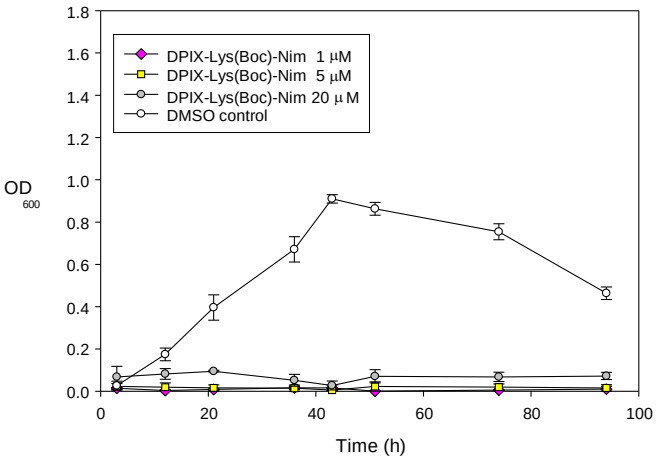
supplementary information

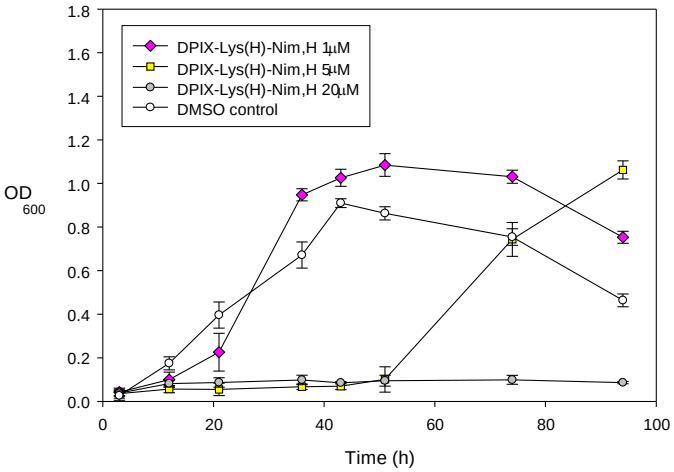
Amino acid-linked porphyrin-nitroimidazole antibiotics targeting *Porphyromonas gingivalis*†

Simon A. Dingsdag,[^,a,b] Benjamin C-M. Yap,[^,a,c] Neil Hunter[a,b] and Maxwell J. Crossley[*c]

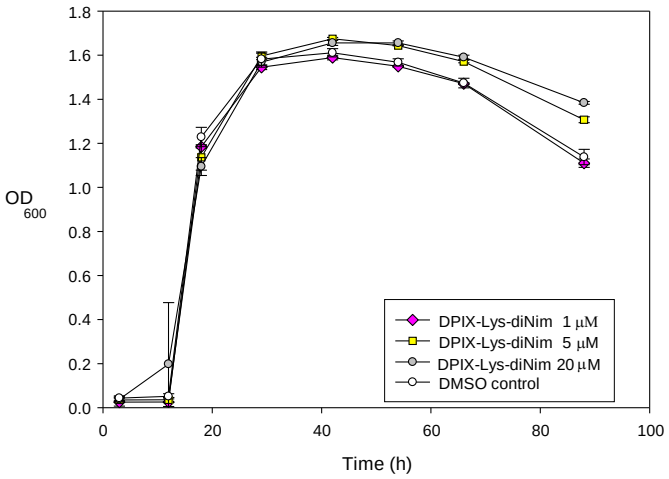
Bacteriology



Supplementary figure 1: Growth inhibitory activity of the mixture of **12a** and **12b** for *P. gingivalis*.



Supplementary figure 2: Growth inhibitory activity of the mixture of **14a** and **14b** for *P. gingivalis*.



Supplementary figure 3: Growth inhibitory activity of the mixture of **17a** and **17b** for *P. gingivalis*.

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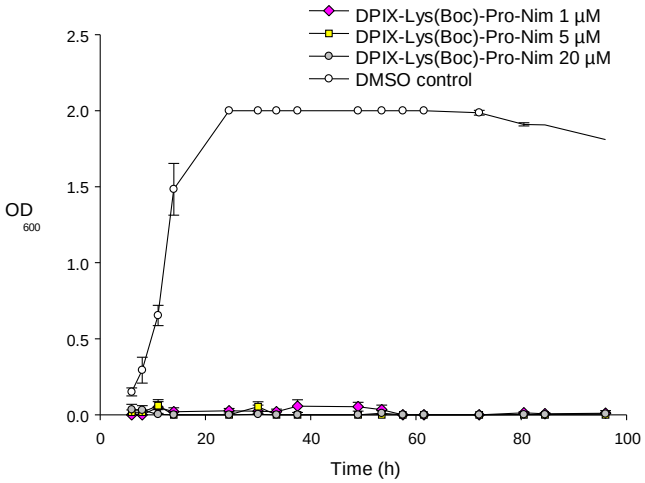
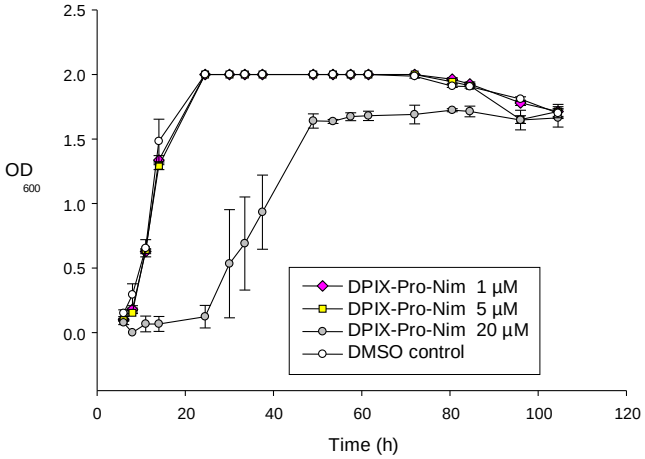
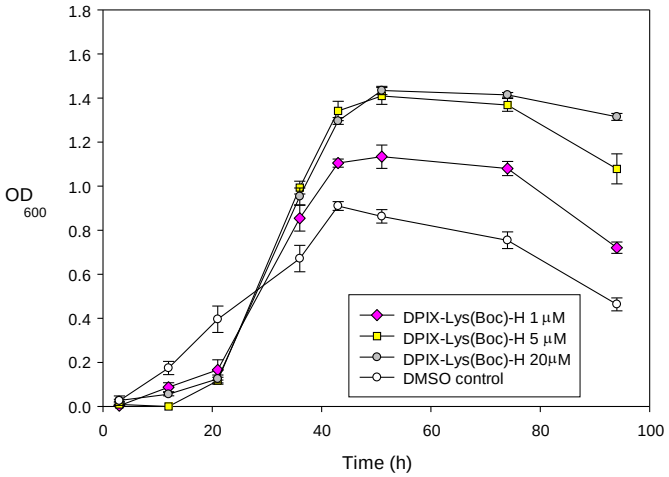


Supplementary figure 4: Growth inhibitory activity of the mixture of **22a** and **22b** for *P. gingivalis***.**



Supplementary figure 5: Growth inhibitory activity of the mixture of **24a** and **24b** for *P. gingivalis*.

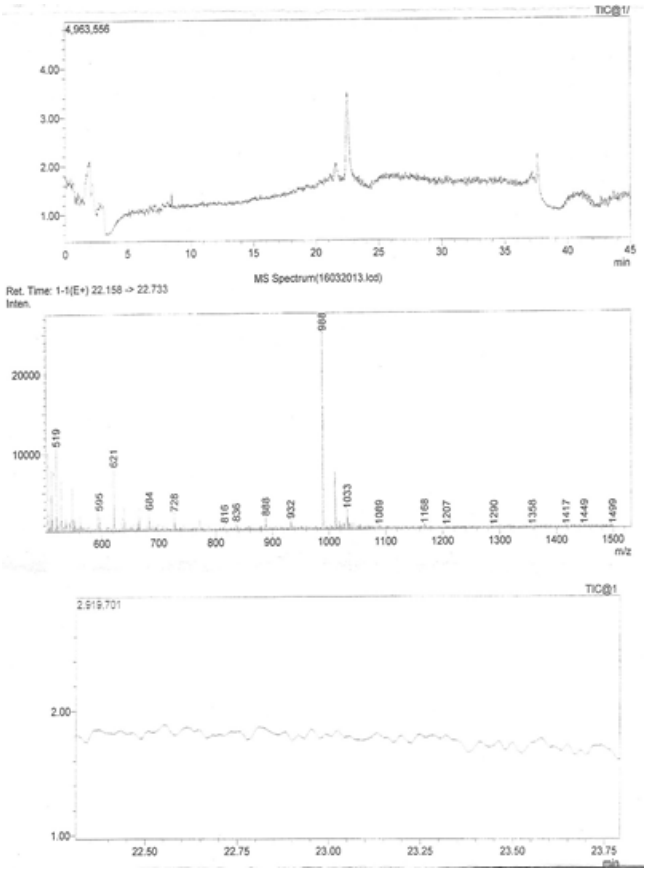


Supplementary figure 6: Growth activity of control mixture of **29a** and **29b** for *P gingivalis*.

Enzyme activity studies

The substrate lysine-para-nitroanilide (KpNA) was used to establish the activity of the lysine-specific gingipain (Kgp, 1 µM). It was shown that 1 µL of Kgp is able to hydrolyse 200 µL of 0.5 mM KpNA with a velocity of 20.2 mOD/min. Kgp (1 µL) was incubated with the DPIX-Lys(Boc)-Pro-Nim adducts **22a** and **22b** (200 µM), with a lysine-proline preferred site of cleavage, and analysis by HPLC-MS showed the complete and successful cleavage of the lysine-proline linkage in the presence of cysteine (1 µM, 1 µL) after 1 h at 37 °C (**Fig. S7c**). The products of the reaction were monitored by HPLC-MS using a solvent system of CH_3CN:H_2O:CF_3CO_2H (10:90:0.5) over a gradient to CH_3CN:H_2O:CF_3CO_2H (60:40:0.5). A control experiment whereby the DPIX-Pro-Mtz adducts **24a** and **24b** were used in place of the DPIX-Lys(Boc)-Pro-Nim adducts **22a** and **22b** showed no cleavage by Kgp. In another control experiment, Kgp was first inactivated with TLCK (4 mM) for 30 min before incubation with DPIX-Lys(Boc)-Pro-Nim adducts **22a** and **22b** (200 µM) in the presence of cysteine (1 µM) for 1 h at 37 °C. HPLC-MS analysis showed no cleavage occurred in these adducts (**Figs. S7a and S7b**). This confirms Kgp has a cleavage preference for a proline next to a lysine and that the Kgp is responsible for the cleavage as Kgp inactivation prevented cleavage of the adducts.

These results indicate the possibility of attaching these amino-acid linked porphyrin-antibiotic adducts to antibodies which are selective to an antigen selectively expressed by the epithelial lining in disease sites (for instance CD24),[14,15] to form depots to increase the availability of porphyrin adduct. The localisation of adduct on epithelial cells would allow for controlled local release of porphyrin adduct for uptake by *P. gingivalis* present within and attached to epithelial cells, following Kgp-mediated cleavage of a lysine-proline linker.



Supplementary figure 7a) LC-MS analysis of DPIX-Lys(Boc)-Pro-Nim adducts **22a** and **22b** initially and with prior inactivation of Kgp with TLCK; **b)** Mass spectrum of product in main peak of TLC chromatogram that eluted at ~23 min; **c)** LC-MS analysis of DPIX-Lys(Boc)-Pro-Nim adducts **22a** and **22b** after incubation with cysteine activated Kgp for 1 h at 37 ºC.

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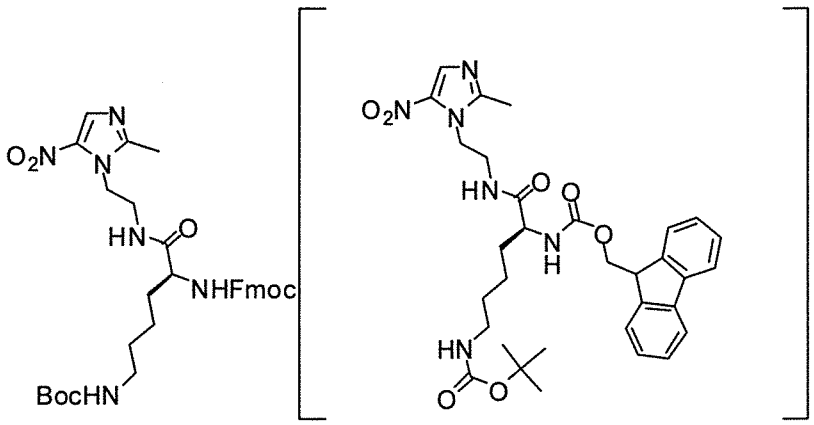

Fmoc-Lys(Boc)-Met amine
Chemical Formula: $C_{32}H_{40}N_6O_7$
Molecular Weight: 620.69600

✓ ^{1}H NMR:

^{13}C NMR:

✓ MS:

✓ Hi Res MS:

UV:

IR:

mp:

Yield:

Experimental:

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MeOH/DCM

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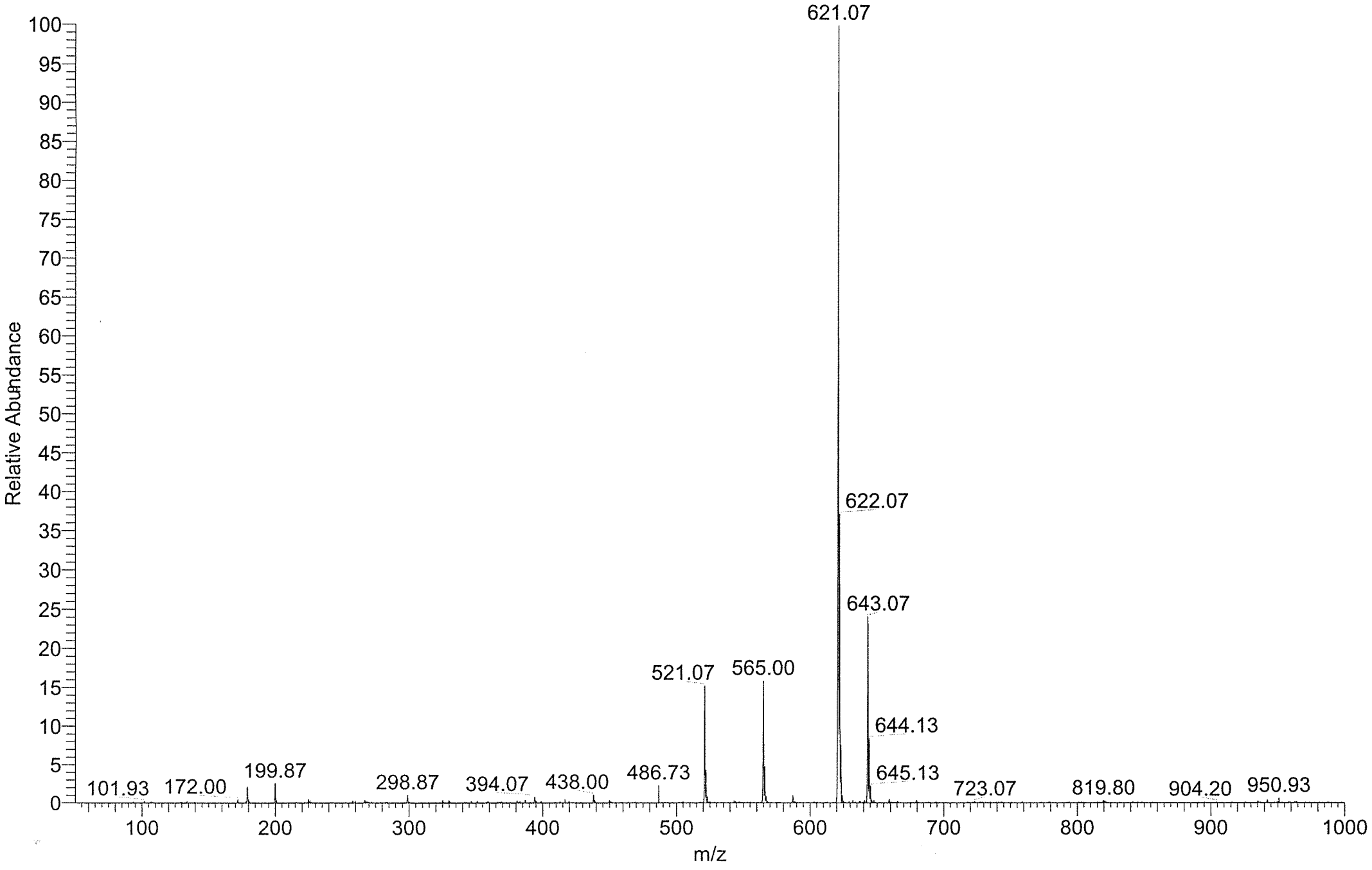
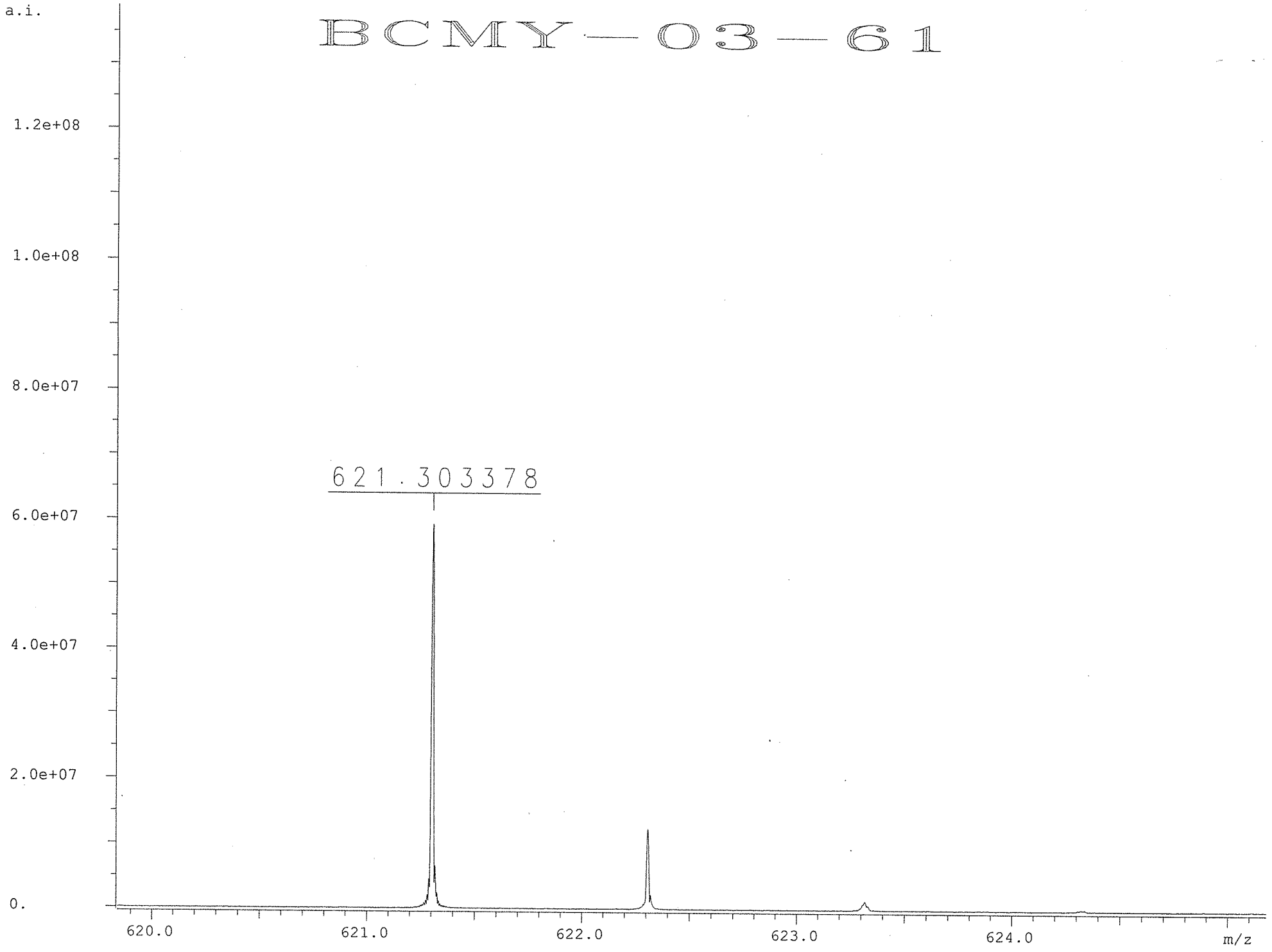
T: + p ESI Full ms [50.00-1000.00]



BCMY—03—61



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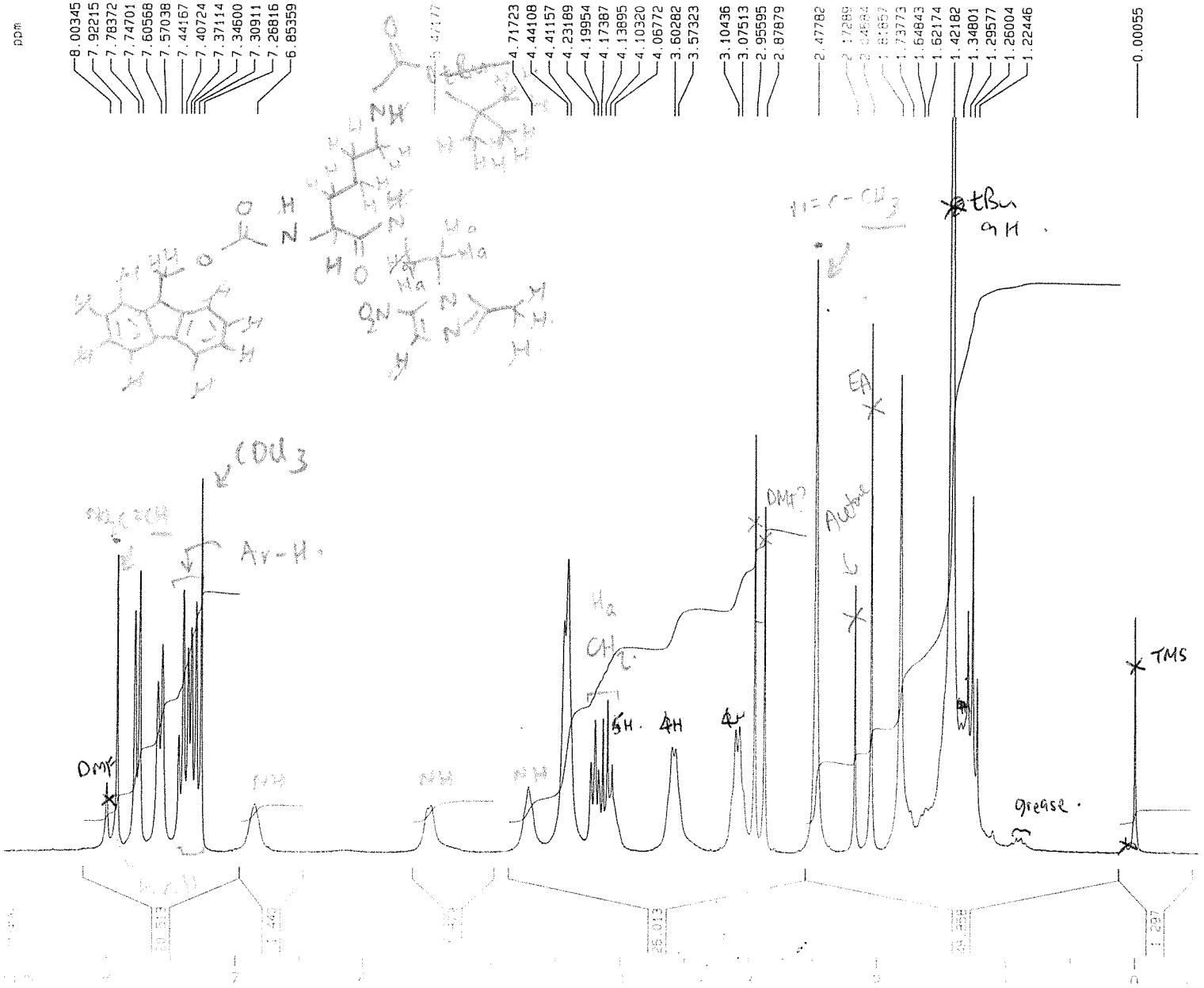

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PROCNO	1

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FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	181
DW	124.800 usec
DE	6.00 usec
TE	295.0 K
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MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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PL1	1.00 dB
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F2 - Processing parameters

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GB	0
PC	1.00

1D NMR plot parameters

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CY	40.00 cm
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F2	-100.06 Hz
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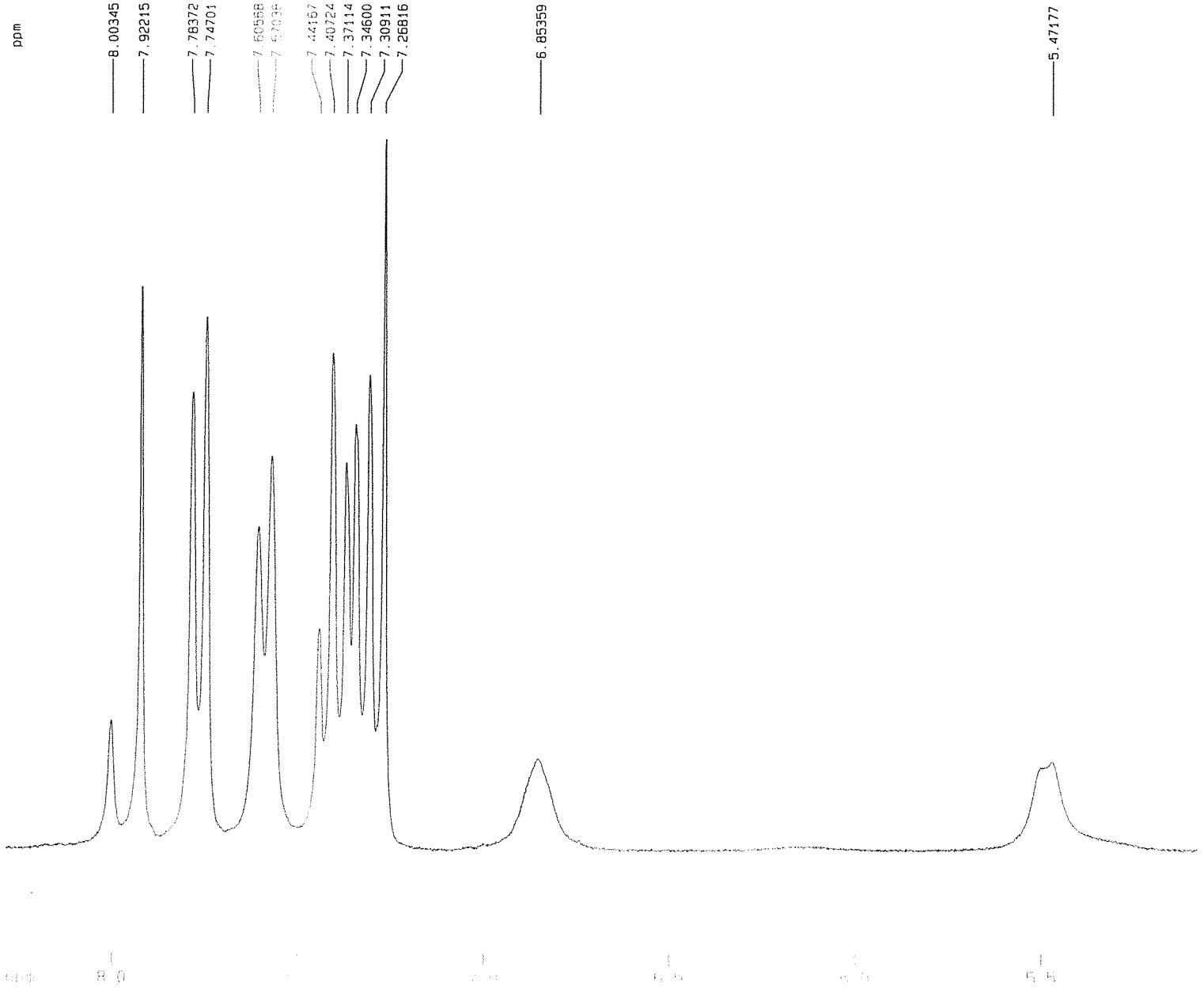

Current Data Parameters

NAME	FmocLysBocMetAmine
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

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TD	32768
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MCWRK	0.01500000 sec

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

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F2 - Processing parameters

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1D NMR plot parameters

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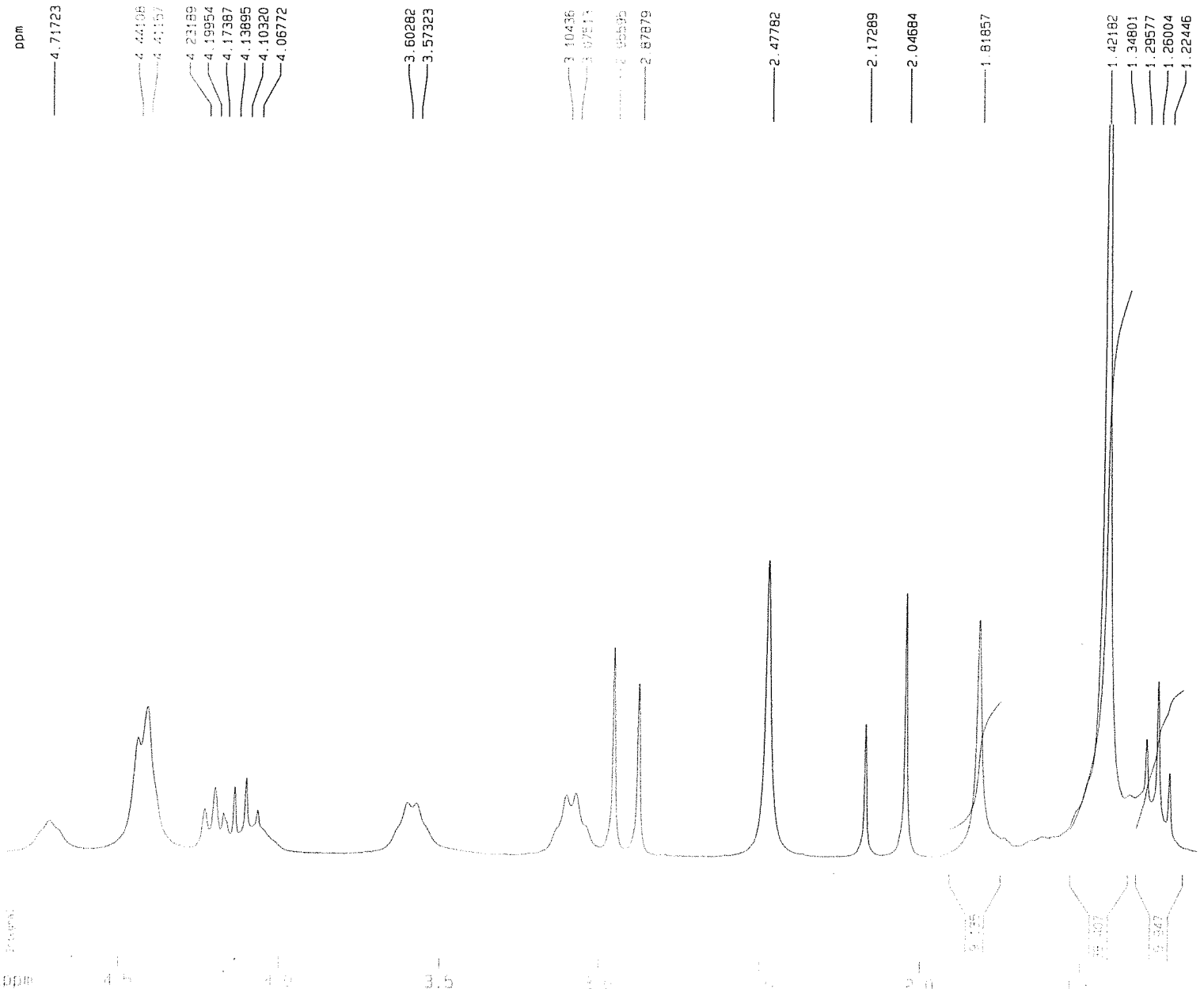

Current Data Parameters

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EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

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RG	181
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TE	295.0 K
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MCREST	0.00000000 sec
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======== CHANNEL f1 ========

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1D NMR plot parameters

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F1	972.34 Hz
F2P	1.136 ppm
F2	227.43 Hz
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Current Data Parameters
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PROCNO 1
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FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 181
DW 124.800 usec
DE 6.00 usec
TE 295.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
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PL1 1.00 dB
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SSB 0
LB 0.10 Hz
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HZCM 34.72490 Hz/cm
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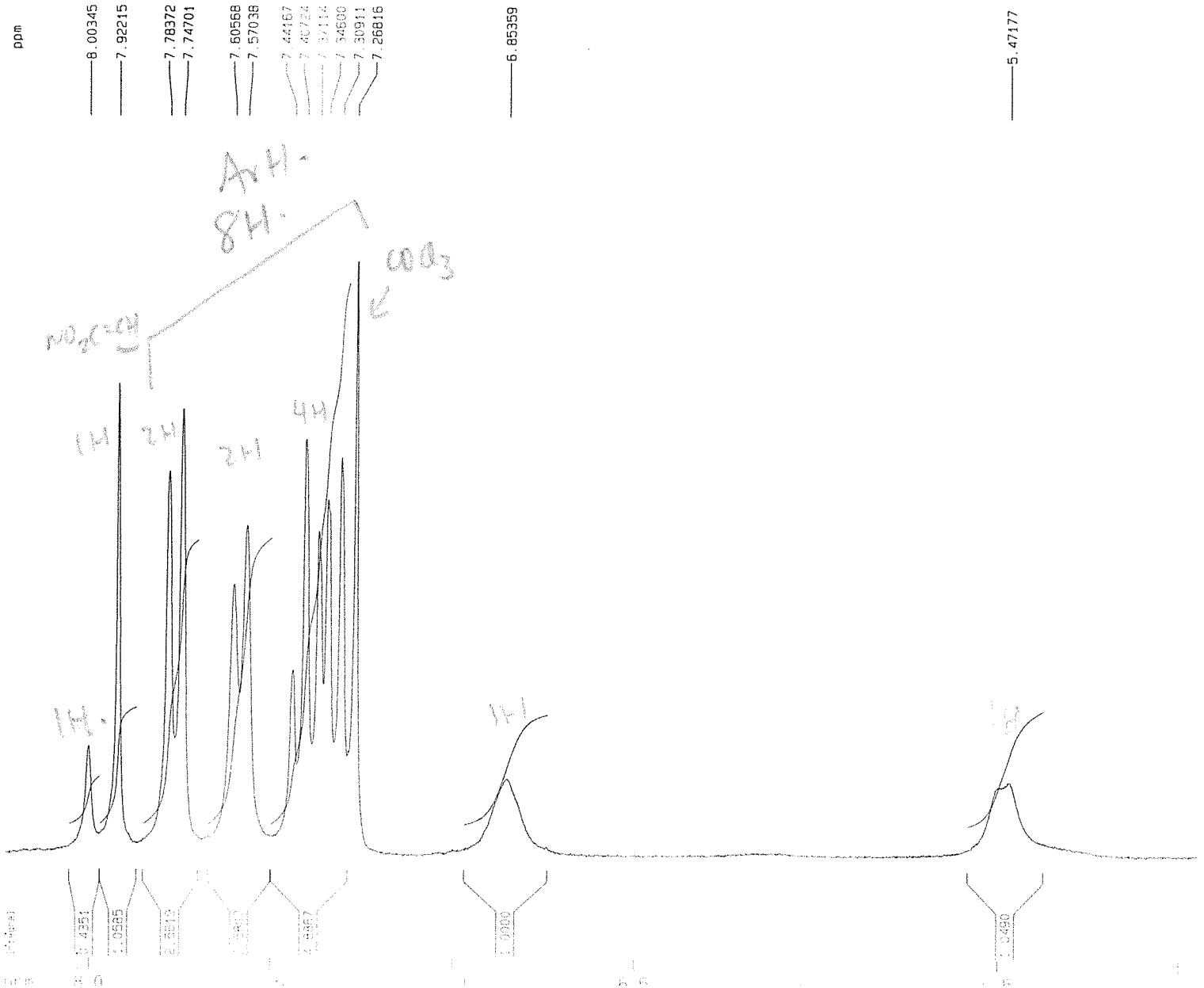


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PROCNO                 1

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PULPROG             zg
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TE              295.0 K
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MCWRK         0.01500000 sec

