

Supporting Information

Rec. Nat. Prod. 11:1 (2017) 43-50

Melilotoside Derivatives from *Artemisia splendens* (Asteraceae)

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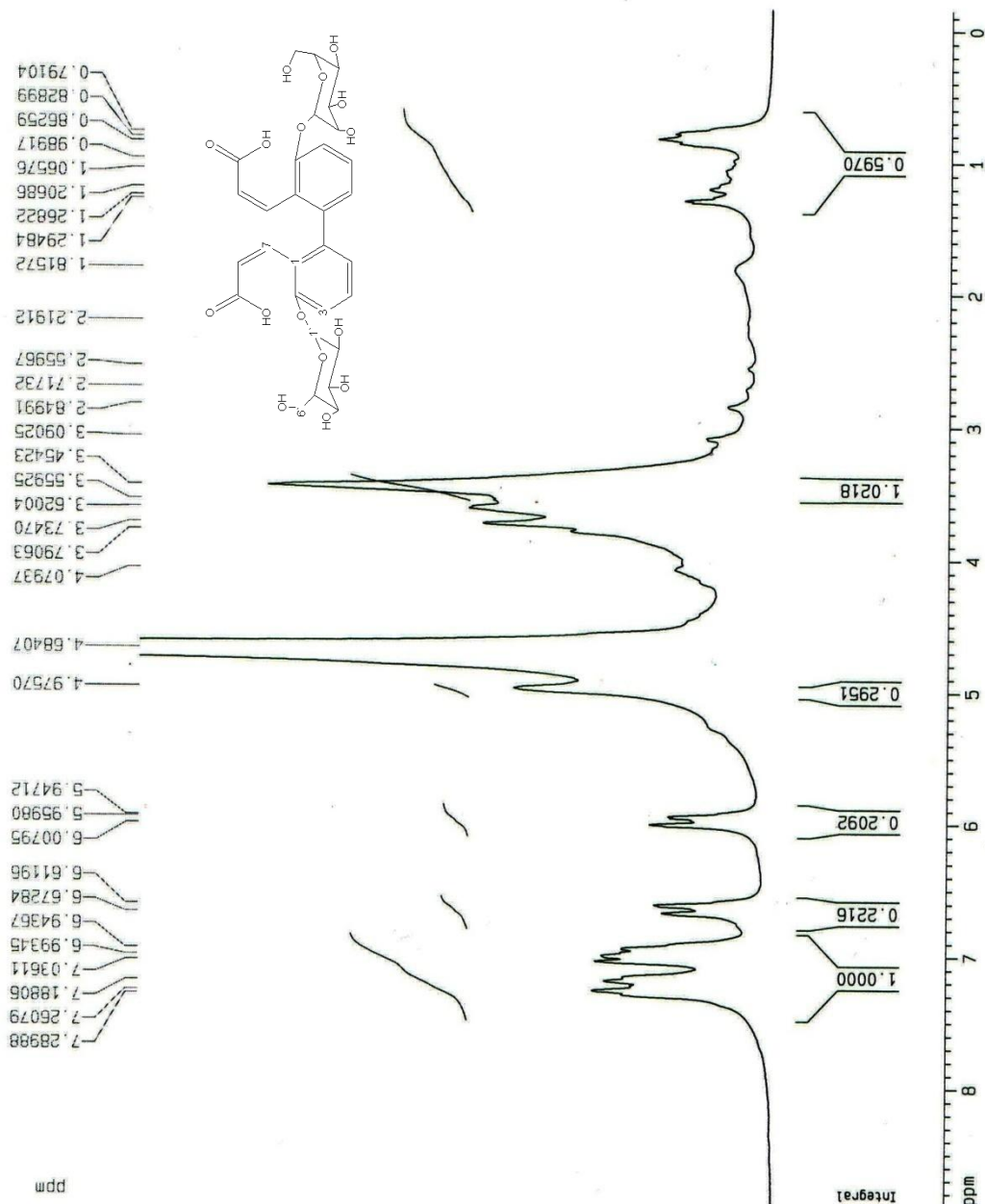
Current Data Parameters
NAME art-splend-10-5
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110209
Time 10.39
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg
TD 32768
SOLVENT D2O
NS 58
DS 0
SMH 2796.421 Hz
FIDRES 0.085340 Hz
AQ 5.8599683 sec
RG 143.7
DM 178.800 usec
DE 6.00 usec
TE 293.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -6.00 dB
SF01 200.1312359 MHz

F2 - Processing parameters
SI 32768
SF 200.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 62.89 cm
F1P 8.880 ppm
F1 1777.13 Hz
F2P -0.154 ppm
F2 -30.77 Hz
PPMCM 0.45168 ppm/ci
HZCM 90.39505 Hz/cm



S1: Bis-Z-melilotoside (^1H NMR) (NMR 200)

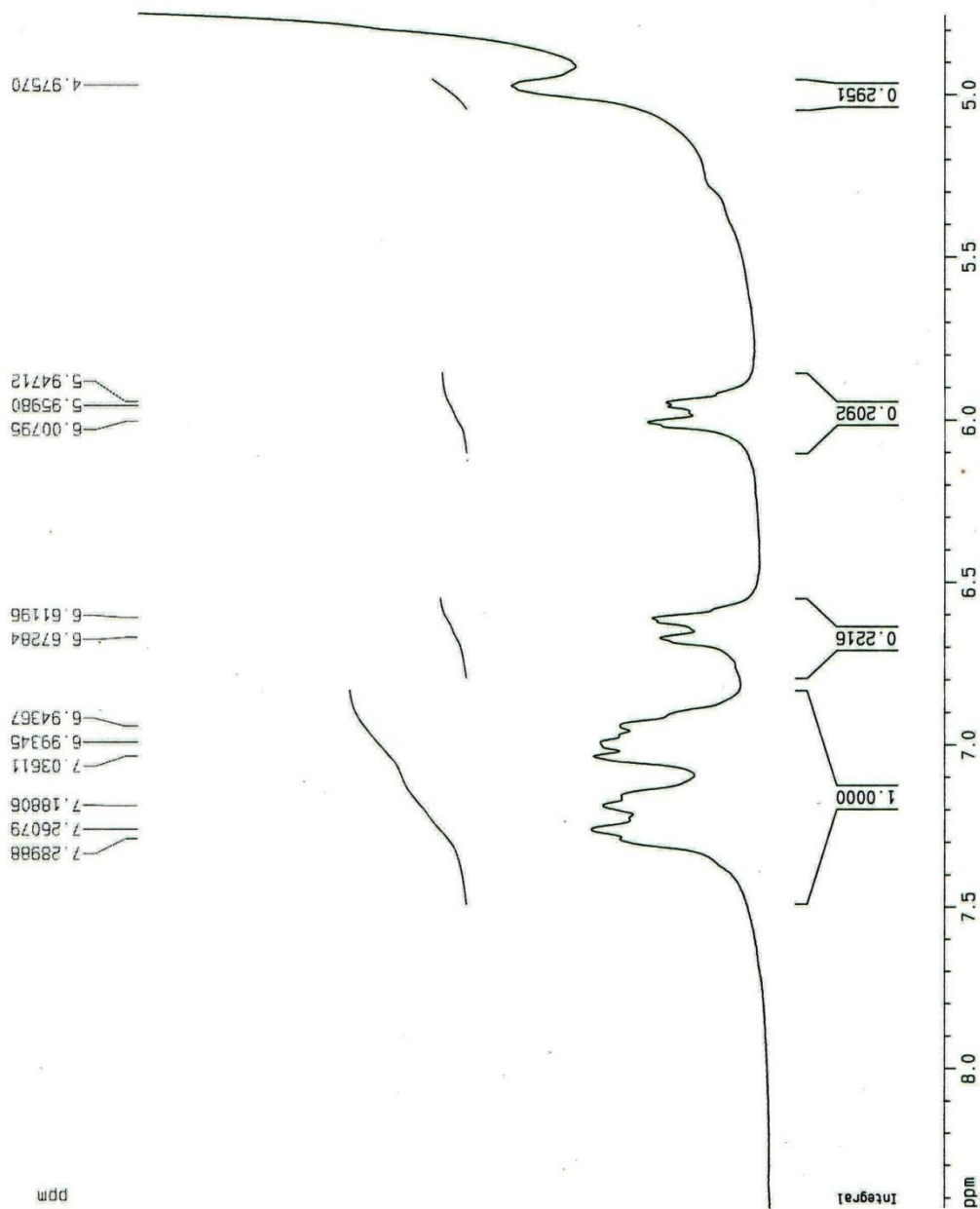
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NAME art-splend-10-5
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 10.39
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PULPROG zg
TD 32768
SOLVENT D2O
NS 58
DS 0
SWH 2796.421 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 143.7
DM 178.800 usec
DE 6.00 usec
TE 293.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRR 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -6.00 dB
SF01 200.1312359 MHz

F2 - Processing parameters
SI 32768
SF 200.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 62.89 cm
FIP 8.431 ppm
F1 1687.22 Hz
F2P 4.752 ppm
F2 950.94 Hz
PPMCH 0.18395 ppm/cm
HZCM 36.81411 Hz/cm



S2: Bis-Z-melilotoside (^1H NMR)

Current Data Parameters
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EXPNO 2
PROCNO 1

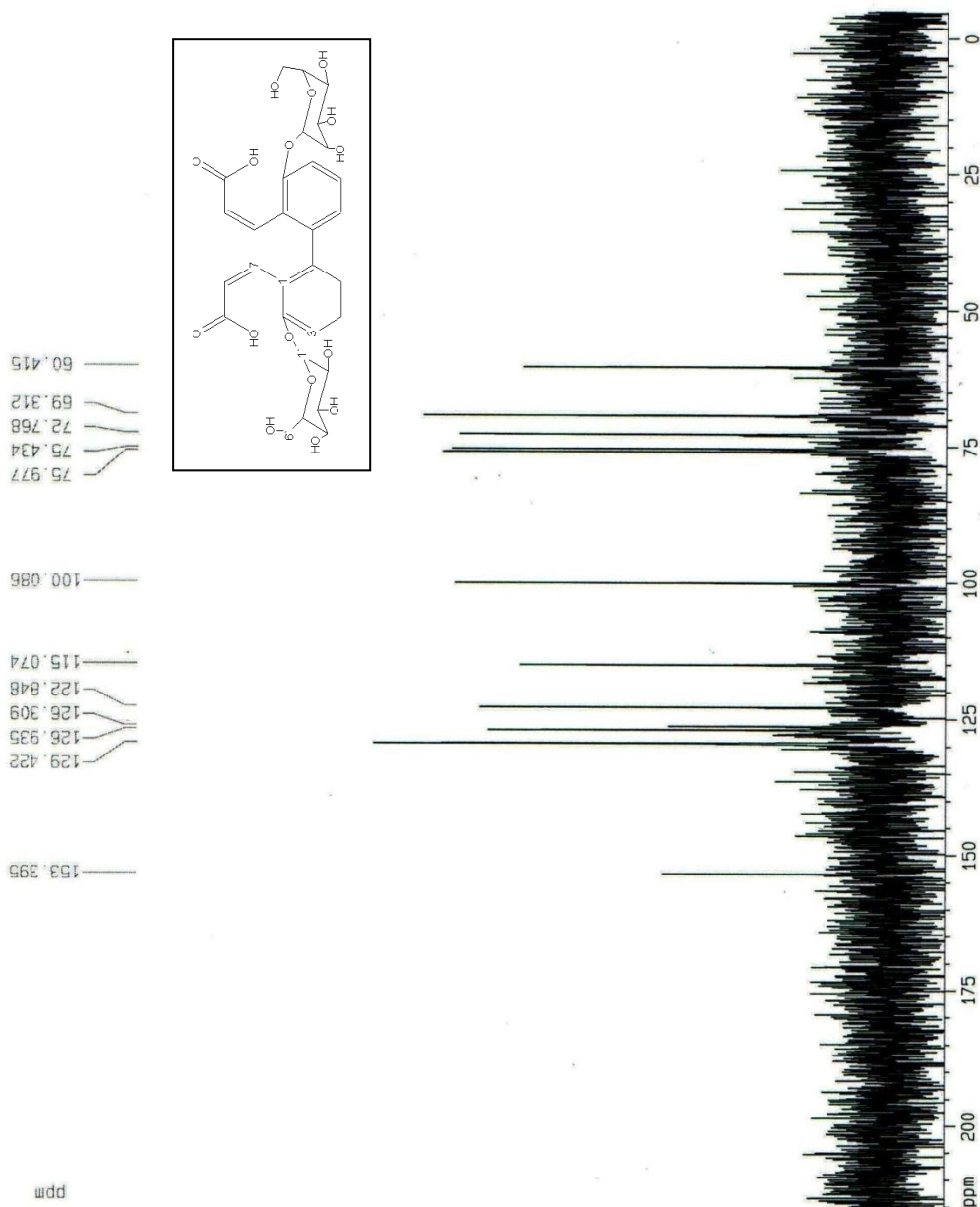
F2 - Acquisition Parameters
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Time 10.47
INSTRUM spect
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PULPROG zgpg
TO 65536
SOLVENT MeOD
NS 304
DS 0
SMH 11990.407 Hz
FIDRES 0.162959 Hz
AQ 2.7329011 sec
RG 50.8
DM 41.700 usec
DE 5.00 usec
TE 293.2 K
D1 5.00000000 sec
d11 0.03000000 sec
DELTA 4.90000010 sec
MCREST 0.00000000 sec
MCIRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 -6.00 dB
SF01 50.3277608 MHz

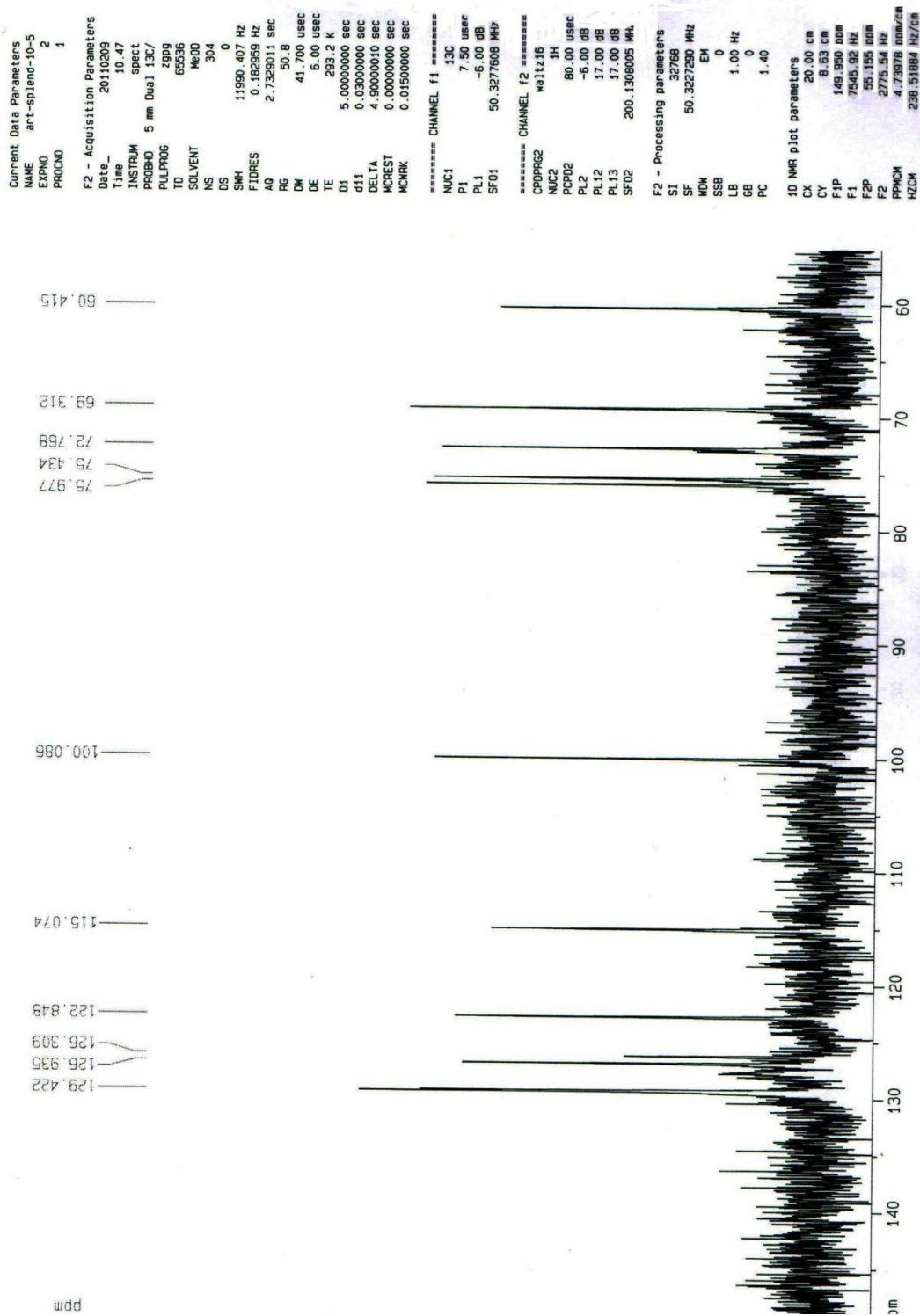
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PCPD2 80.00 usec
PL2 -6.00 dB
PL12 17.00 dB
PL13 17.00 dB
SF02 200.1308005 MHz

