

## Regio- and stereo- selective oxidation of $\beta$ -boswellic acids transformed by filamentous fungi

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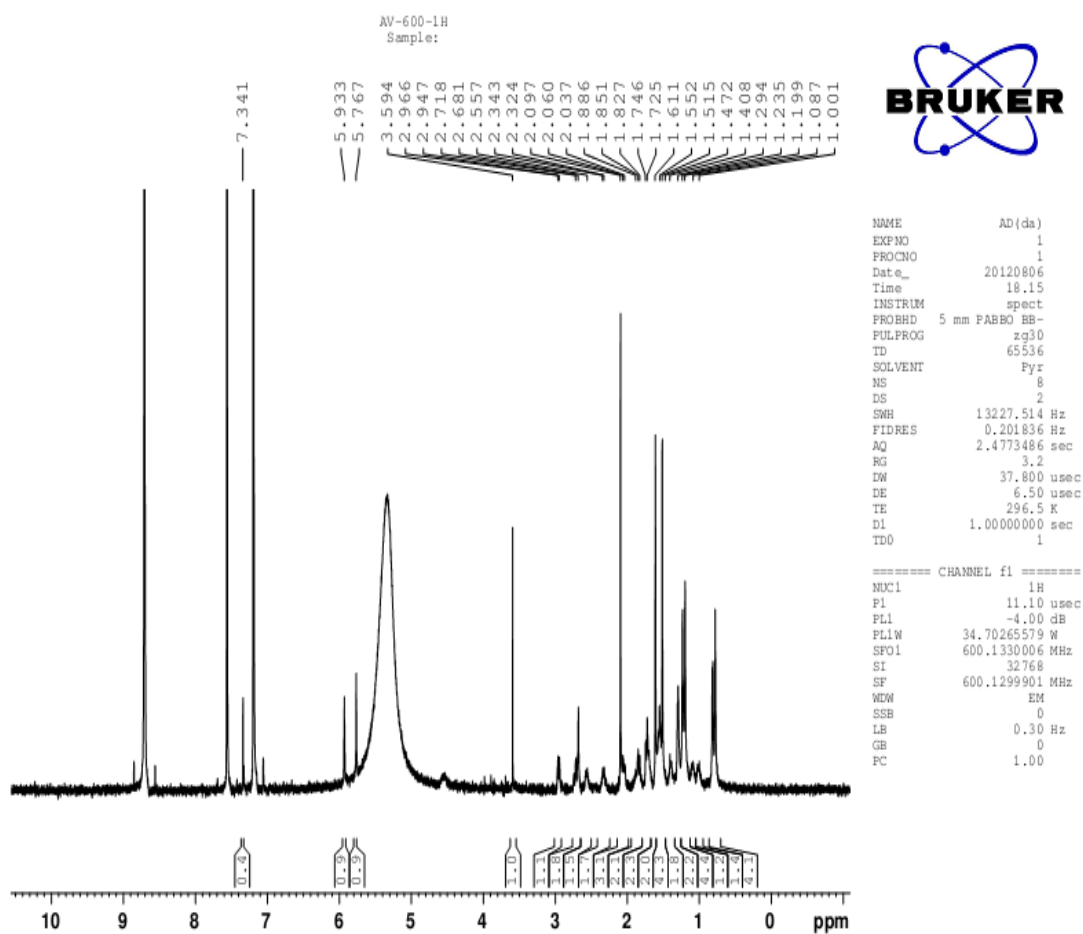
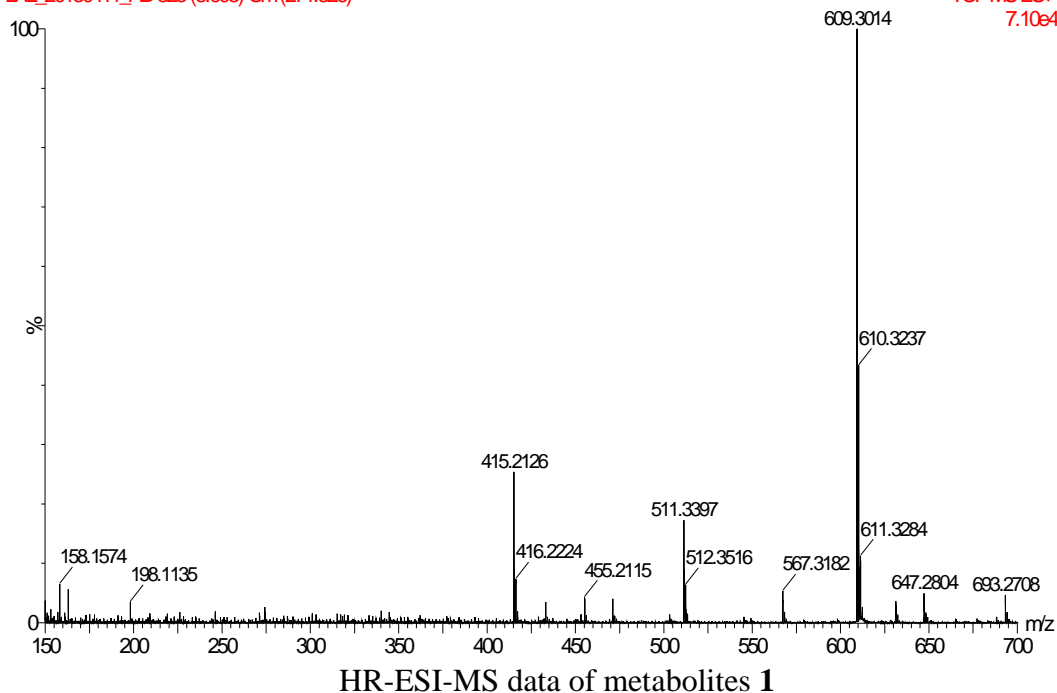
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E-mail: maxc1978@163.com; Tel/fax: +86-411-86110419.

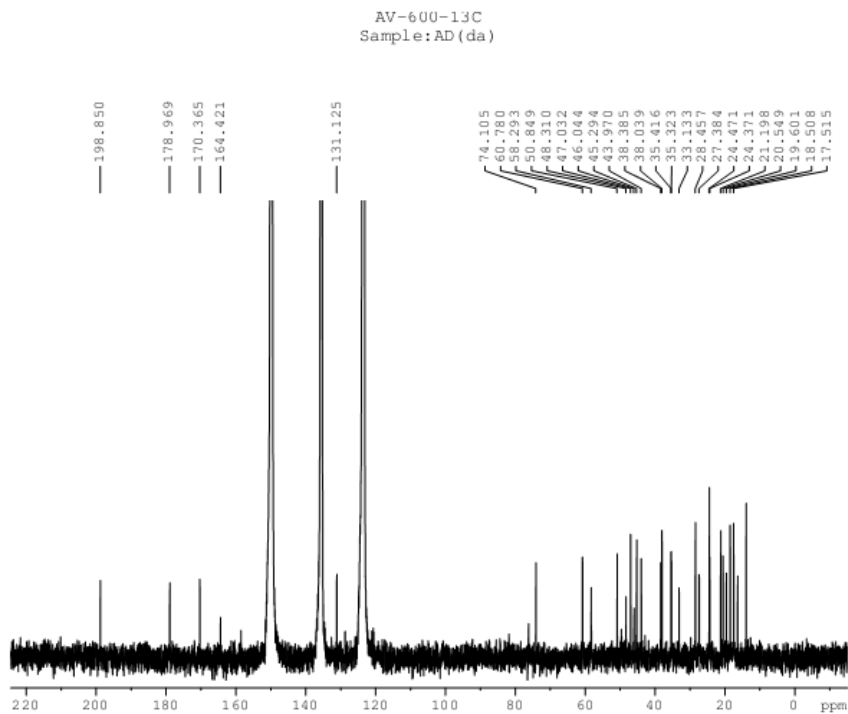
## Supplementary Information

50ACN\_0\_1FA

LXL\_20130411\_AD 325 (5.93) Cm (271:326)



<sup>1</sup>H-NMR data of metabolites 1



```

NAME      AD (da)
EXPNO     2
PROCNO    1
Date_     20120814
Time      7.54
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   Pyr
NS         14307
DS         2
SWH        45454.547 Hz
FIDRES     0.693581 Hz
AQ         0.7209570 sec
RG         11500
DW         11.000 usec
DE         6.50 usec
TE         297.5 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

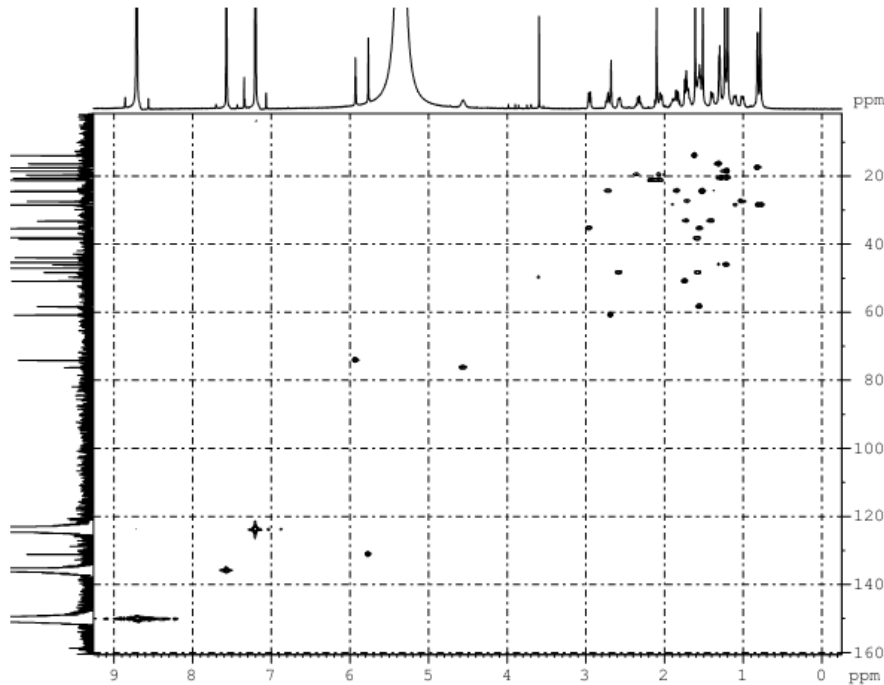
===== CHANNEL f1 =====
NUC1      13C
P1         6.00 usec
PL1        1.00 dB
PL1W       83.2024835 W
SFO1      150.9178993 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        -4.00 dB
PL12       13.16 dB
PL13       16.00 dB
PL2W       34.70265579 W
PL1W       0.66736388 W
PL1W       0.34702653 W
SFO2      600.1324005 MHz
SI         32768
SF         150.9027684 MHz
NUC3      13C
SSB        0
LB         3.00 Hz
GB         0
PC         1.40

```

<sup>13</sup>C NMR data of metabolites 1

AV-600-HSQC  
Sample:



```

NAME      AD (da)
EXPNO     2
PROCNO    1
Date_     20120814
Time      10.50
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         1024
SOLVENT   Pyr
NS         32
DS         14
SWH        7187.809 Hz
FIDRES     7.011318 Hz
AQ         0.1713900 sec
RG         280
DW         69.60 usec
DE         4.50 usec
TE         297.5 K
CPDPRG2   145.0000000
D1         0.00000000 sec
D11        1.50000000 sec
D12        0.00172484 sec
D13        0.00000000 sec
D14        0.00000000 sec
D15        0.00000000 sec
D16        0.00100000 sec
D17        0.00018400 sec
SFO1      400.1360908 MHz

===== CHANNEL f1 =====
NUC1      1H
P1         11.10 usec
PL1        22.20 dB
PL1W       1000.00 usec
PL1W       -4.00 dB
PL1W       34.70265579 W
SFO1      400.1360908 MHz

===== CHANNEL f2 =====
CPDPRG2   gzgpg
NUC2      13C
P2         8.80 usec
PL2        17.40 usec
PL2W       80.00 usec
PL2W       1.00 dB
PL2W       30.17 dB
PL2W       83.2024835 W
SFO2      150.9178993 MHz

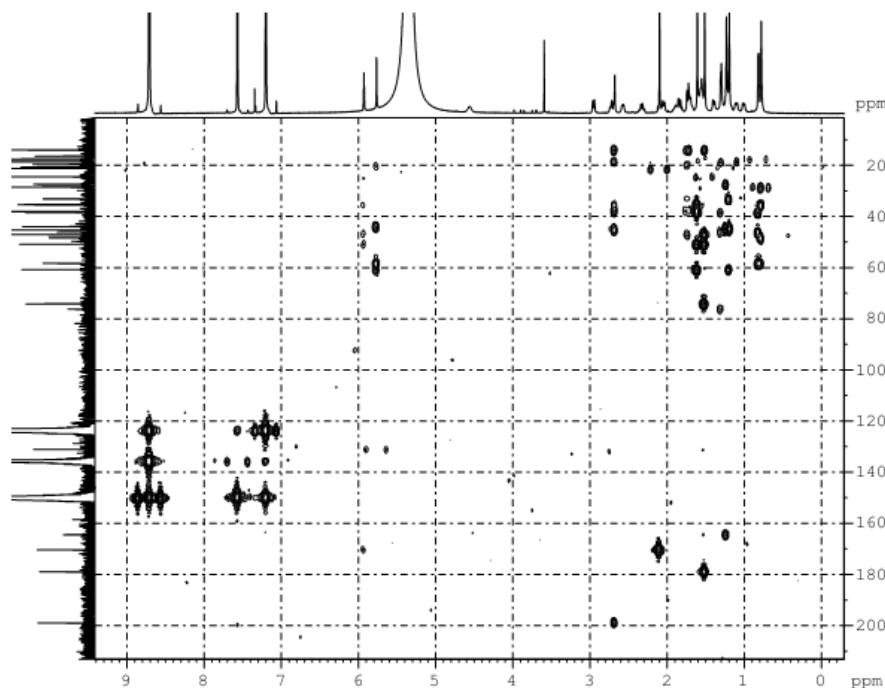
===== CHANNEL f3 =====
CPDPRG2   gzgpg
NUC3      13C
P3         8.80 usec
PL3        17.40 usec
PL3W       80.00 usec
PL3W       1.00 dB
PL3W       30.17 dB
PL3W       83.2024835 W
SFO3      150.9178993 MHz

===== CHANNEL f4 =====
CPDPRG2   gzgpg
NUC4      13C
P4         8.80 usec
PL4        17.40 usec
PL4W       80.00 usec
PL4W       1.00 dB
PL4W       30.17 dB
PL4W       83.2024835 W
SFO4      150.9178993 MHz

```

HMQC data of metabolites 1

AV-600-HMBC  
Sample:



```

NAME      AD(da)
EXPNO     1
PROCNO    1
Date_     20120819
Time      14.43
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   hzgpgp0p01
TD         1024
SOLVENT   Pyz
NS         8
DS         4
SWH        7183.908 Hz
FIDRES     7.015535 Hz
AQ         0.0713900 sec
RG         114
DW         69.600 usec
DE         8.50 usec
TE         296.3 K
CHST2     149.000000
CHST13    5.000000
D0         0.0000000 sec
D1         1.5000000 sec
D2         0.0014800 sec
D3         0.1000000 sec
D4         0.0020000 sec
IN0        0.0001392 sec

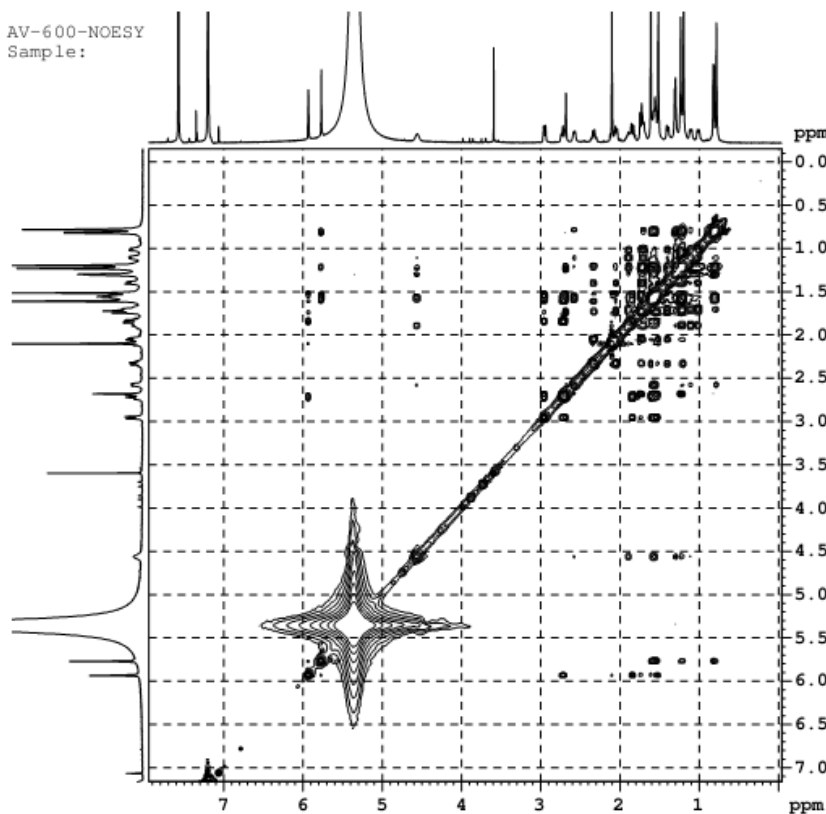
===== CHANNEL f1 =====
NUC1       1H
P1         11.10 usec
PL1        -4.00 dB
PL1W       34.70265579 W
SFO1       600.1336008 MHz
ND0        1
TD         256
SFO1       600.1336 MHz
FIDRES     28.062107 Hz
SW         11.970 ppm
F0MODE     States-TPPI
SI         1024
SF         600.1308896 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.00
SI         1024
MC2        States-TPPI
SF         600.1308910 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0

===== GRABBER CHANNEL =====
GRABM1     SINE.100
GRABM2     SINE.100
GRABM3     SINE.100
GR21       50.00 u
GR22       30.00 u
GR23       40.10 u
PL4         100.00 usec
TD          14
SFO1       150.9184 MHz
FIDRES     232.18170 Hz
SW         220.000 ppm
F0MODE     1024
SF         600.1308883 MHz
WDW        MSINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
SI         1024
MC2        States-TPPI
SF         150.9028778 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0

```

HMBC data of metabolites 1

AV-600-NOESY  
Sample:



```

NAME      AD(da)
EXPNO     6
PROCNO    1
Date_     20120819
Time      9.26
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   noesyph
TD         1024
SOLVENT   Pyz
NS         8
DS         4
SWH        7183.908 Hz
FIDRES     7.015535 Hz
AQ         0.0713900 sec
RG         114
DW         69.600 usec
DE         8.50 usec
TE         296.3 K
D0         0.00005547 sec
D1         2.00000000 sec
D2         0.60000002 sec
IN0        0.00013920 sec

===== CHANNEL f1 =====
NUC1       1H
P1         11.10 usec
PL1        -4.00 dB
PL1W       34.70265579 W
SFO1       600.1336008 MHz
ND0        1
TD         256
SFO1       600.1336 MHz
FIDRES     28.062107 Hz
SW         11.970 ppm
F0MODE     States-TPPI
SI         1024
SF         600.1308896 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.00
SI         1024
MC2        States-TPPI
SF         600.1308910 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0

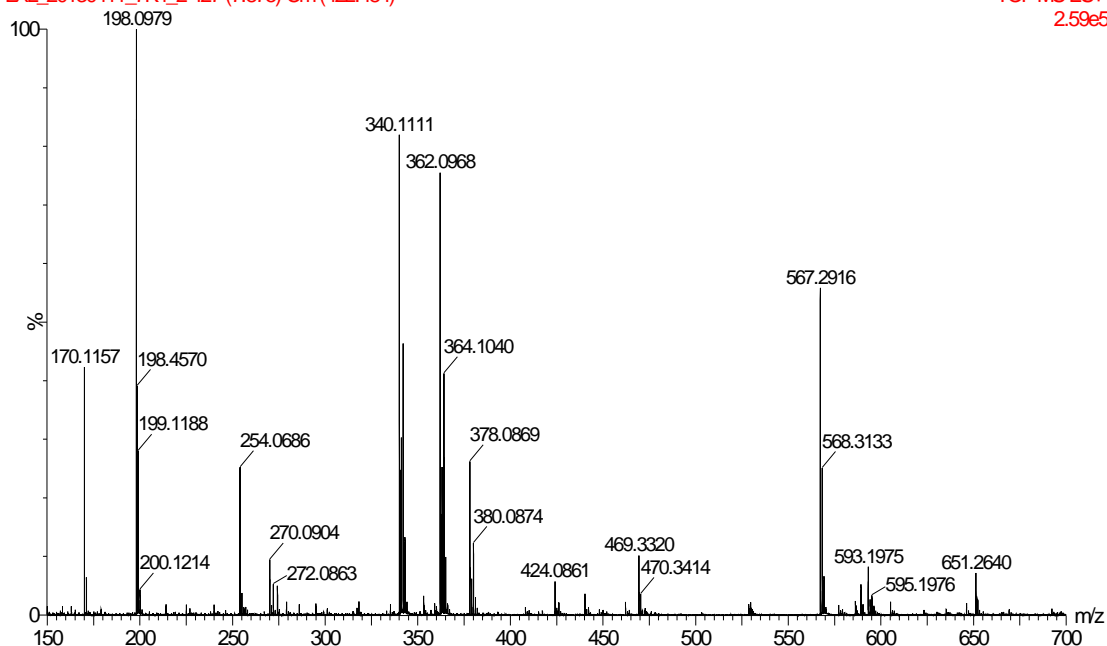
```

NOESY data of metabolites 1

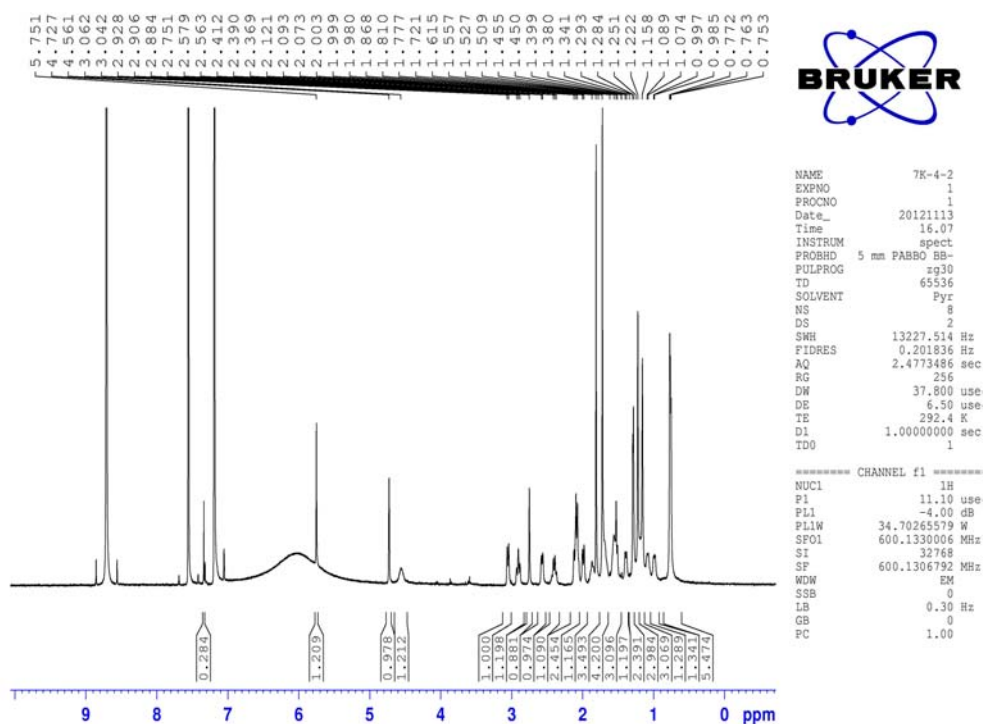
50ACN\_0\_1FA

LXL\_20130411\_7K4\_2.427 (7.875) Cm (422:484)

