

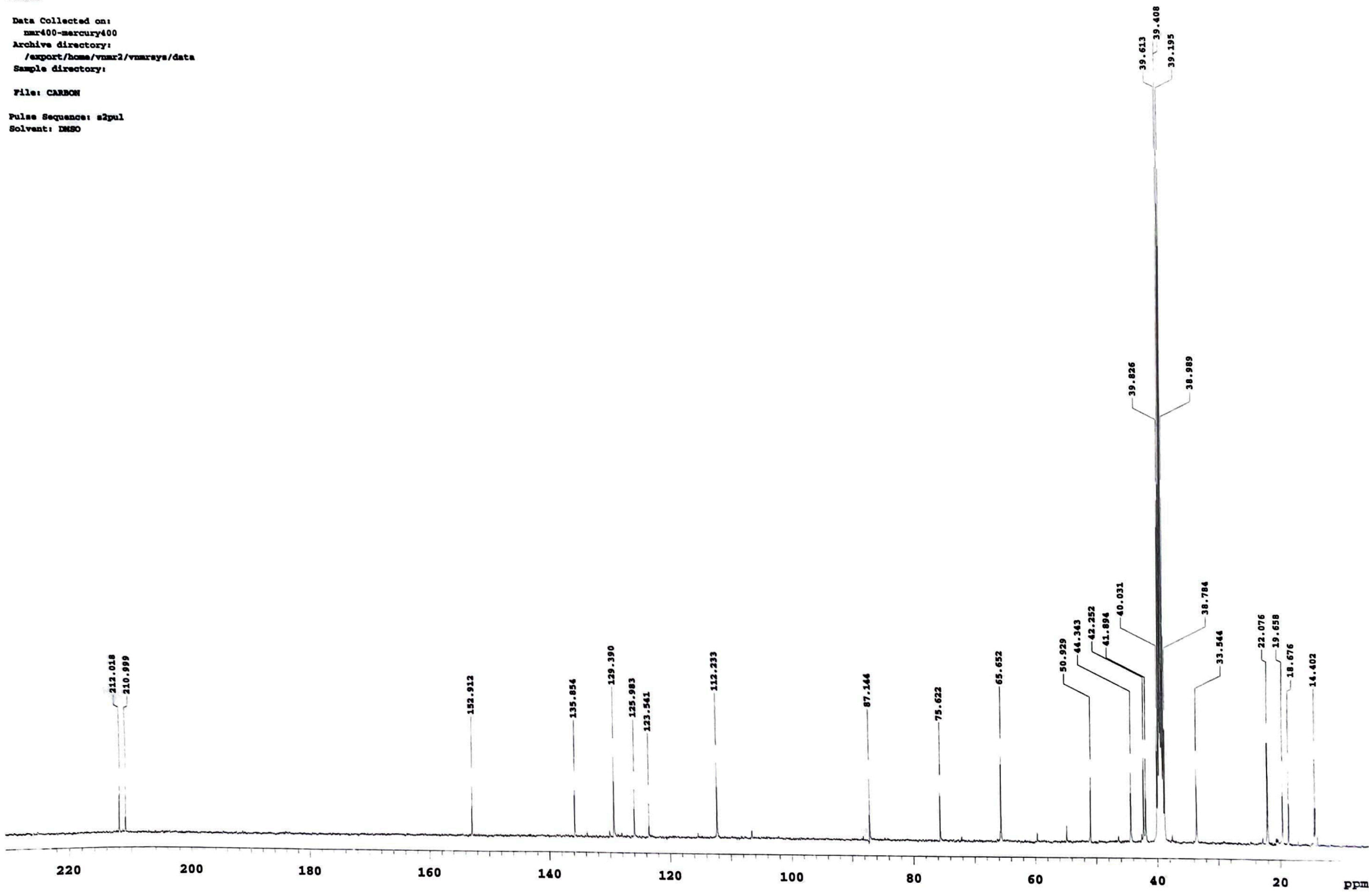
1H-NMR product 6

Fantin

Data Collected on:
nmr400-mercury400
Archive directory:
/export/home/vnmr2/vnmrsws/data
Sample directory:

File: CARBON

Pulse Sequence: s2pul
Solvent: DMSO

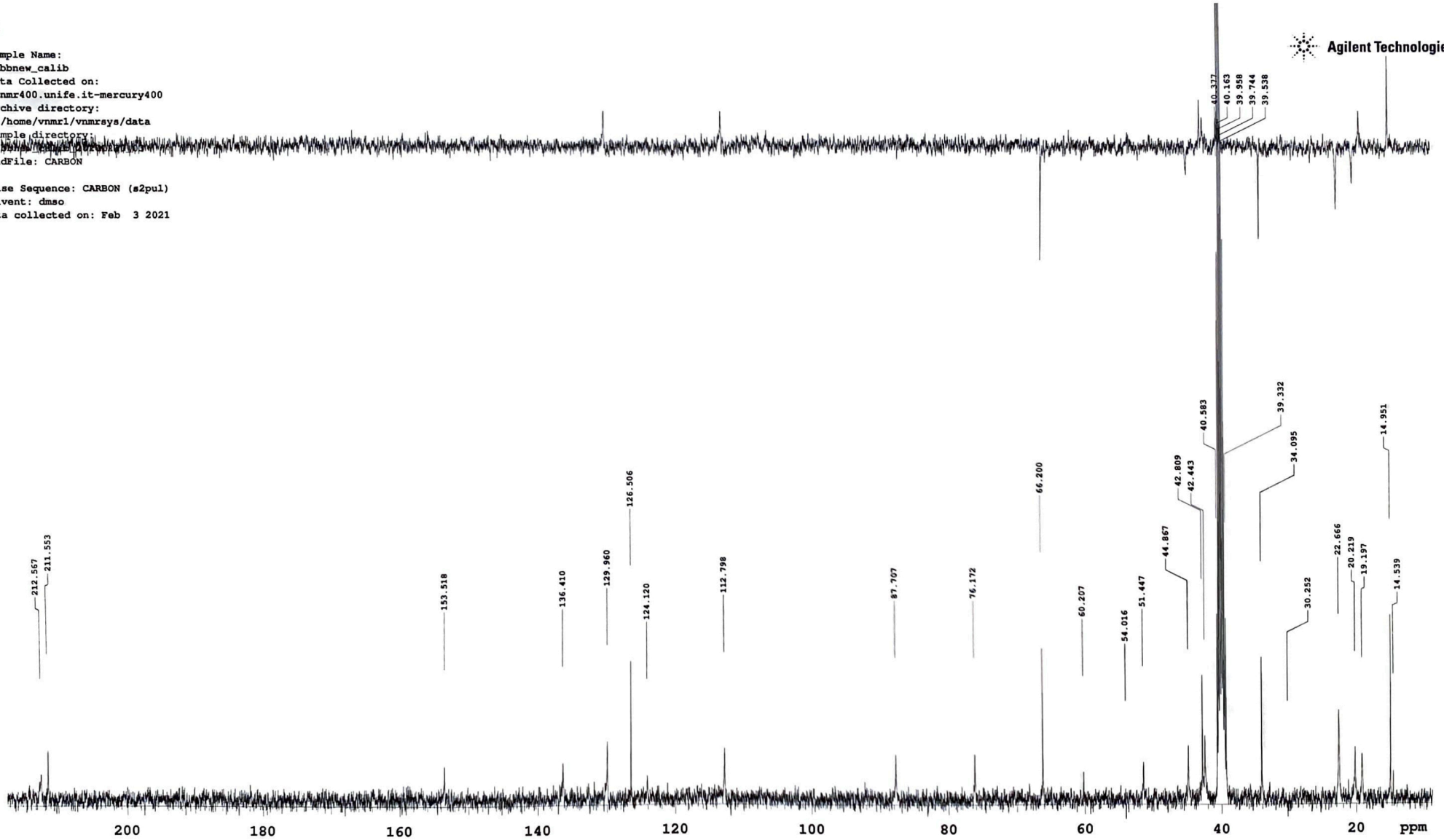


¹³C-NMR product 6

SCA

Sample Name:
bbnew_calib
Data Collected on:
nmr400.unife.it-mercury400
Archive directory:
/home/vnmr1/vnmrSYS/data
Sample directory:
/home/vnmr1/vnmrSYS/data
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: dmsc
Data collected on: Feb 3 2021



DEPT-NMR product 6

bbnew_calib

Sample Name **bbnew_calib**
Date collected **2021-02-03**

Pulse sequence **gCOSY**
Solvent **dmsd**

Temperature **25**
Spectrometer **nmr400.unife.it-mercury400**

Study owner **vnmr1**
Operator **vnmr1**

SCA

SAMPLE

date **Feb 3 2021**
solvent **dmsd**
sample **bbnew_calib_20**
210201_01

FLAGS

hs **nn**
ssol **y**
hsglvl **1104**

SPECIAL

temp **25.0**
gain **22**
spin **0**

ACQUISITION

sw **4081.6**
af **0.150**
np **1224**
fb **2200**
ss **32**
dl **1.000**
rl **1**

F2 PROCESSING

sb **-0.075**
scs **not used**
ln **2048**

2D ACQUISITION

sw1 **4081.6**
nl **256**
dl2 **0**

F1 PROCESSING

sb1 **-0.063**
sbs1 **not used**
proc1 **lp**
ln1 **2048**

PRESATURATION

satmode **n**
wet **n**

DISPLAY

sp **115.0**
vp **3300.4**
sp1 **31.3**
vp1 **3515.6**
rf **-19.3**
rfp **0**
rf1 **-19.3**
rfp1 **0**

