

Antineoplastic Agents 603. Quinstatins. Exceptional Cancer Cell Growth Inhibitors^{1a}

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85287-1604, United States

S1	¹ H NMR (CDCl ₃ , 400 MHz)	Quinstatin 2 (3)
S2	¹³ C NMR (CDCl ₃ , 400 MHz)	Quinstatin 2 (3)
S3	¹ H NMR (CDCl ₃ , 400 MHz)	2-(1'-Ethyl-amido-boc-dap)-quinoline (5)
S4	¹³ C NMR (CDCl ₃ , 400 MHz)	2-(1'-Ethyl-amido-boc-dap)-quinoline (5)
S5	¹ H NMR (CDCl ₃ , 400 MHz)	Quinstatin 3
S6	¹³ C NMR (CDCl ₃ , 400 MHz)	Quinstatin 3
S7	¹ H NMR (CDCl ₃ , 400 MHz)	3-(1'-Ethyl-amido-boc-dap)-quinoline
S8	¹³ C NMR (CDCl ₃ , 400 MHz)	3-(1'-Ethyl-amido-boc-dap)-quinoline
S9	¹ H NMR (CDCl ₃ , 400 MHz)	Quinstatin 4
S10	¹³ C NMR (CDCl ₃ , 400 MHz)	Quinstatin 4

S11	¹ H NMR (CDCl ₃ , 400 MHz)	4-(1'-Ethyl-amido-boc-dap)-quinoline
S12	¹³ C NMR (CDCl ₃ , 400 MHz)	4-(1'-Ethyl-amido-boc-dap)-quinoline
S13	¹ H NMR (CDCl ₃ , 400 MHz)	Quinstatin 5
S14	¹³ C NMR (CDCl ₃ , 400 MHz)	Quinstatin 5
S15	¹ H NMR (CDCl ₃ , 400 MHz)	5-(1'-Ethyl-amido-boc-dap)-quinoline
S16	¹³ C NMR (CDCl ₃ , 400 MHz)	5-(1'-Ethyl-amido-boc-dap)-quinoline
S17	¹ H NMR (CDCl ₃ , 400 MHz)	Quinstatin 6 (4)
S18	¹³ C NMR (CDCl ₃ , 400 MHz)	Quinstatin 6 (4)
S19	¹ H NMR (CDCl ₃ , 400 MHz)	6-(1'-Ethyl-amido-boc-dap)-quinoline (11)
S20	HRAPCIMS	6-(1'-Ethyl-amido-boc-dap)-quinoline (11)
S21	¹ H NMR (CDCl ₃ , 400 MHz)	Quinstatin 7
S22	¹³ C NMR (CDCl ₃ , 400 MHz)	Quinstatin 7
S23	¹ H NMR (CDCl ₃ , 400 MHz)	7-(1'-Ethyl-amido-boc-dap)-quinoline
S24	¹³ C NMR (CDCl ₃ , 400 MHz)	7-(1'-Ethyl-amido-boc-dap)-quinoline
S25	¹ H NMR (CDCl ₃ , 400 MHz)	Quinstatin 8
S26	¹³ C NMR (CDCl ₃ , 400 MHz)	Quinstatin 8
S27	HRAPCIMS	Quinstatin 8
S28	¹ H NMR (CDCl ₃ , 400 MHz)	8-(1'-Ethyl-amido-boc-dap)-quinoline
S29	¹³ C NMR (CDCl ₃ , 400 MHz)	8-(1'-Ethyl-amido-boc-dap)-quinoline

223PNM207

Sample Name:

223PNM207

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 9 2015

Temp. 25.0 C / 298.1 K

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

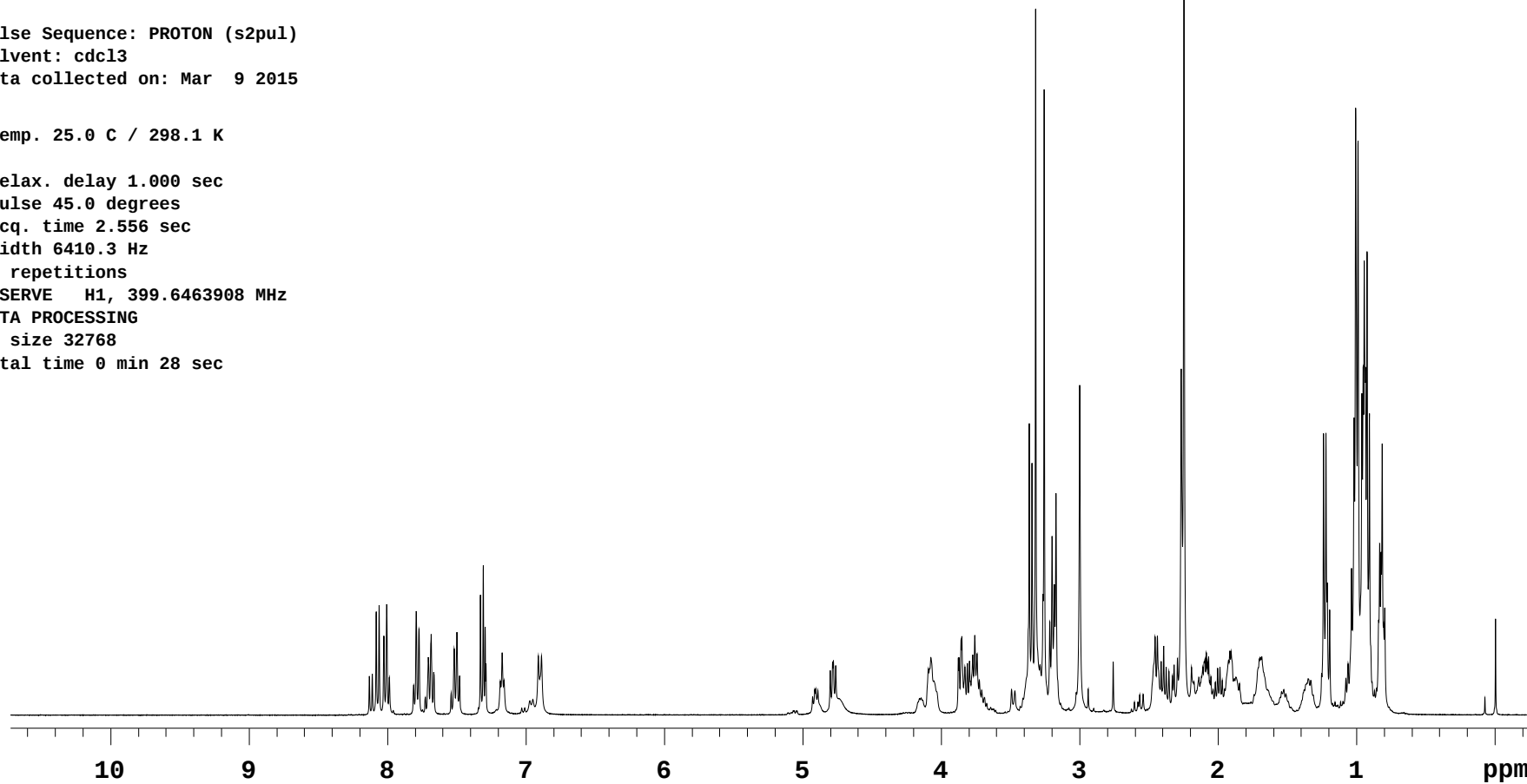
8 repetitions

OBSERVE H1, 399.6463908 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 28 sec



223PNM207

Sample Name:

223PNM207

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Mar 9 2015

Temp. 25.0 C / 298.1 K

User: 1-14-87

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.311 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 100.4911704 MHz

DECOUPLE H1, 399.6484109 MHz

Power 40 dB

continuously on

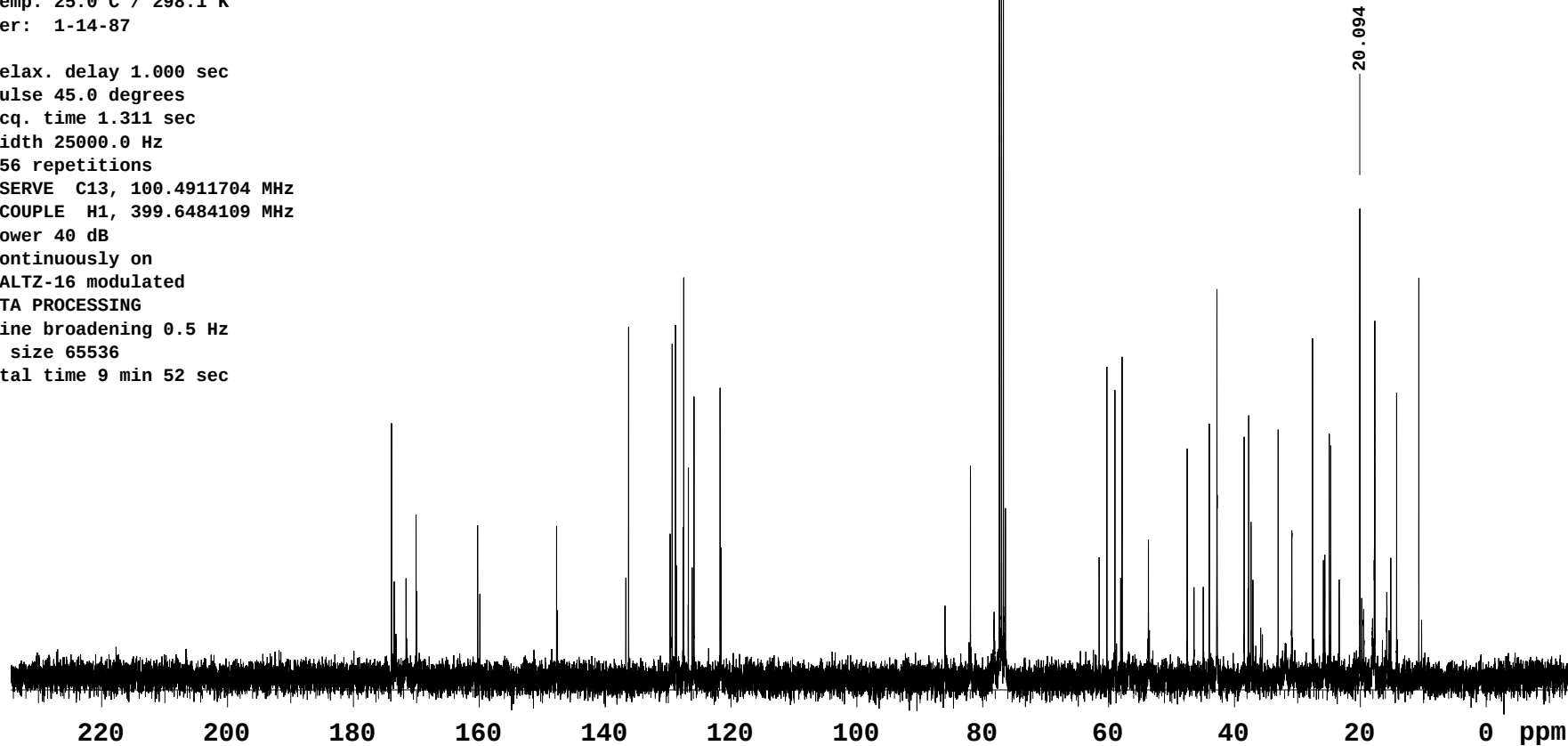
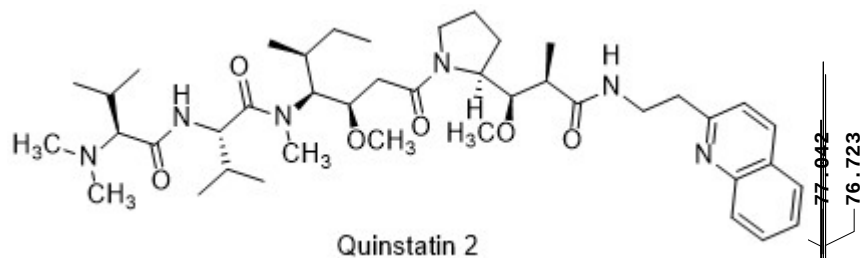
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

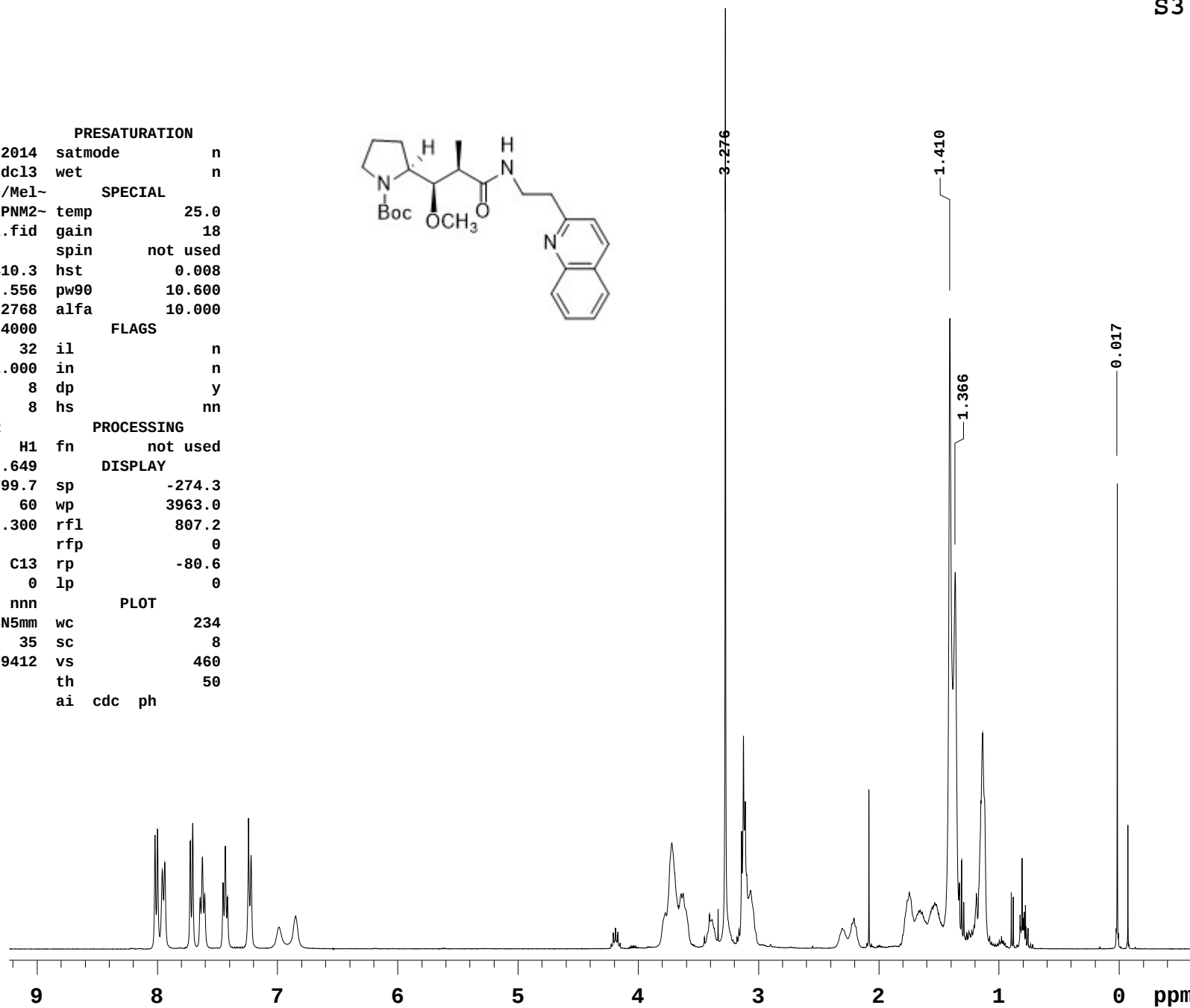
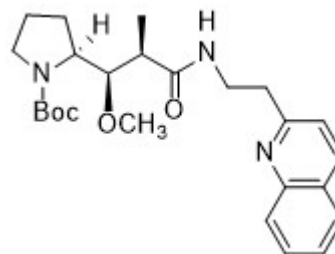
Total time 9 min 52 sec



223PNM201

exp2 PROTON

SAMPLE		PRESATURATION	
date	Dec 8 2014	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel~	SPECIAL	
ody/Book P/223PNM2~	temp	25.0	
01.fid	gain	18	
ACQUISITION		spin	not used
sw	6410.3	hst	0.008
at	2.556	pw90	10.600
np	32768	alfa	10.000
fb	4000	FLAGS	
bs	32	il	n
d1	1.000	in	n
nt	8	dp	y
ct	8	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.649	DISPLAY	
tof	399.7	sp	-274.3
tpwr	60	wp	3963.0
pw	5.300	rfl	807.2
DECOUPLER		rfl	0
dn	C13	rp	-80.6
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_HCN5mm	wc	234
dpwr	35	sc	8
dmf	29412	vs	460
		th	50
		ai	cdc ph



