

11/20/2016 9:29:13 AM

File: MES-I-F31-3  
Sample: RABIA FAROOQ / DR. M. IQBAL  
Instrument: JEOL MS 600H-1

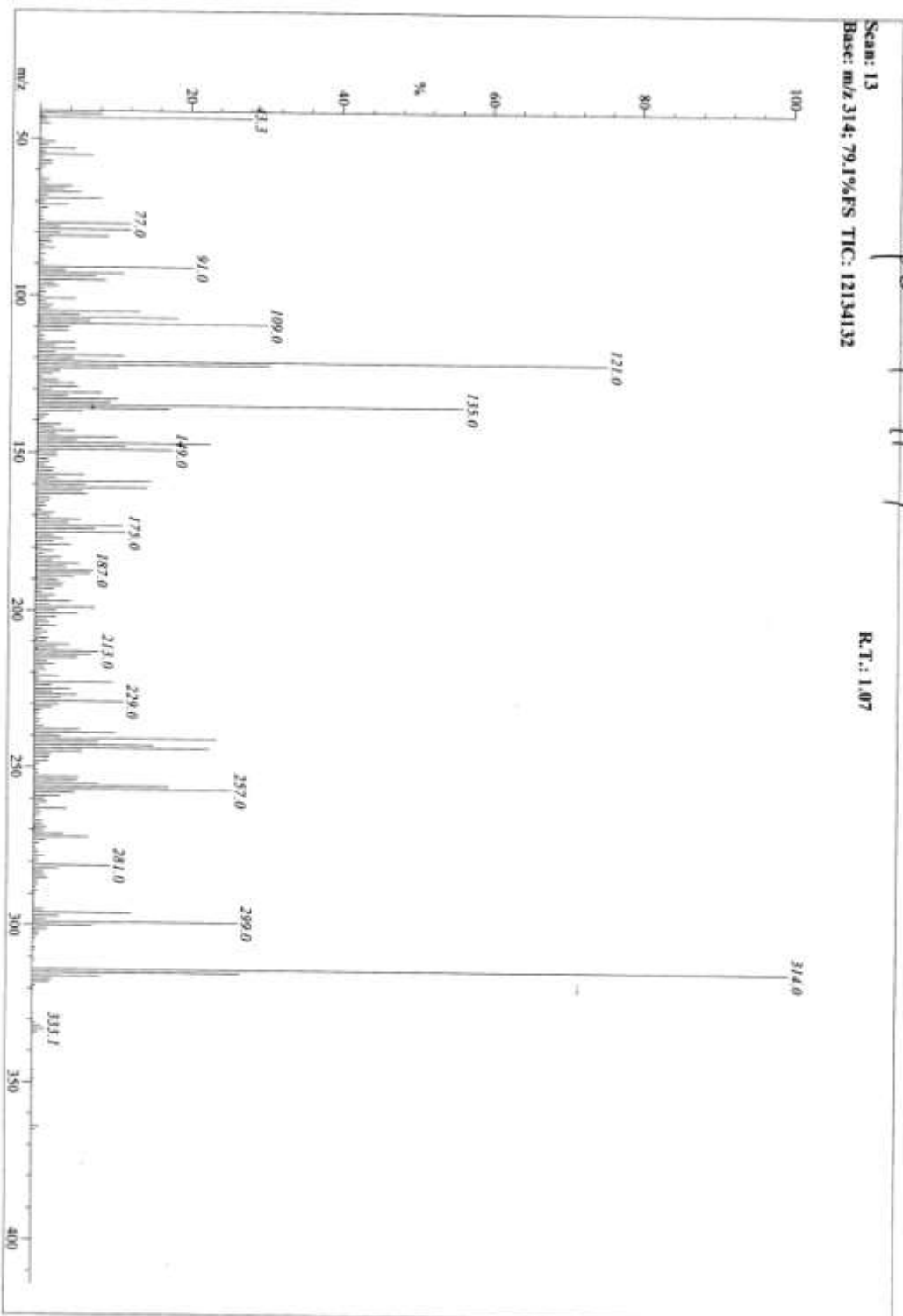
Date Run: 01-13-2016 (Time Run: 09:23:16)

