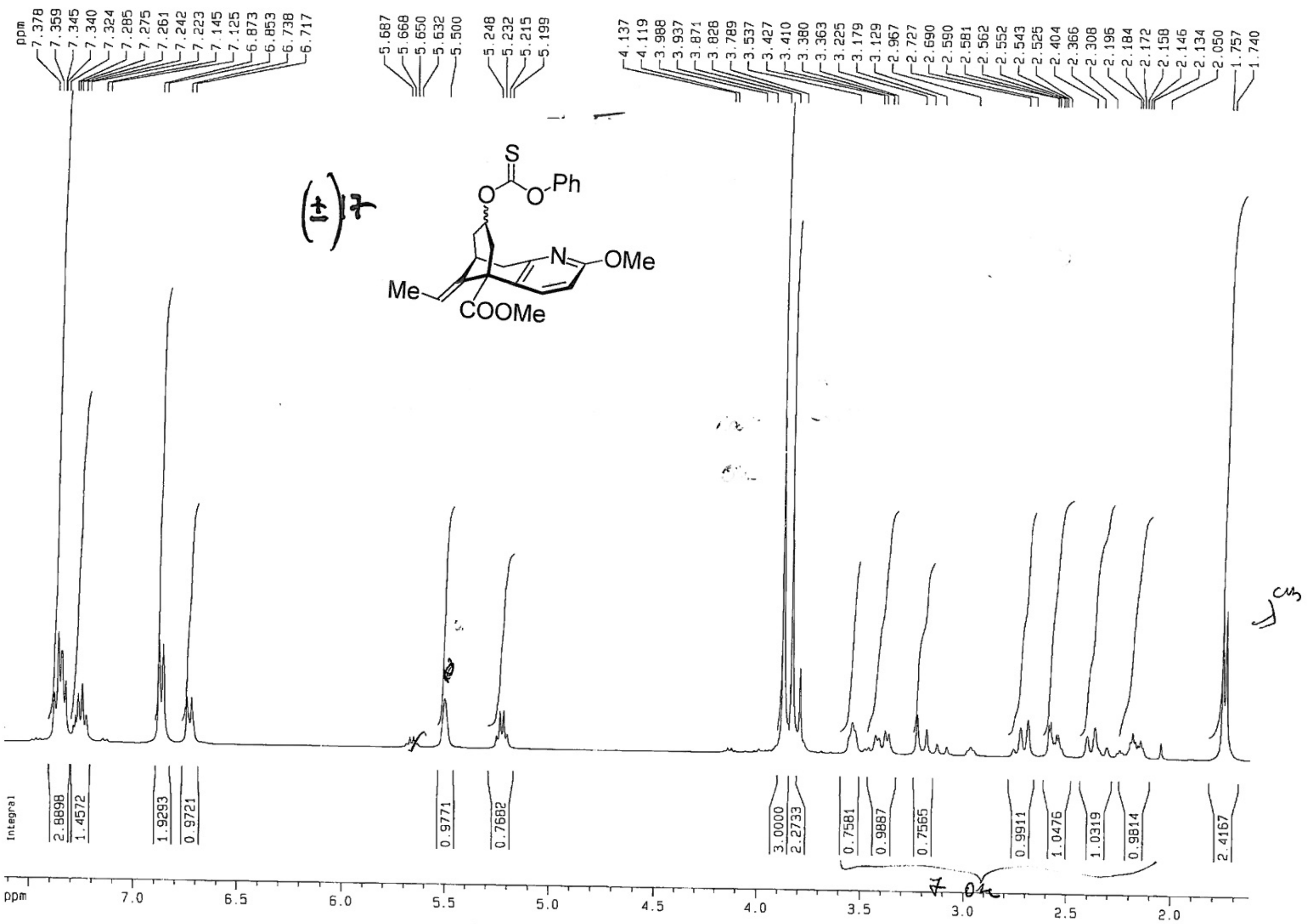
Sample: MF-~~~~~ (±)17
Solvent: c ~~~
Standard 1-D Survey Proton NMR Experiment
Bruker DPX-400 NMR Spectrometer
October 14, 2004 / D. Lankin



Current Data Parameters
NAME marcus
EXPNO 76
PROCNO 1

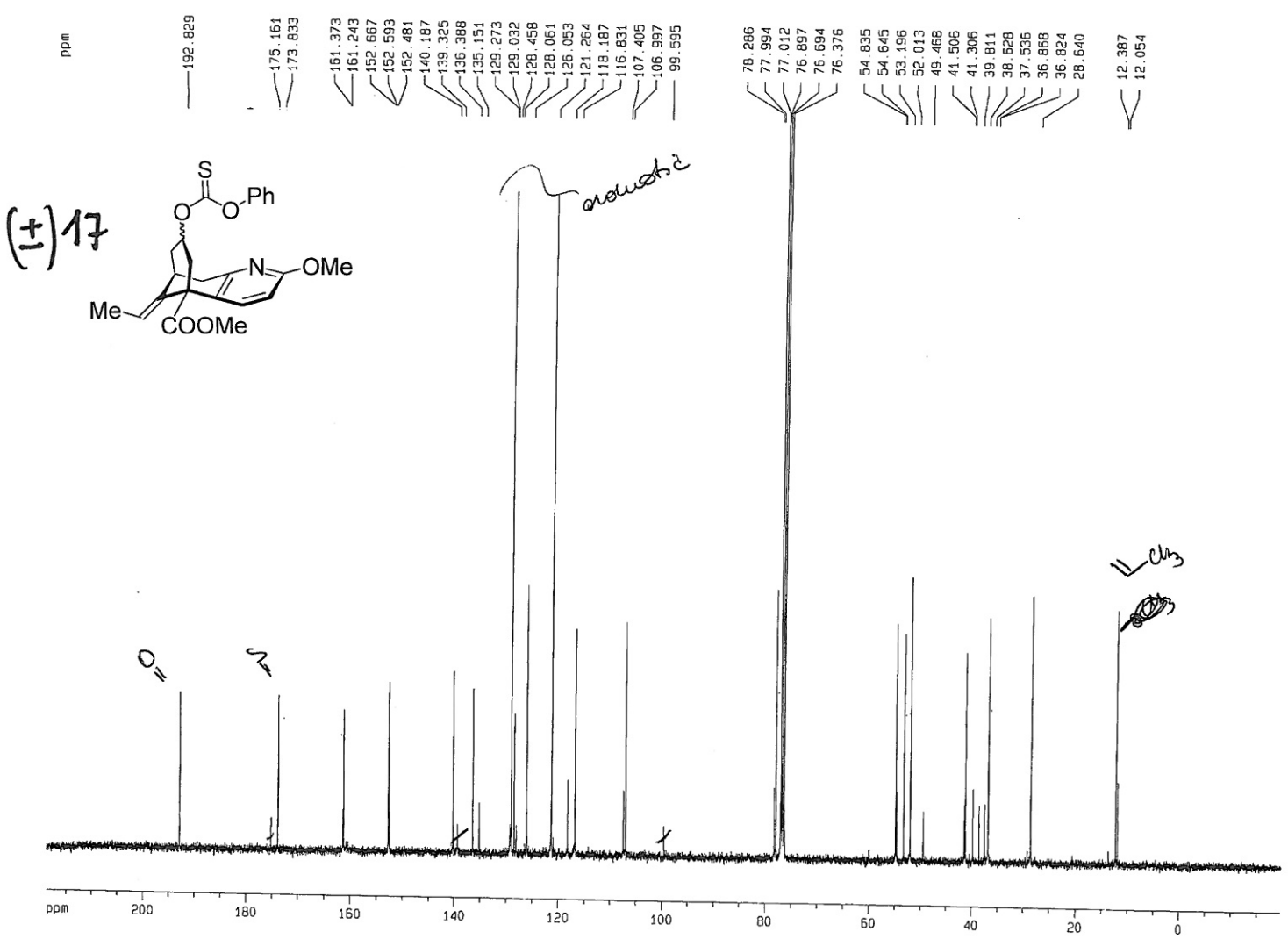
F2 - Acquisition Parameters
Date_ 20101005
Time 15.22
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 64
DW 60.400 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 262144
SF 400.1300037 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 28.00 cm
CY 8.00 cm
F1P 7.617 ppm
F1 3047.78 Hz
F2P 1.625 ppm
F2 650.15 Hz
PPMCM 0.21400 ppm/cm
HZCM 85.62978 Hz/cm

Sample: (±)17
Solvent:
1-D Carbon-13 NMR Spectrum
with Waltz-16 (CPD) Decoupling
Bruker DXP-400 NMR Spectrometer
October 14, 2004 / D. Lankin



Current Data Parameters

NAME	marcus
EXPNO	77
PROCNO	1

F2 - Acquisition Parameters

Date_	20101005
Time	15.28
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1340
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	574.7
DW	20.850 usec
DE	6.00 usec
TE	299.2 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	13C
P1	10.00 usec
PL1	-3.00 dB
SFO1	100.6228303 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6128096 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

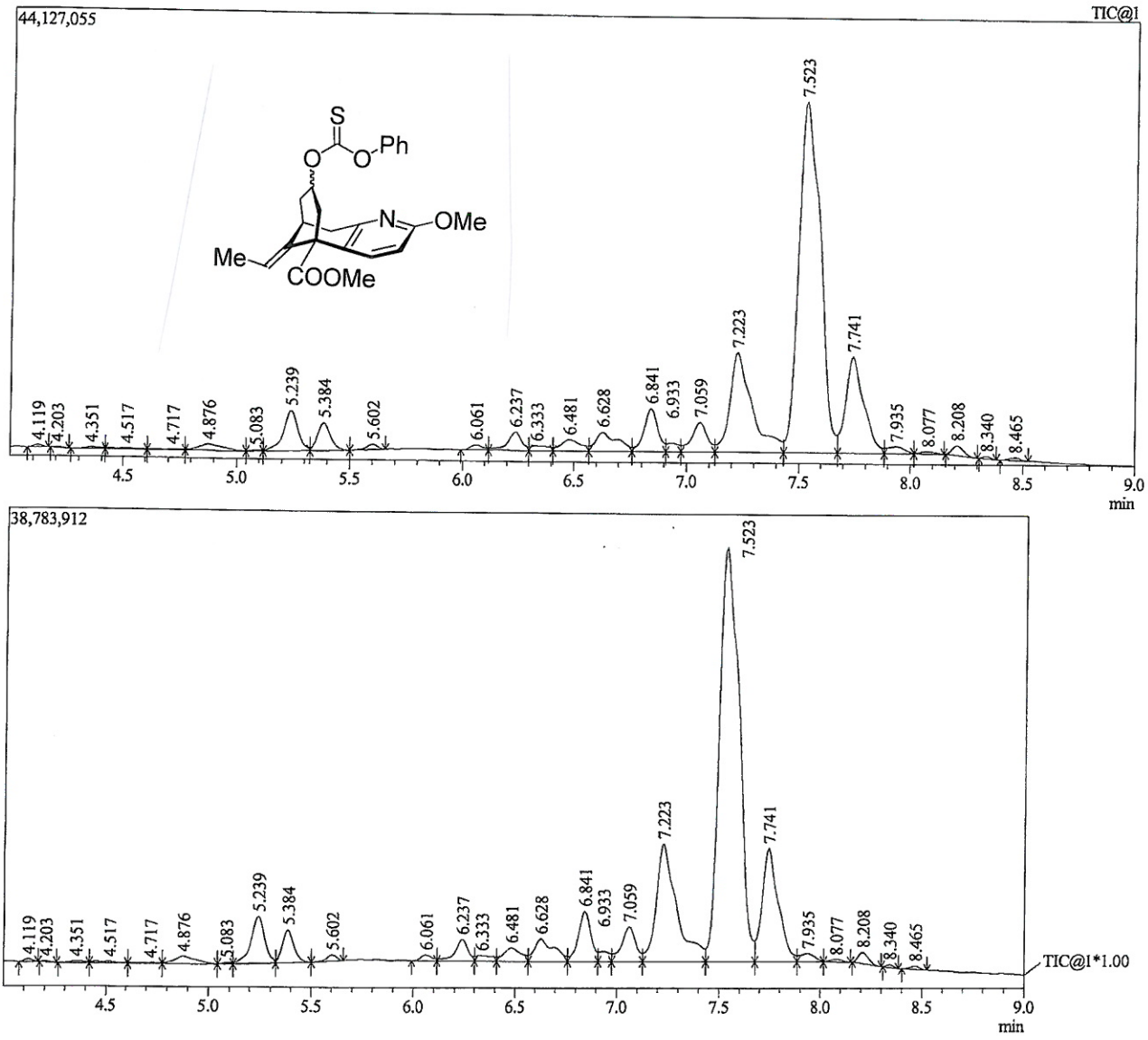
1D NMR plot parameters

CX	28.00 cm
CY	15.00 cm
F1P	218.770 ppm
F1	22011.04 Hz
F2P	-19.578 ppm
F2	-1969.77 Hz
PPMCM	8.51241 ppm/cm
HZCM	856.45770 Hz/cm

MASS# 17

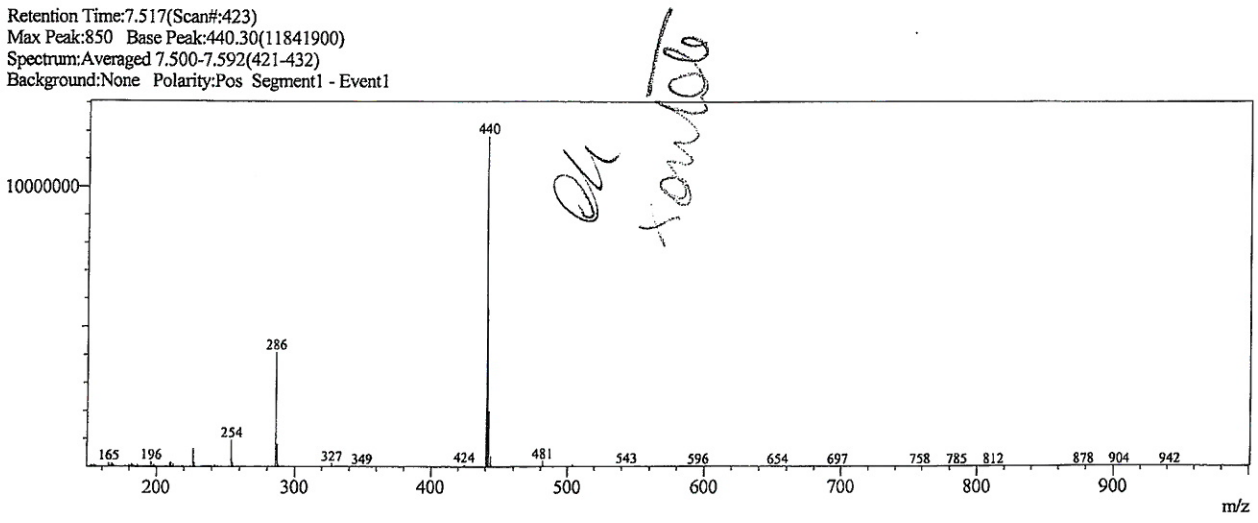
==== Shimadzu LCMSsolution Data Report ====