F2 - Processing parameters
SI 32768
SF 50.3227290 MHz
MDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ID NMR plot parameters
CX 20.00 cm
CY 8.63 cm
FIP 215.000 ppm
F1 10819.39 Hz
F2 -5.000 ppm
F2 -251.51 Hz
PPMCM 11.00000 ppm/1
HZCM 553.54999 Hz/cm

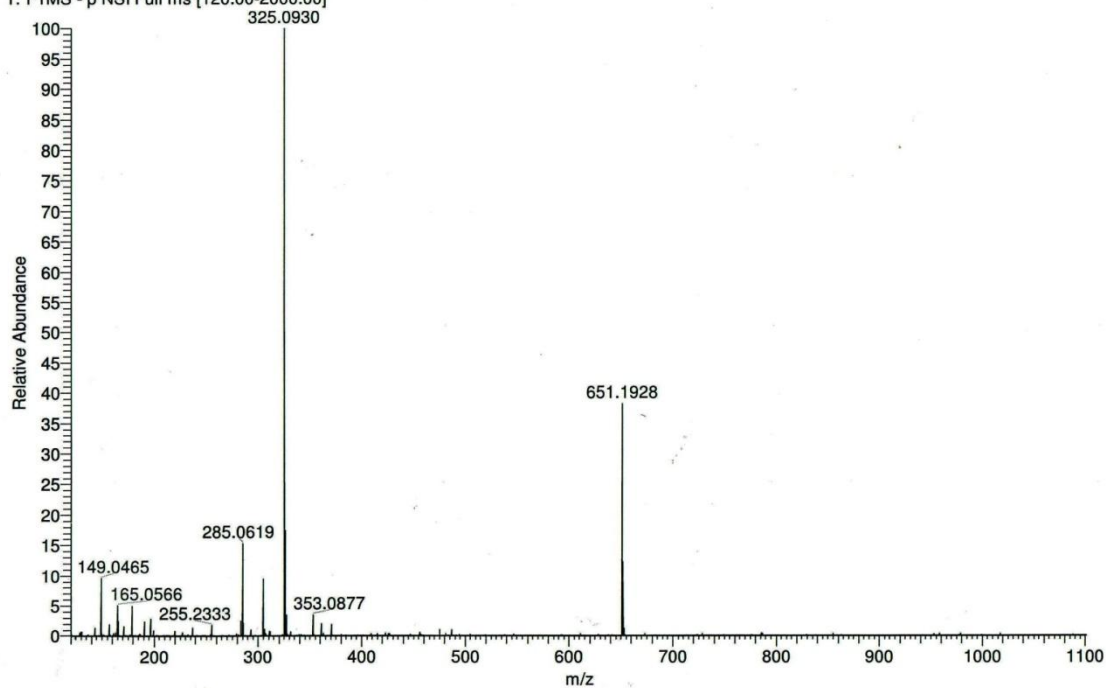


S3: Bis-Z-melilotoside (^{13}C NMR)

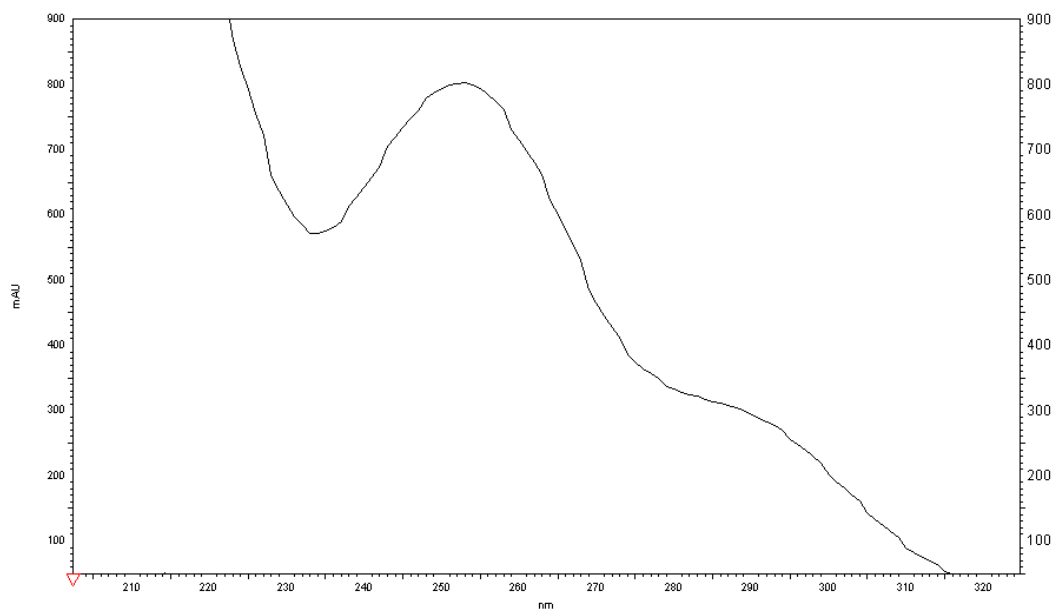


S4: Bis-Z-melilotoside (^{13}C NMR)

WOLSAR090-OV-HNESN #4-6 RT: 0.37-0.49 AV: 3 SM: 7G NL: 5.92E5
T: FTMS - p NSI Full ms [120.00-2000.00]



S5: Bis-Z-melilotoside (MASS)



S6: Bis-Z-melilotoside (UV)

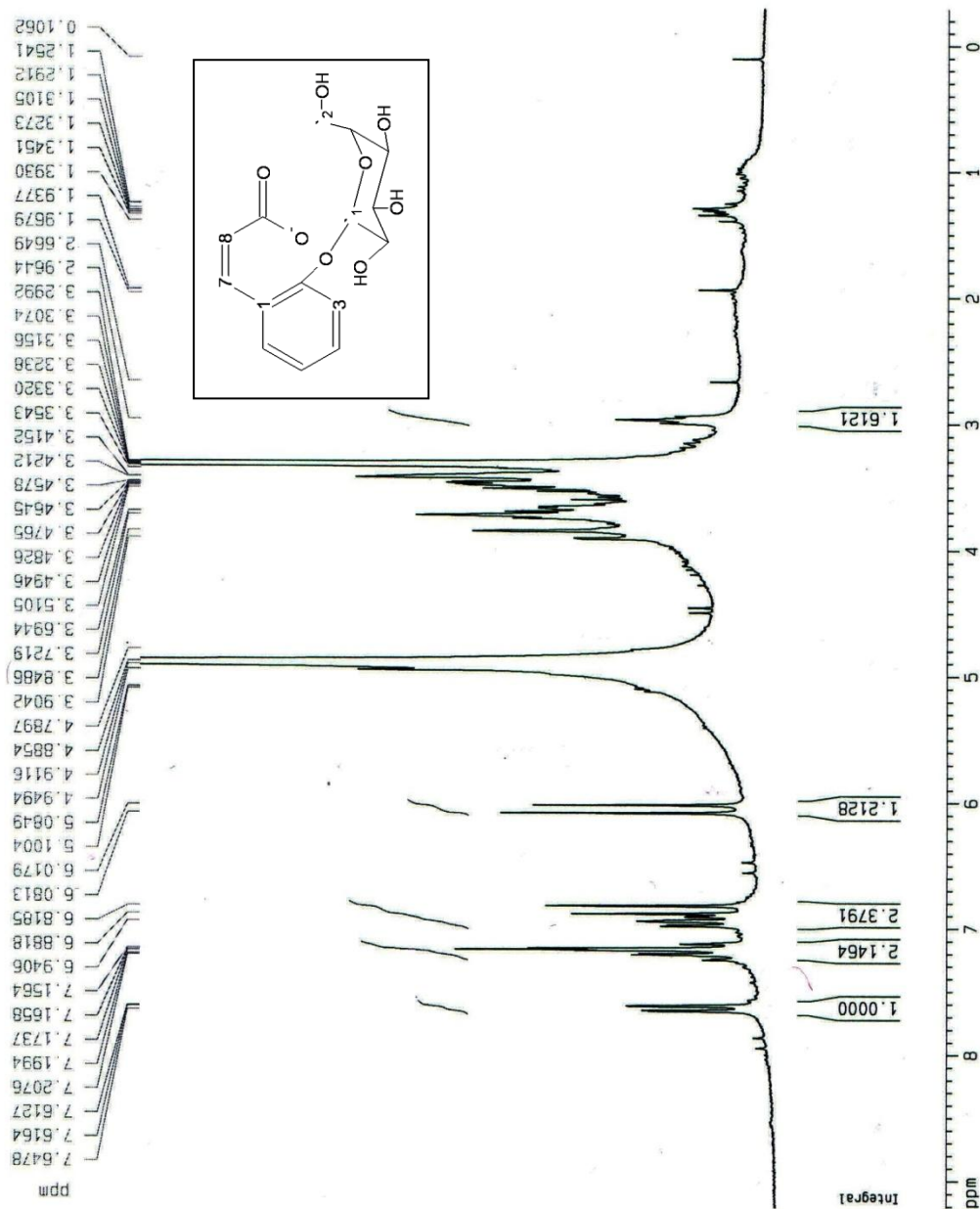
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PROCNO 1

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PULPROG zg
TD 32768
SOLVENT MeOD
NS 195
DS 0
SMH 2795.421 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 1148.4
DM 178.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -6.00 dB
SF01 200.1312359 MHz

F2 - Processing parameters
SI 32768
SF 200.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 192.24 cm
F1P 9.209 ppm
F1 1843.00 Hz
F2P -0.295 ppm
F2 -59.30 Hz
PPMCM 0.47527 ppm/cm
HZCM 95.11510 Hz/cm



S7: Z-melilotoside (¹HNMR)

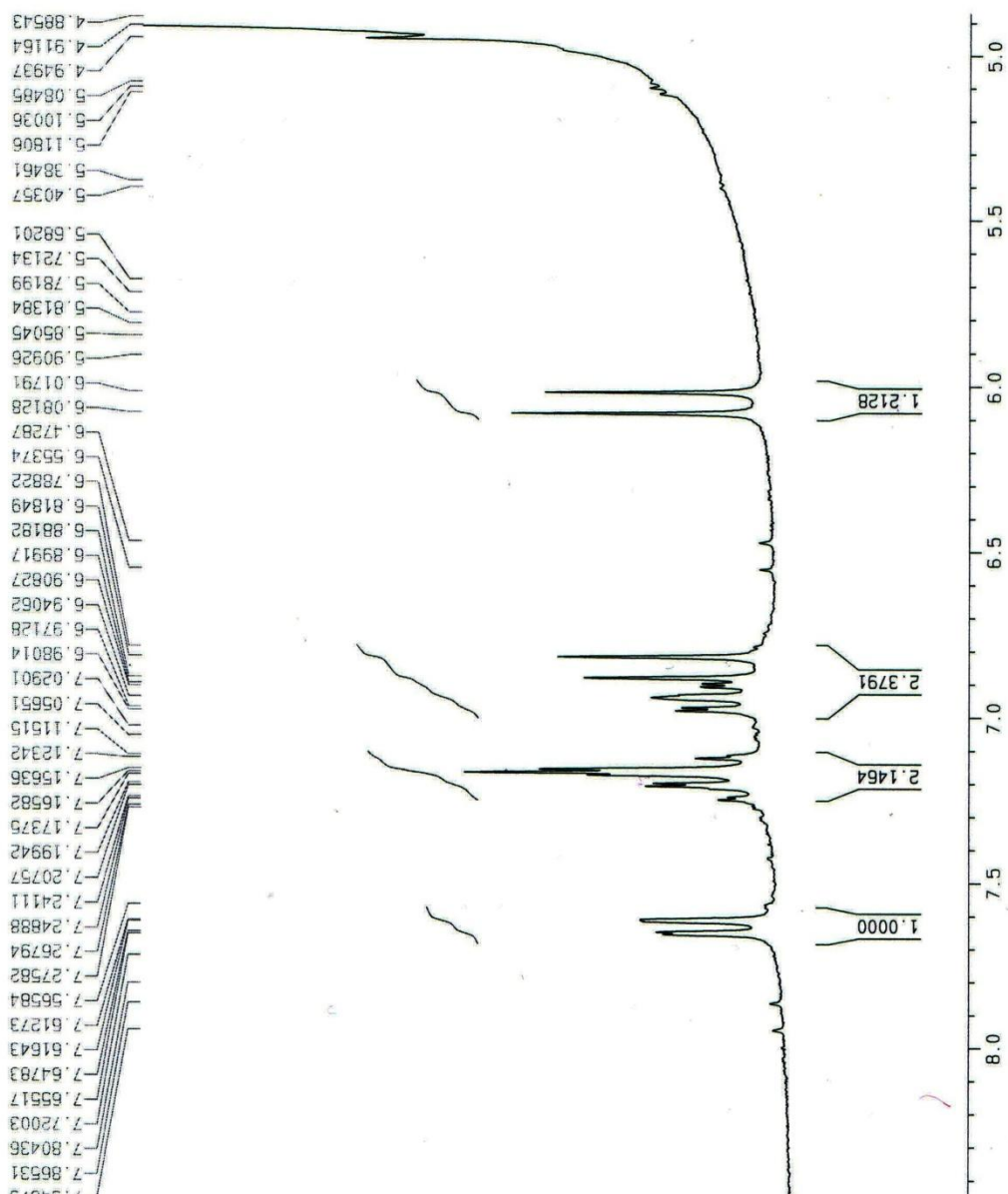
Current Data Parameters
NAME art-splend-20-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110703
Time 9.07
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg
TD 32768
SOLVENT MeOD
NS 195
DS 0
SWH 2796.421 Hz
FIDRES 0.085340 Hz
AQ 5.859683 sec
RG 1149.4
DM 178.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWK 0.01500000 sec

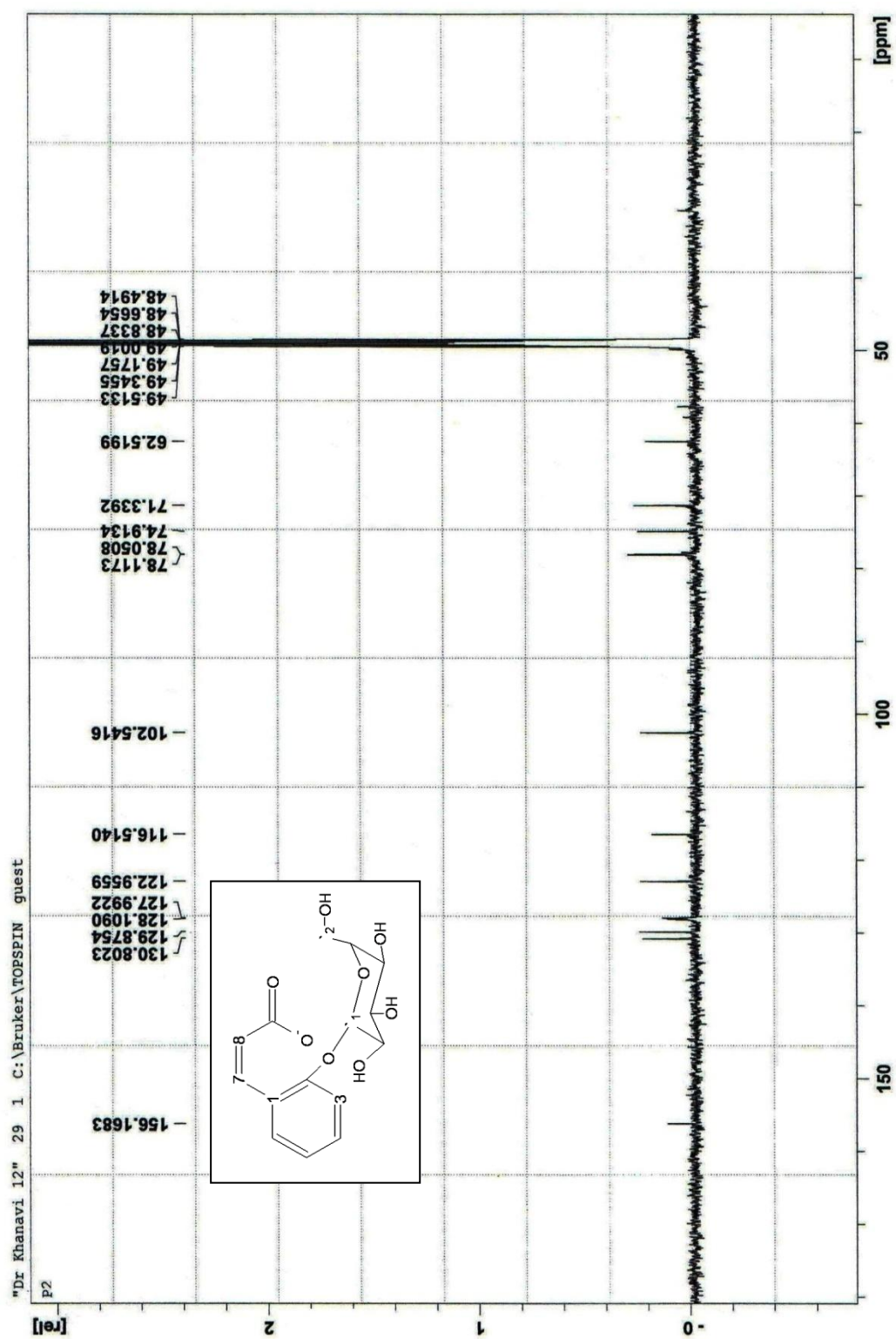
===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -6.00 dB
SF01 200.1312359 MHz

