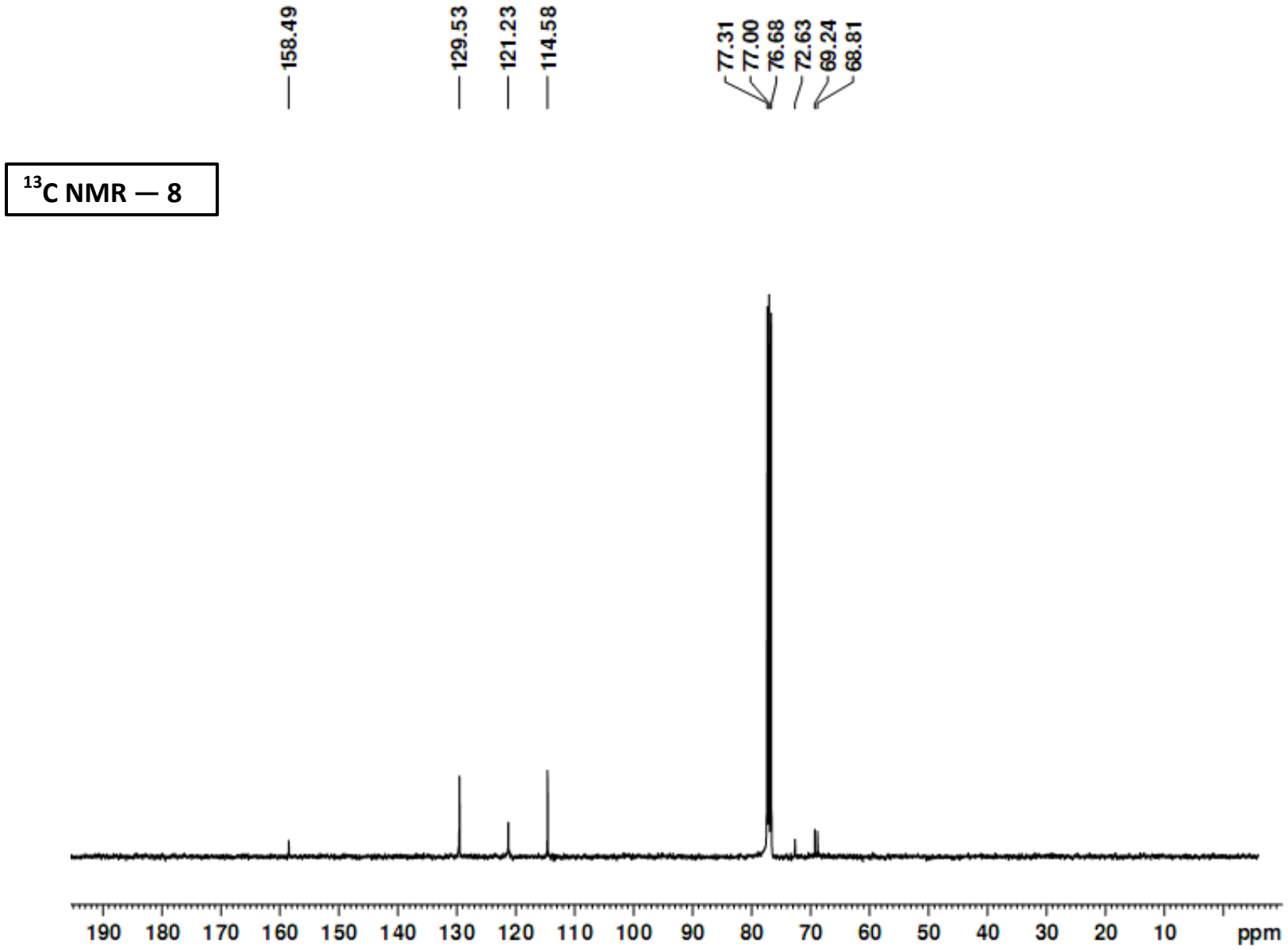
				187745028	12223158			100.00			

OPERATOR





HRMS — 8

Display Report

Analysis Info

Analysis Name	D:\Data\2012\Dr.K.Muralidharan\MAY\HVB-285 R.d	Acquisition Date	5/8/2012 2:52:09 PM
Method	tune_low_Pos.m	Operator	UOH
Sample Name	HVB-285-DCM-ACN	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
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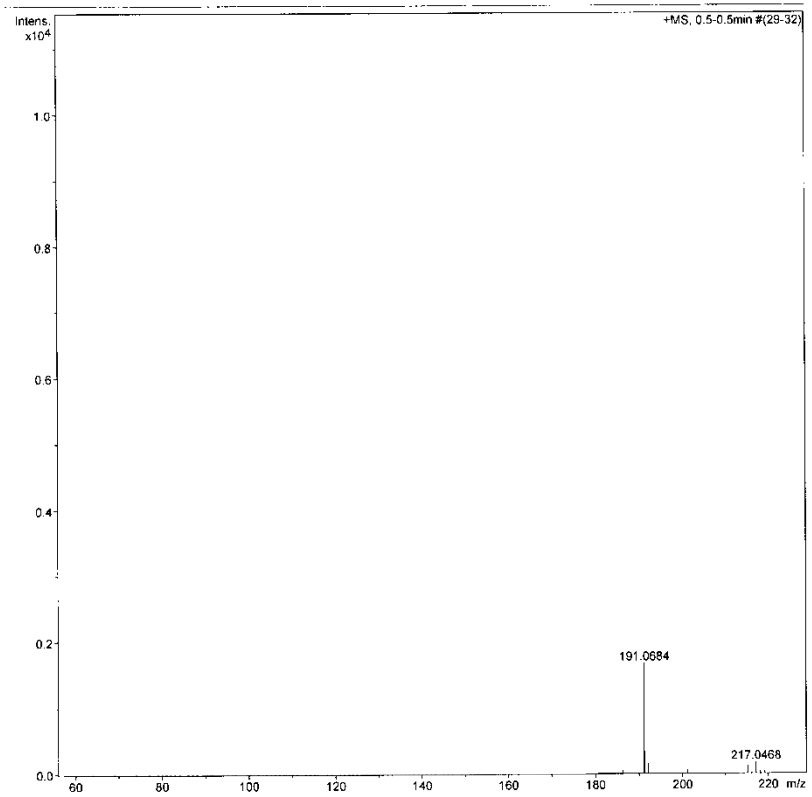
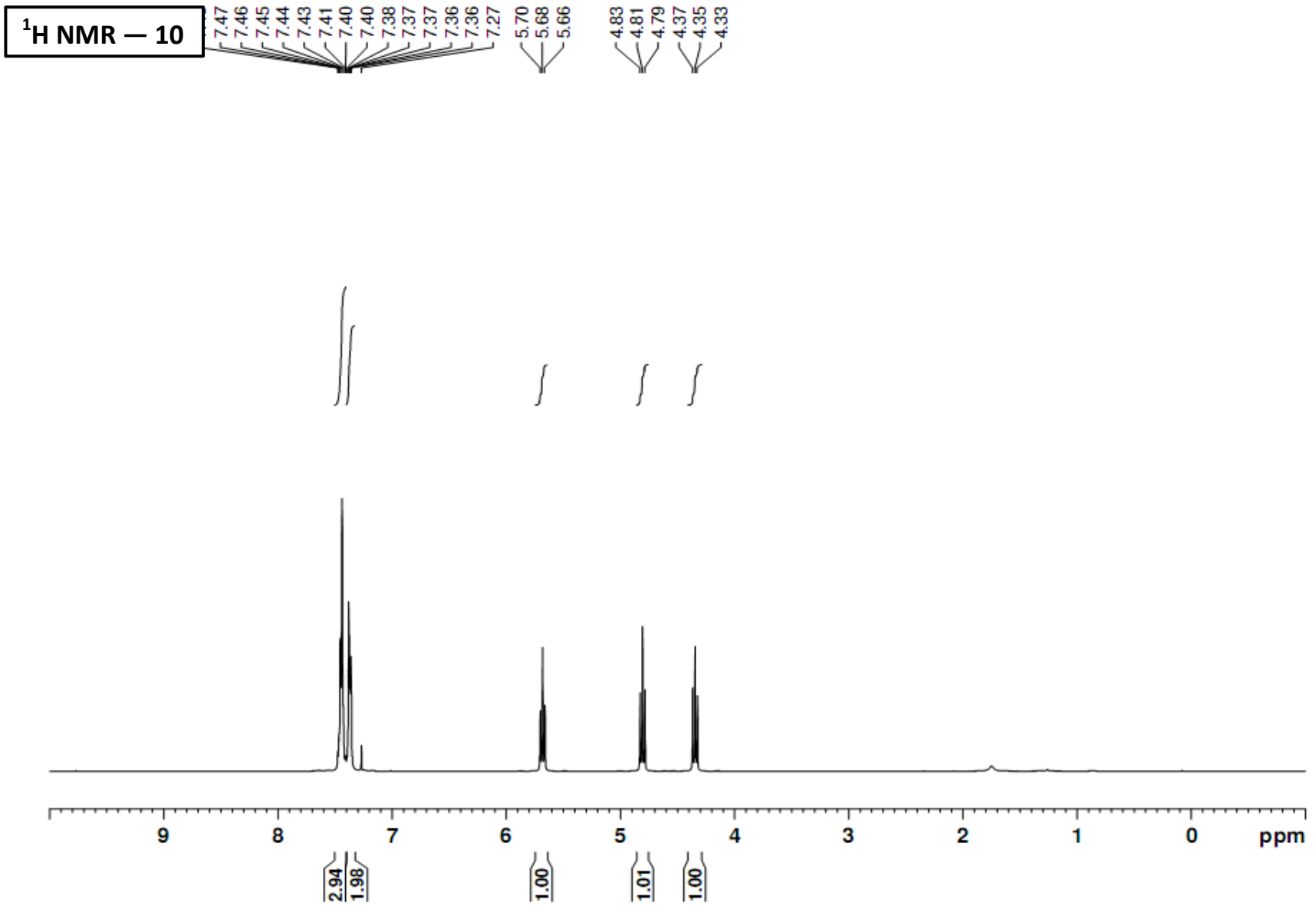
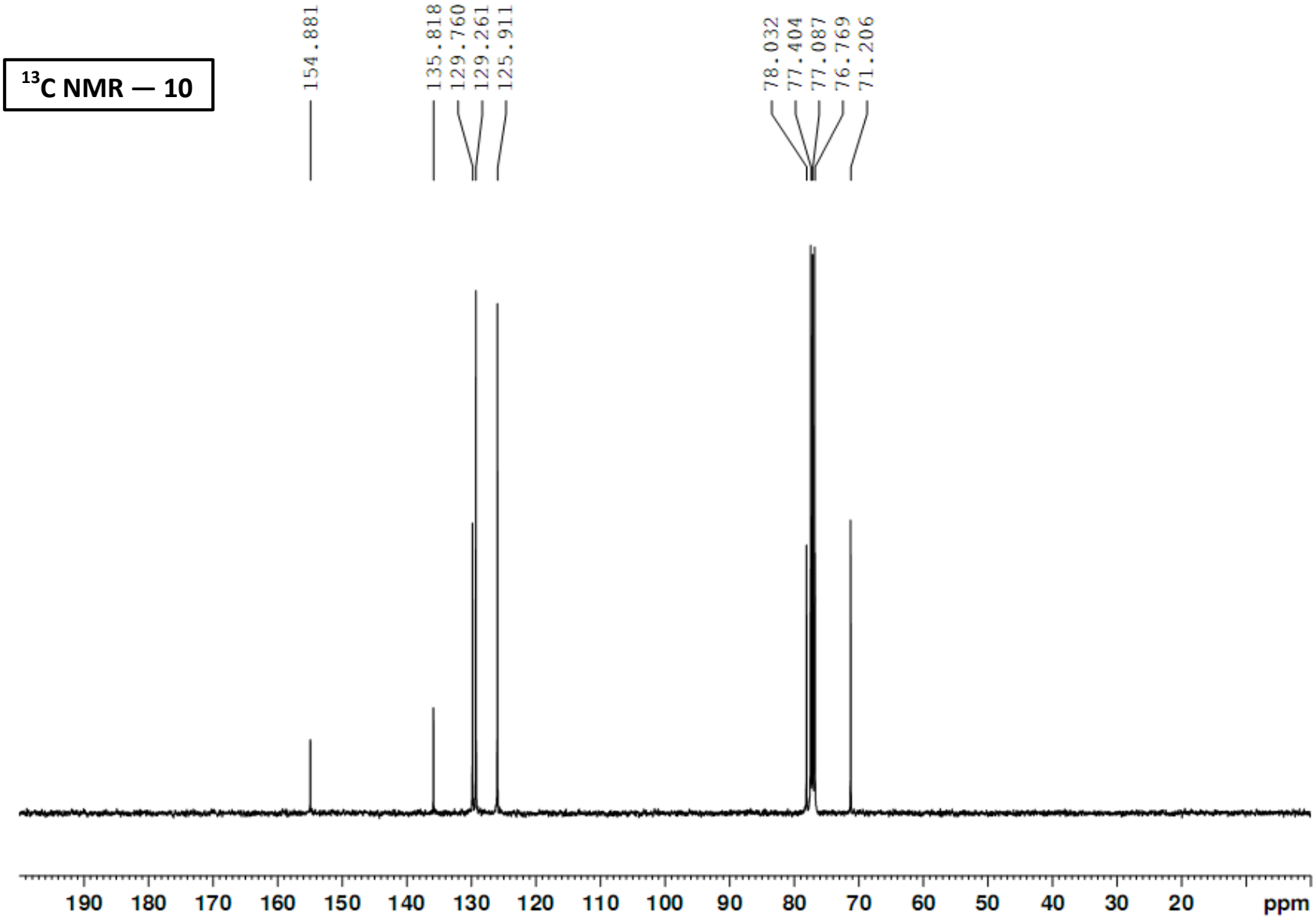
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.0 printed: 5/8/2012 2:59:04 PM Page 1 of 1



