

Supporting Information

**New phenylspirodrimane metabolites MBJ-0030, MBJ-0031, and MBJ-0032  
isolated from the soil fungal strain *Stachybotrys* sp. f23793**

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## Table of Contents

Figure S1	<sup>1</sup> H NMR spectrum of <b>1</b> .	Figure S16	<sup>1</sup> H NMR spectrum of <b>2</b> .
Figure S2	<sup>13</sup> C NMR spectrum of <b>1</b> .	Figure S17	<sup>13</sup> C NMR spectrum of <b>2</b> .
Figure S3	DQF-COSY spectrum of <b>1</b> .	Figure S18	DQF-COSY spectrum of <b>2</b> .
Figure S4	HSQC spectrum of <b>1</b> .	Figure S19	HSQC spectrum of <b>2</b> .
Figure S5	HMBC spectrum of <b>1</b> .	Figure S20	HMBC spectrum of <b>2</b> .
Figure S6	<sup>1</sup> H- <sup>15</sup> N HMBC spectrum of <b>1</b> .	Figure S21	NOESY spectrum of <b>2</b> .
Figure S7	NOESY spectrum of <b>1</b> .	Figure S22	High-resolution mass spectrum of <b>2</b> .
Figure S8	High-resolution mass spectrum of <b>1</b> .	Figure S23	<sup>1</sup> H NMR spectrum of <b>3</b> .
Figure S9	<sup>1</sup> H NMR spectrum of methylated <b>1</b> .	Figure S24	<sup>13</sup> C NMR spectrum of <b>3</b> .
Figure S10	<sup>13</sup> C NMR spectrum of methylated <b>1</b> .	Figure S25	DQF-COSY spectrum of <b>3</b> .
Figure S11	DQF-COSY spectrum of methylated <b>1</b> .	Figure S26	HSQC spectrum of <b>3</b> .
Figure S12	HSQC spectrum of methylated <b>1</b> .	Figure S27	HMBC spectrum of <b>3</b> .
Figure S13	HMBC spectrum of methylated <b>1</b> .	Figure S28	NOESY spectrum of <b>3</b> .
Figure S14	NOESY spectrum of methylated <b>1</b> .	Figure S29	High-resolution mass spectrum of <b>3</b> .
Figure S15	High-resolution mass spectrum of methylated <b>1</b> .		

f23793/T3-3-5  
in CD3OD

Sample Name:  
f23793T335  
Archive directory:  
Sample directory:  
FidFile: f23793T335\_041912\_H

Pulse Sequence: Proton (s2pul)  
Solvent: cd3od  
Data collected on: Apr 19 2012

Temp. 25.0 C / 298.1 K  
Operator: walkup  
VNMR-600 "Agilent-VNS600"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 9615.4 Hz  
16 repetitions  
OBSERVE HL 599.8315746 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
PT size 65536  
Total time 0 min 49 sec

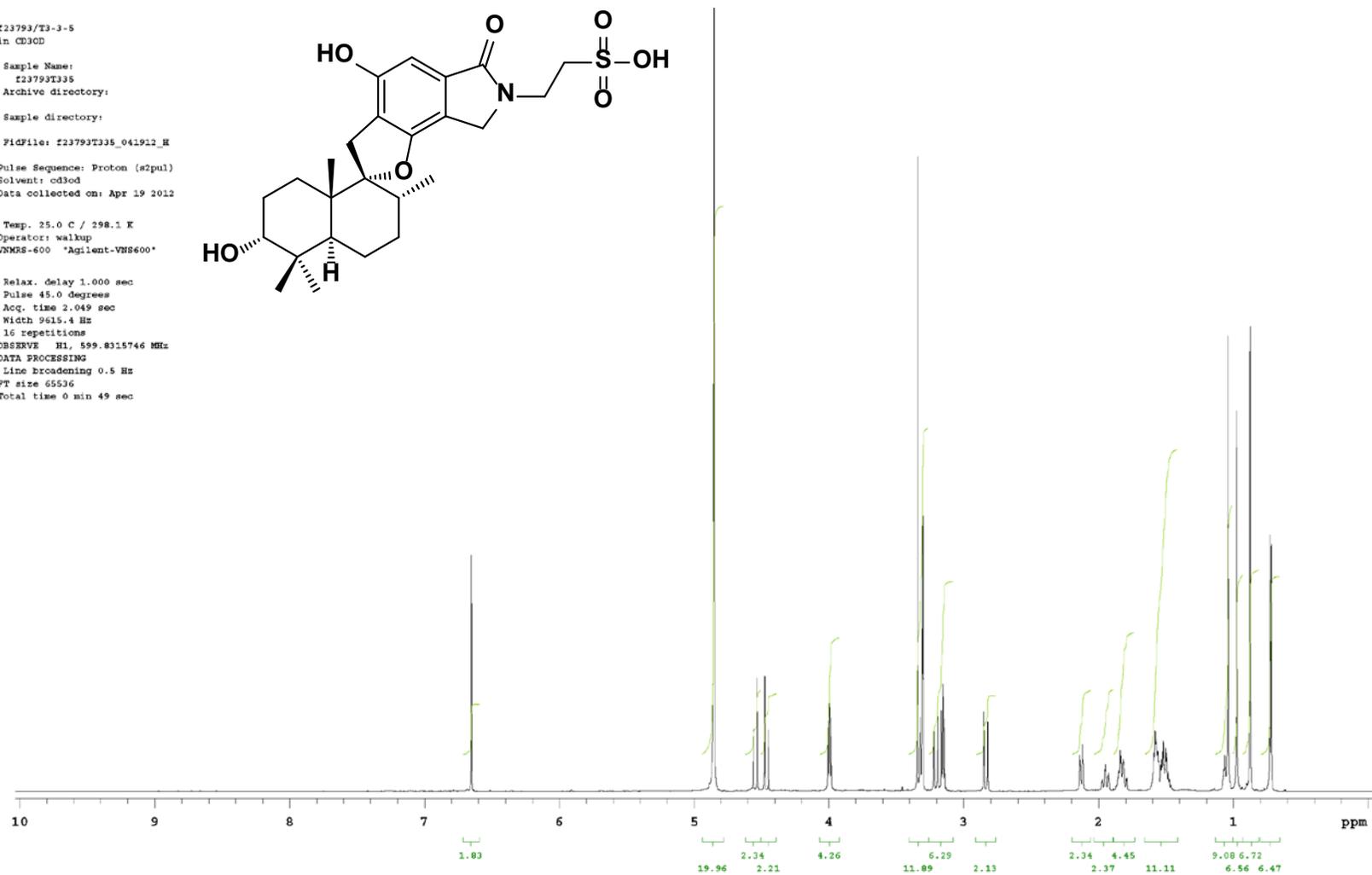
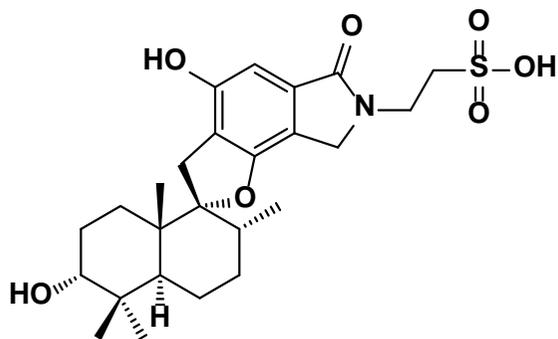


Figure S1

<sup>1</sup>H NMR spectrum of **1**.

f23793/T3-3-5  
in CD3OD  
Sample Name:  
f23793T335  
Archive directory:  
Sample directory:  
FidFile: f23793T335\_041912\_C  
Pulse Sequence: Carbon (s2pul)  
Solvent: cd3od  
Data collected on: Apr 20 2012  
Temp. 25.0 C / 298.1 K  
Operator: walkup  
VNMR5-600 \*Agilent-VNS600\*

Relax. delay 3.500 sec  
Pulse 45.0 degrees  
Acq. time 1.000 sec  
Width 36764.7 Hz  
2240 repetitions  
OBSERVE C13, 150.8277694 MHz  
DECOUPLE H1, 599.8345740 MHz  
Power 32 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 5.0 Hz  
PT size 65536  
Total time 125 hr, 1 min

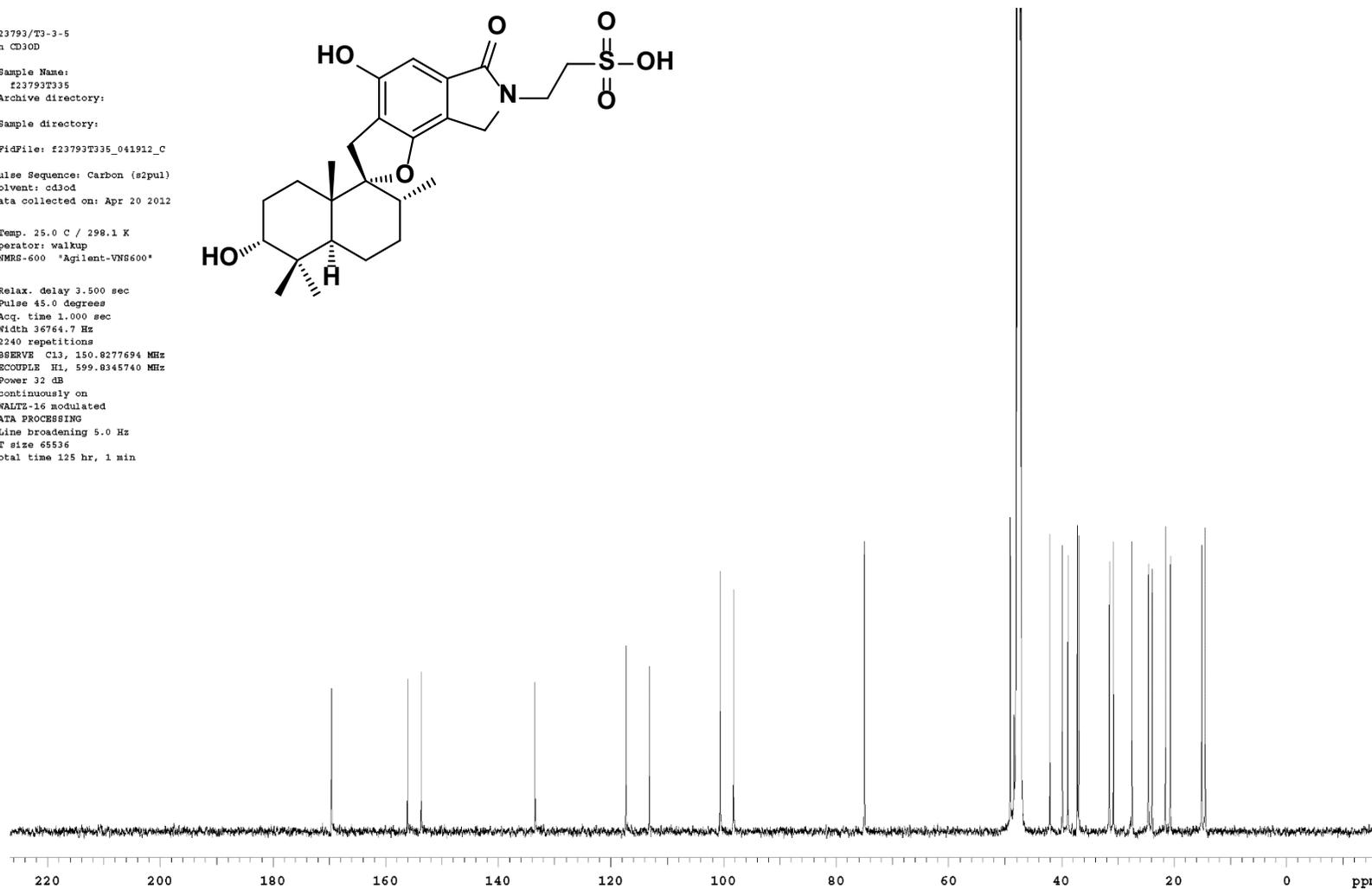
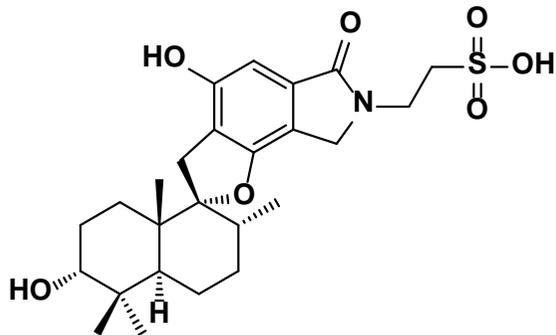


Figure S2 <sup>13</sup>C NMR spectrum of 1.