223PNM201

Sample Name:

223PNM201

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Dec 8 2014

Temp. 25.0 C / 298.1 K

User: 1-14-87

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.311 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 100.4911569 MHz

DECOUPLE H1, 399.6484109 MHz

Power 40 dB

continuously on

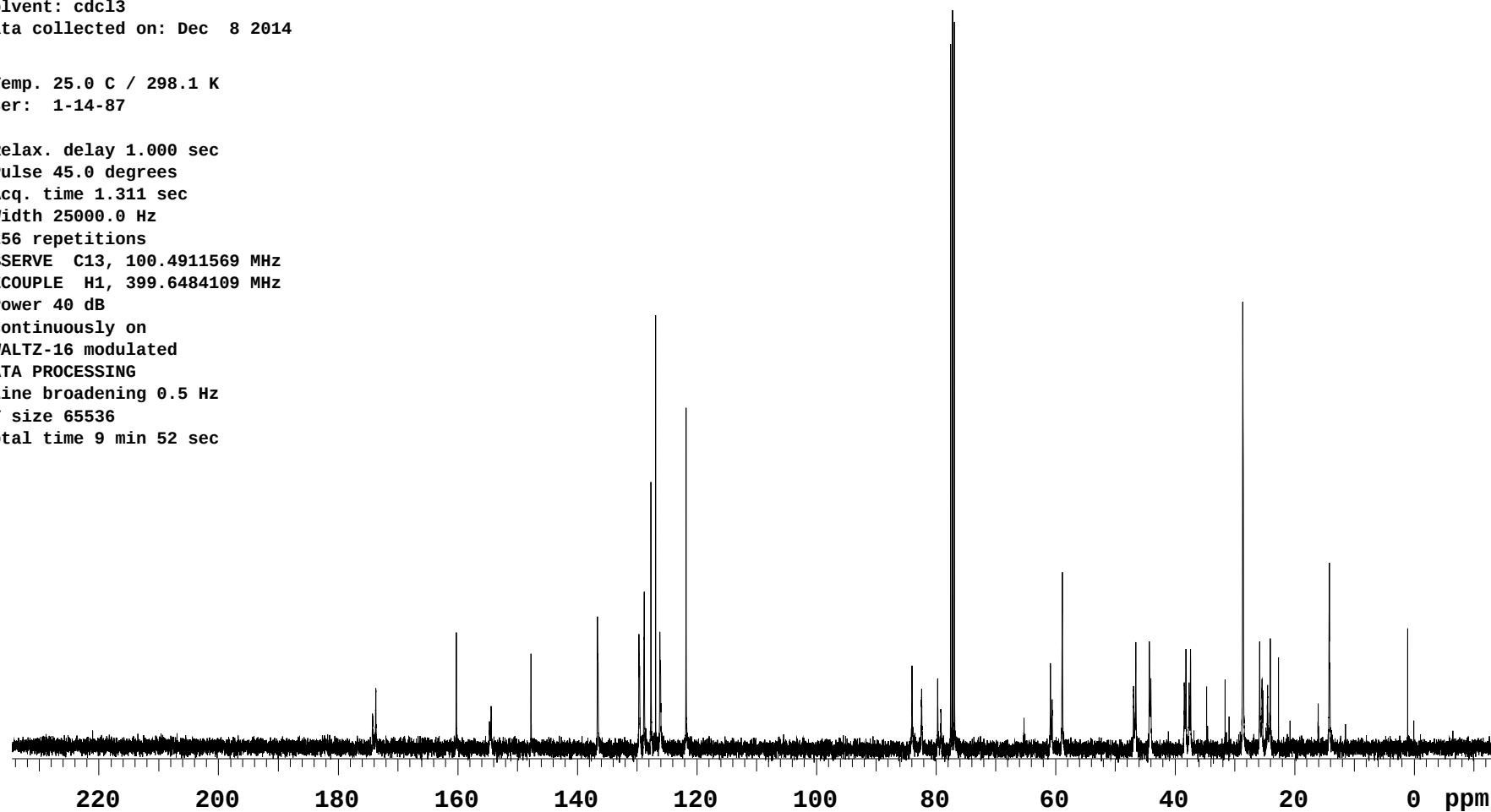
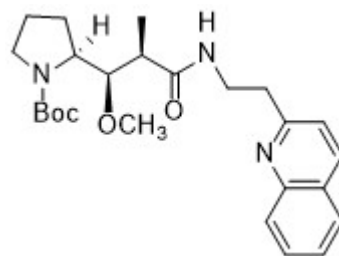
WALTZ-16 modulated

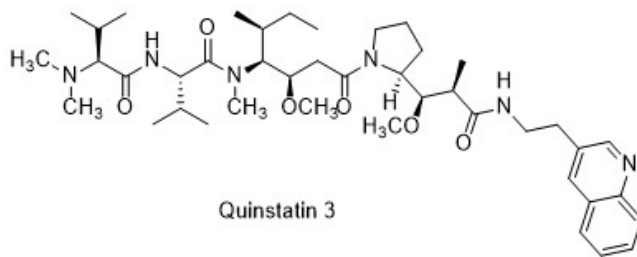
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min 52 sec

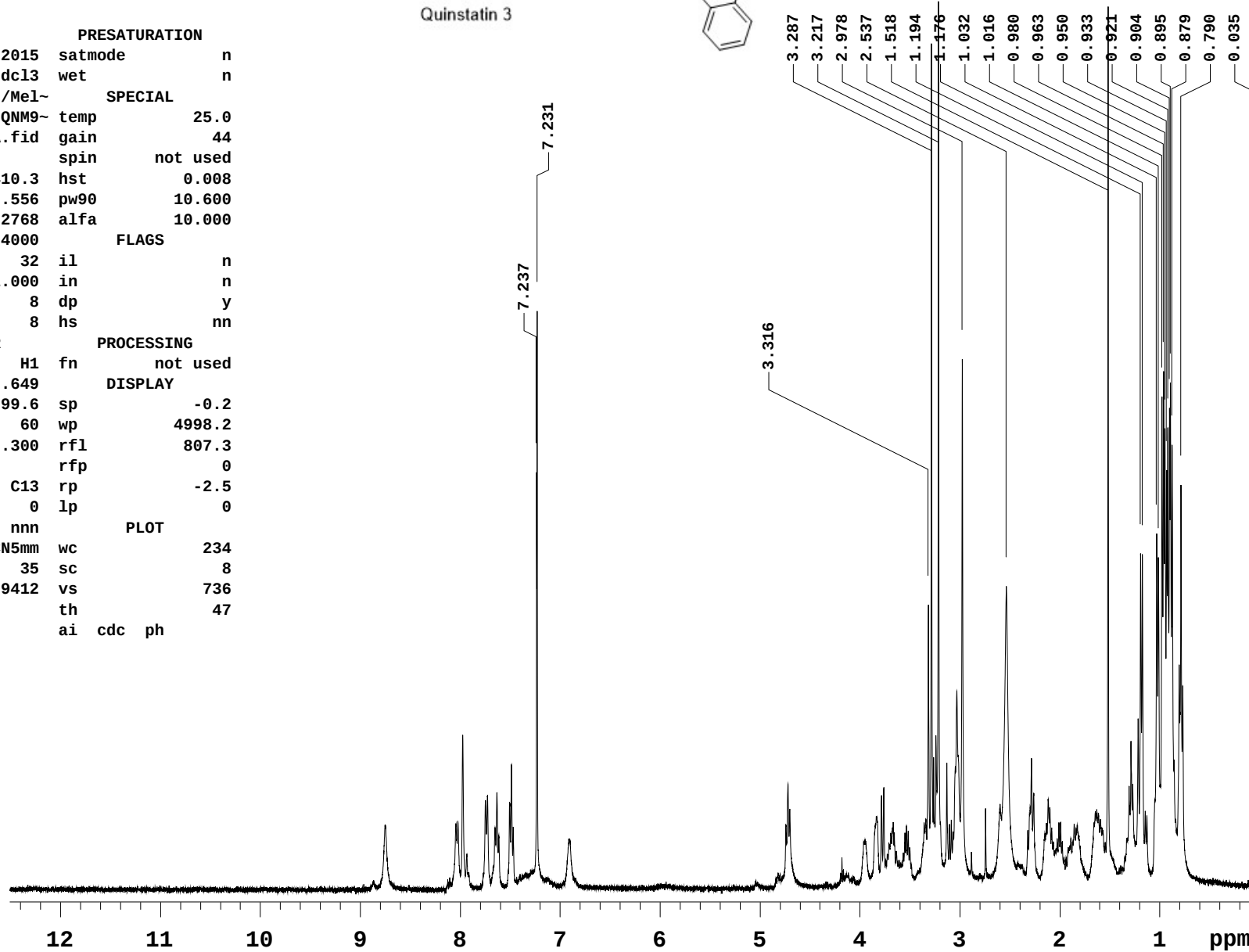




223QNM97F3extracted

exp2 PROTON

SAMPLE		PRESATURATION	
date	Sep 16 2015	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel-	SPECIAL	
ody/Book	Q/223QNM9~	temp	25.0
	7F3_A.fid	gain	44
ACQUISITION		spin	not used
sw	6410.3	hst	0.008
at	2.556	pw90	10.600
np	32768	alfa	10.000
fb	4000	FLAGS	
bs	32	il	n
d1	1.000	in	n
nt	8	dp	y
ct	8	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.649	DISPLAY	
tof	399.6	sp	-0.2
tpwr	60	wp	4998.2
pw	5.300	rfl	807.3
DECOUPLER		rpf	0
dn	C13	rp	-2.5
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_HCN5mm	wc	234
dpwr	35	sc	8
dmf	29412	vs	736
		th	47
		ai	cdc ph

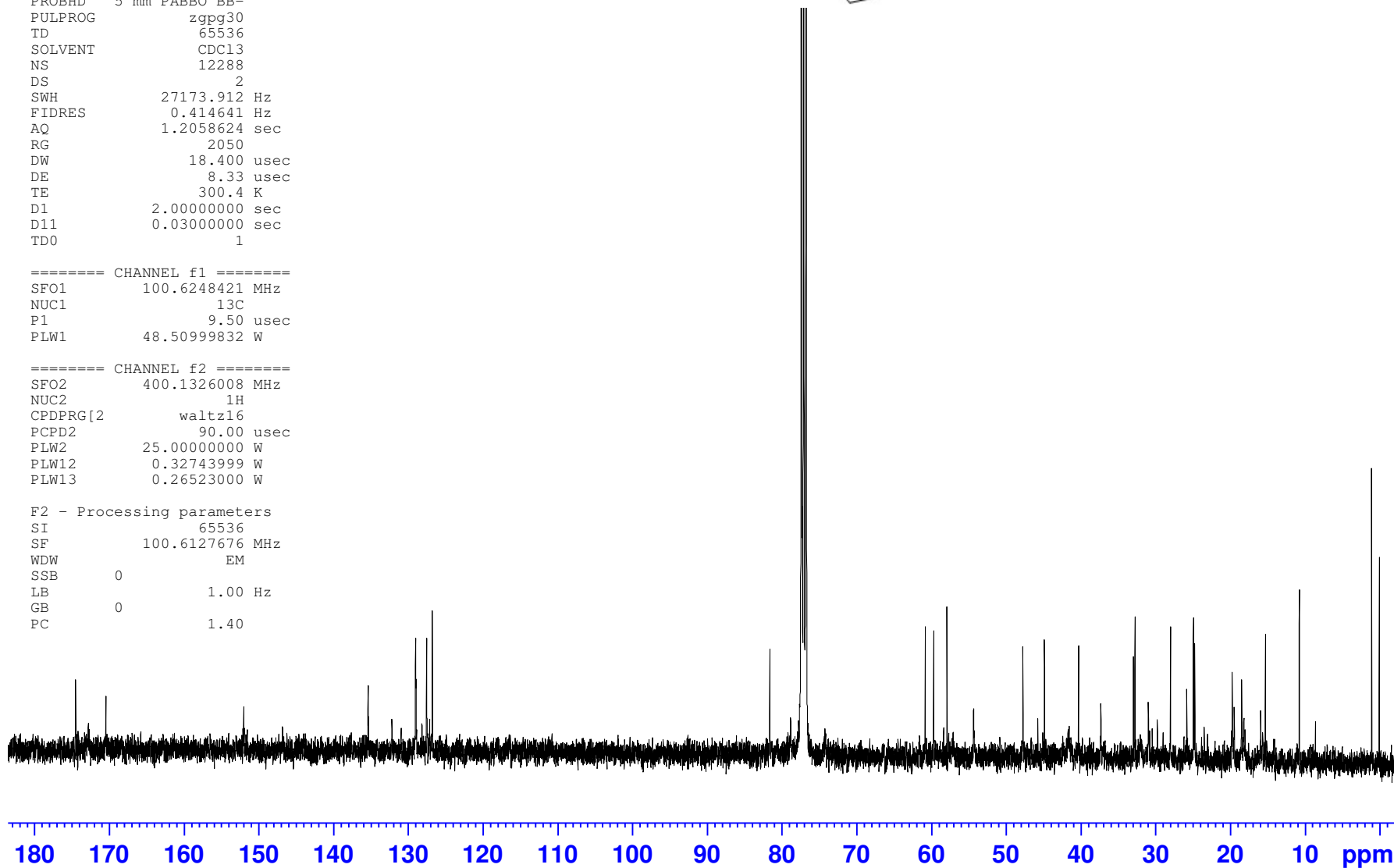
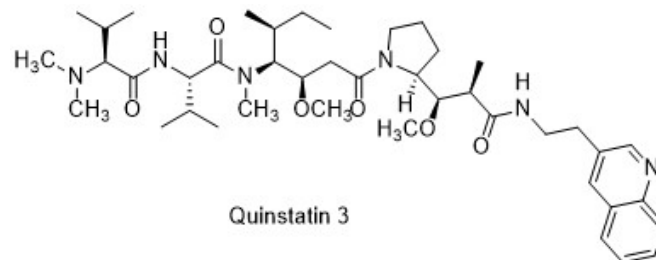


F2 - Acquisition Parameters

```
===== CHANNEL f1 =====
SFO1      100.6248421 MHz
NUC1              13C
P1              9.50 usec
PLW1      48.50999832 W
```

