

Supporting Information

Rec.Nat. Prod. 9:3 (2015) 271-275

Two New Alkaloids from a Marine-derived Fungus *Neosartorya fischeri*

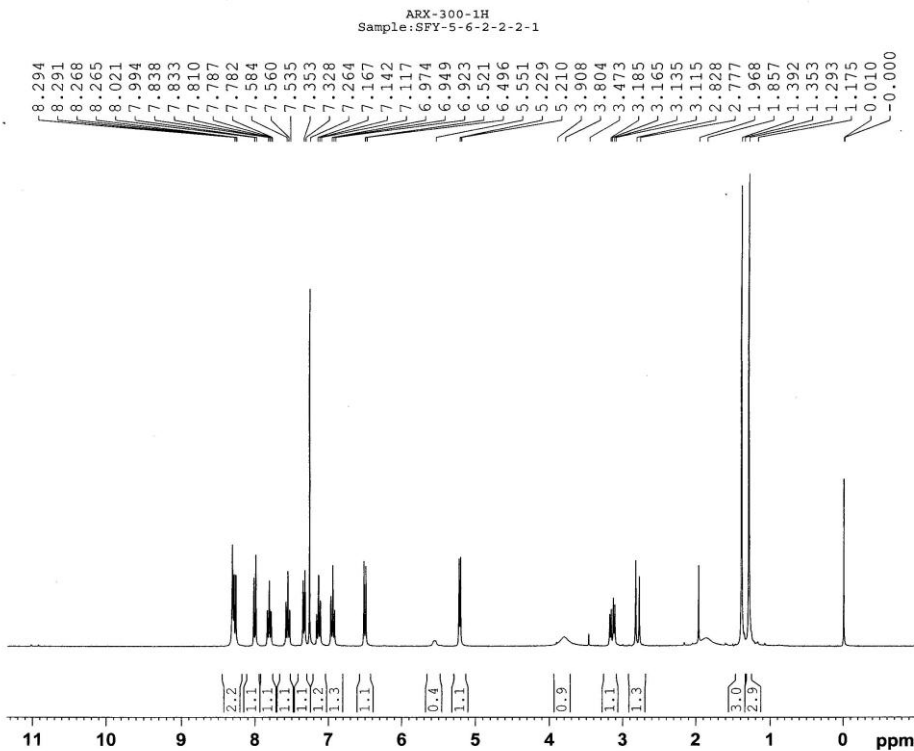