F2 - Processing parameters
SI 32768
SF 200.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

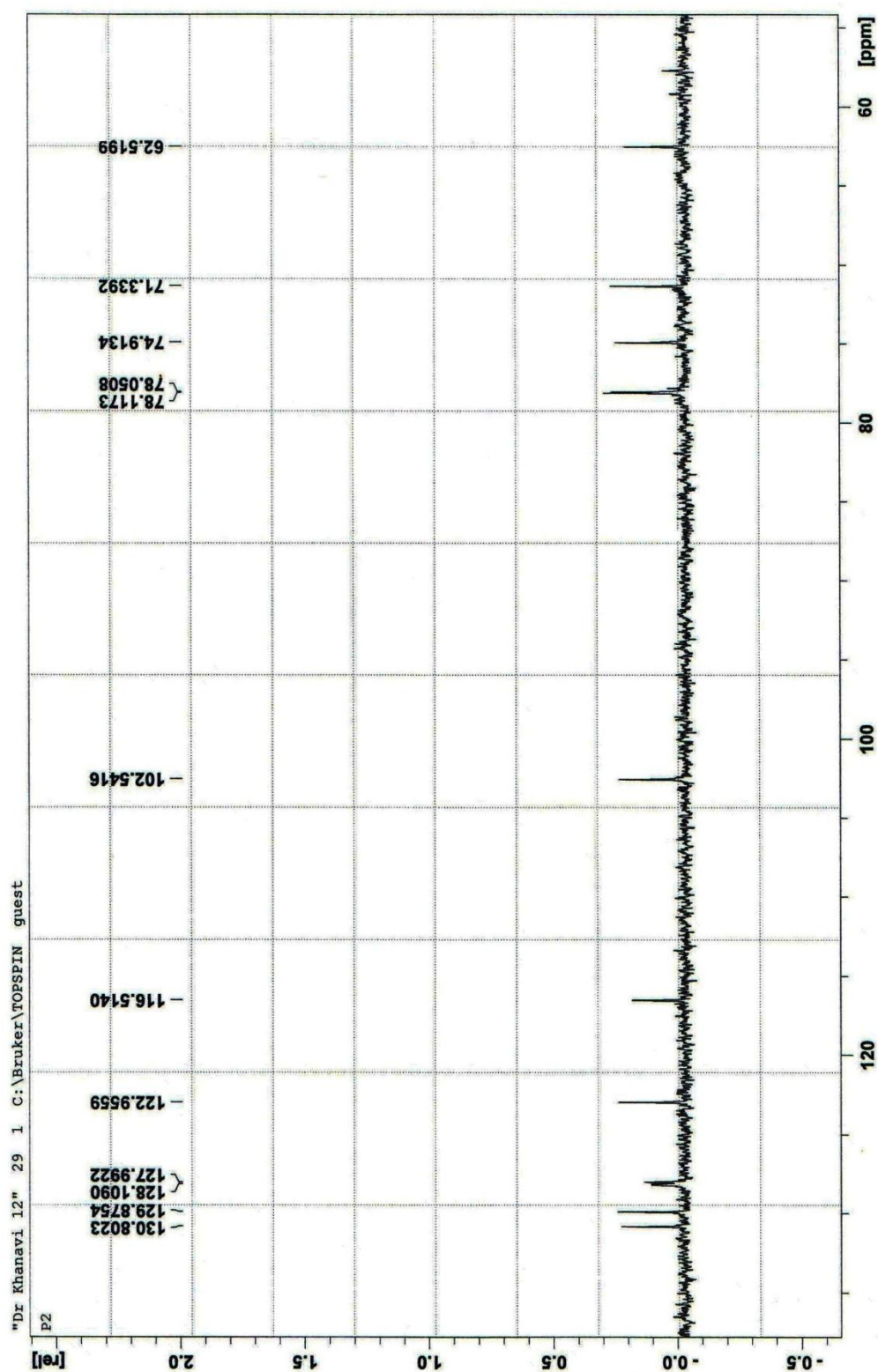
1D NMR plot parameters
CX 20.00 cm
CY 192.24 cm
FIP 8.584 ppm
F1 1717.85 Hz
F2 4.869 ppm
F2 974.45 Hz
PPMCM 0.18573 ppm/cm
HZCM 37.16998 Hz/cm



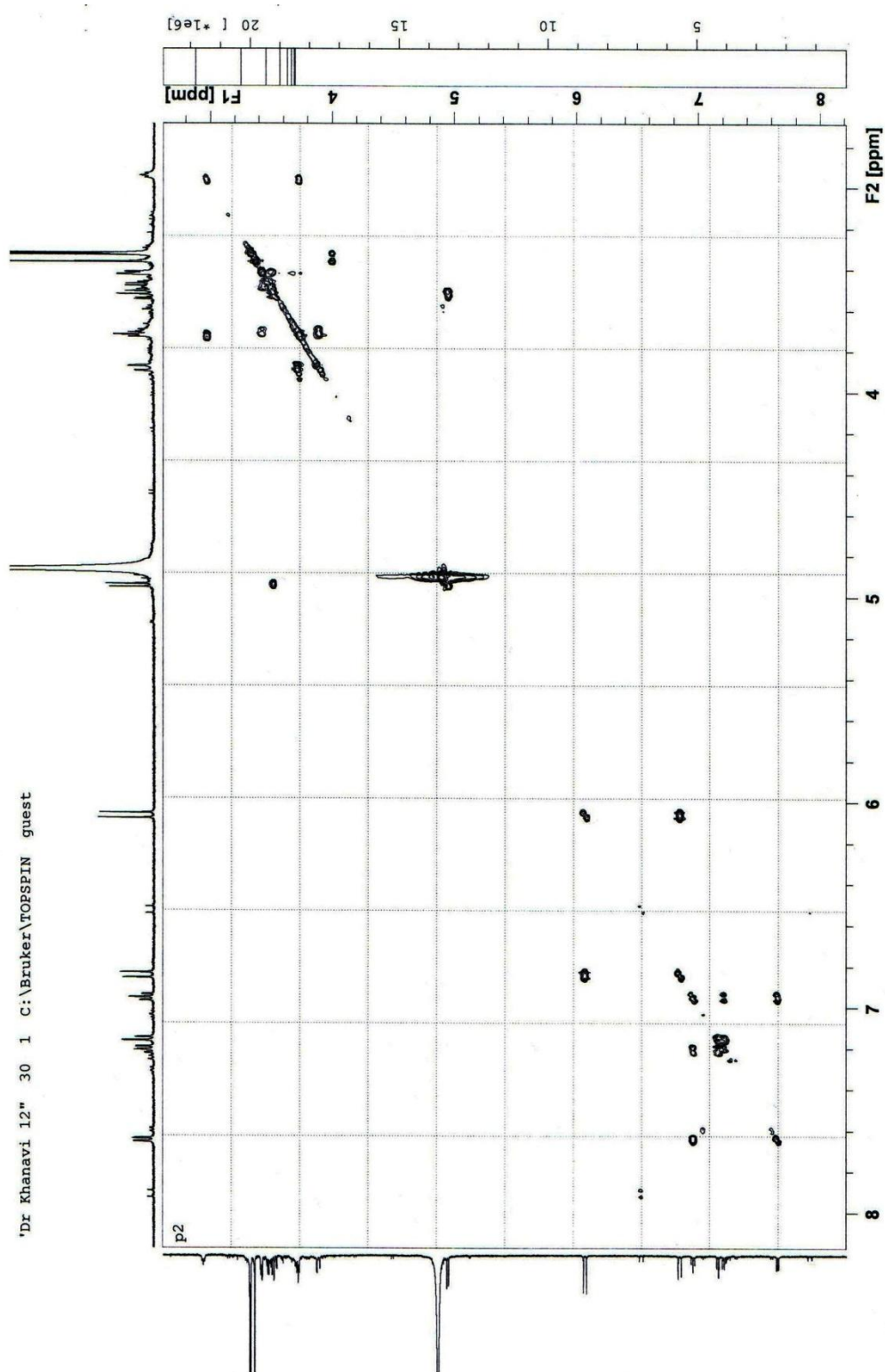
S8: Z-melilotoside (^1H NMR)



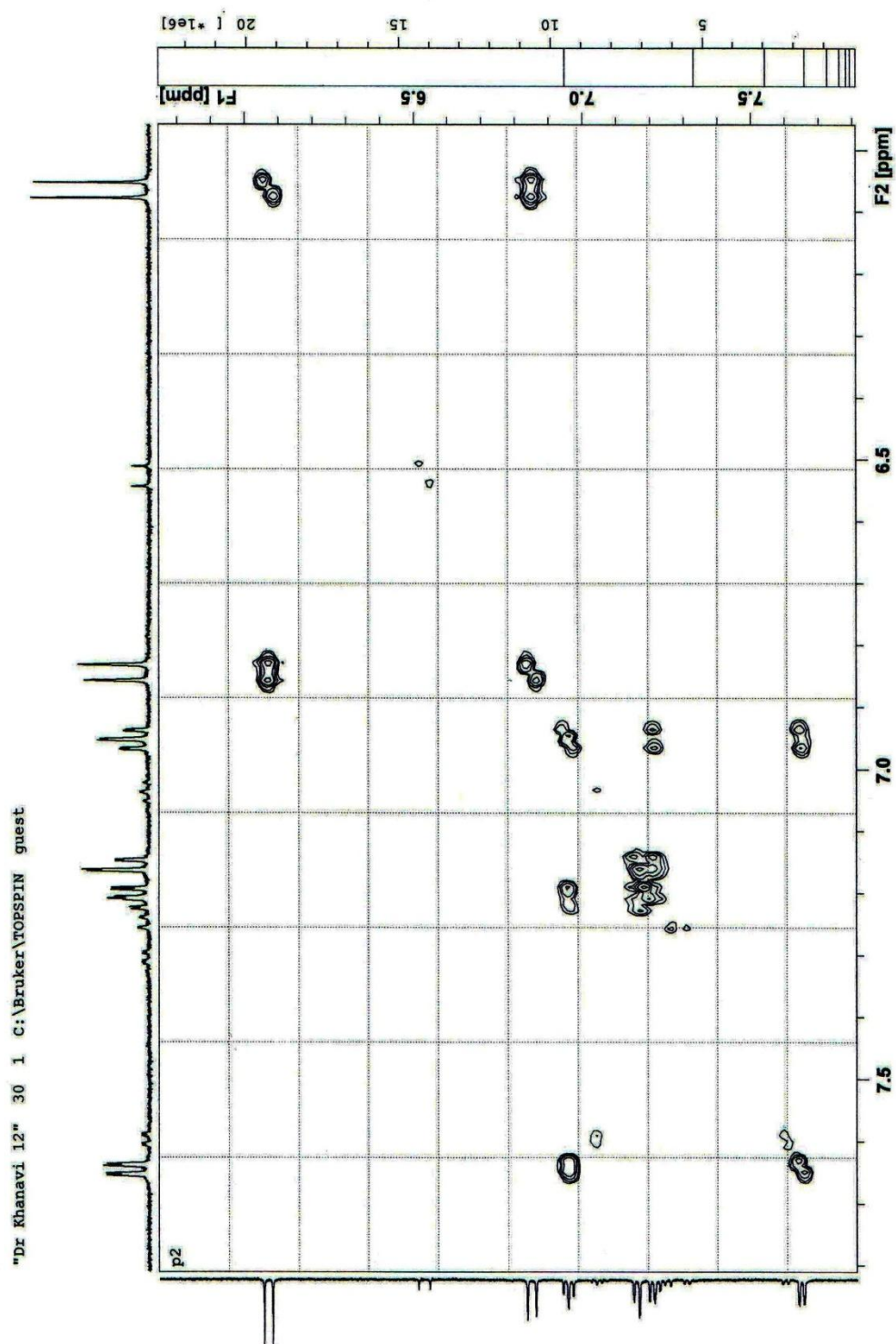
S9: Z-melilotoside (^{13}C NMR)



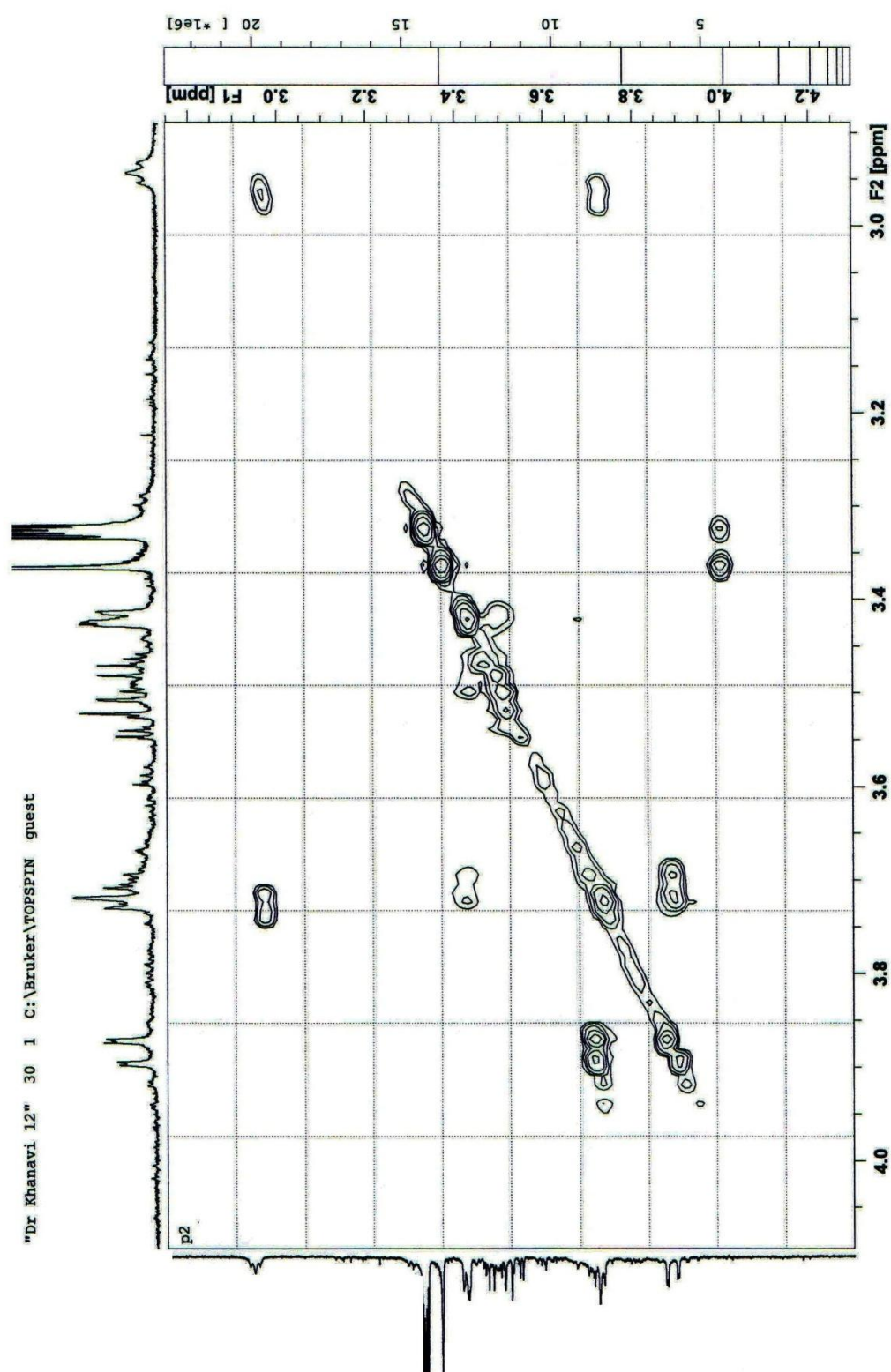
S10: Z-melilotoside (^{13}C NMR)