F2 - Processing parameters

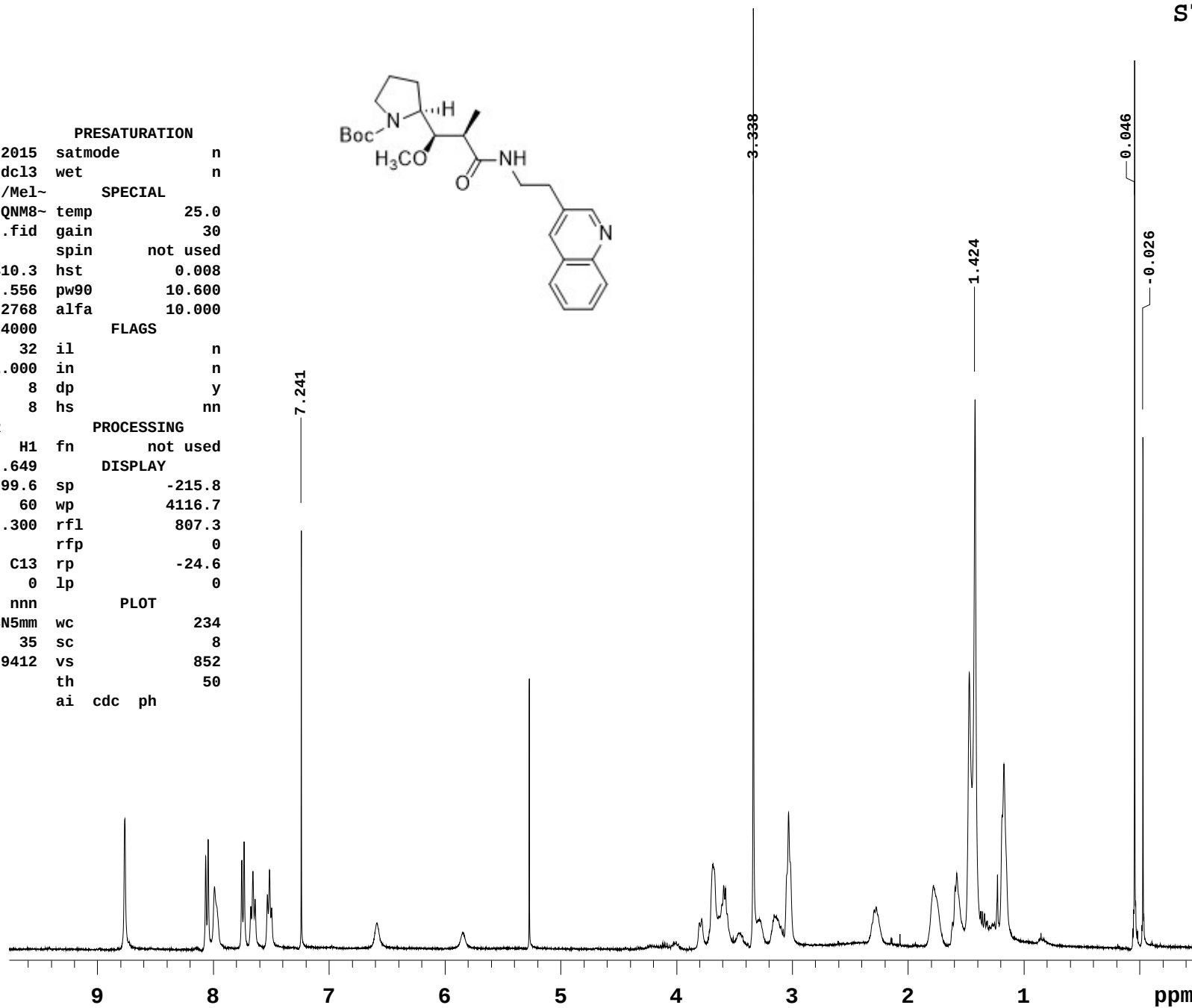
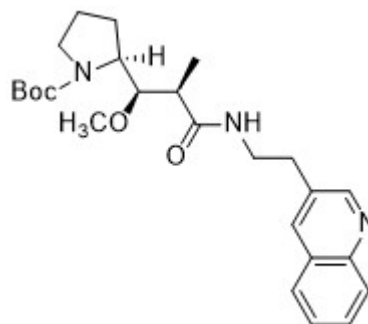
SI		65536
SF		100.6127676 MHz
WDW		EM
SSB	0	
LB		1.00 Hz
GB	0	
PC		1.40

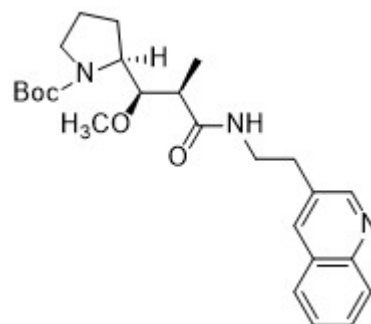


223QNM89F3

exp2 PROTON

SAMPLE		PRESATURATION	
date	Aug 26 2015	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel-	SPECIAL	
ody/Book Q/223QNM8~	temp	25.0	
9F3.fid	gain	30	
ACQUISITION		spin	not used
sw	6410.3	hst	0.008
at	2.556	pw90	10.600
np	32768	alfa	10.000
fb	4000	FLAGS	
bs	32	il	n
d1	1.000	in	n
nt	8	dp	y
ct	8	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.649	DISPLAY	
tof	399.6	sp	-215.8
tpwr	60	wp	4116.7
pw	5.300	rfl	807.3
DECOUPLER		rfl	0
dn	C13	rp	-24.6
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_HCN5mm	wc	234
dpwr	35	sc	8
dmf	29412	vs	852
		th	50
		ai	cdc ph





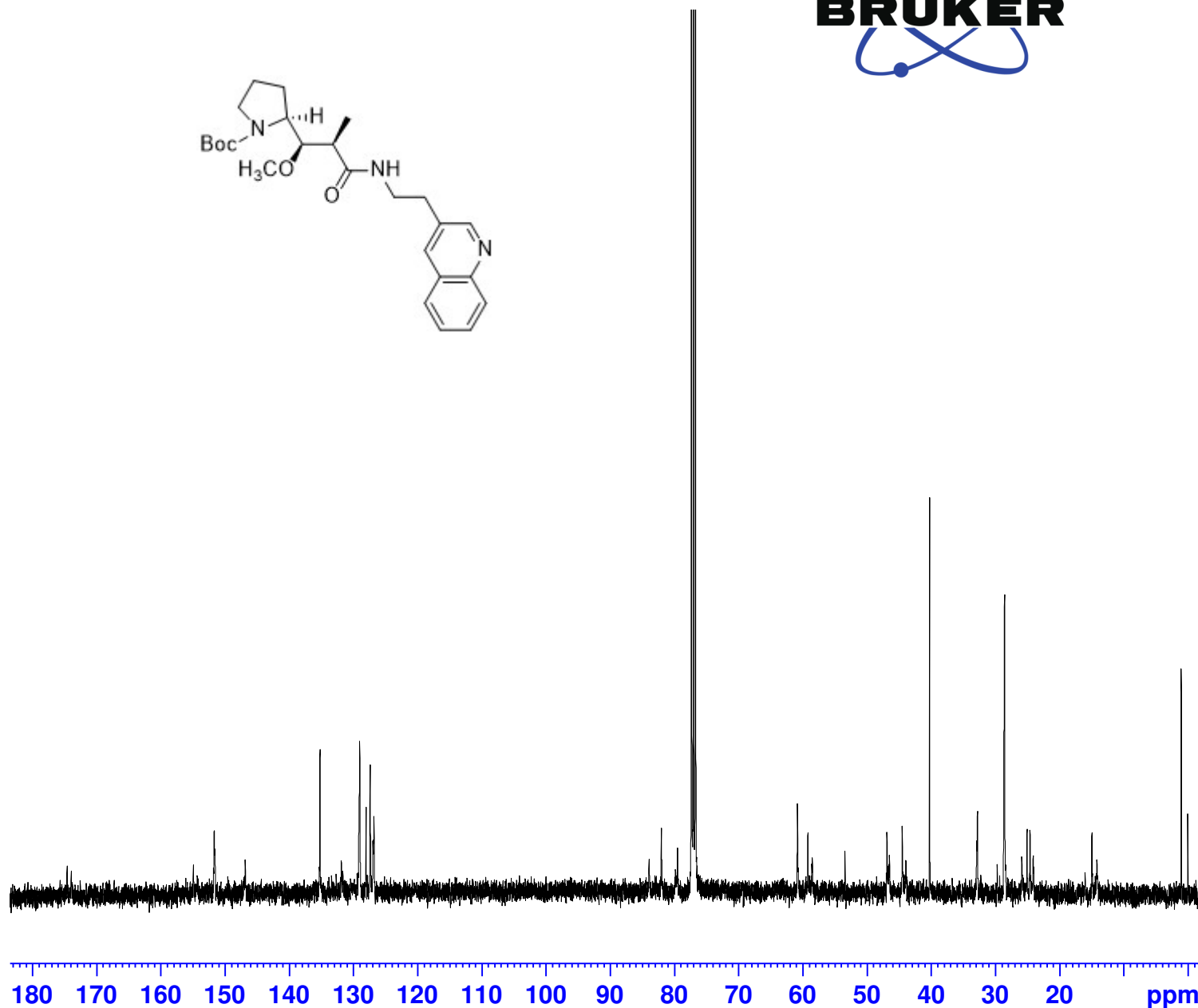
Current Data Parameters
NAME 223QNM89F3
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150827
Time 16.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2058624 sec
RG 2050
DW 18.400 usec
DE 7.87 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6248421 MHz
NUC1 13C
P1 11.70 usec
PLW1 99.00000000 W

===== CHANNEL f2 =====
SFO2 400.1326008 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 25.00000000 W
PLW12 0.32743999 W
PLW13 0.26523000 W

F2 - Processing parameters
SI 65536
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



223RNM15Quinstatin4

Sample Name:

223RNM15Quinstatin4

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: 223RNM15Quinstatin4proton

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Sep 12 2016

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

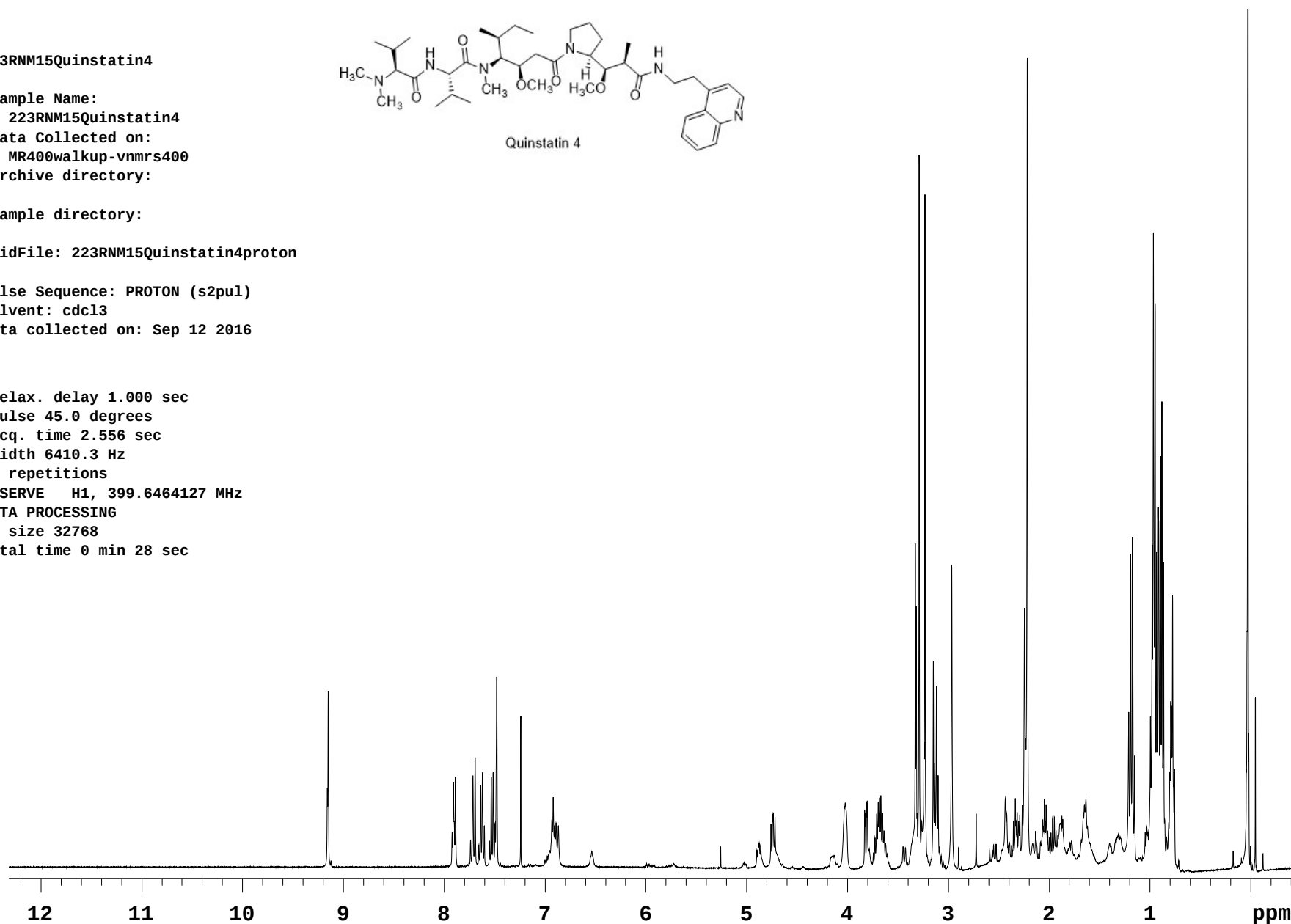
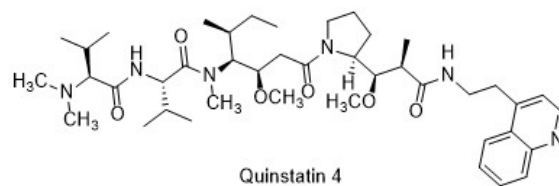
8 repetitions

OBSERVE H1, 399.6464127 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 28 sec



223RNM15Quinstatin4carbon

Sample Name:

223RNM15Q4carbon

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: 223RNM15Quinstatin4carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Sep 12 2016

User: 1-14-87

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.311 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 100.4911493 MHz

DECOUPLE H1, 399.6484109 MHz

Power 40 dB

continuously on

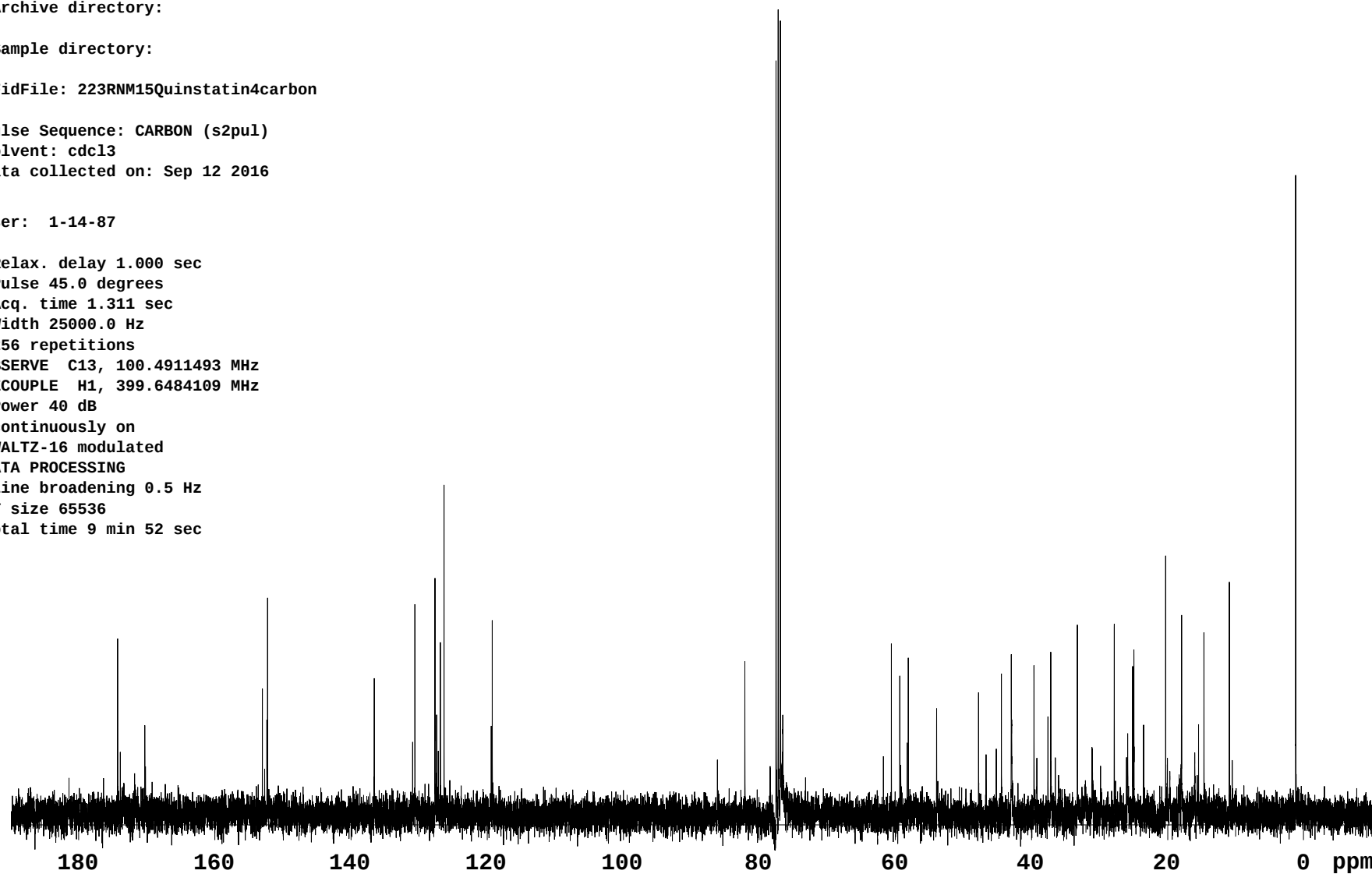
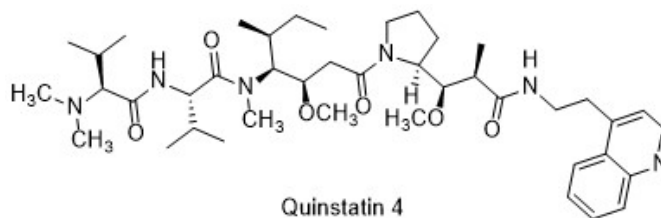
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