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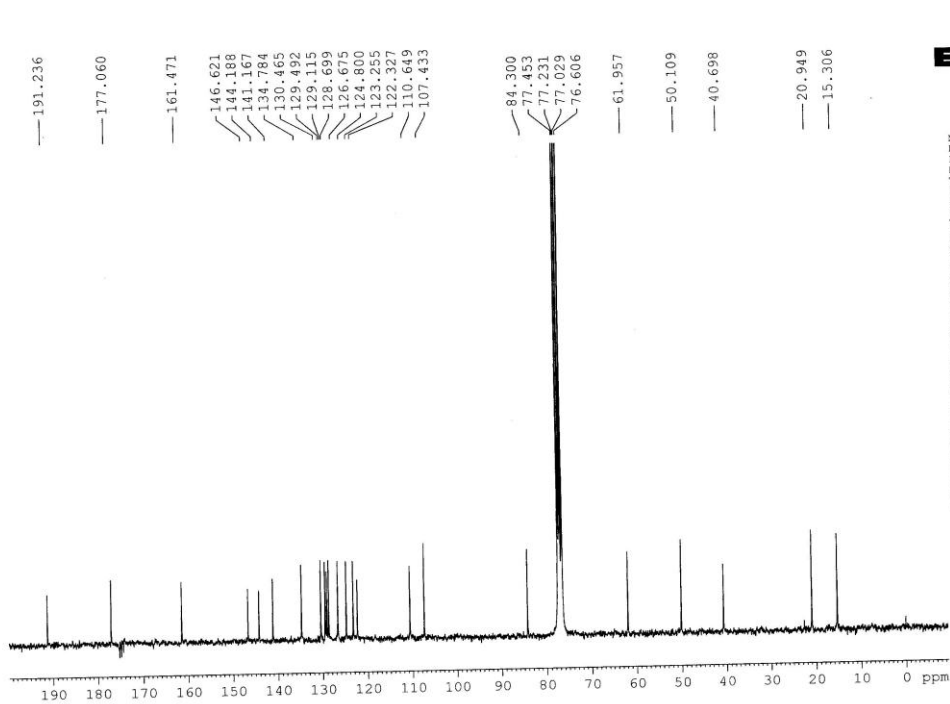
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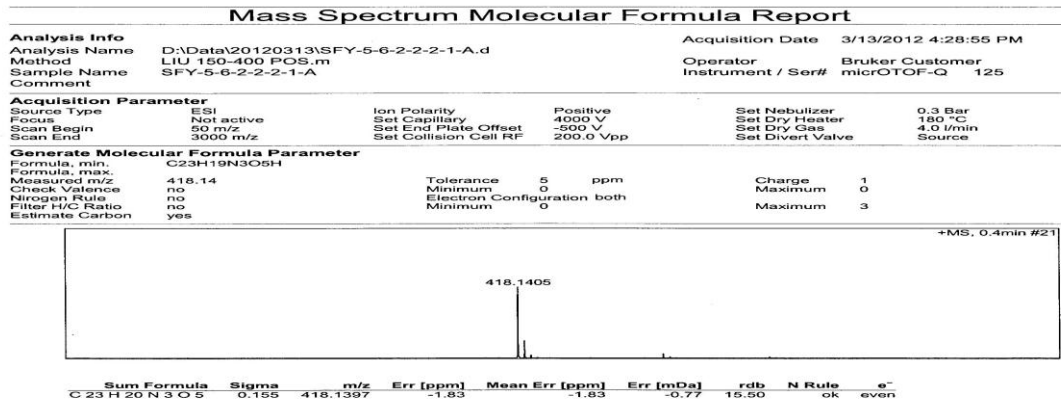