^{13}C NMR — 10



LCMS-2010A DATA REPORT
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Mass Spectra— 10

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Inj. Volume : 5.000
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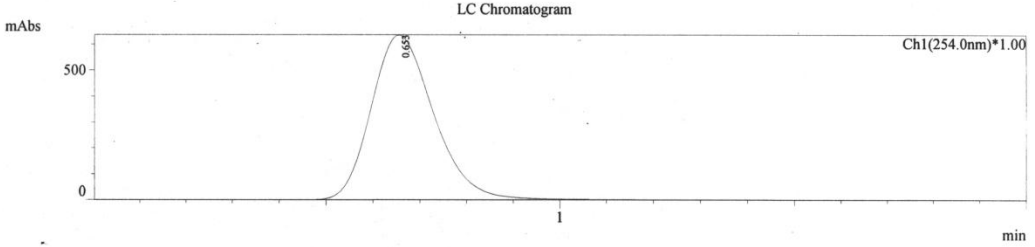
Method Name : C:\LCMSsolution\User\Method\esi.qlm

LC Chromatogram



MS Spectrum

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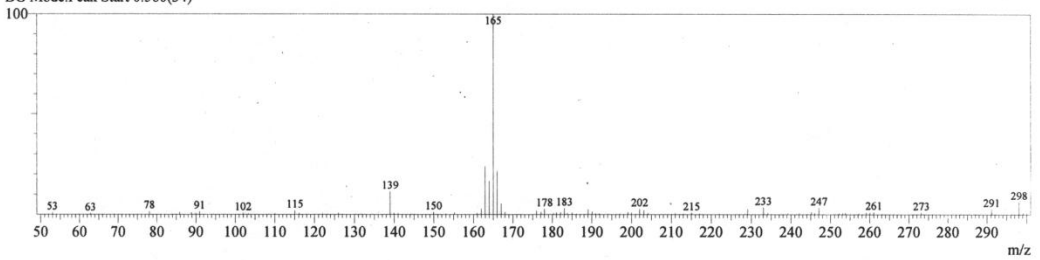
RawMode:Single 0.765(46)
BG Mode:Peak Start 0.560(34)



MS Peak Table

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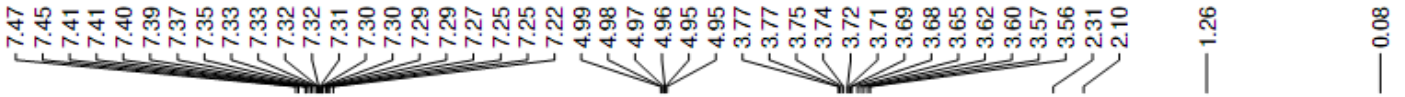
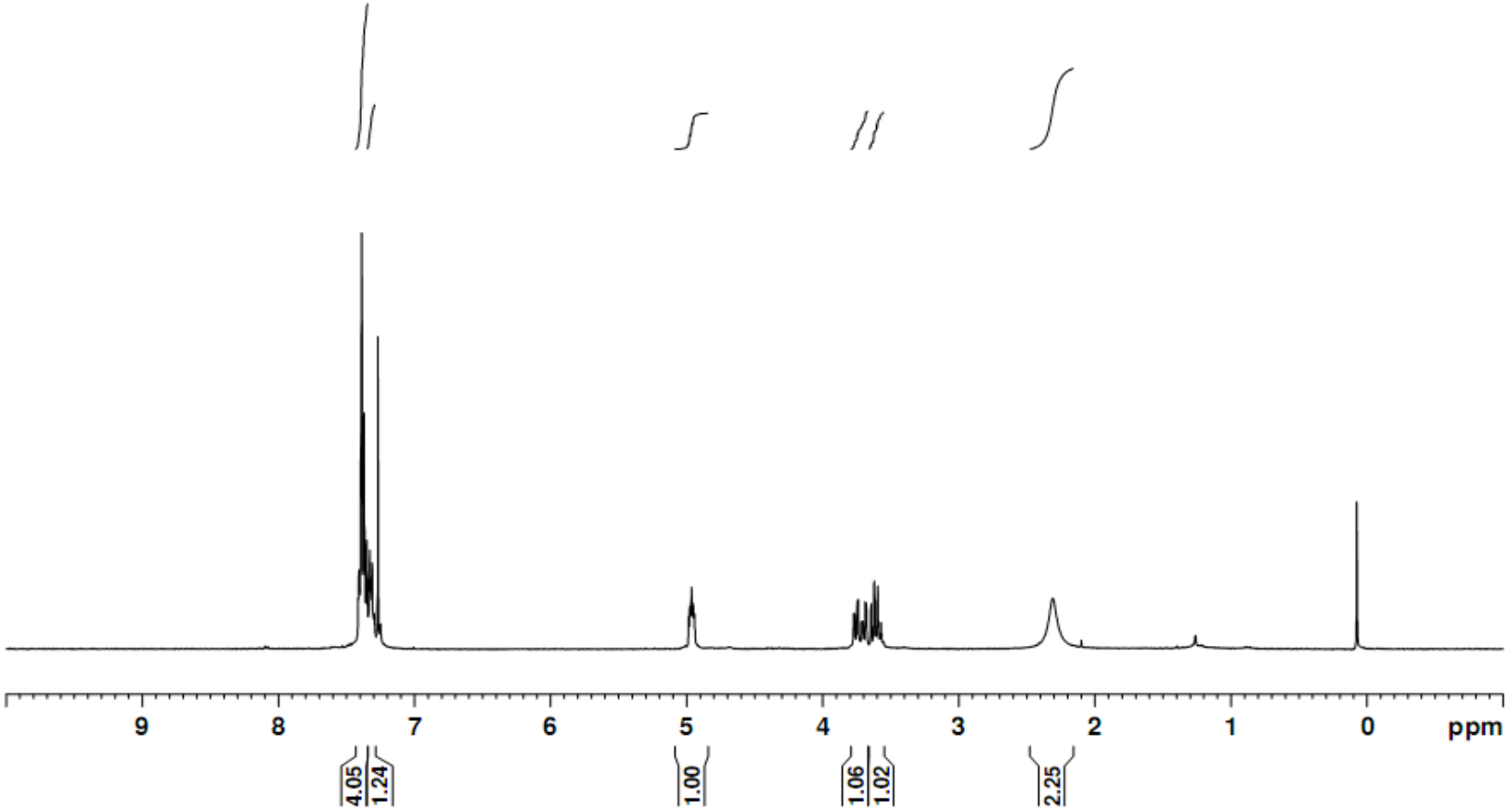
1	0.765	0.560	1.143	678285523	37263095	18.20		100.00		165.00	1862605
				678285523	37263095			100.00			

