

Supporting Information

Dimeric Prenylated C₆-C₃ Compounds from the Stem Bark of *Illicium oligandrum*

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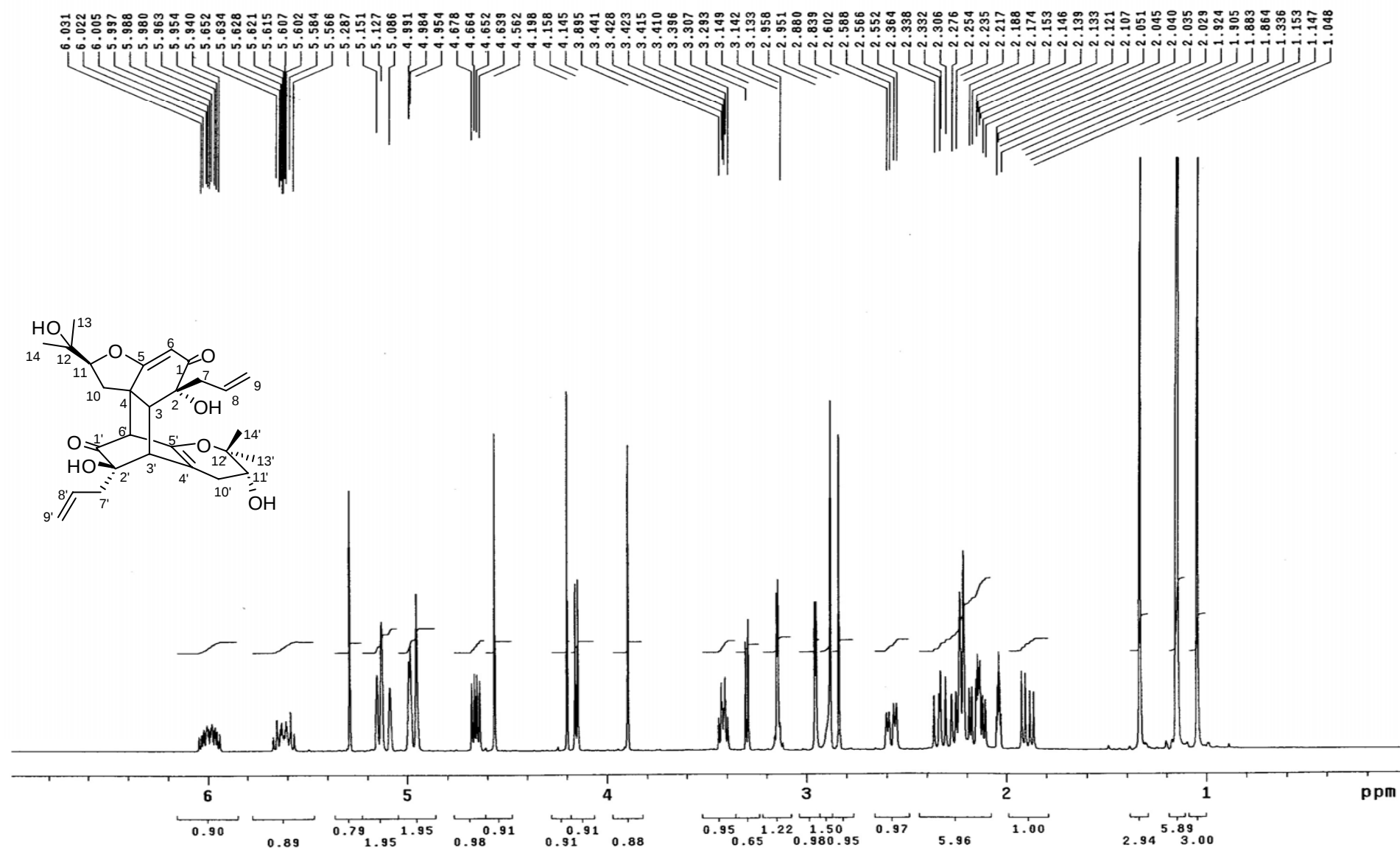
Corresponding author. Tel. 86-10-63165324. Fax: 86-10-63017757

Email address: yushishan@imm.ac.cn

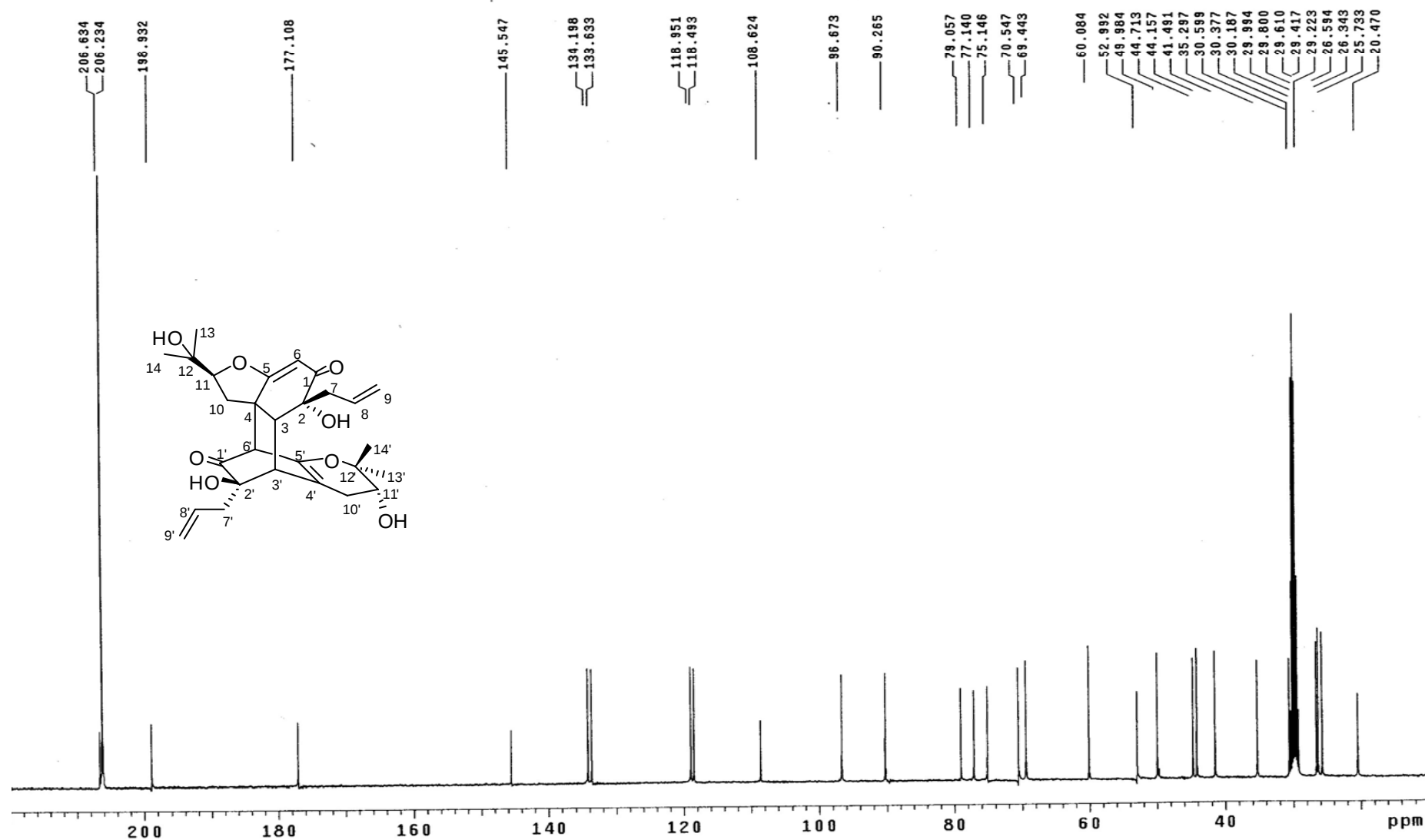
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S1 ^1H NMR spectrum (400 MHz) of compound **1** in acetone- d_6



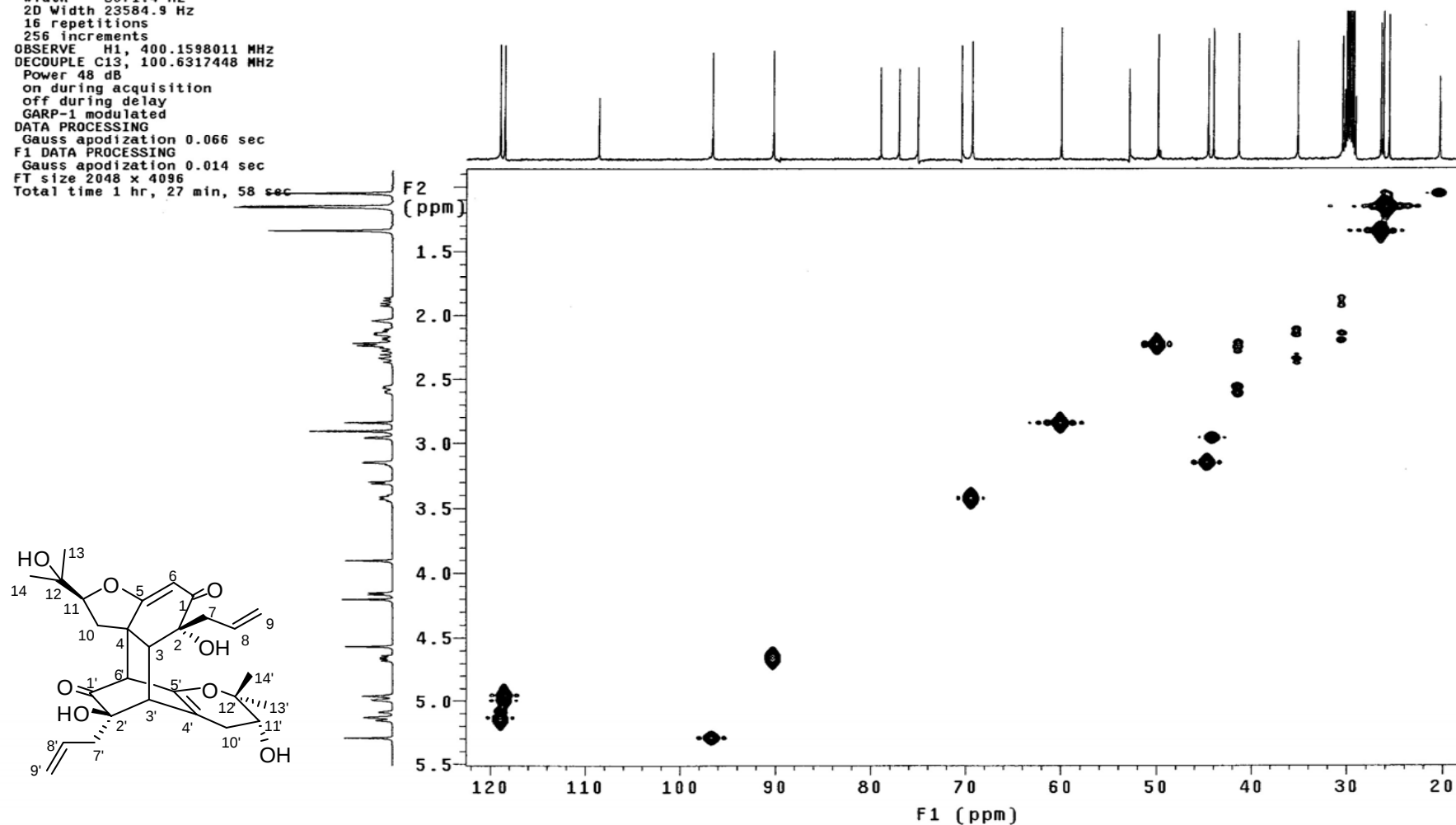
S2 ^{13}C NMR spectrum (100 MHz) of compound **1** in acetone- d_6



