



Supplementary Materials for

Phytochemical investigation on volatile compositions and methoxylated flavonoids of *Agrostis gigantea* Roth

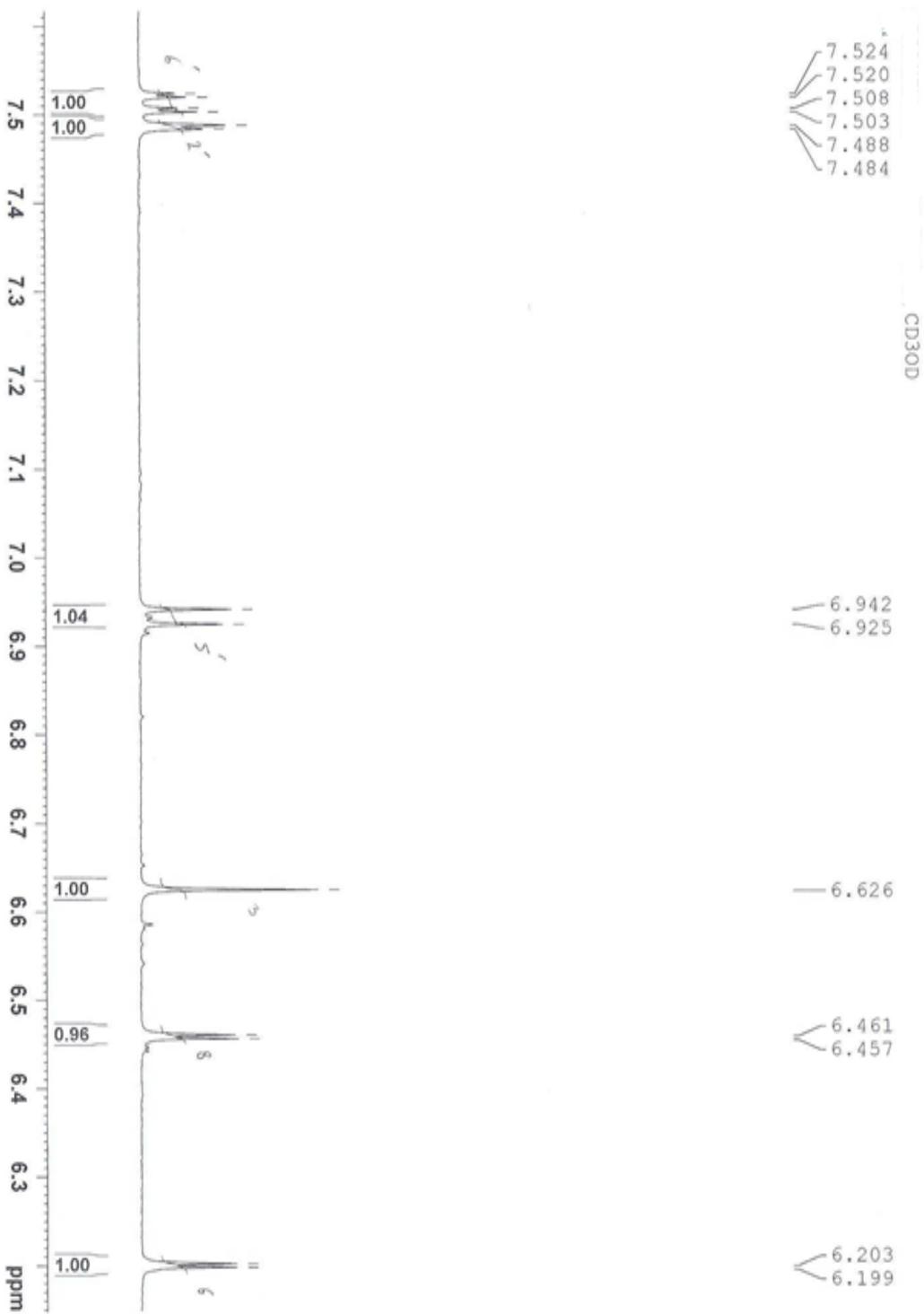
Mahmoud Rafieian-kopaei, Azadeh Hamedi, Ebrahim Soleiman Dehkordi, Arsalan Pasdaran and Aradalan Pasdaran^{*}