The ^1H NMR spectrum of compound **1**

ARX-300-13C
Sample: SFY5-6-2-2-2-1



The ¹³C NMR spectrum of compound 1



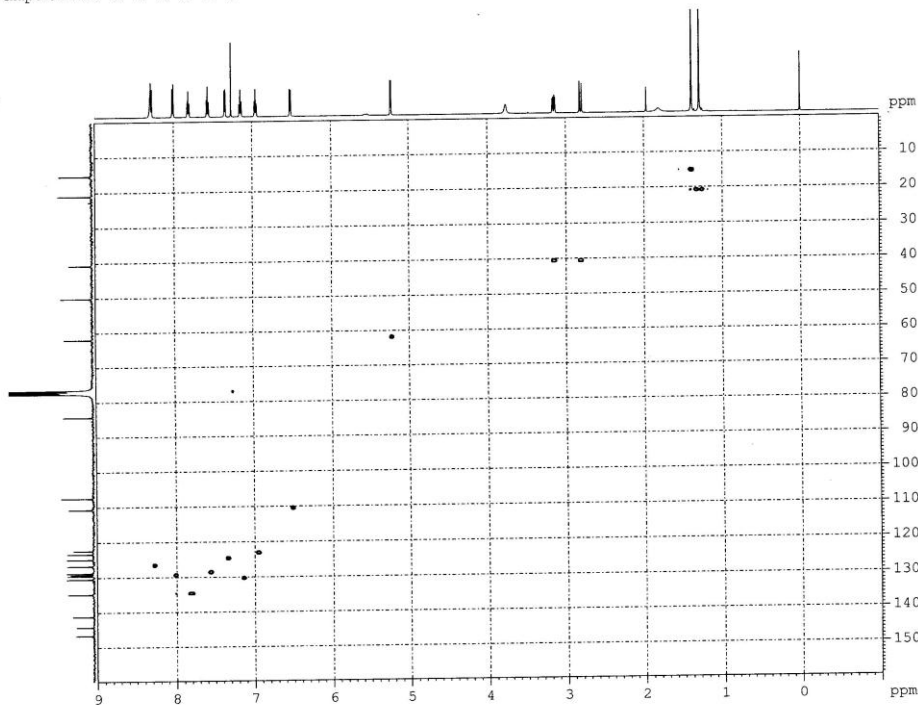
Bruker Daltonics DataAnalysis 3.4

printed: 3/13/2012 4:31:30 PM

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The HRESIMS spectrum of compound 1

AV-600-HSQC
Sample: SFY-5-6-2-2-1



```

NAME SFY-5-6-2-2-1
EXPNO 8
PROCNO 1
Date_ 20111022
Time 9.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 1024
SOLVENT CDCl3
NS 4
DS 1
SWH 6009.615 Hz
FIDRES 5.86876 Hz
AQ 0.0853300 sec
RG 2600
DW 83.200 usec
DE 6.50 usec
TE 298.2 K
CNS2 145.0000000
DO 0.0000300 sec
D1 1.5000000 sec
D4 0.0017414 sec
D11 0.0300000 sec
D13 0.0000400 sec
D15 0.0002000 sec
D24 0.0011000 sec
TD0 0.0000370 sec
ZGPGTNS

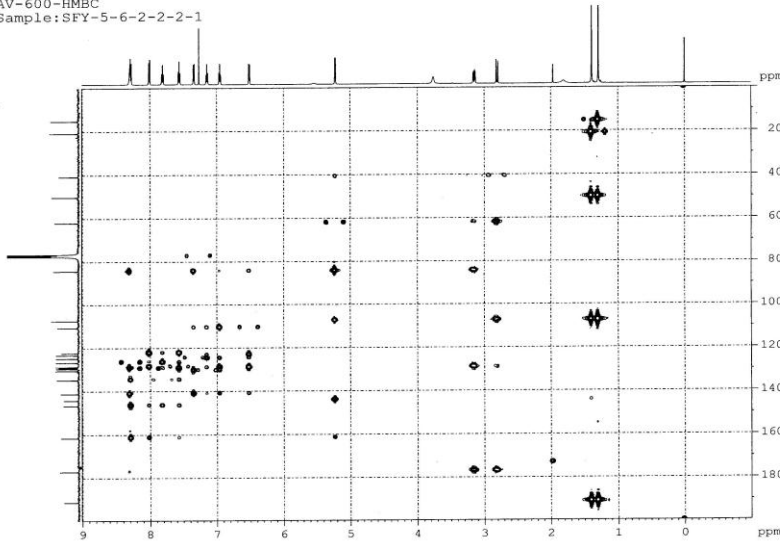
===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 22.20 usec
P2 1000.00 usec
PL2 -4.00 dB
RF1W 34.7026573 MHz
SFO1 600.1324005 MHz

===== CHANNEL f2 =====
CROSS2 94D
NUC2 13C
P3 8.80 usec
P4 17.60 usec
PCPD2 80.00 usec
PL3 1.00 dB
PL12 20.17 dB
P1W 83.2024383 MHz
PL17W 1.0074713 MHz
SFO2 150.9148102 MHz

===== GRADIENT CHANNEL =====
GRNAM1 SINE.100
GRNAM2 SINE.100
GPR1 80.00 Hz
GPR2 80.00 Hz
GPR3 1000.00 usec
P15 256
ND0 2
TD 150.9148 MHz
SFO 150.9148 MHz
FIDRES 94.321800 Hz
SW 160.000 ppm
FMODE Echo-AttLech
SI 1024
SF 600.1300007 MHz
WDW QSHINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.49
SI 1024
MC2 echo-attLech
SF 150.9028267 MHz
WDW QSHINE
SSB 2
LB 0.00 Hz
GB 0
    
```