S3 HSQC spectrum (400 MHz) of compound **1** in acetone-*d*₆

Solvent: Acetone
Temp. 25.0 C / 298.1 K
Mercury-400BB "NMR400"

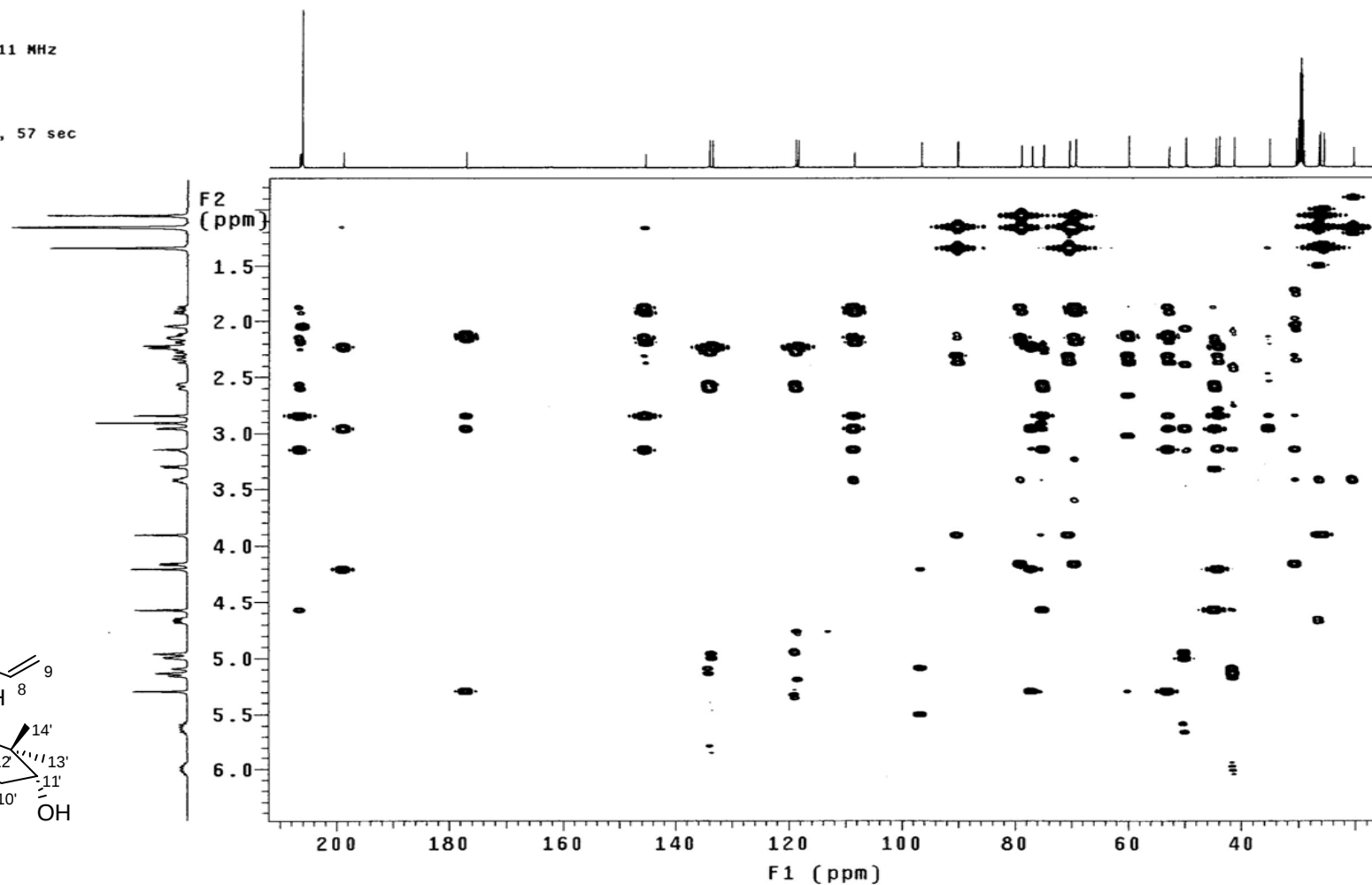
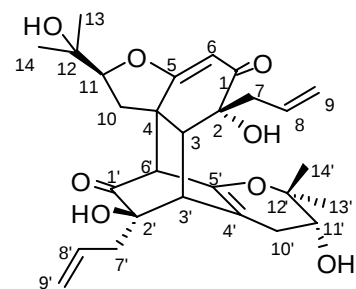
Relax. delay 1.000 sec
Acq. time 0.143 sec
Width 3571.4 Hz
2D Width 23584.9 Hz
16 repetitions
256 increments
OBSERVE H1, 400.1598011 MHz
DECOUPLE C13, 100.6317448 MHz
Power 48 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Gauss apodization 0.066 sec
F1 DATA PROCESSING
Gauss apodization 0.014 sec
FT size 2048 x 4096
Total time 1 hr, 27 min, 58 sec



S4 HMBC spectrum (400 MHz) of compound **1** in acetone-*d*₆

Solvent: Acetone
Temp. 25.0 C / 298.1 K
Mercury-400BB "NMR400"

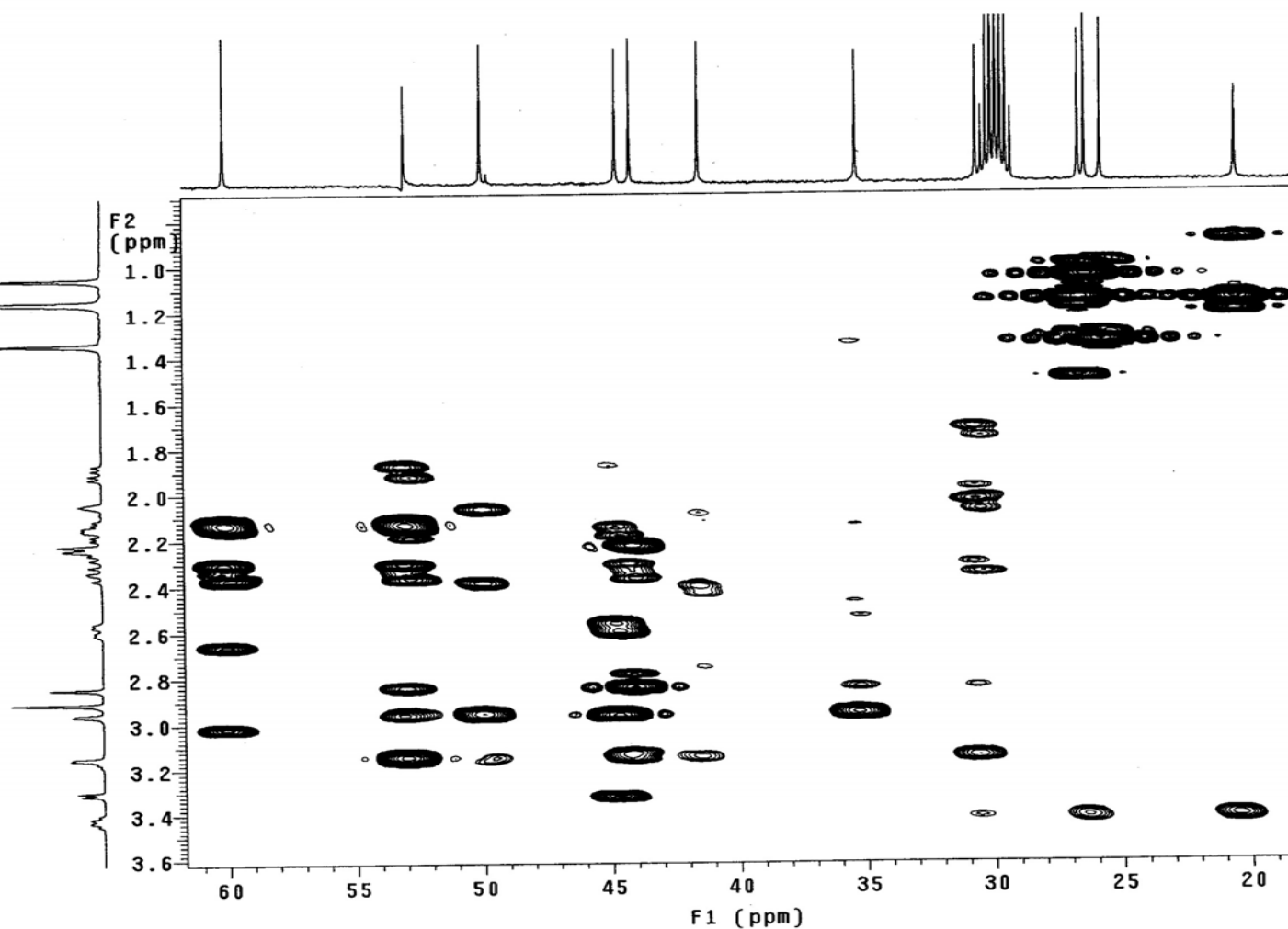
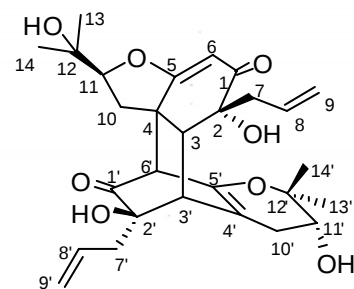
Relax. delay 1.000 sec
Acq. time 0.143 sec
Width 3571.4 Hz
2D Width 23696.7 Hz
32 repetitions
256 increments
OBSERVE H1, 400.1598011 MHz
DATA PROCESSING
Sine bell 0.071 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 4096
Total time 2 hr, 56 min, 57 sec



S4 HMBC spectrum (400 MHz) of compound **1** in acetone- d_6

Solvent: Acetone
Temp. 25.0 C / 298.1 K
Mercury-400BB "NMR400"

