

Supporting Information for

Copper–Catalyzed Huisgen 1,3-Dipolar Cycloaddition

Under Oxidative Conditions: Polymer–Assisted Assembly of

4-Acyl-1-Substituted-1,2,3-Triazoles

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1. Materials and methods

Commercially available starting materials and reagents were purchased and used without further purification from freshly opened containers. Polymer supported reagents (PS-TBD, 2.6 mmol/g, PS-IBX-amide, 0.5-1.0 mmol/g, PS-DIPEA, 3 mmol/g, Tentagel-TBTA, 0.17 mmol/g) were purchased from commercial sources. Acetylenic carbinols were prepared according to the literature²² or purchased from commercial sources. Organic extracts were dried with anhydrous Na₂SO₄. The reactions were monitored by TLC and purified compounds each showed a single spot. Unless stated otherwise, UV light and/or iodine vapour were used for the detection of compounds. The synthesis and purification of all compounds were accomplished using the equipment routinely available in organic chemistry laboratories. Most of the preparative experiments were performed in coated vials on an organic synthesiser with orbital stirring. Purification of isolated products was carried out by column chromatography. Compounds were routinely characterised by spectroscopic and analytical methods. Melting points were determined on a melting point apparatus and are uncorrected. The chemical structures of the obtained compounds were characterized by nuclear magnetic resonance spectroscopy (¹H and ¹³C) and high-resolution mass spectra (HRMS). Unless otherwise quoted, NMR spectra were recorded in CDCl₃. Chemical shifts are given as δ values against tetramethylsilane as internal standard and *J* values are given in Hz.

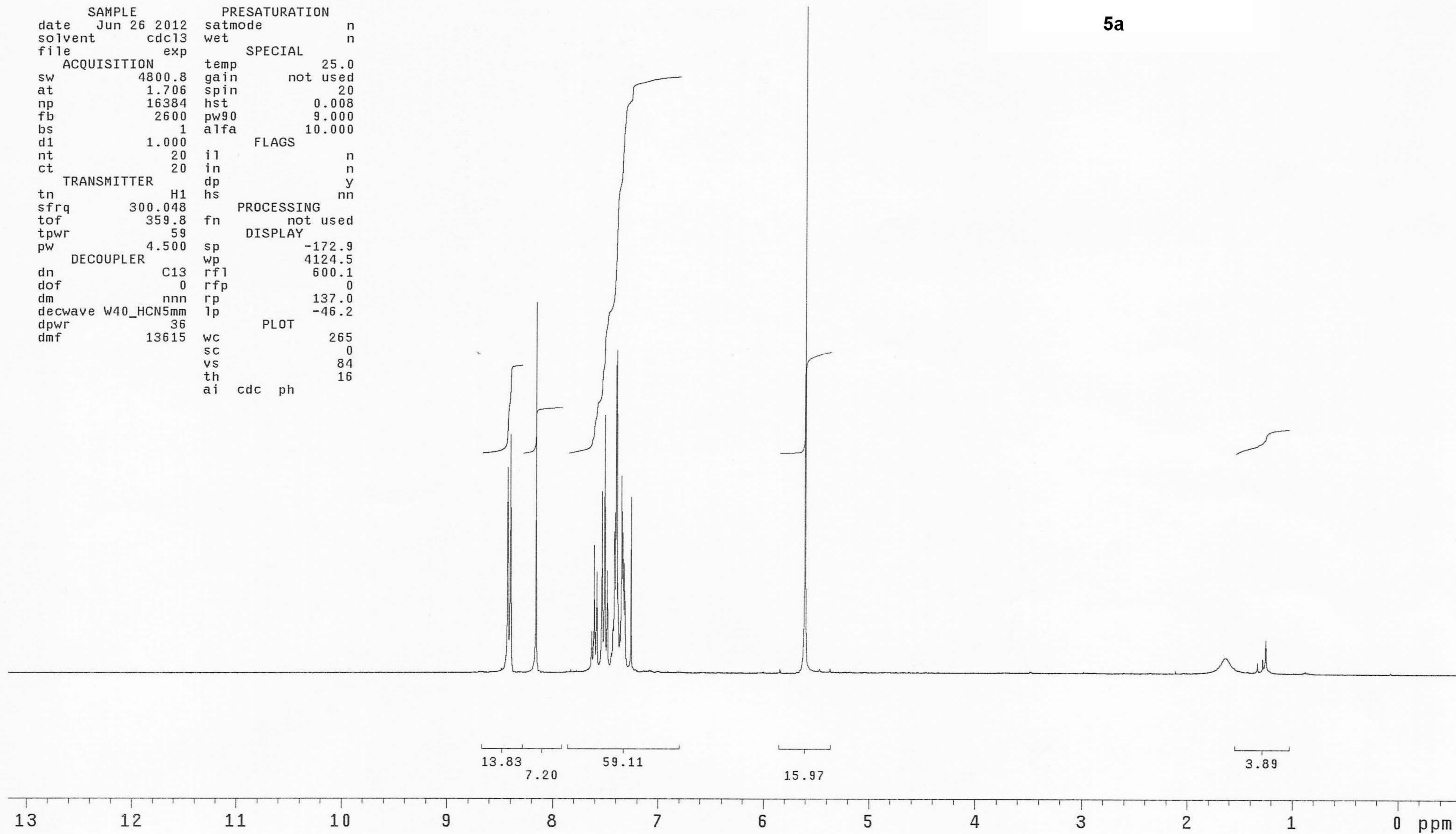
sy1isat139

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bs	1	alfa	10.000
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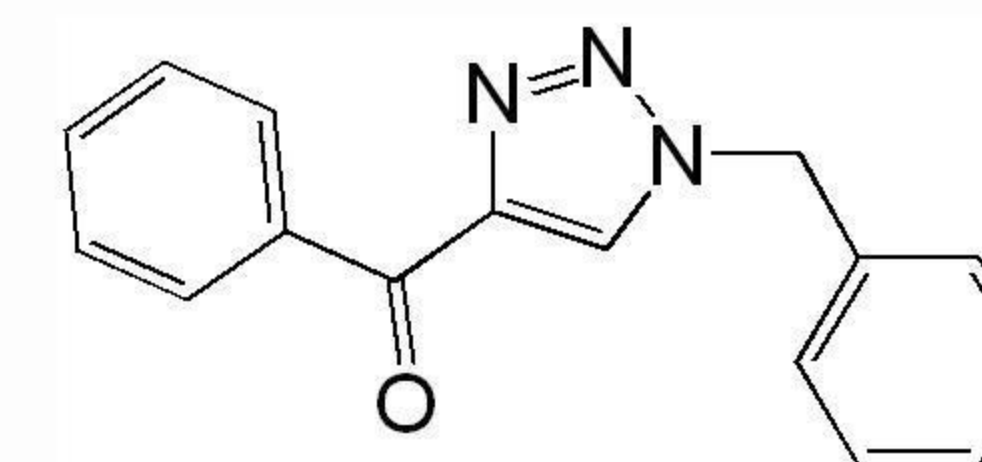
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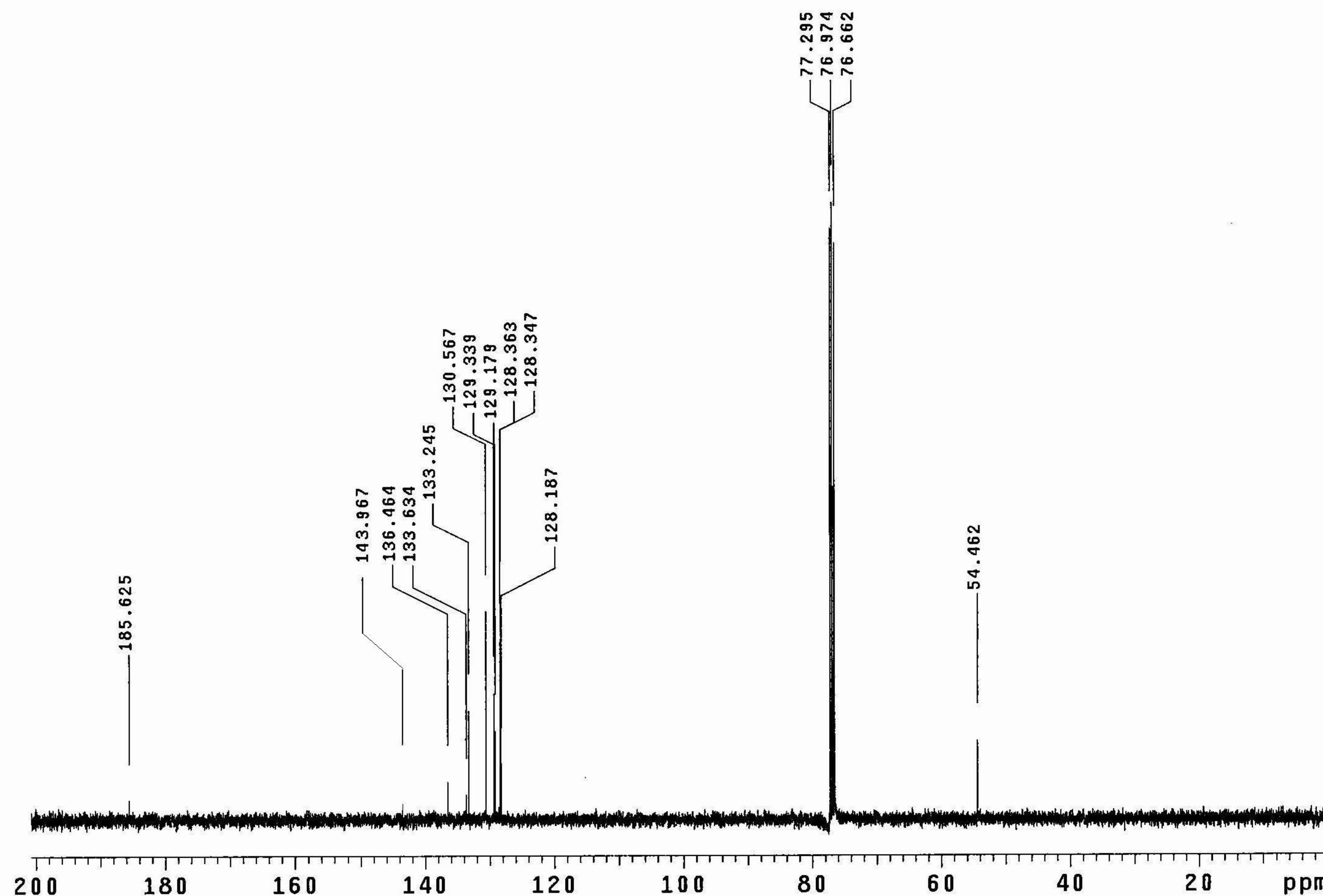
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bs	4	alfa	10.000
d1	1.000	FLAGS	
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tn	C13	hs	nn
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5a

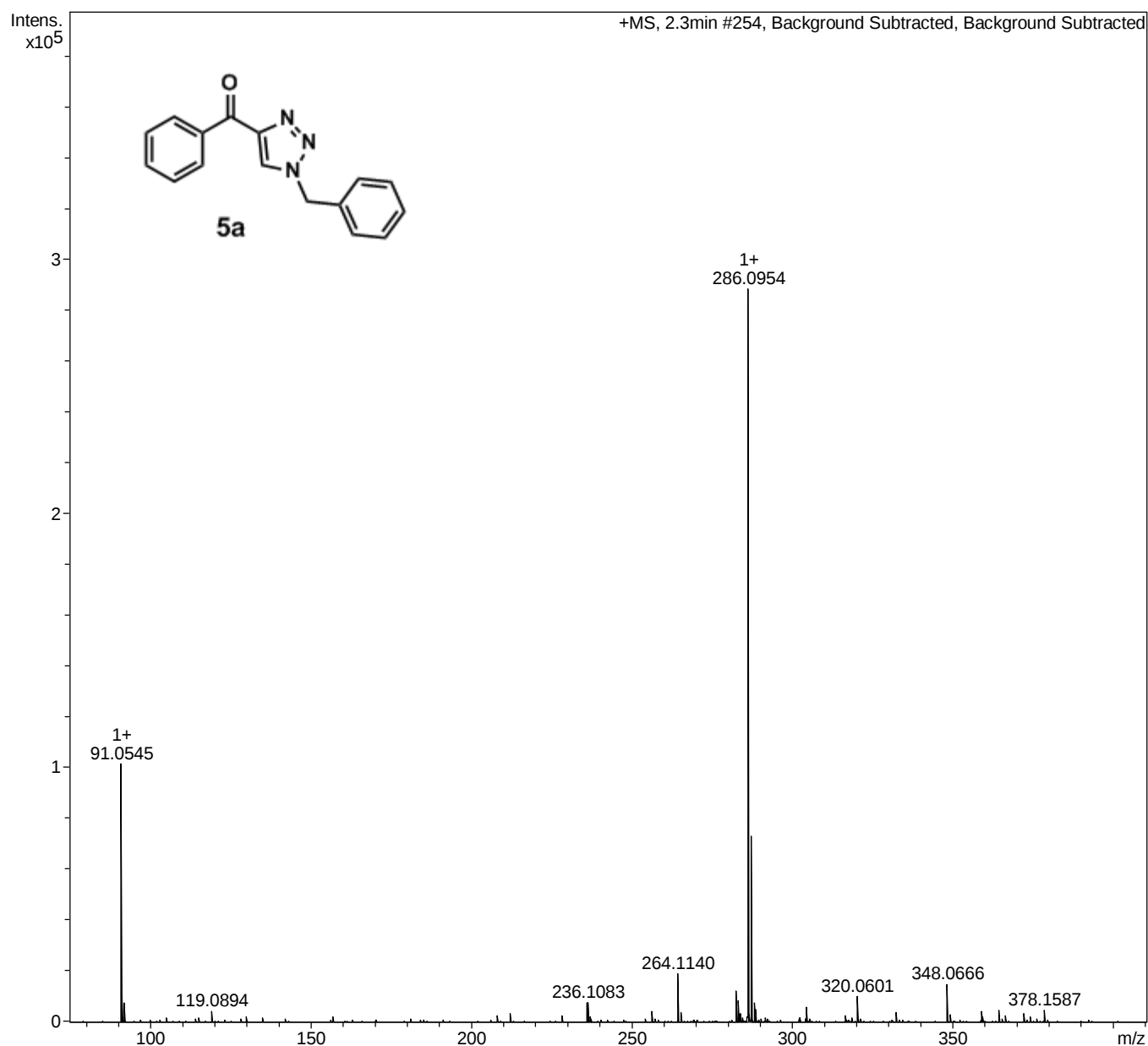


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

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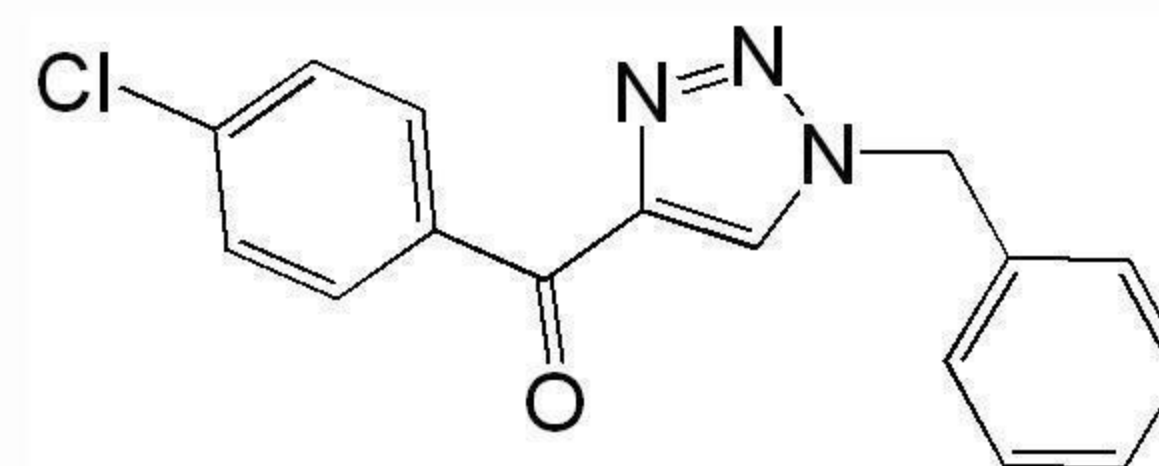
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 Instrument micrOTOF



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5b

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PROCNO 1

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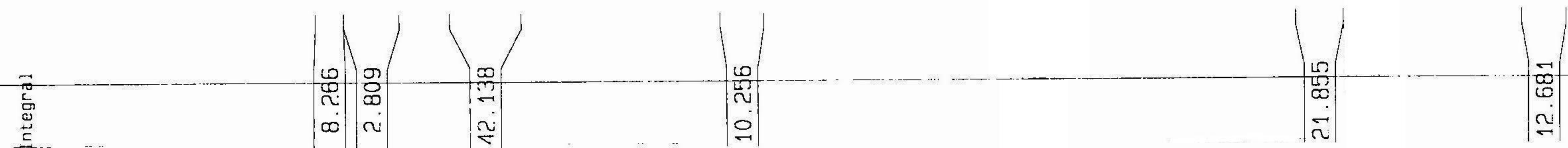
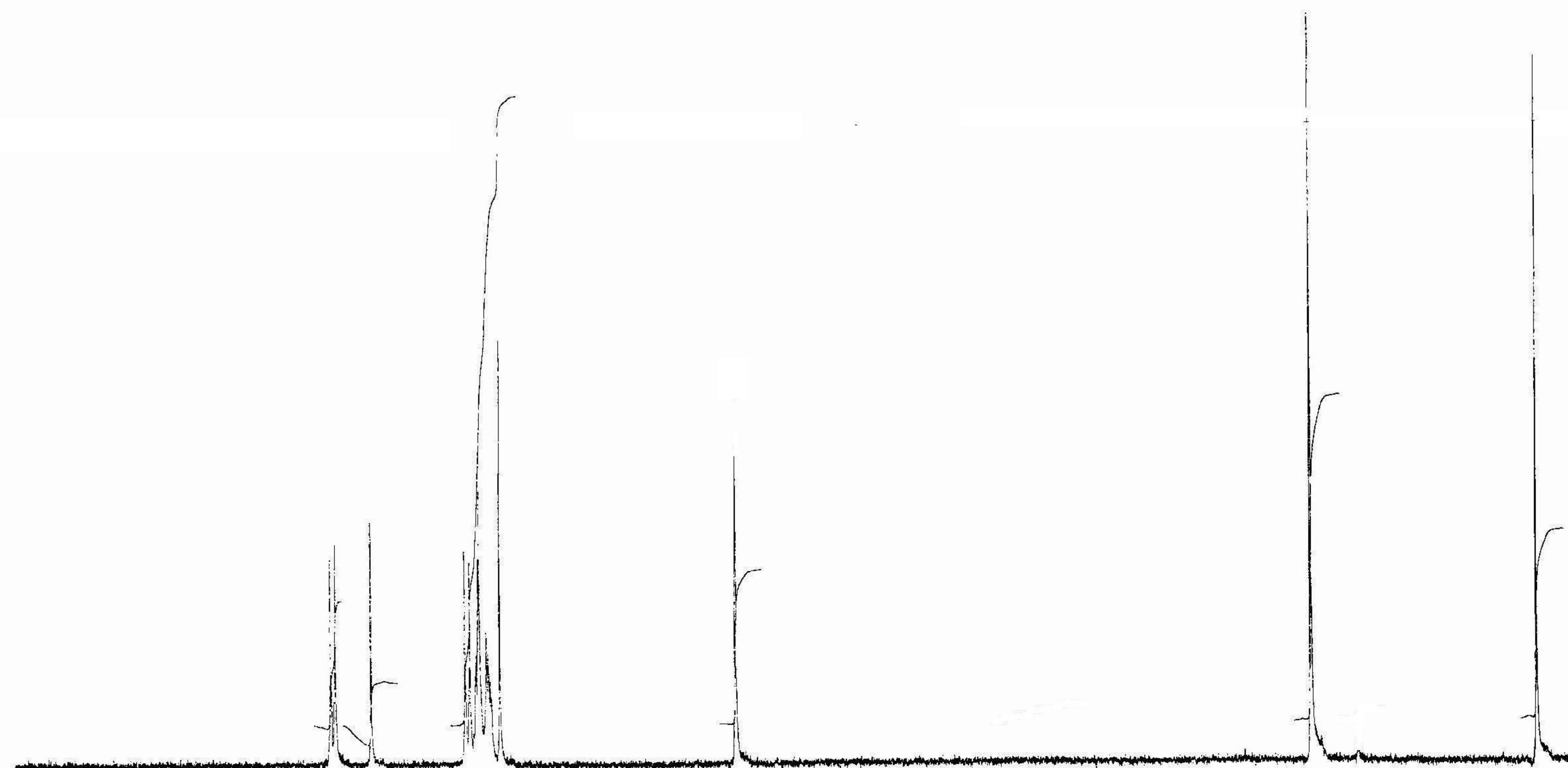
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1D NMR plot parameters

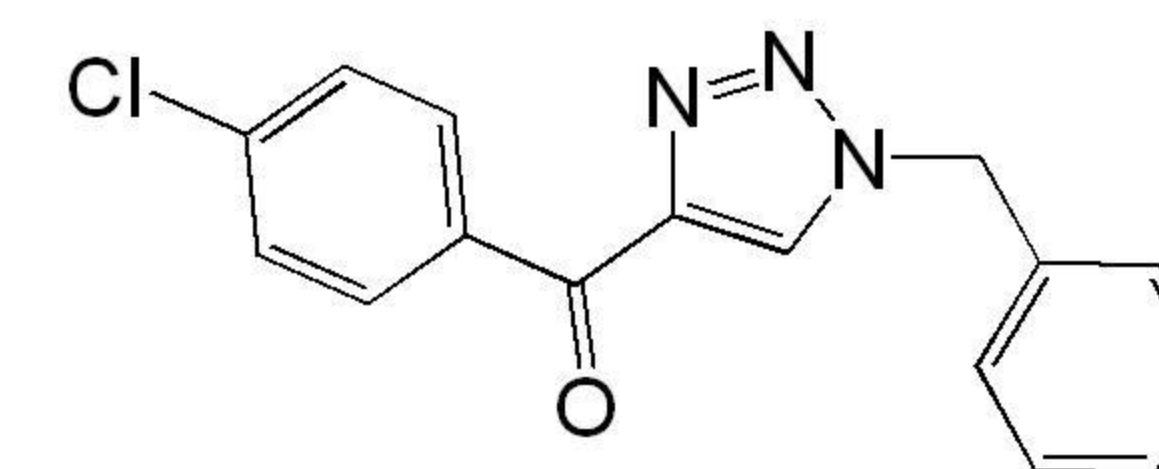
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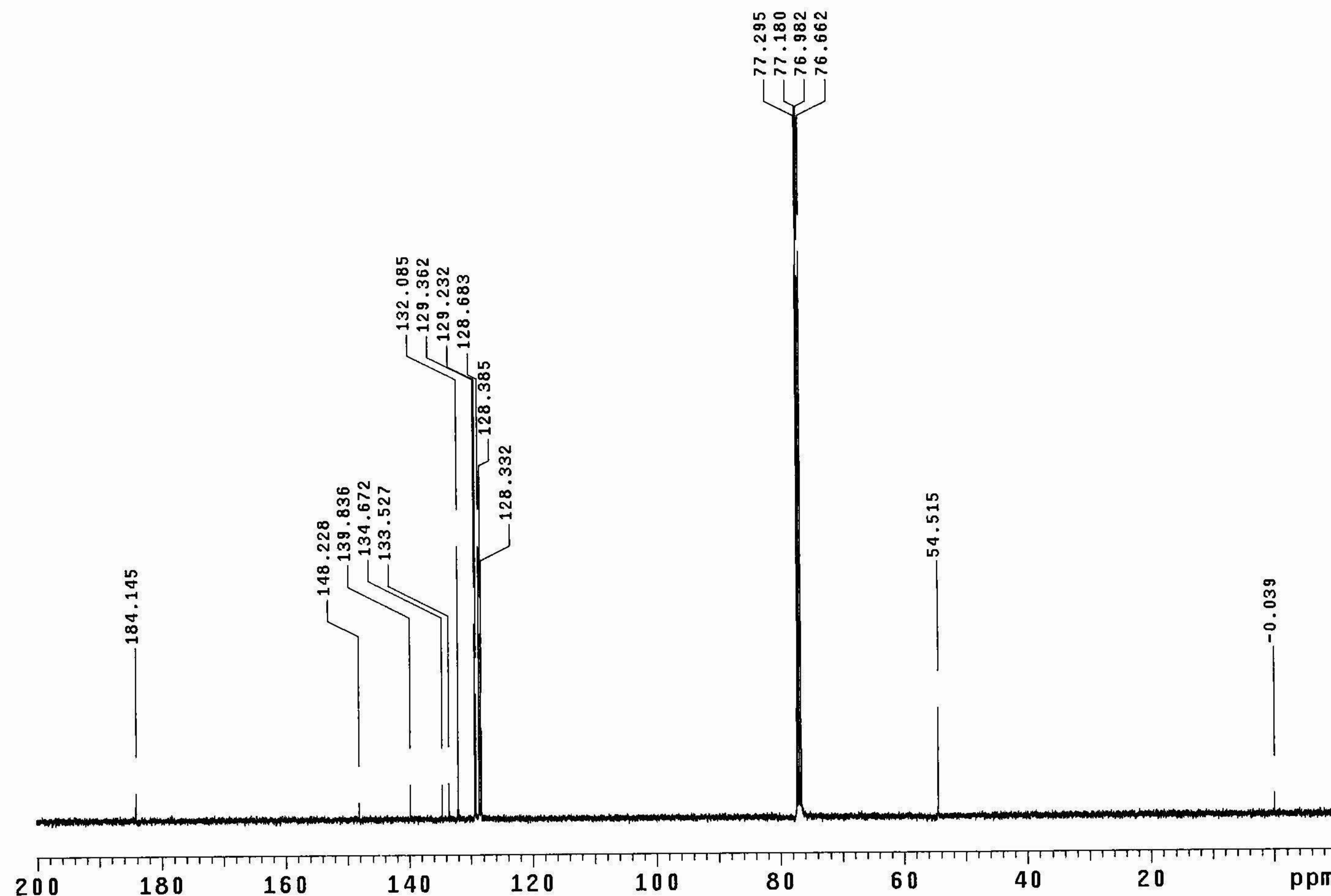
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		ai	ph



5b

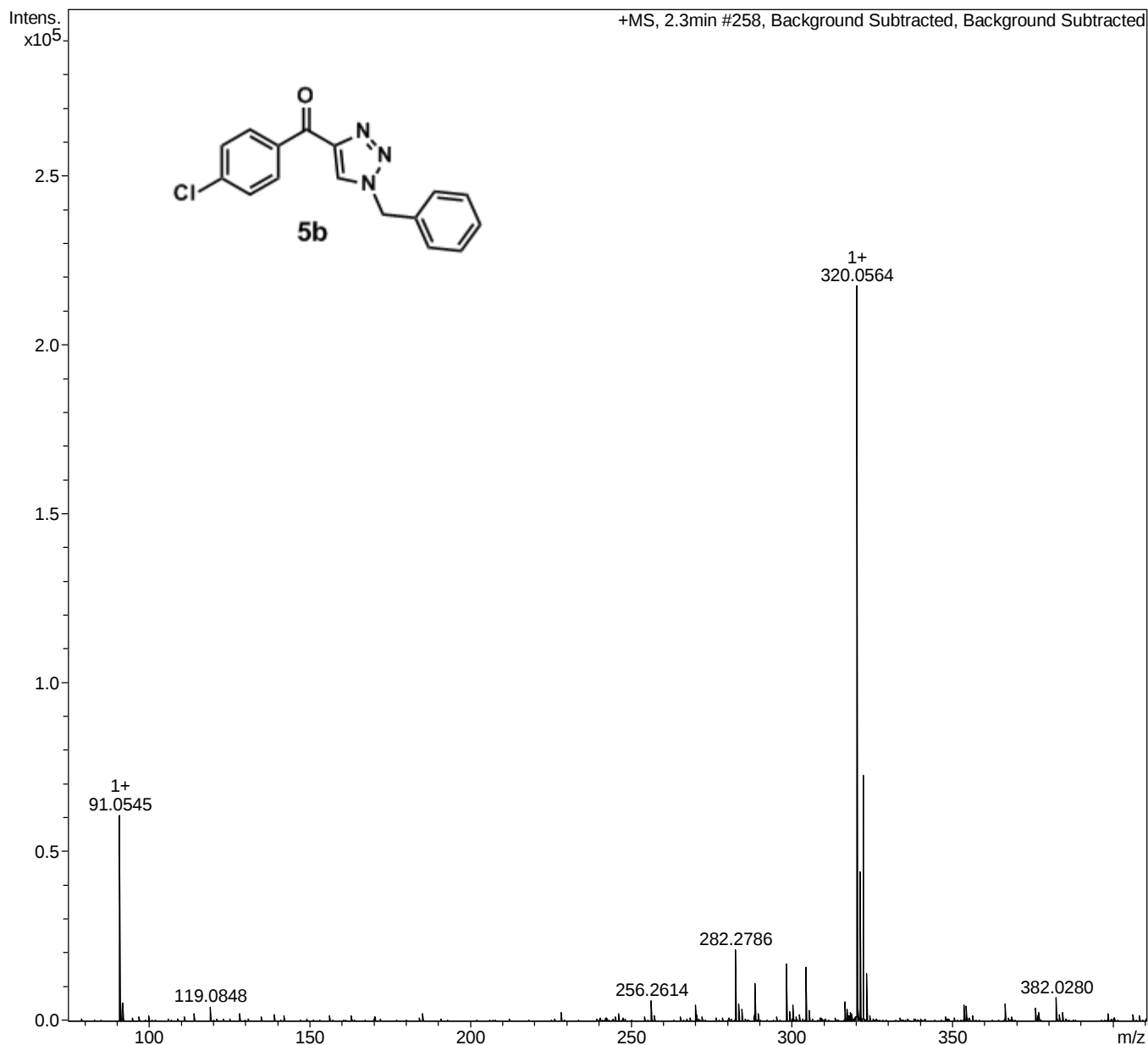


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

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Instrument micrOTOF



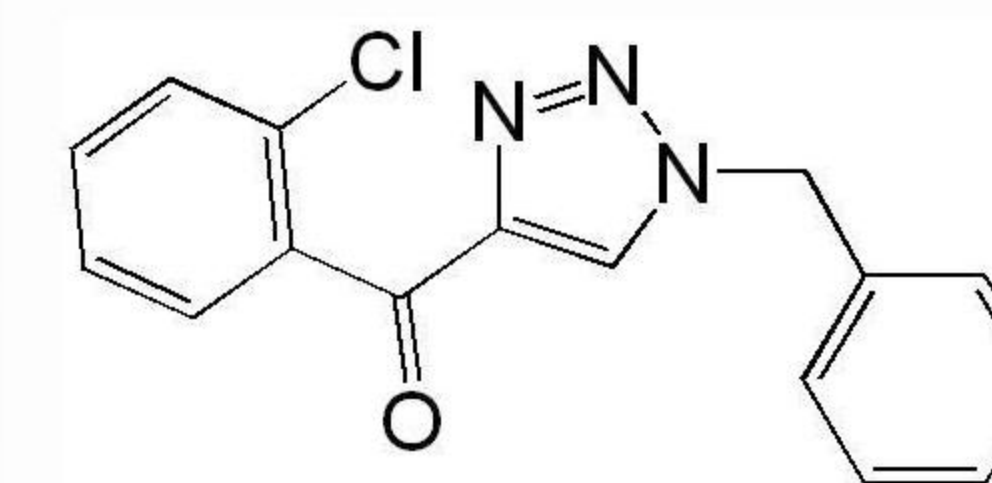
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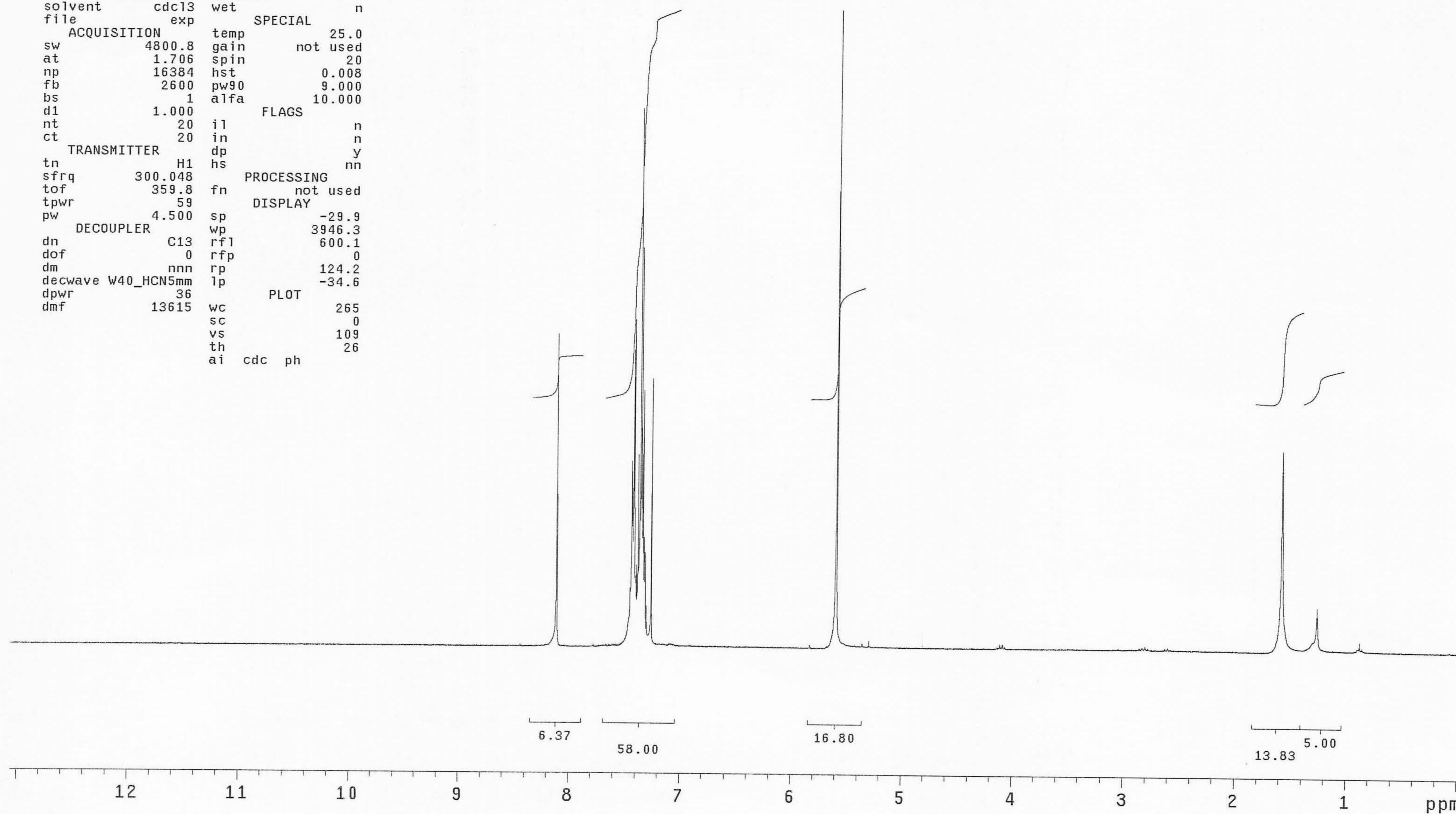
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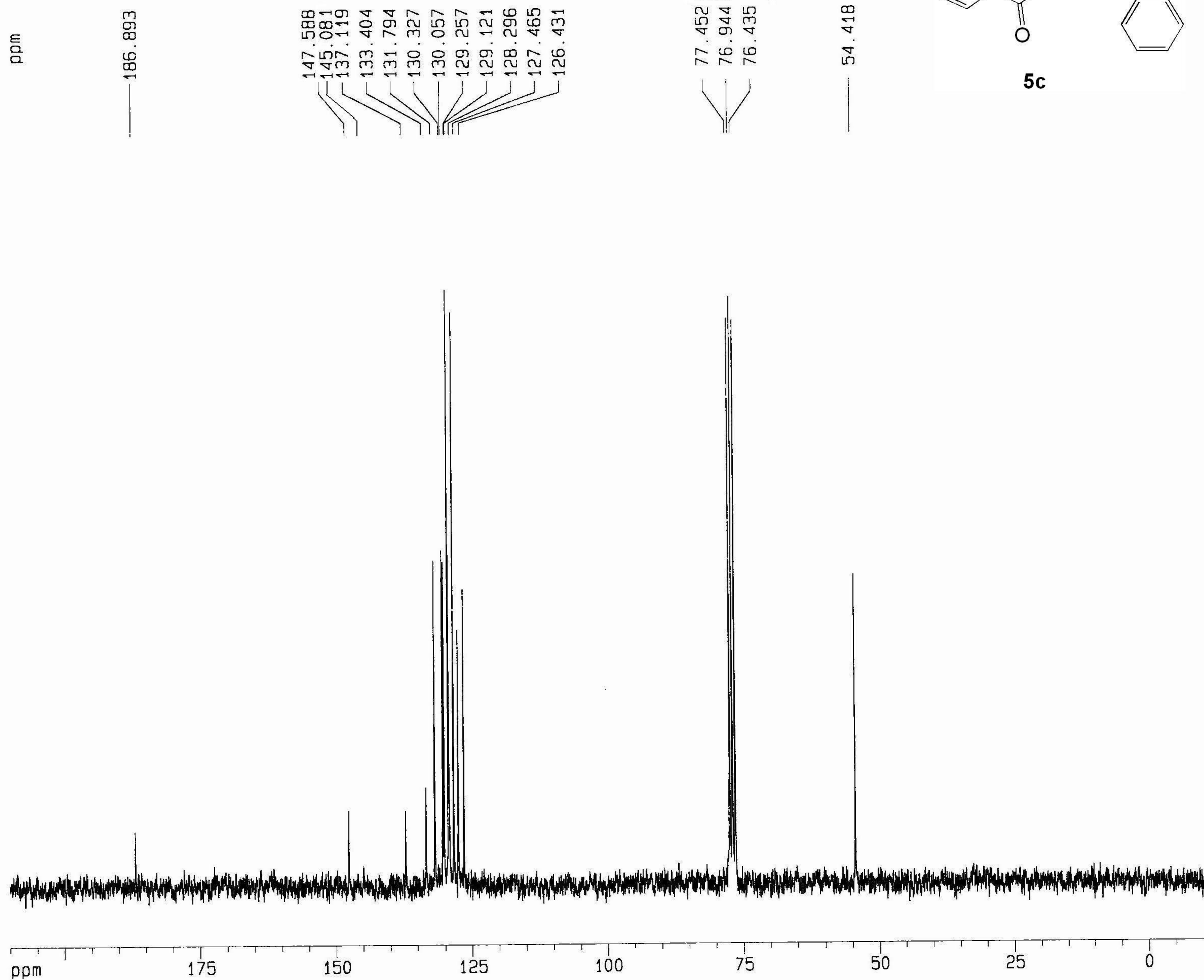
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bs	1	alfa	10.000
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		ai	cdc ph



5c





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 PROCNO 1

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 SOLVENT CDCl3
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 FIDRES 0.287360 Hz
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 RG 8192
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 DE 10.50 usec
 TE 300.0 K
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 D11 0.03000000 sec
 D12 0.00002000 sec

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 PL1 -2.00 dB
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 PL13 15.00 dB
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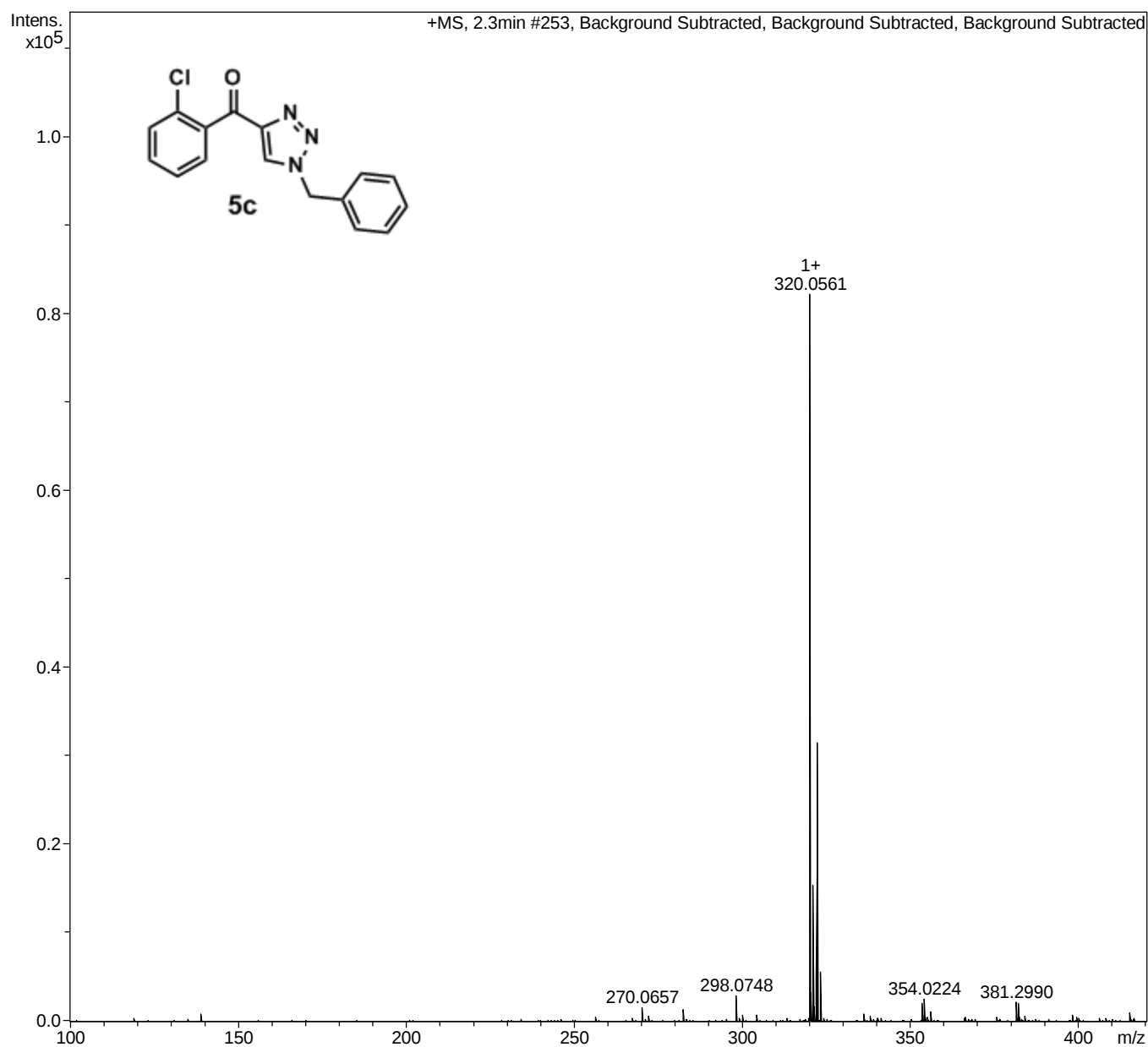
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 F2P -10.000 ppm
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 HZCM 691.84772 Hz/cm

ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

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Method fia_pos_bajo_50-350_egf.m

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Instrument micrOTOF



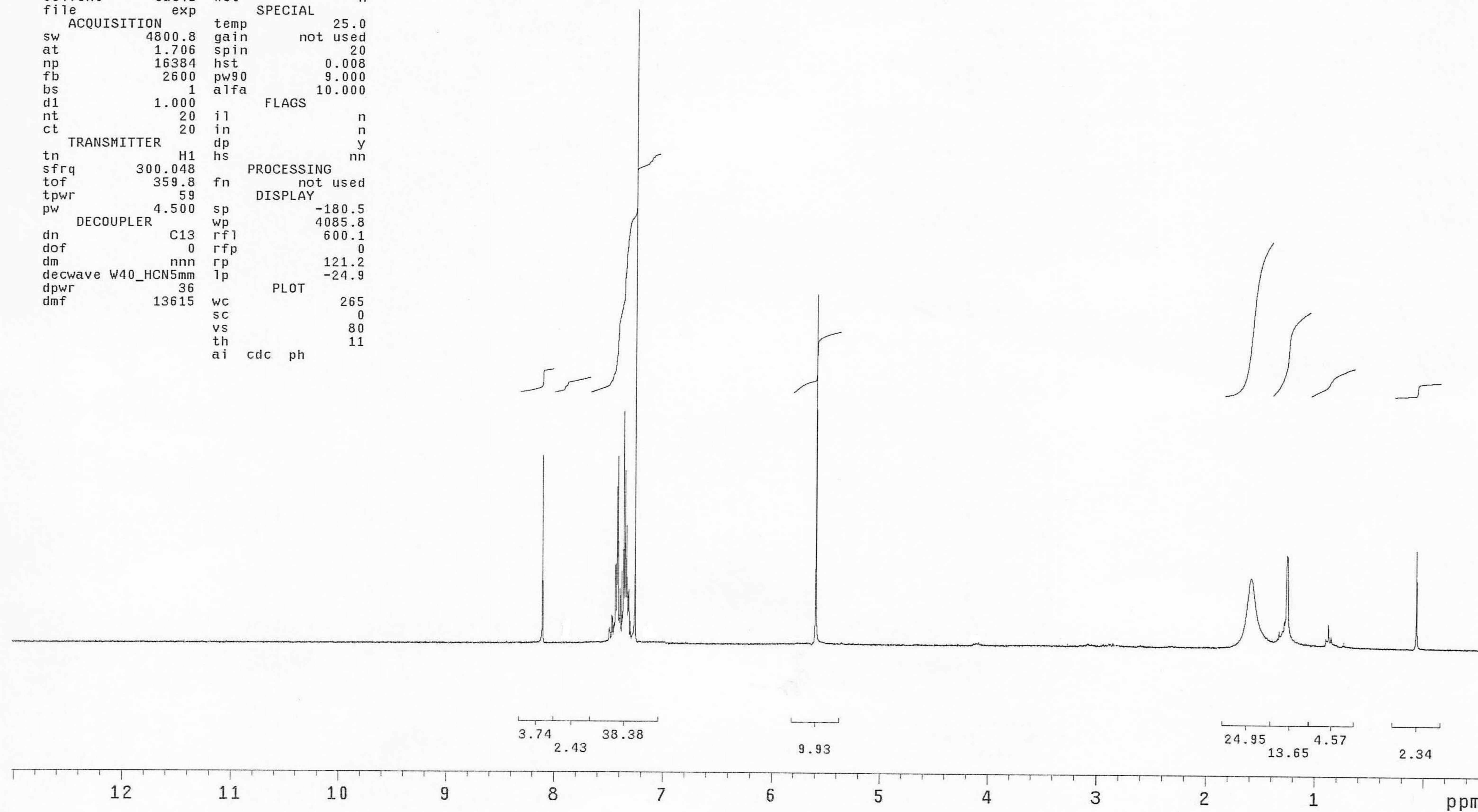
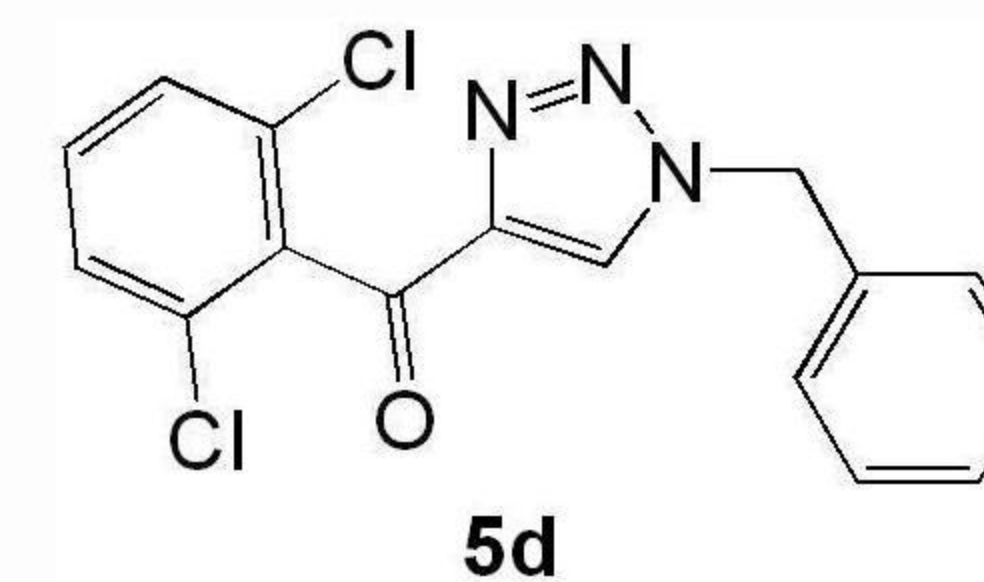
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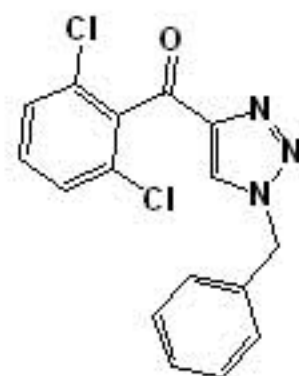
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sy1pa45

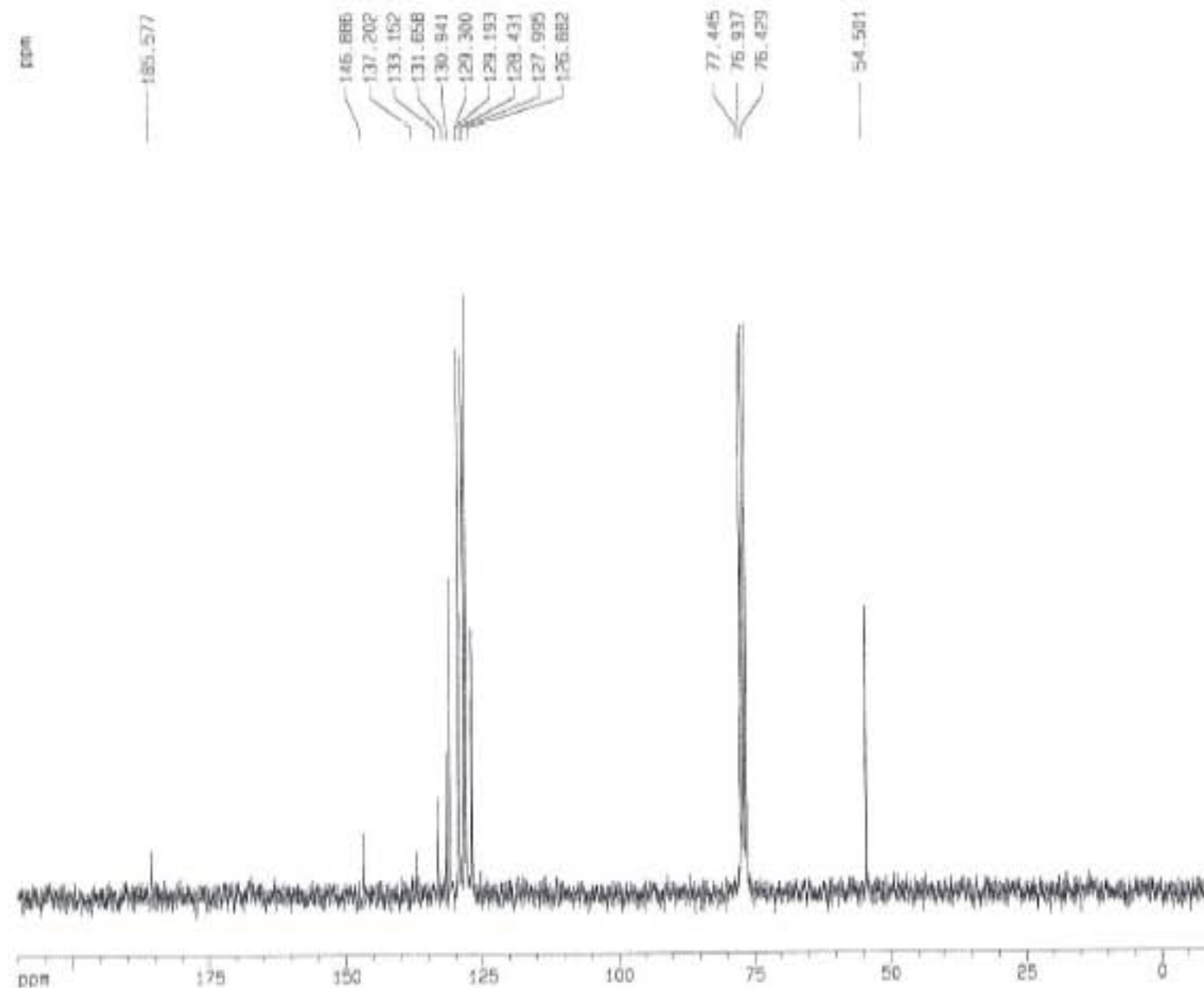
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fb	2600	pw90	9.000
bs	1	alfa	10.000
d1	1.000	FLAGS	
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ct	20	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	300.048	PROCESSING	
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		vs	80
		th	11
		ai	cdc ph





5d



Current Data Parameters
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EXPNO 2
PROCNO 1

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SOLVENT CDCl3
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FIDRES 0.207360 Hz
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RG 8182
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DE 10.50 usec
TE 300.0 K
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D11 0.0300000 sec
D12 0.0002000 sec

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PL1 -2.00 dB
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PCPD2 100.00 usec
PL2 120.00 dB
PL12 15.00 dB
PL13 15.00 dB
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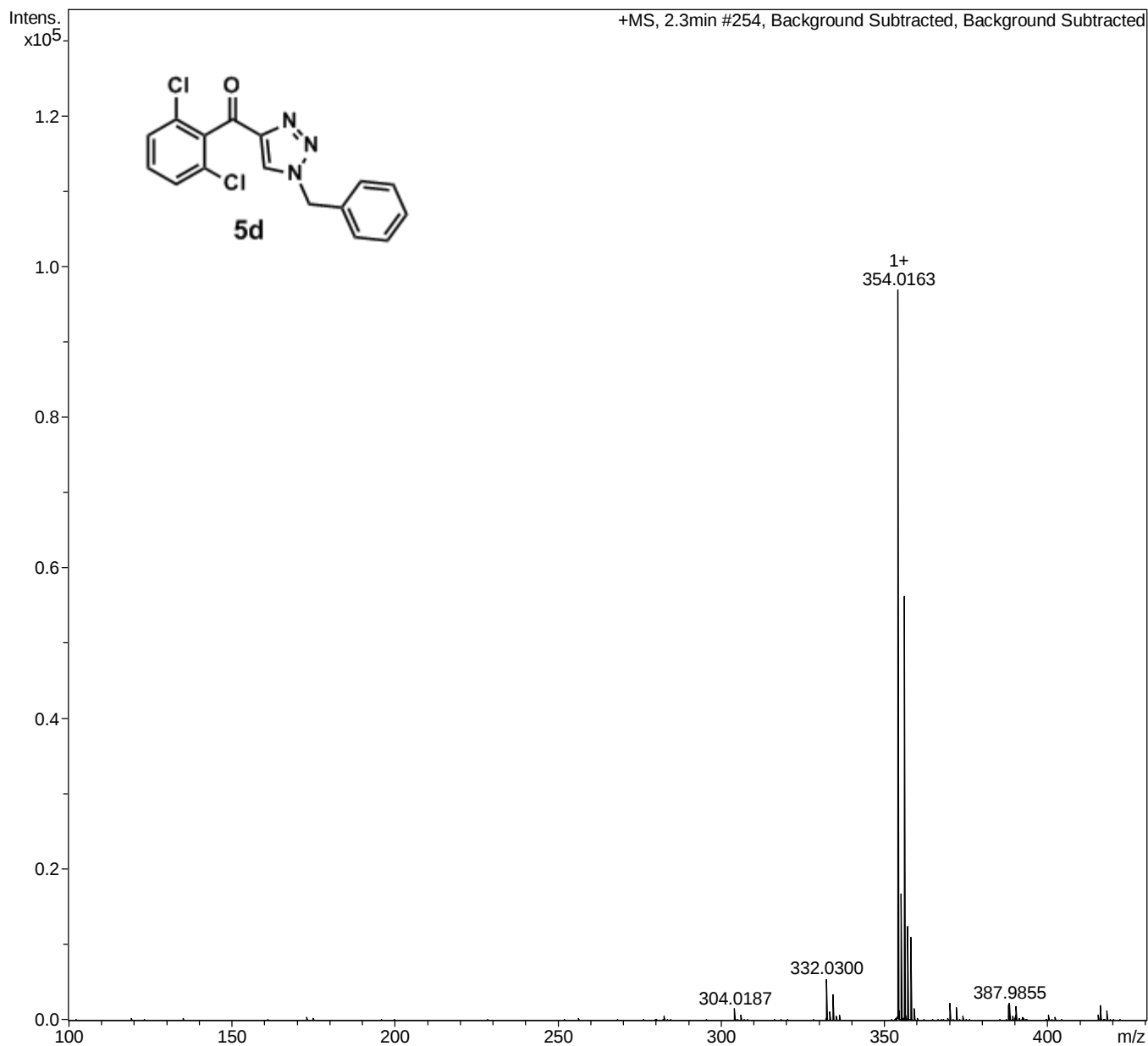
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F2P -10.000 ppm
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H2CM 881.84772 Hz/us

ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

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Instrument microTOF



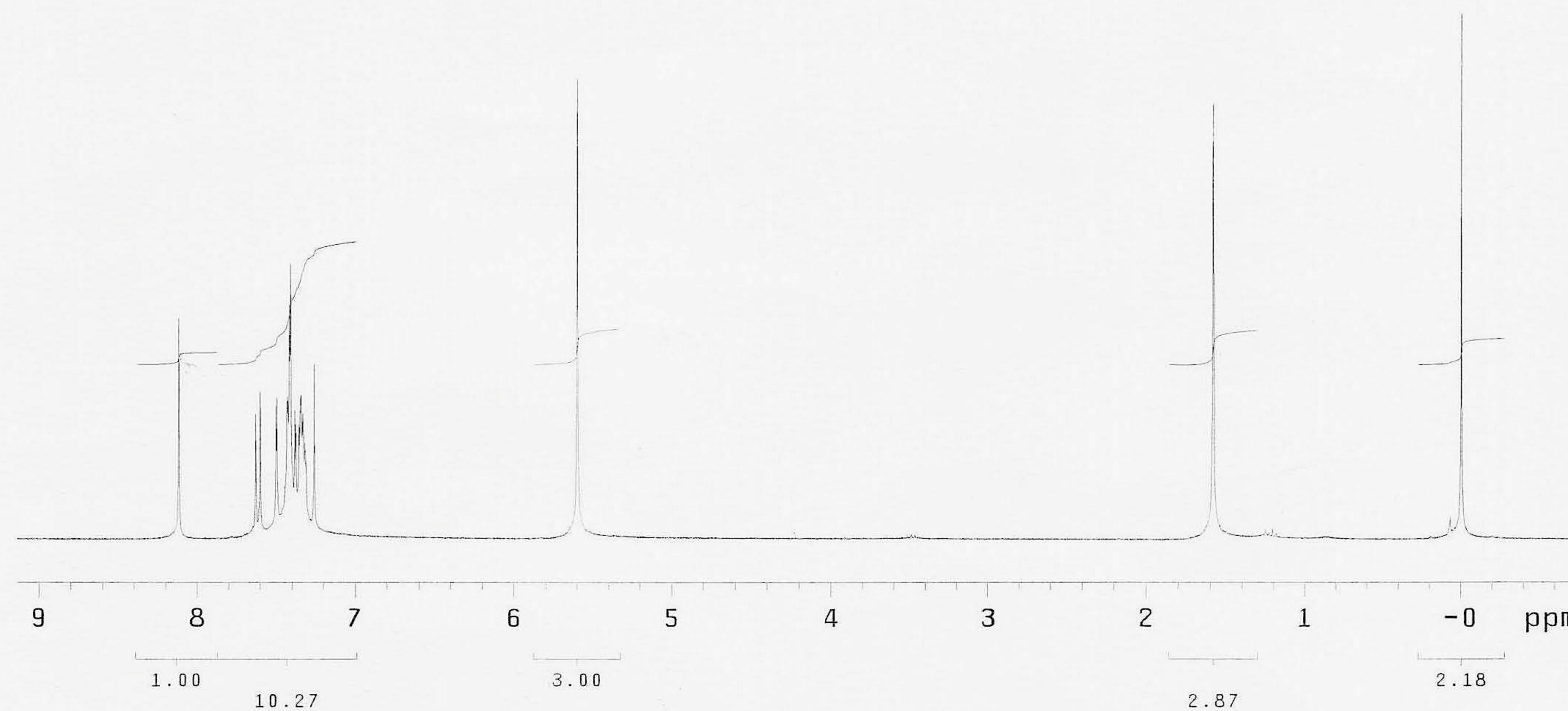
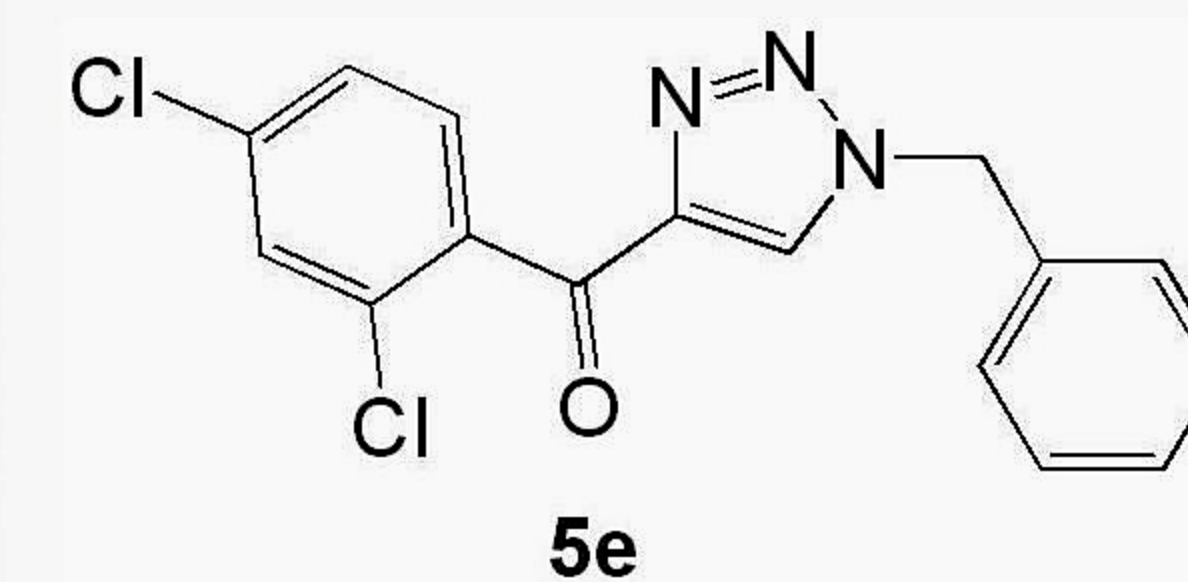
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syipa76

exp100 Proton

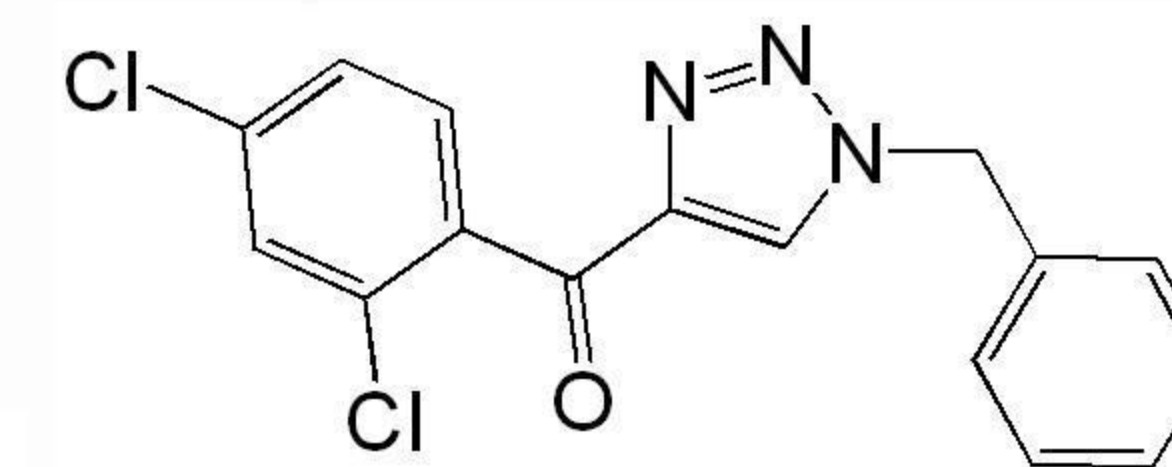
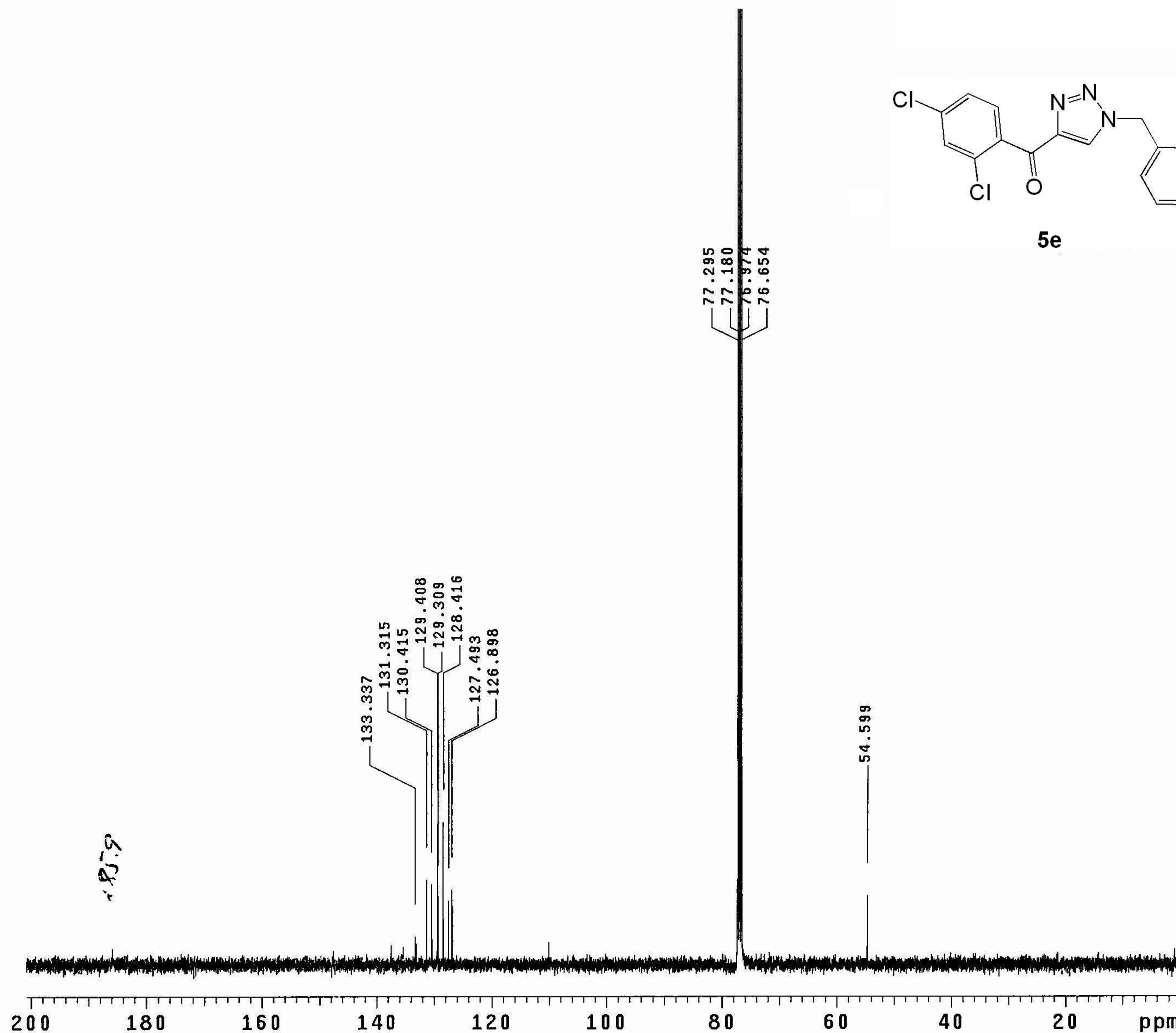
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tn	H1	dmm	c
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sw	6120.0	PROCESSING	
fb	3400	wtfile	
bs	1	proc	ft
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dl	1.000	werr	
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gain	not used		
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in	n		
dp	y		
DISPLAY			
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vs	50		
sc	0		
wc	180		
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th	4		
ins	1.000		
ai	ph		



sy1pt106

exp6 CARBON

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solvent	cdcl3	wet	n
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fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	2.000	FLAGS	
nt	600000	i1	n
ct	16924	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	1.00
tpwr	61	fn	not used
pw	7.300	DISPLAY	
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dn	H1	wp	20311.5
dof	0	rfl	1507.8
dm	yyy	rpf	0
decwave	w	rp	-61.7
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		th	4
		ai	ph



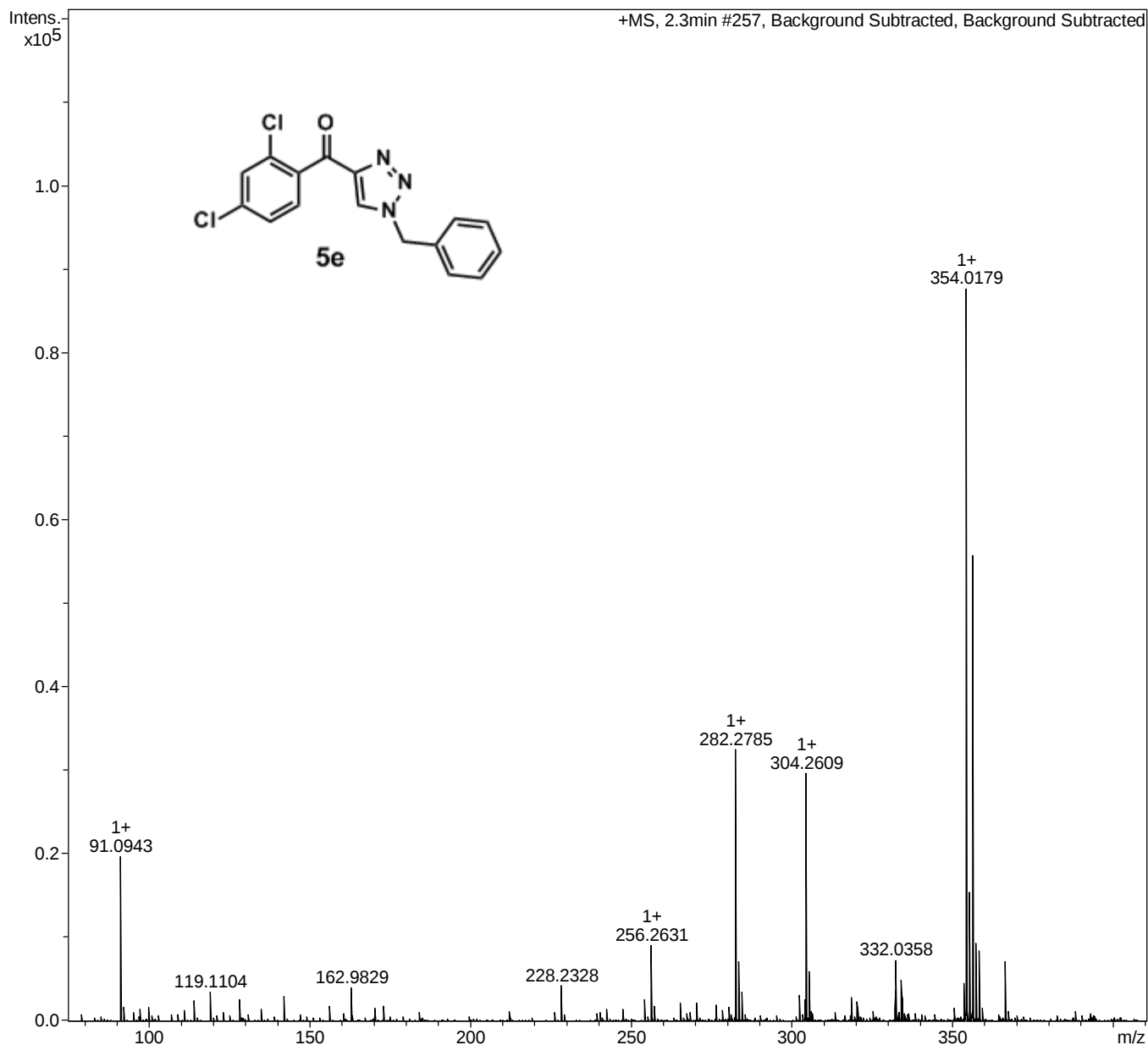
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ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

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 Instrument microTOF



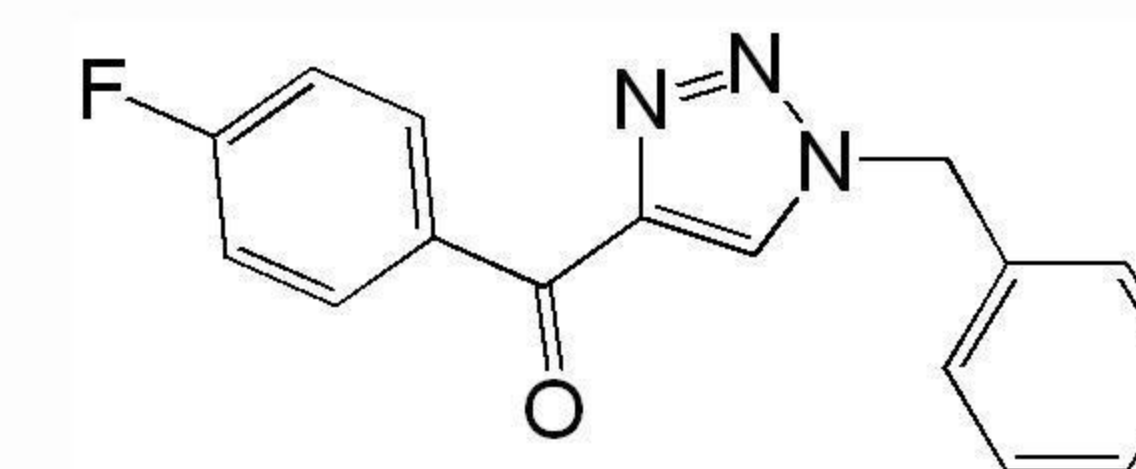
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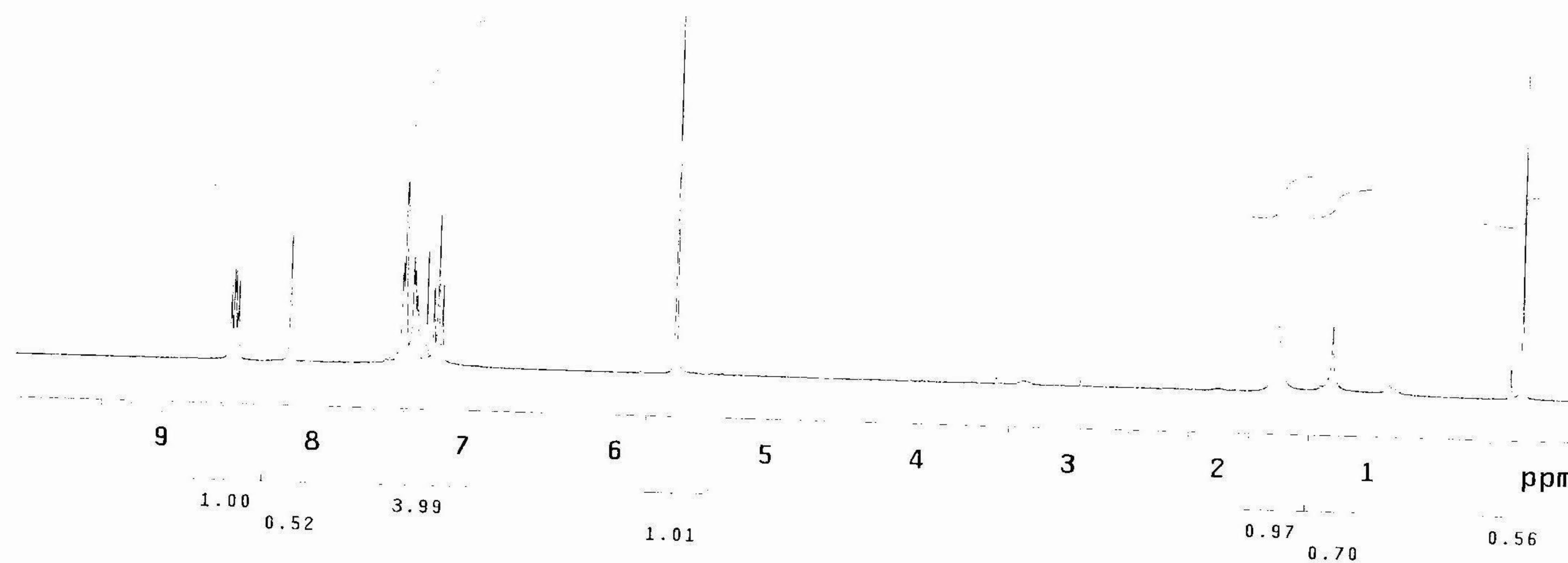
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at	1.706	dmm	c
np	16384	dmf	13900
sw	4800.8	temp	25.0
fb	2600	wtfile	
bs	1	proc	ft
tpwr	59	fn	32768
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d1	1.000	werr	
tof	238.9	wexp	
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ct	20	wnt	
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gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
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wp	3120.0		
vs	45		
sc	0		
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ai	ph		



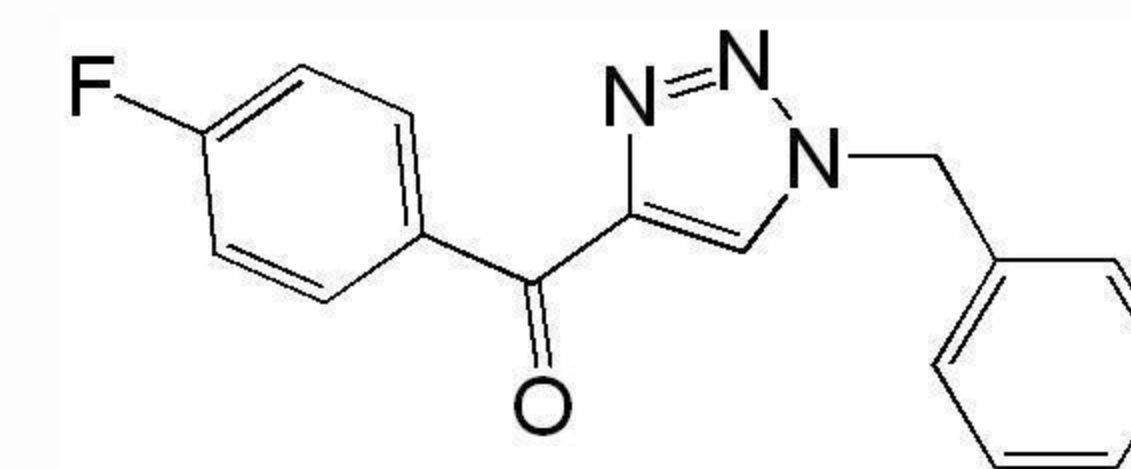
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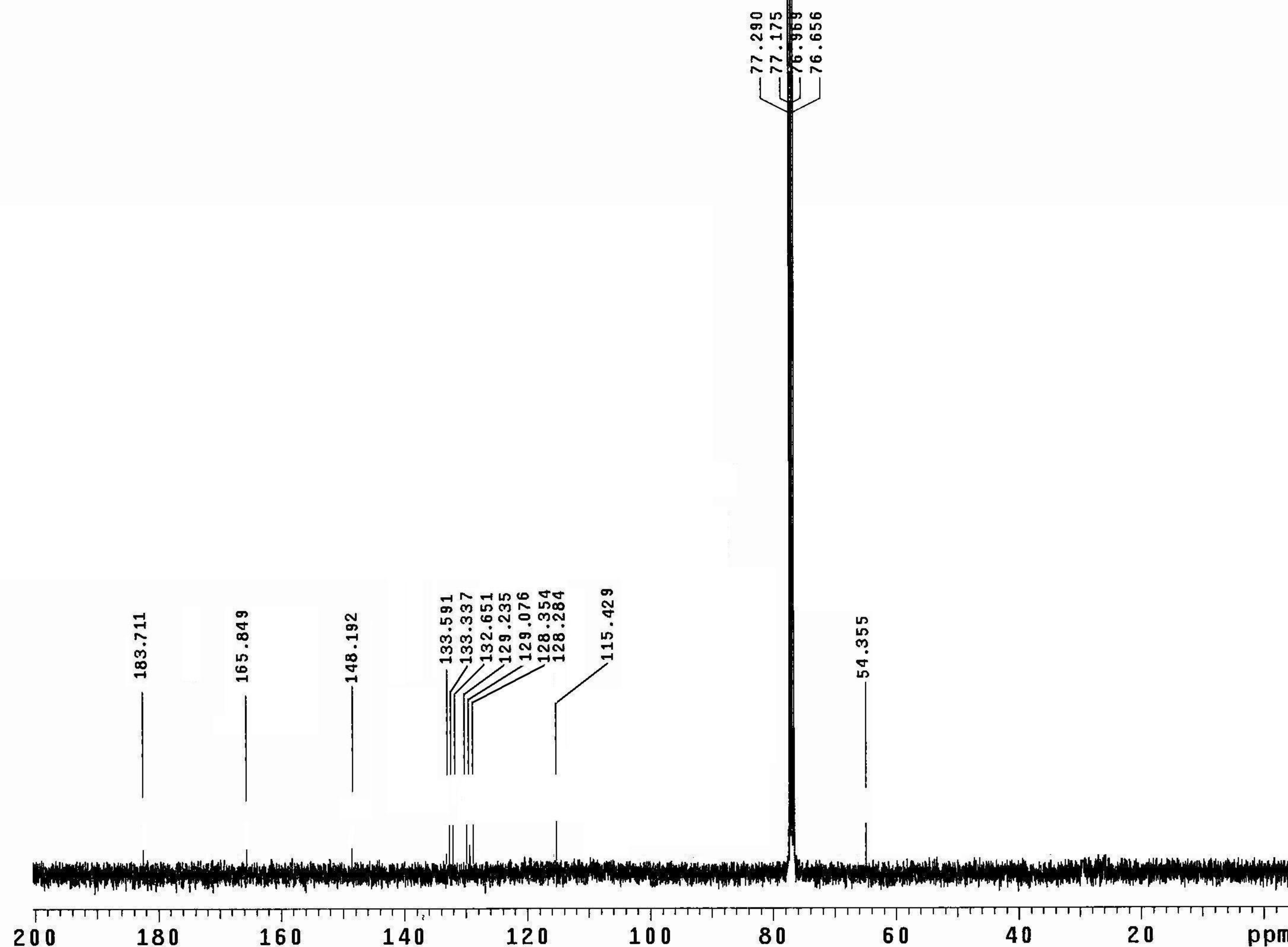
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sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
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ct	129500	in	nn
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tn	C13	hs	nn
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tof	525.0	lb	1.00
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-582.2
dn	H1	wp	20733.5
dof	0	rfl	2514.2
dm	yyy	rfl	0
decwave	w	rp	-32.5
dpwr	29	lp	-316.8
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	13217
		th	3
		ai	ph