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PL1              1.00 dB
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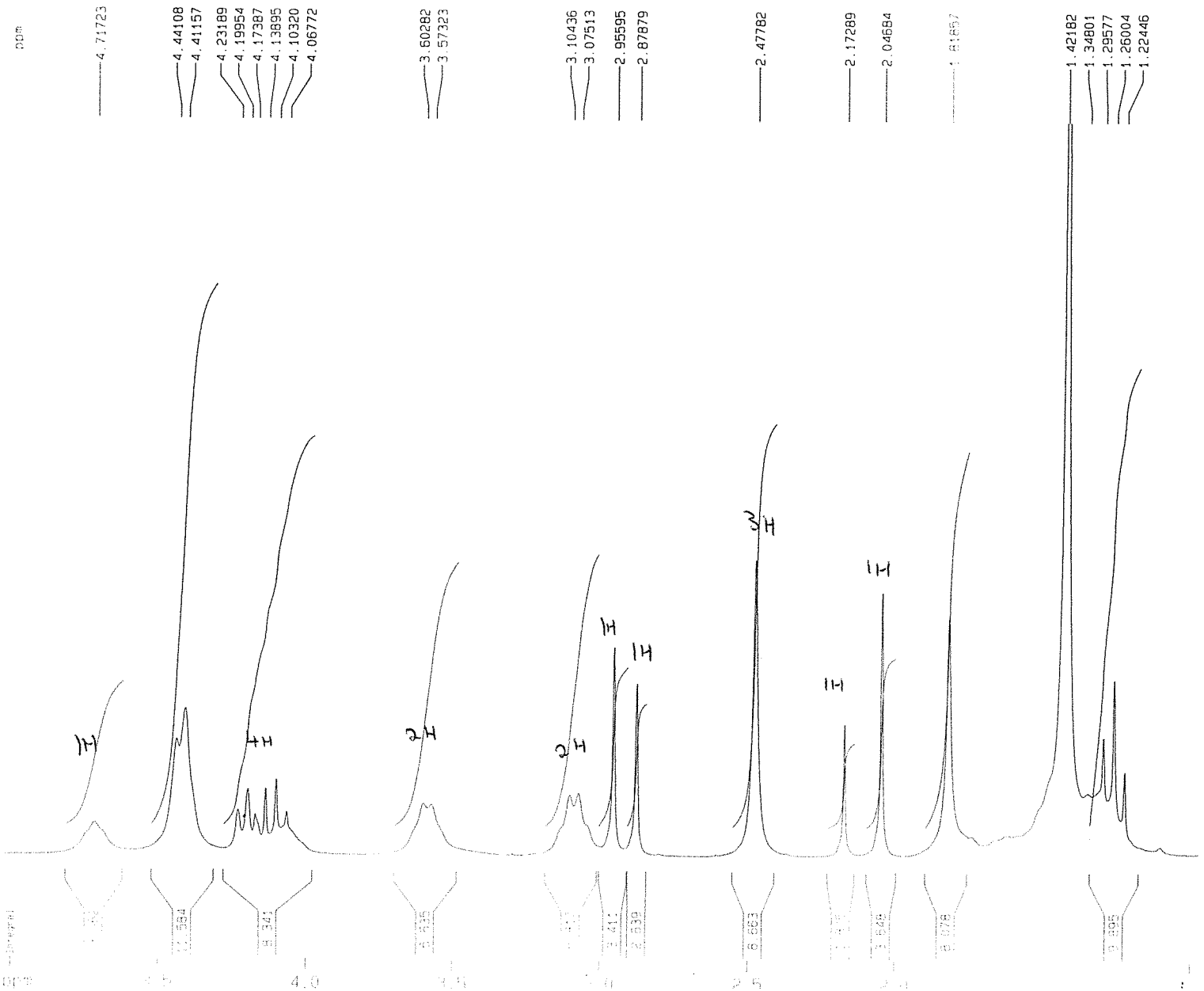

Current Data Parameters

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PROCNO	1

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

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SFO1	200 1310007 MHz

F2 - Processing parameters

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1D NMR plot parameters

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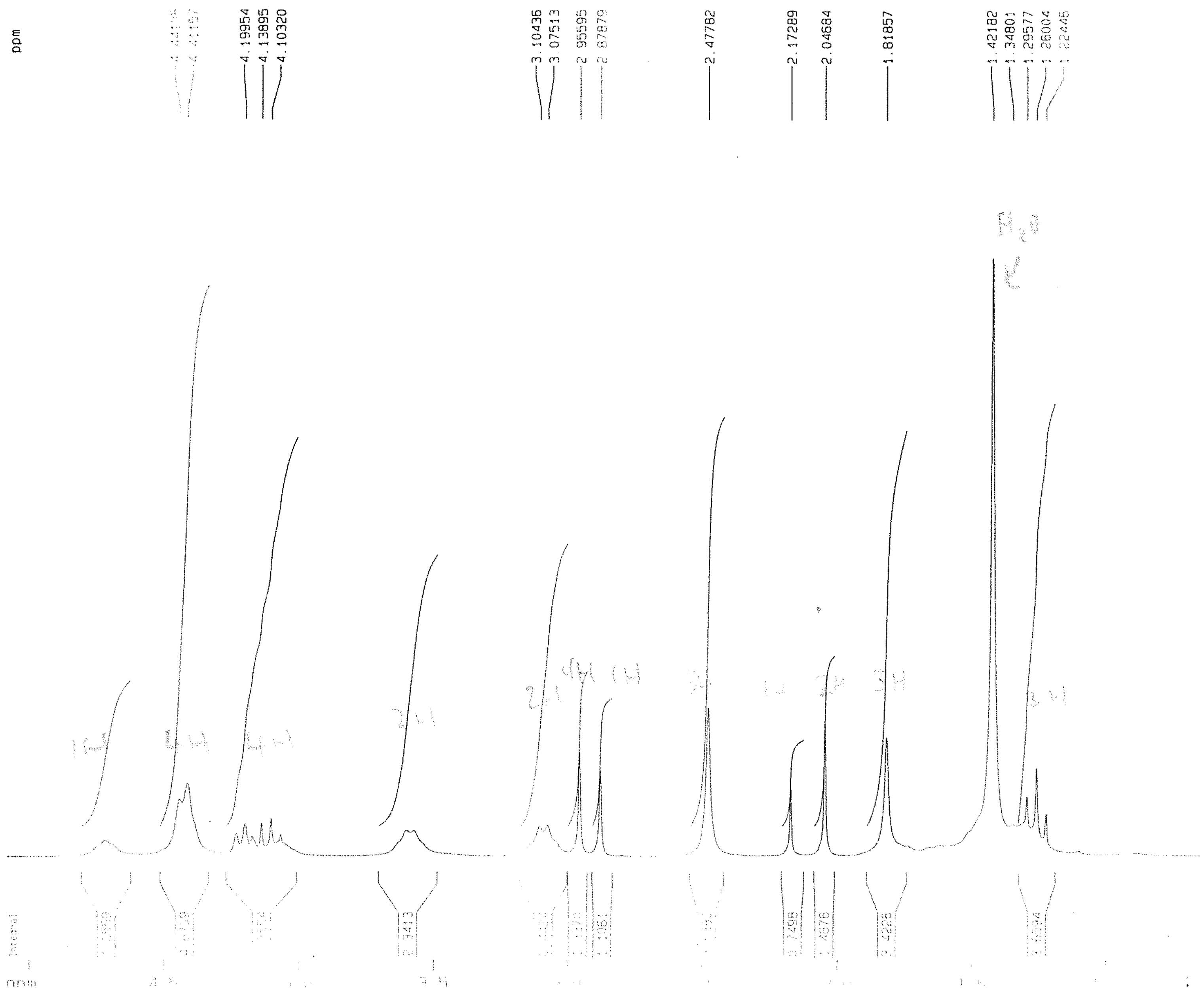

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PROCNO 1

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SOLVENT CDCl3
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DS 0
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 181
DW 124.800 usec
DE 6.00 usec
TE 295.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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PL1 1.00 dB
SFO1 200.1310007 MHz

F2 - Processing parameters
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SSB 0
LB 0.10 Hz
GB 0
PC 1.00

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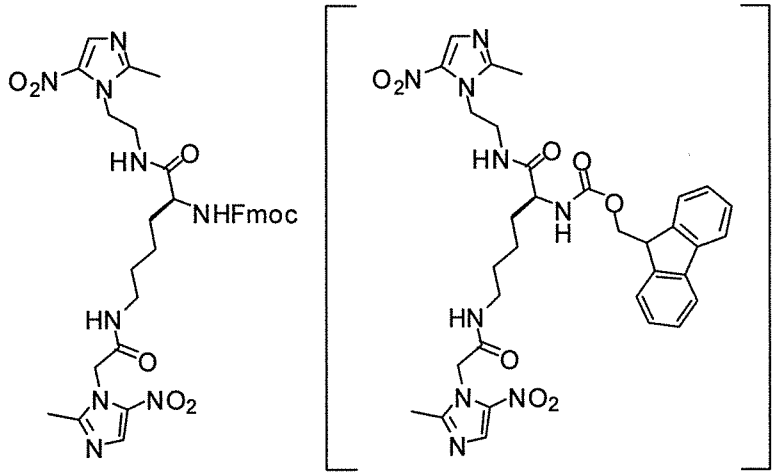
15



Fmoc-Lys(Met acid)-Met amine
Chemical Formula: $C_{33}H_{37}N_9O_8$
Molecular Weight: 687.70238

✓ ^{1}H NMR:

^{13}C NMR:

✓ MS:

✓ Hi Res MS:

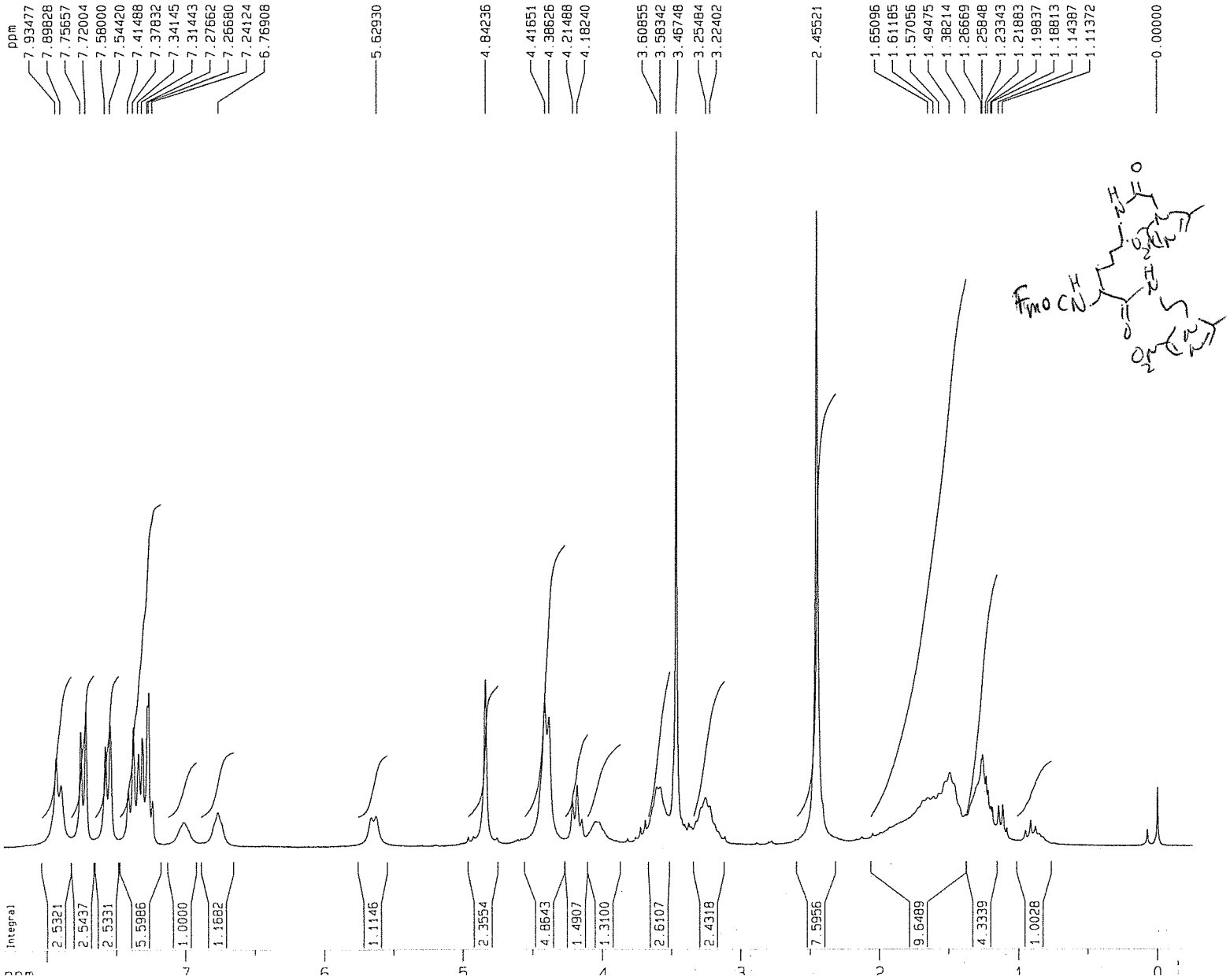
UV:

IR:

mp:

Yield:

Experimental:



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TE	300.4 K
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======== CHANNEL f1 ========

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PL1	1.00 dB
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F2 - Processing parameters

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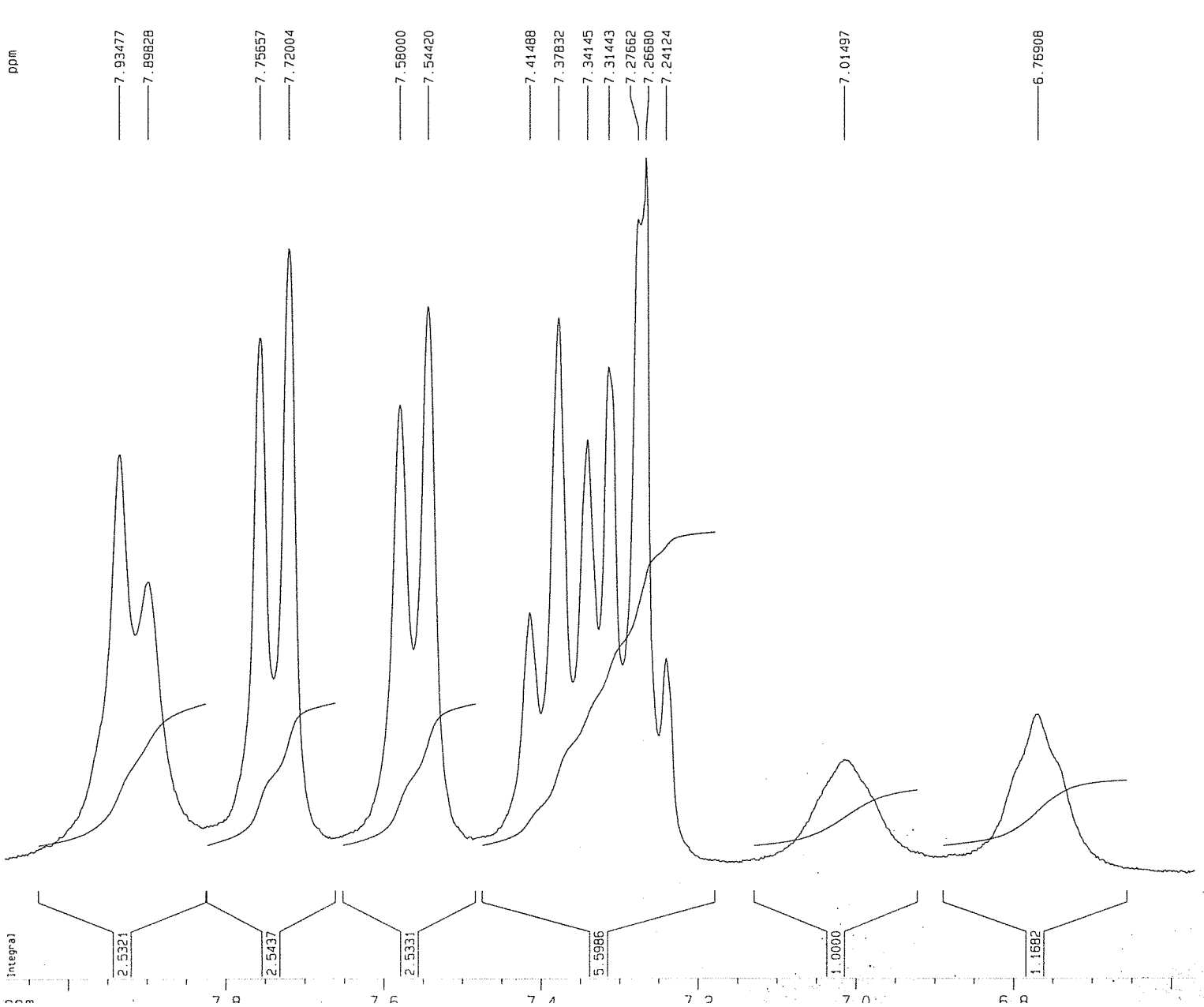

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PROCNO 1

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SOLVENT CDCl3
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FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 161.3
DW 124.800 usec
DE 6.00 usec
TE 300.4 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
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P1 6.35 usec
PL1 1.00 dB
SFO1 200.1310007 MHz

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PC 1.00

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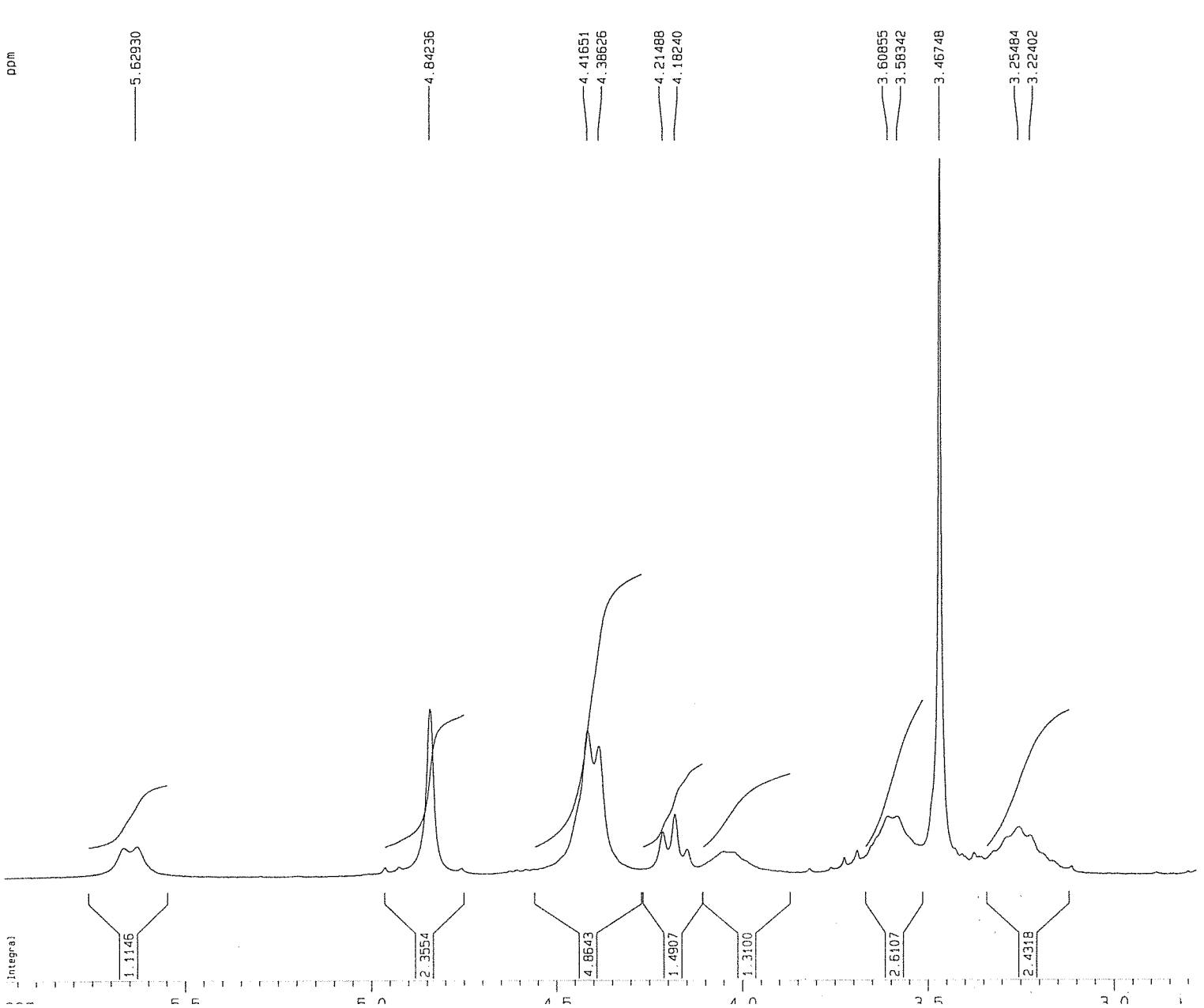

Current Data Parameters

NAME	Fmoc-Lys(Metacid)-Metamine
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PROCNO	1

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SOLVENT	CDCl3
NS	32
DS	2
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DW	124.800 usec
DE	6.00 usec
TE	300.4 K
D1	1.50000000 sec
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MCWRK	0.01500000 sec

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

NUC1	1H
P1	6.35 usec
PL1	1.00 dB
SFO1	200.1310007 MHz

F2 - Processing parameters

SI	16384
SF	200.1300075 MHz
WDW	EM
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LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

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CY	12.00 cm
F1P	5.986 ppm
F1	1197.93 Hz
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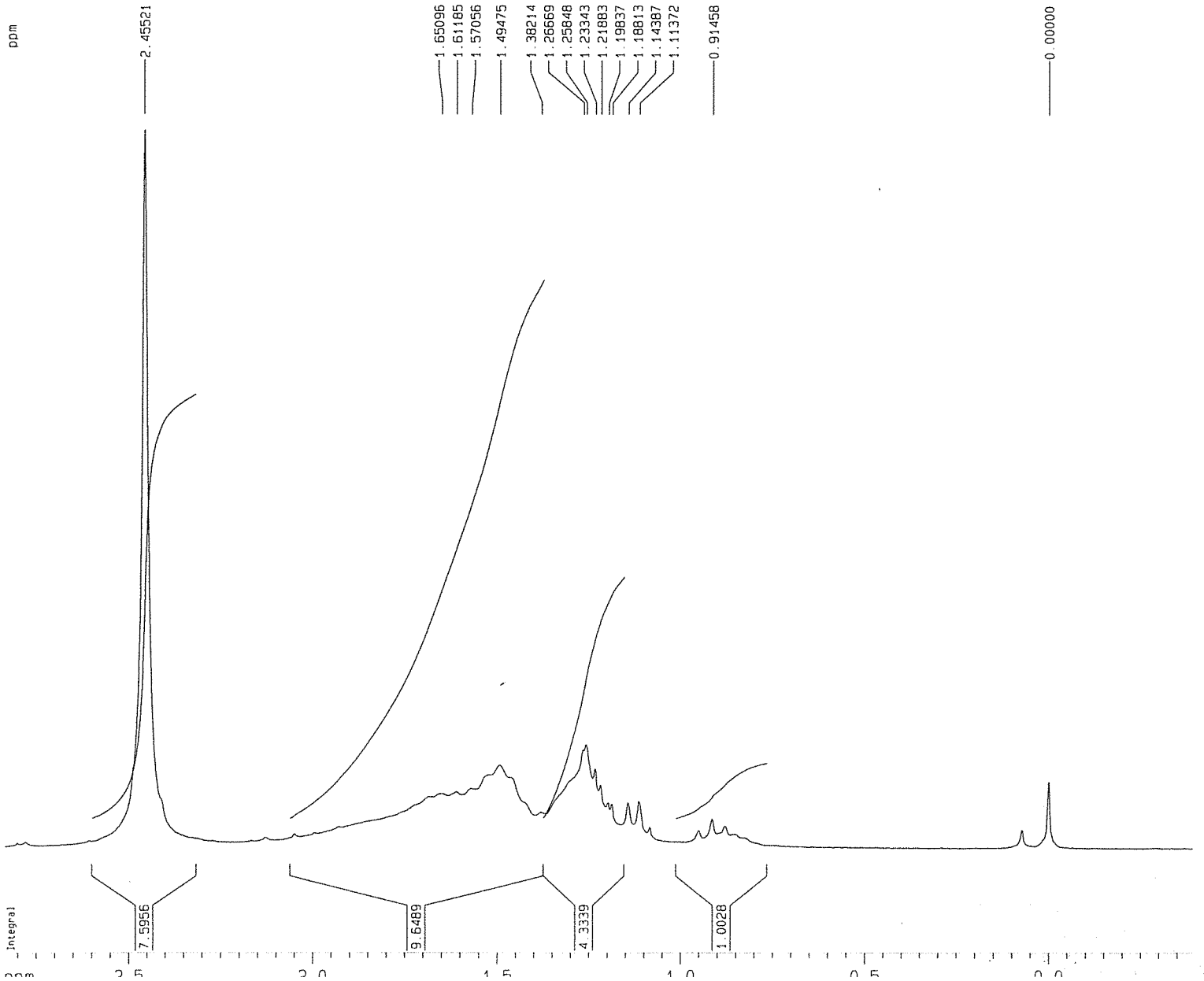

Current Data Parameters

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PROCNO	1

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DW	124.800 usec
DE	6.00 usec
TE	300.4 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	6.35 usec
PL1	1.00 dB
SFO1	200.1310007 MHz

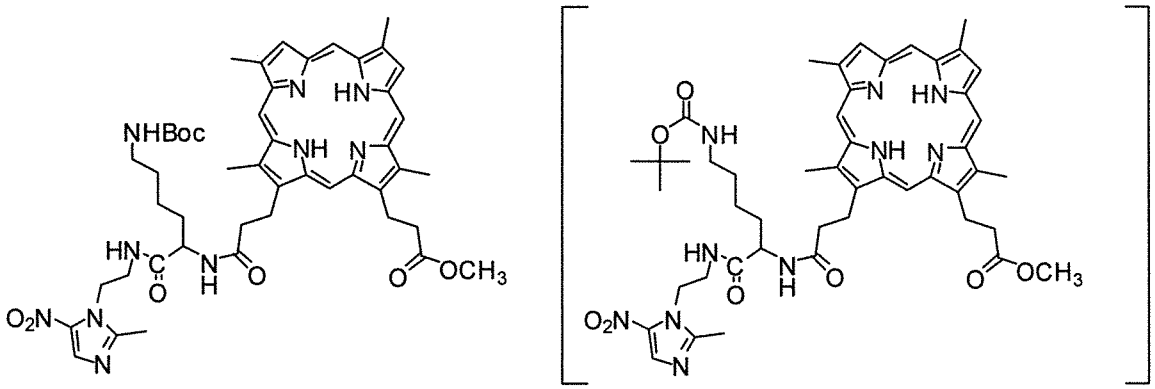
F2 - Processing parameters

SI	16384
SF	200.1300075 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	12.00 cm
F1P	2.836 ppm
F1	567.66 Hz
F2P	-0.393 ppm
F2	-78.66 Hz
PPMCM	0.16148 ppm/cm
HZCM	32.31623 Hz/cm

11a and 11b.



DPIX mono Lys mono Me

Chemical Formula: $C_{48}H_{60}N_{10}O_8$
Molecular Weight: 905.05220

✓ ^{1}H NMR:

^{13}C NMR:

✓ MS:

✓ Hi Res MS:

UV:

IR:

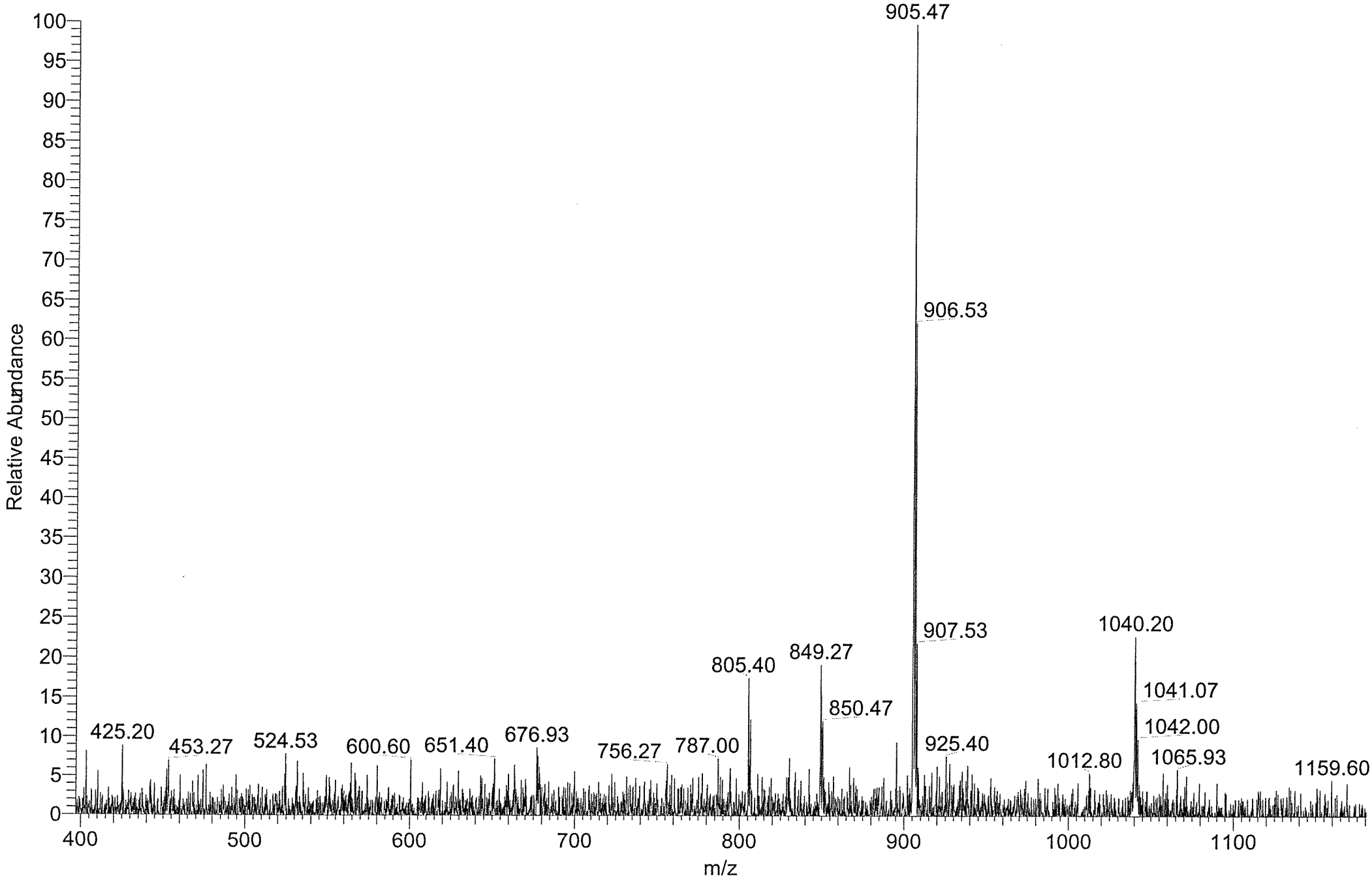
mp:

Yield:

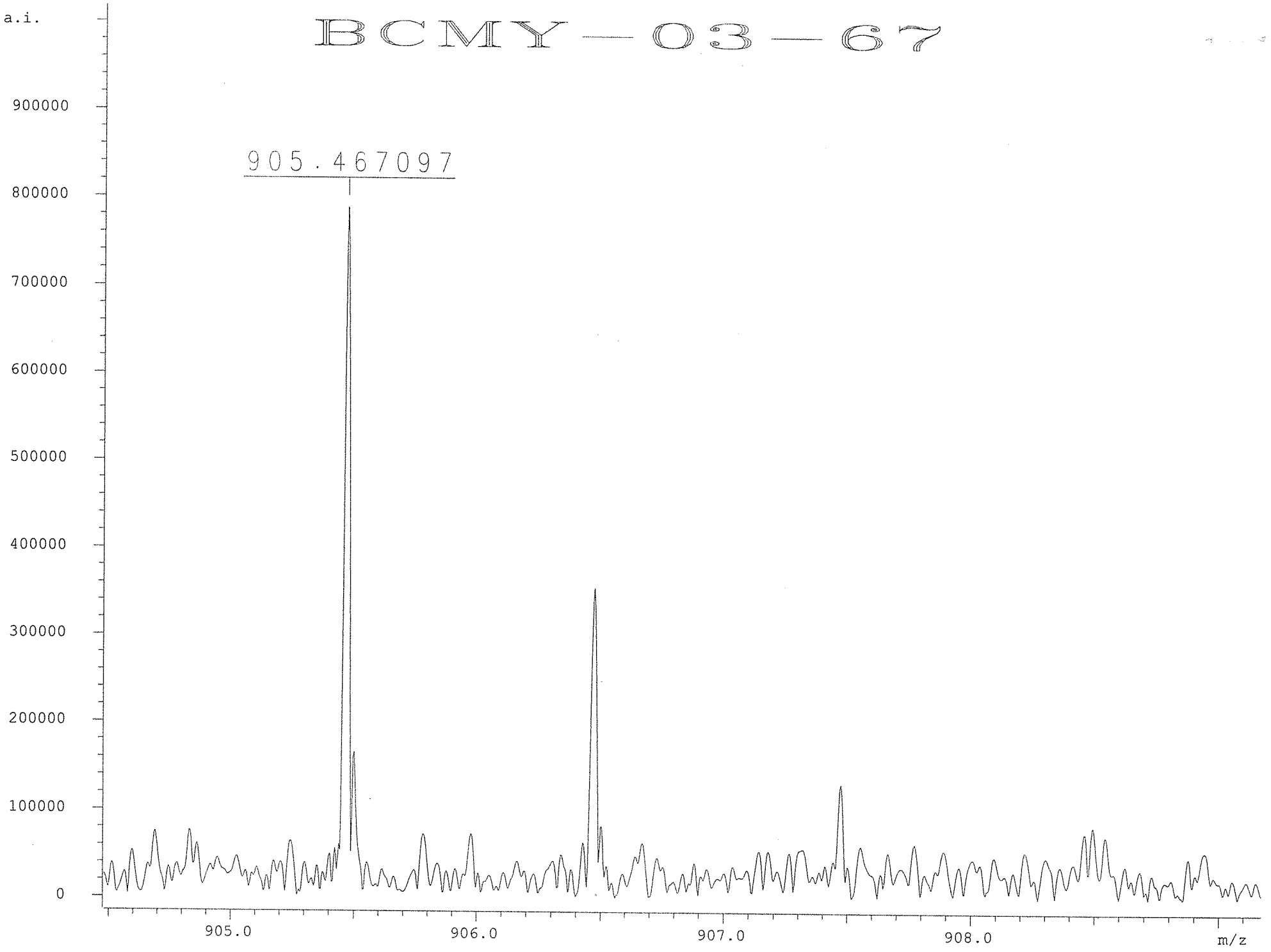
Experimental:

C:\Data\Keith\k24_070924135528 MeOH\DCM\TFA 24/09/2007 1:55:28 PM BCMY-03-67

k24_070924135528 #2-5 RT: 0.06-0.17 AV: 4 NL: 1.32E5
T: + p ESI Full ms [50.00-2000.00]