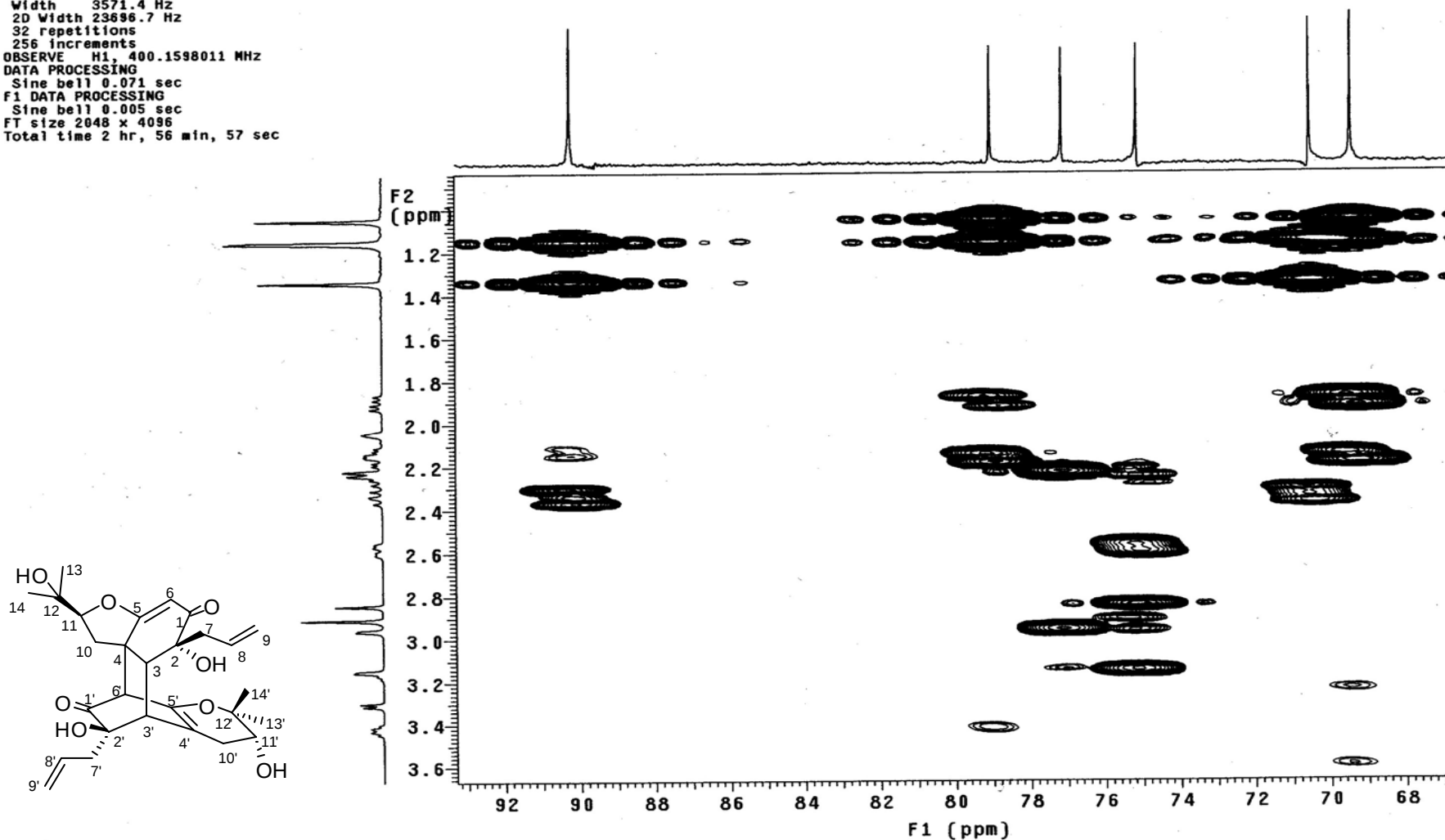
Relax. delay 1.000 sec
Acq. time 0.143 sec
Width 3571.4 Hz
2D Width 23696.7 Hz
32 repetitions
256 increments
OBSERVE H1, 400.1598011 MHz
DATA PROCESSING
Sine bell 0.071 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 4096
Total time 2 hr, 56 min, 57 sec



S4 HMBC spectrum (400 MHz) of compound **1** in acetone- d_6

Solvent: Acetone
Temp. 25.0 C / 298.1 K
Mercury-400BB "NMR400"

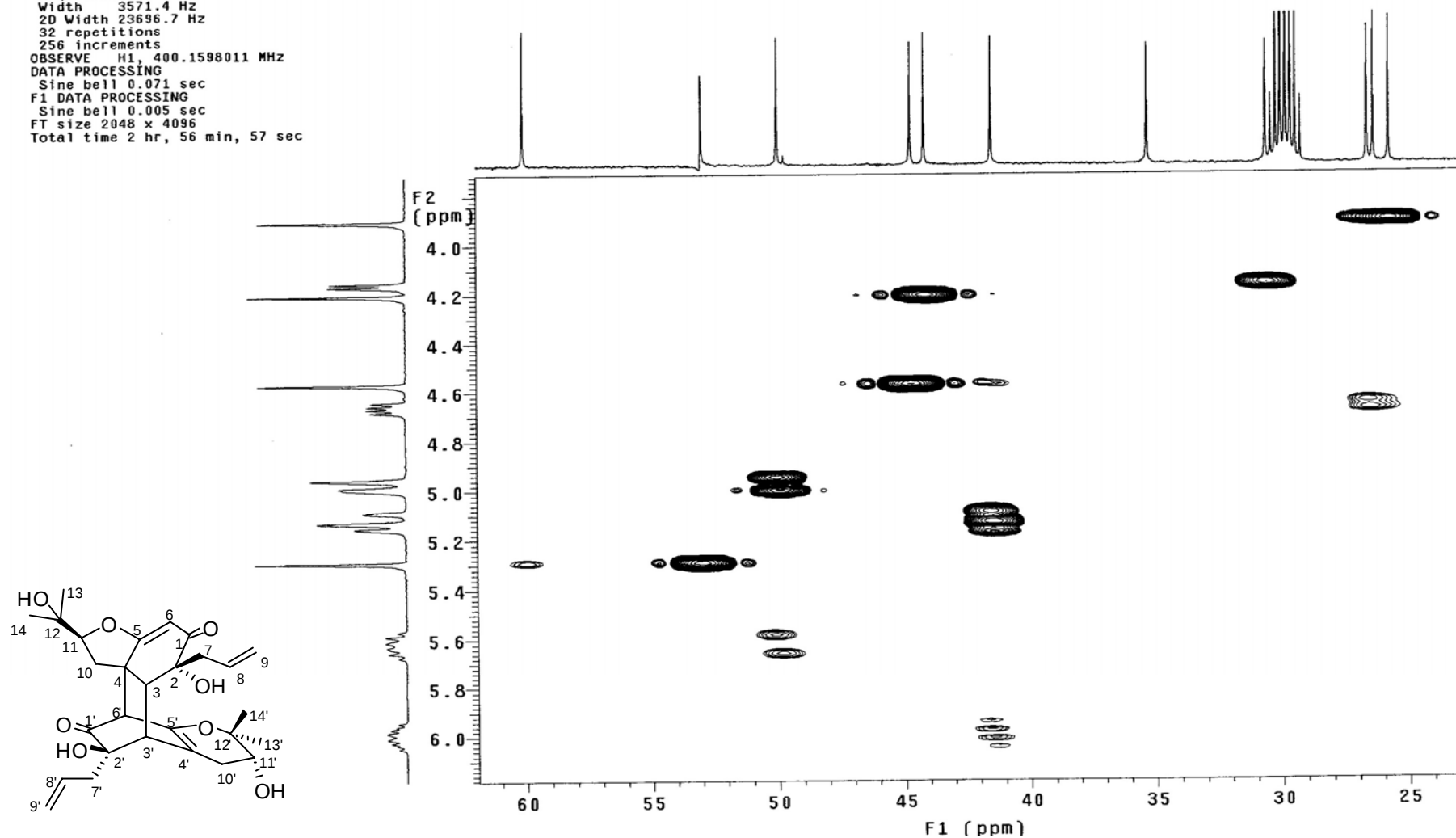
Relax. delay 1.000 sec
Acq. time 0.143 sec
Width 3571.4 Hz
2D Width 23696.7 Hz
32 repetitions
256 increments
OBSERVE H1, 400.1598011 MHz
DATA PROCESSING
Sine bell 0.071 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 4096
Total time 2 hr, 56 min, 57 sec



S4 HMBC spectrum (400 MHz) of compound **1** in acetone- d_6

Solvent: Acetone
Temp. 25.0 C / 298.1 K
Mercury-400BB "NMR400"

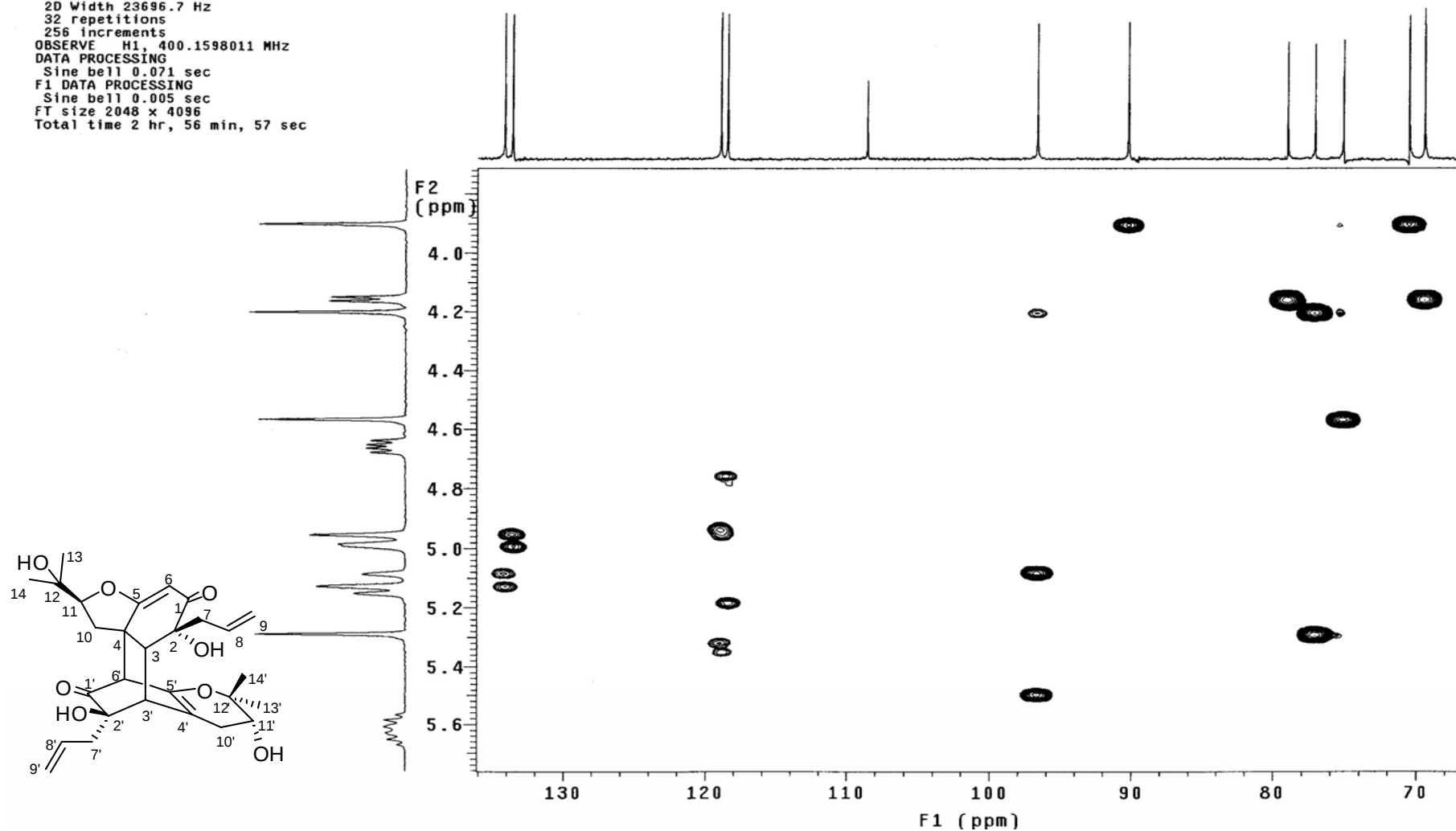
Relax. delay 1.000 sec
Acq. time 0.143 sec
Width 3571.4 Hz
2D Width 23696.7 Hz
32 repetitions
256 increments
OBSERVE H1, 400.1598011 MHz
DATA PROCESSING
Sine bell 0.071 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 4096
Total time 2 hr, 56 min, 57 sec