5f

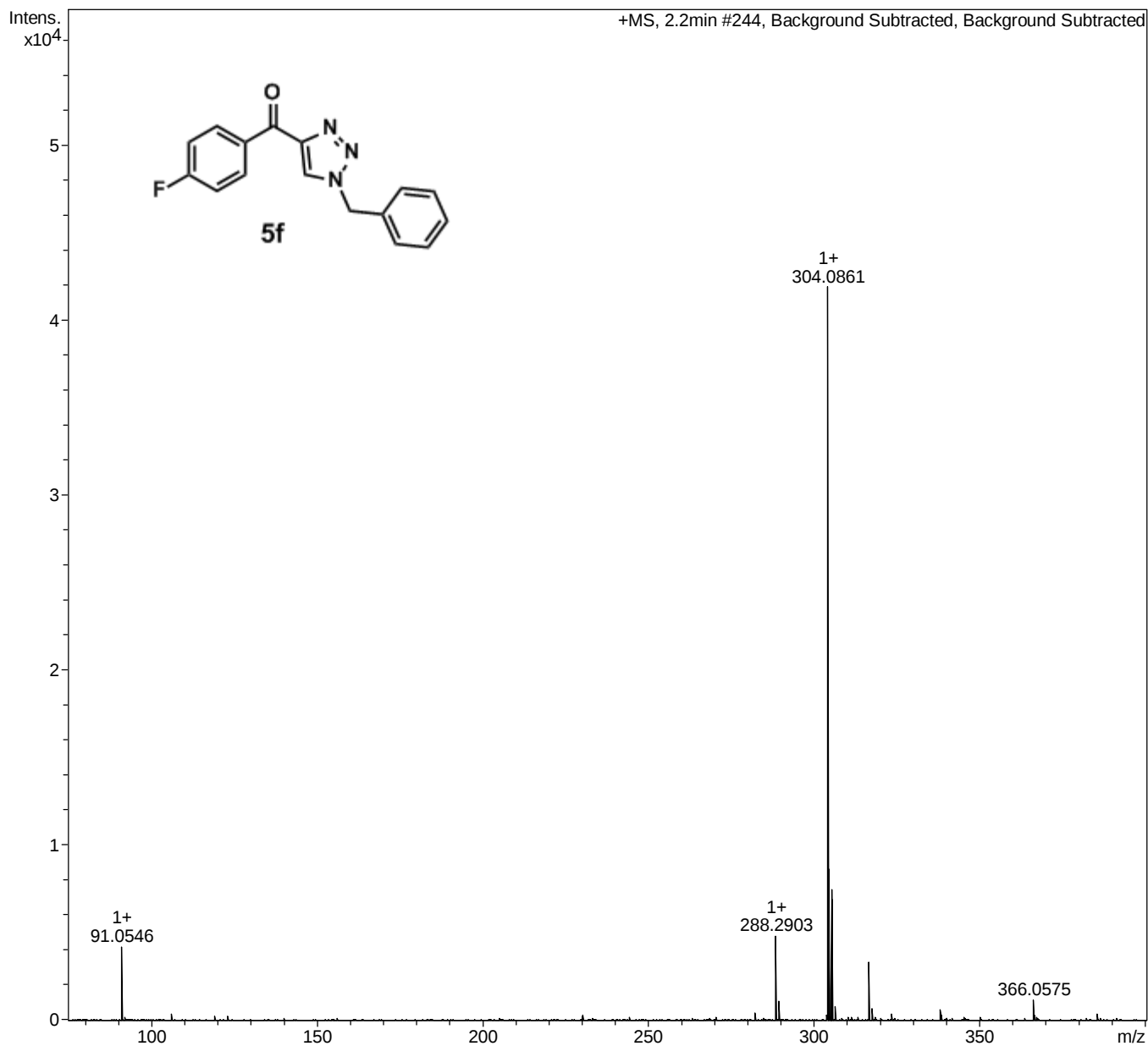


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA58_281_1-H,9_01_3872.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 3/8/2012 1:19:38 PM
Instrument micrOTOF



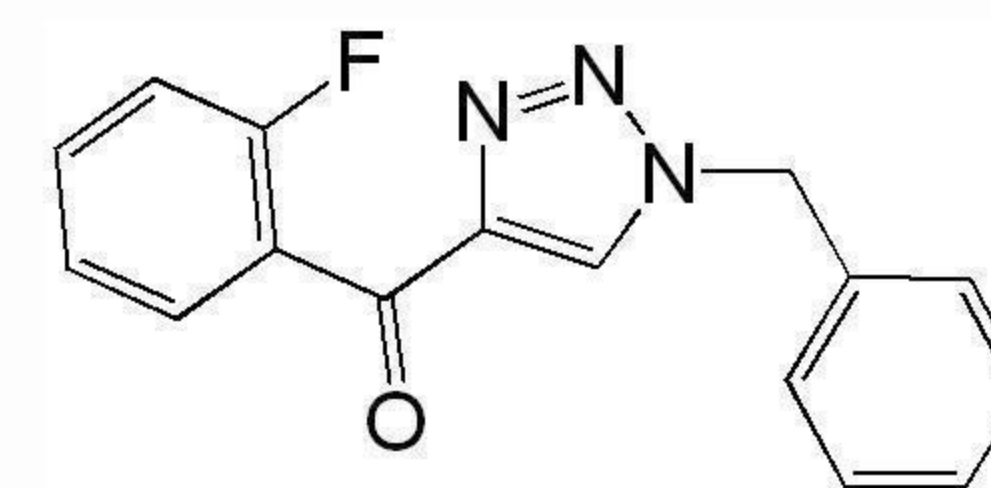
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
304.0861	1	C 16 H 12 F N 3 Na O	100.00	304.0857	-0.5	-1.5	3.8	11.5	even	ok

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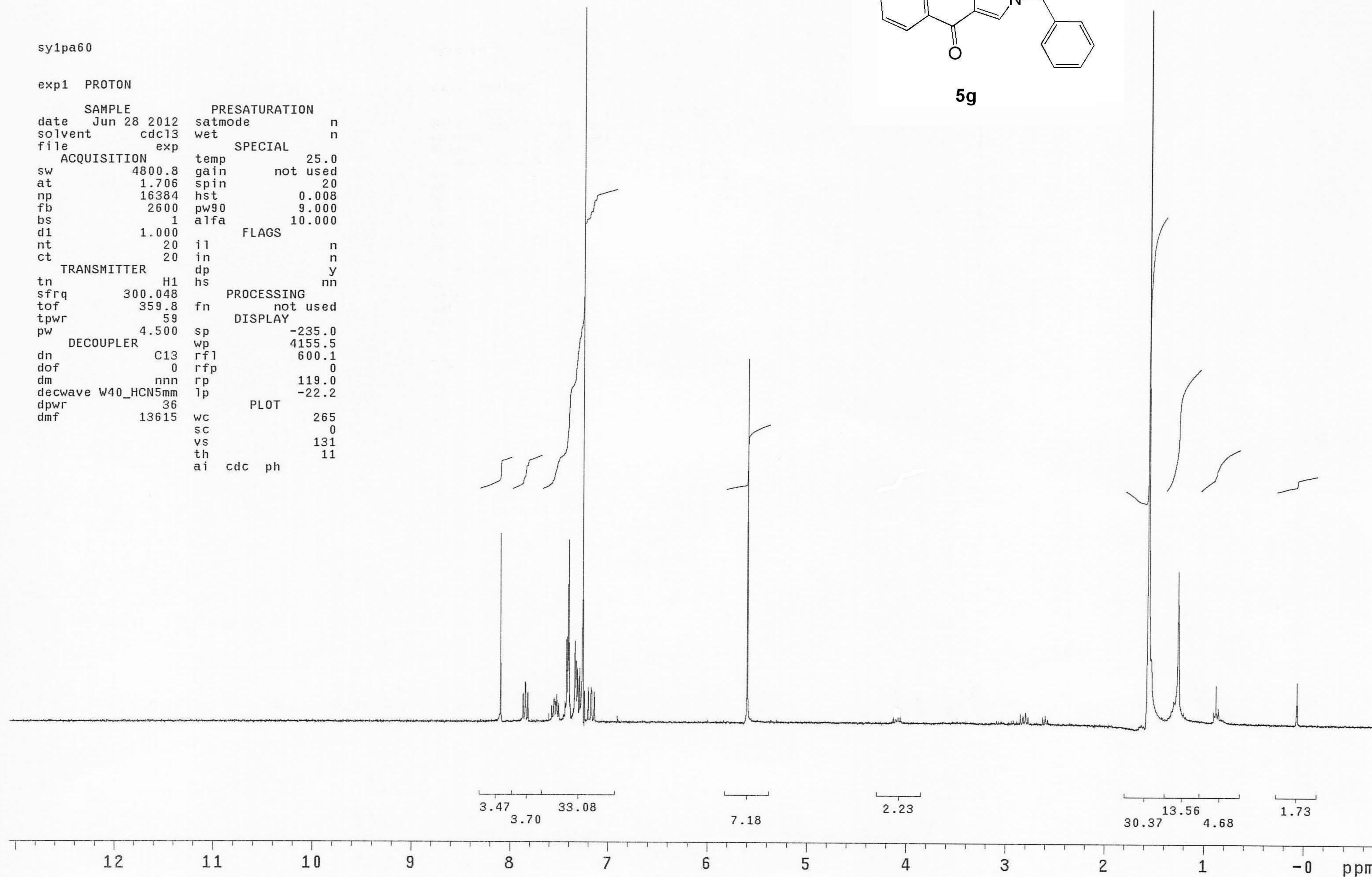
sy1pa60

exp1 PROTON

SAMPLE		PRESATURATION	
date	Jun 28 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	4800.8	gain	not used
at	1.706	spin	20
np	16384	hst	0.008
fb	2600	pw90	9.000
bs	1	alfa	10.000
d1	1.000	FLAGS	
nt	20	il	n
ct	20	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	300.048	PROCESSING	
tof	359.8	fn	not used
tpwr	59	DISPLAY	
pw	4.500	sp	-235.0
DECOUPLER		wp	4155.5
dn	C13	rfl	600.1
dof	0	rfp	0
dm	nnn	rp	119.0
decwave	W40_HCN5mm	lp	-22.2
dpwr	36	PLOT	
dmf	13615	wc	265
		sc	0
		vs	131
		th	11
		ai	cdc ph



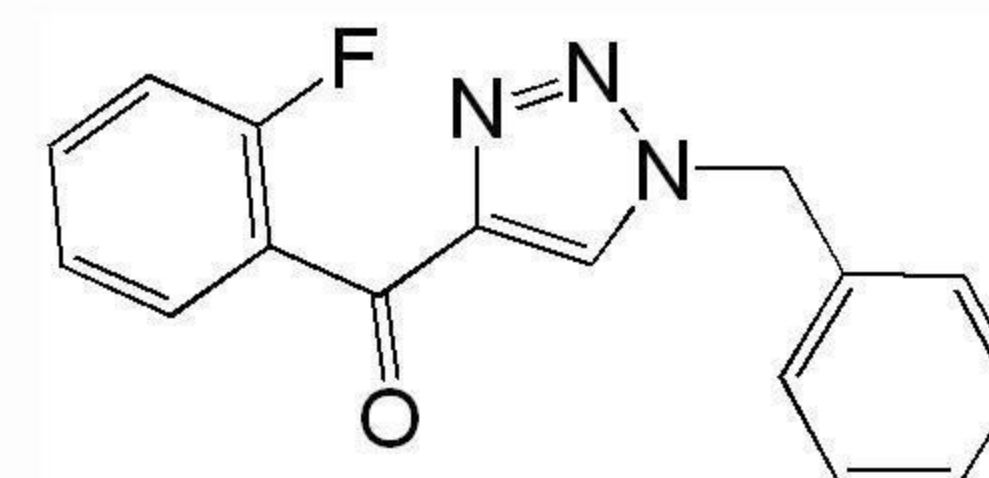
5g



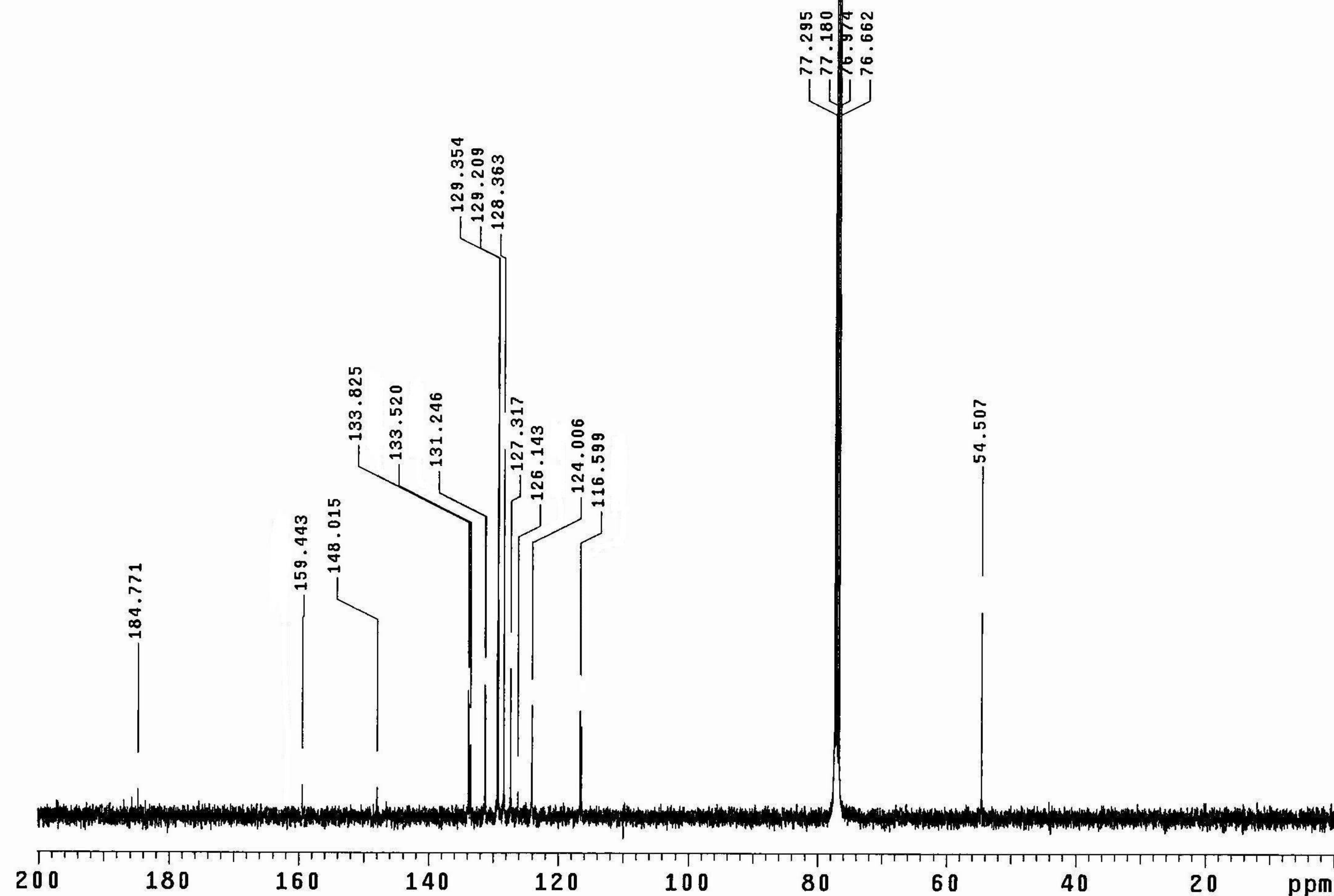
sy11spt70

exp6 CARBON

SAMPLE		PRESATURATION	
date	Feb 29 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	000000	il	n
ct	32472	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	1.00
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-119.0
dn	H1	wp	20250.9
dof	0	rfl	1507.8
dm	yyy	rfl	0
decwave	w	rp	-35.8
dpwr	29	lp	-317.8
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	11380
		th	3
		ai	ph



5g

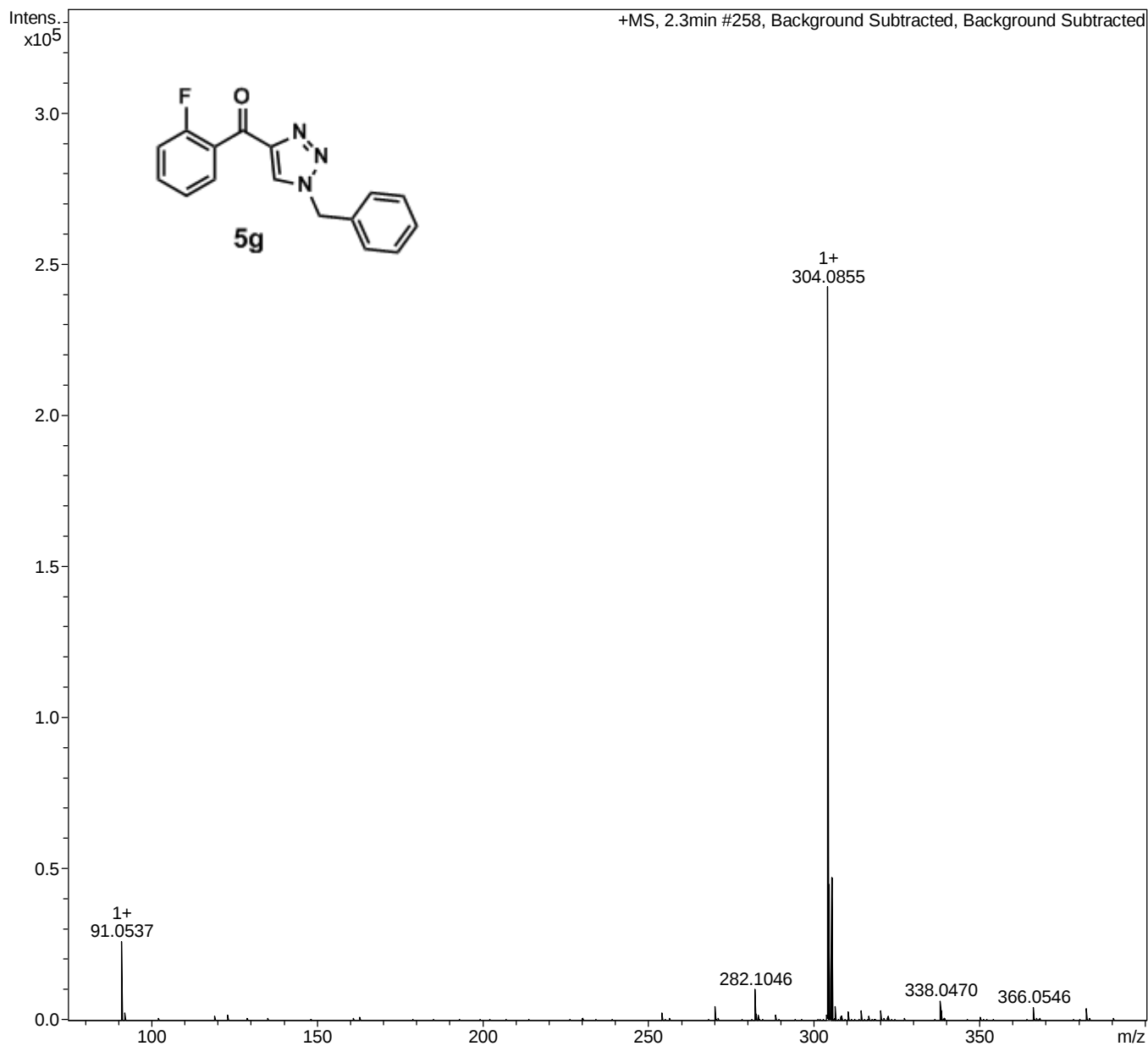


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA60_281_1-G,11_01_3855.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 3/8/2012 10:47:14 AM
Instrument micrOTOF



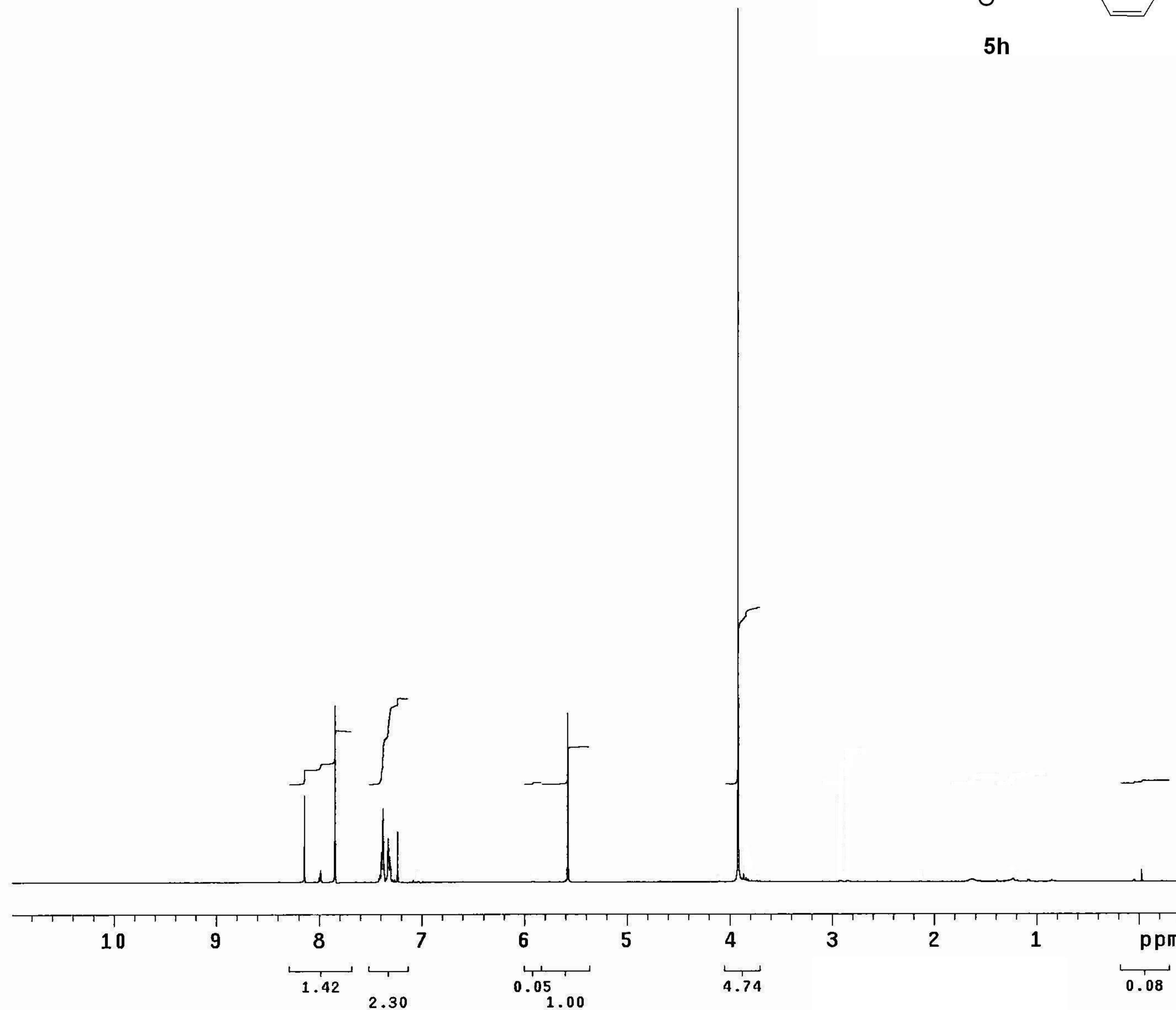
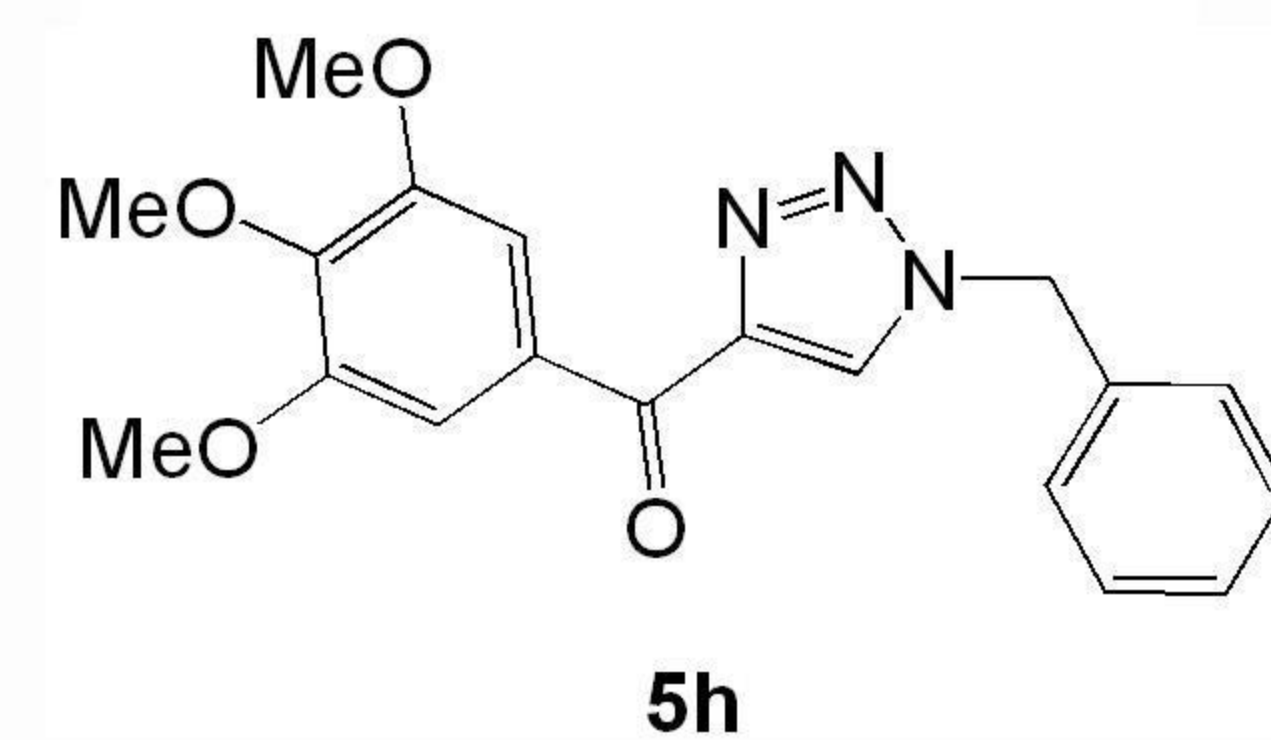
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
304.0855	1	C 16 H 12 F N 3 Na O	100.00	304.0857	0.1	0.4	6.8	11.5	even	ok

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sy1pa6r

exp1 PROTON

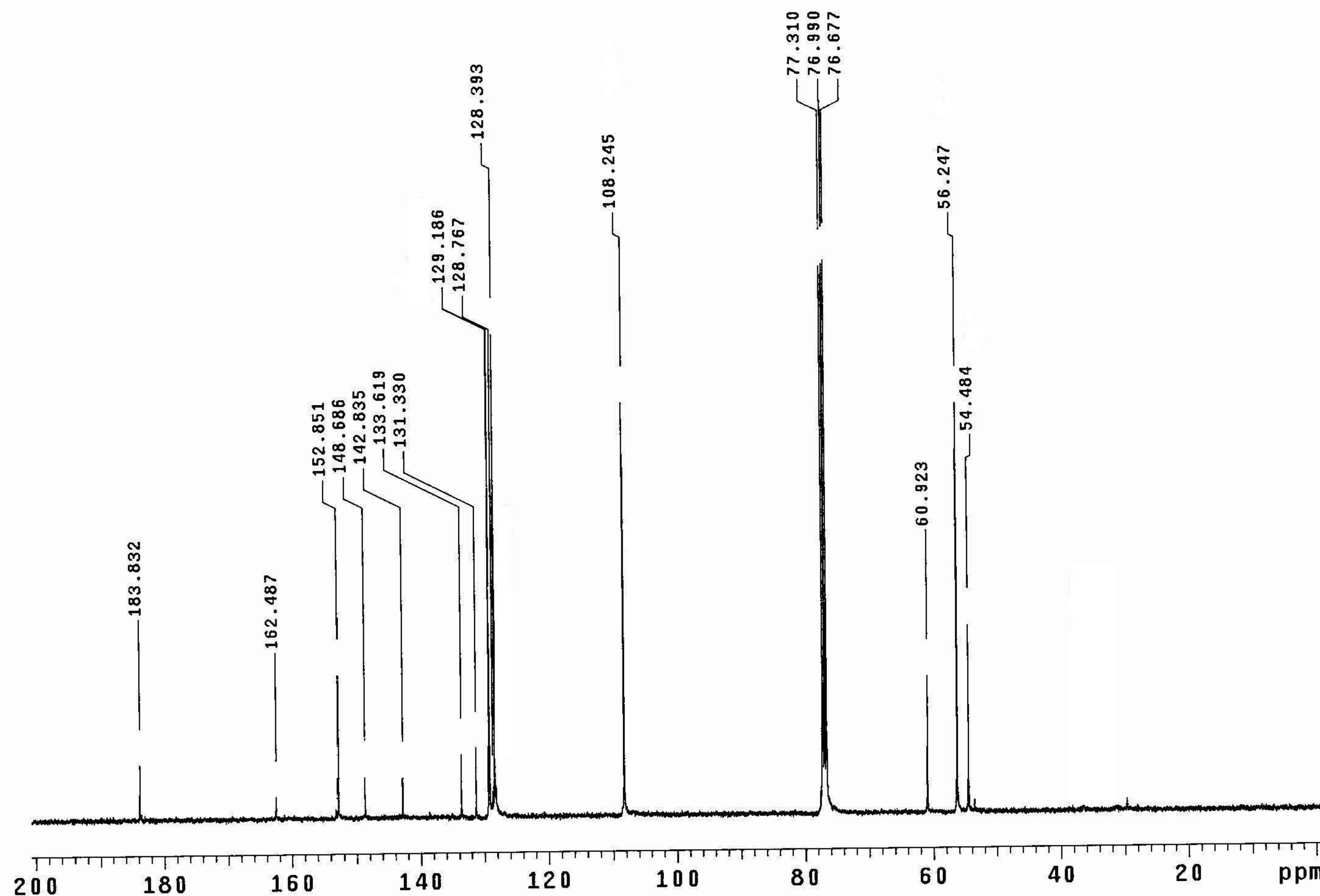
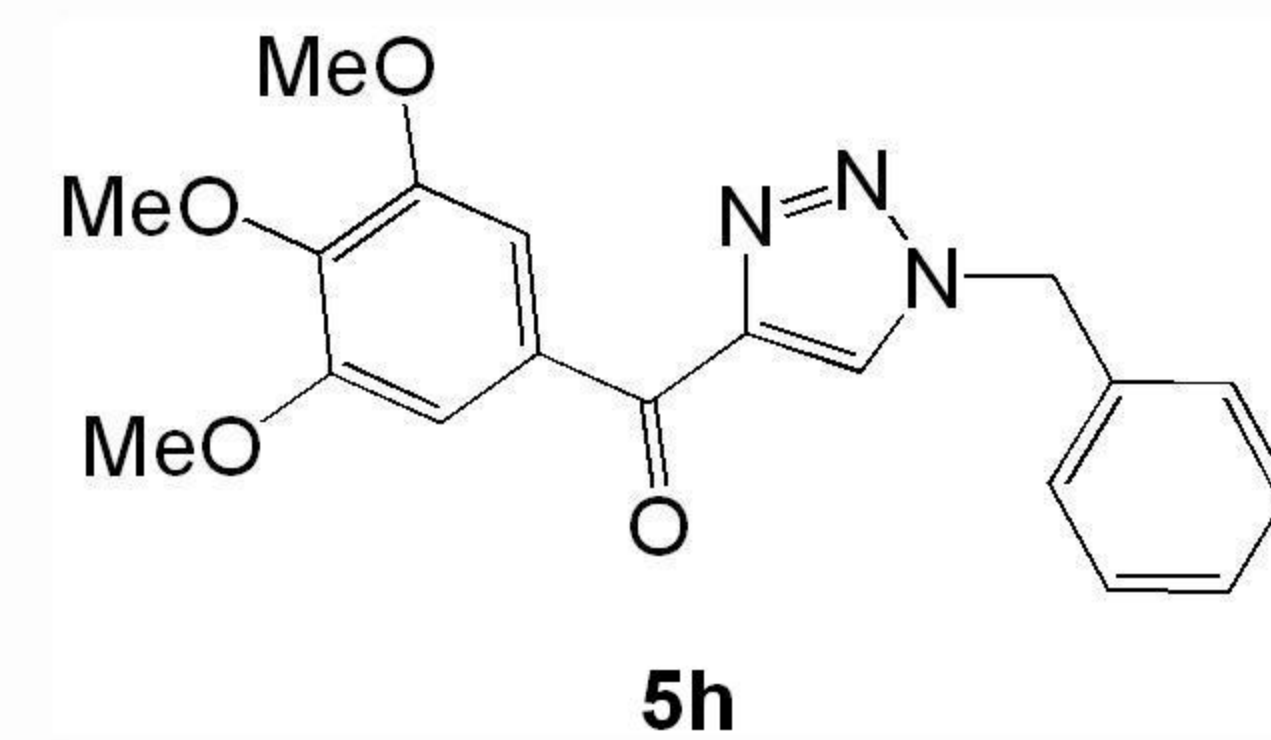
SAMPLE		PRESATURATION	
date	Mar 23 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	7999.2	gain	not used
at	2.048	spin	20
np	32768	hst	0.008
fb	4000	pw90	4.100
bs	1	alfa	6.600
d1	1.000	FLAGS	
nt	400	i1	n
ct	400	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	399.973	PROCESSING	
tof	1199.9	fn	not used
tpwr	56	DISPLAY	
pw	2.050	sp	-192.5
DECOUPLER		wp	4586.9
dn	C13	rfl	799.9
dof	0	rfp	0
dm	nnn	rp	-7.2
decwave	W40_IDPFG~	lp	24.7
	4465	PLOT	
dpwr	46	wc	180
dmf	18500	sc	0
		vs	11
		th	1
		ai	ph



sy1pa6r

exp6 CARBON

SAMPLE		PRESATURATION	
date	Mar 23 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	600000	i1	n
ct	96252	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	1.50
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-234.1
dn	H1	wp	20415.1
dof	0	rfl	1507.8
dm	yyy	rpf	0
decwave	w	rp	-43.3
dpwr	29	lp	-315.4
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	6417
		th	2
		ai	ph

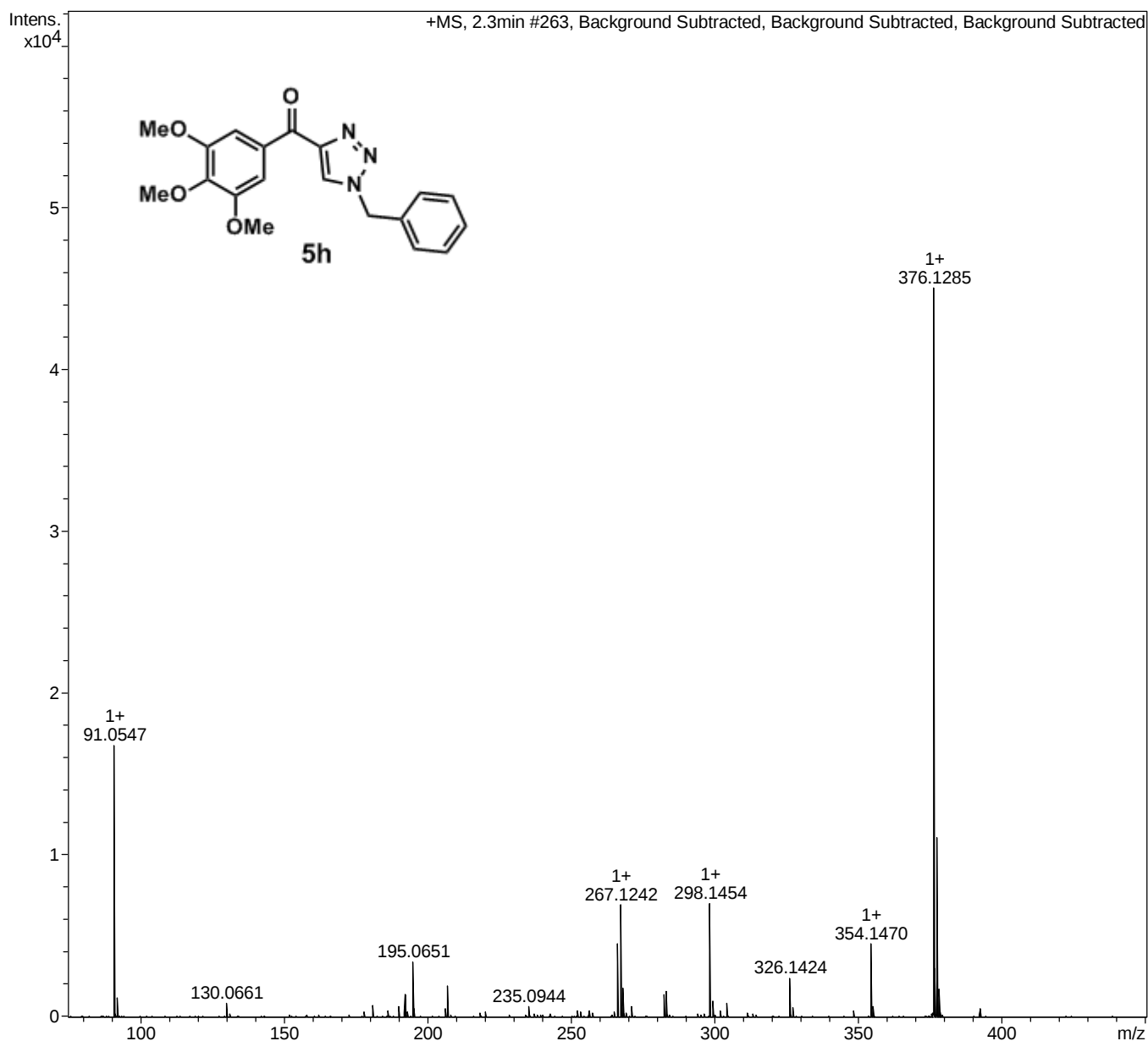


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA6R_353_1-A,12_01_4419.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 4/12/2012 10:59:16 AM
Instrument microTOF



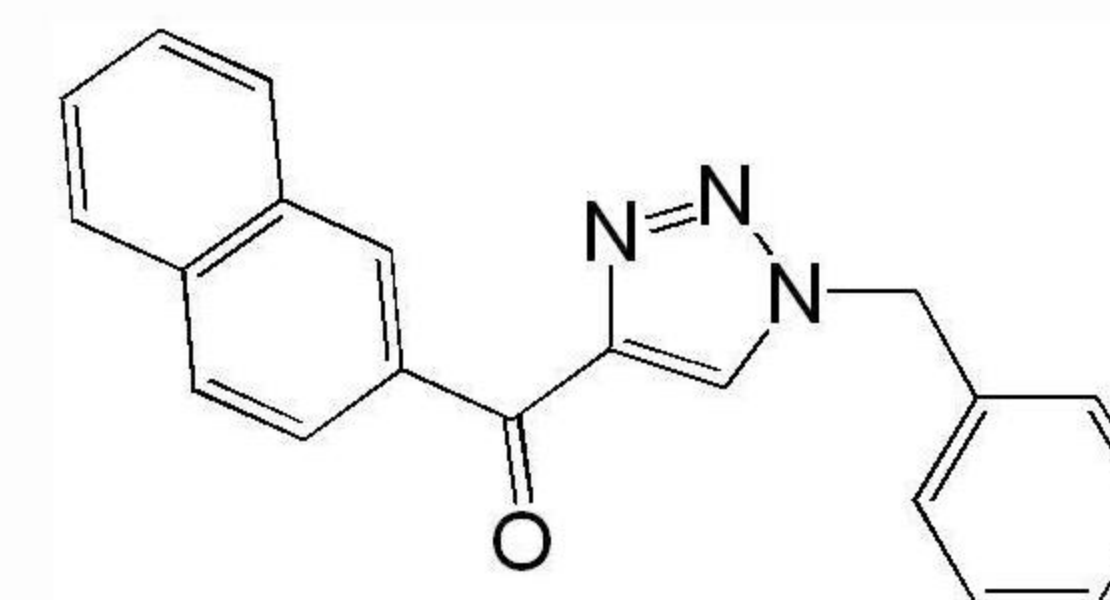
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
376.1285	1	C 19 H 19 N 3 Na O 4	100.00	376.1268	-1.7	-4.5	17.8	11.5	even	ok

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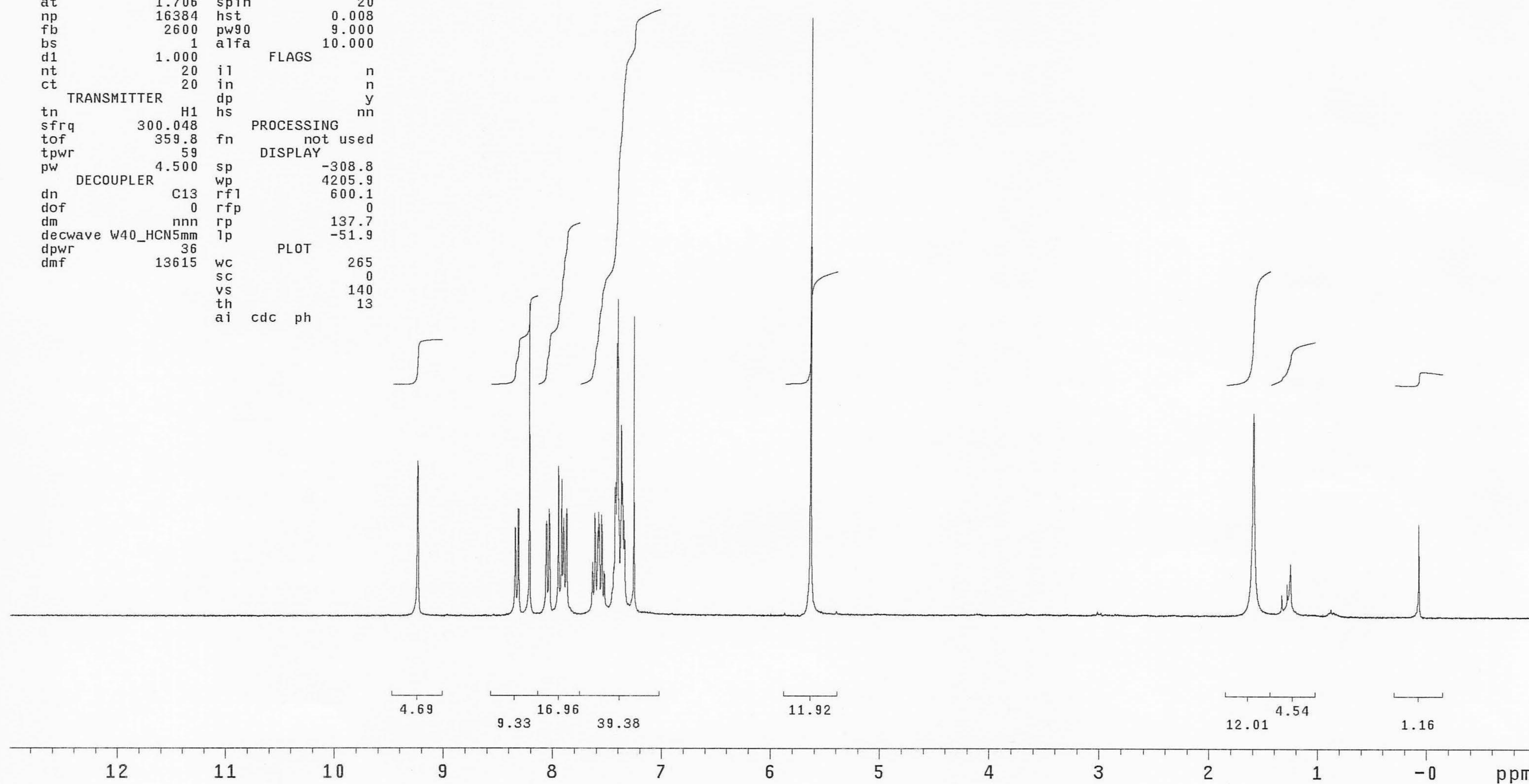
sy1isat158

exp1 PROTON

SAMPLE		PRESATURATION	
date	Jun 26 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	4800.8	gain	not used
at	1.706	spin	20
np	16384	hst	0.008
fb	2600	pw90	9.000
bs	1	alfa	10.000
d1	1.000	FLAGS	
nt	20	il	n
ct	20	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	300.048	PROCESSING	
tof	359.8	fn	not used
tpwr	59	DISPLAY	
pw	4.500	sp	-308.8
DECOUPLER		wp	4205.9
dn	C13	rf1	600.1
dof	0	rfp	0
dm	nnn	rp	137.7
decwave	W40_HCN5mm	lp	-51.9
dpwr	36	PLOT	
dmf	13615	wc	265
		sc	0
		vs	140
		th	13
		ai	cdc ph