The HSQC spectrum of compound 1

AV-600-HMBC
Sample: SFY-5-6-2-2-2-1



```

NAME SFY-5-6-2-2-2-1
EXPNO 5
PROCNO 1
Date_ 20111022
Time 15:23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmcqpl14024
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 6009.615 Hz
FIDRES 5.88165 Hz
AQ 0.082300 sec
RG 251.00
DW 83.200 usec
DE 258.2 K
TE 300.2 K
CST22 145.000000
CST13 5.000000
D0 0.0000000 sec
D1 1.2000000 sec
D2 0.0034889 sec
D3 0.1000000 sec
D4 0.0002000 sec
D5 0.0002500 sec
INO 0.0003500 sec

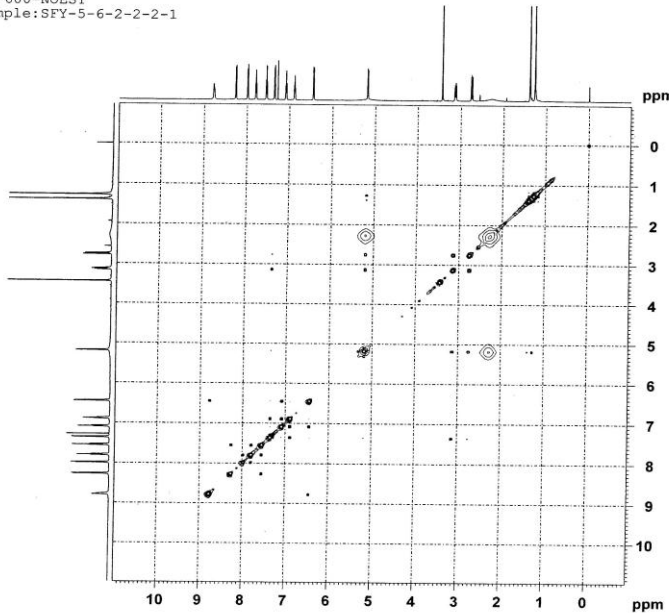
===== CHANNEL f1 =====
NUC1 13
P1 11.10 usec
P2 21.00 usec
PL1 -4.00 dB
PL2 19.00 dB
PL1W 34.7026579 W
SFO1 600.1324005 MHz

===== CHANNEL f2 =====
NUC2 13
P1 1.00 usec
P2 1.00 usec
PL1 83.2024939 W
PL2 150.9178993 MHz

===== GRADIENT CHANNEL =====
GPM1 SINE 100
GPM2 SINE 100
GPM3 SINE 100
GPF1 30.00 %
GPF2 40.00 %
GPF3 100.00 usec
NDO 1
TD 256
SFO1 150.9179 MHz
FIDRES 137.804610 Hz
SFO2 200.000000 MHz
FPMODE Q
SF 600.1299972 MHz
WDW QSI
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 States-TPT
SFO 150.902898 MHz
WDW QSI
SSB 2
LB 0.00 Hz
GB 0
    
```