^{*}To whom correspondence should be addressed

pasdaran@sums.ac.ir

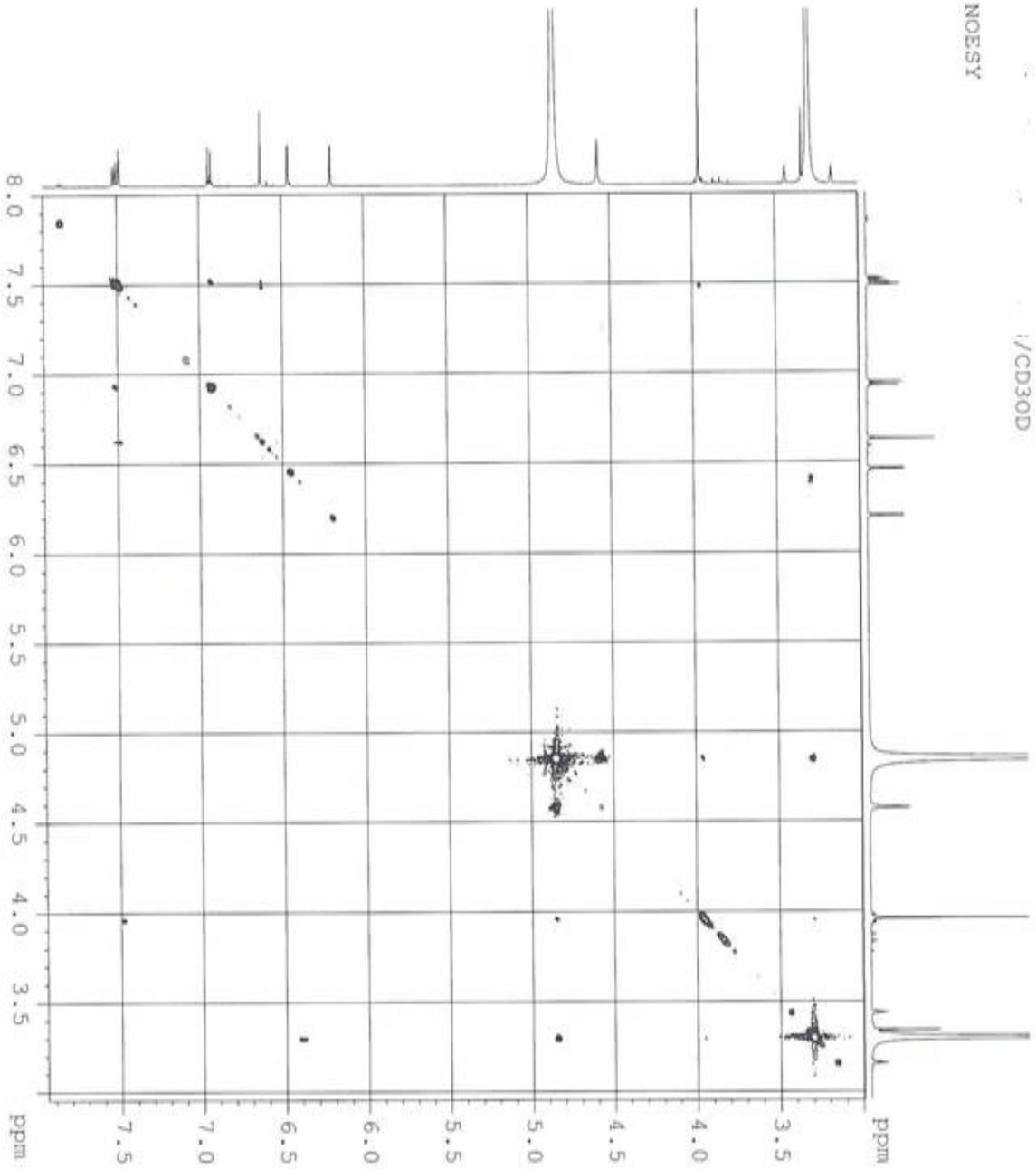
Volume 19, Issue 2 (Spring 2020)