TRANSMITTER

tn **H1**
sfreq **399.972**
tcf **112.7**
tpwr **60**
pM **11.500**

GRADIENTS

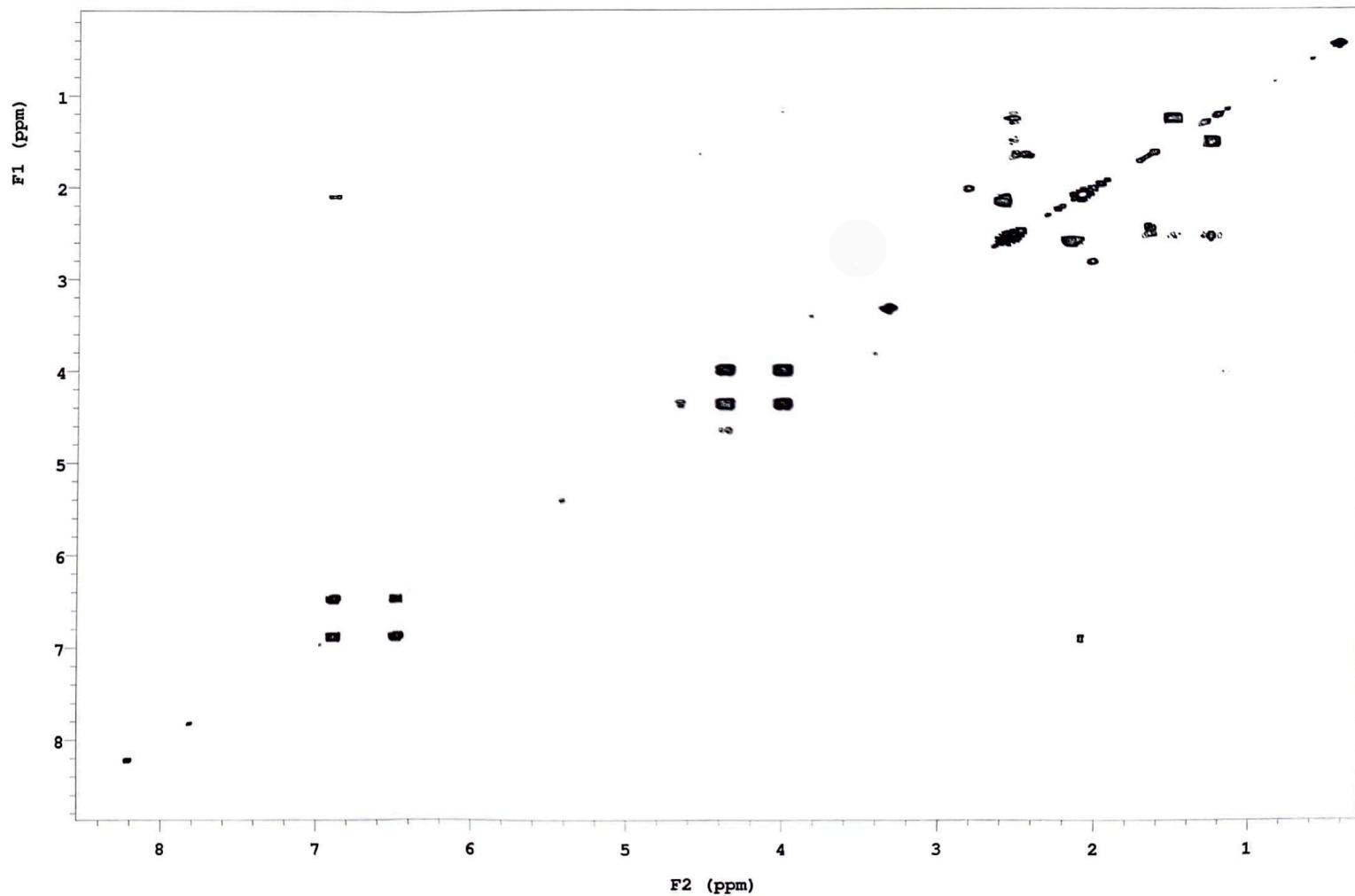
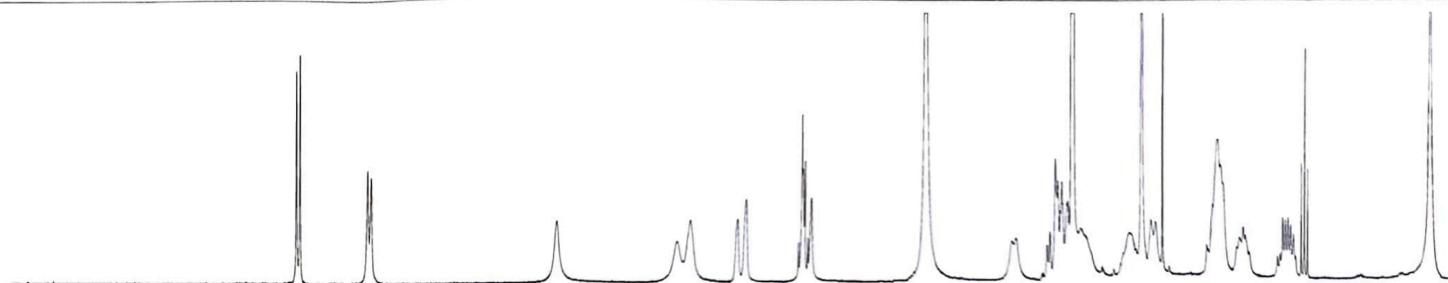
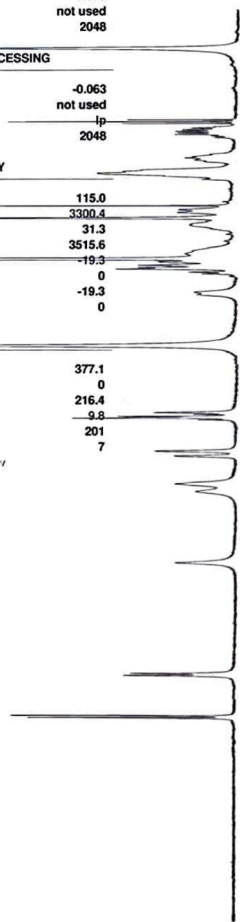
gzME **924**
glE **0.001000**
EDirect **1.000**
grtab **0.000500**

PLOT

wc **377.1**
sc **0**
wc2 **216.4**
sc2 **9.8**
vs **201**
th **7**
ai **odc av**

DECOUPLER

dl **C13**
dl1 **nnn**



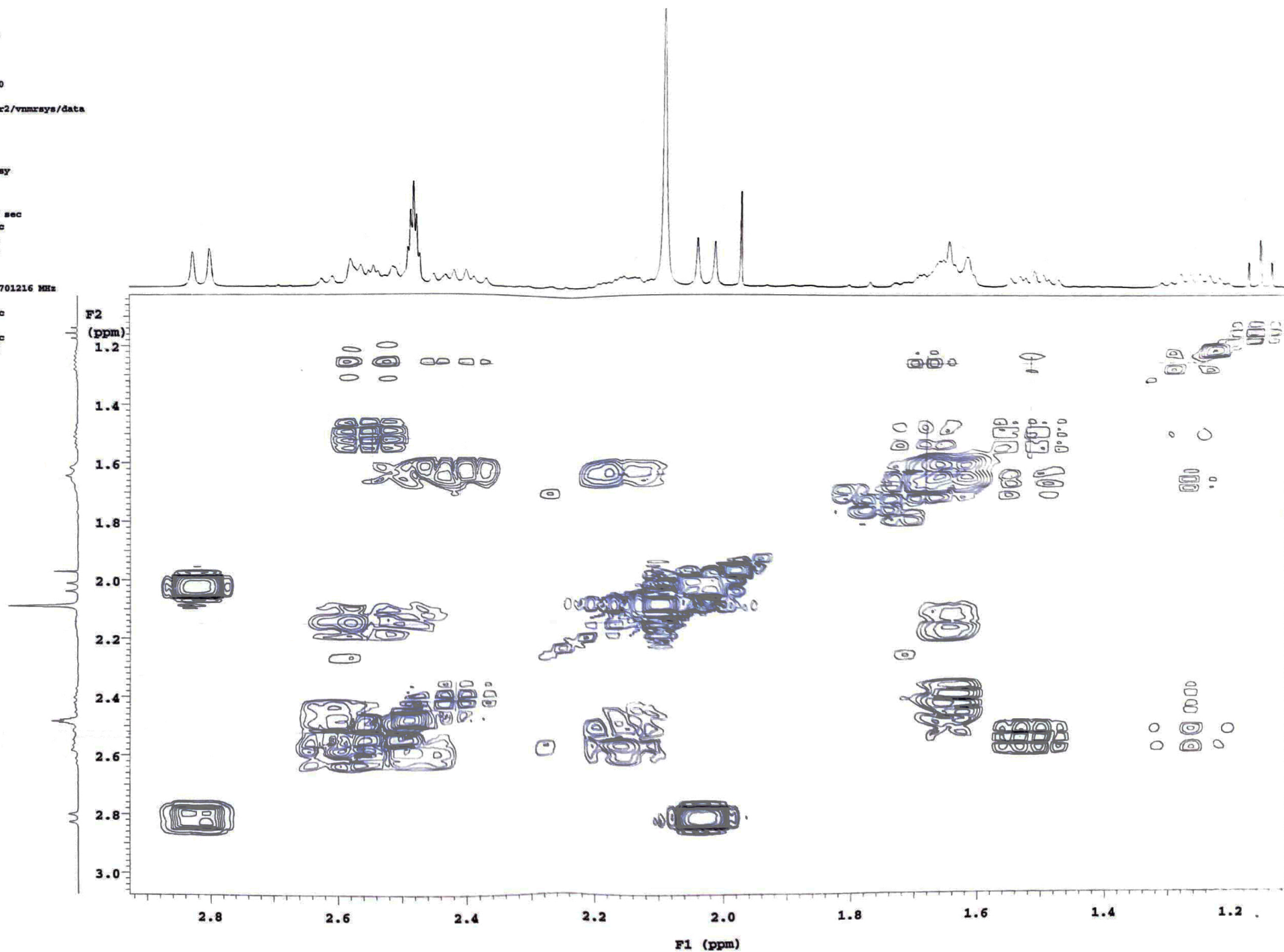
STANDARD IN OBSERVE

Data Collected on:
nmr400-mercury400
Archive directory:
/export/home/vnmr2/vnmrsys/data
Sample directory:

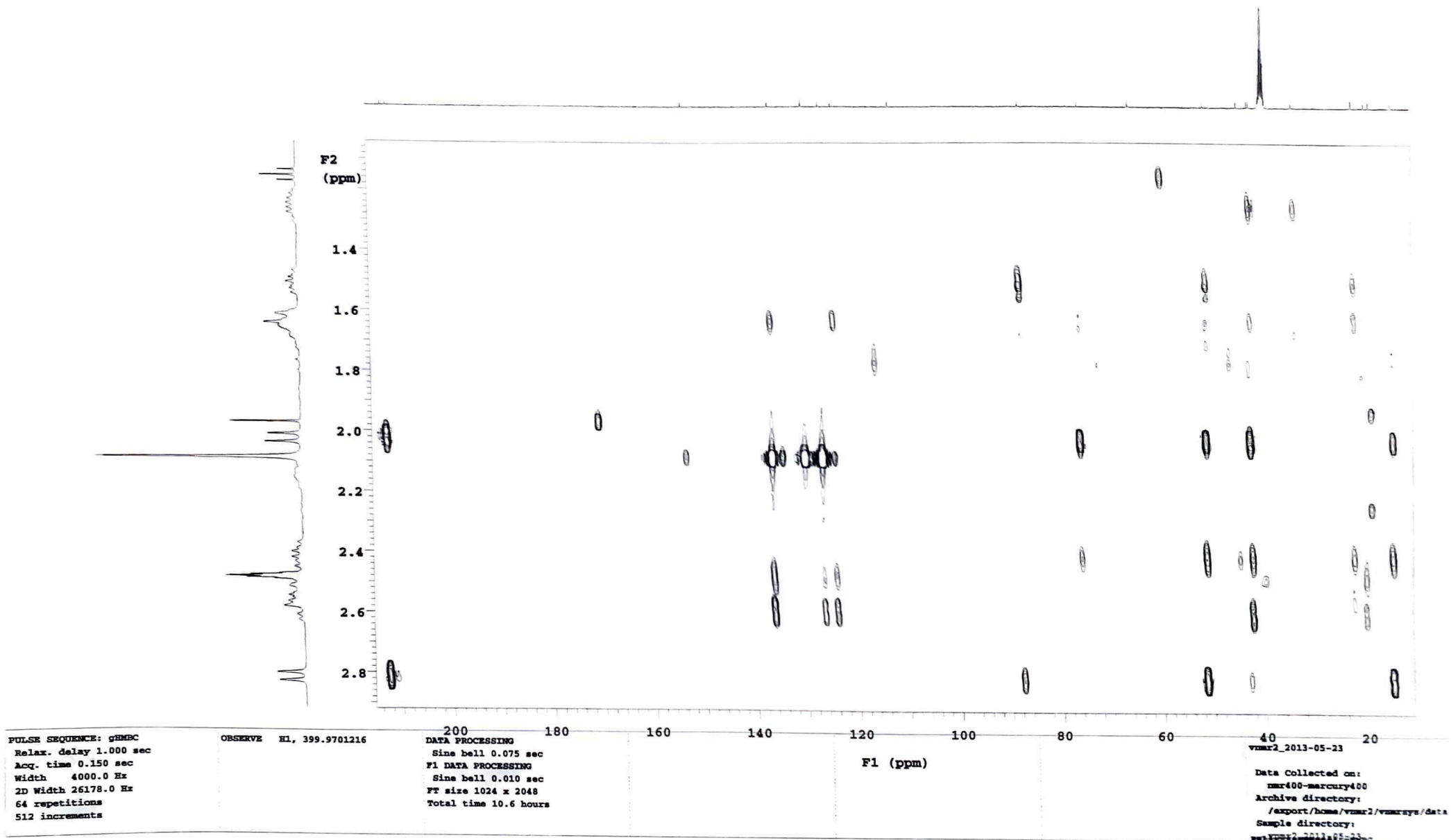
File: gcosy

Pulse Sequence: gcosy
Solvent: DMSO

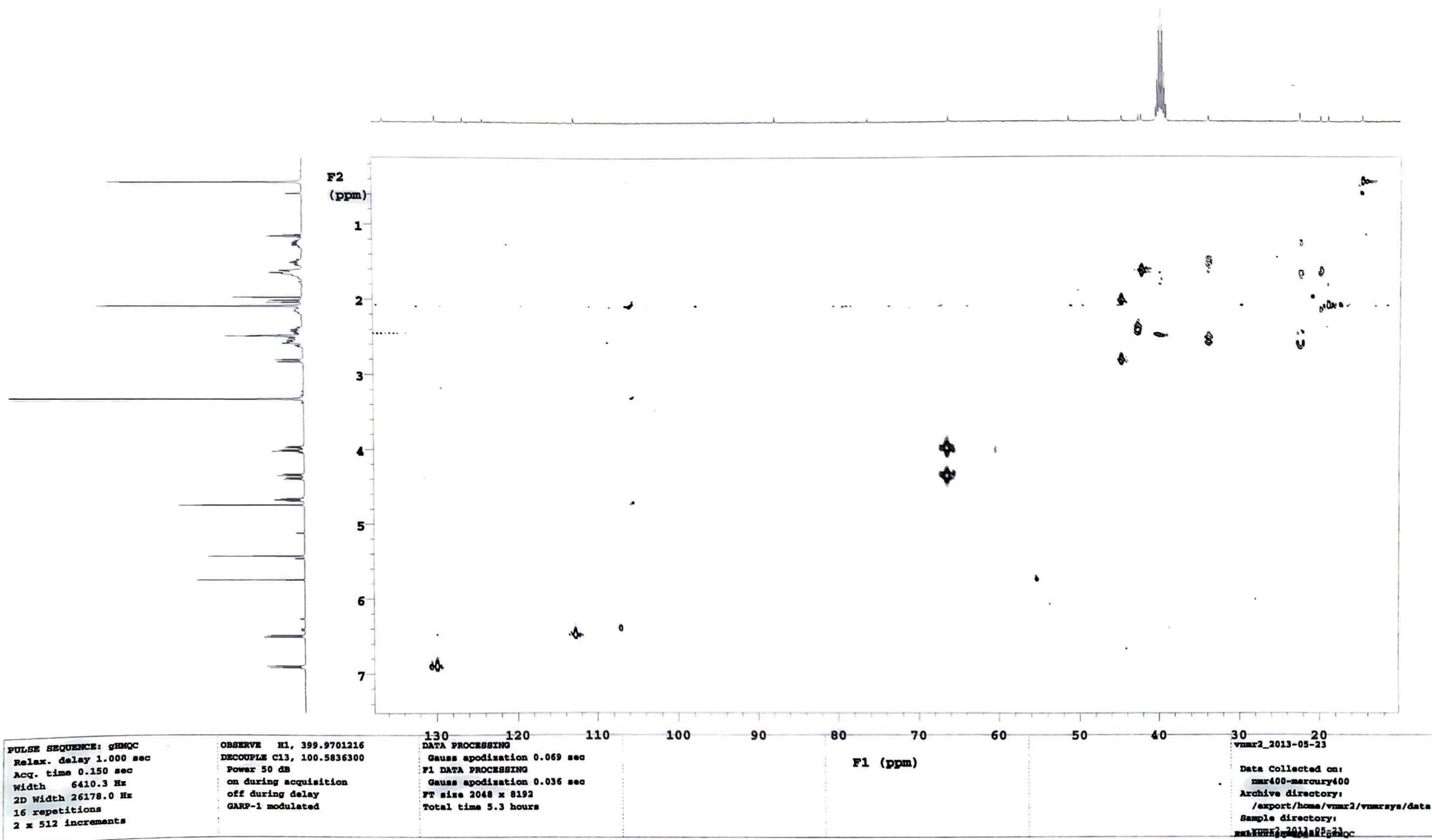
Relax. delay 1.000 sec
Acq. time 0.136 sec
Width 3759.4 Hz
2D Width 3759.4 Hz
Single scan
2048 increments
OBSERVE H1, 399.9701216 MHz
DATA PROCESSING
Sine bell 0.068 sec
F1 DATA PROCESSING
Sine bell 0.034 sec
FT size 4096 x 4096
Total time 1 hr