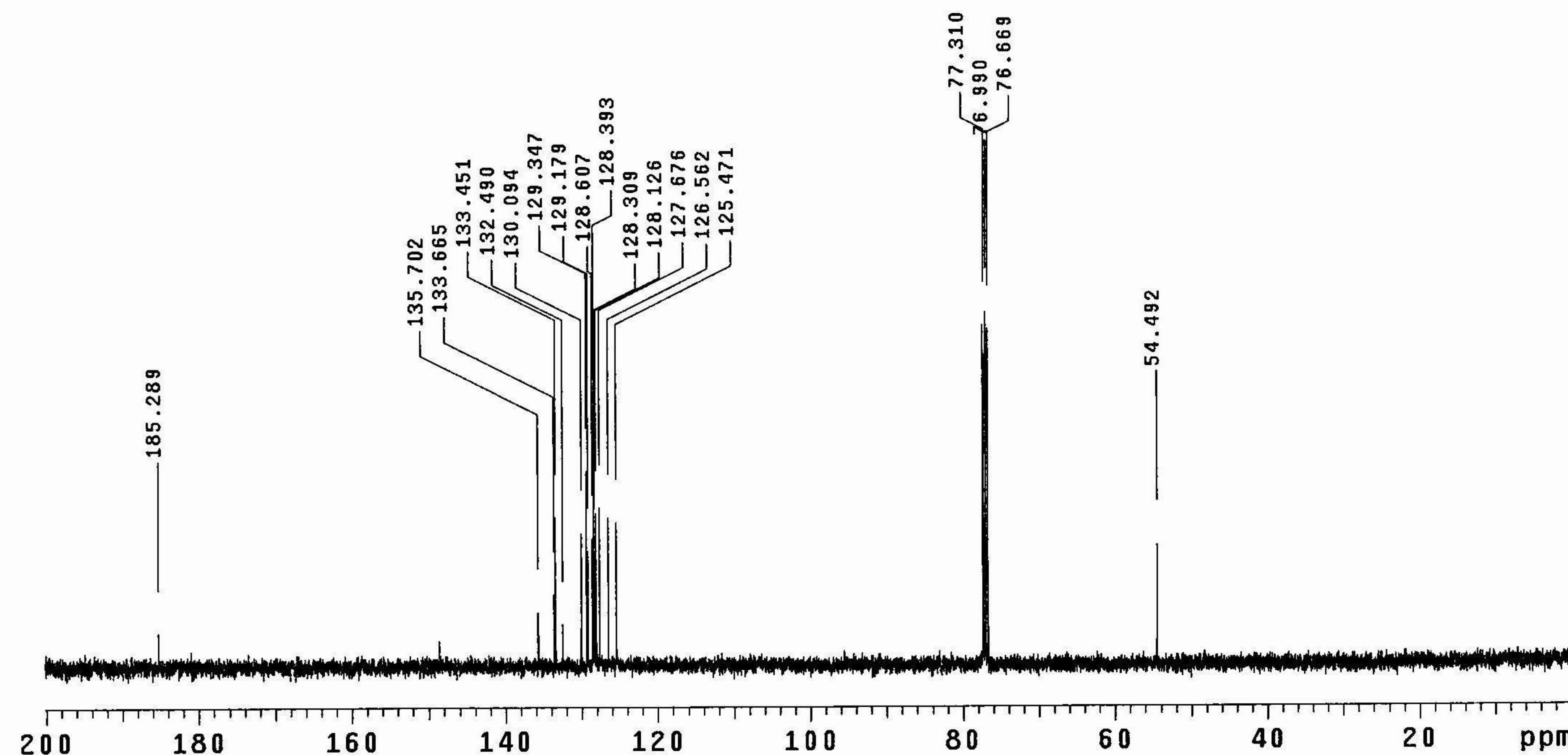
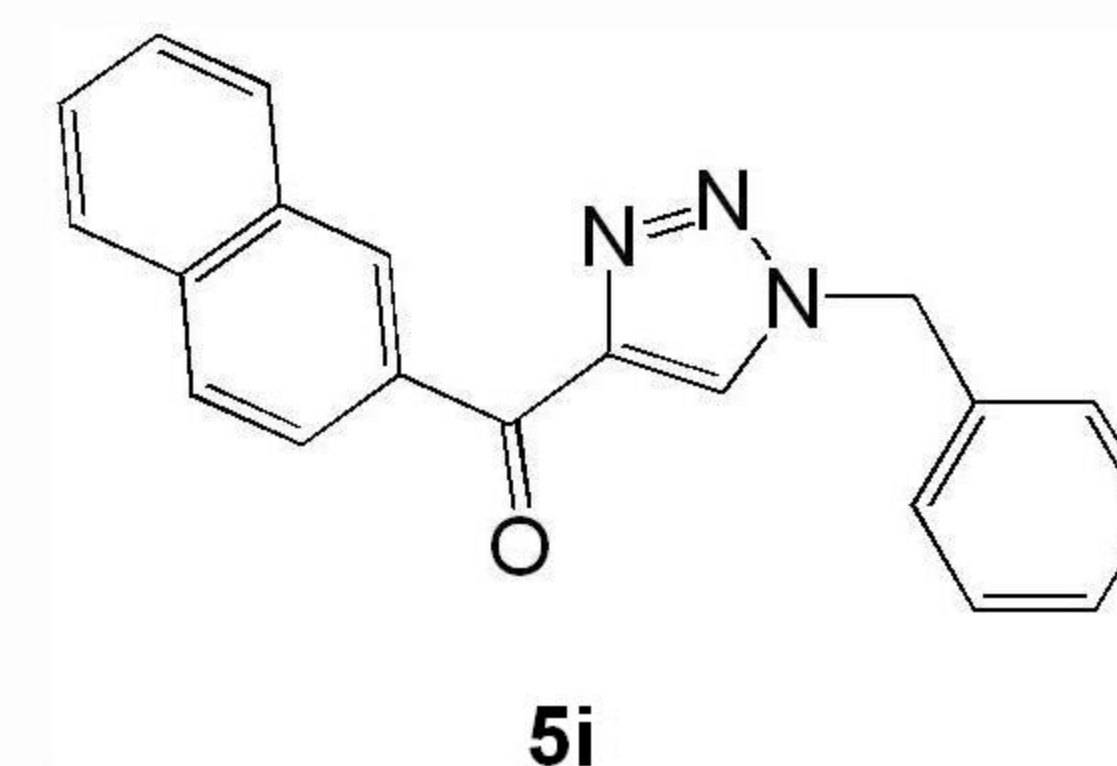
5i



sy1isat158

exp6 CARBON

SAMPLE		PRESATURATION	
date	Mar 1 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	600000	il	n
ct	1178	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	1.00
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-149.7
dn	H1	wp	20280.9
dof	0	rfl	1507.8
dm	yyy	rpf	0
decwave	w	rp	-8.6
dpwr	29	lp	-371.3
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	1624
		th	3
		ai	ph

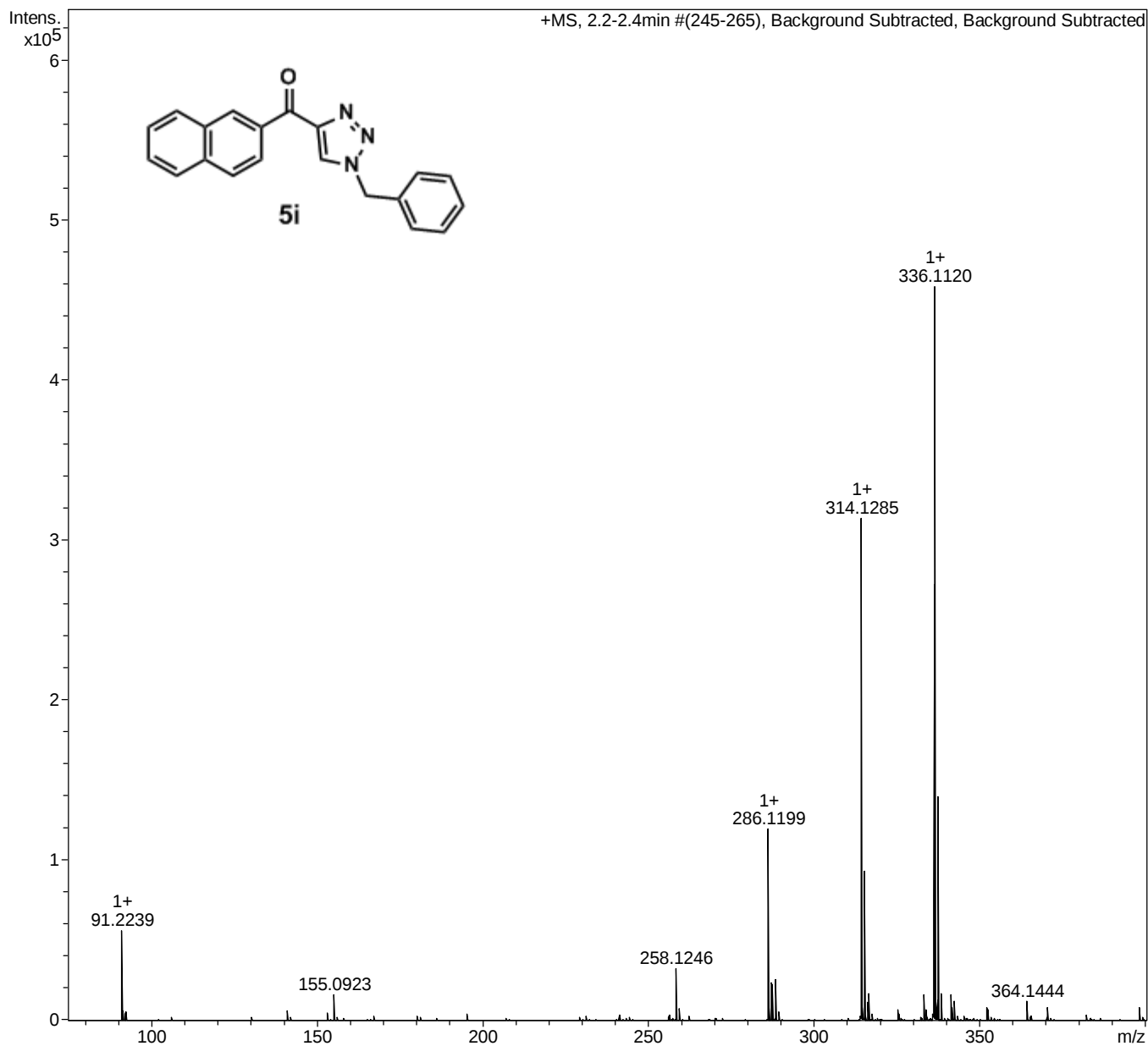


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA53A_313_1-G,12_01_3856.d
 Method fia_pos_bajo_50-350_egf.m

Acquisition Date 3/8/2012 10:56:06 AM
 Instrument microTOF



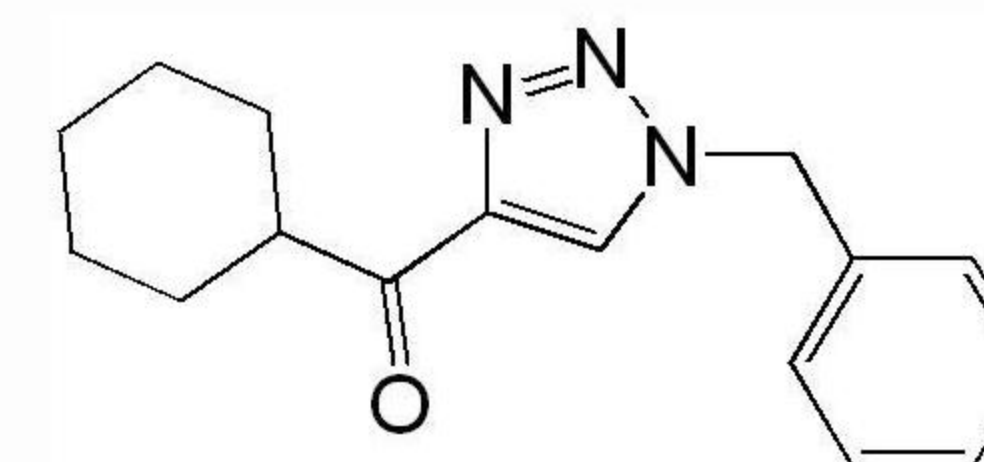
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
314.1285	1	C ₂₀ H ₁₆ N ₃ O	100.00	314.1288	0.3	0.9	41.5	14.5	even	ok

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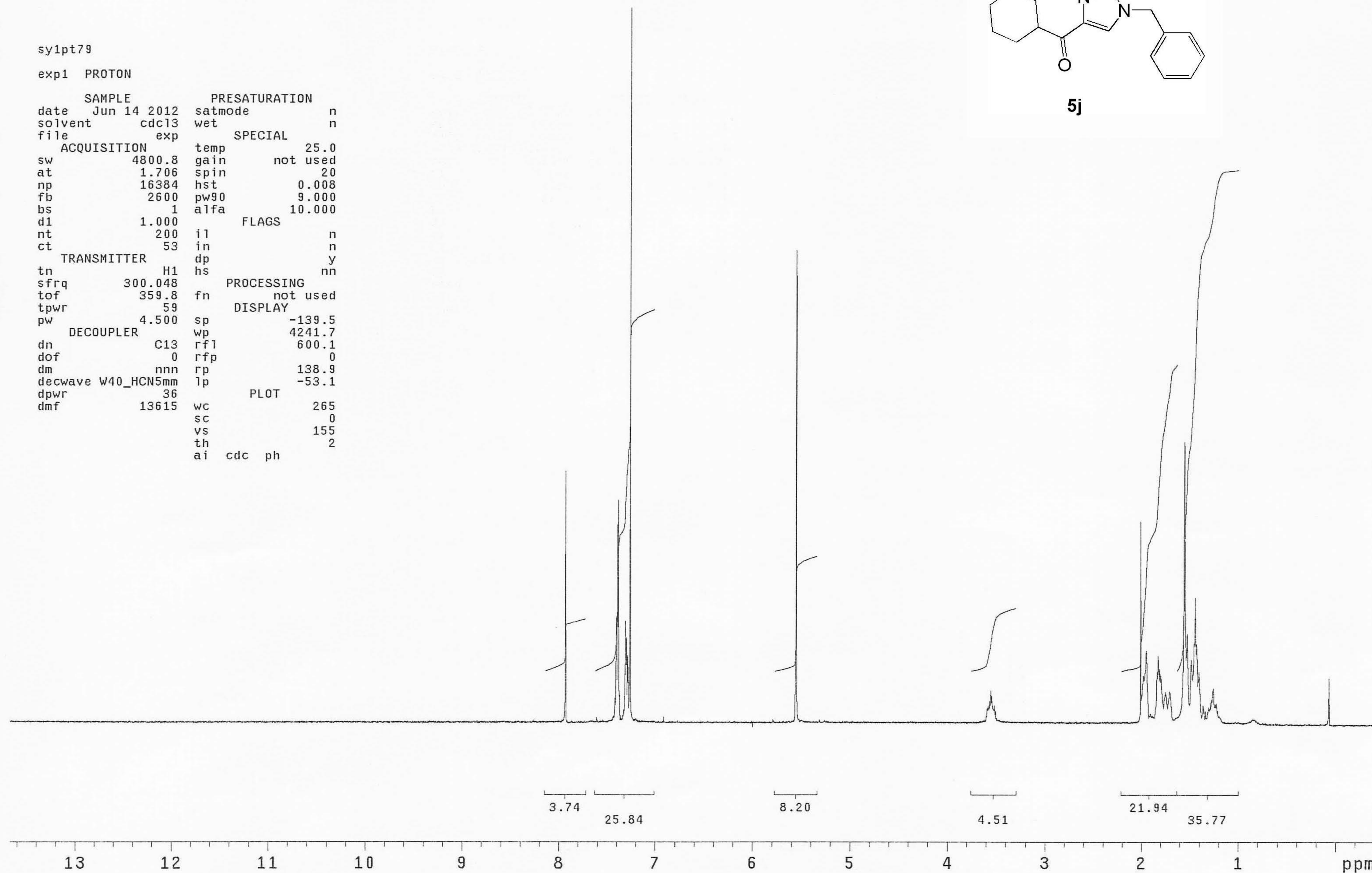
sy1pt79

exp1 PROTON

SAMPLE		PRESATURATION	
date	Jun 14 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	4800.8	gain	not used
at	1.706	spin	20
np	16384	hst	0.008
fb	2600	pw90	9.000
bs	1	alfa	10.000
d1	1.000	FLAGS	
nt	200	il	n
ct	53	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	300.048	PROCESSING	
tof	359.8	fn	not used
tpwr	59	DISPLAY	
pw	4.500	sp	-139.5
DECOUPLER		wp	4241.7
dn	C13	rfl	600.1
dof	0	rfp	0
dm	nnn	rp	138.9
decwave	W40_HCN5mm	lp	-53.1
dpwr	36	PLOT	
dmf	13615	wc	265
		sc	0
		vs	155
		th	2
		ai	cdc ph



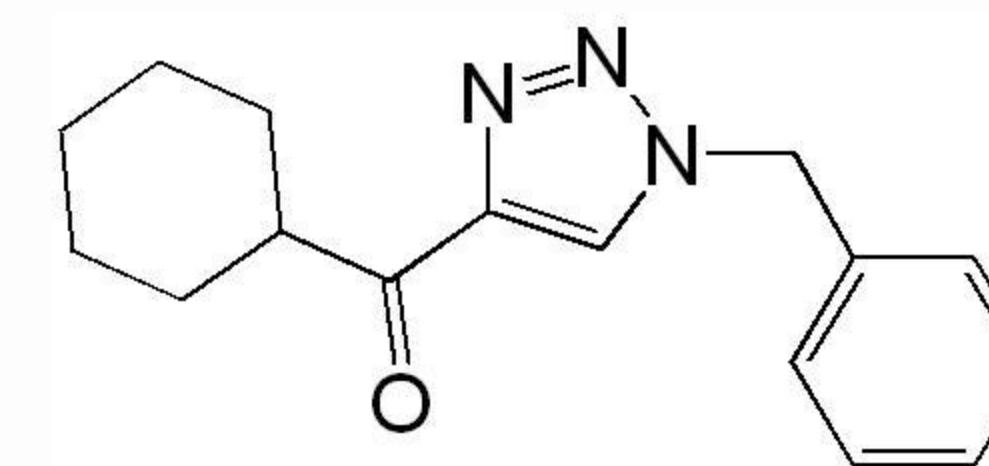
5j



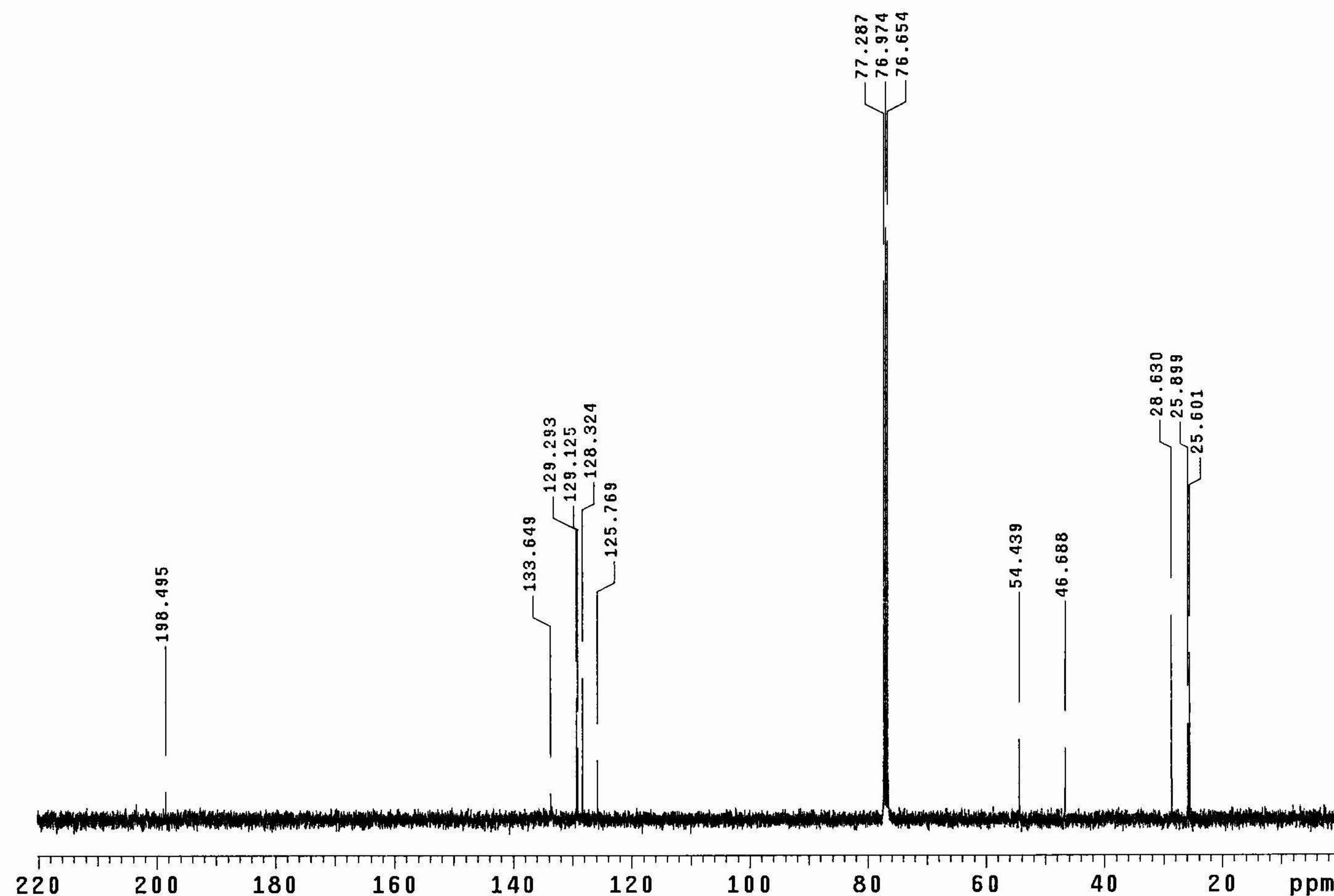
sy1spt97

exp6 CARBON

SAMPLE		PRESATURATION	
date	Feb 15 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	600000	il	n
ct	5016	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	1.00
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-46.1
dn	H1	wp	22188.3
dof	0	rfl	1507.8
dm	yyy	rfp	0
decwave	w	rp	-40.3
dpwr	29	lp	-293.2
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	3731
		th	3
		ai	ph



5j

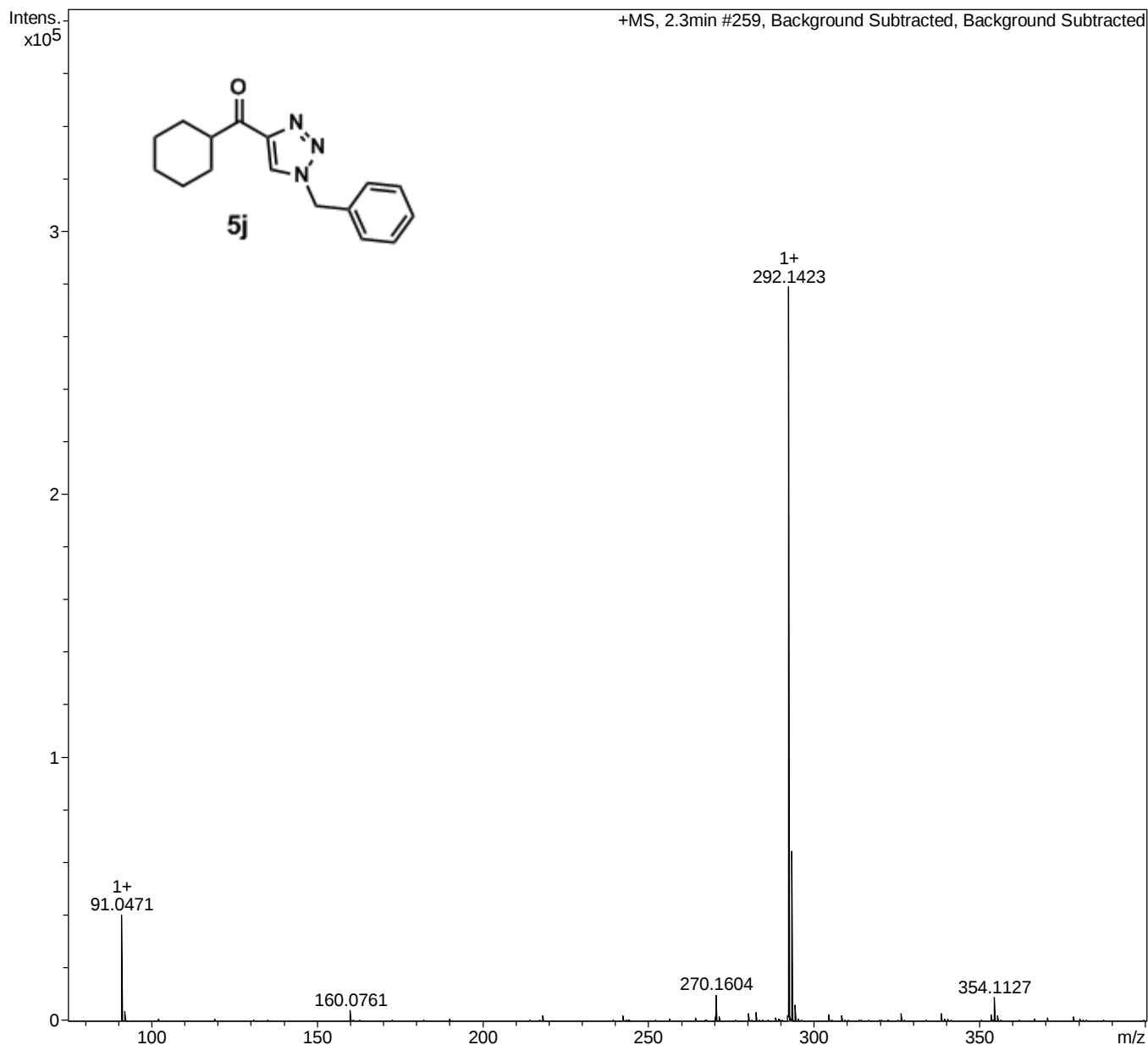


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA97_269_1-H,3_01_3861.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 3/8/2012 11:40:25 AM
Instrument micrOTOF



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
292.1423	1	C 16 H 19 N 3 Na O	100.00	292.1420	-0.3	-0.9	28.0	8.5	even	ok

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5k

Current Data Parameters

NAME sy1pa87
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20090427
Time 17.43
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 25
DS 0
SWH 4251.701 Hz
FIDRES 0.129752 Hz
AQ 3.8535669 sec
RG 724.1
DW 117.600 usec
DE 10.50 usec
TE 300.0 K
D1 1.50000000 sec

===== CHANNEL f1 =====

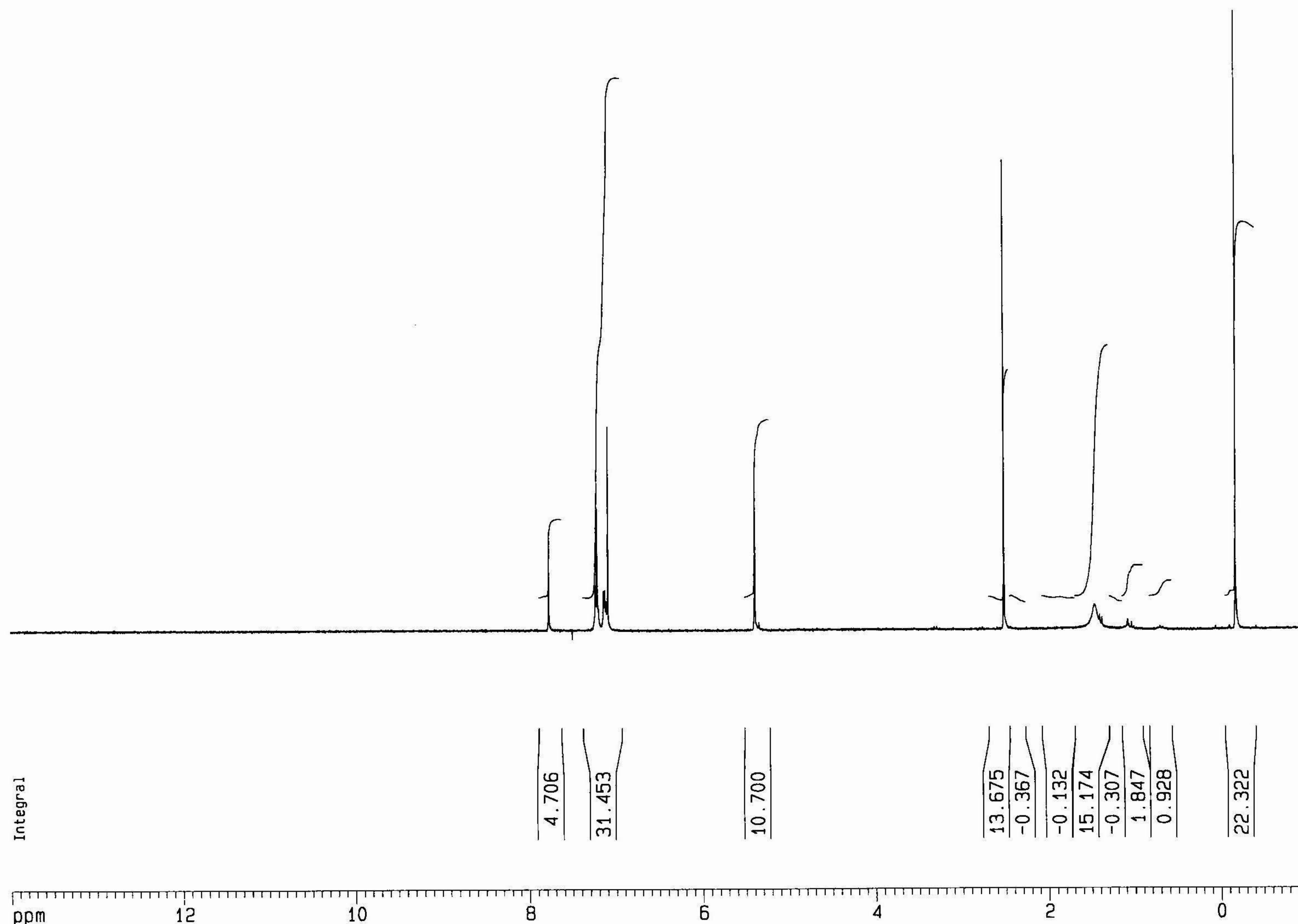
NUC1 1H
P1 9.75 usec
PL1 -6.00 dB
SF01 250.1319258 MHz

F2 - Processing parameters

SI 16384
SF 250.1300498 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

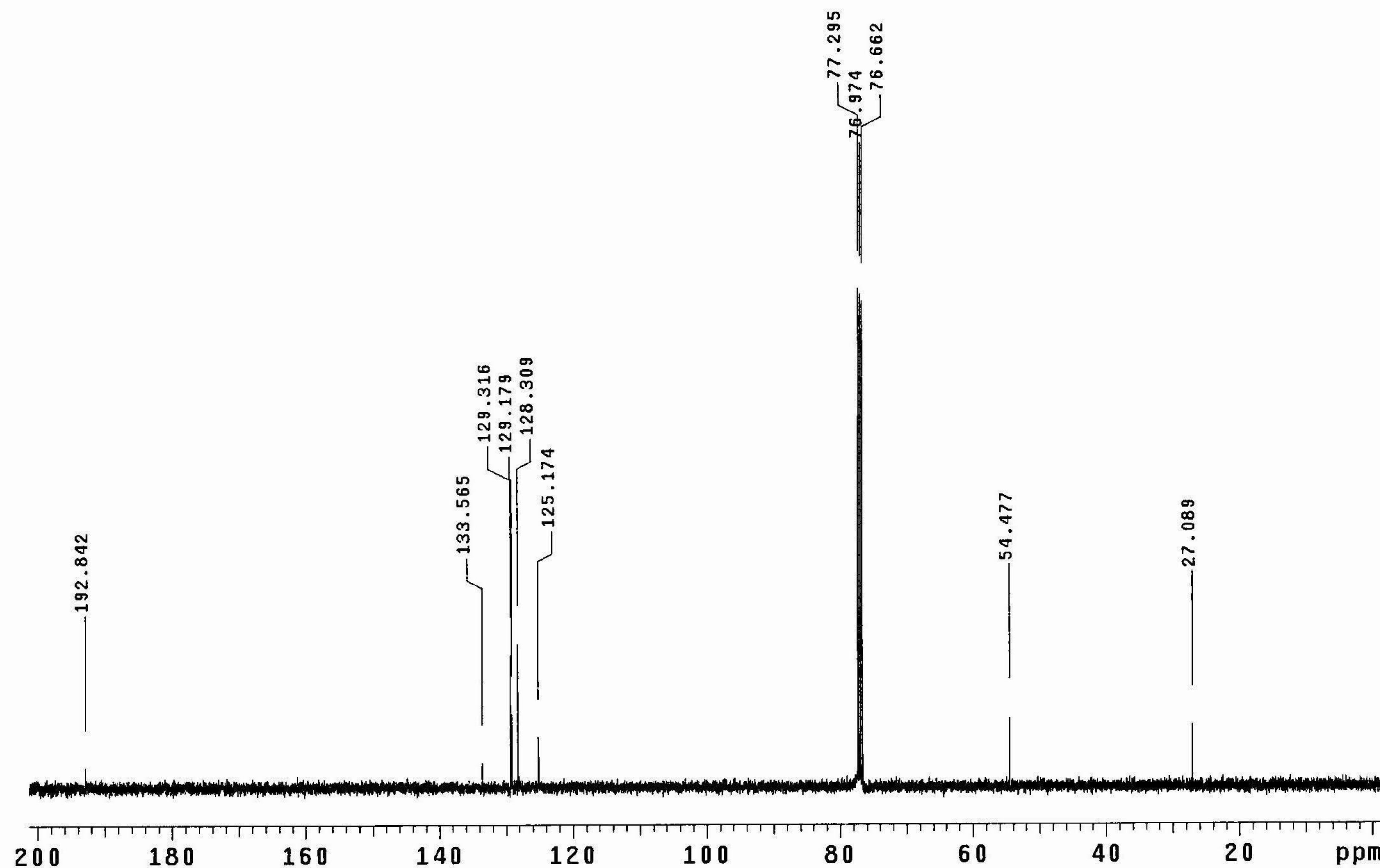
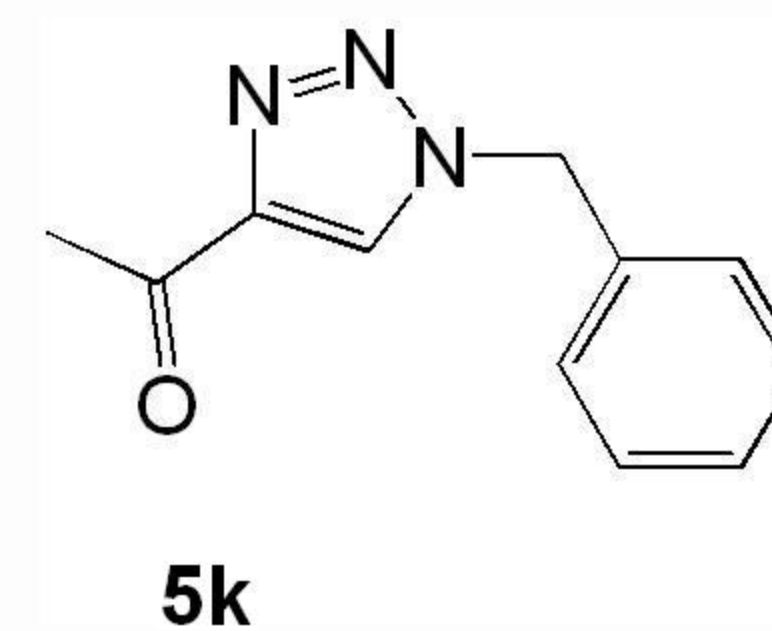
CX 20.00 cm
F1P 14.000 ppm
F1 3501.82 Hz
F2P -1.000 ppm
F2 -250.13 Hz
PPMCM 0.75000 ppm/cm
HZCM 187.59753 Hz/cm



sy1ispt87

exp6 CARBON

SAMPLE		PRESATURATION	
date	Feb 22 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	600000	il	n
ct	4040	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	1.00
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-285.5
dn	H1	wp	20527.9
dof	0	rfl	1507.8
dm	yyy	rfp	0
decwave	w	rp	-5.6
dpwr	29	lp	-368.6
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	2546
		th	2
		ai	ph

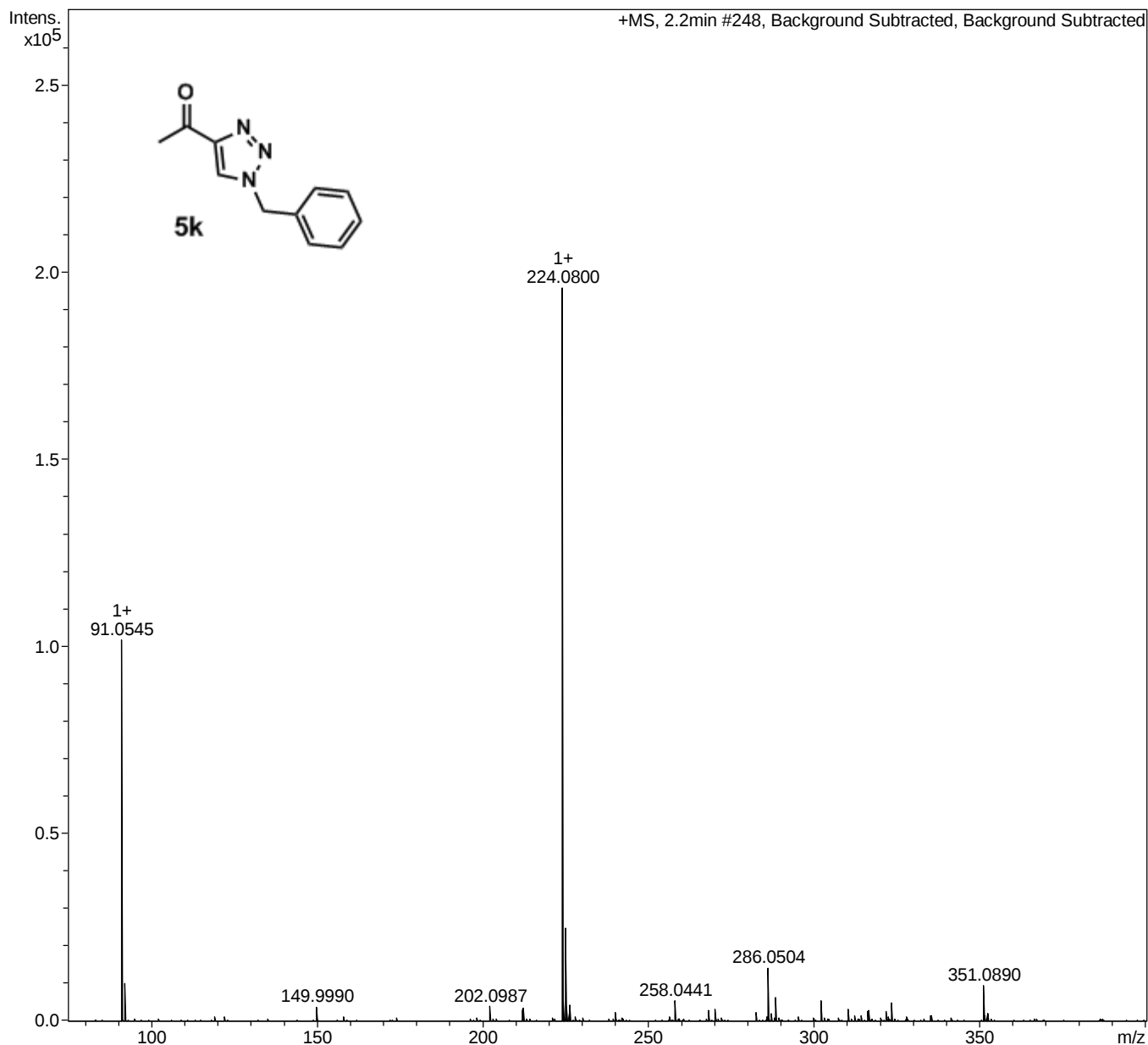


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA87_201_1-H,2_01_3859.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 3/8/2012 11:22:42 AM
Instrument micrOTOF