This PDF file include



NOESY

/CD3OD



AVANCE AV-500
LAB NO:118

```

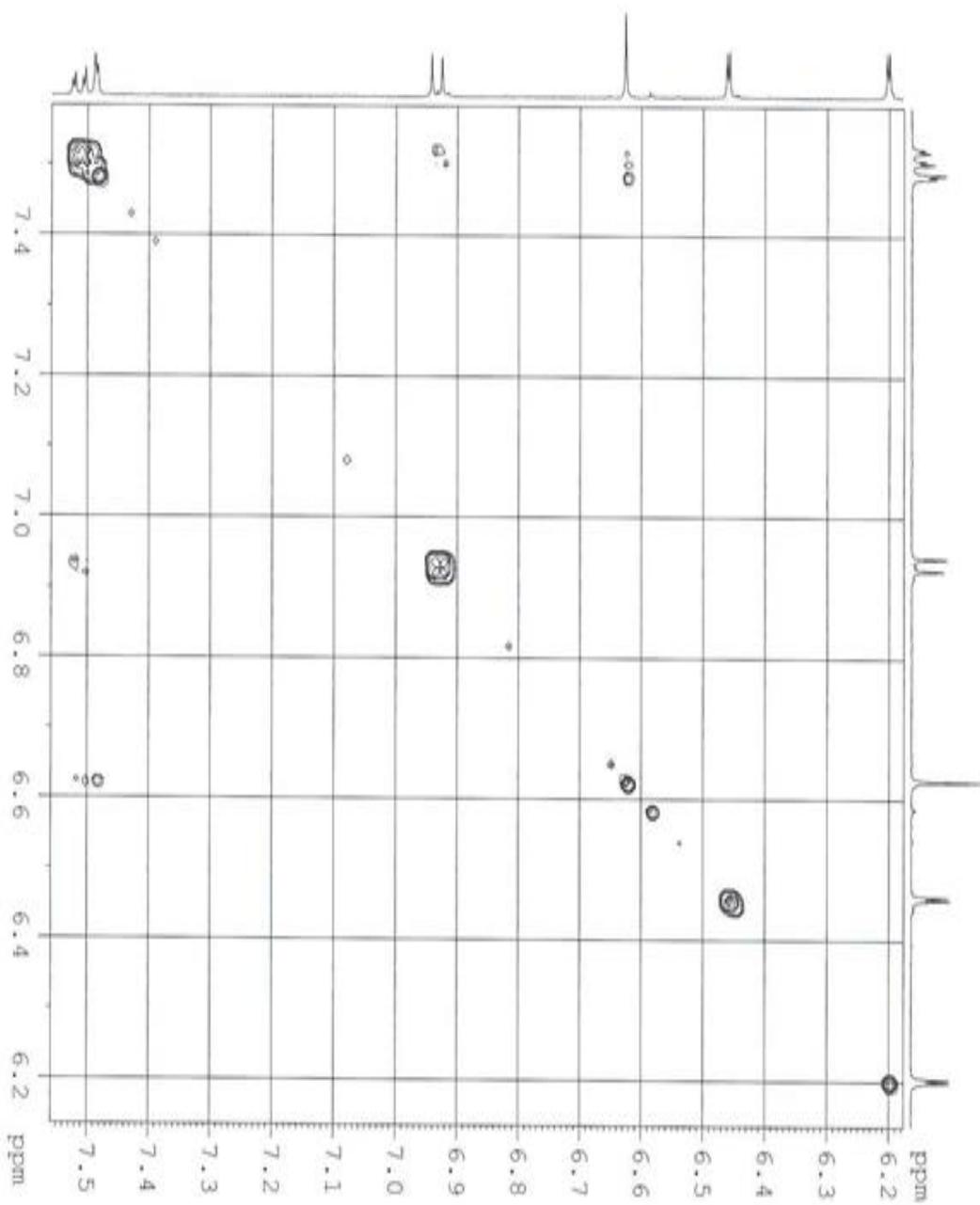
NAME          Jan30-17
EXPNO         4
PROCNO       1
Date_        20170130
Time         12.04
INSTRUM      spect
PROBHD       5 mm PABBI 1H/
PULPROG      noesyzgpgph
TD           2048
SOLVENT      MeOD
NS           16
DS           8
SFR          4084.967 Hz
FIDRES       1.994113 Hz
AQ           0.2508975 sec
RG           812.7
DE           122.900 usec
TE           298.2 K
D0           0.00011218 sec
D1           2.000000000 sec
D8           0.800000001 sec
D16          0.400020000 sec
IN0          0.00024480 sec

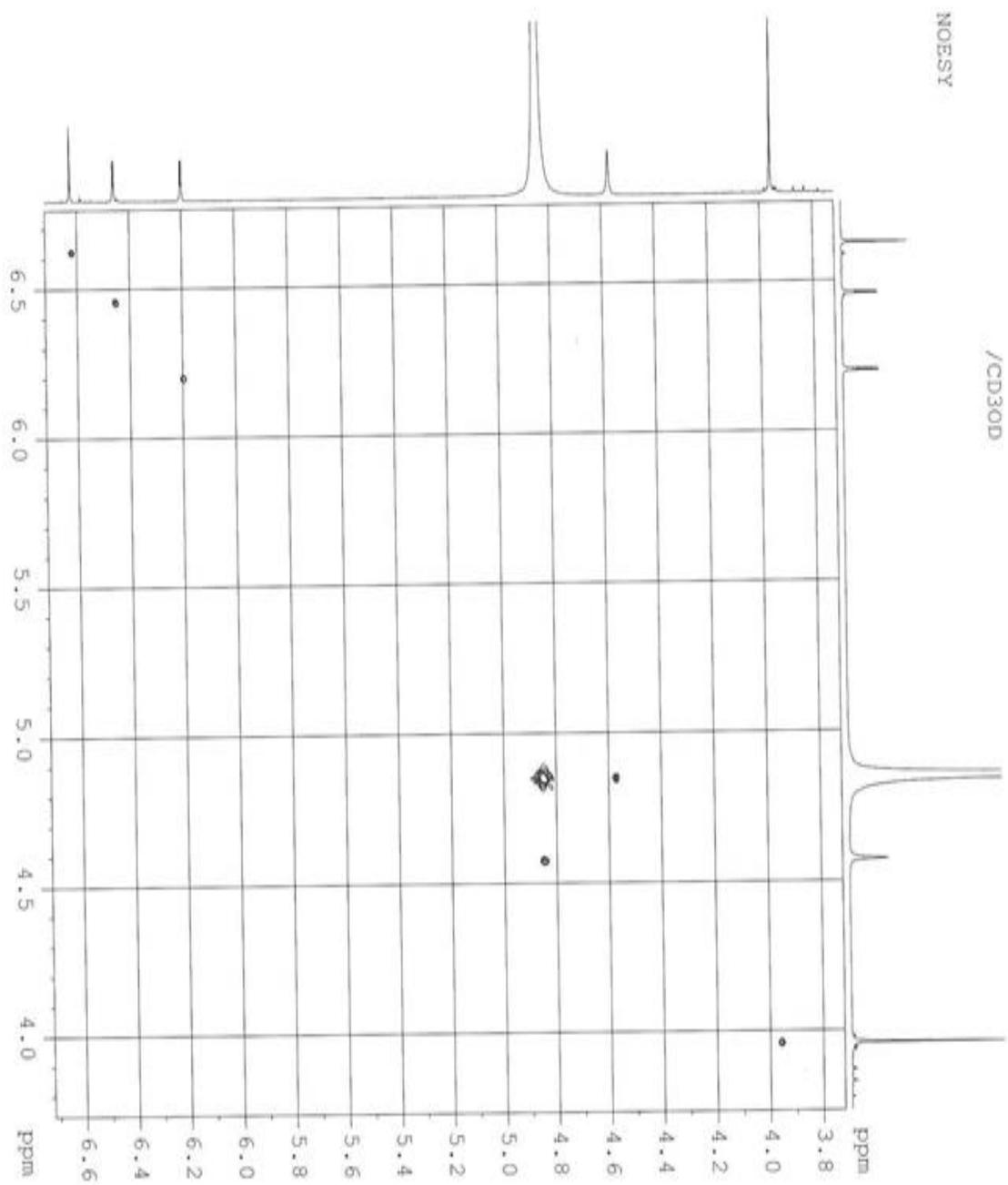
----- CHANNEL f1 -----
NUC1          1H
P1           8.03 usec
P2           16.06 usec
PL1          3.00 dB
SFO1         500.2320509 MHz

----- GRADIENT CHANNEL -----
GENDM1       SINE.100
GPRM1        SINE.100
GE21         40.00 %
GE22         -40.00 %
P16          1000.00 usec
ND0          1
TD           256
SFO1         500.2321 MHz
FIDRES       15.956903 Hz
SW           8.166 Ppm
Fmode        States-TPEI
SI           1024
SF           500.2300118 MHz
AQ           QSINE
MDW          2
SSB          2
LB           0.00 Hz
GB           0
PC           1.00
SI           1024
MC2          States-TPEI
SF           500.2300118 MHz
WDW          QSINE
SSB          2
LB           0.00 Hz
GB           0
  