S4 HMBC spectrum (400 MHz) of compound **1** in acetone-*d*₆

Solvent: Acetone
Temp. 25.0 C / 298.1 K
Mercury-400BB "NMR400"

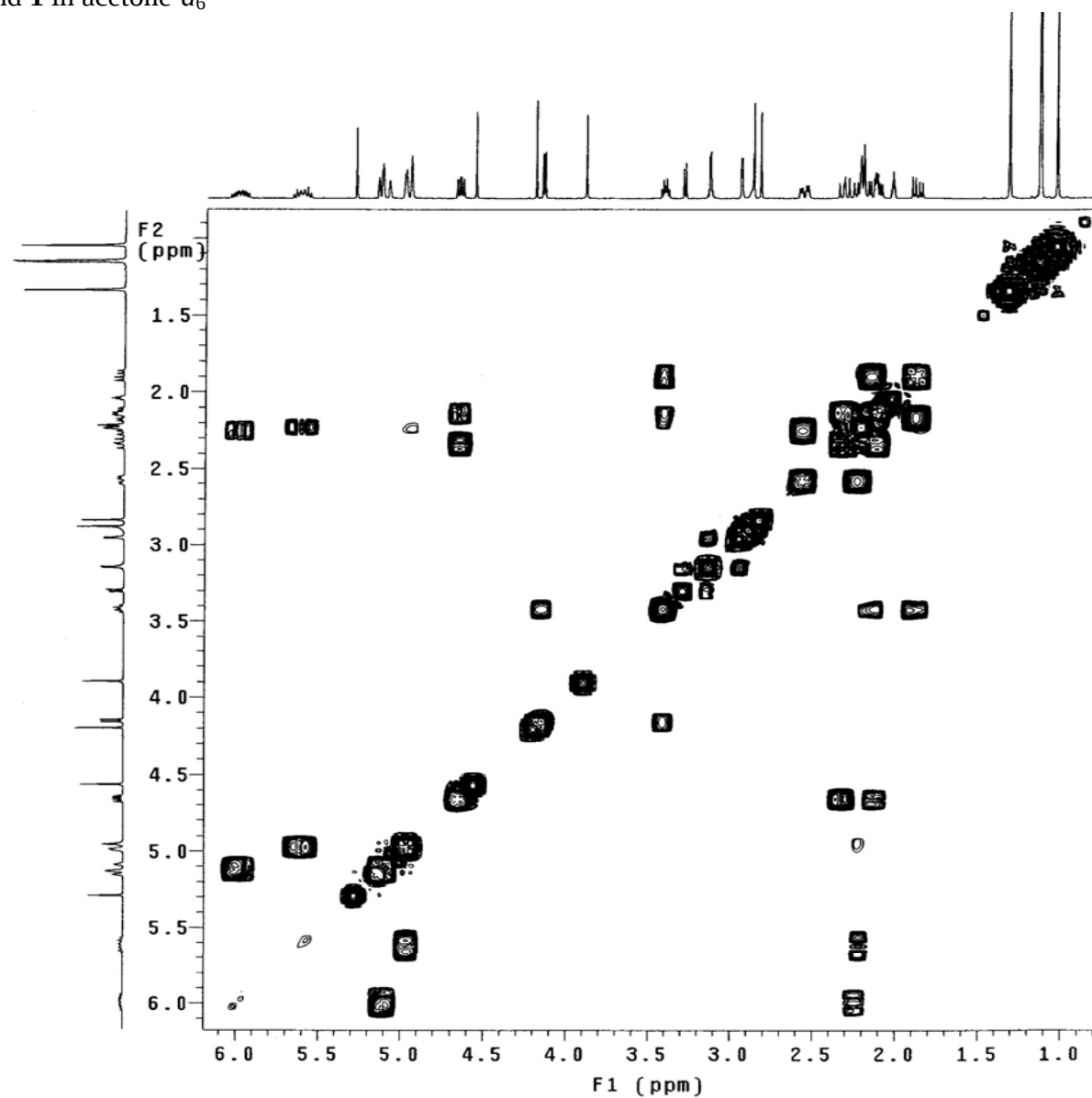
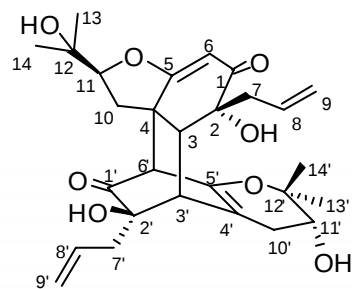
Relax. delay 1.000 sec
Acq. time 0.143 sec
Width 3571.4 Hz
2D Width 23696.7 Hz
32 repetitions
256 increments
OBSERVE H1, 400.1598011 MHz
DATA PROCESSING
Sine bell 0.071 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 4096
Total time 2 hr, 56 min, 57 sec



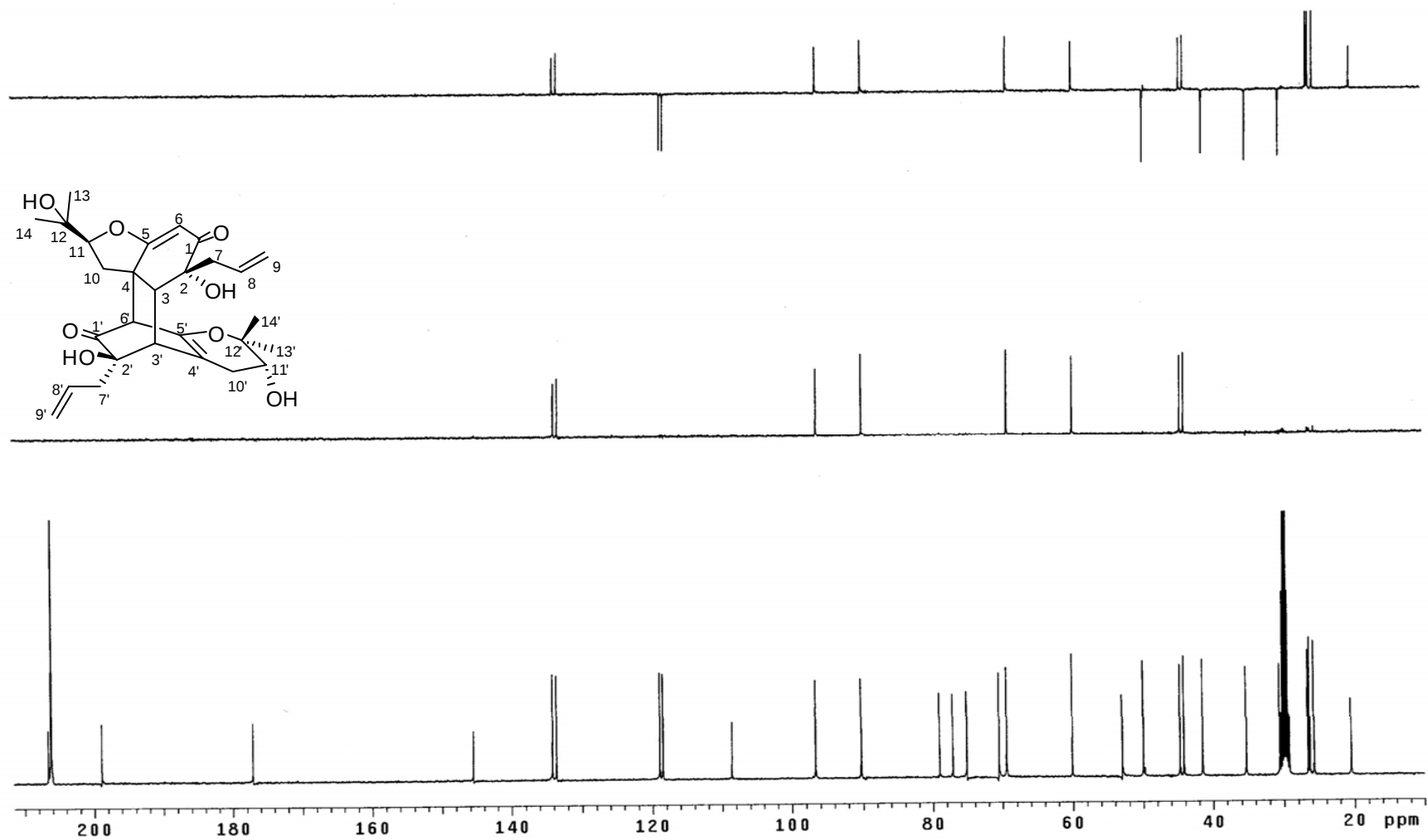
S5 gCOSY spectrum (400 MHz) of compound 1 in acetone- d_6

Solvent: acetone
Temp. 25.0 C / 298.1 K
Mercury-400BB "NMR400"