Ionization mode: EI+

*Compound # 4*

Scan: 13  
Base: m/z 314; 79.1%FS TIC: 12134132

R.T.: 1.07



*Kabin Farcey*

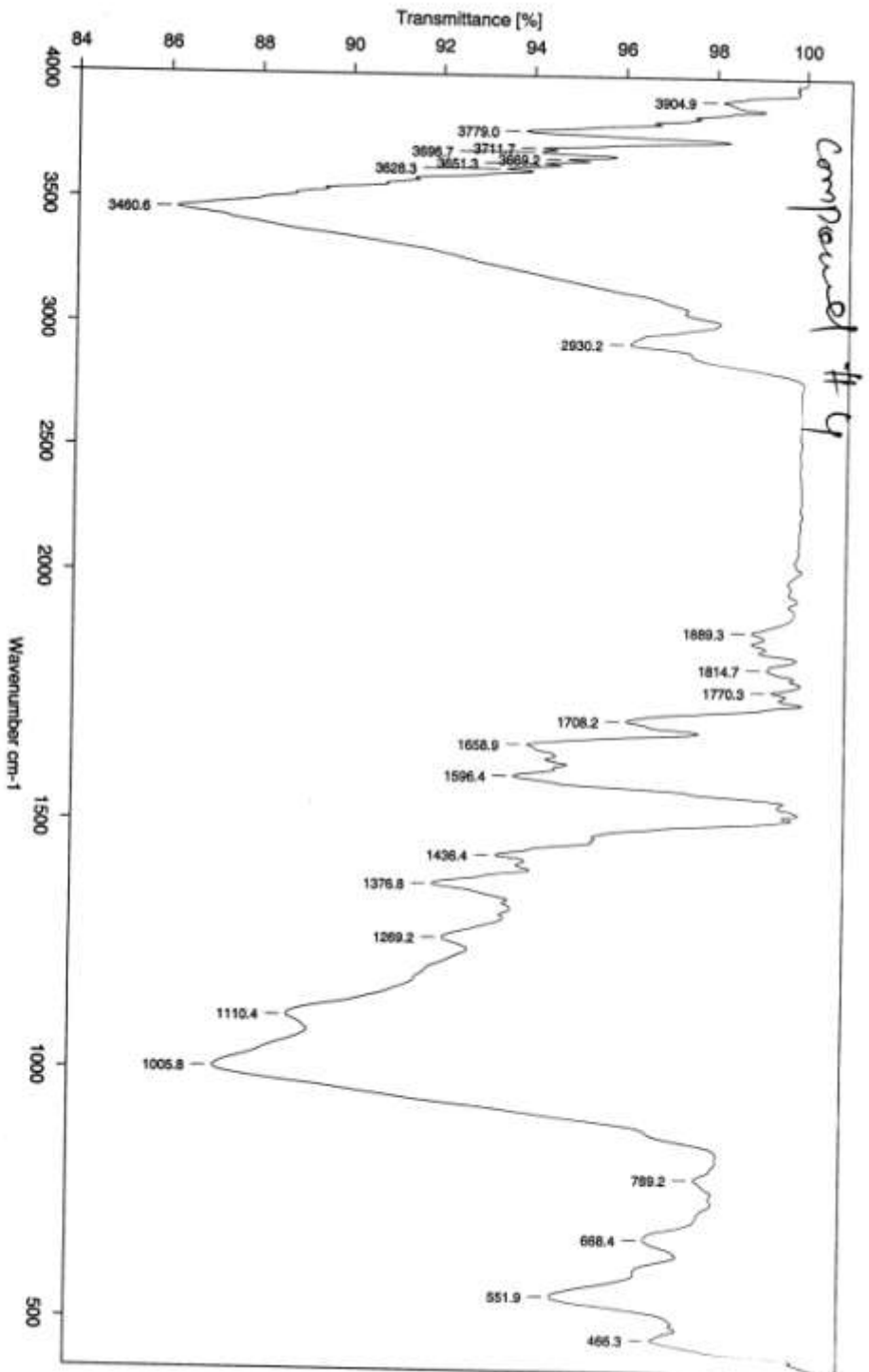
Mass	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
✓ 314.1862	314.1876	-4.6	-1.4	8.0	C <sub>20</sub> H <sub>26</sub> O <sub>3</sub>
299.1629	299.1642	-4.2	-1.3	8.5	C <sub>19</sub> H <sub>23</sub> O <sub>3</sub>
296.1765	296.1771	-2.0	-0.6	9.0	C <sub>20</sub> H <sub>24</sub> O <sub>2</sub>

*Compound # 4*

*Substrate  
304  
C<sub>20</sub> H<sub>32</sub> O<sub>2</sub>*

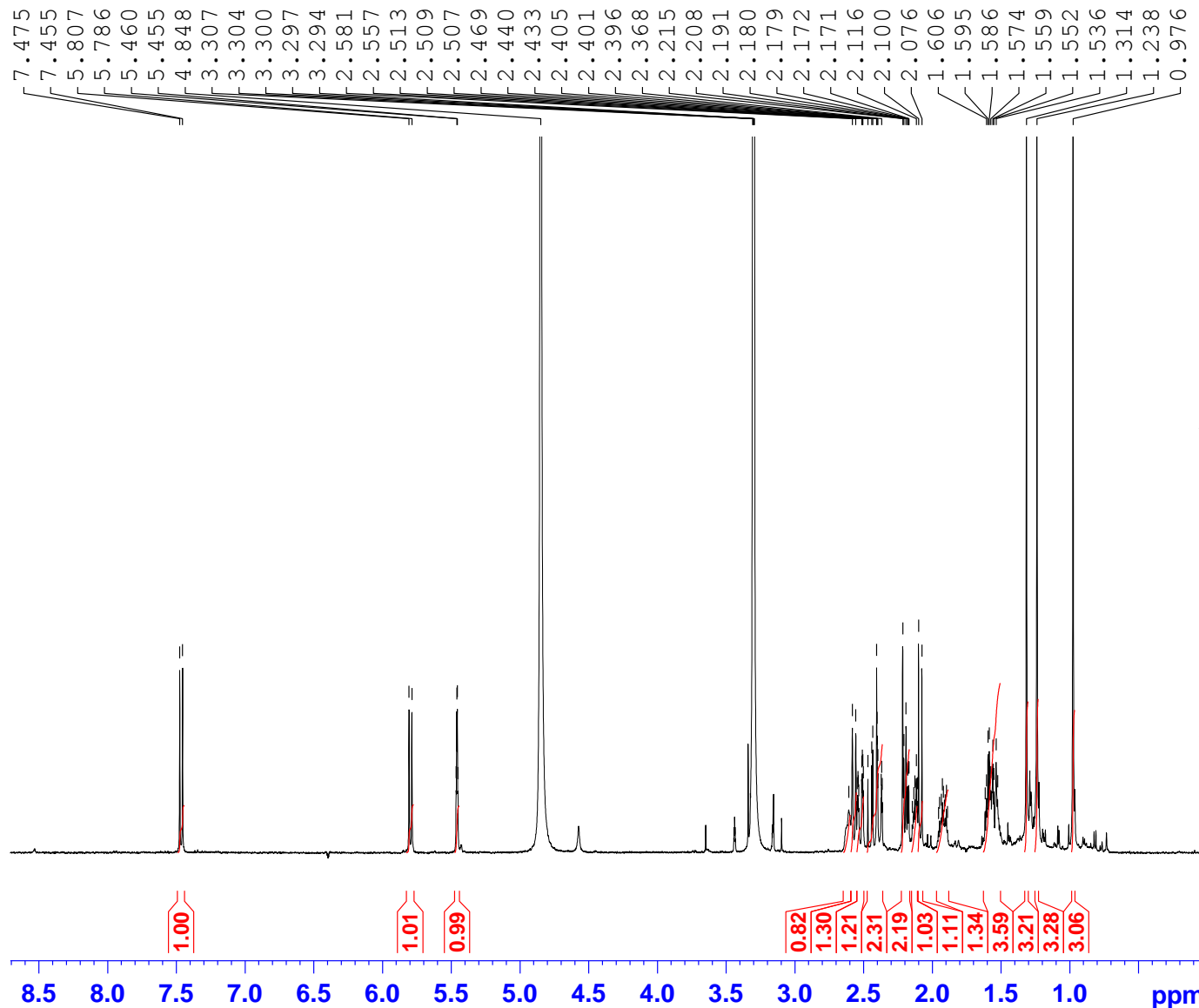
*303 - 304  
329*

*314  
304  
310*



Sample : Mes-J-F31-3/Rabia Farooq/Prof. Dr. M. I. Choudhary  
Measured : 10/11/2016 on VECTOR22  
Resolution : 4 cm<sup>-1</sup> ( 10 scans )  
Spectrum : Mes-J-F31-3.0 (in D:\IRSTUDENT)  
Technic : SOLID  
Analyst : M.Q.sif/ZQ