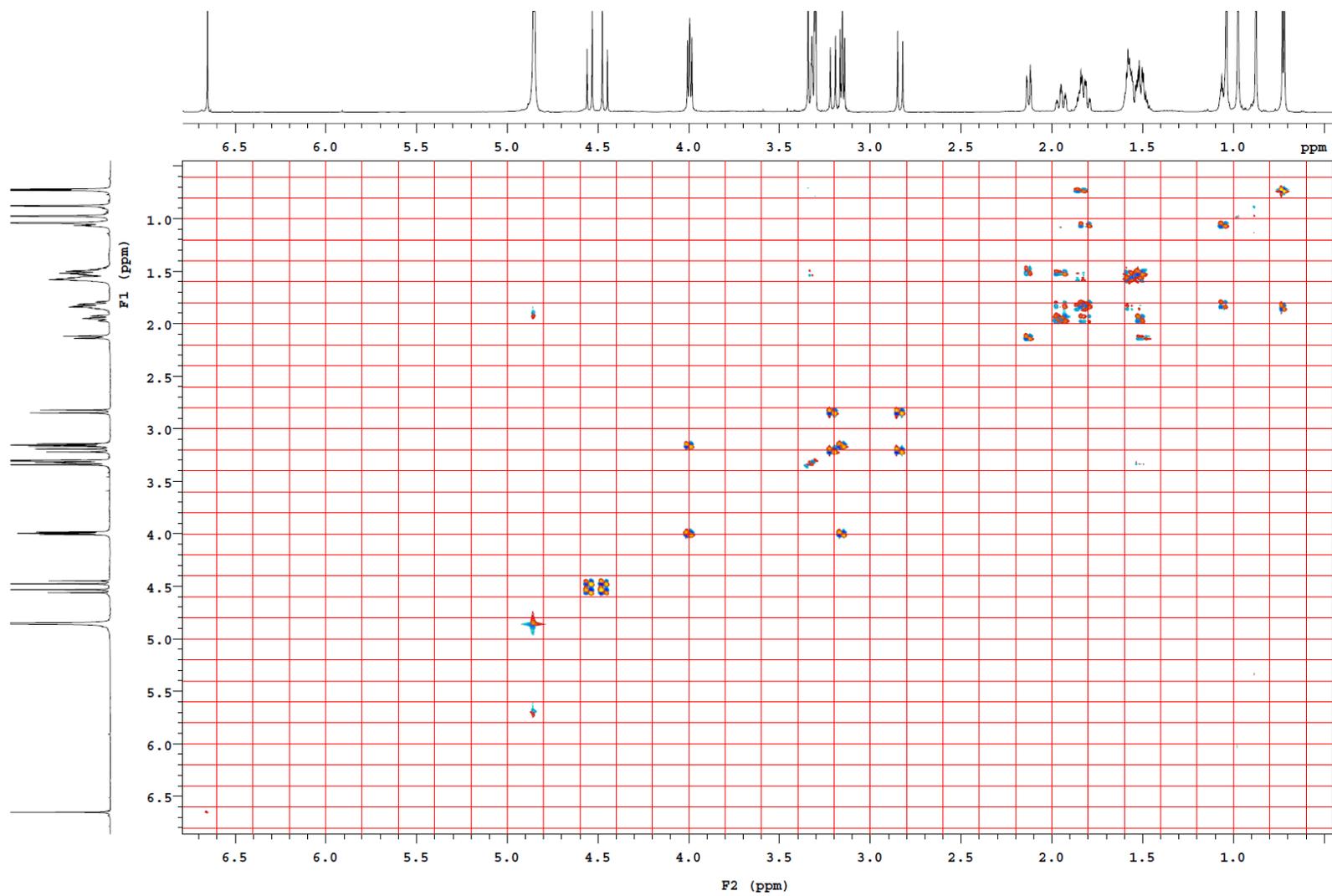


Figure S3 DQF-COSY spectrum of **1**.

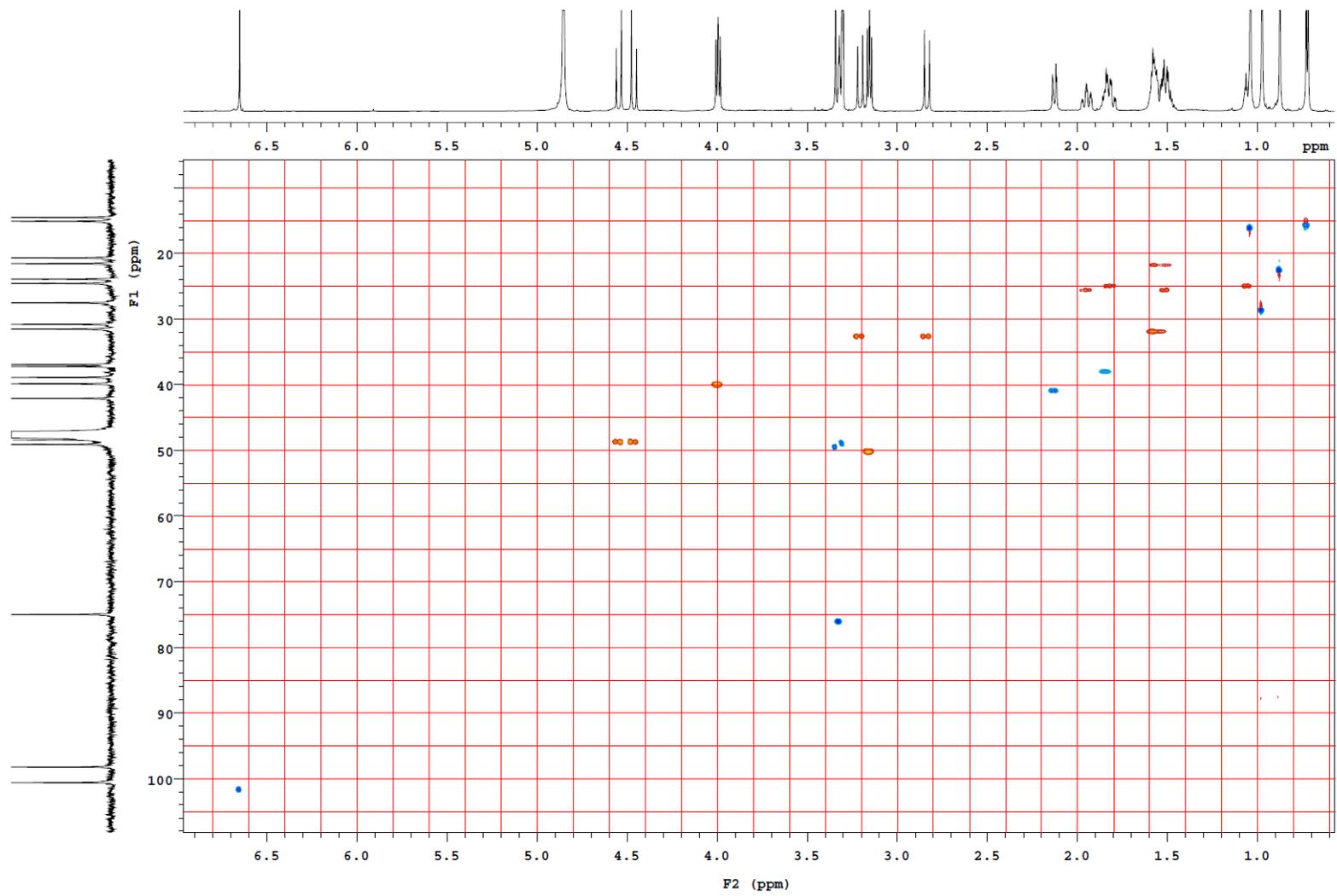


Figure S4 HSQC spectrum of **1**.

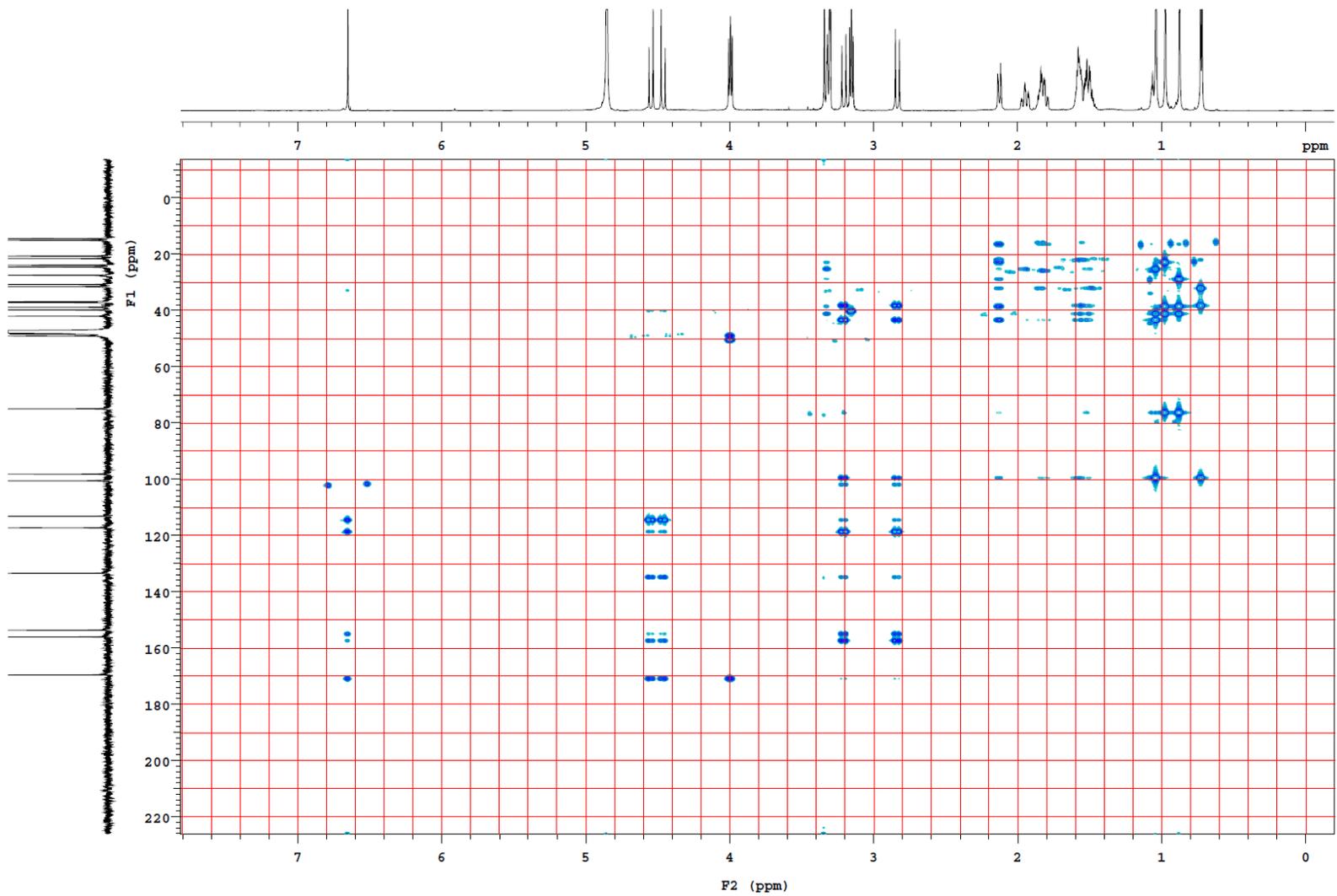


Figure S5 HMBC spectrum of 1.

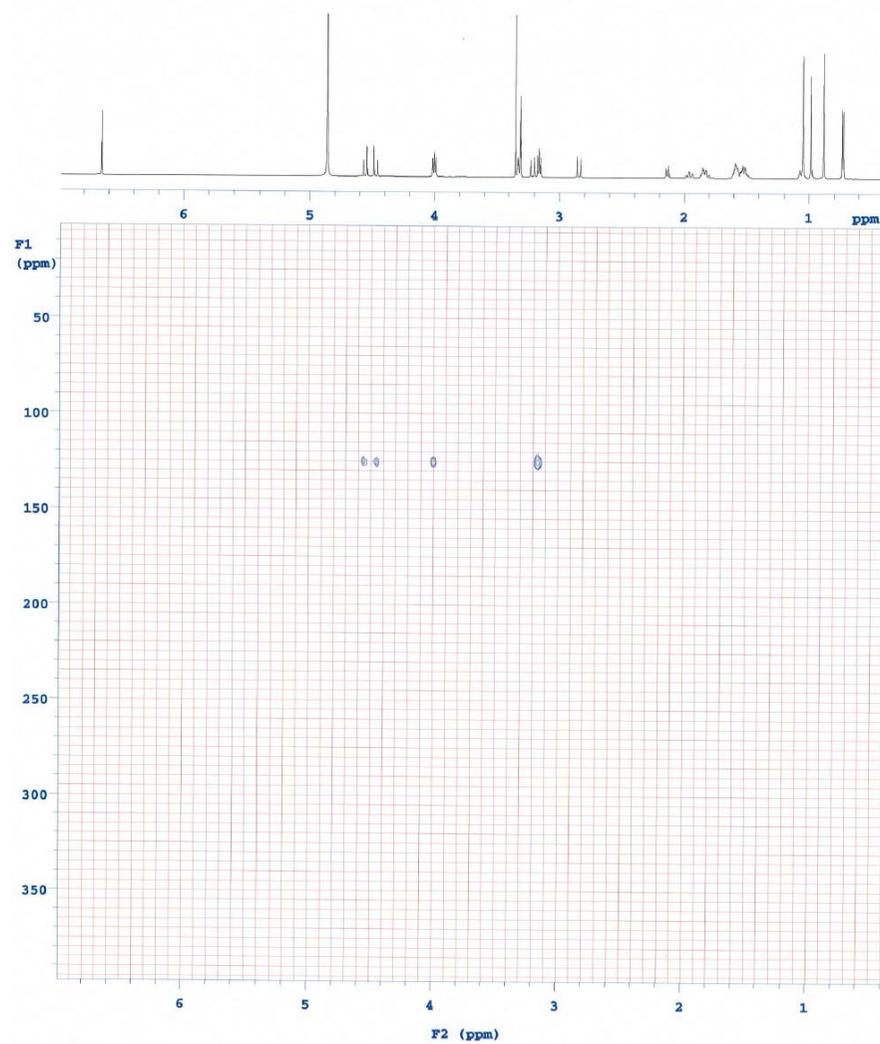


Figure S6  $^1\text{H}$ - $^{15}\text{N}$  HMBC spectrum of **1**.

