

## Supporting information

### ***Andrographis paniculata* elicits anti-invasion activities by suppressing *TM4SF3* gene expression and by anoikis-sensitization in esophageal cancer cells**

Grace Gar-Lee Yue <sup>1,2</sup>, Julia Kin-Ming Lee <sup>1,2</sup>, Lin Li <sup>3</sup>, Kar-Man Chan <sup>1,2</sup>, Eric Chun-Wai Wong<sup>1,2</sup>, Judy Yuet-Wah Chan <sup>1,2</sup>, Kwok-Pui Fung <sup>1,2,4</sup>, Vivian Wai Yan Lui <sup>5,6</sup>, Philip Wai-Yan Chiu <sup>3,\*</sup>, Clara Bik-San Lau <sup>1,2,\*</sup>

<sup>1</sup> Institute of Chinese Medicine; <sup>2</sup> State Key Laboratory of Phytochemistry and Plant Resources in West China (CUHK); <sup>3</sup> Department of Surgery; <sup>4</sup> School of Biomedical Sciences, The Chinese University of Hong Kong, Hong Kong; <sup>5</sup> Department of Pharmacology and Pharmacy, <sup>6</sup> School of Biomedical Sciences, Li Ka Shing Faculty of Medicine, The University of Hong Kong, Hong Kong.

\* Corresponding authors

Clara Bik-San LAU

Address: Institute of Chinese Medicine, E305, Science Centre East Block, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong SAR

Tel: 852 3943 6109 Fax: 852 2603 5248

E-mail address: claralau@cuhk.edu.hk

Philip Wai-Yan CHIU

Address: Department of Surgery, Prince of Wales Hospital, 30-32 Ngan Shing Street, Shatin, New Territories, Hong Kong SAR

Tel: 852 2632 2627 Fax: 852 2637 7974

E-mail address: philipchiu@surgery.cuhk.edu.hk

## Spectroscopic data of isoandrographolide

P.2 HRESIMS

P.3 <sup>1</sup>H NMR

P.4 <sup>13</sup>C NMR

P.5 HSQC

P.6 COSY

P.7 HMBC

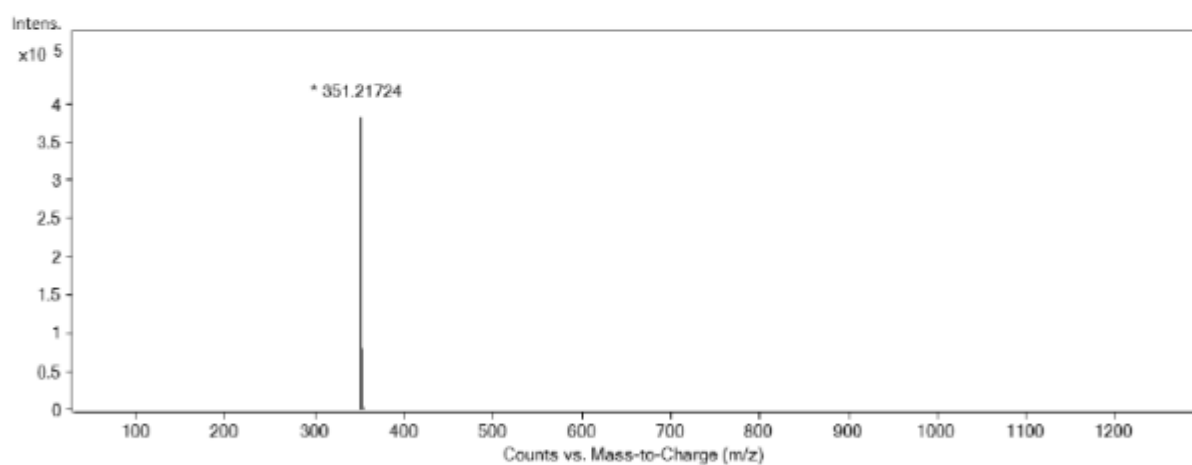
## Mass Spectrum List Report

### Analysis Info

Analysis Name	D:\CUHK3-6530\ERIC\Method\Mass-Test-Column-pos-01.m
Sample Name	CXL 321
Acquisition Date	05/13/2015 11:44:45 AM
Component Model	Agilent Technologies G6530A