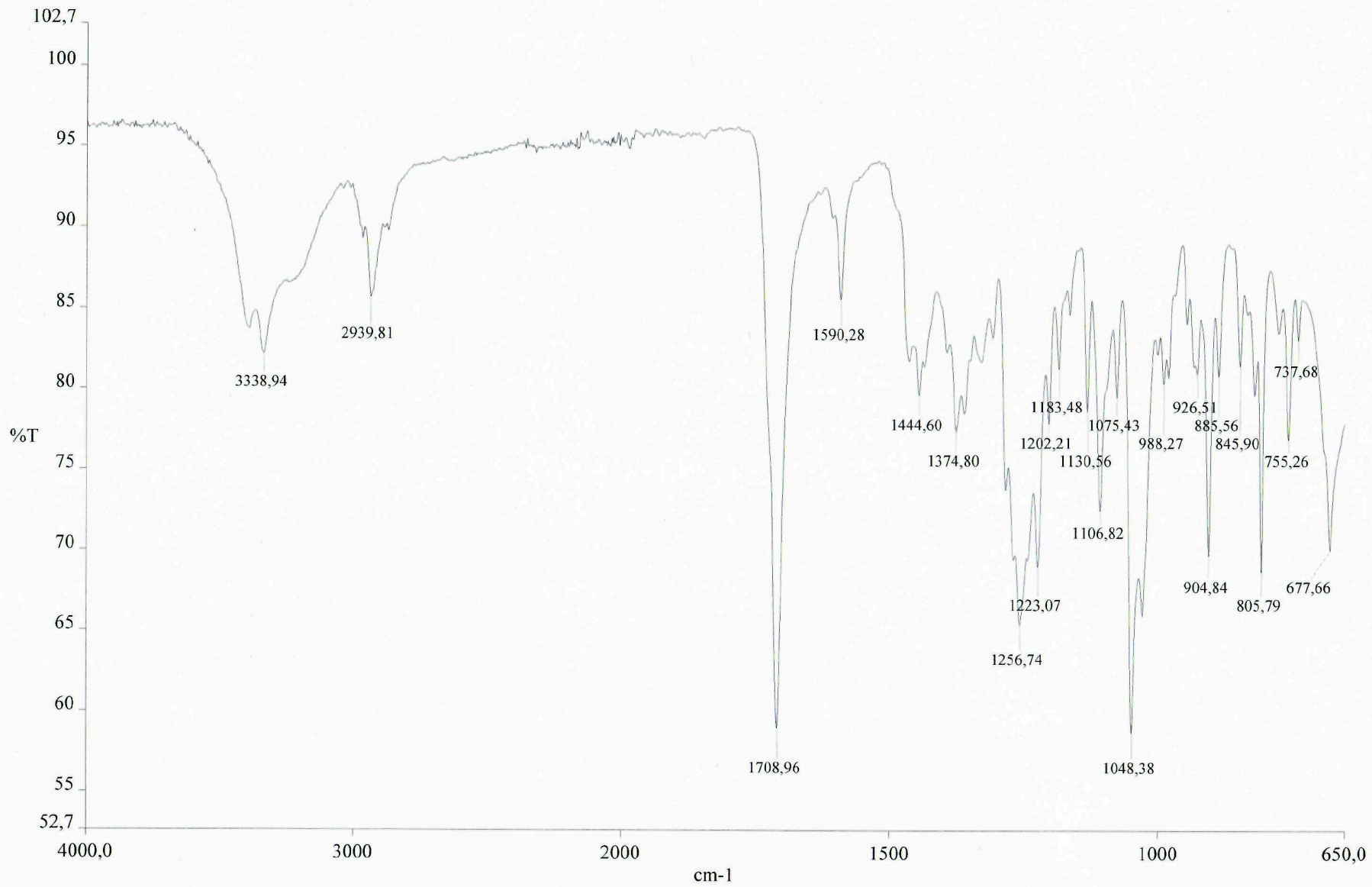
Focused COSY-NMR product 6



HMBC-NMR product 6

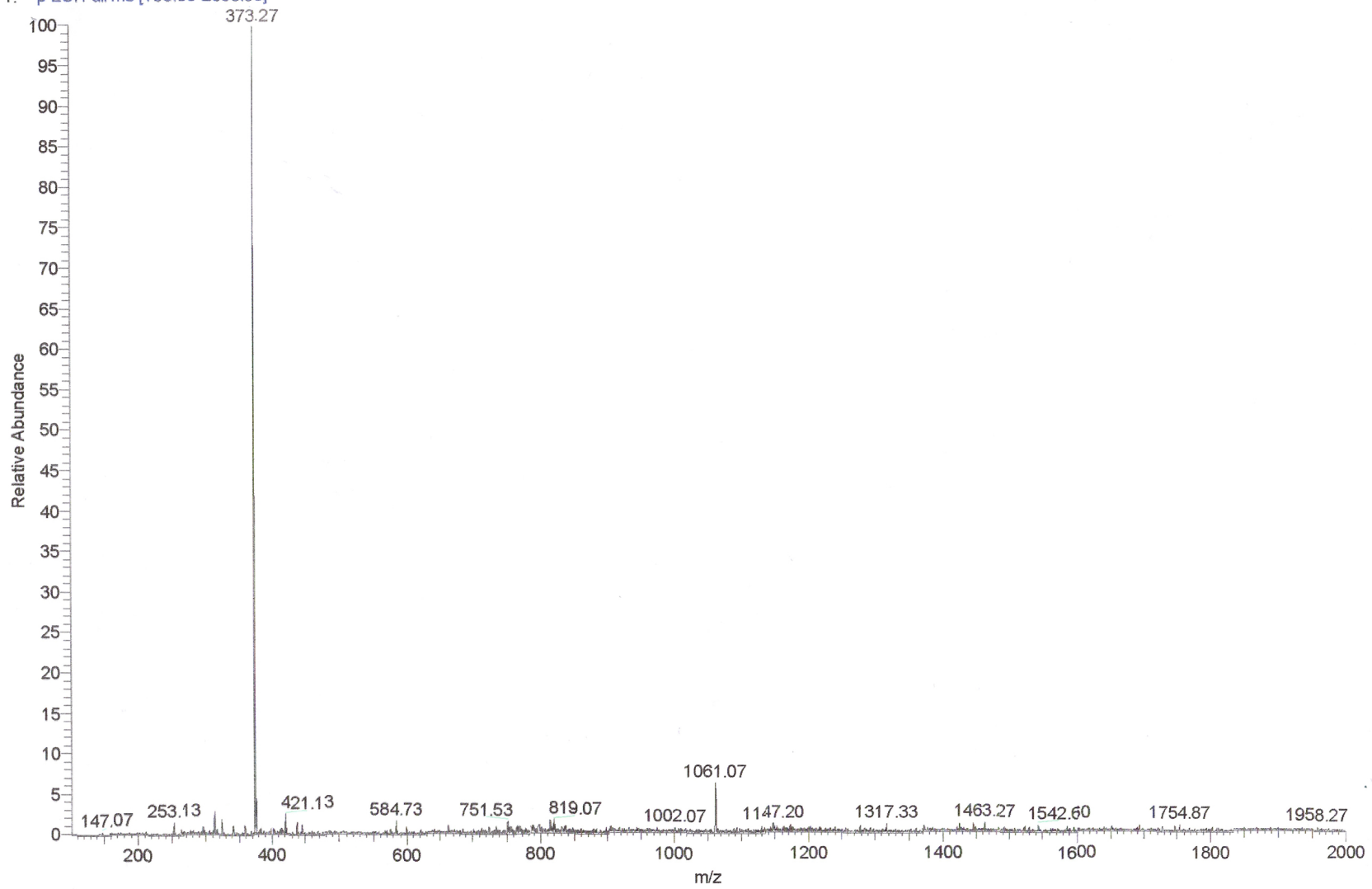


HMQC-NMR product 6

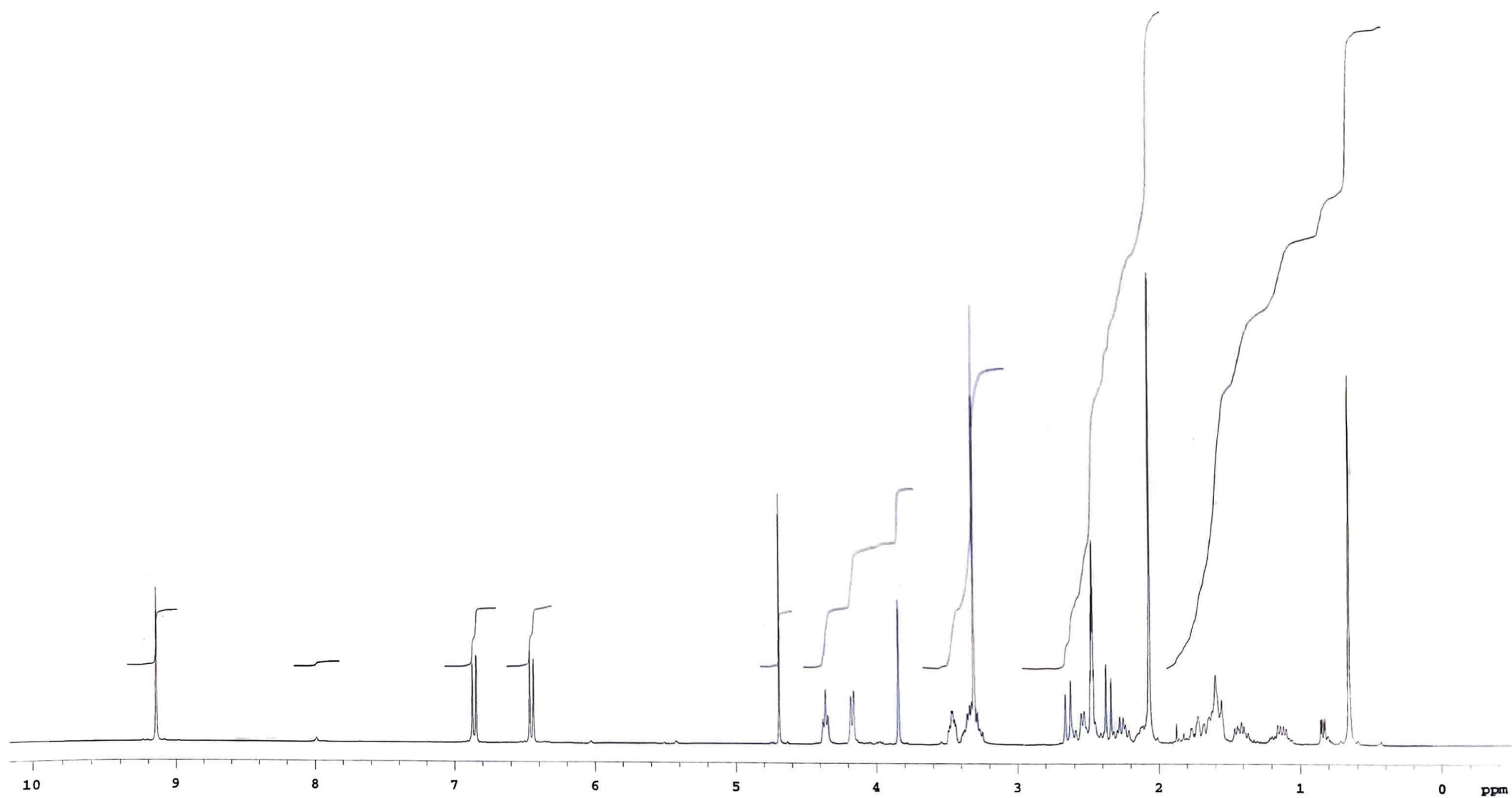


IR product 6

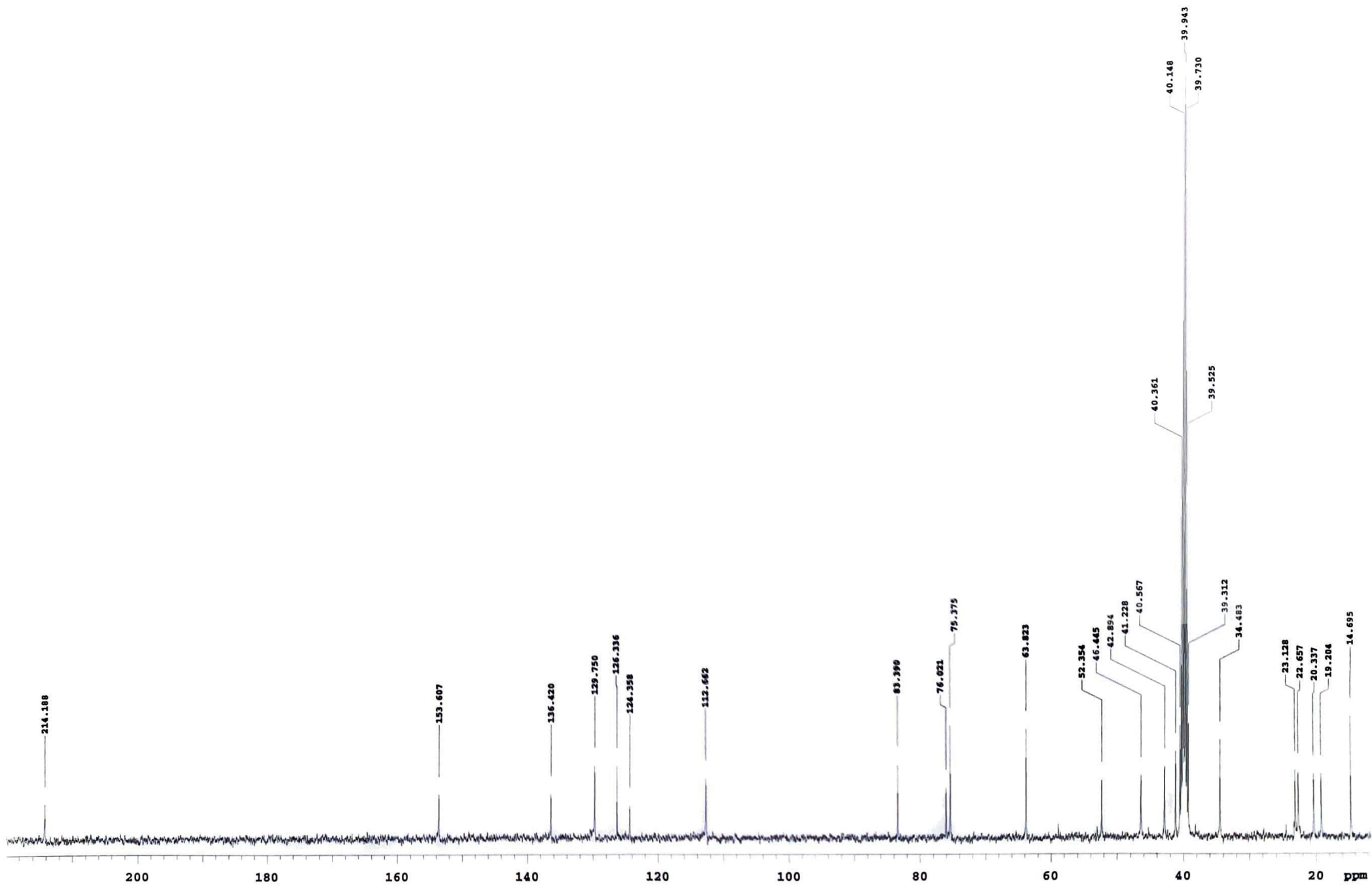
cortisone6 #124-167 RT: 3.53-4.75 AV: 44 NL: 2.87E6
T: -p ESI Full ms [100.00-2000.00]