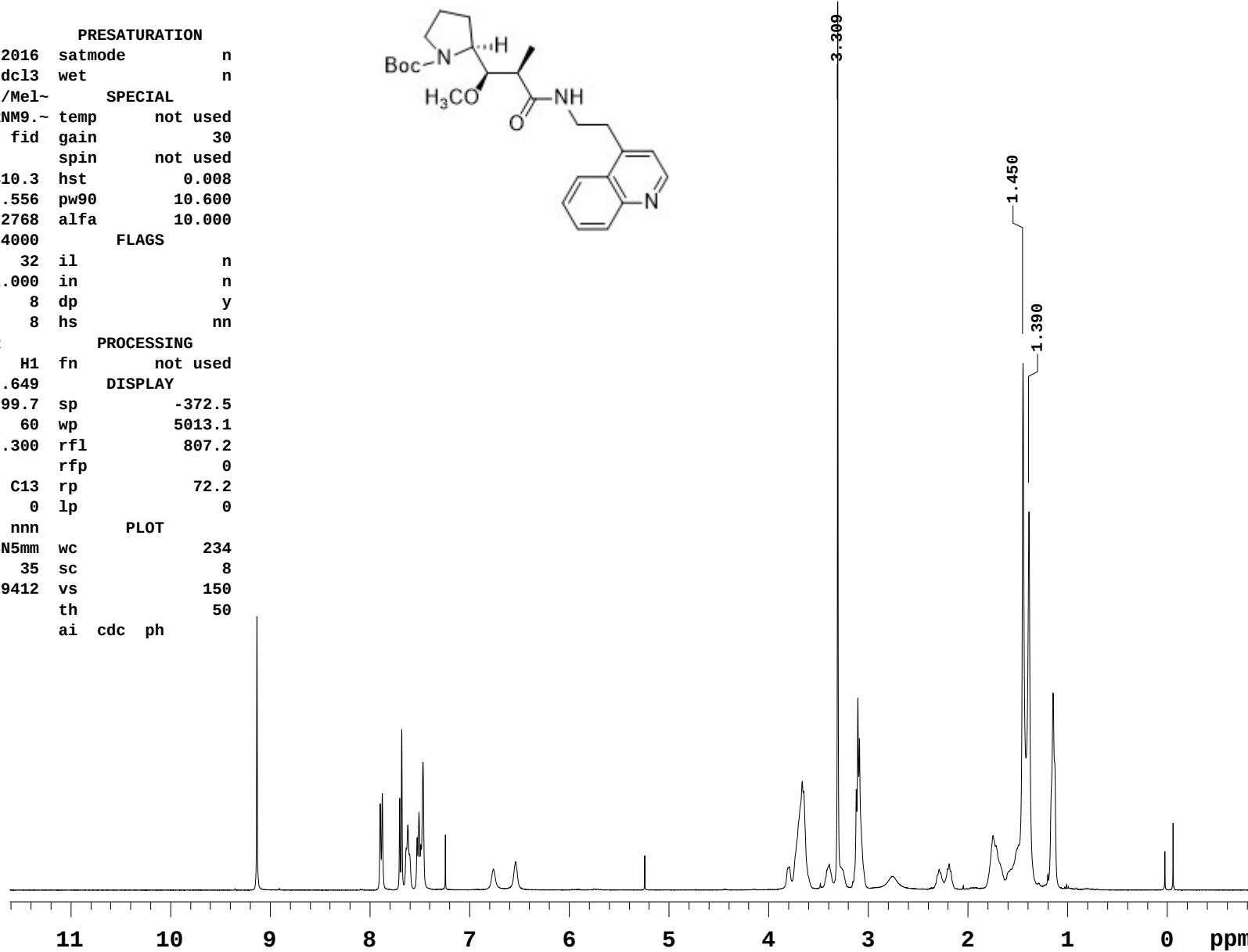
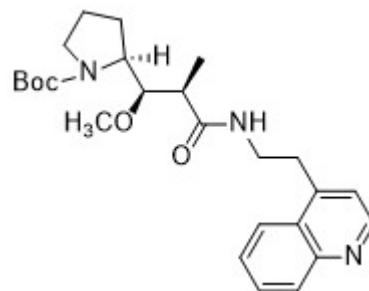
Total time 9 min 52 sec



223RNM9

exp2 PROTON

SAMPLE		PRESATURATION	
date	Aug 29 2016	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel-	SPECIAL	
ody/BookR/223RNM9.~	temp	not used	
	fid	gain	30
ACQUISITION		spin	not used
sw	6410.3	hst	0.008
at	2.556	pw90	10.600
np	32768	alfa	10.000
fb	4000	FLAGS	
bs	32	il	n
d1	1.000	in	n
nt	8	dp	y
ct	8	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.649	DISPLAY	
tof	399.7	sp	-372.5
tpwr	60	wp	5013.1
pw	5.300	rfl	807.2
DECOUPLER		rfp	0
dn	C13	rp	72.2
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_HCN5mm	wc	234
dpwr	35	sc	8
dmf	29412	vs	150
		th	50
		ai	cdc ph



223RNM9

Sample Name:

223RNM9

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: 223RNM9carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Aug 29 2016

User: 1-14-87

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.311 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 100.4911538 MHz

DECOUPLE H1, 399.6484109 MHz

Power 40 dB

continuously on

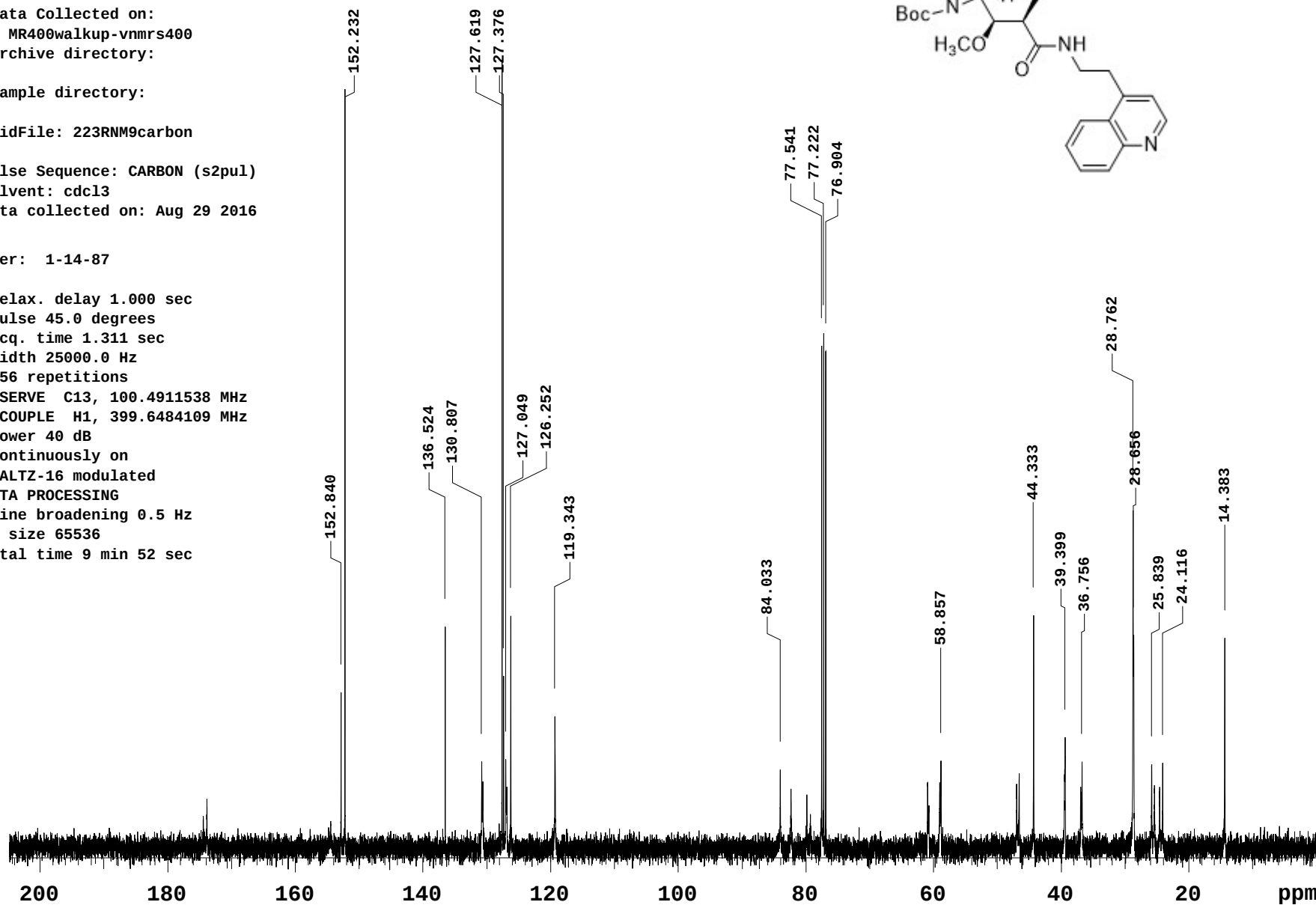
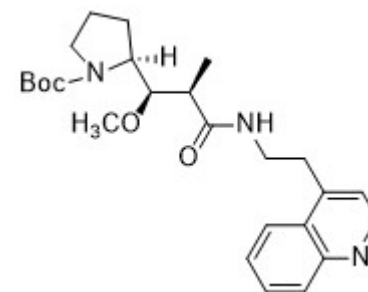
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

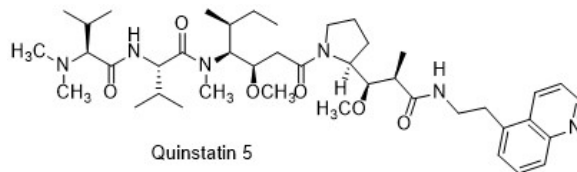
FT size 65536

Total time 9 min 52 sec

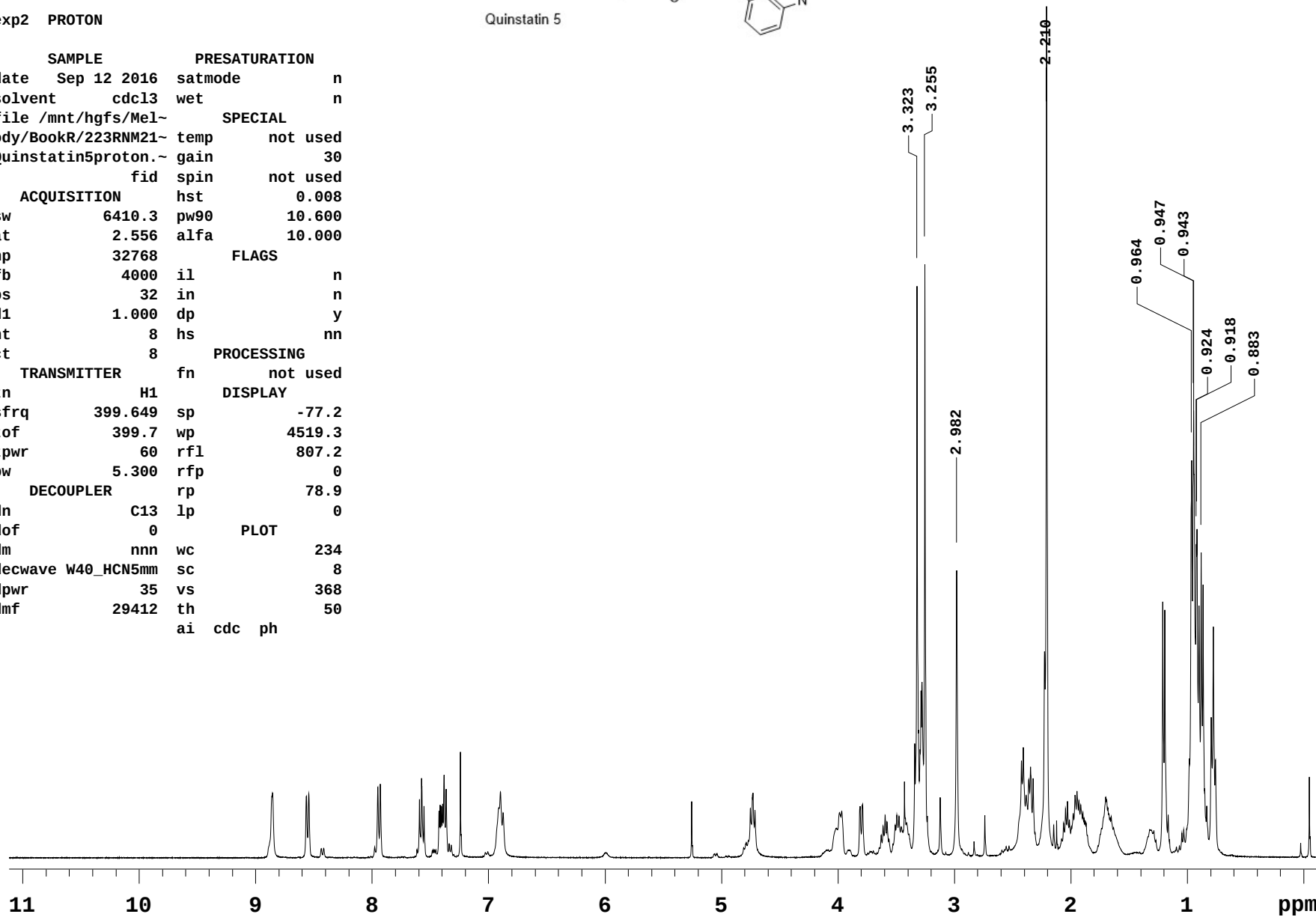


223RNM21Q5

exp2 PROTON



SAMPLE		PRESATURATION	
date	Sep 12 2016	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel~	SPECIAL	
ody/BookR/223RNM21~		temp	not used
Quinstatin5proton.~		gain	30
	fid	spin	not used
ACQUISITION		hst	0.008
sw	6410.3	pw90	10.600
at	2.556	alfa	10.000
np	32768	FLAGS	
fb	4000	il	n
bs	32	in	n
d1	1.000	dp	y
nt	8	hs	nn
ct	8	PROCESSING	
TRANSMITTER		fn	not used
tn	H1	DISPLAY	
sfrq	399.649	sp	-77.2
tof	399.7	wp	4519.3
tpwr	60	rfl	807.2
pw	5.300	rfp	0
DECOUPLER		rp	78.9
dn	C13	lp	0
dof	0	PLOT	
dm	nnn	wc	234
decwave	w40_HCN5mm	sc	8
dpwr	35	vs	368
dmf	29412	th	50
	ai	cdc	ph



223RNM21Q5carbon

Sample Name:

223RNM21Q5carbon

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: 223RNM21Quinstatin5carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Sep 12 2016

User: 1-14-87

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.311 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 100.4911500 MHz