BCMY—03—67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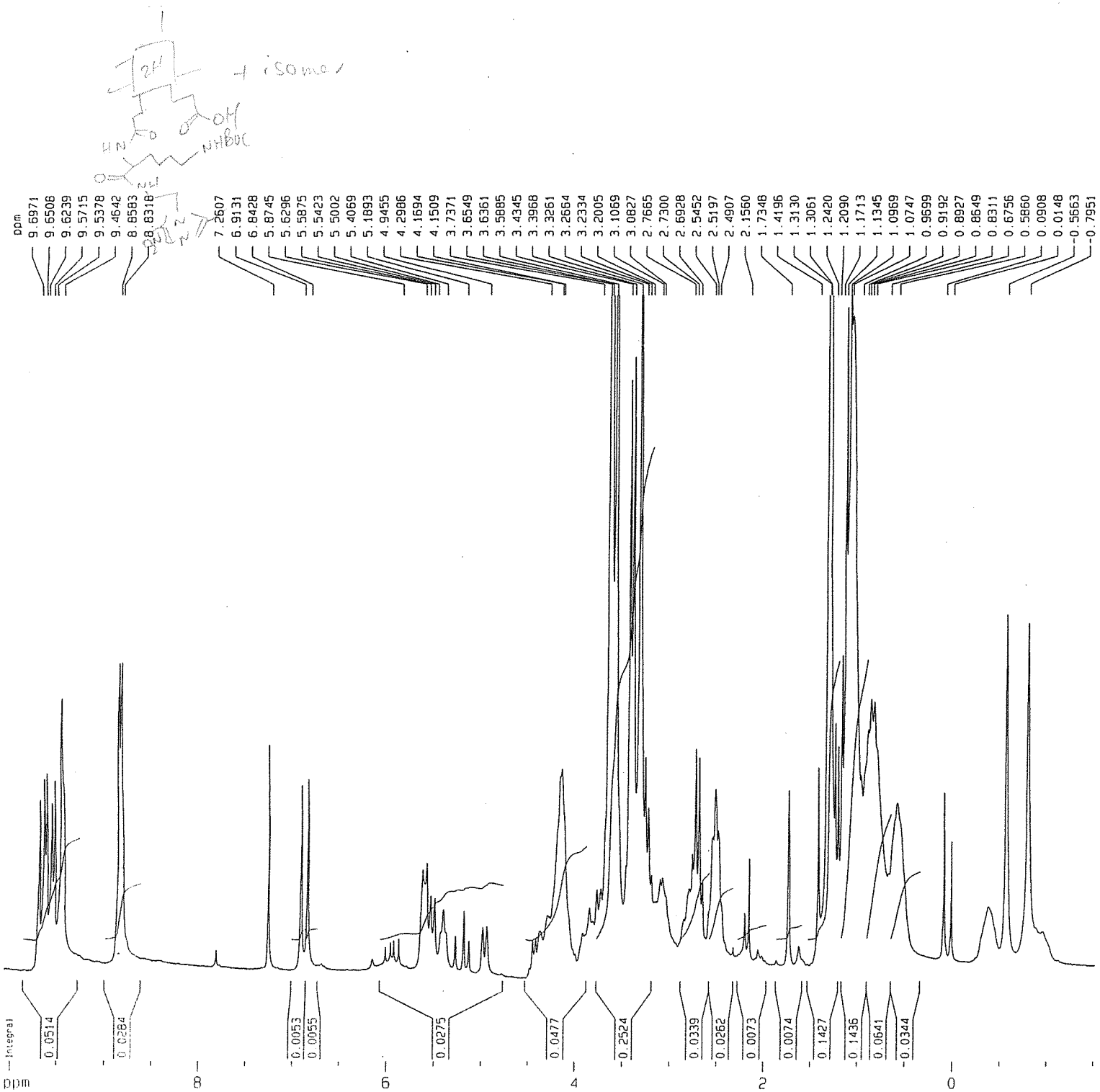
m/z



Current Data Parameters

NAME	BCMY-03-65monoLysmonoMe
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070917
Time	20.47
INSTRUM	spect
PROBHD	5 mm PHOUL 13C
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	71.8
DW	124.800 usec
DE	6.00 usec
TE	300.6 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

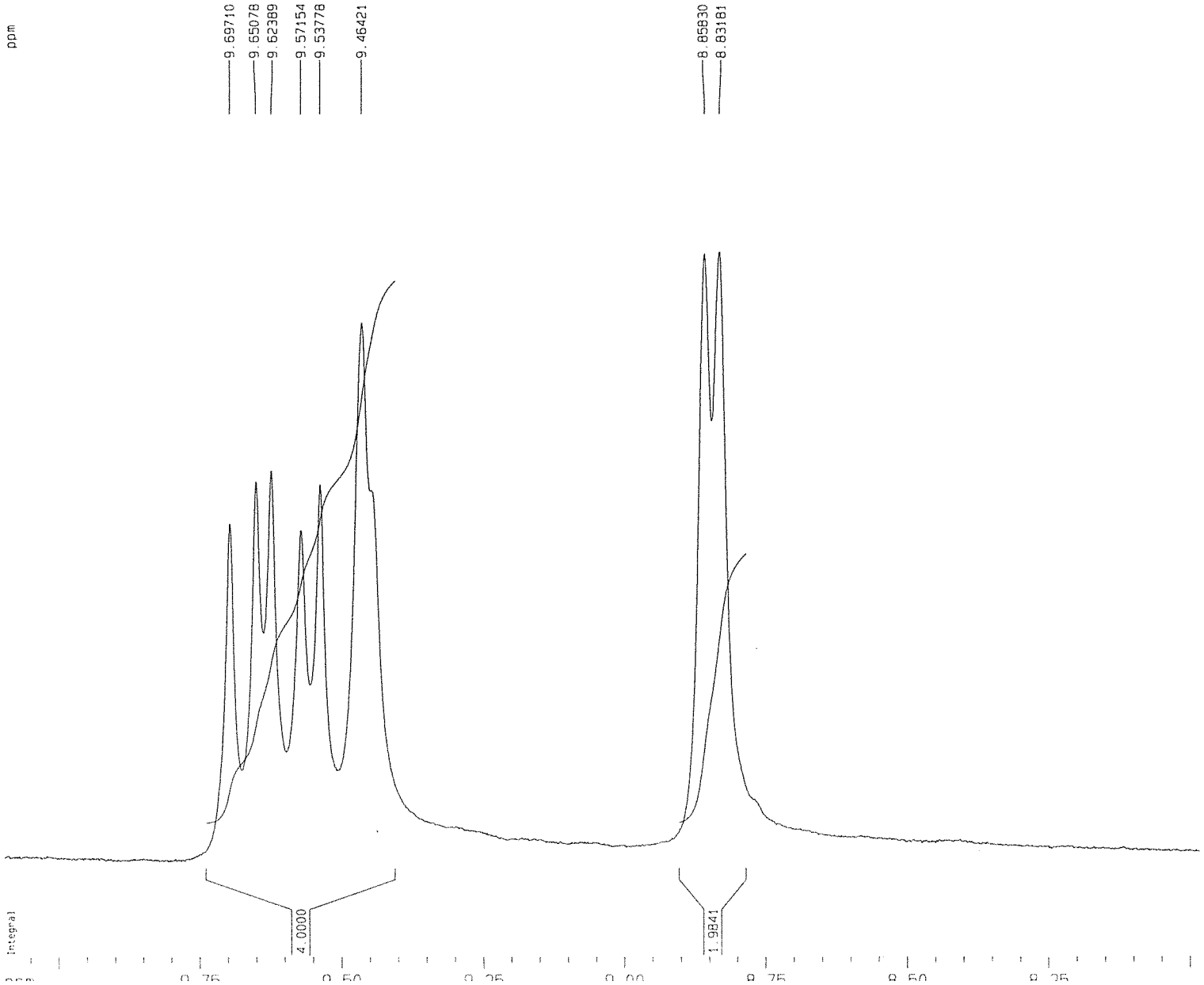
NUC1	1H
P1	6.35 usec
PL1	1.00 dB
SFO1	200.1308005 MHz

F2 - Processing parameters

SI	16384
SF	200.1300083 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	55.00 cm
F1P	10.071 ppm
F1	2015.55 Hz
F2P	-1.517 ppm
F2	-303.68 Hz
PPMCM	0.57943 ppm/cm
HZCM	115.96162 Hz/cm



Current Data Parameters

NAME	BCMY-03-65monoLysmonoMe
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070917
Time	20.47
INSTRUM	spect
PROBHD	5 mm PHDUL 13C
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	71.8
DW	124.800 usec
DE	6.00 usec
TE	300.6 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

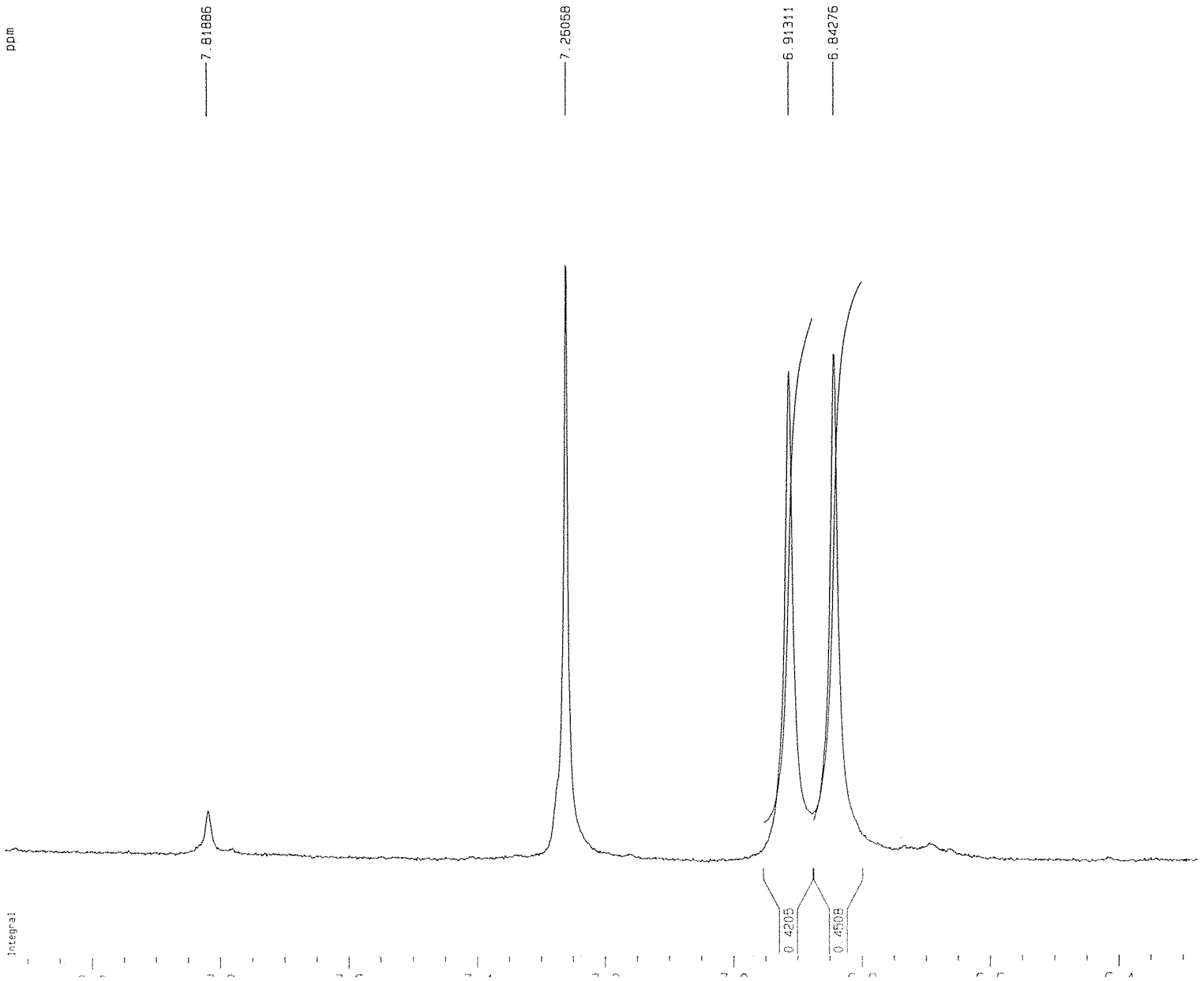
NUC1	1H
P1	6.35 usec
PL1	1.00 dB
SFO1	200.1308005 MHz

F2 - Processing parameters

SI	16384
SF	200.1300083 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	10.00 cm
F1P	10.097 ppm
F1	2020.65 Hz
F2P	7.983 ppm
F2	1597.58 Hz
PPMCM	0.10570 ppm/cm
HZCM	21.15344 Hz/cm



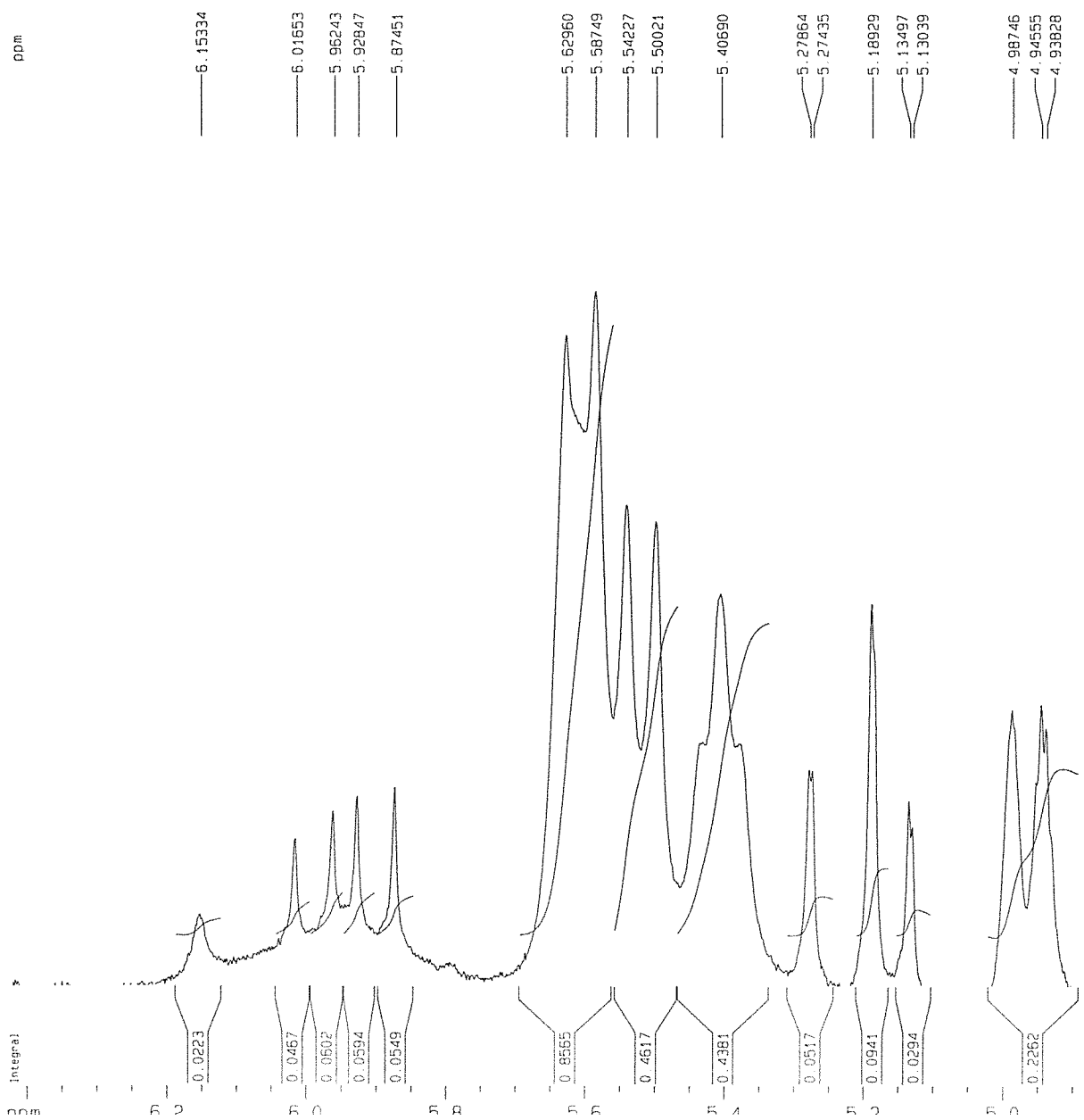
Current Data Parameters
NAME BCMY-03-65monoLysmonoMe
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070917
Time 20.47
INSTRUM spect
PROBHD 5 mm PHDUL 13C
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 71.8
DW 124.800 usec
DE 6.00 usec
TE 300.6 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 6.35 usec
PL1 1.00 dB
SFO1 200.1308005 MHz

F2 - Processing parameters
SI 16384
SF 200.1300083 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 8.136 ppm
F1 1628.16 Hz
F2P 6.276 ppm
F2 1256.07 Hz
PPMCM 0.09296 ppm/cm
HZCM 18.60483 Hz/cm



Current Data Parameters

NAME	BCMY-03-65monoLysmonoMe
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070917
Time	20.47
INSTRUM	spect
PROBHD	5 mm PHOUL 13C
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	71.8
DW	124.800 usec
DE	6.00 usec
TE	300.6 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

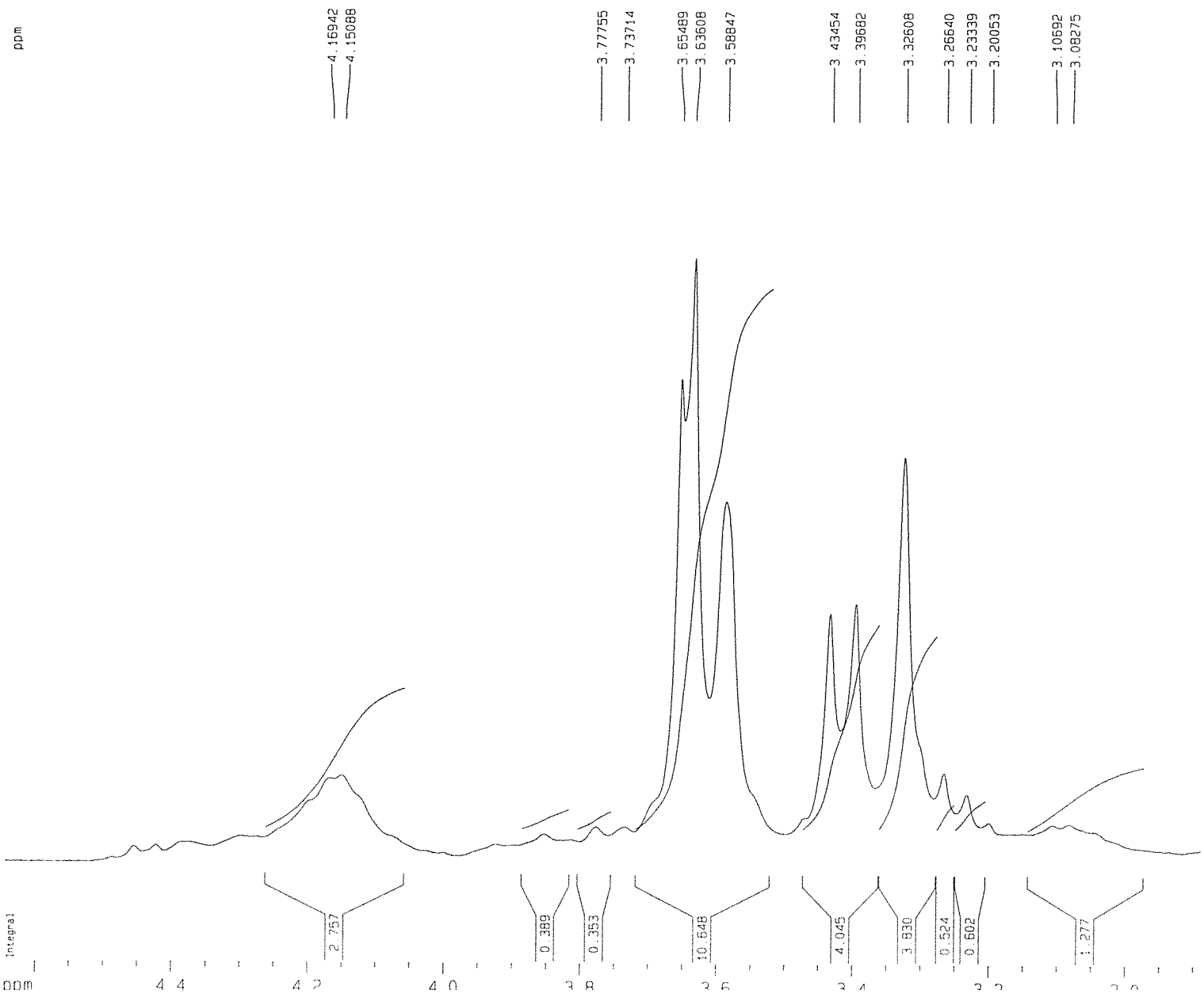
NUC1	1H
P1	6.35 usec
PL1	1.00 dB
SFO1	200.1308005 MHz

F2 - Processing parameters

SI	16384
SF	200.1300083 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	10.00 cm
F1P	6.429 ppm
F1	1286.65 Hz
F2P	4.493 ppm
F2	899.26 Hz
PPMCM	0.09678 ppm/cm
HZCM	19.36942 Hz/cm



Current Data Parameters

NAME	BCMY-03-65monoLysmonoMe
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070917
Time	20.47
INSTRUM	spect
PROBHD	5 mm PHOUL 13C
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	71.8
DW	124.800 usec
DE	6.00 usec
TE	300.6 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

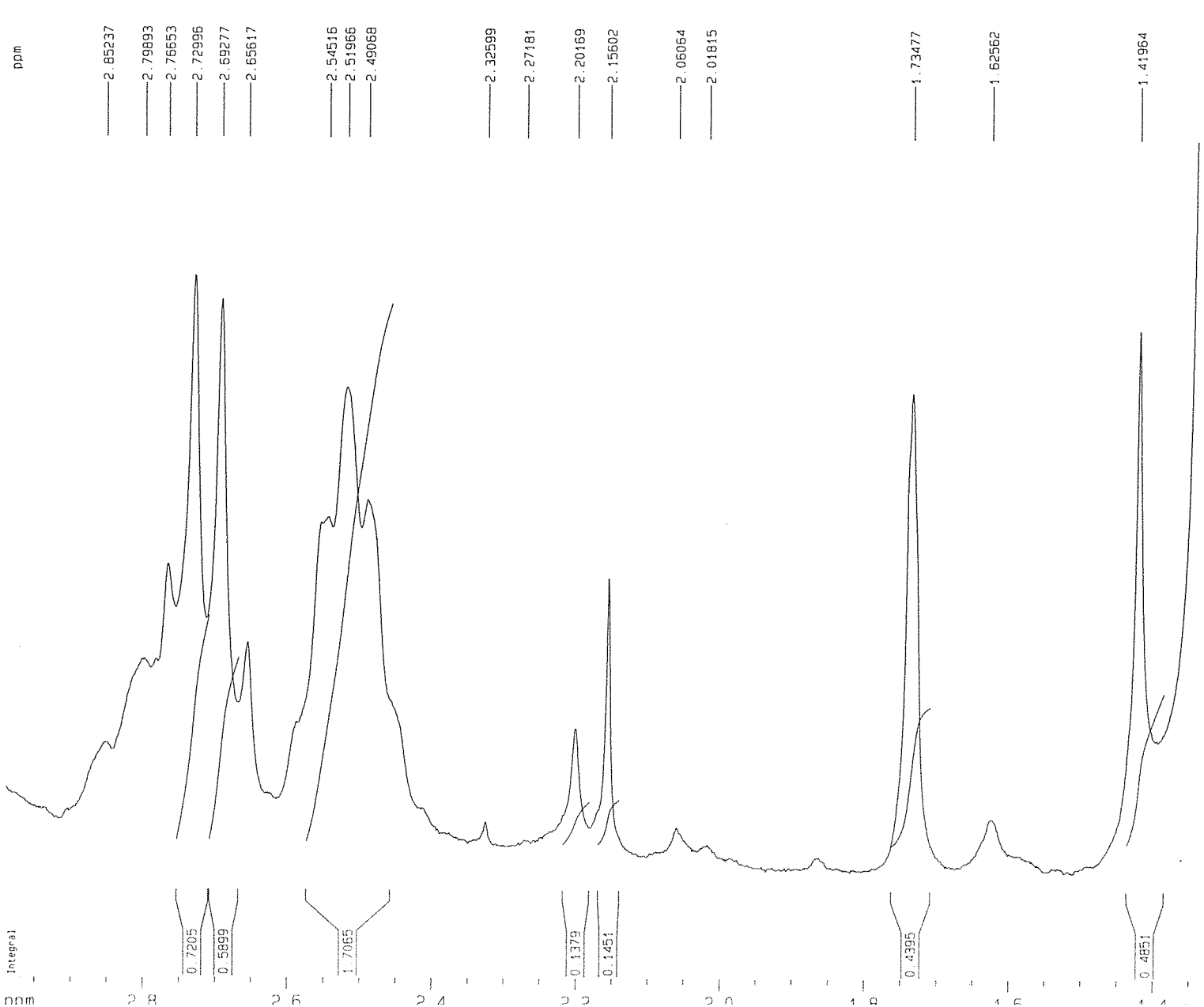
NUC1	1H
P1	6.35 usec
PL1	1.00 dB
SF01	200.1308005 MHz

F2 - Processing parameters

SI	16384
SF	200.1300083 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	10.00 cm
F1P	4.646 ppm
F1	929.84 Hz
F2P	2.889 ppm
F2	578.14 Hz
PPMCM	0.08787 ppm/cm
HZCM	17.58539 Hz/cm



Current Data Parameters

NAME	BCMY-03-65monoLysmonoMe
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070917
Time	20.47
INSTRUM	spect
PROBHD	5 mm PHOUL 13C
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	71.8
DW	124.800 usec
DE	6.00 usec
TE	300.6 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

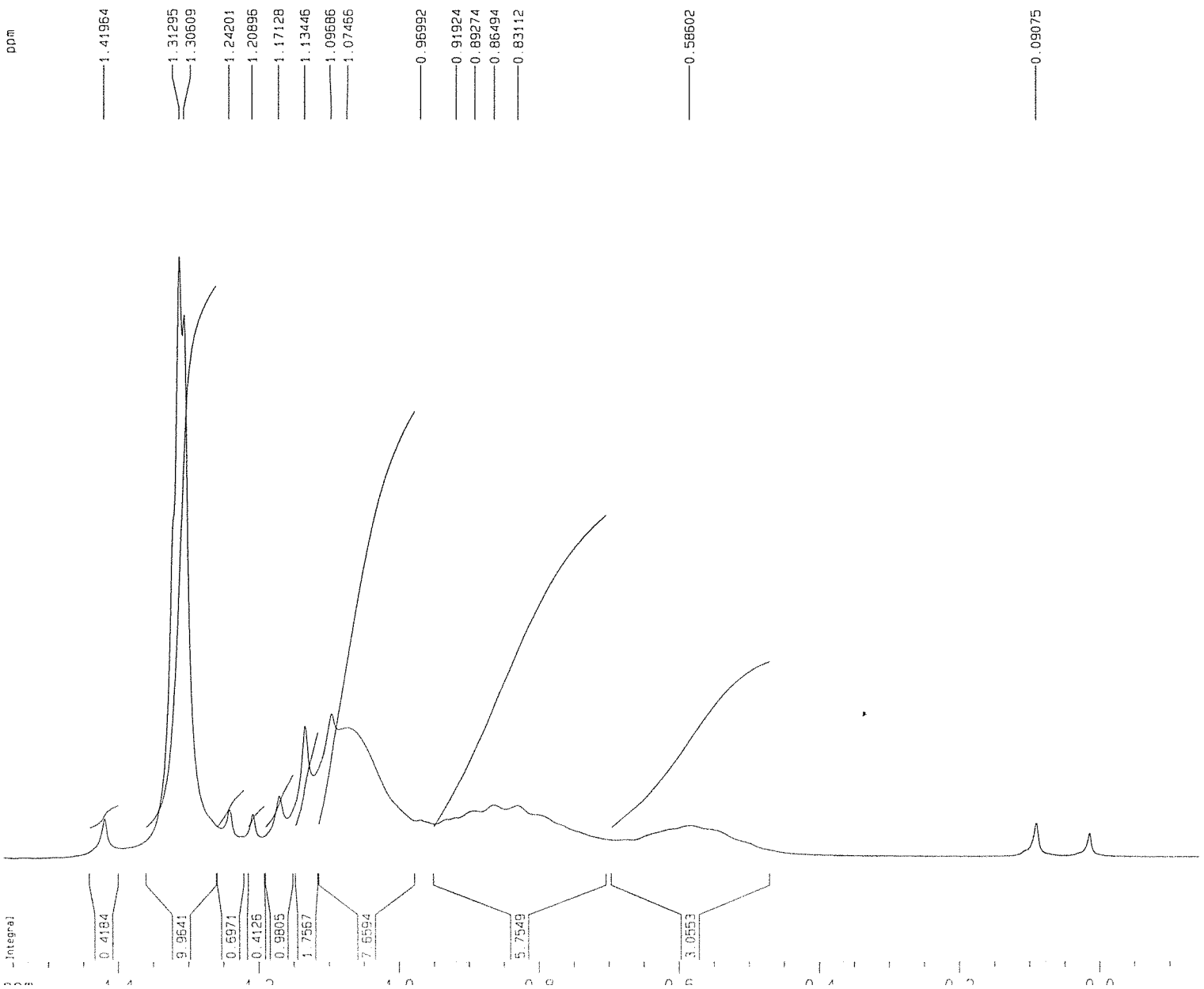
NUC1	1H
P1	6.35 usec
PL1	1.00 dB
SF01	200.1308005 MHz

F2 - Processing parameters

SI	16384
SF	200.1300083 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	10.00 cm
F1P	2.991 ppm
F1	598.52 Hz
F2P	1.335 ppm
F2	267.21 Hz
PPMCM	0.08278 ppm/cm
HZCM	16.56594 Hz/cm



Current Data Parameters

NAME	BCMY-03-65monoLysmonoMe
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070917
Time	20.47
INSTRUM	spect
PROBHD	5 mm PHDUL 13C
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	71.8
DW	124.800 usec
DE	6.00 usec
TE	300.6 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

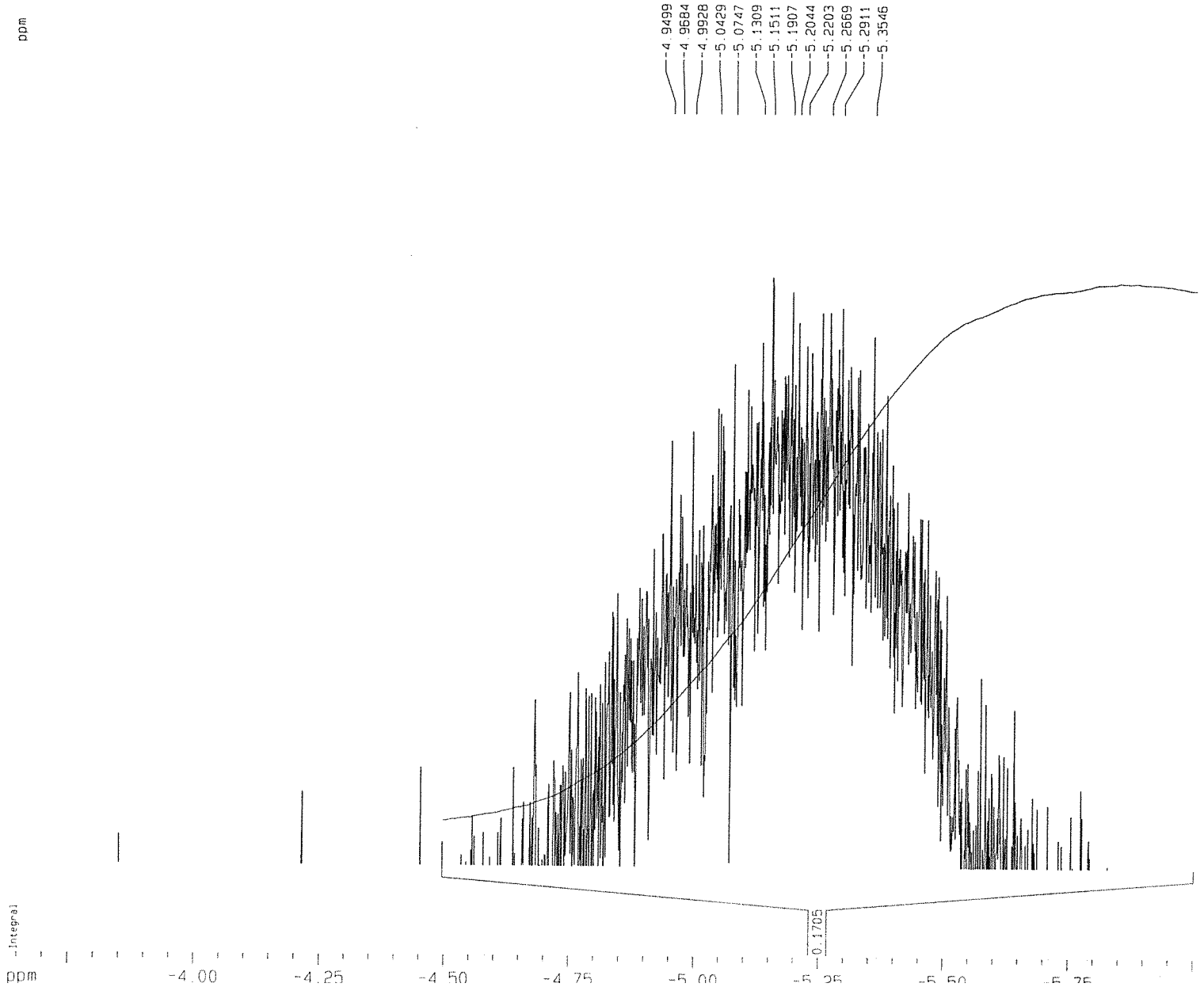
NUC1	1H
P1	6.35 usec
PL1	1.00 dB
SFO1	200.1308005 MHz

F2 - Processing parameters

SI	16384
SF	200.1300083 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	10.00 cm
F1P	1.564 ppm
F1	313.08 Hz
F2P	-0.142 ppm
F2	-28.43 Hz
PPMCM	0.08532 ppm/cm
HZCM	17.07567 Hz/cm



Current Data Parameters

NAME	BCMY-03-65monoLysmonoMe
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070917
Time	20.47
INSTRUM	spect
PROBHD	5 mm PHOUL 13C
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	71.8
DW	124.800 usec
DE	6.00 usec
TE	300.6 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

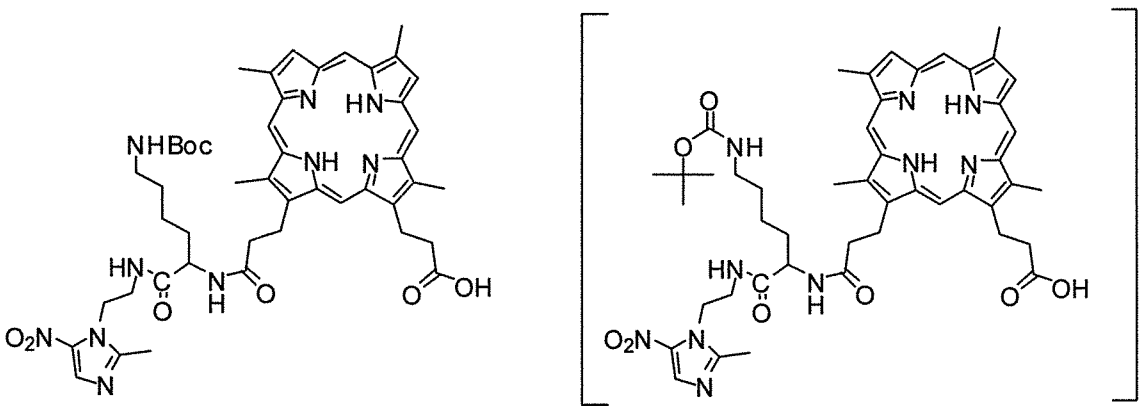
NUC1	1H
P1	6.35 usec
PL1	1.00 dB
SFO1	200.1308005 MHz

F2 - Processing parameters

SI	16384
SF	200.1300083 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	10.00 cm
F1P	-3.631 ppm
F1	-726.75 Hz
F2P	-6.026 ppm
F2	-1205.89 Hz
PPMCM	0.11971 ppm/cm
HZCM	23.95690 Hz/cm



DPIX mono Lys mono H

Chemical Formula: $C_{47}H_{58}N_{10}O_8$
Molecular Weight: 891.02562

✓ ^{1}H NMR:

^{13}C NMR:

✓ MS:

✓ Hi Res MS:

✓ UV:

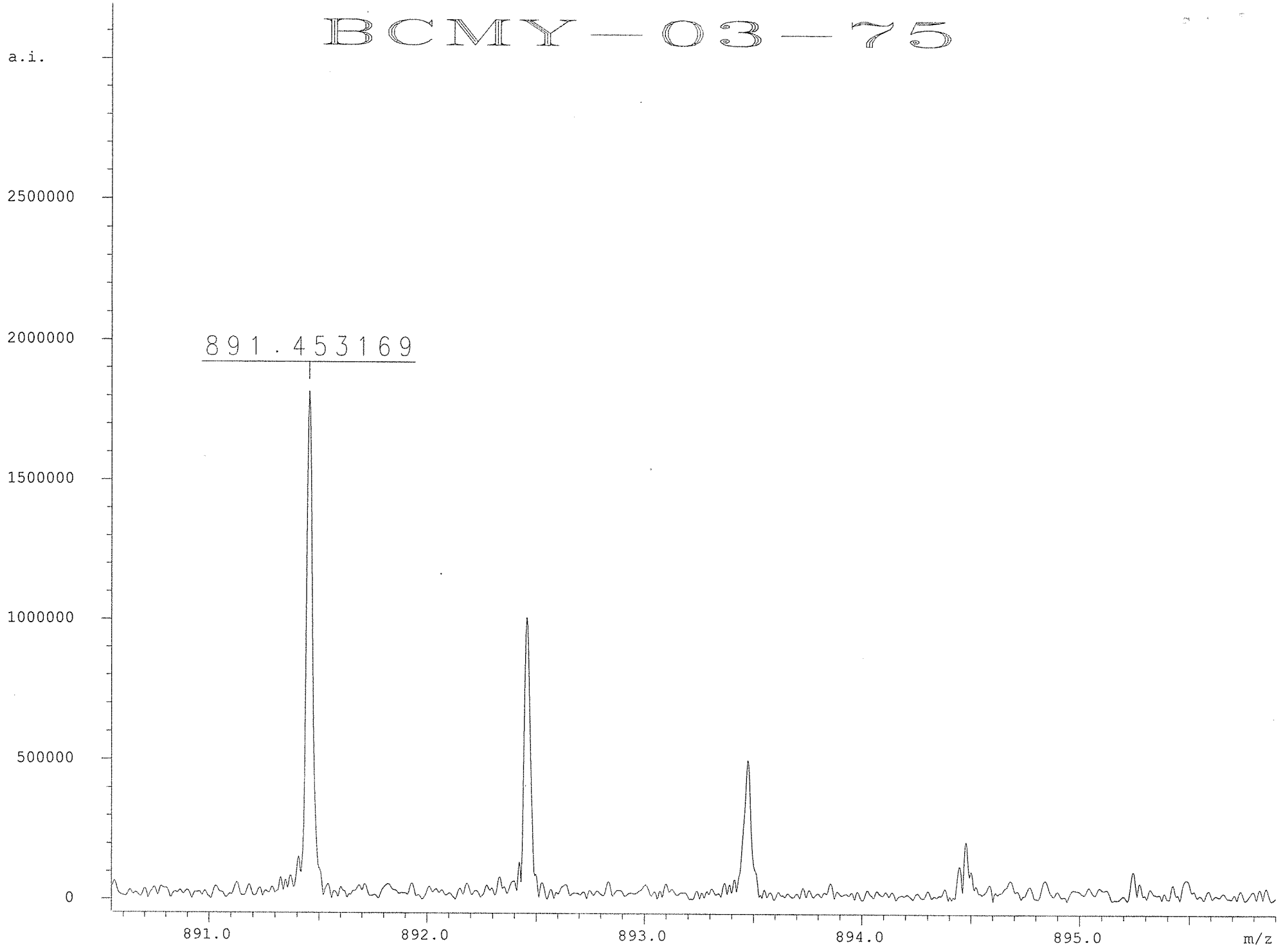
IR:

mp:

Yield:

Experimental:

BCMY-03-75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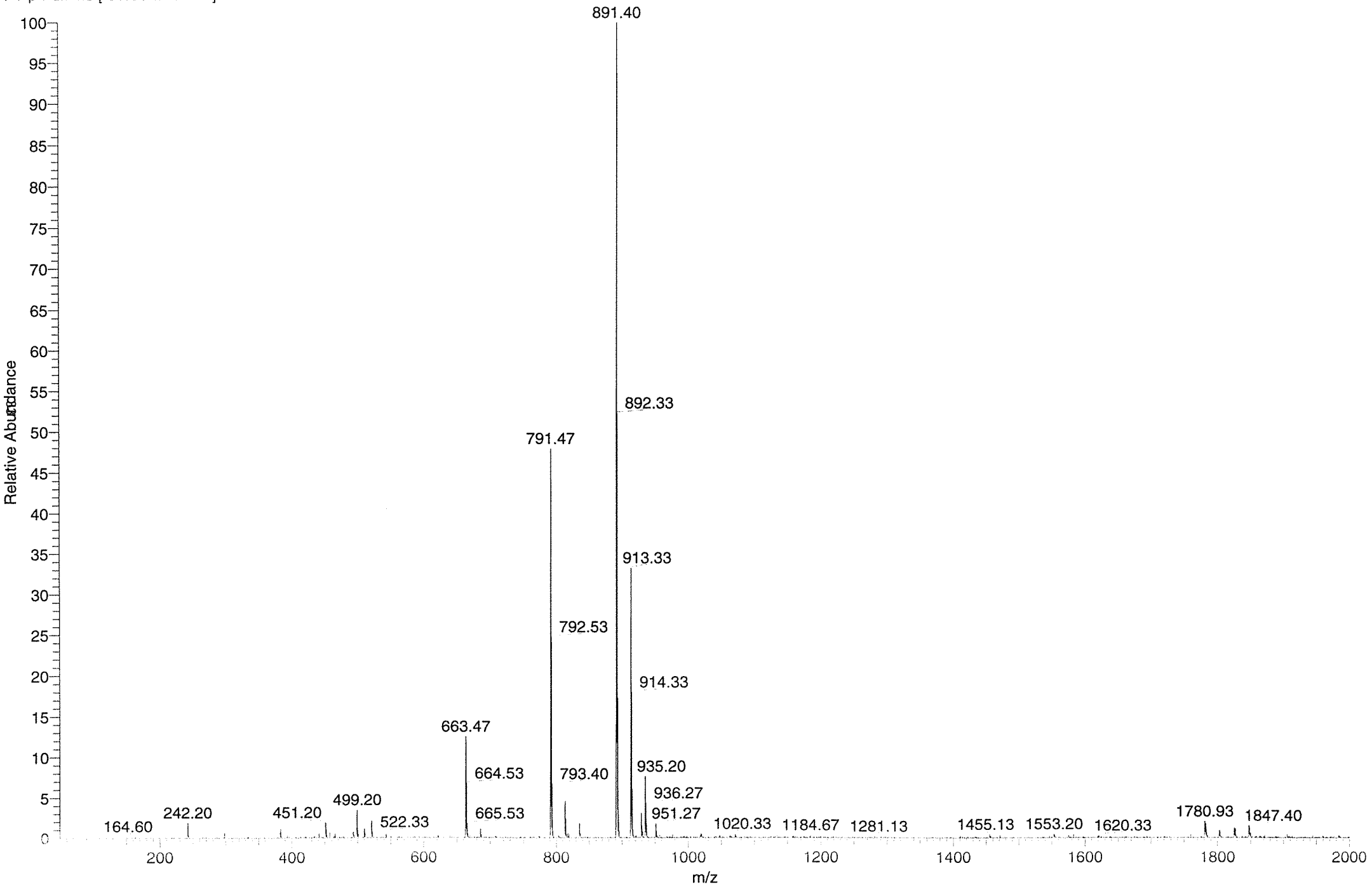
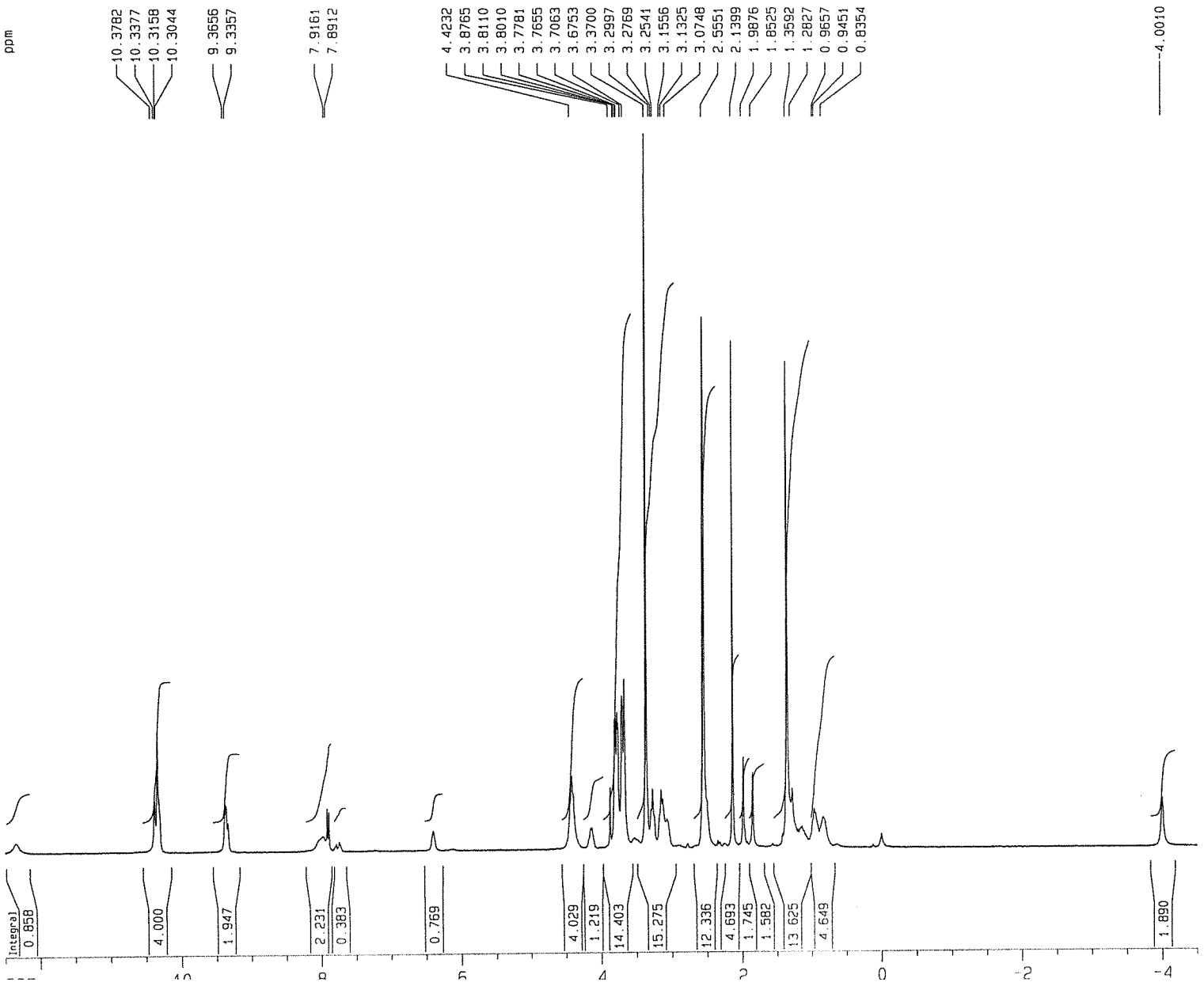
m/z

D:\Crossley\BCMY-03-75monoLysmonoHpure 27/09/07 17:01:53
MeOH/DCM/Formic

BCMY-03-75monoLysmonoHpure #48-53 RT: 1.35-1.49 AV: 6 NL: 3.82E8
F: + p Full ms [50.00-2000.00]





Current Data Parameters

NAME	BCMY-03-75monoLysmonoH
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20071019
Time	15.12
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	322.5
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

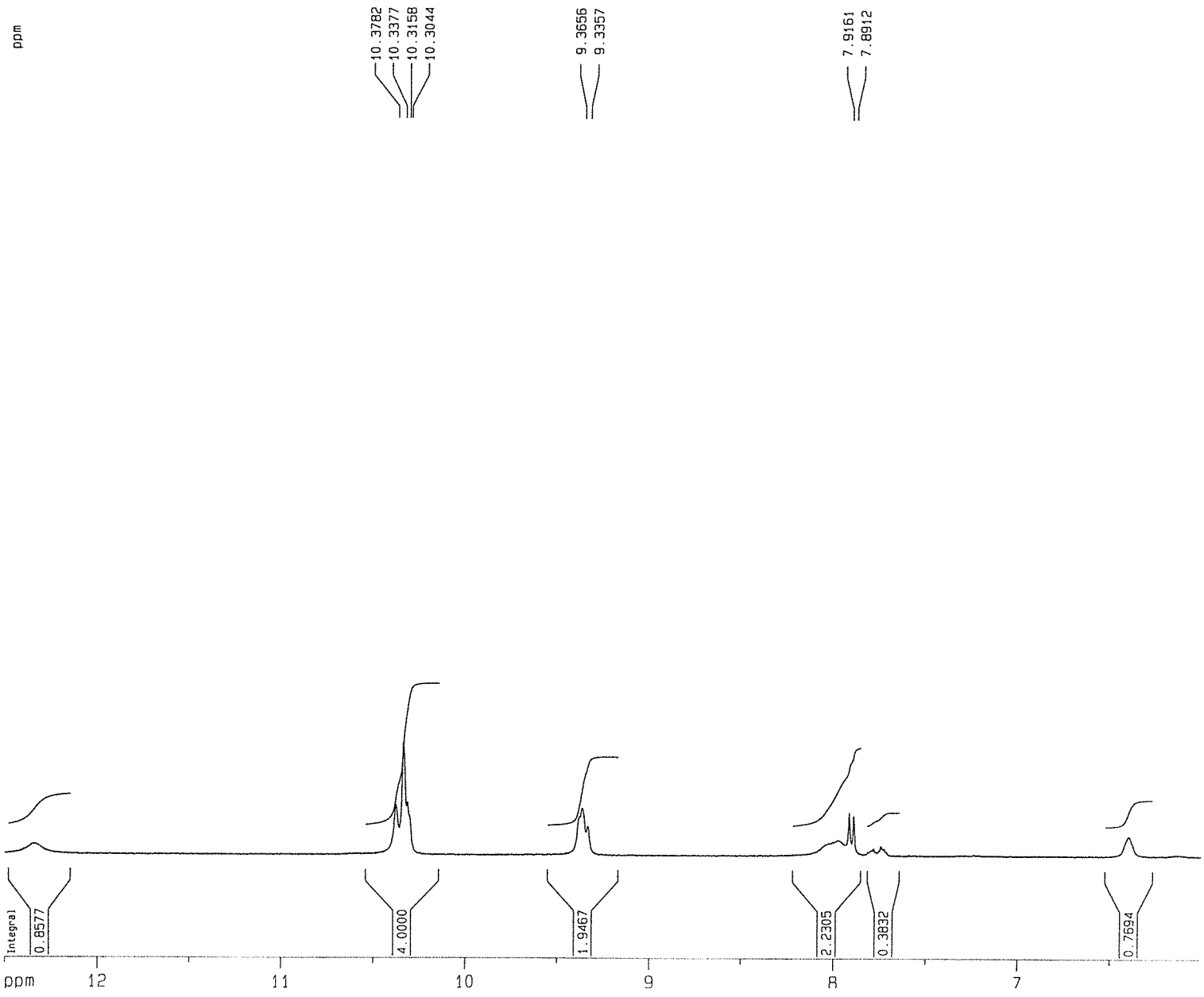
NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1299835 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	11.98 cm
F1P	12.500 ppm
F1	3751.62 Hz
F2P	-4.500 ppm
F2	-1350.59 Hz
PPMCM	0.85000 ppm/cm
HZCM	255.11047 Hz/cm



Current Data Parameters

NAME	BCMY-03-75monoLysmonoH
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20071019
Time	15.12
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	322.5
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

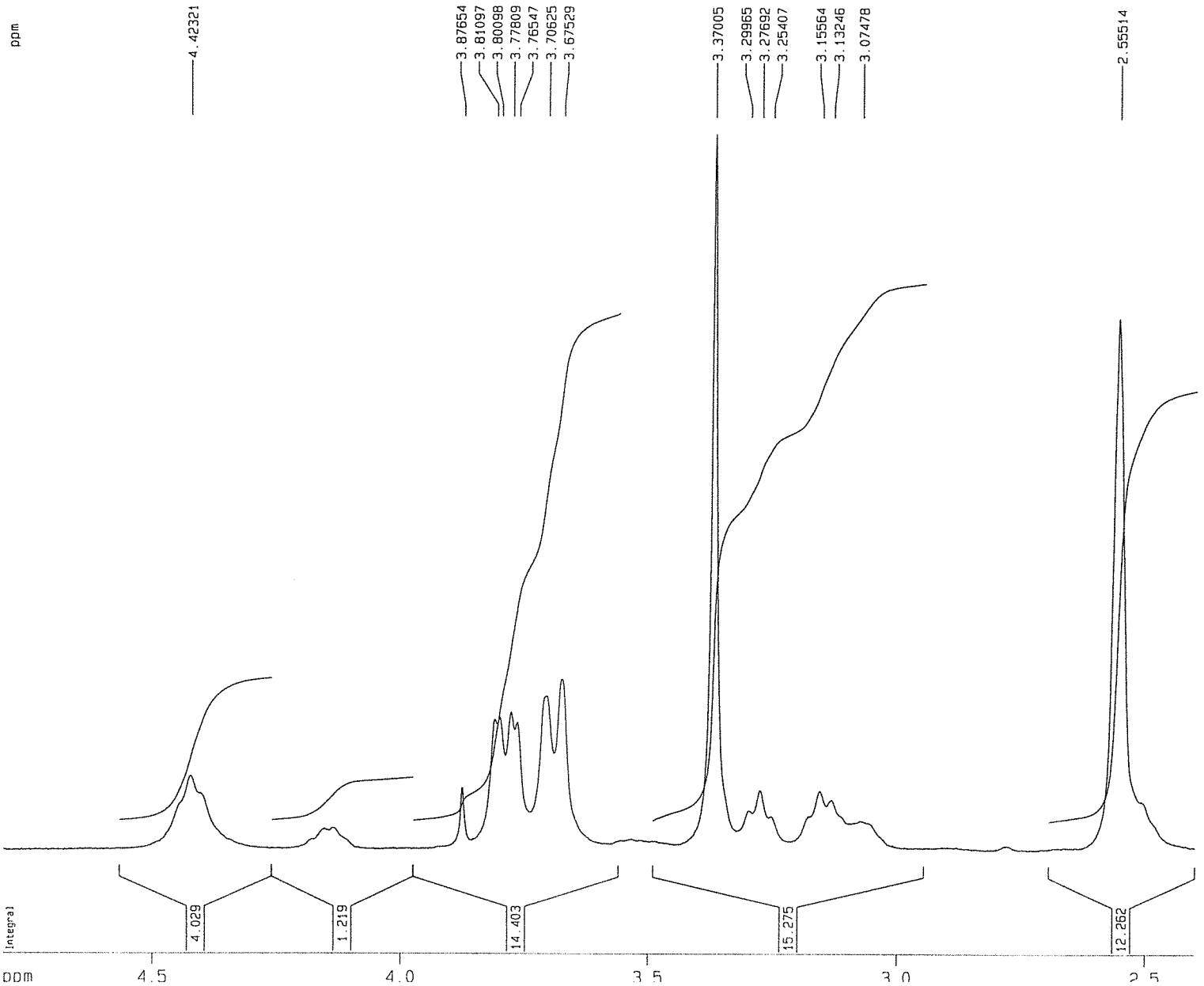
NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1299835 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	11.98 cm
F1P	12.500 ppm
F1	3751.62 Hz
F2P	6.000 ppm
F2	1800.78 Hz
PPMCM	0.32500 ppm/cm
HZCM	97.54224 Hz/cm



Current Data Parameters

NAME	BCMY-03-75monoLysmonoH
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20071019
Time	15.12
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	322.5
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

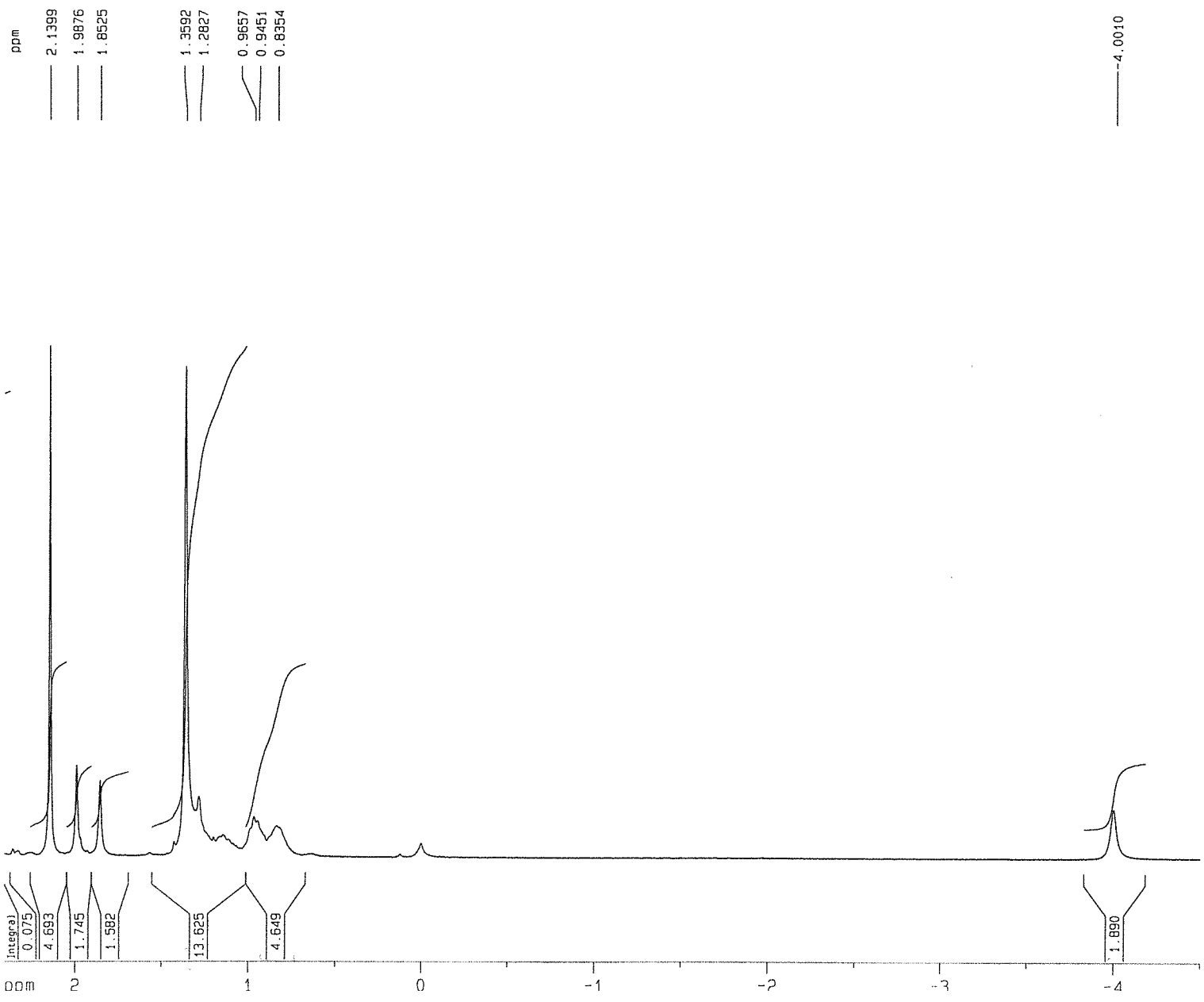
NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1299835 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	11.98 cm
F1P	4.800 ppm
F1	1440.62 Hz
F2P	2.400 ppm
F2	720.31 Hz
PPMCM	0.12000 ppm/cm
HZCM	36.01560 Hz/cm



Current Data Parameters

NAME	BCMY-03-75monoLysmonoH
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20071019
Time	15.12
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	322.5
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1299835 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	11.98 cm
F1P	2.400 ppm
F1	720.31 Hz
F2P	-4.500 ppm
F2	-1350.58 Hz
PPMCM	0.34500 ppm/cm
HZCM	103.54485 Hz/cm

135/136

Chemical Formula: $C_{43}H_{52}N_{10}O_6$
Exact Mass: 804.40713
Molecular Weight: 804.93638
m/z: 804.40713 (100.0%), 805.41048 (46.5%), 806.41384 (10.6%), 805.40416 (3.7%), 806.40752 (1.7%), 807.41719 (1.6%), 806.41138 (1.2%)
Elemental Analysis: C, 64.16; H, 6.51; N, 17.40; O, 11.93

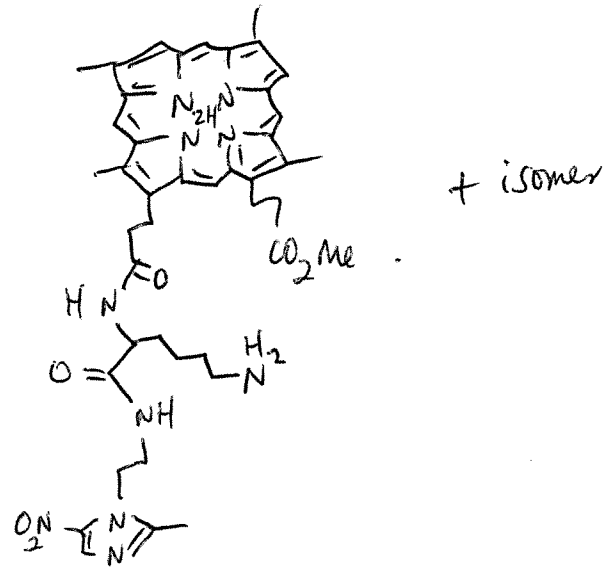
D:\Crossley\By-04-25
MeOH:DCM

02/14/08 01:43:00 PM

DPIX – mono Lys(H) – Met amine mono Me

By-04-25 #32-40 RT: 0.84-1.07 AV: 9 NL: 1.36E8
F: + p Full ms [150.00-2000.00]

13a /13b



+ isomer

Relative Abundance

m/z

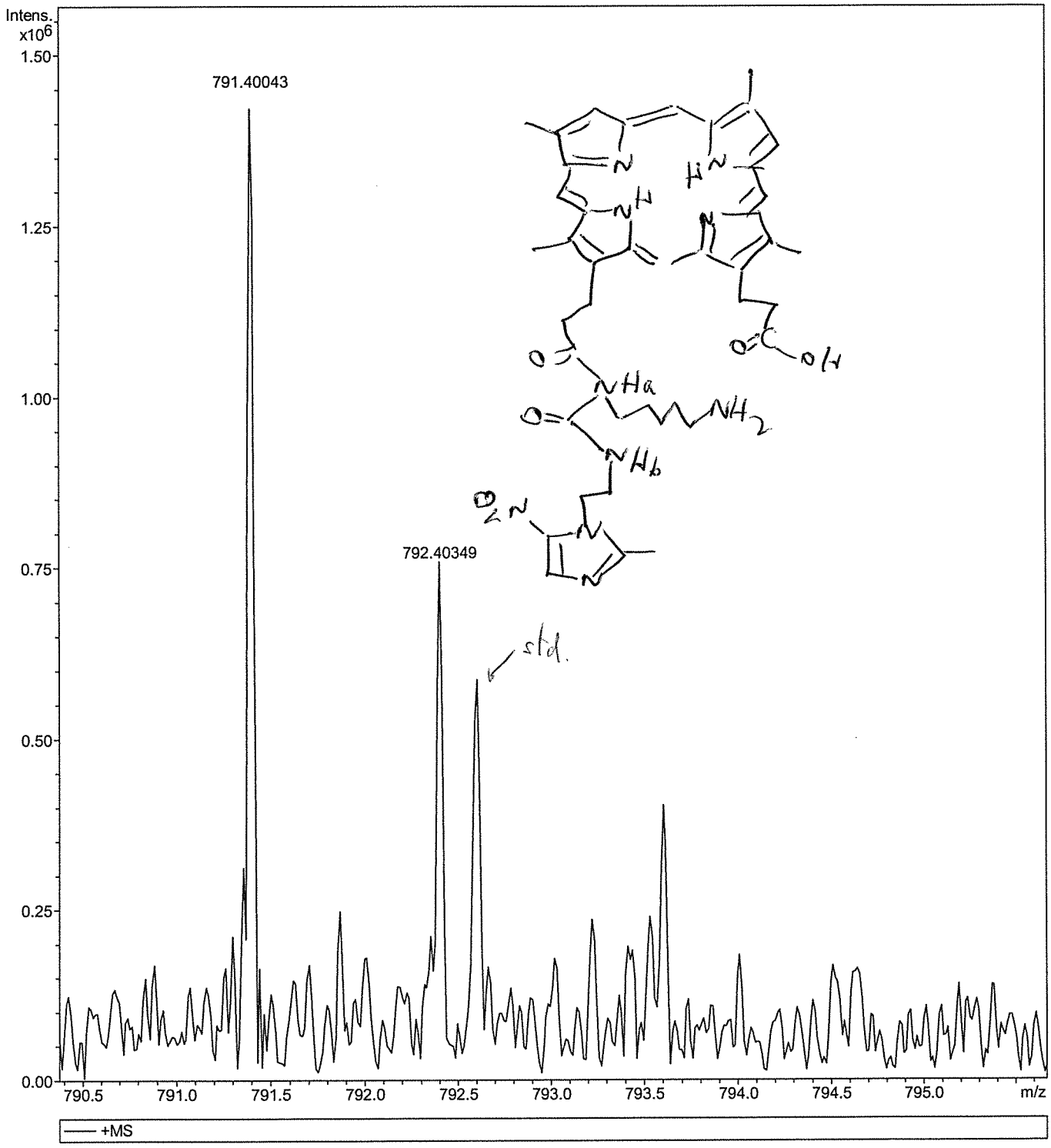
805.47
806.47
857.40
858.47
677.40
804.47
678.47
875.47
403.13
876.40
465.33
788.40
524.20
928.40
331.13
393.20
542.07
699.27
997.47
1089.53
1309.27
1312.67
1313.60
1424.60
1591.67
1630.93
1849.60
1906.20

14a / 145

Generic Display Report

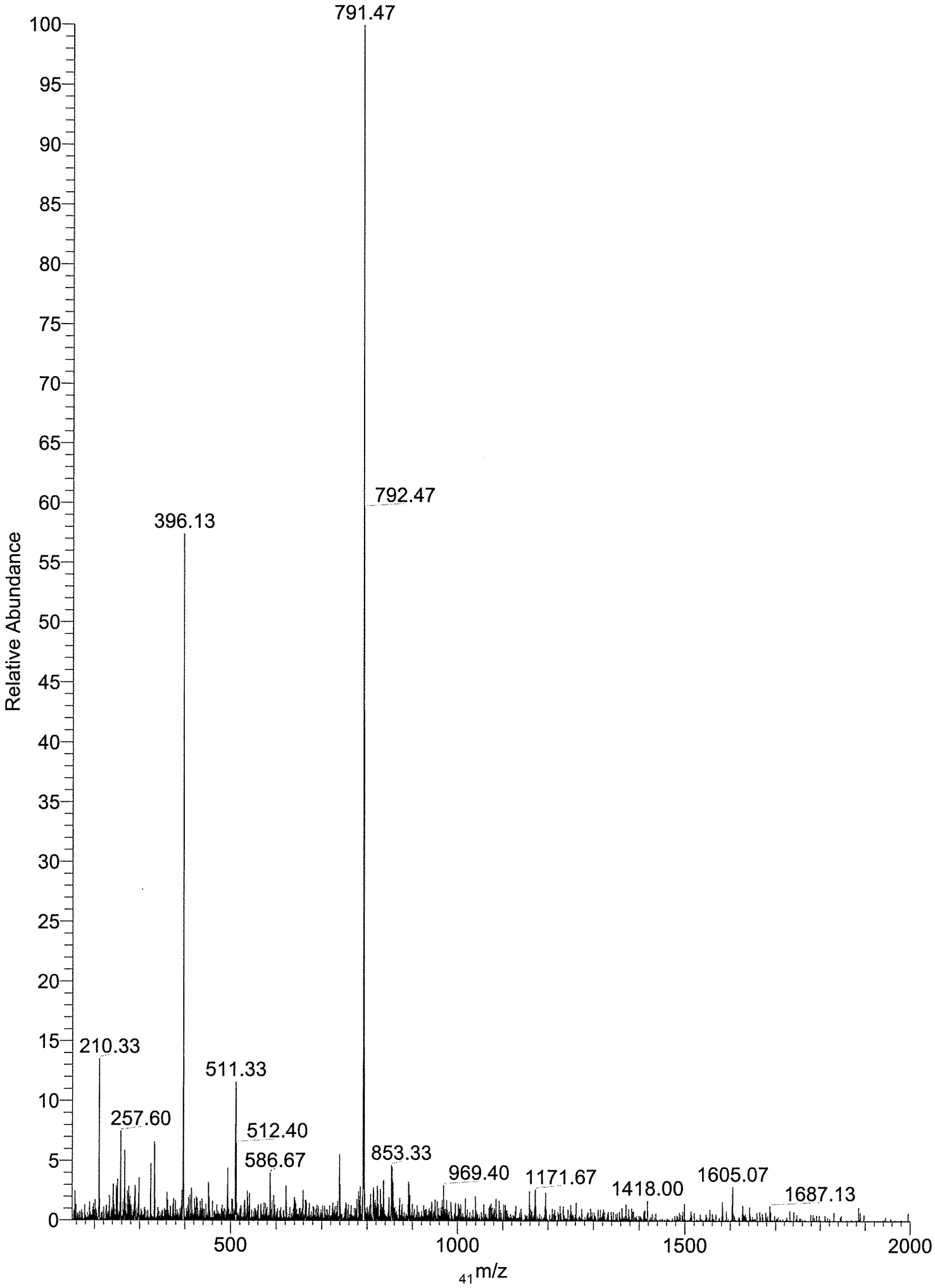
Analysis Info

Analysis Name	D:\Data\K220808-ESI\KF_000012.d	Acquisition Date	8/22/2008 10:30:52 AM
Method	1MW Positive ESI	Operator	Administrator
Sample Name	BY-04-79-5	Instrument	apex-Qe
Comment	RB5-3		

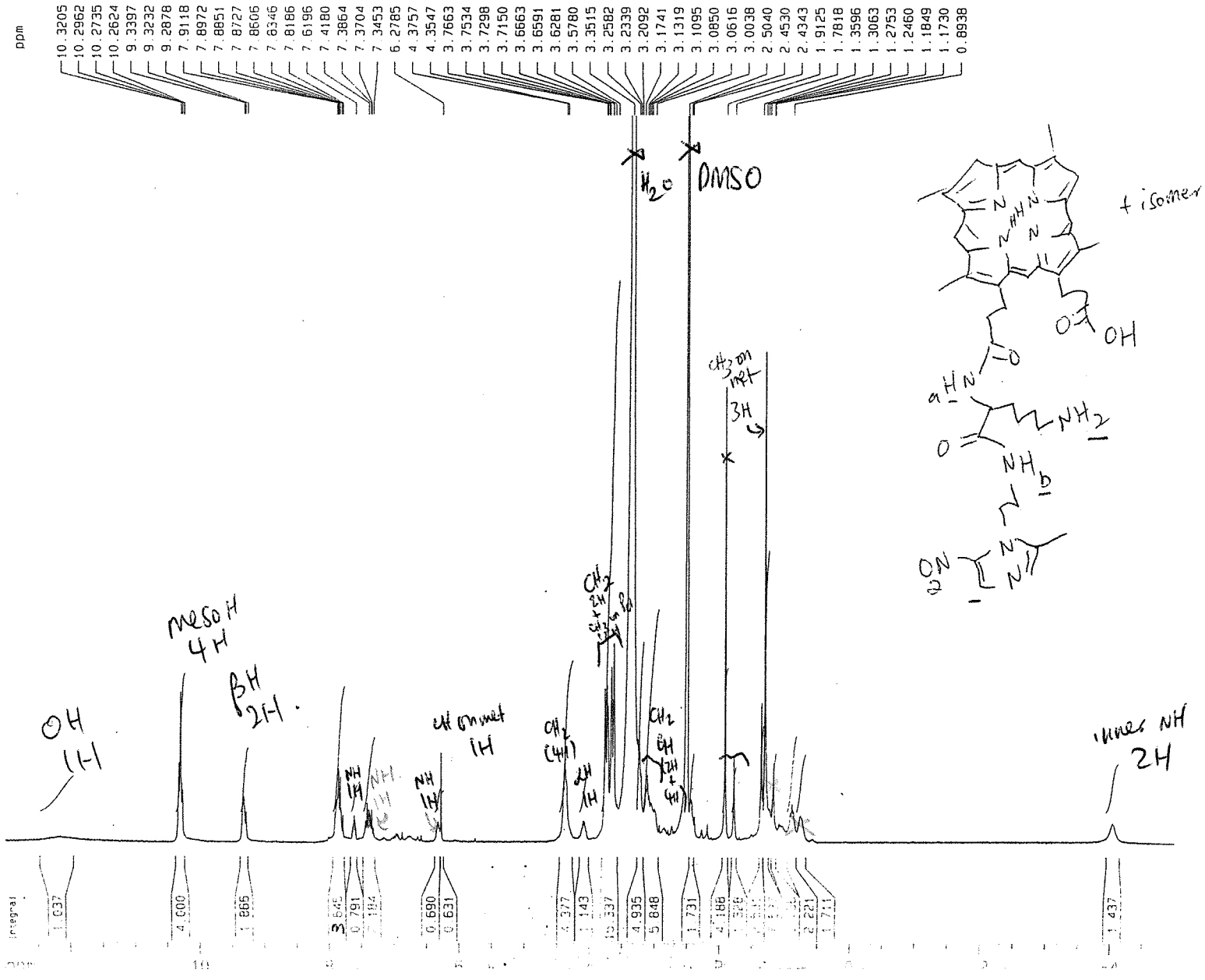


C:\Data\Grace\13_080513135032 13/05/2008 1:50:32 PM BY-04-79-5
meoh (not diluted)