### Acquisition Parameter

Ion Source Type	Dual ESI	Ion Polarity	Positive
Min Range (m/z)	50	VCap	3500
Max Range (m/z)	1700	Fragmentor	150
Scan Rate (spectra/sec)	2.00	Skimmer	65



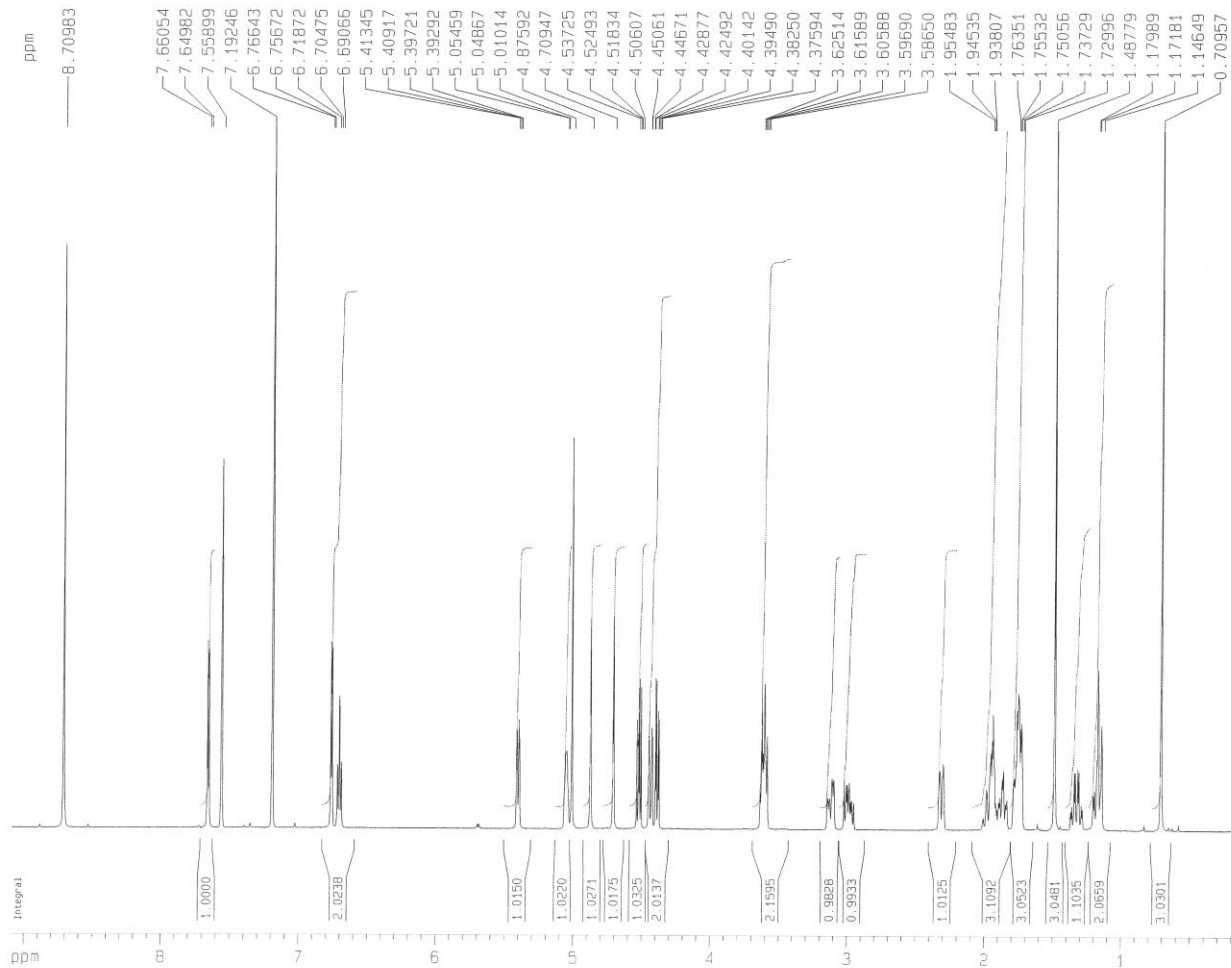
Tolerance = 10PPM

Elements Used: C: 0-200 H: 0-200 O: 0-200

1 result within limits

m/z	m/z (Calc)	Diff (mDa)	Diff (ppm)	Formula
351.21724	351.2166	-0.6	-1.61	C20 H31 O5