```

NOESY

/CD3OD

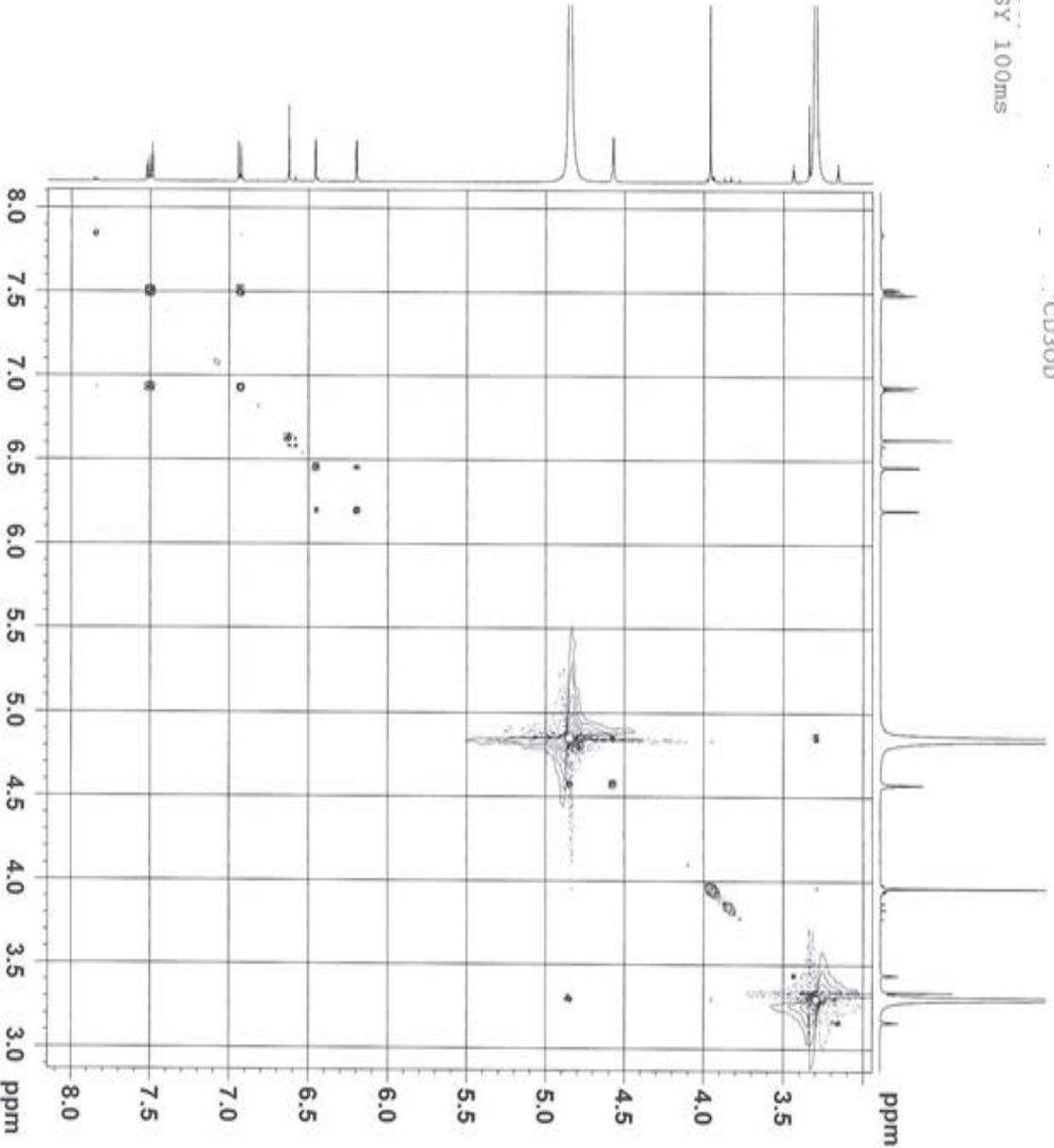




TOCSY 100ms

CD30D

AVANCE AV-500
LXBN0:1B

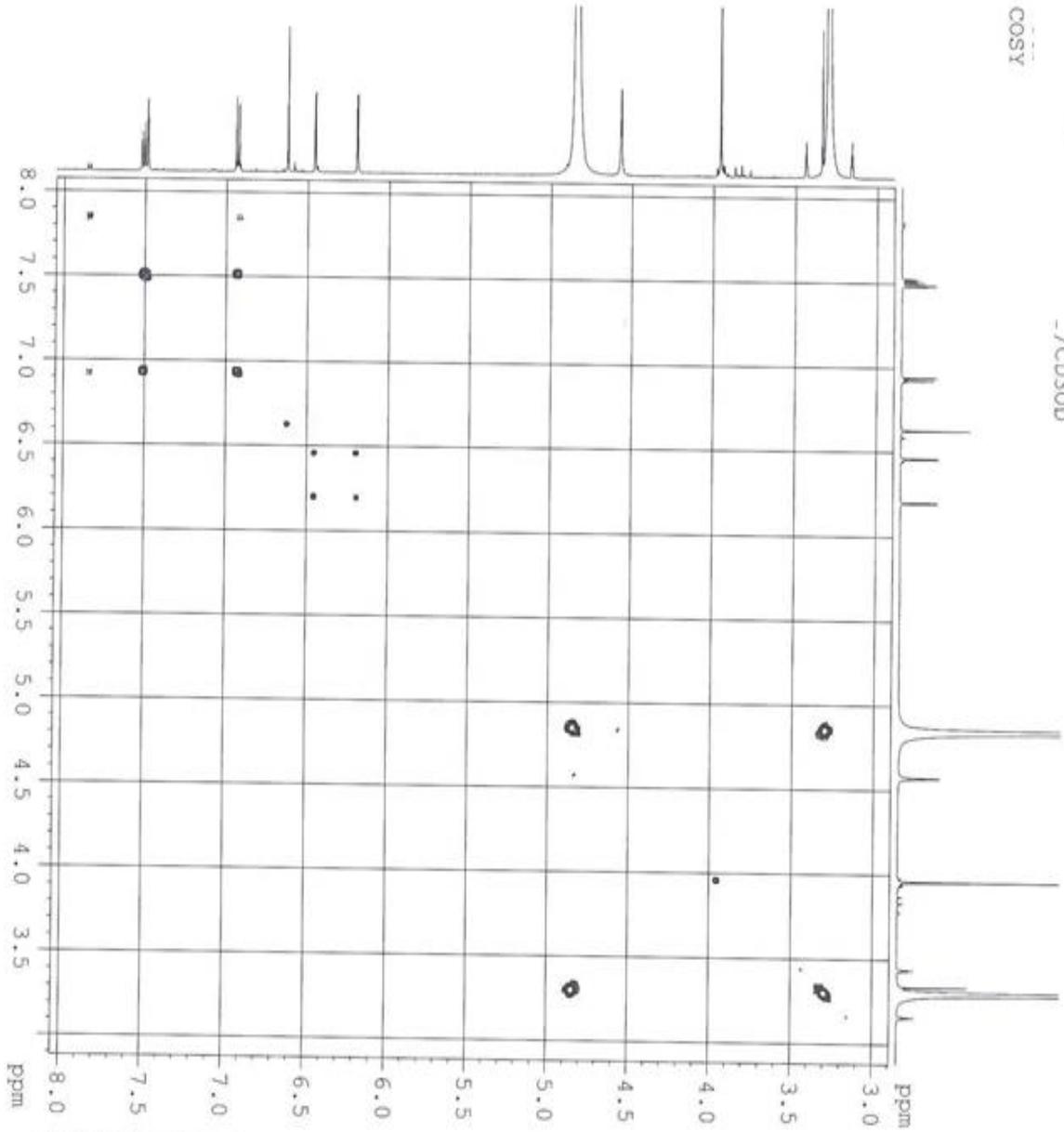


```

NAME          Jan30-17
EXPNO         7
PROCNO       1
Date_         20170130
Time         18.13
INSTRUM      spect
PROBHD       5 mm PABBI 1H/
PULPROG      zgpg30
TD           2048
FIDRES       0.2508476 sec
AQ           812.7
RG           122.400 us/c
DS           4
SS           8
SOLVENT      MeOD
NUC1          1H
NUC2          13C
P1           8.03 usec
P2           21.34 usec
P3           32.00 usec
P4           64.00 usec
P5           2500.00 usec
P6           3.00 dB
P7           14.68 dB
P8           14.68 dB
P9           14.68 dB
P10          14.68 dB
P11          14.68 dB
P12          14.68 dB
P13          14.68 dB
P14          14.68 dB
P15          14.68 dB
P16          14.68 dB
P17          14.68 dB
P18          14.68 dB
P19          14.68 dB
P20          14.68 dB
SFO1         500.230509 MHz
SFO2         125.760325 MHz
SFO3         101.623502 MHz
SFO4         101.623502 MHz
SFO5         101.623502 MHz
SFO6         101.623502 MHz
SFO7         101.623502 MHz
SFO8         101.623502 MHz
SFO9         101.623502 MHz
SFO10        101.623502 MHz
SFO11        101.623502 MHz
SFO12        101.623502 MHz
SFO13        101.623502 MHz
SFO14        101.623502 MHz
SFO15        101.623502 MHz
SFO16        101.623502 MHz
SFO17        101.623502 MHz
SFO18        101.623502 MHz
SFO19        101.623502 MHz
SFO20        101.623502 MHz
WDW          EM
SSB          2
LB           0.00 Hz
GB           0
PC           1.00
SI           1024
SF           500.2300118 MHz
WDW          EM
SSB          2
LB           0.00 Hz
GB           0
  