The HMBC spectrum of compound 1

AV-600-NOESY
Sample: SFY-5-6-2-2-2-1

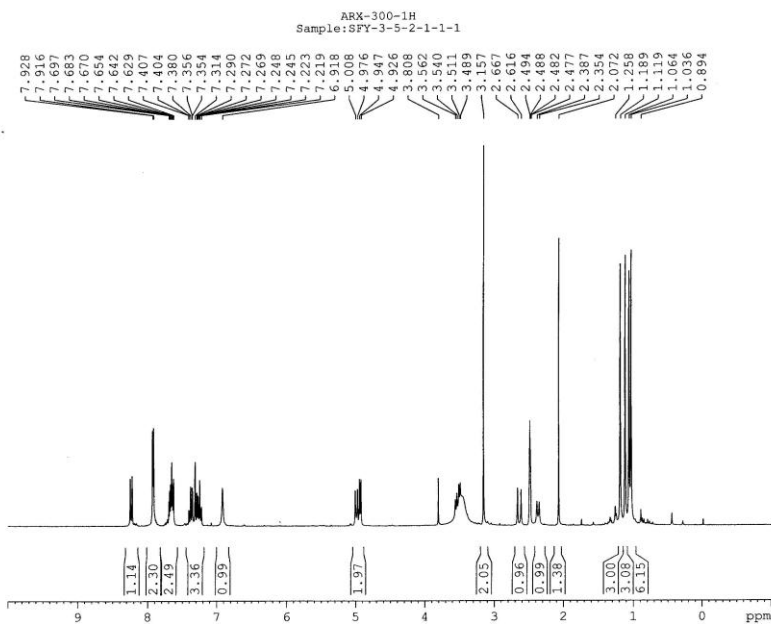


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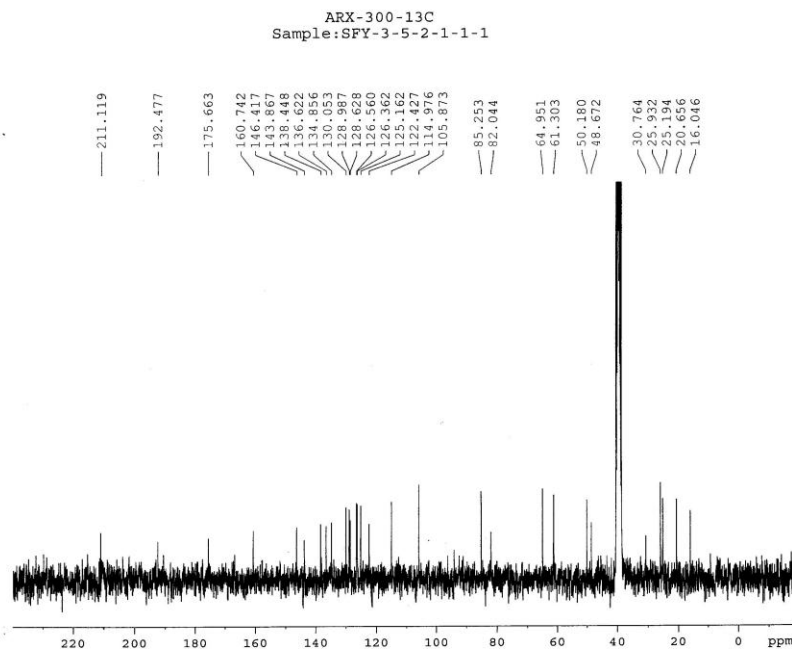
NAME SFY-5-6-2-2-2-1
EXPNO 1
PROCNO 1
Date_ 20120316
Time 16:26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG rdcexptn
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 7183.908 Hz
FIDRES 7.015535 Hz
AQ 0.0713900 sec
RG 90.5
DW 69.600 usec
DE 6.50 usec
TE 293.2 K
D0 0.0005547 sec
D1 2.0000000 sec
D2 0.6000002 sec
D3 0.0001392 sec
D4 0.0001392 sec
INO 0.0001392 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.10 usec
PL1 -4.00 dB
PL1W 34.7026579 W
SFO1 600.1330006 MHz
NDO 1
TD 256
SFO1 600.133 MHz
FIDRES 28.062078 Hz
SW 11.970 ppm
FPMODE States-TPT
SI 1024
SF 600.1299972 MHz
WDW QSI
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPT
SFO 600.1299971 MHz
WDW QSI
SSB 2
LB 0.00 Hz
GB 0
    
