

Sample # 2

File: MES-1-F31-2
Sample: RABIA FAROOQ / DR. M. IQBAL
Instrument: JEOL MS 600H-1

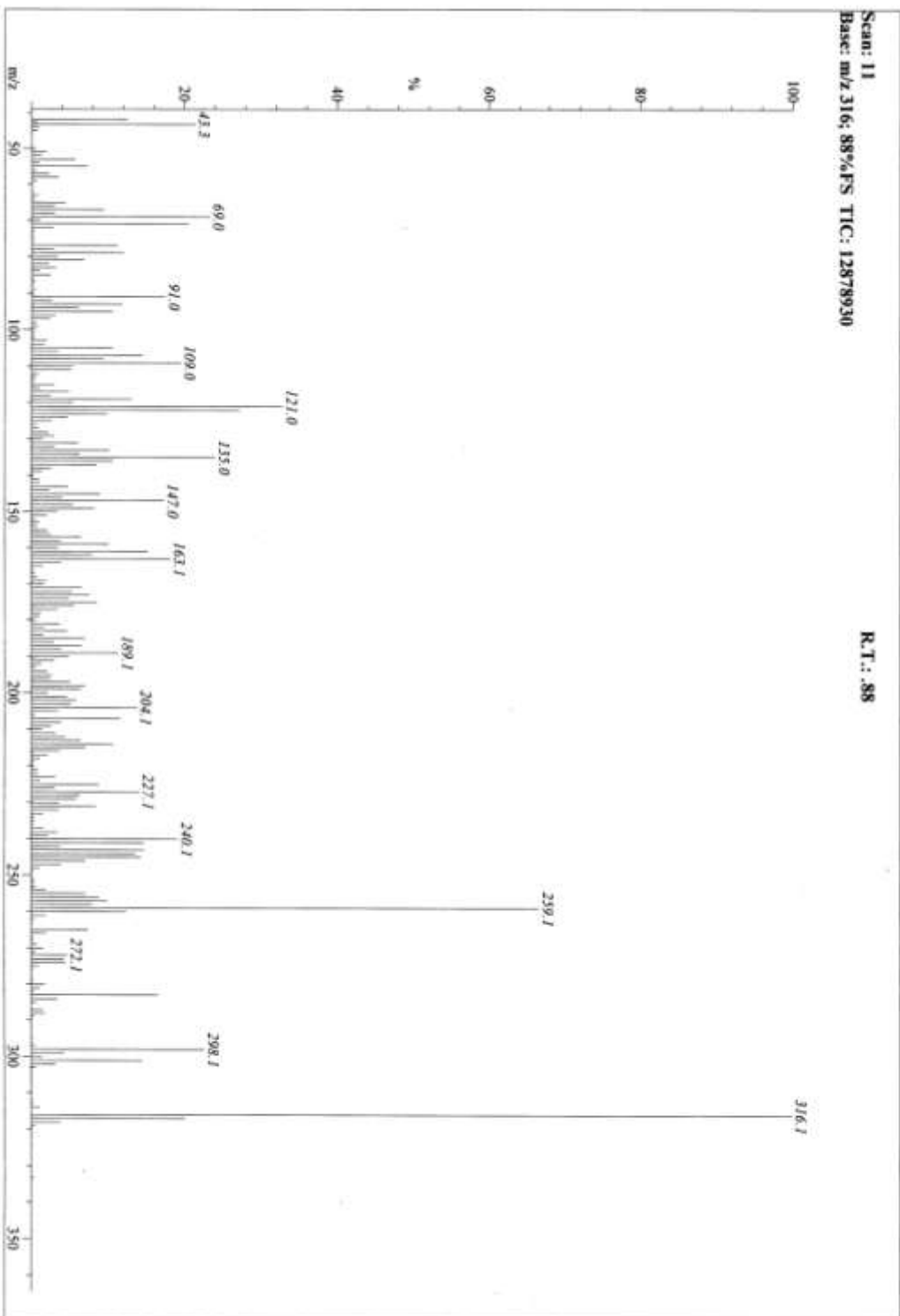
Date Run: 01-13-2016 (Time Run: 09:32:01)

Ionization mode: EI+

Scan: 11

Base: m/z 316; 88%FS TIC: 12879930

R.T.: .88

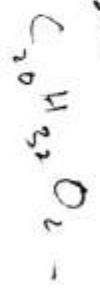


Compound # 2

nicotinic fatty acid

Mass	Theoretical Mass	Delta [ppm]	Delta [amu]	RDB	Composition
316.2039	316.2033	1.9	0.6	7.0	$C_{20}H_{26}O_3$ ✓
301.1806	301.1798	2.6	0.8	7.5	$C_{19}H_{25}O_3$
298.1940	298.1927	4.3	1.3	8.0	$C_{20}H_{26}O_2$

substitute 304.