Bruker Drx-500MHz; cx1321 H c5d5n



Current Data Parameters

NAME ocx1321  
EXPNO 21  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20121221  
Time 19.59  
INSTRUM spect  
PROBHD 5 mm BBI 1H-BB  
PULPROG zg  
TD 32768  
SOLVENT Pyr  
NS 1  
DS 0  
SWH 7002.801 Hz  
FIDRES 0.213709 Hz  
AQ 2.3396852 sec  
RG 57  
DW 71.400 usec  
DE 6.00 usec  
TE 0.0 K  
D1 1.00000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*

NUC1 1H  
P1 9.20 usec  
PL1 -1.00 dB  
SF01 500.1325006 MHz

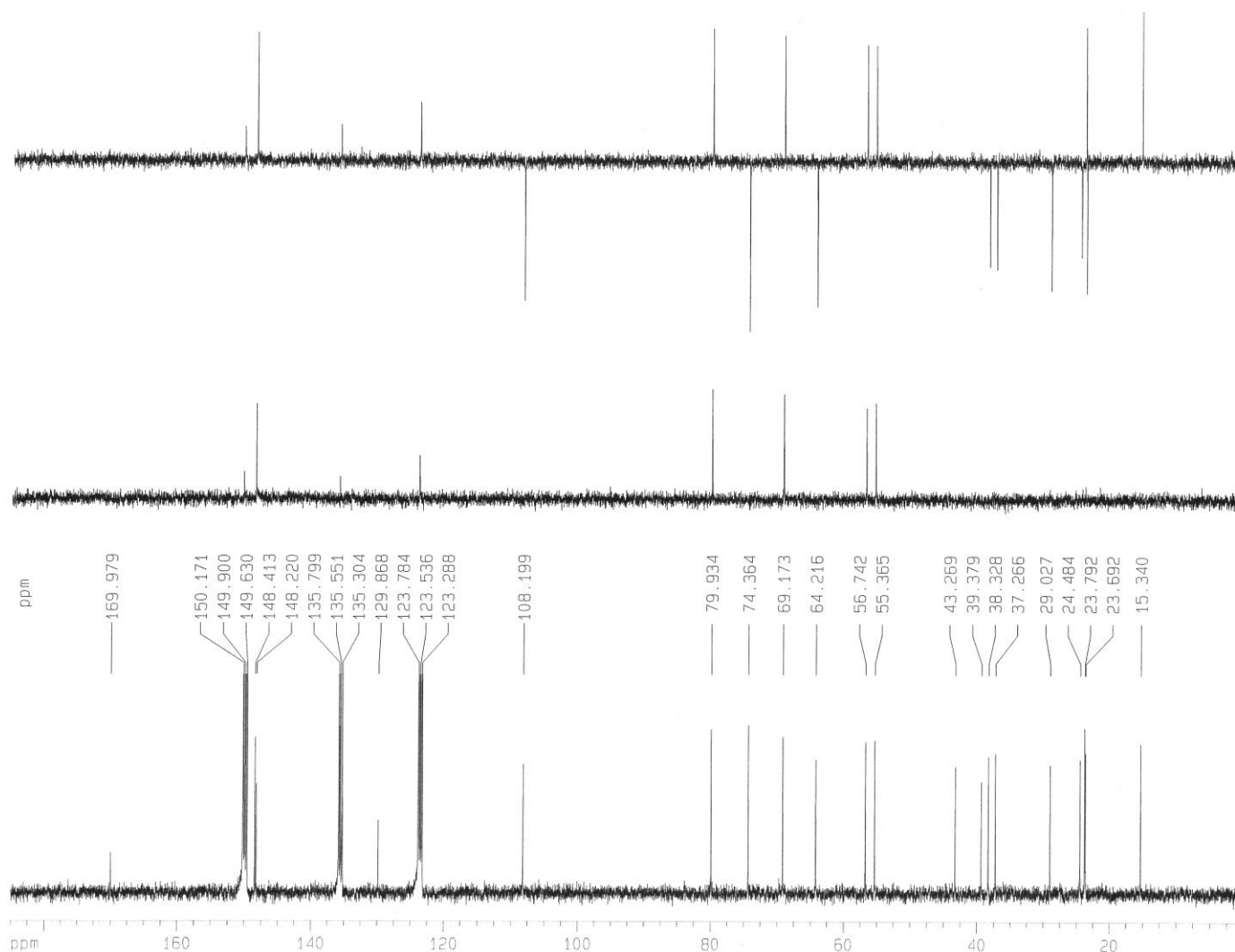
F2 - Processing parameters

SI 16384  
SF 500.1299978 MHz  
WDW GM  
SSB 0  
LB -0.40 Hz  
GB 0.2  
PC 1.00

ID NMR plot parameters

CX 22.00 cm  
CY 21.00 cm  
F1P 9.088 ppm  
F1 4545.33 Hz  
F2P 0.108 ppm  
F2 53.95 Hz  
PPMCM 0.40820 ppm/cm  
HZCM 204.15364 Hz/cm