<Chromatogram>

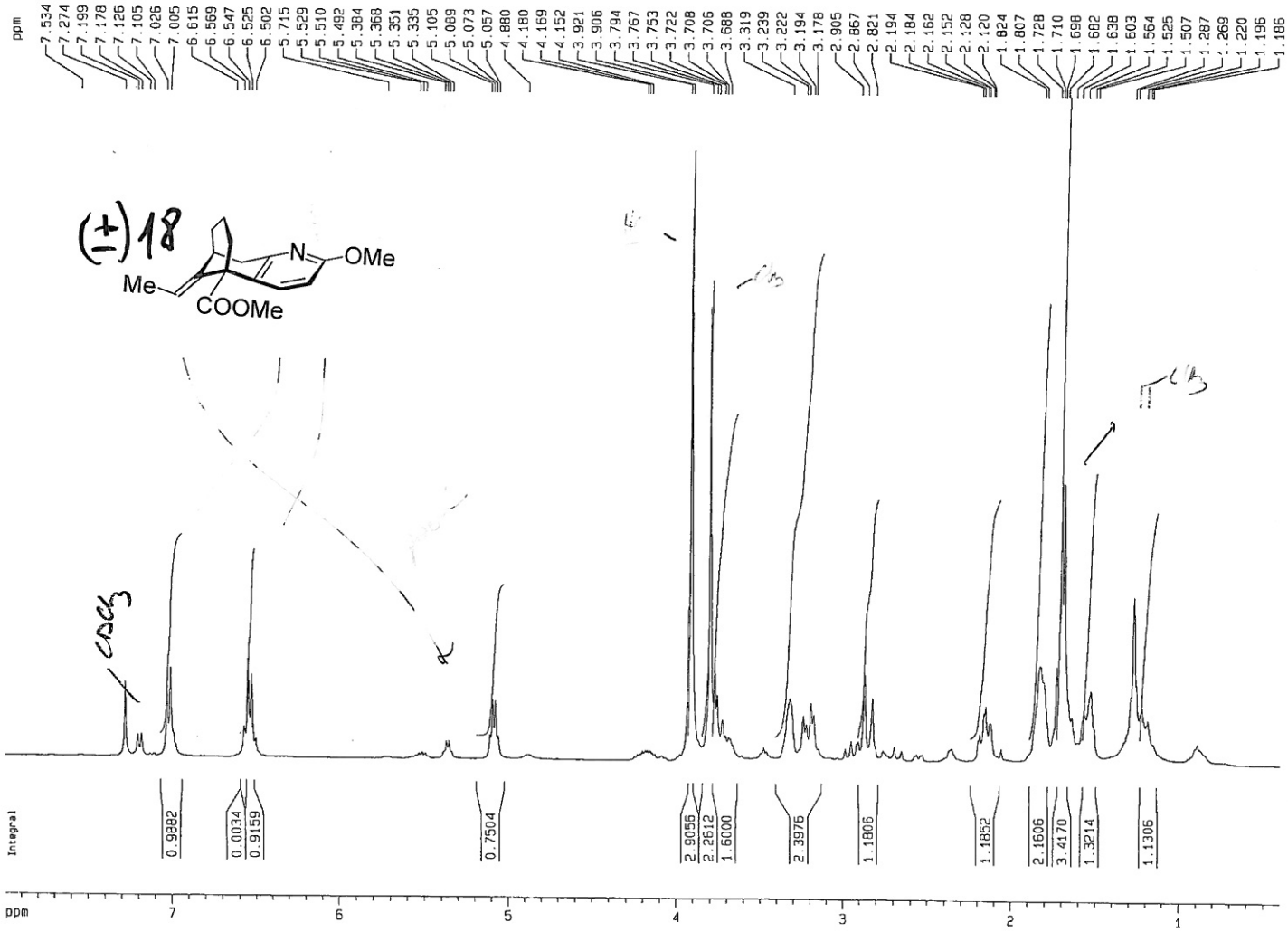


<Spectrum>

Retention Time:7.517(Scan#:423)
Max Peak:850 Base Peak:440.30(11841900)
Spectrum:Averaged 7.500-7.592(421-432)
Background:None Polarity:Pos Segment1 - Event1



Sample: 4 (±) 18
Solvent:
Standard 1-D Survey Proton NMR experiment
Bruker DPX-400 NMR Spectrometer
October 14, 2004 / D. Lankin



Current Data Parameters

NAME	marcus
EXPNO	103
PROCNO	1

F2 - Acquisition Parameters

Date_	20101118
Time	20.16
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	128
DW	60.400 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	12.00 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

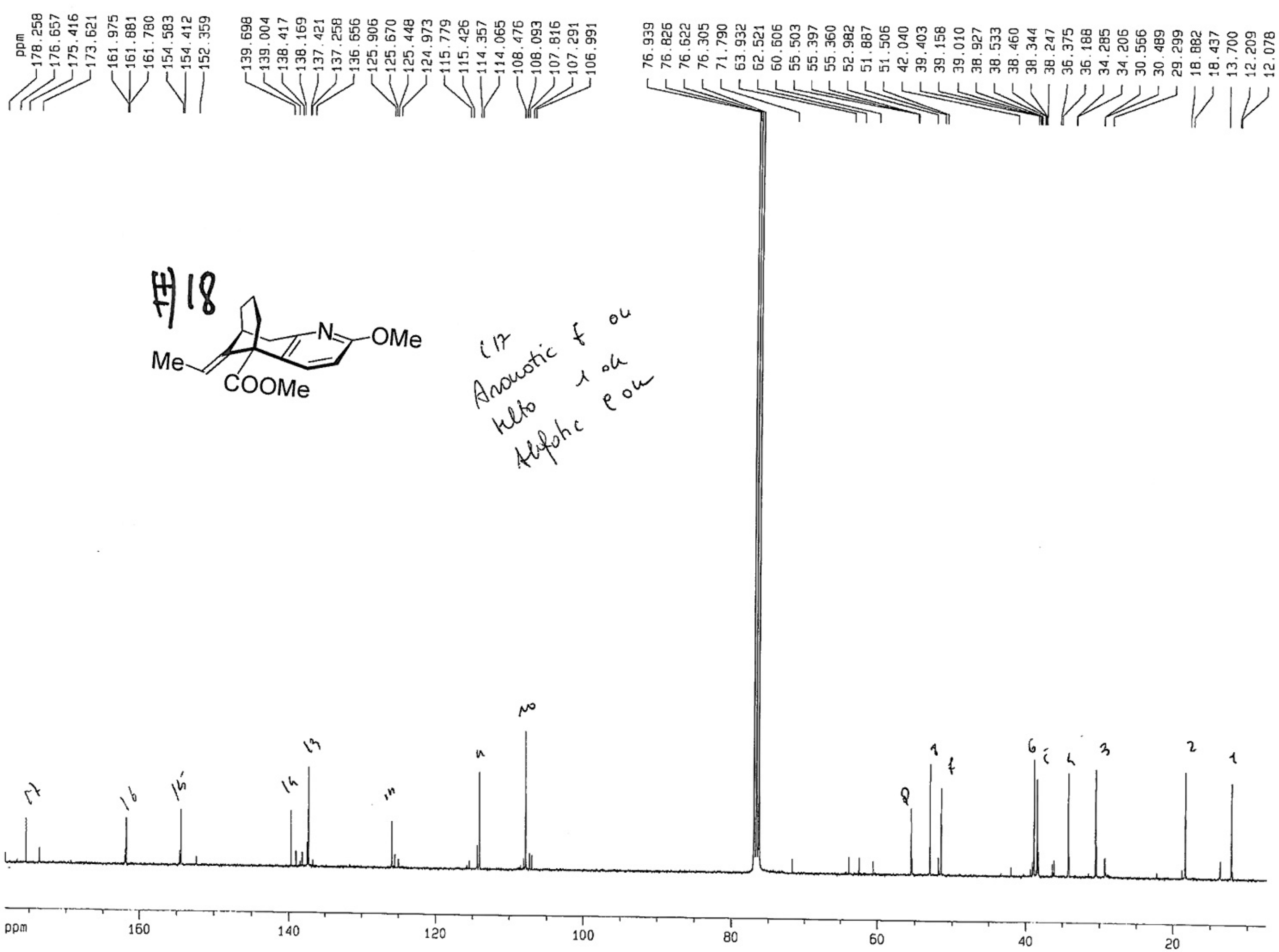
SI	262144
SF	400.1300037 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	28.00 cm
CY	12.00 cm
F1P	7.995 ppm
F1	3199.21 Hz
F2P	0.405 ppm
F2	162.21 Hz
PPMCM	0.27107 ppm/cm
HZCM	108.46438 Hz/cm

(±) 18

Sample:
Solvent:
1-D Carbon-13 NMR Spectrum
with Waltz-16 (CPD) Decoupling
Bruker DXP-400 NMR Spectrometer
October 14, 2004 / D. Lankin



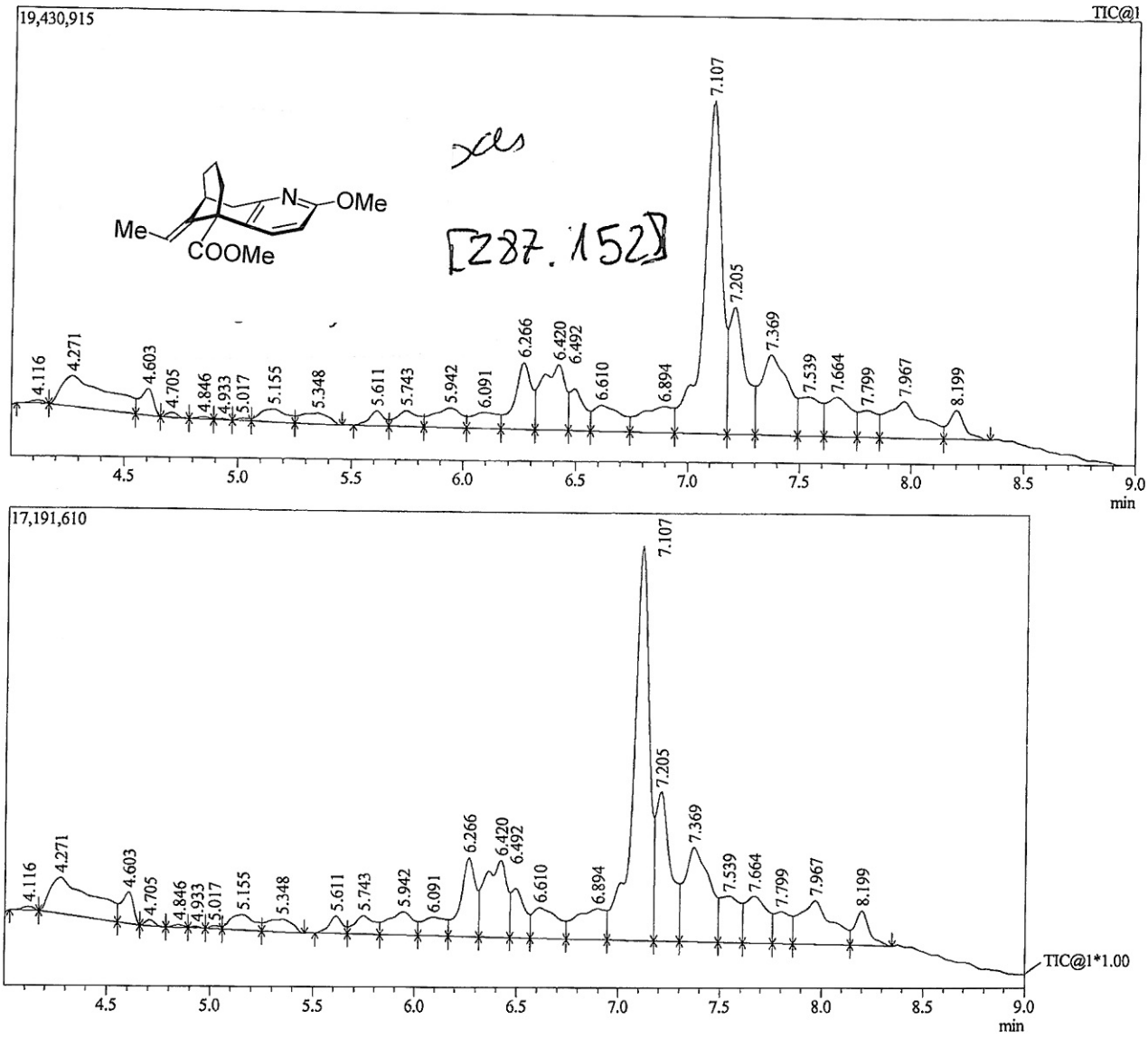
C17
Aromatic 4 CH
Keto 1 CH
Aliphatic 12 CH

Current Data Parameters	
NAME	marcus
EXPNO	104
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101118
Time	20.36
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	15488
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	574.7
DW	20.850 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	-3.00 dB
SFO1	100.6228303 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6128096 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40
1D NMR plot parameters	
CX	28.00 cm
CY	3.00 cm
F1P	178.319 ppm
F1	17941.13 Hz
F2P	7.551 ppm
F2	759.75 Hz
PPMCM	6.09883 ppm/cm
HZCM	613.62061 Hz/cm