metabolite



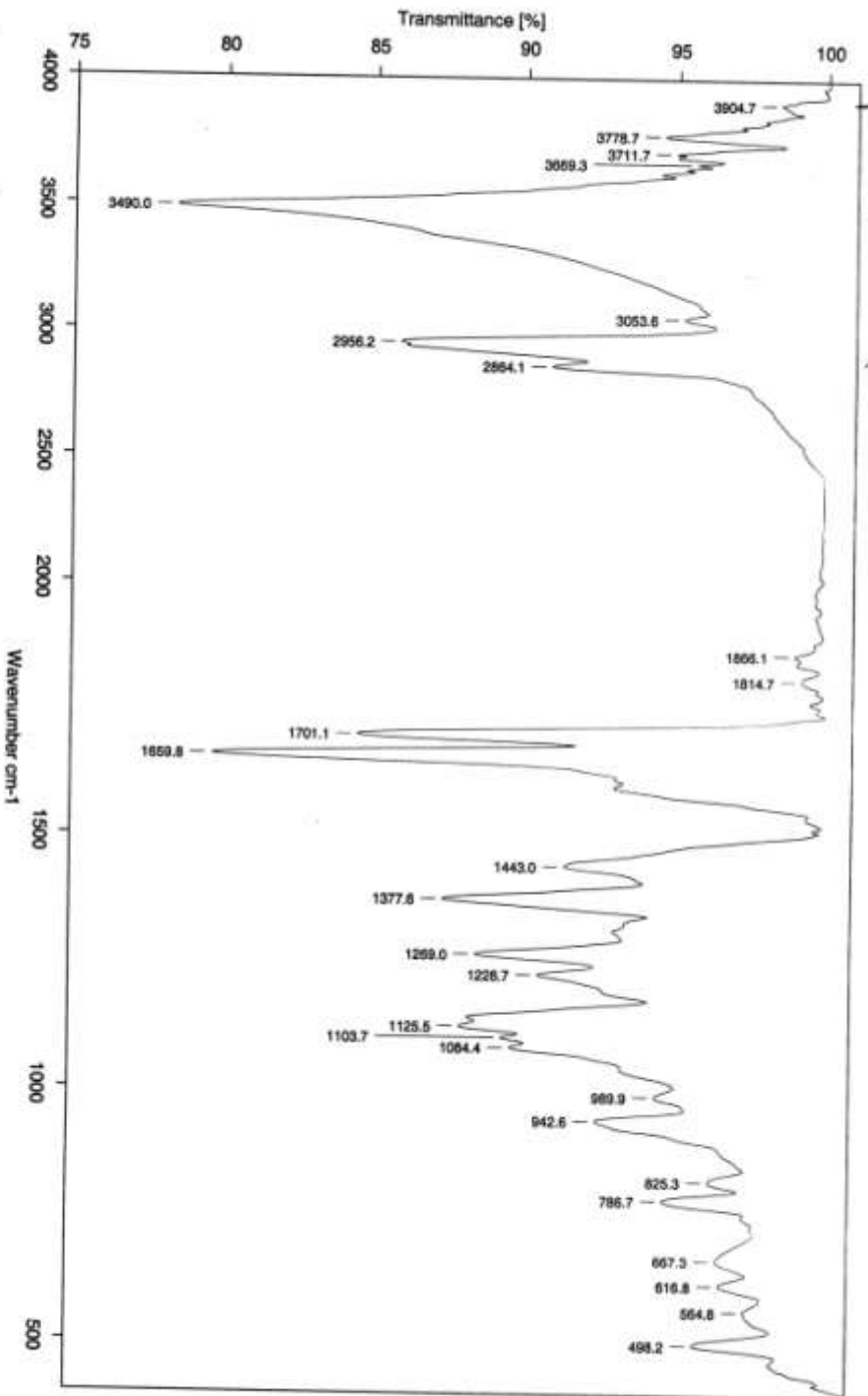
addition of O
loss of u.H.