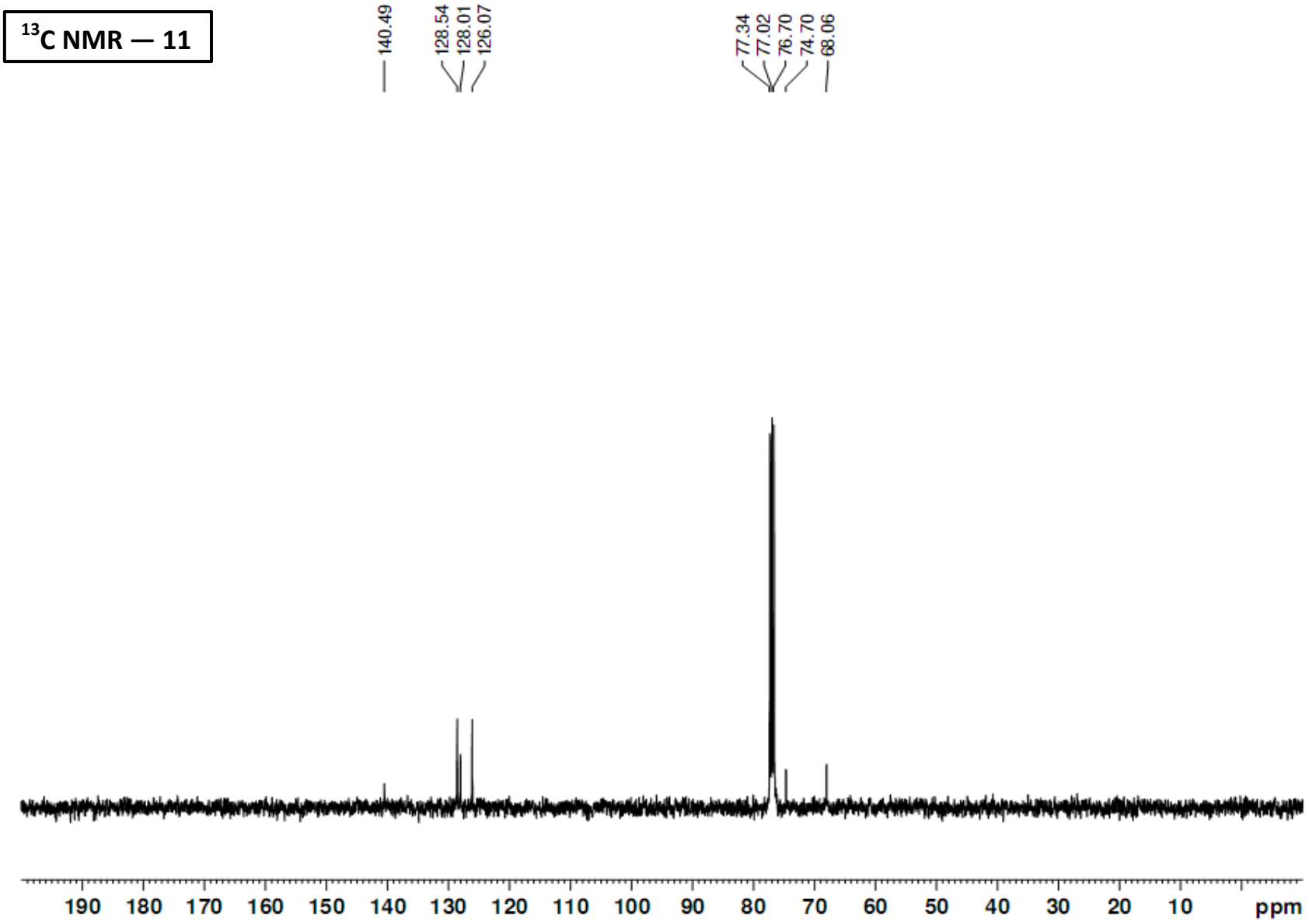
OPERATOR



^{1}H NMR — 11



^{13}C NMR — 11



Mass Spectra — 11

LCMS-2010A DATA REPORT
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Inj. Volume	: 5.000
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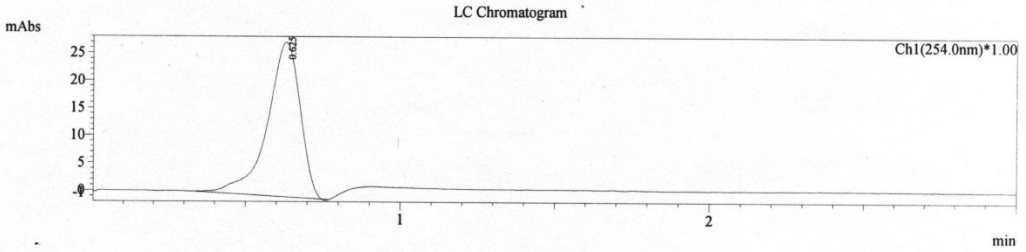
Method Name	: C:\LCMSsolution\User\Method\esi.qlm

LC Chromatogram



MS Spectrum

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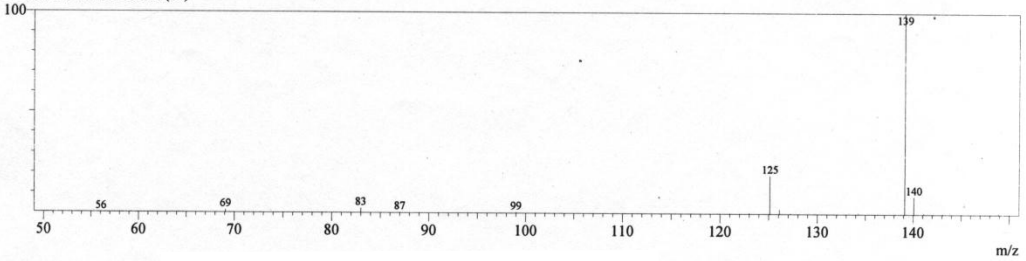
RawMode:Single 0.857(52)
BG Mode:Peak Start 0.527(32)



MS Peak Table

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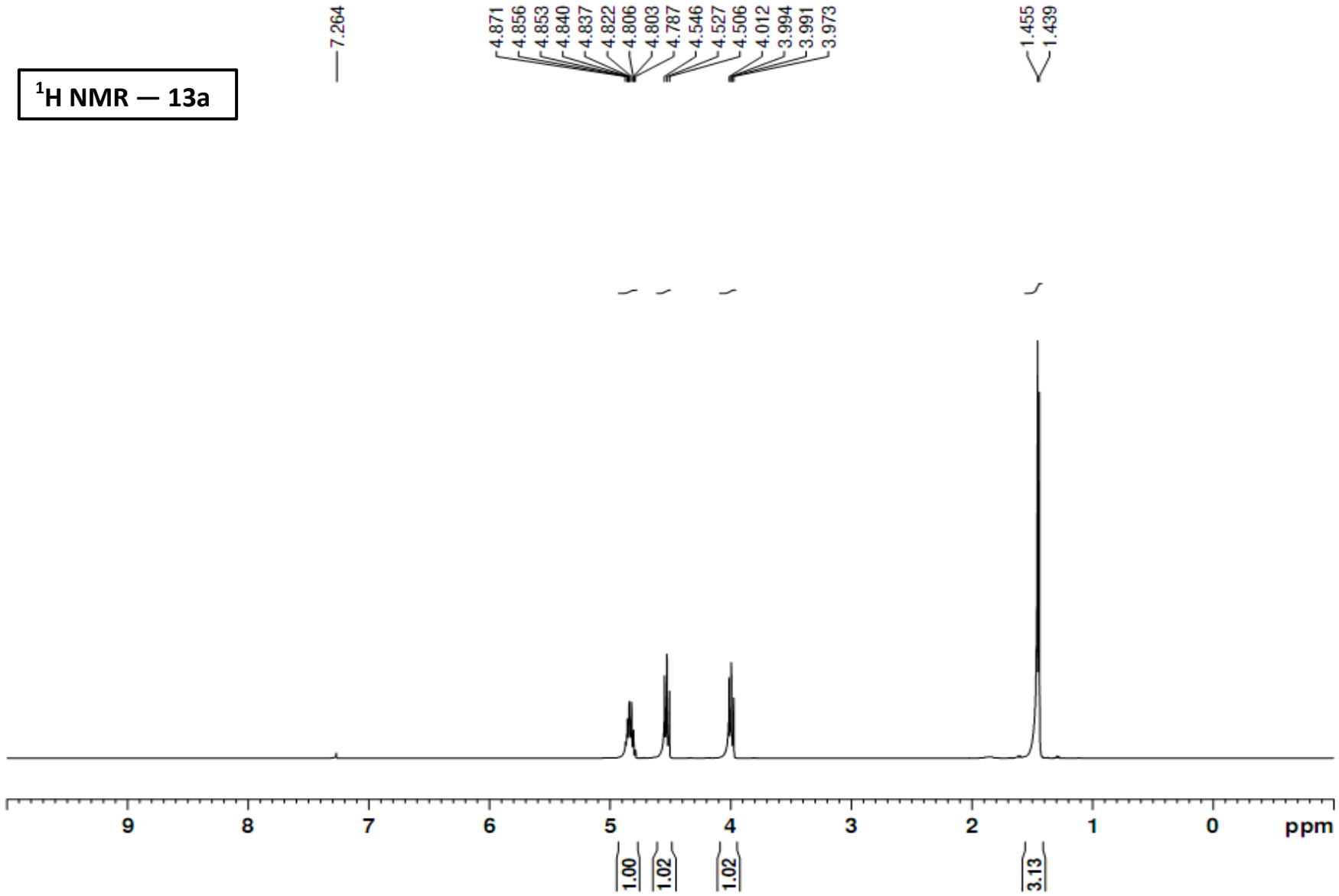
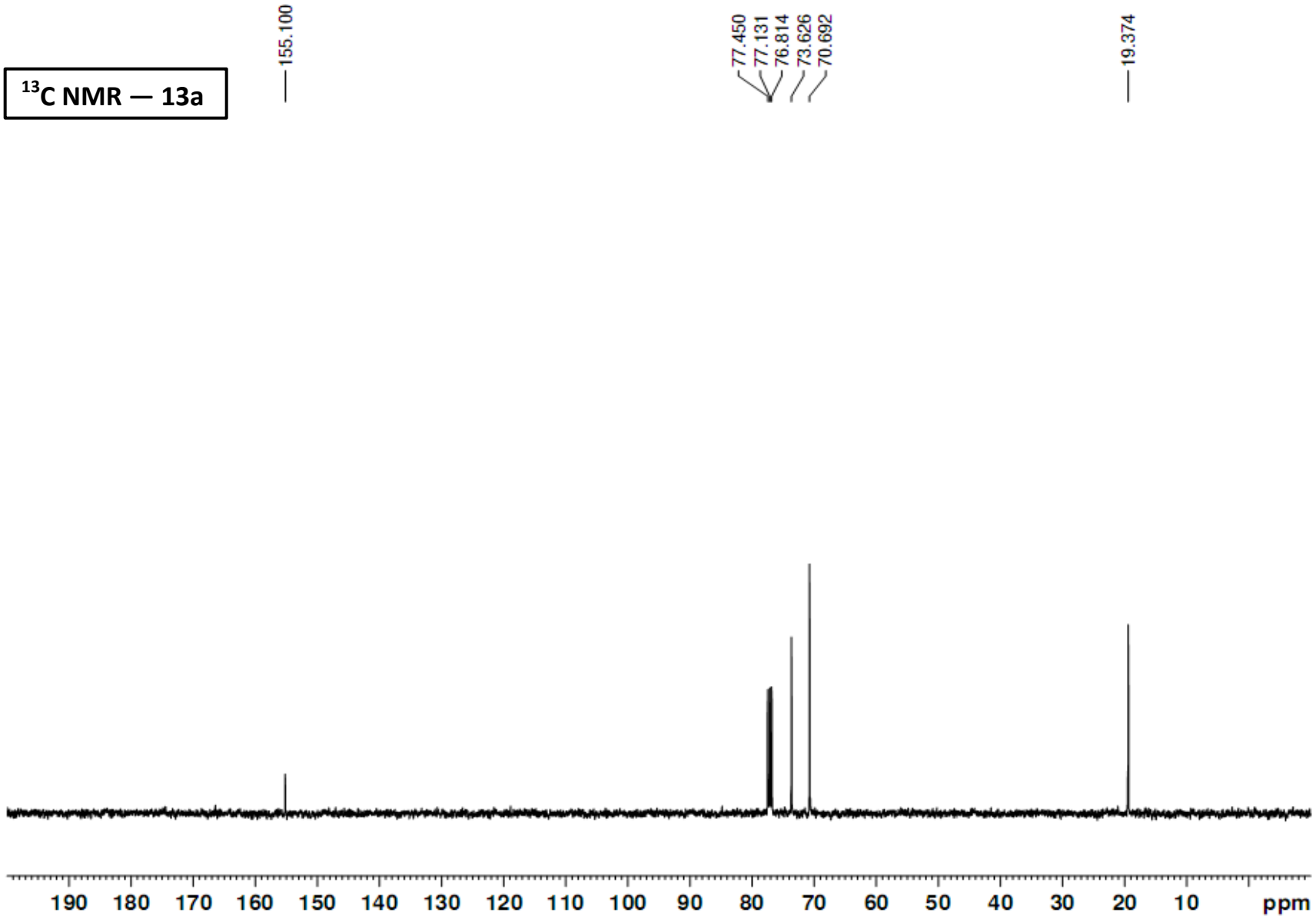
				25687988	1315354			100.00			