```

COSY

-/CD30D

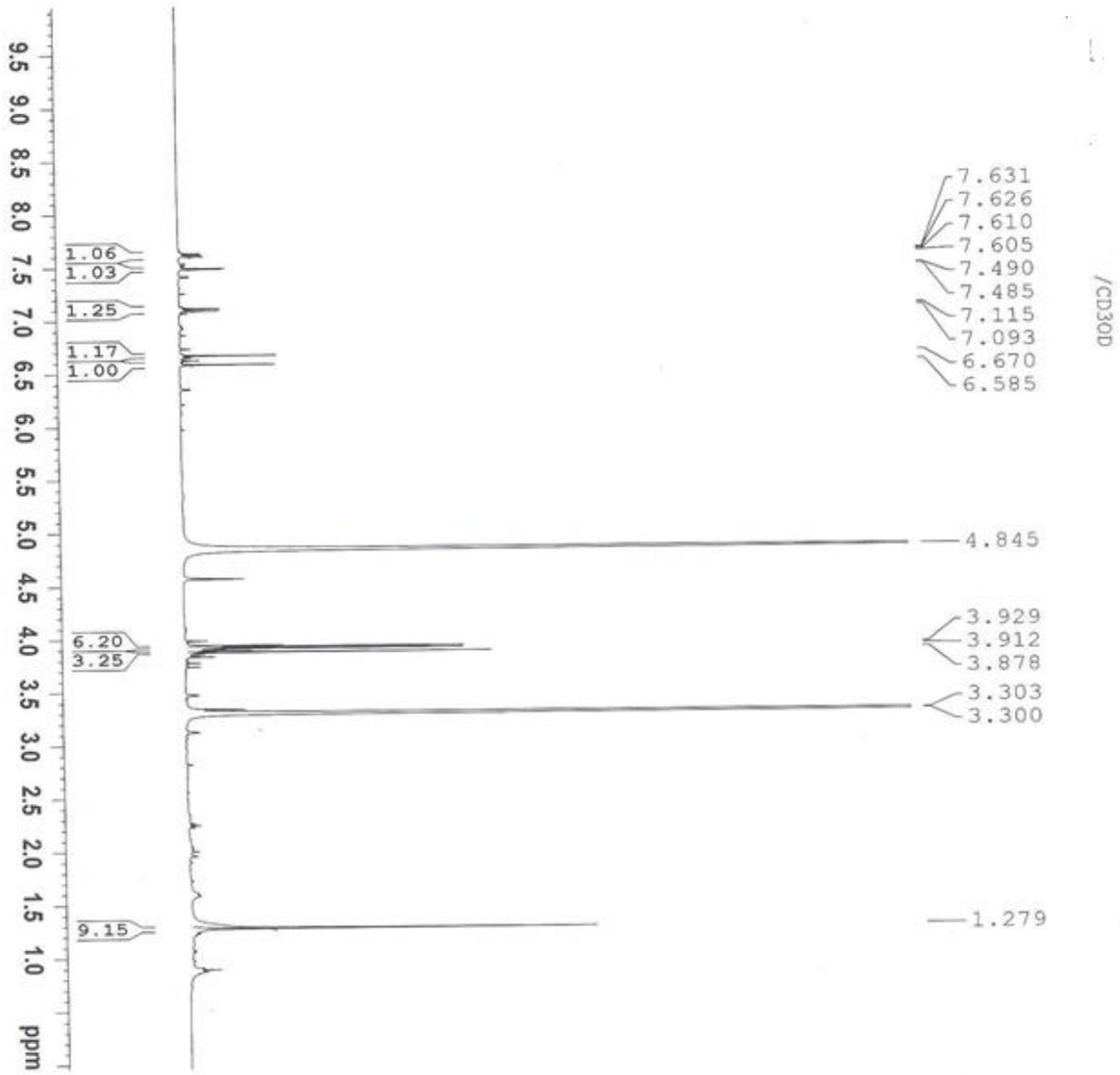


AVANCE AV-500
LAB NO:118

NAME Jan30-17
 EXPNO 3
 PROCNO 1
 Date_ 20170130
 Time 11.02
 INSTRUM spect
 PROBD 5 mm PABBI 1H/
 PULPROG zgpg30
 TD 2048
 SOLVENT MeOD
 NS 8
 DS 8
 SWH 4084.967 Hz
 FIDRES 1.994613 Hz
 AQ 0.2508476 sec
 RG 812.7
 DW 122.400 usec
 DE 6.50 usec
 TE 298.2 K
 D0 0.00000300 sec
 D1 1.50000000 sec
 D13 0.00000400 sec
 D20 0.00000000 sec
 INO 0.00024480 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.03 usec
 P11 3.00 dB
 SFO1 500.2320509 MHz
 NDO 1
 TD 256
 SFO1 500.2321 MHz
 FIDRES 15.956903 Hz
 SW 8.166 ppm
 FHM0DE QF
 SI 1024
 SF 500.2300118 MHz
 KW OSINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00
 SI 1024
 MC2 QF