Distance

14

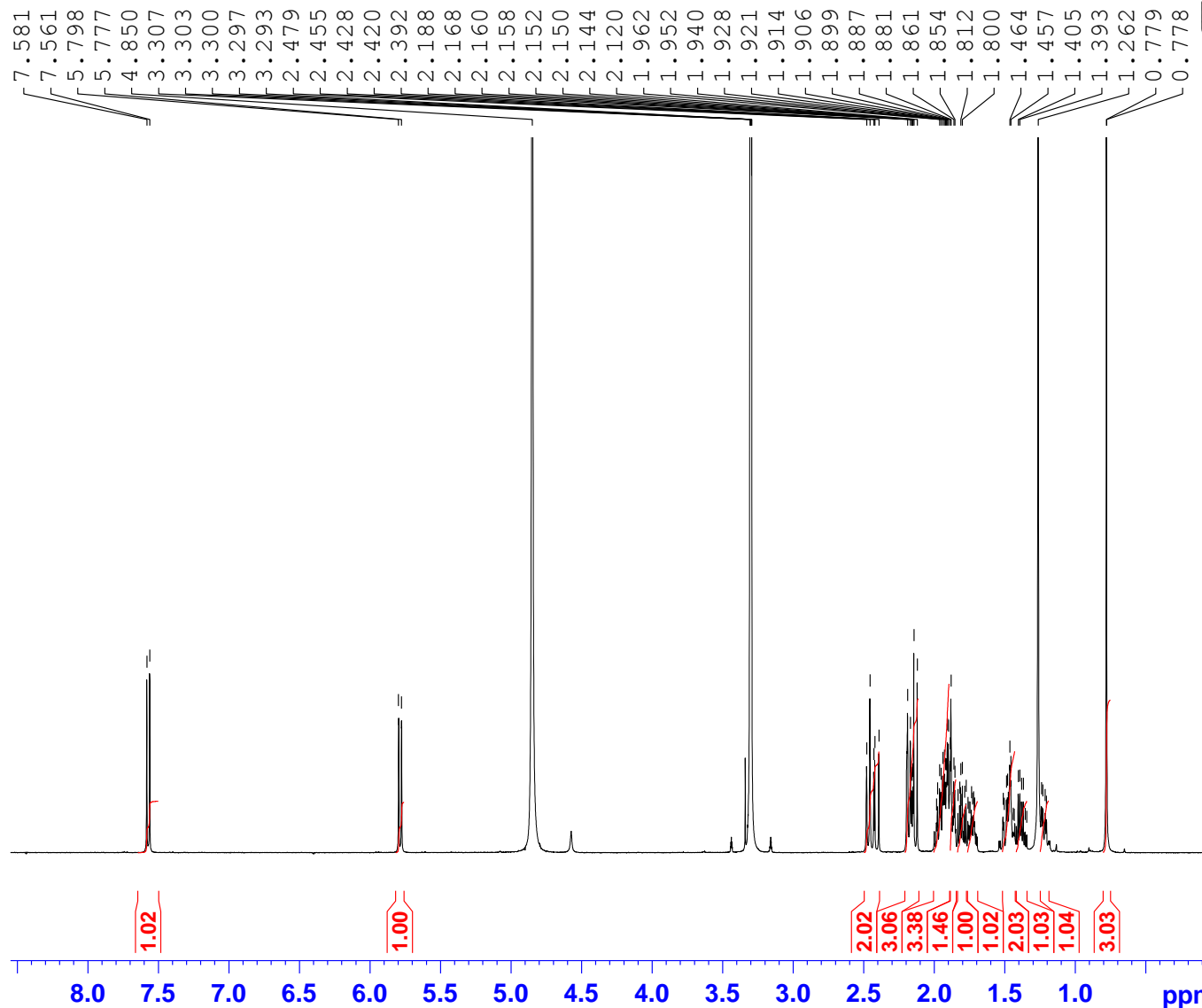
Compound # 2

I. C.C.B.S., University of Kar u Analytical Laboratory - Pakistan



Sample : Mes-J-F31-2/Rabia Farooq/Prof. Dr. M. I. Choudhary
Measured : 10/11/2016 on VECTOR22
Resolution : 4 cm-1 (10 scans)
Spectrum : Mes-J-F31-2.0 (In D:\IRSTUDENT)
Technic : SOLID
Analyst : M.Q.sif/ZQ

RABIA/DR.IQBAL/MES/J/F31-2/CD3OD



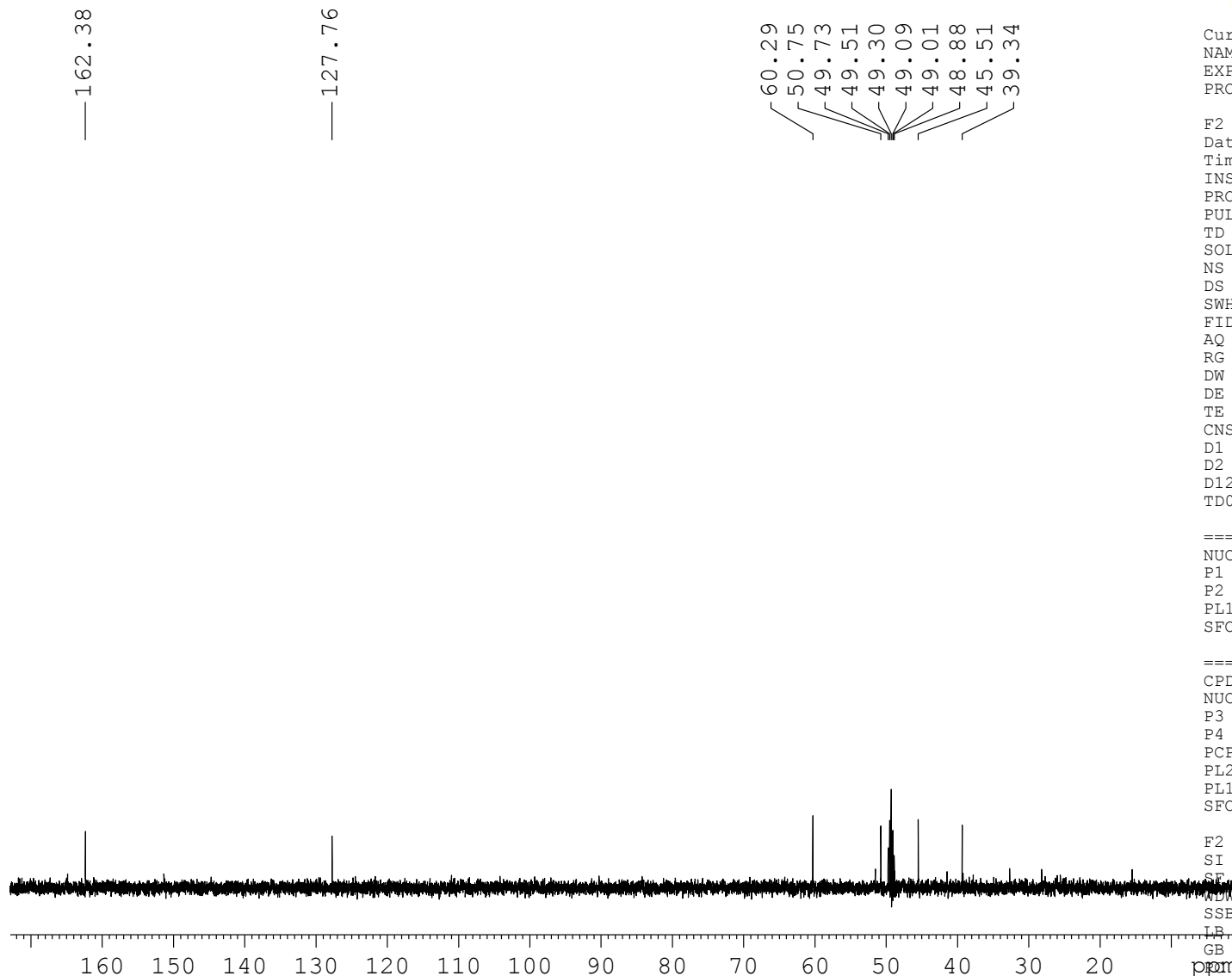
Current Data Parameters
NAME compd 2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160107
Time_ 19.35
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 128
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 256
DW 41.600 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 8.03 usec
PL1 3.00 dB
SFO1 500.2350023 MHz

F2 - Processing parameters
SI 32768
SF 500.2300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