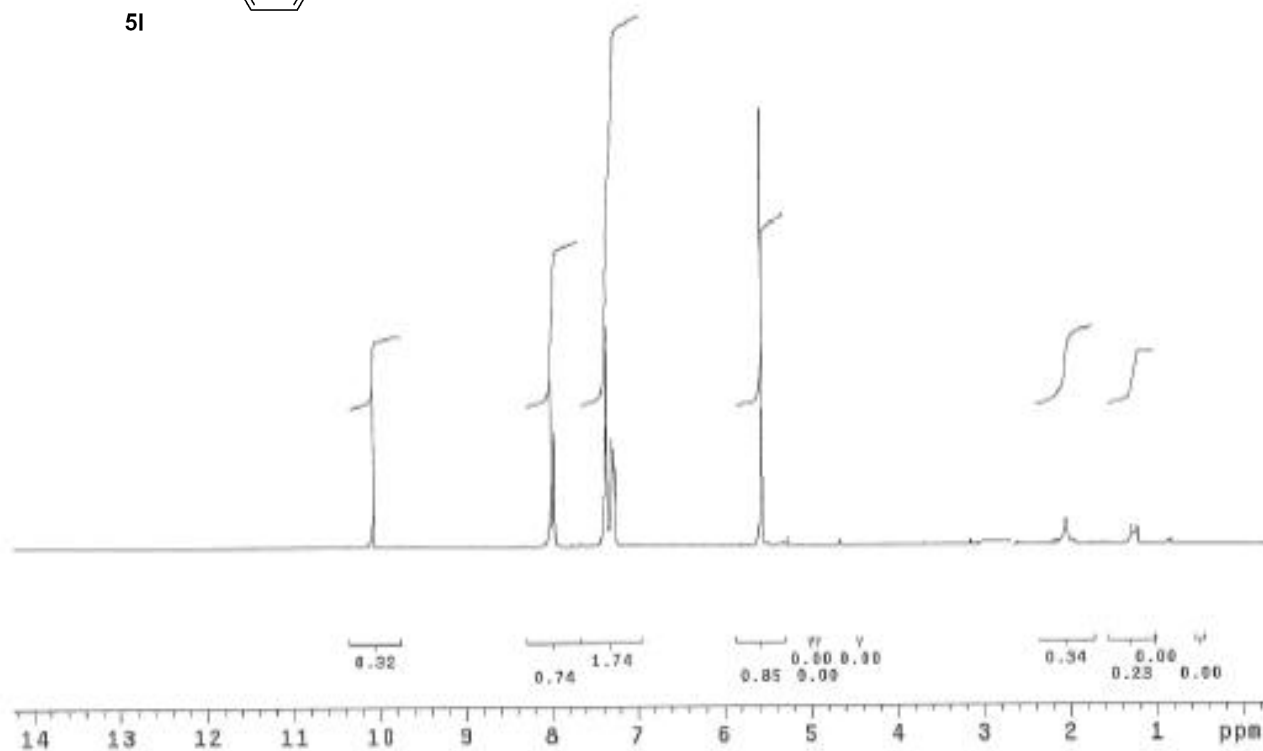
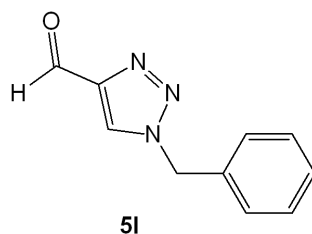
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
224.0800	1	C 11 H 11 N 3 Na O	100.00	224.0794	-0.6	-2.5	8.6	7.5	even	ok

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sy1cof2

expt s2pul

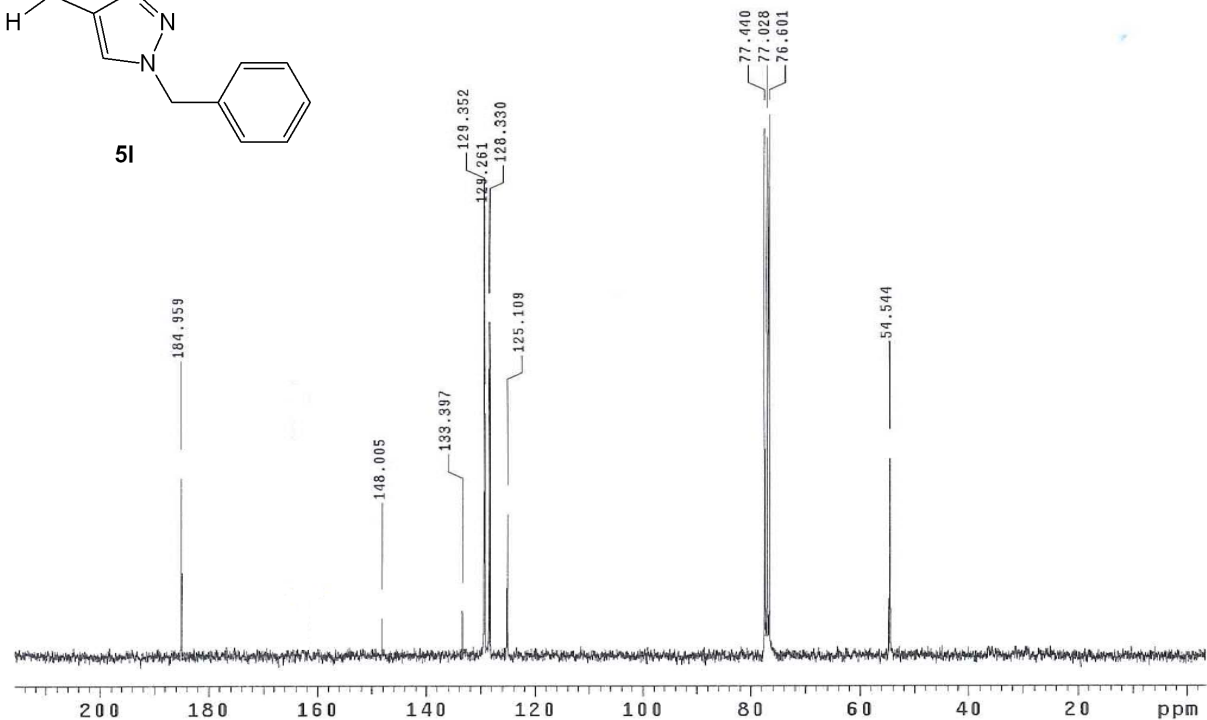
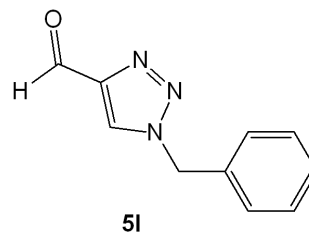
SAMPLE		DEC. & VT	
date	May 8 2012	dfreq	75.454
solvent	cdcl3	dn	C13
file	exp	dpr	37
ACQUISITION		dof	0
sfreq	300.648	dn	nmh
tn	H1	dwn	c
at	1.517	dmp	15500
np	16384	temp	25.0
pw	5395.6	PROCESSING	
fb	3000	lb	0.23
bs	1	wtfile	
tpwr	53	proc	ft
pw	8.0	fn	not used
dl	8.788		
sof	655.7	werr	
nt	298	wexp	
ct	43	wds	
alock	n	wnt	
gain	not used		
FLAOS			
sl	n		
in	n		
dp	y		
DISPLAY			
sp	-92.7		
wp	4365.4		
vs	77		
sc	0		
wc	180		
h2am	24.25		
ic	783.41		
rfl	593.6		
rfp	0		
th	5		
ins	1.000		
al	ph		



sy1C0F2

exp1 CARBON

SAMPLE		PRESATURATION	
date	May 10 2012	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmr2/s~	SPECIAL	
sy1C0F2/13C.fid		temp	25.0
ACQUISITION		gain	not used
sw	18867.9	spin	not used
at	0.868	hst	0.008
np	32768	pw90	7.000
fb	10400	alfa	10.000
bs	2	FLAGS	
d1	1.000	il	n
nt	3000	in	n
ct	1836	dp	y
TRANSMITTER		hs	nn
tn	C13	PROCESSING	
sfrq	75.454	lb	2.50
tof	409.4	fn	not used
tpwr	57	DISPLAY	
pw	3.000	sp	-267.8
DECOUPLER		wp	16550.9
dn	H1	rfl	1889.3
dof	0	rfp	0
dm	yyy	rp	131.3
decwave	w	lp	-285.7
dpwr	37	PLOT	
dmf	8100	wc	180
		sc	0
		vs	290
		th	4
		ai	ph

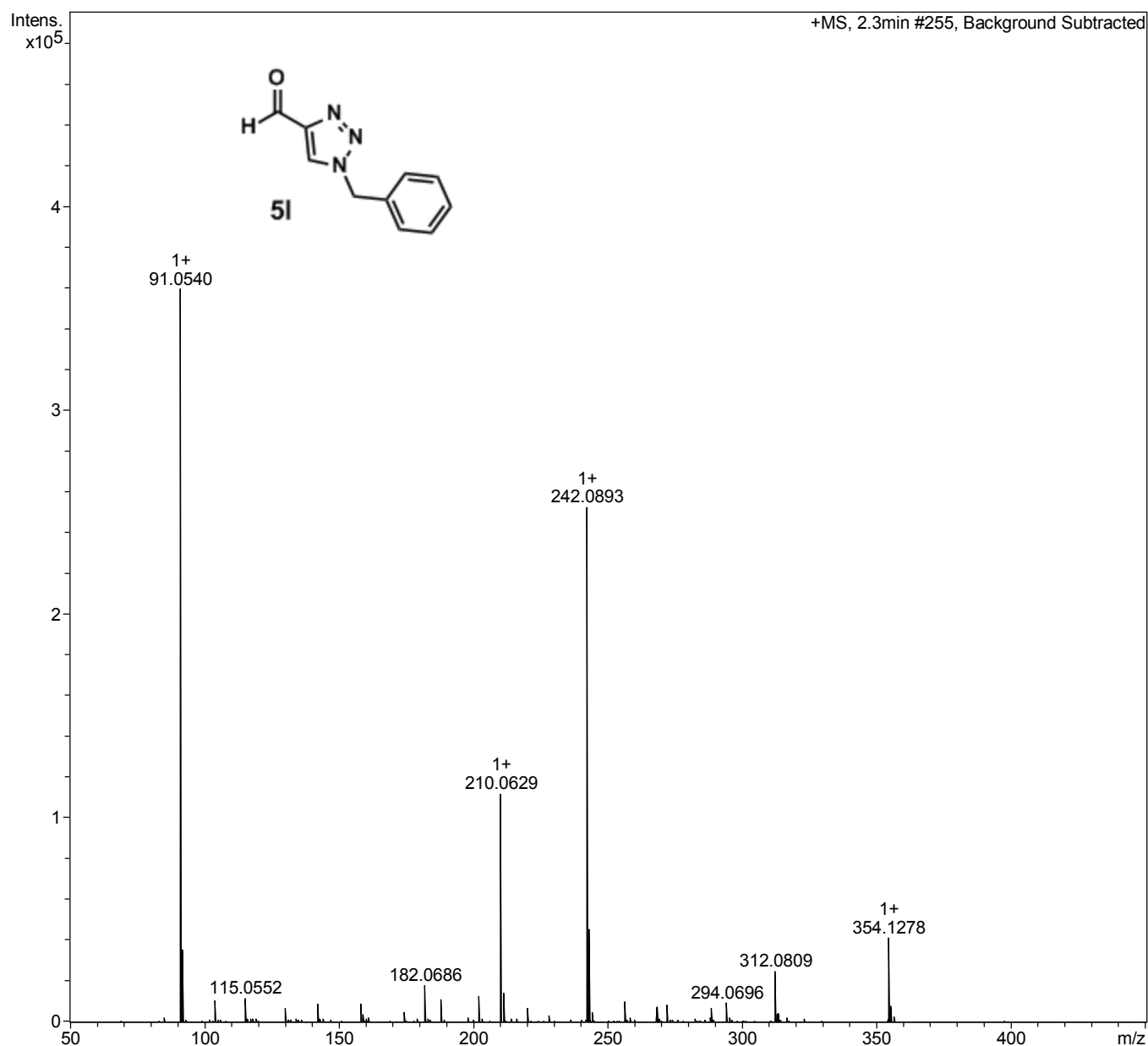


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1COF2_187_1-H,4_01_4906.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 5/11/2012 4:28:25 PM
Instrument micrOTOF



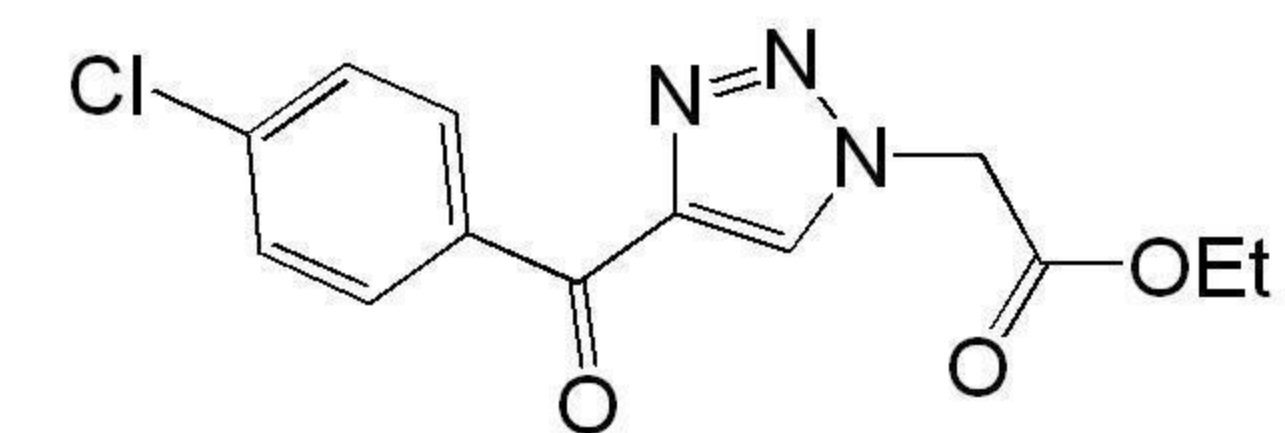
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
210.0629	1	C 10 H 9 N 3 Na O	100.00	210.0638	0.9	4.1	6.2	7.5	even	ok

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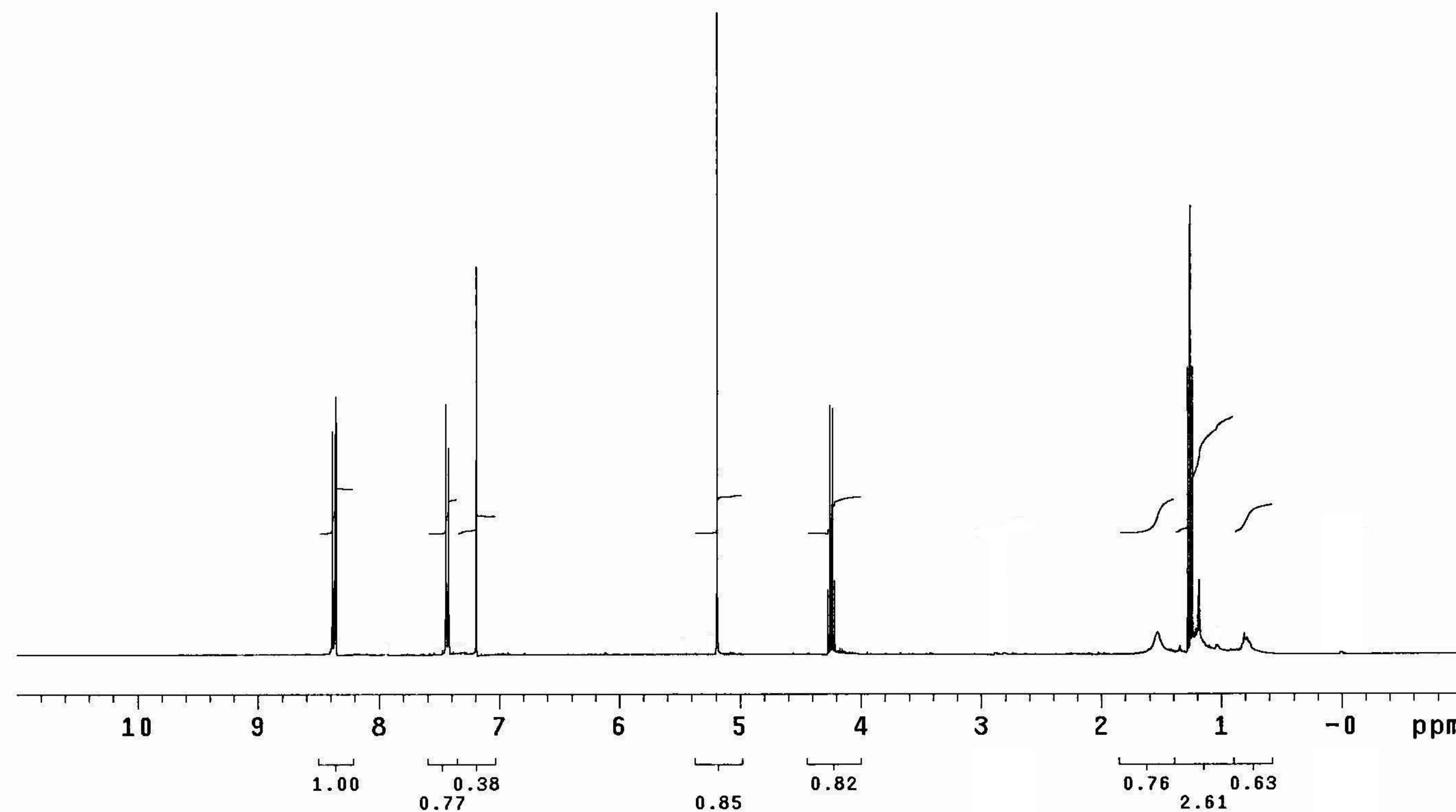
sy1pa6j

exp17 PROTON

SAMPLE		PRESATURATION	
date	Mar 16 2012	satmode	n
solvent	cdcl3	wet	n
file	/home/rgr/sy~	SPECIAL	
	1pa6j/1H.fid	temp	25.0
ACQUISITION		gain	not used
sw	7999.2	spin	20
at	2.048	hst	0.008
np	32768	pw90	4.100
fb	4000	alfa	6.600
bs	1	FLAGS	
d1	1.000	i1	n
nt	128	in	n
ct	128	dp	y
TRANSMITTER		hs	nn
tn	H1	PROCESSING	
sfrq	399.973	fn	not used
tof	1199.9	DISPLAY	
tpwr	56	sp	-432.6
pw	2.050	wp	4831.5
DECOUPLER		rf1	817.8
dn	C13	rfp	0
dof	0	rp	-14.4
dm	nnn	lp	30.3
decwave W40_IDPFG~		PLOT	
	4465	wc	180
dpwr	46	sc	0
dmf	18500	vs	23
		th	2
		ai	ph



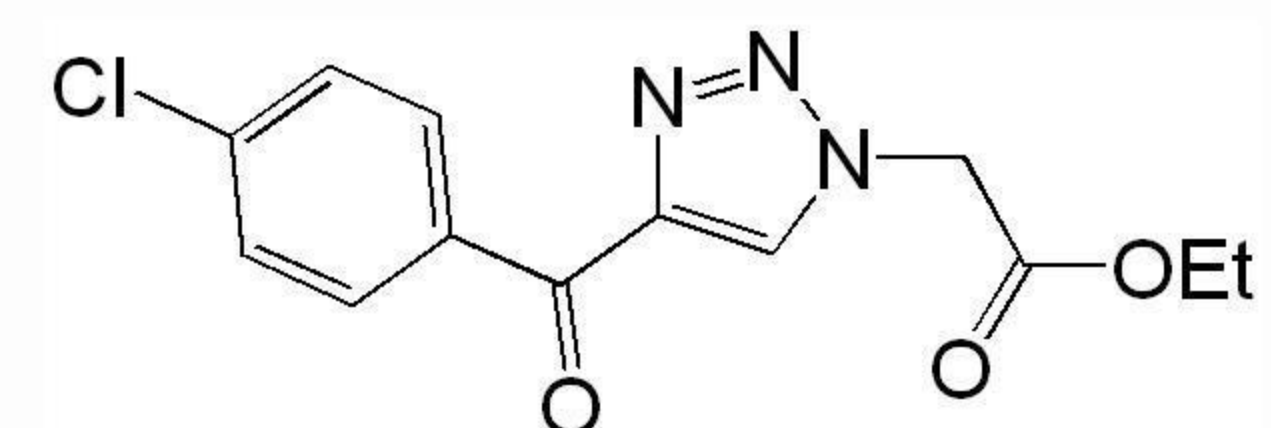
5m



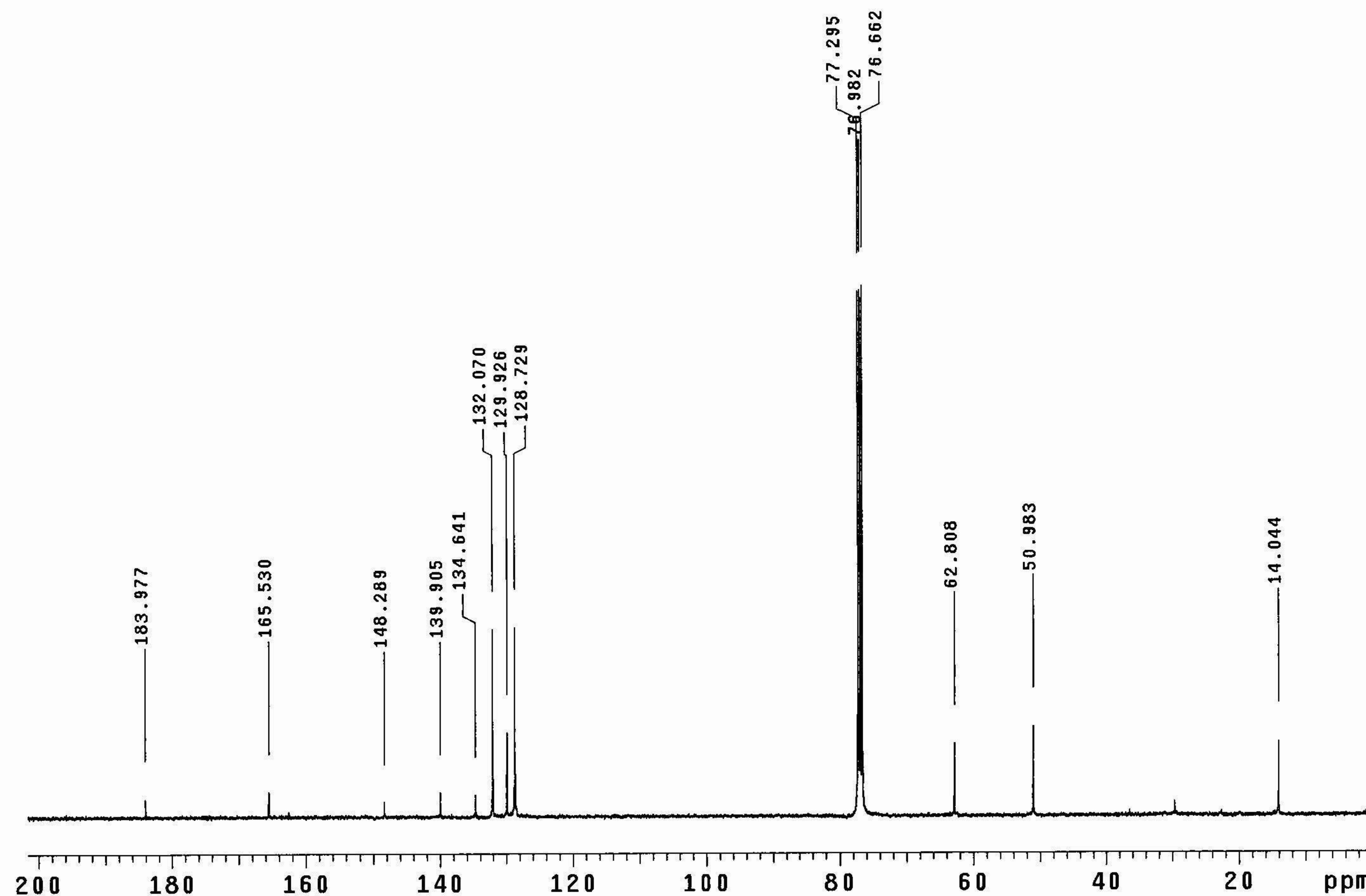
sy1pa6j

exp6 CARBON

SAMPLE		PRESATURATION	
date	Mar 16 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	.4	alfa	10.000
d1	1.000	FLAGS	
nt	600000	il	n
ct	137120	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	2.00
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-109.1
dn	H1	wp	20386.0
dof	0	rfl	1507.8
dm	yyy	rpf	0
decwave	w	rp	-37.8
dpwr	29	lp	-316.4
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	5929
		th	2
		ai	ph



5m

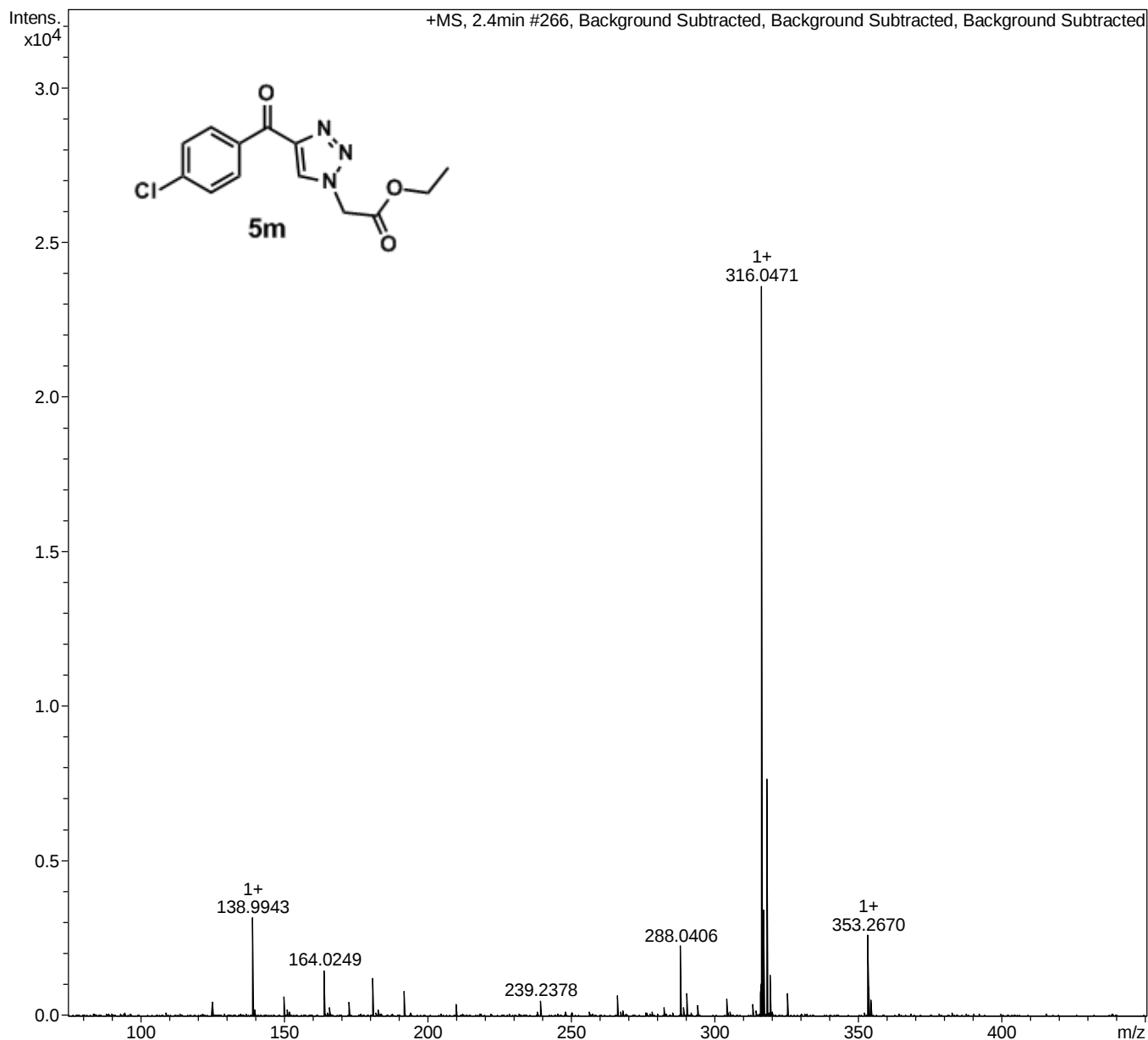


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA6J_293_1-A,10_01_4416.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 4/12/2012 10:32:42 AM
Instrument micrOTOF



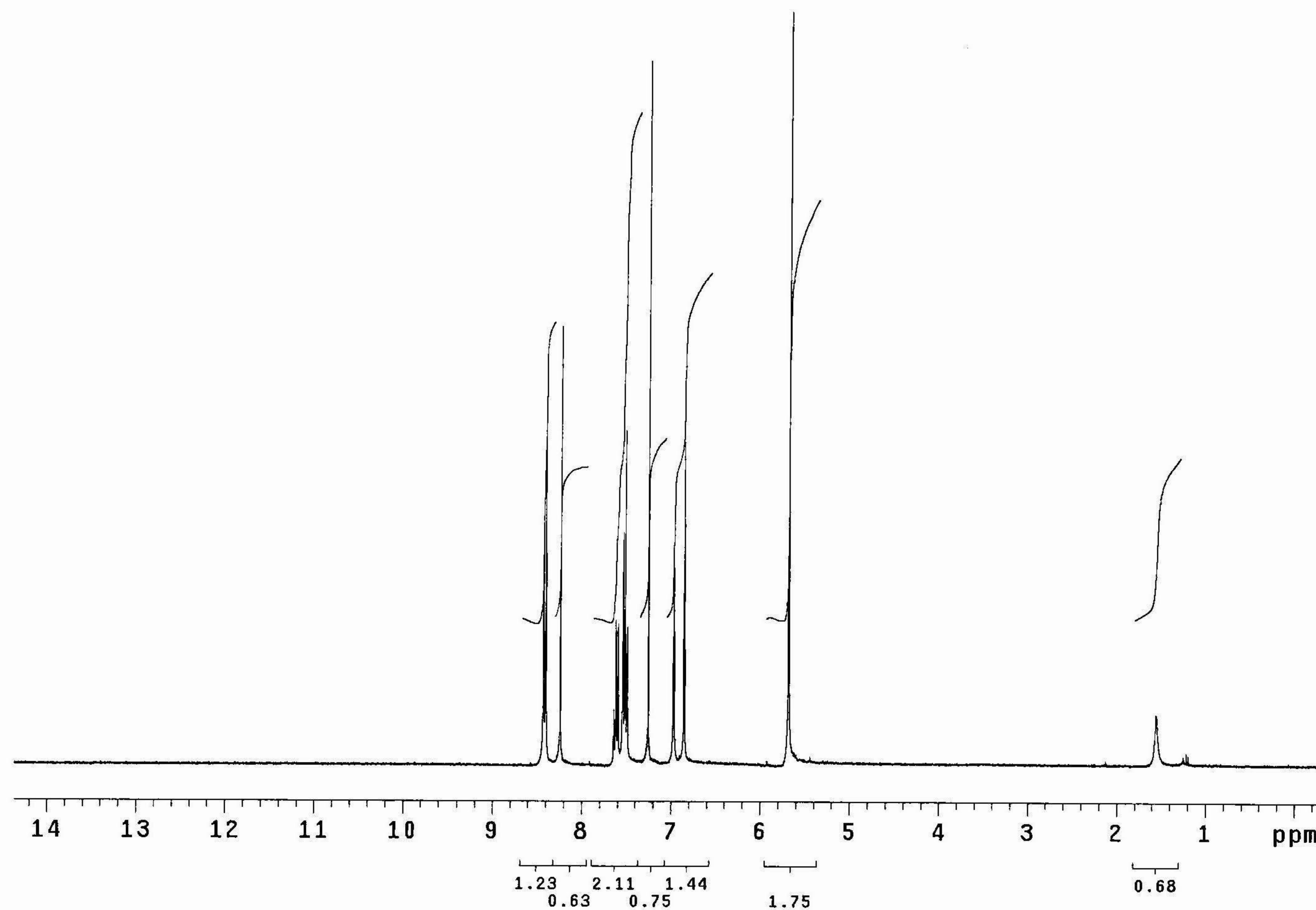
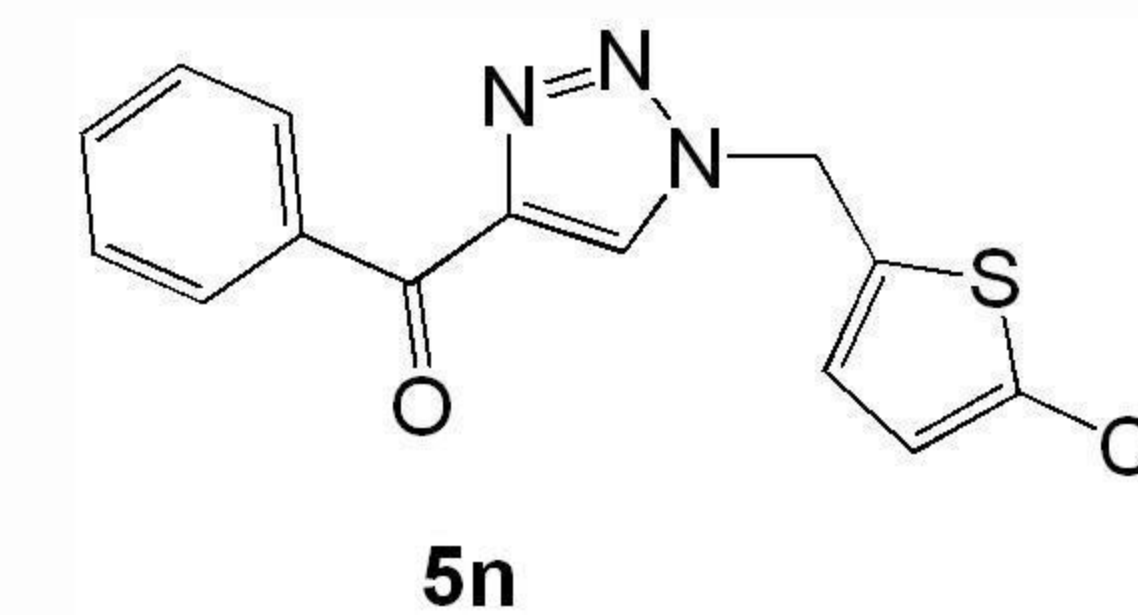
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
316.0471	1	C 13 H 12 Cl N 3 Na O 3	100.00	316.0459	-1.2	-3.7	7.1	8.5	even	ok

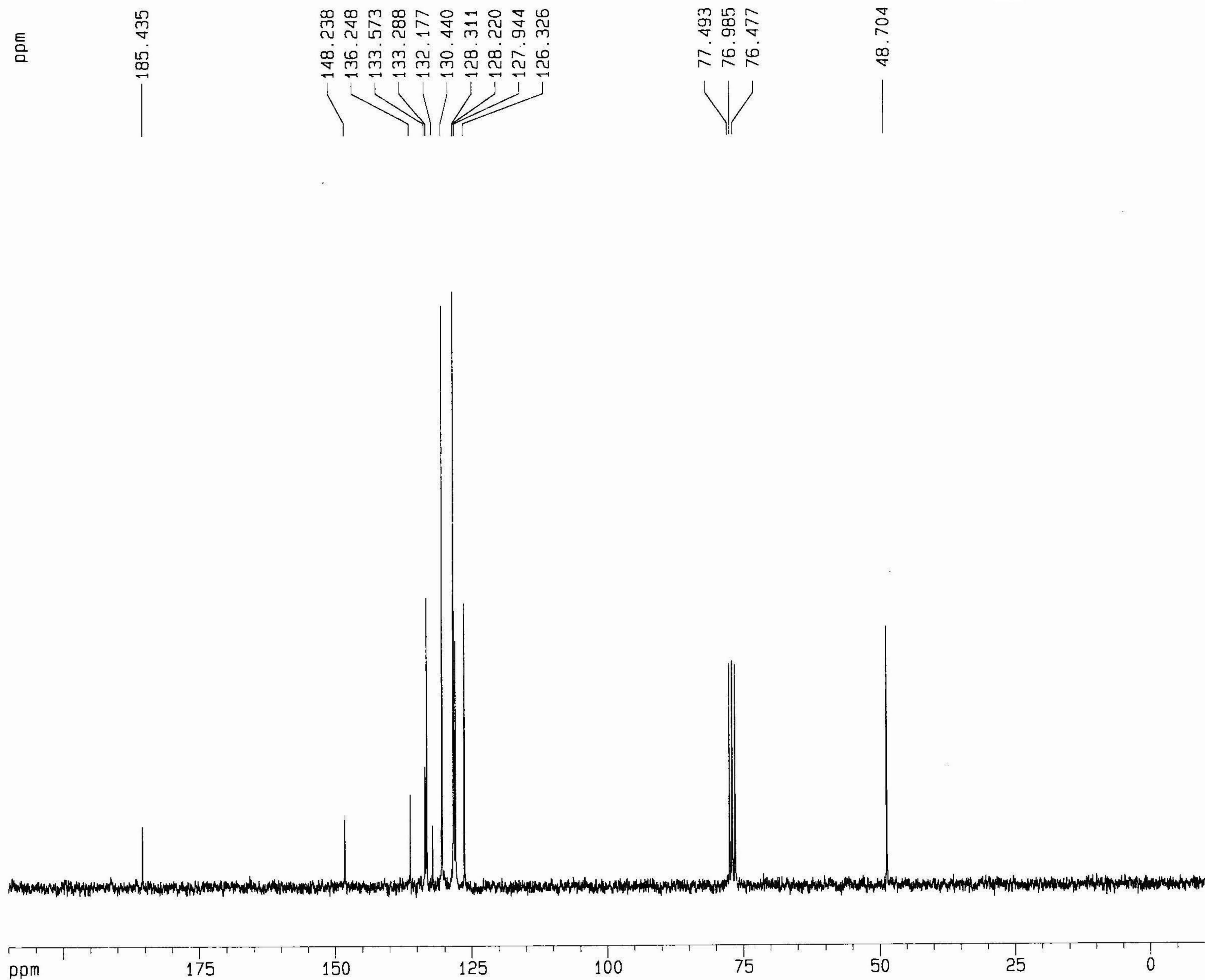
Page 4 of 4

sy11sat141

exp1 s2pu1

SAMPLE		DEC. & VT	
date	Jul 27 2011	dfrq	75.454
solvent	cdc13	dn	C13
file	exp	dpwr	37
ACQUISITION			
sfrq	300.048	dof	0
tn	H1	dm	nnn
at	1.998	dmm	c
np	21576	dmf	13900
sw	5399.6	temp	25.0
PROCESSING			
fb	3000	wtfile	
bs	1	proc	ft
tpwr	59	fn	not used
pw	4.4		
d1	1.000	werr	
tof	659.7	wexp	
nt	100	wbs	
ct	29	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-110.1		
wp	4420.8		
vs	59		
sc	0		
wc	180		
hzmm	24.56		
is	812.38		
rfl	599.5		
rfp	0		
th	9		
ins	1.000		
ai	cdc ph		





Current Data Parameters
NAME sy1isat141
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120203
Time 7.56
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 275
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 8192
DW 26.550 usec
DE 10.50 usec
TE 300.0 K
D1 0.38000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -2.00 dB
SF01 62.9015374 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 15.00 dB
PL13 15.00 dB
SF02 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952479 MHz
WDW EM
SSB 0
LB 2.50 Hz
GB 0
PC 1.40

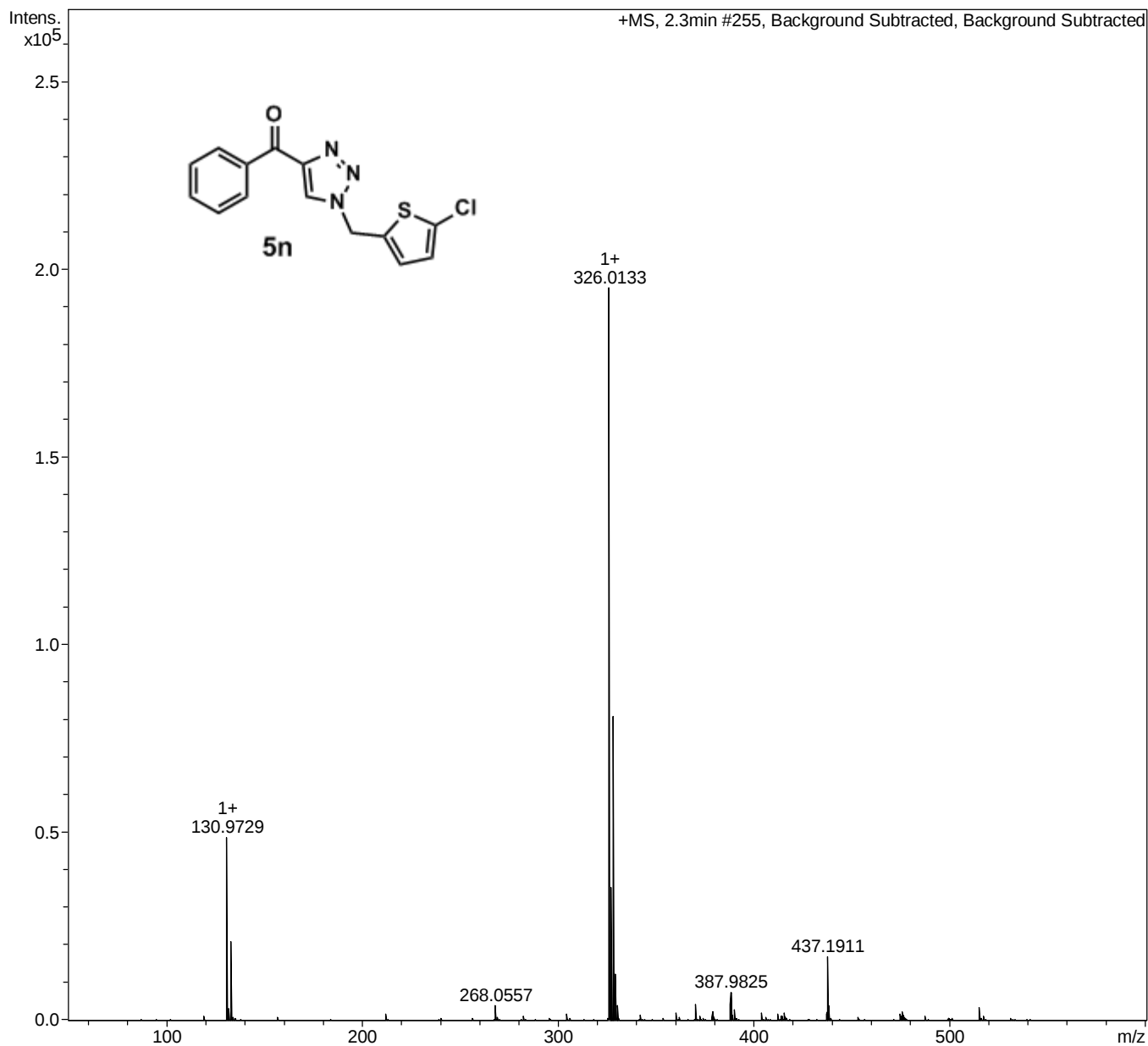
1D NMR plot parameters
CX 20.00 cm
F1P 210.000 ppm
F1 13208.00 Hz
F2P -10.000 ppm
F2 -628.95 Hz
PPMCM 11.00000 ppm/cm
HZCM 691.84772 Hz/cm

ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1ISAT141_303_1-G,8_01_3417.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 2/21/2012 11:42:08 AM
Instrument micrOTOF



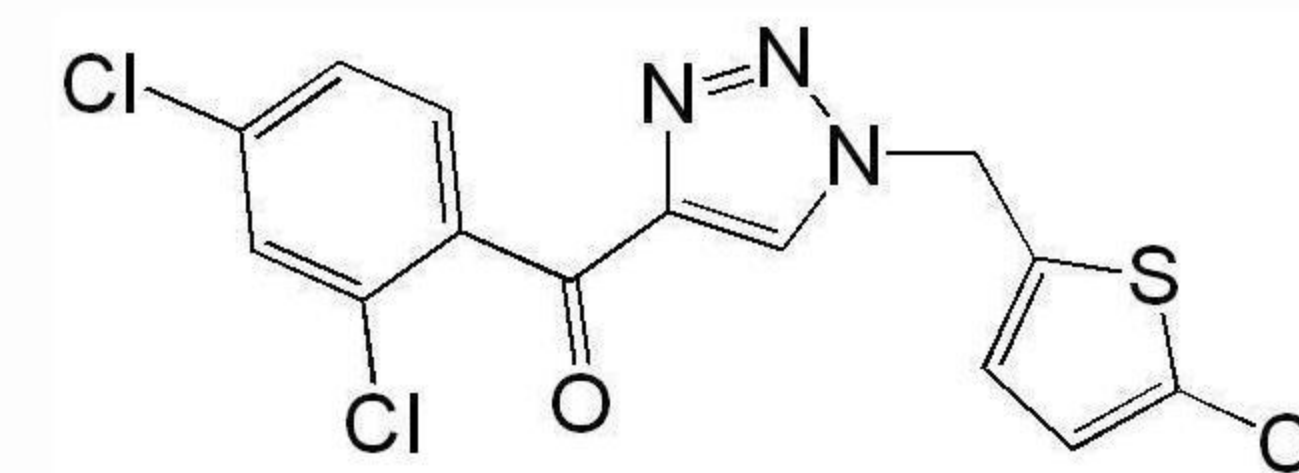
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
326.0133	1	C 14 H 10 Cl N 3 Na O S	100.00	326.0125	-0.8	-2.3	17.0	10.5	even	ok

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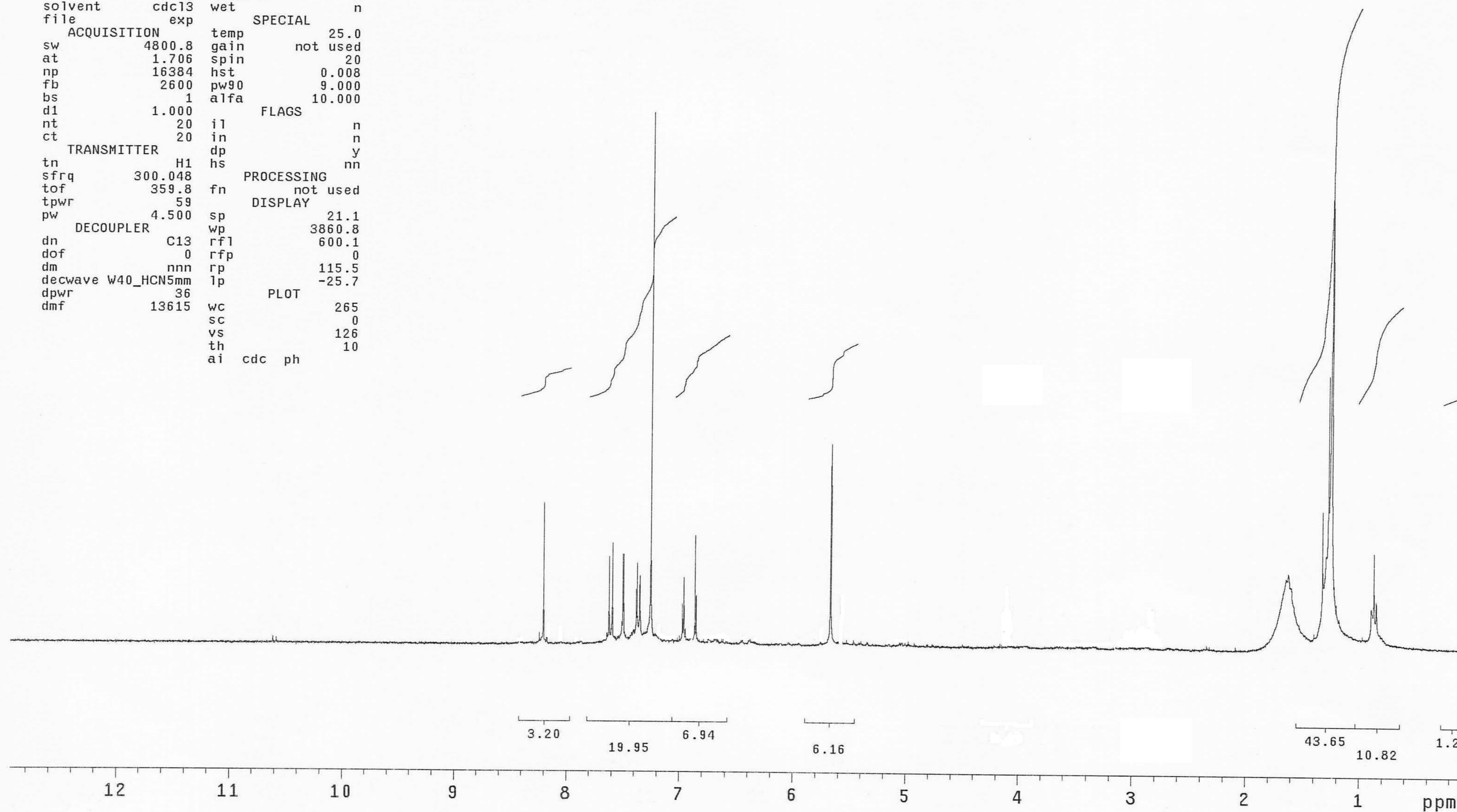
sy1isat147

exp1 PROTON

SAMPLE		PRESATURATION	
date	Jun 28 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	4800.8	gain	not used
at	1.706	spin	20
np	16384	hst	0.008
fb	2600	pw90	9.000
bs	1	alfa	10.000
d1	1.000	FLAGS	
nt	20	il	n
ct	20	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	300.048	PROCESSING	
tof	359.8	fn	not used
tpwr	59	DISPLAY	
pw	4.500	sp	21.1
DECOUPLER		wp	3860.8
dn	C13	rfl	600.1
dof	0	rfl	0
dm	nnn	rp	115.5
decwave	W40_HCN5mm	lp	-25.7
dpwr	36	PLOT	
dmf	13615	wc	265
		sc	0
		vs	126
		th	10
		ai	cdc ph



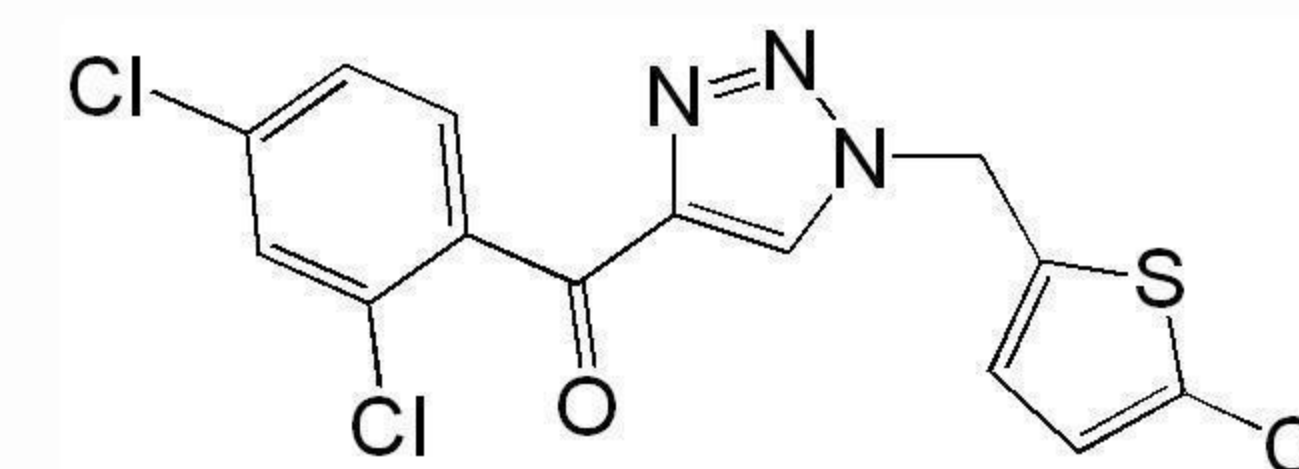
5o



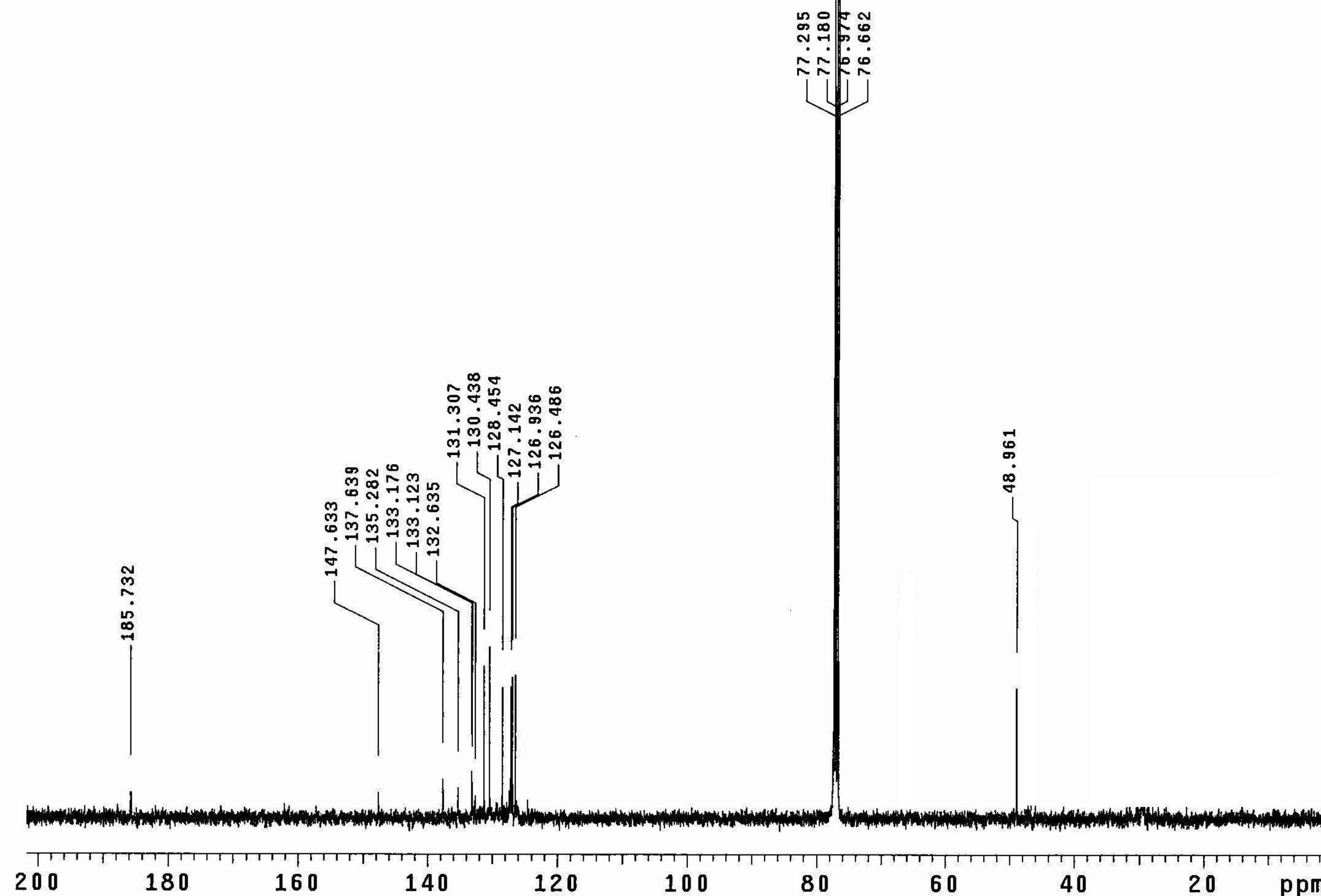
sy11sat147

exp6 CARBON

SAMPLE		PRESATURATION	
date	Feb 14 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	600000	il	n
ct	18562	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	1.40
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-16.2
dn	H1	wp	20300.8
dof	0	rfl	1507.8
dm	yyy	rfp	0
decwave	w	rp	-32.3
dpwr	29	lp	-316.8
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	10670
		th	3
		ai	ph



5o

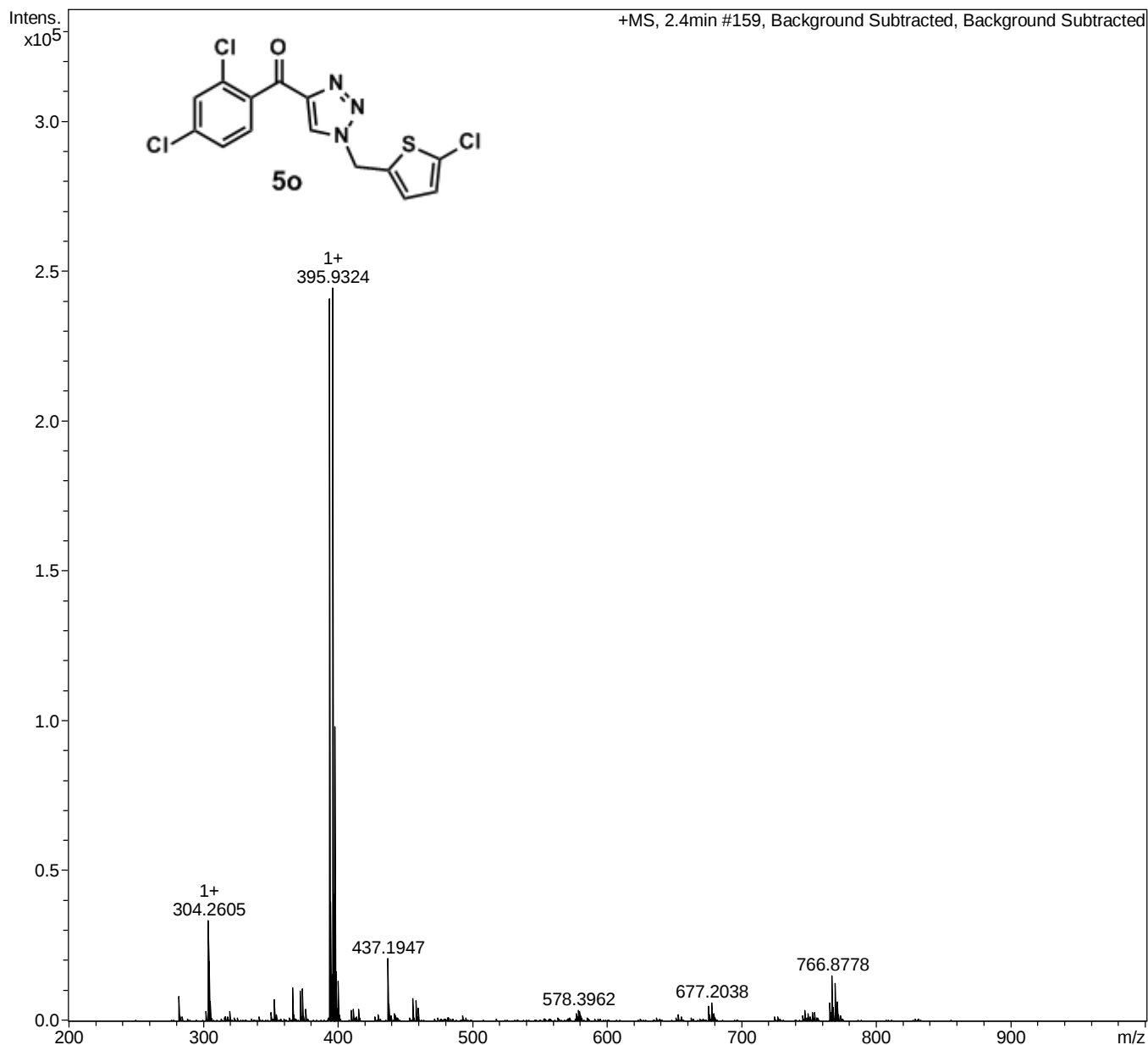


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1ISAT147_372_1-G,6_01_3841.d
 Method fia_pos_medio_350-1500_egf.m

Acquisition Date 3/7/2012 3:21:01 PM
 Instrument micrOTOF



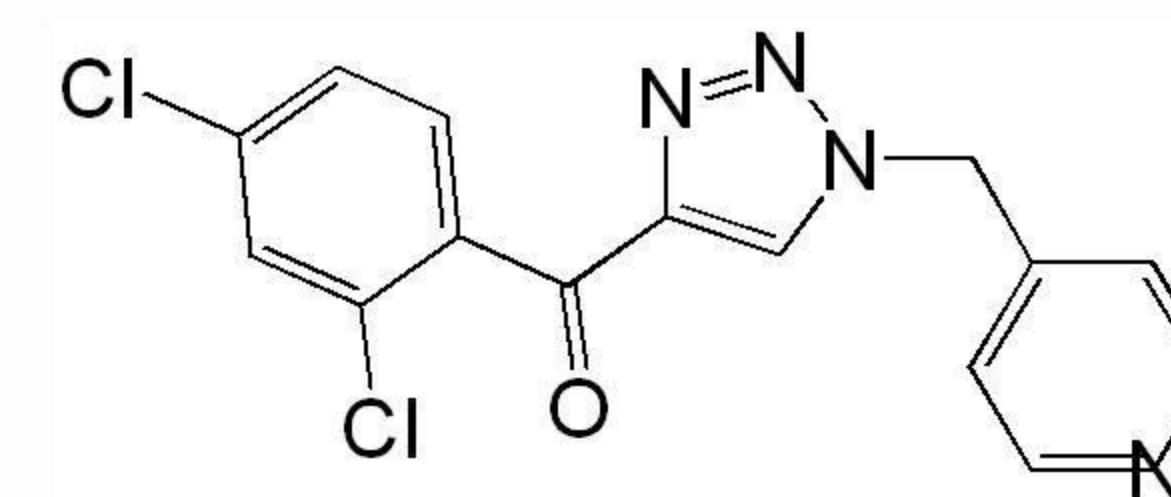
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
393.9351	1	C 14 H 8 Cl 3 N 3 Na O S	100.00	393.9346	-0.5	-1.4	16.4	10.5	even	ok

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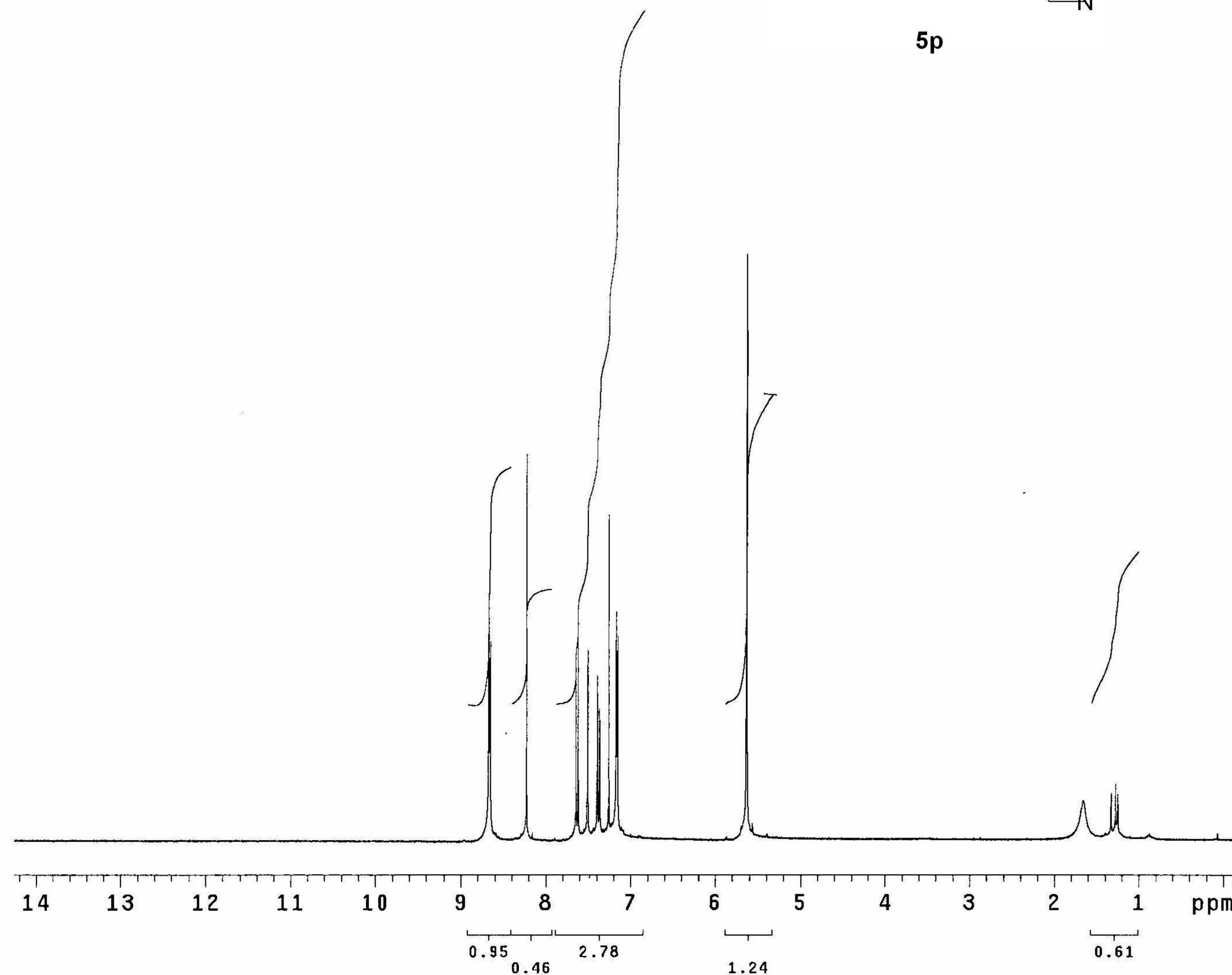
sy1isat148

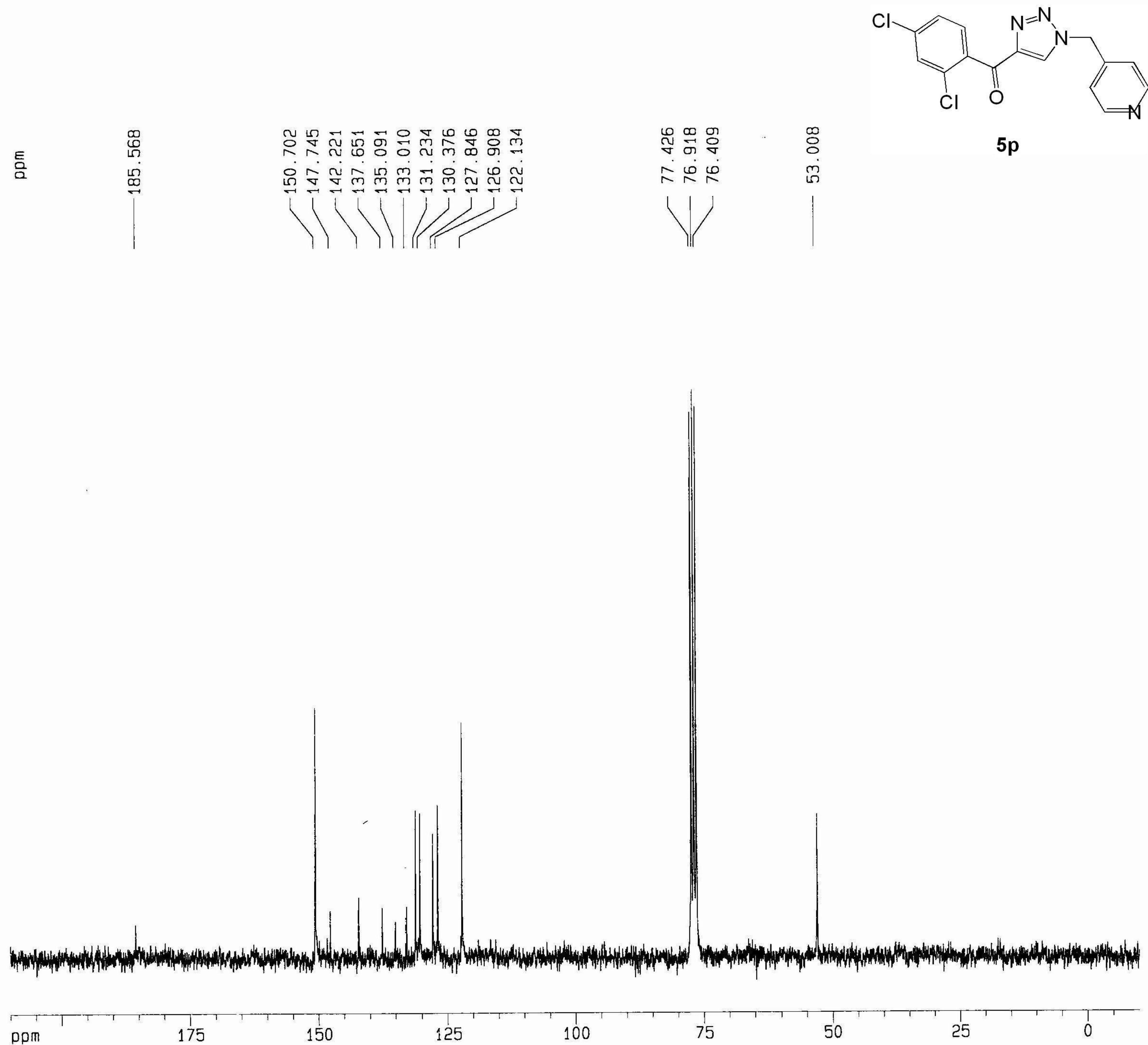
exp1 s2pu1

SAMPLE		DEC. & VT	
date	Jul 27 2011	dfrq	75.454
solvent	cdcl3	dn	C13
file	exp	dpwr	37
ACQUISITION			
sfrq	300.048	dof	0
tn	H1	dm	nnn
at	1.998	dmm	c
np	21576	dmf	13900
sw	5399.6	temp	25.0
PROCESSING			
fb	3000	wtfile	
bs	1	proc	ft
tpwr	59	fn	not used
pw	4.4		
d1	1.000	werr	
tof	659.7	wexp	
nt	100	wbs	
ct	23	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-67.9		
wp	4346.0		
vs	91		
sc	0		
wc	180		
hzmm	24.14		
is	904.71		
rfl	599.5		
rfp	0		
th	4		
ins	1.000		
ai	cdc	ph	



5p





Current Data Parameters
NAME sy11sat148
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120203
Time 8.17
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1023
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 8192
DW 26.550 usec
DE 10.50 usec
TE 300.0 K
D1 0.38000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -2.00 dB
SF01 62.9015374 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 15.00 dB
PL13 15.00 dB
SF02 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952479 MHz
WDW EM
SSB 0
LB 2.50 Hz
GB 0
PC 1.40

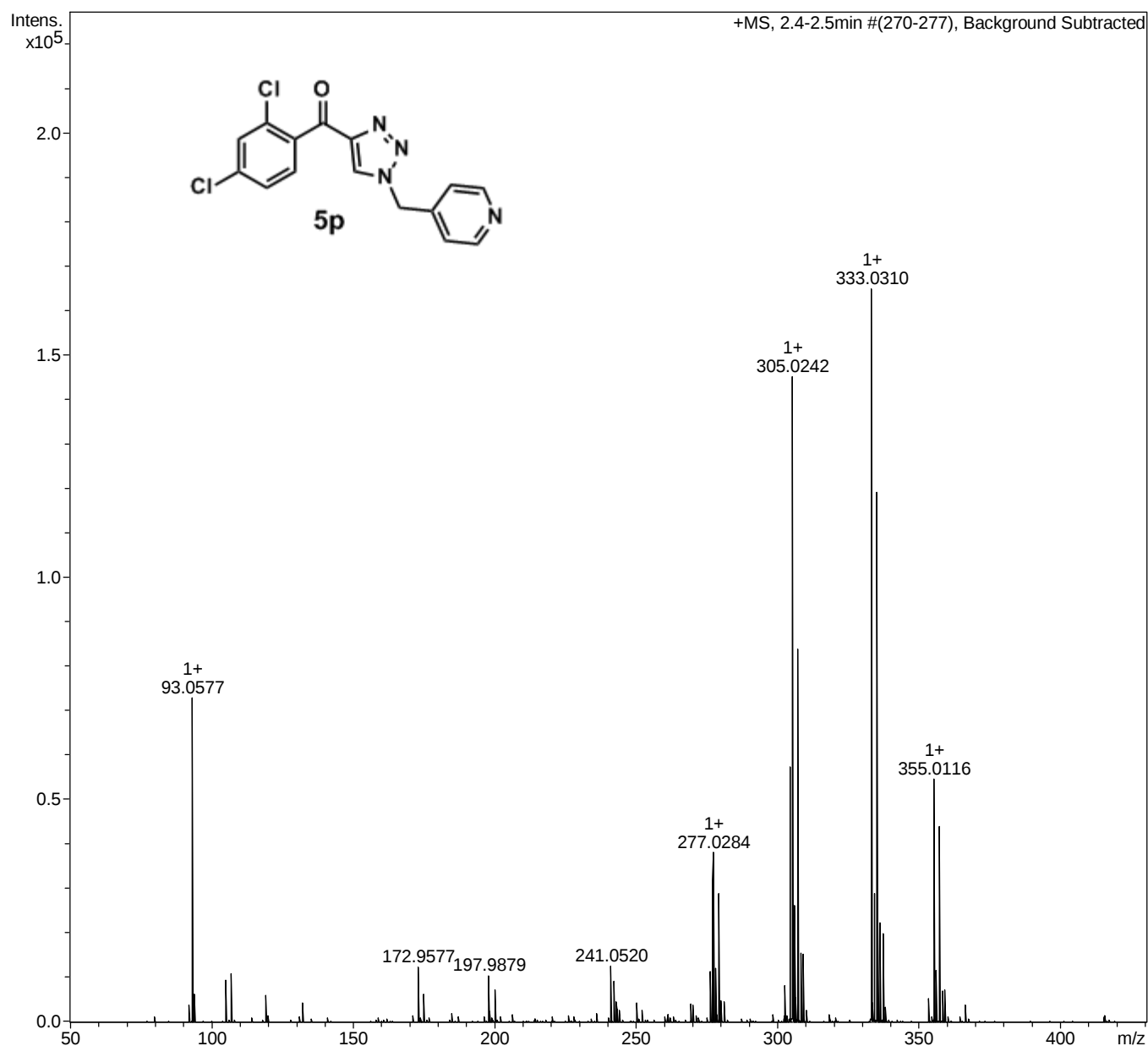
1D NMR plot parameters
CX 20.00 cm
F1P 210.000 ppm
F1 13208.00 Hz
F2P -10.000 ppm
F2 -628.95 Hz
PPMCM 11.00000 ppm/cm
HZCM 691.84772 Hz/cm

ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name S41ISAT148_332_1-H,9_01_3438.d
 Method fia_pos_bajo_50-350_egf.m

Acquisition Date 2/22/2012 11:49:45 AM
 Instrument microTOF



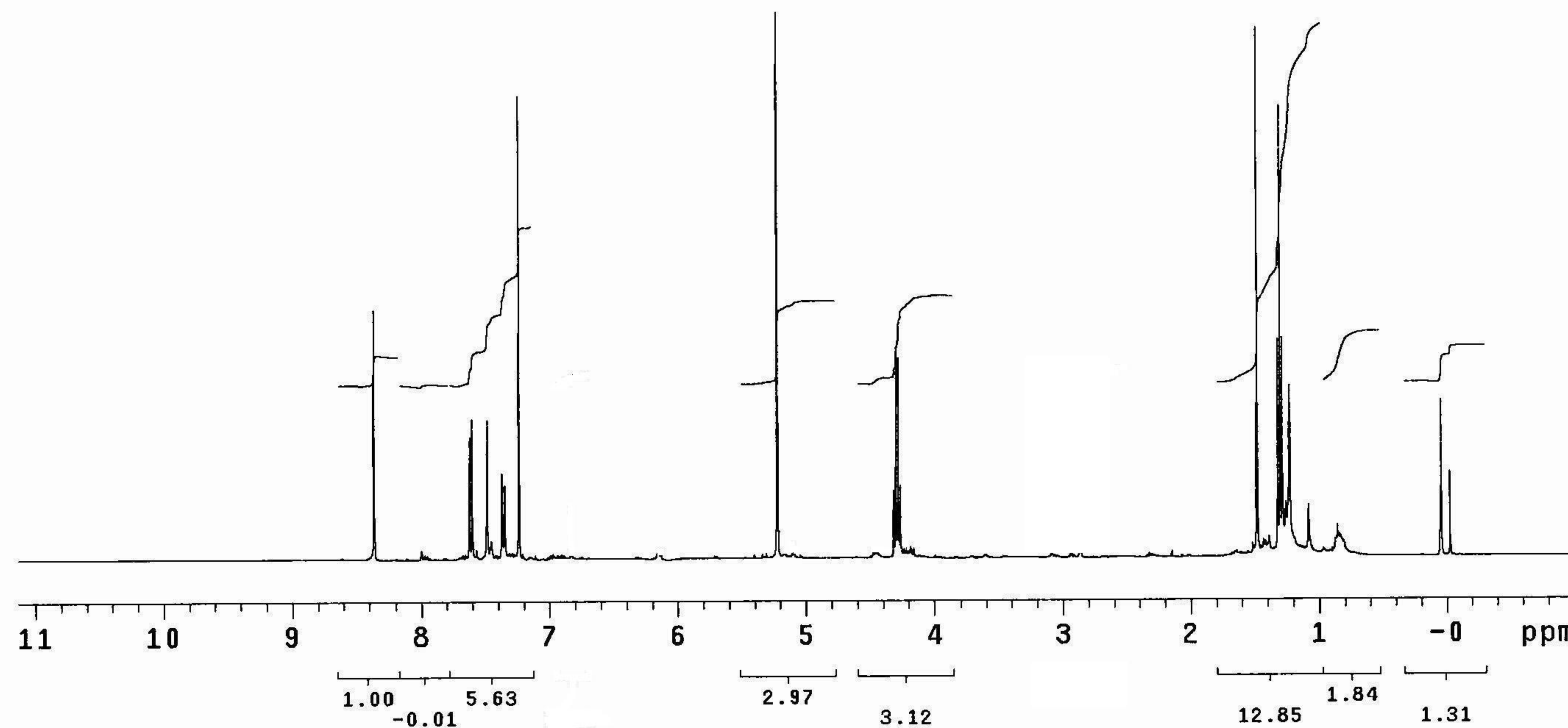
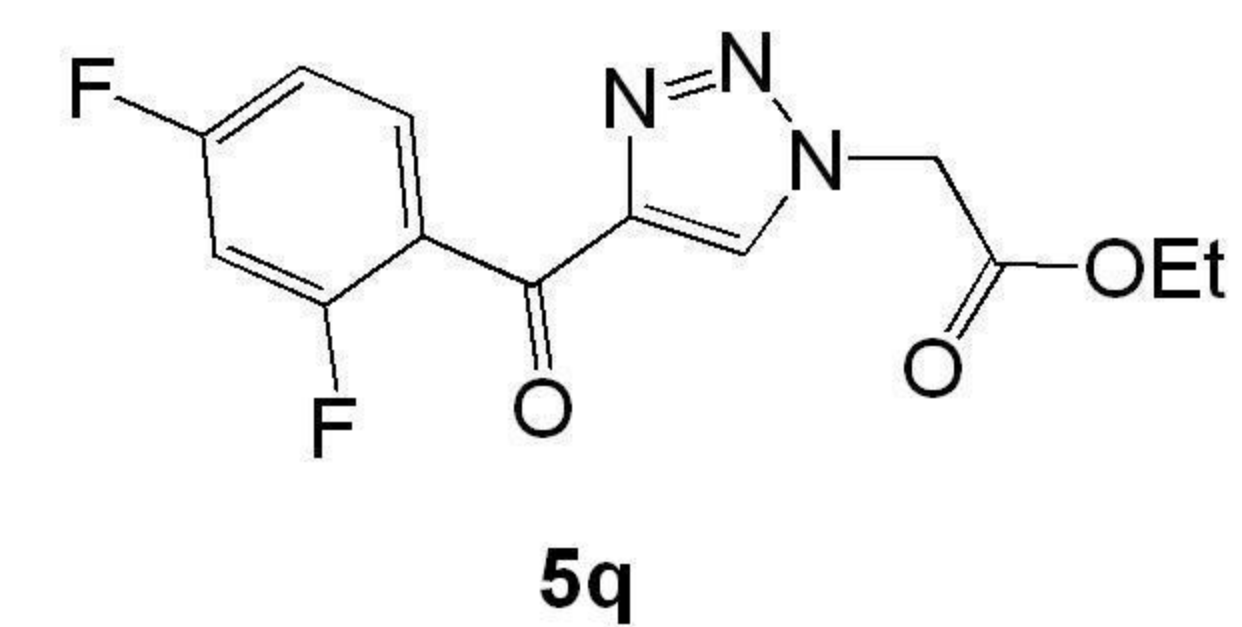
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
333.0310	1	C 15 H 11 Cl 2 N 4 O	100.00	333.0304	-0.5	-1.5	29.5	11.5	even	ok

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sy1pa6t

exp1 PROTON

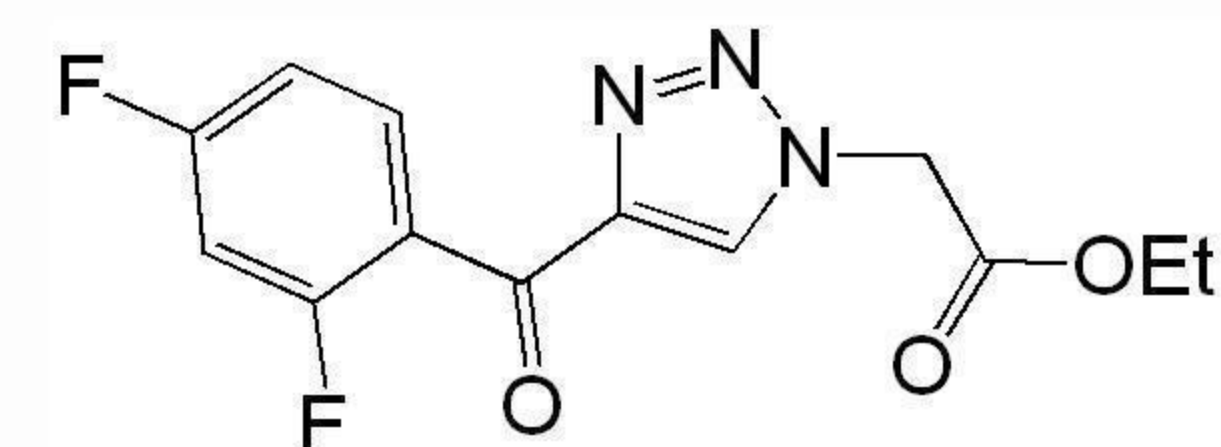
SAMPLE		PRESATURATION	
date	Mar 26 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	7999.2	gain	not used
at	2.048	spin	20
np	32768	hst	0.008
fb	4000	pw90	4.100
bs	1	alfa	6.600
d1	1.000	FLAGS	
nt	128	il	n
ct	128	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq		PROCESSING	
tof	1199.9	lb	0.40
tpwr	56	fn	not used
pw	2.050	DISPLAY	
DECOUPLER		sp	-433.2
dn	C13	wp	4885.7
dof	0	rfl	799.9
dm	nnn	rfl	0
decwave	W40_IDPFG--	rp	-0.3
	4465	lp	16.1
dpwr	46	PLOT	
dmf	18500	wc	180
		sc	0
		vs	48
		th	2
		ai	ph