13_080513135032 #2-7 RT: 0.05-0.21 AV: 6 NL: 1.17E6
T: + p ESI Full ms [150.00-2000.00]



PROTON



Current Data Parameters

NAME	BY-04-79
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	18.03
INSTRUM	spect
PROBHD	5 mm PHONP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	128
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	256
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

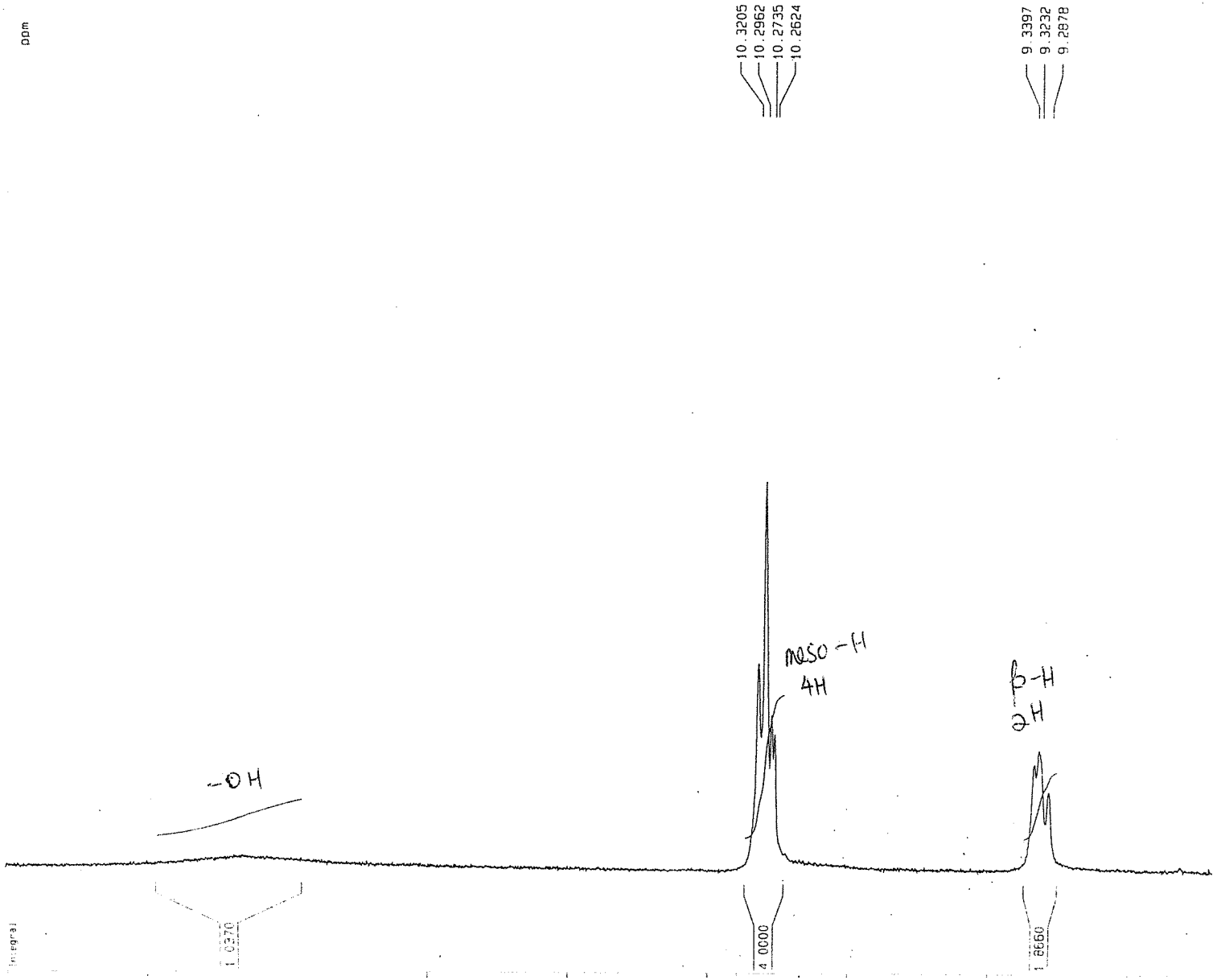
F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	120.00 cm
F1P	13.000 ppm
F1	3901.69 Hz
F2P	-5.000 ppm
F2	-1500.65 Hz
PPMCM	0.90000 ppm/cm
HZCM	270.11700 Hz/cm

PROTON



Current Data Parameters

NAME	BY-04-79
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	18.03
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	128
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	256
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

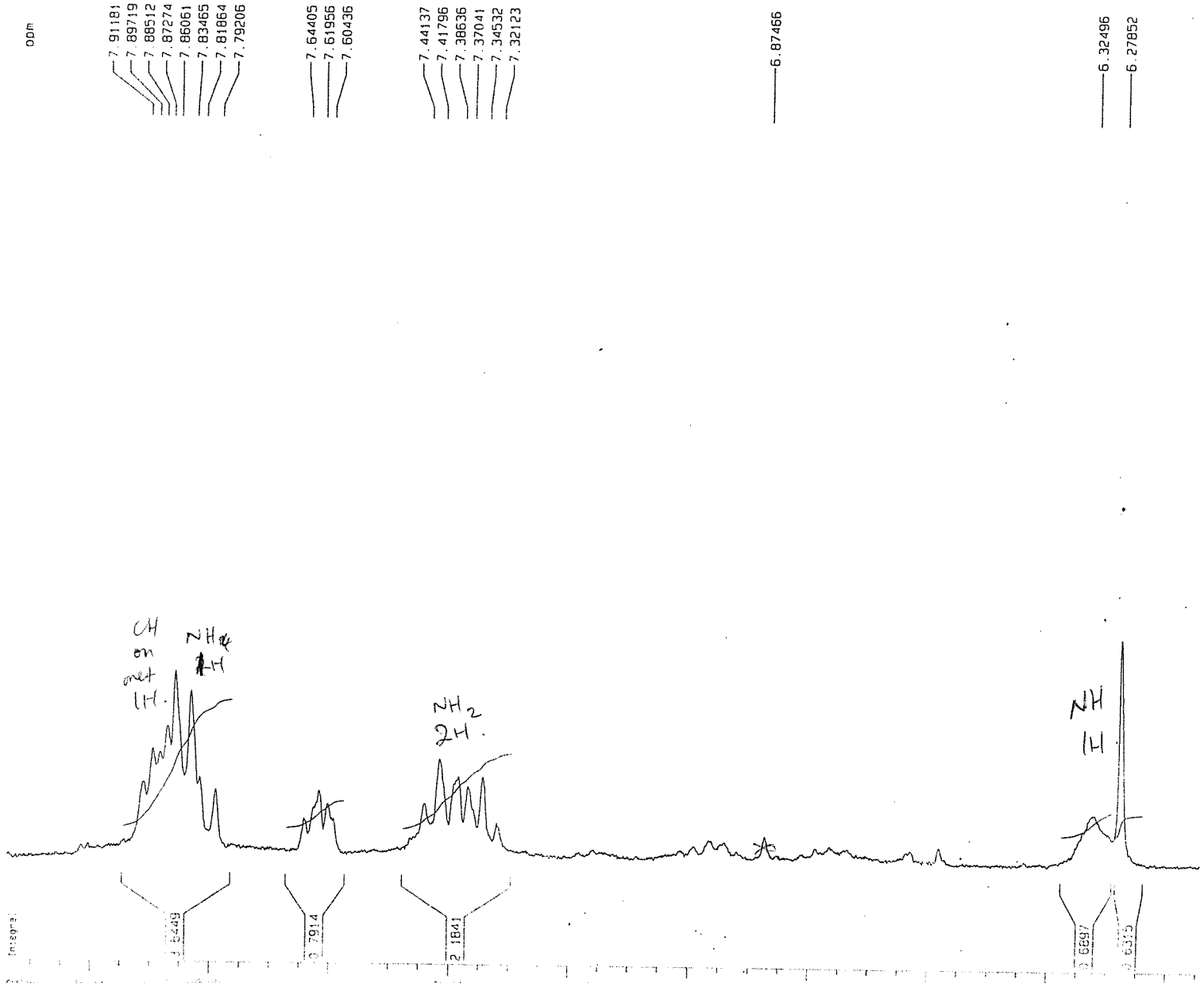
F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	300.00 cm
F1P	13.006 ppm
F1	3903.54 Hz
F2P	8.703 ppm
F2	2611.99 Hz
PPMCM	0.21517 ppm/cm
HZCM	64.57760 Hz/cm

PROTON



Current Data Parameters

NAME	BY-04-79
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	18.03
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	128
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	256
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

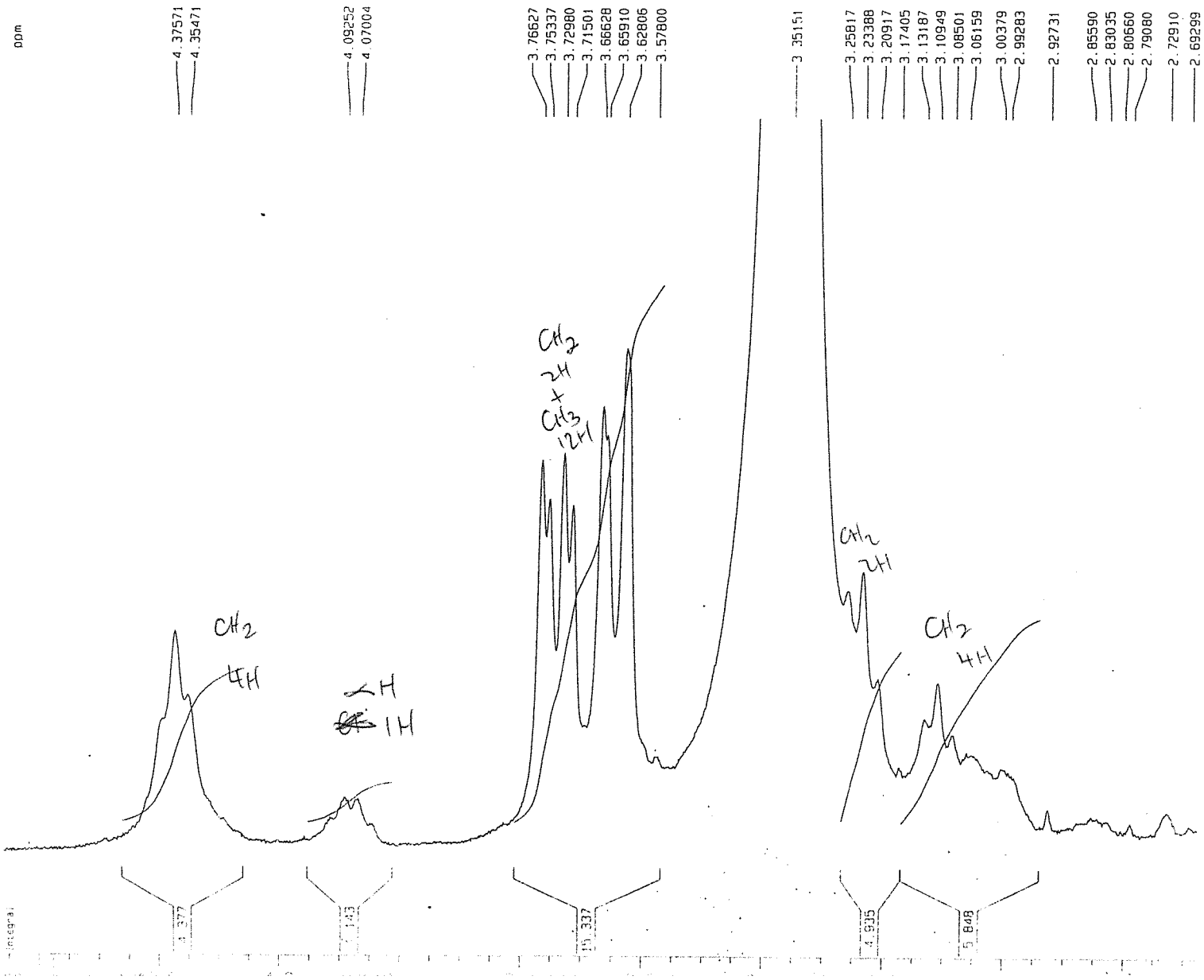
F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	300.00 cm
F1P	8.141 ppm
F1	2443.41 Hz
F2P	6.146 ppm
F2	1844.59 Hz
PPMCM	0.09976 ppm/cm
HZCM	29.94099 Hz/cm

PROTON



Current Data Parameters

NAME	BY-04-79
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	18.03
INSTRUM	spect
PROBHD	5 mm PHONP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	128
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	256
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

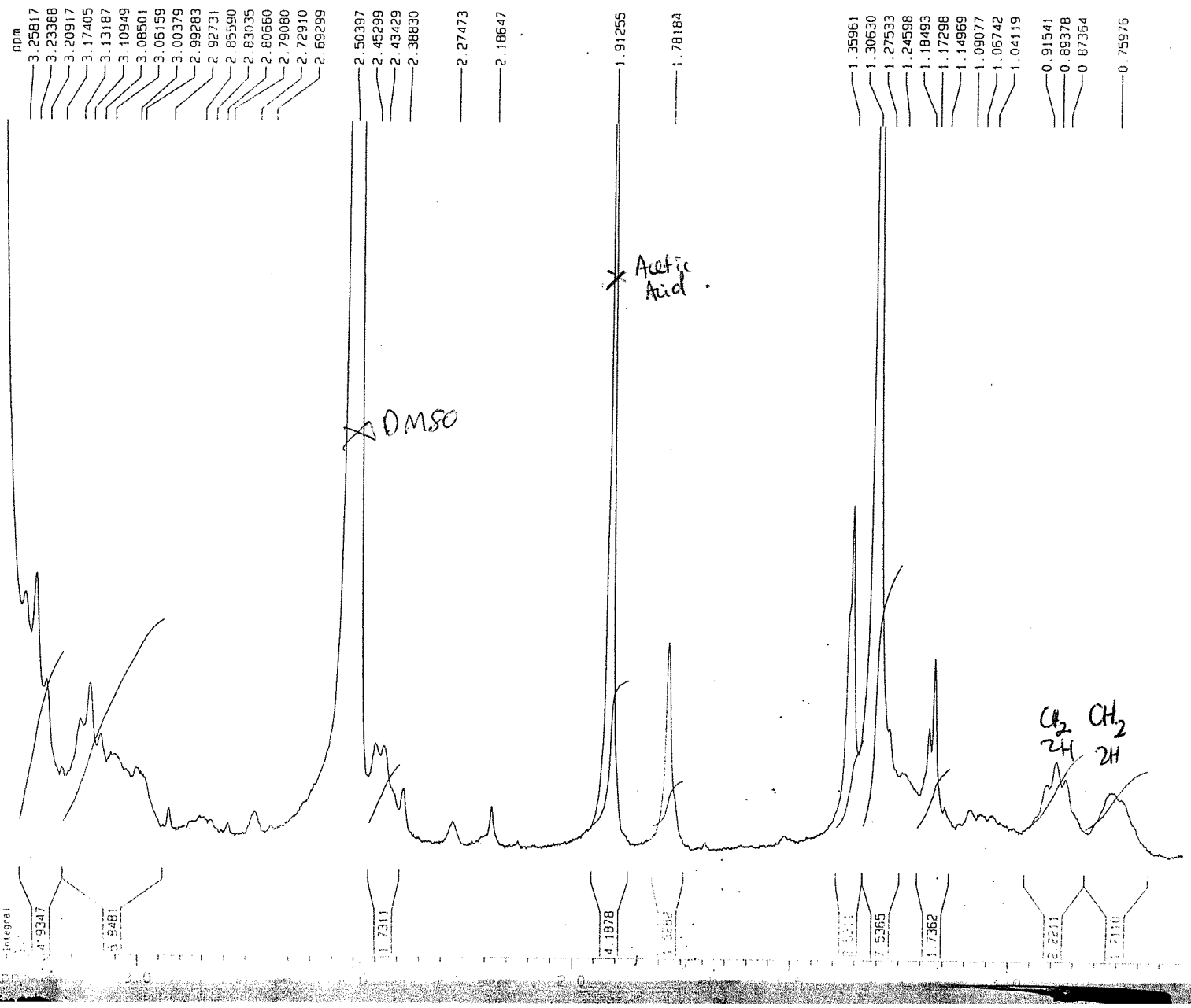
F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	300.00 cm
F1P	4.660 ppm
F1	1398.53 Hz
F2P	2.678 ppm
F2	803.81 Hz
PPMCM	0.09908 ppm/cm
HZCM	29.73573 Hz/cm

PROTON



Current Data Parameters

NAME	BY-04-79
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	18:03
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	128
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	256
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

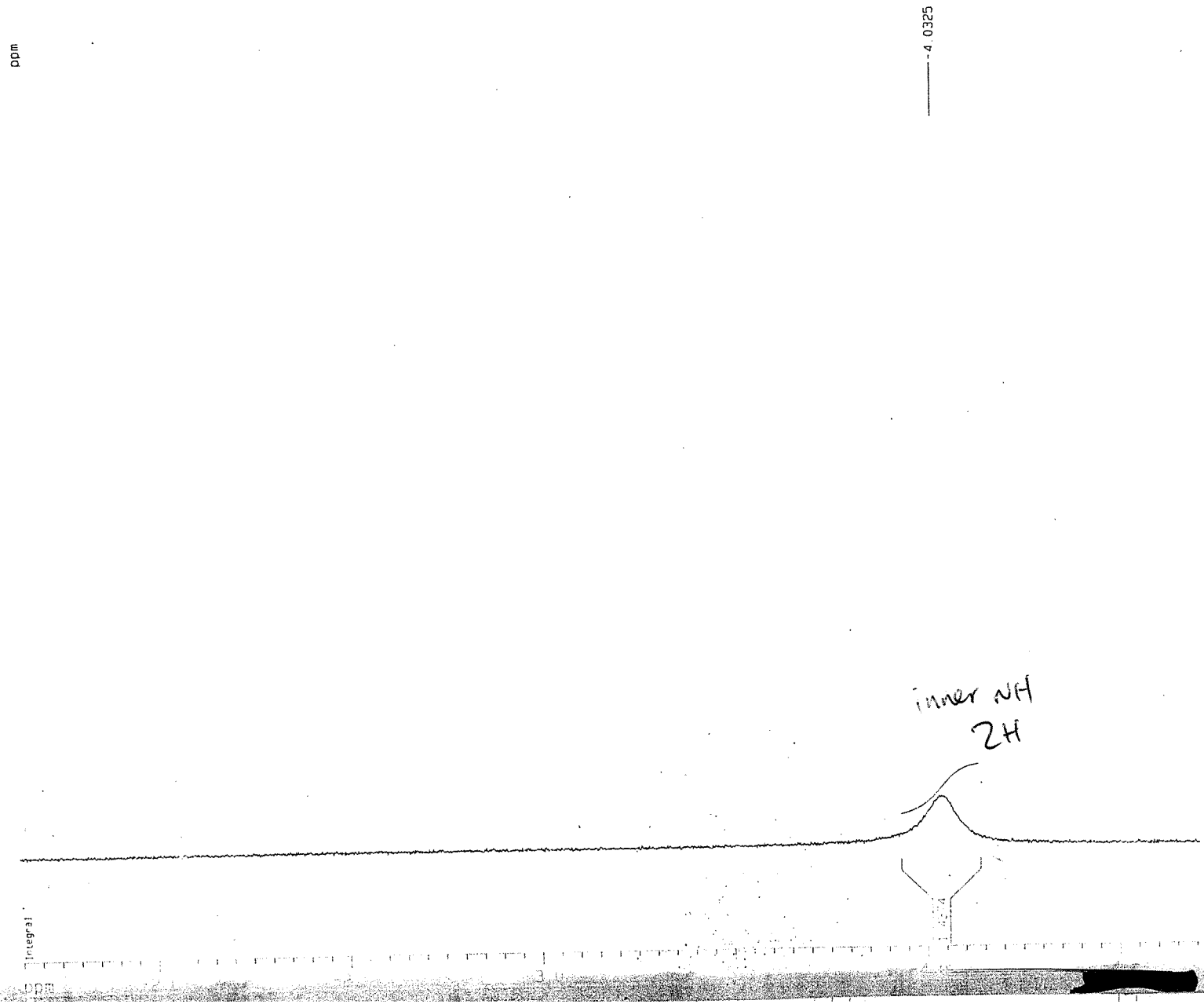
F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	300.00 cm
F1P	3.314 ppm
F1	994.77 Hz
F2P	0.601 ppm
F2	180.27 Hz
PPMCM	0.13569 ppm/cm
HZCM	40.72478 Hz/cm

PROTON



Current Data Parameters

NAME	BY-04-79
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	18.03
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	128
DS	0
SWH	5995.204 Hz
FIDRES	0.182960 Hz
AQ	2.7329011 sec
RG	256
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

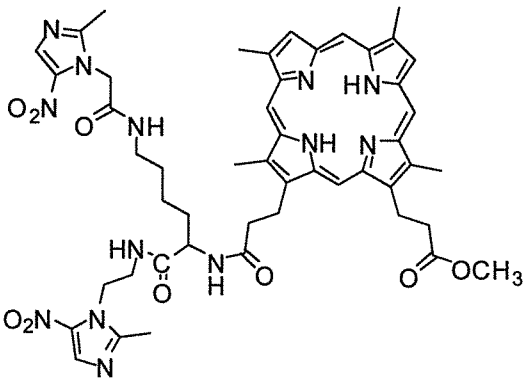
NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	300.00 cm
F1P	-1.645 ppm
F1	-493.75 Hz
F2P	-4.707 ppm
F2	-1412.85 Hz
PPMCM	0.15312 ppm/cm
HZCM	45.95522 Hz/cm



DPIX mono Lys(met acid) mono Me

Chemical Formula: $C_{49}H_{57}N_{13}O_9$

Molecular Weight: 972.05858

^{1}H NMR:

^{13}C NMR:

MS:

Hi Res MS:

UV:

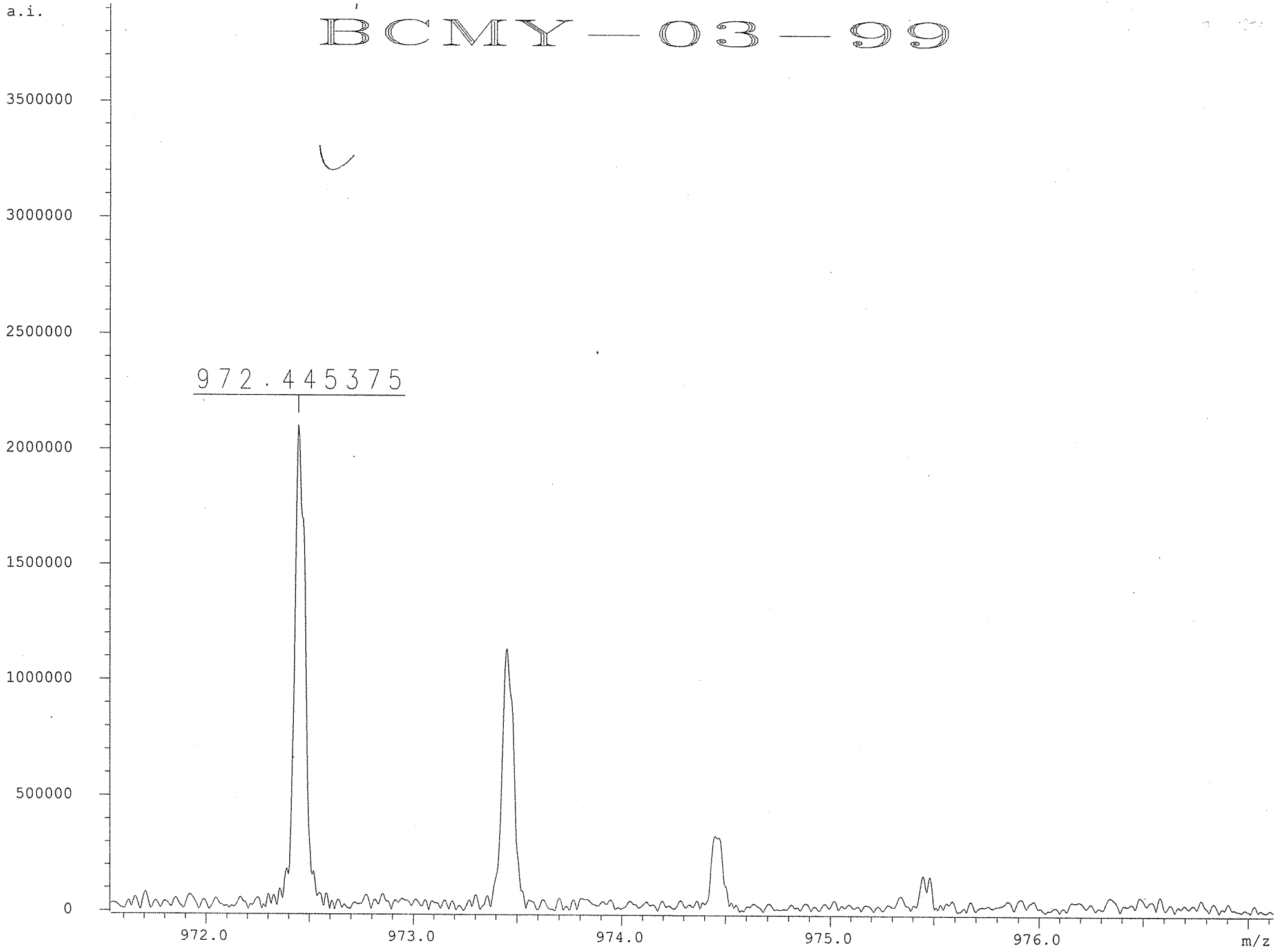
IR:

mp:

Yield:

Experimental:

BCMY—03—99


a.i.
3500000
3000000
2500000
2000000
1500000
1000000
500000
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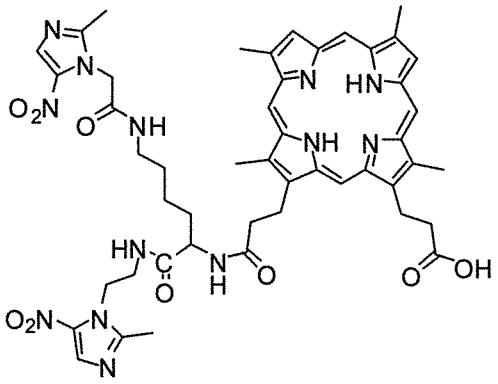
972.445375
972.0
973.0
974.0
975.0
976.0
m/z

17a / 17b



DPIX mono Lys(met acid) mono H

Chemical Formula: $C_{48}H_{55}N_{13}O_9$
Molecular Weight: 958.03200

✓ ^{1}H NMR:

^{13}C NMR:

✓ MS:

✓ Hi Res MS:

UV:

IR:

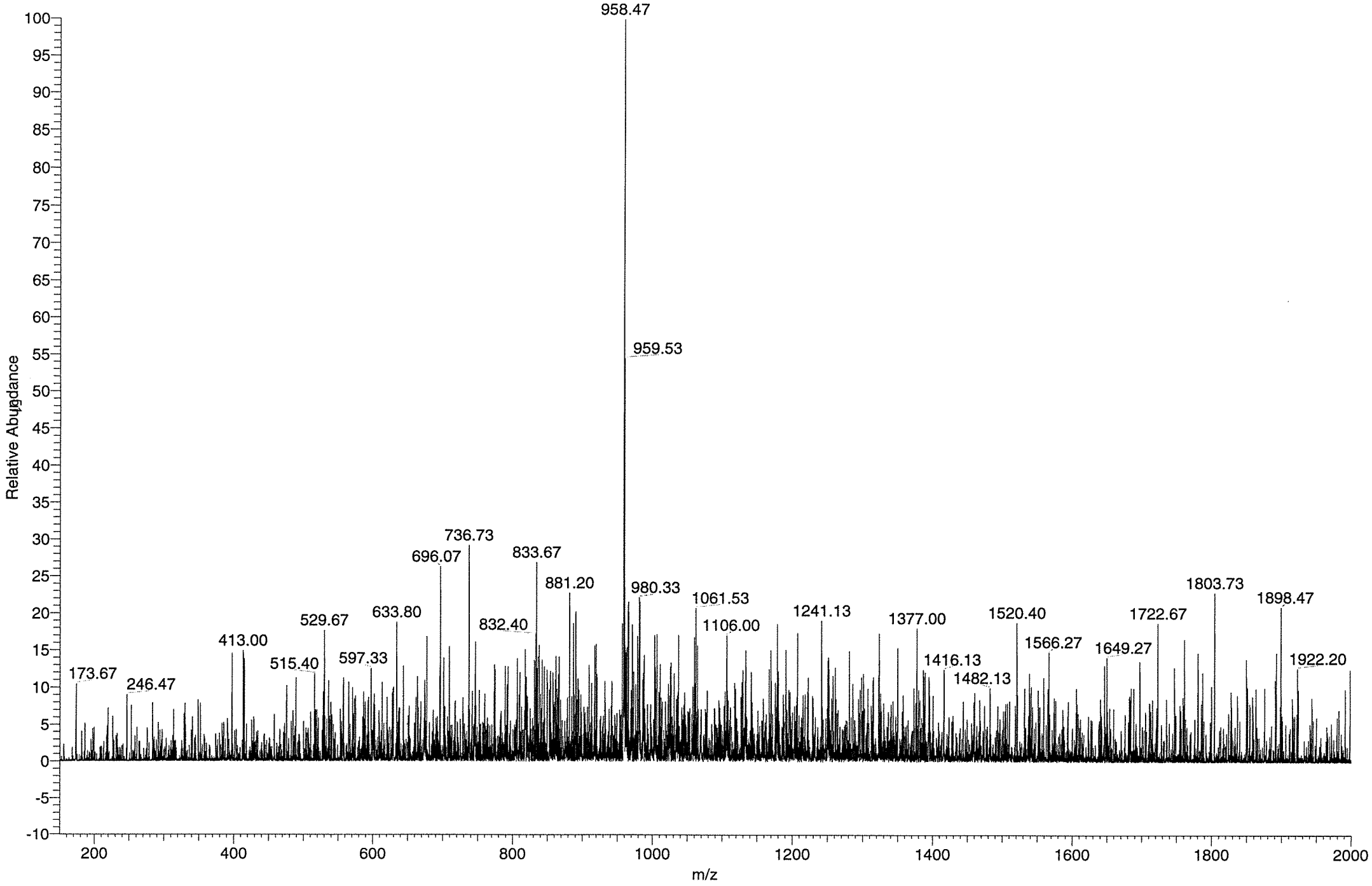
mp:

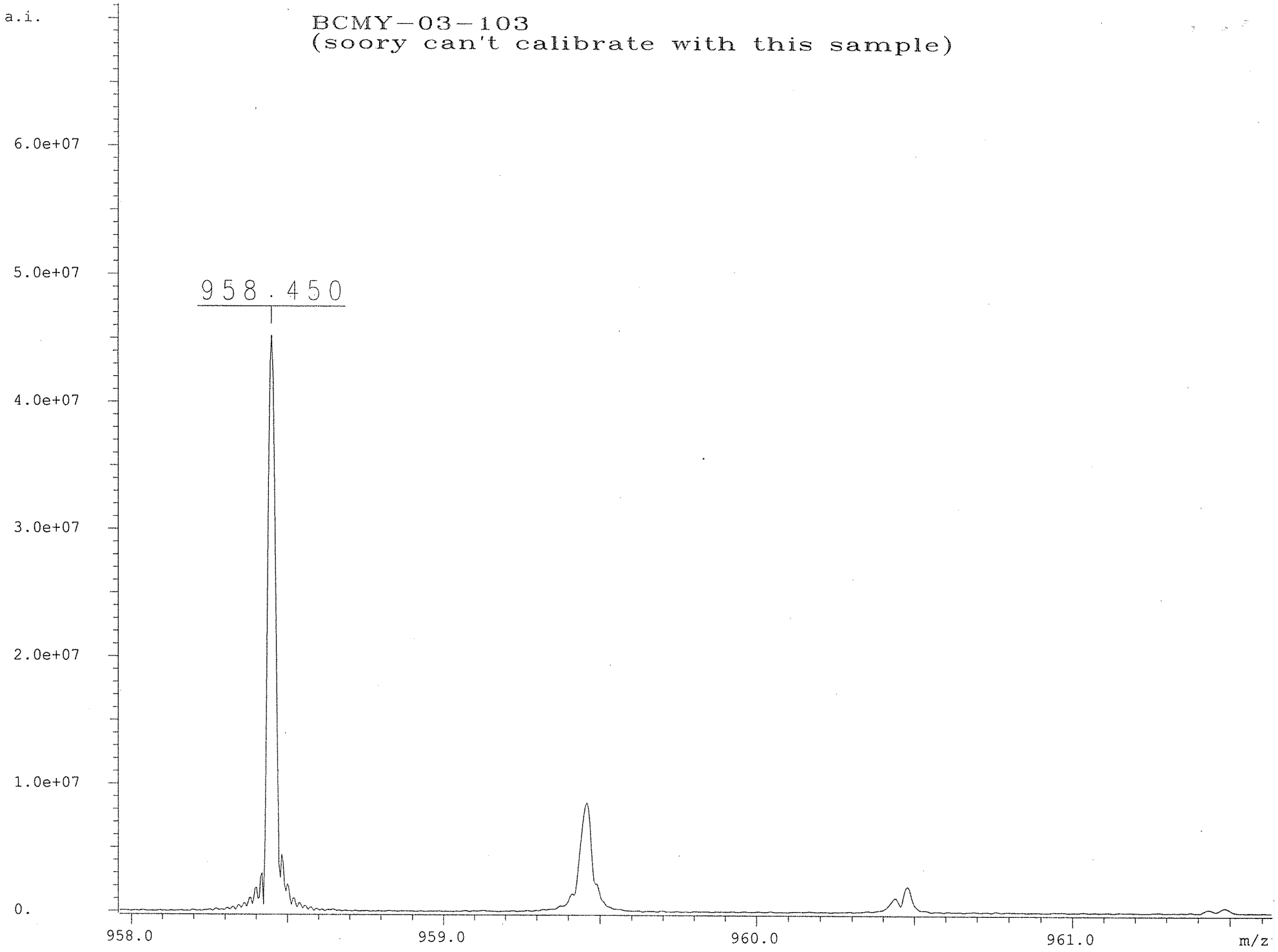
Yield:

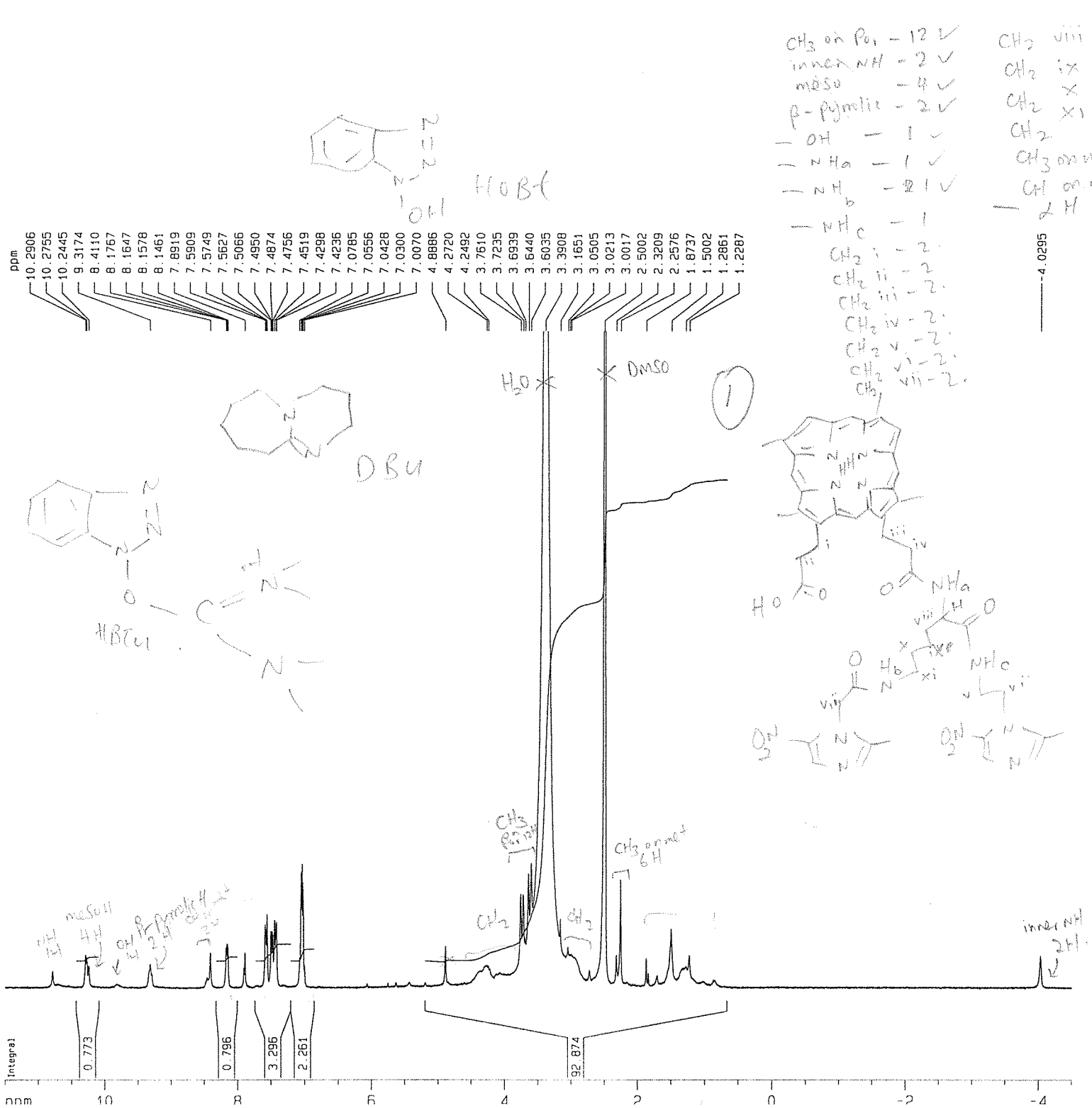
Experimental:

D:\Crossley\Bcmy-03-103 22/11/07 13:14:20
MeOH

BCMY-03-103 #27-28 RT: 0.72-0.75 AV: 2 NL: 8.97E6
T: + p Full ms [150.00-2000.00]




a.i.
BCMY-03-103
(soory can't calibrate with this sample)
958.450
6.0e+07
5.0e+07
4.0e+07
3.0e+07
2.0e+07
1.0e+07
0.
958.0
959.0
960.0
961.0
m/z



Current Data Parameters

NAME	BCMY-03-103
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20071123
Time	11.26
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	64
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	362
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

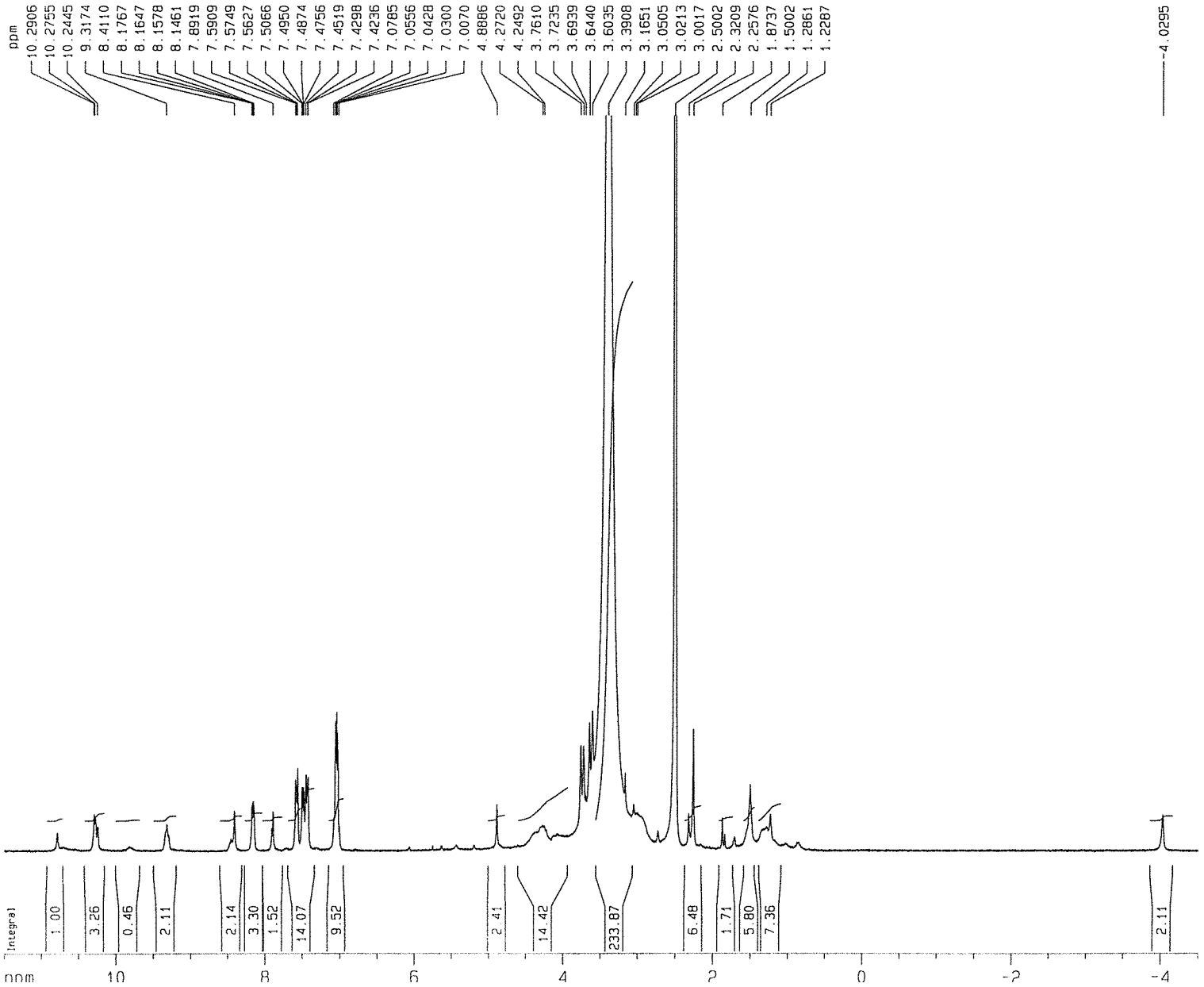
NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	30.00 cm
F1P	11.500 ppm
F1	3451.50 Hz
F2P	-4.500 ppm
F2	-1350.58 Hz
PPMCM	0.80000 ppm/cm
HZCM	240.10400 Hz/cm



Current Data Parameters

NAME	BCMY-03-103
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20071123
Time	11.26
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	64
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	362
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

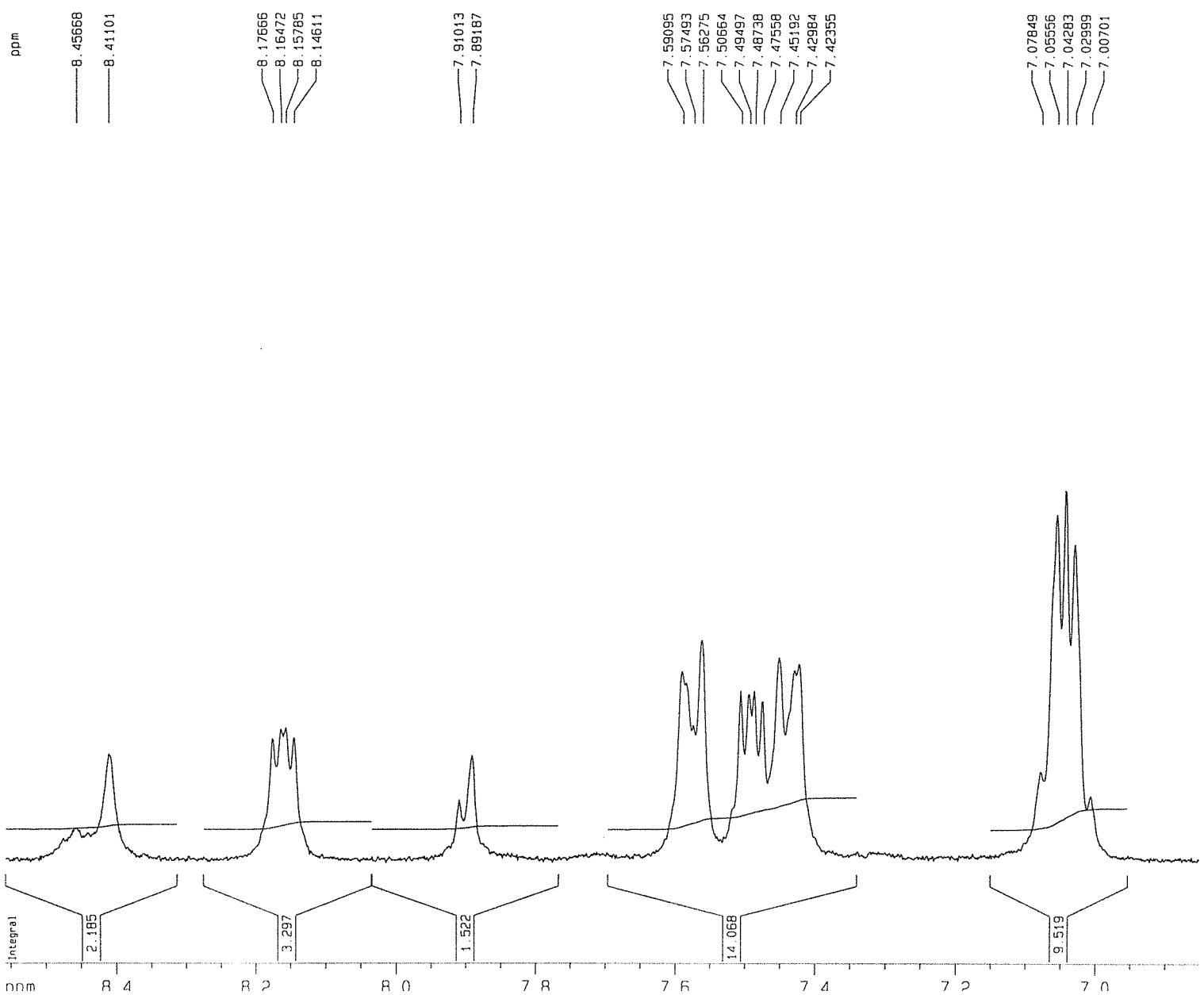
F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	30.00 cm
F1P	11.500 ppm
F1	3451.50 Hz
F2P	-4.500 ppm
F2	-1350.58 Hz
PPMCM	0.80000 ppm/cm
HZCM	240.10400 Hz/cm

Current Data Parameters
NAME BCMY-03-103
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071123
Time 11.26
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 362
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1315007 MHz
F2 - Processing parameters
SI 16384
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 80.00 cm
F1P 8.558 ppm
F1 2568.59 Hz
F2P 6.851 ppm
F2 2056.25 Hz
PPMCM 0.08535 ppm/cm
HZCM 25.61711 Hz/cm
9.3174
9.2974
10.2906
10.2755
10.2445
10.7847
ppm
Integral
0.9995
3.2625
0.4586
2.1145



Current Data Parameters

NAME	BCMY-03-103
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20071123
Time	11.26
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	64
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	362
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

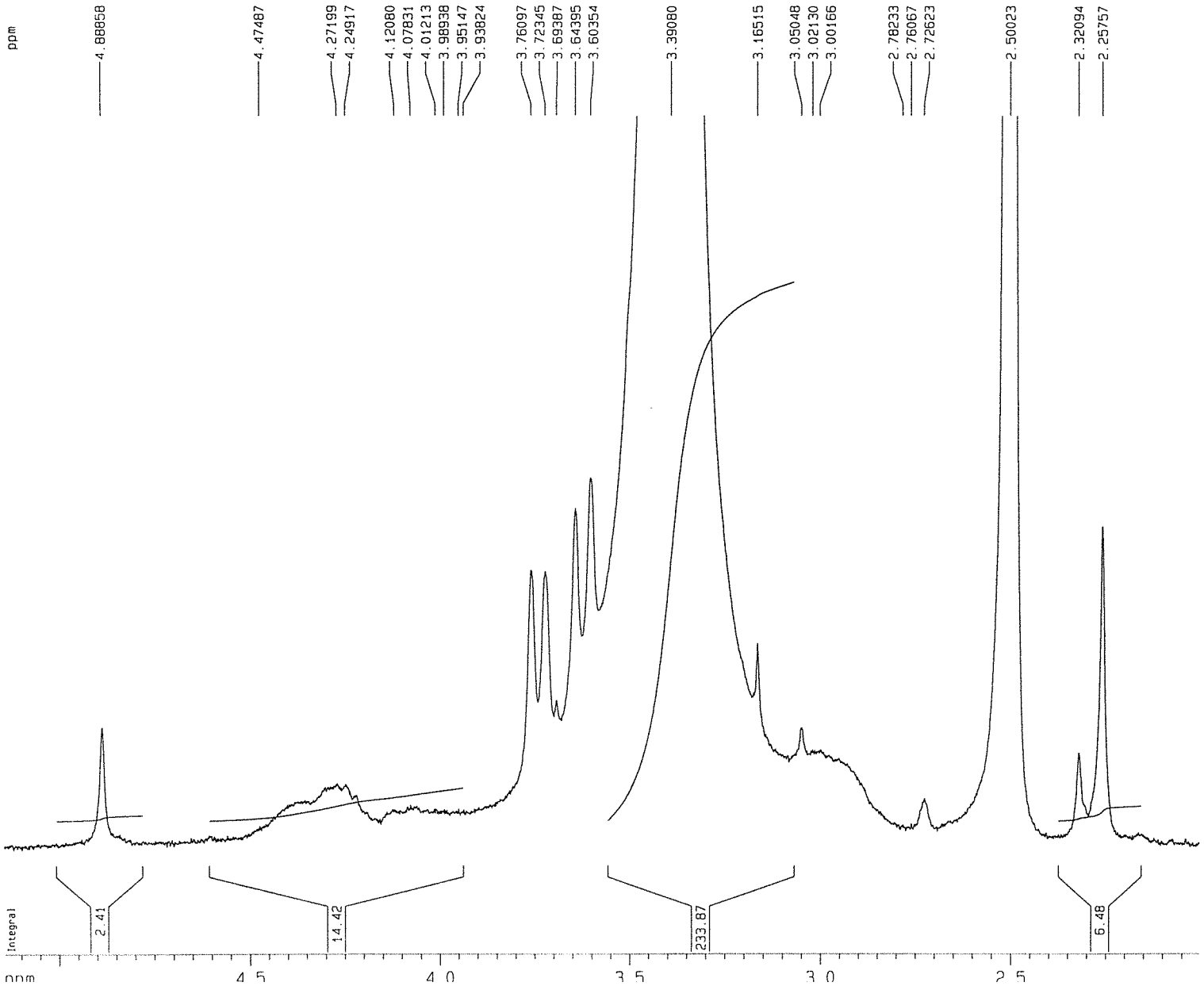
NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	80.00 cm
F1P	5.145 ppm
F1	1544.21 Hz
F2P	2.005 ppm
F2	601.77 Hz
PPMCM	0.15701 ppm/cm
HZCM	47.12214 Hz/cm



Current Data Parameters

NAME	BCMY-03-103
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20071123
Time	11.26
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	64
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	362
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

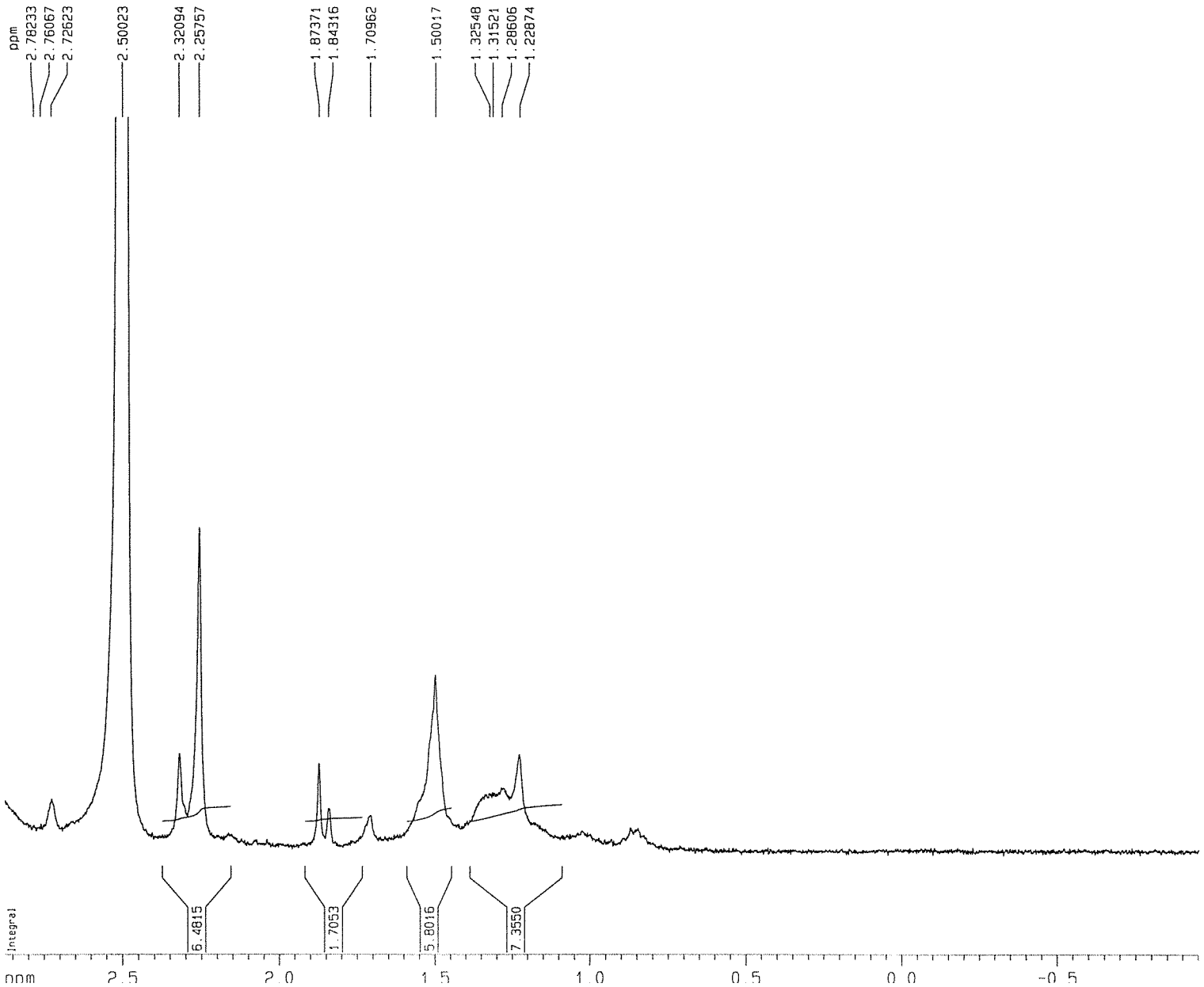
NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	80.00 cm
F1P	5.145 ppm
F1	1544.21 Hz
F2P	2.005 ppm
F2	601.77 Hz
PPMCM	0.15701 ppm/cm
HZCM	47.12214 Hz/cm



Current Data Parameters

NAME	BCMY-03-103
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20071123
Time	11.26
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	64
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	362
DW	83.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	5.80 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

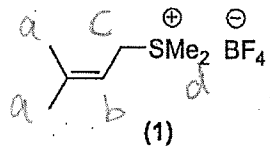
SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

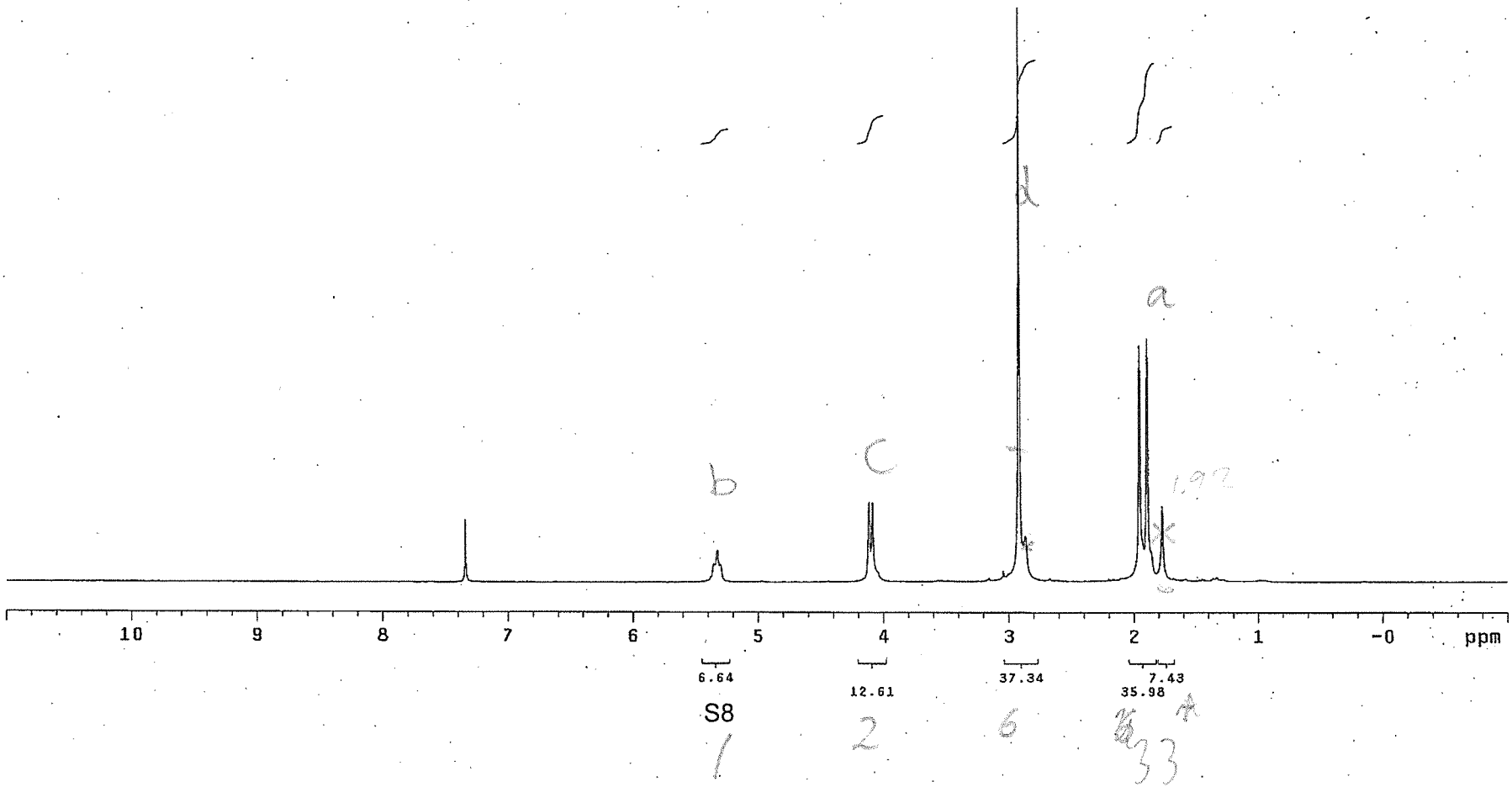
CX	20.00 cm
CY	80.00 cm
F1P	-2.402 ppm
F1	-720.82 Hz
F2P	-4.803 ppm
F2	-1441.51 Hz
PPMCM	0.12006 ppm/cm
HZCM	36.03459 Hz/cm

Current Data Parameters
NAME BCMY-03-103
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071123
Time 11.26
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 362
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1315007 MHz
F2 - Processing parameters
SI 16384
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 80.00 cm
F1P -2.402 ppm
F1 -720.82 Hz
F2P -4.803 ppm
F2 -1441.51 Hz
PPMCM 0.12006 ppm/cm
HZCM 36.03459 Hz/cm
-4.0295
2.1067
integral
ppm
-2.75
-3.00
-3.25
-3.50
-3.75
-4.00
-4.25
-4.50

26


a
c
SMe2
BF4
a
b
d

(1)


b
c
d
a
1.92
10
9
8
7
6
5
4
3
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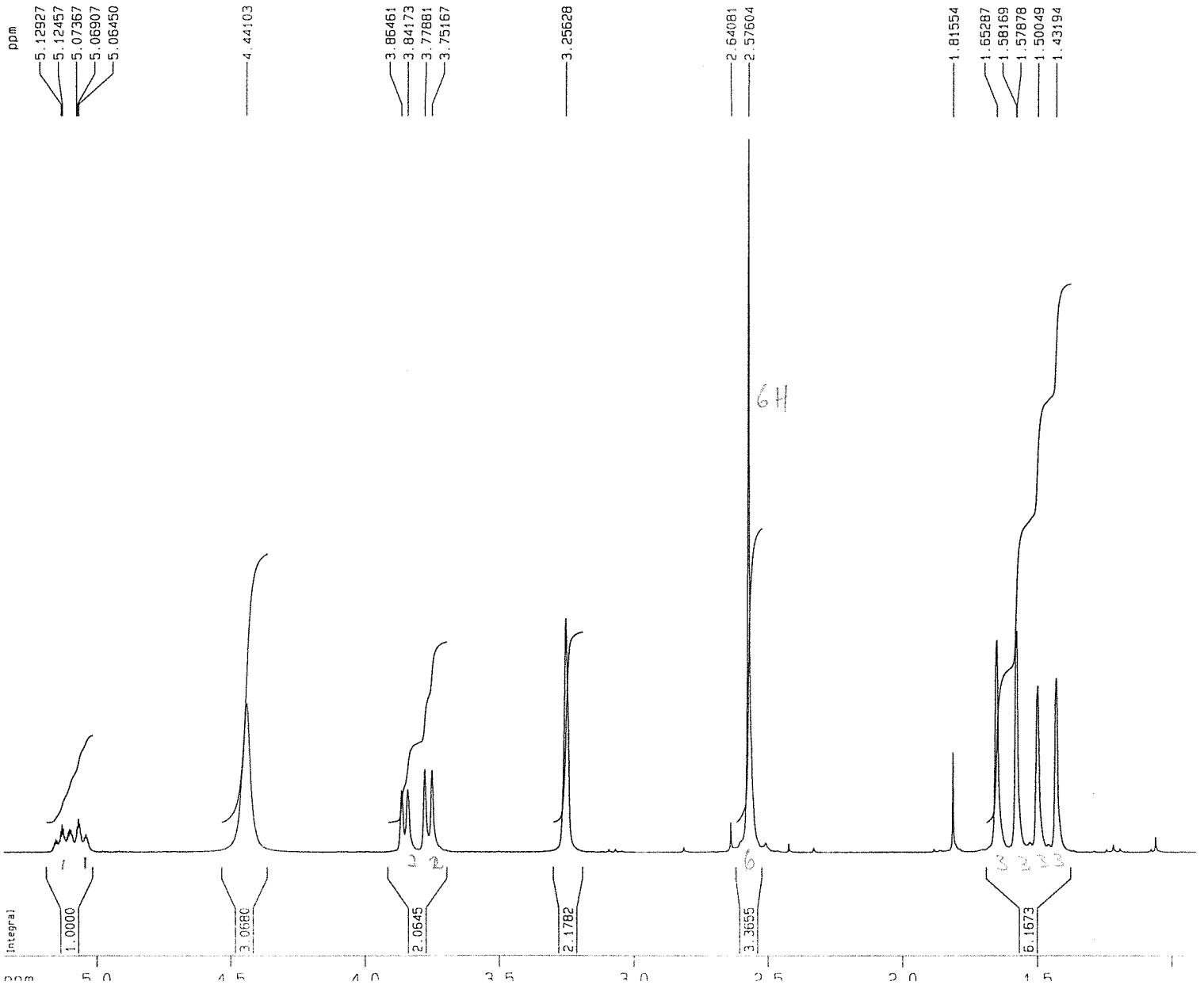
1
-0
ppm
6.64
12.61
37.34
7.43
35.98
S8
1
2
6
33



Current Data Parameters

NAME	BY-04-45
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20080331
Time	13.56
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	2997.602 Hz
FIDRES	0.091480 Hz
AQ	5.4657526 sec
RG	11.3
DW	166.800 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

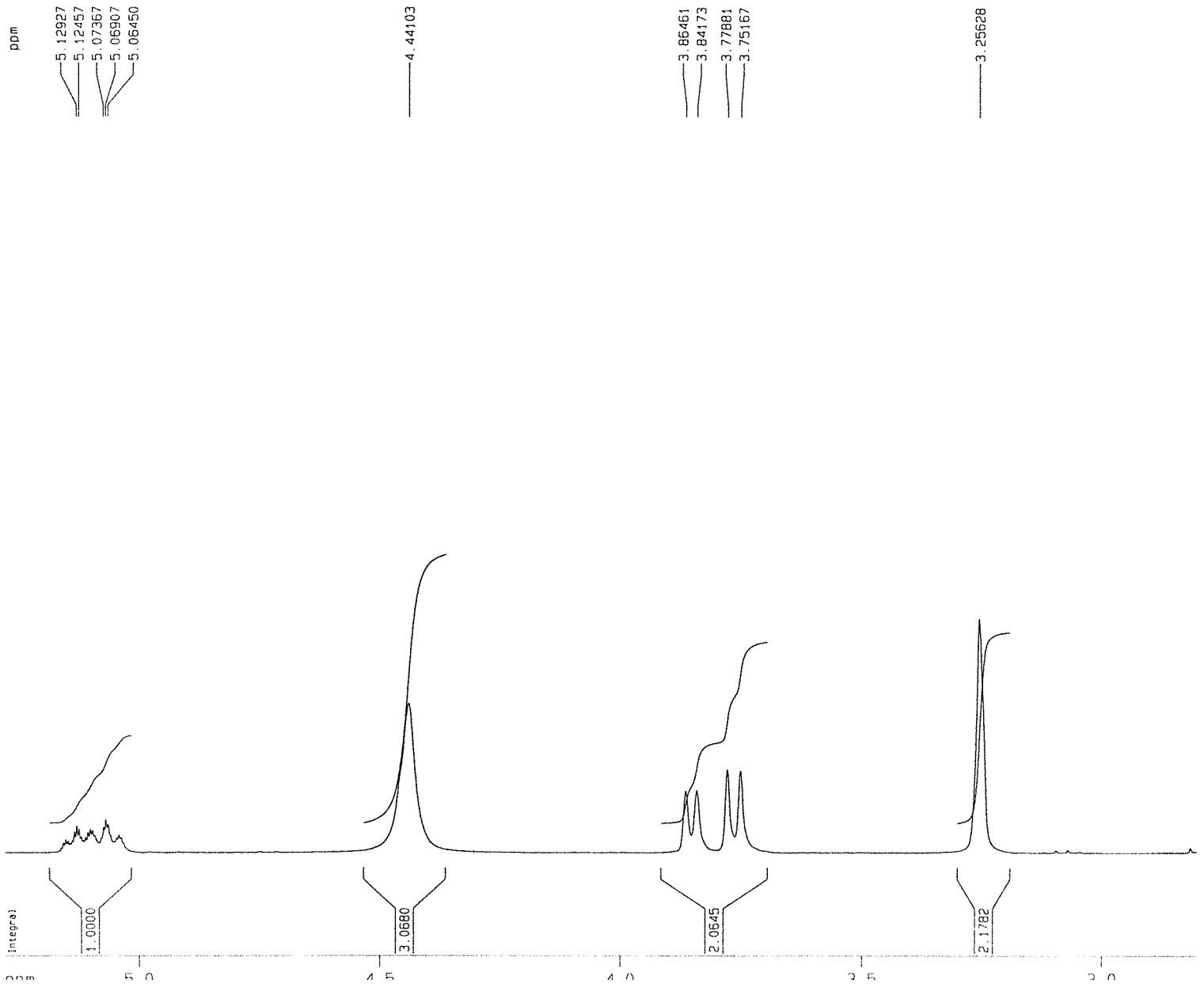
NUC1	1H
P1	10.10 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	11.98 cm
F1P	5.345 ppm
F1	1604.27 Hz
F2P	0.906 ppm
F2	272.00 Hz
PPMCM	0.22195 ppm/cm
HZCM	66.61337 Hz/cm



Current Data Parameters

NAME	BY-04-45
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20080331
Time	13.56
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	2997.602 Hz
FIDRES	0.091480 Hz
AQ	5.4657526 sec
RG	11.3
DW	166.800 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

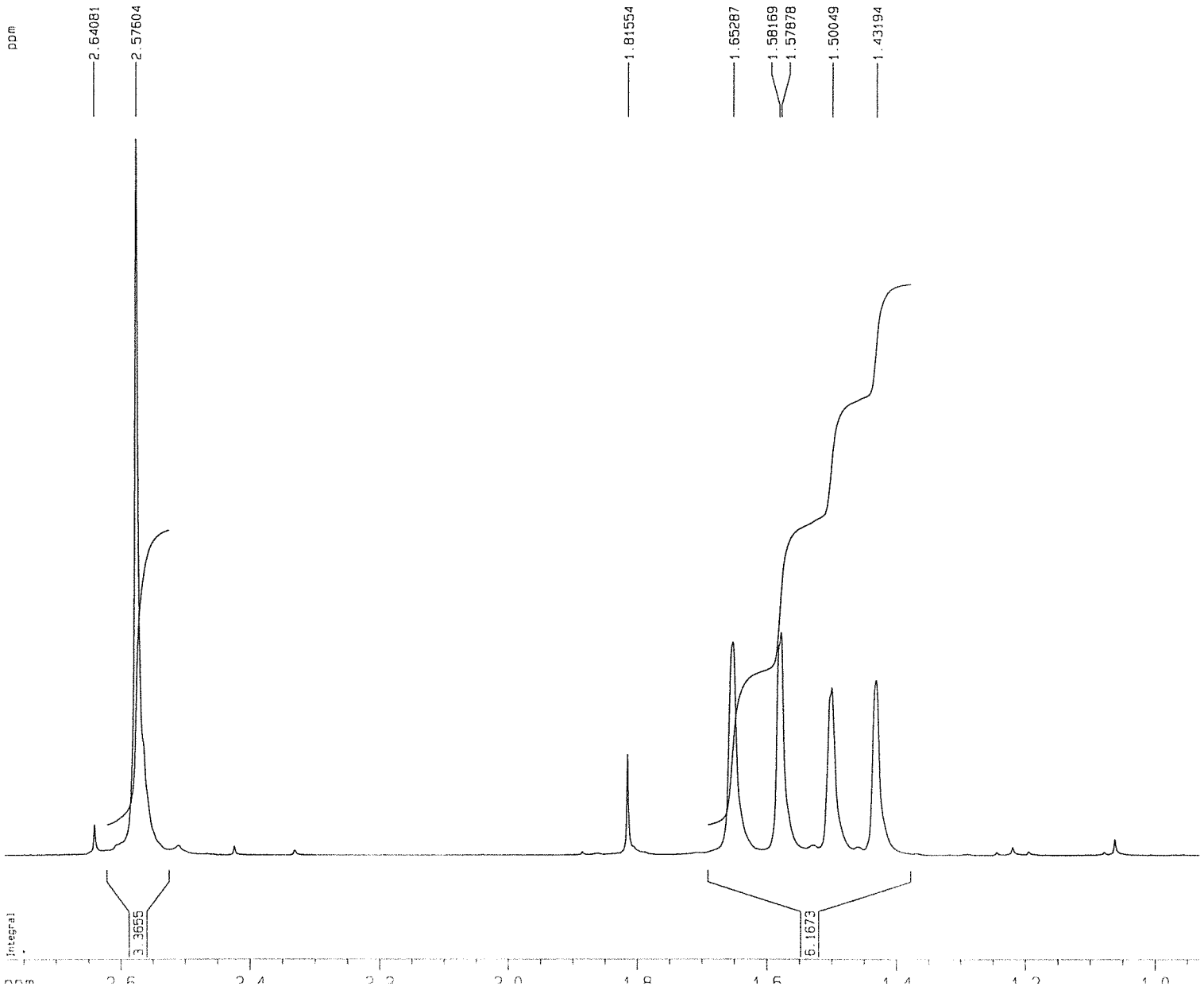
NUC1	1H
P1	10.10 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	11.98 cm
F1P	2.781 ppm
F1	834.52 Hz
F2P	0.931 ppm
F2	279.40 Hz
PPMCM	0.09248 ppm/cm
HZCM	27.75557 Hz/cm



Current Data Parameters

NAME	BY-04-45
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20080331
Time	13.56
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	2997.602 Hz
FIDRES	0.091480 Hz
AQ	5.4657526 sec
RG	11.3
DW	166.800 usec
DE	6.00 usec
TE	300.0 K
D1	1.50000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