RABIA FAROOQ/DR, IQBAL/Mes/J/F31-2/
ICCBS, U.O.K/DEPT-90



Current Data Parameters
NAME compd 2
EXPNO 5
PROCNO 1

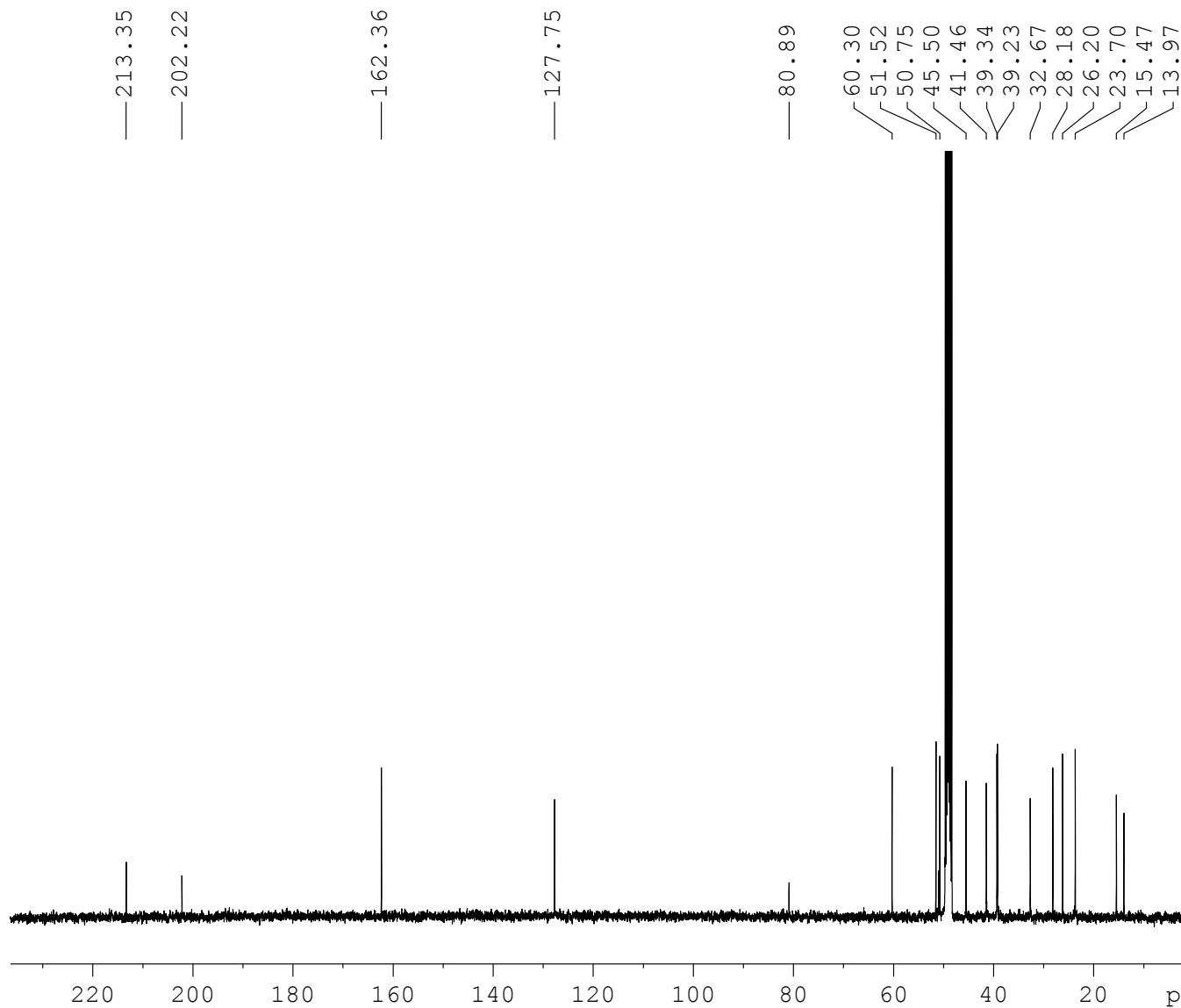
F2 - Acquisition Parameters
Date_ 20160607
Time_ 11.36
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept90
TD 32768
SOLVENT MeOD
NS 1271
DS 2
SWH 19157.088 Hz
FIDRES 0.584628 Hz
AQ 0.8552448 sec
RG 32768
DW 26.100 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 3

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
P2 16.20 usec
PL1 7.00 dB
SFO1 100.6220254 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
P3 9.80 usec
P4 19.60 usec
PCPD2 80.00 usec
PL2 0 dB
PL12 20.00 dB
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 100.6126252 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

RABIA FAROOQ/DR, IQBAL/Mes/J/F31-2/
ICCBS, U.O.K/BB/



Current Data Parameters
NAME compd 2
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160606
Time 15.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
TD 32768
SOLVENT MeOD
NS 20480
DS 2
SWH 24154.590 Hz
FIDRES 0.737140 Hz
AQ 0.6782976 sec
RG 32768
DW 20.700 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 20

==== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 7.00 dB
SFO1 100.6243395 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 100.6126252 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.00

RABIA FAROOQ/DR, IQBAL/Mes/J/F31-2/
ICCBS, U.O.K/DEPT 135

— 162.38

— 127.76

60.29
51.52
50.75
49.73
49.51
49.30
49.09
49.01
48.87
45.51
41.47
39.34
39.22
32.68
28.19
26.21
23.70
15.48
13.98