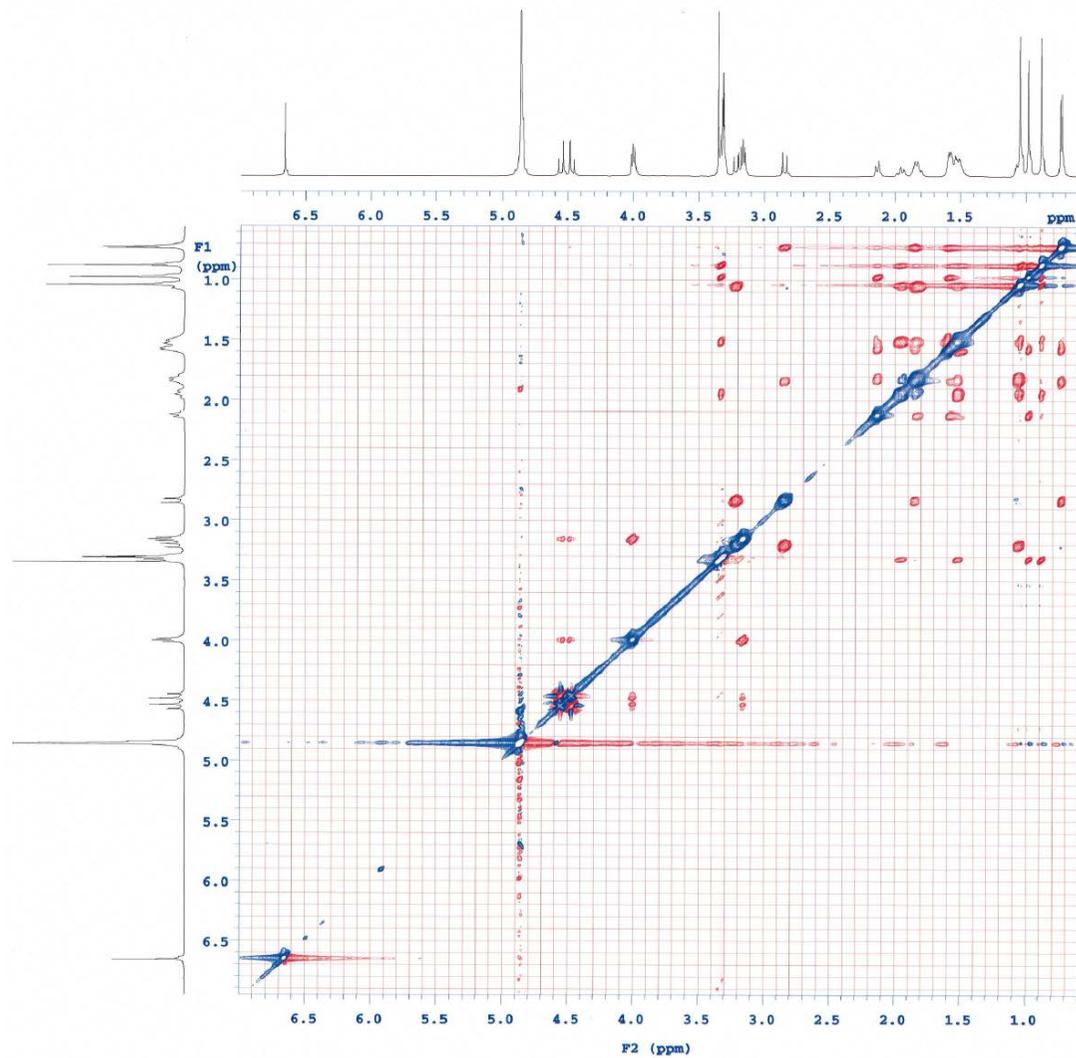


Figure S7 NOESY spectrum of **1**.

T3-3-5  
f23793\_003 36 (2.582) Cm (34:38)

1: TOF MS ES-  
3.84e+005

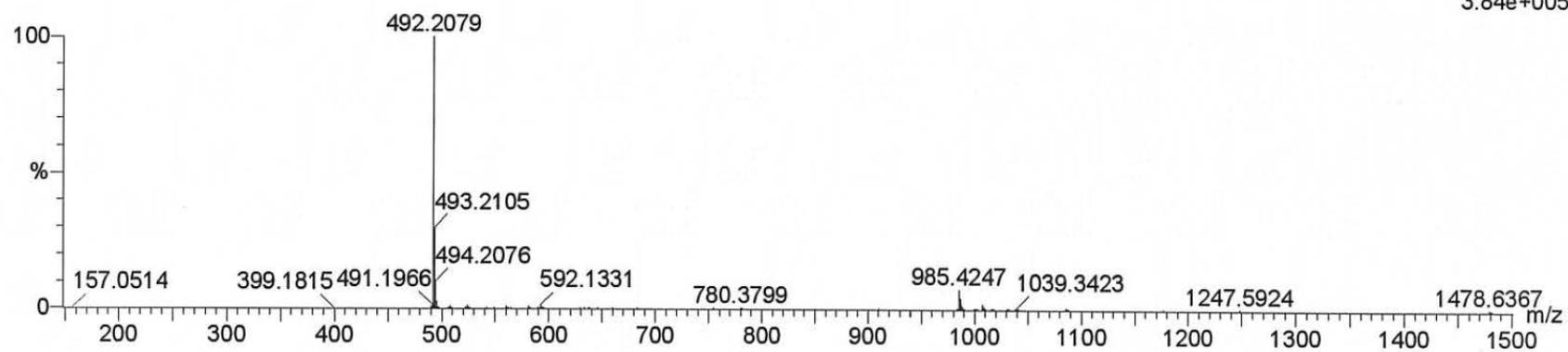


Figure S8 High-resolution mass spectrum of **1** (Negative ion mode).

f23793/73-3-5/Me-0427  
in CD3OD

Automation directory: /home/walkup/vnmrdata/auto\_2011.06.02\_01  
File: exp  
Sample id: tmpstudy  
Sample: f237937335Me0427

Pulse Sequence: s2pul  
Solvent: cd3od  
Temp: 25.0 C / 298.1 K  
Operator: walkup  
VNMRS-500 "cbnmr1.d.aist.go.jp"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 8012.8 Hz  
16 repetitions  
OBSERVE H1, 499.7244690 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65336  
Total time 0 min, 55 sec

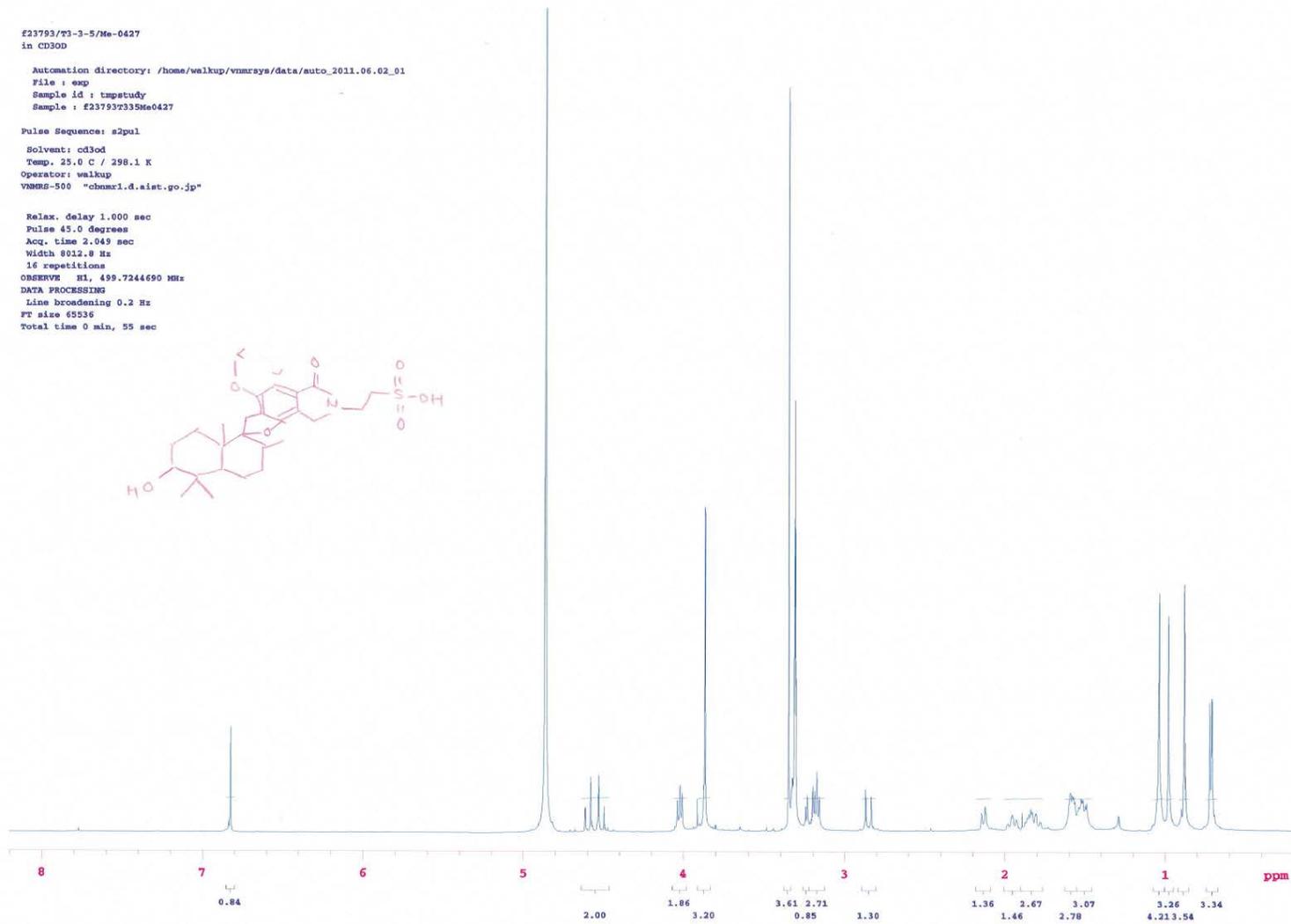
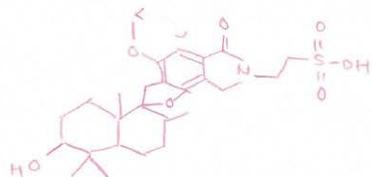


Figure S9 <sup>1</sup>H NMR spectrum of methylated **1**.

f23793/T1-3-5/Me-0427  
in CD3OD

Automation directory: /home/walkup/vnmrsys/data/auto\_2011.06.02\_01  
File : exp  
Sample id : tmpstudy  
Sample : f23793f335Me0427

Pulse Sequence: s2pul  
Solvent: cd3od  
Temp. 25.0 C / 298.1 K  
Operator: walkup  
VNMRS-500 "cbnmr1.d.siat.go.jp"

Relax. delay 3.500 sec  
Pulse 45.0 degrees  
Acq. time 1.000 sec  
Width 30487.8 Hz  
12300 repetitions  
OBSERVE C13, 125.6556389 MHz  
DECOUPLE H1, 499.7269709 MHz  
Power 31 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 65536  
Total time 125 hr, 16 min, 1 sec

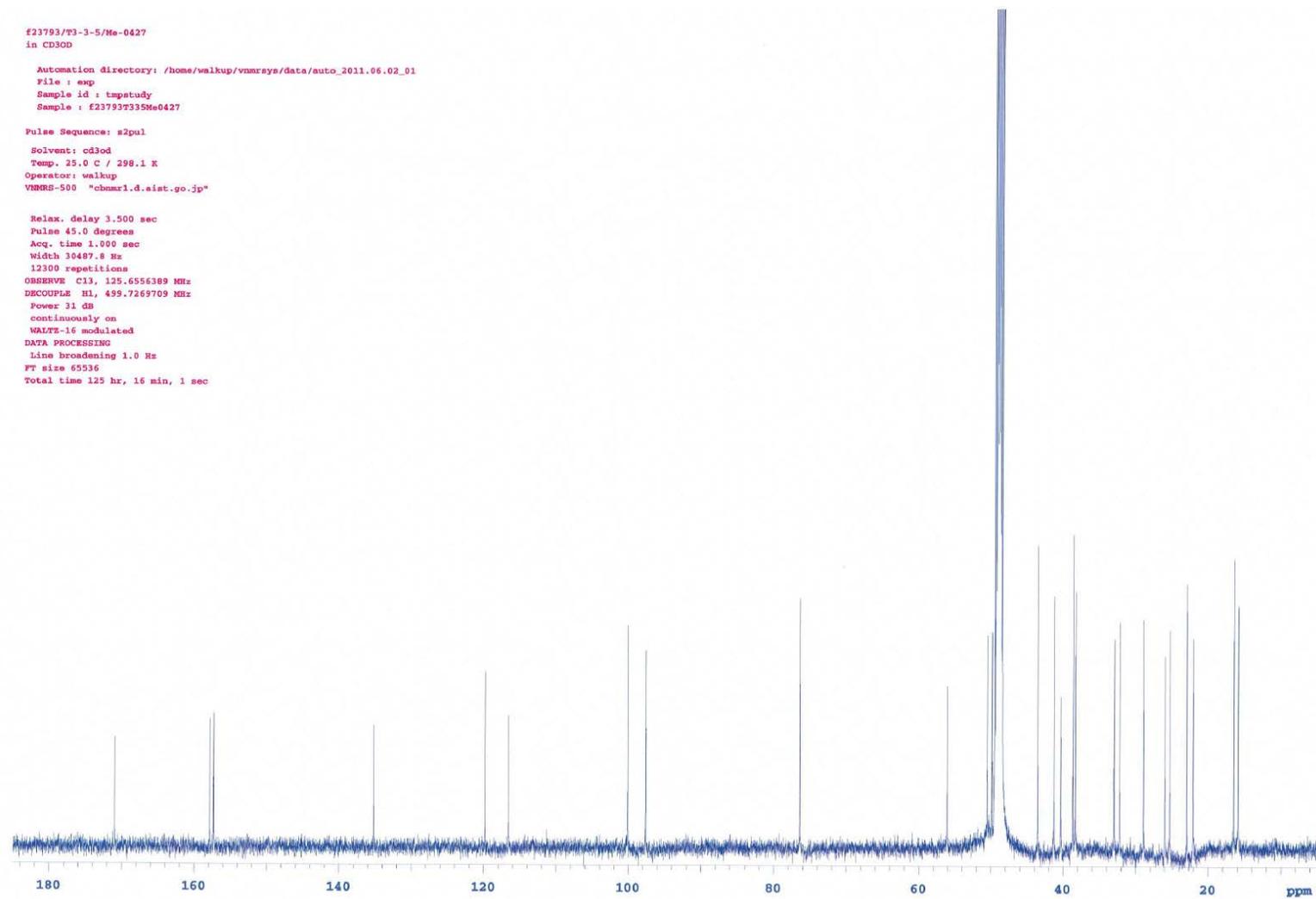


Figure S10  $^{13}\text{C}$  NMR spectrum of methylated **1**.