MASS 18

==== Shimadzu LCMSsolution Data Report ====

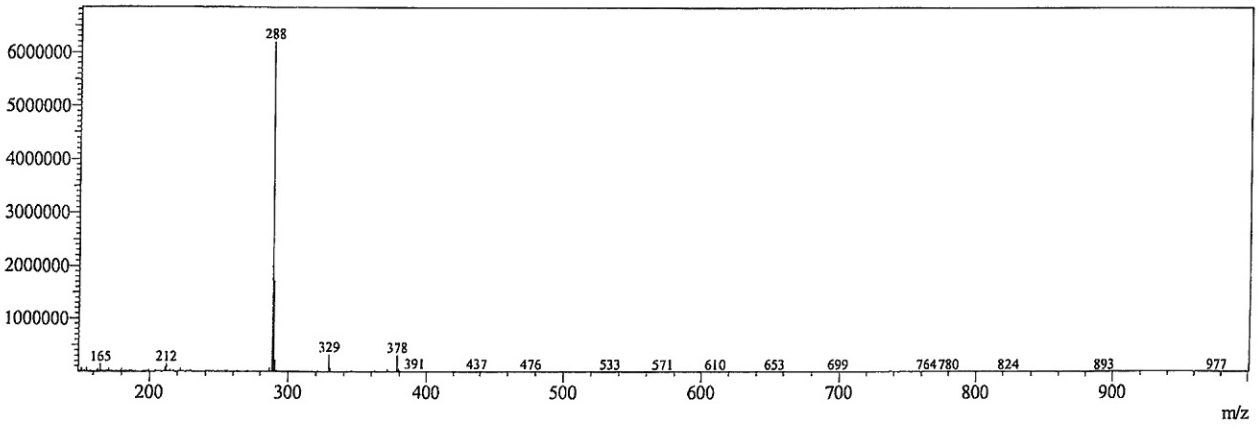
<Chromatogram>



<Spectrum>

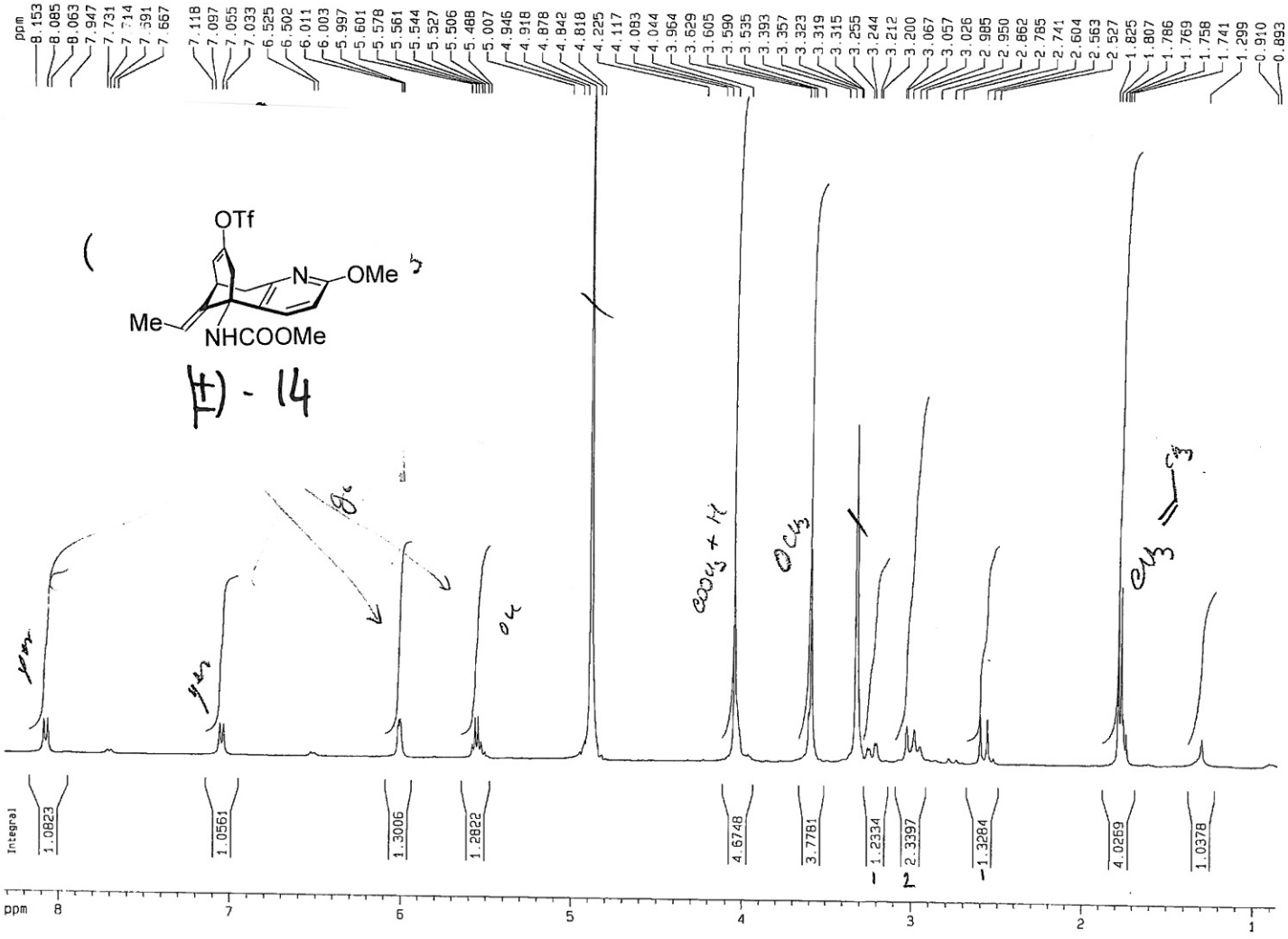
Retention Time:7.100(Scan#:373)
Max Peak:851 Base Peak:288.25(6202411)
Spectrum:Averaged 7.075-7.167(370-381)
Background:None Polarity:Pos Segment1 - Event1

la resolución es OK



Sample: ~~[illegible]~~ (±)14
Solvent: MeOD
Standard 1-D Survey Proton NMR Experiment
Bruker DPX-400 NMR Spectrometer
October 14, 2004 / D. Lankin

MeOD



Current Data Parameters

NAME	marcus
EXPNO	128
PROCNO	1

F2 - Acquisition Parameters

Date_	20101119
Time	10.44
INSTRUM	spect
PROBHD	5 mm GNP 1H/1
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	406.4
DW	60.400 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	12.00 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

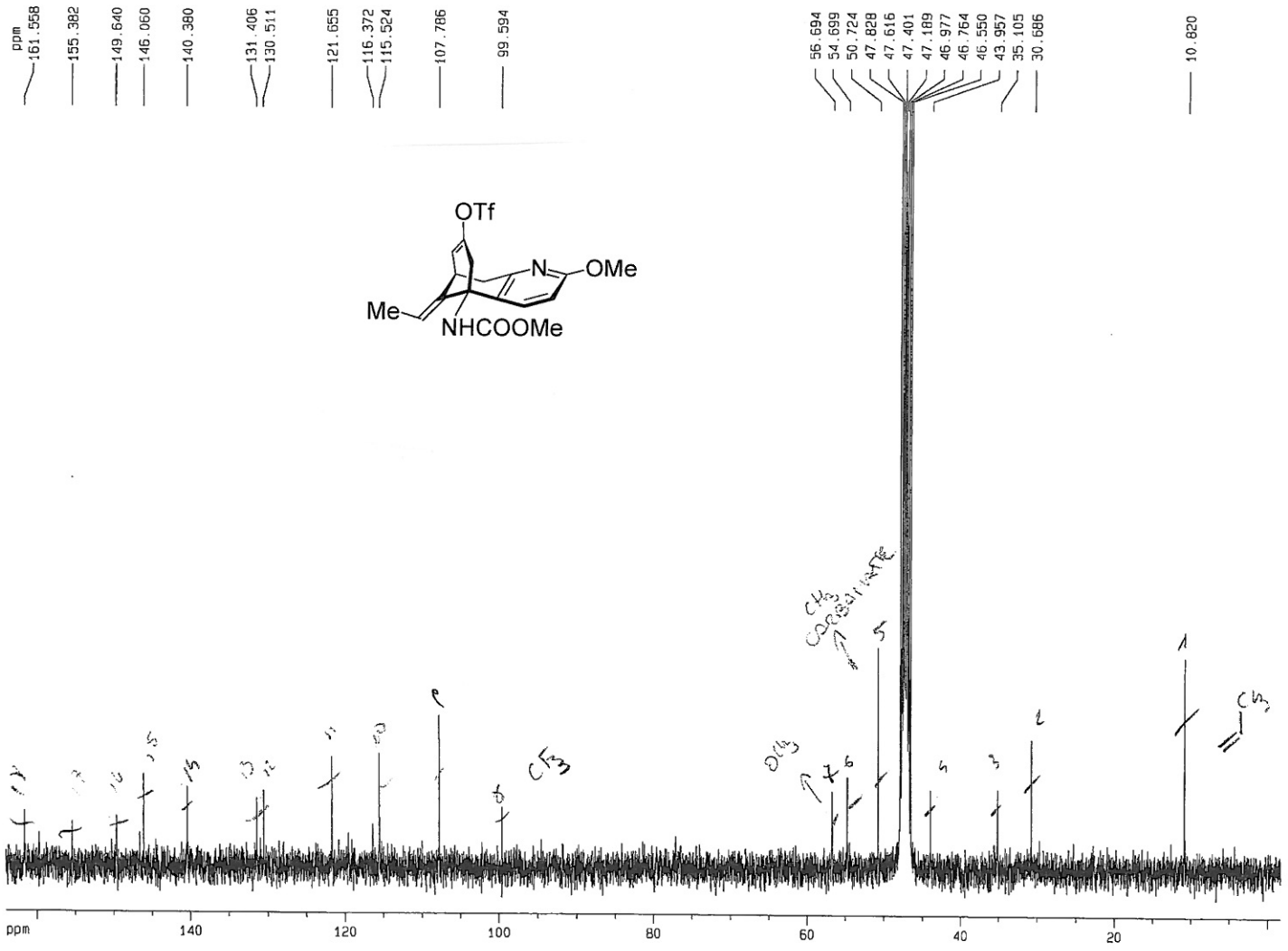
F2 - Processing parameters

SI	262144
SF	400.1300037 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	28.00 cm
CY	19.00 cm
F1P	8.316 ppm
F1	3327.57 Hz
F2P	0.862 ppm
F2	344.89 Hz
PPMCM	0.26622 ppm/cm
HZCM	106.52425 Hz/cm

Sample: Inactive (±)14
Solvent: CD3OD
1-D Carbon-13 NMR Spectrum
with Waltz-16 (CPD) Decoupling
Bruker DXP-400 NMR Spectrometer
October 14, 2004 / D. Lankin



Current Data Parameters

NAME	marcus
EXPNO	129
PROCNO	1

F2 - Acquisition Parameters

Date_	20101119
Time	10.55
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30
TD	65536
SOLVENT	MeOD
NS	2436
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3654756 sec
RG	2580.3
DW	20.850 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	13C
P1	10.00 usec
PL1	-3.00 dB
SFO1	100.6228303 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

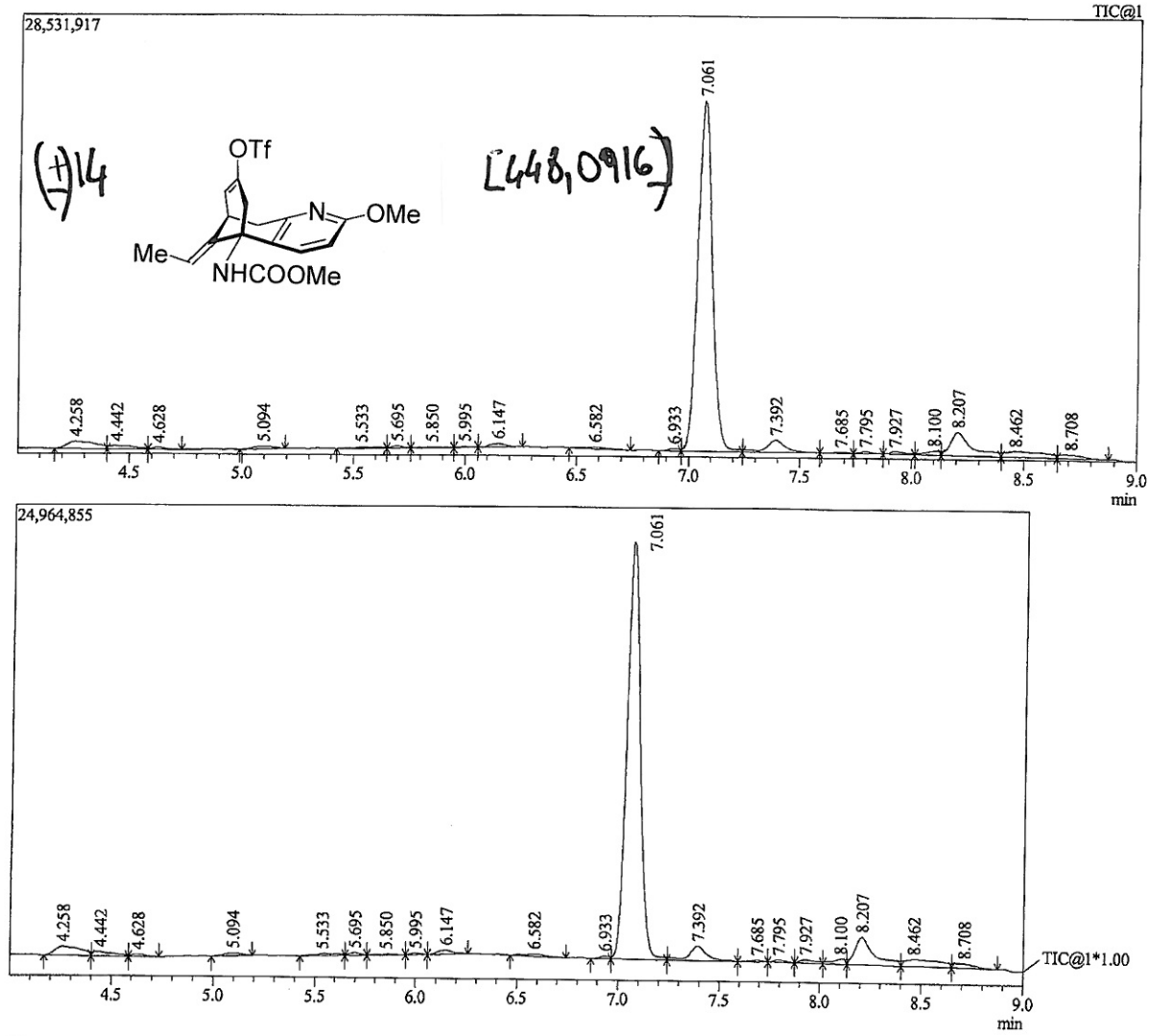
SI	32768
SF	100.6128096 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	28.00 cm
CY	250.00 cm
F1P	164.027 ppm
F1	16503.25 Hz
F2P	-1.653 ppm
F2	-166.33 Hz
PPMCM	5.91716 ppm/cm
HZCM	595.34247 Hz/cm

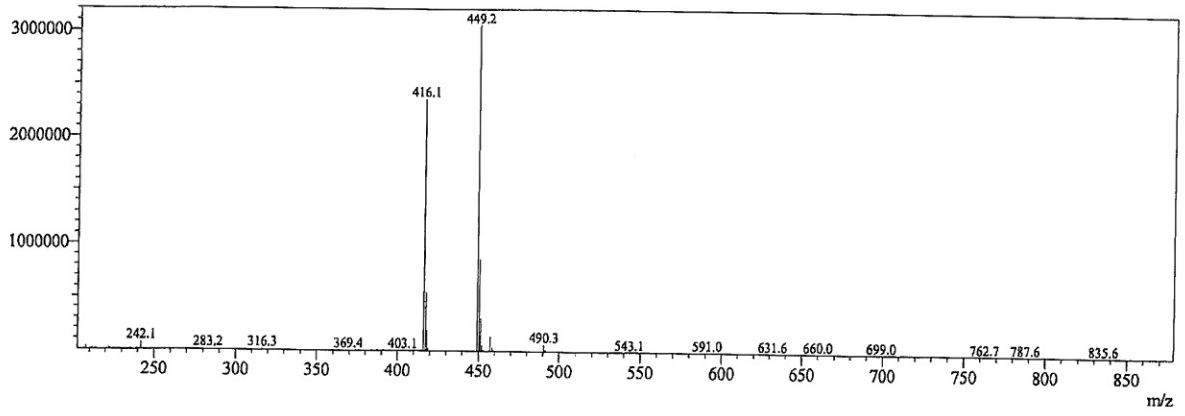
==== Shimadzu LCMSsolution Data Report ====

<Chromatogram>

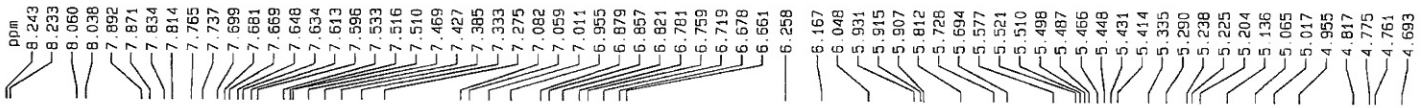


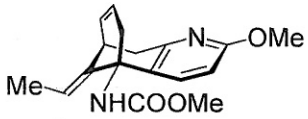
<Spectrum>

Retention Time:7.058(Scan#:368)
Max Peak:851 Base Peak:449.15(3054161)
Spectrum:Averaged 6.992-7.192(360-384)
Background:None Polarity:Pos Segment1 - Event1