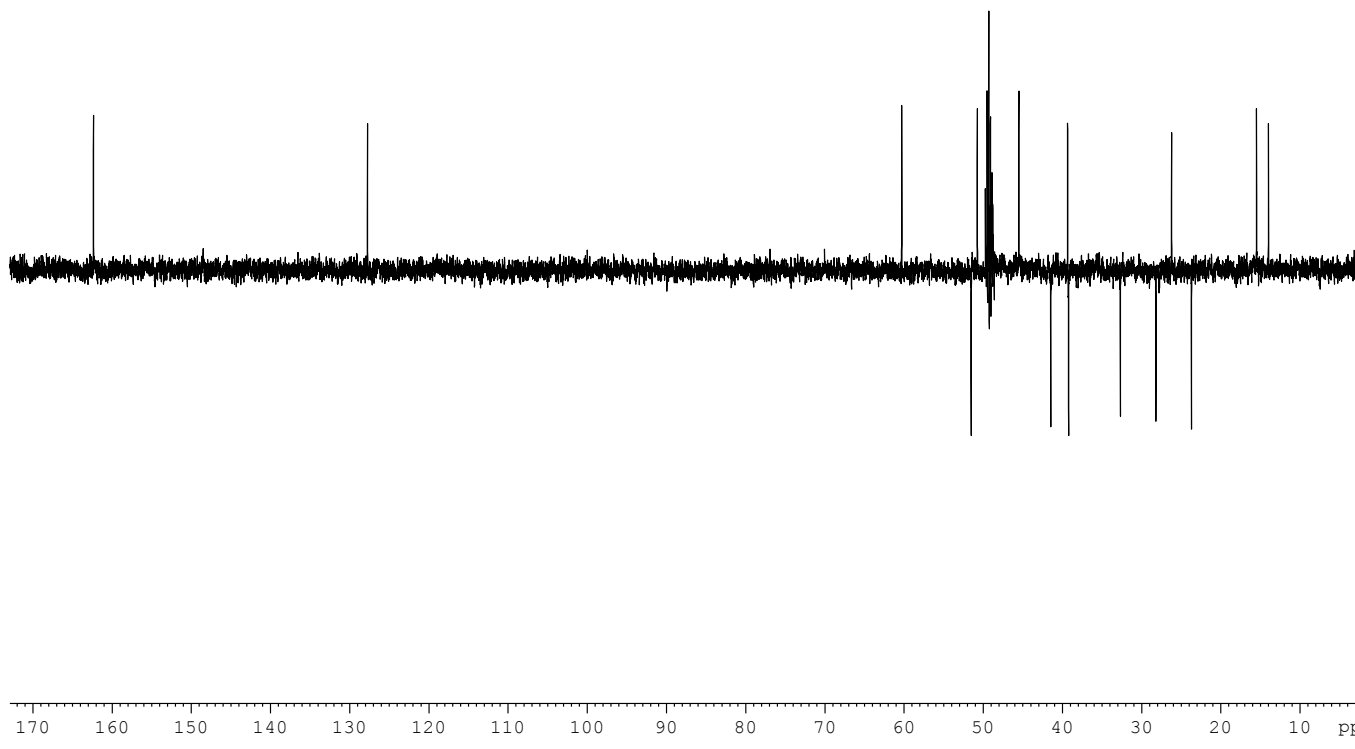
Current Data Parameters
NAME compd 2
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date 20160607
Time 7.22
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 32768
SOLVENT MeOD
NS 6414
DS 2
SWH 19157.088 Hz
FIDRES 0.584628 Hz
AQ 0.8552448 sec
RG 32768
DW 26.100 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 9

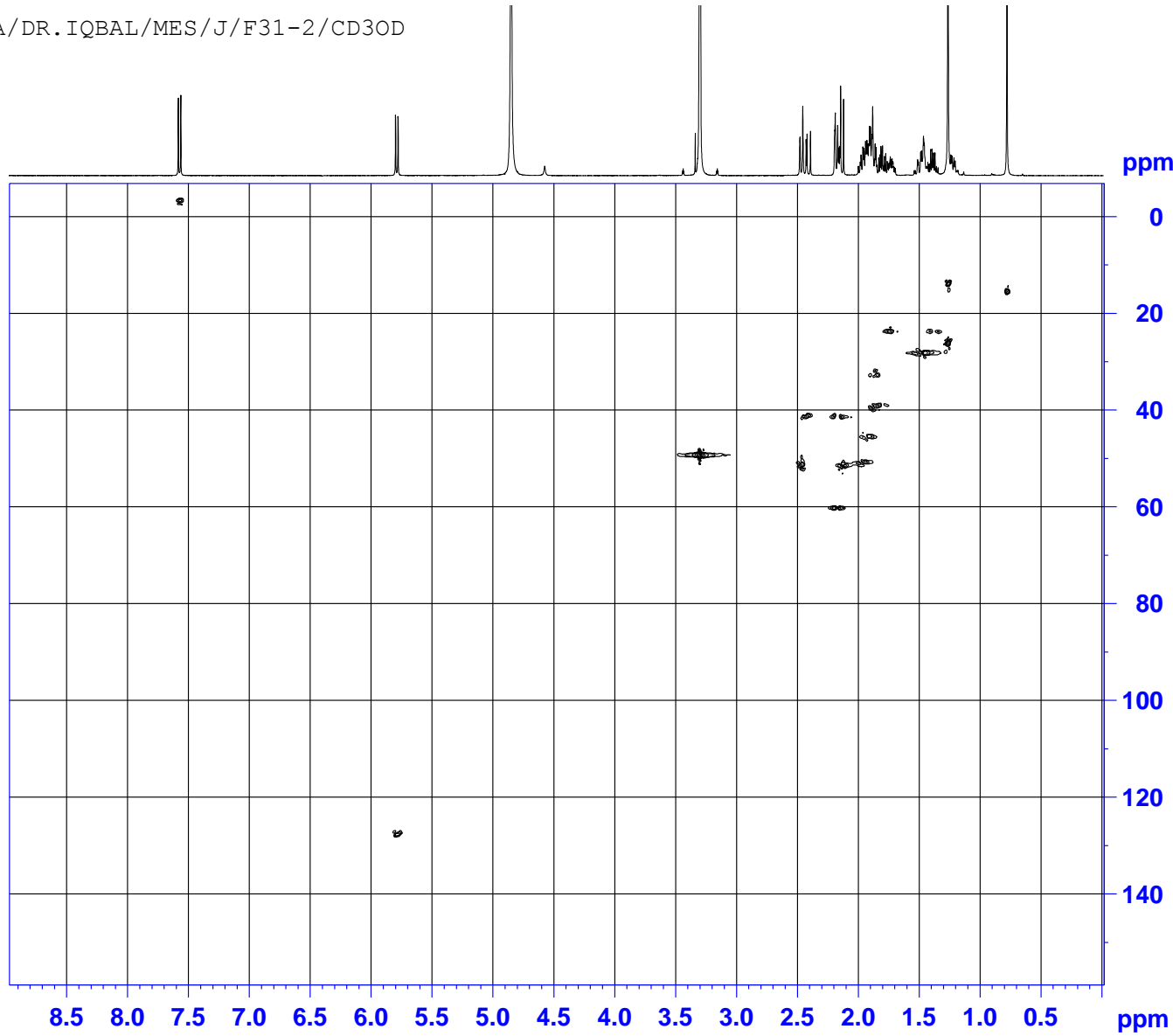
==== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
P2 16.20 usec
PL1 7.00 dB
SFO1 100.6220254 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
P3 9.80 usec
P4 19.60 usec
PCPD2 80.00 usec
PL2 0 dB
PL12 20.00 dB
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 100.6126252 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40