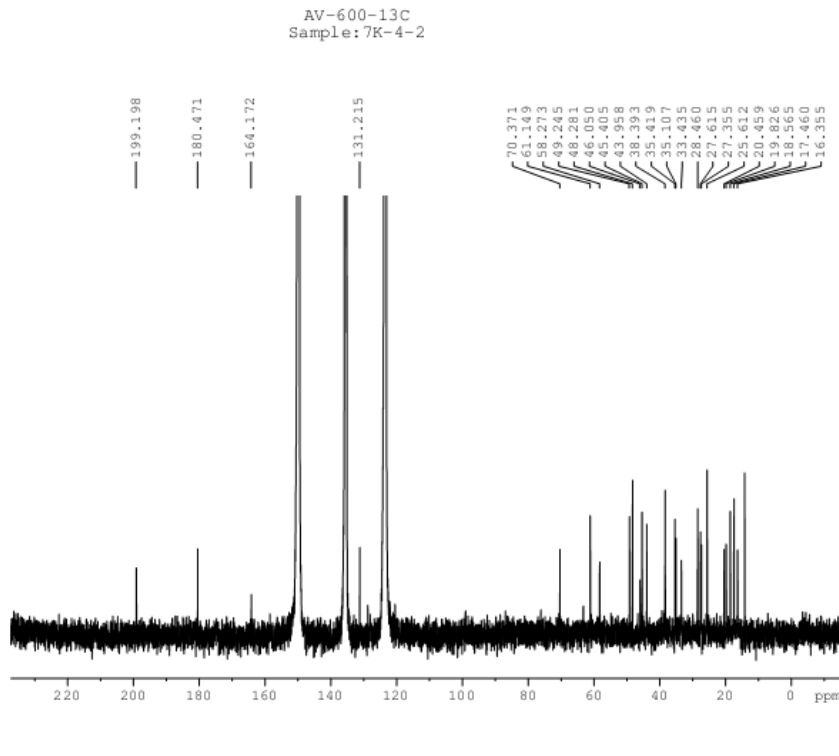
TOF MS ES+  
2.59e5



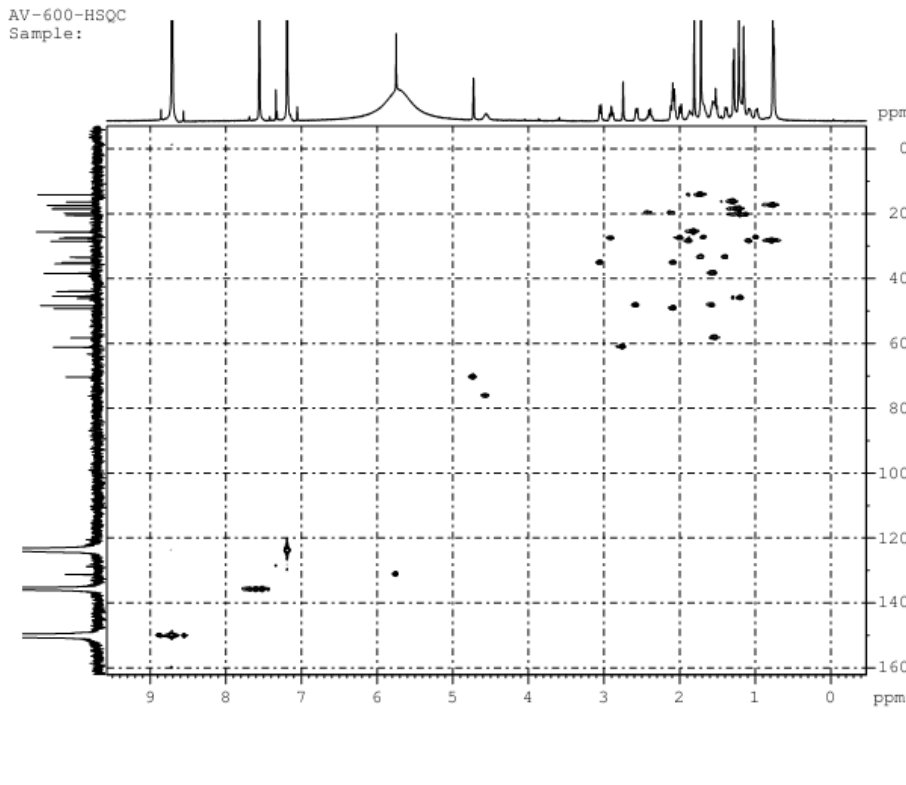
HR-ESI-MS data of metabolites 2



<sup>1</sup>H-NMR data of metabolites 2

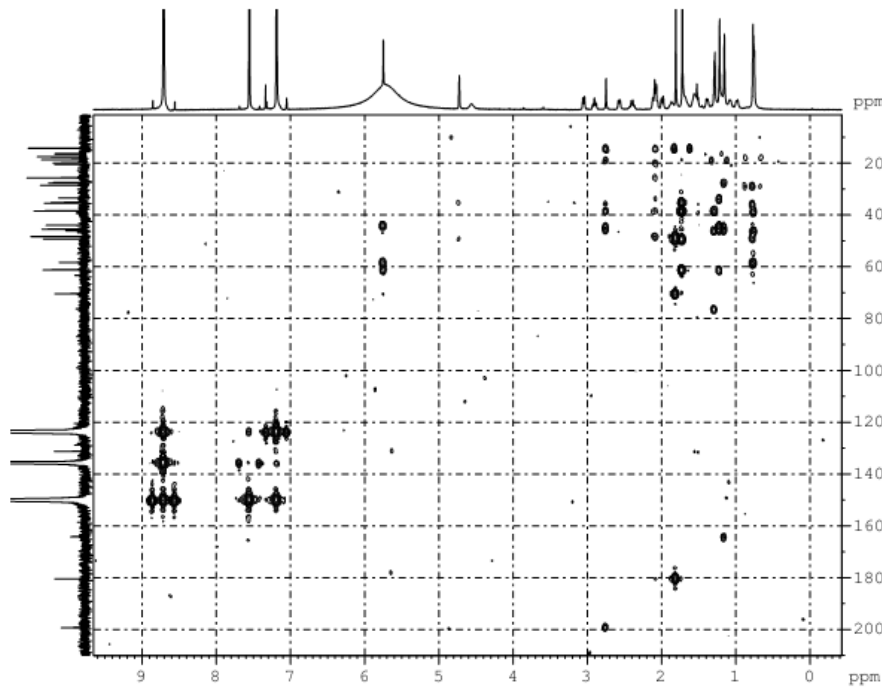


<sup>13</sup>C NMR data of metabolites 2



HMQC data of metabolites 2

AV-600-HMBC  
Sample:



```

NAME       7K-4-2
EXPNO     1
PROCNO    1
Date_     20121123
Time      23.07
INSTRUM   spect
PROBHD    5 mm FAMBQ BB-
PULPROG   hsbcp4ppm2f
TD        1024
SOLVENT   Pyr
NS        256
DS        4
SWH       7183.908 Hz
FIDRES    7.015535 Hz
AQ        0.0713901 sec
RG        2500
DM        69.600 usec
DE        6.50 usec
TE        292.2 K
CST2      145.000000
CST13     1.000000
D0        0.0000000 sec
D1        1.5000000 sec
D2        0.0034482 sec
D3        0.0000000 sec
D4        0.1000000 sec
D5        0.0020000 sec
D6        0.0001001 sec
IN0       0.0001001 sec

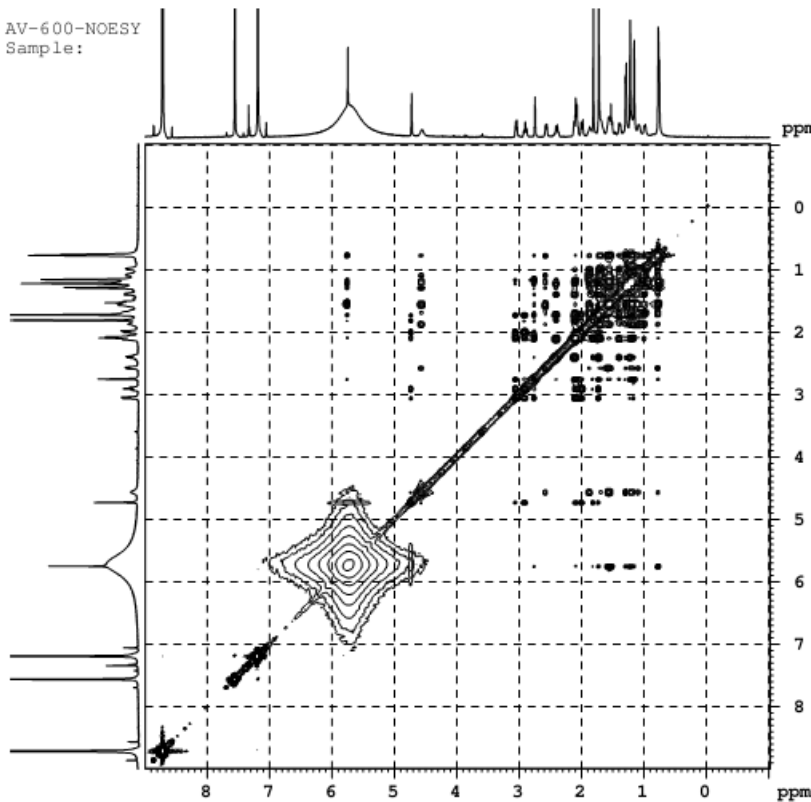
===== CHANNEL f1 =====
NUC1      1H
P1        11.10 usec
P2        22.20 usec
PL1       -4.00 dB
PL12      34.70245379 W
SFO1      600.1330006 MHz

===== CHANNEL f2 =====
NUC2      13C
P3        8.80 usec
PL3       -1.00 dB
PL12      83.20241819 W
SFO2      150.9194081 MHz

===== GRABBER CHANNEL =====
GRAB1     SINE.100
GRAB2     SINE.100
GRAB3     SINE.100
OP1       30.00 kHz
OP2       30.00 kHz
OP3       40.10 kHz
P16       1000.00 usec
NS2       160
TD        160
SFO1      150.9194 MHz
FIDRES    397.314191 Hz
SW        220.000 ppm
F0MODE    1024
SF        600.1306748 MHz
WDW       SINE
SSB       2
LB        0.00 Hz
GB        0
FC        1.00
SI        1024
MC2       States-TFPI
SF        600.1306753 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
  
```

HMBC data of metabolites 2

AV-600-NOESY  
Sample:



```

NAME       7K-4-2
EXPNO     6
PROCNO    1
Date_     20121123
Time      17.50
INSTRUM   spect
PROBHD    5 mm FAMBQ BB-
PULPROG   noesyph
TD        1024
SOLVENT   Pyr
NS        8
DS        4
SWH       7183.908 Hz
FIDRES    7.015535 Hz
AQ        0.0713900 sec
RG        181
DM        69.600 usec
DE        6.50 usec
TE        292.2 K
D0        0.00005547 sec
D1        2.00000000 sec
D2        0.60000002 sec
D3        0.00000000 sec
D4        0.00000000 sec
IN0       0.00013920 sec

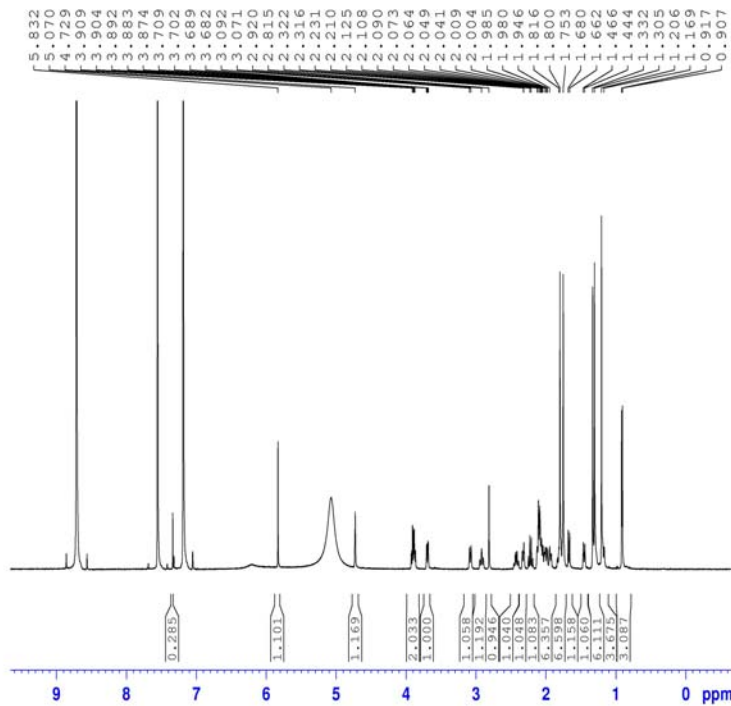
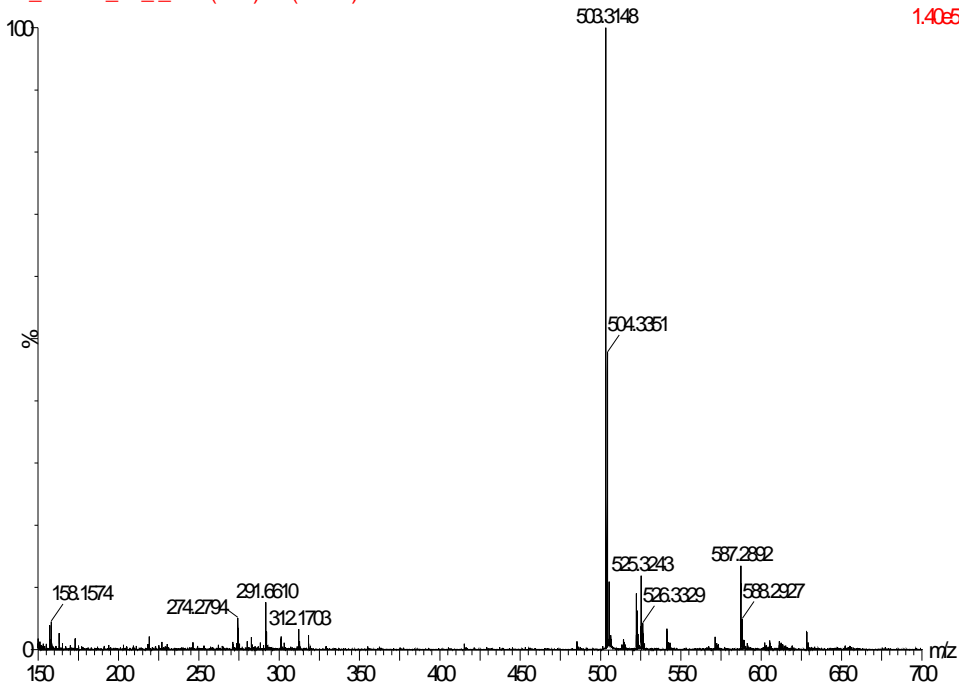
===== CHANNEL f1 =====
NUC1      1H
P1        11.10 usec
PL1       -4.00 dB
PL12      34.70265579 W
SFO1      600.1330006 MHz
TD        1
SFO1      600.133 MHz
FIDRES    28.062078 Hz
SW        11.970 ppm
F0MODE    States-TFPI
SI        1024
SF        600.1306748 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
FC        1.00
SI        1024
MC2       States-TFPI
SF        600.1306753 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
  
```

NOESY data of metabolites 2

50ACN.0\_1FA

LX\_20130411\_7K6\_2\_1428(7.893)Om(387.441)

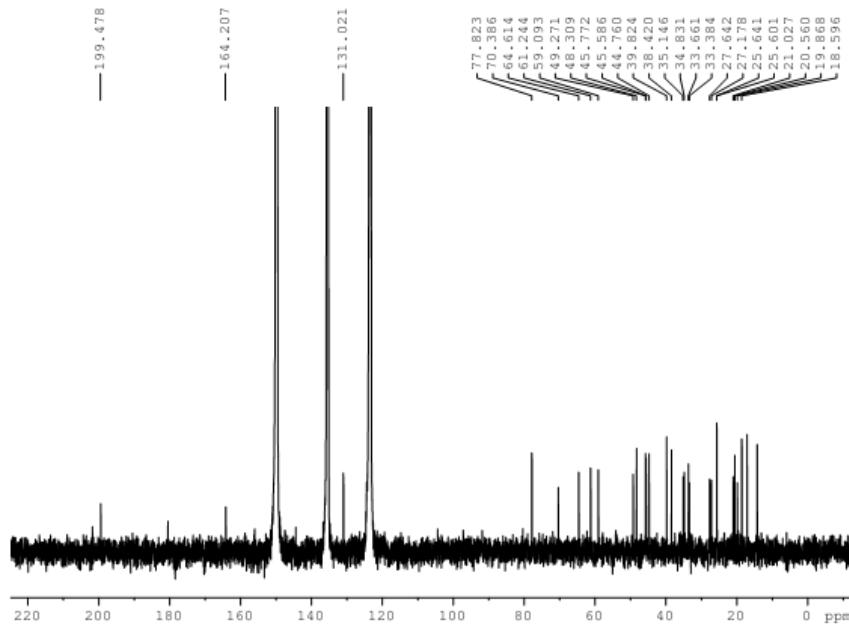
TOF/MS+  
1.40e5



```
NAME       7K-6-2-1
EXPNO      1
PROCNO     1
Date_      20121113
Time       9.53
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zg30
TD          65536
SOLVENT    Pyr
NS          8
DS          2
SWH         13227.514 Hz
FIDRES     0.201836 Hz
AQ          2.4773486 sec
RG          256
DW          37.800 use
DE          6.50 use
TE          292.2 K
D1          1.00000000 sec
TDO         1
----- CHANNEL f1 -----
NUC1       1H
P1         11.10 use
PL1        -4.00 dB
PL1W       34.70265579 W
SFO1       600.1330006 MHz
SI         32768
SF         600.1308989 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



AV-600-13C  
Sample:



**BRUKER**

```

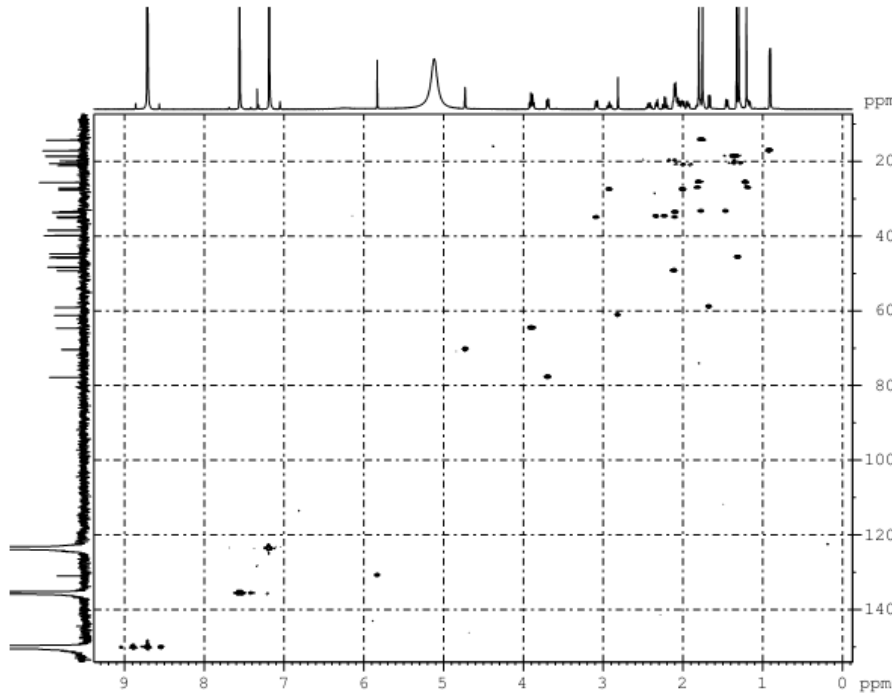
NAME       7K-6-2-1
EXPNO      2
PROCNO     1
Date_      20121114
Time       18.31
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD          65536
SOLVENT    Pyr
NS          4478
DS          2
SWH         45454.547 Hz
FIDRES     0.693581 Hz
AQ          0.7209570 sec
RG          13000
ZW          11.000 usec
DE          6.50 usec
TE          293.4 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1

===== CHANNEL f1 =====
NUC1        13C
P1          6.00 usec
PL1         1.00 dB
PL1W        83.20243835 W
SFO1        150.9178993 MHz

===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2        1H
PCPD2       80.00 usec
PL2         -4.00 dB
PL12        13.16 dB
PL13        16.00 dB
PL2W        34.70265579 W
PL12W       0.66736388 W
PL13W       0.34702653 W
SFO2        600.1324005 MHz
SF          32768
SF          150.9029432 MHz
WDW         EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40
  
```

<sup>13</sup>C-NMR data of metabolites 3

AV-600-HSQC  
Sample:



**BRUKER**

```

NAME       7K-6-2-1
EXPNO      2
PROCNO     1
Date_      20121114
Time       18.31
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD          65536
SOLVENT    Pyr
NS          4478
DS          2
SWH         45454.547 Hz
FIDRES     0.693581 Hz
AQ          0.7209570 sec
RG          13000
ZW          11.000 usec
DE          6.50 usec
TE          293.4 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1

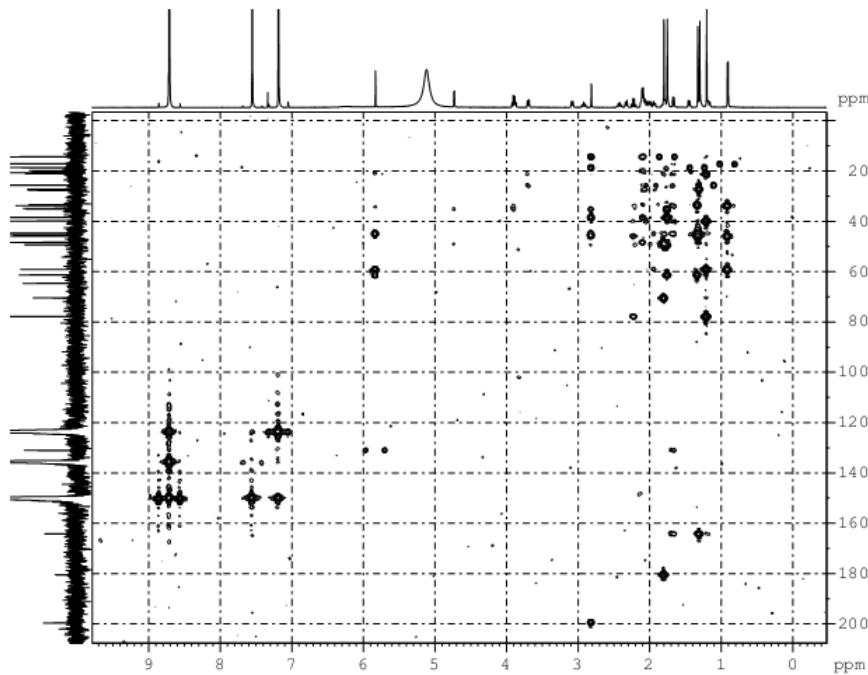
===== CHANNEL f1 =====
NUC1        1H
P1          11.10 usec
PL1         20.00 dB
PL1W        1000.00 usec
SFO1        400.1468012 MHz

===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2        13C
PCPD2       80.00 usec
PL2         17.40 dB
PL12        13.16 dB
PL13        16.00 dB
PL2W        34.70265579 W
PL12W       0.66736388 W
PL13W       0.34702653 W
SFO2        600.1324005 MHz
SF          32768
SF          150.9029432 MHz

===== GRADIENT CHANNEL =====
GRANAL     30.00 Hz
GRANAL2    30.00 Hz
GRPE1      30.00 Hz
GRPE2      30.00 Hz
P14         1000.00 usec
NUC3        13C
TD          384
SFO3        150.914818 MHz
FIDRES3    62.881189 Hz
SF         140.000 MHz
PULPROG3   Rho-AntiCo
SF         400.1299883 MHz
NS          68 DDC
DS          2
LB          0.00 Hz
GB          0
PC          1.40
MCP        rho-anti-co
SFO        150.9029432 MHz
NS          68 DDC
DS          2
LB          0.00 Hz
GB          0
  
```

HSQC data of metabolites 3

AV-600-HMBC  
Sample:



```

NAME       7K-6-2-1
EXPNO     1
PROCNO    1
Date_     20121123
Time      17.15
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   hmcpcpprogf
TD        1024
SOLVENT   Pyz
NS         4
DS         4
SWH       7788.162 Hz
FIDRES    7.605627 Hz
AQ        0.0458550 sec
RG        287
DW        64.200 usec
DE        6.50 usec
TE        291.8 K
D0        0.0000000 sec
D1        1.5000000 sec
D2        0.0034428 sec
D8        0.1000000 sec
D16       0.0002000 sec
IN0       0.0000180 sec

===== CHANNEL f1 =====
NUC1      1H
P1        11.10 usec
PL1       -4.00 dB
PL1W     34.7026579 W
SFO1     600.1327000 MHz

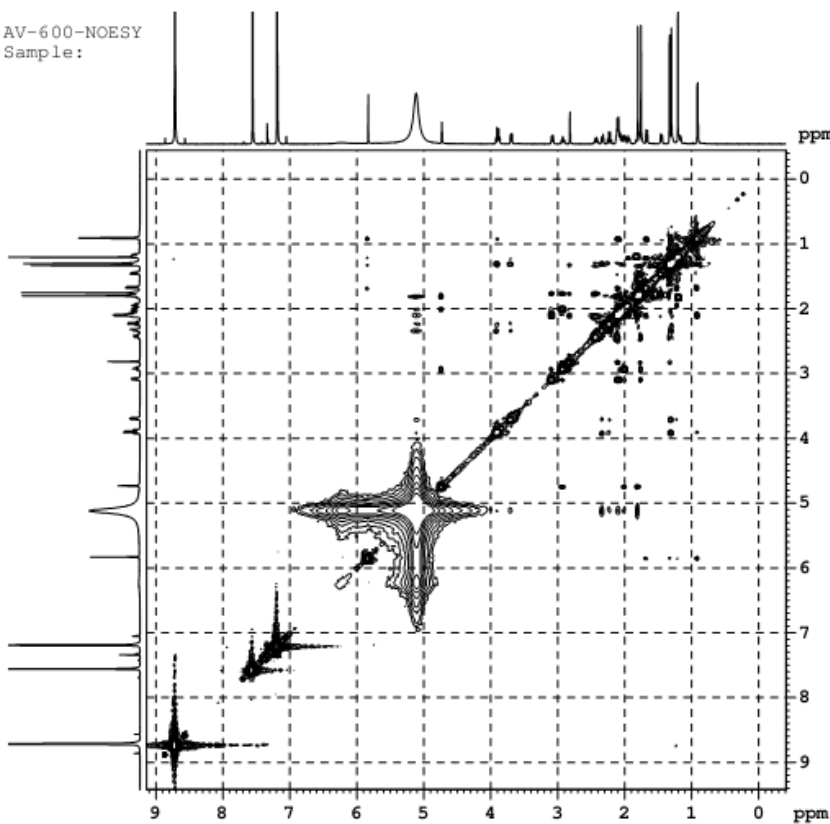
===== CHANNEL f2 =====
NUC2      13C
P2        8.10 usec
PL2       1.00 dB
PL2W     83.2043135 W
SFO2     150.9193090 MHz