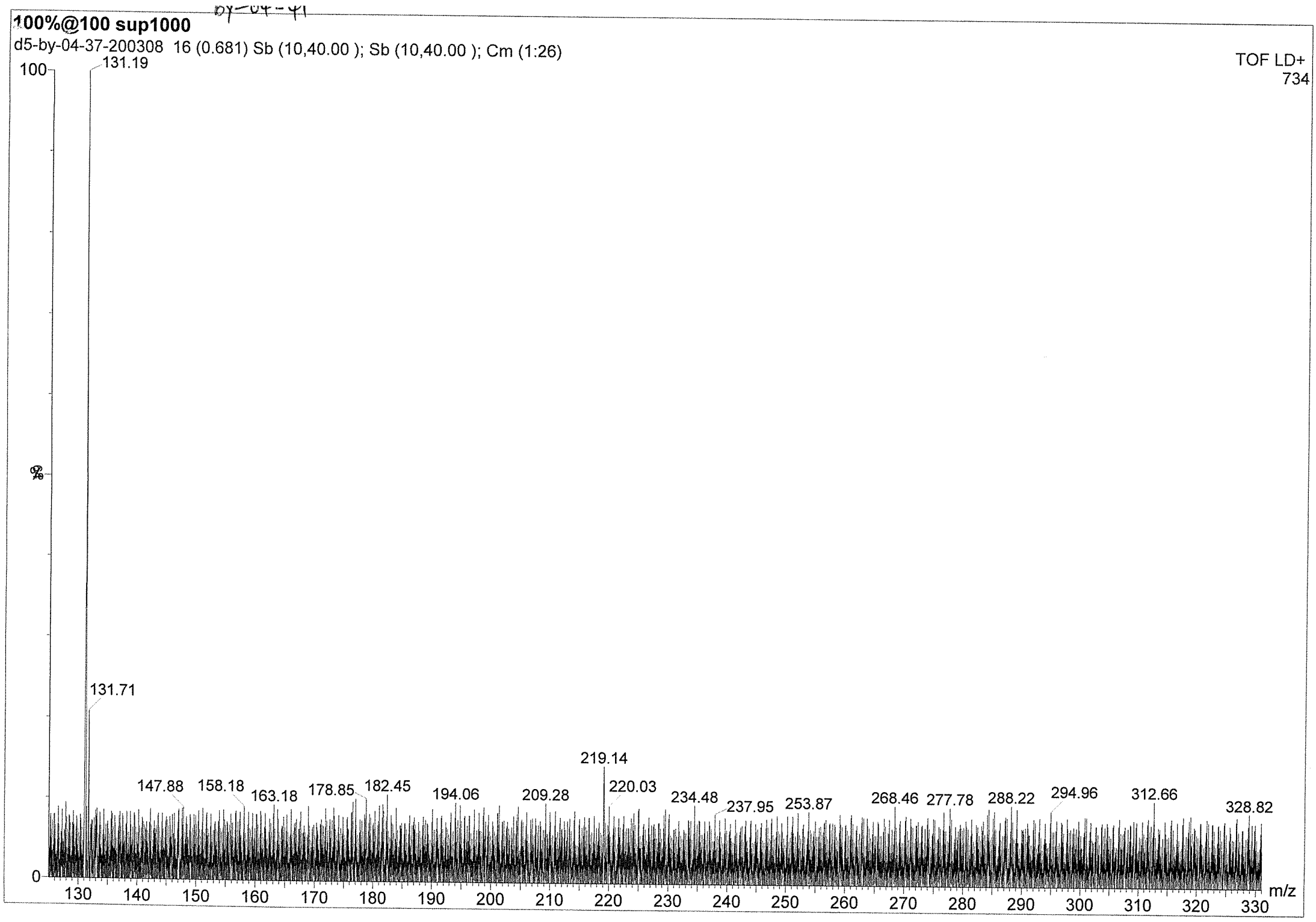
NUC1	1H
P1	10.10 usec
PL1	-3.00 dB
SFO1	300.1315007 MHz

F2 - Processing parameters

SI	16384
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

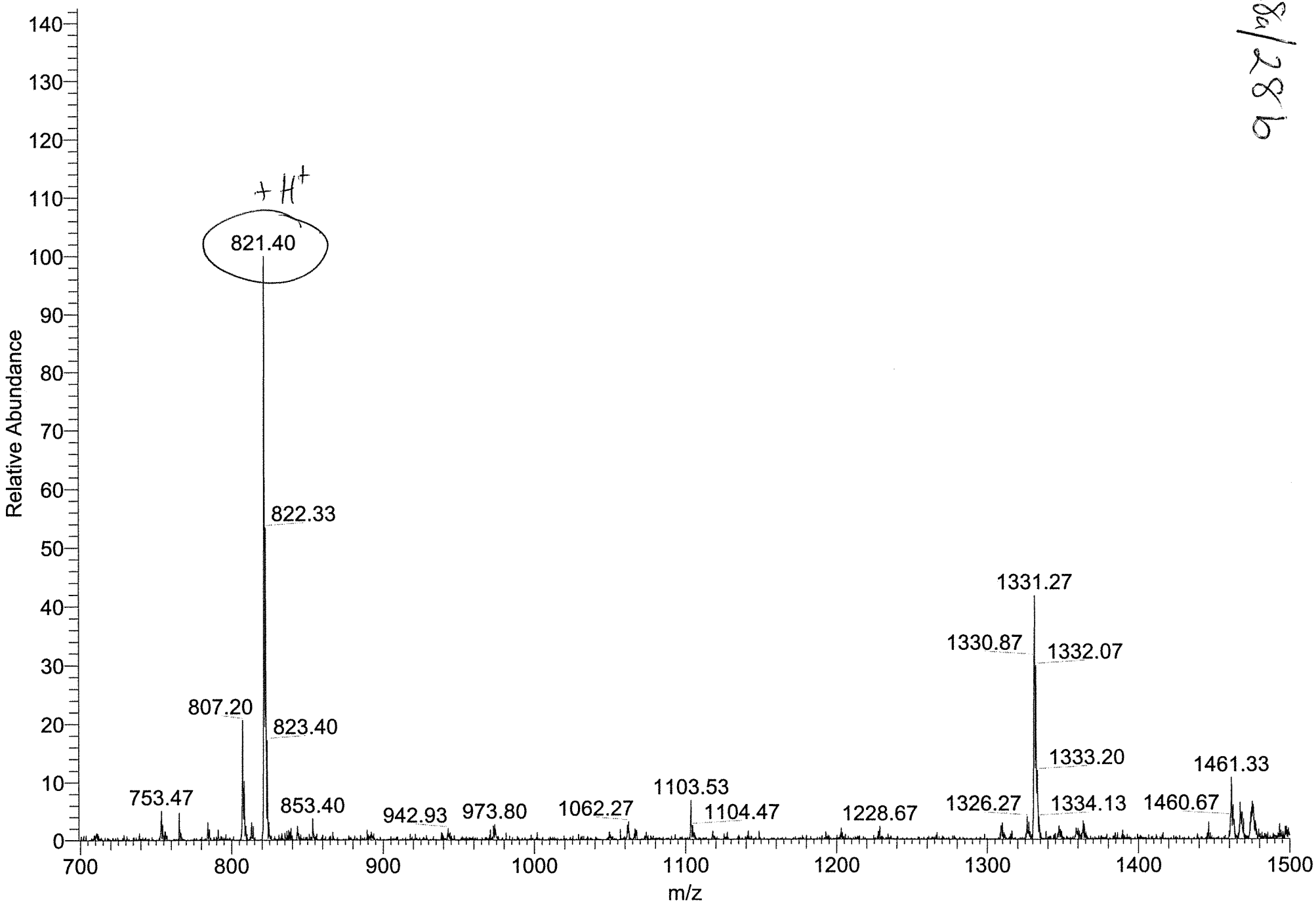
CX	20.00 cm
CY	11.98 cm
F1P	2.781 ppm
F1	834.52 Hz
F2P	0.931 ppm
F2	279.40 Hz
PPMCM	0.09248 ppm/cm
HZCM	27.75557 Hz/cm


100%@100 sup1000
d5-by-04-37-200308 16 (0.681) Sb (10,40.00); Sb (10,40.00); Cm (1:26)
TOF LD+
734
100
%
0
131.19
131.71
147.88
158.18
163.18
178.85
182.45
194.06
209.28
219.14
220.03
234.48
237.95
253.87
268.46
277.78
288.22
294.96
312.66
328.82
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320
330
m/z

C:\Data\Fargo\BY-04-67_080826161511 26/08/2008 4:15:11 PM
MeOH/DCM/TFA

BY-04-67_080826161511 #2-9 RT: 0.05-0.22 AV: 8 NL: 3.45E6
T: + p ESI Full ms [200.00-1500.00]

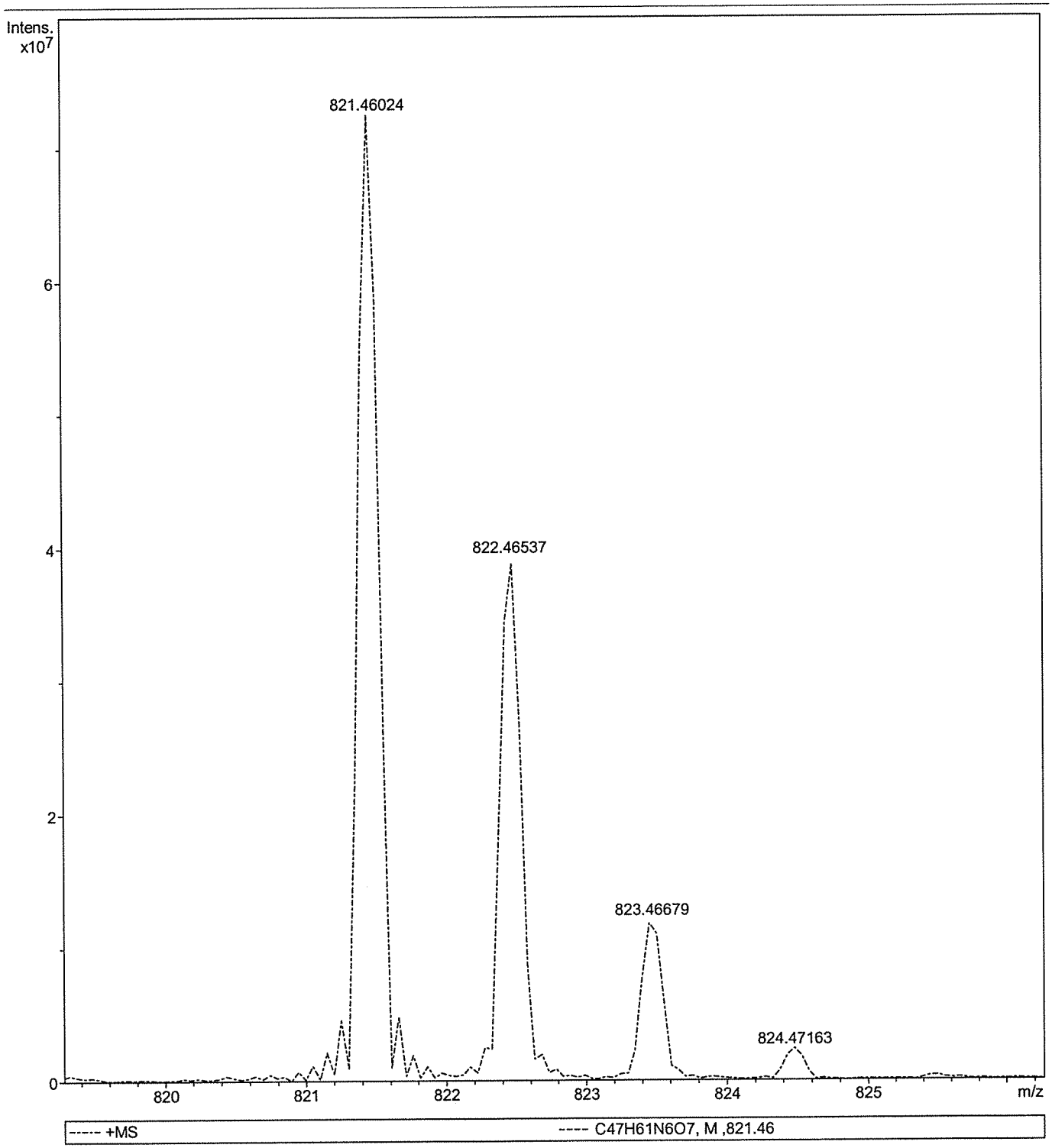
284/286



Generic Display Report

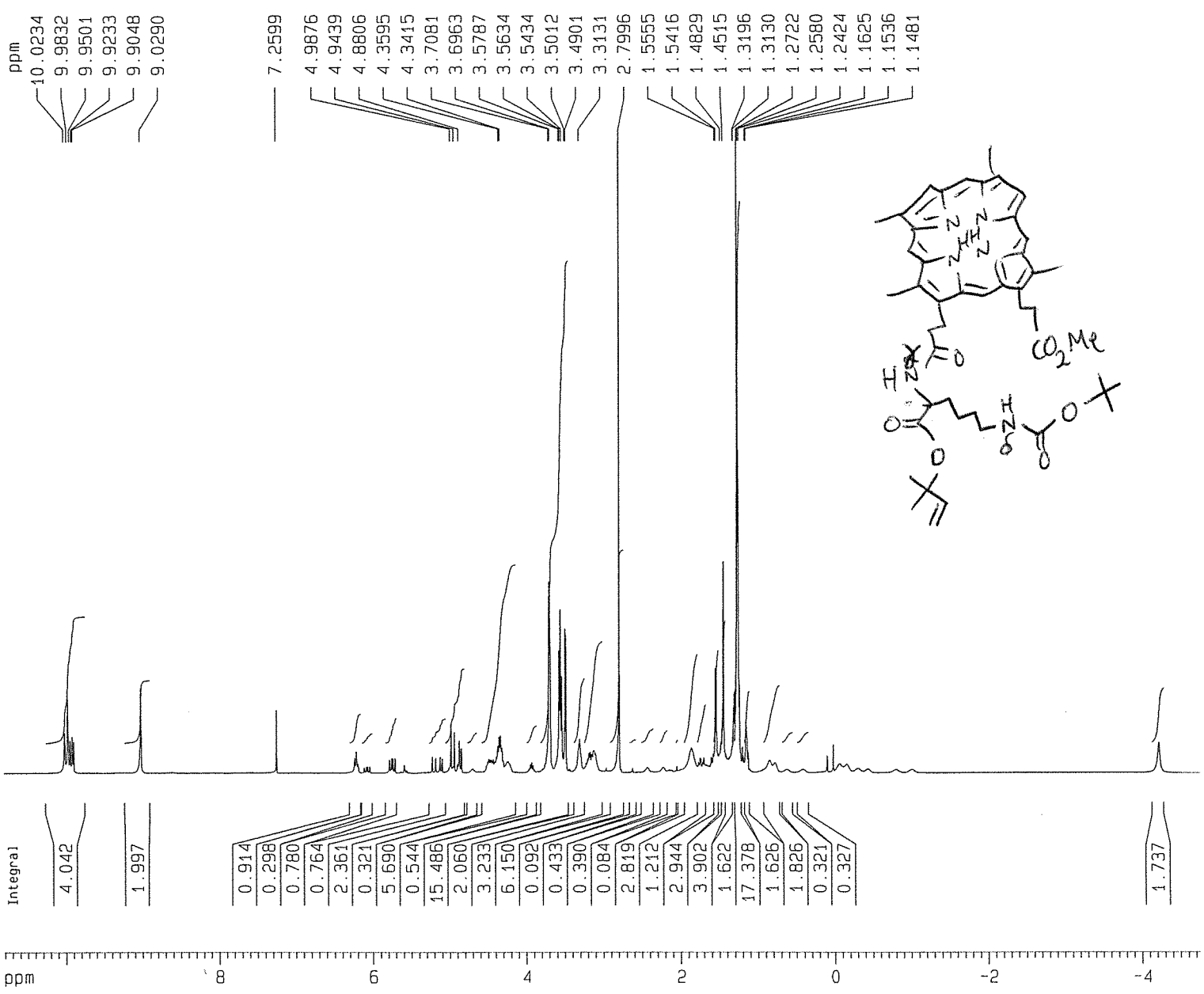
Analysis Info

Analysis Name	D:\Data\K270808a-ESI\KF_000005.d	Acquisition Date	8/27/2008 10:38:35 AM
Method	1MW Positive ESI	Operator	Administrator
Sample Name	BY-04-67	Instrument	apex-Qe
Comment			



+ 23 + 1.5 + .5 + 1.6

PROTON
sw: 20ppm
17--3



Current Data Parameters
NAME by-04-49
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080418
Time 17.48
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 25.4
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 400.1320007 MHz

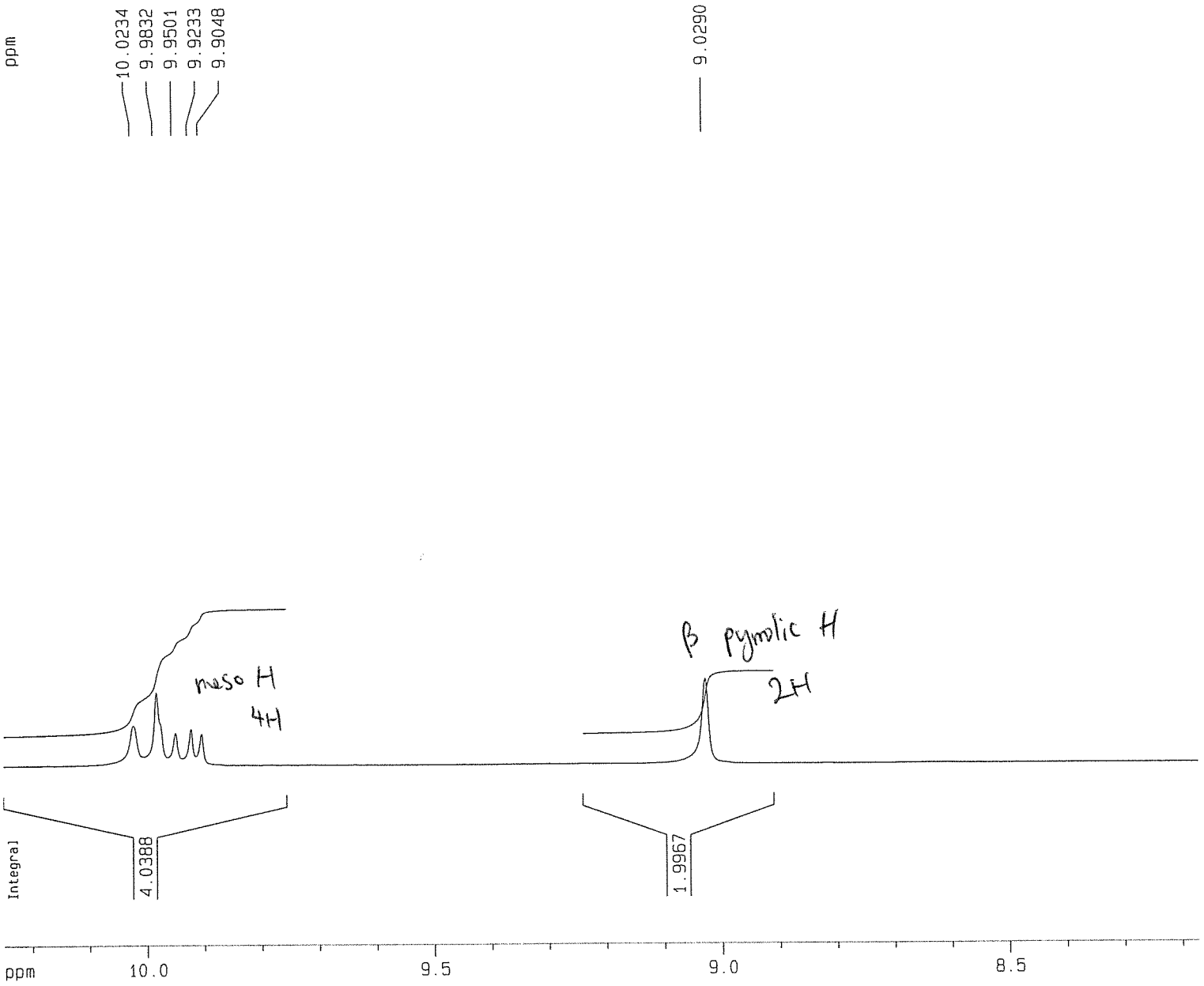
F2 - Processing parameters
SI 32768
SF 400.1300100 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.822 ppm
F1 4330.31 Hz
F2P -4.748 ppm
F2 -1899.90 Hz
PPMCM 0.77852 ppm/cm
HZCM 311.51062 Hz/cm

28a / 286

67

PROTON
sw: 20ppm
17--3



Current Data Parameters
NAME by-04-49
EXPNO 2
PROCNO 1

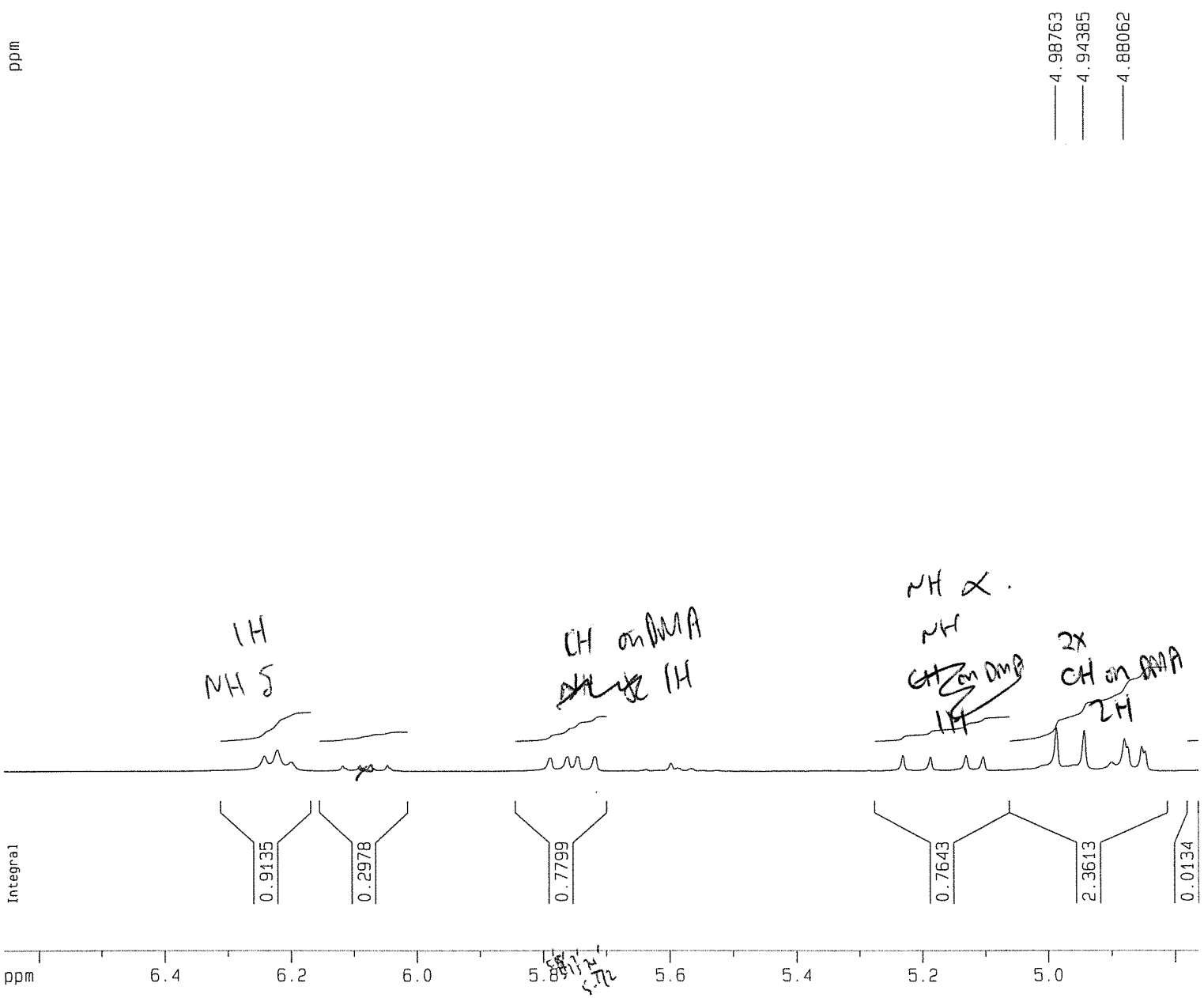
F2 - Acquisition Parameters
Date_ 20080418
Time 17.48
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 25.4
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300100 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.251 ppm
F1 4101.61 Hz
F2P 8.172 ppm
F2 3270.00 Hz
PPMCM 0.10392 ppm/cm
HZCM 41.58095 Hz/cm

PROTON
sw: 20ppm
17--3



Current Data Parameters

NAME	by-04-49
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20080418
Time	17.48
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	25.4
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

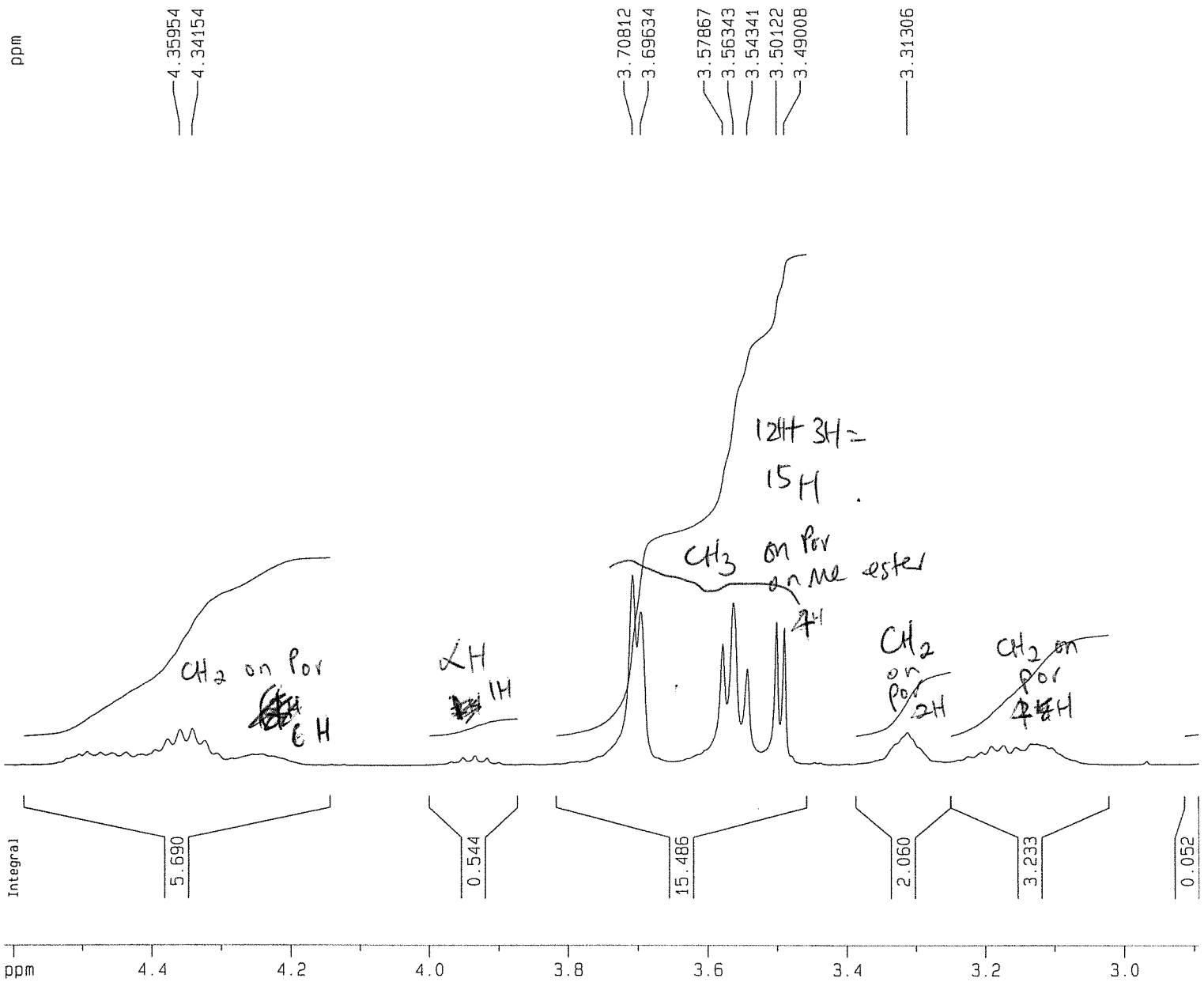
F2 - Processing parameters

SI	32768
SF	400.1300100 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	12.50 cm
F1P	6.657 ppm
F1	2663.57 Hz
F2P	4.763 ppm
F2	1905.96 Hz
PPMCM	0.09467 ppm/cm
HZCM	37.88041 Hz/cm

PROTON
sw: 20ppm
17--3



Current Data Parameters

NAME	by-04-49
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20080418
Time	17.48
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	25.4
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

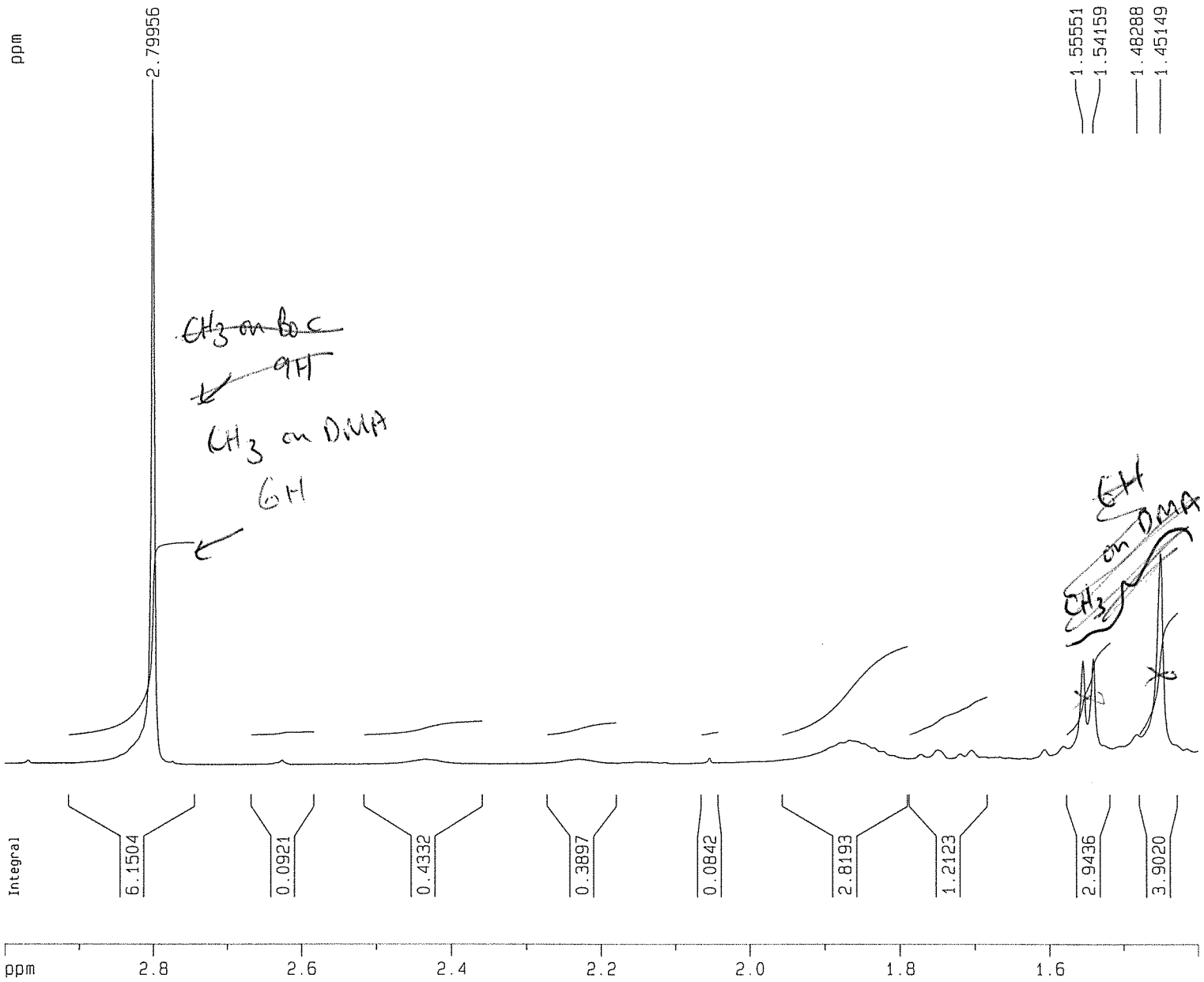
F2 - Processing parameters

SI	32768
SF	400.1300100 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	12.50 cm
F1P	4.614 ppm
F1	1846.14 Hz
F2P	2.894 ppm
F2	1157.78 Hz
PPMCM	0.08602 ppm/cm
HZCM	34.41780 Hz/cm

PROTON
sw: 20ppm
17--3



Current Data Parameters

NAME	by-04-49
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20080418
Time	17.48
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	25.4
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

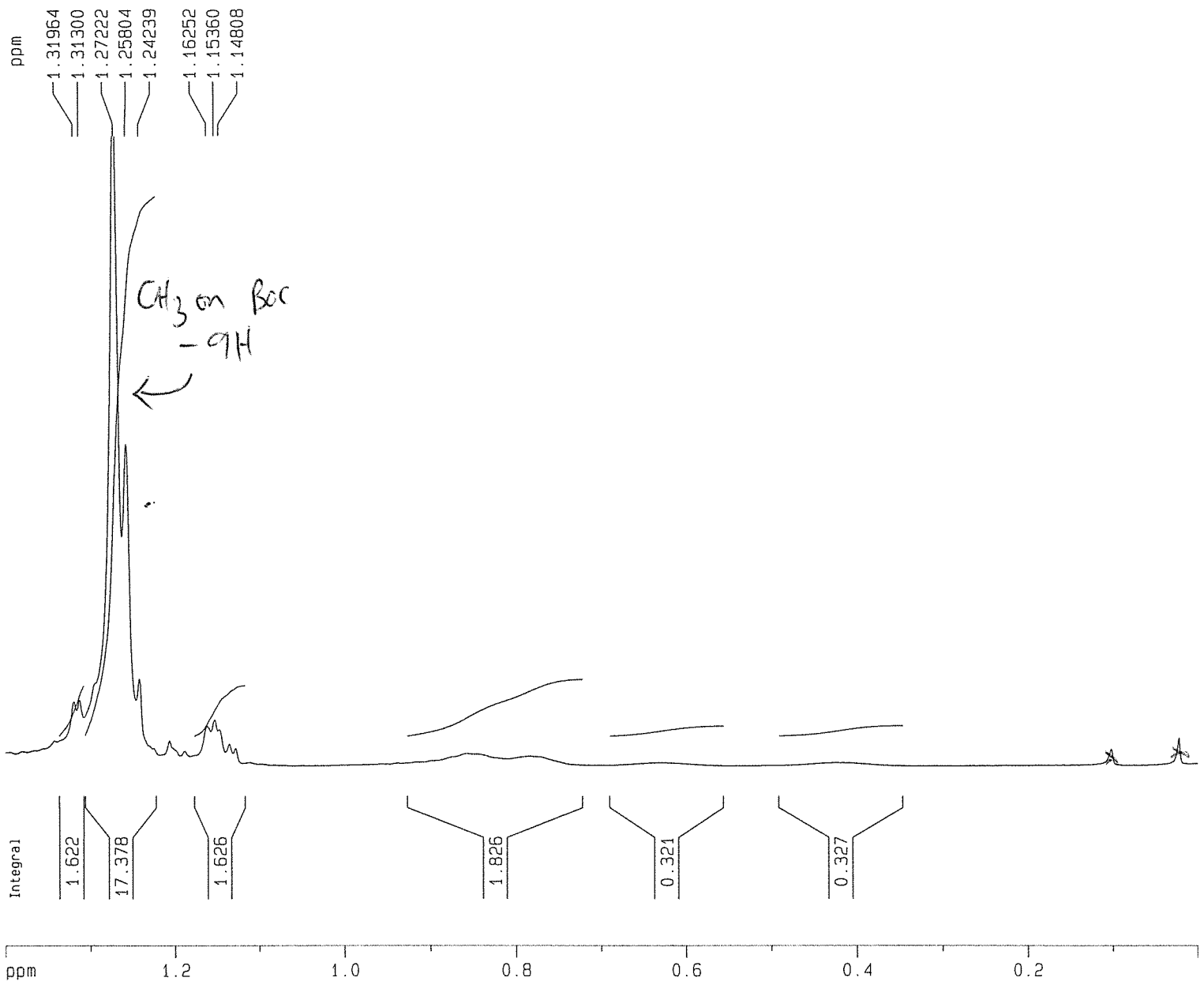
F2 - Processing parameters

SI	32768
SF	400.1300100 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	12.50 cm
F1P	3.000 ppm
F1	1200.39 Hz
F2P	1.400 ppm
F2	560.18 Hz
PPMCM	0.08000 ppm/cm
HZCM	32.01040 Hz/cm