RABIA/DR.IQBAL/MES/J/F31-2/CD3OD



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Current Data Parameters
NAME      compd 2
EXPNO    13
PROCNO   1

F2 - Acquisition Parameters
Date_    20160108
Time     0.05
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  hsqcedetgp
TD       1024
SOLVENT  MeOD
NS       32
DS       16
SWH      4496.403 Hz
FIDRES   4.391018 Hz
AQ       0.1138688 sec
RG       18390.4
DW       111.200 usec
DE       6.50 usec
TE       295.9 K
CNST2    145.0000000
D0       0.00000300 sec
D1       1.50000000 sec
D4       0.00172414 sec
D11      0.03000000 sec
D13      0.00000400 sec
D16      0.00020000 sec
D21      0.00345000 sec
IN0      0.00002400 sec
ZGOFPTS

===== CHANNEL f1 =====
NUC1     1H
P1       8.03 usec
P2       16.06 usec
P28      1000.00 usec
PL1      3.00 dB
SFO1     500.2322510 MHz

===== CHANNEL f2 =====
CPDPRG2  garp
NUC2     13C
P3       13.35 usec
P4       26.70 usec
PCPD2    70.00 usec
PL2      -3.00 dB
PL12     10.00 dB
SFO2     125.7923151 MHz

===== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1     80.00 %
GPZ2     20.10 %
P16      1000.00 usec

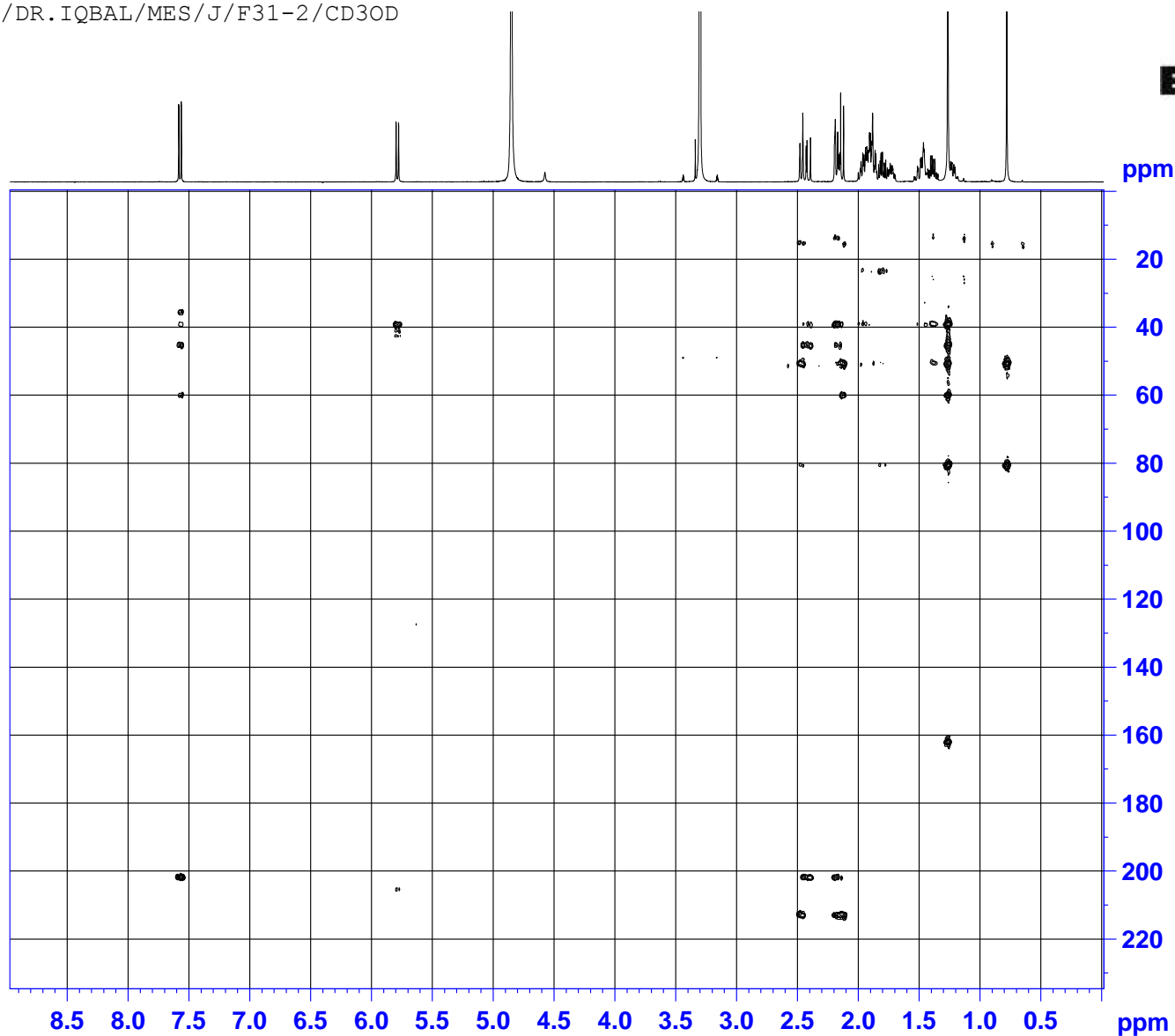
F1 - Acquisition parameters
TD       256
SFO1     125.7923 MHz
FIDRES   162.782379 Hz
SW       165.639 ppm
FnMODE   Echo-Antiecho