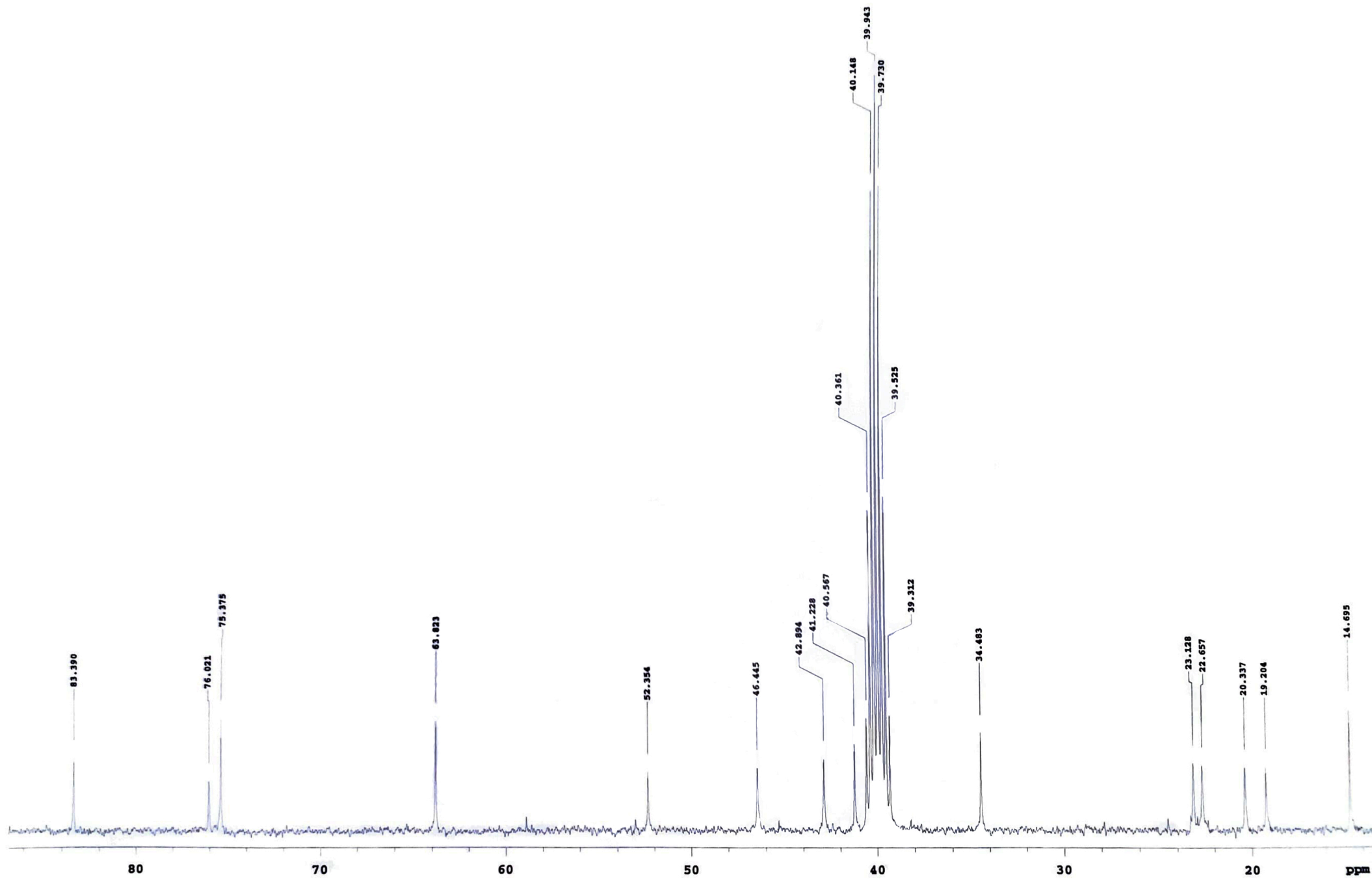
MS product 6



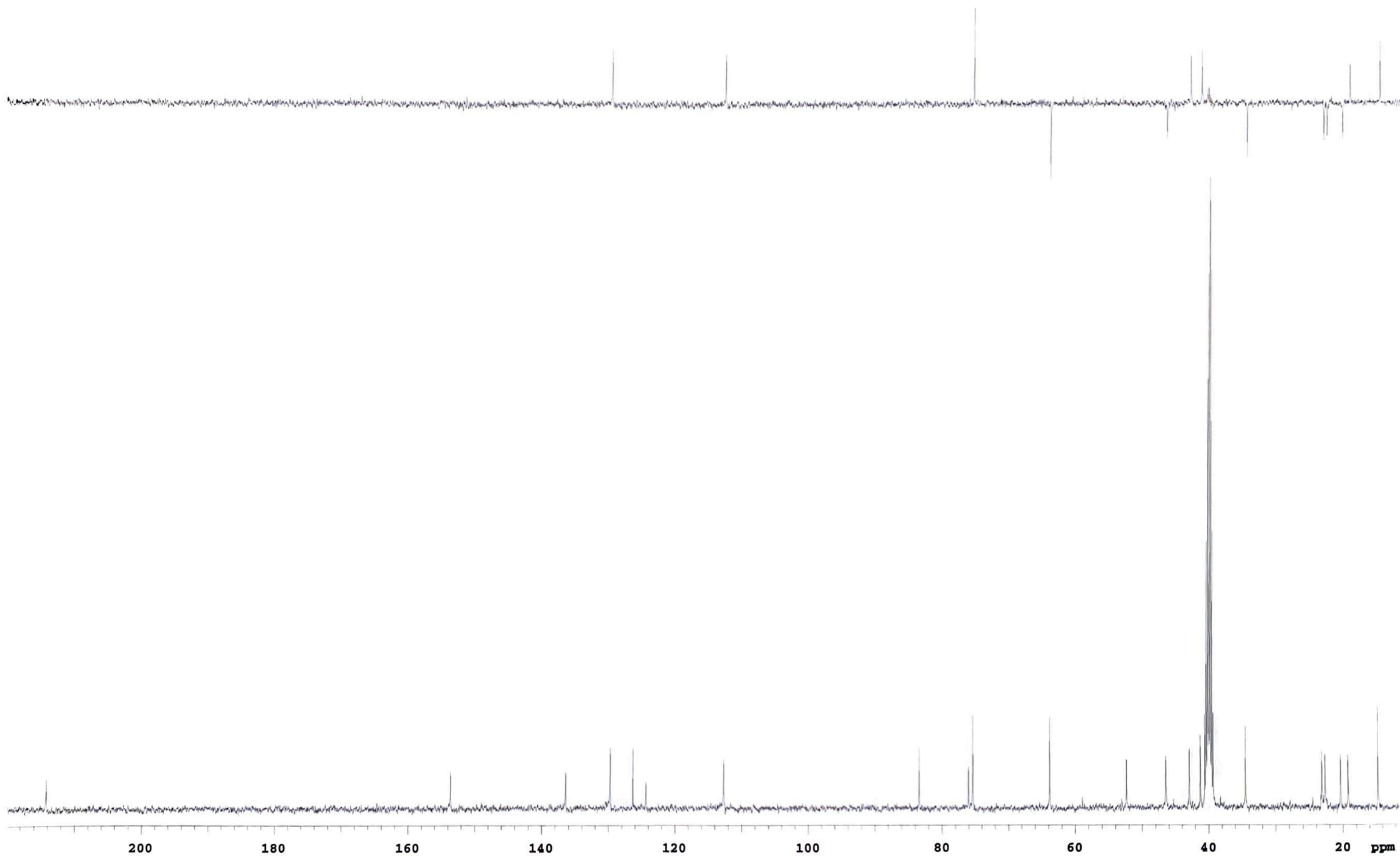
$^1\text{H-NMR}$ product 7



¹³C-NMR product 7



Focused ^{13}C -NMR product 7



DEPT-NMR product 7

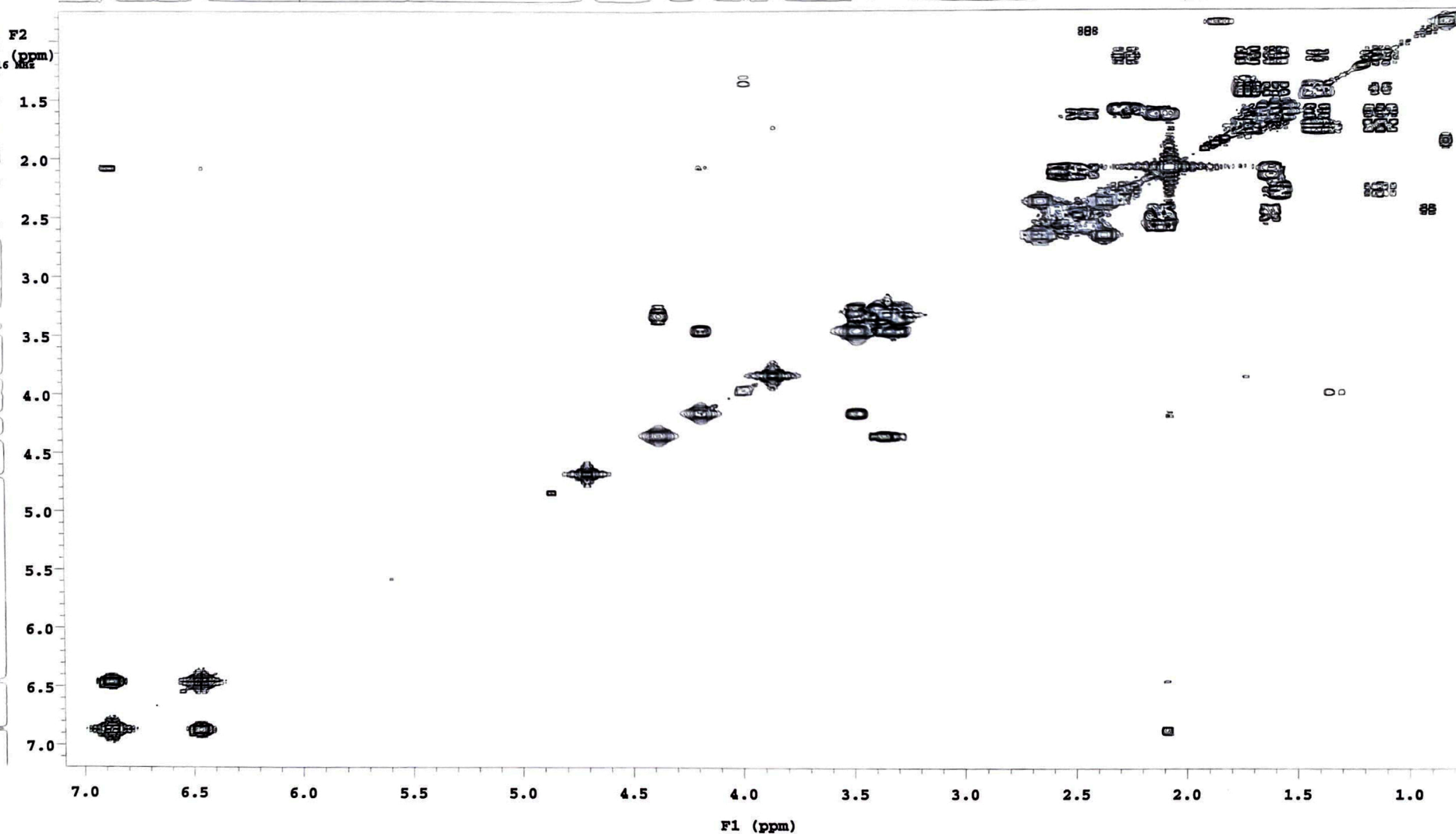
STANDARD 1H OBSERVE

Data Collected on:
mmr400-mercury400
Archive directory:
/export/home/vnmr2/vnmrsys/data