 SF 500.2300118 MHz
 KW OSINE
 SSB 0
 LB 0.00 Hz
 GB 0

1D, 2D NMR data of cirsilineol.

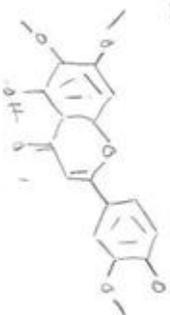


AVANCE AV-III HD
400 MHz
LAB #109A

Current Data Parameters
NAME Jan30-17
EXPTNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170130
Time 11.42 h
INSTRUM spect
PROBHD 28247_0039 (SE)
PULPROG zg30
TD 32768
SOLVENT MeOD
NS 128
DS 0
SMH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 2.0447233 sec
RG 180.09
TW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.50000000 sec
TD0 1
SFO1 400.3331626 MHz
NUC1 1H
P1 6.70 usec
PLM1 20.00000000 W

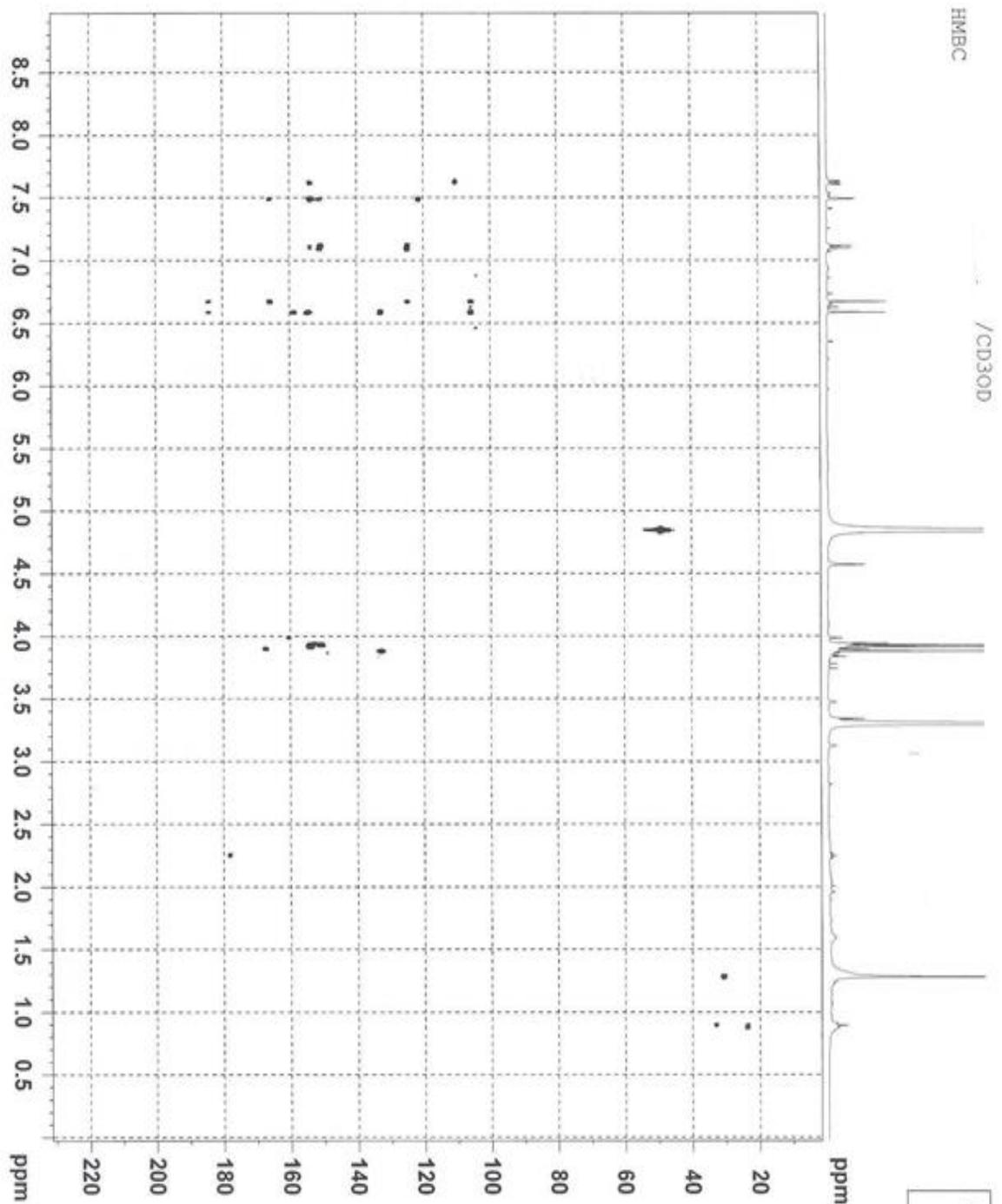
F2 - Processing parameters
SI 32768
SF 400.3300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Cirsilineol