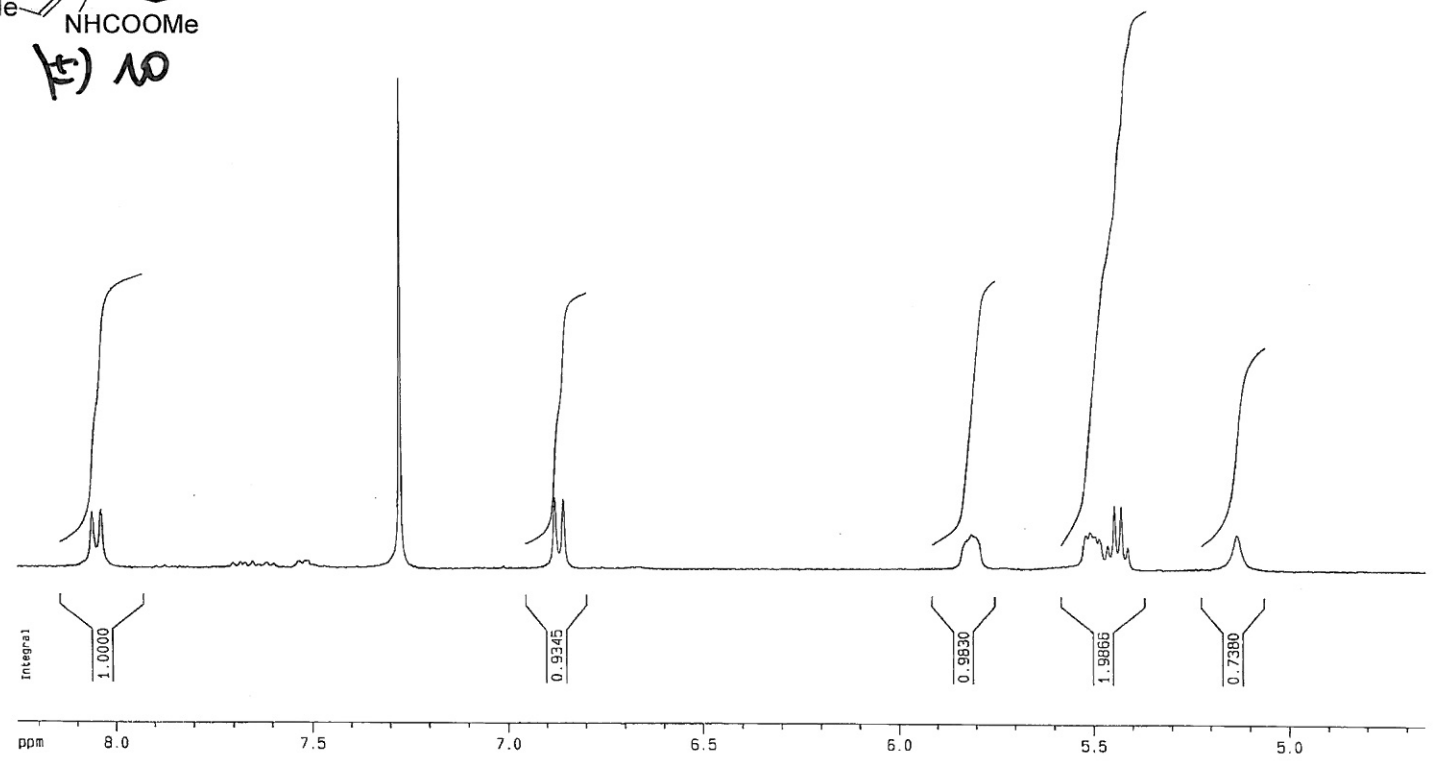


Sample: ~~MPV-12~~ (±) 10 $CDCl_3$
Solvent: ~~Cdcl3~~
Standard 1-D Survey Proton NMR Experiment
Bruker DPX-400 NMR Spectrometer
October 14, 2004 / D. Lankin





(±) 10



Current Data Parameters
NAME marcus
EXPNO 69
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100217
Time 17.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 812.7
DW 60.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

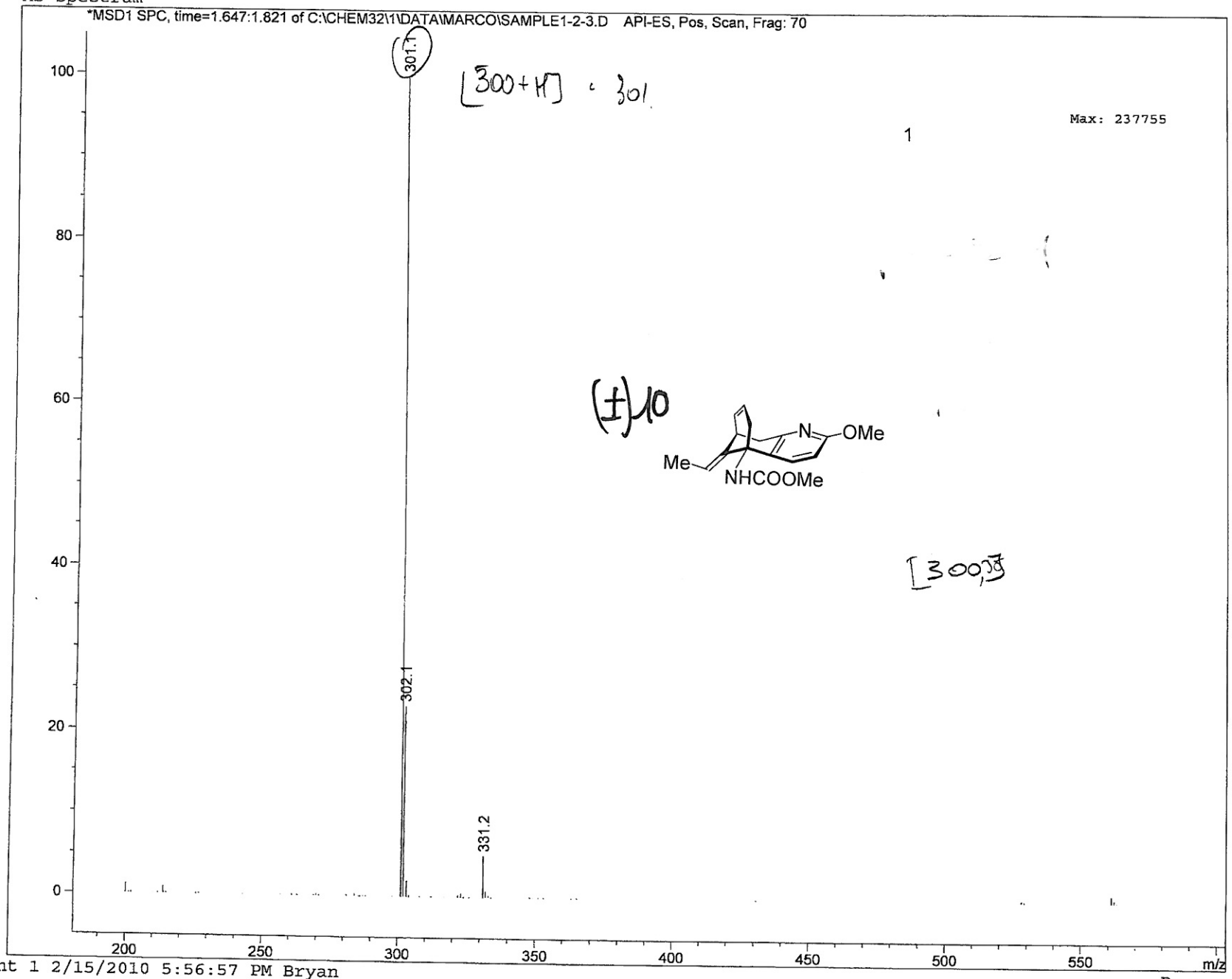
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 262144
SF 400.1300037 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 28.00 cm
CY 10.00 cm
F1P 8.254 ppm
F1 3302.73 Hz
F2P 4.654 ppm
F2 1862.21 Hz
PPMCM 0.12858 ppm/cm
HZCM 51.44730 Hz/cm

Print of window 80: MS Spectrum (±) 10

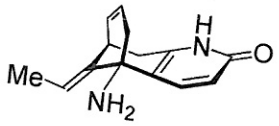
MS Spectrum



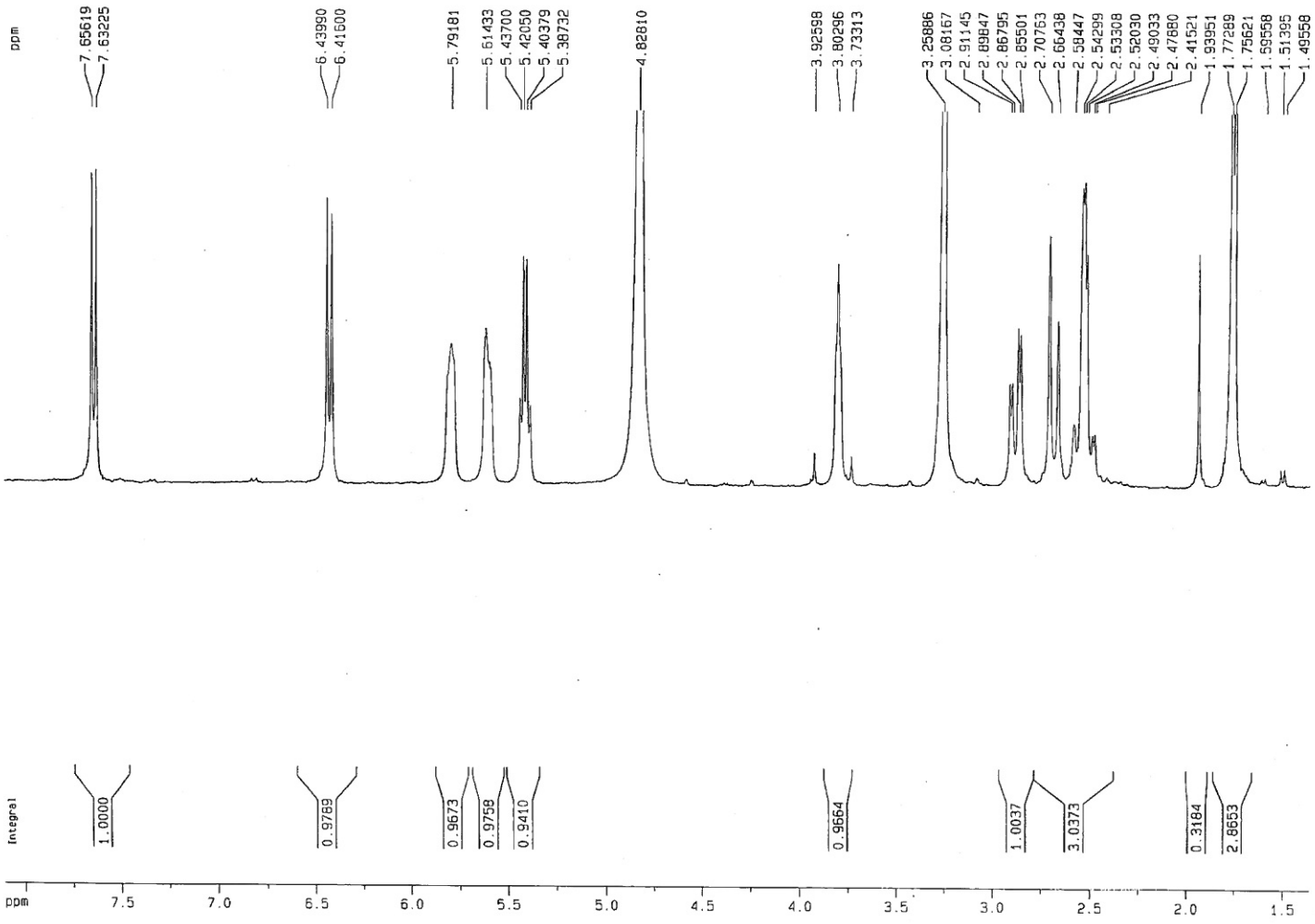
Instrument 1 2/15/2010 5:56:57 PM Bryan

Sample:
Solvent:
Survey 1-D APT Experiment
C, CH2-up / CH, CH3-down
Bruker DPX-400 NMR Spectrometer
June 8, 2005 / D. Lankin

(+)
5



MeOD



Current Data Parameters

NAME	marcus
EXPNO	314
PROCNO	1

F2 - Acquisition Parameters

Date_	20101220
Time	15.35
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	512
DW	60.400 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	12.00 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

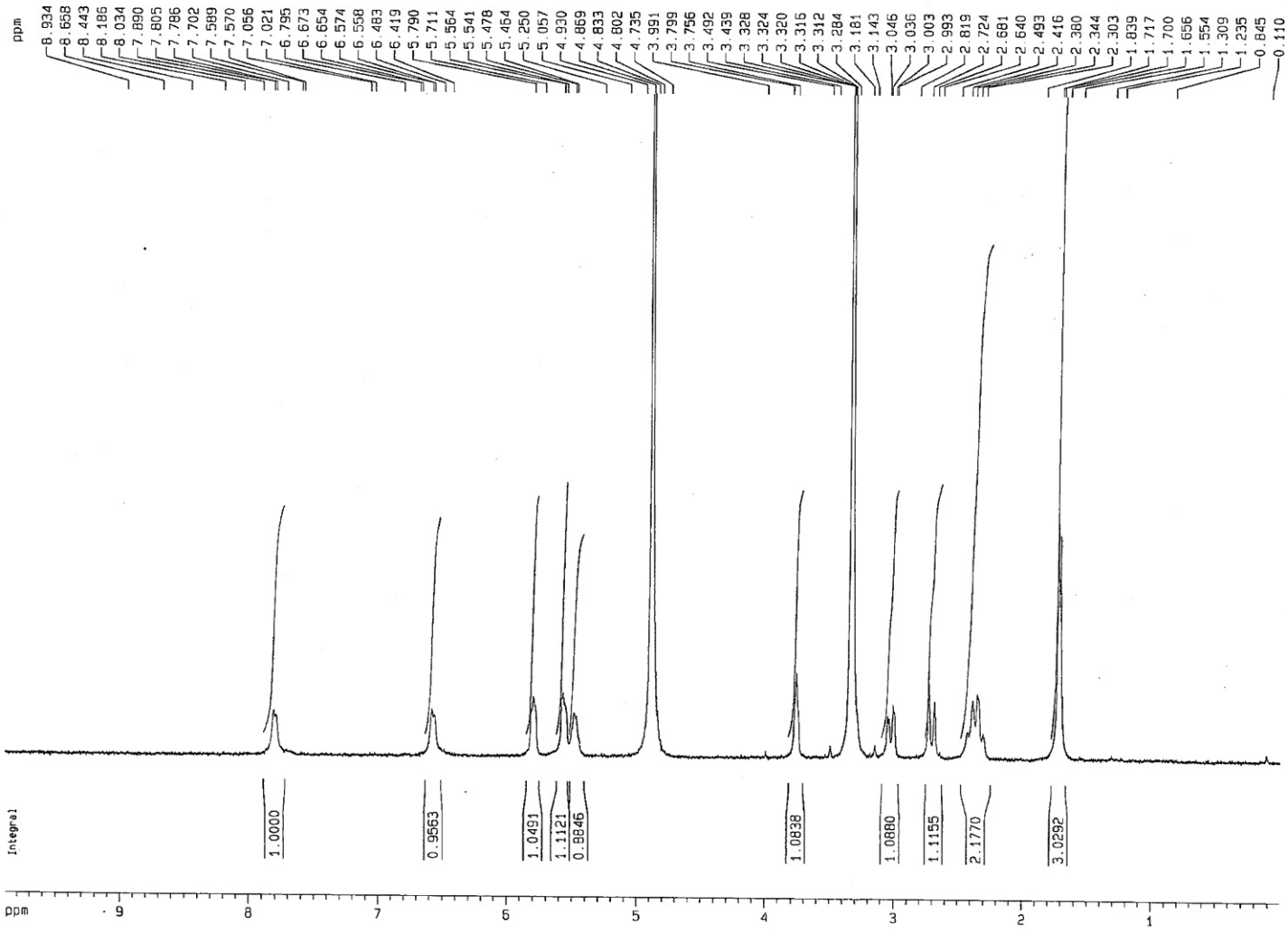
SI	65536
SF	400.1300280 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	28.00 cm
CY	50.00 cm
F1P	8.113 ppm
F1	3246.43 Hz
F2P	1.364 ppm
F2	545.94 Hz
PPMCM	0.24104 ppm/cm
HZCM	96.44616 Hz/cm