Sample directory:

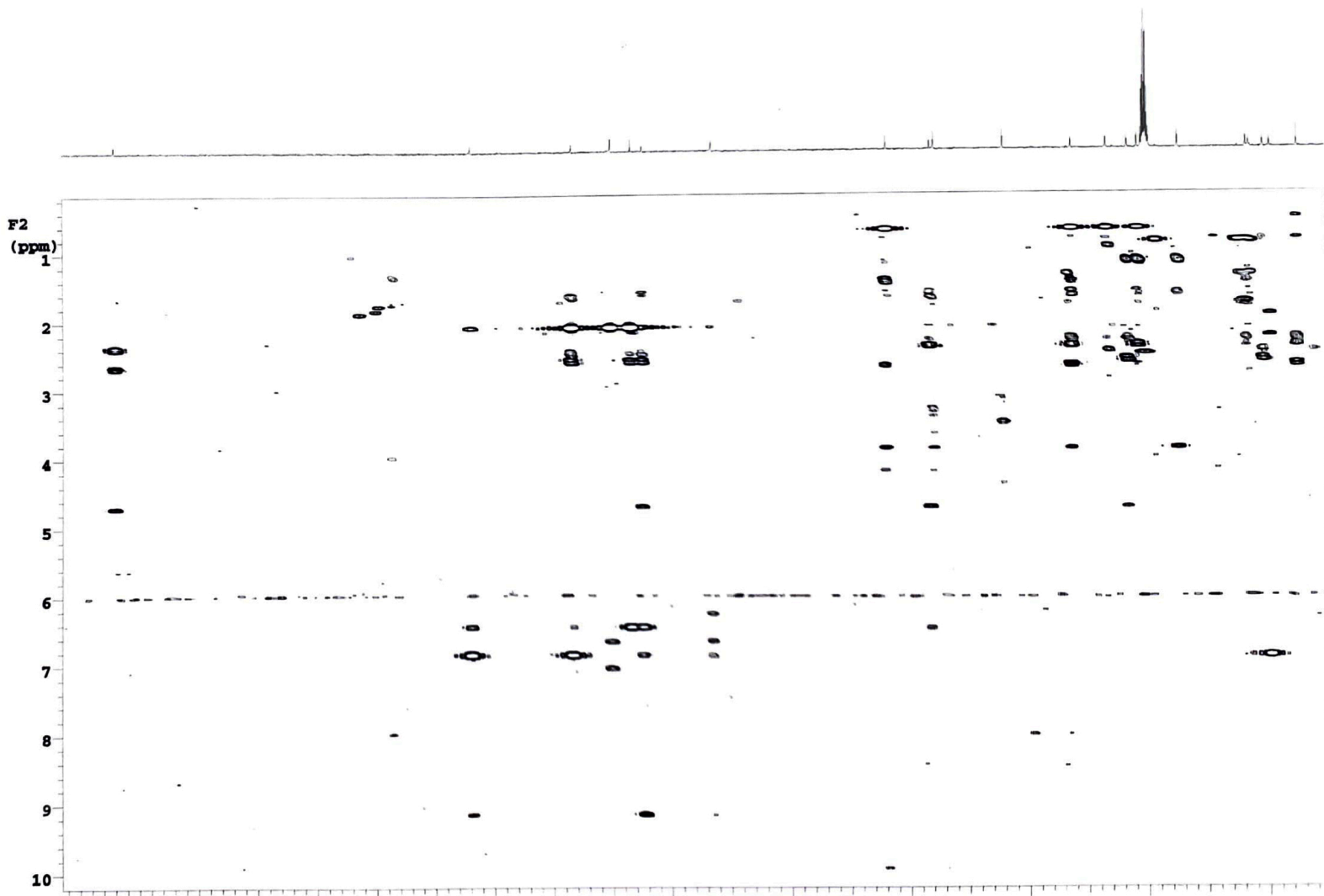
File: gcosy

Pulse Sequence: gcosy
Solvent: DMSO

Relax. delay 1.000 sec
Acq. time 0.142 sec
Width 3623.2 Hz
2D Width 3623.2 Hz
Single scan
1024 increments
OBSERVE H1, 399.9701216 MHz
DATA PROCESSING
Sine bell 0.071 sec
F1 DATA PROCESSING
Sine bell 0.035 sec
FT size 4096 x 4096
Total time 28 min