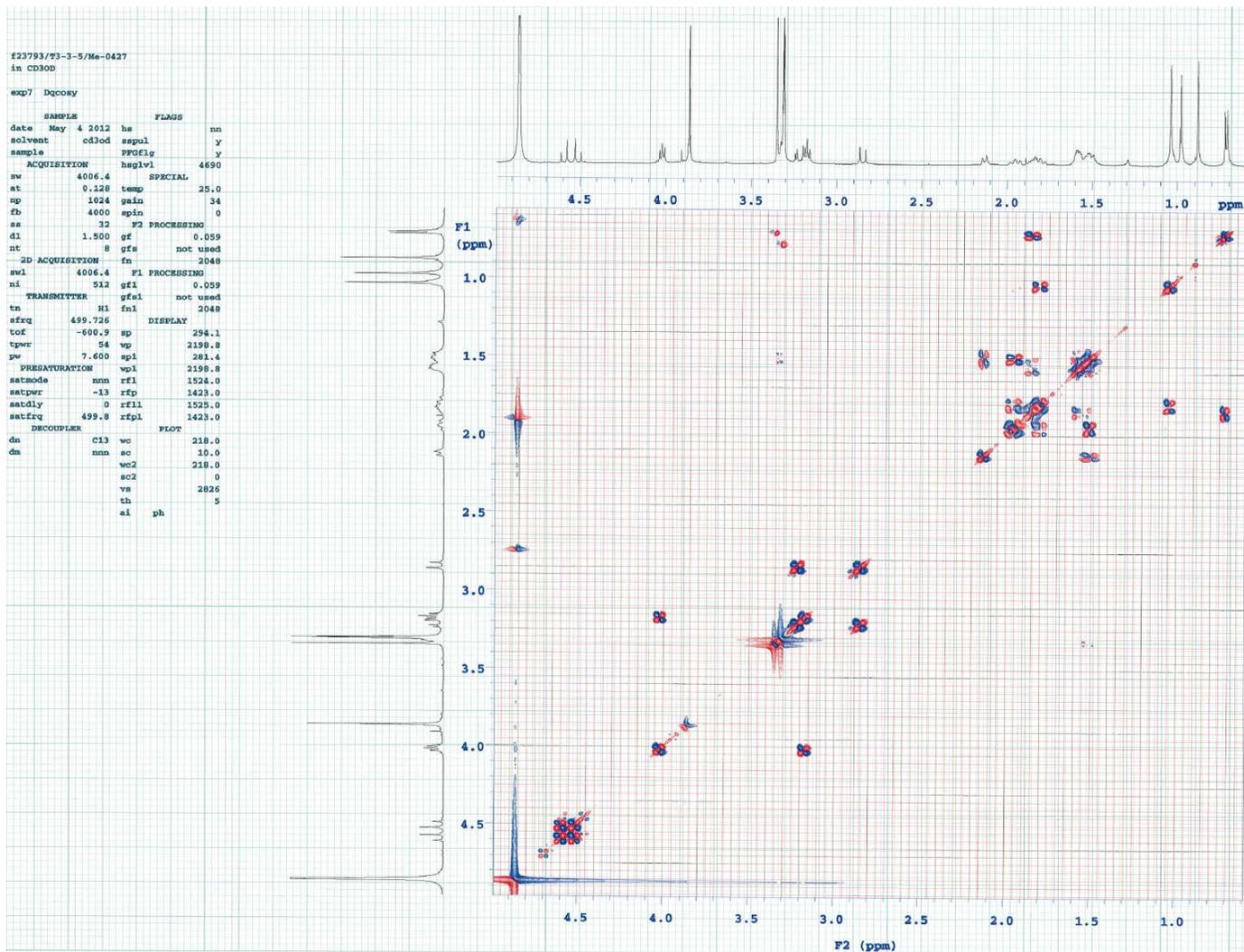


Figure S11 DQF-COSY spectrum of methylated **1**.

ACQUISITION ARRAYS  
array phase  
arraydim 1024  
  
i phase  
1 1  
2 2

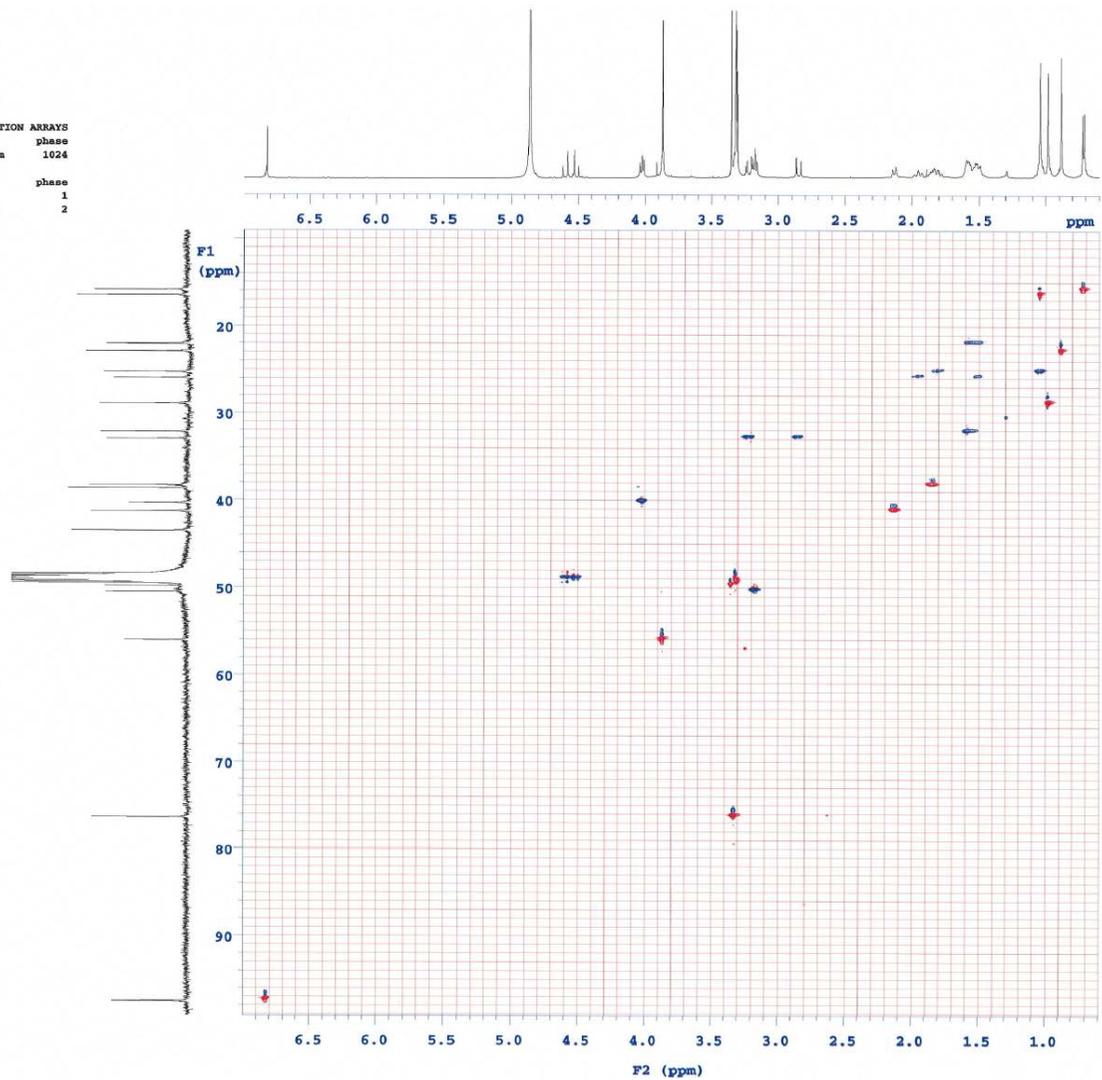


Figure S12 HSQC spectrum of methylated **1**.

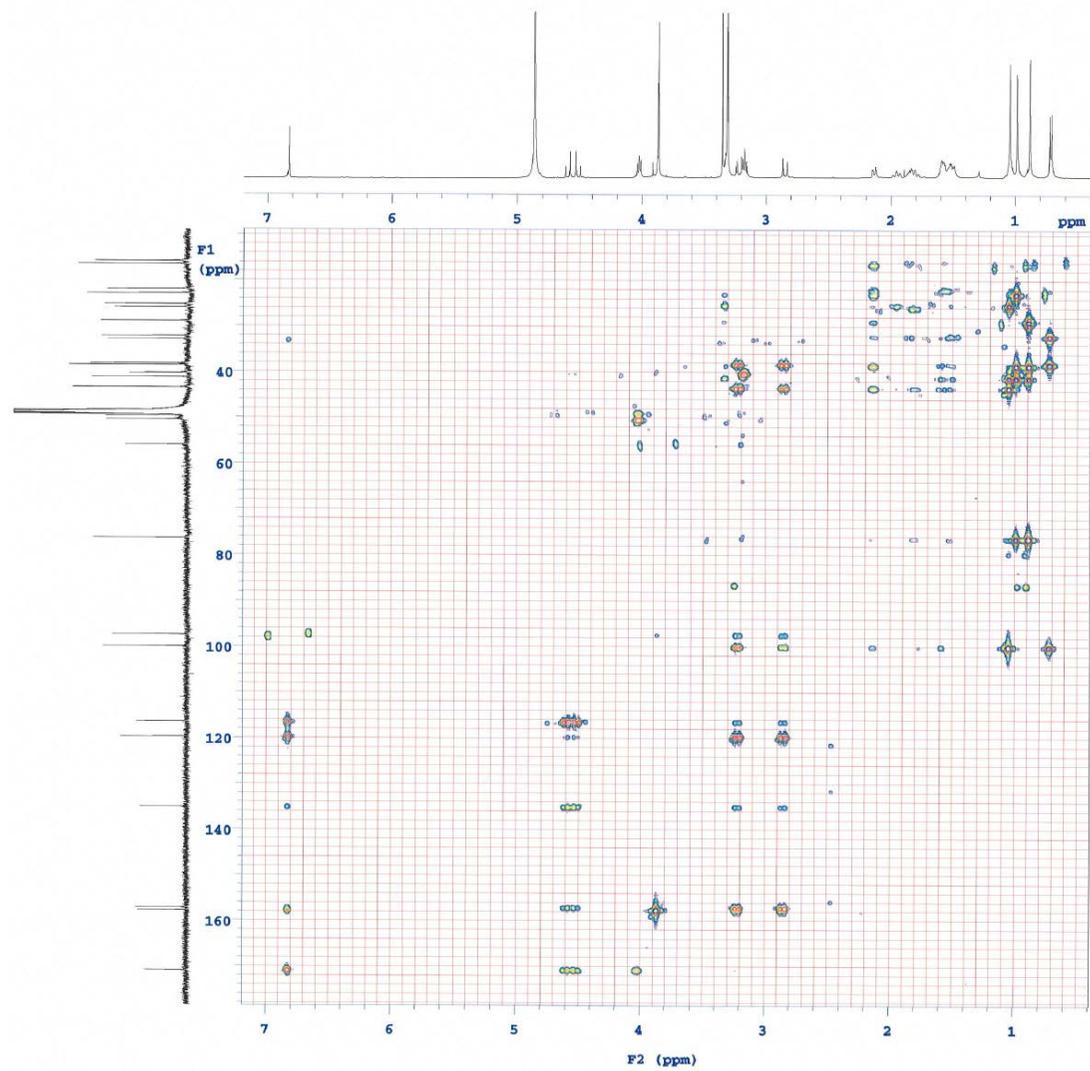


Figure S13 HMBC spectrum of methylated **1**.

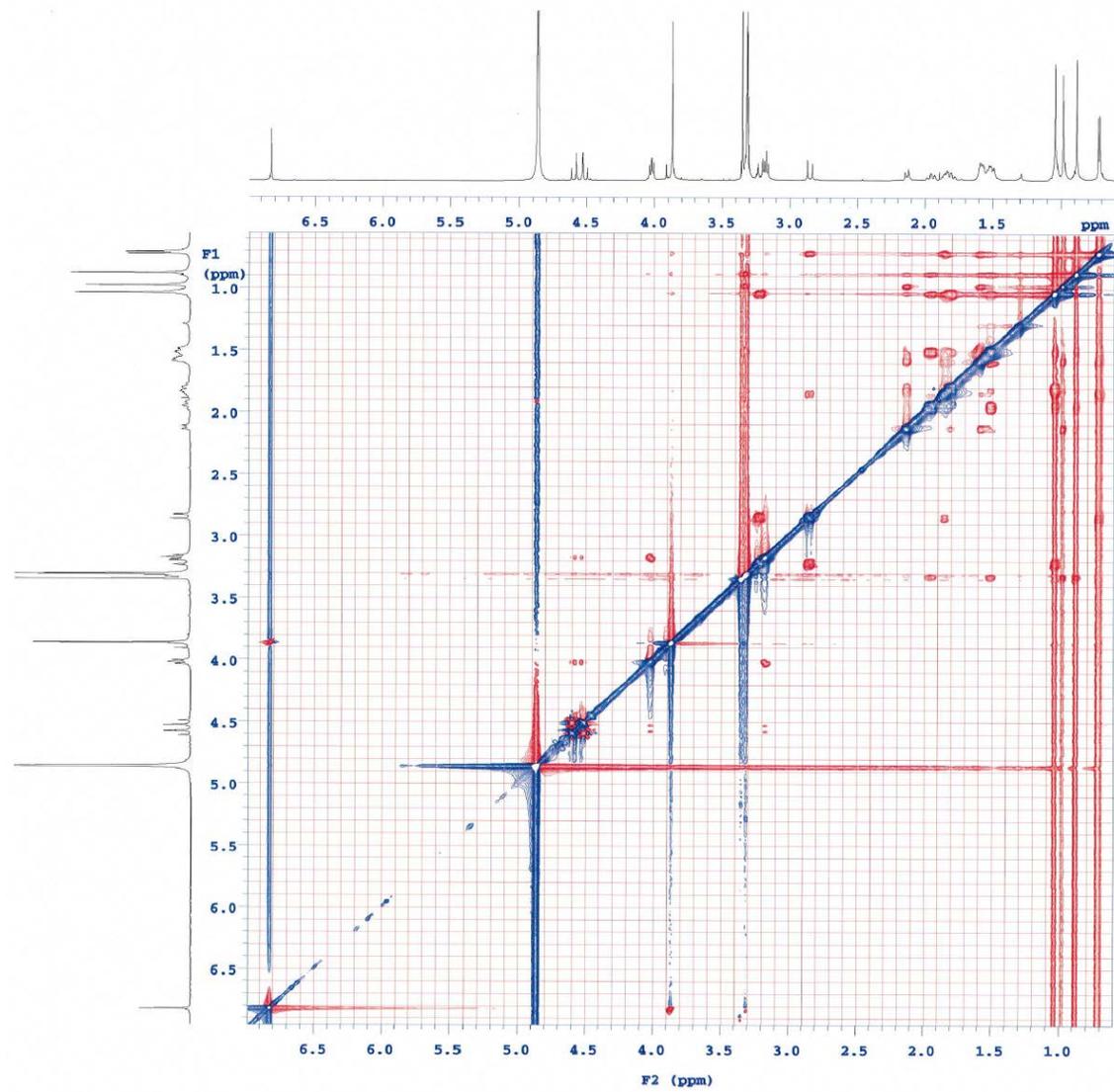


Figure S14 NOESY spectrum of methylated 1.