F2 - Processing parameters
SI       1024
SF       500.2300120 MHz
WDW      QSINE
SSB      2
LB       0 Hz
GB       0
PC       0.80

F1 - Processing parameters
SI       1024
MC2      echo-antiecho
SF       125.7827558 MHz
WDW      QSINE
SSB      2
LB       0 Hz
GB       0
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RABIA/DR.IQBAL/MES/J/F31-2/CD3OD

HMBC



Current Data Parameters
NAME comp1 2
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160108
Time 3.51
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG hmbcgp1pndqf
TD 2048
SOLVENT MeOD
NS 64
DS 16
SWH 4496.403 Hz
FIDRES 2.195509 Hz
AQ 0.2277376 sec
RG 20642.5
DW 111.200 usec
DE 6.50 usec
TE 295.4 K
CNST2 145.000000
CNST13 10.000000
D0 0.0000000 sec
D1 2.0000000 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
IN0 0.00001690 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.03 usec
P2 16.06 usec
PL1 3.00 dB
SFO1 500.2322510 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 13.35 usec
PL2 -3.00 dB
SFO2 125.7974871 MHz

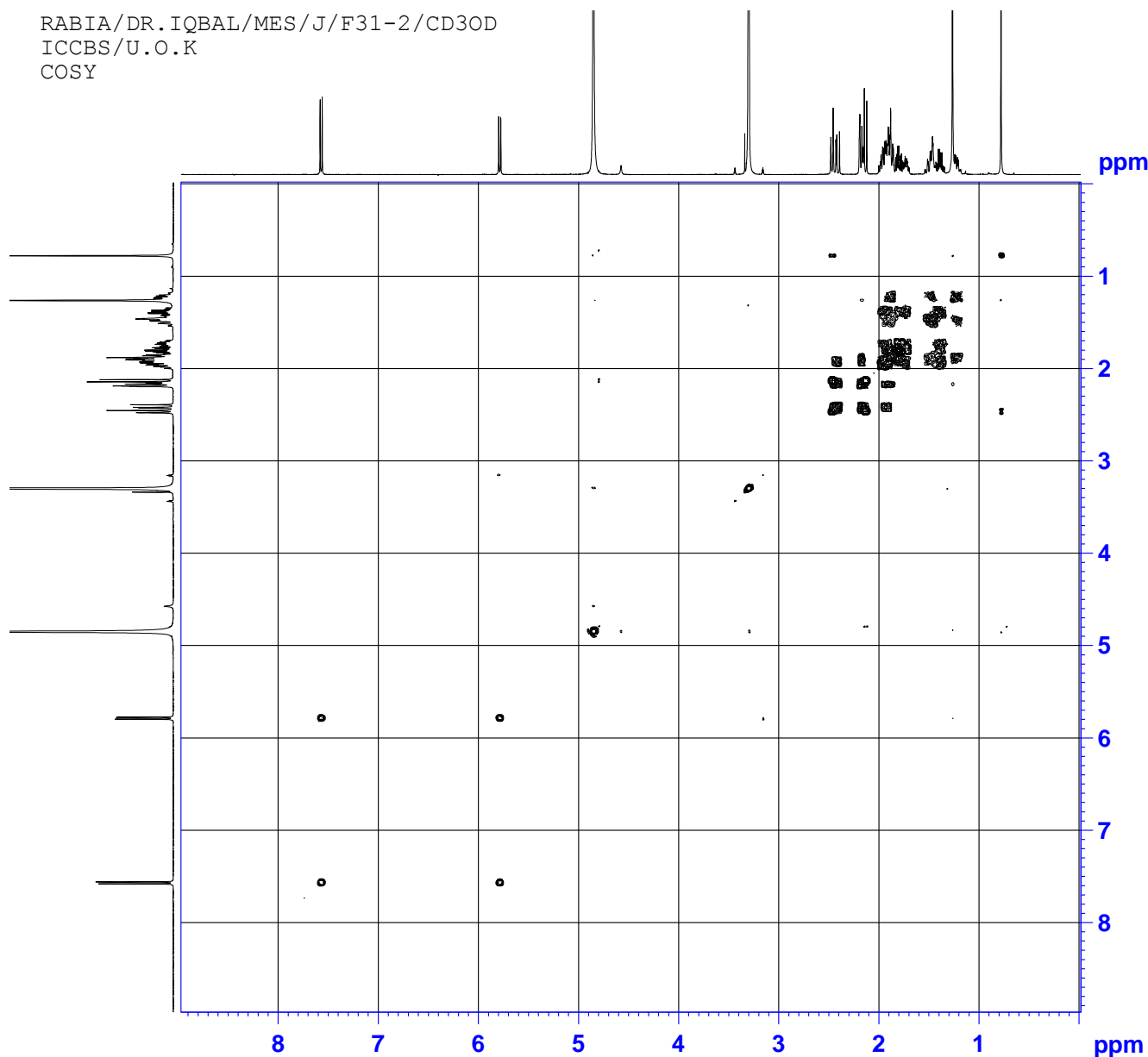
===== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPNAM[3] SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 125.7975 MHz
FIDRES 230.956329 Hz
SW 235.000 ppm
FhMODE QF

F2 - Processing parameters
SI 1024
SF 500.2300120 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
FC 1.00

F1 - Processing parameters
SI 512
MC2 QF
SF 125.7827558 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

RABIA/DR. IQBAL/MES/J/F31-2/CD3OD
ICCBS/U.O.K
COSY



Current Data Parameters
NAME compd 2
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160107
Time 19.35
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG cosydfqf
TD 2048
SOLVENT MeOD
NS 8
DS 8
SWH 4496.403 Hz
FIDRES 2.195509 Hz
AQ 0.2277376 sec
RG 574.7
DW 111.200 usec
DE 6.50 usec
TE 298.0 K
D0 0.00000300 sec
D1 1.50000000 sec
D13 0.00000400 sec
D20 0 sec
IN0 0.00022240 sec