OPERATOR

^{1}H NMR — 13a



^{13}C NMR — 13a



HRMS — 13a

Display Report

Analysis Info

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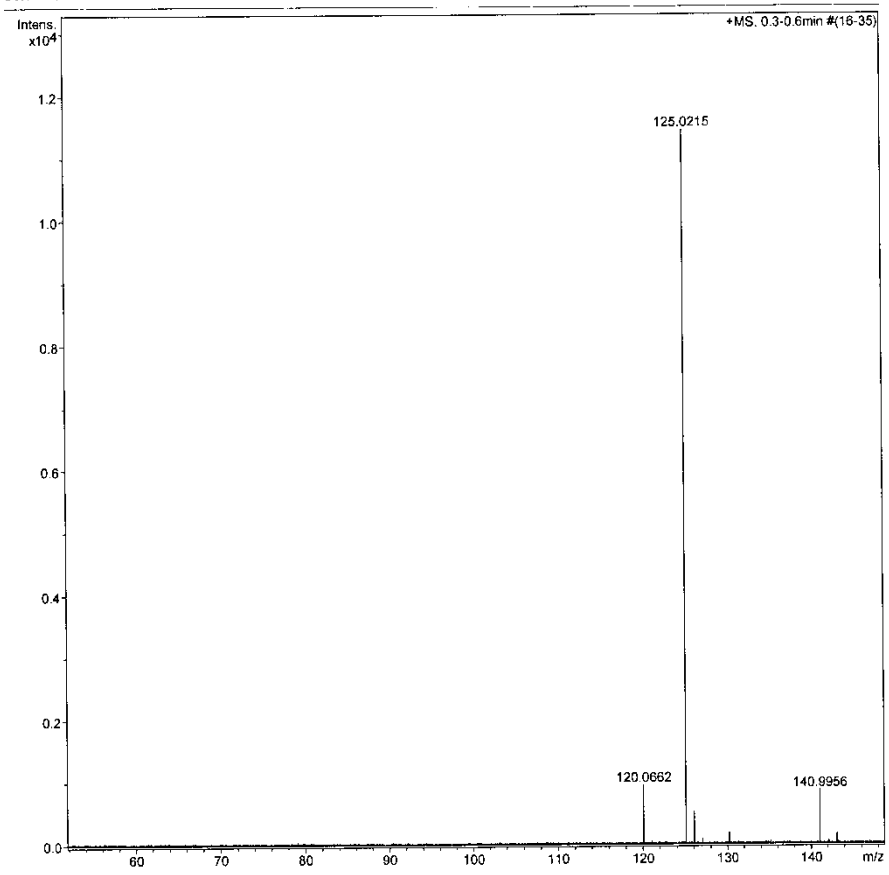
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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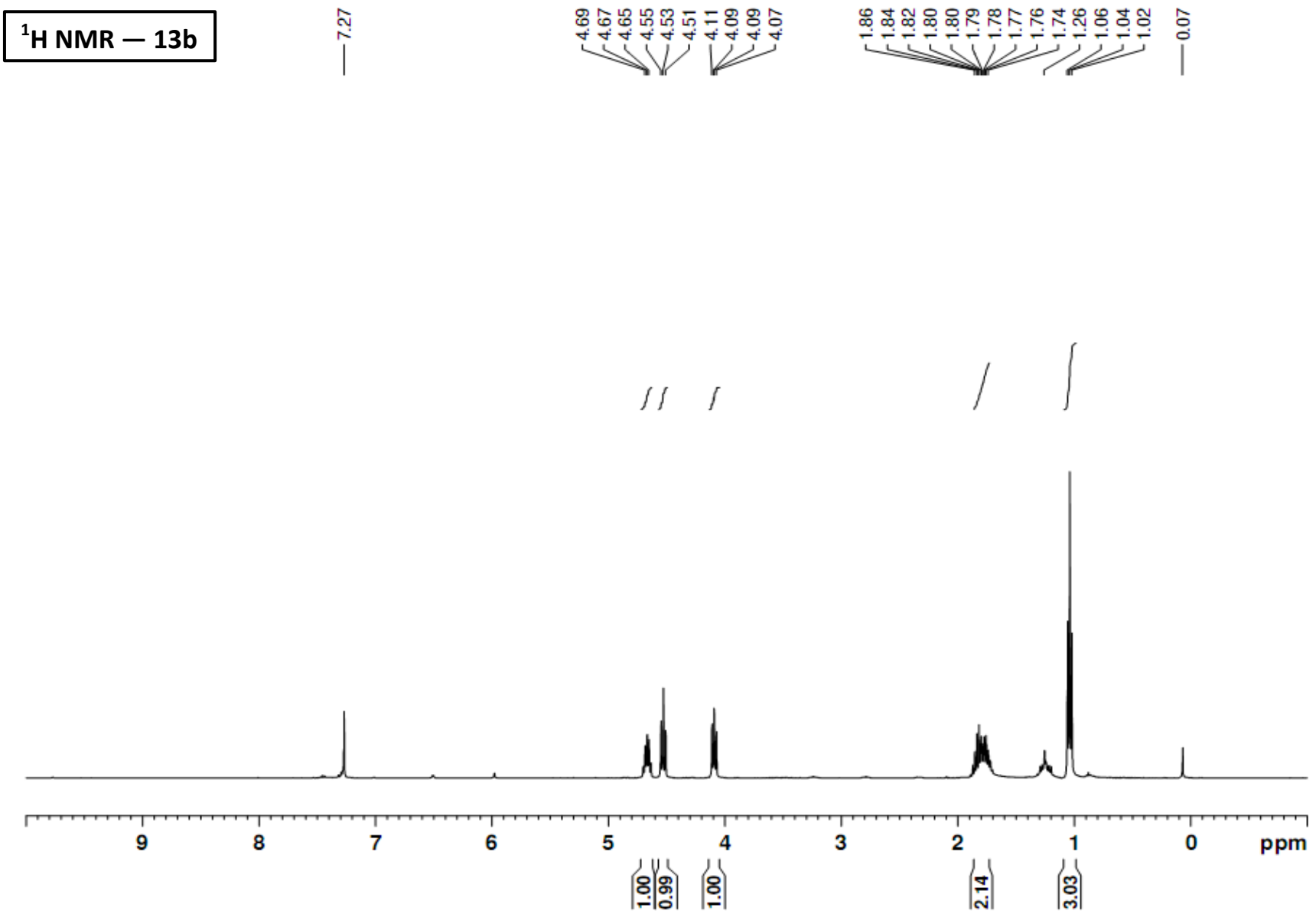
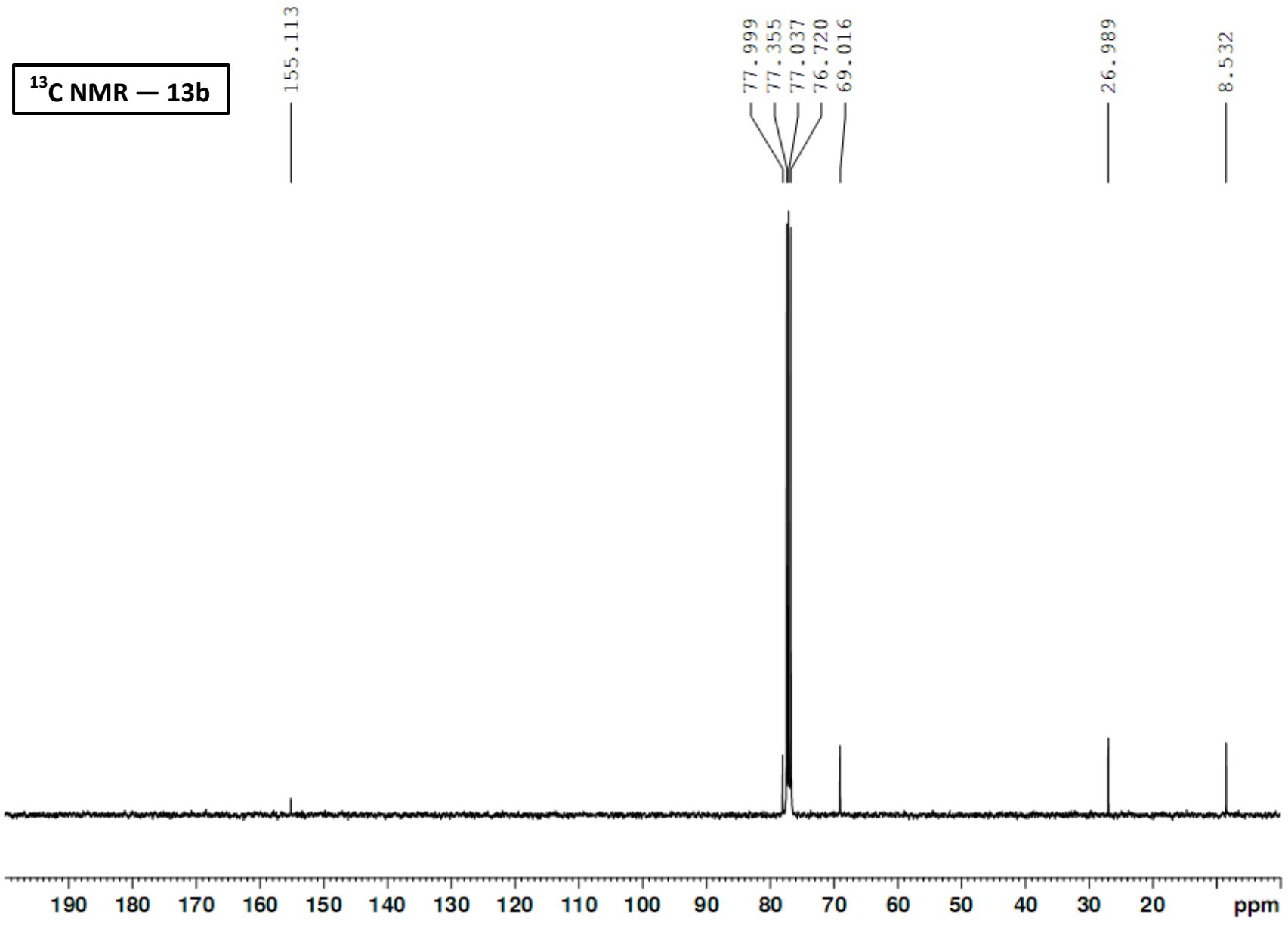
^{1}H NMR — 13b