HMBC

/CD3OD



AVANCE AV-III HD
400 MHz
LAB #109A

Current Data Parameters
 NAME JMBP-17
 EXNO 8
 PROCNO 1

F2 - Acquisition Parameters
 DATE_ 20170131
 TIME 6:01 B
 INSTRUM spect
 PROBR0 5Q241 503.9 MHz
 PULPROG hmcgprndet
 TD 2048
 SOLVENT MeOD
 NS 64
 DS 16
 SFR 3403.149 Hz
 AQ 2.1118189 sec
 FIDRES 0.7138853 MHz
 B0 202.75
 DM 138.647 usec
 DE 6.50 usec
 TE 298.0 K

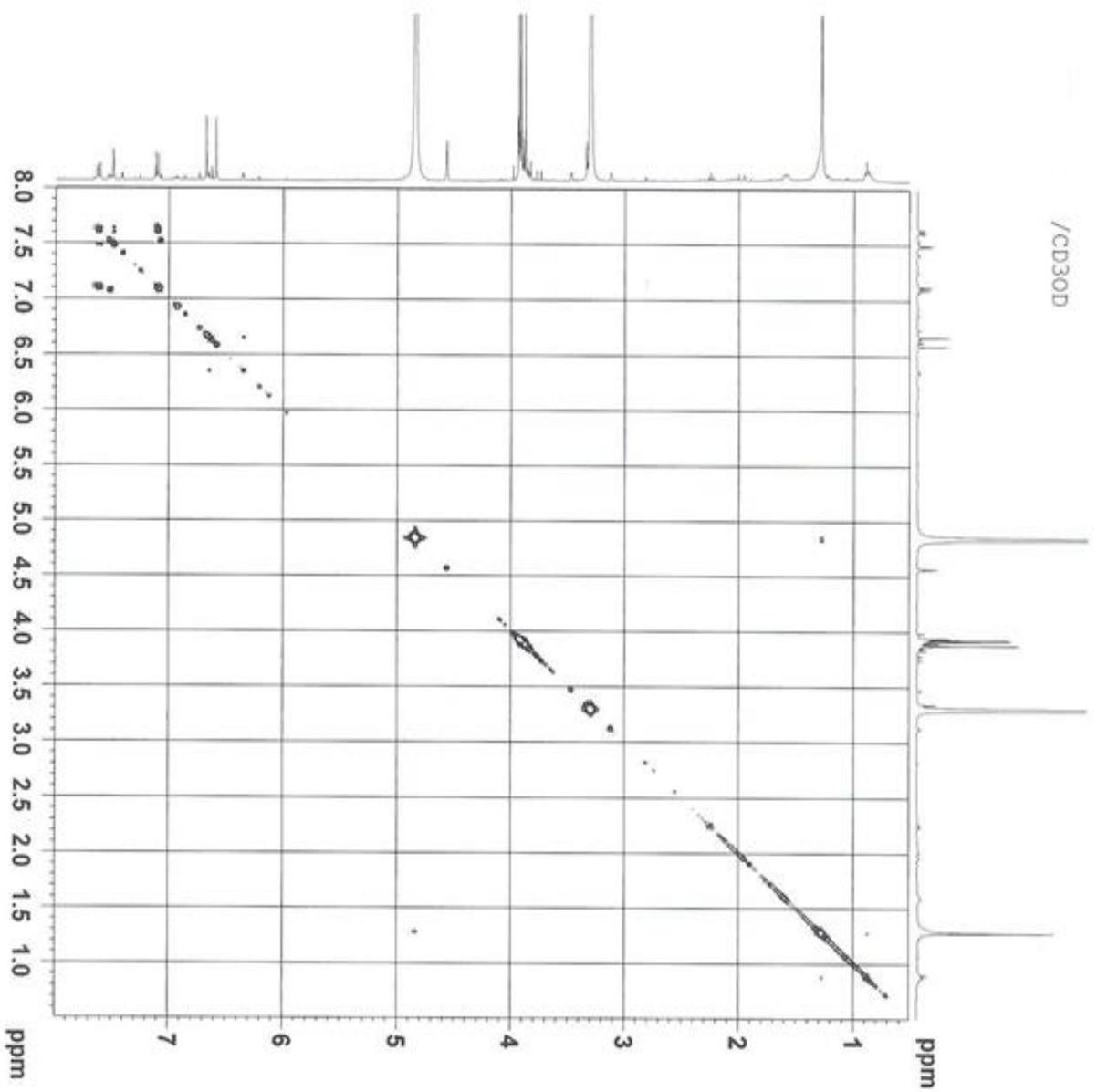
CH3T2 145.0000000
 D0 0.0000000
 D1 0.0000000
 D2 6.00344828 sec
 D3 0.01000000 sec
 D4 0.00070000 sec
 D5 0.00002160 sec
 T0 1
 T1 450.3180112 MHz
 T2 1
 F1 6.70 usec
 F2 13.40 usec
 F3 20.00000000 W
 F4 150.6746353 MHz
 POC2 13C
 POC1 13C
 F2 11.00 usec
 P1 150.0000000
 P2 150.0000000
 GSI1 50.00 %
 GRN1 20.00 %
 GRN2 10.00 %
 GRN3 40.00 %
 GRN4 100.00 usec

F1 - Acquisition parameters
 TD 16
 SFO1 160.6746 MHz
 FIDRES 236.205597 Hz
 SFO 229.350 SPM
 P1 11.00 usec

F2 - Processing parameters
 SI 32768
 SF 400.3180117 MHz
 KMC 1
 SSB 0
 LA 0
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 32768
 SF 100.6429168 MHz
 KMC 1
 SSB 0
 LA 0
 GB 0