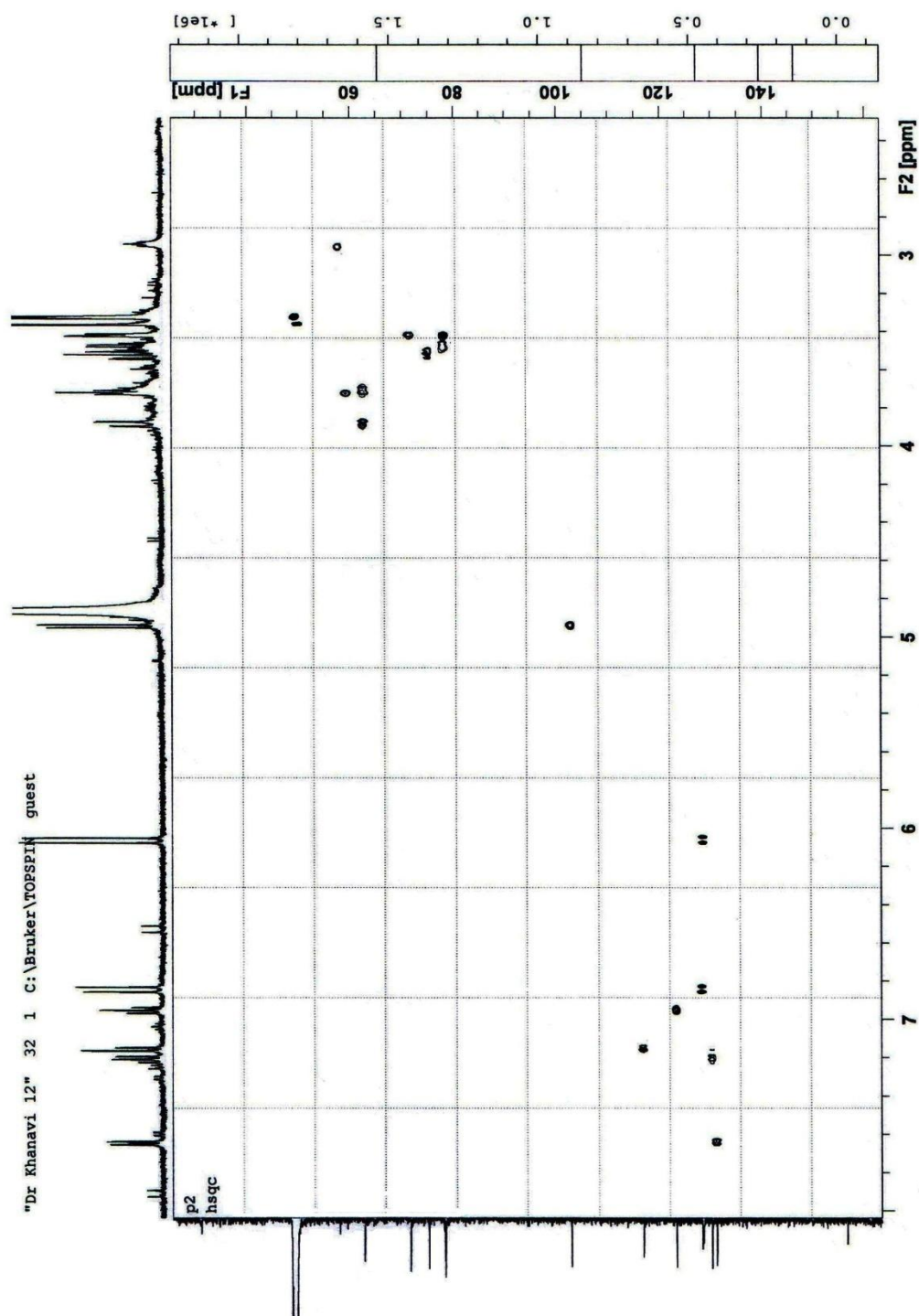
S11: Z-melilotoside(COSY)



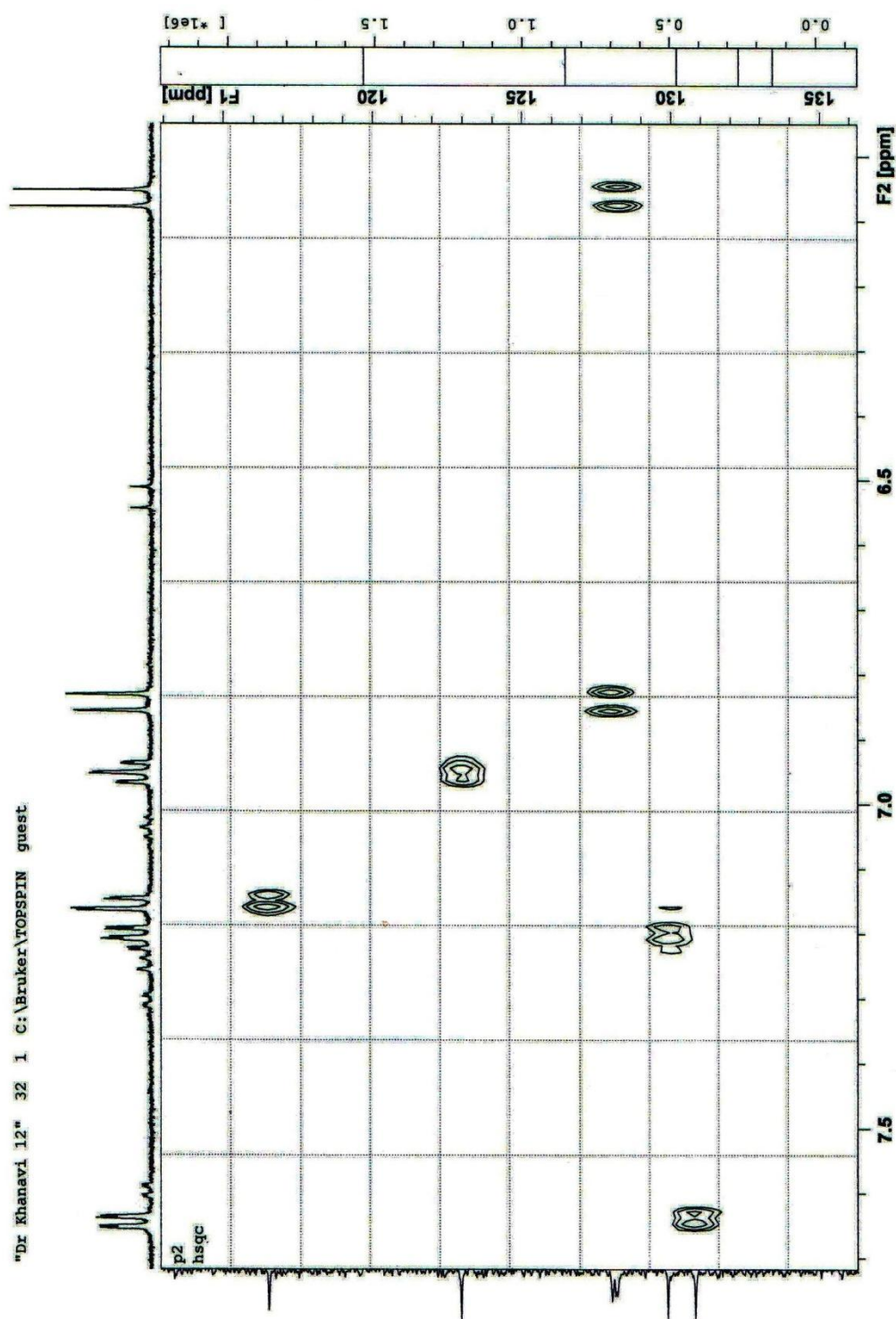
S12: Z-melilotoside (COSY)



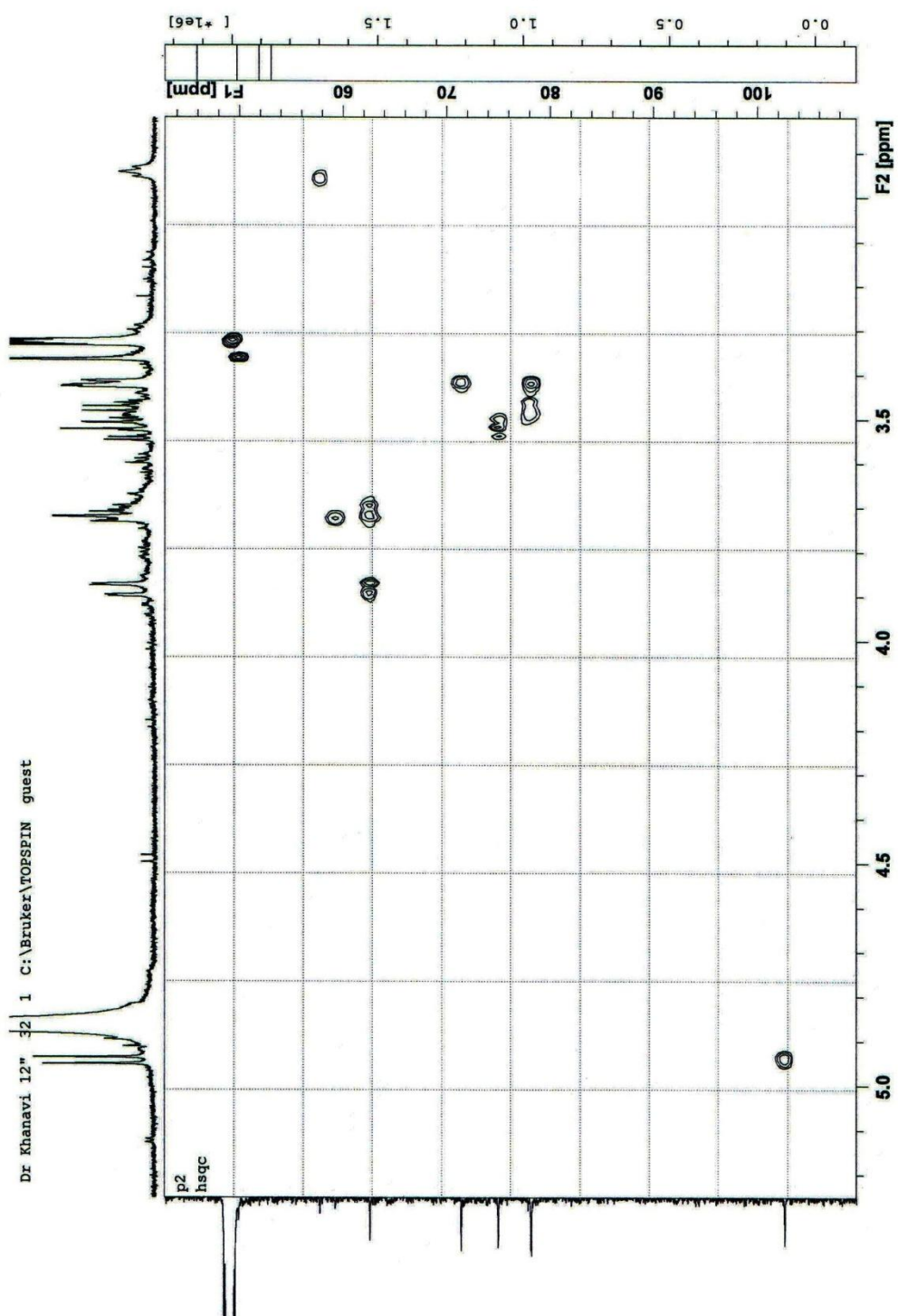
S13: Z-melilotoside COSY)



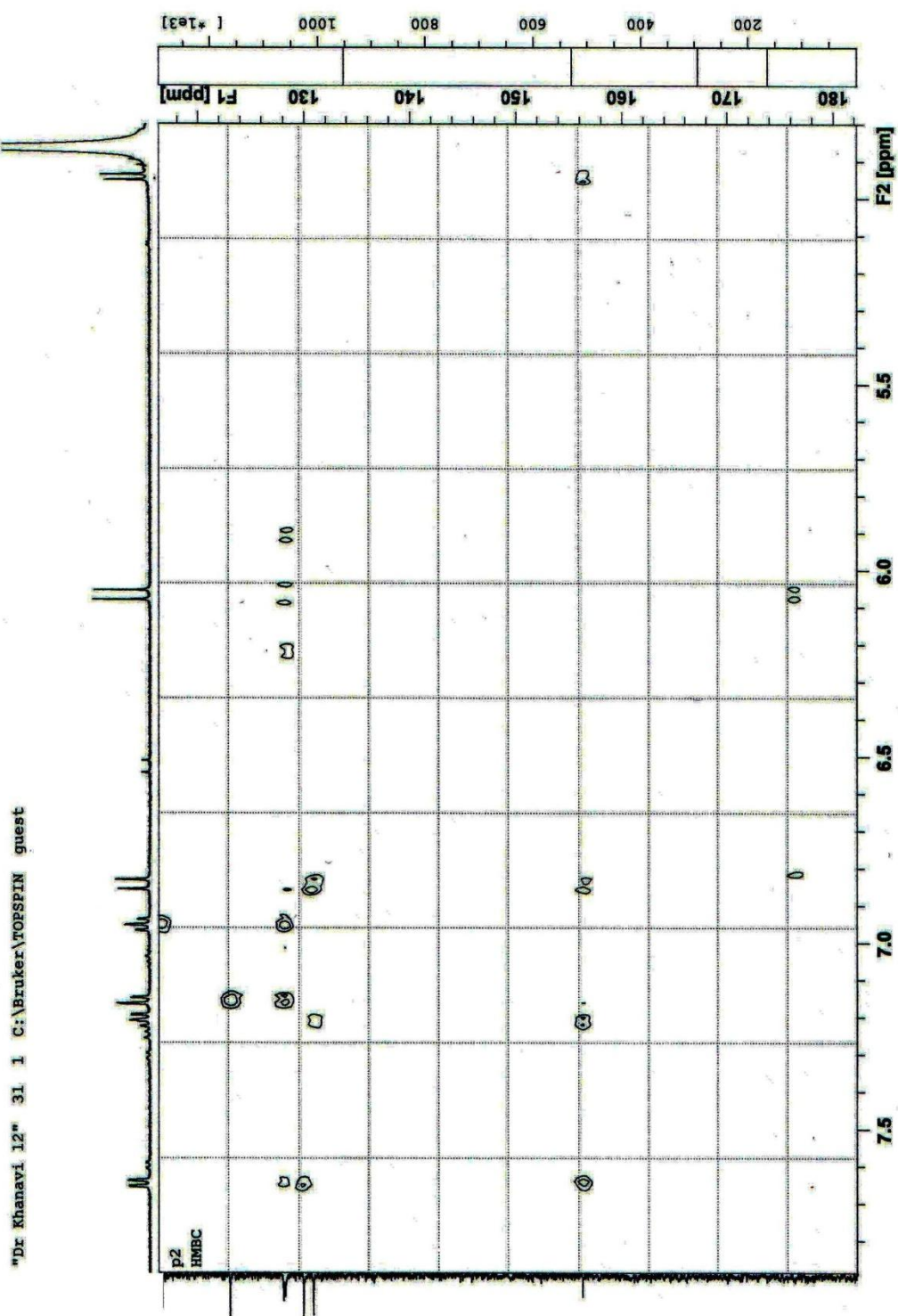
S14: Z-melilotoside (HSQC)



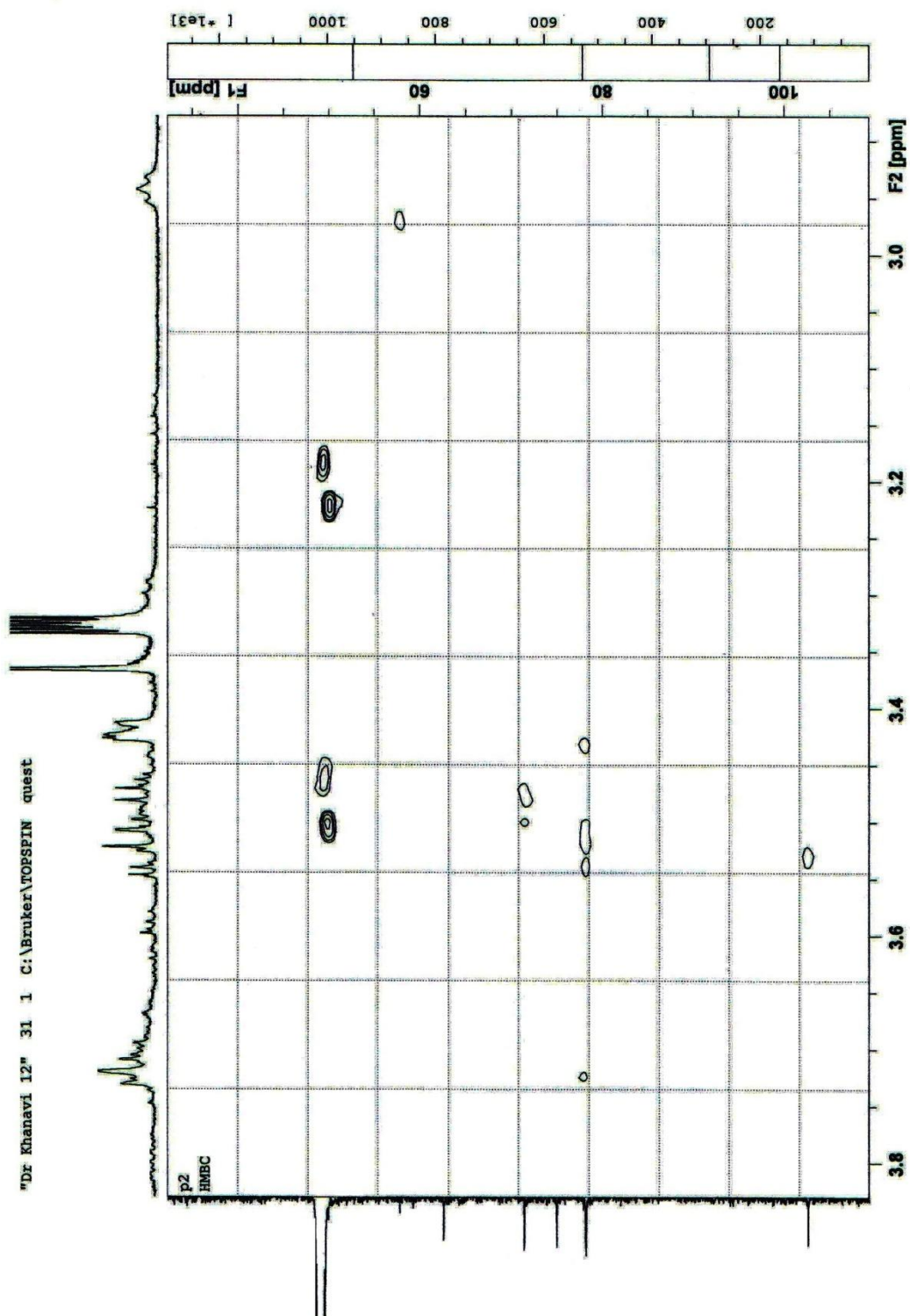
S15:Z-melilotoside (HSQC)