^{13}C NMR — 13b



HRMS — 13b

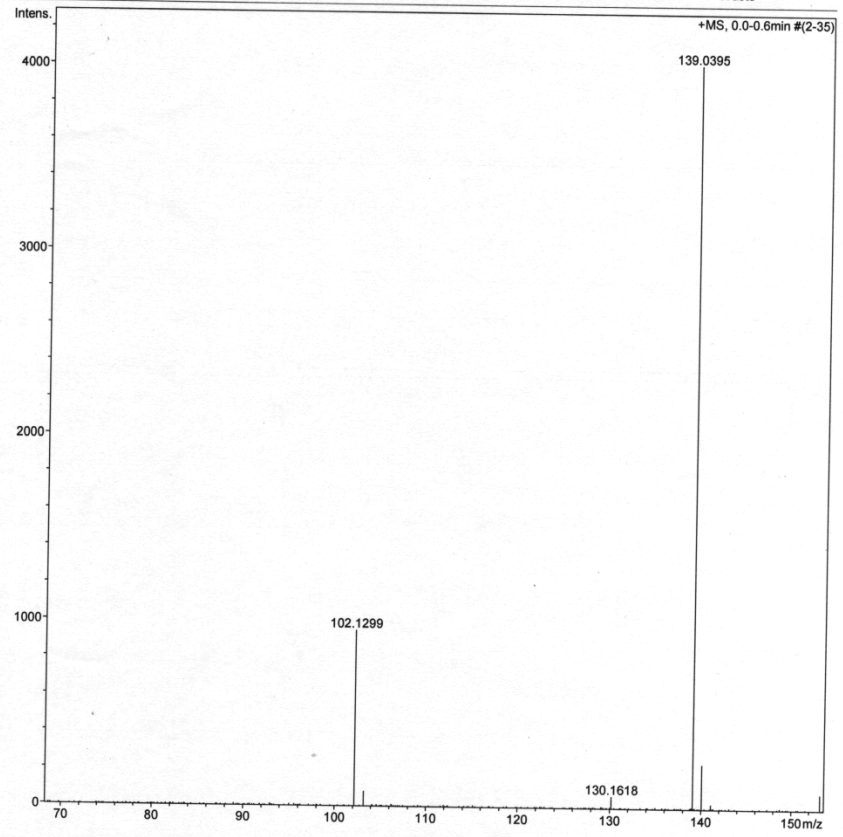
Display Report

Analysis Info

Analysis Name	D:\Data\2012\Dr.K.Muralidharan\JAN\KPK-V-238.d	Acquisition Date	1/31/2012 4:15:10 PM
Method	tune_low_Pos.m		
Sample Name	KPK-V-238-DCM-ACN	Operator	UOH
Comment		Instrument	maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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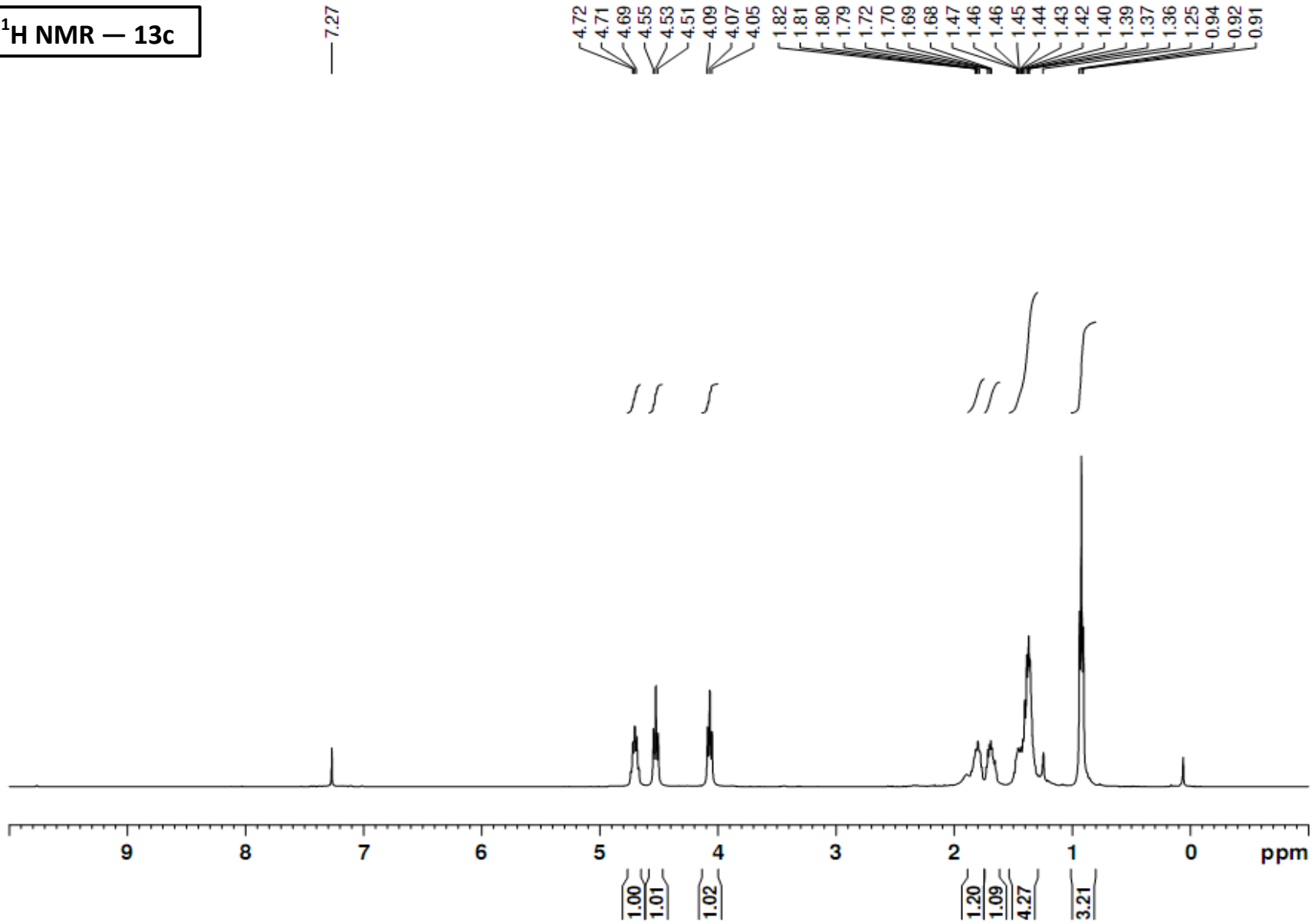
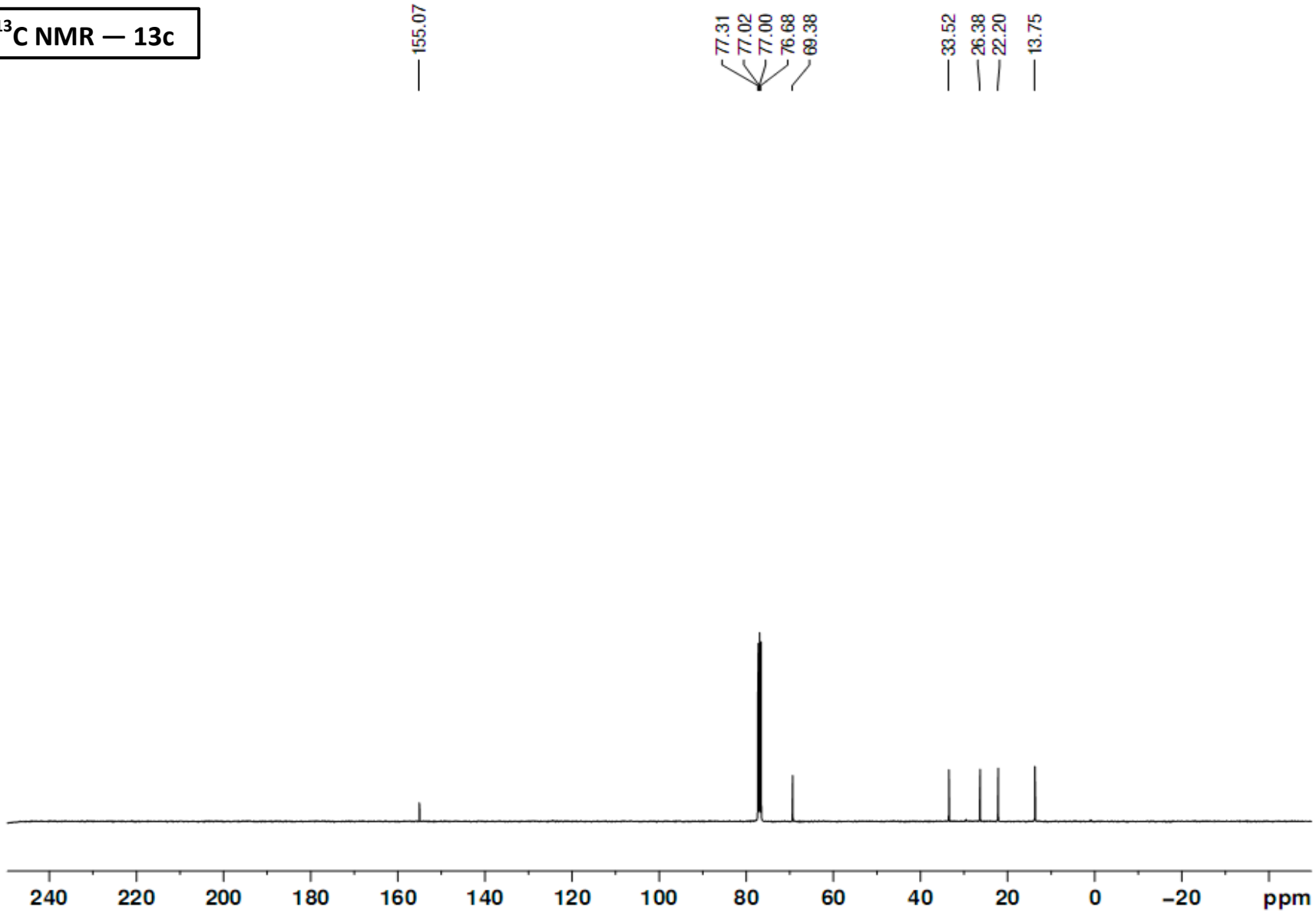
^{1}H NMR — 13c