COSY-NMR product 7



PULSE SEQUENCE: ghmhc
 Relax. delay 1.000 sec
 Acq. time 0.150 sec
 Width 6410.3 Hz
 2D Width 24154.6 Hz
 16 repetitions
 256 increments

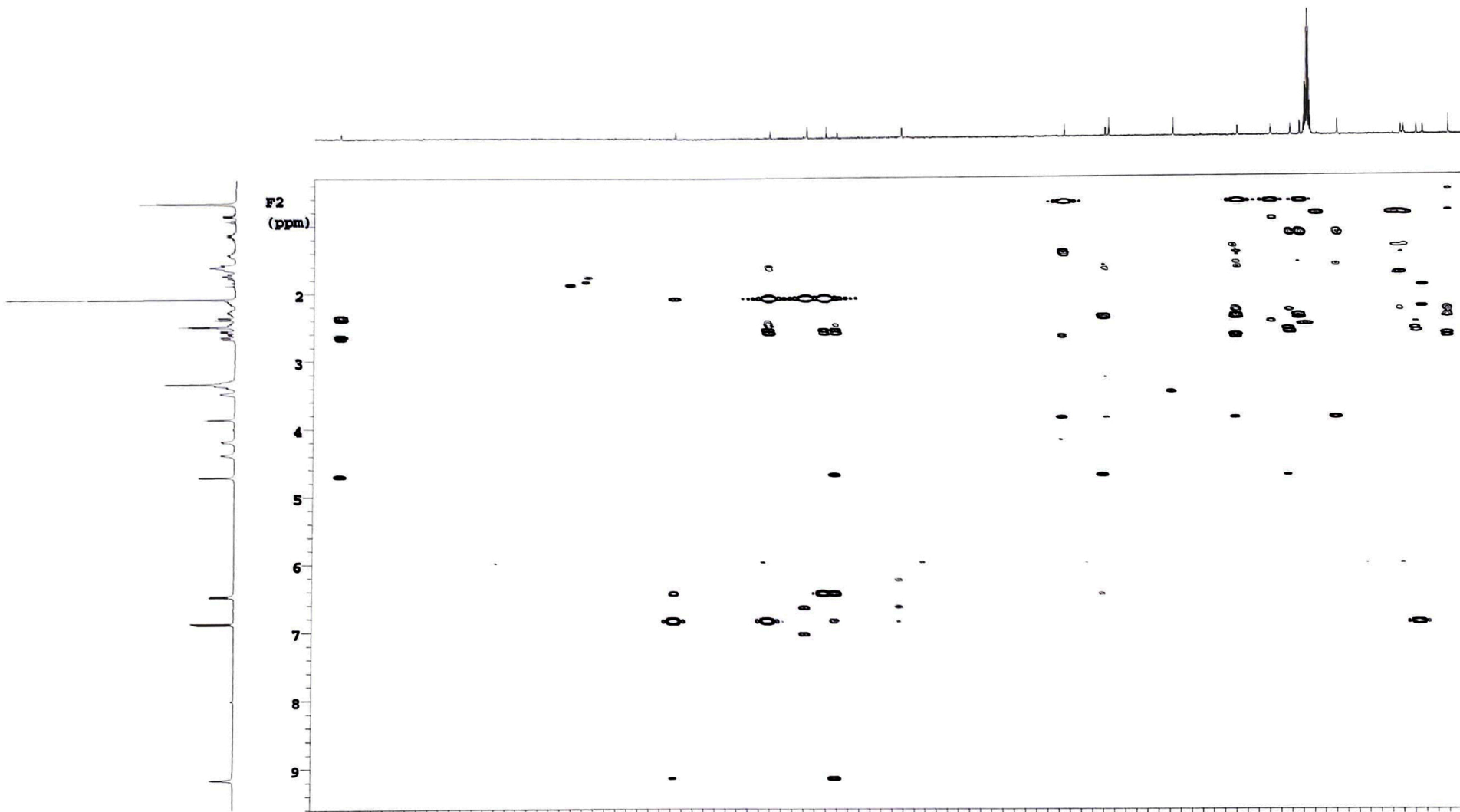
OBSERVE H1, 399.9701216

DATA PROCESSING
 Sine bell 0.075 sec
 F1 DATA PROCESSING
 Sine bell 0.005 sec
 FT size 2048 x 2048
 Total time 79 minutes

F1 (ppm)

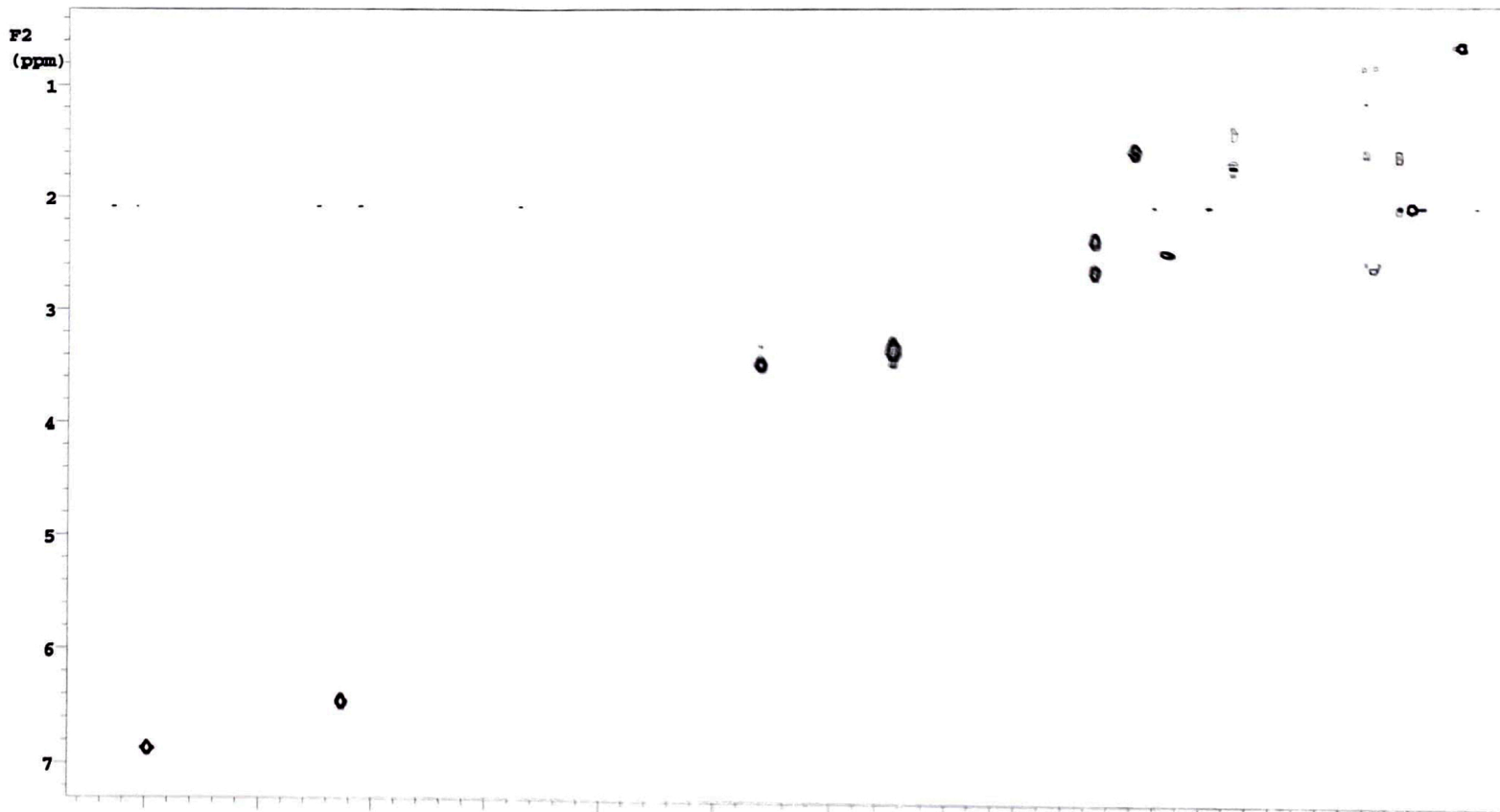
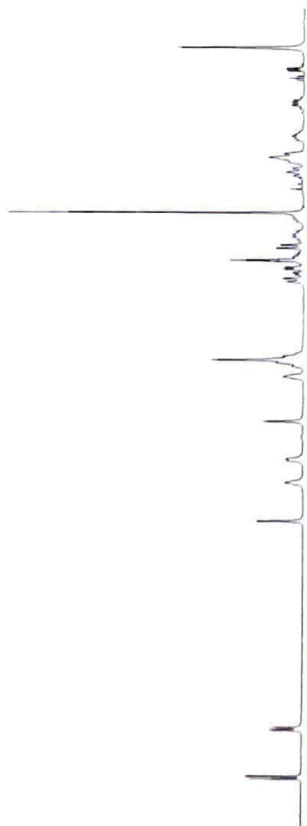
nmr2_2013-06-05
 Data Collected on:
 nmr400-mercury400
 Archive directory:
 /export/home/vnmr2/vnmrsys/data
 Sample directory:
 nmr400-2013-06-05