S16: Z-melilotoside (HSQC)



S17: Z-melilotoside (HMBC)



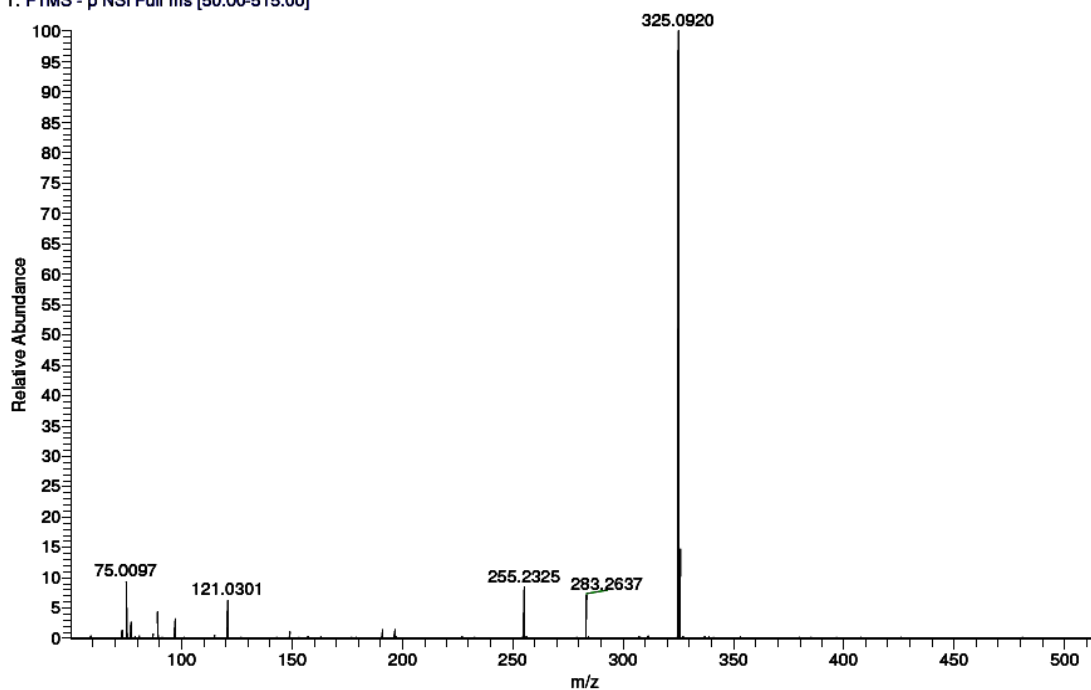
S18: Z-melilotoside (HMBC)

20.2 MW-?
(MeOH)/MeOH

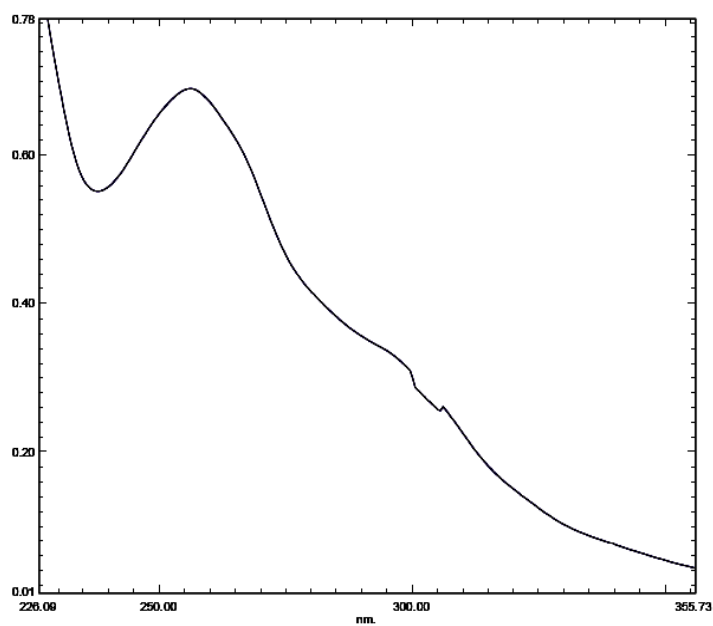
EPSRC National Centre Swansea
LTQ Orbitrap XL

Prof S Sarker
30/08/2012 14:25:09

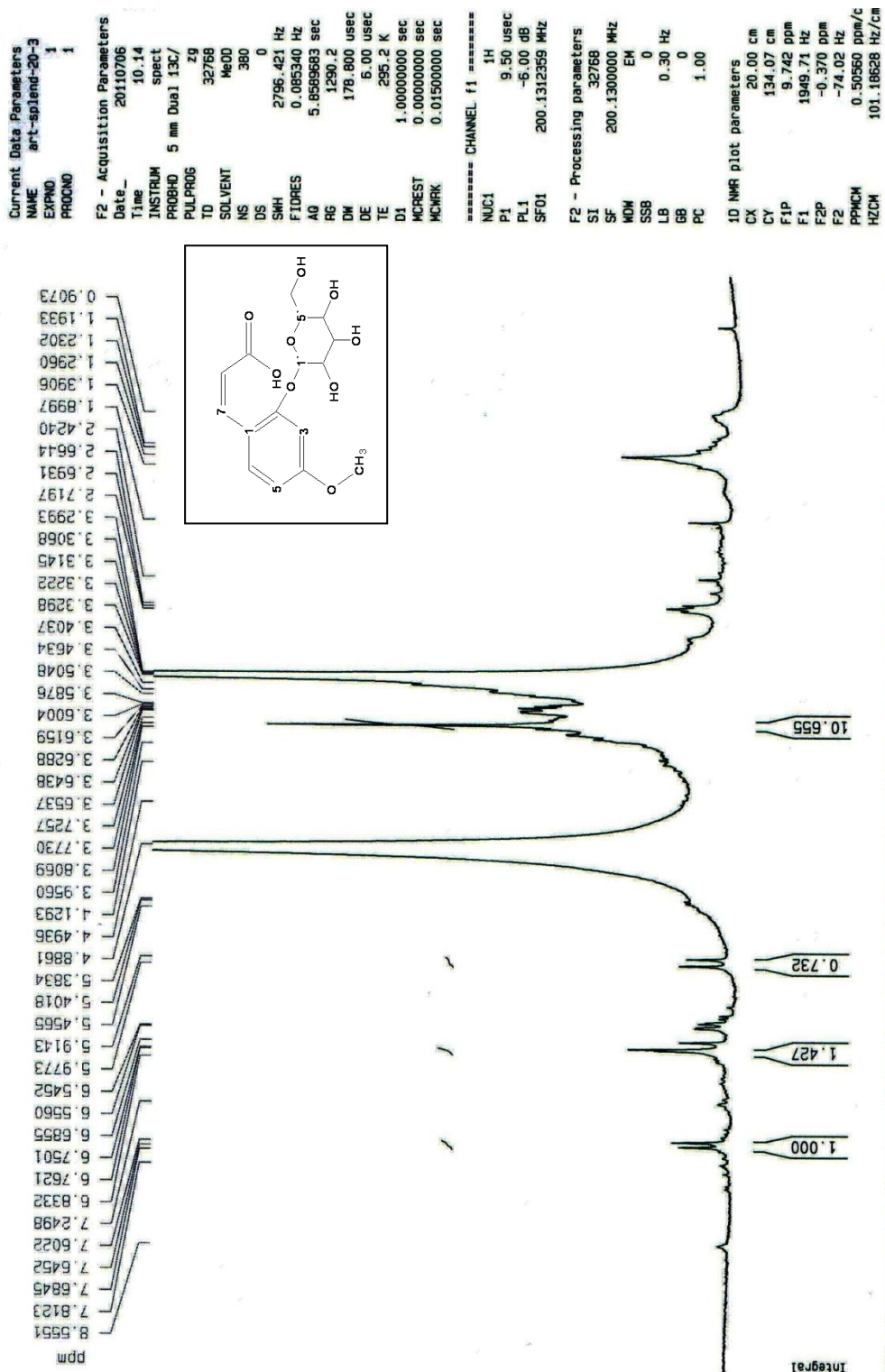
WOLSA089-OV-HNESN-2 #34-40 RT: 1.13-1.48 AV: 7 SM: 7G NL: 5.82E6
T: FTMS - p NSI Full ms [50.00-515.00]



S19: Z-melilotoside (MASS)



S20: Z-melilotoside (UV)



S21: 4-methoxy-Z-melilotoside (¹HNMR)

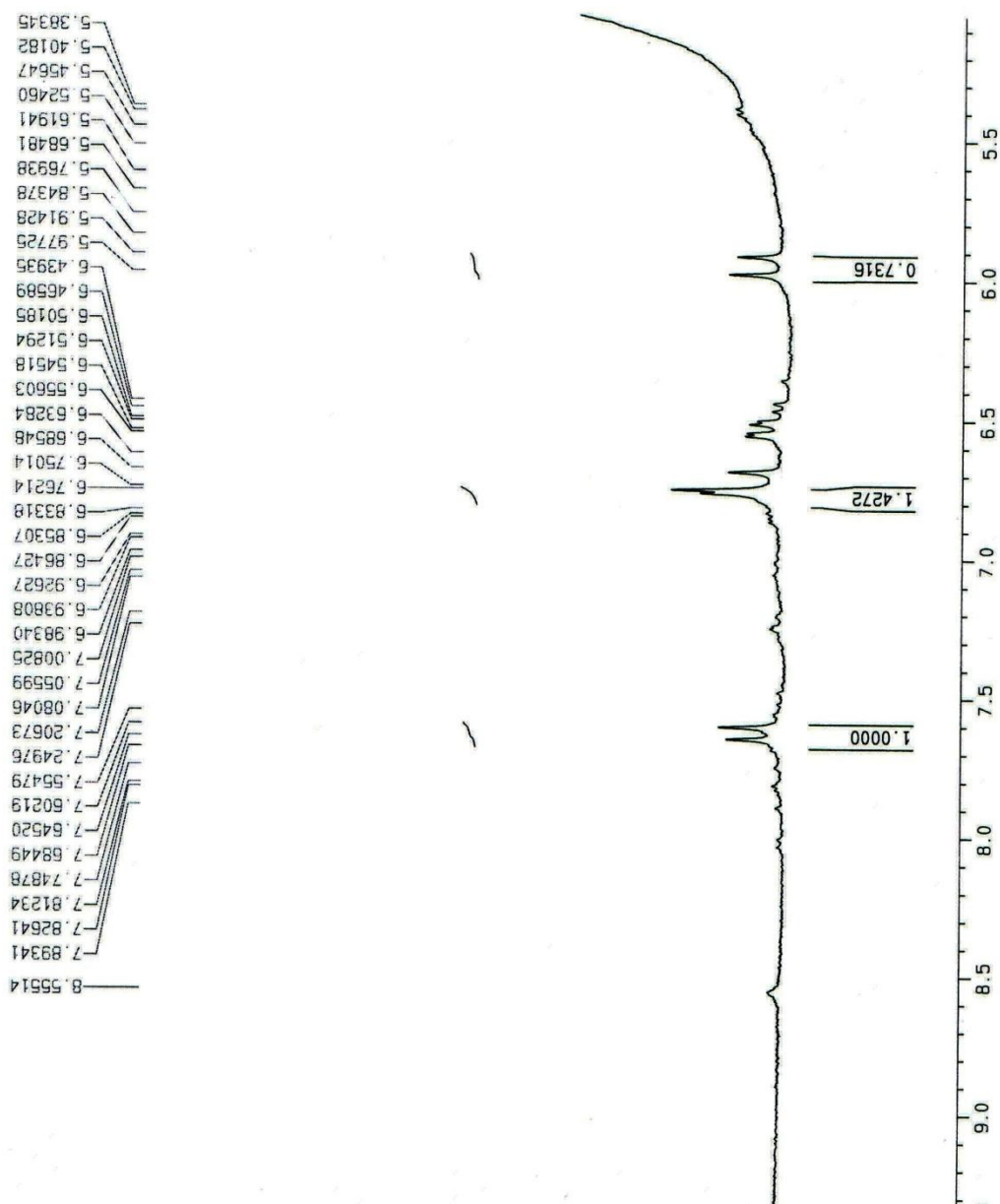
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EXPNO 1
PROCNO 1

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PROBHD 5 mm Dual 13C/
PULPROG zg
TD 32768
SOLVENT MeOD
NS 380
DS 0
SWH 2796.421 Hz
FIDRES 0.085340 Hz
AQ 5.8569683 sec
RG 1290.2
DM 178.800 use
DE 6.00 use
TE 295.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -6.00 dB
SF01 200.1312359 MHz

F2 - Processing parameters
SI 32768
SF 200.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 134.07 cm
F1P 9.423 ppm
F1 1885.80 Hz
F2P 5.045 ppm
F2 1009.74 Hz
PPMCH 0.21887 ppm/cm
HZCH 43.80301 Hz/cm



S22: 4-methoxy-Z-melilotoside (^1H NMR)

Current Data Parameters
NAME ant-splend-20-3
EXPNO 2
PROCNO 1

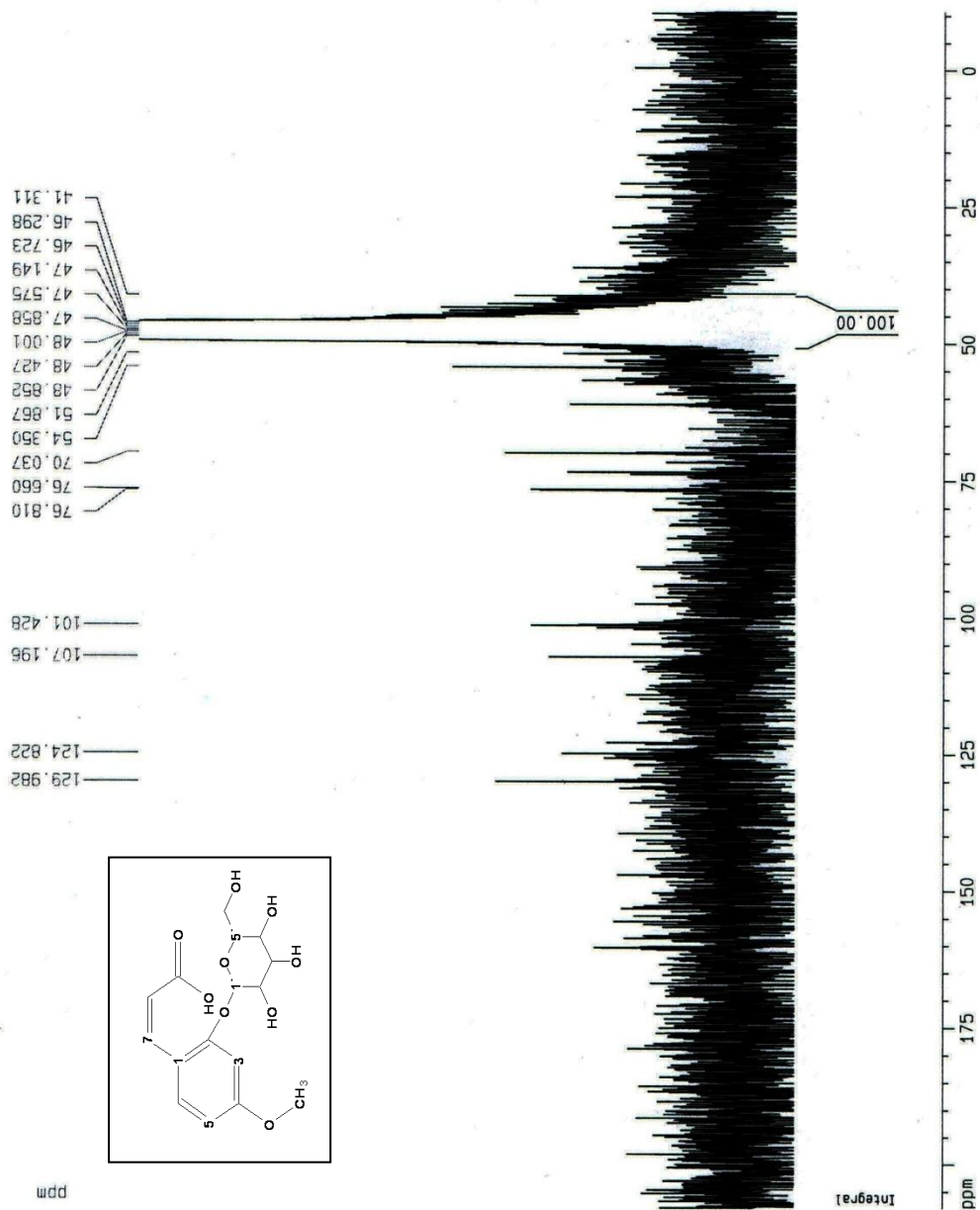
F2 - Acquisition Parameters
Date_ 20110720
Time 10.42
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg
TD 65536
SOLVENT MeOD
NS 33255
DS 0
SWH 12562.814 Hz
FIDRES 0.191693 Hz
AQ 2.6083827 sec
RG 161.3
DM 39.800 usec
DE 6.00 usec
TE 296.2 K
D1 5.0000000 sec
d11 0.0300000 sec
DELTA 4.9000010 sec
MCREST 0.0000000 sec
MCIRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 -6.00 dB
SF01 50.3277608 MHz