PROTON
sw: 20ppm
17--3



Current Data Parameters

NAME	by-04-49
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20080418
Time	17.48
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	25.4
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

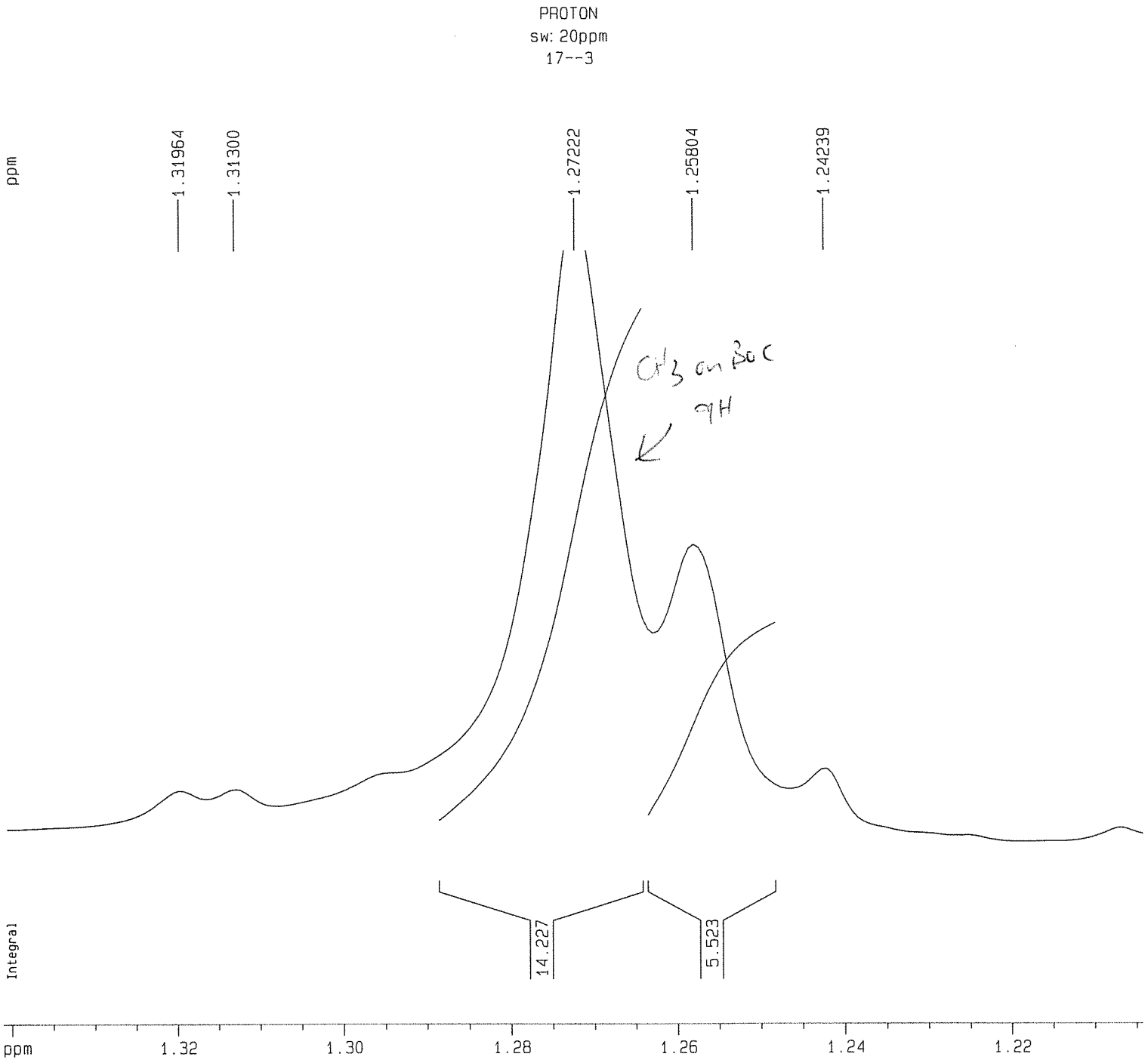
NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SI	32768
SF	400.1300100 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	12.50 cm
F1P	1.400 ppm
F1	560.18 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	0.07000 ppm/cm
HZCM	28.00910 Hz/cm



Current Data Parameters

NAME	by-04-49
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20080418
Time	17.48
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	25.4
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

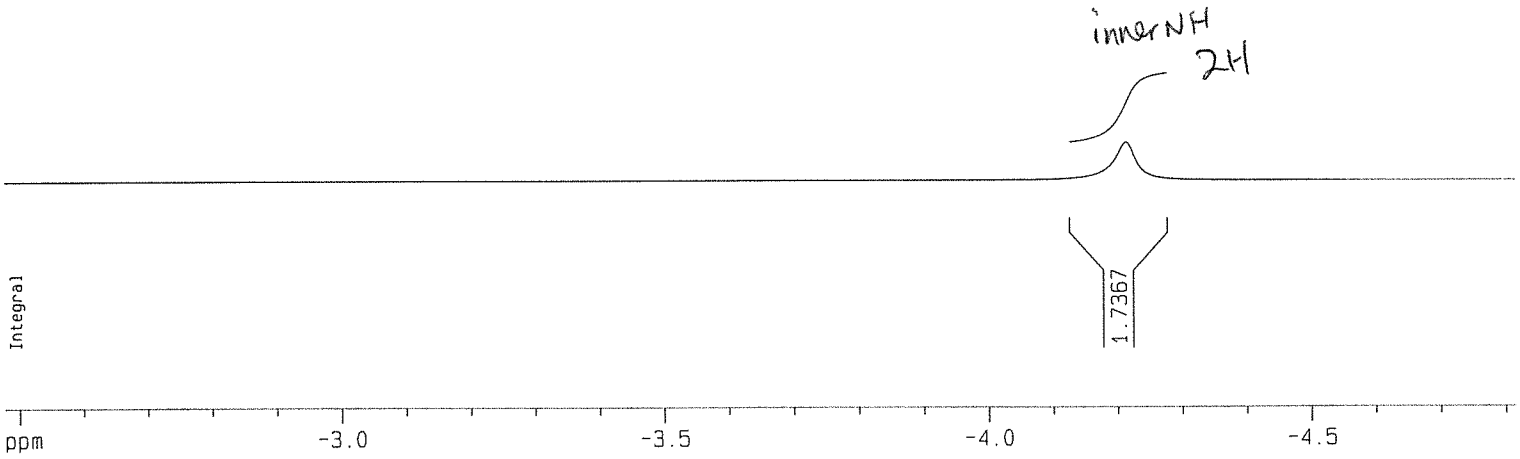
F2 - Processing parameters

SI	32768
SF	400.1300100 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	12.50 cm
F1P	1.341 ppm
F1	536.63 Hz
F2P	1.204 ppm
F2	481.86 Hz
PPMCM	0.00684 ppm/cm
HZCM	2.73859 Hz/cm

PROTON
sw: 20ppm
17--3



Current Data Parameters

NAME	by-04-49
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20080418
Time	17.48
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	25.4
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SI	32768
SF	400.1300100 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

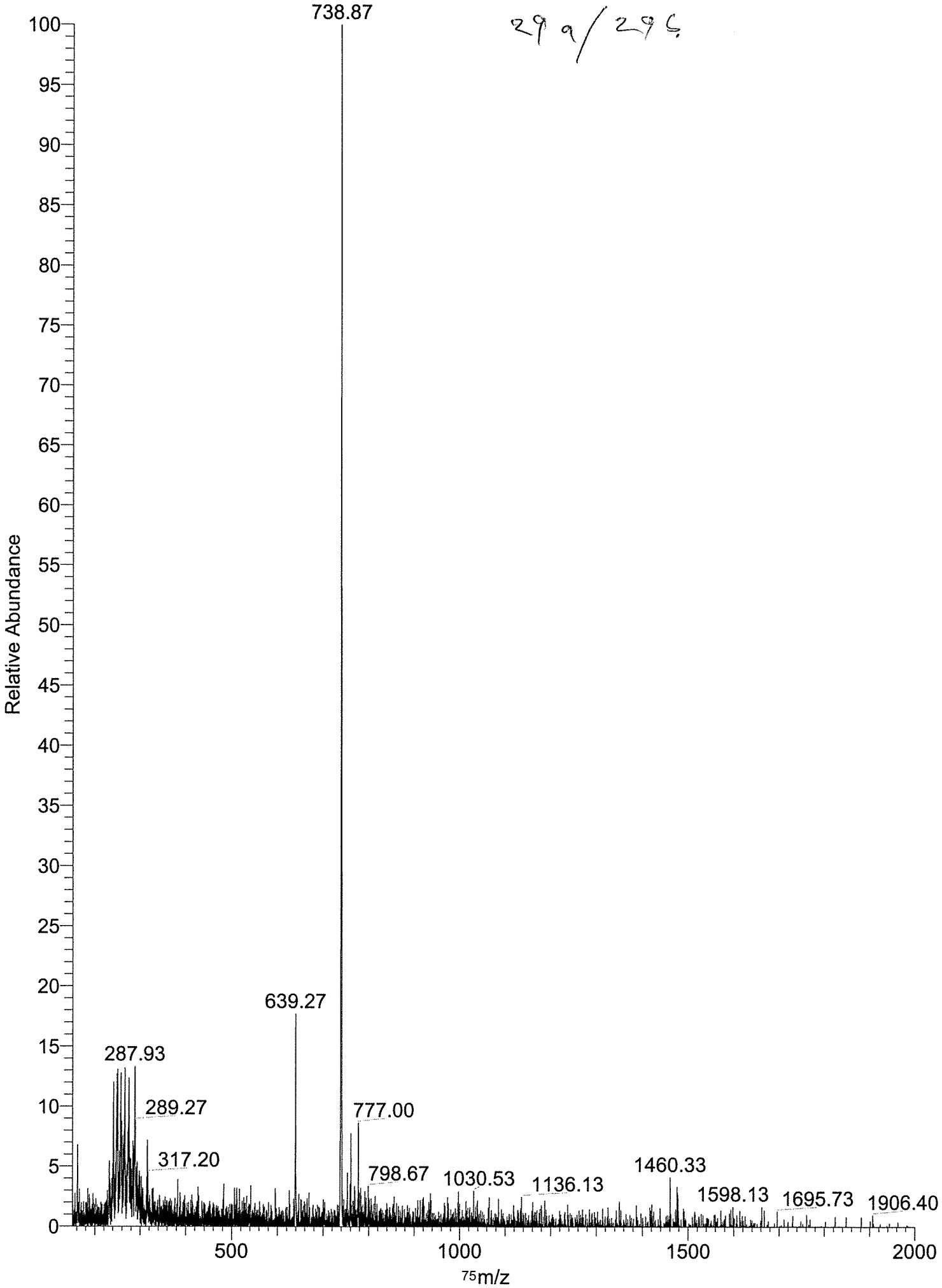
1D NMR plot parameters

CX	20.00 cm
CY	12.50 cm
F1P	-2.476 ppm
F1	-990.77 Hz
F2P	-4.815 ppm
F2	-1926.64 Hz
PPMCM	0.11695 ppm/cm
HZCM	46.79345 Hz/cm

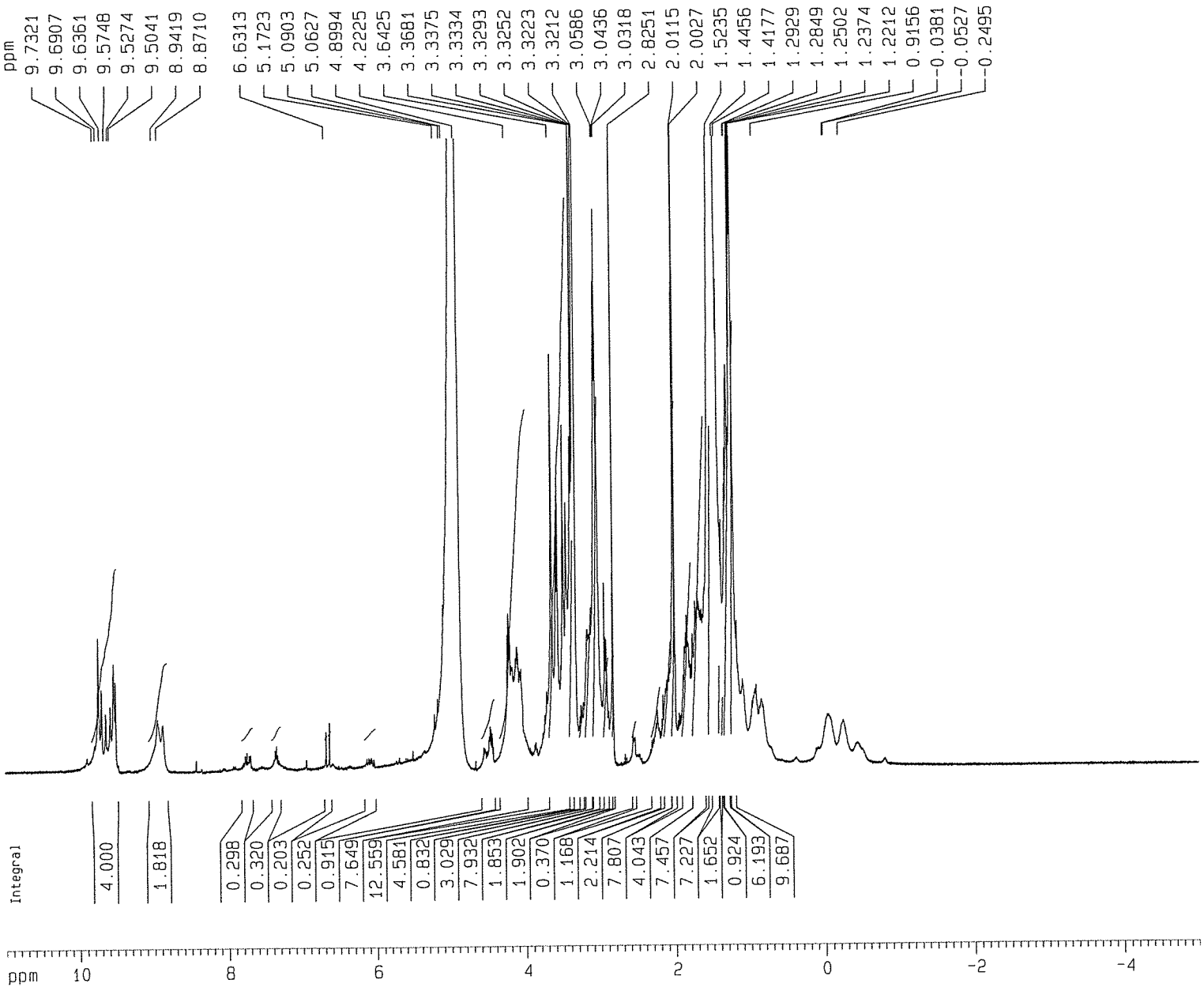
C:\Data\Fargol\BY-04-65_080501090554 1/05/2008 9:05:54 AM
MeOh

BY-04-65_080501090554 #2-7 RT: 0.07-0.23 AV: 6 NL: 7.64E5
T: + p ESI Full ms [150.00-2000.00]

29 a / 29 c



PROTON
sw: 20ppm
17--3



Current Data Parameters

NAME	BY-04-75a
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	12.20
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	MeOD
NS	32
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	50.8
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

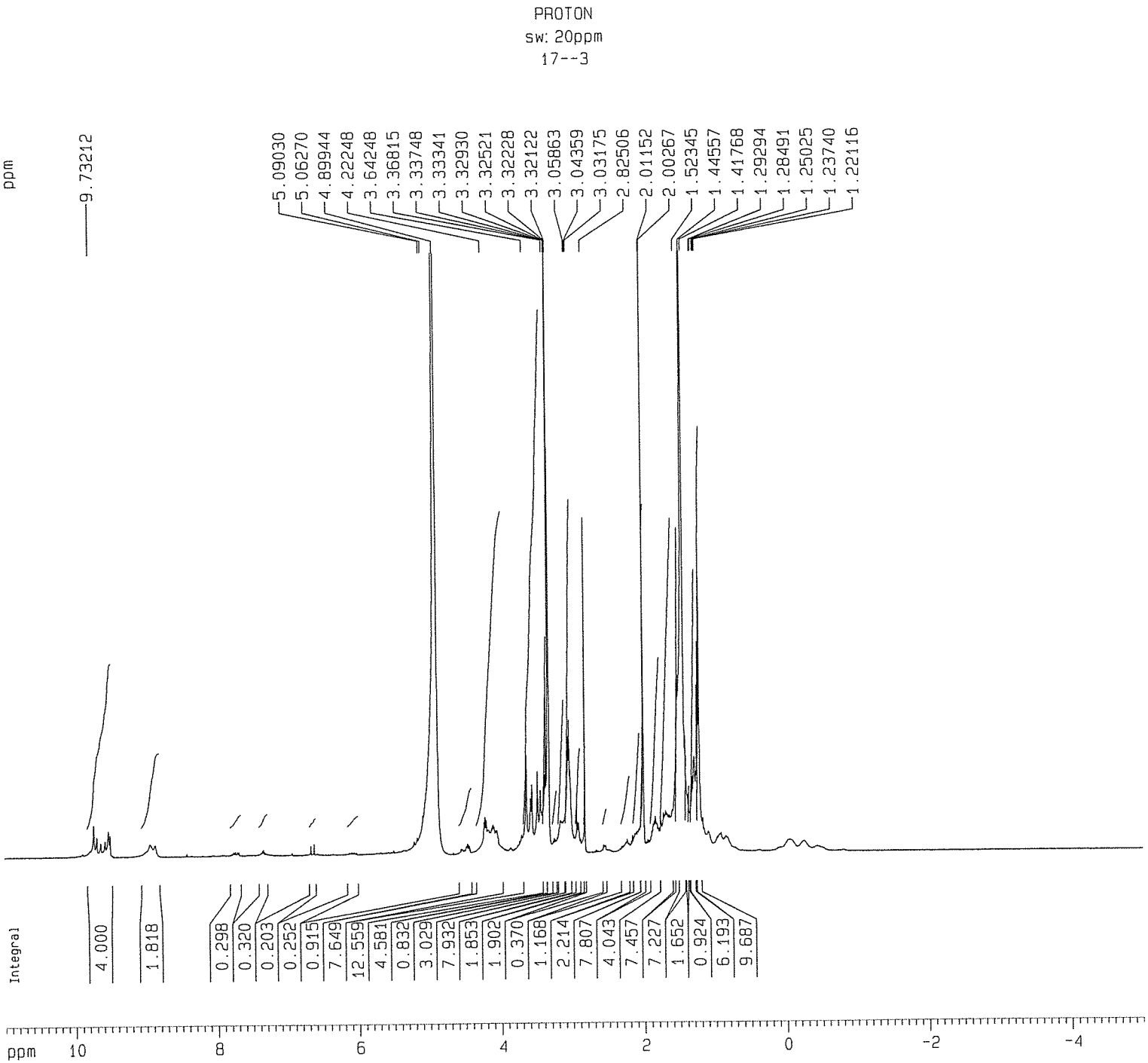
NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	200.00 cm
F1P	11.000 ppm
F1	4401.43 Hz
F2P	-5.000 ppm
F2	-2000.65 Hz
PPMCM	0.80000 ppm/cm
HZCM	320.10400 Hz/cm



Current Data Parameters

NAME	BY-04-75a
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	12.20
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	MeOD
NS	32
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	50.8
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

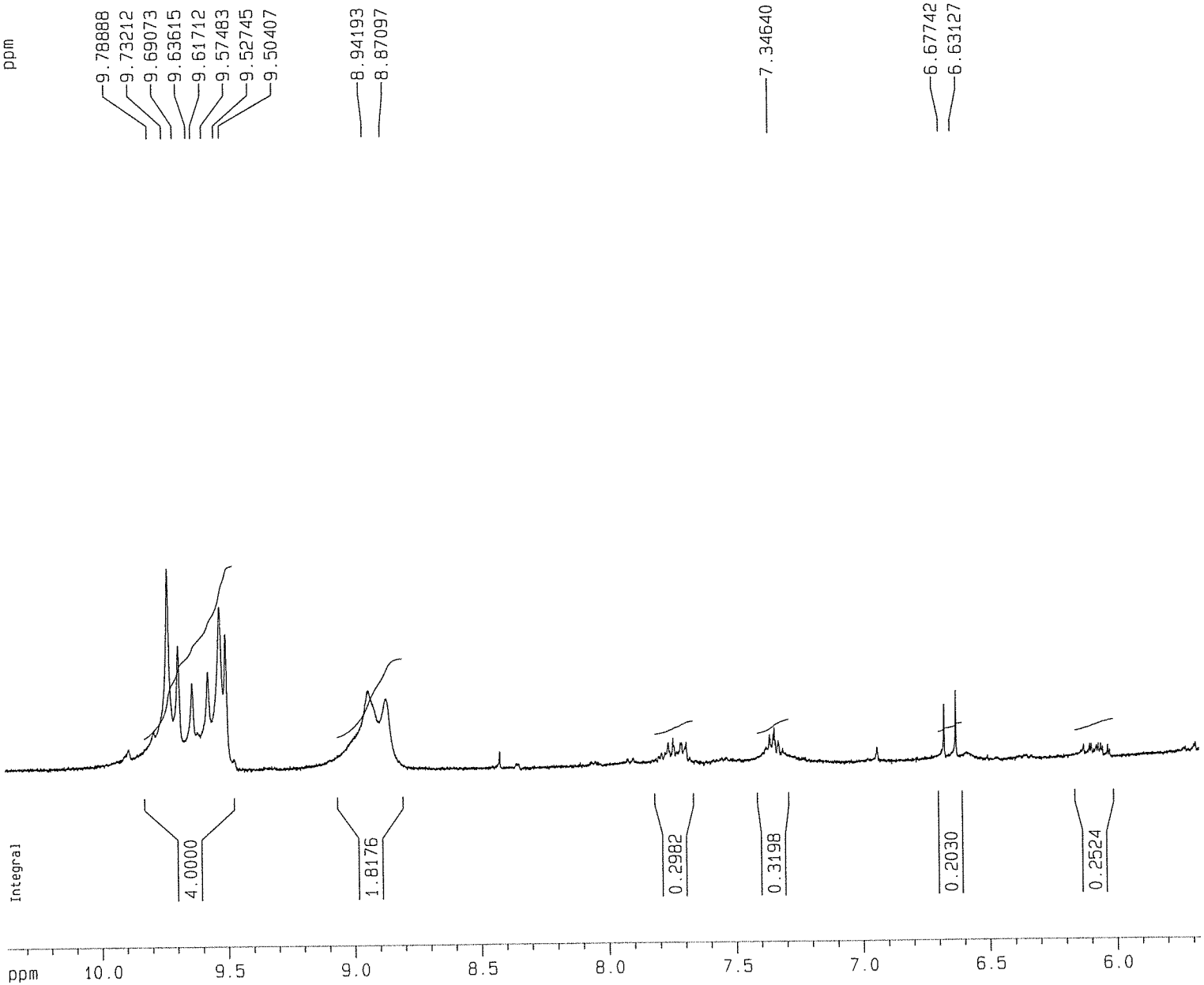
F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	50.00 cm
F1P	11.000 ppm
F1	4401.43 Hz
F2P	-5.000 ppm
F2	-2000.65 Hz
PPMCM	0.80000 ppm/cm
HZCM	320.10400 Hz/cm

PROTON
sw: 20ppm
17--3



Current Data Parameters

NAME	BY-04-75a
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	12.20
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	MeOD
NS	32
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	50.8
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

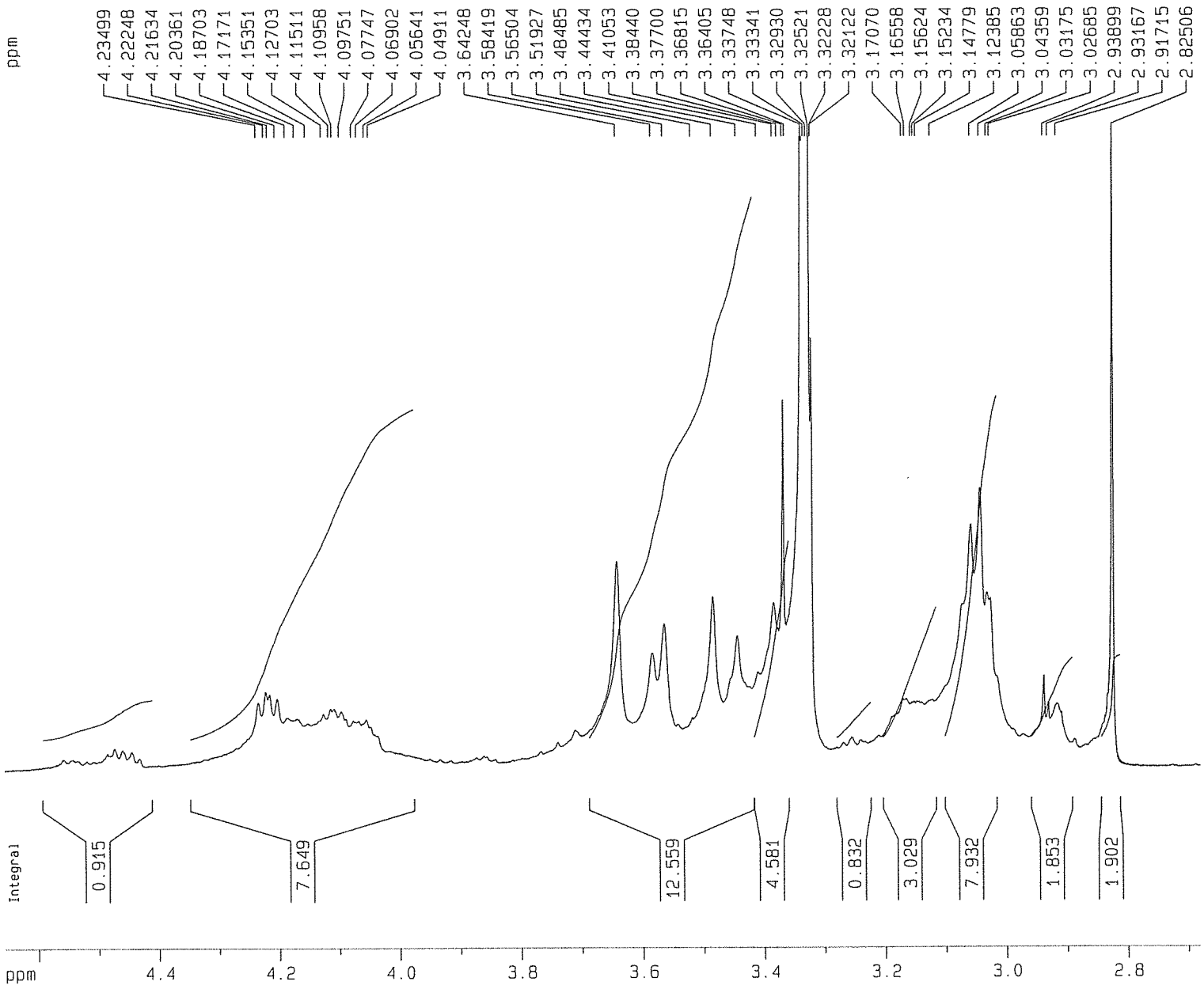
F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	300.00 cm
F1P	10.379 ppm
F1	4152.93 Hz
F2P	5.675 ppm
F2	2270.85 Hz
PPMCM	0.23518 ppm/cm
HZCM	94.10406 Hz/cm

PROTON
sw: 20ppm
17--3



Current Data Parameters

NAME	BY-04-75a
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	12.20
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	MeOD
NS	32
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	50.8
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

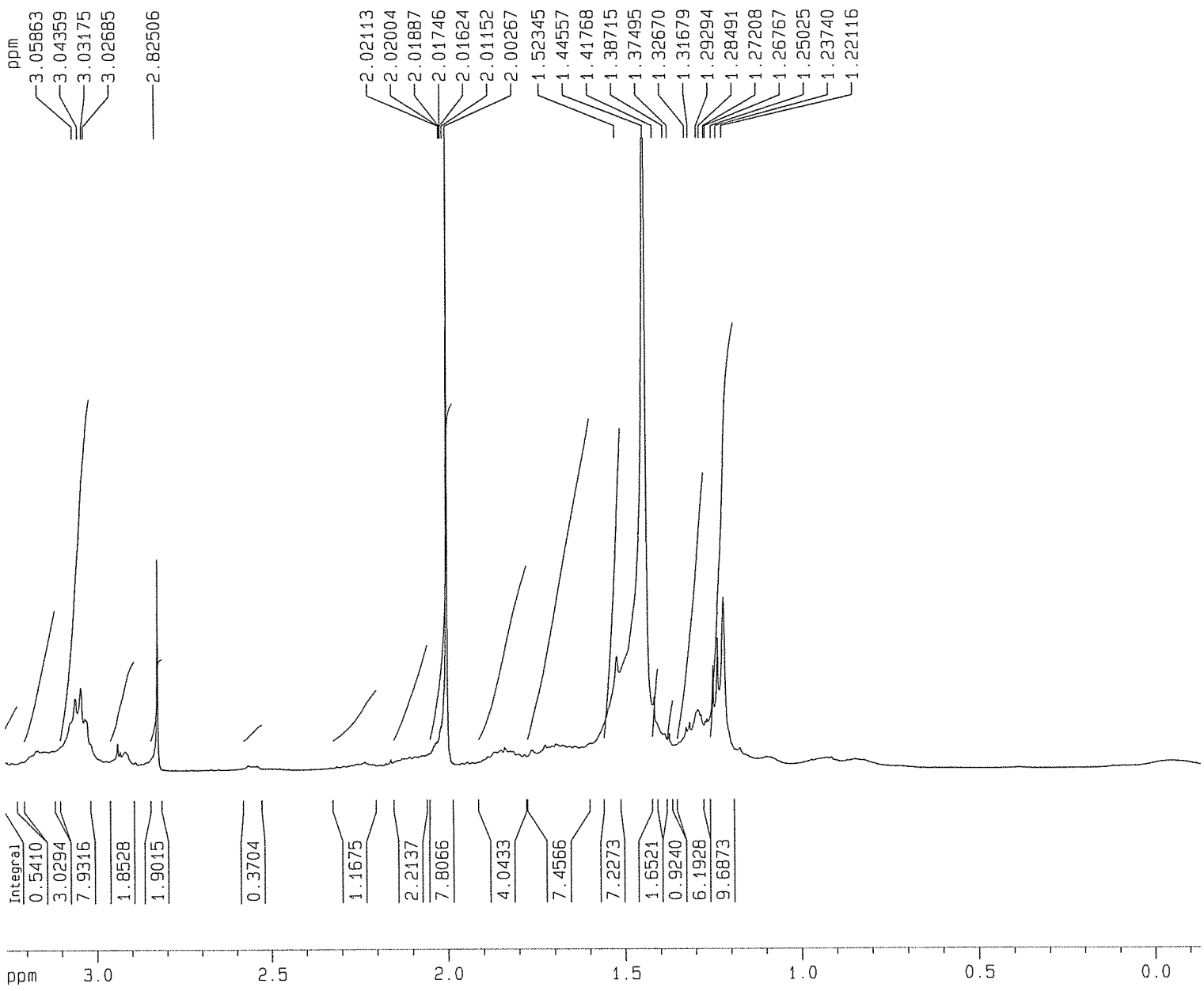
F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	100.00 cm
F1P	4.657 ppm
F1	1863.21 Hz
F2P	2.681 ppm
F2	1072.72 Hz
PPMCM	0.09878 ppm/cm
HZCM	39.52457 Hz/cm

PROTON
sw: 20ppm
17--3



Current Data Parameters

NAME	BY-04-75a
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	12.20
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	MeOD
NS	32
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	50.8
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

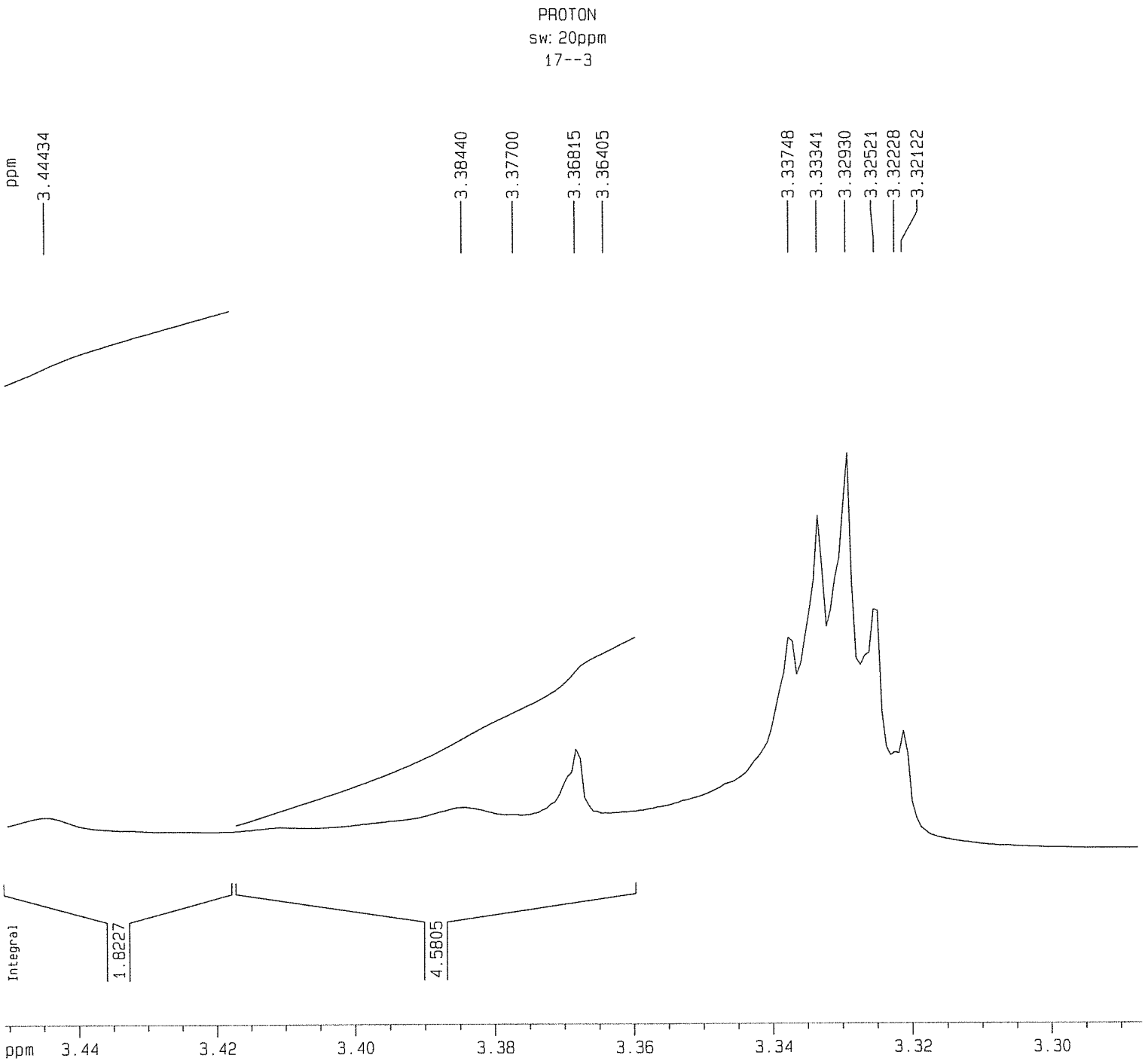
NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	30.00 cm
F1P	3.259 ppm
F1	1304.05 Hz
F2P	-0.129 ppm
F2	-51.66 Hz
PPMCM	0.16941 ppm/cm
HZCM	67.78504 Hz/cm



Current Data Parameters

NAME	BY-04-75a
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080508
Time	12.20
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	MeOD
NS	32
DS	0
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	2.0447731 sec
RG	50.8
DW	62.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	1H
P1	8.20 usec
PL1	-3.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	30.00 cm
F1P	3.451 ppm
F1	1380.75 Hz
F2P	3.287 ppm
F2	1315.24 Hz
PPMCM	0.00819 ppm/cm
HZCM	3.27544 Hz/cm