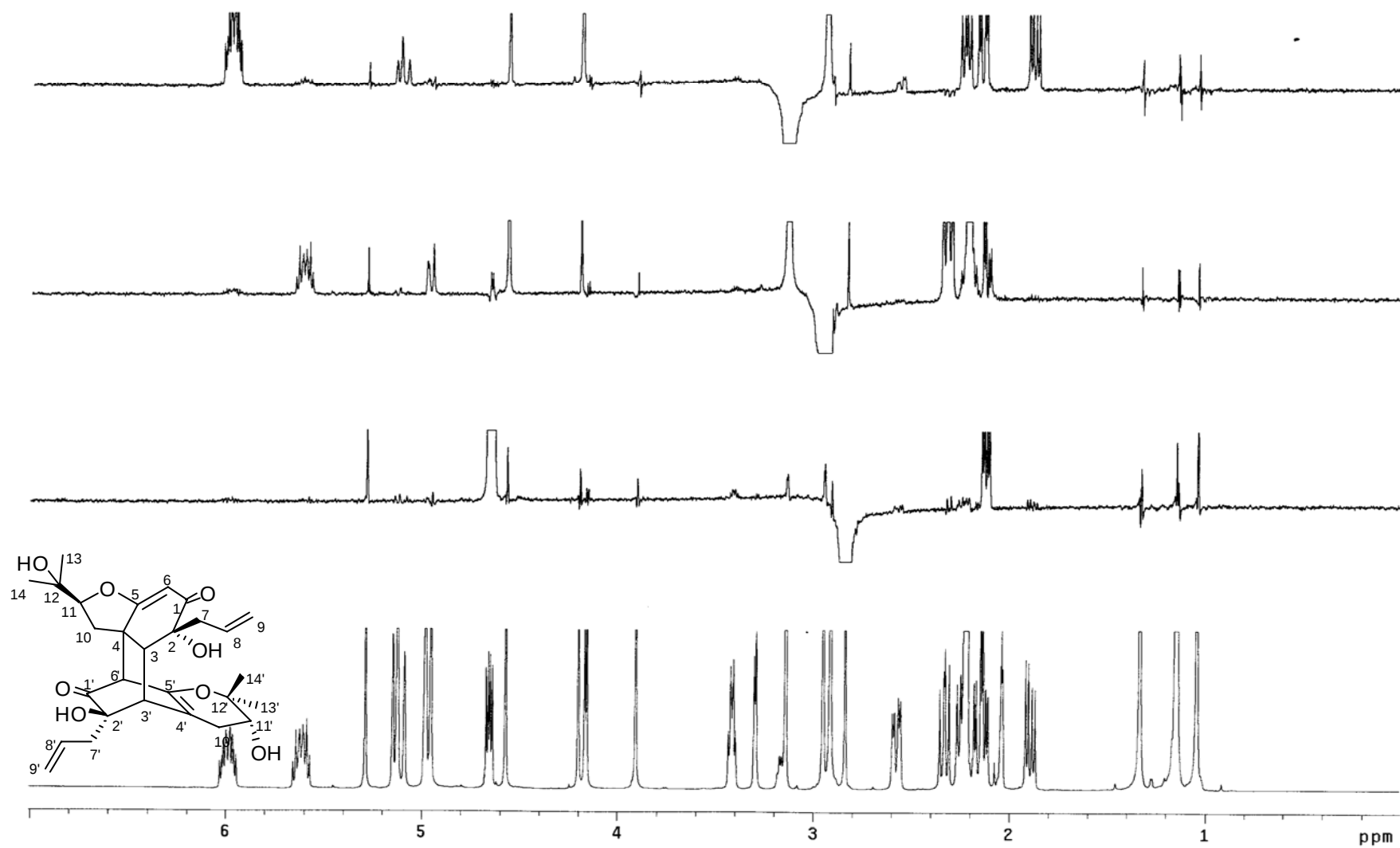
Relax. delay 1.000 sec
Acq. time 0.155 sec
Width 3301.4 Hz
2D Width 3301.4 Hz
8 repetitions
128 increments
OBSERVE H1, 400.1598012 MHz
DATA PROCESSING
Sq. sine bell 0.043 sec
F1 DATA PROCESSING
Sq. sine bell 0.021 sec
FT size 2048 x 2048
Total time 21 min, 40 sec



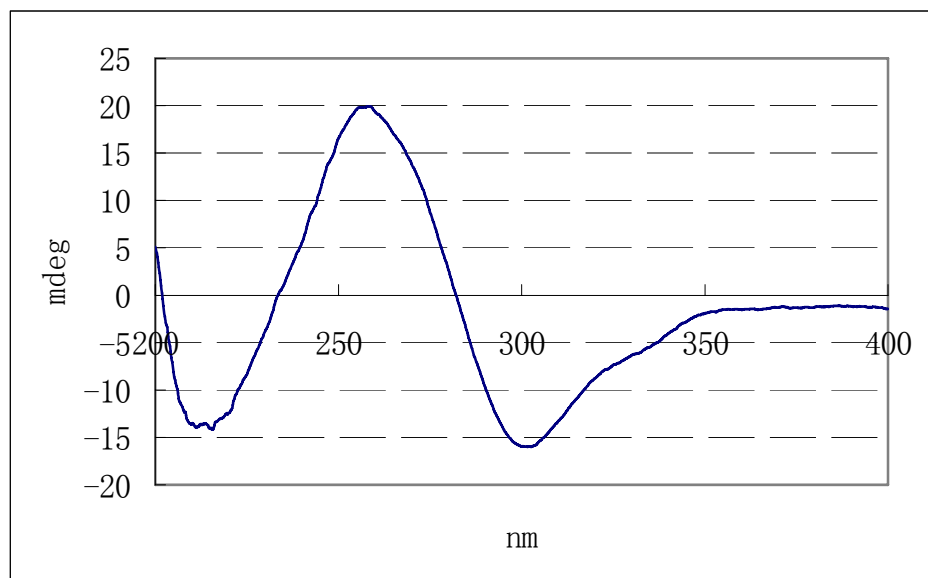
S6 DEPT spectrum (400 MHz) of compound **1** in acetone- d_6



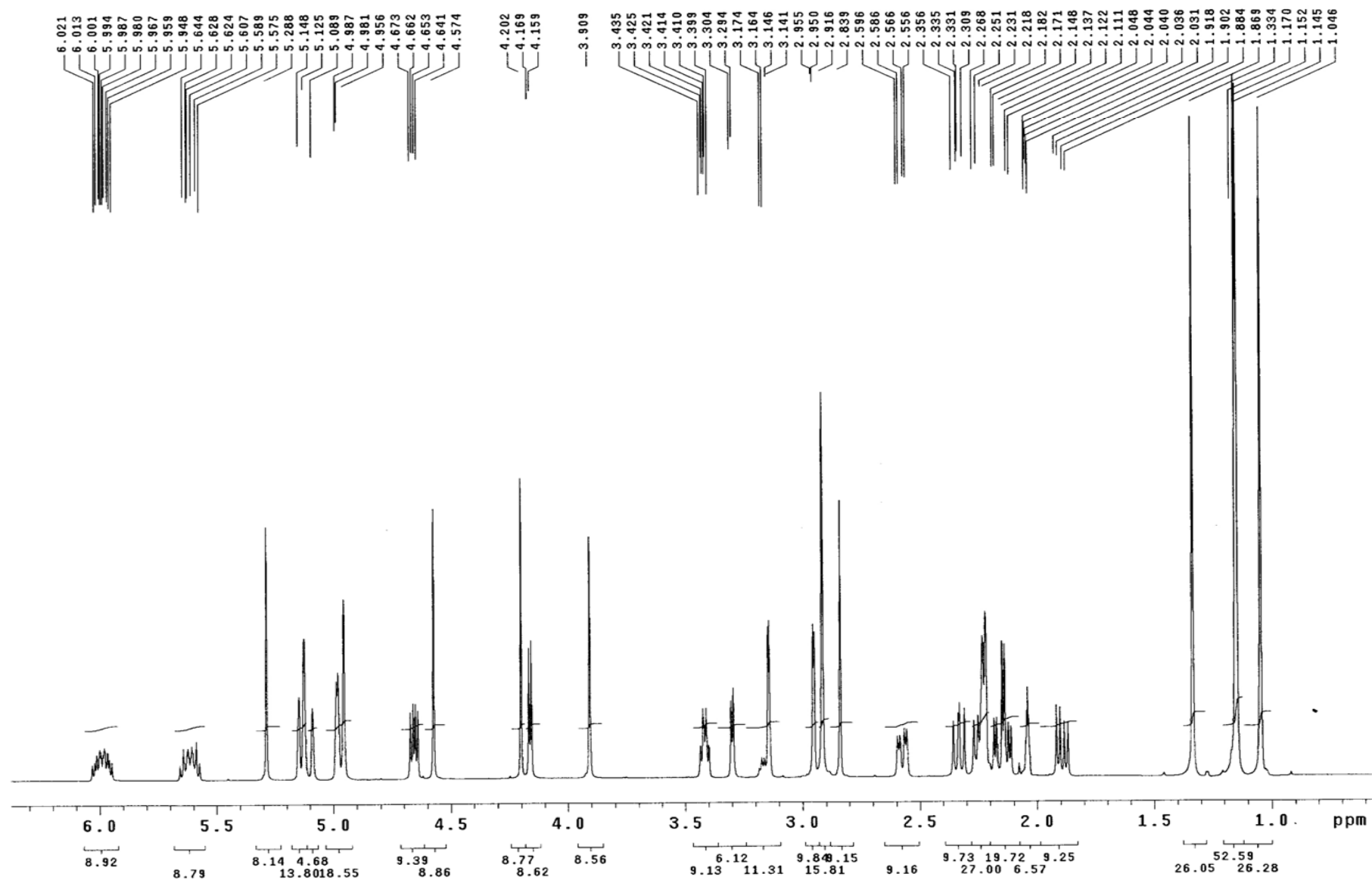
S7 Deference NOE spectrum (400 MHz) of compound **1**



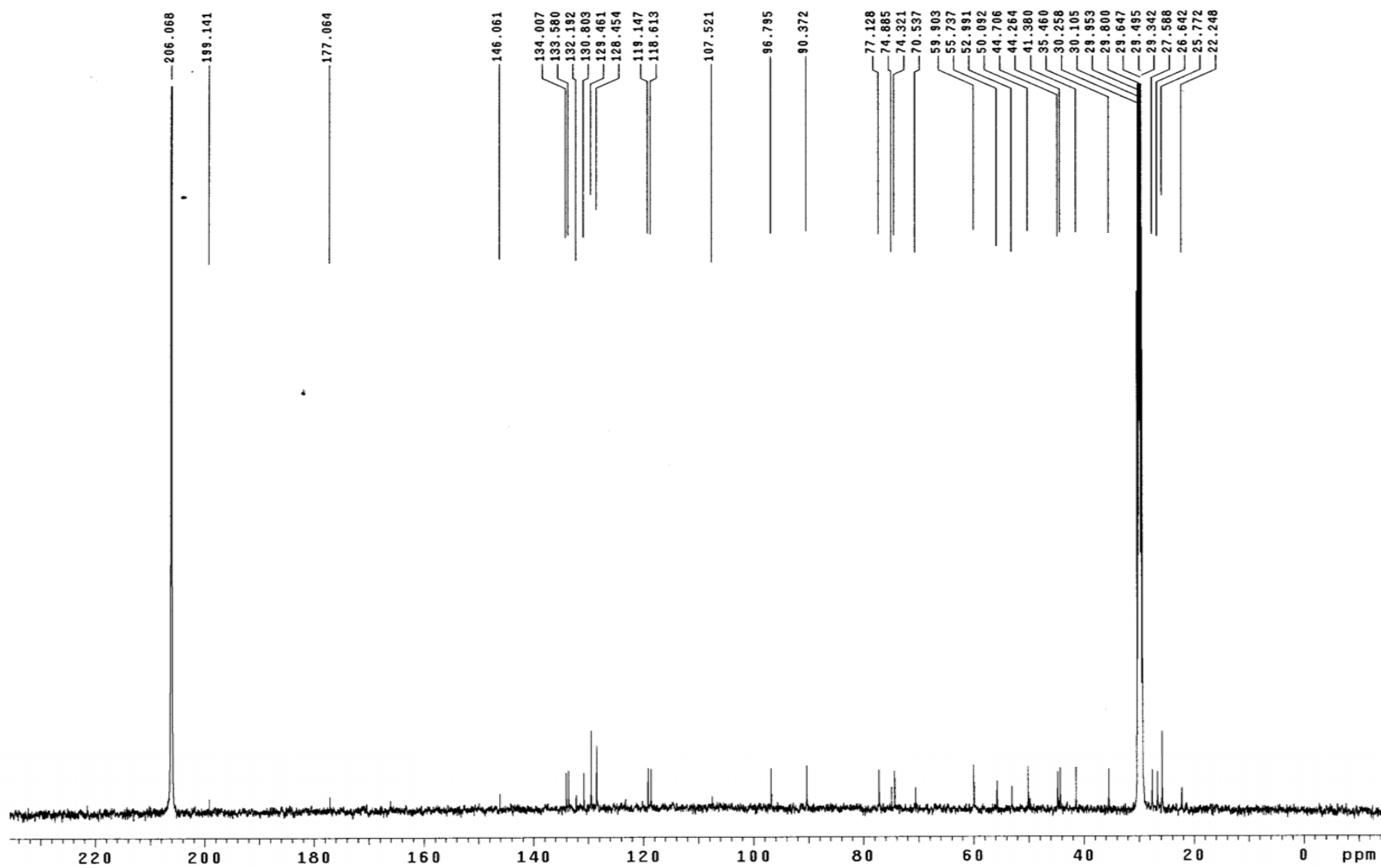
S8 CD spectrum of compound **1** in MeOH