^{13}C NMR — 13c



HRMS — 13c

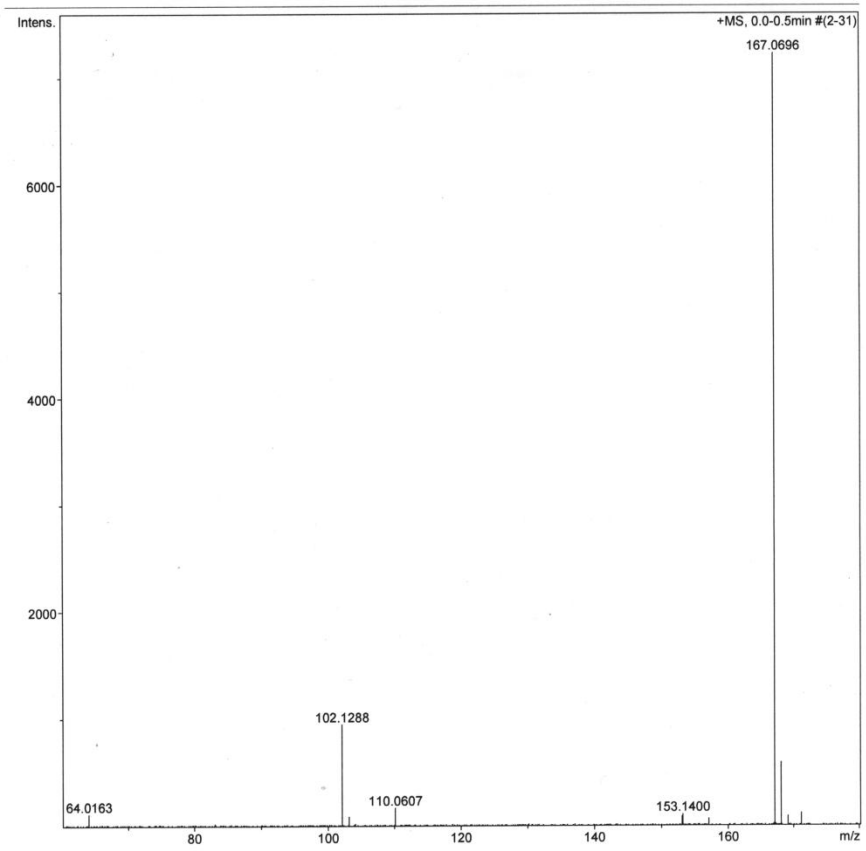
Display Report

Analysis Info

Analysis Name	D:\Data\2012\Dr.K.Muralidharan\JAN\KPK-V-239.d	Acquisition Date	1/31/2012 4:27:14 PM
Method	tune_low_Pos.m	Operator	UOH
Sample Name	KPK-V-239-DCM-ACN	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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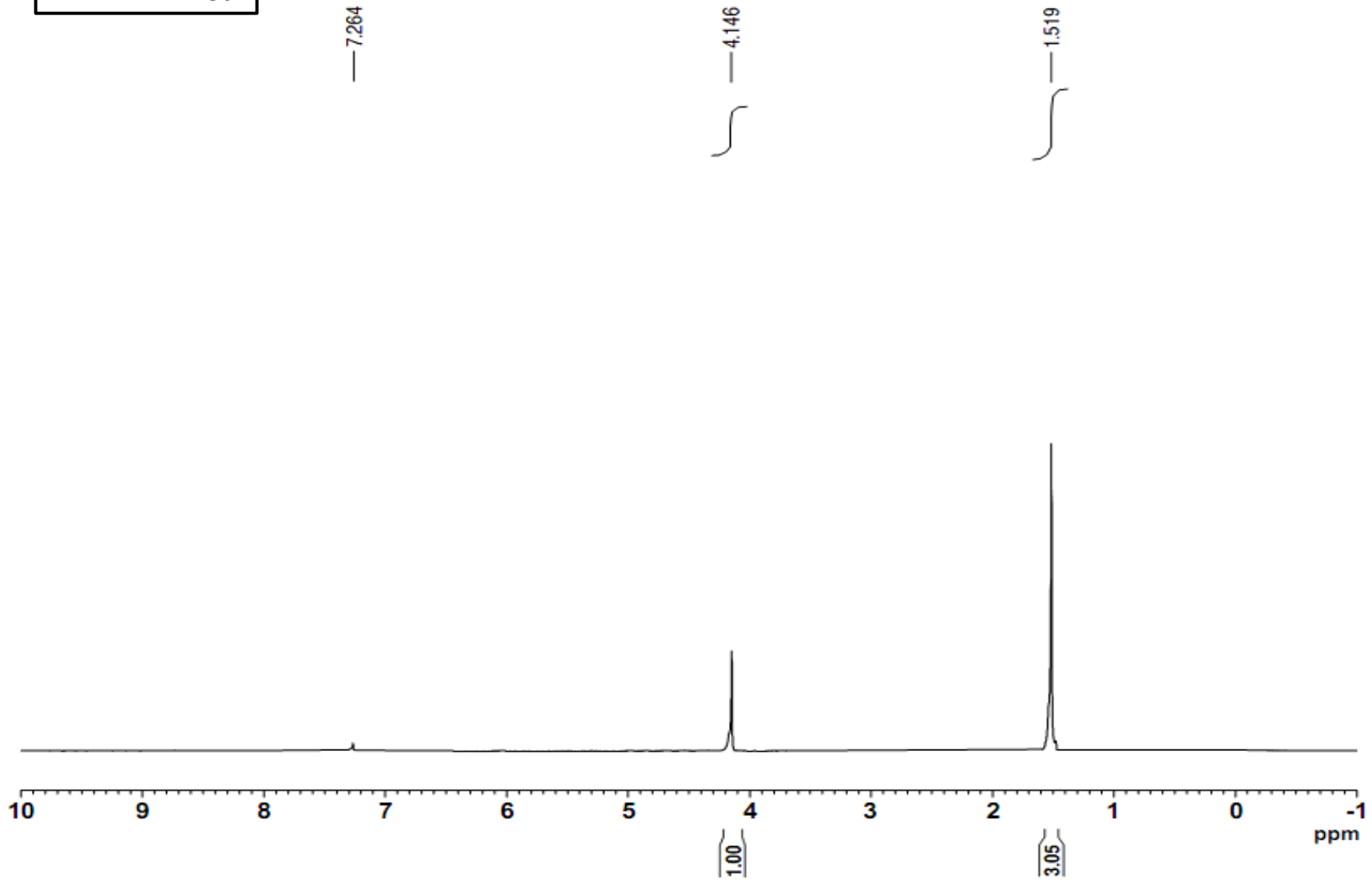
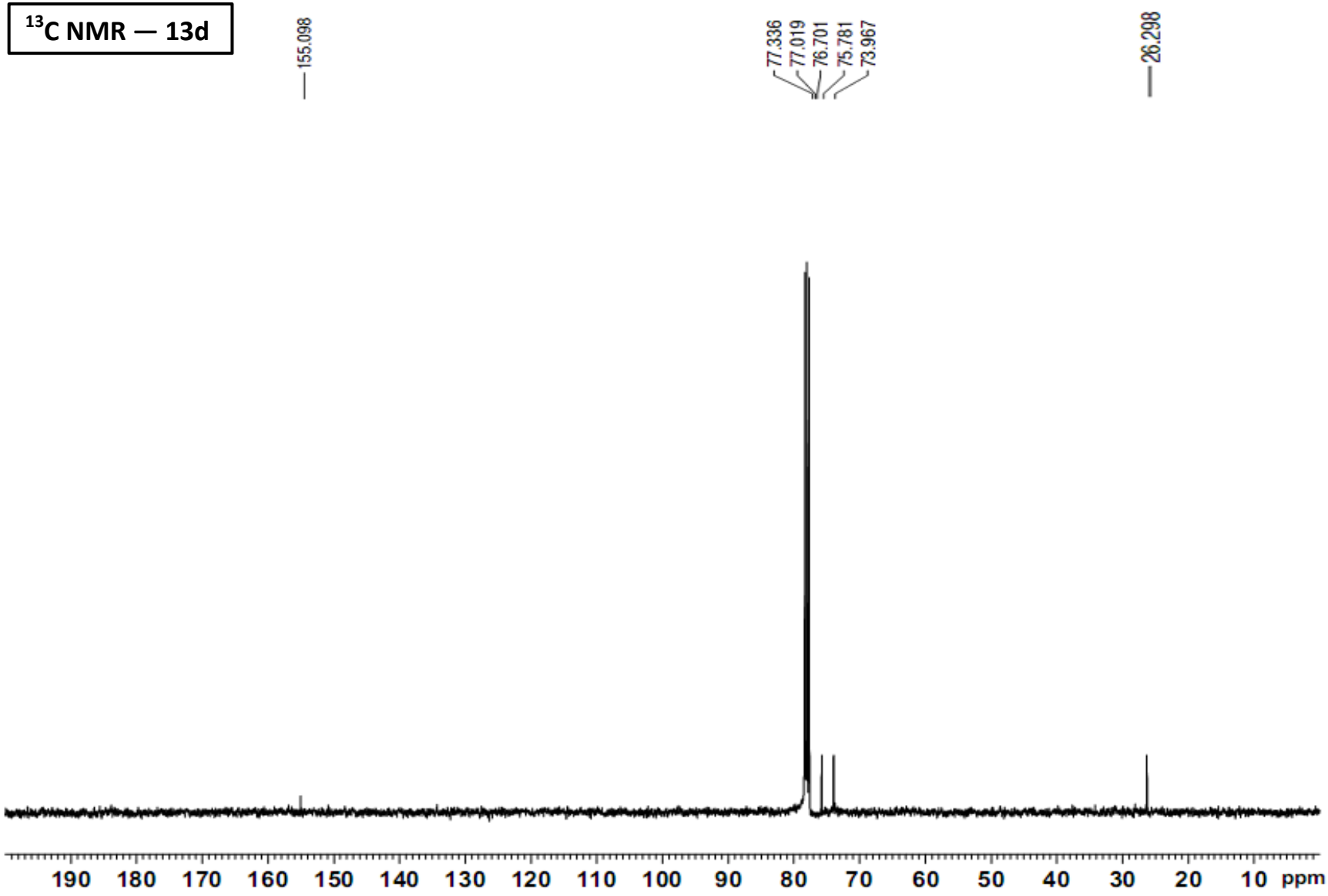
^{1}H NMR — 13d