Sample: MeOD + D_2O
Solvent:
Standard 1-D Survey Proton NMR Experiment
Bruker DPX-400 NMR Spectrometer
October 14, 2004 / D. Lankin

(+)5 MeOD + D_2O



Current Data Parameters

NAME	marcus
EXPNO	316
PROCNO	1

F2 - Acquisition Parameters

Date_	20110110
Time	10.29
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	724.1
DW	60.400 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	12.00 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

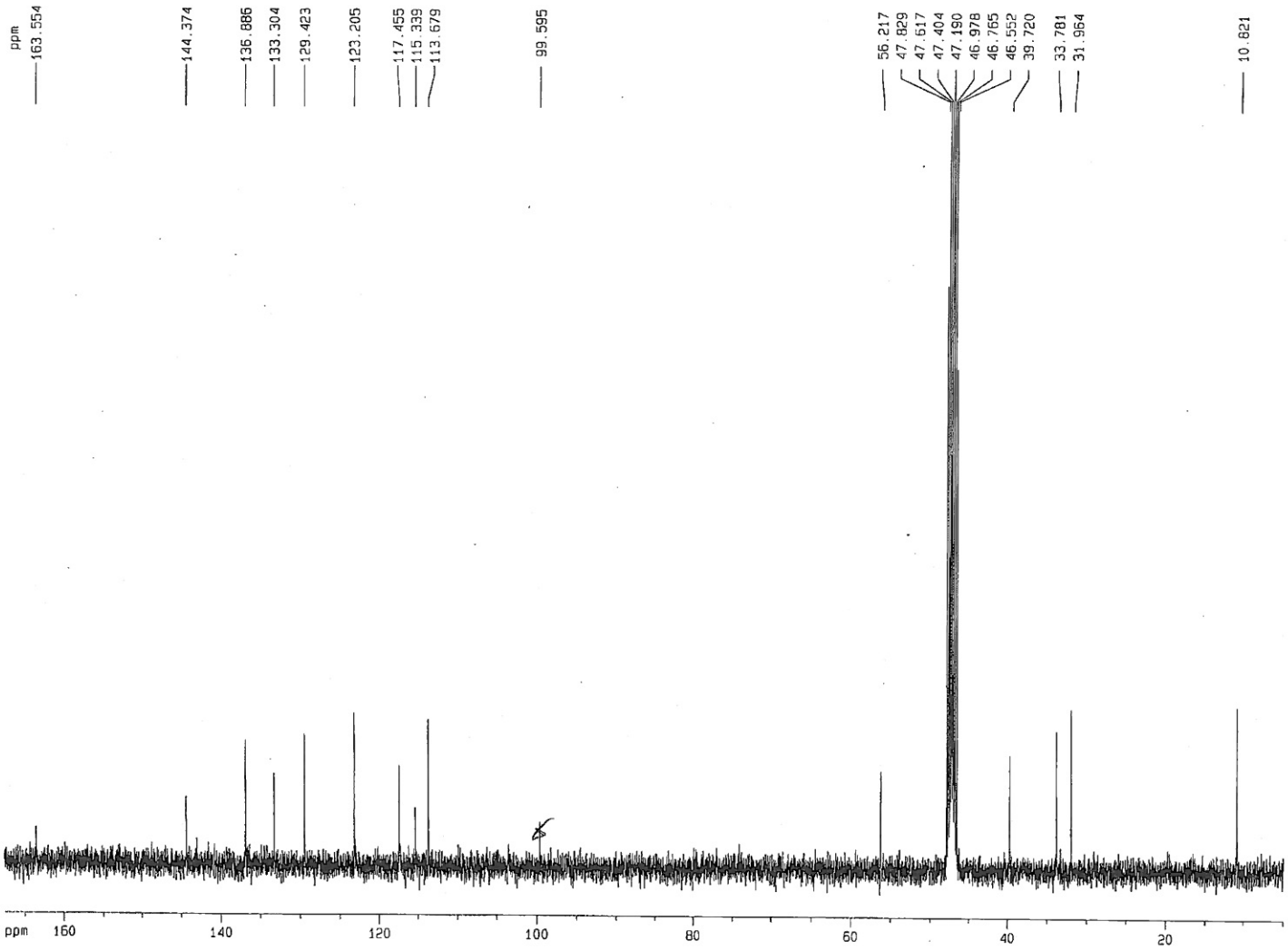
SI	262144
SF	400.1300037 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	28.00 cm
CY	80.00 cm
F1P	9.888 ppm
F1	3956.36 Hz
F2P	0.006 ppm
F2	2.37 Hz
PPMCM	0.35292 ppm/cm
HZCM	141.21402 Hz/cm

Sample:
Solvent:
1-D Carbon-13 NMR Spectrum
with Waltz-16 (CPD) Decoupling
Bruker DXP-400 NMR Spectrometer
October 14, 2004 / D. Lankin

(+)5
MeOD



Current Data Parameters

NAME	marcus
EXPNO	326
PROCNO	1

F2 - Acquisition Parameters

Date_	20110119
Time	13.33
INSTRUM	spect
PROBHD	5 mm GNP 1H/1
PULPROG	zgpg30
TD	65536
SOLVENT	MeOD
NS	1289
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	2298.8
DW	20.850 usec
DE	6.00 usec
TE	299.2 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	13C
P1	10.00 usec
PL1	-3.00 dB
SFO1	100.6228303 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

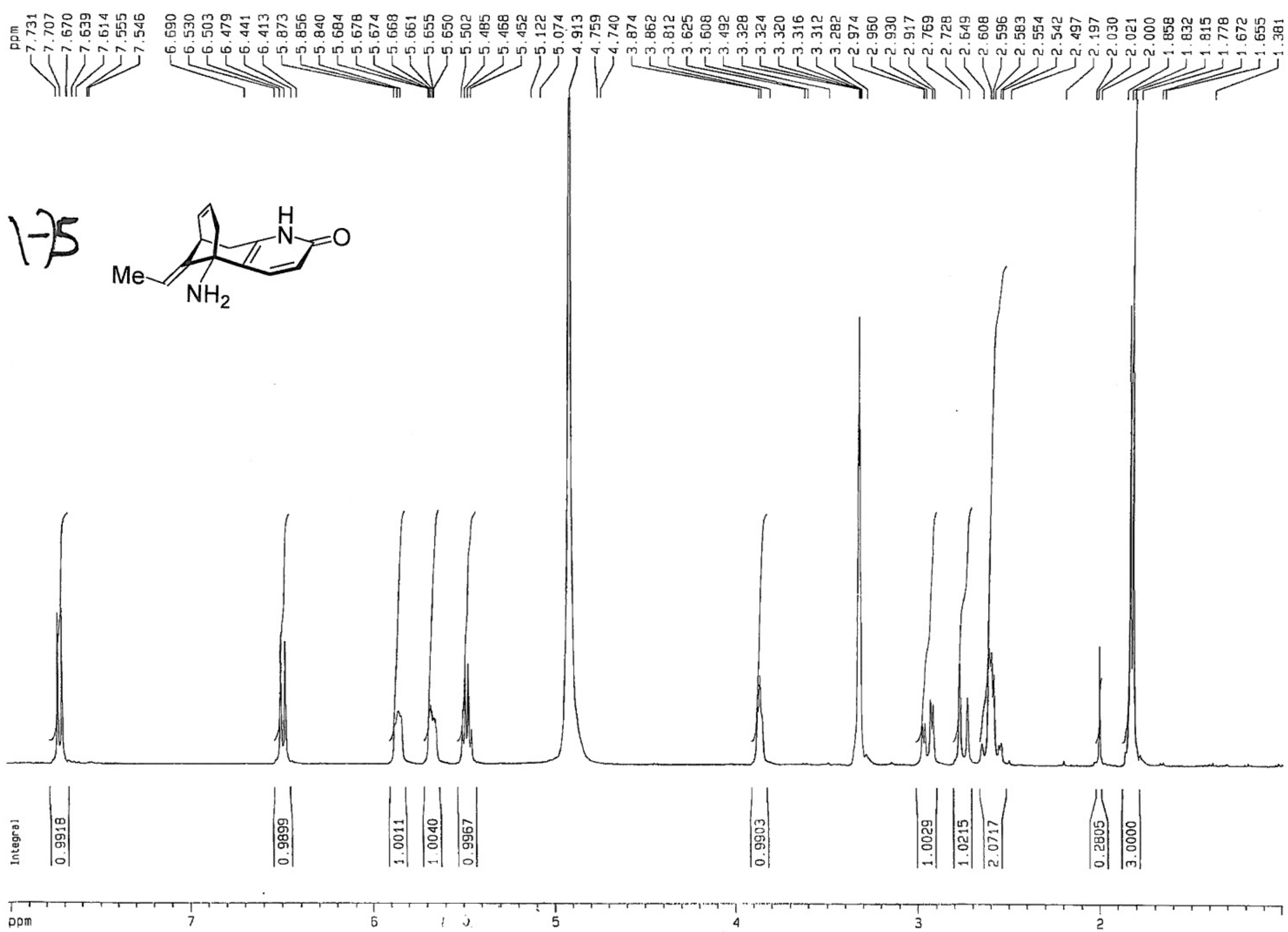
SI	32768
SF	100.6128095 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	28.00 cm
CY	85.00 cm
F1P	167.633 ppm
F1	16866.07 Hz
F2P	4.979 ppm
F2	500.99 Hz
PPMCM	5.80907 ppm/cm
HZCM	584.46716 Hz/cm

Sample: [struck through]
Solvent: [struck through]
Standard 1-D Survey Proton NMR Experiment
Bruker DPX-400 NMR Spectrometer
October 14, 2004 / D. Lankin

1-35 MeOD

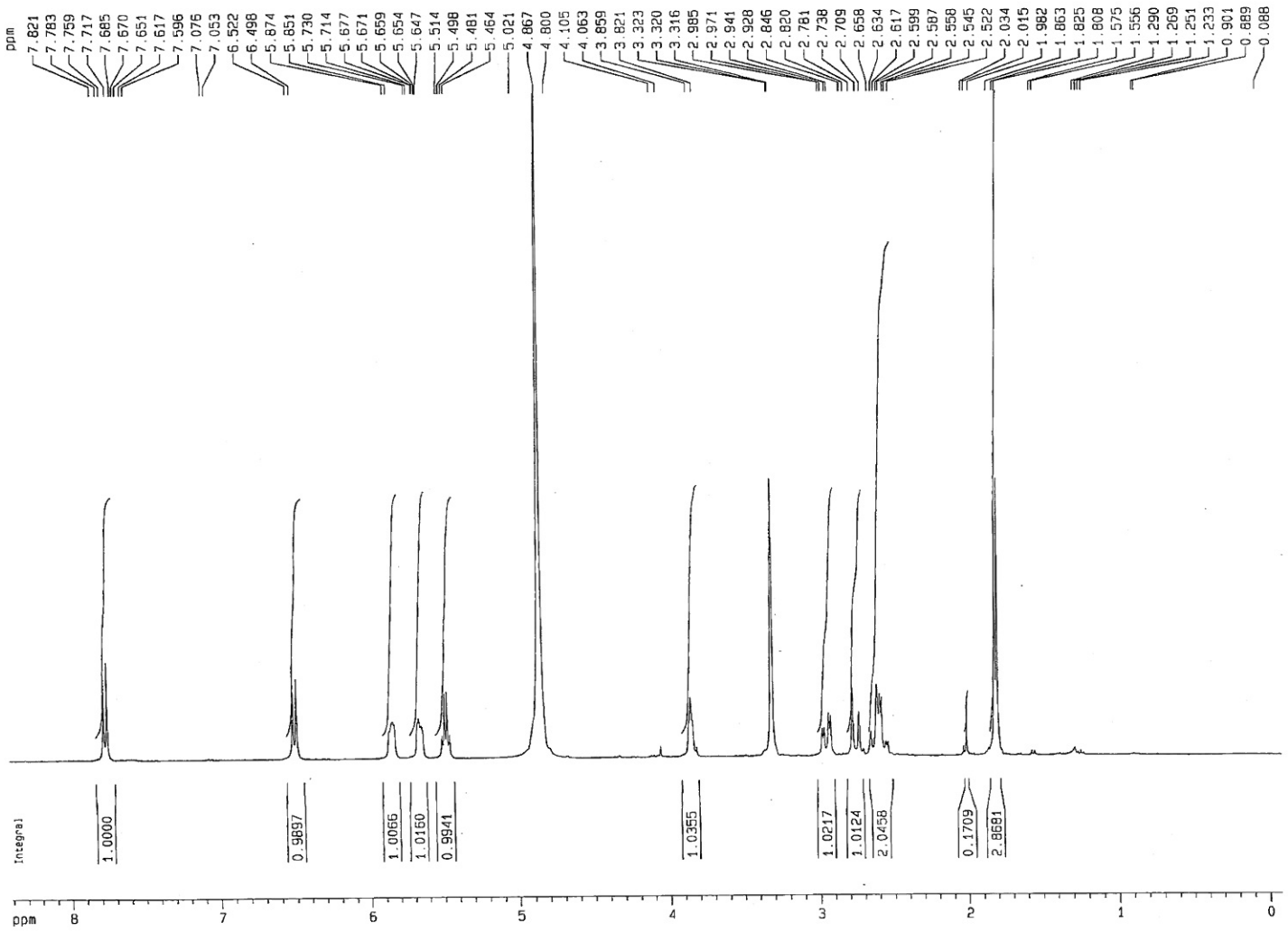


Current Data Parameters	
NAME	marcus
EXPNO	319
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110110
Time	10.55
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	362
DW	60.400 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.00 usec
PL1	0.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	262144
SF	400.1300037 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
1D NMR plot parameters	
CX	28.00 cm
CY	19.00 cm
F1P	8.016 ppm
F1	3207.62 Hz
F2P	0.994 ppm
F2	397.77 Hz
PPMCM	0.25080 ppm/cm
HZCM	100.35209 Hz/cm

Sample:
Solvent:
Standard 1-D Survey Proton NMR Experiment
Bruker DPX-400 NMR Spectrometer
October 14, 2004 / D. Lankin