S9 ^1H NMR spectrum (500 MHz) of compound **1** in acetone- d_6



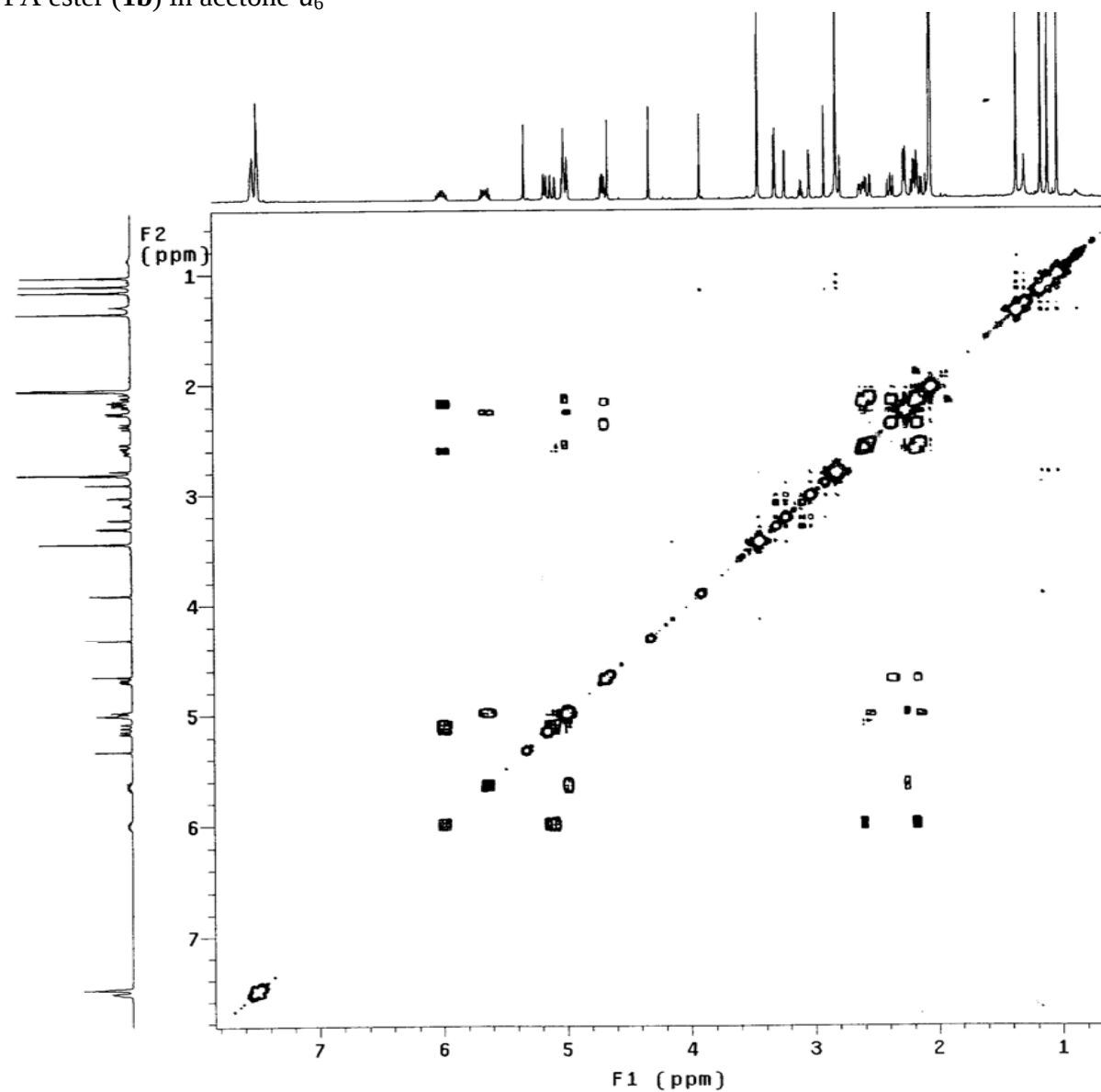
S11 ^{13}C NMR spectrum (125 MHz) of (*S*)-MTPA ester (**1b**) in acetone- d_6



S12 gCOSY spectrum (500 MHz) of (S)-MTPA ester (**1b**) in acetone- d_6

Solvent: Acetone
Temp. 25.0 C / 298.1 K
INOVA-500 "IMM-501"

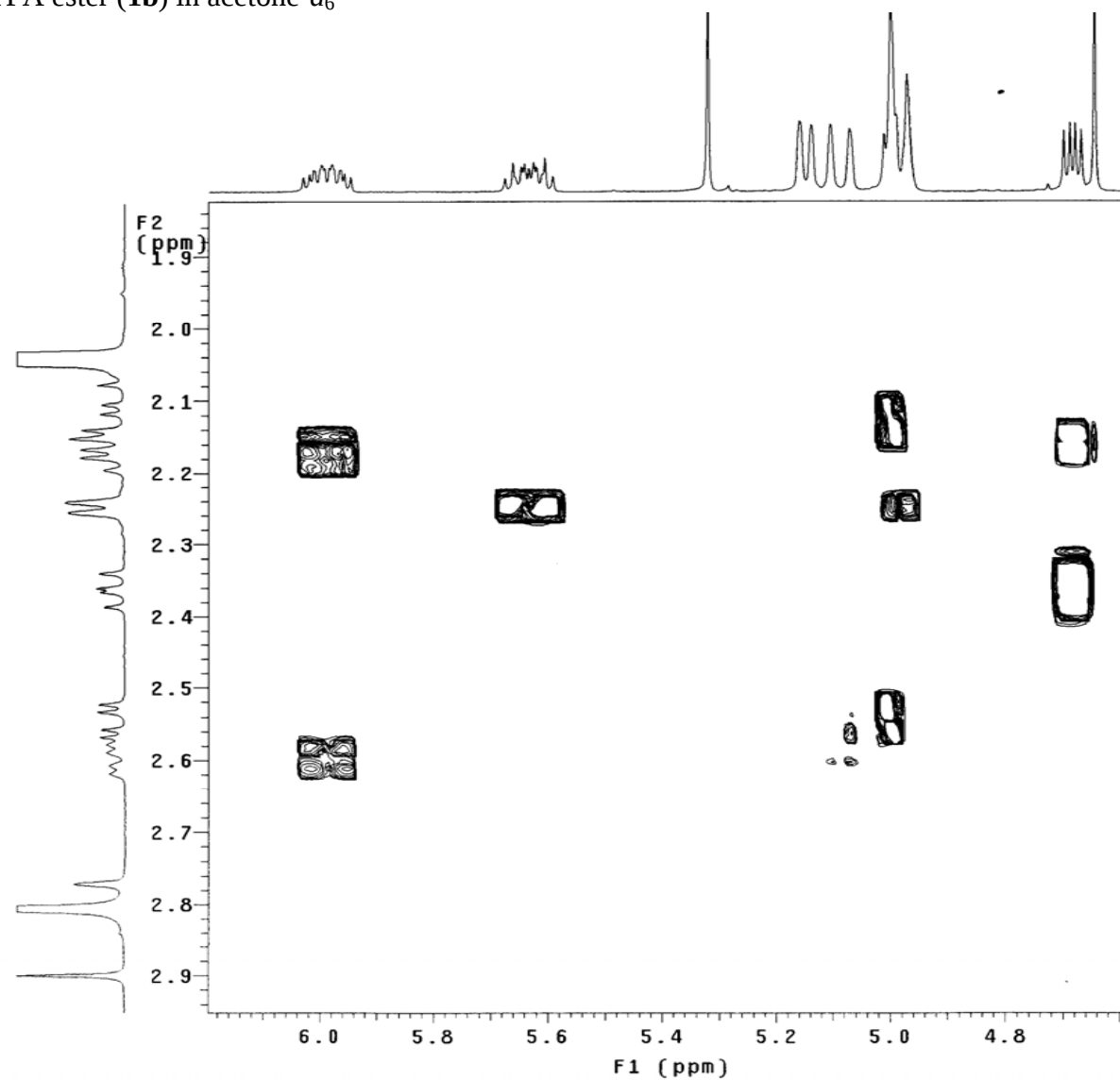
Relax. delay 1.000 sec
Acq. time 0.247 sec
Width 4149.4 Hz
2D Width 4149.4 Hz
2 repetitions
256 increments
OBSERVE H1, 499.7728089 MHz
DATA PROCESSING
Sine bell 0.123 sec
F1 DATA PROCESSING
Sine bell 0.031 sec
FT size 2048 x 2048
Total time 11 min, 20 sec