^{13}C NMR — 13d



HRMS — 13d

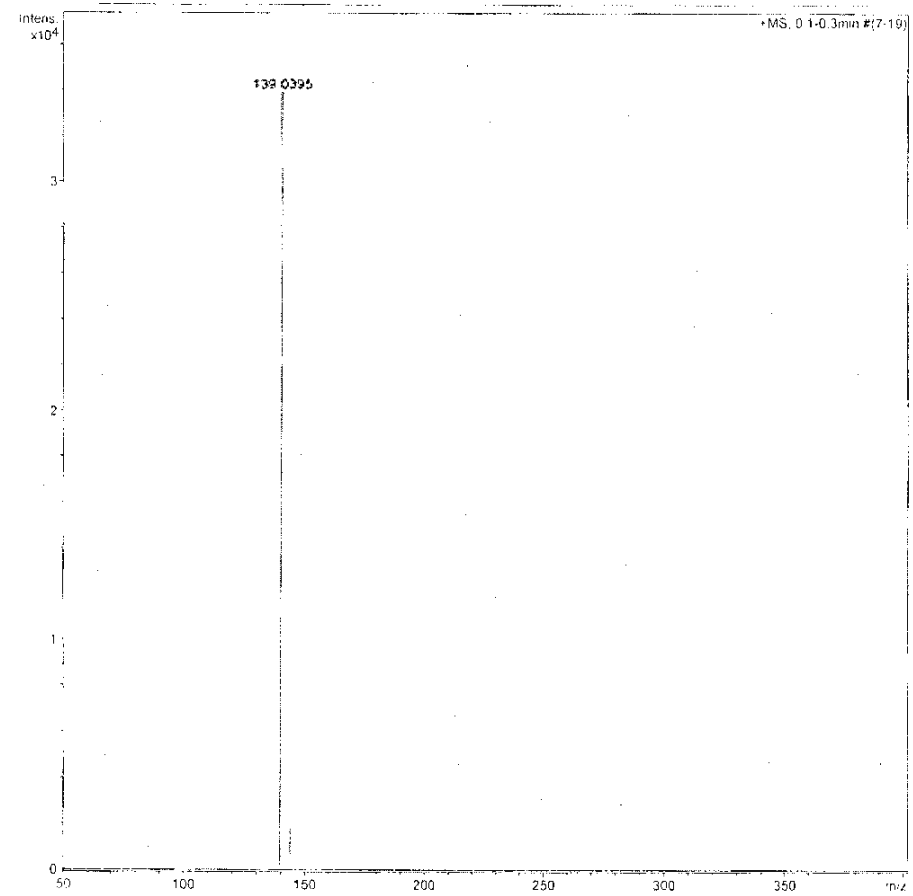
Display Report

Analysis Info

Analysis Name	D:\Data\2012\Dr.K.Muralidharan\MAY\HVB-277.d	Acquisition Date	5/8/2012 10:49:24 AM
Method	tune_low_Pos.m	Operator	UOH
Sample Name	HVB-277-DCM-ACN	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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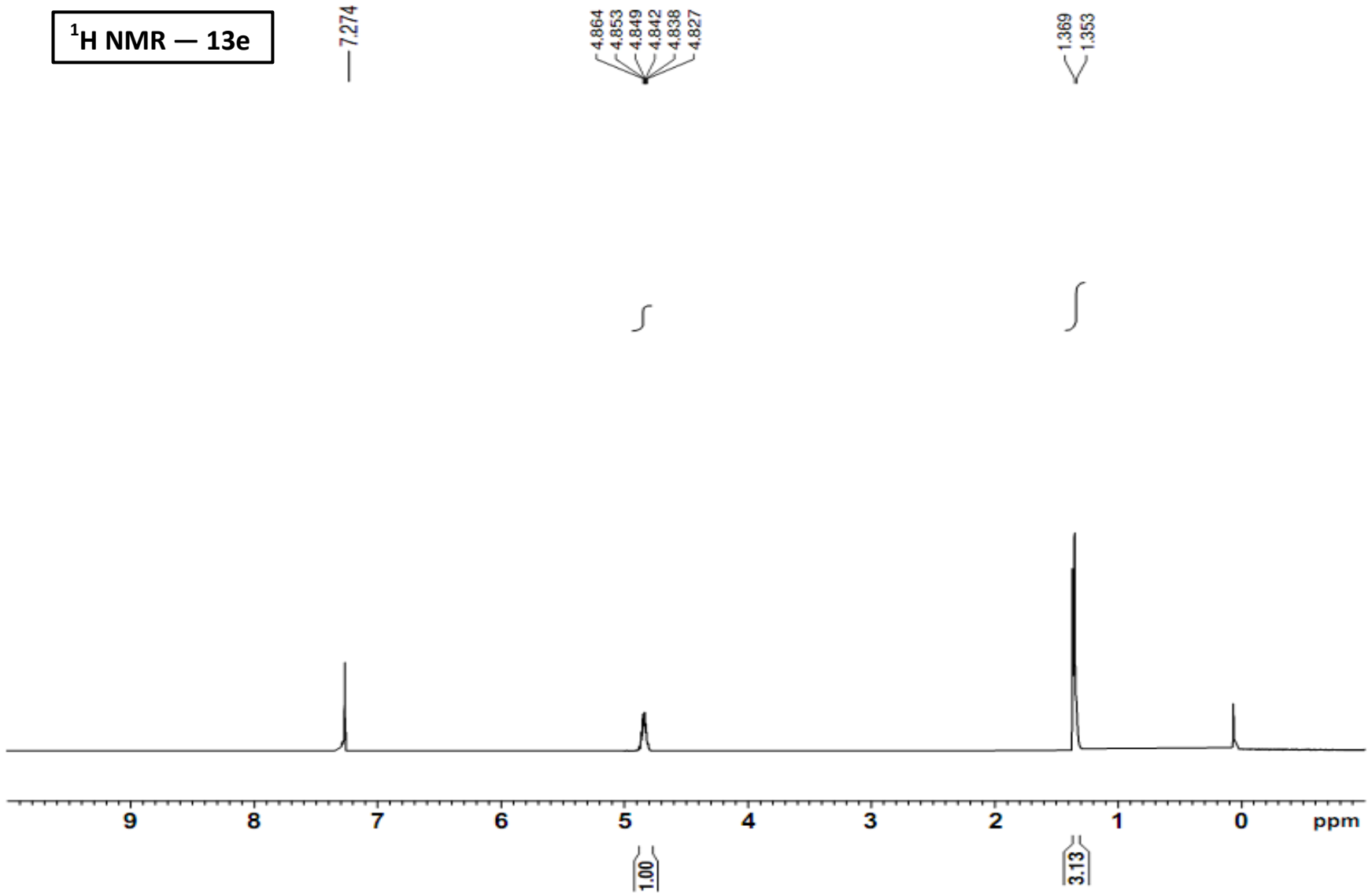
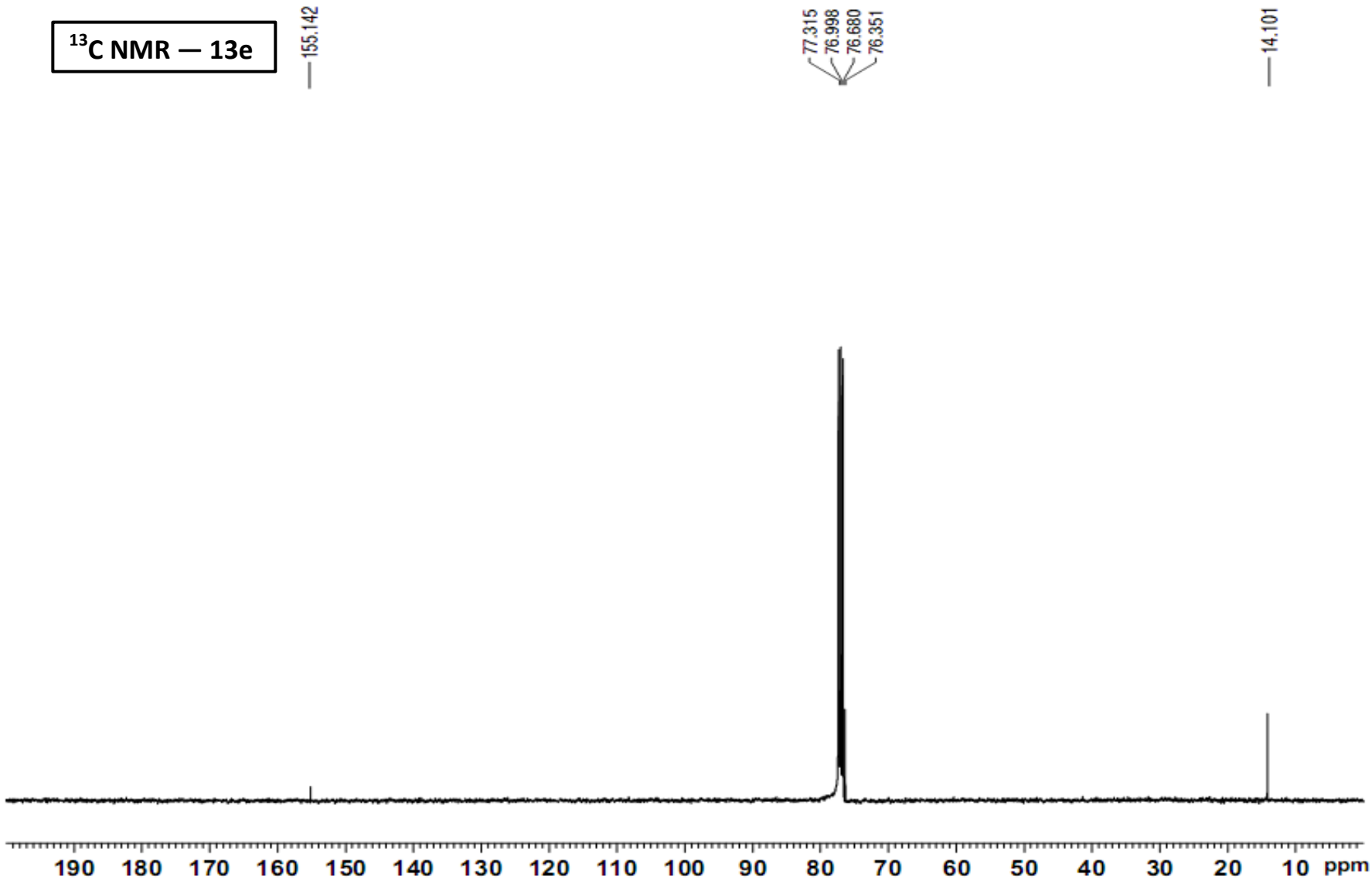
^{1}H NMR — 13e