```

The NOE spectrum of compound 1



The ^1H NMR spectrum of compound 2



The ^{13}C NMR spectrum of compound 2

Mass Spectrum Molecular Formula Report

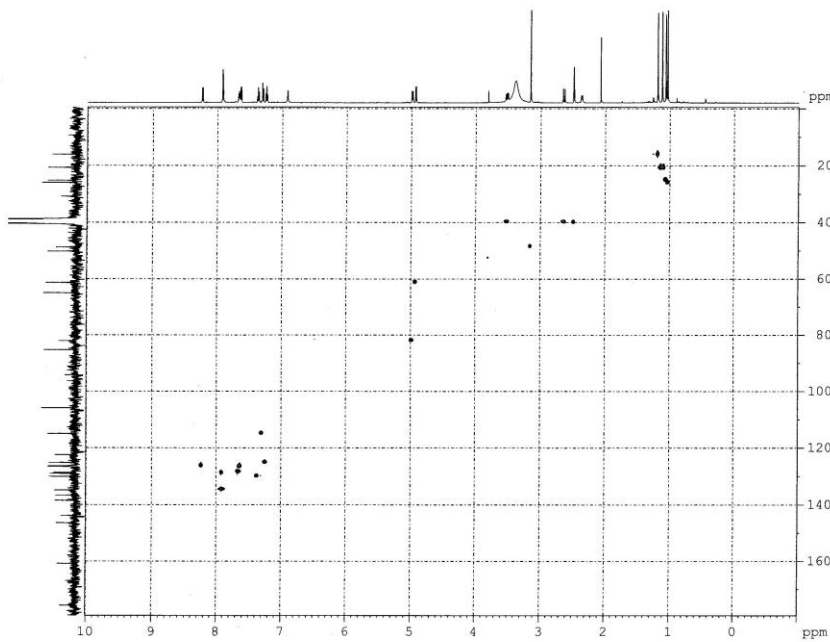
Analysis Info		Acquisition Date		3/13/2012 4:16:31 PM	
Analysis Name	D:\Data\20120313\SFY-3-5-2-1-1-1.d	Operator	Bruker Customer		
Method	LIU 150-400 POS.m	Instrument / Ser#	micrOTOF-Q 125		
Sample Name	SFY-3-5-2-1-1-1	Comment			
Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source
Generate Molecular Formula Parameter					
Formula, min.	C27H27N4O5	Tolerance	5 ppm	Charge	1
Formula, max.		Minimum	0	Maximum	0
Measured m/z	487.197	Electron Configuration both		Maximum	3
Check Valence	no	Minimum	0		
Nitrogen Rule	no				
Filter H/C Ratio	no				
Estimate Carbon	yes				



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C27H27N4O5	0.183	487.1976	1.74	1.74	0.85	16.50	ok	even

The HRESIMS spectrum of compound 2

AV-600-HSQC
Sample: SFY-3-5-2-1-1-1

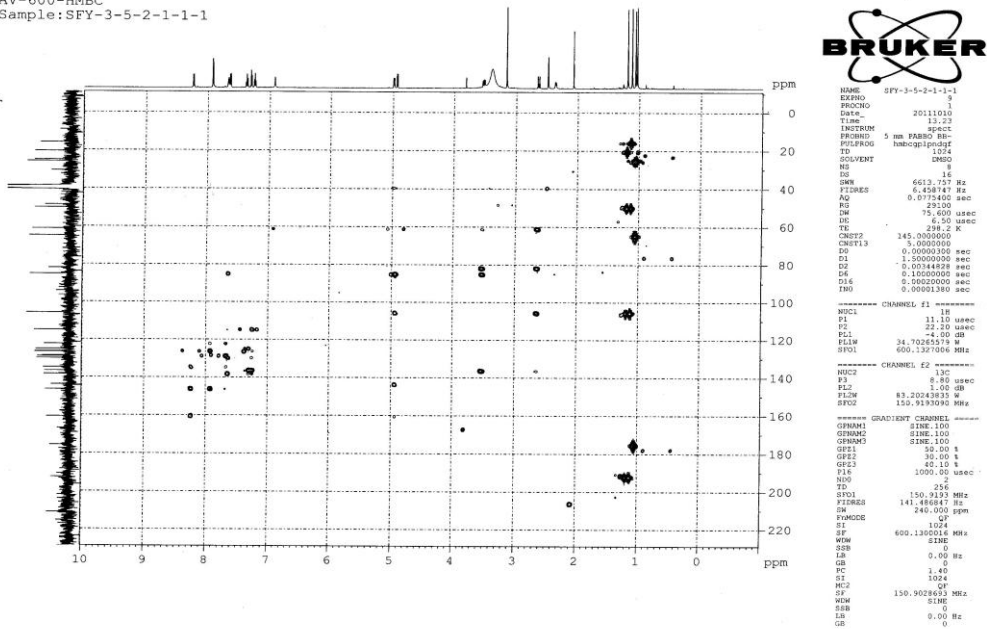