RABIA FAROOQ/DR.IQBAL/MES/J/F31-3/CD3OD



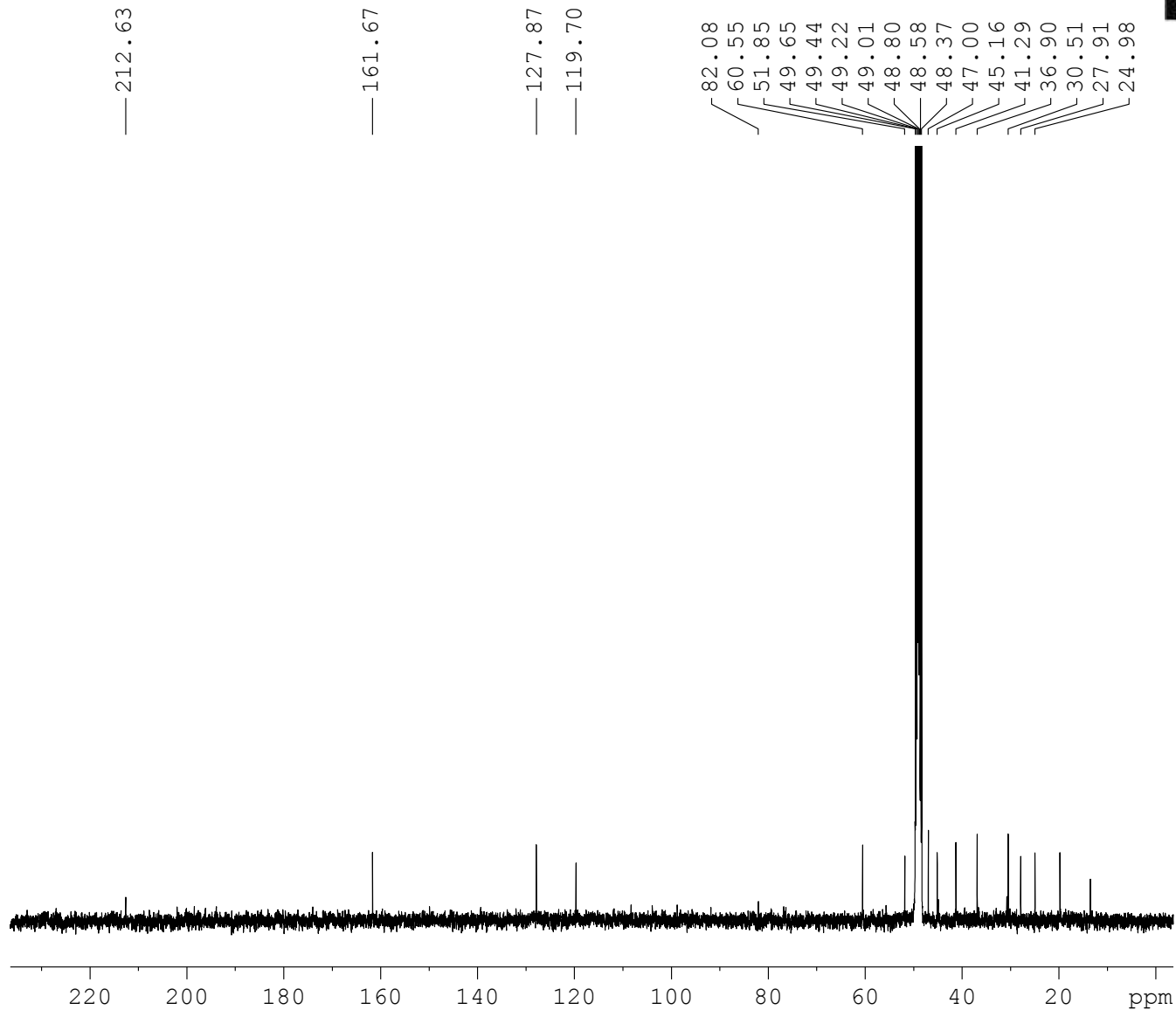
Current Data Parameters  
NAME compud 4  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20151216  
Time\_ 18.51  
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 228.1  
DW 41.600 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.50000000 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 500.2300118 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