Bruker AV-400MHz; cx1321 c13 and dept c5d5n



Current Data Parameters  
 NAME cx1321  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20121221  
 Time 19.00  
 INSTRUM av400  
 PROBHD 5 mm QNP 1H/15  
 PULPROG zgpg30  
 TO 32768  
 SOLVENT Pyr  
 NS 195  
 DS 2  
 SWH 23148.148 Hz  
 FIDRES 0.706425 Hz  
 AQ 0.7078388 sec  
 RG 18  
 DW 21.600 usec  
 DE 6.00 usec  
 TE 293.8 K  
 D1 4.50000000 sec  
 d11 0.03000000 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec

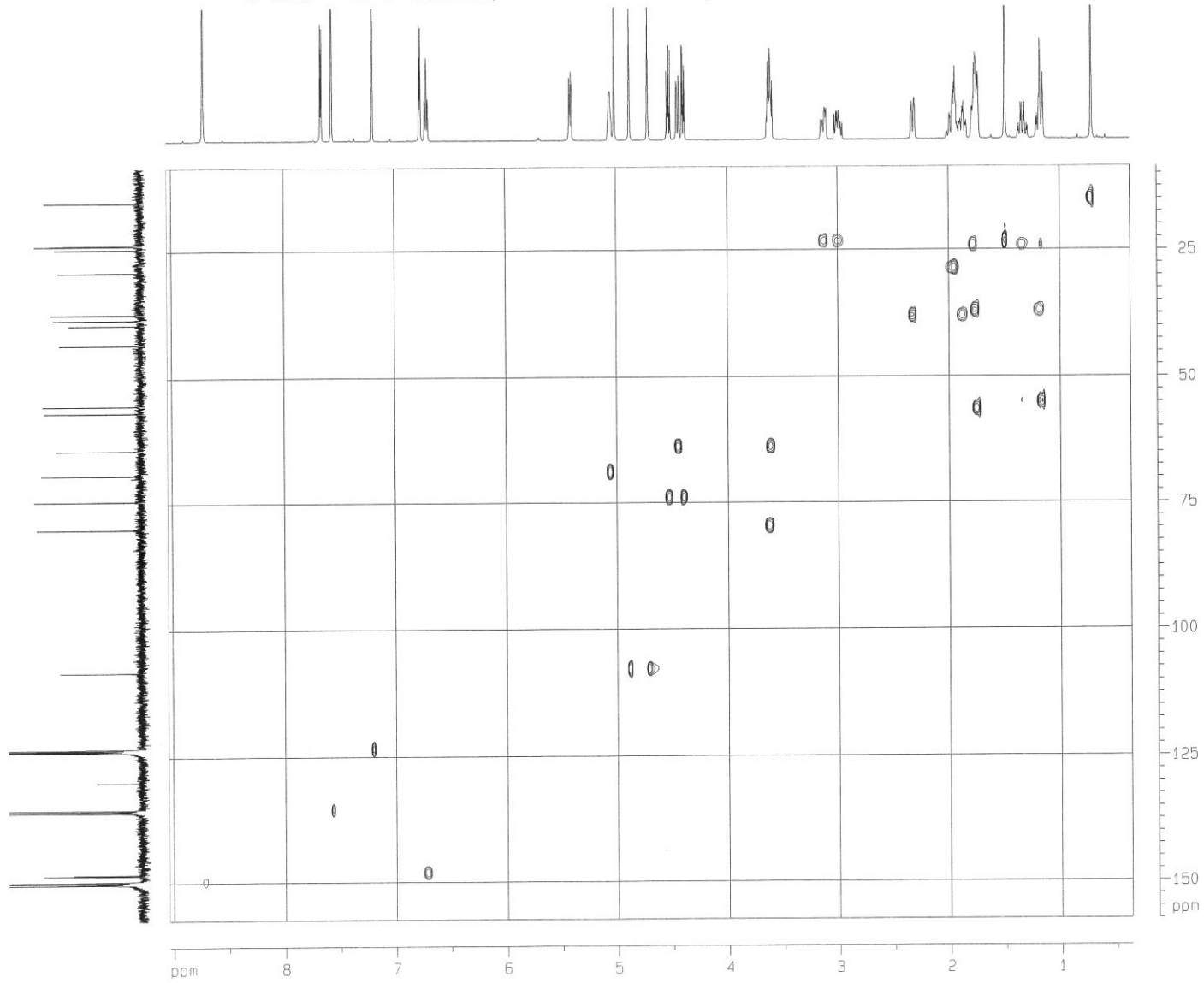
\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 9.40 usec  
 PL1 -4.00 dB  
 SFO1 100.6236958 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -3.00 dB  
 PL12 14.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127437 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 22.00 cm  
 CY 12.00 cm  
 F1P 185.000 ppm  
 F1 18813.36 Hz  
 F2P -0.000 ppm  
 F2 -0.00 Hz  
 PPMCM 8.40909 ppm/cm  
 HZCM 846.06177 Hz/cm