~~MeOH~~ + D_2O

H5 MeOD + D_2O



Current Data Parameters

NAME	marcus
EXPNO	327
PROCNO	1

F2 - Acquisition Parameters

Date_	20110119
Time	14.30
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	322.5
DW	60.400 usec
DE	6.00 usec
TE	299.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	12.00 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

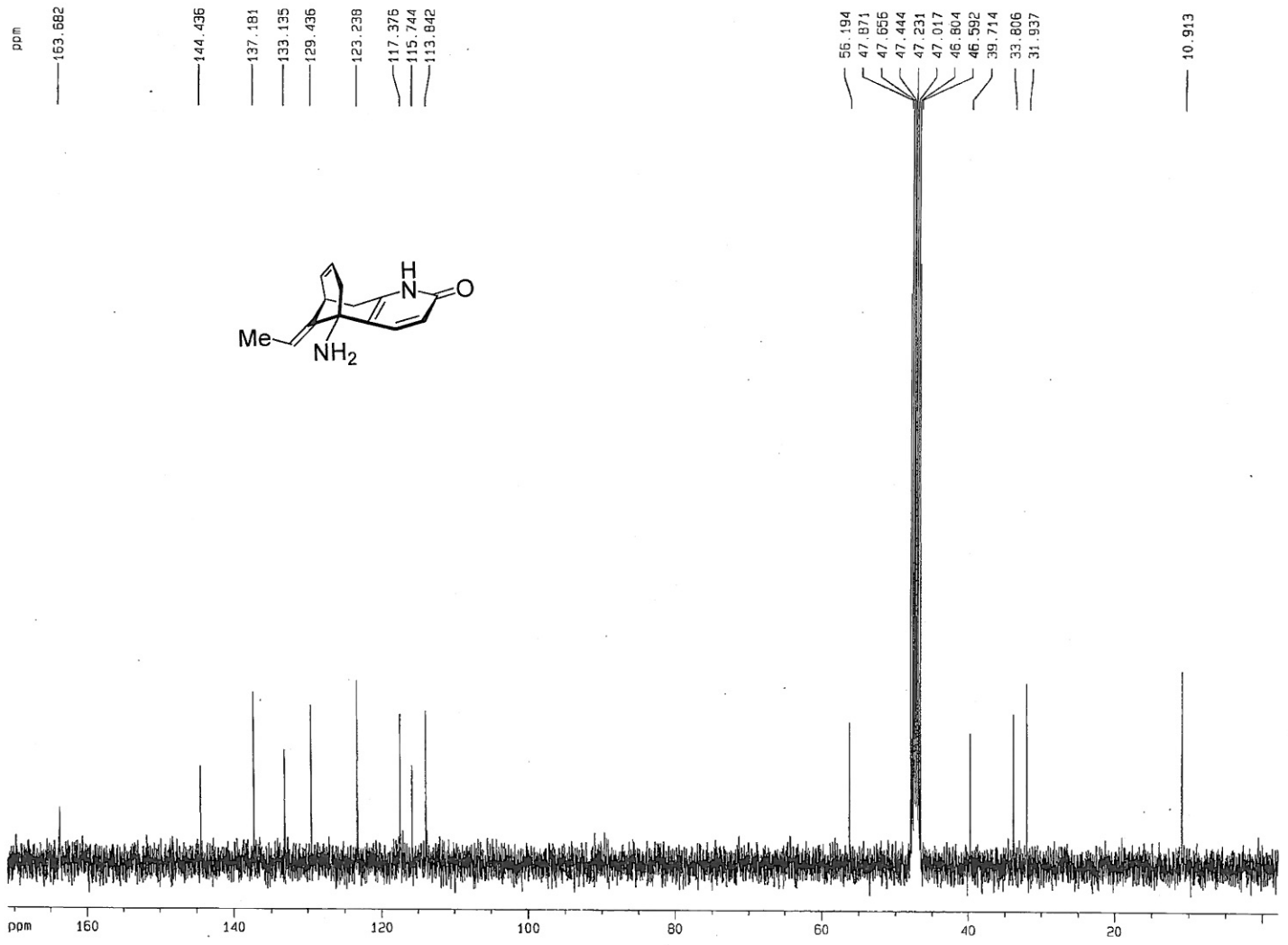
SI	262144
SF	400.1300037 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	28.00 cm
CY	19.00 cm
F1P	8.416 ppm
F1	3367.47 Hz
F2P	-0.078 ppm
F2	-31.28 Hz
PPMCM	0.30336 ppm/cm
HZCM	121.38396 Hz/cm

(-)5 MeOD

Sample:
Solvent:
1-D Carbon-13 NMR Spectrum
with Waltz-16 (CPD) Decoupling
Bruker DXP-400 NMR Spectrometer
October 14, 2004 / D. Lankin



Current Data Parameters

NAME	marcus
EXPNO	332
PROCNO	1

F2 - Acquisition Parameters

Date_	20110119
Time	19.28
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30
TD	65536
SOLVENT	MeOD
NS	1338
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	2048
DW	20.850 usec
DE	6.00 usec
TE	299.2 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	13C
P1	10.00 usec
PL1	-3.00 dB
SFO1	100.6228303 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

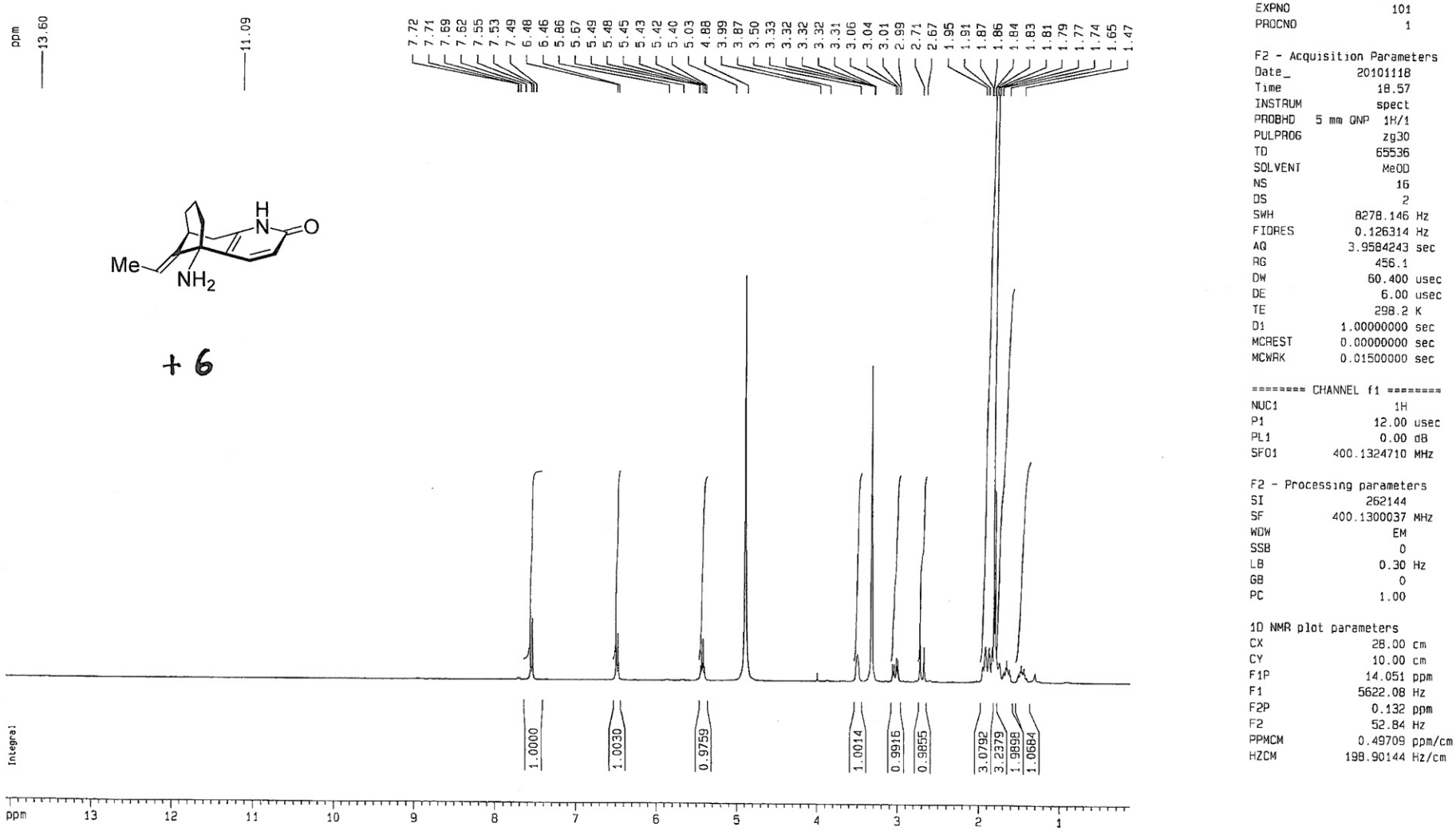
SI	32768
SF	100.6128096 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	28.00 cm
CY	90.00 cm
F1P	170.810 ppm
F1	17185.64 Hz
F2P	-2.138 ppm
F2	-215.08 Hz
PPMCM	6.17669 ppm/cm
HZCM	621.45404 Hz/cm

Sample: [redacted]
Solvent: [redacted]
Standard 1-D Survey Proton NMR Experiment
Bruker DPX-400 NMR Spectrometer
October 14, 2004 / D. Lankin

(+) 6
MeOD



+ 6

Current Data Parameters

NAME	marcus
EXPNO	101
PROCNO	1

F2 - Acquisition Parameters

Date_	20101118
Time	18.57
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	456.1
DW	60.400 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	12.00 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

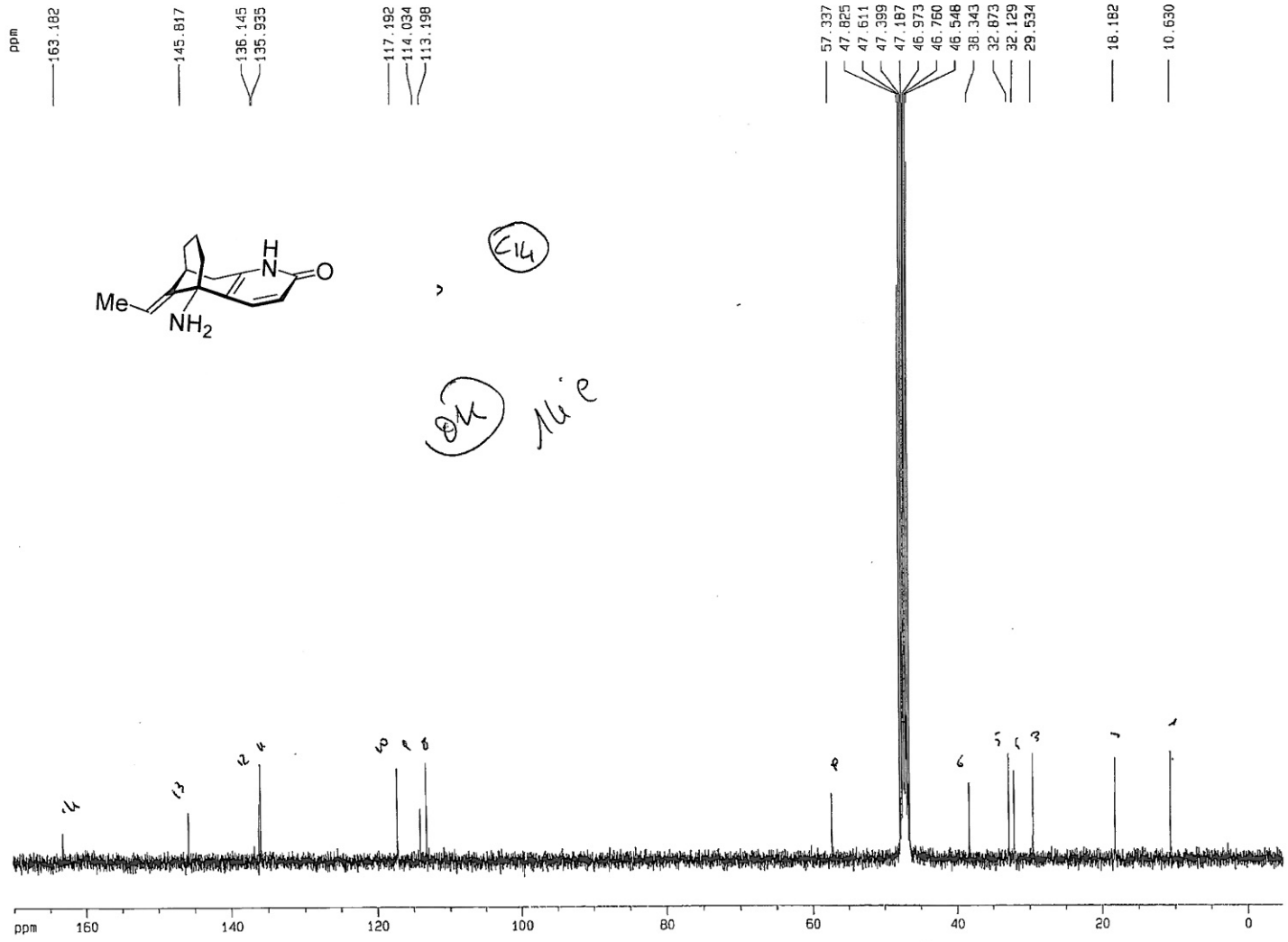
F2 - Processing parameters

SI	262144
SF	400.1300037 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	28.00 cm
CY	10.00 cm
F1P	14.051 ppm
F1	5622.08 Hz
F2P	0.132 ppm
F2	52.84 Hz
PPMCM	0.49709 ppm/cm
HZCM	198.90144 Hz/cm

Sample: ~~KDH15~~ (+)6
Solvent: ~~MeOD~~ MeOD
1-D Carbon-13 NMR Spectrum
with Waltz-16 (CPD) Decoupling
Bruker DXP-400 NMR Spectrometer
October 14, 2004 / D. Lankin



Current Data Parameters

NAME	marcus
EXPNO	102
PROCNO	1

F2 - Acquisition Parameters

Date_	20101118
Time	19.05
INSTRUM	spect
PROBHD	5 mm GNP 1H/1
PULPROG	zgpg30
TD	65536
SOLVENT	MeOD
NS	1695
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	1625.5
DW	20.850 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	13C
P1	10.00 usec
PL1	-3.00 dB
SFO1	100.6228303 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