RABIA FAROOQ/DR, IQBAL/Mes/J/F31-3/  
ICCBS, U.O.K/BB/



Current Data Parameters  
NAME compud 4  
EXPNO 7  
PROCNO 1

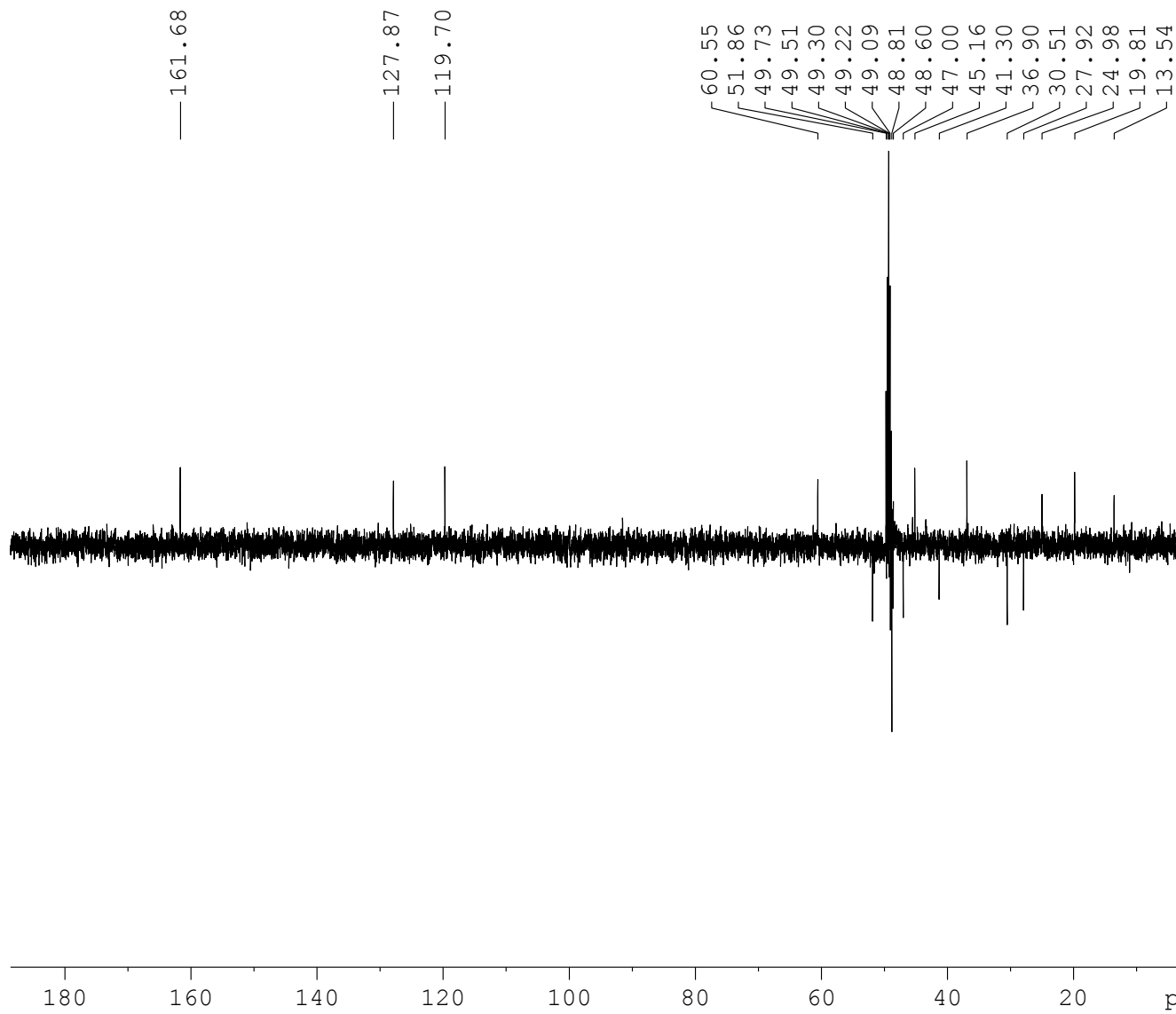
F2 - Acquisition Parameters  
Date\_ 20160609  
Time\_ 17.48  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg  
TD 32768  
SOLVENT MeOD  
NS 25083  
DS 2  
SWH 24154.590 Hz  
FIDRES 0.737140 Hz  
AQ 0.6782976 sec  
RG 32768  
DW 20.700 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 30

==== 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/F31-3/  
ICCBS, U.O.K/DEPT 135



Current Data Parameters  
NAME comput 4  
EXPNO 8  
PROCNO 1

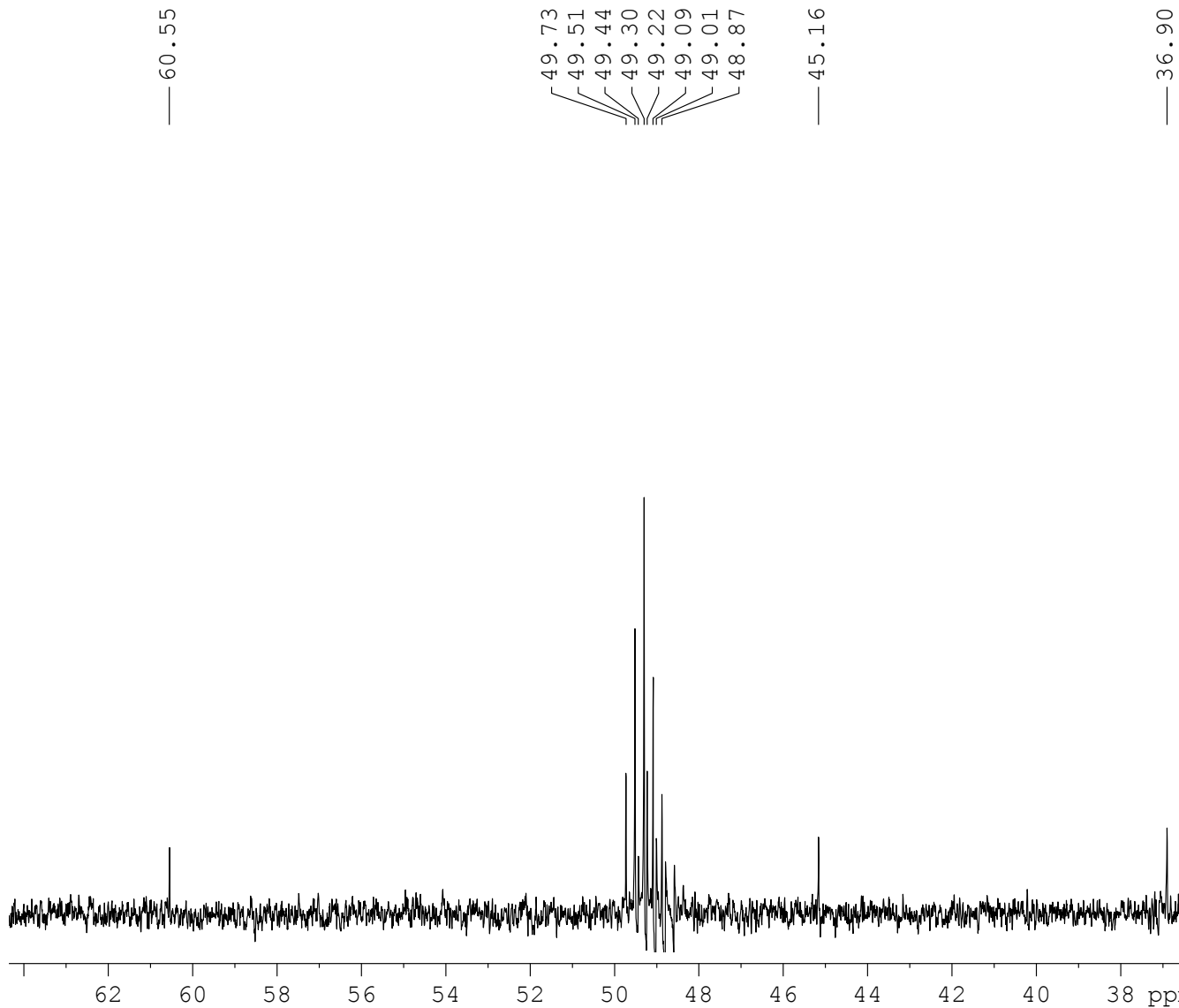
F2 - Acquisition Parameters  
Date\_ 20160609  
Time\_ 6.02  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG dept135  
TD 32768  
SOLVENT MeOD  
NS 9216  
DS 2  
SWH 19157.088 Hz  
FIDRES 0.584628 Hz  
AQ 0.8552448 sec  
RG 32768  
DW 26.100 usec  
DE 6.50 usec  
TE 300.0 K  
CNST2 145.0000000  
D1 1.5000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
FID0 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 FAROOQ/DR, IQBAL/Mes/J/F31-3/  
ICCBS, U.O.K/DEPT-90