===== GRABF2 CHANNEL =====
GPRM1     SINE.100
GPRM2     SINE.100
GPRM3     SINE.100
GP21      50.00 %
GP22      30.00 %
GP23      40.00 %
P16       1000.00 usec
TD        256
SFO1     150.9193 MHz
FIDRES    141.48647 Hz
SW        240.000 ppm
FMODE     QP
SI        1024
SF        600.1299829 MHz
WDW       QSI
SSB       2
LB        0.00 Hz
GB        0
PC        1.00
SI        1024
MC1      600.1299798 MHz
SF        150.9027155 MHz
WDW       QSI
SSB       2
LB        0.00 Hz
GB        0

```

HMBC data of metabolites 3

AV-600-NOESY  
Sample:



```

NAME       7K-6-2-1
EXPNO     5
PROCNO    1
Date_     20121123
Time      7.04
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   noesyph
TD        1024
SOLVENT   Pyz
NS         6
DS         4
SWH       7788.162 Hz
FIDRES    7.605627 Hz
AQ        0.0658550 sec
RG        287
DW        64.200 usec
DE        6.50 usec
TE        291.8 K
D0        0.00004996 sec
D1        2.0000000 sec
D8        0.6000000 sec
IN0       0.00012820 sec

===== CHANNEL f1 =====
NUC1      1H
P1        11.10 usec
PL1       -4.00 dB
PL1W     34.70265579 W
SFO1     600.1327000 MHz
ND0       1
TD        256
SFO1     600.1327 MHz
FIDRES    30.475489 Hz
SW        13.000 ppm
FMODE     States-TPPI
SI        1024
SF        600.1299829 MHz
WDW       QSI
SSB       2
LB        0.00 Hz
GB        0
PC        1.00
SI        1024
MC2      States-TPPI
SF        600.1299798 MHz
WDW       QSI
SSB       2
LB        0.00 Hz
GB        0

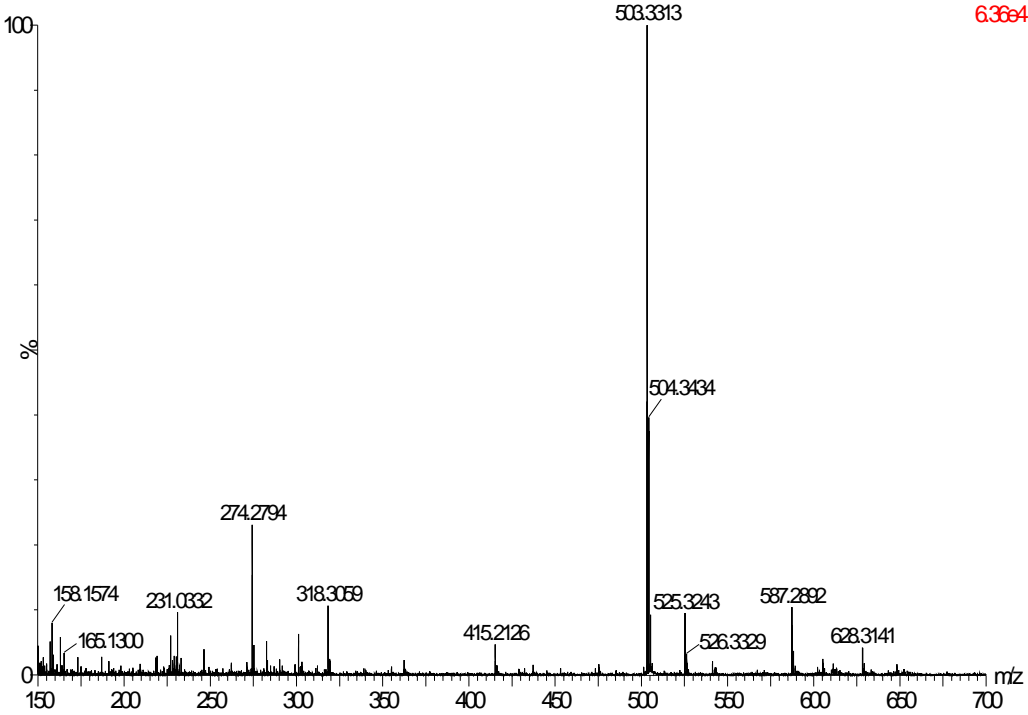
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NOESY data of metabolites 3

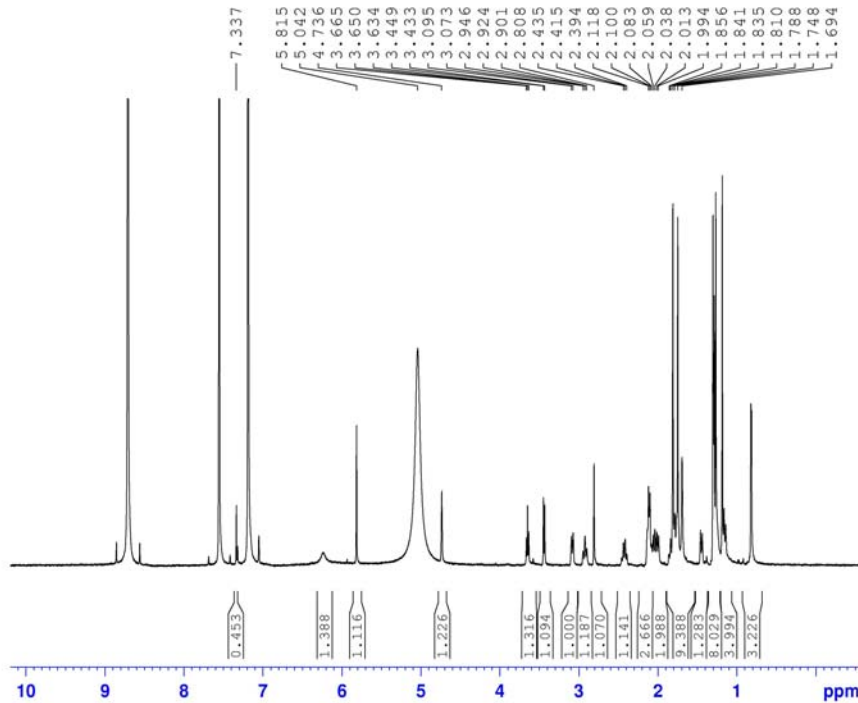
50ACN\_0\_1FA

LXI\_20130411\_746\_3\_1425(7.837) Om(382-437)

TOFMS/ESI+  
6.36e4



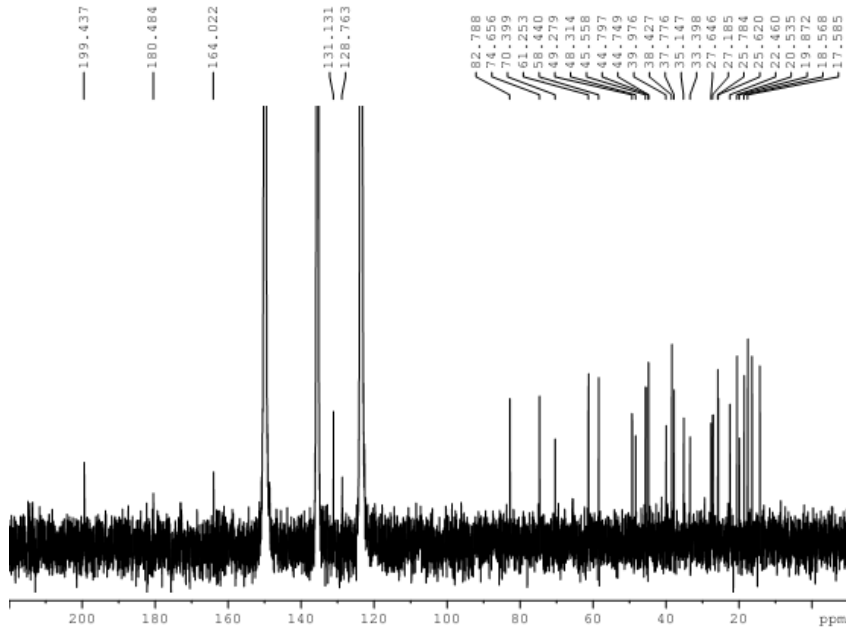
HR-ESI-MS data of metabolites 4



```
NAME          7K-6-3-1
EXPNO         1
PROCNO        1
Date_         20121113
Time          9.35
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       Pyr
NS            8
DS            2
SWH           13227.514 Hz
FIDRES        0.201836 Hz
AQ            2.4773486 sec
RG            322
DW            37.800 usec
DE            6.50 usec
TE            292.3 K
D1            1.00000000 sec
TD0           1
***** CHANNEL f1 *****
NUC1          1H
P1            11.10 usec
PL1           -4.00 dB
PL1W          34.70265579 W
SFOL          600.1330006 MHz
SI            32768
SF            600.1306801 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

<sup>1</sup>H-NMR data of metabolites 4

AV-600-13C  
Sample:



```

NAME       7K-6-3-1
EXFNO     2
PROCNO    1
Date_     20121115
Time      21.17
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   Pyr
NS        4273
DS        2
SWH       45454.547 Hz
FIDRES    0.693581 Hz
AQ        0.7209570 sec
RG        13000
LW        11.000 usec
DE        6.50 usec
TE        294.4 K
D1        2.0000000 sec
D11       0.0300000 sec
TD0       1
  
```

```

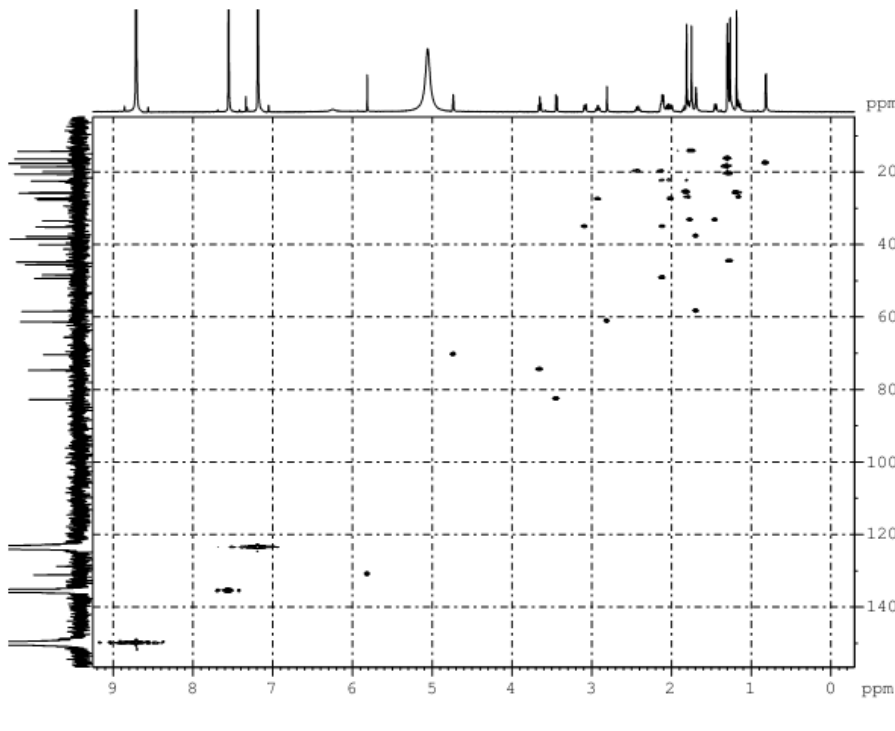
===== CHANNEL f1 =====
NUC1      13C
P1        6.00 usec
PL1       1.00 dB
PL1W     83.20243835 W
SF01     150.9178993 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -4.00 dB
PL12     13.16 dB
PL13     16.00 dB
PL2W     34.70265579 W
PL12W    0.66736388 W
PL13W    0.34702653 W
SFO2     600.1324005 MHz
SI        32768
SF       150.9027684 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40
  
```

<sup>13</sup>C-NMR data of metabolites 4

AV-600-HSQC  
Sample:



```

NAME       7K-6-3-1
EXFNO     7
PROCNO    1
Date_     20121122
Time      7.13
INSTRUM   spect
PROBHD    5 mm F4BBO BB-
PULPROG   hsqcetpgp1
TD        1024
SOLVENT   Pyr
NS        4
DS        16
SWH       7788.142 Hz
FIDRES    7.825818 Hz
AQ        0.0492550 sec
RG        25000
LW        44.200 usec
DE        291.4 K
D1        1.4500000 sec
D11       0.0000000 sec
D12       1.5000000 sec
D13       0.0000000 sec
D14       0.0000000 sec
D15       0.0000000 sec
D16       0.0000000 sec
D17       0.0000000 sec
D18       0.0000000 sec
D19       0.0000000 sec
D20       0.0000000 sec
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        11.10 usec
PL1       22.20 dB
PL1W     1000.00 usec
SF01     34.7026579 MHz
  
```

```

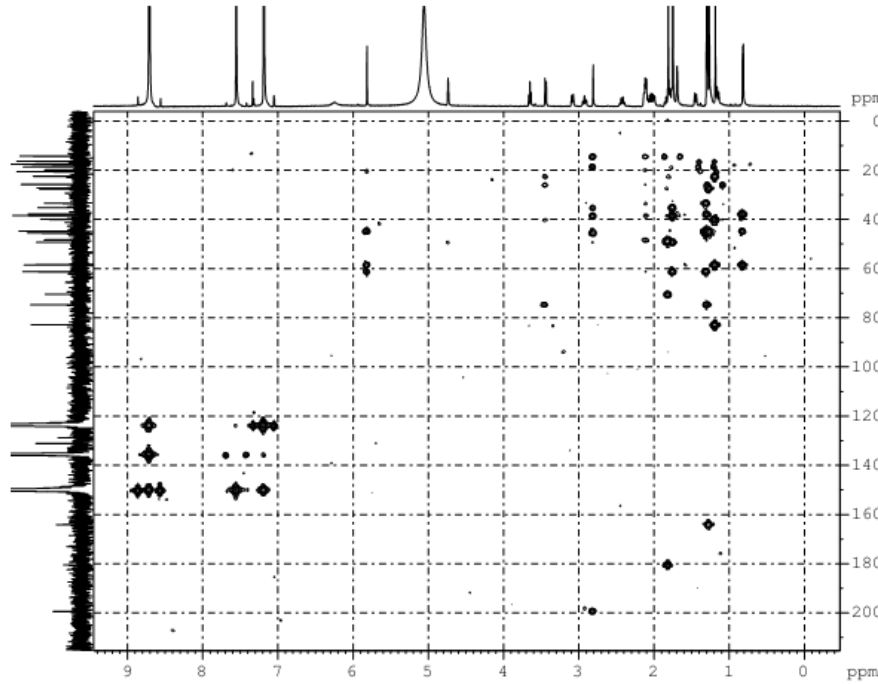
===== CHANNEL f2 =====
CPDPRG2   gqrq
NUC2      13C
P2        8.80 usec
PL2       17.60 dB
PL2W     80.00 usec
SF02     150.9178993 MHz
  
```

```

===== GRADIENT CHANNEL =====
GRNAM1    SINE_100
GRNAM2    SINE_100
GPR1      80.00 Hz
GPR2      20.10 Hz
GPR3      1000.00 usec
SI        2048
SF01     150.9149 MHz
FIDRES    42.861199 Hz
SI        140.0000 ppm
P1PROG    Echo-AntiEcho
SI        400.1299883 MHz
NS        2
DS        2
SSB       0
LB        0.00 Hz
GB        0
PC        1.024
  
```

HSQC data of metabolites 4

AV-600-HMBC  
Sample:



```

NAME          7K-6-3-1
EXPNO         1
PROCNO        1
Date_         20121121
Time          17.12
INSTRUM       spect
PROBHD        5 mm FAPBO BB-
PULPROG       hmcgcp1p024
TD            1024
SOLVENT       Pyr
NS            128
DS            16
SWH           7788.162 Hz
FIDRES        7.605627 Hz
AQ            0.0658550 sec
RG            6100
DW            64.200 usec
DE            6.50 usec
TE            291.2 K
CHFT2         145.000000
CHFT13        5.000000
D0            0.0000000 sec
D1            1.5000000 sec
D2            0.0014482 sec
D4            0.1000000 sec
D16           0.0020000 sec
IN0           0.0001380 sec

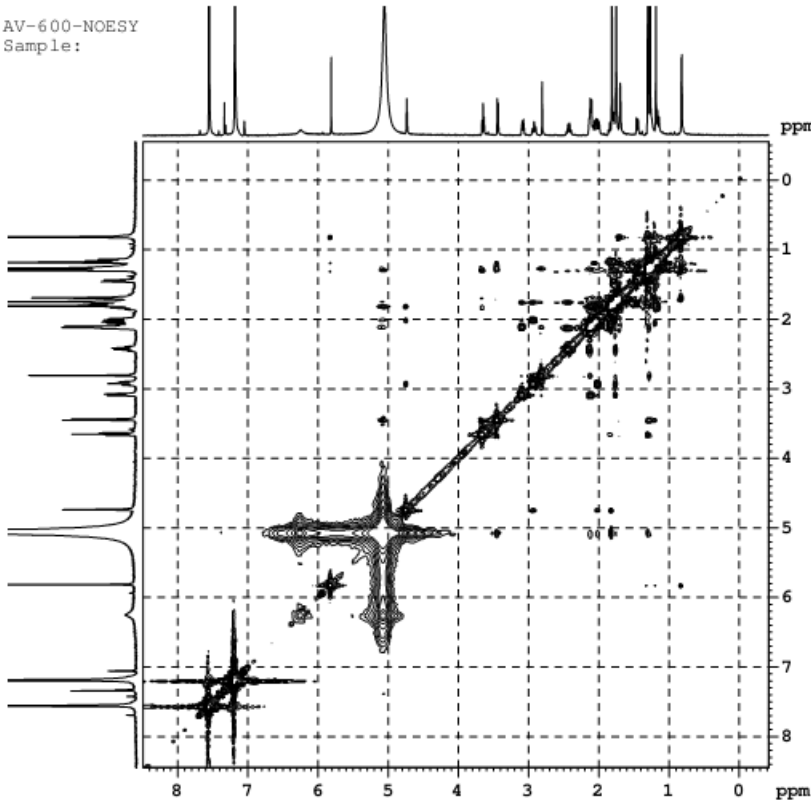
===== CHANNEL f1 =====
NUC1          1H
P1            11.10 usec
P2            23.20 usec
PL1           -4.00 dB
PL1W          34.7024379 W
SFO1          600.1327000 MHz

===== CHANNEL f2 =====
NUC2          13C
P3            8.80 usec
P4            1.00 dB
P4W           81.2024379 W
SFO2          100.6181080 MHz

===== GRABUNT CHANNEL =====
GRABM1        SDR:100
GRABM2        SDR:100
GRABM3        SDR:100
GP21          50.00 k
GP22          30.00 k
GP23          40.10 k
P16           1000.00 usec
ND0           2
TD            256
SFO1          100.6181080 MHz
FIDRES        141.484897 Hz
SW            240.000 ppm
FRMODE        SI
SI            1024
SF            600.1299829 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
SI            1024
MC2           States-TPPI
SF            600.1299798 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
  
```

HMBC data of metabolites 4

AV-600-NOESY  
Sample:



```

NAME          7K-6-3-1
EXPNO         6
PROCNO        1
Date_         20121122
Time          6.04
INSTRUM       spect
PROBHD        5 mm FAPBO BB-
PULPROG       noesyph
TD            1024
SOLVENT       Pyr
NS            6
DS            4
SWH           7788.162 Hz
FIDRES        7.605627 Hz
AQ            0.0658550 sec
RG            228
DW            64.200 usec
DE            6.50 usec
TE            291.4 K
D0            0.00004996 sec
D1            2.00000000 sec
D8            0.60000002 sec
IN0           0.00012820 sec

===== CHANNEL f1 =====
NUC1          1H
P1            11.10 usec
PL1           -4.00 dB
PL1W          34.70265579 W
SFO1          600.1327000 MHz
ND0           1
TD            256
SFO1          600.1327000 MHz
FIDRES        30.475489 Hz
SW            13.000 ppm
FRMODE        States-TPPI
SI            1024
SF            600.1299829 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
SI            1024
MC2           States-TPPI
SF            600.1299798 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
  
```

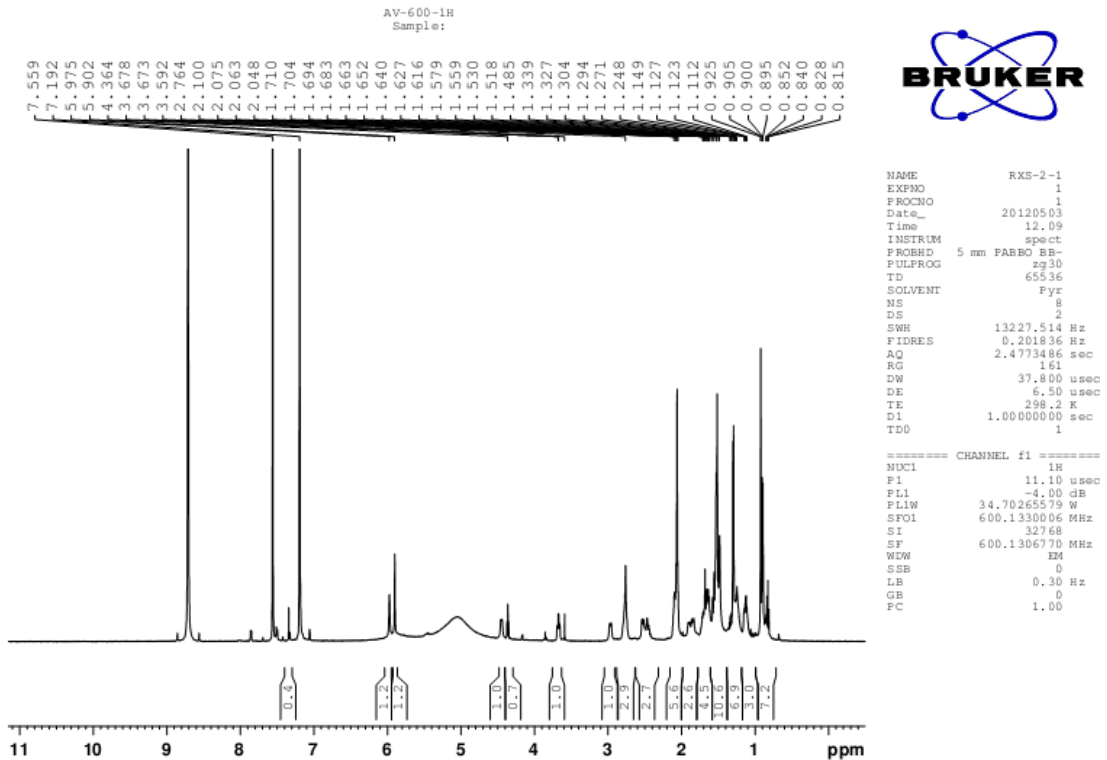
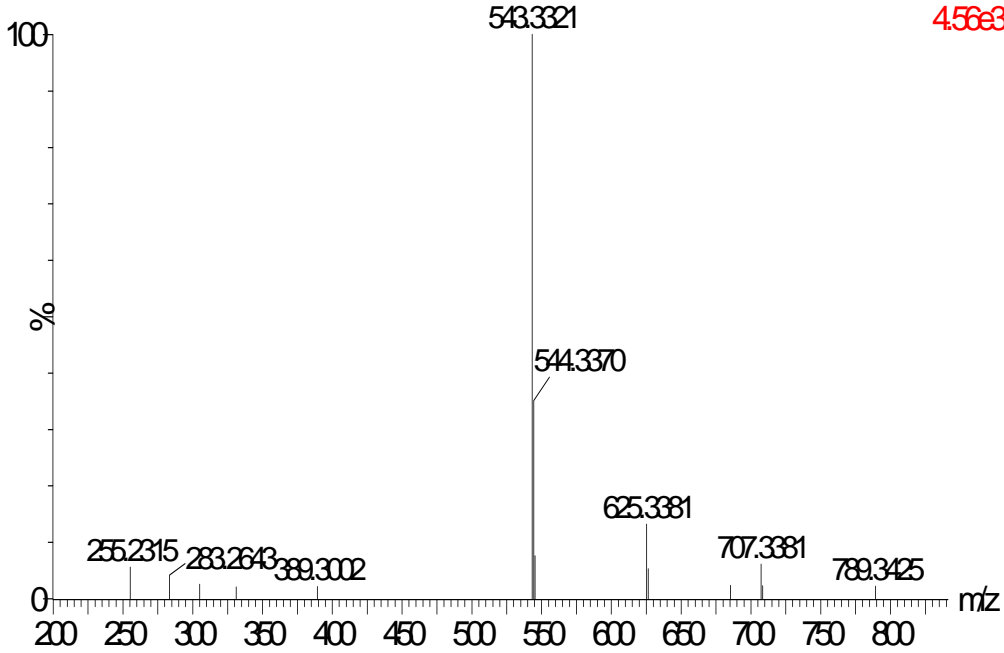
NOESY data of metabolites 4

RMS2

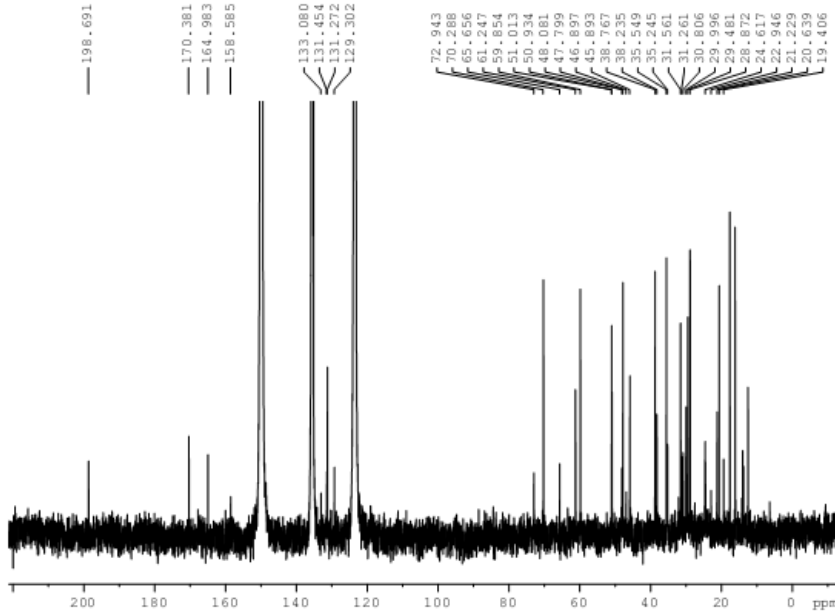
10:45:03

1203281663(1.172) AM(Cen,2, 80.00, H,5000.0,0.00,1.00); Sm(Mh, 2x1.00); Cm(47:73)

4.56e3



AV-600-13C  
Sample:



```

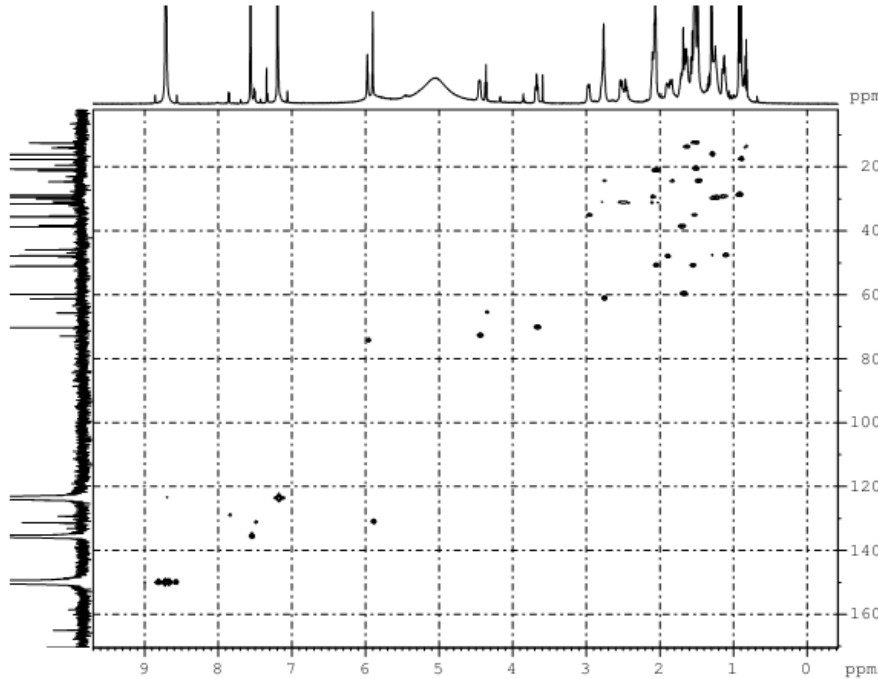
NAME      RXS-2-1
EXPNO    2
PROCNO   1
Date_    20120505
Time     20.03
INSTRUM  spect
PROBHD   5 mm FAPBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  Pyr
NS        8309
DS        2
SWH       45454.547 Hz
FIDRES   0.693581 Hz
AQ        0.7209570 sec
RG         13000
DW         11.000 usec
DE         6.50 usec
TE         298.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO       1

===== CHANNEL f1 =====
NUC1      13C
P1         6.00 usec
PL1        1.00 dB
PL1W       83.20243835 W
SFO1      150.9178993 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        -4.00 dB
PL12       13.16 dB
PL13       16.00 dB
PL2W       34.70265579 W
PL12W      0.66736388 W
PL13W      0.3472653 W
SFO2      600.1324005 MHz
SI         32768
SF         150.9027684 MHz
WDW        EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40
  
```

<sup>13</sup>C NMR data of metabolites 5

AV-600-HSQC  
Sample:RXS-2-1



```

NAME      RXS-2-1
EXPNO    2
PROCNO   1
Date_    20120505
Time     20.52
INSTRUM  spect
PROBHD   5 mm FAPBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  Pyr
NS        8309
DS        2
SWH       7183.958 Hz
FIDRES   7.015335 Hz
AQ        0.9712965 sec
RG         24000
DW         69.400 usec
DE         6.50 usec
TE         298.2 K
CPDPRG2   145.0000000 usec
D1         0.00000000 sec
D11        1.50000000 sec
D12        0.0117841 sec
D13        0.03000000 sec
D14        0.00000000 sec
D15        0.00000000 sec
D16        0.00000000 sec
D17        0.01110000 sec
D18        0.00000000 sec
SFO1      150.9162903 MHz

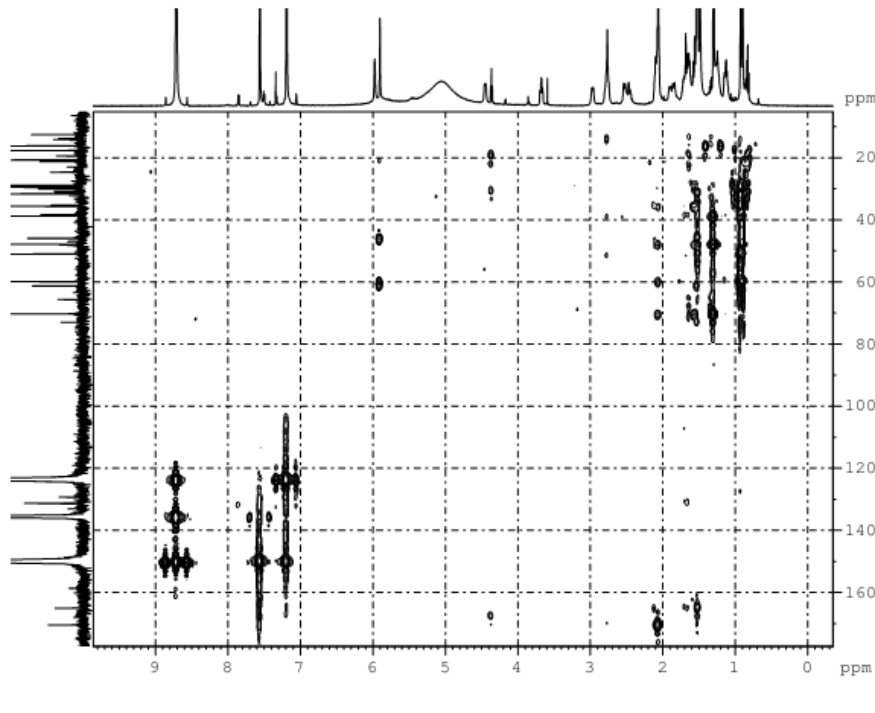
===== CHANNEL f1 =====
NUC1      1H
P1         11.10 usec
PL1        2.00 dB
PL1W       1000.00 usec
SFO1      400.1330006 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       13C
PCPD2     80.00 usec
PL2        17.00 dB
PL12       13.16 dB
PL13       16.00 dB
PL2W       34.70265579 W
PL12W      0.66736388 W
PL13W      0.3472653 W
SFO2      150.9162903 MHz

===== GRABBER CHANNEL =====
OPRAME1   8388.100
OPRAME2   8388.100
OP1        80.00 Hz
OP2        20.10 Hz
TD         10000.00 usec
TE         298.2 K
SFO1      150.9162903 MHz
FIDRES    106.111025 Hz
SI         65536.0000 usec
SF         400.1330006 MHz
WDW        EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40
SFO2      150.9162903 MHz
SI         65536.0000 usec
SF         150.9162903 MHz
WDW        EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40
  
```

HSQC data of metabolites 5

AV-600-HMBC  
Sample:RXS-2-1



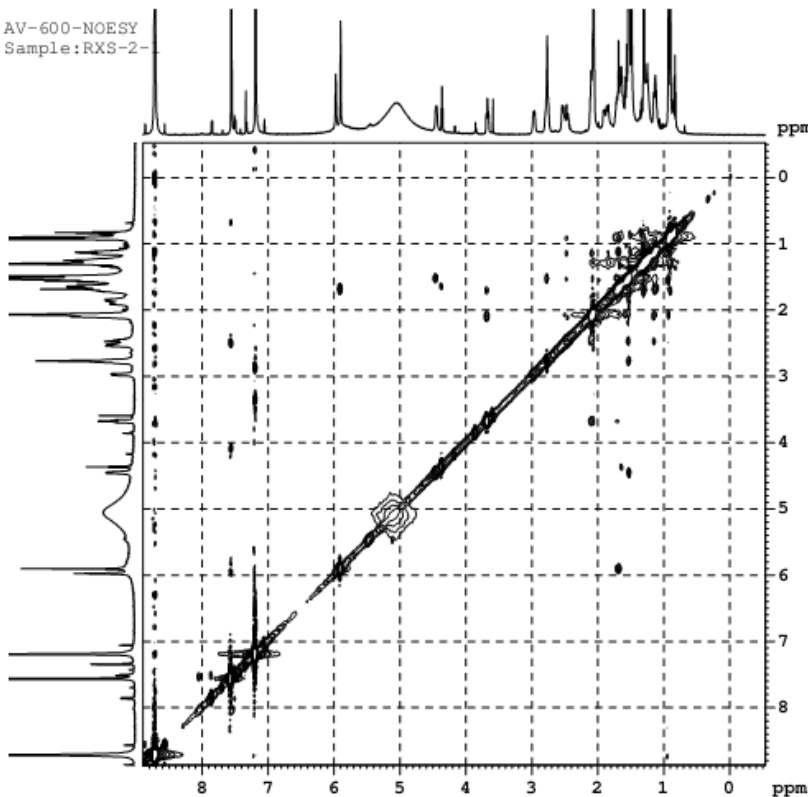
```

NAME          RXS-2-1
EXPNO         6
PROCNO        1
Date_         20120527
Time          22.43
INSTRUM       spect
PROBHD        5 mm FAPBO BB-
PULPROG       hsbcp1p2d4f
TD            1024
SOLVENT       Pyr
NS            128
DS            4
SWH           7183.908 Hz
FIDRES        7.015535 Hz
AQ            0.0713900 sec
RG            101
DW            69.600 usec
DE            5.50 usec
TE            298.2 K
D0            0.0000000 sec
D1            1.0000000 sec
D2            0.0034428 sec
D3            0.1000000 sec
D4            0.0000000 sec
D5            0.0000000 sec
D6            0.0000000 sec
D7            0.0000000 sec
D8            0.0000000 sec
D9            0.0000000 sec
D10           0.0000000 sec
===== CHANNEL f1 =====
NUC1          1H
P1            11.10 usec
PL1           -4.00 dB
PL12          34.7026577 W
PL13          150.1330006 MHz
PL14          600.1330006 MHz
===== CHANNEL f2 =====
NUC2          13C
P2            6.80 usec
PL2           -4.00 dB
PL22          83.2024937 W
PL23          150.1330006 MHz
===== GRADIENT CHANNEL =====
GRNAME        SINE-100
GRPROG        SINE-100
Time          218.100 usec
GRD1          50.00 %
GRD2          30.00 %
GRD3          40.10 %
P14           1000.00 usec
TD            1
NS            256
DS            2
SWH           150.8184 MHz
FIDRES        215.399152 Hz
AQ            0.0713900 sec
RG            101
DW            69.600 usec
DE            5.50 usec
TE            298.2 K
D0            0.0000000 sec
D1            2.000000000 sec
D2            0.600000002 sec
D3            0.00013920 sec
D4            0.00013920 sec
D5            0.00013920 sec
D6            0.00013920 sec
D7            0.00013920 sec
D8            0.00013920 sec
D9            0.00013920 sec
D10           0.00013920 sec
===== CHANNEL f1 =====
NUC1          1H
P1            11.10 usec
PL1           -4.00 dB
PL12          34.7026577 W
PL13          150.1330006 MHz
===== CHANNEL f2 =====
NUC2          13C
P2            6.80 usec
PL2           -4.00 dB
PL22          83.2024937 W
PL23          150.1330006 MHz
===== GRADIENT CHANNEL =====
GRNAME        SINE-100
GRPROG        SINE-100
Time          218.100 usec
GRD1          50.00 %
GRD2          30.00 %
GRD3          40.10 %
P14           1000.00 usec
TD            1
NS            256
DS            2
SWH           150.8184 MHz
FIDRES        215.399152 Hz
AQ            0.0713900 sec
RG            101
DW            69.600 usec
DE            5.50 usec
TE            298.2 K
D0            0.0000000 sec
D1            2.000000000 sec
D2            0.600000002 sec
D3            0.00013920 sec
D4            0.00013920 sec
D5            0.00013920 sec
D6            0.00013920 sec
D7            0.00013920 sec
D8            0.00013920 sec
D9            0.00013920 sec
D10           0.00013920 sec

```

HMBC data of metabolites 5

AV-600-NOESY  
Sample:RXS-2-



```

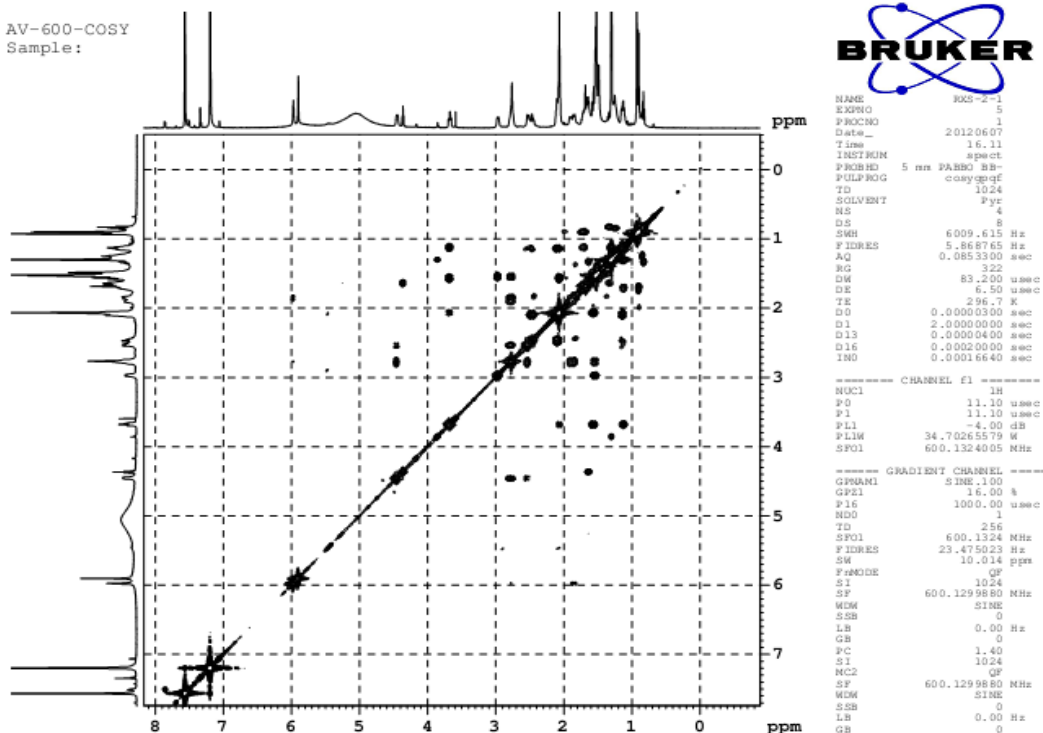
NAME          RXS-2-1
EXPNO         6
PROCNO        1
Date_         20120527
Time          20.05
INSTRUM       spect
PROBHD        5 mm FAPBO BB-
PULPROG       noesyph
TD            1024
SOLVENT       Pyr
NS            128
DS            4
SWH           7183.908 Hz
FIDRES        7.015535 Hz
AQ            0.0713900 sec
RG            101
DW            69.600 usec
DE            5.50 usec
TE            298.2 K
D0            0.0000000 sec
D1            2.000000000 sec
D2            0.600000002 sec
D3            0.00013920 sec
D4            0.00013920 sec
D5            0.00013920 sec
D6            0.00013920 sec
D7            0.00013920 sec
D8            0.00013920 sec
D9            0.00013920 sec
D10           0.00013920 sec
===== CHANNEL f1 =====
NUC1          1H
P1            11.10 usec
PL1           -4.00 dB
PL12          34.7026577 W
PL13          150.1330006 MHz
===== CHANNEL f2 =====
NUC2          1H
P2            11.10 usec
PL2           -4.00 dB
PL22          34.7026577 W
PL23          150.1330006 MHz
===== GRADIENT CHANNEL =====
GRNAME        States-TFPI
GRPROG        States-TFPI
Time          218.100 usec
GRD1          2
GRD2          2
GRD3          2
P14           1024
NS            256
DS            2
SWH           600.1299907 MHz
FIDRES        28.062078 Hz
AQ            0.0713900 sec
RG            101
DW            69.600 usec
DE            5.50 usec
TE            298.2 K
D0            0.0000000 sec
D1            2.000000000 sec
D2            0.600000002 sec
D3            0.00013920 sec
D4            0.00013920 sec
D5            0.00013920 sec
D6            0.00013920 sec
D7            0.00013920 sec
D8            0.00013920 sec
D9            0.00013920 sec
D10           0.00013920 sec
===== CHANNEL f1 =====
NUC1          1H
P1            11.10 usec
PL1           -4.00 dB
PL12          34.7026577 W
PL13          150.1330006 MHz
===== CHANNEL f2 =====
NUC2          1H
P2            11.10 usec
PL2           -4.00 dB
PL22          34.7026577 W
PL23          150.1330006 MHz
===== GRADIENT CHANNEL =====
GRNAME        States-TFPI
GRPROG        States-TFPI
Time          218.100 usec
GRD1          2
GRD2          2
GRD3          2
P14           1024
NS            256
DS            2
SWH           600.1299907 MHz
FIDRES        28.062078 Hz
AQ            0.0713900 sec
RG            101
DW            69.600 usec
DE            5.50 usec
TE            298.2 K
D0            0.0000000 sec
D1            2.000000000 sec
D2            0.600000002 sec
D3            0.00013920 sec
D4            0.00013920 sec
D5            0.00013920 sec
D6            0.00013920 sec
D7            0.00013920 sec
D8            0.00013920 sec
D9            0.00013920 sec
D10           0.00013920 sec

```

NOESY data of metabolites 5



AV-600-COSY  
Sample:

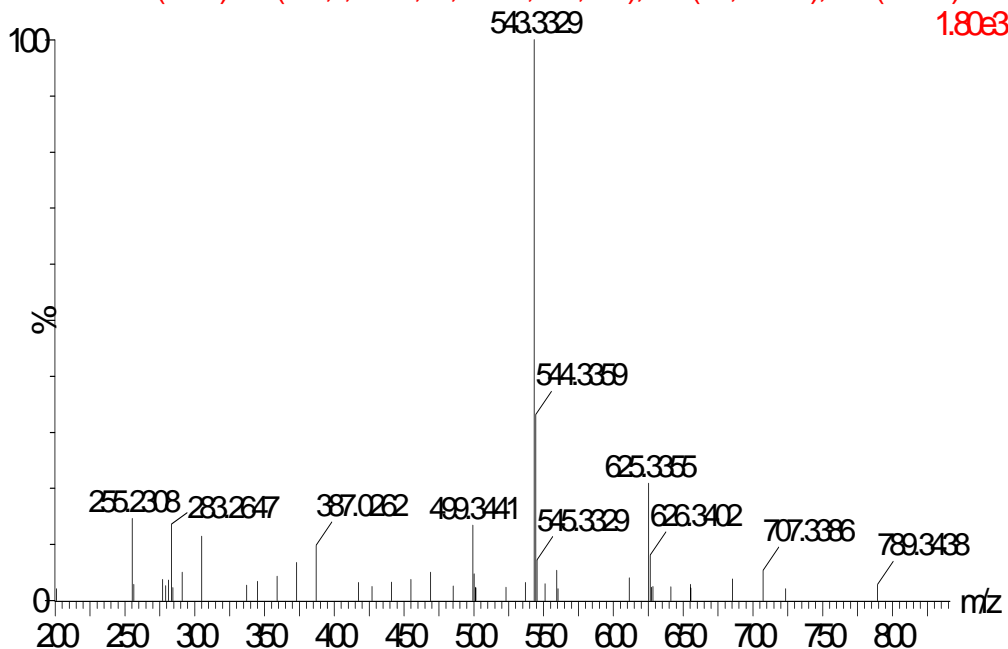


<sup>1</sup>H-<sup>1</sup>H COSY data of metabolites 5

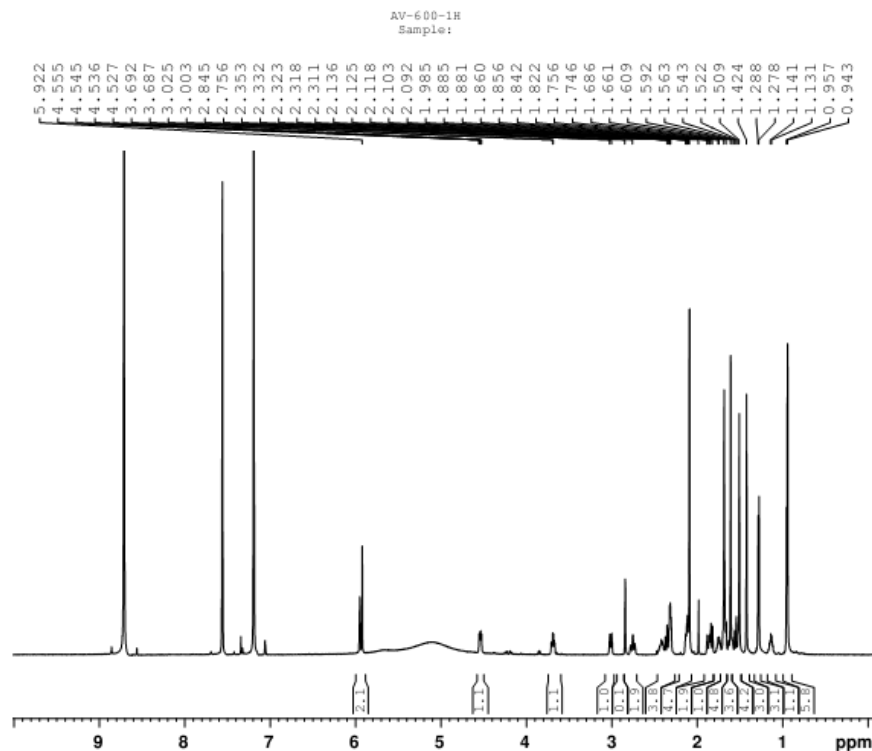
R2

10:39:26

12032815 103 (1.909) AM(Cen,2, 80.00, H,5000.0,0.00,1.00); Sm(Mh, 2x1.00); Cm(86:117)



HR-ESI-MS data of metabolites 6



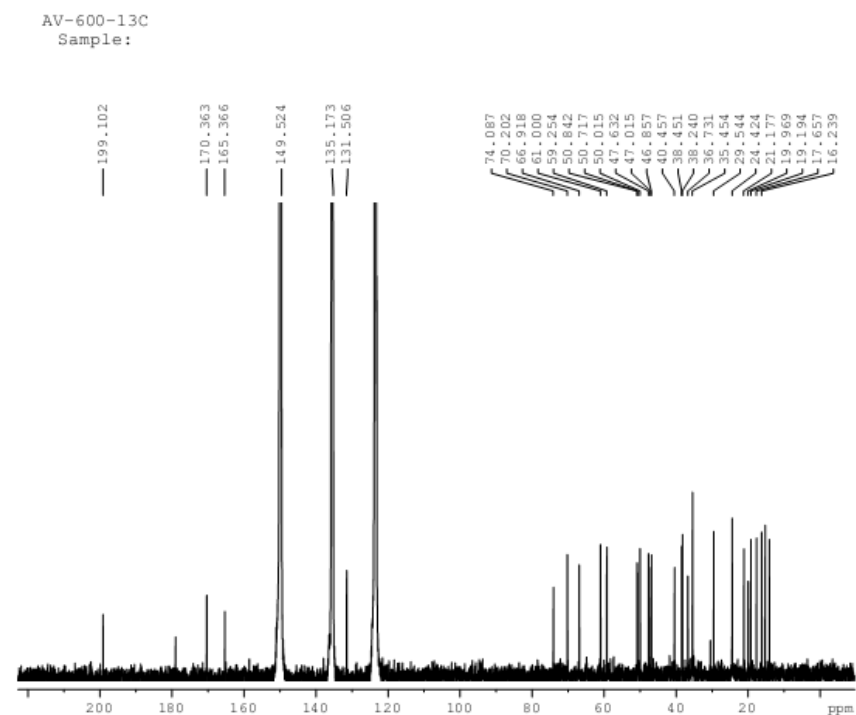
```

NAME          R-2
EXPNO         1
PROCNO        1
Date_         20111214
Time          15.19
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       Pyr
NS            8
DS            2
SWH           13227.514 Hz
FIDRES        0.201836 Hz
AQ            2.4773486 sec
RG            287
EW            37.800 usec
DE            6.50 usec
TE            298.2 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            11.10 usec
PL1           -4.00 dB
PL1W          34.70265579 W
SFO1          600.1330006 MHz
SI            32768
SF            600.1306777 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