HMBC-NMR product 7



<p>PULSE SEQUENCE: gHMBC Relax. delay 1.000 sec Acq. time 0.150 sec Width 6410.3 Hz 2D Width 24154.6 Hz 16 repetitions 256 increments</p>	<p>OBSERVE H1, 399.9701216</p>	<p>DATA PROCESSING Sine bell 0.075 sec F1 DATA PROCESSING Sine bell 0.005 sec FT size 2048 x 2048 Total time 79 minutes</p>	<p>200 180 160 140 120 100 80 60 40 20</p>	<p>F1 (ppm)</p>	<p>200 180 160 140 120 100 80 60 40 20</p>	<p>vmnr2_2013-06-05 Data Collected on: mxr400-mercury400 Archive directory: /export/home/vmnr2/vmnrays/data Sample directory: vmnr2_2013-06-05</p>
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Focused HMBC-NMR product 7



PULSE SEQUENCE: ghmqc
 Relax. delay 1.000 sec
 Acq. time 0.150 sec
 Width 4000.0 Hz
 2D Width 24154.6 Hz
 8 repetitions
 2 x 256 increments

OBSERVE H1, 399.9701216
 DECOUPLE C13, 100.5831272
 Power 50 dB
 on during acquisition
 off during delay
 GARP-1 modulated

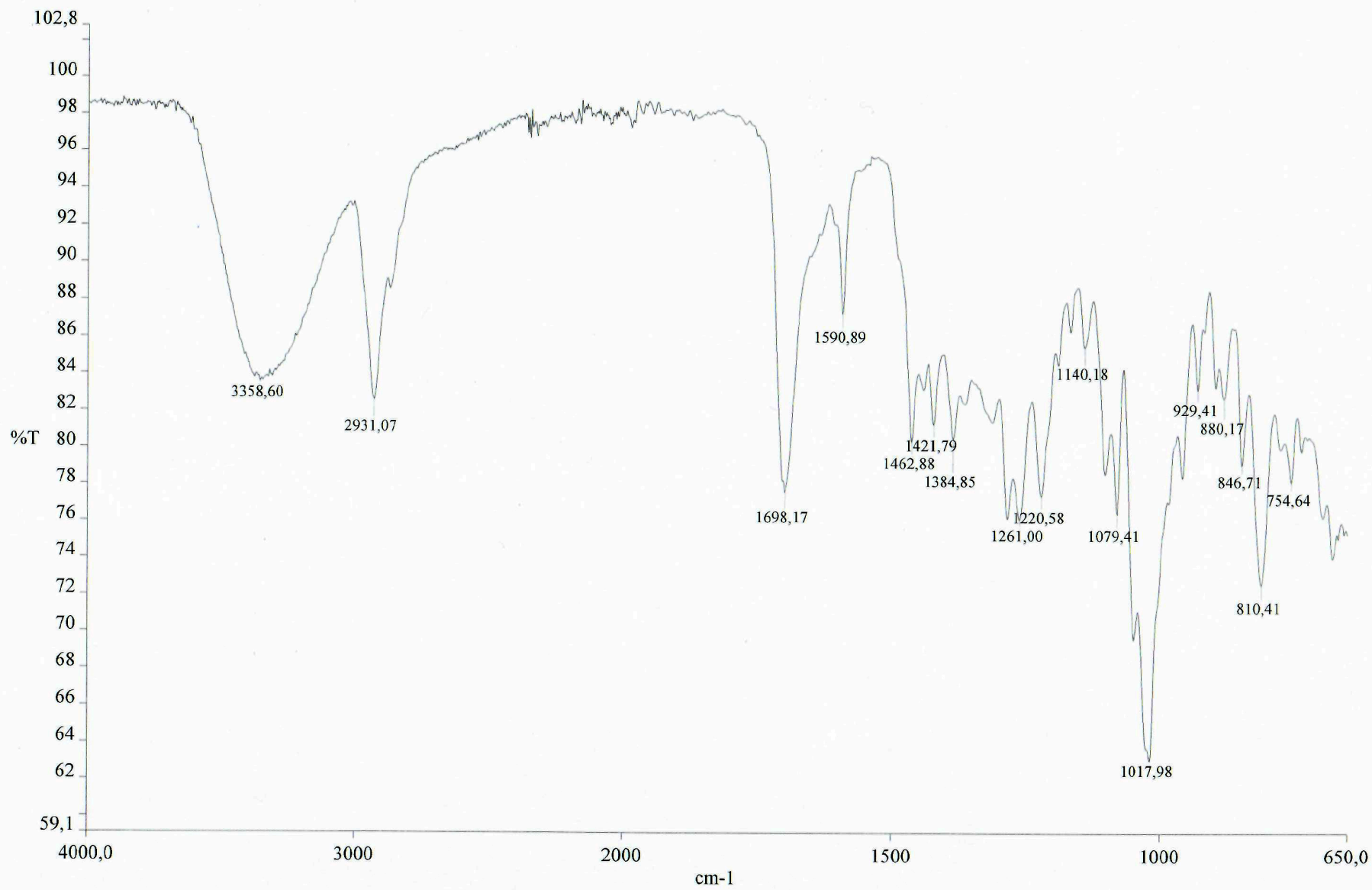
130 120 110 100 90 80 70 60 50 40 30 20
 DATA PROCESSING
 Gauss apodisation 0.069 sec
 F1 DATA PROCESSING
 Gauss apodisation 0.020 sec
 FT size 1024 x 4096
 Total time 79 minutes

F1 (ppm)

30 20
 vnmr2_2013-06-05

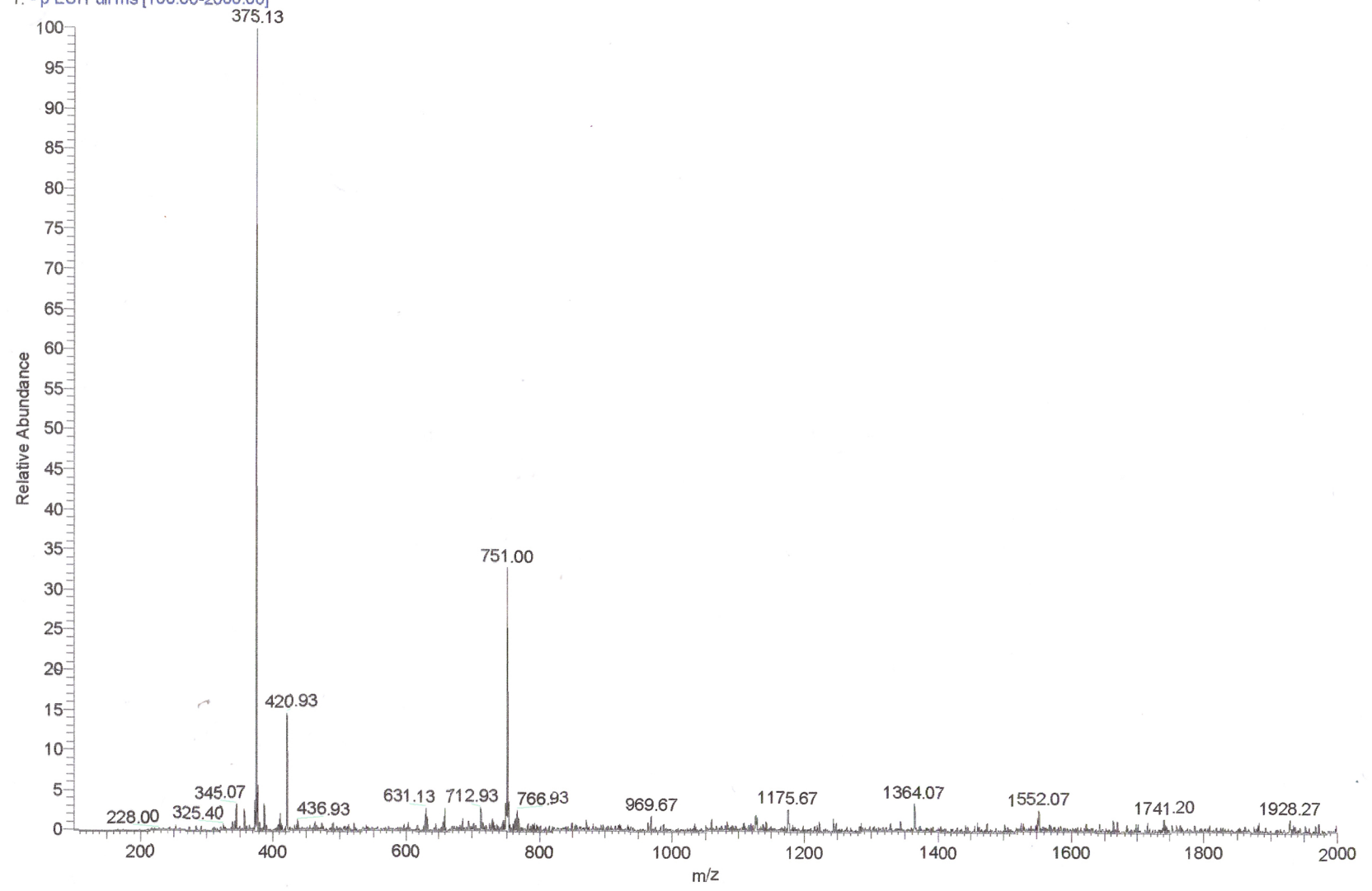
Data Collected on:
 nmr400-mercury400
 Archive directory:
 /export/home/vnmr2/vnmrays/data
 Sample directory:
 nmr400-2013-06-05

HMQC-NMR product 7



IR product 7

cortisone7 #97-114 RT: 2.75-3.23 AV: 18 NL: 8.62E5
T: - p ESI Full ms [100.00-2000.00]



MS product 7