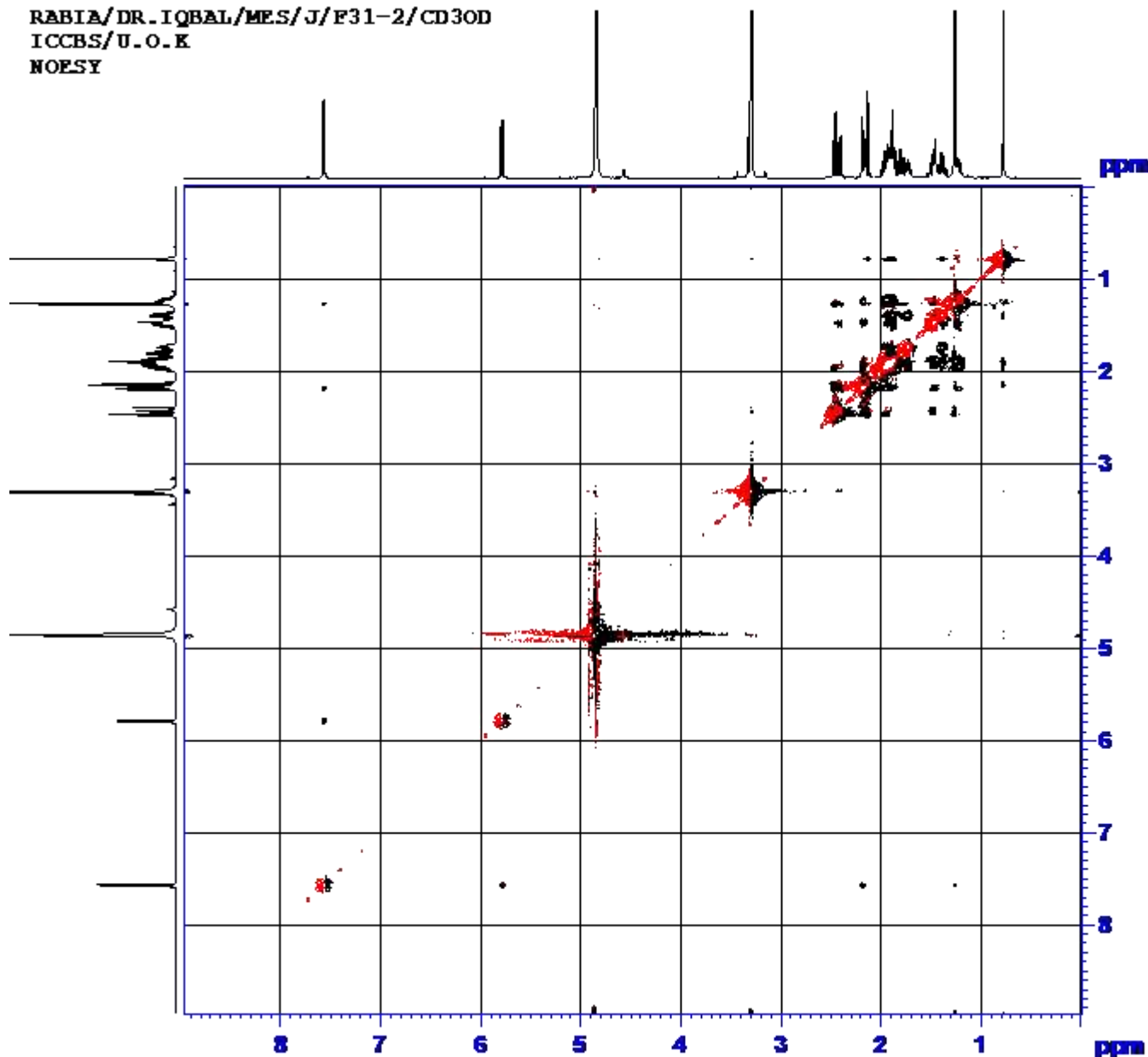
===== CHANNEL f1 =====
NUC1 1H
P1 8.03 usec
PL1 3.00 dB
SFO1 500.2322510 MHz

F1 - Acquisition parameters
TD 256
SFO1 500.2323 MHz
FIDRES 35.128147 Hz
SW 8.989 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 500.2300120 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.2300120 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

RABIA/DR. IQBAL/MES/J/F31-2/CD3OD
 ICCBS/U.O.K
 NOESY



Current Data Parameters
 NAME comp2
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150107
 Time_ 20.37
 INSTRUM spect
 PROCNO 5 nm F300 1H/
 PULPROG zgpg30
 TD 2048
 SOLVENT MeOD
 NS 16
 DS 8
 SSB 4496.403 Hz
 FIDRES 2.193309 Hz
 AQ 0.2277376 sec
 RC 1523.5
 RM 111.200 msec
 DE 6.50 msec
 TE 297.7 K
 D0 0.0000038 sec
 D1 2.0000000 sec
 D2 0.8000000 sec
 D15 0.0002000 sec
 LBD 0.0002240 sec

CHANNEL f1
 NUCL 1H
 P1 8.03 msec
 P2 16.06 msec
 PFL 3.00 dB
 SFO1 500.2322510 MHz

GRADIENT CHANNEL
 CHOM[1] SIDE 1.00
 CHOM[2] SIDE 1.00
 CEN1 40.00 G
 CEN2 -40.00 G
 P15 1000.00 msec

F1 - Acquisition parameters
 TD 256
 SFO1 500.2323 MHz
 FIDRES 35.128147 Hz
 SN 8.989 ppm
 PPMODE States-TFPI

F2 - Processing parameters
 SI 1024
 SF 500.2300120 MHz
 WM GSIW
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 States-TFPI
 SF 500.2300120 MHz
 WM GSIW
 SSB 2
 LB 0 Hz
 GB 0