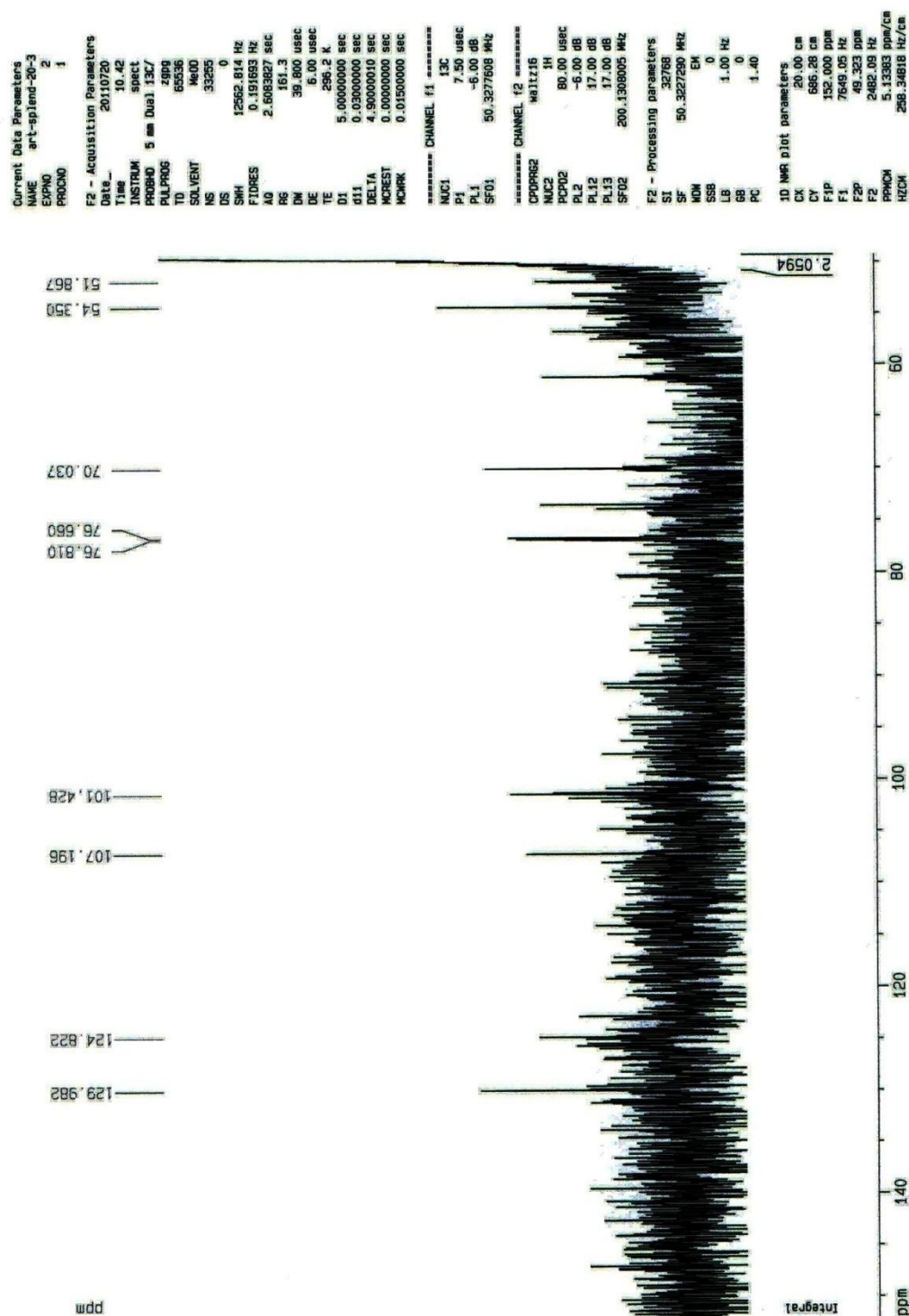
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CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 17.00 dB
PL13 17.00 dB
SF02 200.1308005 MHz

F2 - Processing parameters
SI 32768
SF 50.327290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

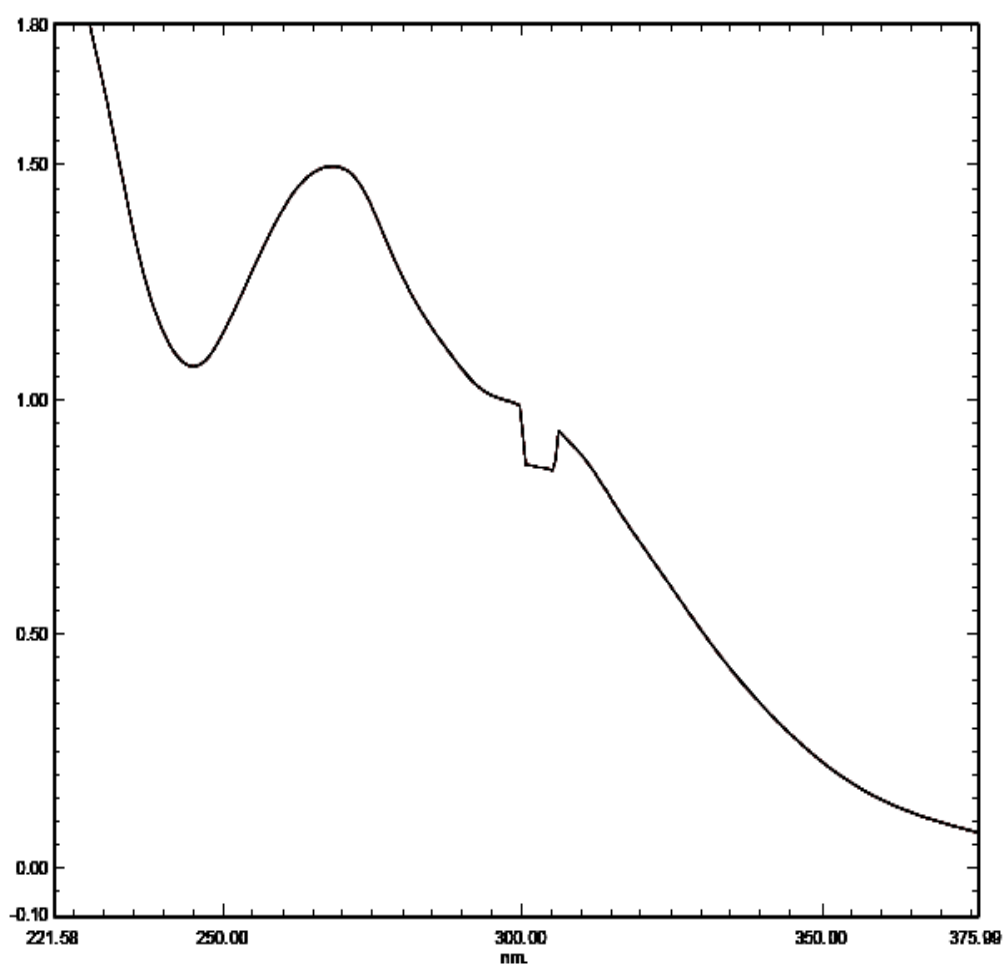
1D NMR plot parameters
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CY 666.28 cm
FIP 208.036 ppm
F1 10468.93 Hz
F2 -10.739 ppm
F2 -540.42 Hz
PPMCM 10.93874 ppm/cm
HZCM 550.46735 Hz/cm



S23: 4-methoxy-Z-melilotoside (^{13}C NMR)



S24: 4-methoxy-Z-melilotoside (¹³CNMR)



S25: 4-methoxy-Z-melilotoside (UV)

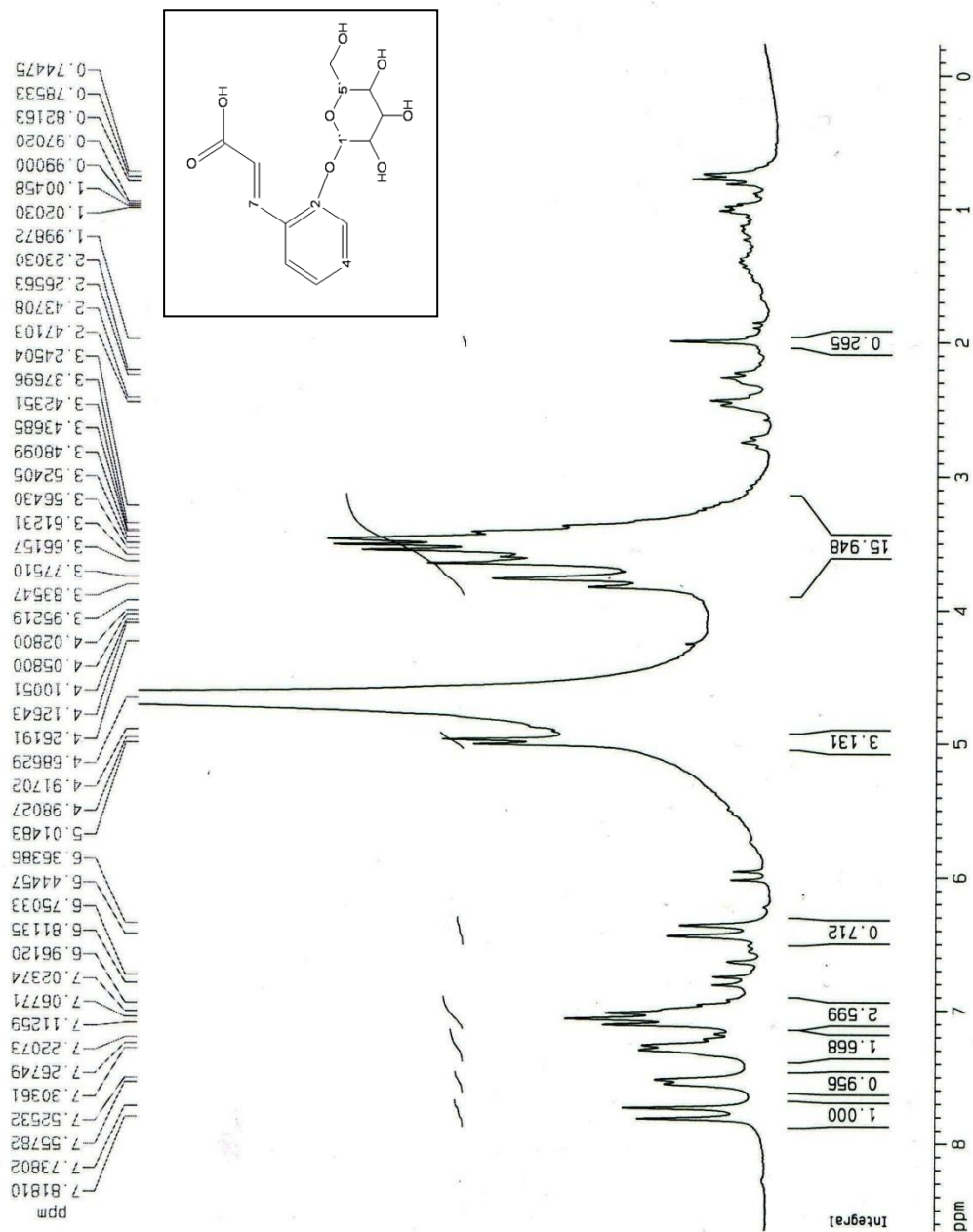
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EXPNO 1
PROCNO 1

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Time 11.12
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg
TD 32768
SOLVENT D2O
NS 291
DS 0
SWH 2796.421 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 362
DM 178.800 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -6.00 dB
SF01 200.1312359 MHz

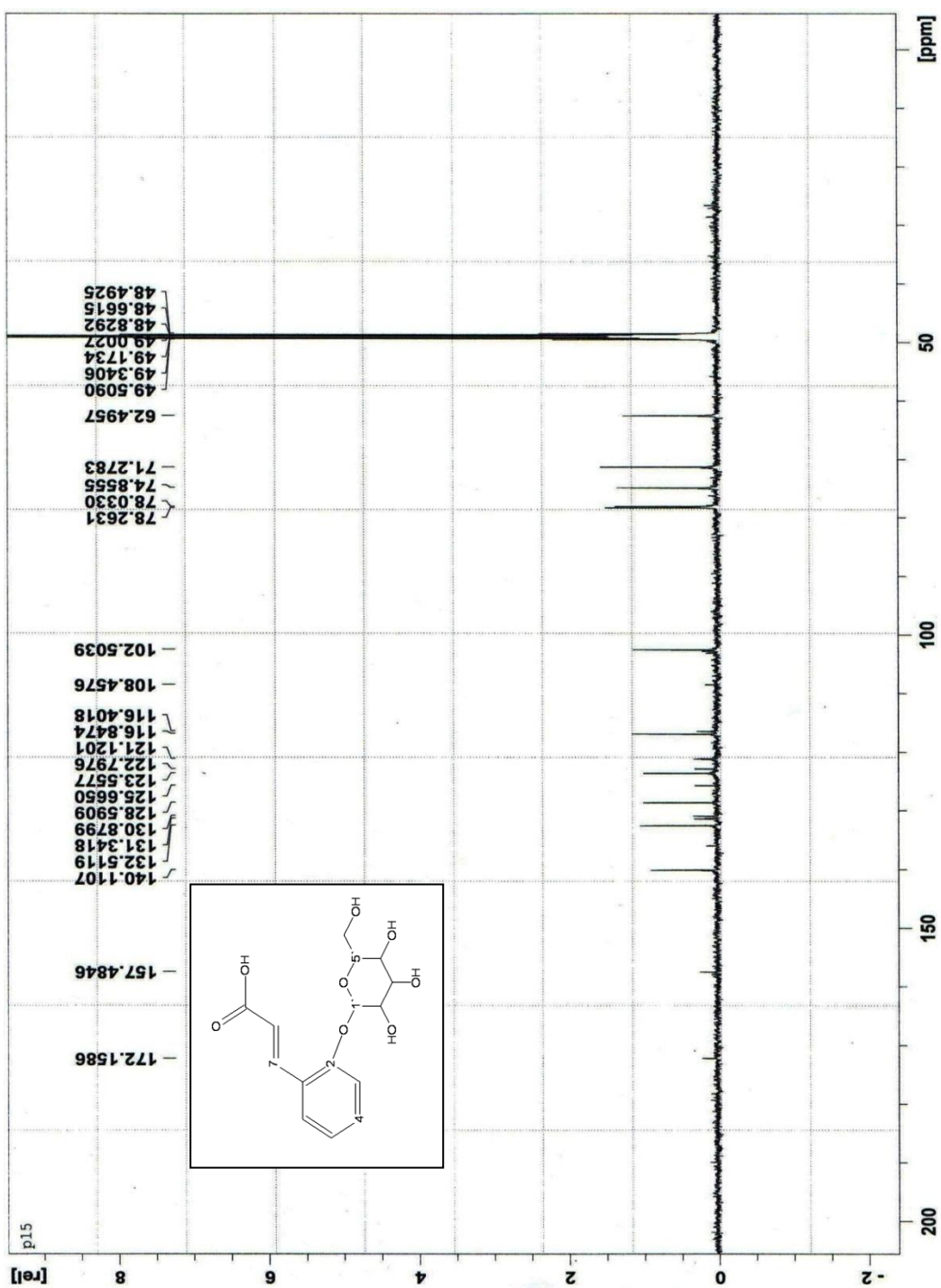
F2 - Processing parameters
SI 32768
SF 200.1300000 MHz
WDW EN
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 339.48 cm
F1P 8.651 ppm
F1 1731.40 Hz
F2P -0.235 ppm
F2 -47.09 Hz
PPMCM 0.44433 ppm/cm
HZCM 88.92463 Hz/cm