T3-3-5Me\_0427P1  
f23793\_011 42 (3.042) Cm (41:44)

1: TOF MS ES-  
7.30e+005

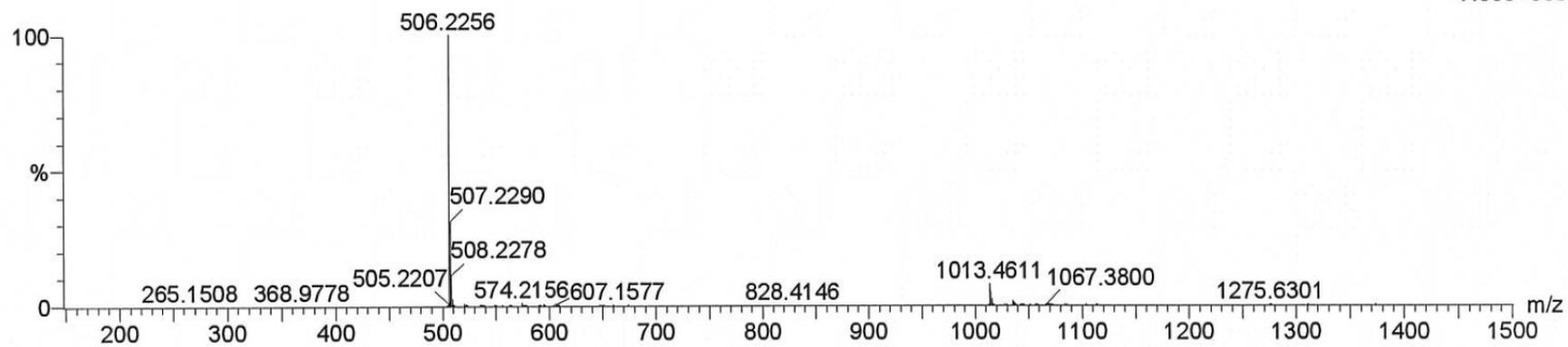


Figure S15 High-resolution mass spectrum of methylated **1** (Negative ion mode).

f23793/T3-3-8  
in CD3OD

Sample Name:  
f23793T338  
Archive directory:  
Sample directory:  
FidFile: f23793T338\_042912\_H

Pulse Sequence: Proton (s2pul)  
Solvent: cd3od  
Data collected on: Apr 29 2012

Temp. 25.0 C / 298.1 K  
Operator: walkup  
VNMR5-500 \*Agilent-VNMR500\*

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 8012.8 Hz  
16 repetitions  
OBSERVE H1. 499.7244722 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 0 min 55 sec

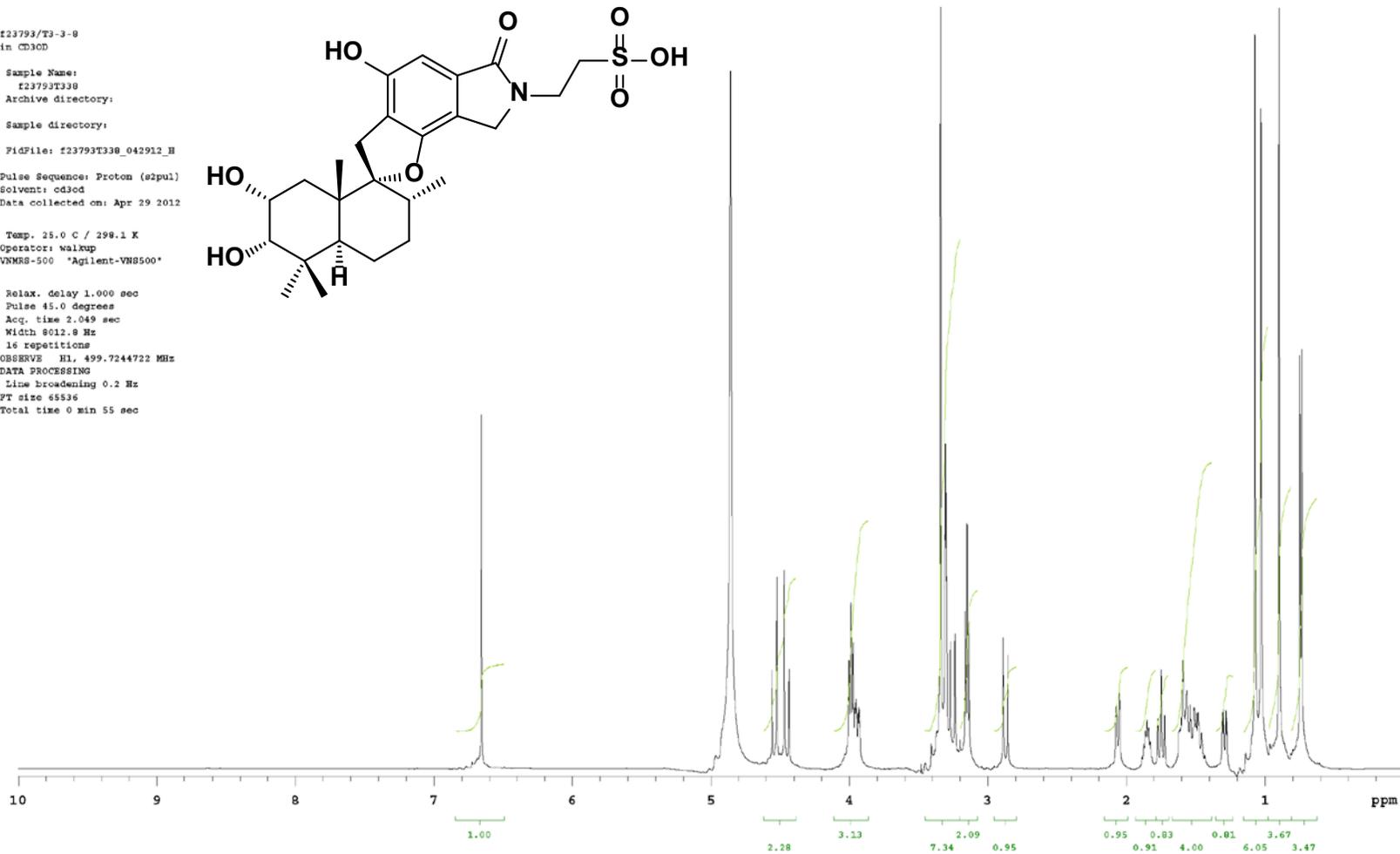
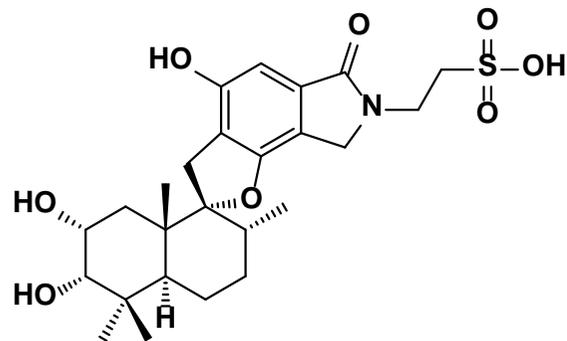


Figure S16 <sup>1</sup>H NMR spectrum of 2.

f23793/T3-3-8  
in CD3OD  
Sample Name:  
f23793T338  
Archive directory:  
Sample directory:  
FIDFile: f23793T338\_042912\_C  
Pulse Sequence: Carbon (s2pul)  
Solvent: cd3od  
Data collected on: Apr 29 2012  
Temp. 25.0 C / 298.1 K  
Operator: walkup  
VNMR-500 "Agilent-VNMR500"  
Relax. delay 3.500 sec  
Pulse 45.0 degrees  
Acq. time 1.000 sec  
Width 30487.8 Hz  
1820 repetitions  
OBSERVE C13, 125.6550185 MHz  
DECOUPLE H1, 499.7269709 MHz  
Power 31 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 65536  
Total time 125 hr, 1 min

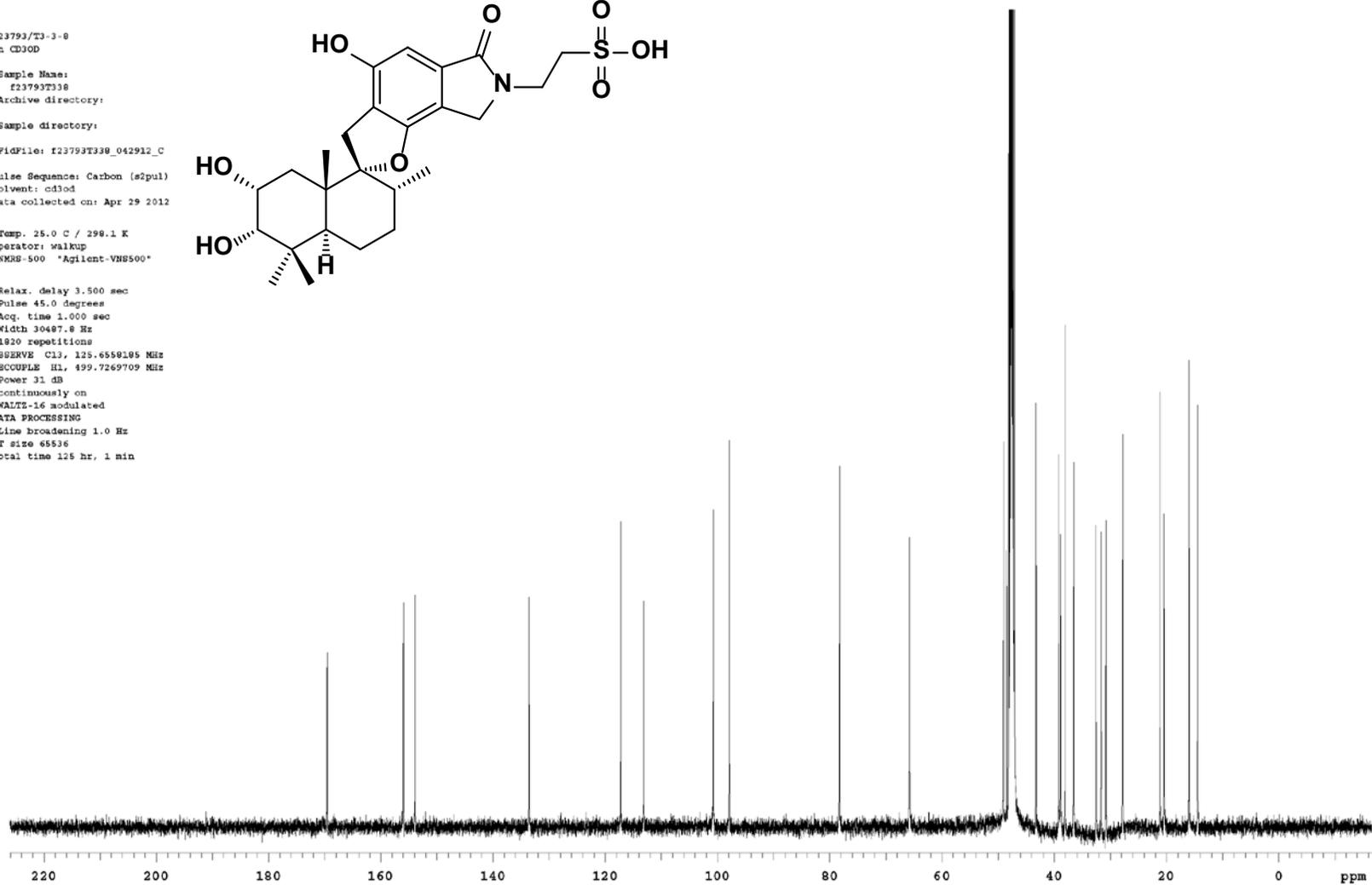
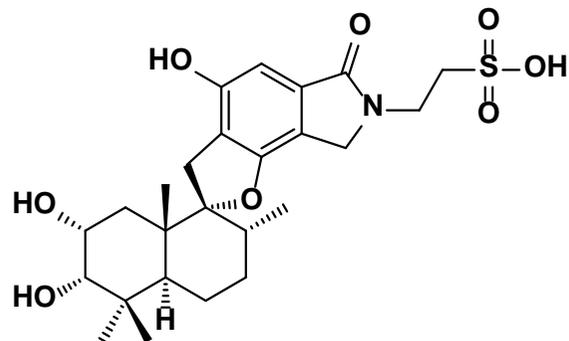


Figure S17 <sup>13</sup>C NMR spectrum of 2.

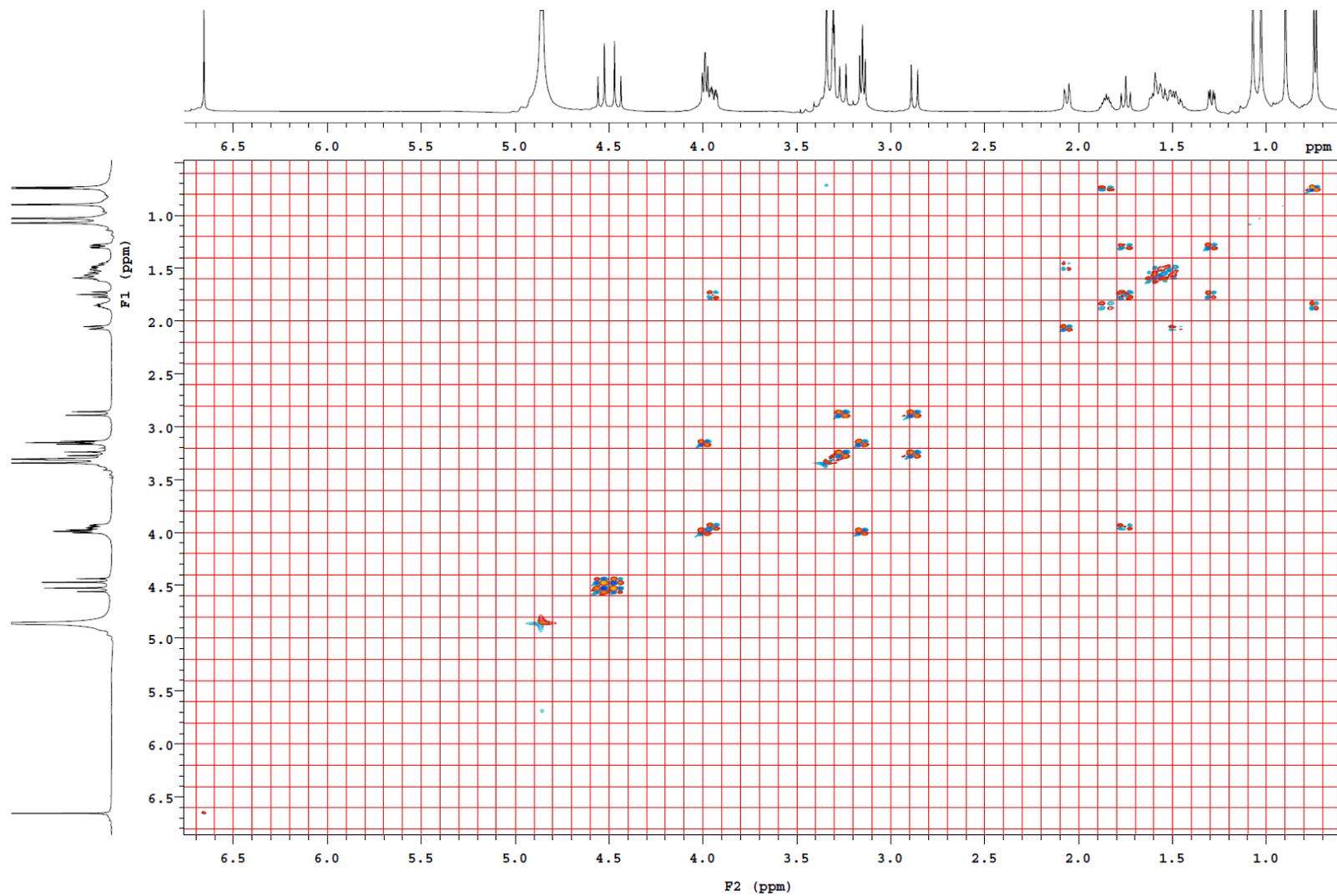


Figure S18 DQF-COSY spectrum of **2**.