DECOUPLE H1, 399.6484109 MHz

Power 40 dB

continuously on

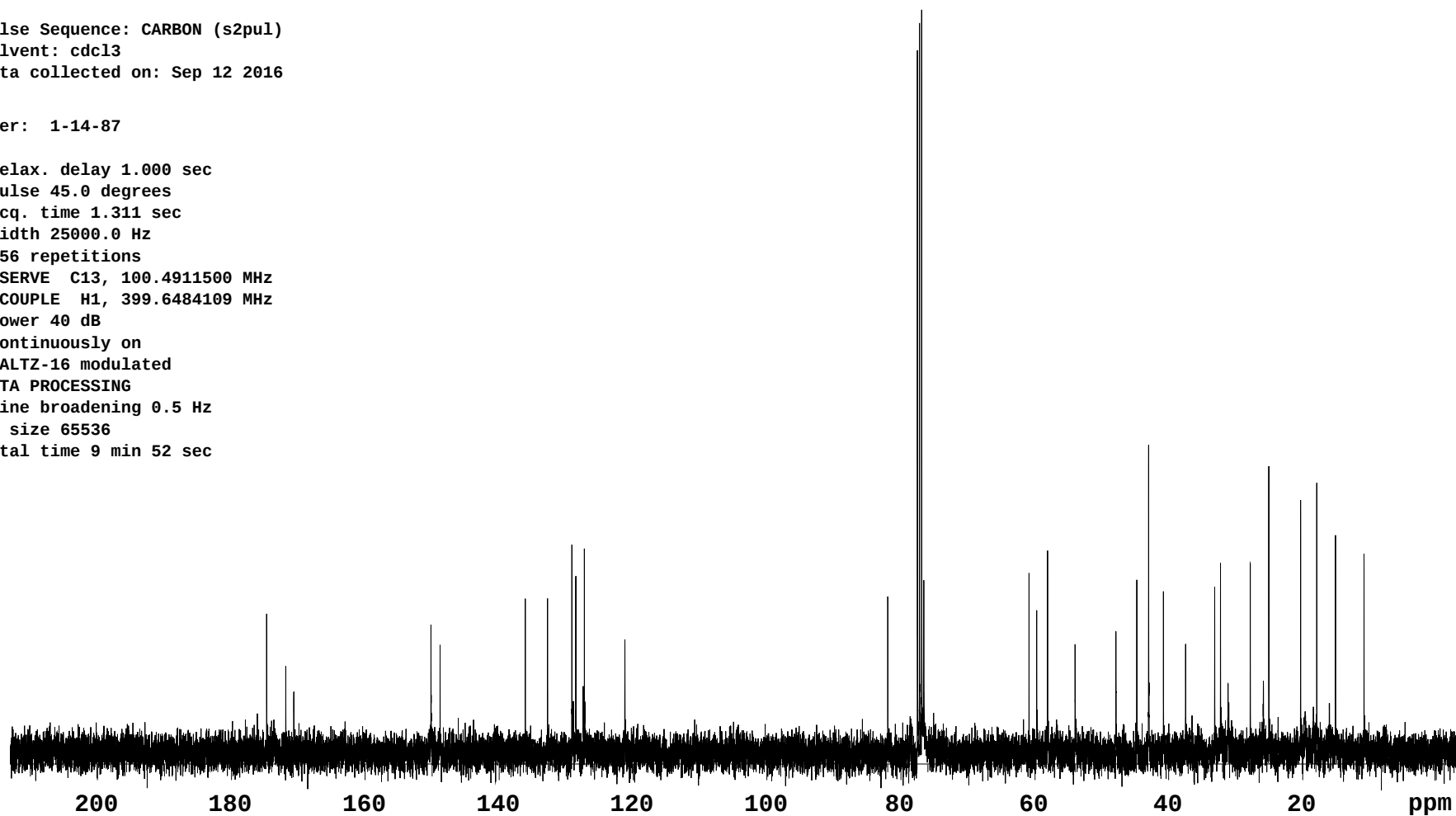
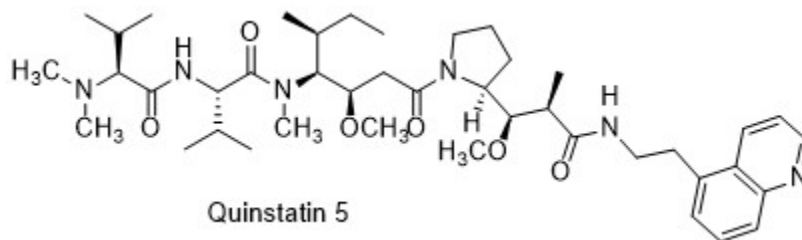
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

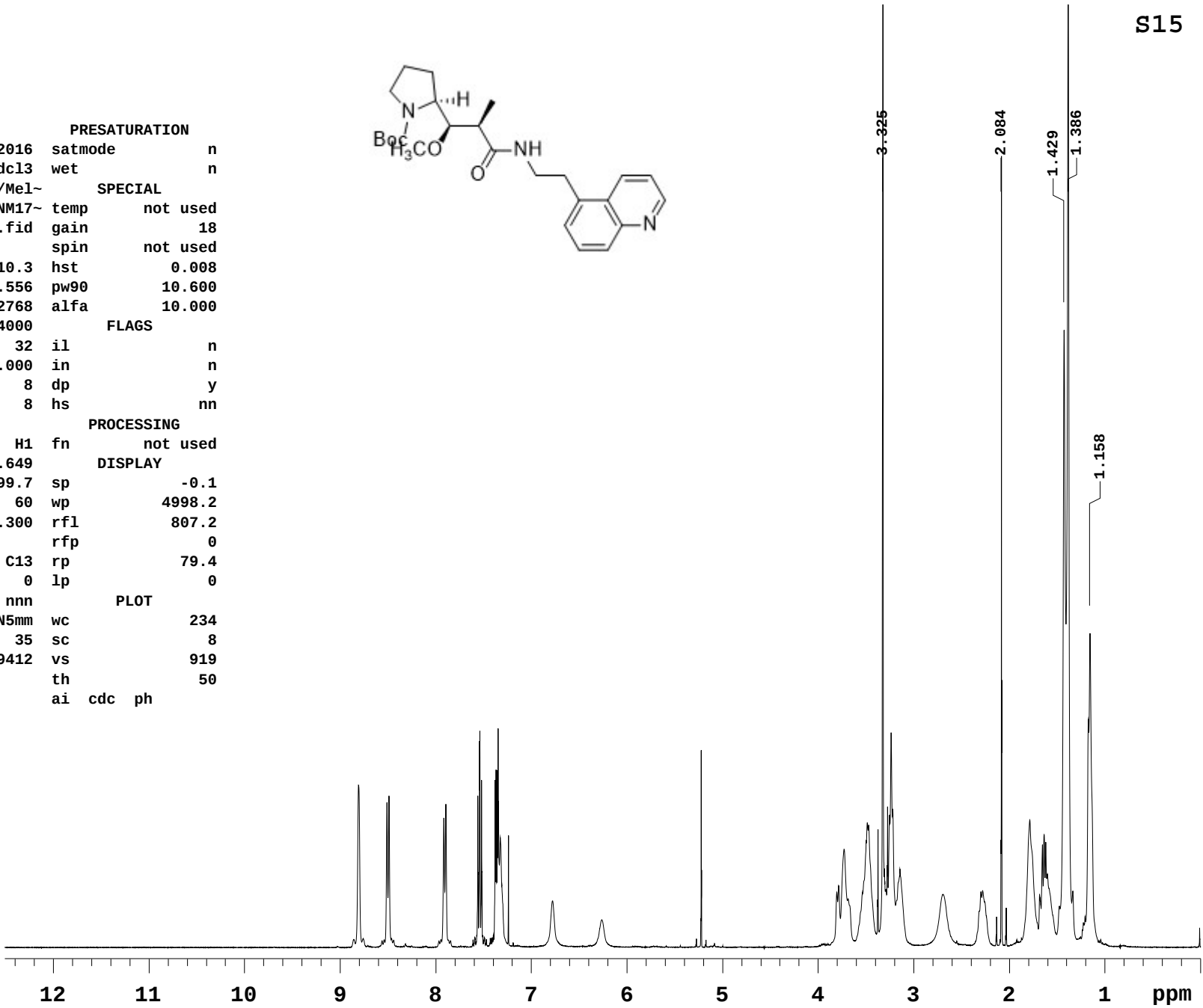
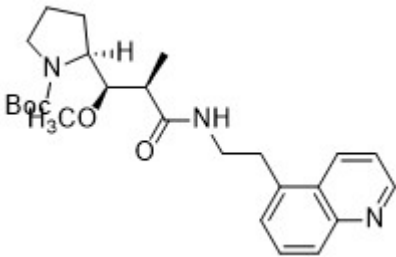
Total time 9 min 52 sec



223RNM17

exp2 PROTON

SAMPLE		PRESATURATION	
date	Sep 7 2016	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel-	SPECIAL	
ody/BookR/223RNM17~	temp	not used	
proton.fid	gain	18	
ACQUISITION		spin	
sw	6410.3	hst	0.008
at	2.556	pw90	10.600
np	32768	alfa	10.000
fb	4000	FLAGS	
bs	32	il	n
d1	1.000	in	n
nt	8	dp	y
ct	8	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.649	DISPLAY	
tof	399.7	sp	-0.1
tpwr	60	wp	4998.2
pw	5.300	rfl	807.2
DECOUPLER		rfl	0
dn	C13	rp	79.4
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_HCN5mm	wc	234
dpwr	35	sc	8
dmf	29412	vs	919
		th	50
		ai	cdc ph



223RNM17carbon

S16

Sample Name:

223RNM17carbon

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: 223RNM17carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Sep 7 2016

User: 1-14-87

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.311 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 100.4911554 MHz

DECOUPLE H1, 399.6484109 MHz

Power 40 dB

continuously on

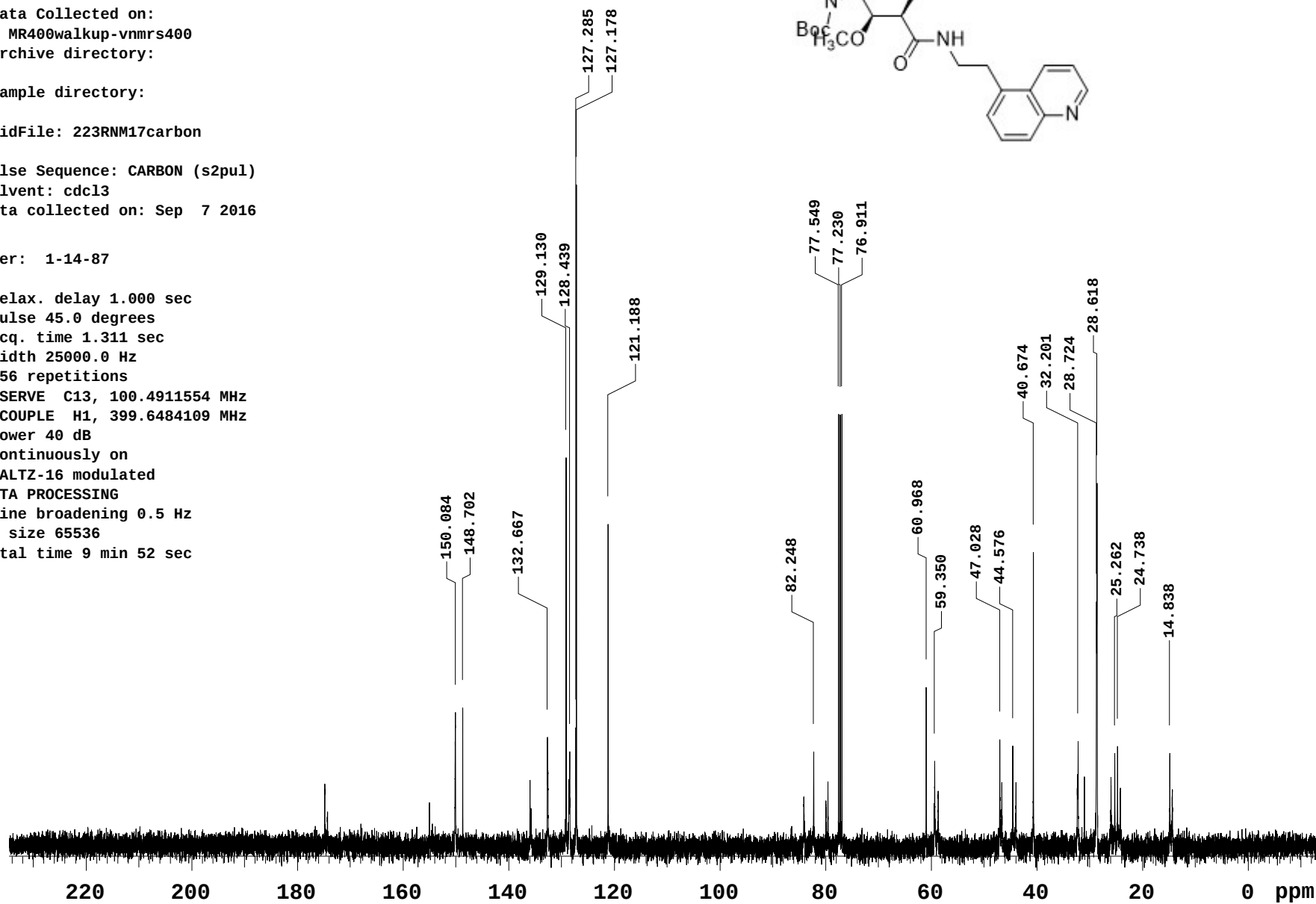
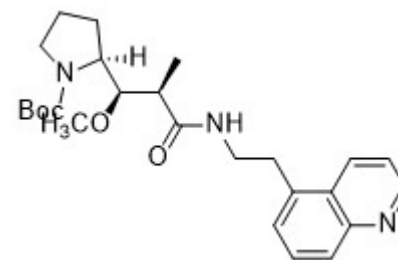
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

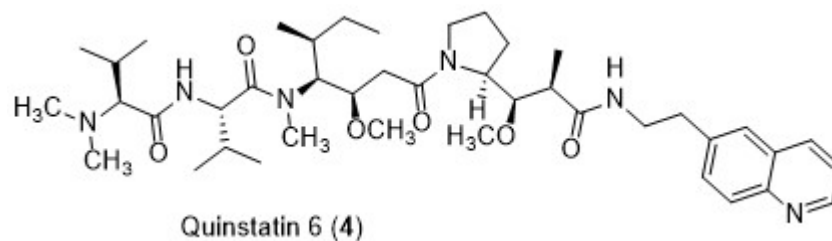
FT size 65536

Total time 9 min 52 sec

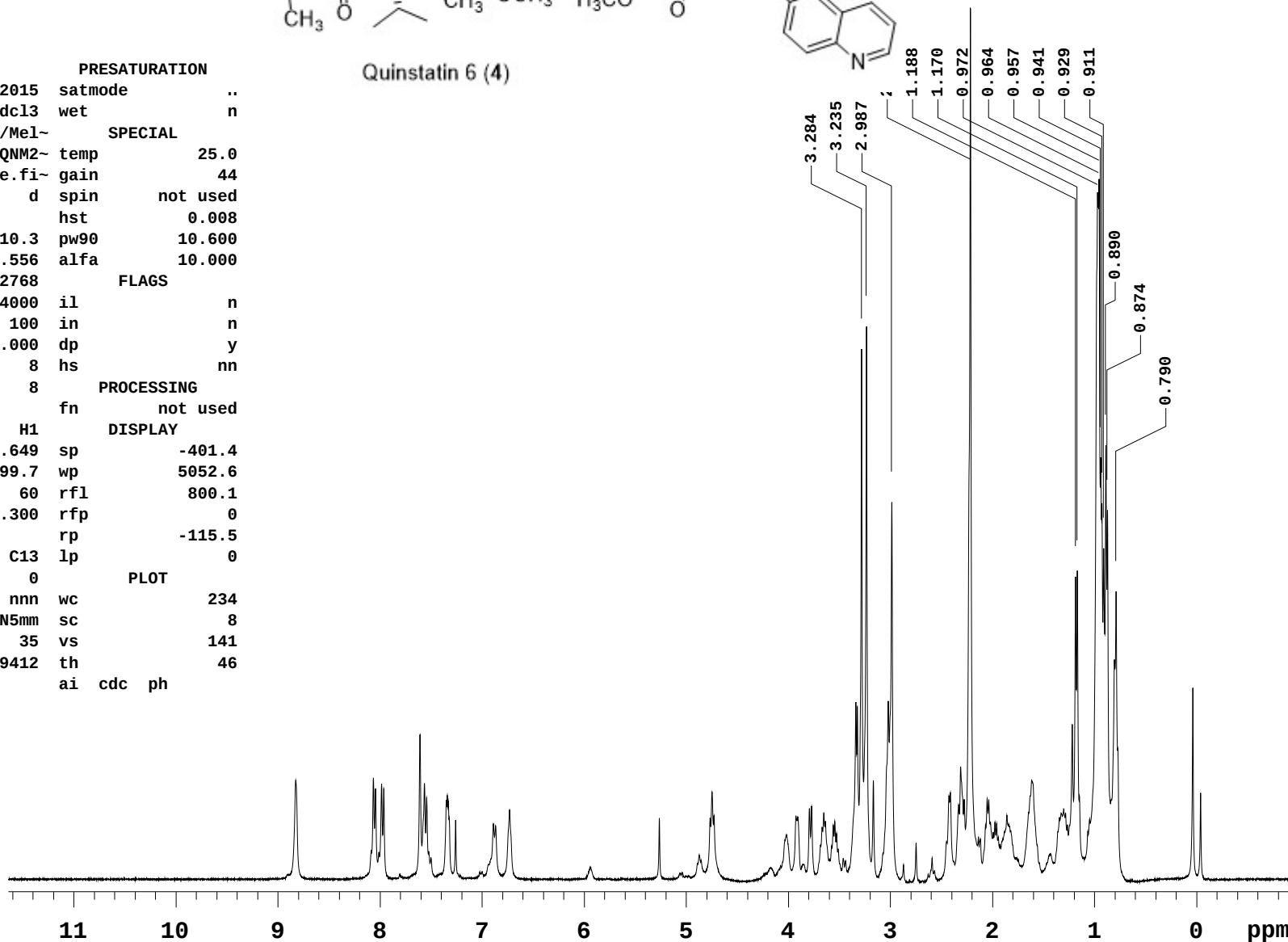


223QNM23F2

exp2 PROTON



SAMPLE		PRESATURATION	
date	May 4 2015	satmode	..
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel-	SPECIAL	
ody/Book Q/223QNM2~	temp	25.0	
3F2largersample.fi~	gain	44	
d	spin	not used	
ACQUISITION		hst	0.008
sw	6410.3	pw90	10.600
at	2.556	alfa	10.000
np	32768	FLAGS	
fb	4000	il	n
bs	100	in	n
d1	1.000	dp	y
nt	8	hs	nn
ct	8	PROCESSING	
TRANSMITTER		fn	not used
tn	H1	DISPLAY	
sfrq	399.649	sp	-401.4
tof	399.7	wp	5052.6
tpwr	60	rfl	800.1
pw	5.300	rpf	0
DECOUPLER		rp	-115.5
dn	C13	lp	0
dof	0	PLOT	
dm	nnn	wc	234
decwave	W40_HCN5mm	sc	8
dpwr	35	vs	141
dmf	29412	th	46
	ai	cdc	ph