Bruker Drx-500MHz; cx1321 Hsqc c5d5n



```

Current Data Parameters
NAME      cx1321
EXPNO    26
PROCNO   1

F2 - Acquisition Parameters
Date_    20120221
Time     22.03
INSTRUM  spect
PROBHD   5 mm BBI 1H-60
PULPROG  zgpg30
TD       1024
SOLVENT  Py
NS       2
DS       16
SWH      4466.403 Hz
FIDRES   4.391018 Hz
AQ       0.112096 sec
RG       8192
DM       111.200 usec
DE       6.00 usec
TE       0.0 K
DCHTR    145.000000
d0       0.0000300 sec
d1       1.0000000 sec
d4       0.0017444 sec
d11      0.0300000 sec
d13      0.0000400 sec
d18      0.0000000 sec
d24      0.0006207 sec
DELTA    0.0021440 sec
DELTA1   0.0010000 sec
DELTA2   0.0006207 sec
DELTA3   0.0005414 sec
IND      0.0002485 sec
MCREST   0.0000000 sec
MCMK     0.1666700 sec
STICENT  64

***** CHANNEL f1 *****
NUC1      1H
P1        9.20 usec
P2        18.40 usec
P3        2000.00 usec
PL1       -1.00 dB
PL2       -1.00 dB
PL3       15.50 dB
PL4       15.50 dB
SFO1      500.1323506 MHz

***** CHANNEL f2 *****
CPDPRG2   gpgp
NUC2      13C
P3        12.00 usec
P4        24.00 usec
P5        25.00 usec
PL2       -1.00 dB
PL3       15.50 dB
PL4       15.50 dB
SFO2      125.7651011 MHz

***** GRADIENT CHANNEL *****
GRNAM1    SINE 100