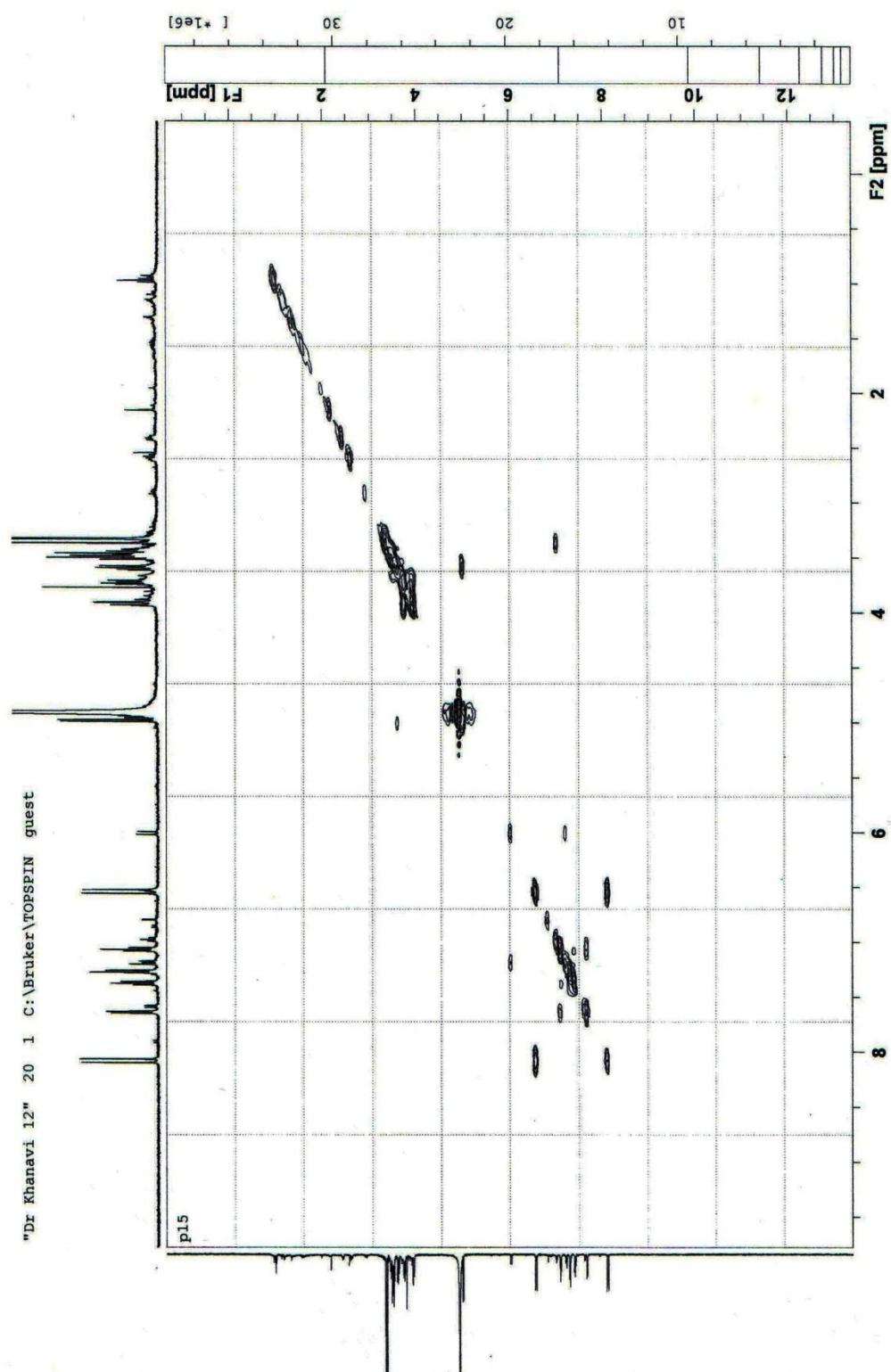


S26: E-melilotoside (¹H NMR)

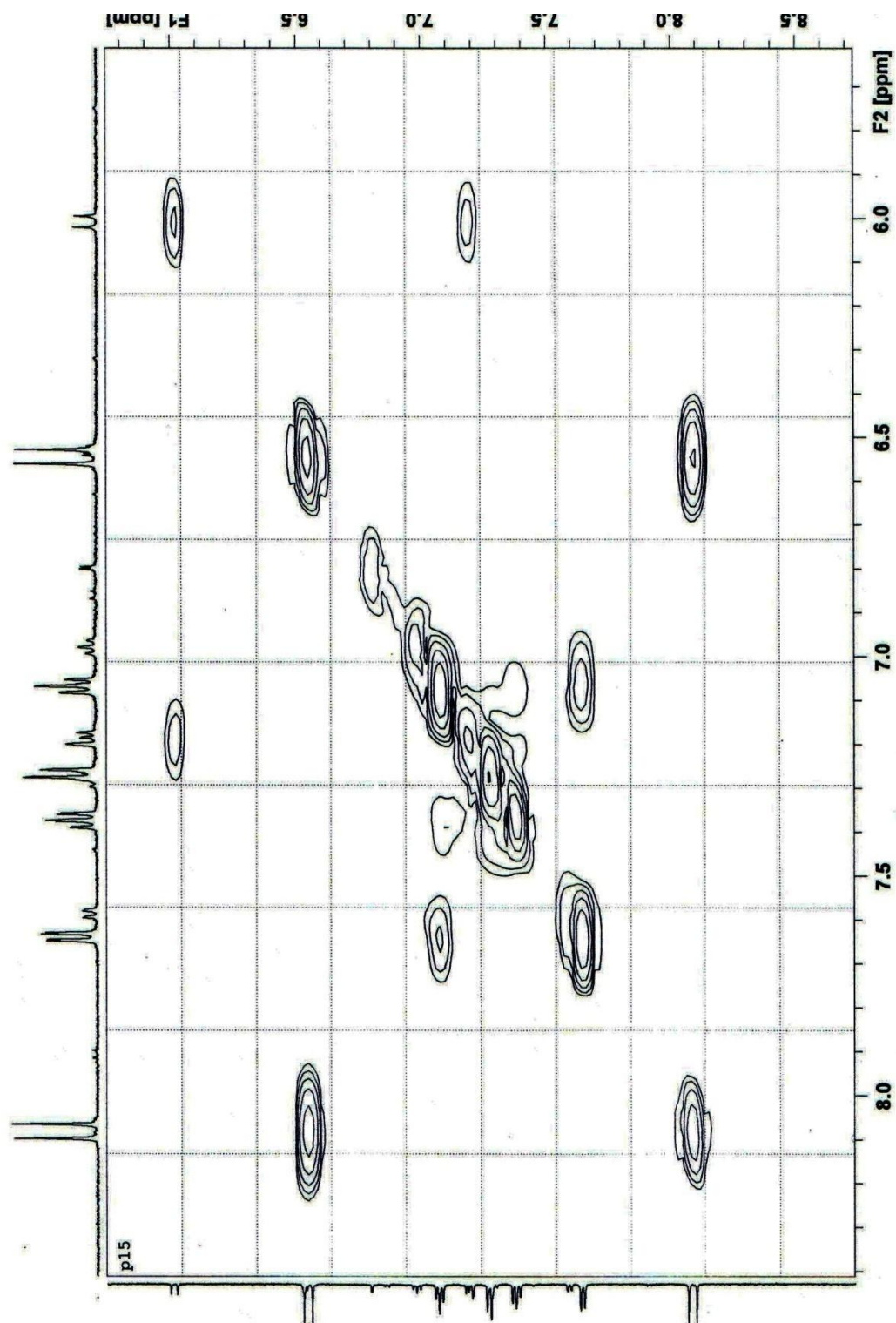
(NMR400MHz و در حلال متانول)



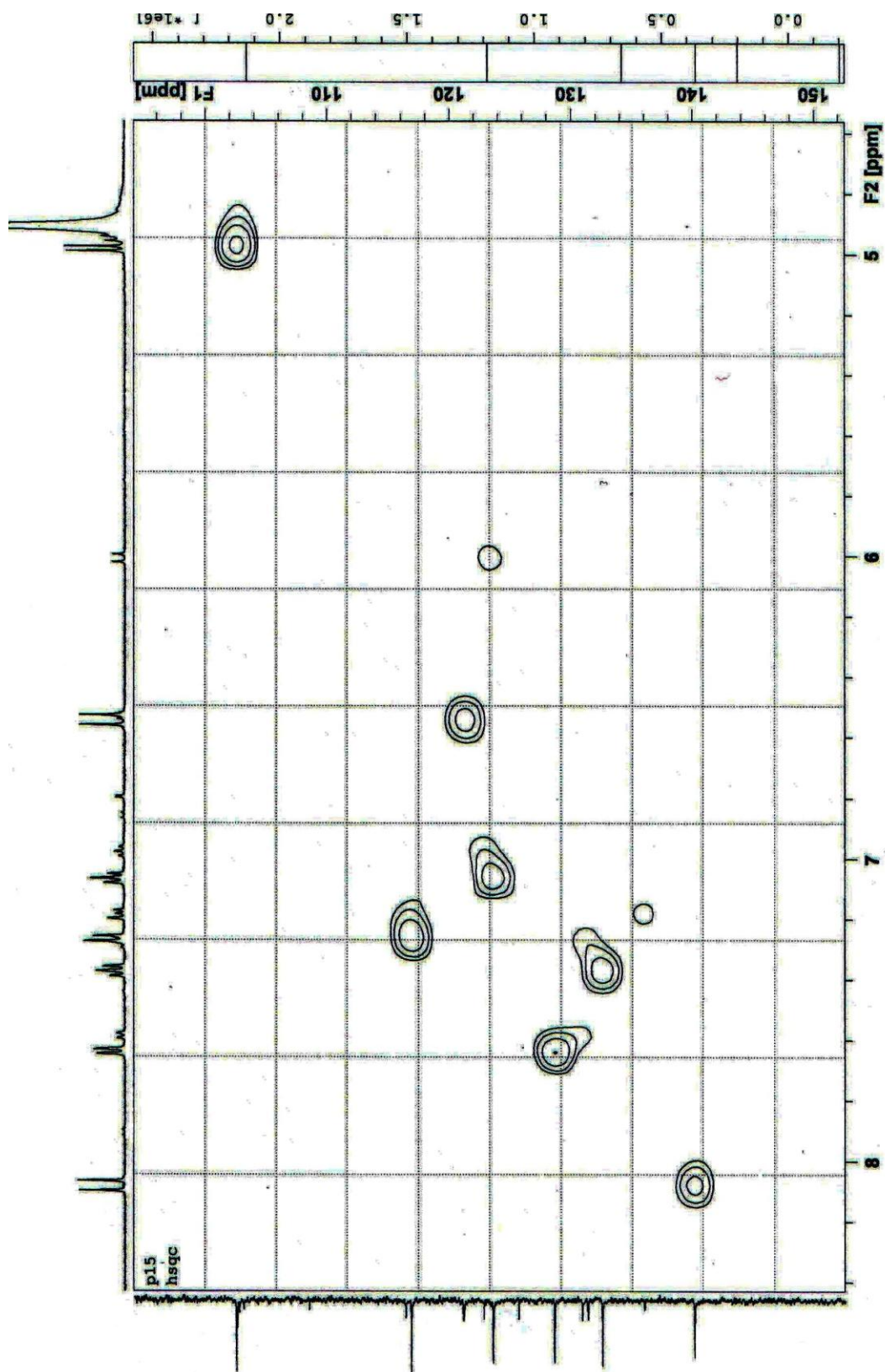
S27: E-melilotoside (¹³CNMR)



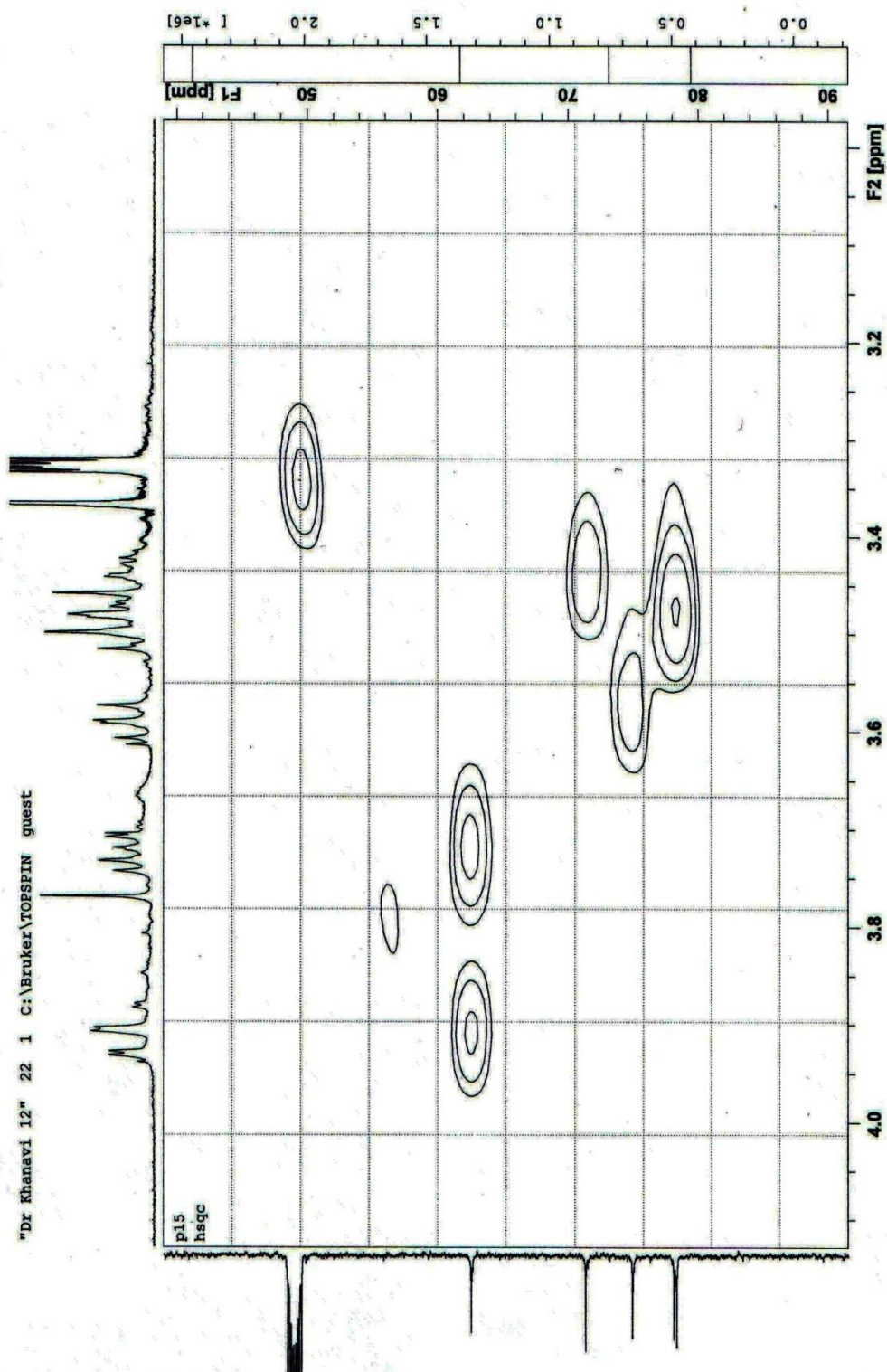
S28: E-melilotoside (COSY)



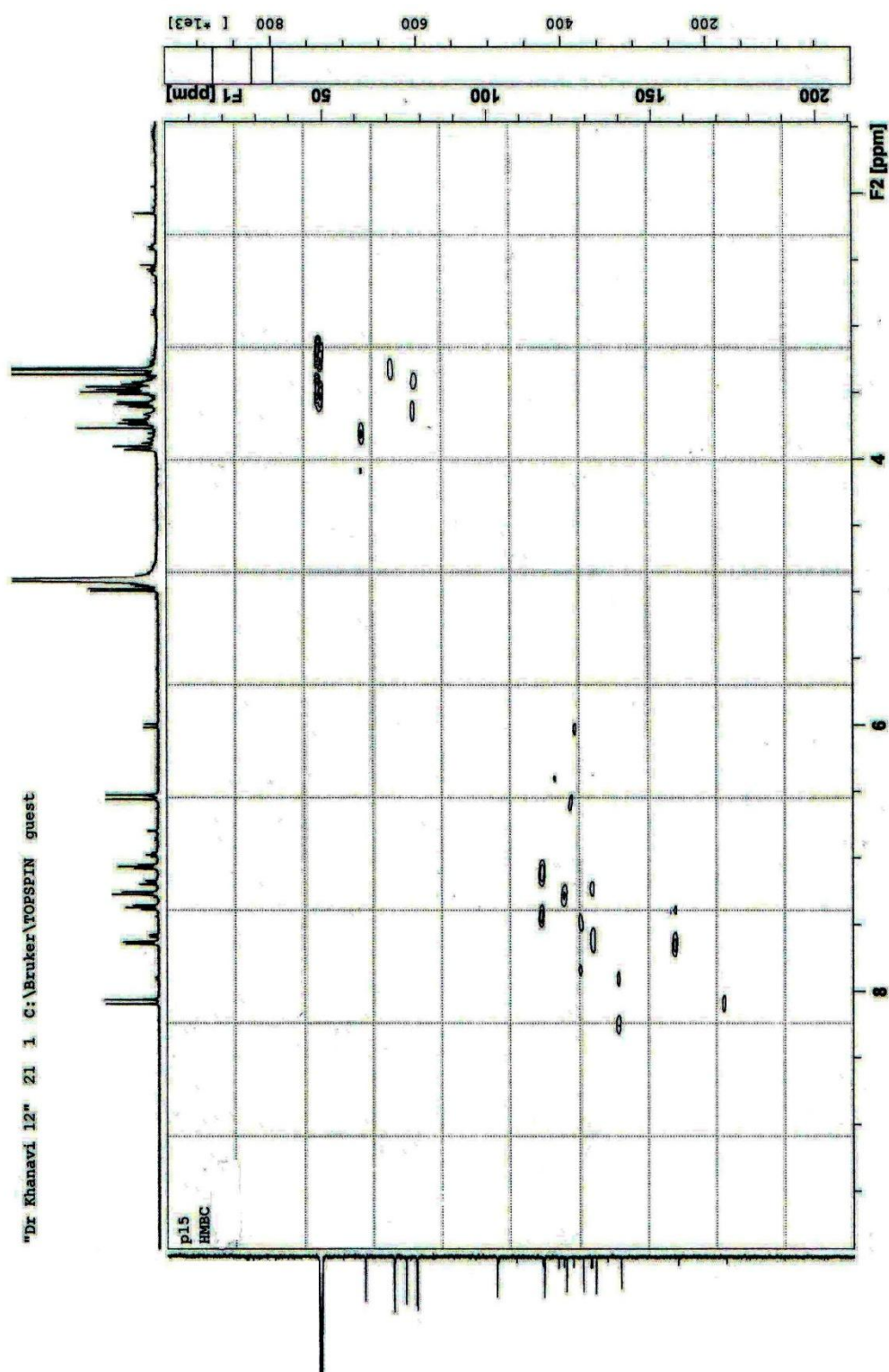
S29: E-melilotoside (COSY)