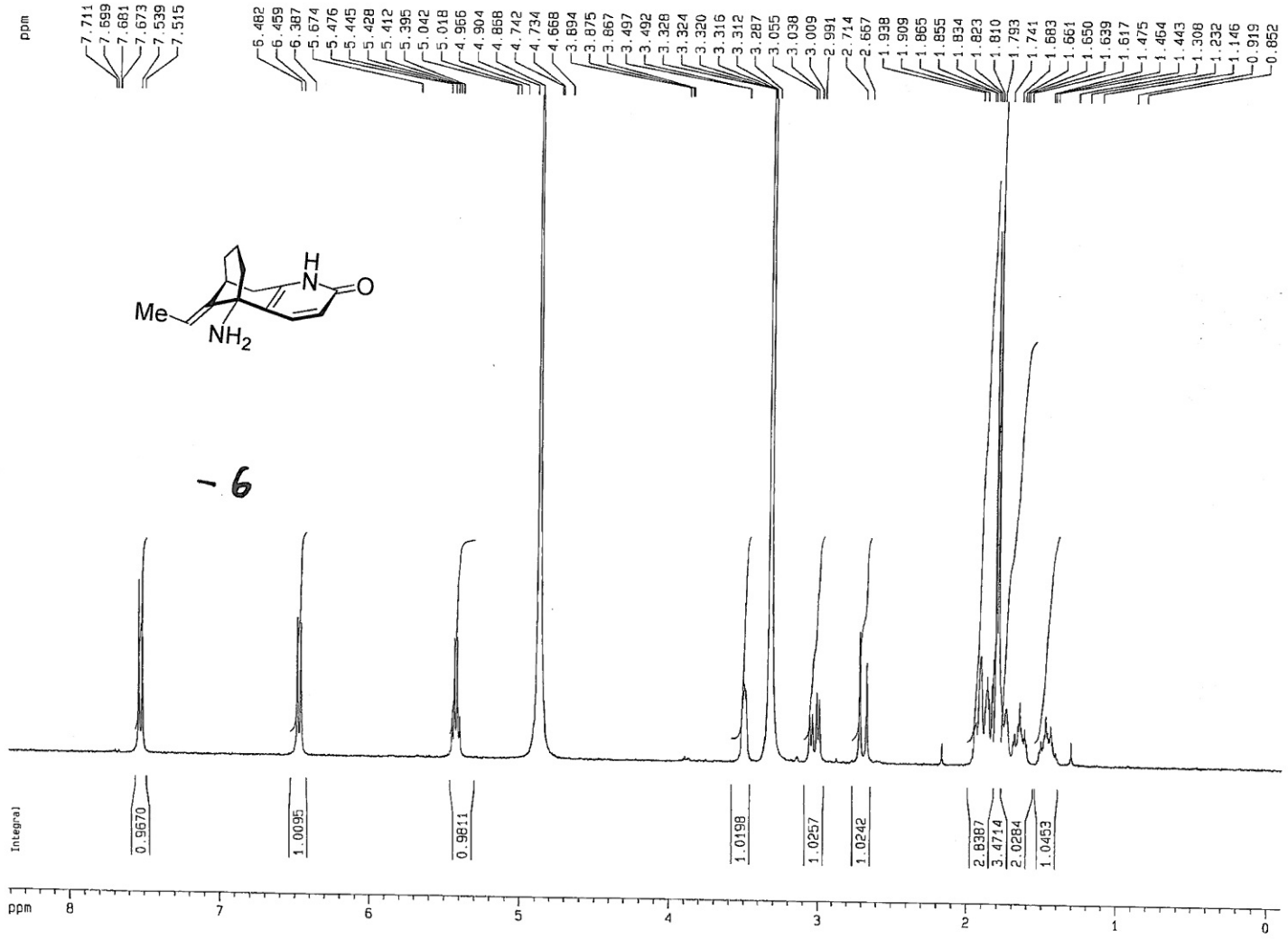
SI	32768
SF	100.6128096 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	28.00 cm
CY	100.00 cm
F1P	170.083 ppm
F1	17112.53 Hz
F2P	-4.802 ppm
F2	-483.15 Hz
PPMCM	6.24590 ppm/cm
HZCM	628.41711 Hz/cm

Sample: [redacted]
Solvent: [redacted]
Standard 1-D Survey Proton NMR Experiment
Bruker DPX-400 NMR Spectrometer
October 14, 2004 / D. Lankin

(-)6
MeOD



Current Data Parameters

NAME	marcus
EXPNO	108
PROCNO	1

F2 - Acquisition Parameters

Date_	20101119
Time	7.00
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	645.1
DW	60.400 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	12.00 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

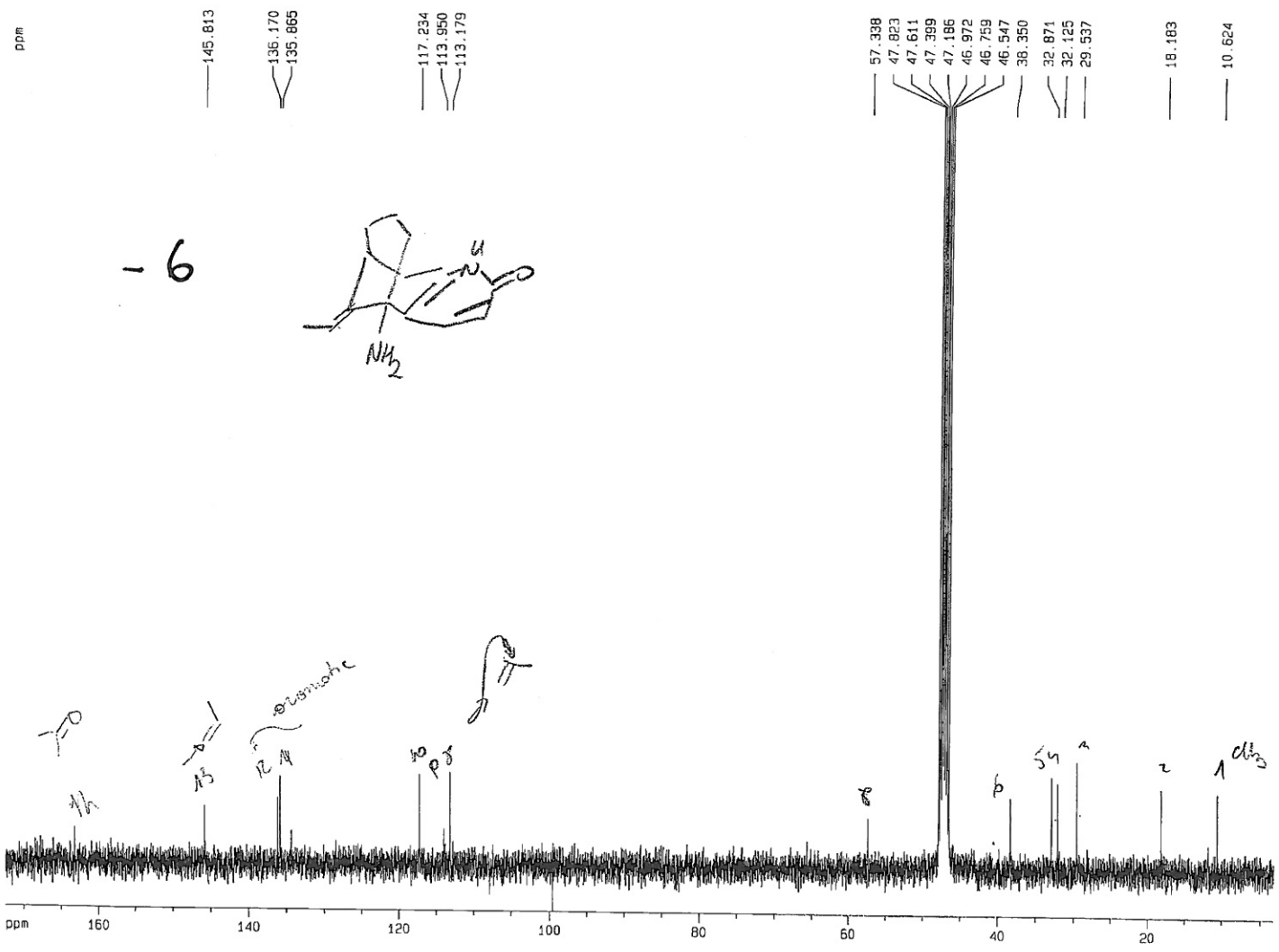
SI	262144
SF	400.1300037 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	28.00 cm
CY	50.00 cm
F1P	8.416 ppm
F1	3367.47 Hz
F2P	-0.099 ppm
F2	-39.70 Hz
PPMCM	0.30411 ppm/cm
HZCM	121.68442 Hz/cm

Sample: [redacted]
Solvent: [redacted]
1-D Carbon-13 NMR Spectrum
with Waltz-16 (CPD) Decoupling
Bruker DXP-400 NMR Spectrometer
October 14, 2004 / D. Lankin

P(-)6
MeOD



Current Data Parameters

NAME	marcus
EXPNO	125
PROCNO	1

F2 - Acquisition Parameters

Date_	20101119
Time	8.36
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30
TD	65536
SOLVENT	MeOD
NS	3125
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	3251
DW	20.850 usec
DE	6.00 usec
TE	299.2 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	13C
P1	10.00 usec
PL1	-3.00 dB
SFO1	100.6228303 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
SFO2	400.1316005 MHz

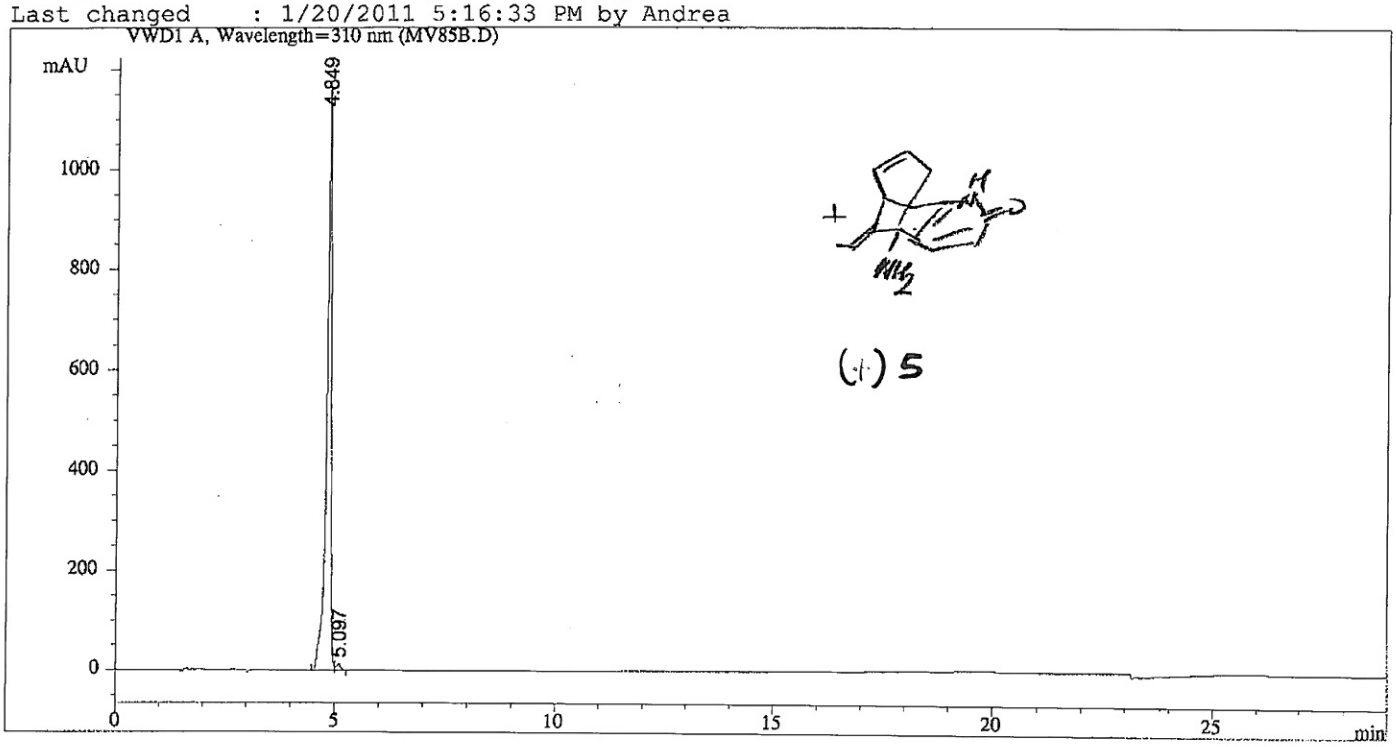
F2 - Processing parameters

SI	32768
SF	100.6128096 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	28.00 cm
CY	150.00 cm
F1P	172.505 ppm
F1	17356.23 Hz
F2P	3.191 ppm
F2	321.08 Hz
PPMCM	6.04693 ppm/cm
HZCM	608.39825 Hz/cm

```
Injection Date  : 1/20/2011 8:05:11 PM          Seq. Line :   8
Sample Name     : m-v-85                        Location : Vial 72
Acq. Operator   : Andrea                           Inj :   1
                                                Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 15 µl
Method          : C:\HPCHEM\1\METHODS\3AQHUP.M
Last changed    : 1/20/2011 5:16:33 PM by Andrea
```



(+) 5

Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=310 nm

Peak RetTime Type  Width     Area       Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   4.849 BV    0.0904 7734.23242 1168.01196  98.9103
   2   5.097 VV    0.0882   85.21005   13.23517   1.0897

Totals :                  7819.44247 1181.24714

 Results obtained with enhanced integrator!
```

*** End of Report ***

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Mass Spectrometry
SINGLE ANALYSIS REPORT

Room 109A SES, M/C 337
845 W. Taylor St.
Chicago, IL 60607-7058
Office: (312) 355-2124
Art@uic.edu Lab: (312) 996-6849

MSL Log# 024430

Logged in 01/13/2011 01:32:24 PM

RRC Account No YG3340
UserName Marco Pieroni
Affiliation UIC
Phone **FAX**
Email piero@uic.edu
SampleLabel MP-V-85
ProjectName
Formula C14 H16 N2 O1
Mono-isotopic Mass 228.12626 **M.W.** 228.29

Advisor Gaysin
Department Medicinal Chemistry and

Analysis Requested	
Analysis Type	Accurate Mass
Resolution	HR
LR spect attach?	No
Chromatography	None
Ionization	ESI
Polarity	Positive
m/z Range	150 -2000
OtherAnalysis	None

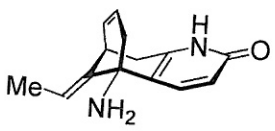
Operator Comments

Instrument Shimadzu LCMSITTOF
Source, deg C 220 **Gas** Ar
Acc. Volt. 9100 **Resolution** 10,300
ScanRange 100-1000
Solvent MeOH
Matrix
Ref. dG

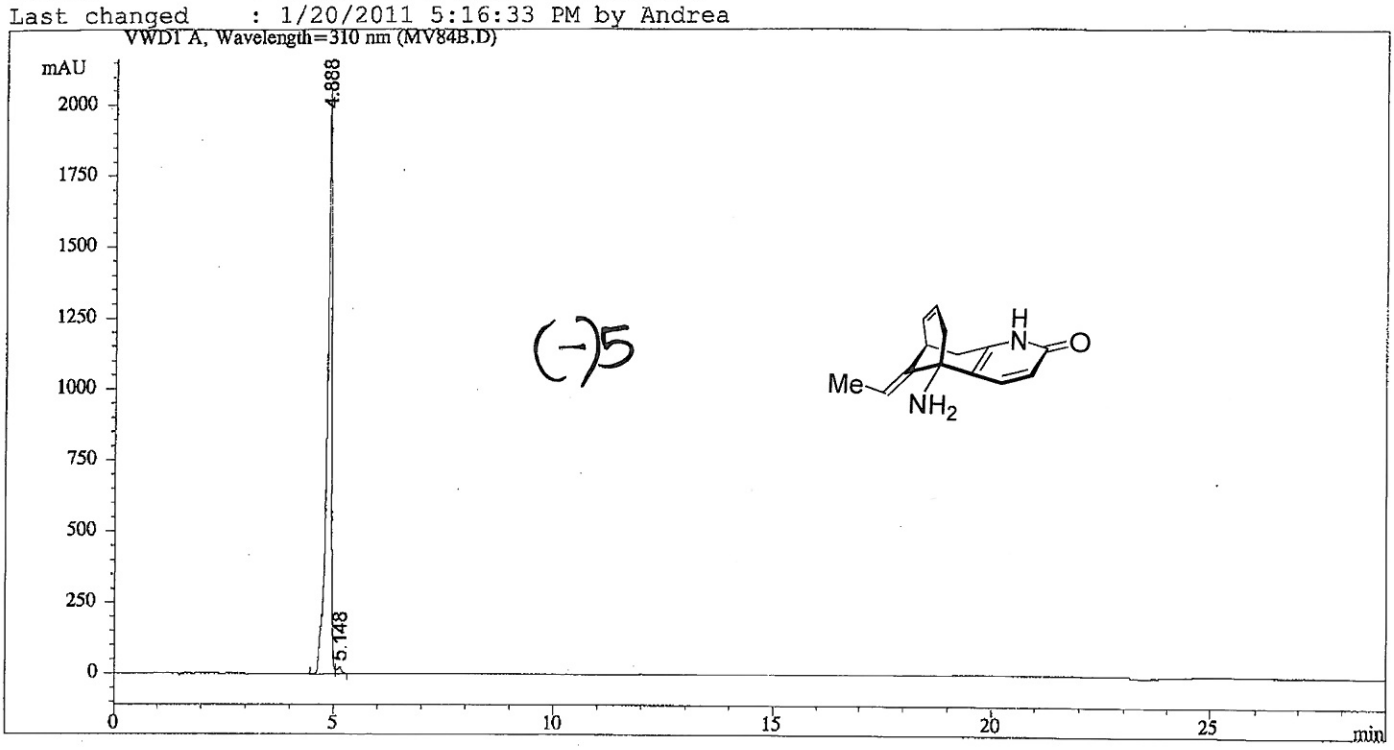
Ion	Expected	Observed	ppm Error
M - H	227.11899	227.1190	0.06

MSL Log#	Analyst	Date	Analysis Performed	Rate	Quantity	Total	N/C	
024430	Bryan M. Zahakaylo	1/18/2011	HRESI	$35.00	1	$35.00		

(+) 5