GRNAM2    SINE 100
GRNAM3    SINE 100
GRNAM4    SINE 100
GP1       0.00 %
GP2       0.00 %
GP3       0.00 %
GP4       0.00 %
GP5       0.00 %
GP6       0.00 %
GP7       0.00 %
GP8       0.00 %
GP9       0.00 %
GP10      0.00 %
GP11      0.00 %
GP12      0.00 %
GP13      0.00 %
GP14      0.00 %
GP15      0.00 %
GP16      0.00 %
GP17      0.00 %
GP18      0.00 %
GP19      0.00 %
P16       1000.00 usec
P19       600.00 usec

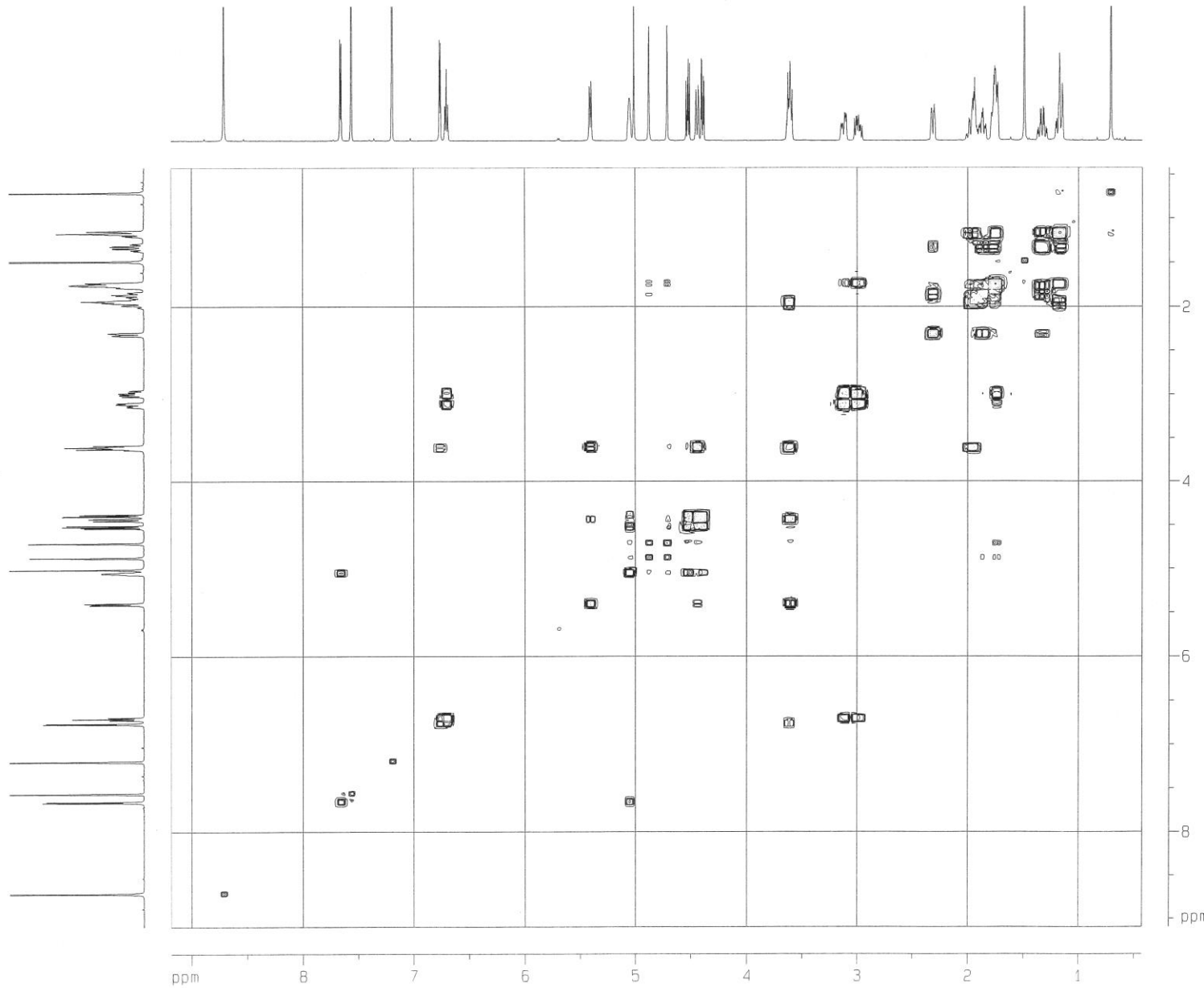
F1 - Acquisition parameters
NUC1      1H
TD        64
SFO1      125.7416 MHz
FIDRES    214.65026 Hz
SW        160.016 ppm
FHM000    Echo-Antiecho

F2 - Processing parameters
SI        1024
SF        500.120026 MHz
WDW       DSINE
SSB       0
LB        0.00 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
MC2       echo-antiecho
SF        125.732735 MHz
WDW       DSINE
SSB       0
LB        0.00 Hz
GB        0

2D NMR plot parameters
CX2       18.00 cm
CX1       14.00 cm
F2PLO     9.041 ppm
F2LO      4501.80 Hz
F2PHI     0.367 ppm
F2HI      183.47 Hz
F1PLO     157.540 ppm
F1LO      19827.71 Hz
F1PHI     8.606 ppm
F1HI      1862.00 Hz
F2PPMCM   0.48191 ppm/cm
F1PPMCM   241.01814 Hz/cm
F2HZCM    10.03813 ppm/cm
F1HZCM    1337.04568 Hz/cm
    
```