$^1\text{H}$ -NMR data of metabolites **6**



```

NAME          R-2
EXPNO         2
PROCNO        1
Date_         20120107
Time          18.15
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       Pyr
NS            5228
DS            2
SWH           45454.547 Hz
FIDRES        0.693581 Hz
AQ            0.7209570 sec
RG            13000
EW            11.000 usec
DE            6.50 usec
TE            298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

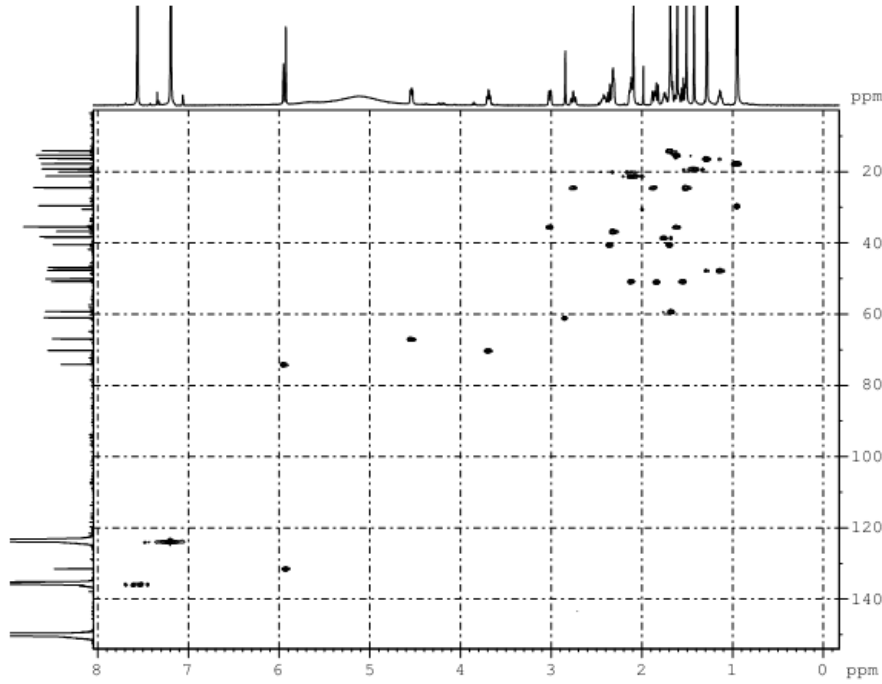
===== CHANNEL f1 =====
NUC1          13C
P1            6.00 usec
PL1           1.00 dB
PL1W          83.20243835 W
SFO1          150.9178993 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -4.00 dB
PL12          13.16 dB
PL13          16.00 dB
PL2W          34.70265579 W
PL12W         0.66736388 W
PL13W         0.34702653 W
SFO2          600.1324005 MHz
SI            32768
SF            150.9027690 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.40

```

$^{13}\text{C}$ -NMR data of metabolites **6**

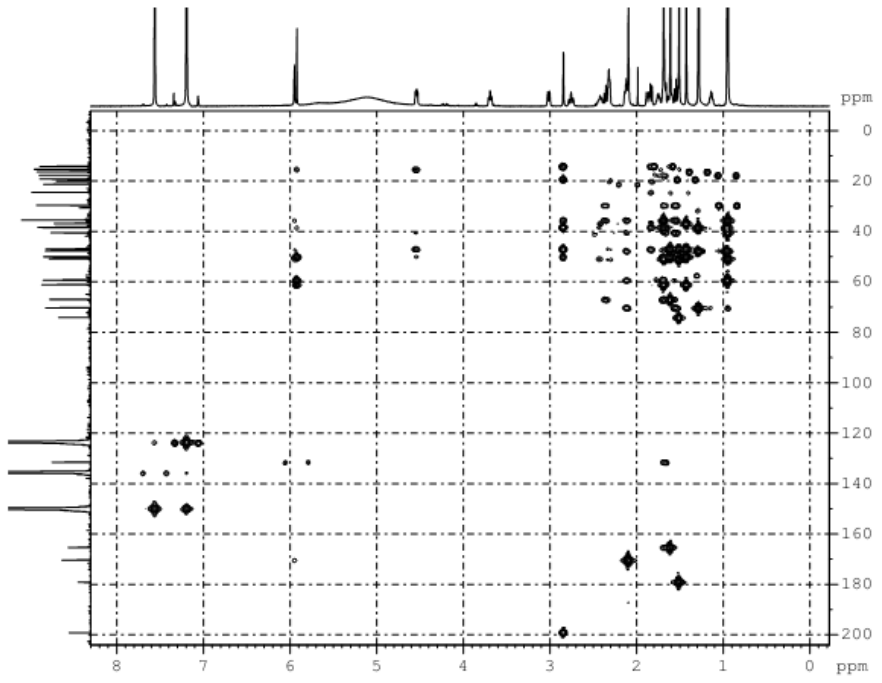
AV-600-HSQC  
Sample:



```
NAME      B-2
EXPNO     1
PROCNO    1
Date_    20120314
Time      4.10
INSTRUM   spect
PROBHD    5 mm QNP1H
PULPROG   zgpg30
TD         65536
SOLVENT   Pyz
NS         14
DS         2
SWH        4413.757 Hz
FIDRES     4.452747 Hz
AQ         0.0775400 sec
RG         24000
DW         75.400 usec
DE         4.50 usec
TE         298.2 K
CHFT2     145.0000000
D0         0.0000000 sec
D1         1.0000000 sec
D2         0.0017444 sec
D3         0.0000000 sec
D4         0.0000000 sec
D5         0.0000000 sec
D6         0.0011000 sec
D7         0.0000000 sec
D8         0.0011000 sec
D9         0.0000000 sec
ZDELTA    2.0000000
===== CHANNEL f1 =====
NUC1       13C
P1         11.10 usec
PC         22.20 usec
P2         100.00 usec
P3         1.00 usec
PL1W      34.7024573 W
PL2W      400.1327000 MHz
===== CHANNEL f2 =====
NUC2       1H
P1         1.30 usec
PC         2.80 usec
P2         17.40 usec
P3         90.00 usec
P4         1.00 usec
PL1W      24.10 W
PL2W      500.1360992 MHz
===== GRADIENT CHANNEL =====
GPRAME     SINE.100
GPRAMD     SINE.100
OP1        30.00 %
OP2        30.00 %
OP3        40.10 %
P14        100.00 usec
RG0        2
RG1         0
RG2         0
RG3         0
RG4         0
RG5         0
RG6         0
RG7         0
RG8         0
RG9         0
RG10        0
RG11        0
RG12        0
RG13        0
RG14        0
RG15        0
RG16        0
RG17        0
RG18        0
RG19        0
RG20        0
RG21        0
RG22        0
RG23        0
RG24        0
RG25        0
RG26        0
RG27        0
RG28        0
RG29        0
RG30        0
RG31        0
RG32        0
RG33        0
RG34        0
RG35        0
RG36        0
RG37        0
RG38        0
RG39        0
RG40        0
RG41        0
RG42        0
RG43        0
RG44        0
RG45        0
RG46        0
RG47        0
RG48        0
RG49        0
RG50        0
RG51        0
RG52        0
RG53        0
RG54        0
RG55        0
RG56        0
RG57        0
RG58        0
RG59        0
RG60        0
RG61        0
RG62        0
RG63        0
RG64        0
RG65        0
RG66        0
RG67        0
RG68        0
RG69        0
RG70        0
RG71        0
RG72        0
RG73        0
RG74        0
RG75        0
RG76        0
RG77        0
RG78        0
RG79        0
RG80        0
RG81        0
RG82        0
RG83        0
RG84        0
RG85        0
RG86        0
RG87        0
RG88        0
RG89        0
RG90        0
RG91        0
RG92        0
RG93        0
RG94        0
RG95        0
RG96        0
RG97        0
RG98        0
RG99        0
RG100       0
```

HMQC data of metabolites 6

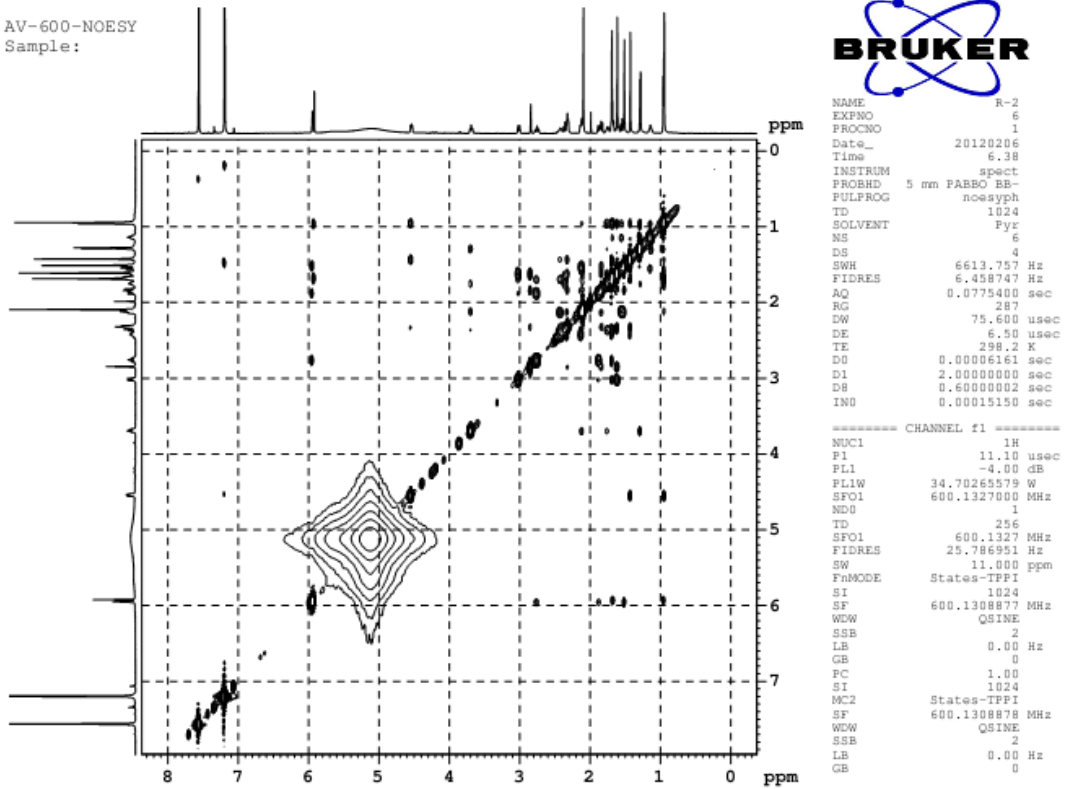
AV-600-HMBC  
Sample:



```
NAME      B-2
EXPNO     1
PROCNO    1
Date_    20120314
Time      10.59
INSTRUM   spect
PROBHD    5 mm QNP1H
PULPROG   zgpg30
TD         65536
SOLVENT   Pyz
NS         14
DS         2
SWH        4413.757 Hz
FIDRES     4.452747 Hz
AQ         0.0775400 sec
RG         24000
DW         75.400 usec
DE         4.50 usec
TE         298.2 K
CHFT2     145.0000000
D0         0.0000000 sec
D1         1.0000000 sec
D2         0.0034428 sec
D3         0.1000000 sec
D4         0.0000000 sec
D5         0.0000000 sec
D6         0.0000000 sec
D7         0.0000000 sec
D8         0.0000000 sec
D9         0.0000000 sec
D10        0.0000000 sec
D11        0.0000000 sec
D12        0.0000000 sec
D13        0.0000000 sec
D14        0.0000000 sec
D15        0.0000000 sec
D16        0.0000000 sec
D17        0.0000000 sec
D18        0.0000000 sec
D19        0.0000000 sec
D20        0.0000000 sec
D21        0.0000000 sec
D22        0.0000000 sec
D23        0.0000000 sec
D24        0.0000000 sec
D25        0.0000000 sec
D26        0.0000000 sec
D27        0.0000000 sec
D28        0.0000000 sec
D29        0.0000000 sec
D30        0.0000000 sec
D31        0.0000000 sec
D32        0.0000000 sec
D33        0.0000000 sec
D34        0.0000000 sec
D35        0.0000000 sec
D36        0.0000000 sec
D37        0.0000000 sec
D38        0.0000000 sec
D39        0.0000000 sec
D40        0.0000000 sec
D41        0.0000000 sec
D42        0.0000000 sec
D43        0.0000000 sec
D44        0.0000000 sec
D45        0.0000000 sec
D46        0.0000000 sec
D47        0.0000000 sec
D48        0.0000000 sec
D49        0.0000000 sec
D50        0.0000000 sec
D51        0.0000000 sec
D52        0.0000000 sec
D53        0.0000000 sec
D54        0.0000000 sec
D55        0.0000000 sec
D56        0.0000000 sec
D57        0.0000000 sec
D58        0.0000000 sec
D59        0.0000000 sec
D60        0.0000000 sec
D61        0.0000000 sec
D62        0.0000000 sec
D63        0.0000000 sec
D64        0.0000000 sec
D65        0.0000000 sec
D66        0.0000000 sec
D67        0.0000000 sec
D68        0.0000000 sec
D69        0.0000000 sec
D70        0.0000000 sec
D71        0.0000000 sec
D72        0.0000000 sec
D73        0.0000000 sec
D74        0.0000000 sec
D75        0.0000000 sec
D76        0.0000000 sec
D77        0.0000000 sec
D78        0.0000000 sec
D79        0.0000000 sec
D80        0.0000000 sec
D81        0.0000000 sec
D82        0.0000000 sec
D83        0.0000000 sec
D84        0.0000000 sec
D85        0.0000000 sec
D86        0.0000000 sec
D87        0.0000000 sec
D88        0.0000000 sec
D89        0.0000000 sec
D90        0.0000000 sec
D91        0.0000000 sec
D92        0.0000000 sec
D93        0.0000000 sec
D94        0.0000000 sec
D95        0.0000000 sec
D96        0.0000000 sec
D97        0.0000000 sec
D98        0.0000000 sec
D99        0.0000000 sec
D100       0.0000000 sec
===== CHANNEL f1 =====
NUC1       13C
P1         11.10 usec
PC         22.20 usec
P2         100.00 usec
P3         1.00 usec
PL1W      34.7024573 W
PL2W      400.1327000 MHz
===== CHANNEL f2 =====
NUC2       1H
P1         1.30 usec
PC         2.80 usec
P2         17.40 usec
P3         90.00 usec
P4         1.00 usec
PL1W      24.10 W
PL2W      500.1360992 MHz
===== GRADIENT CHANNEL =====
GPRAME     SINE.100
GPRAMD     SINE.100
OP1        30.00 %
OP2        30.00 %
OP3        40.10 %
P14        100.00 usec
RG0        2
RG1         0
RG2         0
RG3         0
RG4         0
RG5         0
RG6         0
RG7         0
RG8         0
RG9         0
RG10        0
RG11        0
RG12        0
RG13        0
RG14        0
RG15        0
RG16        0
RG17        0
RG18        0
RG19        0
RG20        0
RG21        0
RG22        0
RG23        0
RG24        0
RG25        0
RG26        0
RG27        0
RG28        0
RG29        0
RG30        0
RG31        0
RG32        0
RG33        0
RG34        0
RG35        0
RG36        0
RG37        0
RG38        0
RG39        0
RG40        0
RG41        0
RG42        0
RG43        0
RG44        0
RG45        0
RG46        0
RG47        0
RG48        0
RG49        0
RG50        0
RG51        0
RG52        0
RG53        0
RG54        0
RG55        0
RG56        0
RG57        0
RG58        0
RG59        0
RG60        0
RG61        0
RG62        0
RG63        0
RG64        0
RG65        0
RG66        0
RG67        0
RG68        0
RG69        0
RG70        0
RG71        0
RG72        0
RG73        0
RG74        0
RG75        0
RG76        0
RG77        0
RG78        0
RG79        0
RG80        0
RG81        0
RG82        0
RG83        0
RG84        0
RG85        0
RG86        0
RG87        0
RG88        0
RG89        0
RG90        0
RG91        0
RG92        0
RG93        0
RG94        0
RG95        0
RG96        0
RG97        0
RG98        0
RG99        0
RG100       0
```

HMBC data of metabolites 6

AV-600-NOESY  
Sample:



```

NAME R-2
EXPNO 6
PROCNO 1
Date_ 20120206
Time 6.38
INSTRUM spect
PROBHD 5 mm F4BBO BB-
PULPROG noesyph
TD 1024
SOLVENT Pyr
NS 6
DS 4
SWH 6613.757 Hz
FIDRES 6.458747 Hz
AQ 0.0775400 sec
RG 287
DW 75.600 usec
DE 6.50 usec
TE 298.2 K
D0 0.00006161 sec
D1 2.00000000 sec
D8 0.60000002 sec
IN0 0.00015150 sec

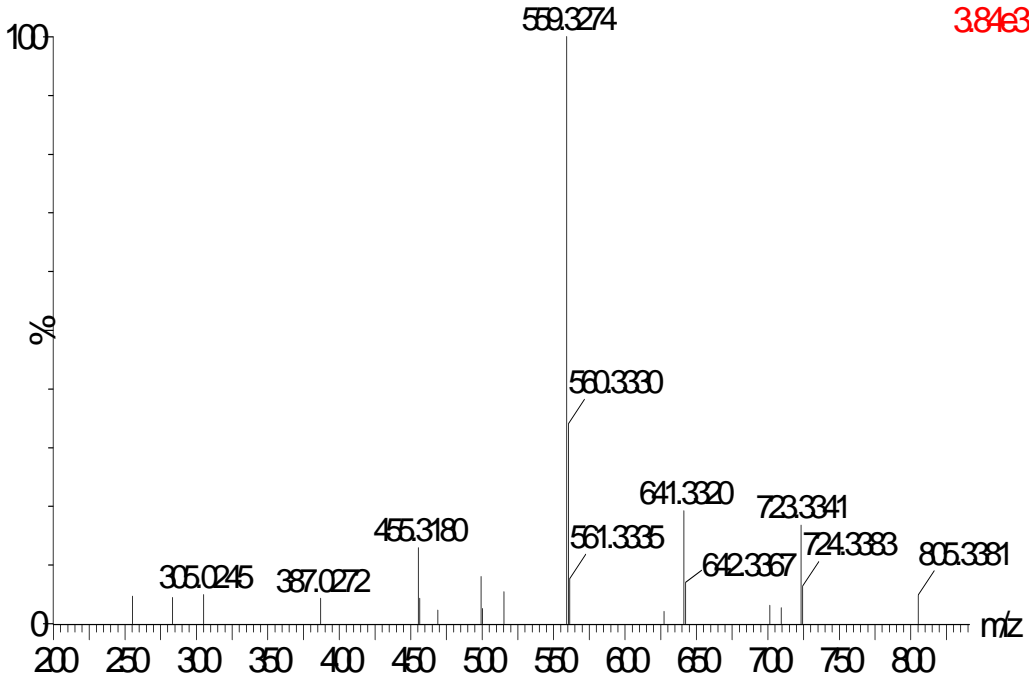
===== CHANNEL f1 =====
NUC1 1H
P1 11.10 usec
PL1 -4.00 dB
PL1W 34.70265579 W
SFO1 600.1327000 MHz
ND0 1
TD 256
SFO1 600.1327 MHz
FIDRES 25.786951 Hz
SW 11.000 ppm
FMODE States-TPPI
SI 1024
SF 600.1308877 MHz
WDB QSIINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPPI
SF 600.1308878 MHz
WDB QSIINE
SSB 2
LB 0.00 Hz
GB 0
  
```

NOESY data of metabolites 6

R1

10:34:57

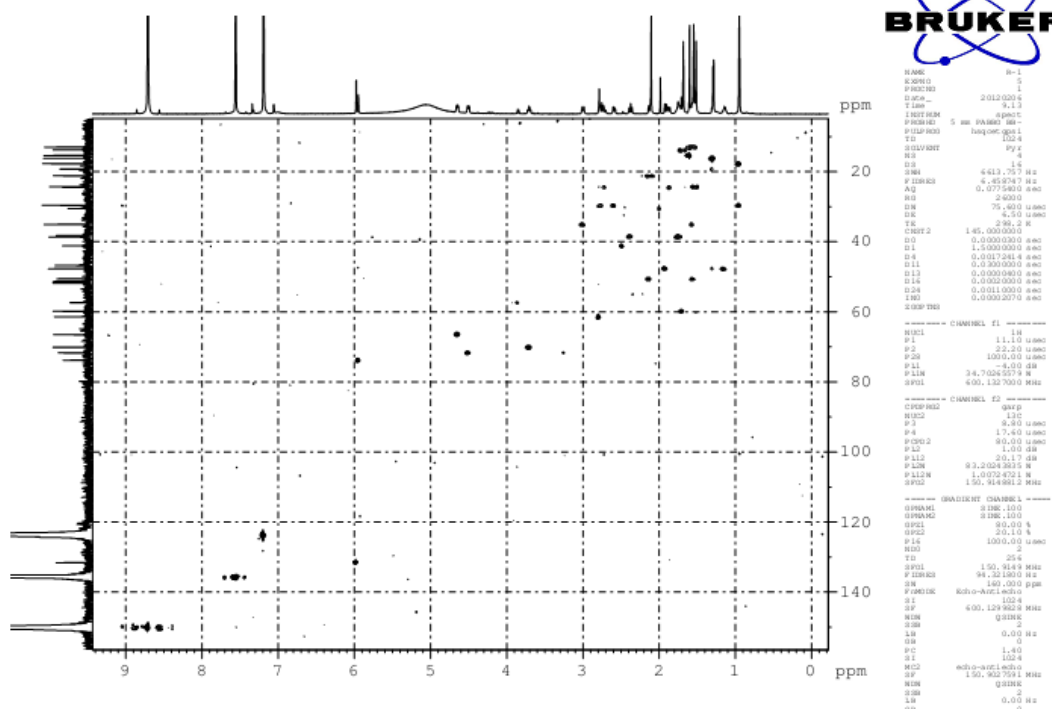
1203281436 (0.670) AM(Cen,2, 80.00, H,5000.0,0.00,1.00); Sm(Mh, 2x1.00); Cm(22.42)



HR-ESI-MS data of metabolites 7

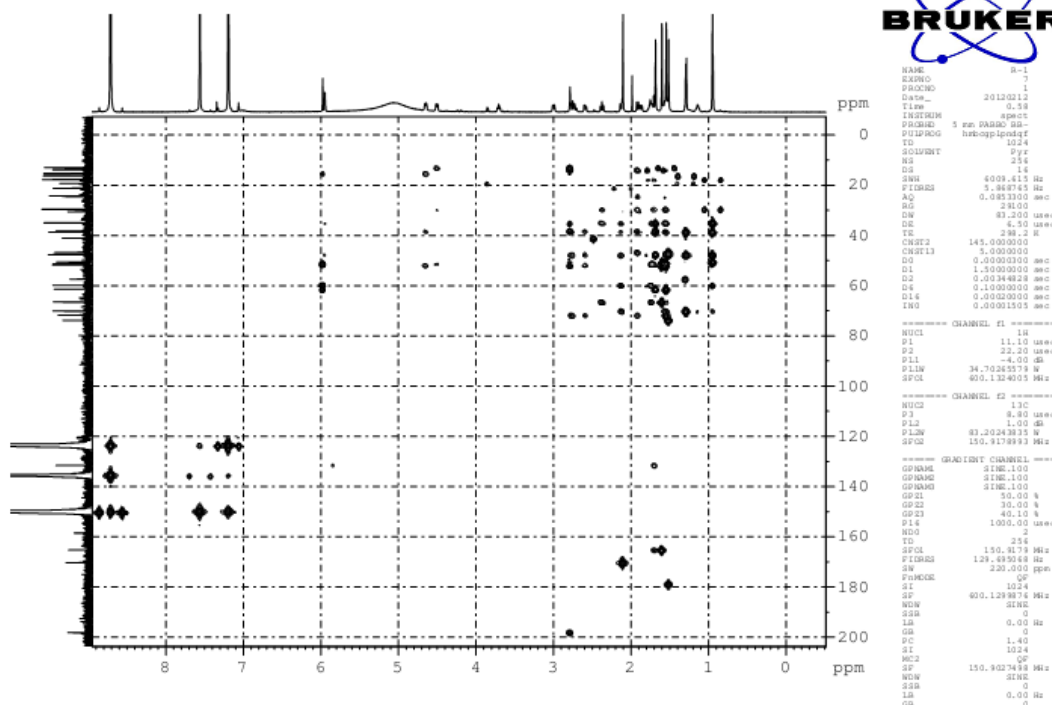


AV-600-HSQC  
Sample:

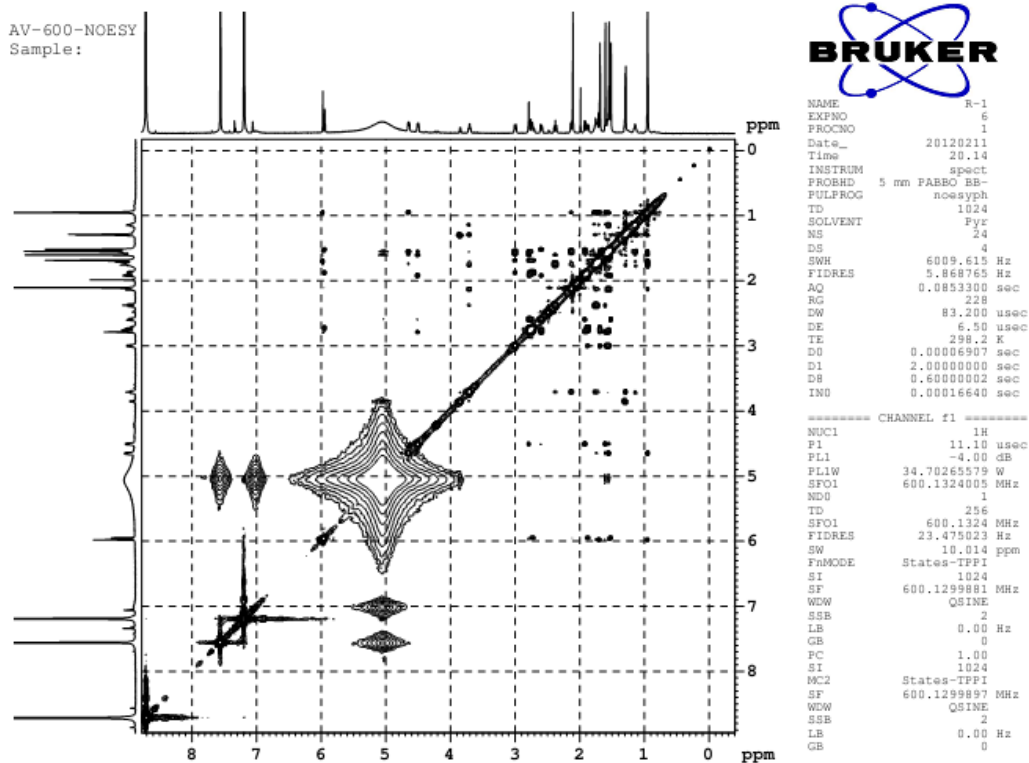


HMQC data of metabolites 7

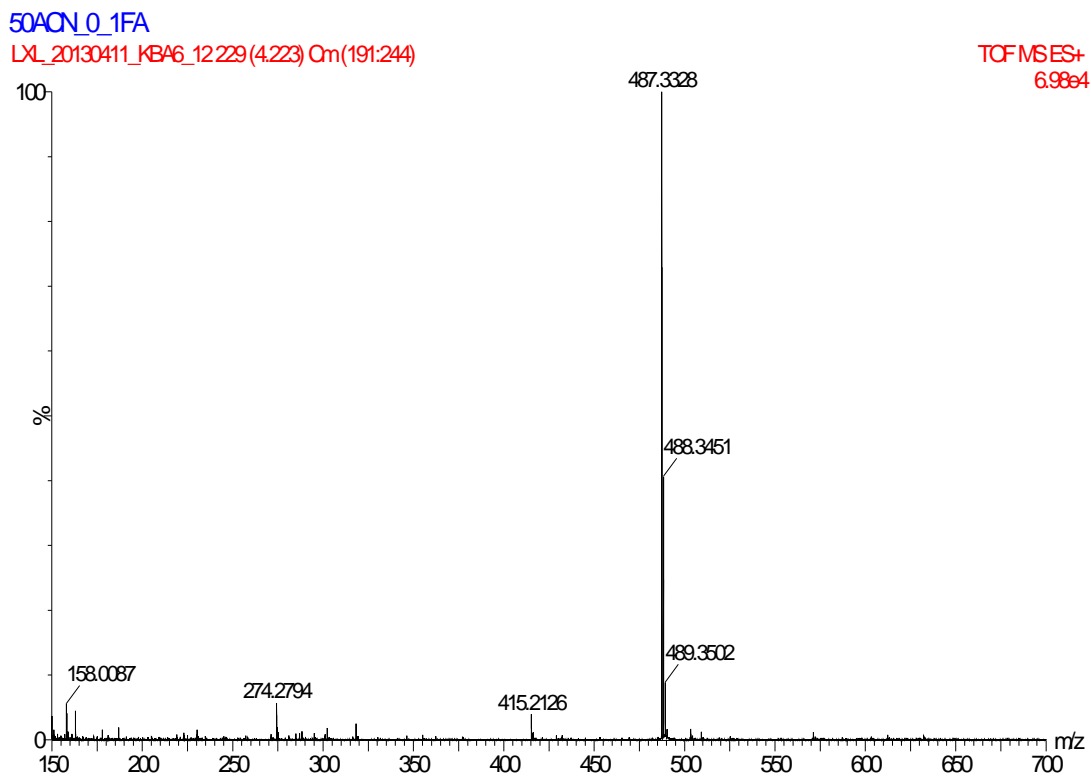
AV-600-HMBC  
Sample:



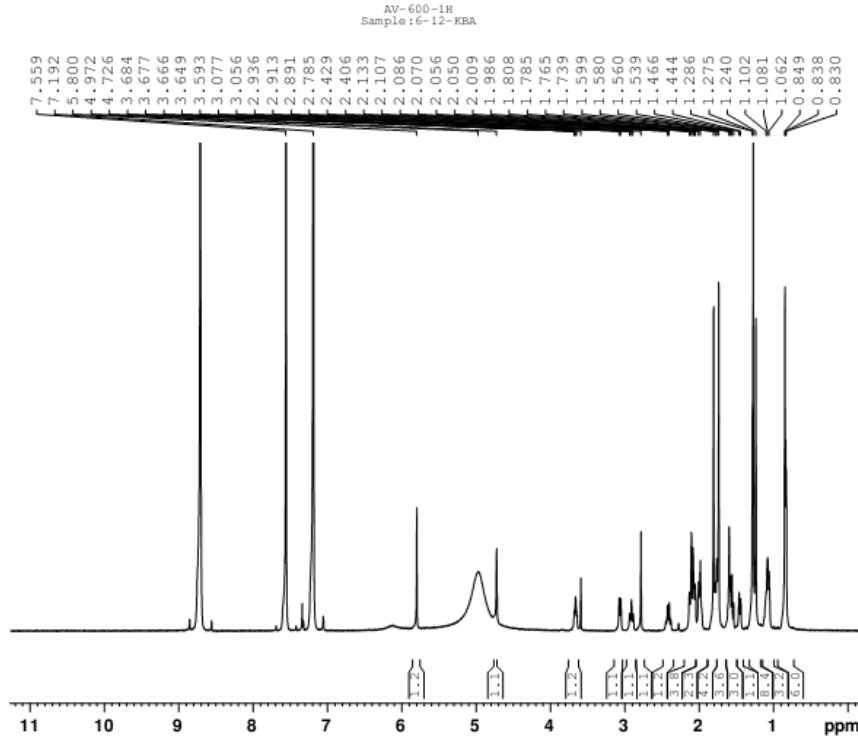
HMBC data of metabolites 7



NOESY data of metabolites 7



HR-ESI-MS data of metabolites 8



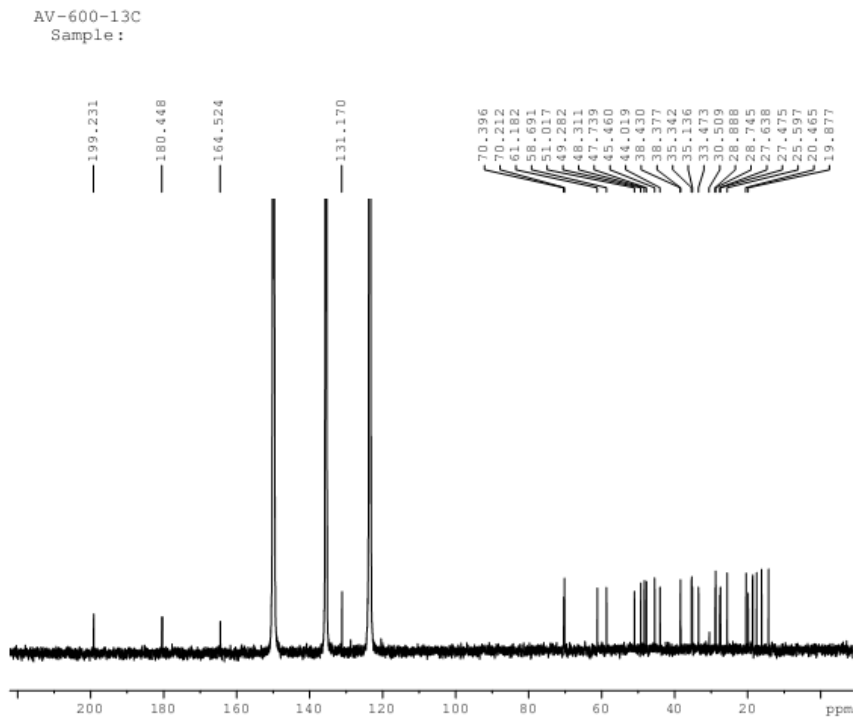
```

NAME          6-12KBA
EXPNO         1
PROCNO        1
Date_         20120503
Time          10.49
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       Pyr
NS            8
DS            2
SWH           12019.230 Hz
FIDRES        0.183399 Hz
AQ            2.7263892 sec
RG            297
DW            41.600 usec
DE            6.50 usec
TE            298.2 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
F1            11.10 usec
PL1           -4.00 dB
PL1W          34.70265579 W
SFO1          600.1341700 MHz
SI            32768
SF            600.1299904 MHz
WVW           EM
SSB           0
LB            0.30 Hz
GB            0
FC            1.00

```

<sup>1</sup>H-NMR data of metabolites 8



```

NAME          6-12KBA
EXPNO         2
PROCNO        1
Date_         20120505
Time          14.25
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       Pyr
NS            6896
DS            2
SWH           45454.547 Hz
FIDRES        0.693581 Hz
AQ            0.7209570 sec
RG            13000
DW            11.000 usec
DE            6.50 usec
TE            298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
F1            6.00 usec
PL1           1.00 dB
PL1W          83.20243835 W
SFO1          150.9178993 MHz

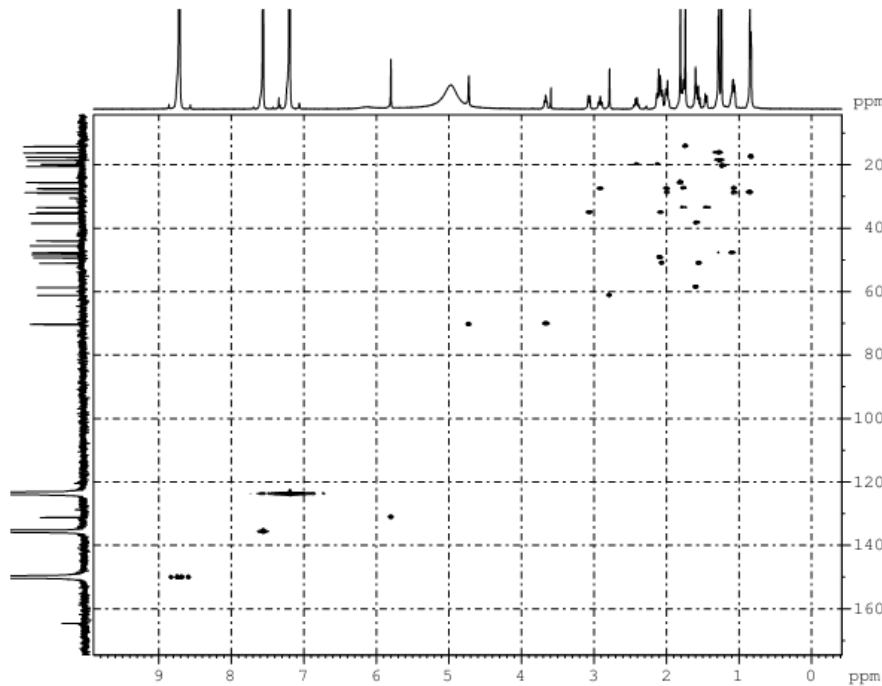
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -4.00 dB
PL12          13.16 dB
PL13          16.00 dB
PL2W          34.70265579 W
PL12W         0.66736388 W
PL13W         0.34702653 W
SFO2          600.1324005 MHz
SI            32768
SF            150.9027684 MHz
WVW           EM
SSB           0
LB            3.00 Hz
GB            0
FC            1.40

```

<sup>13</sup>C-NMR data of metabolites 8



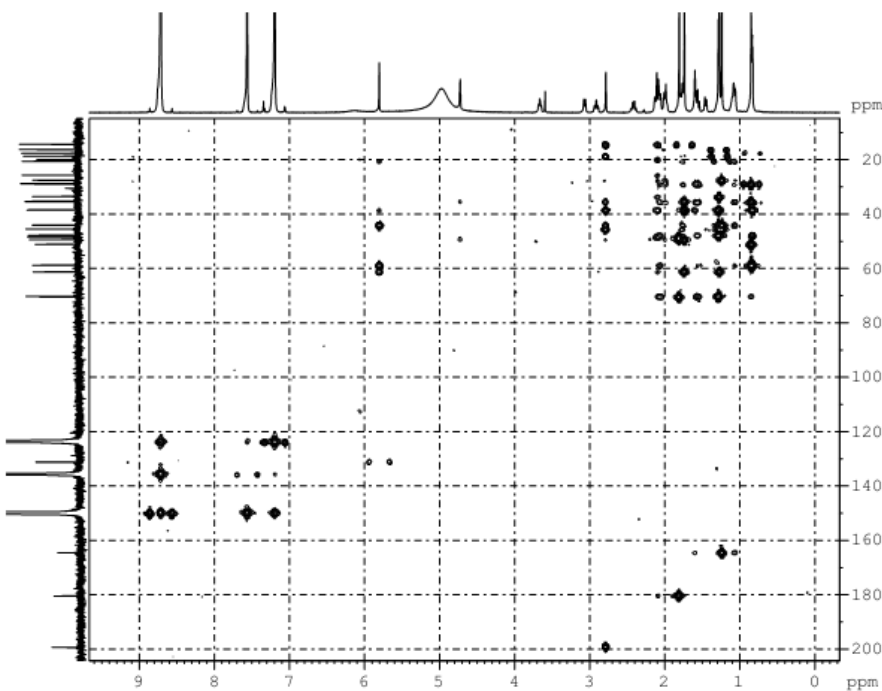
AV-600-HSQC  
Sample:6-12KBA



```
NAME 6-12KBA
EXPNO 2
PROCNO 1
Date_ 20120524
Time 14.15
INSTRUM spect
PROBHD 5 mm QNP1H1
PULPROG zgpg30
TD 1024
SOLVENT Pyz
NS 8
DS 4
SWH 7183.908 Hz
FIDRES 7.215375 Hz
AQ 0.0713900 sec
RG 25100
DE 6.50 usec
TE 298.2 K
CMT2 145.000000 sec
DO 0.0000000 sec
D1 1.5000000 sec
D11 0.0017484 sec
D12 0.0300000 sec
D13 0.0000000 sec
D14 0.0020000 sec
D15 0.0011000 sec
D16 0.0001940 sec
===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
P2 22.20 usec
PL1 -4.00 dB
PL2 19.00 dB
PLW 34.7024315 W
SFO1 600.1330006 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 8.80 usec
P4 17.40 usec
PCPD2 90.00 usec
P5 1.00 dB
PL3 20.17 dB
PLW 83.2024315 W
PLW2 1.0024211 W
SFO2 150.9149813 MHz
===== GRADIENT CHANNEL =====
GDPRG1 SINE.100
GDPRG2 SINE.100
GDPRG3 SINE.100
OP1 50.00 %
OP2 30.00 %
OP3 40.10 %
P15 1000.00 usec
RG 256
TD 256
SFO1 150.9149813 MHz
FIDRES 70.3400000 Hz
SW 180.000 ppm
F1F2 waltz16
SI 1024
SF 600.1330006 MHz
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 0
SFO 150.9020018 MHz
WDW 0
SSB 0
LA 0.00 Hz
GB 0
```

HMOC data of metabolites 8

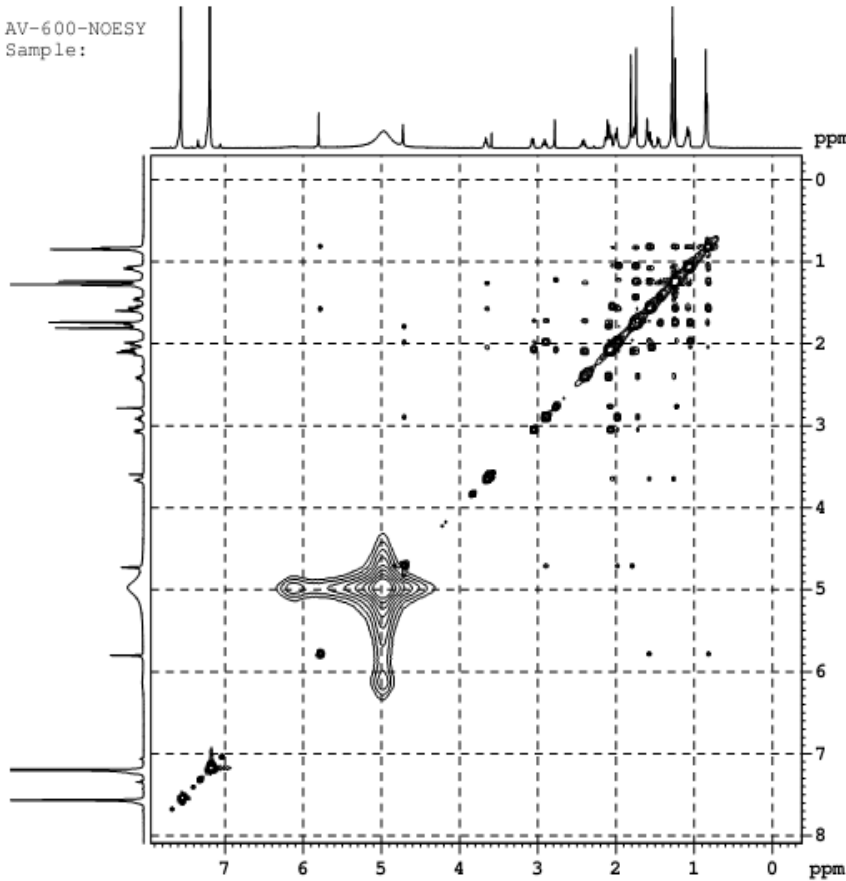
AV-600-HMBC  
Sample:6-12KBA



```
NAME 6-12KBA
EXPNO 2
PROCNO 1
Date_ 20120524
Time 22.20
INSTRUM spect
PROBHD 5 mm QNP1H1
PULPROG zgpg30
TD 1024
SOLVENT Pyz
NS 8
DS 4
SWH 7183.908 Hz
FIDRES 7.215375 Hz
AQ 0.0713900 sec
RG 25100
DE 6.50 usec
TE 298.2 K
CMT2 145.000000 sec
DO 0.0000000 sec
D1 1.5000000 sec
D11 0.0014488 sec
D12 0.1000000 sec
D13 0.0020000 sec
D14 0.0001940 sec
===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
P2 22.20 usec
PL1 -4.00 dB
PL2 19.00 dB
PLW 34.7024315 W
SFO1 600.1330006 MHz
===== CHANNEL f2 =====
NUC2 1H
P3 8.80 usec
P4 17.40 usec
PL3 20.17 dB
PLW 83.2024315 W
PLW2 1.0024211 MHz
SFO2 150.9149813 MHz
===== GRADIENT CHANNEL =====
GDPRG1 SINE.100
GDPRG2 SINE.100
GDPRG3 SINE.100
OP1 50.00 %
OP2 30.00 %
OP3 40.10 %
P15 1000.00 usec
RG 256
TD 256
SFO1 150.9149813 MHz
FIDRES 139.494365 Hz
SW 220.000 ppm
F1F2 waltz16
SI 1024
SF 600.1330006 MHz
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 0
SFO 150.9020018 MHz
WDW 0
SSB 0
LA 0.00 Hz
GB 0
```

HMBC data of metabolites 8

AV-600-NOESY  
Sample:



```
NAME 6-12KBA
EXPNO 6
PROCNO 1
Date_ 20120524
Time 17.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesyph
TD 1024
SOLVENT Pyr
NS 4
DS 4
SWH 7183.908 Hz
FIDRES 7.015535 Hz
AQ 0.0713900 sec
RG 128
DW 69.600 usec
DE 6.50 usec
TE 298.2 K
D0 0.00005547 sec
D1 2.00000000 sec
D8 0.60000002 sec
IND 0.00013920 sec
```

```
===== CHANNEL f1 =====
NUC1 1H
P1 11.10 usec
PL1 -4.00 dB
PLLW 34.70265579 W
SFO1 600.1330006 MHz
ND0 1
TD 256
SFO1 600.133 MHz
FIDRES 28.062078 Hz
SW 11.970 ppm
FRMODE States-TPPI
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPPI
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
```

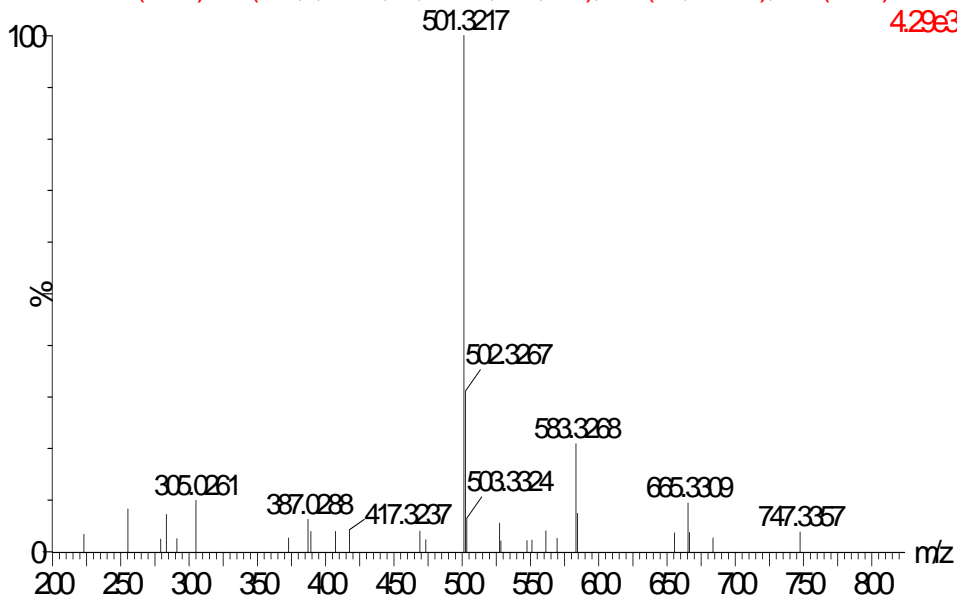
NOESY data of metabolites 8

**KBA6-32**

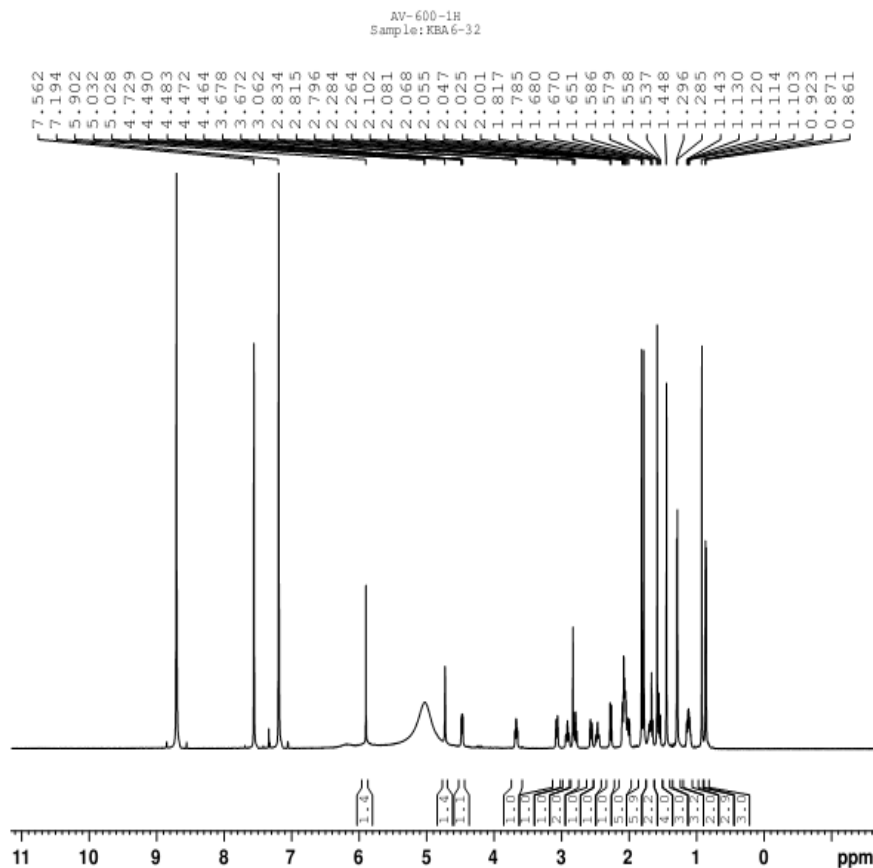
**09:53:28**

12032808 14 (0.260) AM(Cen,2, 80.00, H,5000,0,0,0,1.00); Sm(Mh, 2x1.00); Cm(12.31)