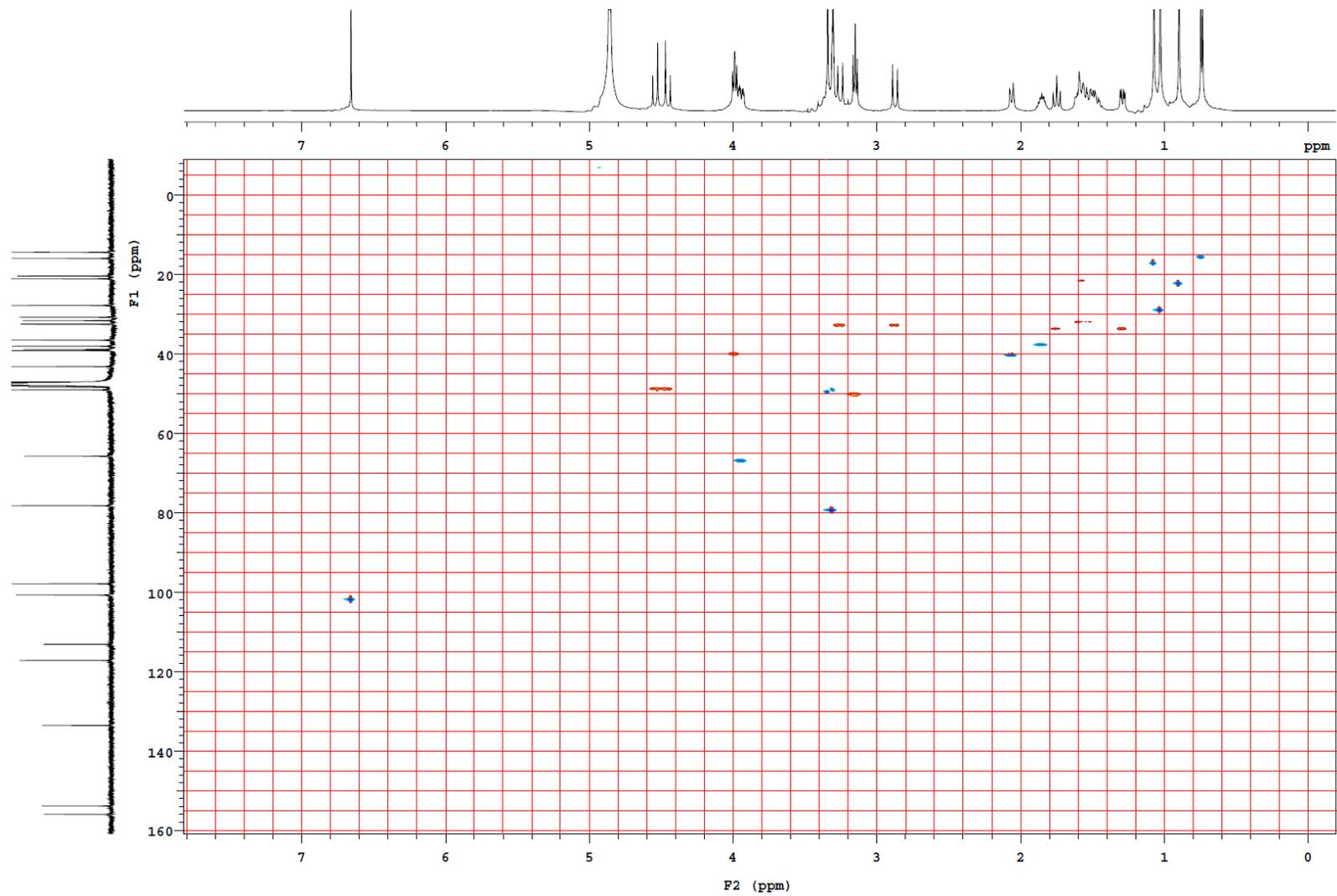


Figure S19 HSQC spectrum of **2**.

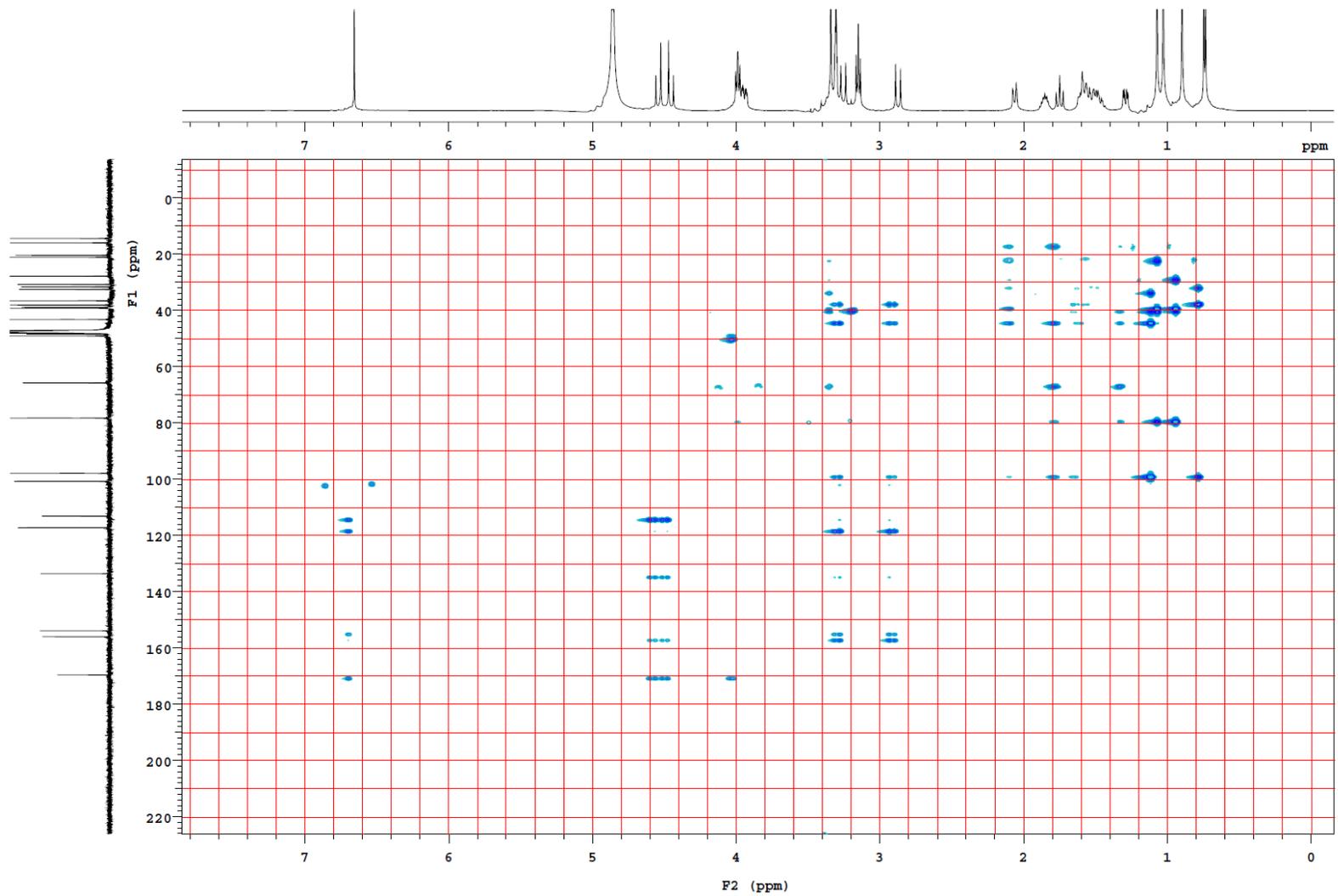


Figure S20 HMBC spectrum of 2.

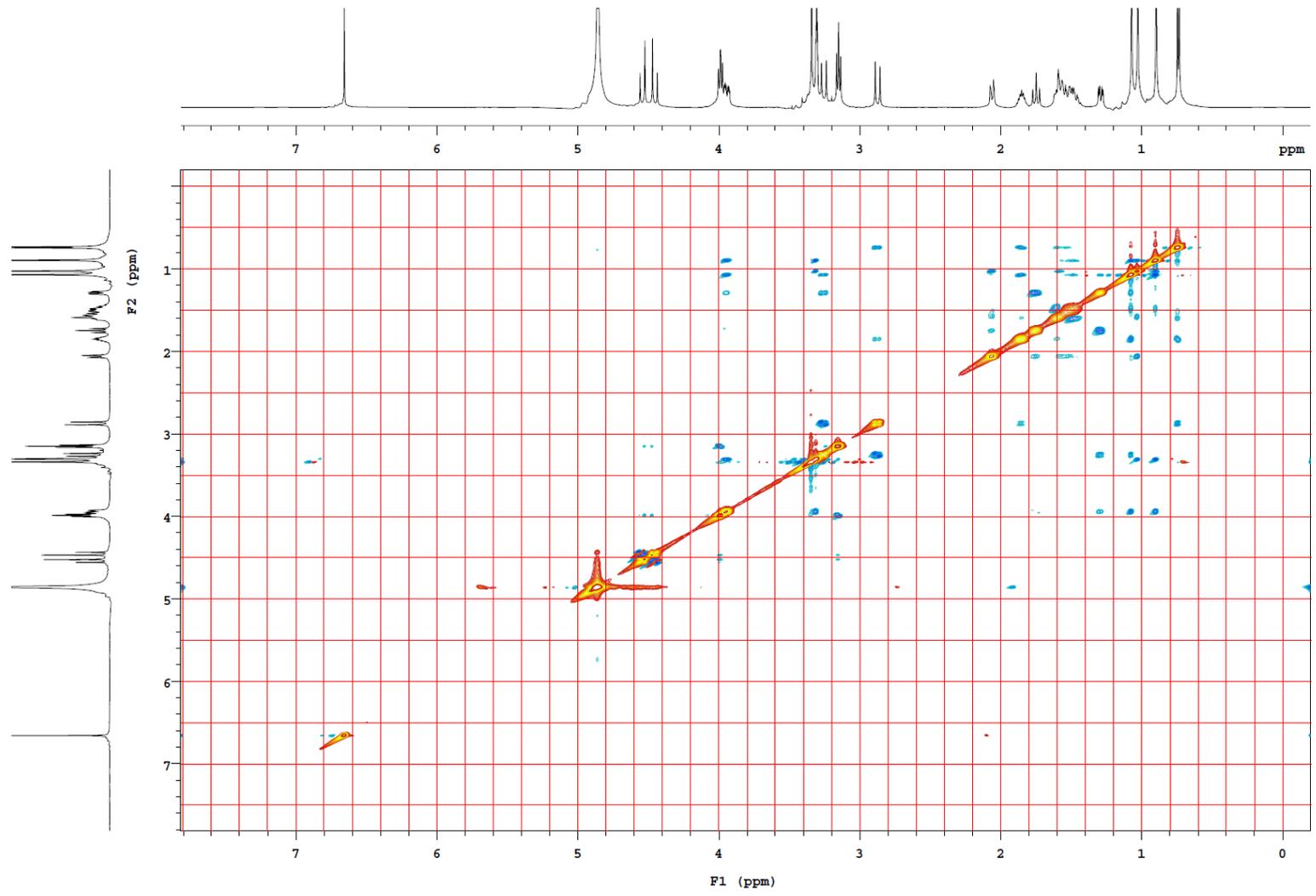


Figure S21 NOESY spectrum of **2**.

f23793\_001 31 (2.235) Cm (30:31)

1: TOF MS ES-  
2.40e+005

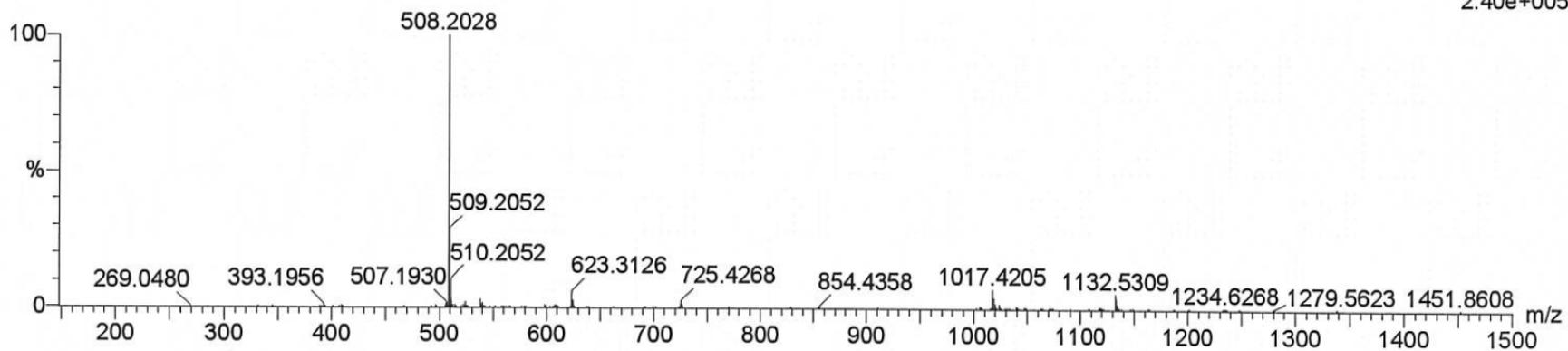


Figure S22 High-resolution mass spectrum of **2** (Negative ion mode).