^{13}C NMR — 13e



HRMS — 13e

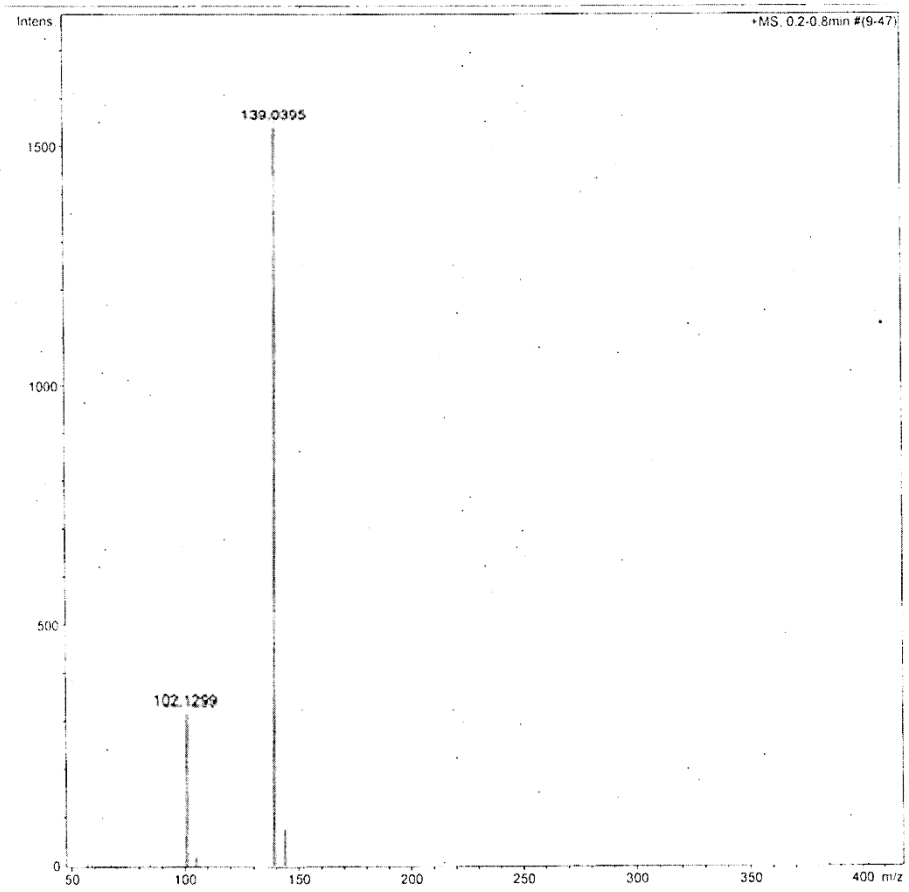
Display Report

Analysis Info

Analysis Name	D:\Data\2012\Dr.K.Muralidharan\MAY\HVB-275.d	Acquisition Date	5/8/2012 10:27:10 AM
Method	tune_low.m	Operator	UOH
Sample Name	HVB-275-DCM-ACN	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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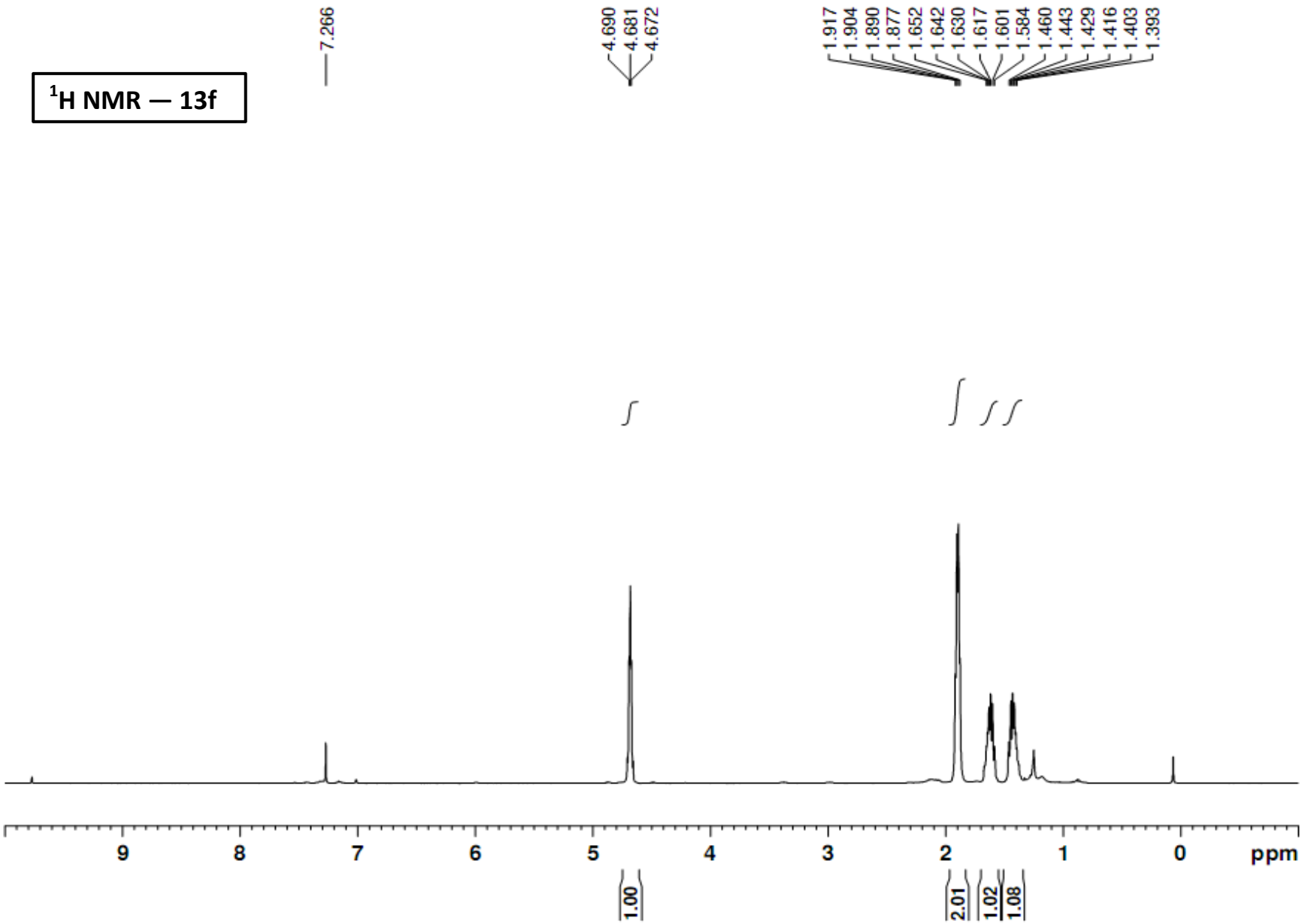
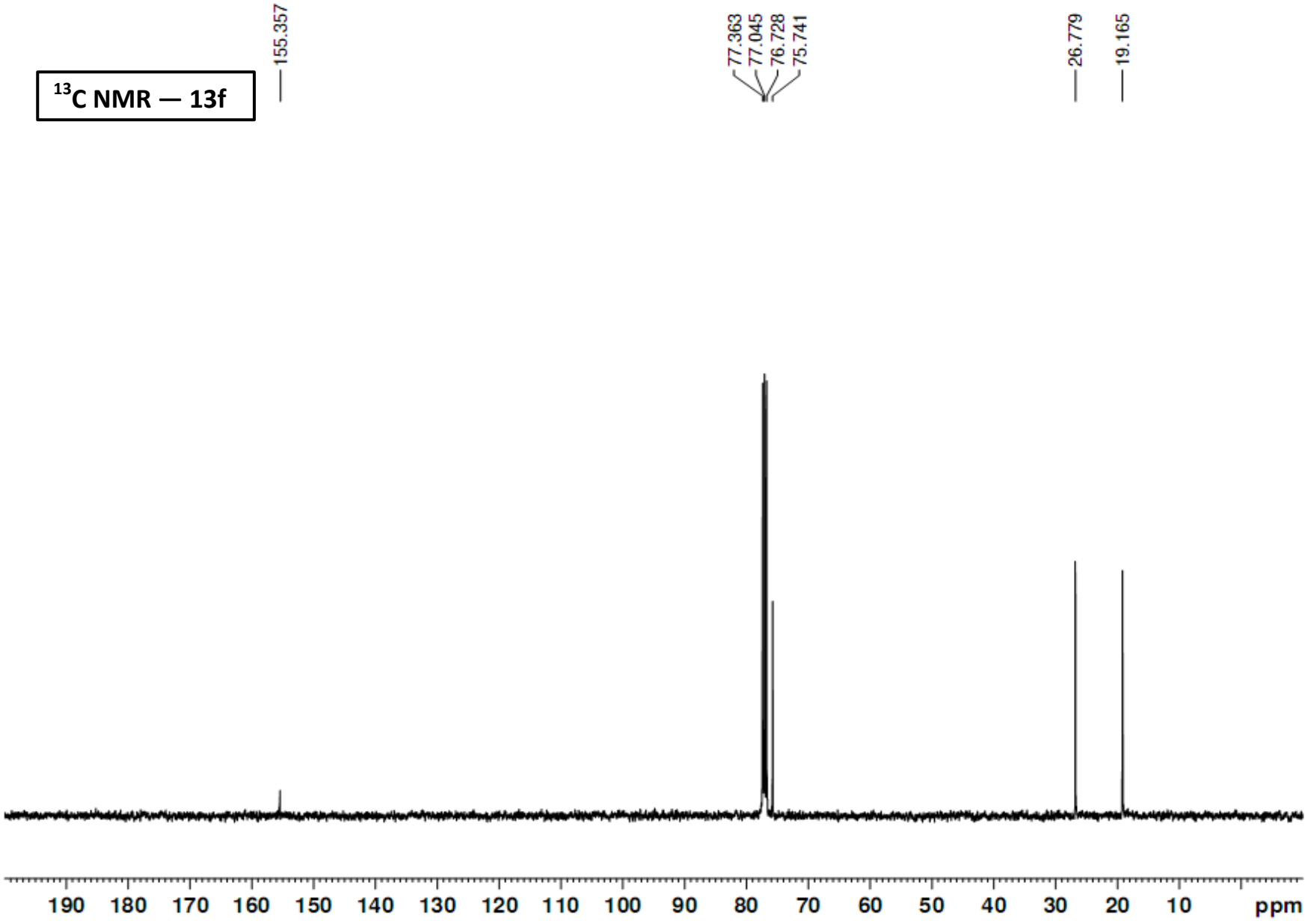
^{1}H NMR — 13f



^{13}C NMR — 13f



HRMS — 13f

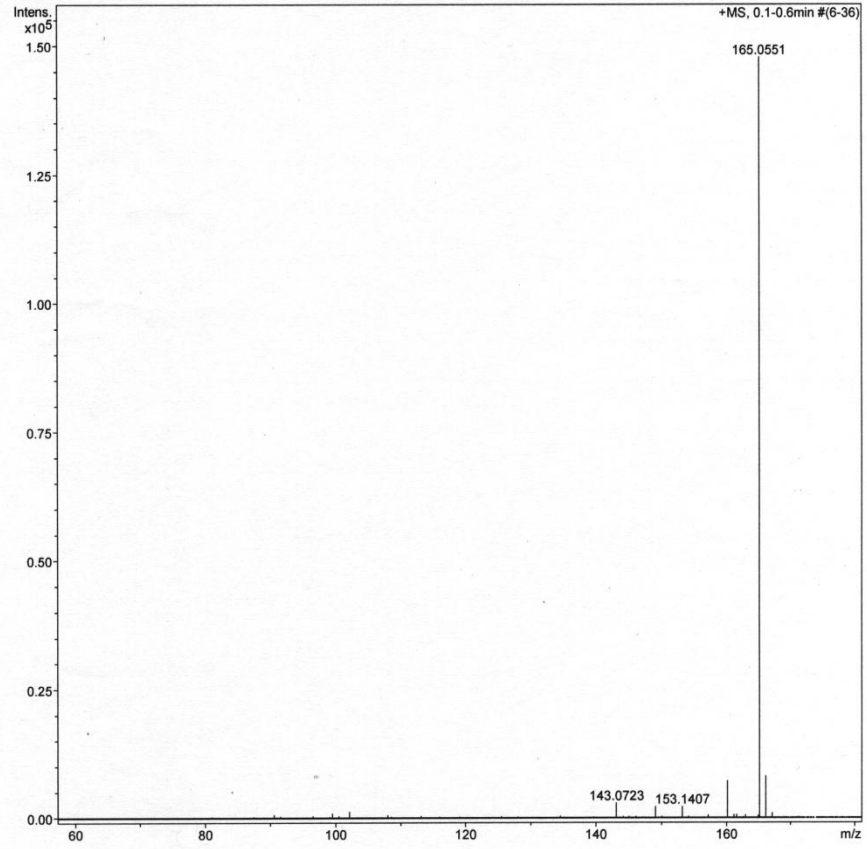
Display Report

Analysis Info

Analysis Name	D:\Data\2012\Dr.K.Muralidharan\FEB\KPK-V1.d	Acquisition Date	2/7/2012 3:38:57 PM
Method	tune_low_Pos.m	Operator	UOH
Sample Name	KPK-V1-DCM-ACN	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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