223QNM23F2carbon

Sample Name:

223QNM23F2carbon

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: May 4 2015

Temp. 25.0 C / 298.1 K

User: 1-14-87

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.311 sec

Width 25000.0 Hz

512 repetitions

OBSERVE C13, 100.4911500 MHz

DECOUPLE H1, 399.6484109 MHz

Power 40 dB

continuously on

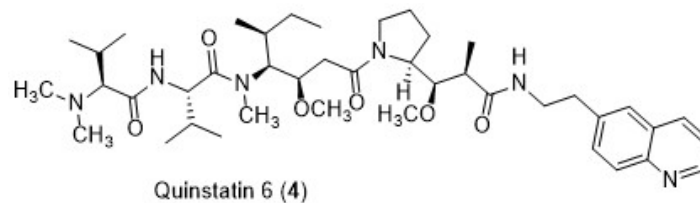
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

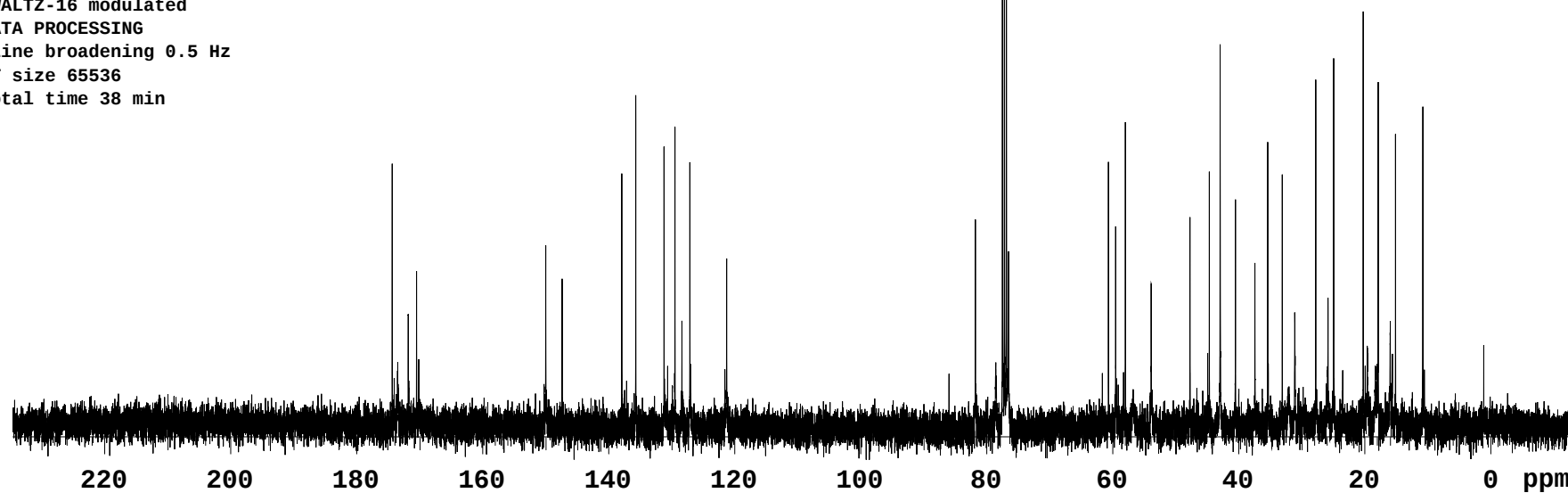
Total time 38 min



Quinstatin 6 (4)

77.549
77.290
76.911

S18

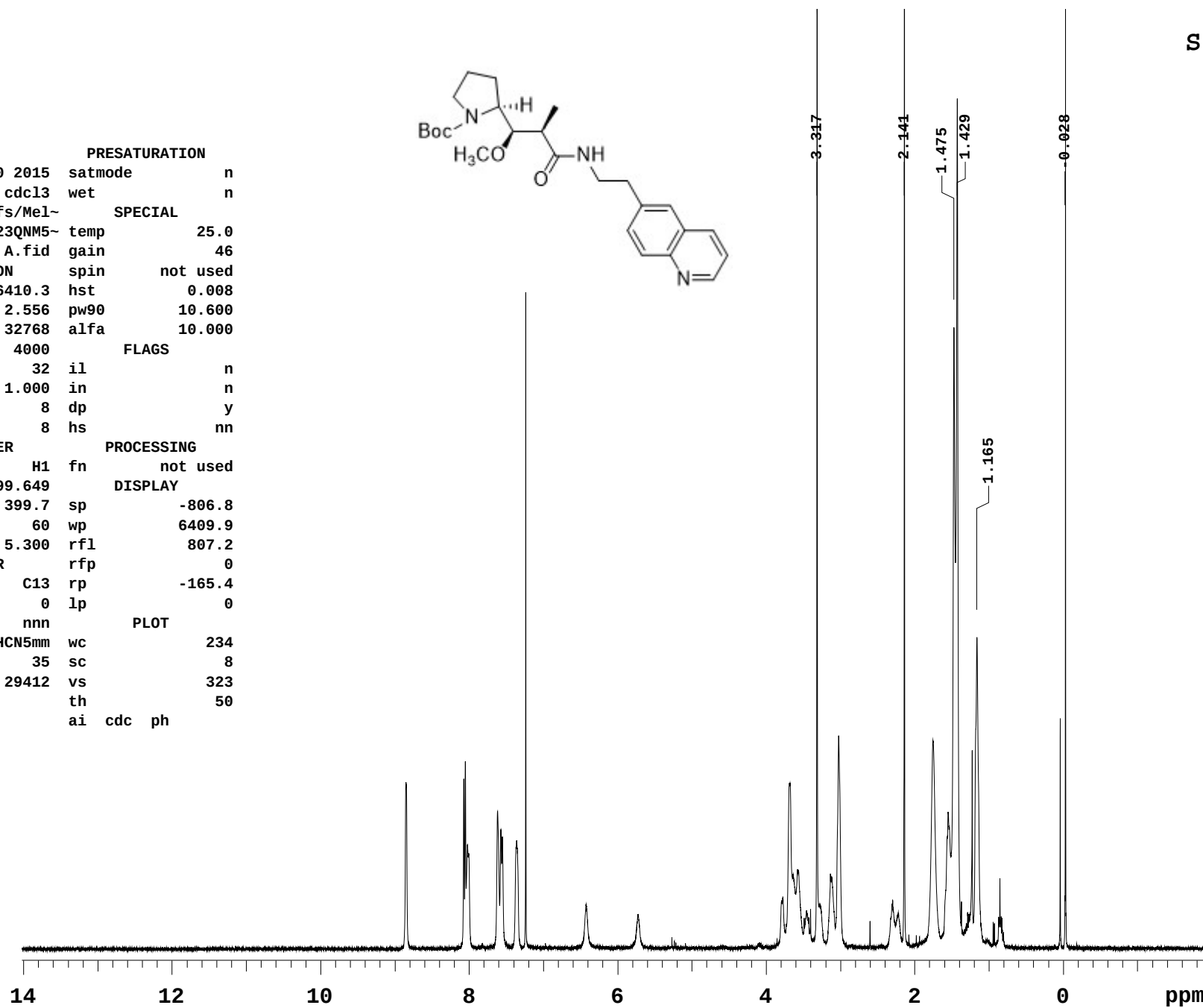
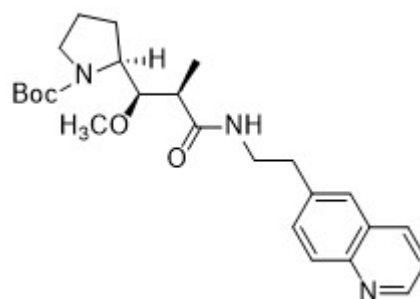


223QNM5A

S19

exp2 PROTON

SAMPLE		PRESATURATION	
date	Apr 20 2015	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel~	SPECIAL	
ody/Book Q/223QNM5~	temp	25.0	
A.fid	gain	46	
ACQUISITION		spin	not used
sw	6410.3	hst	0.008
at	2.556	pw90	10.600
np	32768	alfa	10.000
fb	4000	FLAGS	
bs	32	il	n
d1	1.000	in	n
nt	8	dp	y
ct	8	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.649	DISPLAY	
tof	399.7	sp	-806.8
tpwr	60	wp	6409.9
pw	5.300	rfl	807.2
DECOUPLER		rfp	0
dn	C13	rp	-165.4
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_HCN5mm	wc	234
dpwr	35	sc	8
dmf	29412	vs	323
		th	50
		ai	cdc ph

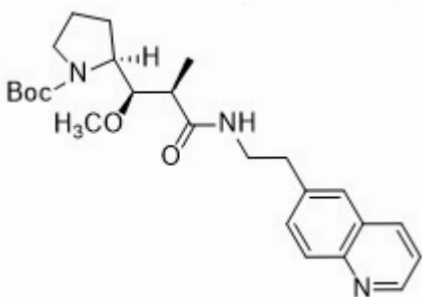


S20

File: 223QNM5A_run1 Date Run: 04-29-2015 (Time Run: 15:45:28)
Sample: Sample in DCM/ MeOH; apci400-1000p
Instrument: JEOL LCmate

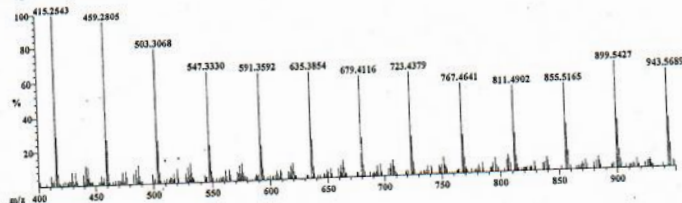
Run By: Zolotova/Knight

Ionization mode: APCI+



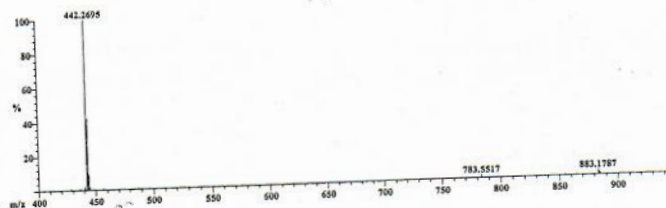
Scan: 6-19 R.T.: .52
Base: m/z 415; 1.3%FS TIC: 335920 (Max Inten : 13571)
(Background)

#Ions: 395



Scan: 21-52 (6-19) R.T.: 1.48
Base: m/z 442; 18.6%FS TIC: 344344 (Max Inten : 195428)

#Ions: 172



Selected Isotopes: $\text{CHN}_{0.3}\text{O}_{0.4}$

Error Limit: 3 ppm

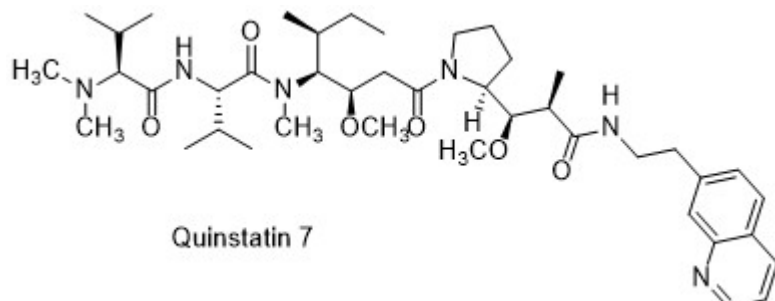
Unsaturation Limits: 1 to 40

Measured Mass	% Base	Formula	Calculated Mass	Error	Unsaturation
442.2695	100.0%	$\text{C}_{25}\text{H}_{36}\text{N}_3\text{O}_4$	442.2706	-2.4	9.5

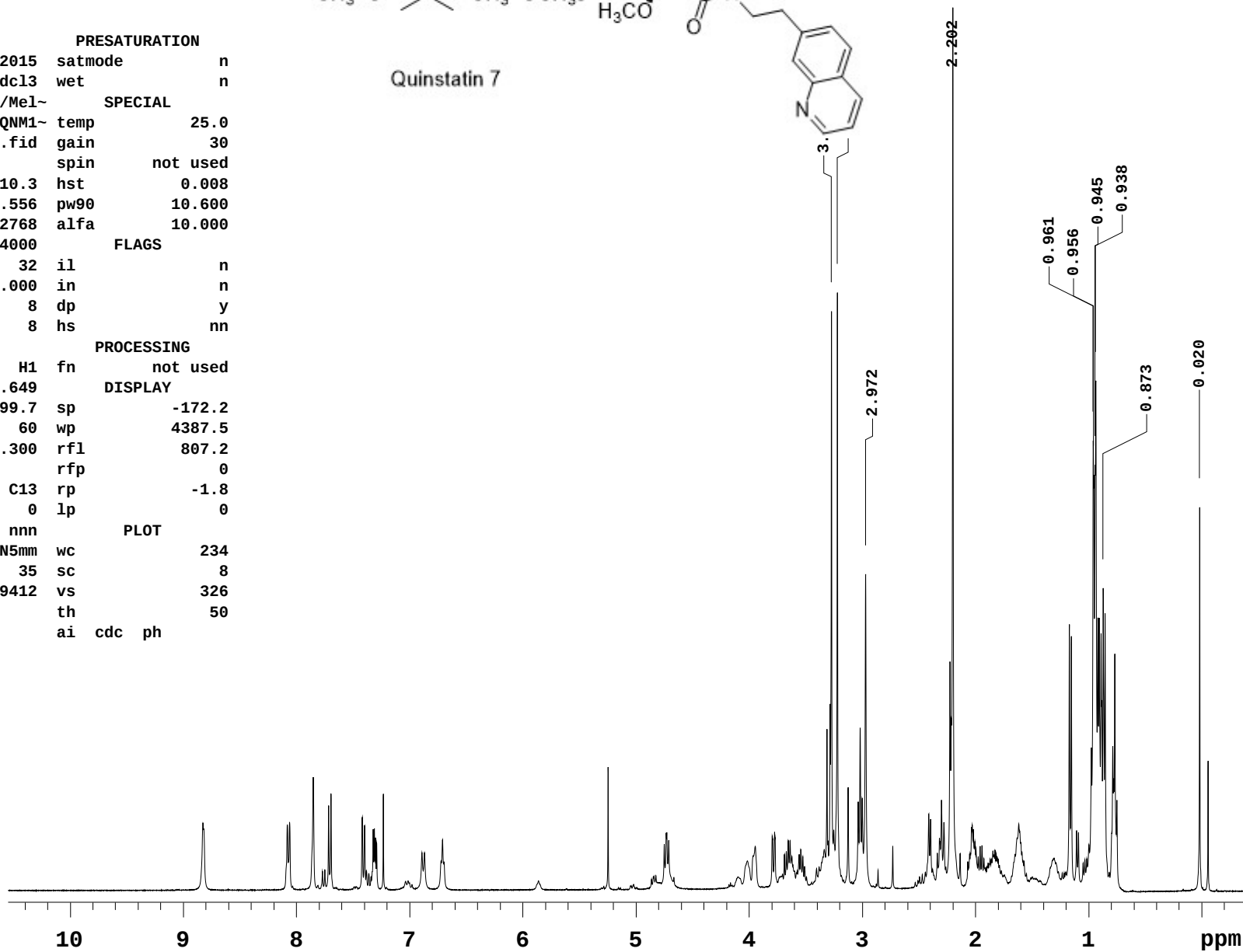


exp2 PROTON

SAMPLE		PRESATURATION	
date	Sep 21 2015	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel-	SPECIAL	
ody/Book	Q/223QNM1~	temp	25.0
	11F2.fid	gain	30
ACQUISITION		spin	not used
sw	6410.3	hst	0.008
at	2.556	pw90	10.600
np	32768	alfa	10.000
fb	4000	FLAGS	
bs	32	il	n
d1	1.000	in	n
nt	8	dp	y
ct	8	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.649	DISPLAY	
tof	399.7	sp	-172.2
tpwr	60	wp	4387.5
pw	5.300	rfl	807.2
DECOUPLER		rfp	0
dn	C13	rp	-1.8
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_HCN5mm	wc	234
dpwr	35	sc	8
dmf	29412	vs	326
		th	50
		ai	cdc ph