f23793/T3-3-12  
in CD3OD

Sample Name:  
f23793T3312  
Archive directory:

Sample directory:

FidFile: f23793T3312\_051612\_H

Pulse Sequence: Proton (s2pul)  
Solvent: cd3od  
Data collected on: May 16 2012

Temp: 25.0 C / 298.1 K  
Operator: walkup  
VNMR-600 \*Agilent-VNMR600\*

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 9615.4 Hz  
16 repetitions  
OBSERVE CH: 599.8115746 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min 49 sec

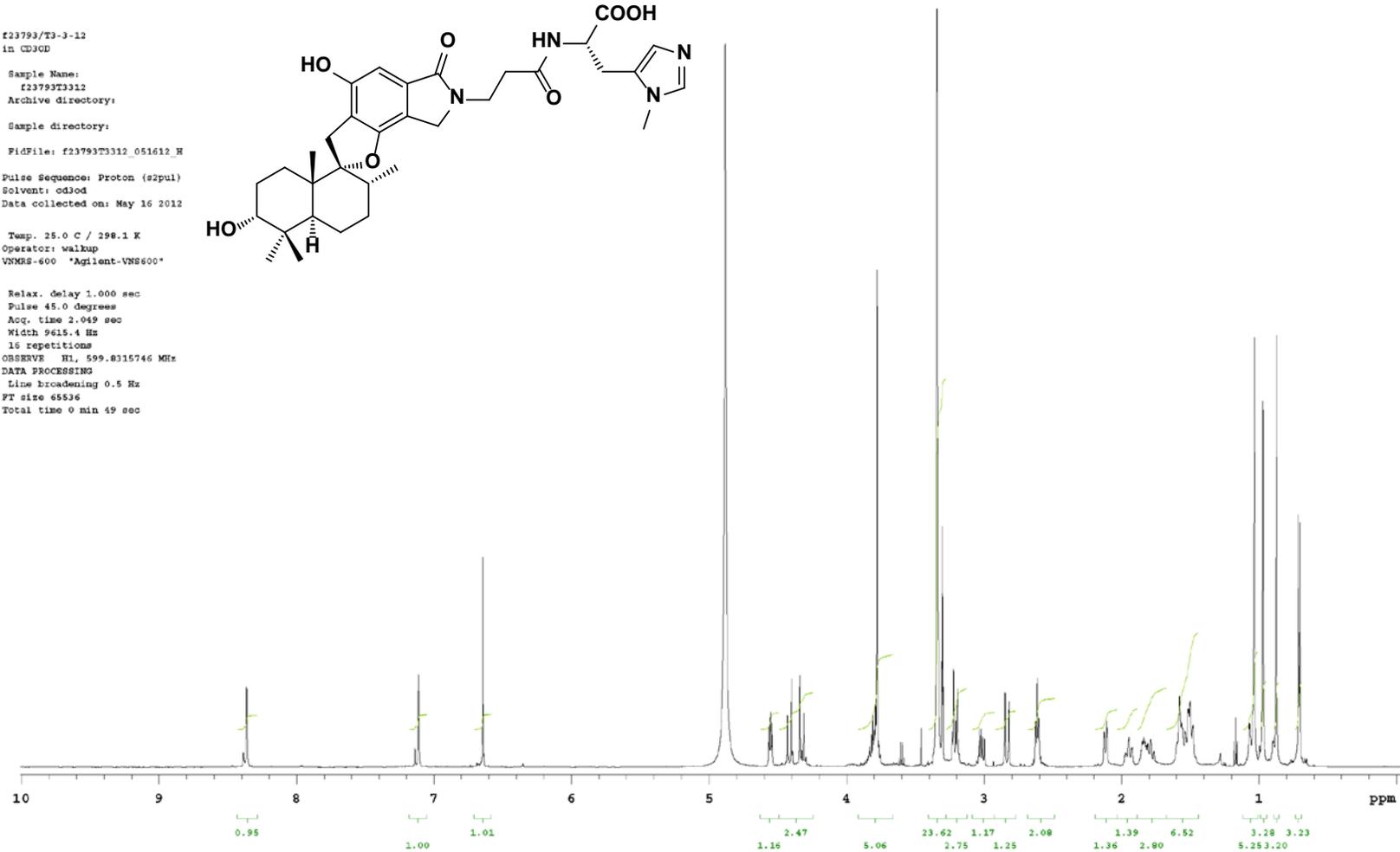
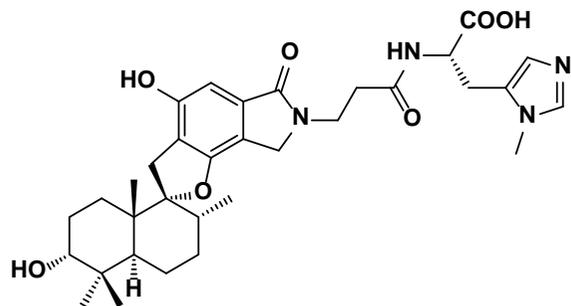


Figure S23  $^1\text{H}$  NMR spectrum of **3**.

f23793/T3-3-12  
in CD3OD

Sample Name:  
f23793T3312  
Archive directory:

Sample directory:

FidFile: f23793T3312\_051712\_C

Pulse Sequence: Carbon (s2pul)  
Solvent: cd3od  
Data collected on: May 16 2012

Temp. 25.0 C / 298.1 K  
Operator: walkup  
VNMR5-600 "Agilent-VNMR600"

Relax. delay 3.500 sec  
Pulse 45.0 degrees  
Acq. time 1.000 sec  
Width 36764.7 Hz  
4288 repetitions  
OBSERVE C13, 150.8277694 MHz  
DECOUPLE H1, 599.8345740 MHz  
Power 32 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 5.0 Hz  
FT size 65536  
Total time 125 hr, 1 min

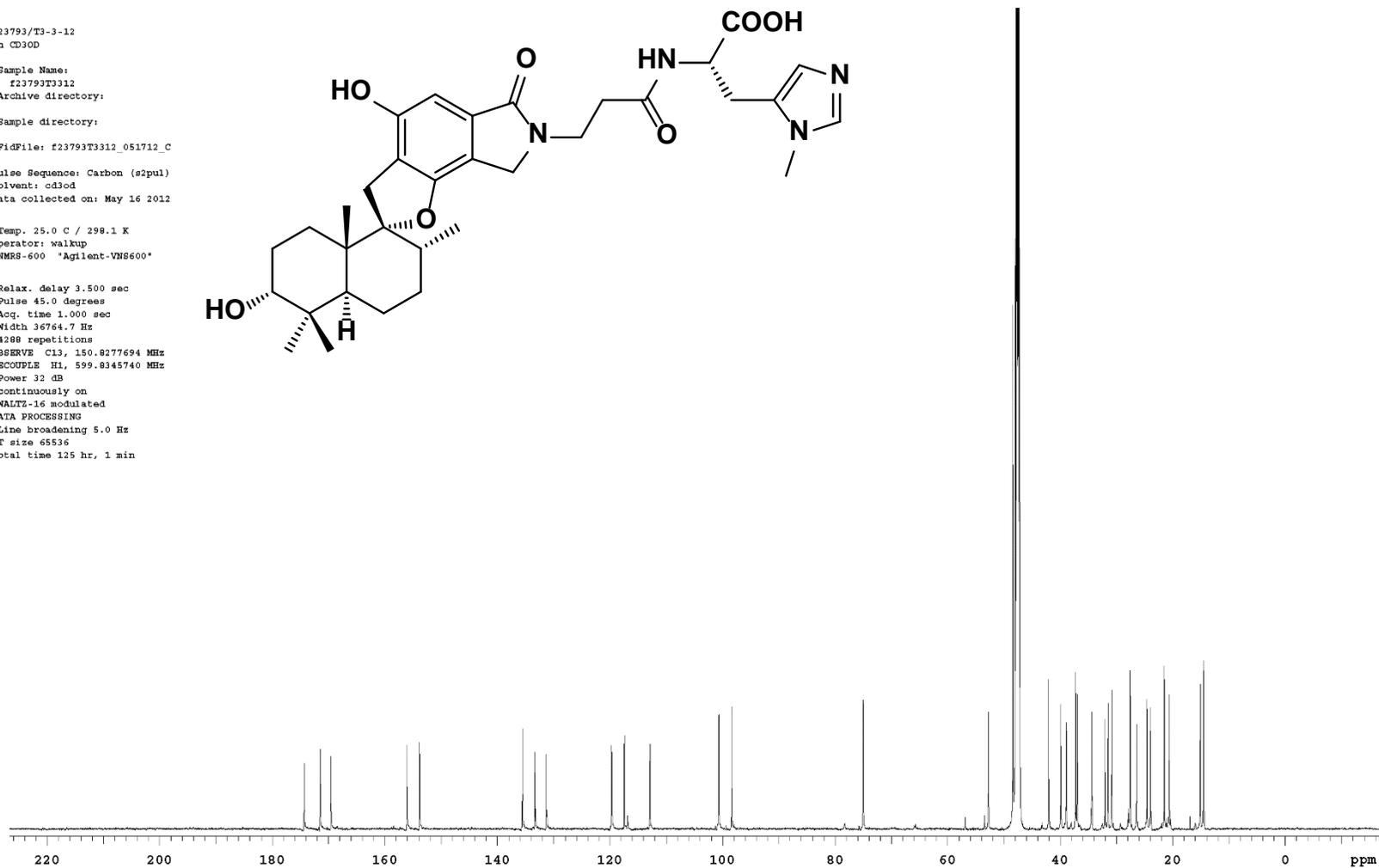
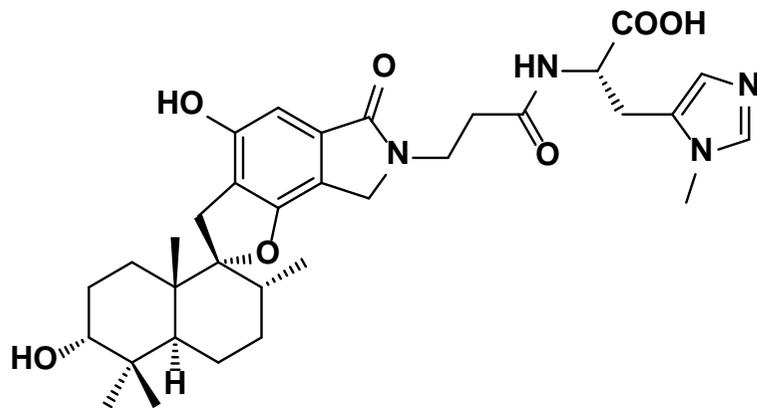


Figure S24 <sup>13</sup>C NMR spectrum of 3.

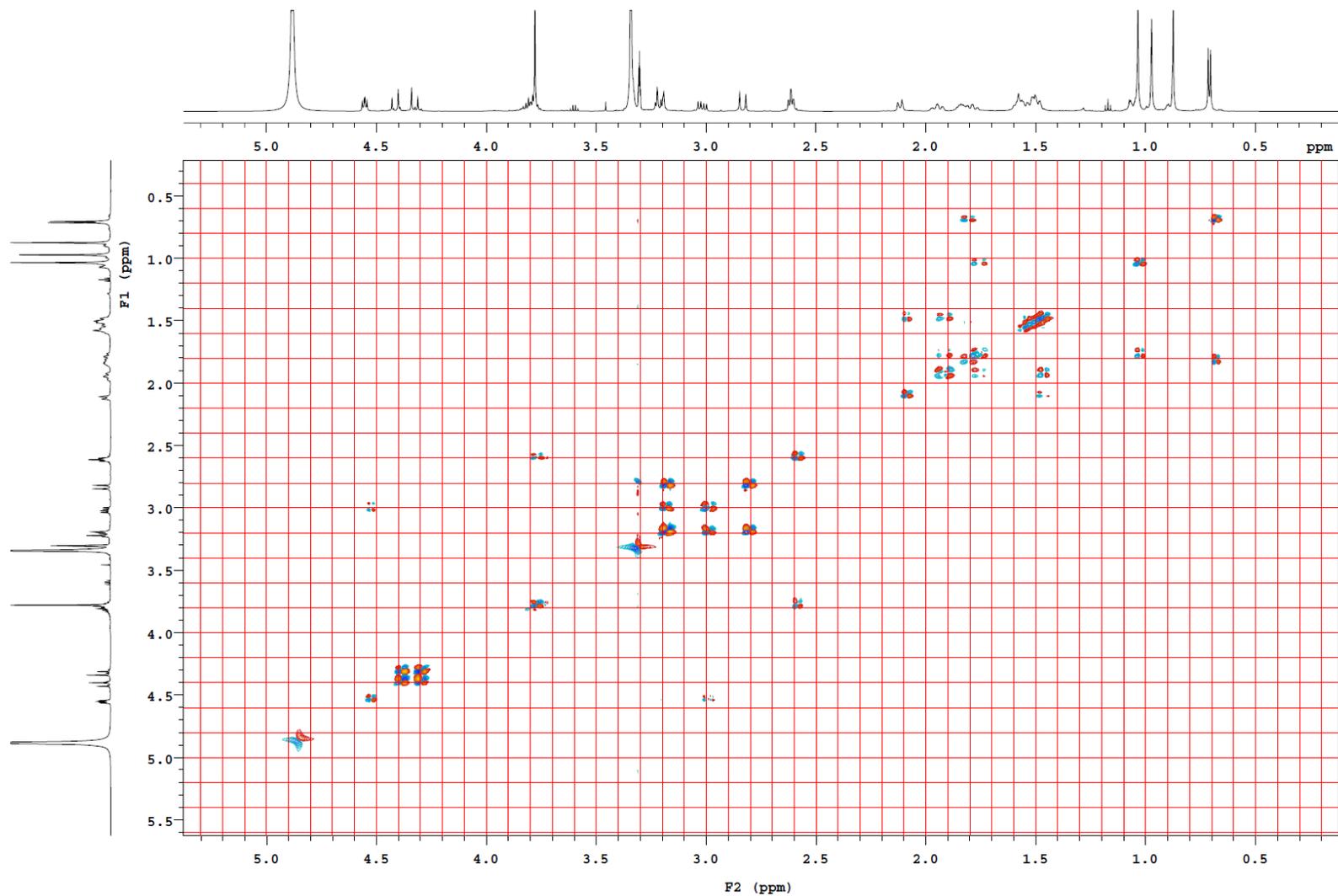


Figure S25 DQF-COSY spectrum of **3**.