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Current Data Parameters
NAME          comput 4
EXPNO         9
PROCNO        1

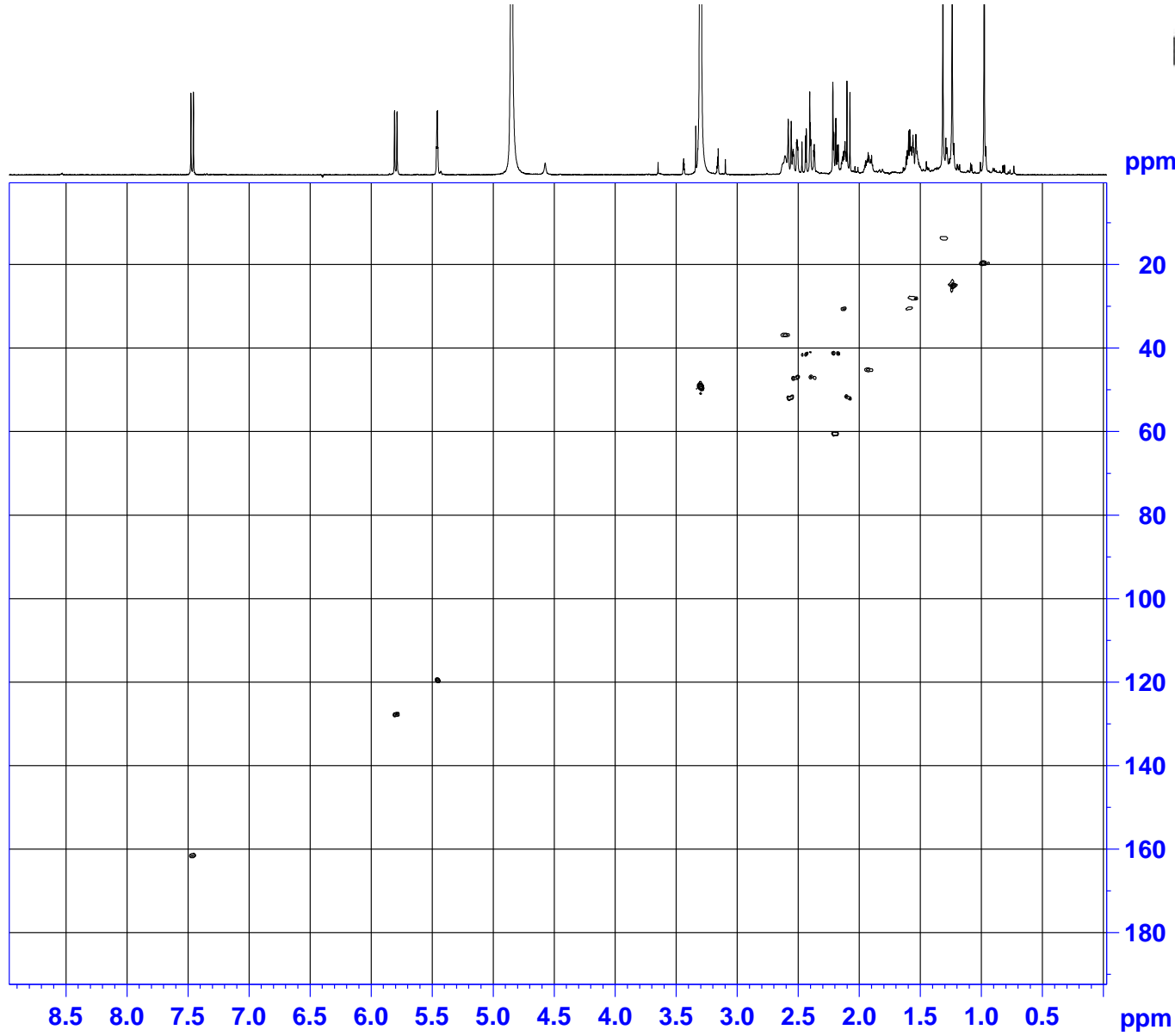
F2 - Acquisition Parameters
Date_         20160609
Time_         12.11
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       dept90
TD            32768
SOLVENT       MeOD
NS            4096
DS            2
SWH           19157.088 Hz
FIDRES        0.584628 Hz
AQ            0.8552448 sec
RG            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
TDO           4