S21



223QNM111F2carbon

Sample Name:

223QNM111F2carbon

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Sep 21 2015

Temp. 25.0 C / 298.1 K

User: 1-14-87

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.311 sec

Width 25000.0 Hz

448 repetitions

OBSERVE C13, 100.4911485 MHz

DECOUPLE H1, 399.6484109 MHz

Power 40 dB

continuously on

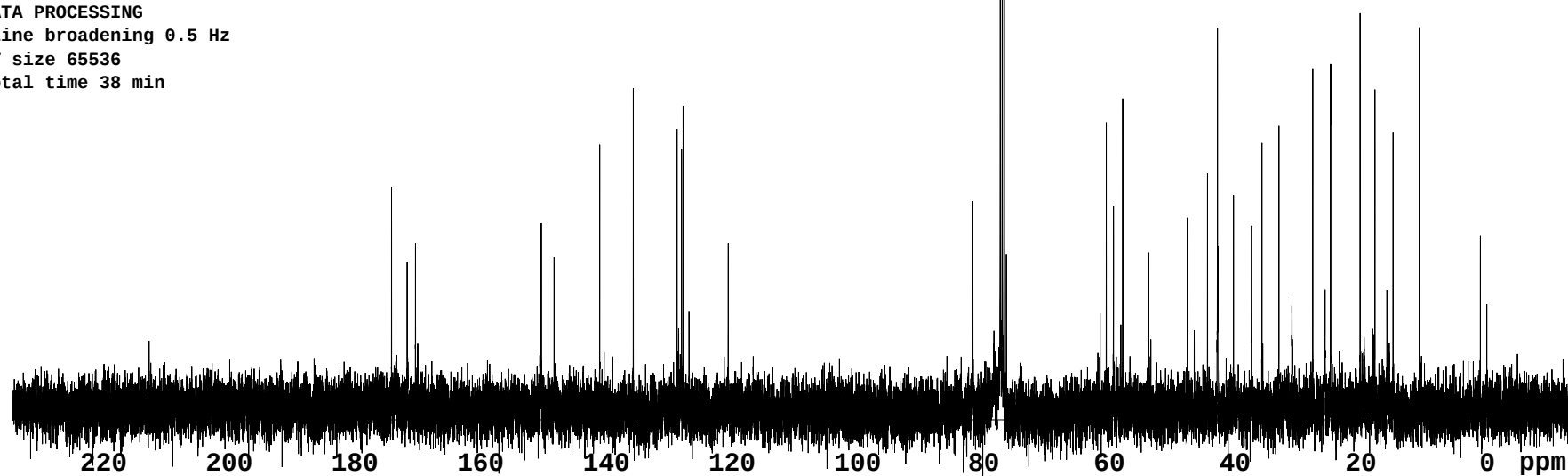
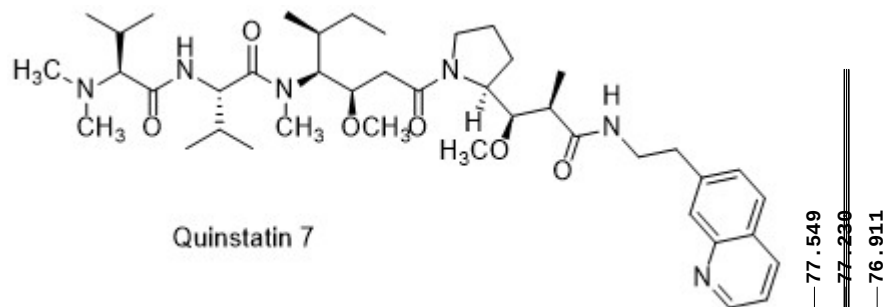
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

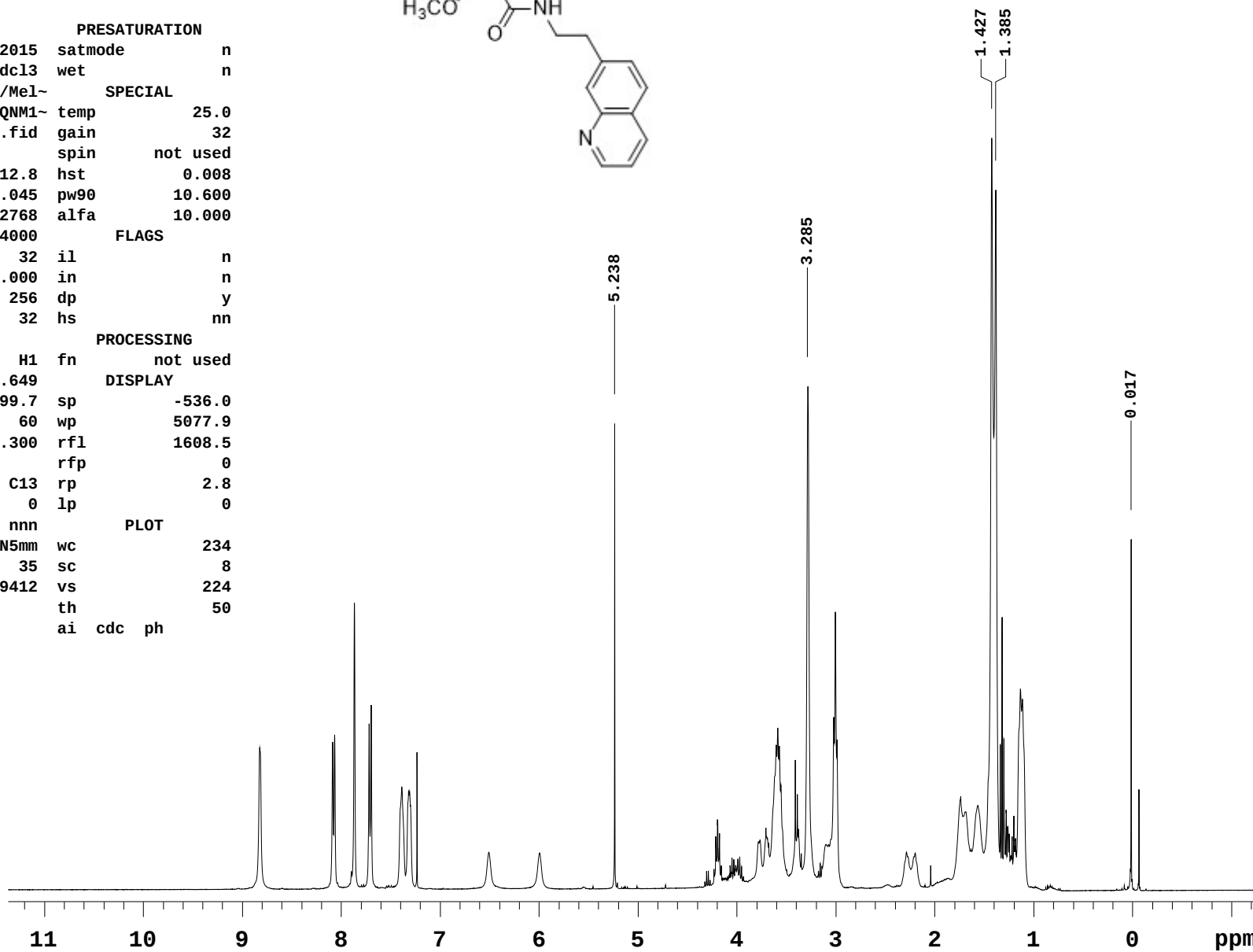
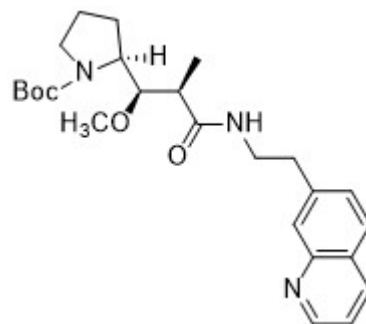
Total time 38 min



223QNM107F2

exp2 PROTON

SAMPLE		PRESATURATION	
date	Sep 17 2015	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel-	SPECIAL	
ody/Book Q/223QNM1~	temp	25.0	
07F2bocdapQ7.fid	gain	32	
ACQUISITION		spin	not used
sw	8012.8	hst	0.008
at	2.045	pw90	10.600
np	32768	alfa	10.000
fb	4000	FLAGS	
bs	32	il	n
d1	1.000	in	n
nt	256	dp	y
ct	32	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.649	DISPLAY	
tof	399.7	sp	-536.0
tpwr	60	wp	5077.9
pw	5.300	rfl	1608.5
DECOUPLER		rfl	0
dn	C13	rp	2.8
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_HCN5mm	wc	234
dpwr	35	sc	8
dmf	29412	vs	224
		th	50
		ai	cdc ph



223QNM107F2carbon

S24

Sample Name:

223QNM107F2carbon

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Sep 17 2015

Temp. 25.0 C / 298.1 K

User: 1-14-87

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.311 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 100.4911508 MHz

DECOUPLE H1, 399.6484109 MHz

Power 40 dB

continuously on

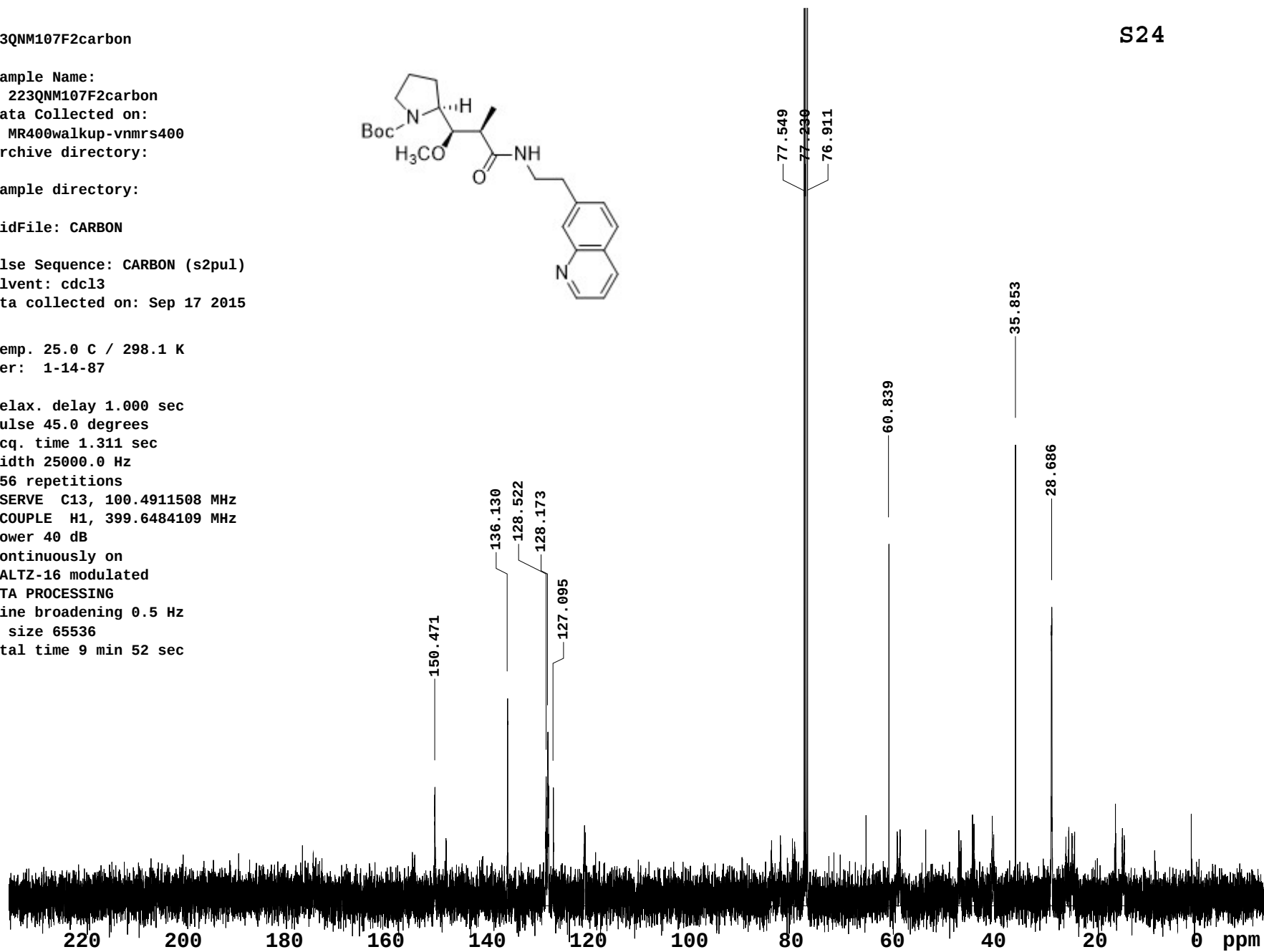
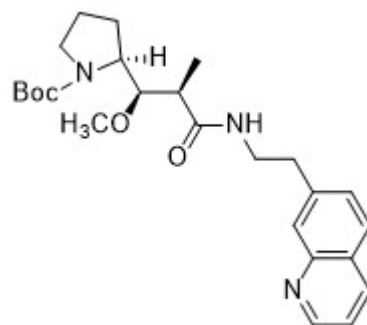
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

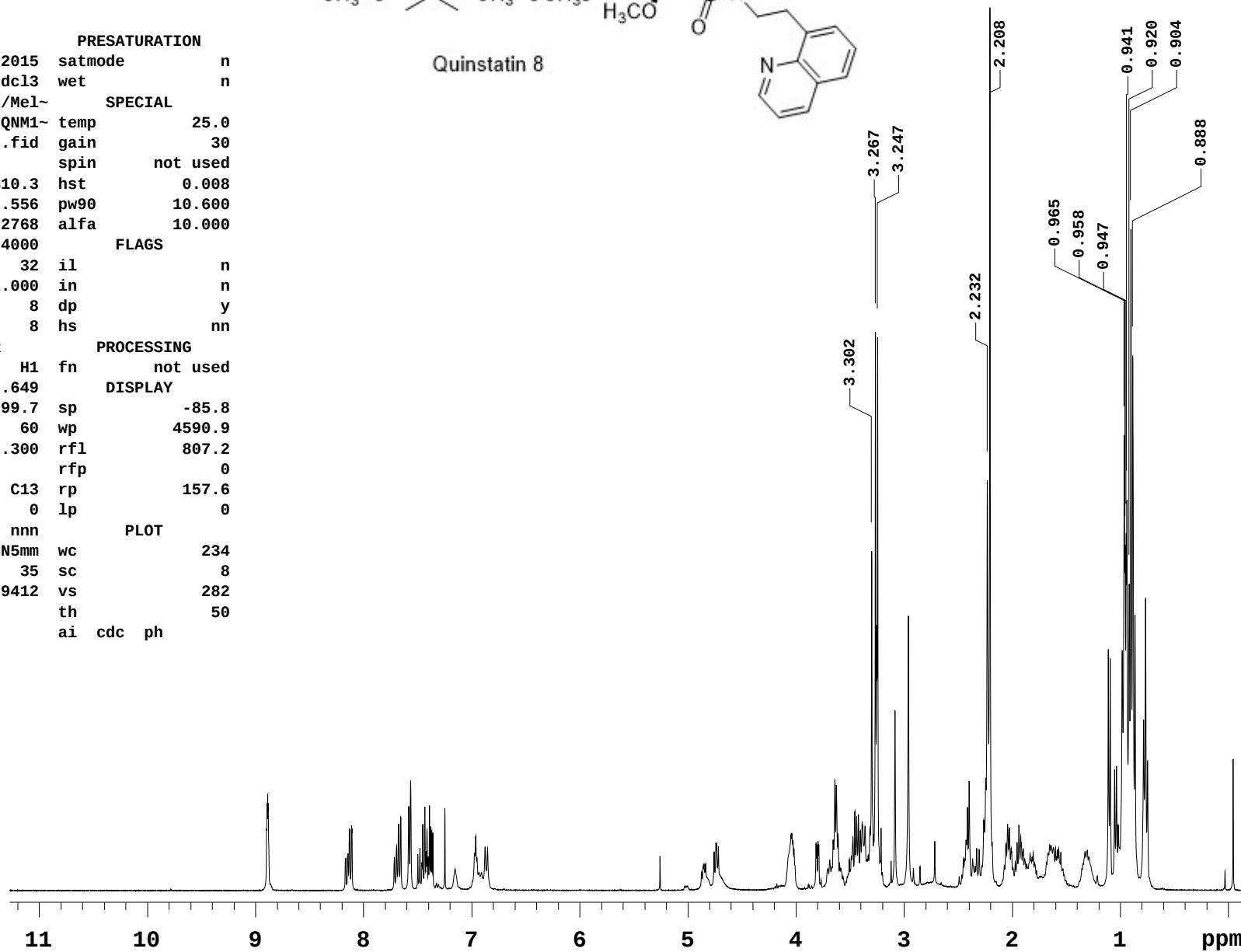
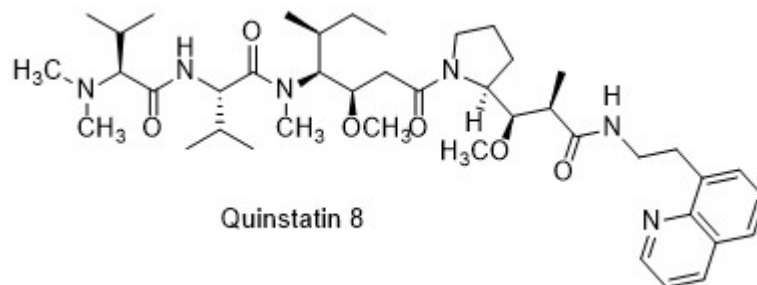
Total time 9 min 52 sec