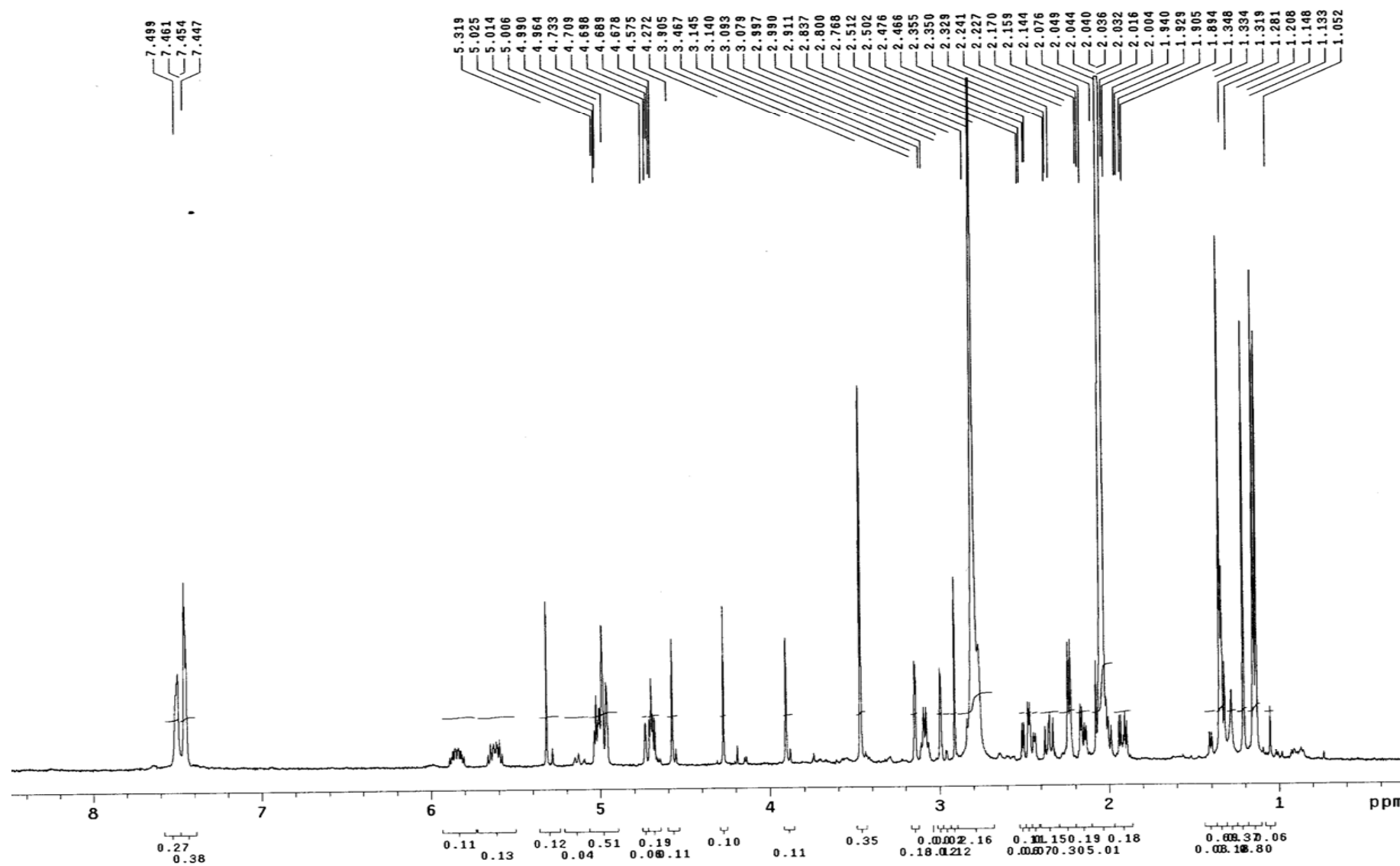
S12 gCOSY spectrum (500 MHz) of (S)-MTPA ester (**1b**) in acetone- d_6

Solvent: Acetone
Temp. 25.0 C / 298.1 K
INOVA-500 "IMM-501"

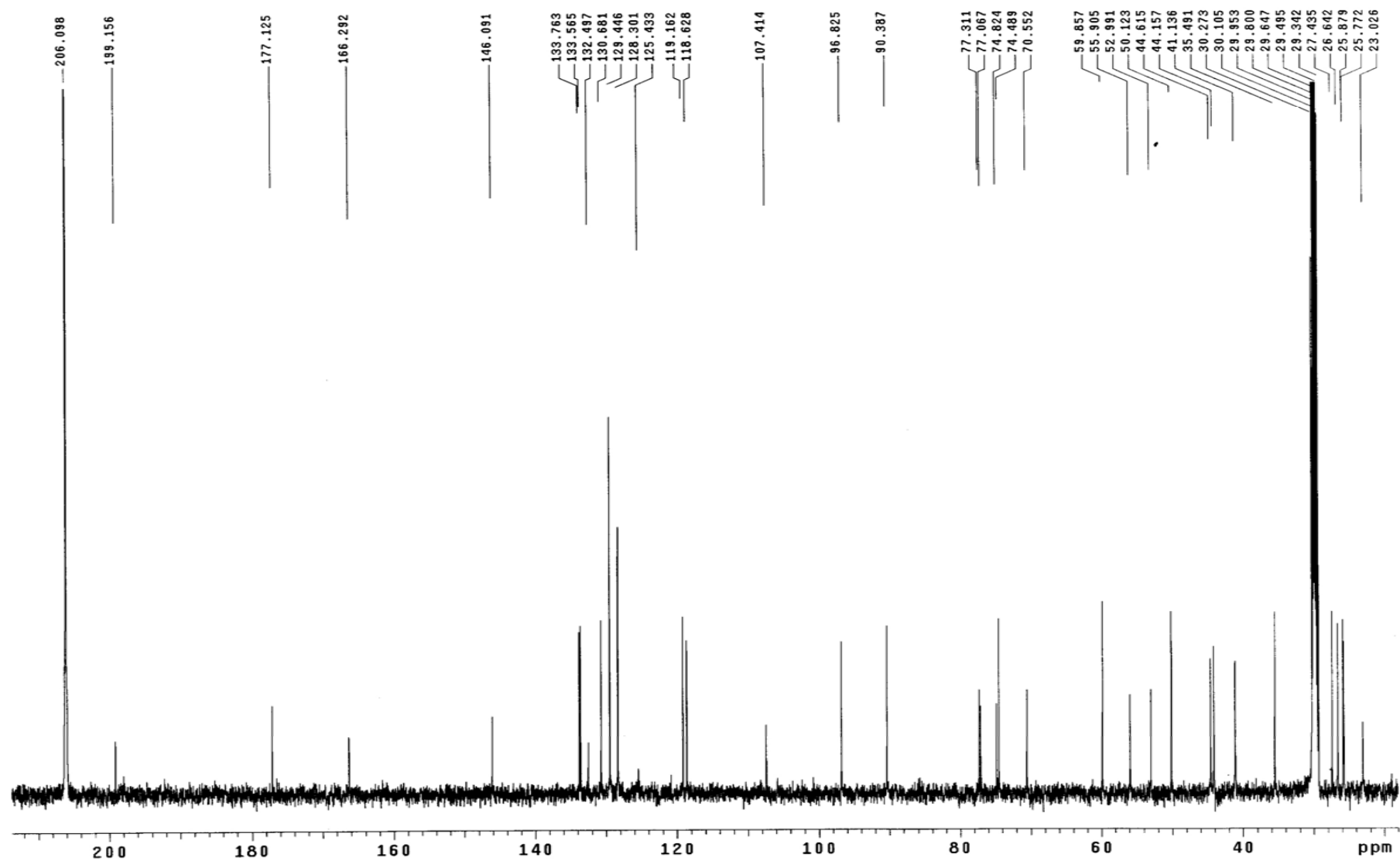
Relax. delay 1.000 sec
Acq. time 0.247 sec
Width 4149.4 Hz
2D Width 4149.4 Hz
2 repetitions
256 increments
OBSERVE H1, 499.7728089 MHz
DATA PROCESSING
Sine bell 0.123 sec
F1 DATA PROCESSING
Sine bell 0.031 sec
FT size 2048 x 2048
Total time 11 min, 20 sec



S13 ^1H NMR spectrum (500 MHz) of (*R*)-MTPA ester (**1a**) in acetone- d_6



S14 ^{13}C NMR spectrum (125 MHz) of (*R*)-MTPA ester (**1a**) in acetone- d_6

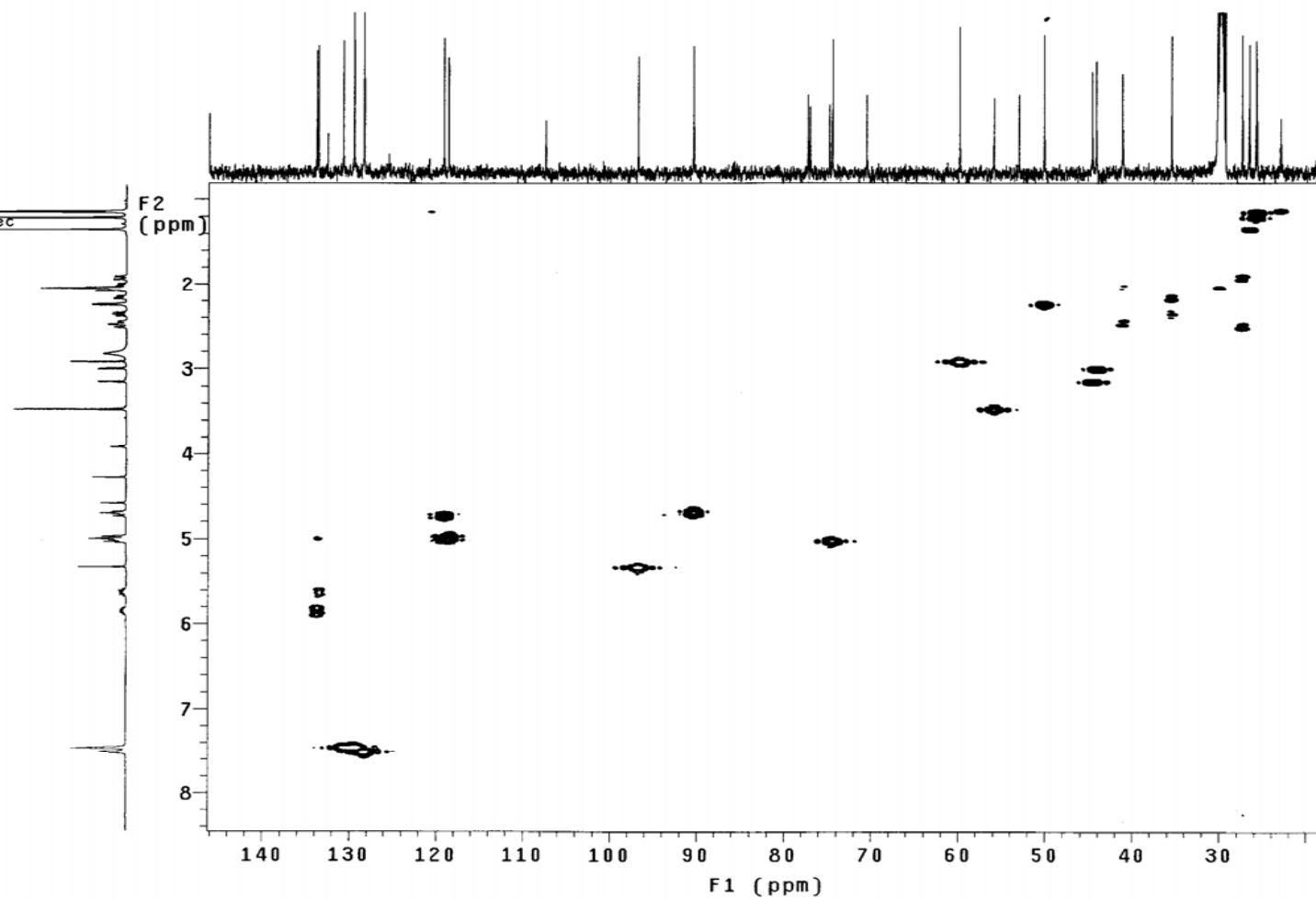


S15 HSQC spectrum (500 MHz) of (R)-MTPA ester (**1a**) in acetone-*d*₆

Solvent: Acetone
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: HSQCD3C0CD30418-T18-41S
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.234 sec
Width 4369.4 Hz
2D Width 25624.6 Hz
32 repetitions
256 increments
OBSERVE H1, 499.7728089 MHz
DECOUPLE C13, 125.6822004 MHz
Power 48 dB
on during acquisition
off during delay
GARP-1 modulated