===== 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/F31-3/CD3OD



ppm  
20  
40  
60  
80  
100  
120  
140  
160  
180  
ppm

```
Current Data Parameters
NAME          compud 4
EXPNO        5
PROCNO       1

F2 - Acquisition Parameters
Date_        20160106
Time         23.58
INSTRUM      spect
PROBHD       5 mm BBI 1H/D-
PULPROG      hsqcedetgp
TD           1024
SOLVENT      MeOD
NS           32
DS           8
SWH          4496.403 Hz
FIDRES       4.391018 Hz
AQ           0.1138688 sec
RG           26008
DW           111.200 usec
DE           6.50 usec
TE           297.9 K
CNST2        145.0000000
DO           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D13          0.00000400 sec
D16          0.00020000 sec
D21          0.00350000 sec
INO          0.00002070 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1         1H
P1           8.00 usec
P2           16.00 usec
PZ8          1000.00 usec
PL1          -1.00 dB
SF01         500.1322506 MHz

===== CHANNEL f2 =====
CPDPRG[2]   garp
NUC2         13C
P3           12.70 usec
P4           25.40 usec
PCPD2        65.00 usec
PL2          -3.00 dB
PL12         11.67 dB
SF02         125.7697360 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
SF01        125.7697 MHz
FIDRES      188.654602 Hz
SW          192.000 ppm
FnMODE      Echo-Antiecho

F2 - Processing parameters
SI          1024
SF          500.1300158 MHz
WDW         QSINE
SSB         2
LB          0 Hz
GB          0
PC          4.00

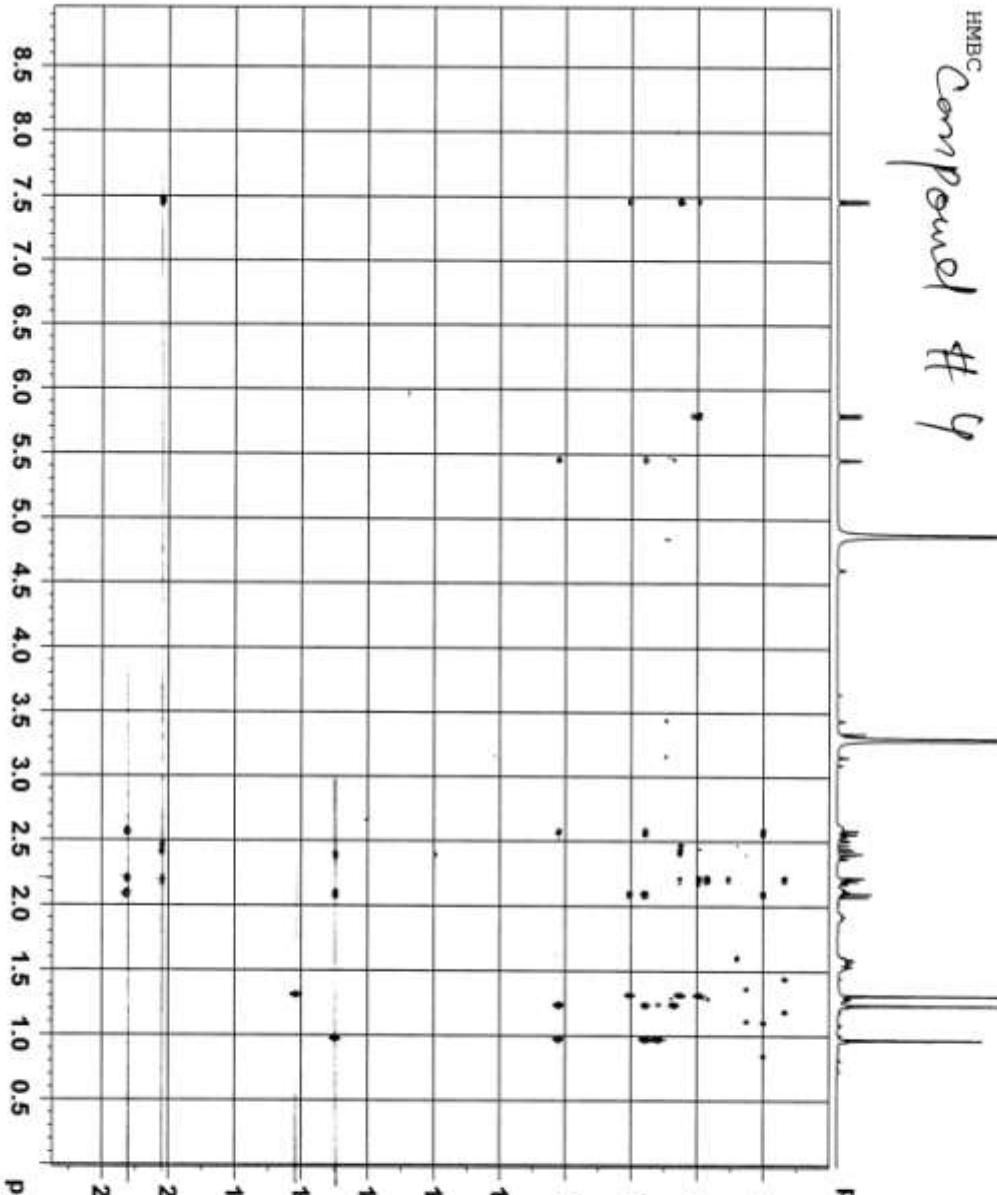
F1 - Processing parameters
SI          1024
MC2         echo-antiecho
SF          125.7576112 MHz
WDW         QSINE
SSB         2
LB          0 Hz
GB          0
```