Bruker Drx-500MHz; cx1321 cosy c5d5n



```

Current Data Parameters
NAME      cx1321
EXPNO    25
PROCNO    1

F2 - Acquisition Parameters
Date_    20121221
Time     20.00
INSTRUM  spect
PROBHD   5 mm BB1 JH-BB
PULPROG  cosygpm/qf
TD       1024
SOLVENT  Pyr
NS       7
DS       15
SWH      5000.000 Hz
FIDRES   4.882812 Hz
AQ       0.1024500 sec
RG       4096
DW       100.000 usec
DE       6.00 usec
TE       0.0 K
D0       0.00000300 sec
D1       1.00000000 sec
d13      0.00000400 sec
D16      0.00020000 sec
JN0      0.00019999 sec
MCREST   0.00000000 sec
MCWRK    1.00000000 sec

***** CHANNEL f1 *****
NUC1     1H
P1       9.20 usec
PL1      -1.00 dB
SF01     500.1323506 MHz

***** GRADIENT CHANNEL *****
GPNAM1   sine.100
GPNAM2   sine.100
GPNAM3   sine.100
GPX1     0.00 %
GPX2     0.00 %
GPX3     0.00 %
GPY1     0.00 %
GPY2     0.00 %
GPY3     0.00 %
GPZ1     16.00 %
GPZ2     12.00 %
GPZ3     40.00 %
PT6      1000.00 usec

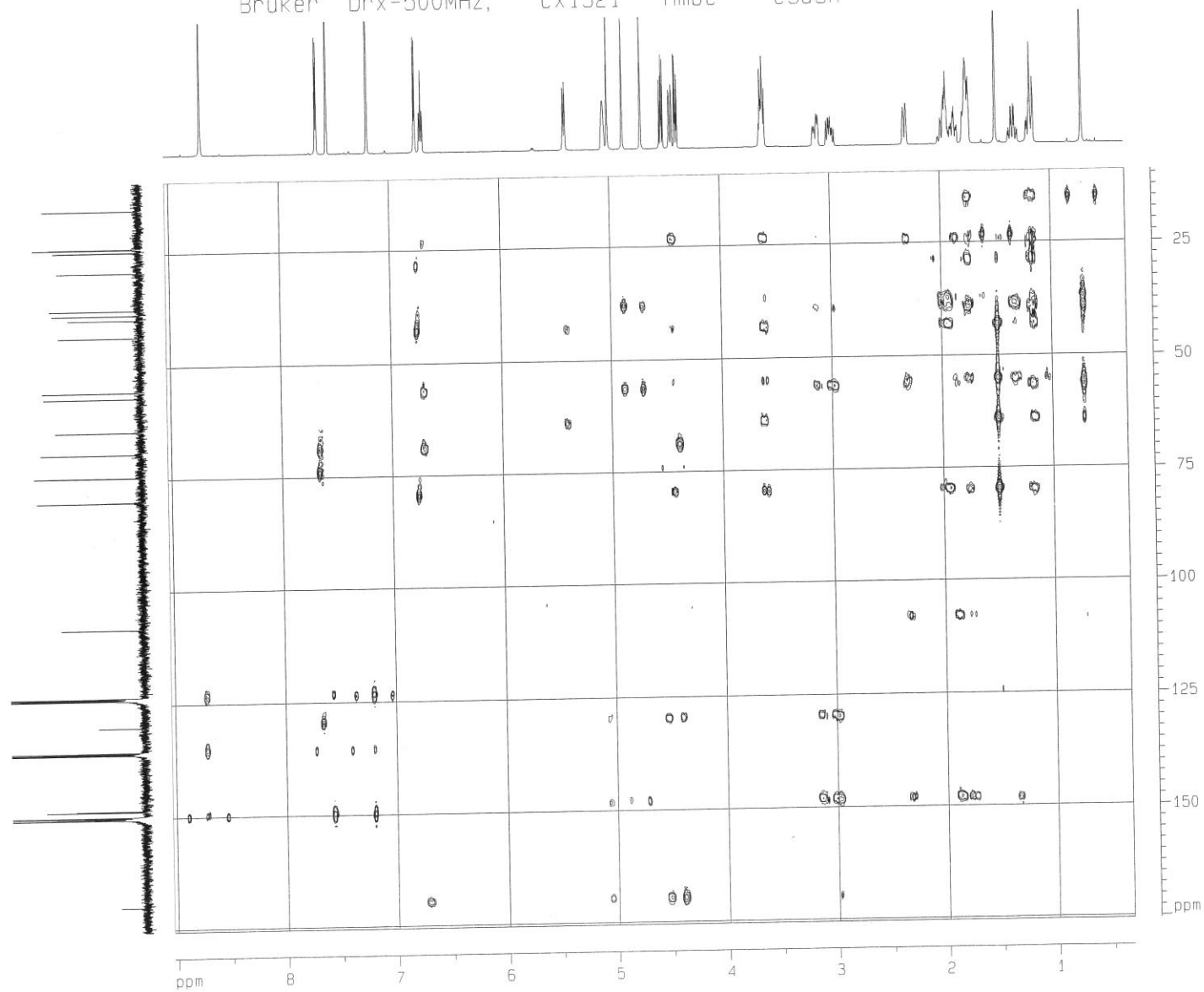
F1 - Acquisition parameters
ND0      1
TD       128
SF01     500.0318 MHz
FIDRES   39.064941 Hz
SW       10.000 ppm
FAMODE   gf

F2 - Processing parameters
SI       1024
SF       500.1299978 MHz
WDW      SINE
SSB      0
LB       0.00 Hz
GB       0
PC       1.00

F1 - Processing parameters
SI       1024
HC2      gf
SF       500.0293985 MHz
WDW      SINE
SSB      0
LB       0.00 Hz
GB       0

2D NMR plot parameters
CX2      18.00 cm
CX1      14.00 cm
F2PLO    9.186 ppm
F2LO     4594.02 Hz
F2PH1    0.428 ppm
F2H1     214.14 Hz
F1PLO    9.098 ppm
F1LO     4549.03 Hz
F1PH1    0.426 ppm
F1H1     212.82 Hz
F2PPMCM  0.48653 ppm/cm
F2HZCM   243.32683 Hz/cm
F1PPMCM  0.61942 ppm/cm
F1HZCM   309.72919 Hz/cm
    
```