```
Injection Date  : 1/20/2011 7:02:05 PM          Seq. Line :   6
Sample Name     : m-v-84                        Location : Vial 71
Acq. Operator   : Andrea                           Inj :   1
                                                Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 15 µl
Method          : C:\HPCHEM\1\METHODS\3AQHUP.M
Last changed    : 1/20/2011 5:16:33 PM by Andrea
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=310 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.888	VV	0.0949	1.41962e4	2062.13892	98.7996
2	5.148	VV	0.0955	172.47617	24.41029	1.2004
Totals :				1.43687e4	2086.54921	

Results obtained with enhanced integrator!

*** End of Report ***

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Office: (312) 355-2124
Art@uic.edu Lab: (312) 996-6849

MSL Log# 024429

Logged in 01/13/2011 01:31:16 PM

RRC Account No YG3340
UserName Marco Pieroni
Affiliation UIC
Phone **FAX**
Email piero@uic.edu
SampleLabel MP-V-86
ProjectName
Formula C14 H16 N2 O1
Mono-isotopic Mass 228.12626 **M.W.** 228.29

Advisor Gaysin
Department Medicinal Chemistry and

Analysis Requested	
Analysis Type	Accurate Mass
Resolution	HR
LR spect attach?	No
Chromatography	None
Ionization	ESI
Polarity	Positive
m/z Range	150 -2000
OtherAnalysis	None

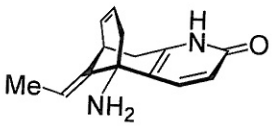
Operator Comments

Instrument Shimadzu LCMSITTOF
Source, deg C 220 **Gas** Ar
Acc. Volt. 9100 **Resolution** 10,300
ScanRange 100-1000
Solvent MeOH
Matrix
Ref. dG

Ion	Expected	Observed	ppm Error
M - H	227.11899	227.1201	4.90

MSL Log#	Analyst	Date	Analysis Performed	Rate	Quantity	Total	N/C	
024429	Bryan M. Zahakaylo	1/18/2011	HRESI	$35.00	1	$35.00		

(-)5



Data File C:\HPCHEM\1\DATA\MPV74.D Sample Name: mpv74

```
Injection Date  : 10/22/2010 1:36:15 PM          Seq. Line :   1
Sample Name     : mpv74                        Location : Vial 21
Acq. Operator   : Andrea                           Inj :   1
                                               Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 20 µl
Method          : C:\HPCHEM\1\METHODS\3AQ280.M
Last changed    : 12/18/2008 5:15:31 PM
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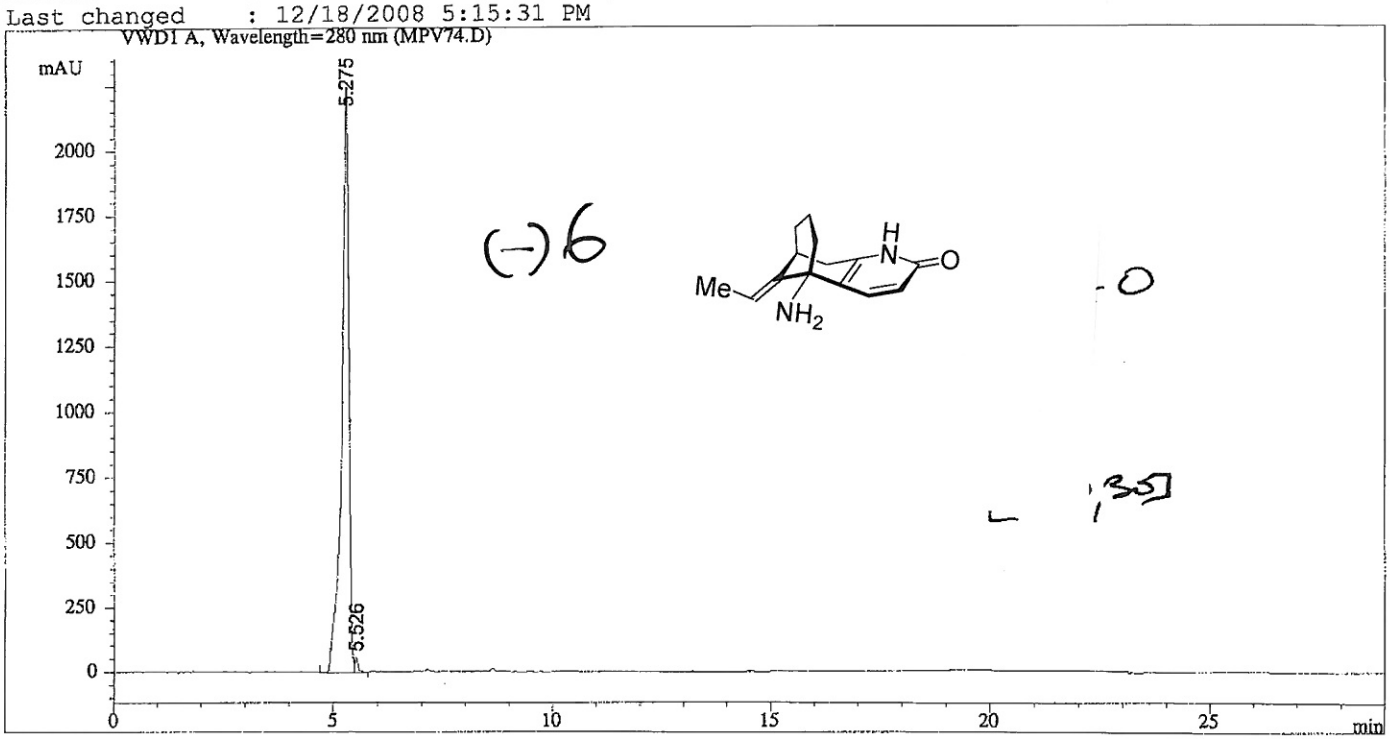

(-)6

-O

L 1305

Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=280 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   5.275 VV    0.1569 2.49399e4  2250.98779  98.7195
   2   5.526 VV    0.0768  323.48666   59.97657   1.2805

Totals :                  2.52634e4  2310.96436

 Results obtained with enhanced integrator!
```

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Room 109A SES, M/C 337
845 W. Taylor St.
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Office: (312) 355-2124
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MSL Log# 024428

Logged in 01/13/2011 01:30:26 PM

RRC Account No YG3340
UserName Marco Pieroni
Affiliation UIC
Phone **FAX**
Email piero@uic.edu
SampleLabel MP-V-74
ProjectName
Formula C14 H18 N2 O1
Mono-isotopic Mass 230.14191 **M.W.** 230.31

Advisor Gaysin
Department Medicinal Chemistry and

Analysis Requested	
Analysis Type	Accurate Mass
Resolution	HR
LR spect attach?	No
Chromatography	None
Ionization	ESI
Polarity	Positive
m/z Range	150 -2000
OtherAnalysis	None

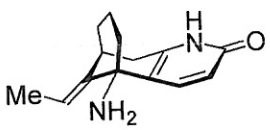
Operator Comments

Instrument Shimadzu LCMSITTOF
Source, deg C 220 **Gas** Ar
Acc. Volt. 9100 **Resolution** 10,300
ScanRange 100-1000
Solvent MeOH
Matrix
Ref. dG

Ion	Expected	Observed	ppm Error
M + H	231.14919	231.1495	1.34

MSL Log#	Analyst	Date	Analysis Performed	Rate	Quantity	Total	N/C	
024428	Bryan M. Zahakaylo	1/18/2011	HRESI	$35.00	1	$35.00		

(-) 6



```
Injection Date  : 11/16/2010 11:17:21 AM        Seq. Line :   2
Sample Name     : mpv75                          Location : Vial 2
Acq. Operator   : Andrea                             Inj :   1
                                                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 10 µl
Acq. Method     : C:\HPCHEM\1\METHODS\3AQ280.M
Last changed    : 12/18/2008 5:15:31 PM
Analysis Method : C:\HPCHEM\1\METHODS\1AQ100MM.M
Last changed    : 8/8/2008 12:31:58 PM
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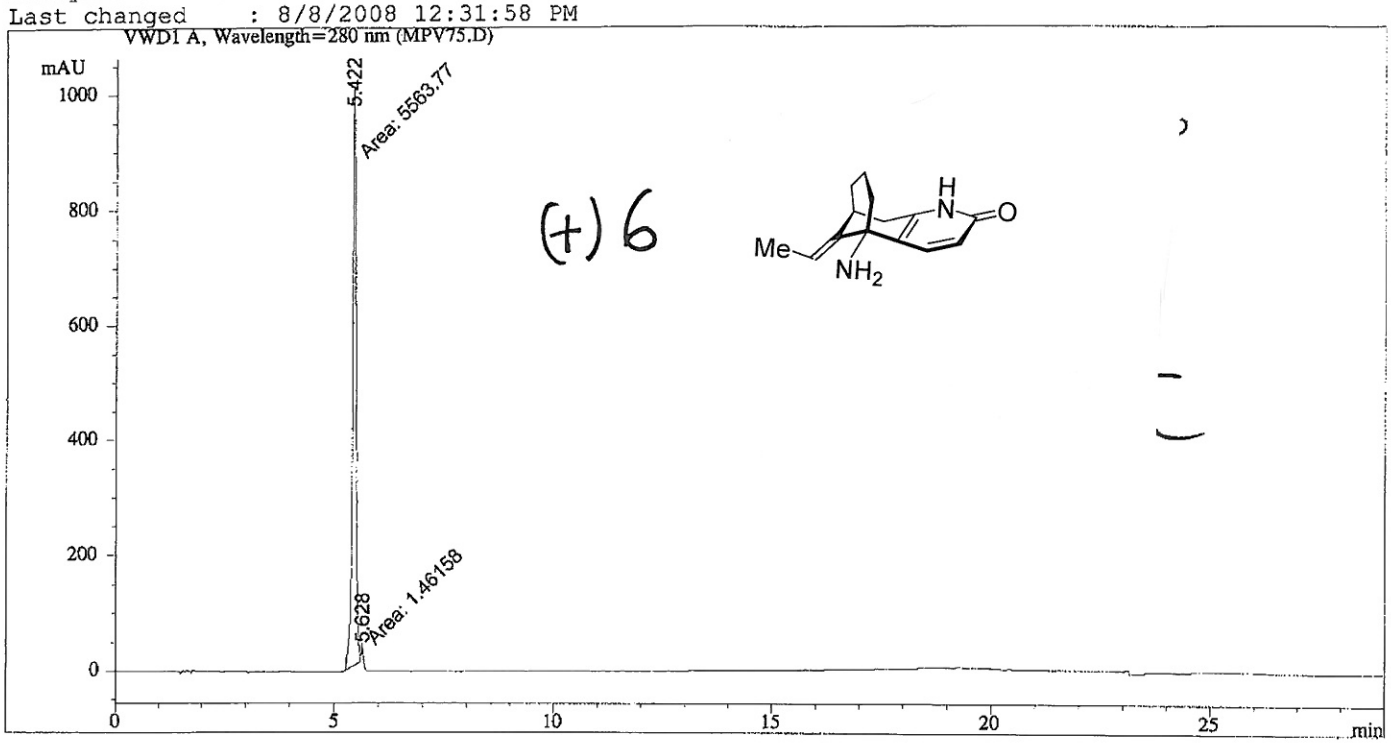

(+) 6

Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=280 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]  mAU   *s   [mAU   ]      %
-----|-------|----|-------|----------|----------|--------|
   1   5.422 MM    0.0923 5563.77197 1004.79272  99.9737
   2   5.628 MM    0.0113    1.46158    2.15683   0.0263

Totals :                  5565.23355 1006.94955

 Results obtained with enhanced integrator!
```

*** End of Report ***

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Mass Spectrometry
SINGLE ANALYSIS REPORT

Room 109A SES, M/C 337
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Office: (312) 355-2124
Art@uic.edu Lab: (312) 996-6849

MSL Log# 024427

Logged in 01/13/2011 01:28:33 PM

RRC Account No YG3340
UserName Marco Pieroni
Affiliation UIC
Phone **FAX**
Email piero@uic.edu
SampleLabel MP-V-75
ProjectName
Formula C14 H18 N2 O1
Mono-isotopic Mass 230.14191 **M.W.** 230.31

Advisor Gaysin
Department Medicinal Chemistry and

Analysis Requested	
Analysis Type	Accurate Mass
Resolution	HR
LR spect attach?	No
Chromatography	None
Ionization	ESI
Polarity	Positive
***m/z* Range**	150 -2000
OtherAnalysis	None

Operator Comments

Instrument Shimadzu LCMSITTOF
Source, deg C 220 **Gas** Ar
Acc. Volt. 9100 **Resolution** 10,300
ScanRange 100-1000
Solvent MeOH
Matrix
Ref. dG

Ion	Expected	Observed	ppm Error
M + H	231.14919	231.1495	1.34

MSL Log#	Analyst	Date	Analysis Performed	Rate	Quantity	Total	N/C	
024427	Bryan M. Zahakaylo	1/18/2011	HRESI	$35.00	1	$35.00		

(+) 6