RABIA FAROOQ/DR. IQBAL/MES/J/F31-3/CD30D  
 ICCBS/U.O.K

HMBc  
 Compound # 9

AVANCE AV-500  
 LAB NO: 109B

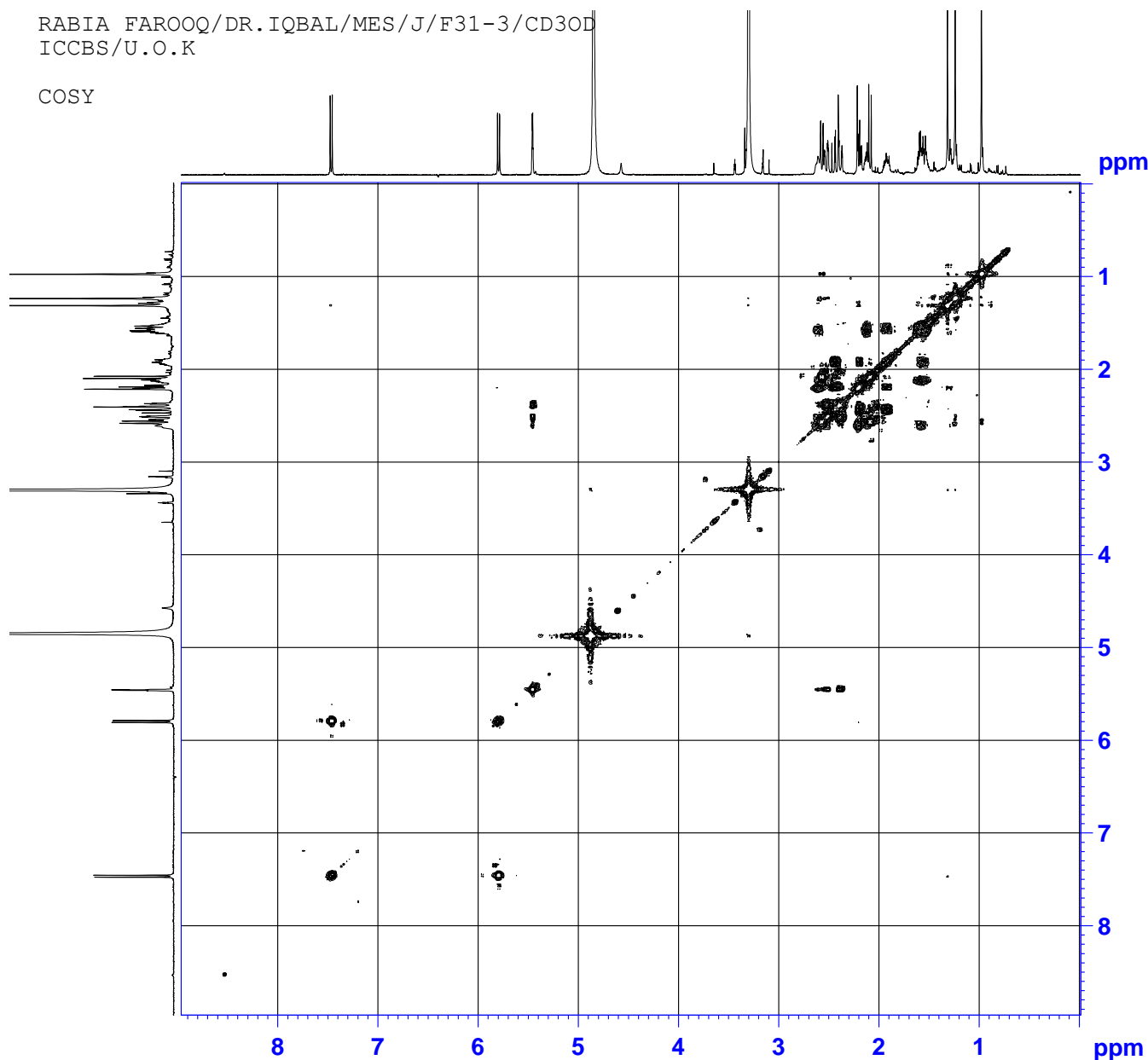


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NAME          1an06-16
EXPNO         4
PROCNO       20160101
Date_         23-43
INSTRUM      5 mm BBI 1H/13
PROBHD       hmcgpr125
PULPROG      zgpg30
TD           2048
SFO          125.761
AQ           0.04
RG           655
SC-VENT      2048
SI           6
DS           6
SWH          4496.403 Hz
FIDRES      2.195509 Hz
AQ          0.227898 sec
RG          111.100
DS          5.50 usec
SE          289.0 K
TE          145.0000000
CNSRTY      10.0000000
SOLVENT      DMS
D1          2.0000000 sec
D2          2.0000000 sec
D3          0.00344428 sec
D4          0.05000000 sec
D5          0.00020000 sec
D6          0.00020000 sec
D7          0.00016900 sec
D8          0.00016900 sec
D9          0.00016900 sec
D10         0.00016900 sec
D11         0.00016900 sec
D12         0.00016900 sec
D13         0.00016900 sec
D14         0.00016900 sec
D15         0.00016900 sec
D16         0.00016900 sec
D17         0.00016900 sec
D18         0.00016900 sec
D19         0.00016900 sec
D20         0.00016900 sec
D21         0.00016900 sec
D22         0.00016900 sec
D23         0.00016900 sec
D24         0.00016900 sec
D25         0.00016900 sec
D26         0.00016900 sec
D27         0.00016900 sec
D28         0.00016900 sec
D29         0.00016900 sec
D30         0.00016900 sec
D31         0.00016900 sec
D32         0.00016900 sec
D33         0.00016900 sec
D34         0.00016900 sec
D35         0.00016900 sec
D36         0.00016900 sec
D37         0.00016900 sec
D38         0.00016900 sec
D39         0.00016900 sec
D40         0.00016900 sec
D41         0.00016900 sec
D42         0.00016900 sec
D43         0.00016900 sec
D44         0.00016900 sec
D45         0.00016900 sec
D46         0.00016900 sec
D47         0.00016900 sec
D48         0.00016900 sec
D49         0.00016900 sec
D50         0.00016900 sec
D51         0.00016900 sec
D52         0.00016900 sec
D53         0.00016900 sec
D54         0.00016900 sec
D55         0.00016900 sec
D56         0.00016900 sec
D57         0.00016900 sec
D58         0.00016900 sec
D59         0.00016900 sec
D60         0.00016900 sec
D61         0.00016900 sec
D62         0.00016900 sec
D63         0.00016900 sec
D64         0.00016900 sec
D65         0.00016900 sec
D66         0.00016900 sec
D67         0.00016900 sec
D68         0.00016900 sec
D69         0.00016900 sec
D70         0.00016900 sec
D71         0.00016900 sec
D72         0.00016900 sec
D73         0.00016900 sec
D74         0.00016900 sec
D75         0.00016900 sec
D76         0.00016900 sec