Bruker Drx-500MHz; cx1321 Hmbc c5d5n



```

Current Data Parameters
NAME      cx1321
EXPNO    27
PROCNO   1

F2 - Acquisition Parameters
Date_    20121221
Time     20.08
INSTRUM  spect
PROBHD   5 mm BBI 1H-BS
PULPROG  invgpp1r1mdd1
TD        2048
SOLVENT  Pyr
NS        8
DS        16
SWH       4056.403 Hz
FIDRES    2.195598 Hz
AQ        0.227876 sec
RG         6192
DM        111.200 usec
DE         6.00 usec
TE         0.0 K
CNG12     145.000000
d0        0.00000300 sec
d1        1.29999995 sec
d2        0.00344829 sec
d5        0.08340000 sec
d13       0.00000400 sec
d16       0.00000000 sec
TWO       0.00002209 sec
MCREST1  0.00000000 sec
MCMRK     1.29999995 sec

***** CHANNEL f1 *****
NUC1      1H
P1        9.20 usec
p2        18.40 usec
PL1       -1.00 dB
SFO1      500.1323506 MHz

***** CHANNEL f2 *****
NUC2      13C
P3        12.00 usec
PL2       -1.00 dB
SFO2      125.7696102 MHz

***** GRADIENT CHANNEL *****
GPHAM1    SINE 100
GPHAM2    SINE 100
GPHAM3    SINE 100
GPX1      0.00 %
GPX2      0.00 %
GPX3      0.00 %
GPY1      0.00 %
GPY2      0.00 %
GPY3      0.00 %
GR21      50.00 %
GR22      30.00 %
GR23      40.10 %
P15       1000.00 usec

F1 - Acquisition parameters
NUC       2
TD        128
SFO1      125.7448 MHz
FIDRES    176.853424 Hz
SH        180.005 ppm
FHMNDE    GF

F2 - Processing parameters
SI         1024
SF         500.1299953 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         512
MC2        GF
SF         125.7330239 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0

20 NMR plot parameters
CX2       18.00 cm
CX1       14.00 cm
F2PLO     9.038 ppm
F2L0      4520.07 Hz
F2PHI     0.328 ppm
F2H1      164.18 Hz
F1PLO     175.560 ppm
F1L0      22073.64 Hz
F1PHI     9.225 ppm
F1H1      1160.73 Hz
F2PPMCM   0.48386 ppm/cm
F2HZCM    241.88395 Hz/cm
F1PPMCM   11.88057 ppm/cm
F1HZCM    1493.77979 Hz/cm
    
```