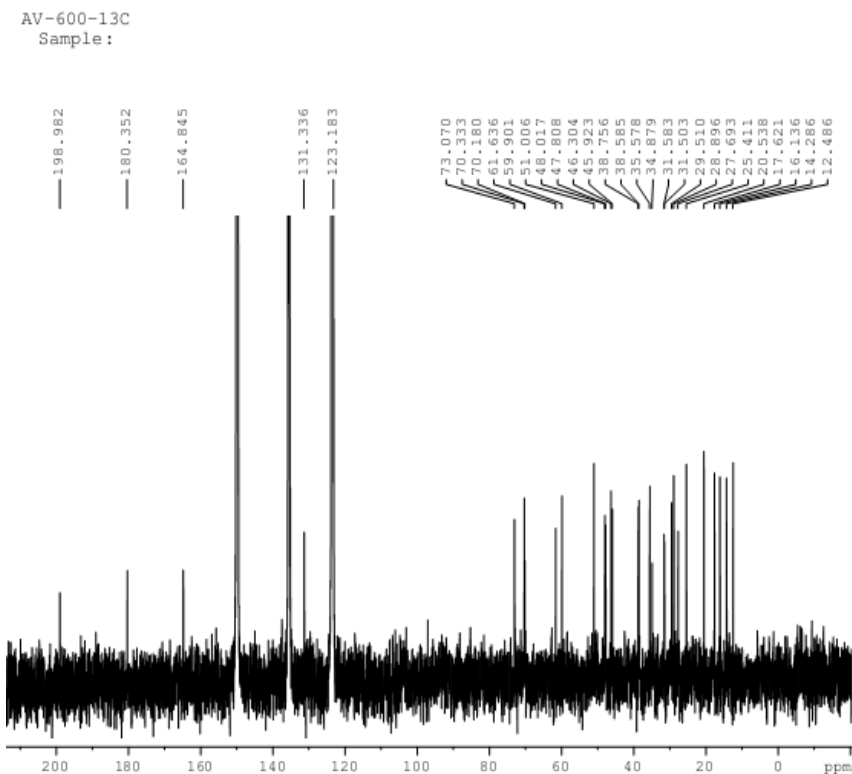
4.29e3



HR-ESI-MS data of metabolites 9

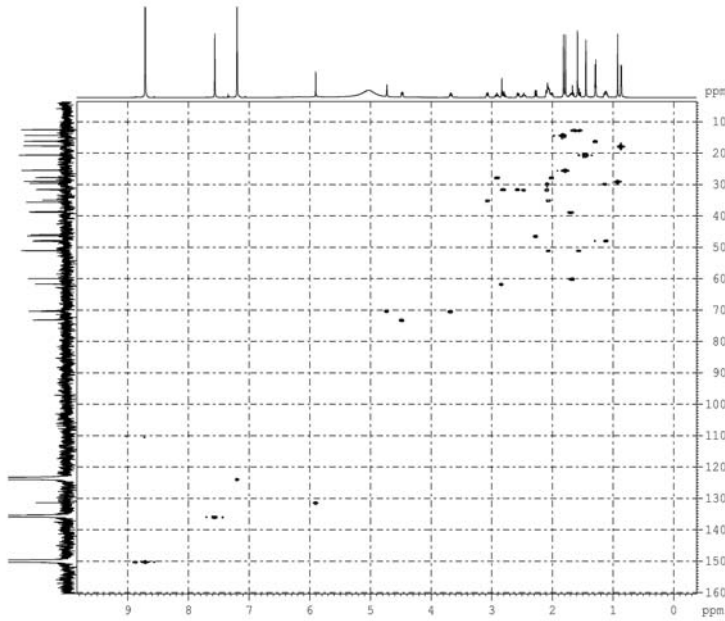


<sup>1</sup>H-NMR data of metabolites 9



<sup>13</sup>C-NMR data of metabolites 9

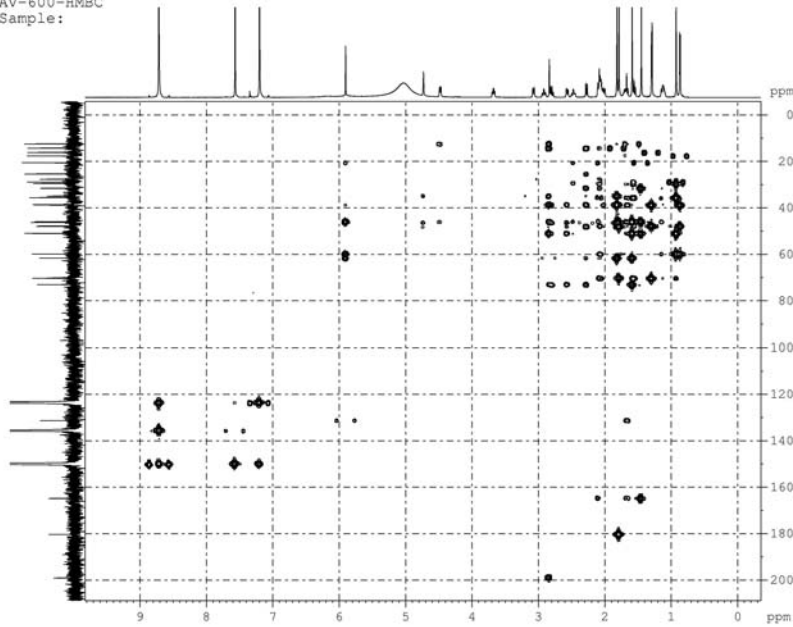
AV-600-HSQC  
Sample:



```
NAME K3AA-12
EXPNO 1
PROCNO 1
Date_ 20120117
Time 9.43
INSTRUM spect
PROBHD 5 mm ZAGX001
PULPROG zgpg30
TD 65536
SOLVENT H2O
NS 16
DS 4
SWH 7183.408 Hz
FIDRES 7.01533 Hz
AQ 0.0713900 sec
RG 24000
AQ 49.400 usec
DE 6.50 usec
TE 298.2 K
CNS1 145.000000 sec
D1 0.0000000 sec
D2 1.5000000 sec
D3 0.0012414 sec
D4 0.0000000 sec
D5 0.0000000 sec
D6 0.0000000 sec
D7 0.0011000 sec
IND 0.0000000 sec
SFO100
===== CHANNEL F1 =====
NUC1 13C
P1 11.10 usec
PL1 22.00 dB
PL2 1900.00 usec
PL3 34.7024378 W
PL4 400.130000 MHz
===== CHANNEL F2 =====
NUC2 1H
P2 8.80 usec
PL2 17.40 dB
PL3 90.00 usec
PL4 1.00 dB
PL5 201.140 W
PL6 83.2024383 W
PL7 150.9148812 MHz
===== GRADIENT CHANNEL =====
GPMAX1 8190.100
GPMAX2 8190.100
GPD1 50.00 %
GPD2 30.00 %
GPD3 40.10 %
P14 1000.00 usec
NS0 2
TD 324
SFO1 150.9149 MHz
FIDRES 47.48139 Hz
SW 240.000 ppm
FWDI 800-Axis1
SI 1024
SF 400.130000 MHz
MCW 8190
GB 0
GB 0.00 Hz
PC 1.40
SI 1024
SF 150.9149 MHz
MCW 8190
GB 0
GB 0.00 Hz
```

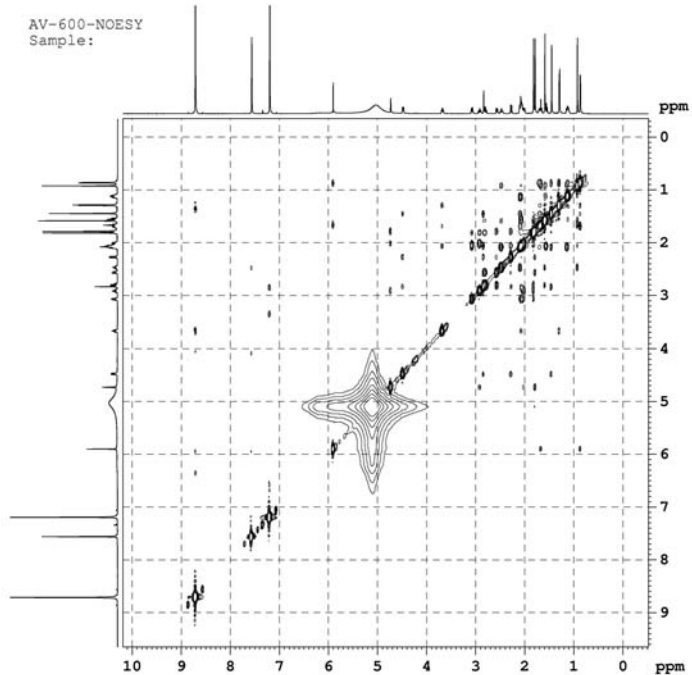
HMQC data of metabolites 9

AV-600-HMBC  
Sample:



```
NAME K3AA-12
EXPNO 1
PROCNO 1
Date_ 20120117
Time 10.87
INSTRUM spect
PROBHD 5 mm ZAGX001
PULPROG zgpg30
TD 65536
SOLVENT H2O
NS 16
DS 4
SWH 7183.408 Hz
FIDRES 7.01533 Hz
AQ 0.0713900 sec
RG 24000
AQ 49.400 usec
DE 6.50 usec
TE 298.2 K
CNS1 145.000000 sec
D1 0.0000000 sec
D2 1.5000000 sec
D3 0.0012414 sec
D4 0.0000000 sec
D5 0.0000000 sec
D6 0.0000000 sec
D7 0.0011000 sec
IND 0.0000000 sec
SFO100
===== CHANNEL F1 =====
NUC1 13C
P1 11.10 usec
PL1 22.00 dB
PL2 1900.00 usec
PL3 34.7024378 W
PL4 400.130000 MHz
===== CHANNEL F2 =====
NUC2 1H
P2 8.80 usec
PL2 17.40 dB
PL3 90.00 usec
PL4 1.00 dB
PL5 201.140 W
PL6 83.2024383 W
PL7 150.9148812 MHz
===== GRADIENT CHANNEL =====
GPMAX1 8190.100
GPMAX2 8190.100
GPD1 50.00 %
GPD2 30.00 %
GPD3 40.10 %
P14 1000.00 usec
NS0 2
TD 324
SFO1 150.9149 MHz
FIDRES 47.48139 Hz
SW 240.000 ppm
FWDI 800-Axis1
SI 1024
SF 400.130000 MHz
MCW 8190
GB 0
GB 0.00 Hz
PC 1.40
SI 1024
SF 150.9149 MHz
MCW 8190
GB 0
GB 0.00 Hz
```

HMBC data of metabolites 9



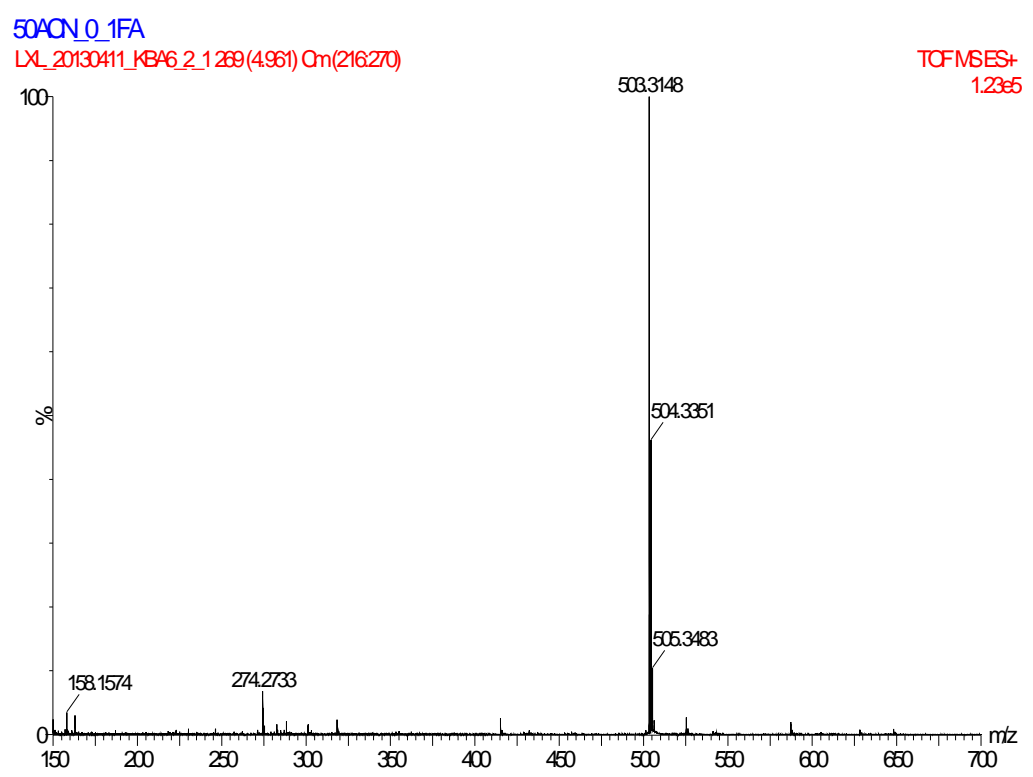
```

NAME      KBA6-32
EXPNO    7
PROCNO   1
Date_    20120117
Time     8.59
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  noesyph
TD       1024
SOLVENT  Pyr
NS       4
DS       4
SWH      7183.908 Hz
FIDRES   7.015535 Hz
AQ       0.0713900 sec
RG       80.6
DW       69.600 usec
DE       6.50 usec
TE       298.2 K
DO       0.00005510 sec
D1       2.00000000 sec
D8       0.60000002 sec
IND      0.00013885 sec

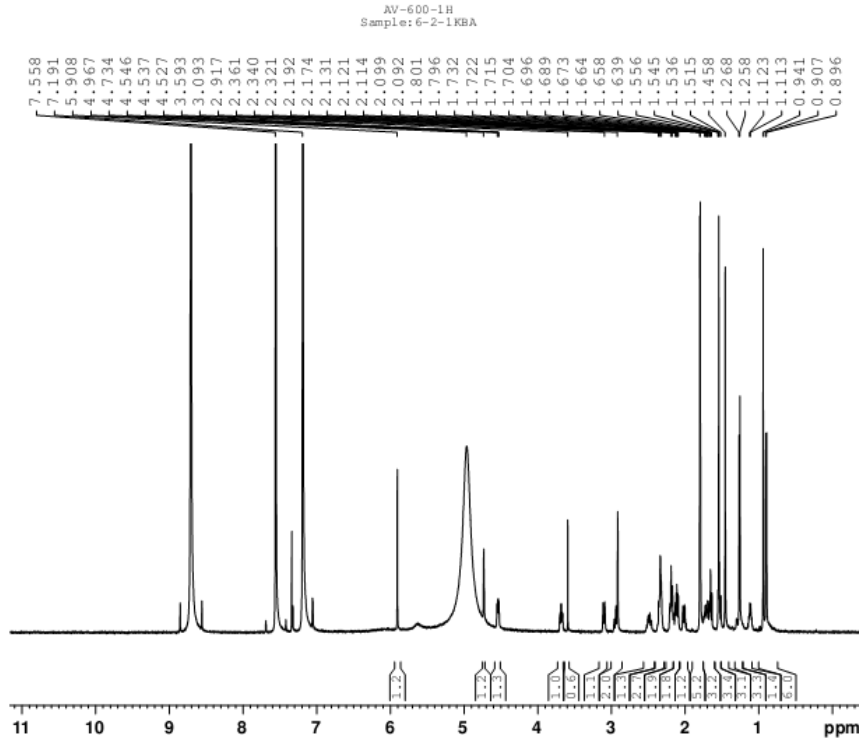
===== CHANNEL f1 =====
NUC1     1H
P1       11.10 usec
PL1     -4.00 dB
PL1W    34.70265579 W
SFO1    600.1330000 MHz
ND0     1
TD      256
SFO1    600.133 MHz
FIDRES   28.131235 Hz
SW      12.000 ppm
FeMODE   States-TPPI
SI       1024
SF      600.1299852 MHz
WDW      QSINE
SSB      2
LB       0.00 Hz
GB       0
PC       1.00
SI       1024
MC2     States-TPPI
SF      600.1299875 MHz
WDW      QSINE
SSB      2
LB       0.00 Hz
GB       0

```

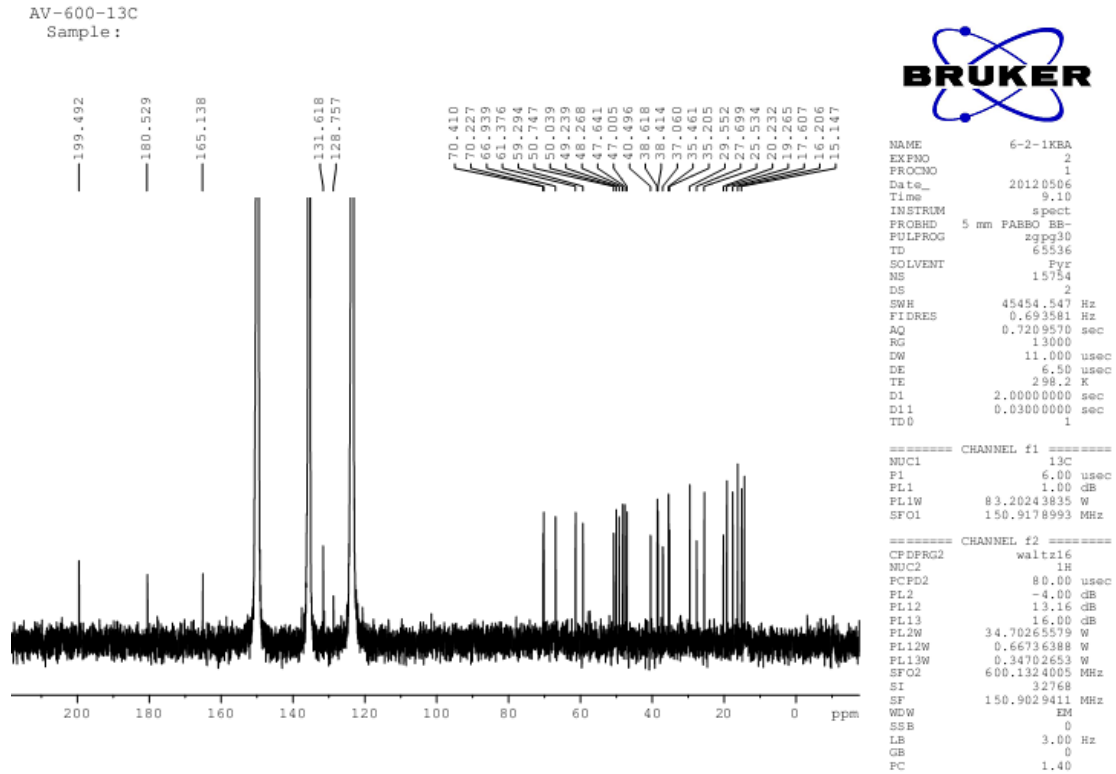
NOESY data of metabolites 9



HR-ESI-MS data of metabolites 10

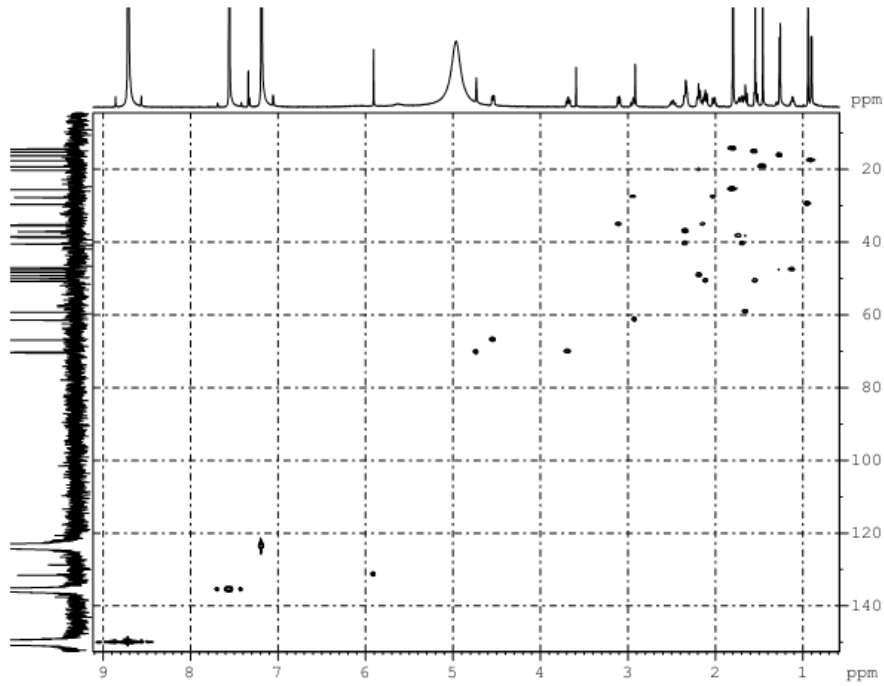


<sup>1</sup>H-NMR data of metabolites **10**



<sup>13</sup>C-NMR data of metabolites **10**

AV-600-HSQC  
Sample:6-2-1-KAB

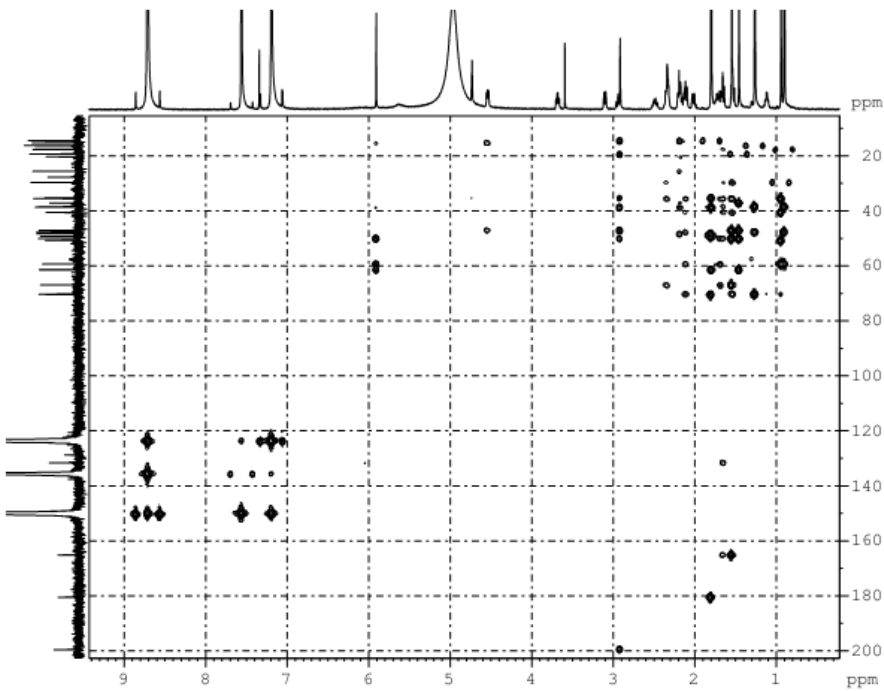


```

NAME      6-2-100A
EXPNO     1
PROCNO    1
Date_     20120524
Time      18.40
INSTRUM   spect
PROBHD    5 mm QNP90 1H-
PULPROG   zgpg30
TD         65536
SOLVENT   DMS
NS         16
DS         4
SWH        6009.415 Hz
F2 (MHz)  150.914813 Hz
AQ         0.0853300 sec
RG         26000
DE         81.200 usec
TE         298.2 K
CHFT2     145.000000 sec
D1         0.0000000 sec
D2         1.5000000 sec
D4         0.00172414 sec
D13        0.0000000 sec
D14        0.0000000 sec
D24        0.0010000 sec
TAD        0.0002070 sec
===== CHANNEL f1 =====
NUC1       13C
P1         11.10 usec
P2         22.20 usec
P12        1.00 dB
P13        4.00 dB
P14        34.70245779 Hz
SFO1       600.1330006 MHz
===== CHANNEL f2 =====
NUC2       1H
P1         8.80 usec
P2         17.60 usec
P12        1.00 dB
P13        20.17 dB
P14        81.20245779 Hz
SFO2       400.1464000 MHz
===== GRADIENT CHANNEL =====
GRHM1      SINC.100
GRHM2      SINC.100
GRHM3      SINC.100
GSP1       30.00 Hz
GSP2       30.00 Hz
GSP3       40.10 Hz
P14        1000.00 usec
WDW         2
TE         298.2 K
SFO1       150.914813 Hz
F2 (MHz)  150.914813 Hz
SW         140.000 ppm
PULPROG   zgpg30
SF         600.1330006 MHz
SI         1024
WDW        SINC
SSB        0
LB         0.00 Hz
GB         0
PC         1.40
SFO        150.9077563 MHz
SF         600.1330006 MHz
WDW        SINC
SSB        0
LB         0.00 Hz
GB         0
  