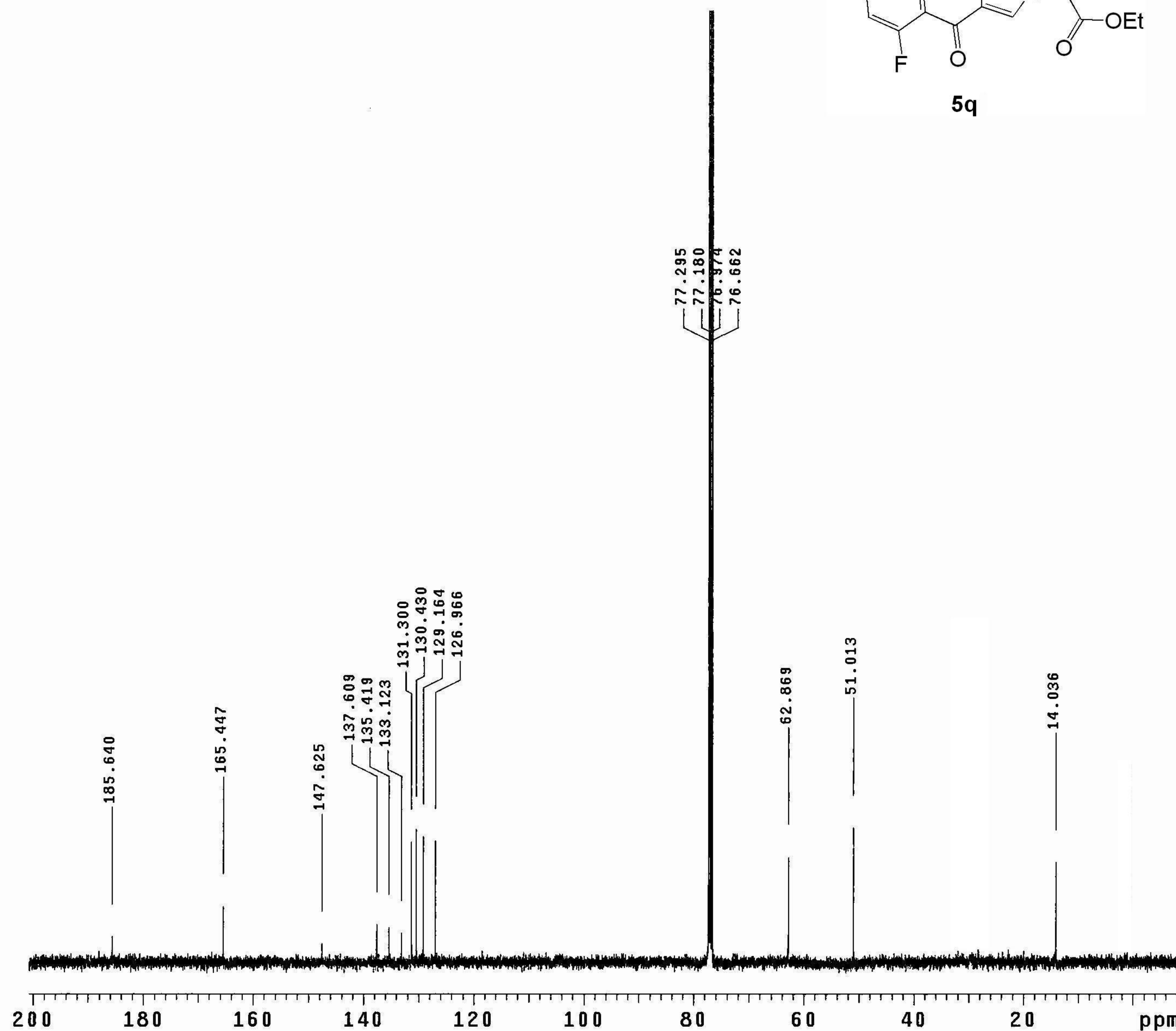
sy1pa6t

exp6 CARBON

SAMPLE		PRESATURATION	
date	Mar 26 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	600000	il	n
ct	24140	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	1.00
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-992.2
dn	H1	wp	21172.4
dof	0	rfl	1507.8
dm	yyy	rfl	0
decwave	w	rp	-29.7
dpwr	29	lp	-324.3
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	7250
		th	2
		ai	ph



5q

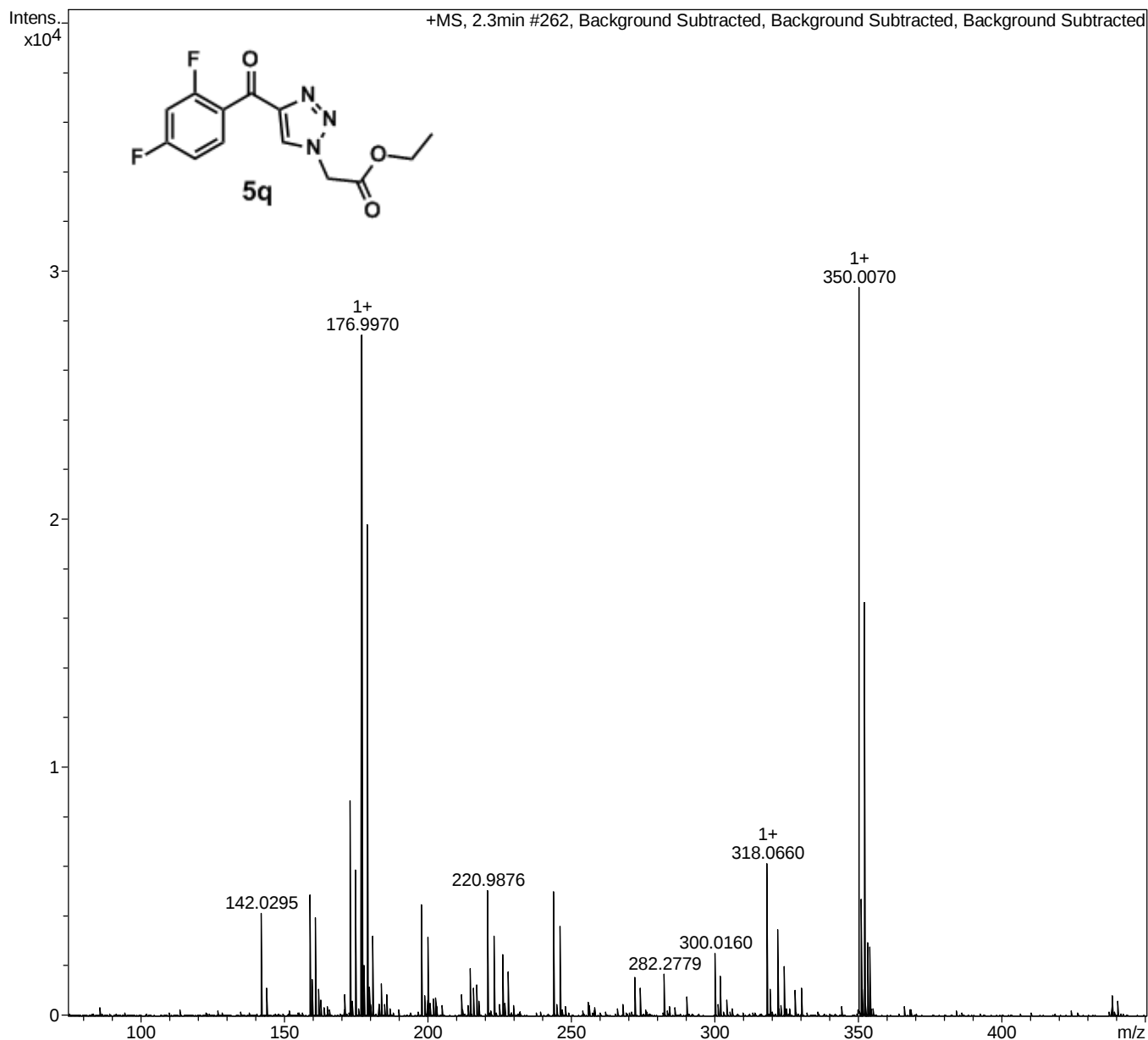


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA6T_295_1-A,11_01_4418.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 4/12/2012 10:50:24 AM
Instrument microTOF



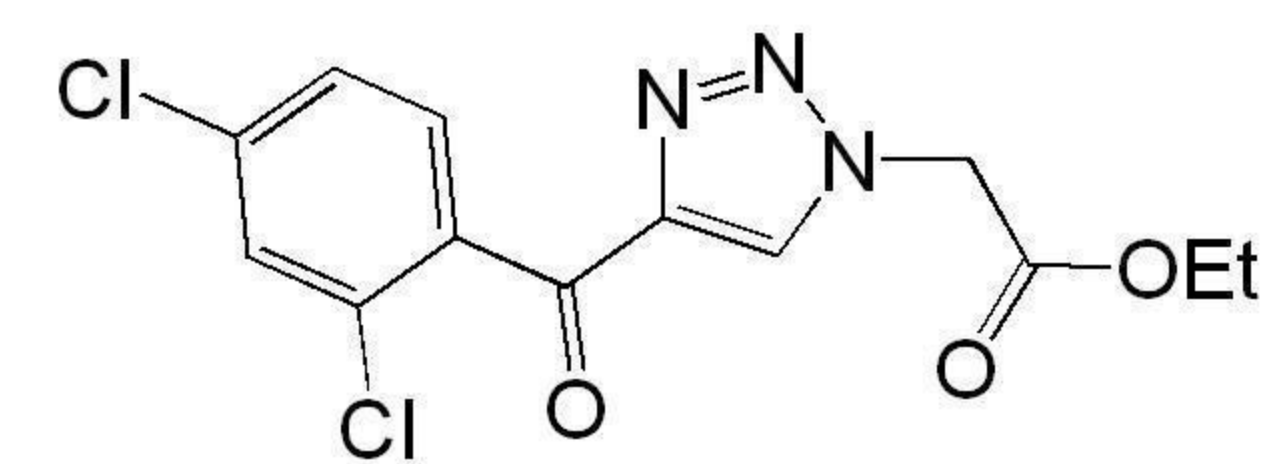
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
318.0660	1	C 13 H 11 F 2 N 3 Na O 3	100.00	318.0661	0.1	0.3	19.7	8.5	even	ok

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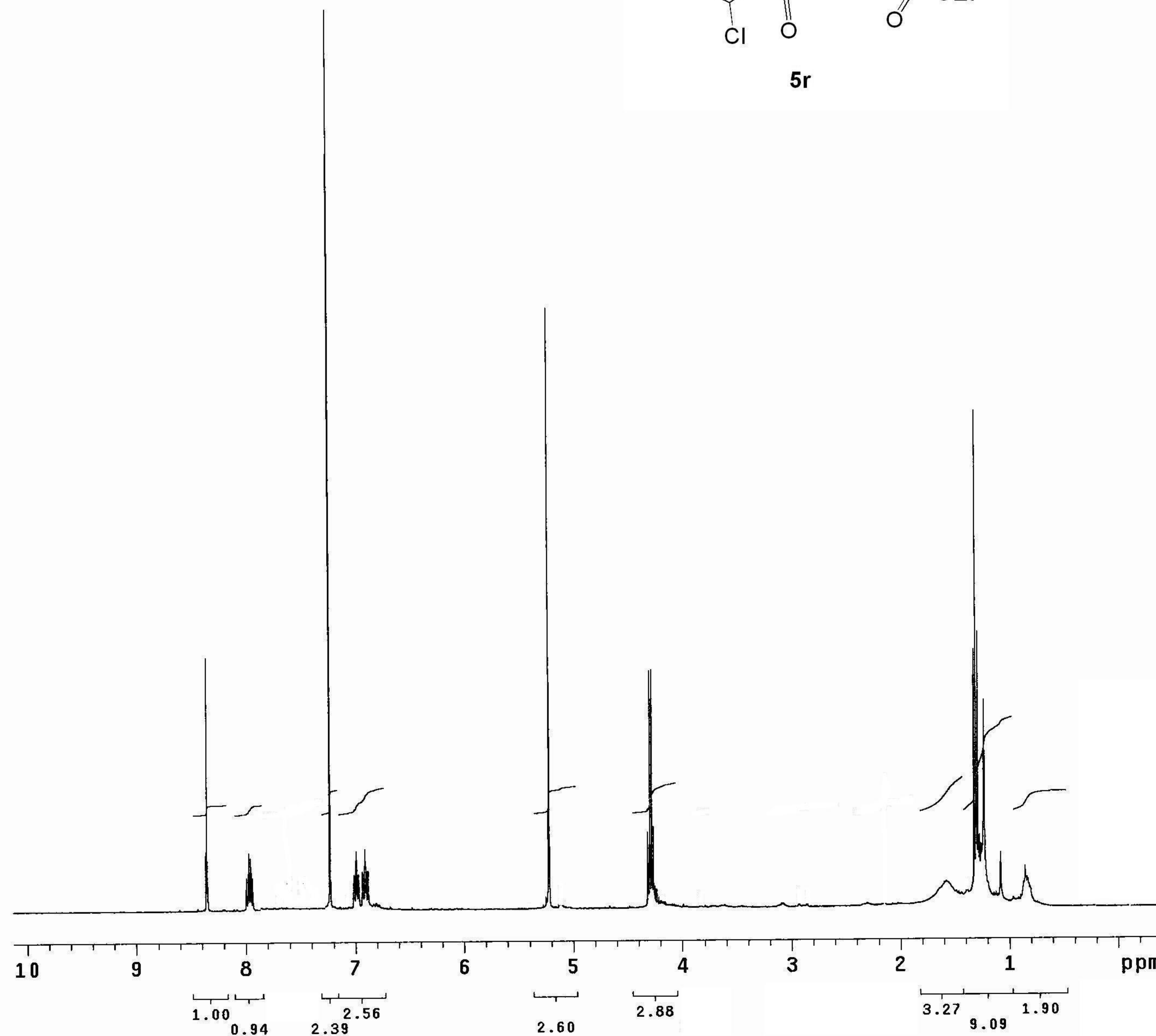
sy1pa6s

exp1 PROTON

SAMPLE		PRESATURATION	
date	Mar 21 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	7999.2	gain	not used
at	2.048	spin	20
np	32768	hst	0.008
fb	4000	pw90	4.100
bs	1	alfa	6.600
d1	1.000	FLAGS	
nt	128	il	n
ct	128	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
PROCESSING		fn	not used
sfrq	399.973		
tof	1199.9		
tpwr	56		
DISPLAY		sp	-183.7
pw	2.050	wp	4234.9
DECOUPLER		rf1	799.9
dn	C13	rfp	0
dof	0	rp	-61.3
dm	nnn	lp	-4.1
decwave W40_IDPFG~			
	4465	PLOT	
dpwr	46	wc	180
dmf	18500	sc	0
		vs	73
		th	1
		ai	ph



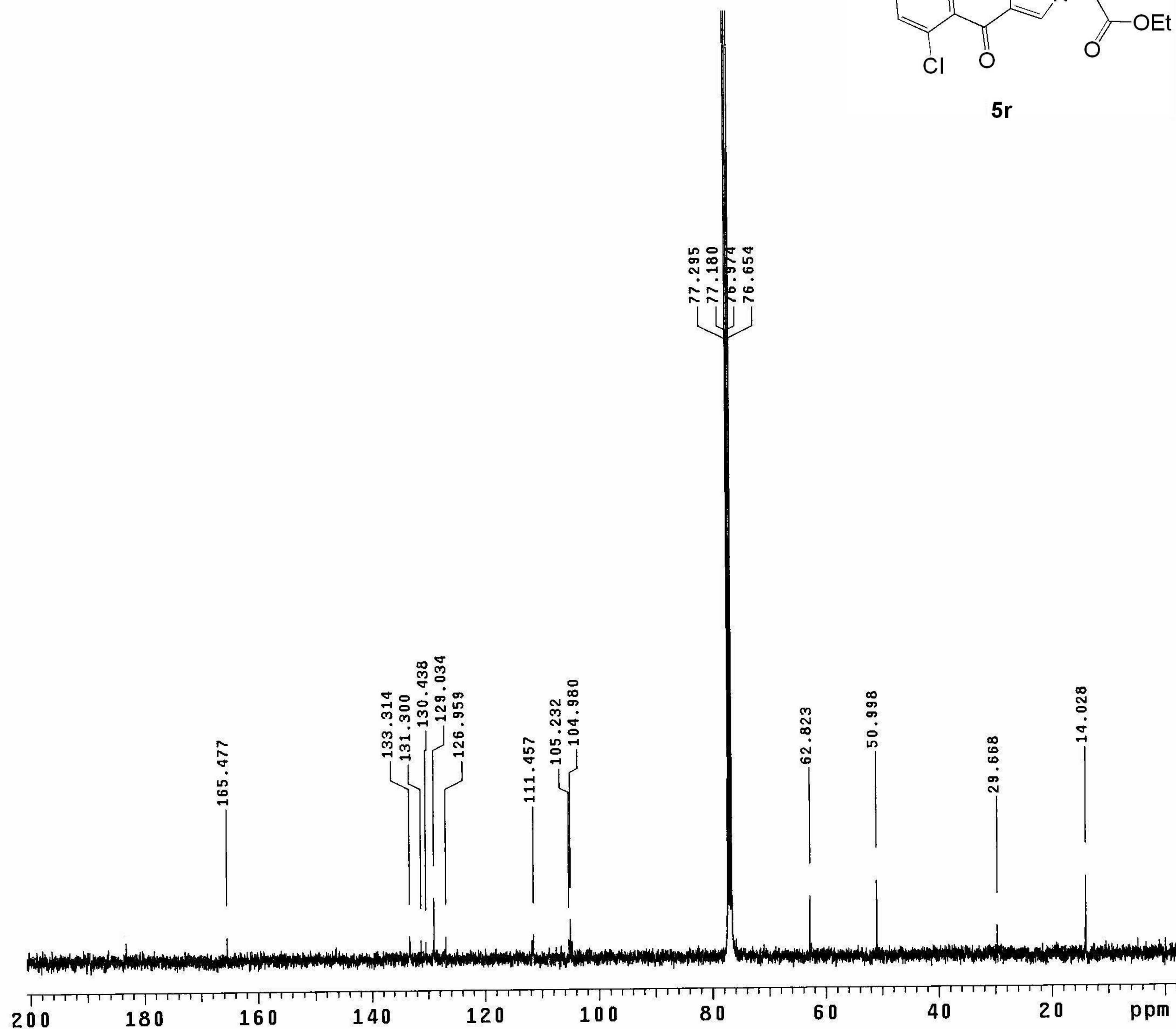
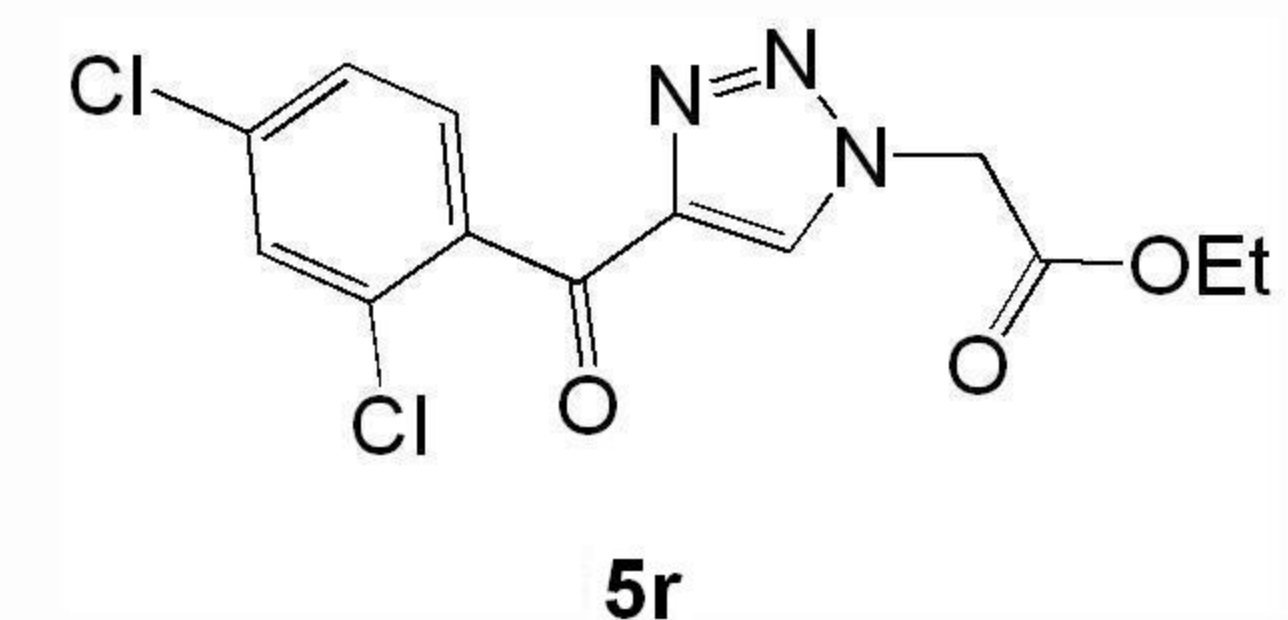
5r



sy1pa6s

exp6 CARBON

SAMPLE		PRESATURATION	
date	Mar 21 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	600000	il	n
ct	23796	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	1.50
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-208.8
dn	H1	wp	20390.6
dof	0	rfl	1507.8
dm	yyy	rff	0
decwave	w	rp	-36.6
dpwr	29	lp	-316.8
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	10445
		th	2
		ai	ph

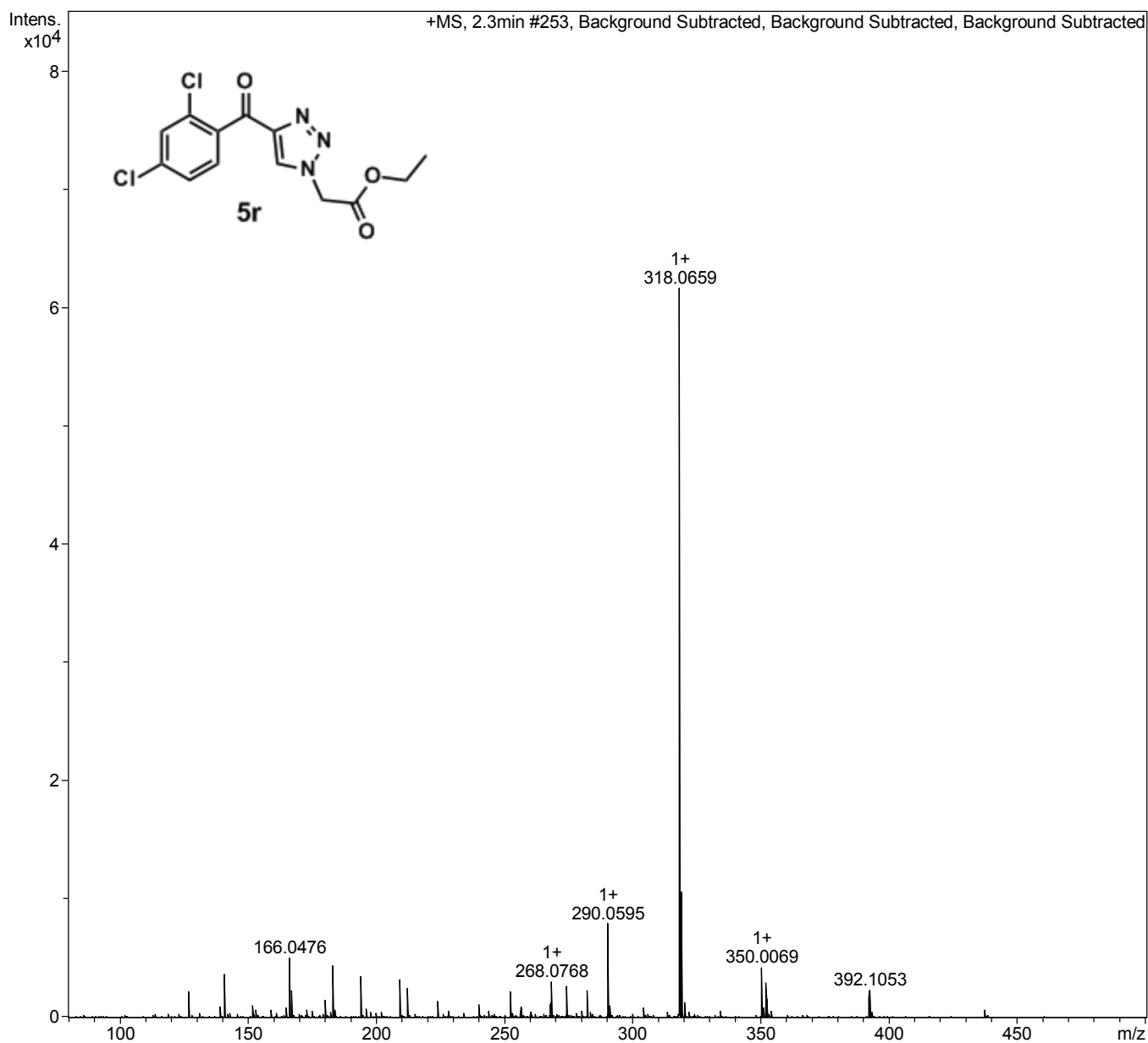


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

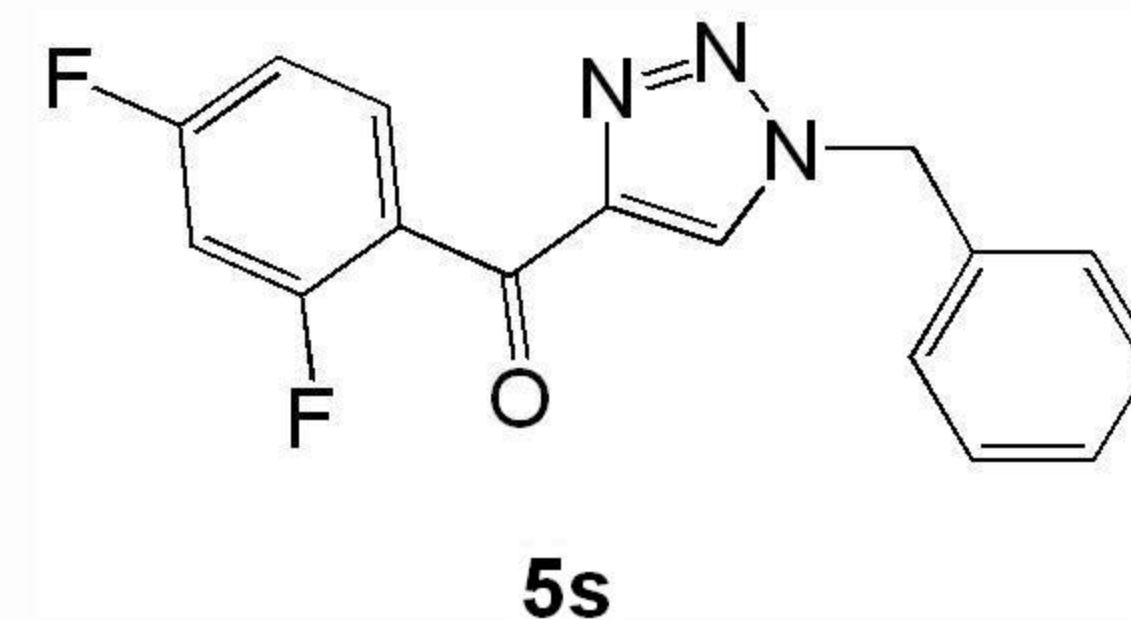
Sample Name SY1PA65_327_1-A,9_01_4415.d
 Method fia_pos_bajo_50-350_egf.m

Acquisition Date 4/12/2012 10:23:50 AM
 Instrument micrOTOF



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
350.0069	1	C 13 H 11 Cl 2 N 3 Na O 3	100.00	350.0070	0.1	0.3	26.9	8.5	even		ok

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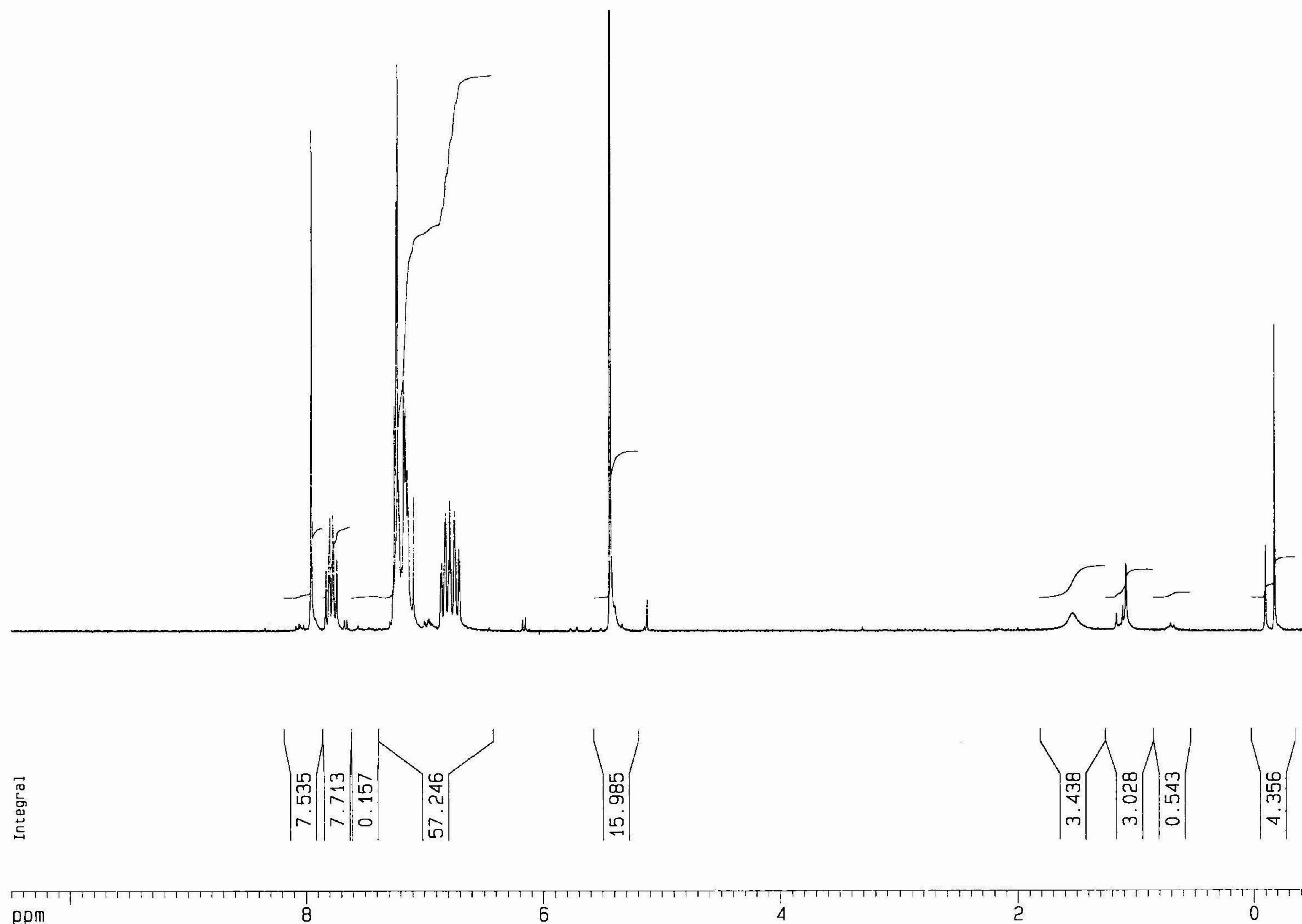
Current Data Parameters
 NAME syipa63
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081211
 Time 12.13
 INSTRUM spect
 PROBHD 5 mm Dual 13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 362
 DW 111.200 usec
 DE 10.50 usec
 TE 300.0 K
 D1 1.50000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 -6.00 dB
 SF01 250.1315581 MHz

F2 - Processing parameters
 SI 16384
 SF 250.1300498 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

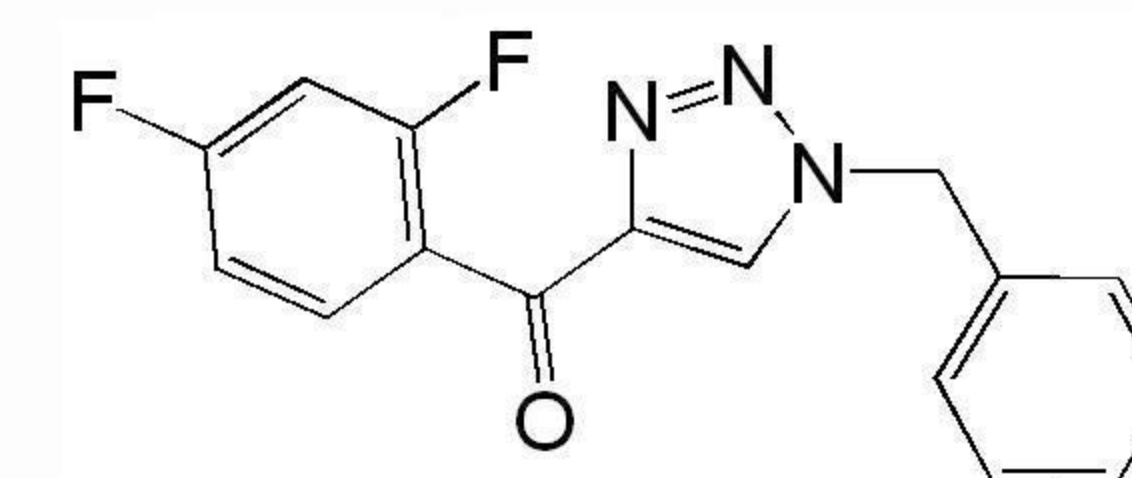
1D NMR plot parameters
 CX 20.00 cm
 F1P 10.500 ppm
 F1 2626.37 Hz
 F2P -0.500 ppm
 F2 -125.07 Hz
 PPMCM 0.55000 ppm/cm
 HZCM 137.57153 Hz/cm



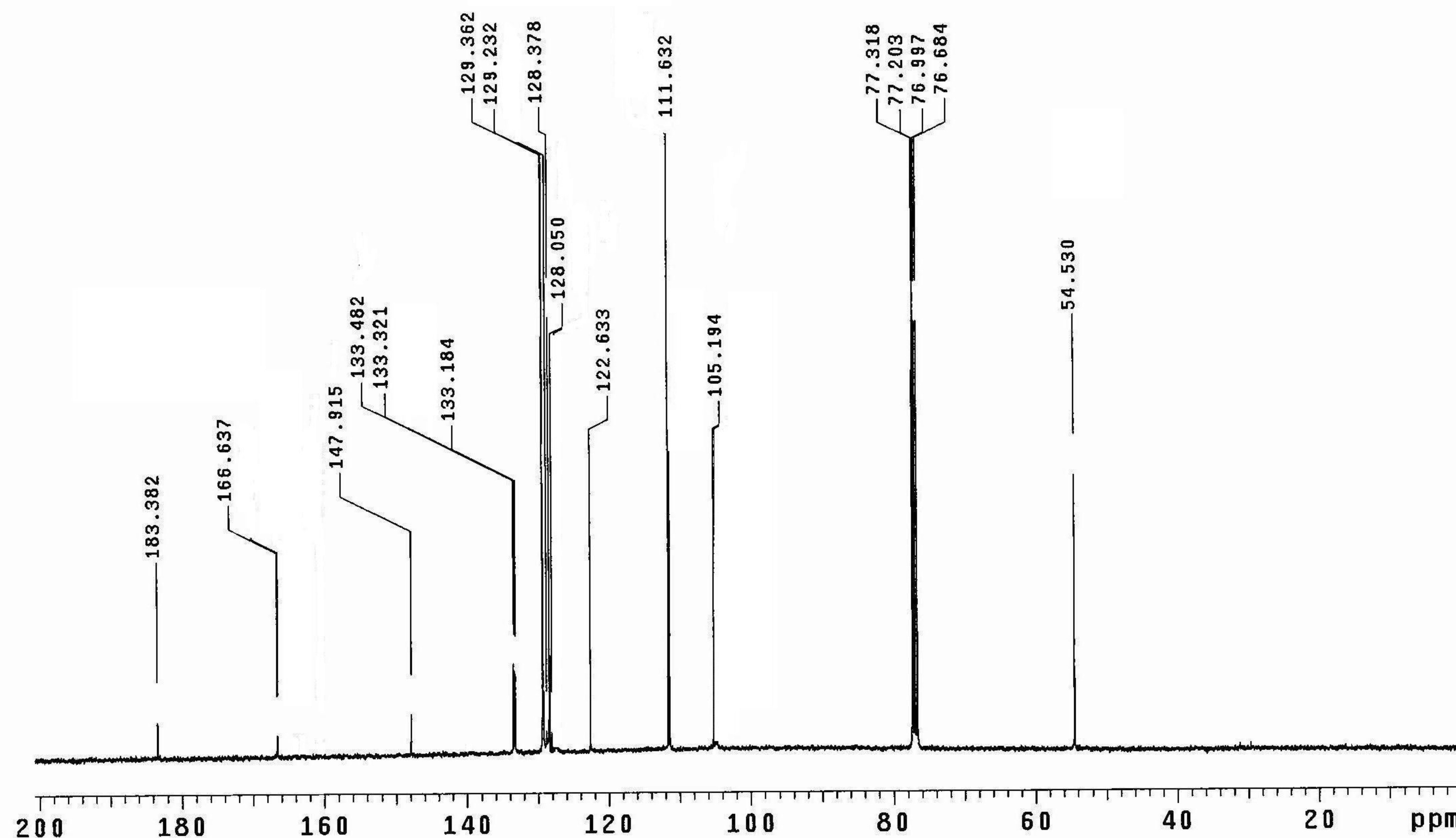
sy1pa64

exp6 CARBON

SAMPLE		PRESATURATION	
date	Mar 20 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	600000	il	n
ct	23072	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	2.00
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-117.5
dn	H1	wp	20300.0
dof	0	rfl	1507.8
dm	yyy	rfl	0
decwave	w	rp	-36.0
dpwr	29	lp	-309.7
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	3179
		th	2
		ai	ph



5s

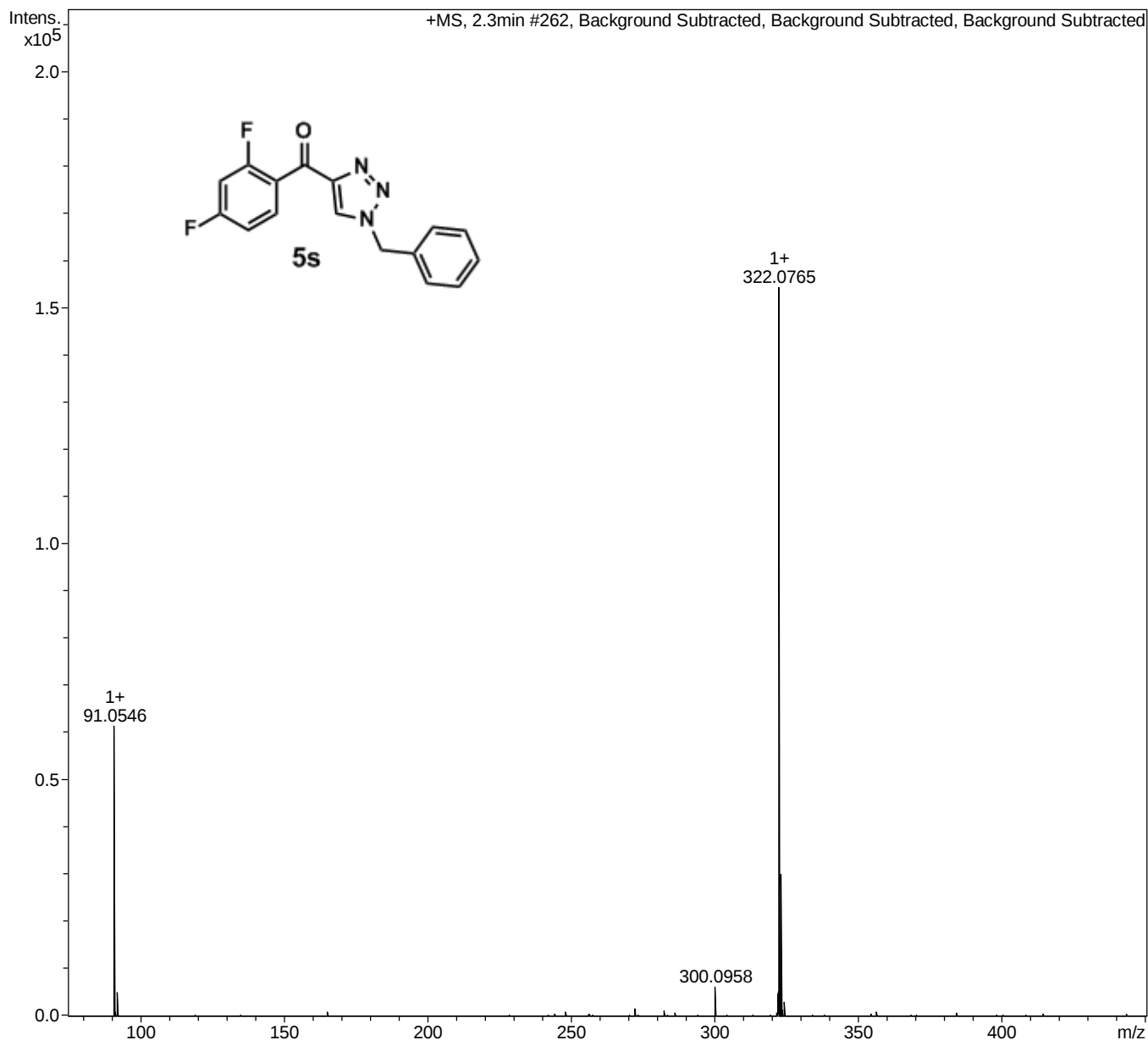


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA6H_299_1-B,1_01_4421.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 4/12/2012 11:16:59 AM
Instrument micrOTOF



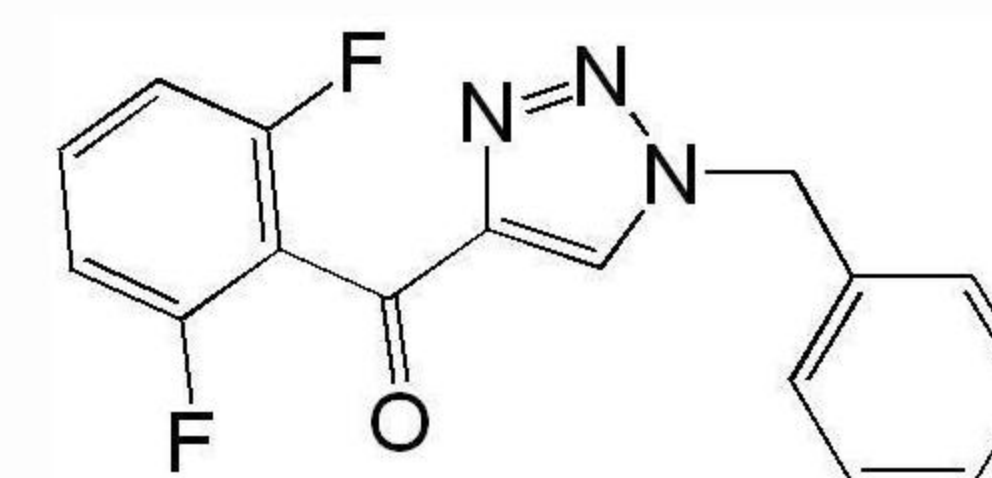
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
322.0765	1	C 16 H 11 F 2 N 3 Na O	100.00	322.0762	-0.3	-0.9	6.5	11.5	even	ok