```

NAME SFY-3-5-2-1-1-1
EXPNO 6
PROCNO 20111010
Time 13.09
Timepoint 4
PROBHD 5 mm FARGO BB-
PULPROG zgpg30
TD 65536
SOLVENT H2O
NS 2
DS 2
SWH 6613.707 Hz
FIDRES 6.458747 Hz
AQ 0.0775400 sec
RG 24000
DM 75.600 usec
DE 6.50 usec
TE 298.2 K
CRST2 145.0000000 sec
DO 0.00000000 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D14 0.00020000 sec
D16 0.00110640 sec
D18 0.0001482 sec
EGGPRG
----- CHANNEL F1 -----
NUC1 1H
P1 11.10 usec
P2 12.20 usec
P3 1900.00 usec
PL1 0.00 dB
PL12 18.7000000 W
PL13 600.1327006 MHz
SFO1 600.1327006 MHz
----- CHANNEL F2 -----
CROSSP2 981P
NUC2 13C
P4 8.10 usec
P5 17.60 usec
P6 90.00 usec
PL2 1.00 dB
PL3 20.17 dB
PL4 83.20243835 W
PL14 1.0012411 W
PL15 150.9163903 MHz
SFO2 150.9163903 MHz
----- GRADIENT CHANNEL -----
GPRM1 SINE 100
GPRM2 SINE 100
GPF1 80.00 V
GPF2 25.10 V
RF 1000.00 usec
NU0 2
SFO3 526
SFO4 150.9164 MHz
FIDRES 106.113094 Hz
SW 180.000 PPM
PRMODE Echo-AntiEcho
SI 1624
NEW 600.1300016 MHz
SFB 2
SB 0.00 Hz
PC 1.40
SI 1824
NC2 echo-MT1&ch3
SI 150.9029882 MHz
NEW QSHZ
SSB 2
SB 0.00 Hz
SM 0
    
```

The HSQC spectrum of compound 2

AV-600-HMBC
Sample: SFY-3-5-2-1-1-1



```

NAME SFY-3-5-2-1-1-1
EXPNO 3
PROCNO 1
Date_ 20111010
Time 11.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmcqplp1dprgr
TD 1224
SOLVENT DMSO
NS 8
DS 15
SWH 6613.757 Hz
FIDRES 6.458747 Hz
AQ 0.0775400 sec
RG 228
DW 75.600 usec
DE 6.50 usec
TE 293.1 K
D0 0.00000000 sec
D1 0.00000000 sec
D2 0.00000000 sec
D3 0.00184838 sec
D4 0.10000000 sec
D5 0.00000000 sec
D6 0.00001380 sec
IN0 0.00001380 sec