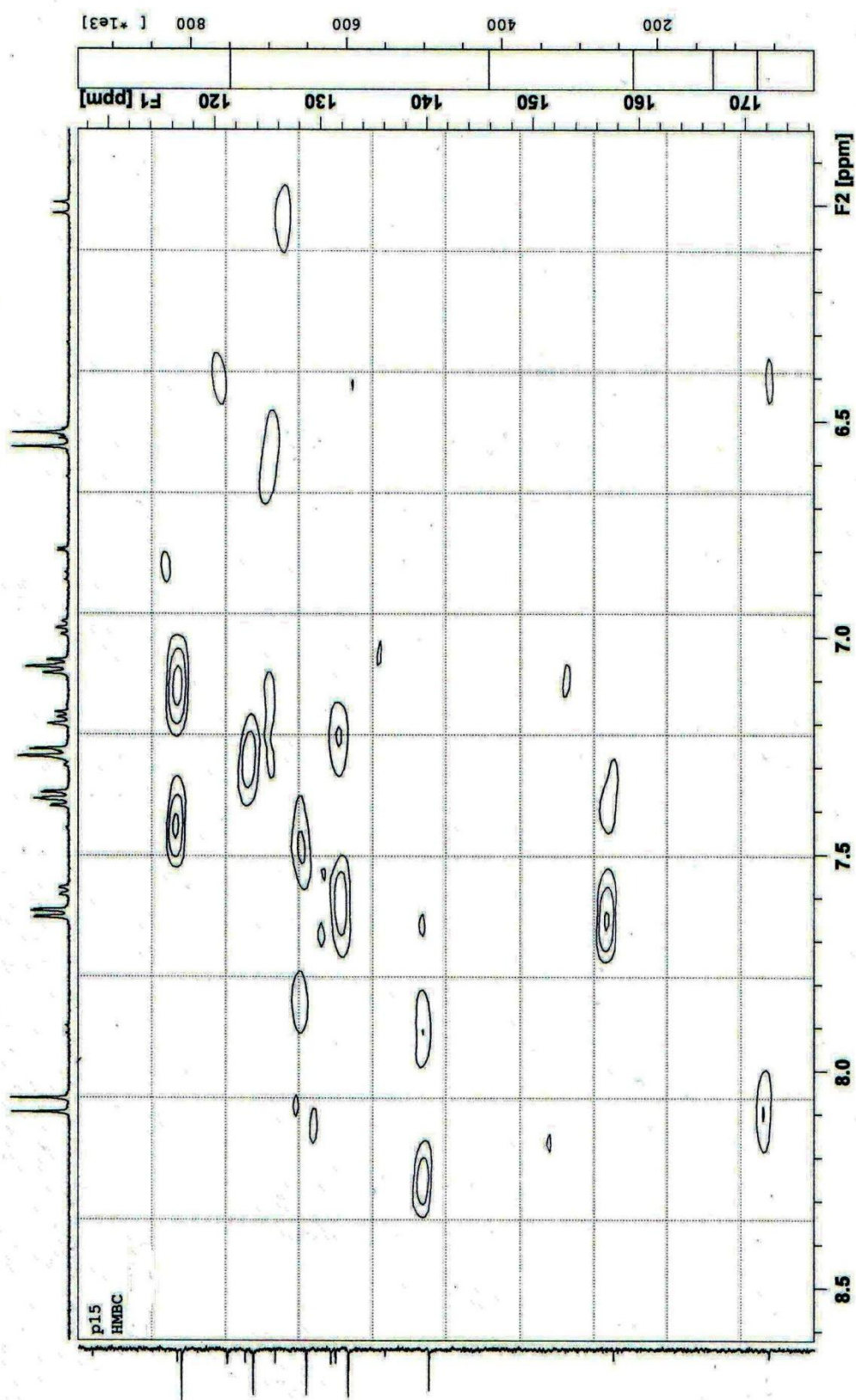
S30: E-melilotoside(HSQC)



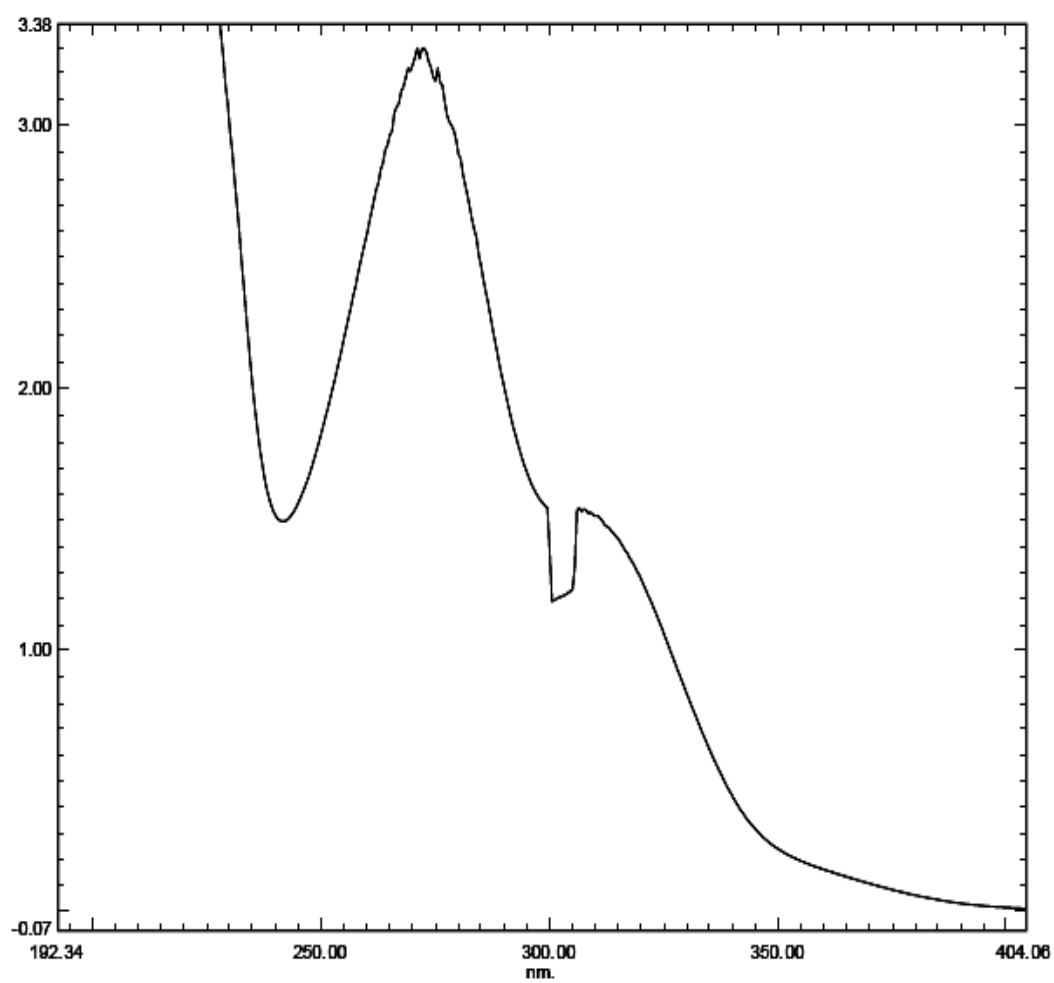
S31: E-melilotoside (HSQC)



S32: E-melilotoside(HMBC)



S33: E-melilotoside(HMBC)



S34: E-melilotoside(UV)

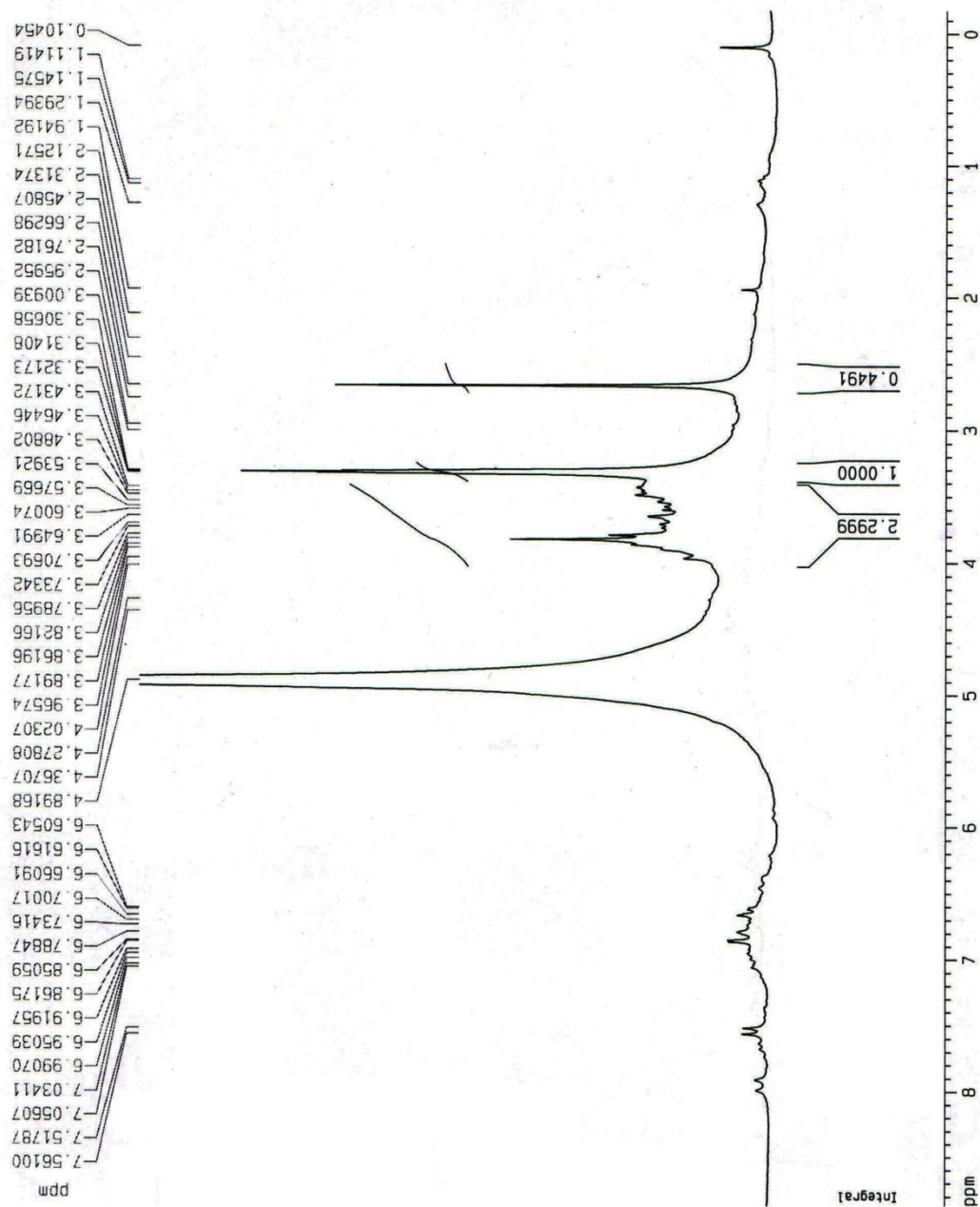
NAME ant-sp1end-40-5 (1)
EXPNO
PROCNO

F2 - Acquisition Parameters
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INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg
TD 32768
SOLVENT MeOD
NS 127
DS 0
SH 2796.421 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 512
DW 178.800 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCNPK 0.01500000 sec

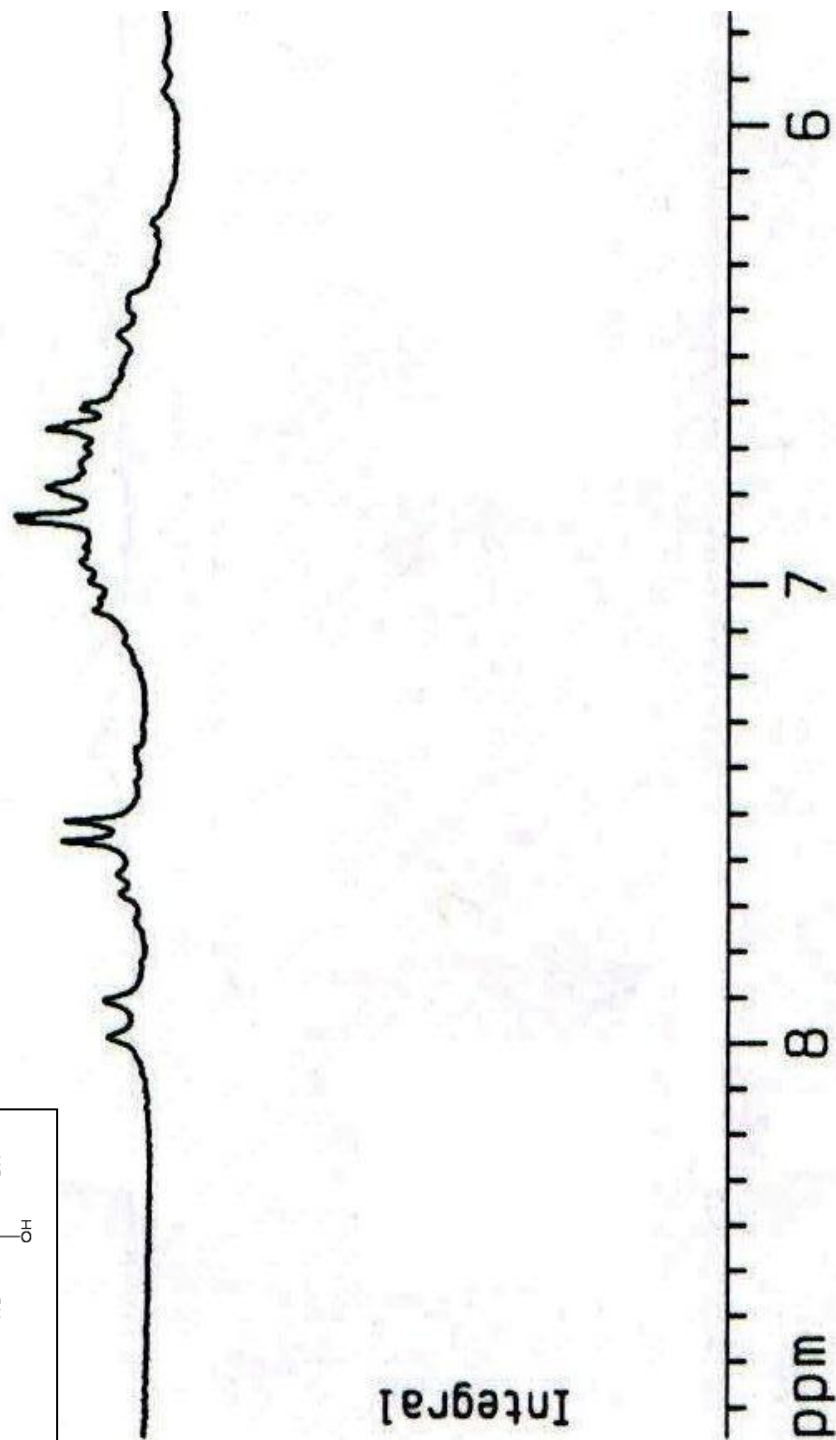
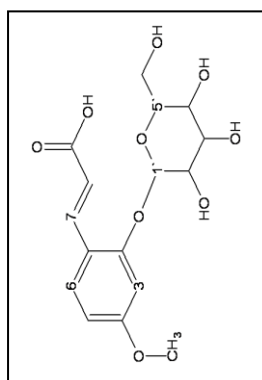
===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -6.00 dB
SF01 200.1312359 MHz

F2 - Processing parameters
SI 32768
SF 200.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 61.86 cm
F1P 8.868 ppm
F1 1774.78 Hz
F2P -0.174 ppm
F2 -34.88 Hz
PPMCM 0.45212 ppm/cm
HZCM 90.48314 Hz/cm



S35: 4-methoxy-E-melilotoside (^1H NMR)



S36: 4-methoxy-E-melilotoside (^1H NMR)