COSY /CD3OD



AVANCE AV-III HD
400 MHz
LAB #109A

```

Current Data Parameters
NAME      Jan30-17
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20170130
Time      11.43 h
INSTRUM   spect
PROBHD    zgpg30
PULPROG   coyyppqf
TD        2048
SOLVENT   MeOD
NS         16
DS         4
SFR       3605.769 Hz
FIDRES    3.521259 Hz
AQ         0.2839893 sec
RG         202.75
TW         138.667 usec
DE         6.50 usec
TE         298.0 K
D0         0.00000360 sec
D1         1.500000000 sec
D13        0.00000400 sec
D16        0.00020000 sec
IND0       0.00027740 sec
TD0AV      1
SFO1       400.318015 MHz
RG01       18
RG02       6.70 usec
RG03       6.70 usec
F1         20.00000000 W
GPMV(1)    10.00
GPR1       1000.00 usec
P16

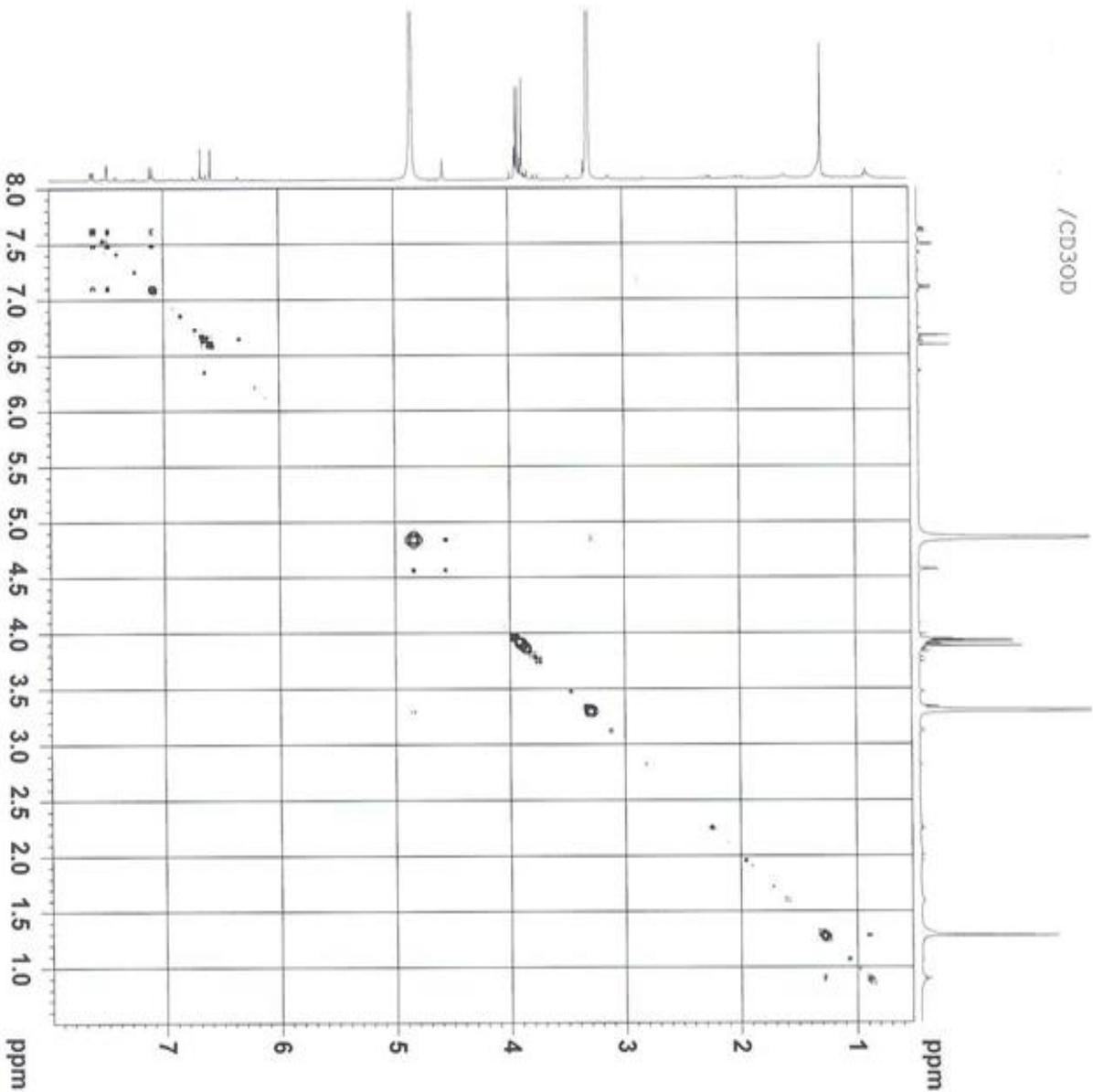
F1 - Acquisition parameters
TD         256
SFO1       400.318 MHz
FIDRES     28.16301 Hz
SK         9.005 ppm
FHM0000   Op

F2 - Processing parameters
SI         400.3180117 MHz
SF         400.3180117 MHz
WDW        QSINE
SSB        0
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         2048
MC2        OR
SF         400.3180117 MHz
WDW        QSINE
SSB        0
LB         0 Hz
GB         0
  
```

TOCSY100

/CD3OD



AVANCE AV-III HD
400 MHz
LAB #109A

Current Data Parameters
 NAME Jan30-17
 EXPRNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20170130
 Time_ 18.04 h
 INSTRUM spect
 PROBRD zgpg30
 PULPROG zgpg30
 TD 65536
 SFO 400.136250
 SOLVENT MeOD
 NS 16
 DS 4
 SWH 3895.169 Hz
 FIDRES 3.321259 Hz
 AQ 0.2839893 sec
 RG 202.75
 DW 202.75
 DE 6.50 usec
 TE 298.2 K

DO 0.00013037 sec
 D1 1.50000000 sec
 D2 0.10000000 sec
 D12 0.00020000 sec
 ING 0.00027740 sec
 L1 48
 TDav 1
 SFO1 400.3318015 MHz
 NUC1 1H
 FI 6.80 usec
 FS 20.01 usec
 FD 30.00 usec
 FT 60.00 usec
 F17 2500.00 usec
 PLM1 20.00000000 M
 PLM10 1.02760000 M

F1 - Acquisition Parameters
 TD 256
 SFO1 400.3318 MHz
 FIDRES 28.163301 Hz
 SW 9.005 ppm
 FWHM 5.005 ppm
 STAKE 5.005 ppm

F2 - Processing Parameters
 SI 2048
 SF 400.3300117 MHz
 WDM 0
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing Parameters
 SI 2048
 MC1 512
 SC 400.3300117 MHz
 MSB 0
 MSX 0
 MSY 0
 MSZ 0
 GB 0
 PC 1.40

NOESY

/CD3OD