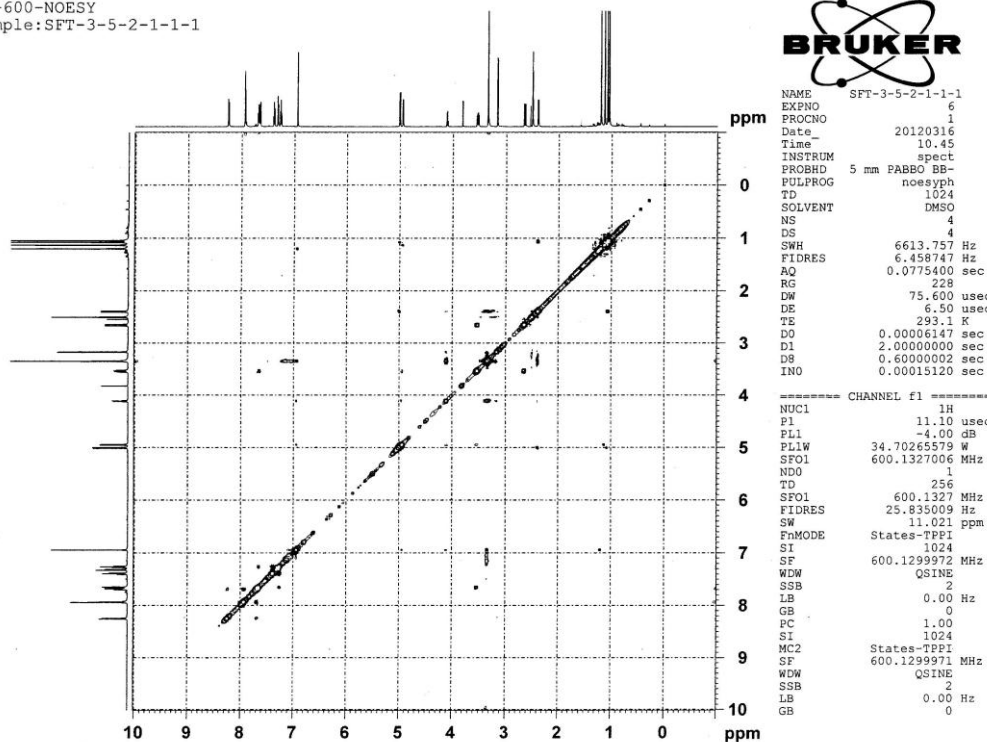
===== CHANNEL f1 =====
NUC1 13
P1 11.10 usec
PC 4.00 dB
PL1 34.7026579 W
PLW 34.7026579 W
SF01 600.1327006 MHz

===== CHANNEL f2 =====
NUC2 1H
P2 9.80 usec
PC 0.00 dB
PL2 83.3004889 W
PLW 150.9193093 MHz

===== GRADIENT CHANNEL =====
GPM1 SINE.100
GPM2 SINE.100
GPM3 SINE.100
GPF1 50.00 %
GPF2 30.00 %
GPF3 40.10 %
GFB 1000.00 usec
ND0 256
SF01 600.1327 MHz
FIDRES 25.835009 Hz
SW 11.021 ppm
FMODE States-TPPI
SI 1024
SF 600.1299972 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPPI
SF 600.1299971 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
    
```

The HMBC spectrum of compound 2

AV-600-NOESY
Sample: SFT-3-5-2-1-1-1



```

NAME SFT-3-5-2-1-1-1
EXPNO 6
PROCNO 1
Date_ 20120316
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesyph
TD 1024
SOLVENT DMSO
NS 4
DS 4
SWH 6613.757 Hz
FIDRES 6.458747 Hz
AQ 0.0775400 sec
RG 228
DW 75.600 usec
DE 6.50 usec
TE 293.1 K
D0 0.00006147 sec
D1 2.00000000 sec
D2 0.60000002 sec
D3 0.00015120 sec
IN0 0.00015120 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.10 usec
PC 4.00 dB
PL1 34.7026579 W
PLW 34.7026579 W
SF01 600.1327006 MHz
TD 1
ND0 256
SF01 600.1327 MHz
FIDRES 25.835009 Hz
SW 11.021 ppm
FMODE States-TPPI
SI 1024
SF 600.1299972 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPPI
SF 600.1299971 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
    
```

The NOE spectrum of compound 2