223QNM129Quinstatin 8

exp2 PROTON

SAMPLE		PRESATURATION	
date	Oct 29 2015	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel~	SPECIAL	
ody/Book Q/223QNM1~	temp	25.0	
29Quinstatin8.fid	gain	30	
ACQUISITION		spin	not used
sw	6410.3	hst	0.008
at	2.556	pw90	10.600
np	32768	alfa	10.000
fb	4000	FLAGS	
bs	32	il	n
d1	1.000	in	n
nt	8	dp	y
ct	8	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.649	DISPLAY	
tof	399.7	sp	-85.8
tpwr	60	wp	4590.9
pw	5.300	rfl	807.2
DECOUPLER		rfl	0
dn	C13	rp	157.6
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_HCN5mm	wc	234
dpwr	35	sc	8
dmf	29412	vs	282
		th	50
		ai	cdc ph



223QNM129Quinstatin 8carbon

Sample Name:

223QNM129carbon

Data Collected on:

MR400walkup-vnmrs400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Oct 29 2015

Temp. 25.0 C / 298.1 K

User: 1-14-87

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.311 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 100.4911515 MHz

DECOUPLE H1, 399.6484109 MHz

Power 40 dB

continuously on

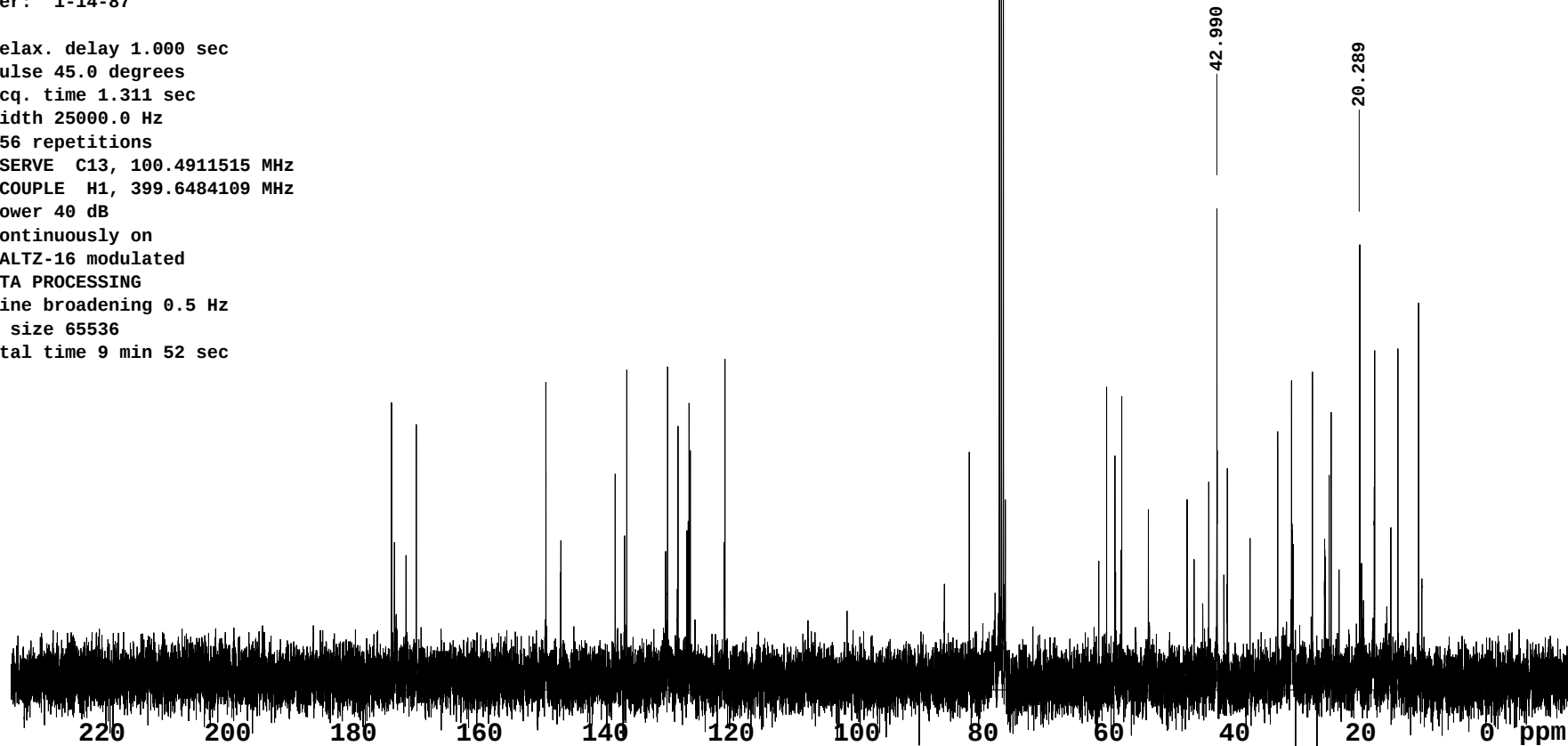
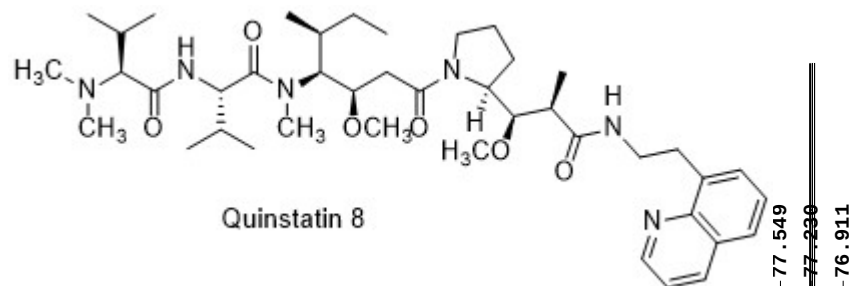
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min 52 sec



File: 223Q-NM-129-run2 Date Run: 11-05-2015 (Time Run: 15:10:56)

Sample: Sample in MeCl₂/MeOH

Instrument: JEOL LCmate

Run By: Zolotova/Knight

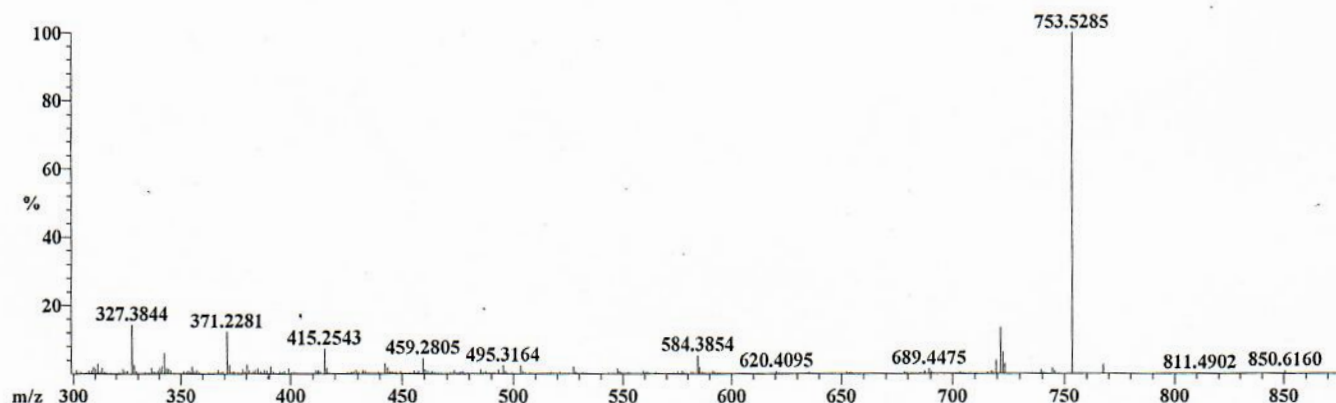
Ionization mode: APCI+

Scan: 98-104

R.T.: 4.02

Base: m/z 754; 86.8%FS TIC: 3485632 (Max Inten : 910160)

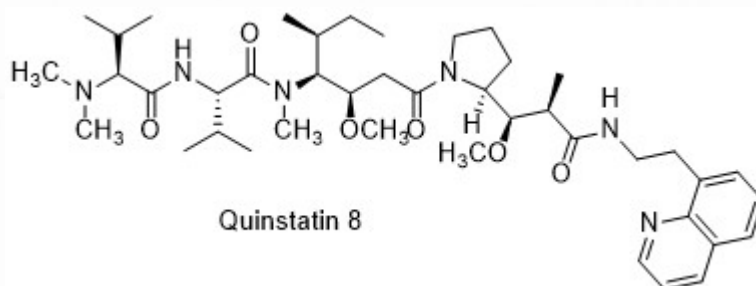
#Ions: 392

Selected Isotopes : CHN₆O₆

Error Limit : 100 ppm

Unsaturation Limits : 4 to 20

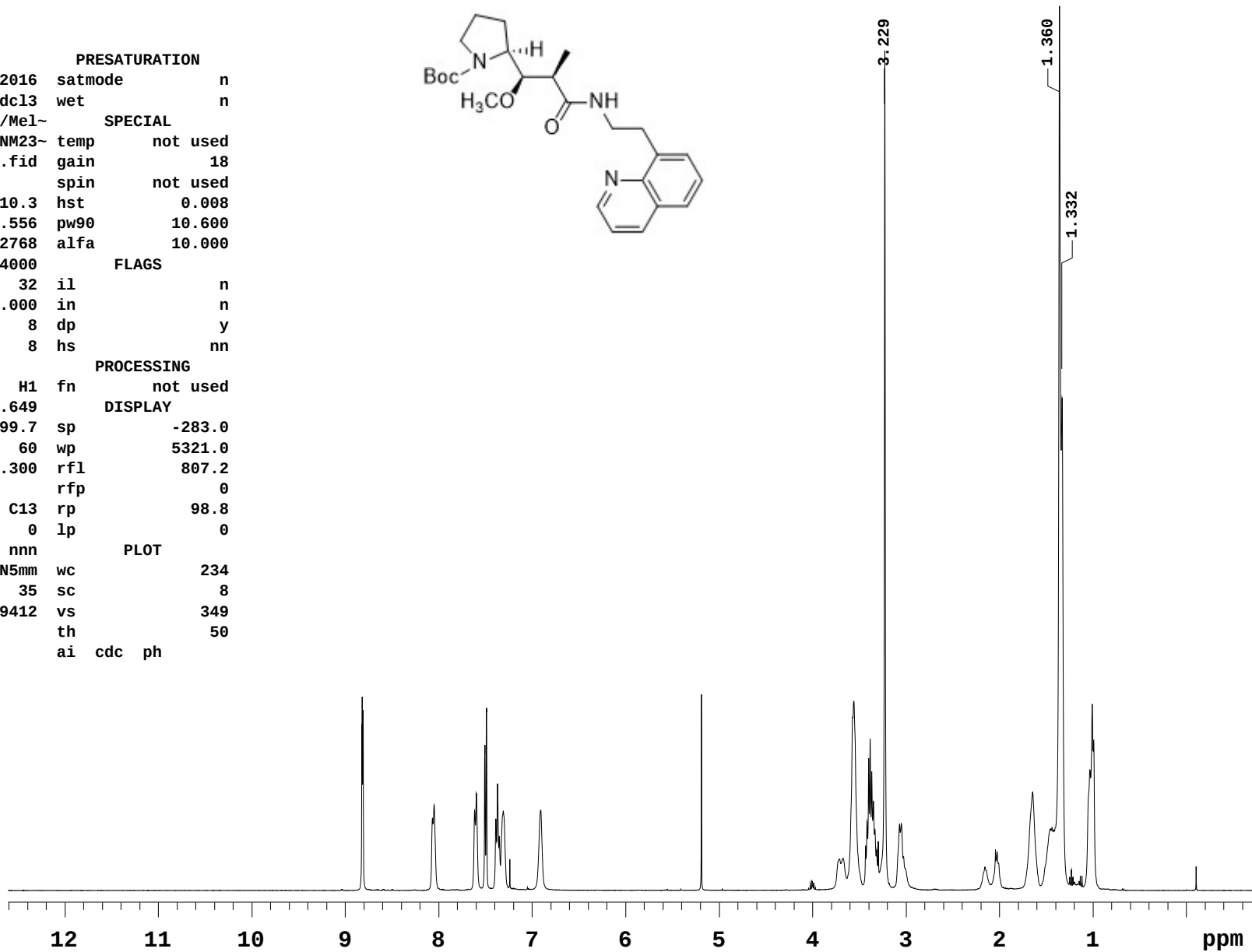
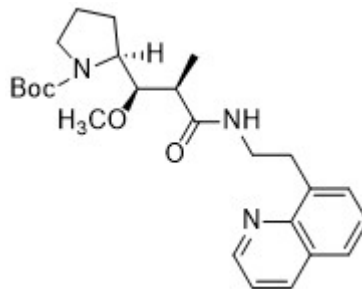
<u>Measured Mass</u>	<u>% Base</u>	<u>Formula</u>	<u>Calculated Mass</u>	<u>Error</u>	<u>Unsaturation</u>
753.5285	100.0%	C ₄₂ H ₆₉ N ₆ O ₆	753.5279	0.8	11.5



223RNM23

exp2 PROTON

SAMPLE		PRESATURATION	
date	Sep 13 2016	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel~	SPECIAL	
ody/BookR/223RNM23~		temp	not used
.fid		gain	18
ACQUISITION		spin	not used
sw	6410.3	hst	0.008
at	2.556	pw90	10.600
np	32768	alfa	10.000
fb	4000	FLAGS	
bs	32	il	n
d1	1.000	in	n
nt	8	dp	y
ct	8	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.649	DISPLAY	
tof	399.7	sp	-283.0
tpwr	60	wp	5321.0
pw	5.300	rfl	807.2
DECOUPLER		rfp	0
dn	C13	rp	98.8
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_HCN5mm	wc	234
dpwr	35	sc	8
dmf	29412	vs	349
		th	50
		ai	cdc ph



223RNM23carbon

exp2 CARBON

SAMPLE		PRESATURATION	
date	Sep 13 2016	satmode	n
solvent	cdcl3	wet	n
file	/mnt/hgfs/Mel~	SPECIAL	
ody/BookR/223RNM23~		temp	not used
bocDapQ8carbon.fid		gain	30
ACQUISITION		spin	not used
sw	25000.0	hst	0.008
at	1.311	pw90	13.750
np	65536	alfa	10.000
fb	17000	FLAGS	
bs	64	il	n
d1	1.000	in	n
nt	256	dp	y
ct	256	hs	nn
TRANSMITTER		PROCESSING	
tn	C13	lb	0.50
sfrq	100.502	fn	not used
tof	1530.2	DISPLAY	
tpwr	57	sp	-198.8
pw	6.875	wp	20928.2
DECOUPLER		rfl	9200.3
dn	H1	rfp	7760.9
dof	0	rp	-84.7
dm	yyy	lp	0
decwave	w	PLOT	
dpwr	40	wc	234
dmf	9311	sc	8
		vs	87899
		th	16
		ai	cdc ph