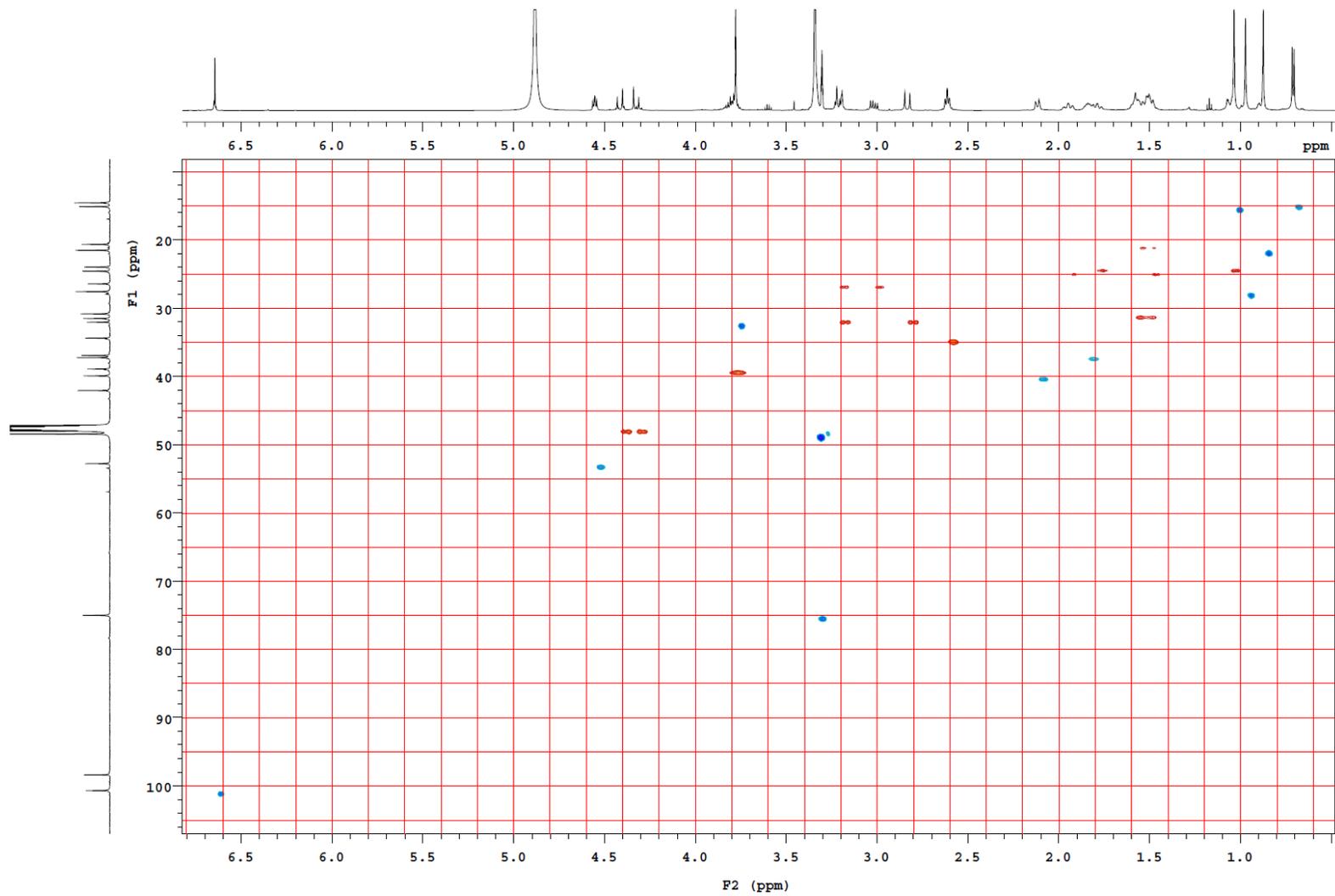


Figure S26 HSQC spectrum of **3**.

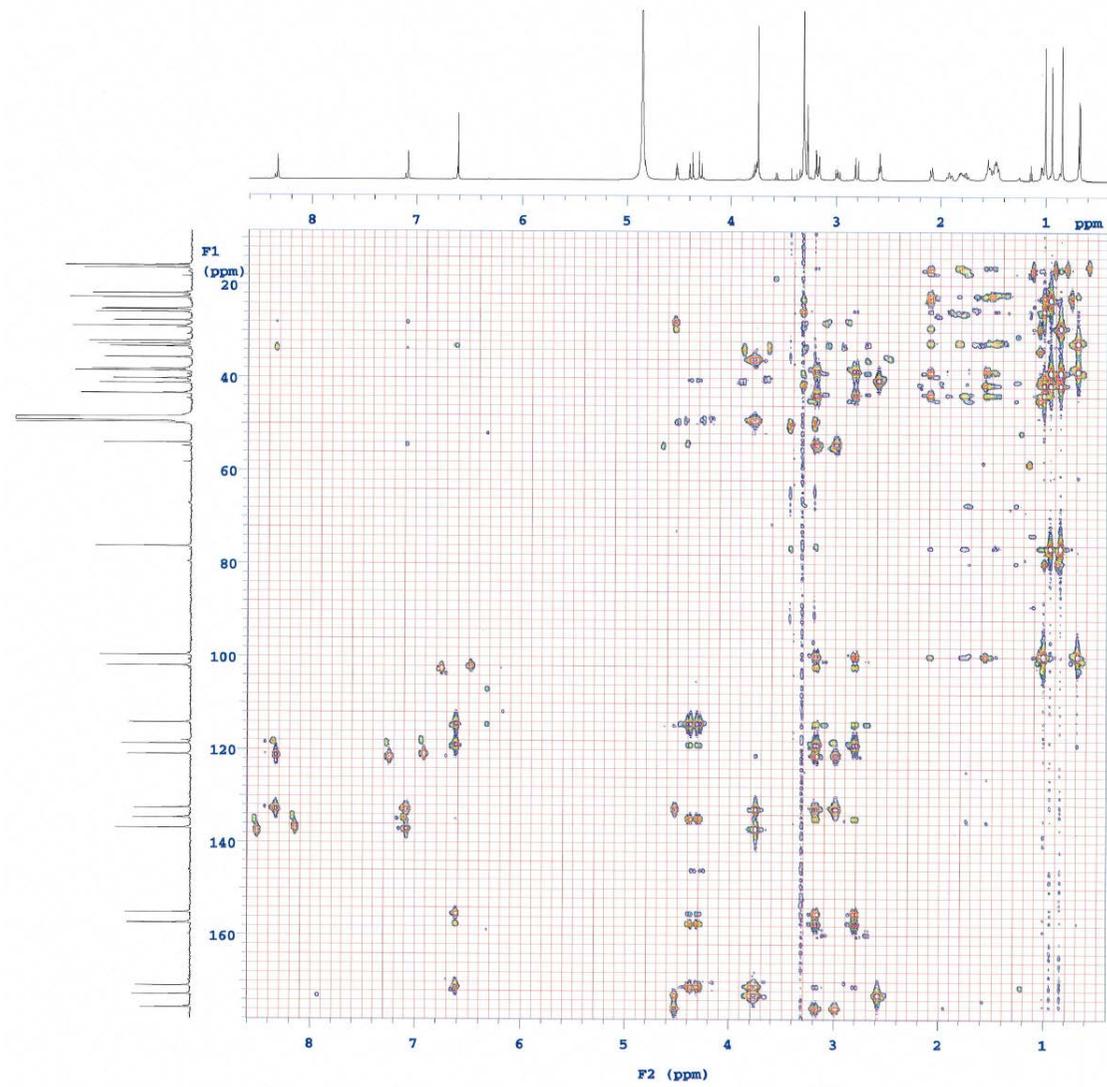


Figure S27 HMBC spectrum of 3.

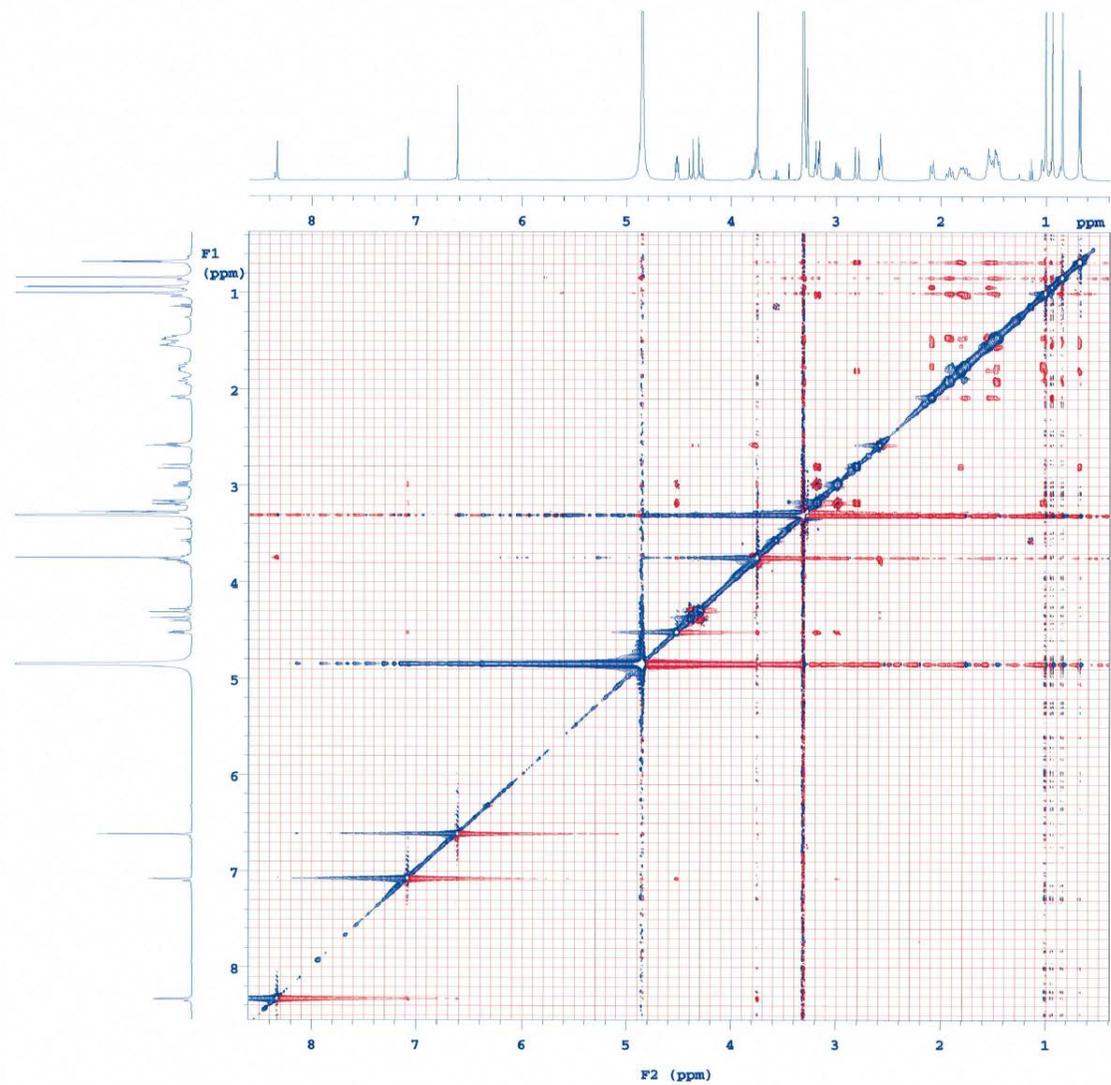


Figure S28 NOESY spectrum of 3.

T3-3-12  
f23793\_017 35 (2.522)

1: TOF MS ES-  
1.21e+005

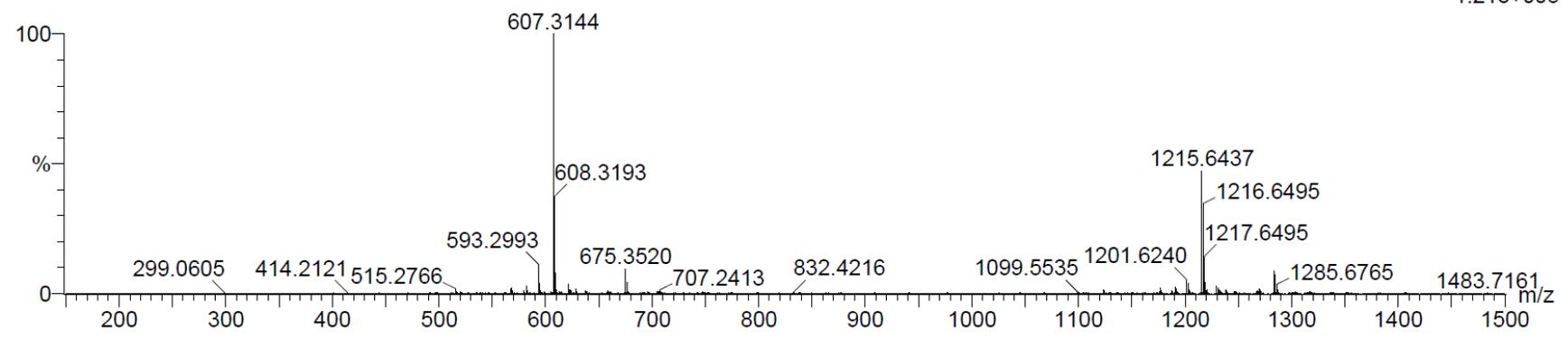


Figure S29 High-resolution mass spectrum of **3** (Negative ion mode).