D77         0.00016900 sec
D78         0.00016900 sec
D79         0.00016900 sec
D80         0.00016900 sec
D81         0.00016900 sec
D82         0.00016900 sec
D83         0.00016900 sec
D84         0.00016900 sec
D85         0.00016900 sec
D86         0.00016900 sec
D87         0.00016900 sec
D88         0.00016900 sec
D89         0.00016900 sec
D90         0.00016900 sec
D91         0.00016900 sec
D92         0.00016900 sec
D93         0.00016900 sec
D94         0.00016900 sec
D95         0.00016900 sec
D96         0.00016900 sec
D97         0.00016900 sec
D98         0.00016900 sec
D99         0.00016900 sec
D100        0.00016900 sec
  
```

RABIA FAROOQ/DR. IQBAL/MES/J/F31-3/CD3OD  
ICCBS/U.O.K

COSY



ppm

ppm

Current Data Parameters  
NAME compud 4  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160106  
Time 19.29  
INSTRUM spect  
PROBHD 5 mm BBI 1H/D-  
PULPROG cosygpgrf  
TD 2048  
SOLVENT MeOD  
NS 8  
DS 8  
SWH 4496.403 Hz  
FIDRES 2.195509 Hz  
AQ 0.2277376 sec  
RG 1625.5  
DW 111.200 usec  
DE 6.50 usec  
TE 294.6 K  
DO 0.00000300 sec  
D1 1.50000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
INO 0.00022240 sec

===== CHANNEL f1 =====  
NUC1 1H  
PO 8.00 usec  
PL 8.00 usec  
PL1 -1.00 dB  
SFO1 500.1322506 MHz

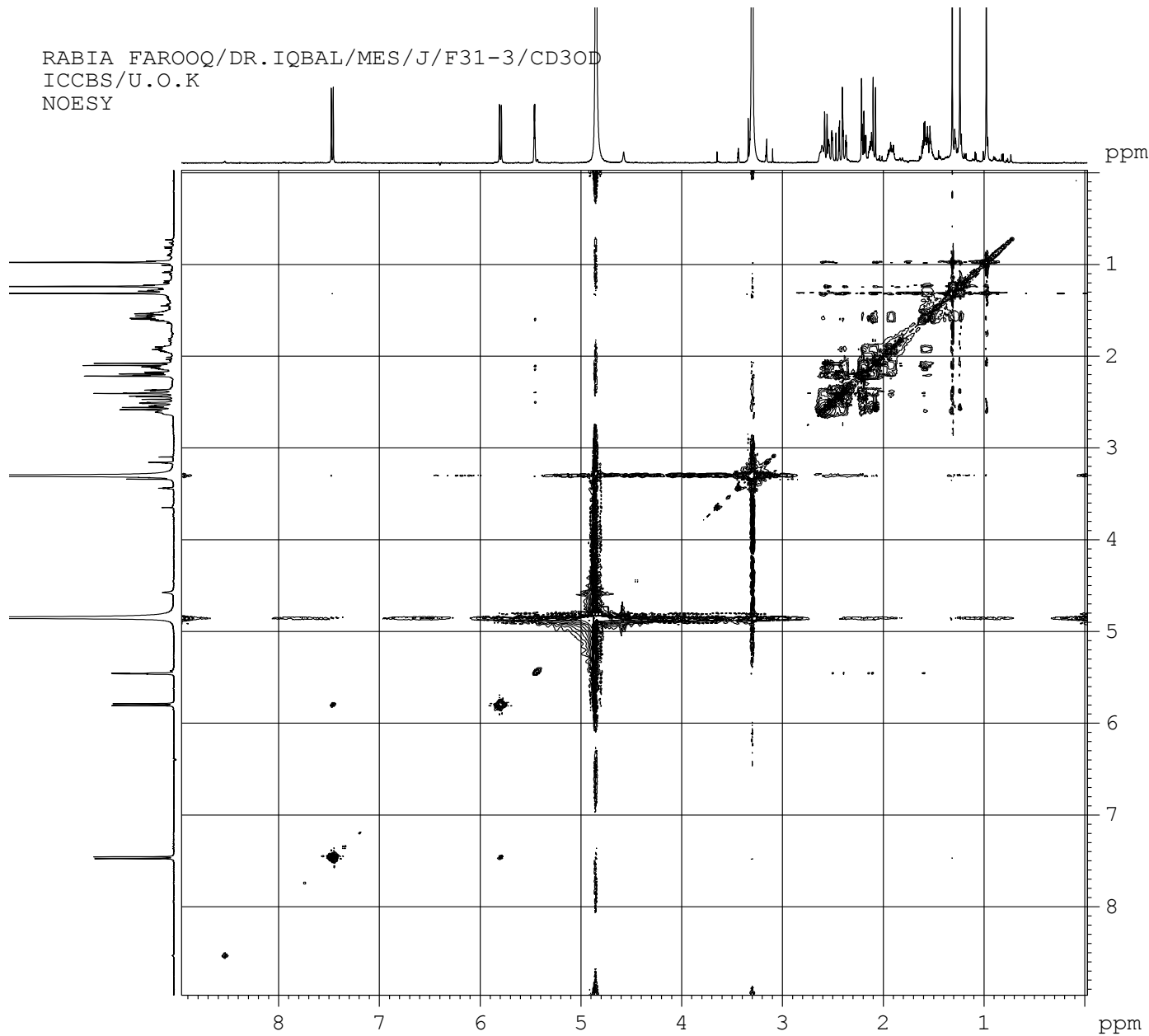
===== GRADIENT CHANNEL =====  
GPNAM[1] SINE.100  
GPZ1 10.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SFO1 500.1323 MHz  
FIDRES 35.128147 Hz  
SW 8.990 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 500.1300158 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 4.00

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 500.1300158 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

RABIA FAROOQ/DR. IQBAL/MES/J/F31-3/CD3OD  
ICCBS/U.O.K  
NOESY



Current Data Parameters  
NAME comput 4  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160106  
Time 20.30  
INSTRUM spect  
PROBHD 5 mm BBI 1H/D-  
PULPROG noesygp  
TD 2048  
SOLVENT MeOD  
NS 16  
DS 2  
SWH 4496.403 Hz  
FIDRES 2.195509 Hz  
AQ 0.2277376 sec  
RG 362  
DW 111.200 usec  
DE 6.50 usec  
TE 294.9 K  
D0 0.00010101 sec  
D1 2.00000000 sec  
D8 0.80000001 sec  
D16 0.00020000 sec  
IN0 0.00022240 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 8.00 usec  
P2 16.00 usec  
PL1 -1.00 dB  
SFO1 500.1322506 MHz

===== GRADIENT CHANNEL =====  
GPNAM[1] SINE.100  
GPZ1 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SFO1 500.1323 MHz  
FIDRES 35.128147 Hz  
SW 8.990 ppm  
FnMODE States-TPPI

F2 - Processing parameters  
SI 1024  
SF 500.1300158 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 4.00

F1 - Processing parameters  
SI 1024  
MC2 States-TPPI  
SF 500.1300158 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0