```

HMQC data of metabolites 10

AV-600-HMBC  
Sample:6-2-1-KAB

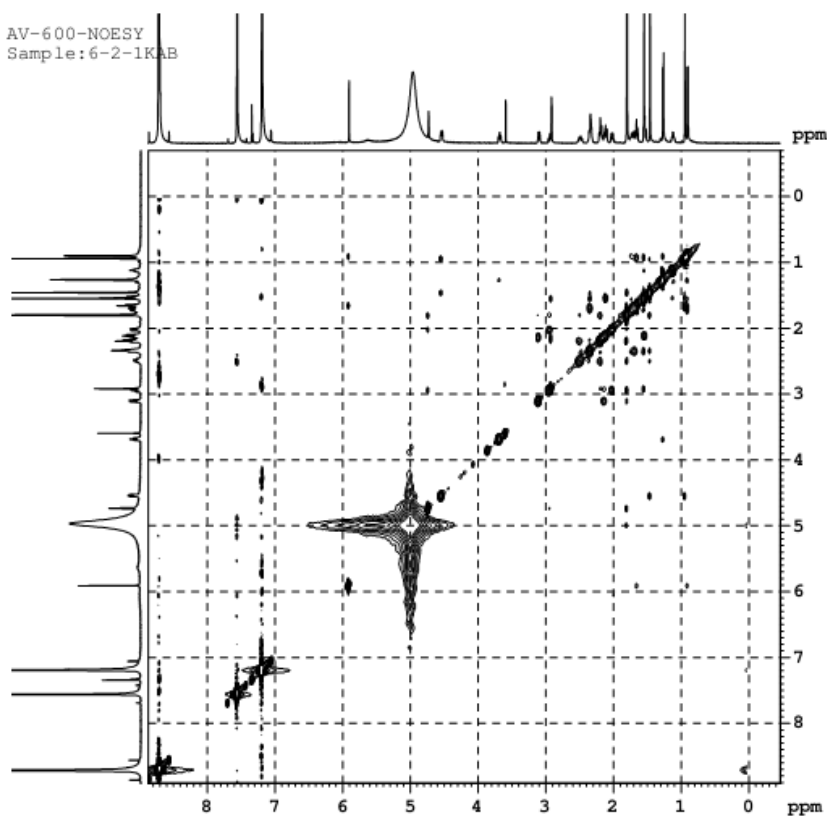


```

NAME      6-2-100A
EXPNO     1
PROCNO    1
Date_     20120524
Time      21.34
INSTRUM   spect
PROBHD    5 mm QNP90 1H-
PULPROG   zgpg30
TD         65536
SOLVENT   DMS
NS         16
DS         4
SWH        6009.415 Hz
F2 (MHz)  150.914813 Hz
AQ         0.0853300 sec
RG         26000
DE         81.200 usec
TE         298.2 K
CHFT2     145.000000 sec
CHFT13    5.0000000 sec
D1         0.0000000 sec
D2         1.5000000 sec
D4         0.00172414 sec
D13        0.0000000 sec
D14        0.0002000 sec
TAD        0.0002000 sec
===== CHANNEL f1 =====
NUC1       13C
P1         11.10 usec
P2         22.20 usec
P12        1.00 dB
P13        4.00 dB
P14        34.70245779 Hz
SFO1       600.1330006 MHz
===== CHANNEL f2 =====
NUC2       1H
P1         8.80 usec
P2         17.60 usec
P12        1.00 dB
P13        20.17 dB
P14        81.20245779 Hz
SFO2       400.1464000 MHz
===== GRADIENT CHANNEL =====
GRHM1      SINC.100
GRHM2      SINC.100
GRHM3      SINC.100
GSP1       30.00 Hz
GSP2       30.00 Hz
GSP3       40.10 Hz
P14        1000.00 usec
WDW         2
TE         298.2 K
SFO1       150.914813 Hz
F2 (MHz)  150.914813 Hz
SW         140.000 ppm
PULPROG   zgpg30
SF         600.1330006 MHz
SI         1024
WDW        SINC
SSB        0
LB         0.00 Hz
GB         0
PC         1.40
SFO        150.9077563 MHz
SF         600.1330006 MHz
WDW        SINC
SSB        0
LB         0.00 Hz
GB         0
  
```

HMBC data of metabolites 10

AV-600-NOESY  
Sample: 6-2-1KAB



```

NAME          6-2-1KBA
EXPNO         6
PROCNO        1
Date_         20120526
Time          18.53
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       noesyph
TD            1024
SOLVENT       Fyr
NS            4
DS            4
SWH           6009.615 Hz
FIDRES        5.868765 Hz
AQ            0.0853300 sec
RG            406
DW            83.200 usec
DE            6.50 usec
TE            298.2 K
D0            0.00006907 sec
D1            2.00000000 sec
D8            0.60000002 sec
IN0           0.00016640 sec

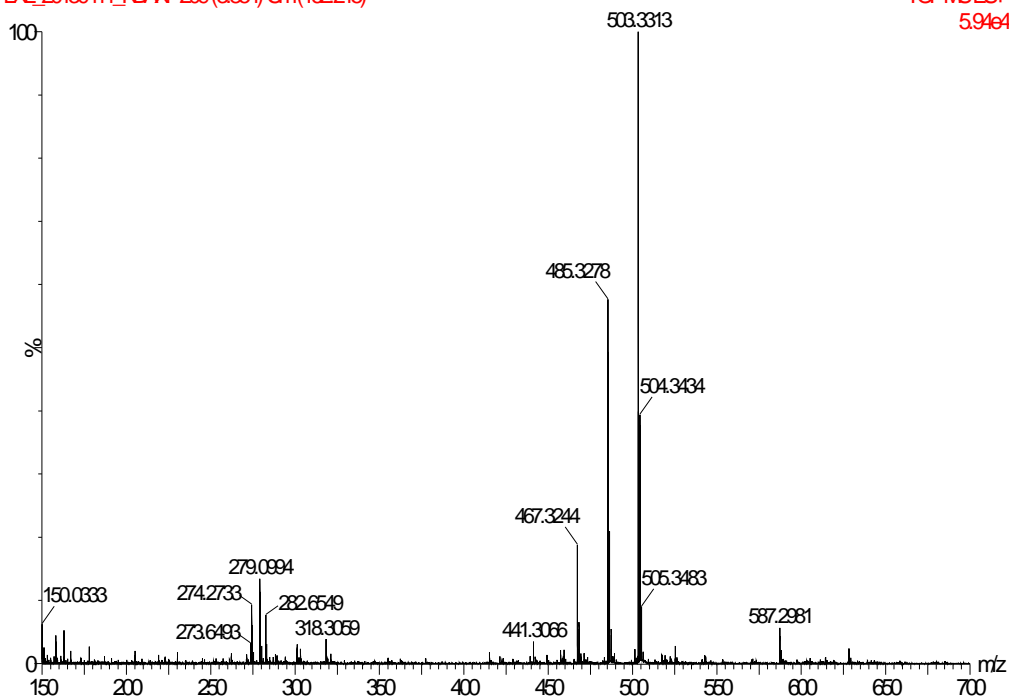
===== CHANNEL f1 =====
NUC1          1H
P1            11.10 usec
PL1           -4.00 dB
PL1W         34.70265579 W
SFO1         600.1330006 MHz
ND0           1
TD            256
SFO1         600.133 MHz
FIDRES        23.475046 Hz
SW            10.014 ppm
PRMODE        States-TFPI
SI            1024
SF            600.1299874 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
SI            1024
MC2           States-TFPI
SF            600.1299869 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
  
```

NOESY data of metabolites **10**

50ACN\_0\_1FA

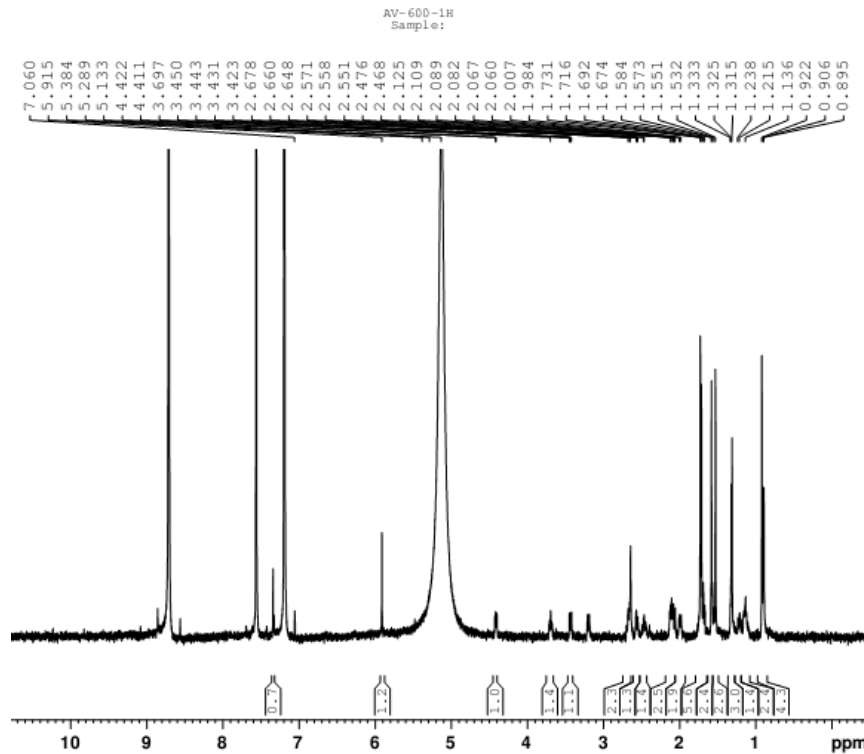
LXL\_20130411\_KBAXF209(3.854)Om(162215)

TCFMSES+  
5.9464



HR-ESI-MS data of metabolites **11**



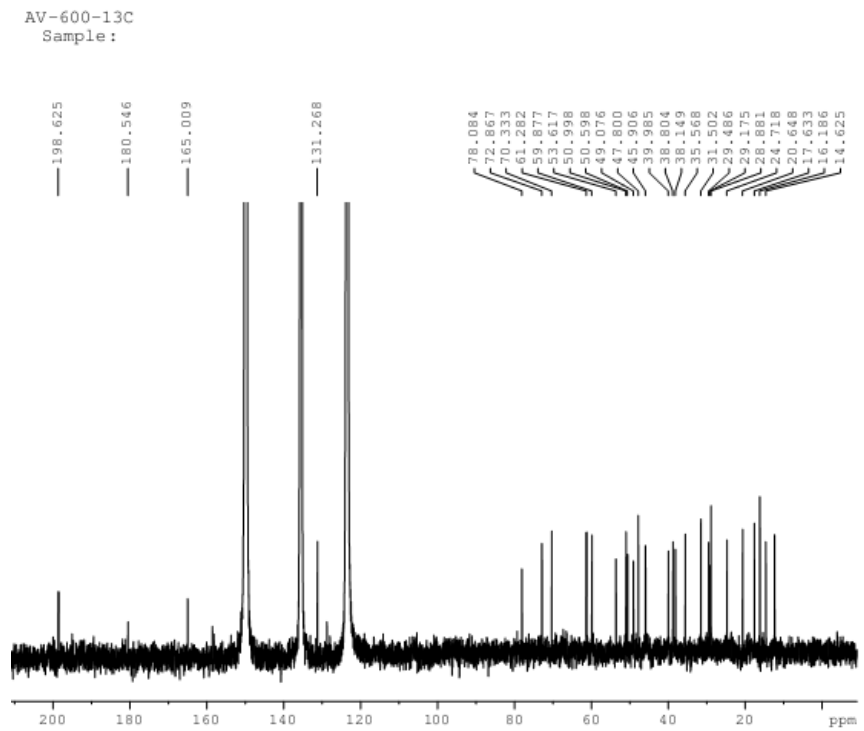


```

NAME           KBAXF
EXPNO          1
PROCNO        1
Date_         20120806
Time          18.19
INSTRUM       spect
PROBHD        5 mm FAPBO BB-
PULPROG       zg30
TD            65536
SOLVENT       Pyr
NS            8
DS            2
SWH           13227.514 Hz
FIDRES        0.201836 Hz
AQ            2.4773486 sec
RG            3.2
DW            37.800 usec
DE            6.50 usec
TE            296.5 K
D1            1.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1           1H
P1             11.10 usec
PL1            -4.00 dB
PL1W           34.70265579 W
SFO1           600.1330006 MHz
SI             32768
SF             600.1299899 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB             0
PC             1.00
  
```



```

NAME           KBAXF
EXPNO          2
PROCNO        1
Date_         20120806
Time          18.23
INSTRUM       spect
PROBHD        5 mm FAPBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       Pyr
NS            18389
DS            2
SWH           45454.547 Hz
FIDRES        0.693581 Hz
AQ            0.7209570 sec
RG            14600
DW            11.000 usec
DE            6.50 usec
TE            296.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
```

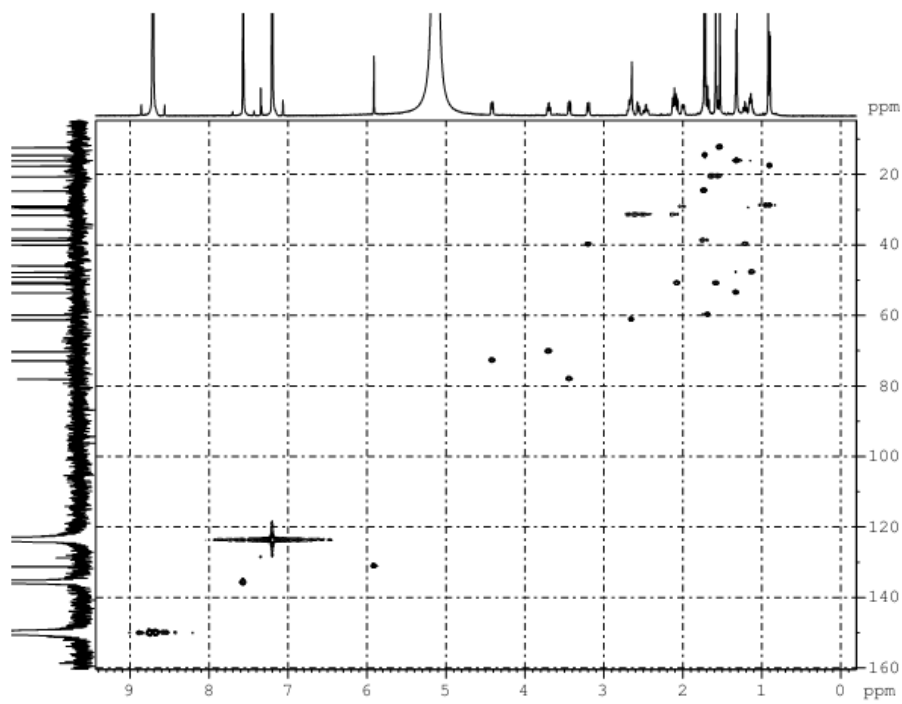
```

===== CHANNEL f1 =====
NUC1           13C
P1             6.00 usec
PL1            1.00 dB
PL1W           83.20243835 W
SFO1           150.9178993 MHz
  
```

```

===== CHANNEL f2 =====
CFDPRG2       waltr16
NUC2           1H
PCPD2         80.00 usec
PL2            -4.00 dB
PL12          13.16 dB
PL13          16.00 dB
PL2W           34.70265579 W
PL12W         0.66736388 W
PL13W         0.34702653 W
SFO2           600.1324005 MHz
SI             32768
SF             150.9027676 MHz
WDW            EM
SSB            0
LB             3.00 Hz
GB             0
PC             1.40
  
```

AV-600-HSQC  
Sample:

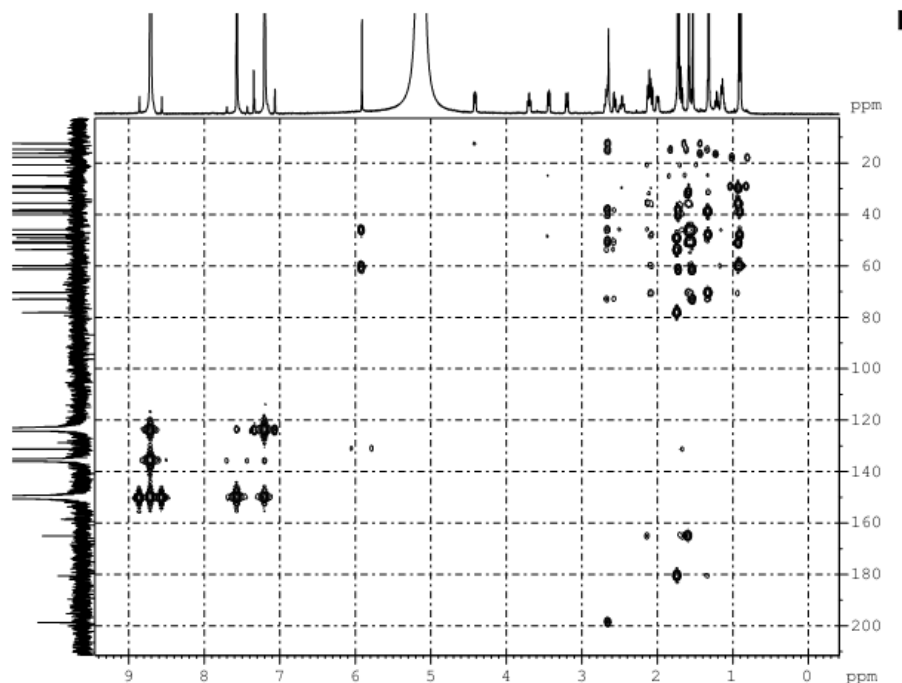


```

NAME          HSQC2
EXPNO         7
PROCNO        1
Date_         20120818
Time          12:48
INSTRUM       spect
PROBHD        5 mm PABBO MM-
PULPROG       zgpg30p1
TD            1024
SOLVENT       Pyz
NS            12
DS            14
FIDRES        7183.908 Hz
AQ            0.0713900 sec
RG            25000
CW            69.600 usec
DE            4.50 usec
TE            294.5 K
===== CHANNEL f1 =====
NUC1          13C
P1            11.10 usec
P2            22.20 usec
P3            22.20 usec
P4            17.40 usec
P5            24.7024579 Hz
P6            400.133608 MHz
===== CHANNEL f2 =====
CPDPRG2       zgpg30
NUC2          1H
P7            8.80 usec
P8            17.40 usec
P9            80.00 usec
P10           1.00 usec
P11           20.17 dB
P12           97.2024925 Hz
P13           1.0024925 Hz
P14           150.9143903 MHz
===== GRADIENT CHANNEL =====
GPMAG1        SINE.100
GPMAG2        SINE.100
GPD1          50.00 %
GPD2          30.00 %
GPD3          40.10 %
GPD4          1000.00 usec
ND0           2
TD            654
SFO1          150.9194 MHz
FIDRES        104.111091 Hz
AQ            150.000 usec
P1PROG        Echo-AntiEcho
SI            0
SF            600.1306467 MHz
WDW           EM
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           Echo-AntiEcho
SF            150.9029219 MHz
WDW           EM
SSB           2
LB            0.00 Hz
GB            0
  
```

HMQC data of metabolites 11

AV-600-HMBC  
Sample:

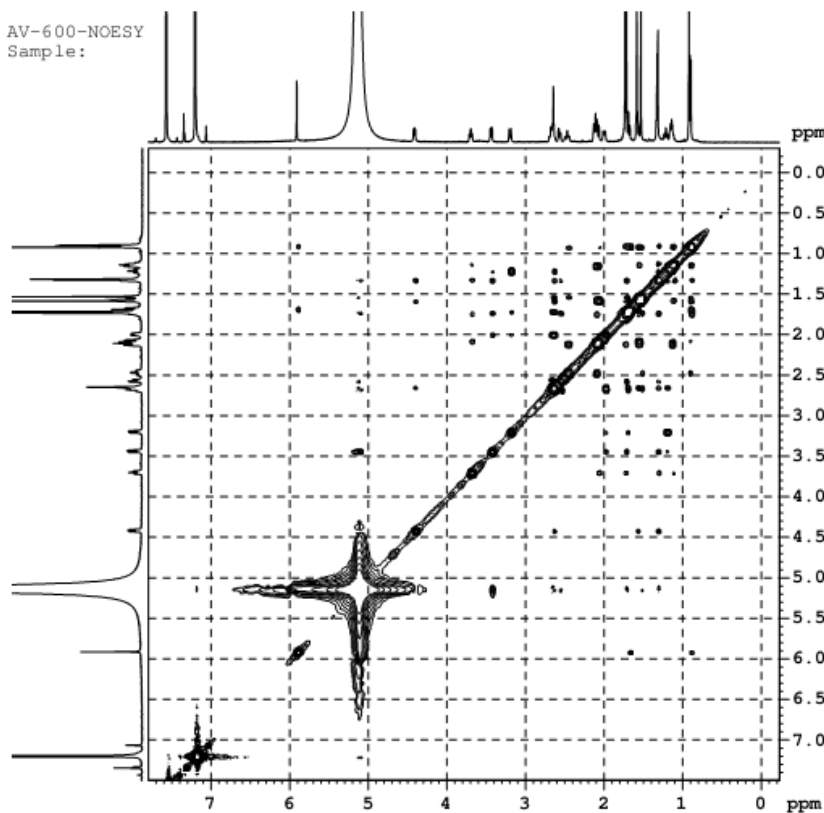


```

NAME          HSQC2
EXPNO         8
PROCNO        1
Date_         20120818
Time          14:14
INSTRUM       spect
PROBHD        5 mm PABBO MM-
PULPROG       zgpg30p1
TD            1024
SOLVENT       Pyz
NS            12
DS            14
FIDRES        7183.908 Hz
AQ            0.0713900 sec
RG            25000
CW            69.600 usec
DE            4.50 usec
TE            294.5 K
===== CHANNEL f1 =====
NUC1          13C
P1            11.10 usec
P2            22.20 usec
P3            22.20 usec
P4            17.40 usec
P5            24.7024579 Hz
P6            400.133608 MHz
===== CHANNEL f2 =====
NUC2          1H
P7            8.80 usec
P8            17.40 usec
P9            80.00 usec
P10           1.00 usec
P11           20.17 dB
P12           97.2024925 Hz
P13           1.0024925 Hz
P14           150.9143903 MHz
===== GRADIENT CHANNEL =====
GPMAG1        SINE.100
GPMAG2        SINE.100
GPMAG3        SINE.100
GPD1          50.00 %
GPD2          30.00 %
GPD3          40.10 %
GPD4          1000.00 usec
ND0           2
TD            654
SFO1          150.9194 MHz
FIDRES        212.283588 Hz
AQ            250.000 usec
P1PROG        SF
SI            0
SF            600.1306467 MHz
WDW           EM
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           SF
SF            150.9029219 MHz
WDW           EM
SSB           2
LB            0.00 Hz
GB            0
  
```

HMBC data of metabolites 11

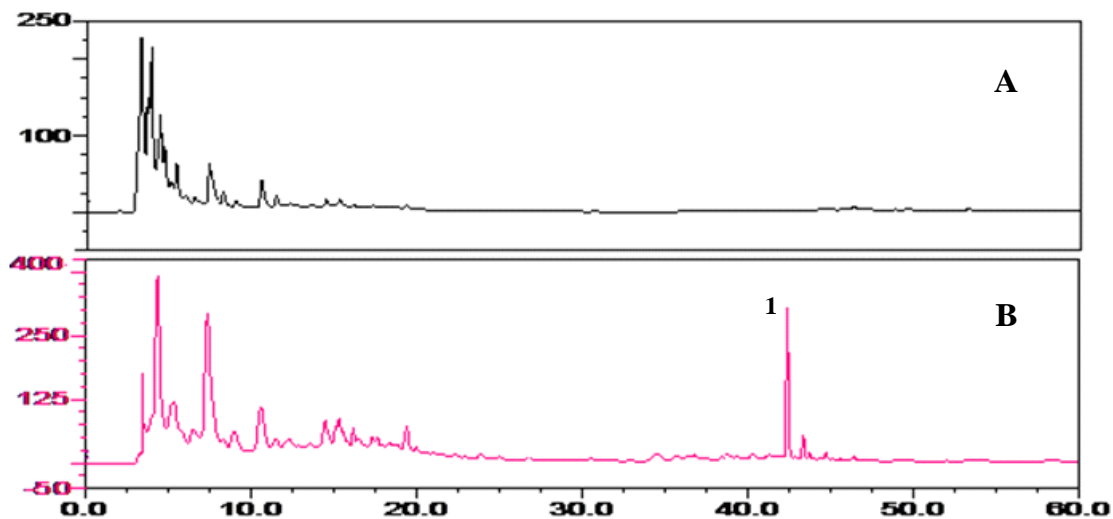
AV-600-NOESY  
Sample:



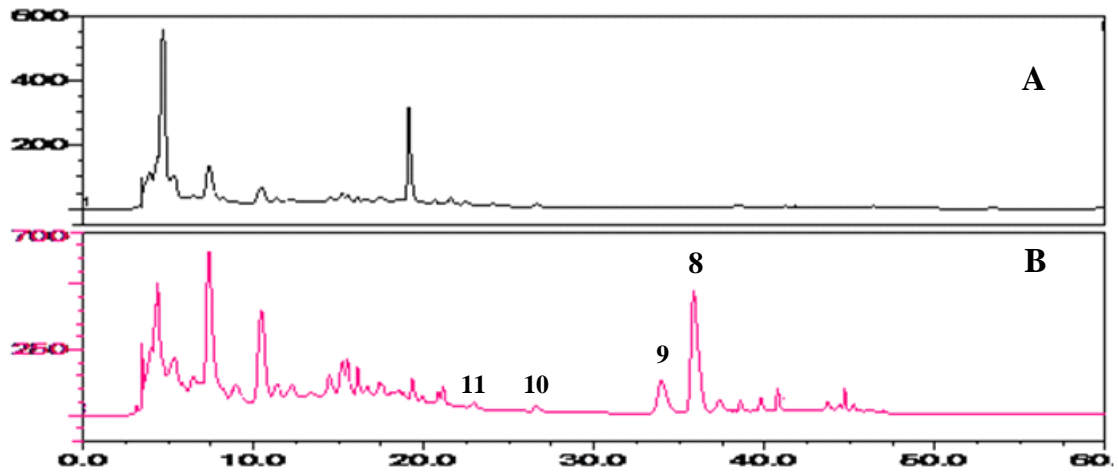
```
NAME          KBAXF
EXPNO         6
PROCNO        1
Date_         20120818
Time          9.17
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       noesyph
TD            1024
SOLVENT       Pyr
NS            8
DS            4
SWH           7183.908 Hz
FIDRES        7.015535 Hz
AQ            0.0713900 sec
RG            128
DW            69.600 usec
DE            6.50 usec
TE            296.7 K
D0            0.00005547 sec
D1            2.00000000 sec
D8            0.60000002 sec
IN0           0.00013920 sec

===== CHANNEL f1 =====
NUC1          1H
P1            11.10 usec
PL1          -4.00 dB
PL1W         34.70265579 W
SFO1         600.1330006 MHz
ND0          1
TD           256
SFO1         600.133 MHz
FIDRES        28.062078 Hz
SW           11.970 ppm
FMODE         States-TFPI
SI           1024
SF           600.1306871 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
SI           1024
MC2          States-TFPI
SF           600.1306654 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
```

NOESY data of metabolites **11**



The HPLC chromatogram (254 nm) of the metabolite of AKBA transformed by *Penicillium janthinellum* AS 3.510.



The HPLC chromatogram (254 nm) of the metabolites of KBA transformed by *Cunninghamella elegans* AS 3.1207.