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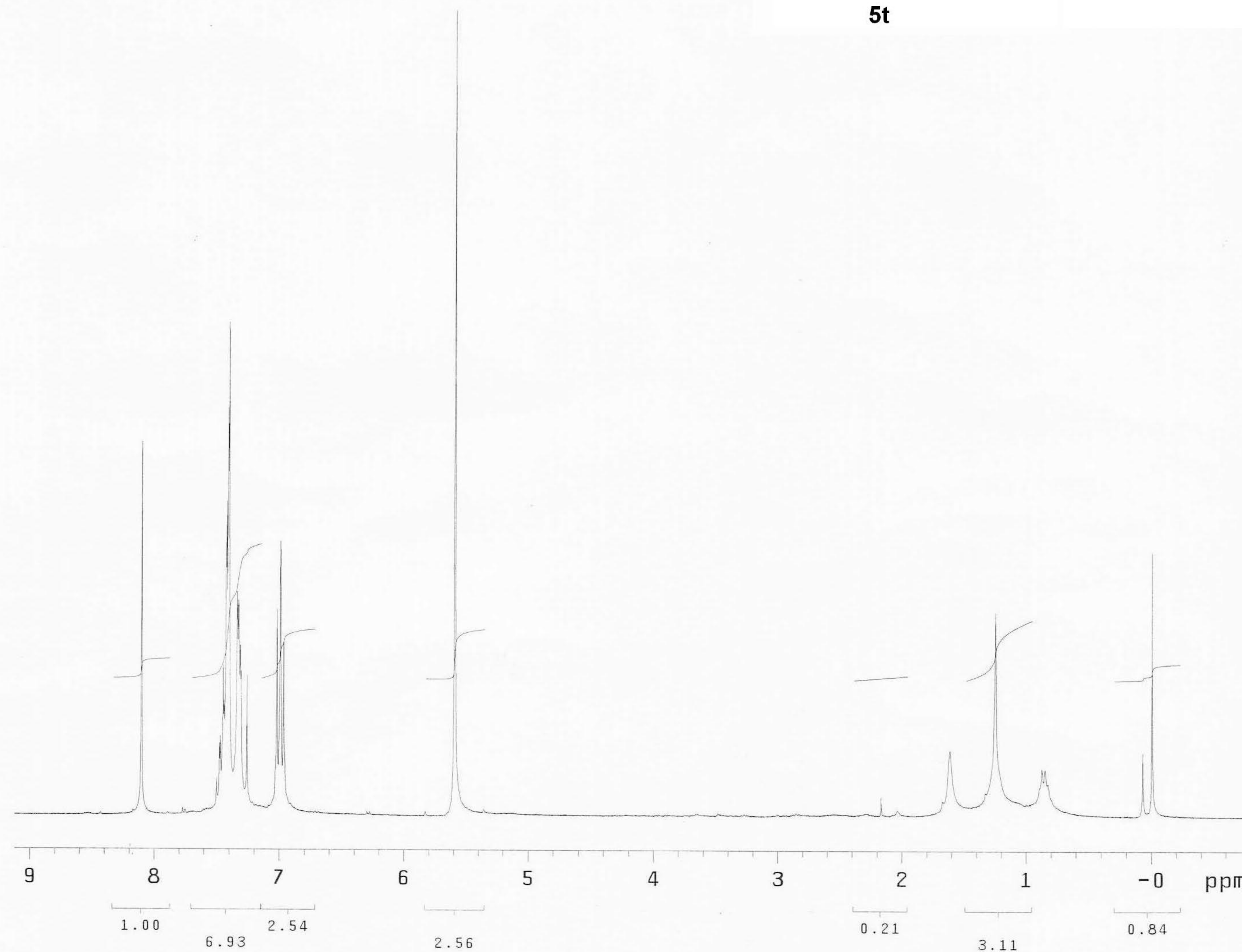
sy1pa73b

exp100 Proton

SAMPLE		DEC. & VT	
date	Jan 21 2009	dfrq	75.454
solvent	cdcl3	dn	C13
file	exp	dpwr	37
ACQUISITION		PROCESSING	
sfrq	300.048	dof	0
tn	H1	dm	nnn
at	1.706	dmm	c
np	16384	dmf	13900
sw	4800.8	temp	25.0
fb	2600	wtfile	
bs	1	proc	ft
tpwr	59	fn	32768
pw	4.4		
d1	1.000	werr	
tof	238.9	wexp	
nt	400	wbs	
ct	33	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-248.2		
wp	2985.2		
vs	143		
sc	0		
wc	180		
hzmm	16.58		
is	159.10		
rfl	720.8		
rfl	0		
th	4		
ins	1.000		
ai	ph		



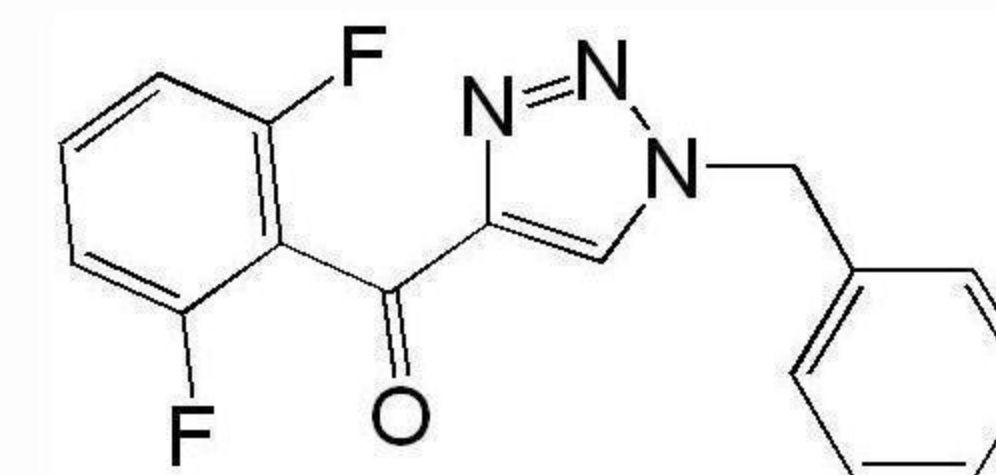
5t



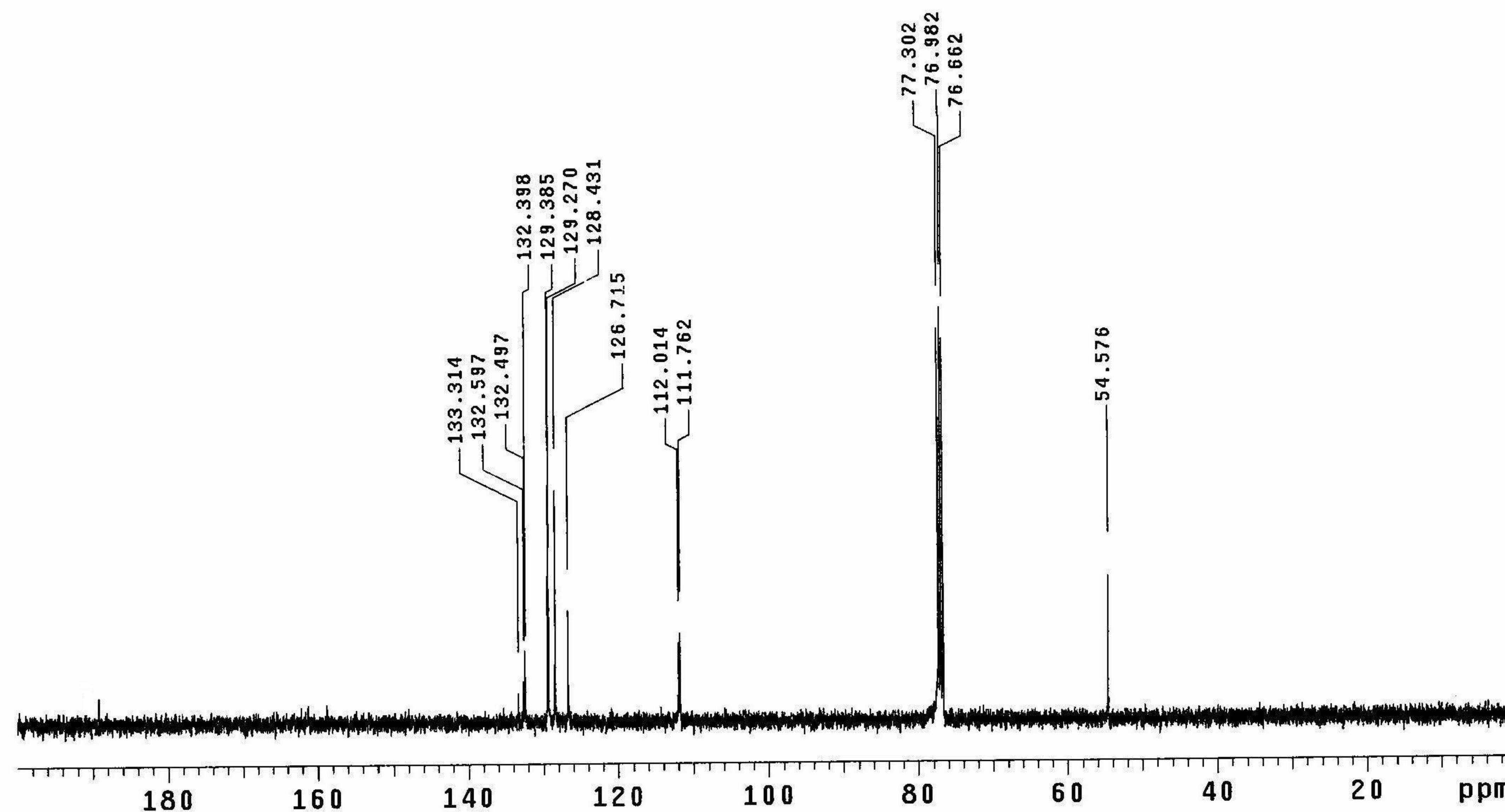
sy1spt73

exp6 CARBON

SAMPLE		PRESATURATION	
date	Feb 15 2012	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25141.4	gain	not used
at	1.303	spin	20
np	65536	hst	0.008
fb	14000	pw90	14.600
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	600000	il	n
ct	7380	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	100.583	PROCESSING	
tof	1531.4	lb	1.00
tpwr	61	fn	not used
pw	7.300	DISPLAY	
DECOUPLER		sp	-46.1
dn	H1	wp	20158.1
dof	0	rfl	1507.8
dm	YYY	rpf	0
decwave	w	rp	2.8
dpwr	29	lp	-387.5
dmf	9700	PLOT	
		wc	180
		sc	0
		vs	4471
		th	3
		ai	ph



5t

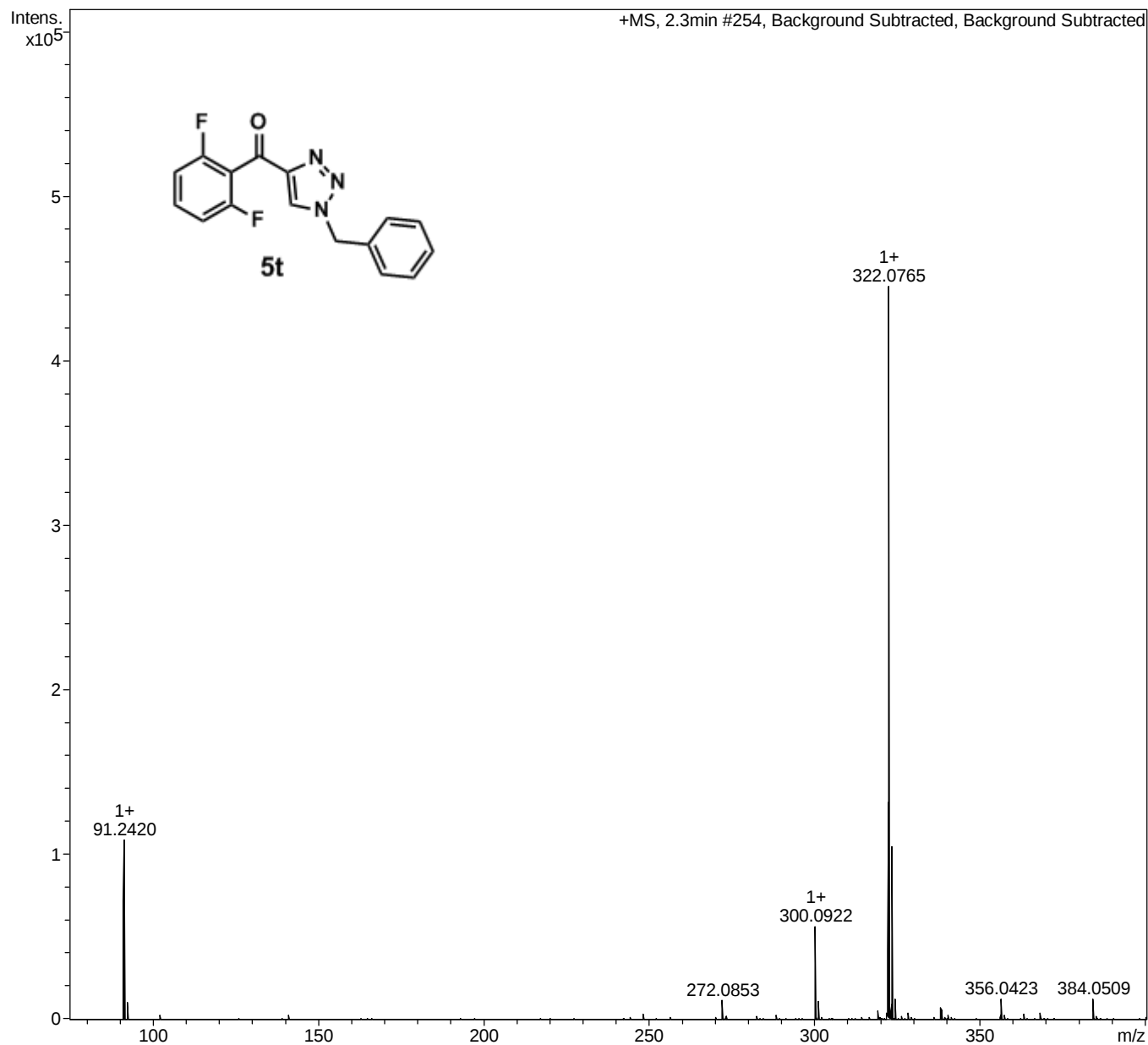


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA73B_299_1-H,1_01_3858.d
 Method fia_pos_bajo_50-350_egf.m

Acquisition Date 3/8/2012 11:13:50 AM
 Instrument micrOTOF



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
322.0765	1	C 16 H 11 F 2 N 3 Na O	100.00	322.0762	-0.2	-0.8	31.1	11.5	even	ok

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5u

Current Data Parameters

NAME sy1pa90b
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20090504
Time 17.46
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 0
SWH 3742.515 Hz
FIDRES 0.114212 Hz
AQ 4.3778548 sec
RG 512
DW 133.600 usec
DE 10.50 usec
TE 300.0 K
D1 1.50000000 sec

===== CHANNEL f1 =====

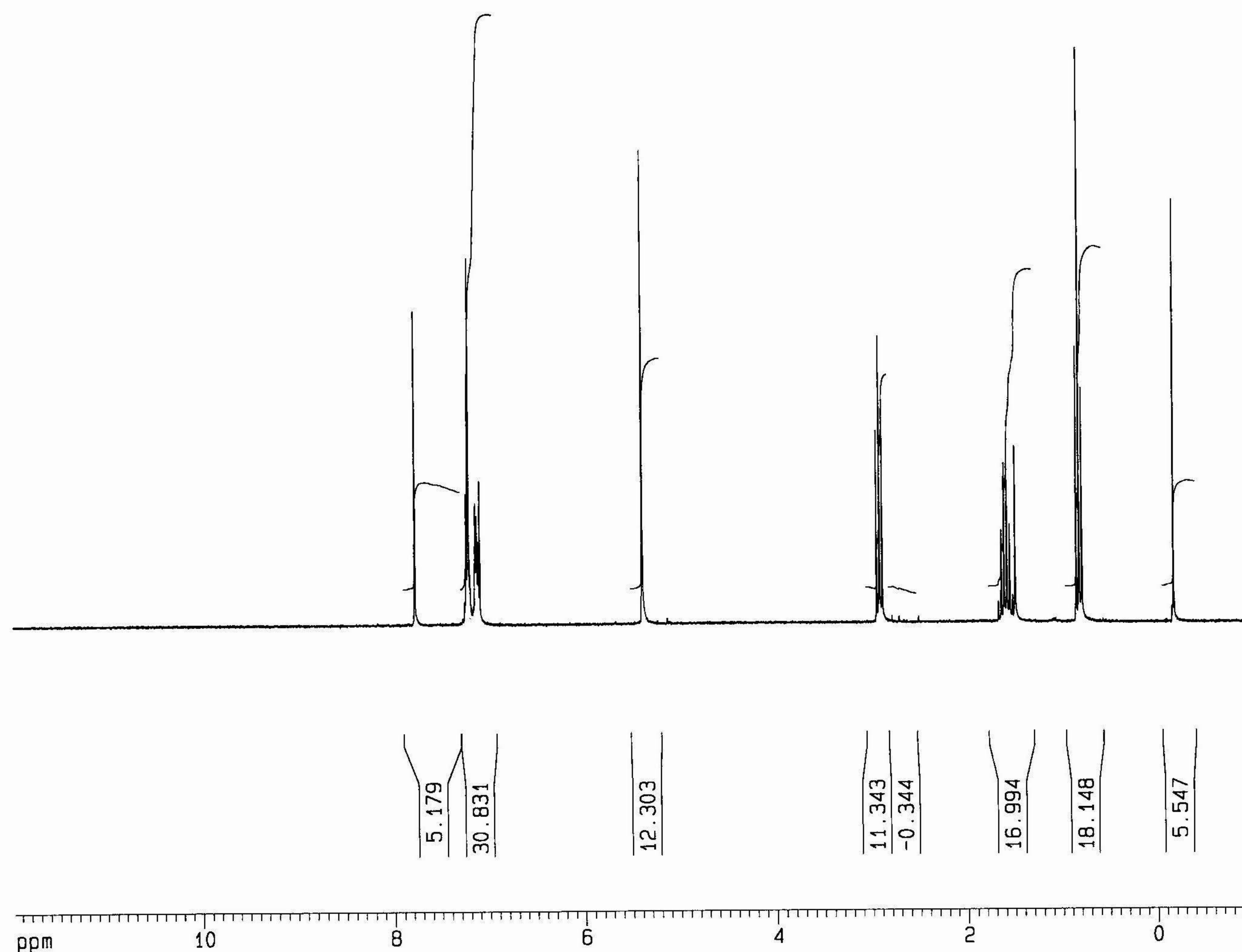
NUC1 1H
P1 9.75 usec
PL1 -6.00 dB
SF01 250.1311754 MHz

F2 - Processing parameters

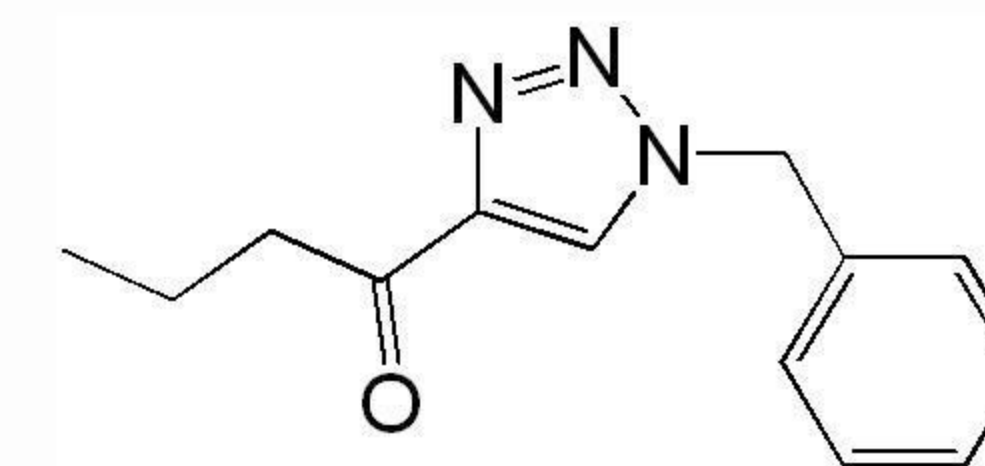
SI 16384
SF 250.1300498 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

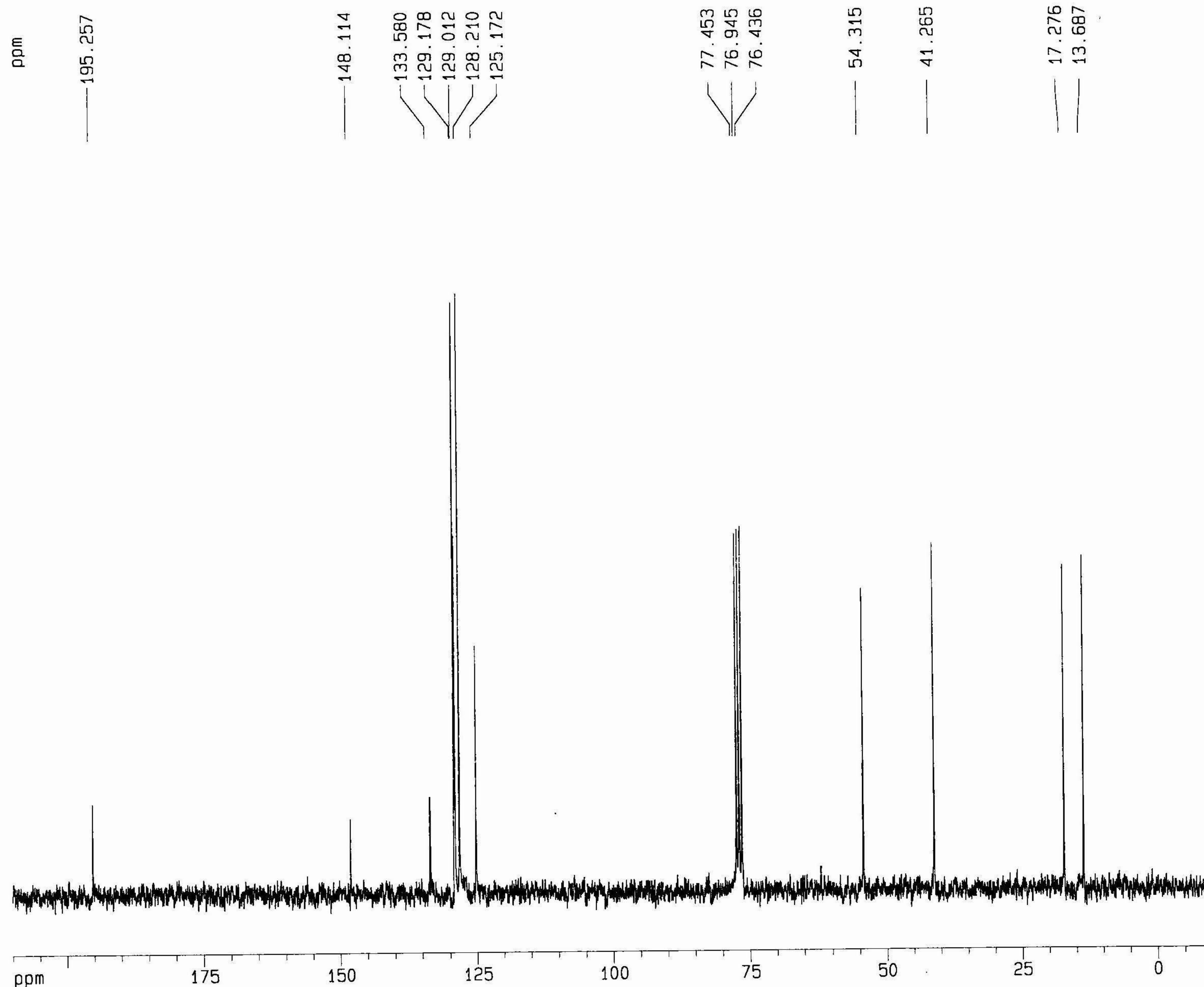
CX 20.00 cm
F1P 14.000 ppm
F1 3501.82 Hz
F2P -1.000 ppm
F2 -250.13 Hz
PPMCM 0.75000 ppm/cm
HZCM 187.59753 Hz/cm



Integral



5u



Current Data Parameters
 NAME sy1ispt90
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120131
 Time 8.16
 INSTRUM spect
 PROBHD 5 mm Dual 13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 8192
 DW 26.550 usec
 DE 10.50 usec
 TE 300.0 K
 D1 0.38000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -2.00 dB
 SF01 62.9015374 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 15.00 dB
 PL13 15.00 dB
 SF02 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8952479 MHz
 WDW EM
 SSB 0
 LB 2.50 Hz
 GB 0
 PC 1.40

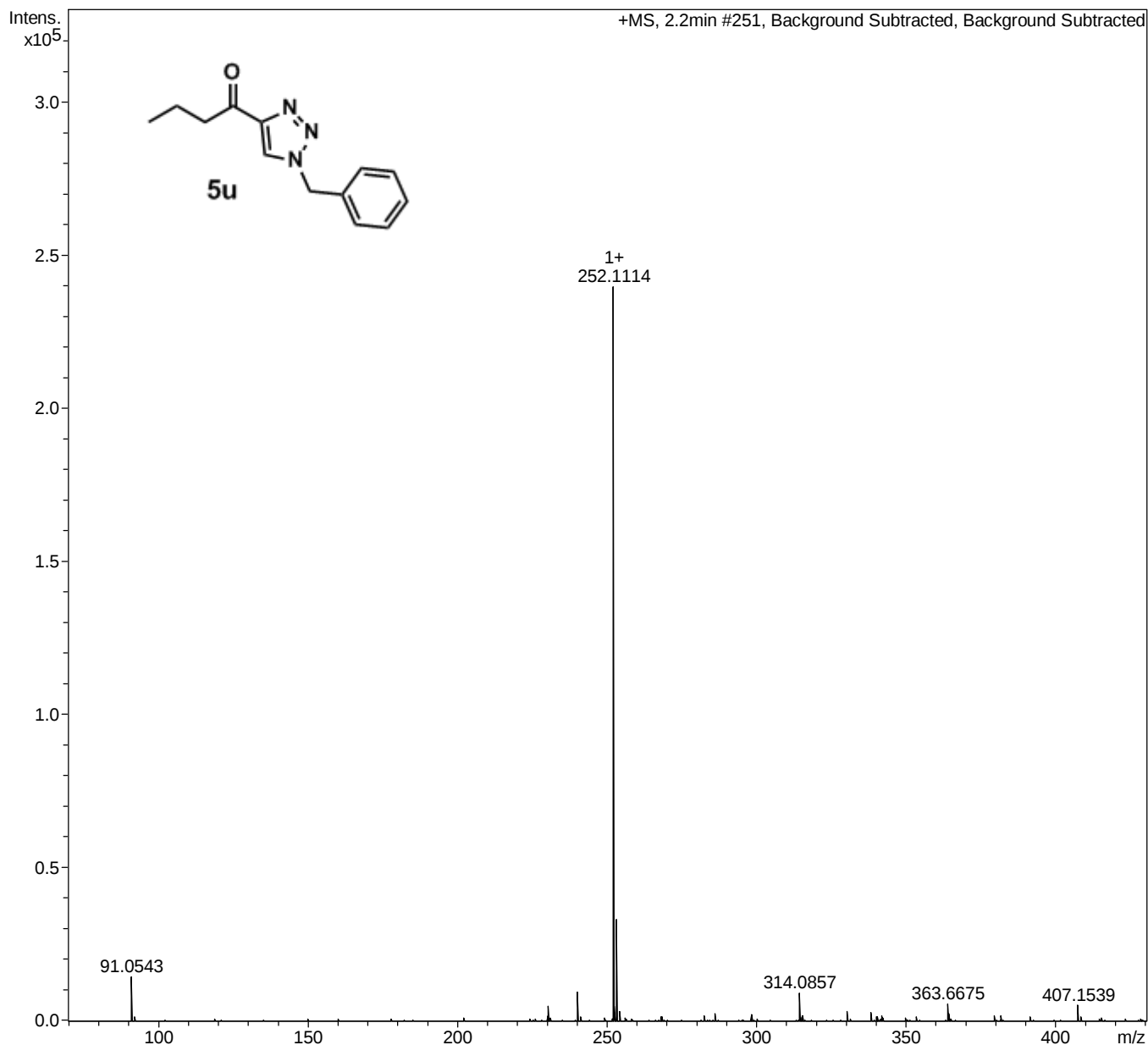
1D NMR plot parameters
 CX 20.00 cm
 F1P 210.000 ppm
 F1 13208.00 Hz
 F2P -10.000 ppm
 F2 -628.95 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 691.84772 Hz/cm

ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1PA90B_229_1-F,2_01_3386.d
Method fia_pos_bajo_50-350_egf.m

Acquisition Date 2/20/2012 4:15:19 PM
Instrument micrOTOF



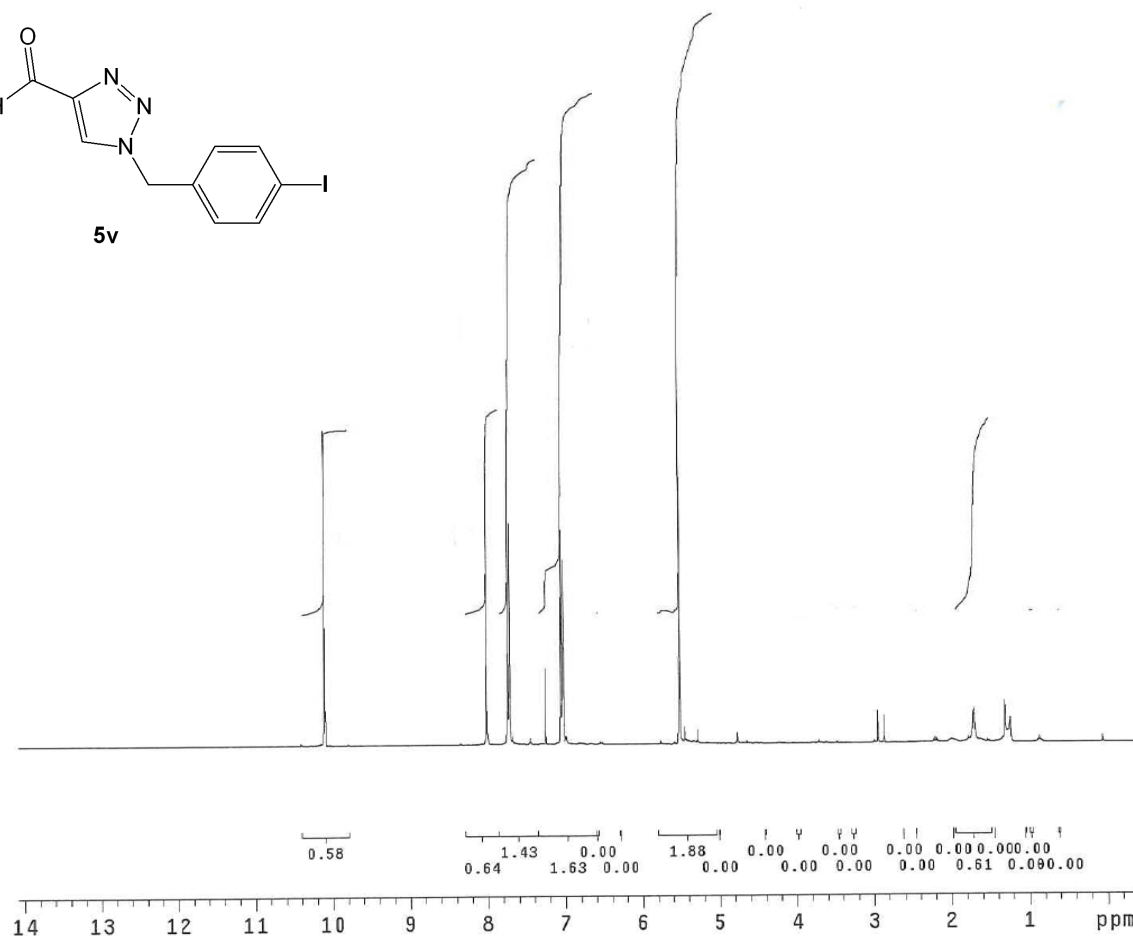
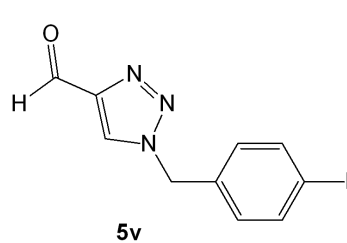
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
252.1114	1	C 13 H 15 N 3 Na O	100.00	252.1107	-0.6	-2.6	7.6	7.5	even	ok

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sy1cof1

exp1 s2pu1

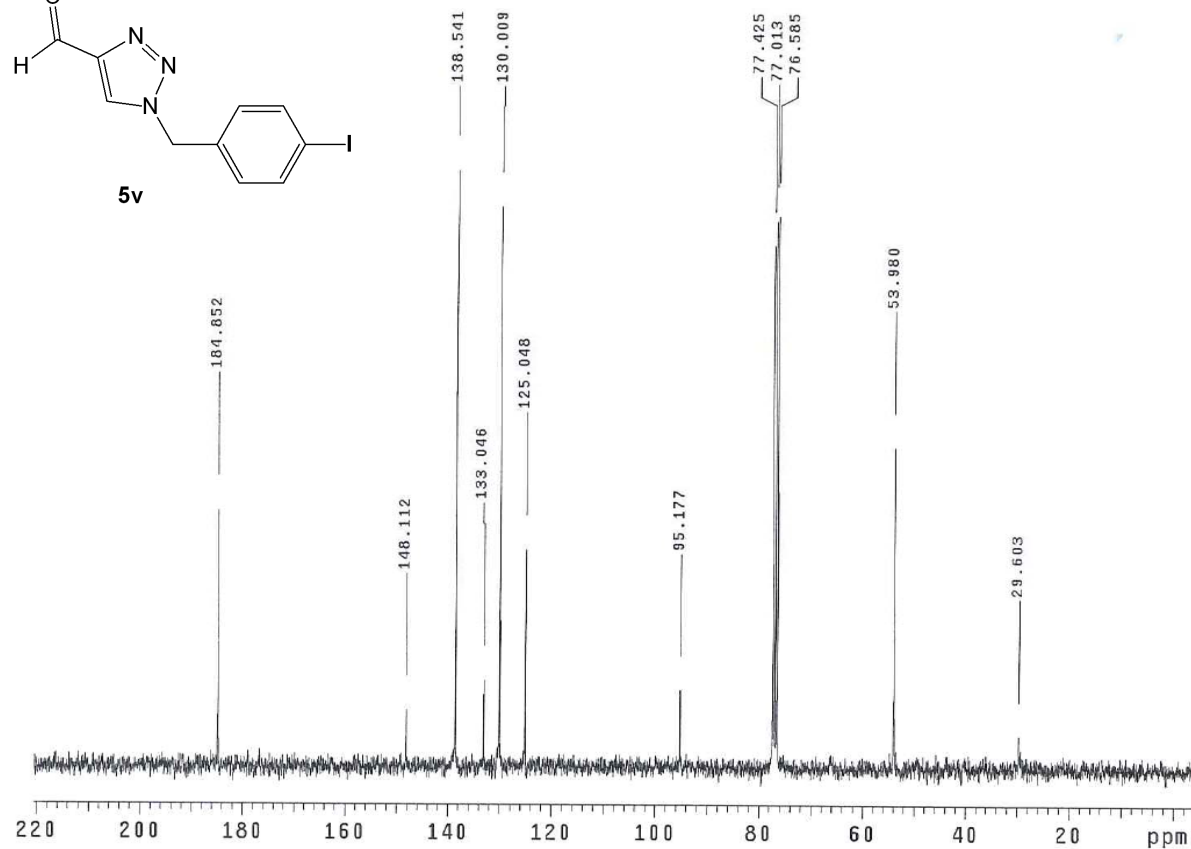
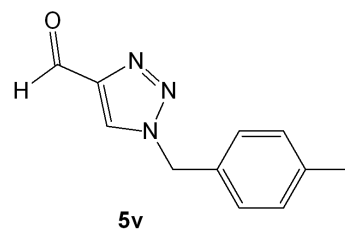
SAMPLE		DEC. & VT	
date	May 8 2012	dfrq	75.454
solvent	cdc13	dn	C13
file	exp	dpwr	37
ACQUISITION		dof	0
sfrq	300.048	dm	nnn
tn	H1	dmm	c
at	1.517	dmf	13900
np	16384	temp	25.0
sw	5399.6	PROCESSING	
fb	3000	lb	0.23
bs	1	wtfile	
tpwr	59	proc	ft
pw	6.0	fn	not used
d1	0.700		
tof	659.7	werr	
nt	200	wexp	
ct	52	wbs	
alock	n	wnt	
gain	not used		
FLAGS			
il	n		
ln	n		
dp	y		
DISPLAY			
sp	-131.6		
wp	4358.8		
vs	44		
sc	0		
wc	180		
hzmm	24.22		
is	1193.40		
rfl	599.6		
rfl	0		
th	5		
ins	1.000		
ai	ph		



sy1C0F1

exp2 CARBON

SAMPLE		PRESATURATION	
date	May 10 2012	satmode	n
solvent	cdc13	wet	n
file	exp	SPECIAL	
ACQUISITION		SPECIAL	
sw	18867.9	temp	25.0
at	0.868	gain	not used
np	32768	spin	not used
fb	10400	hst	0.008
bs	2	pw90	7.000
d1	1.000	alfa	10.000
nt	3000	FLAGS	
ct	1524	il	n
TRANSMITTER		in	n
tn	C13	dp	y
sfrq	75.454	hs	nn
tof	409.4	lb	2.50
tpwr	57	fn	not used
pw	3.000	DISPLAY	
DECOUPLER		sp	-328.9
dn	H1	wp	16951.7
dof	0	rfl	1889.3
dm	yyy	rfl	0
decwave	w	rp	109.8
dpwr	37	lp	-290.6
dmf	8100	PLOT	
		wc	180
		sc	0
		vs	551
		th	4
		ai	ph

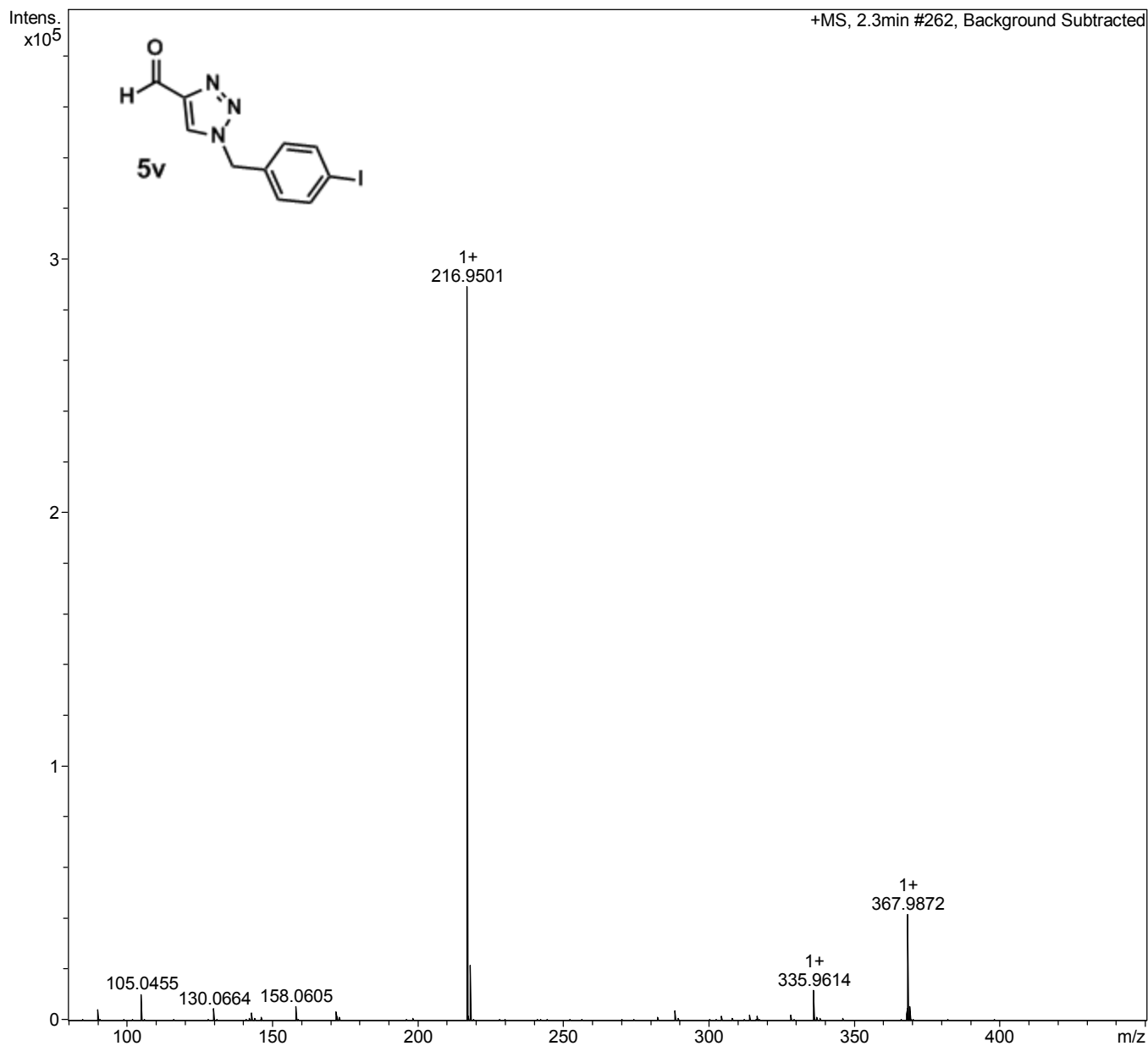


ESPECTRO ESI-FIA-TOF-Medida de Masas Exactas

Analysis Info

Sample Name SY1COF1_312_1-H,3_01_4905.d
 Method fia_pos_bajo_50-350_egf.m

Acquisition Date 5/11/2012 4:18:58 PM
 Instrument micrOTOF



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
335.9614	1	C 10 H 8 I N 3 Na O	100.00	335.9604	-1.0	-2.9	37.3	7.5	even	ok

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