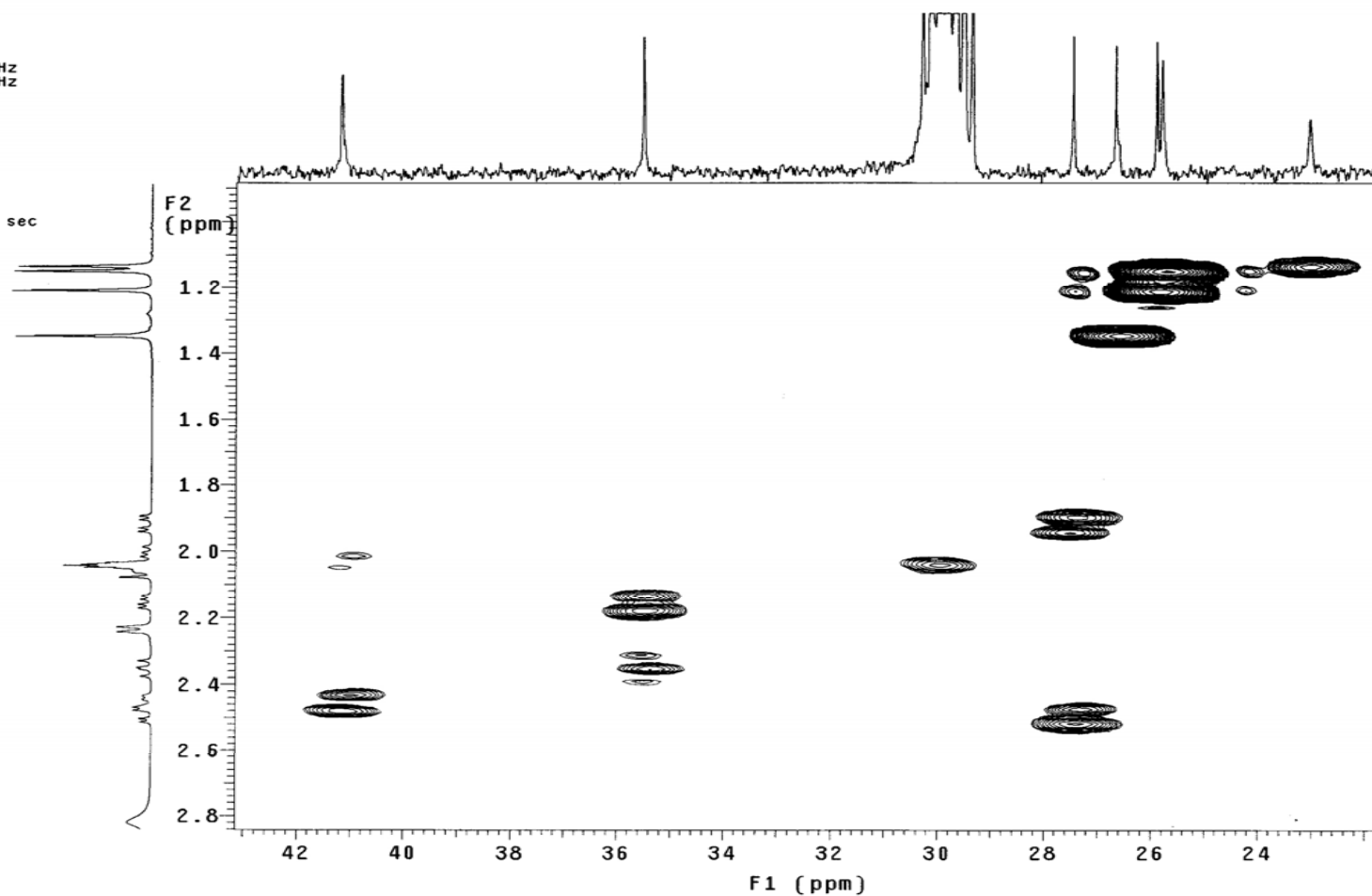
DATA PROCESSING
Sine bell 0.038 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 4096
Total time 2 hr, 59 min, 15 sec



S15 HSQC spectrum (500 MHz) of (*R*)-MTPA ester (**1a**) in acetone-*d*₆

Solvent: Acetone
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: HSQCCD3C0CD30418-TIB-41S
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.234 sec
Width 4369.4 Hz
2D Width 25624.6 Hz
32 repetitions
256 increments
OBSERVE H1, 499.7728089 MHz
DECOUPLE C13, 125.6822004 MHz
Power 48 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.038 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 4096
Total time 2 hr, 59 min, 15 sec



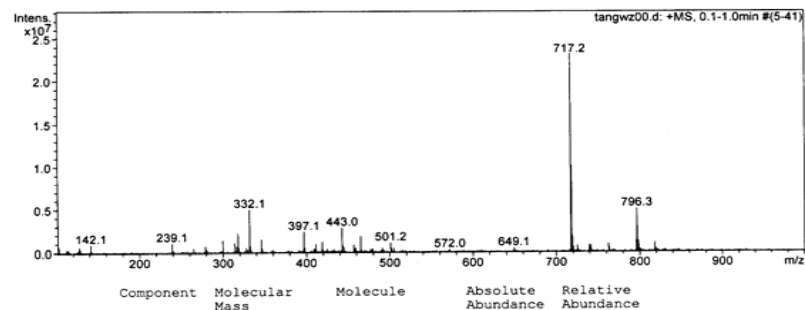
S16 ESI MS spectrum of (S)-MTPA ester (1b)

Single Mass Spectrum Deconvolution Report

Analysis Name: tangwz00.d **Instrument:** LC-MSD-Trip-SL **Print Date:** 3/15/2007 11:12:38 AM
Method: TEST.MS **Operator:** Administrator **Acq. Date:** 3/15/2007 10:57:41 AM
Sample Name: TIB-41a
Analysis Info:

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	58.2	Scan Begin	100 m/z
Ion Polarity	Positive	Octopole RF Amplitude	150.0 Vpp	Scan End	1000 m/z
Ion Source Type	ESI	Capillary Exit	117.3 Volt	Averages	5 Spectra
Dry Temp (Set)	325 °C	Skimmer	40.0 Volt	Max. Accu Time	300000 µs
Nebulizer (Set)	15.00 psi	Oct 1 DC	12.00 Volt	ICC Target	-1
Dry Gas (Set)	6.00 l/min	Oct 2 DC	2.00 Volt	Charge Control	on



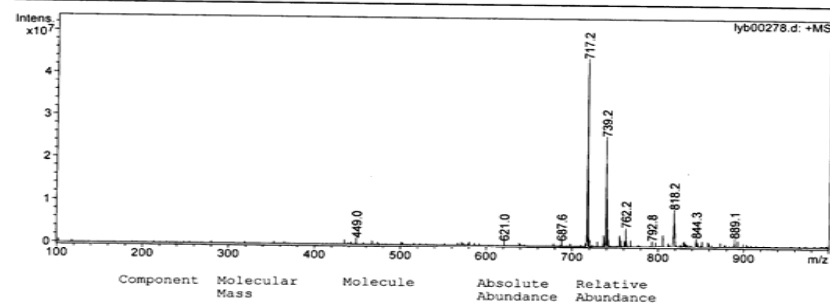
S17 ESI MS spectrum of (R)-MTPA ester (1a)

Single Mass Spectrum Deconvolution Report

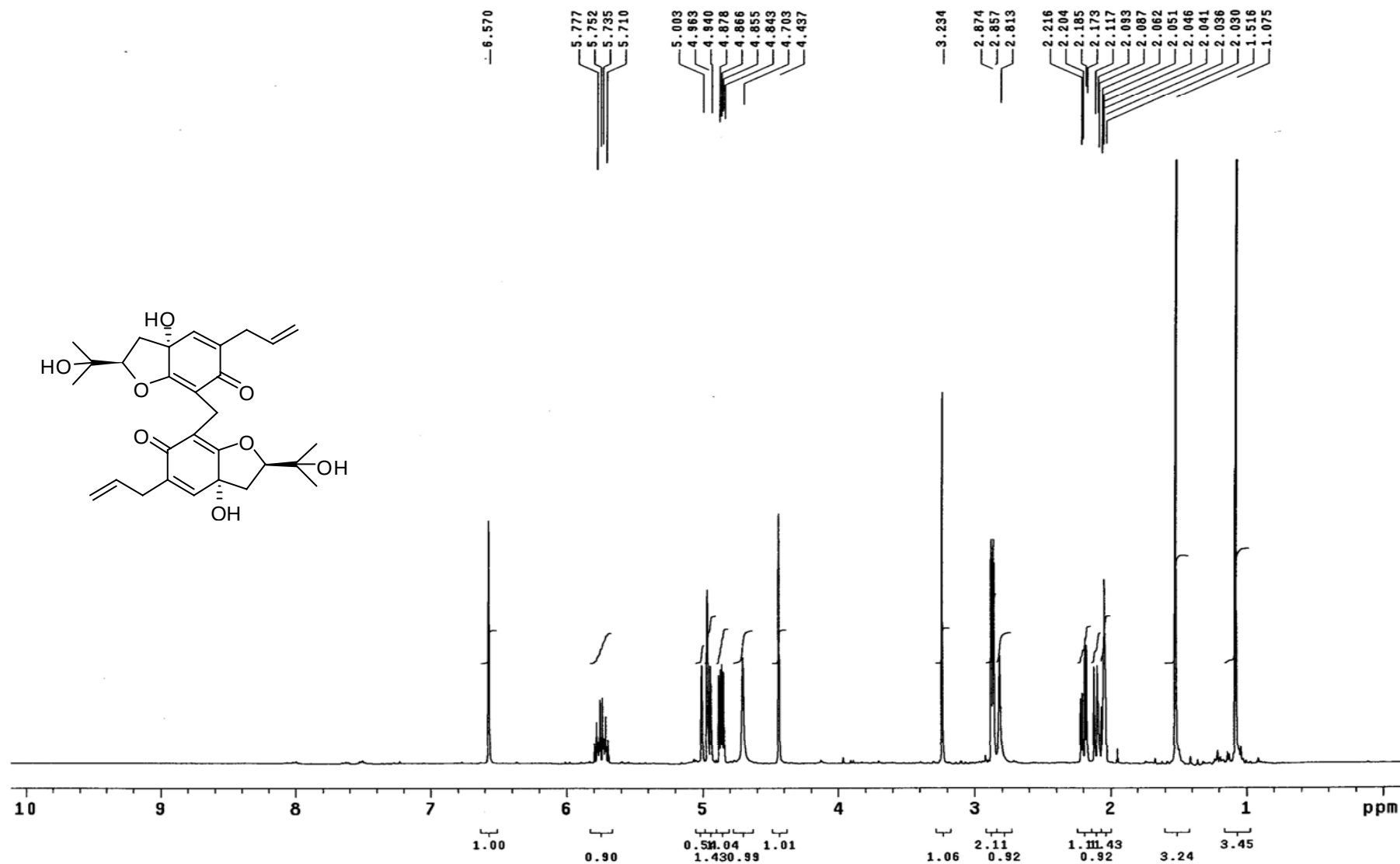
Analysis Name: lyb00278.d **Instrument:** LC-MSD-Trip-SL **Print Date:** 4/18/2007 2:00:27 PM
Method: TEST.MS **Operator:** Administrator **Acq. Date:** 4/17/2007 1:59:16 PM
Sample Name: H-4
Analysis Info:

Acquisition Parameter:

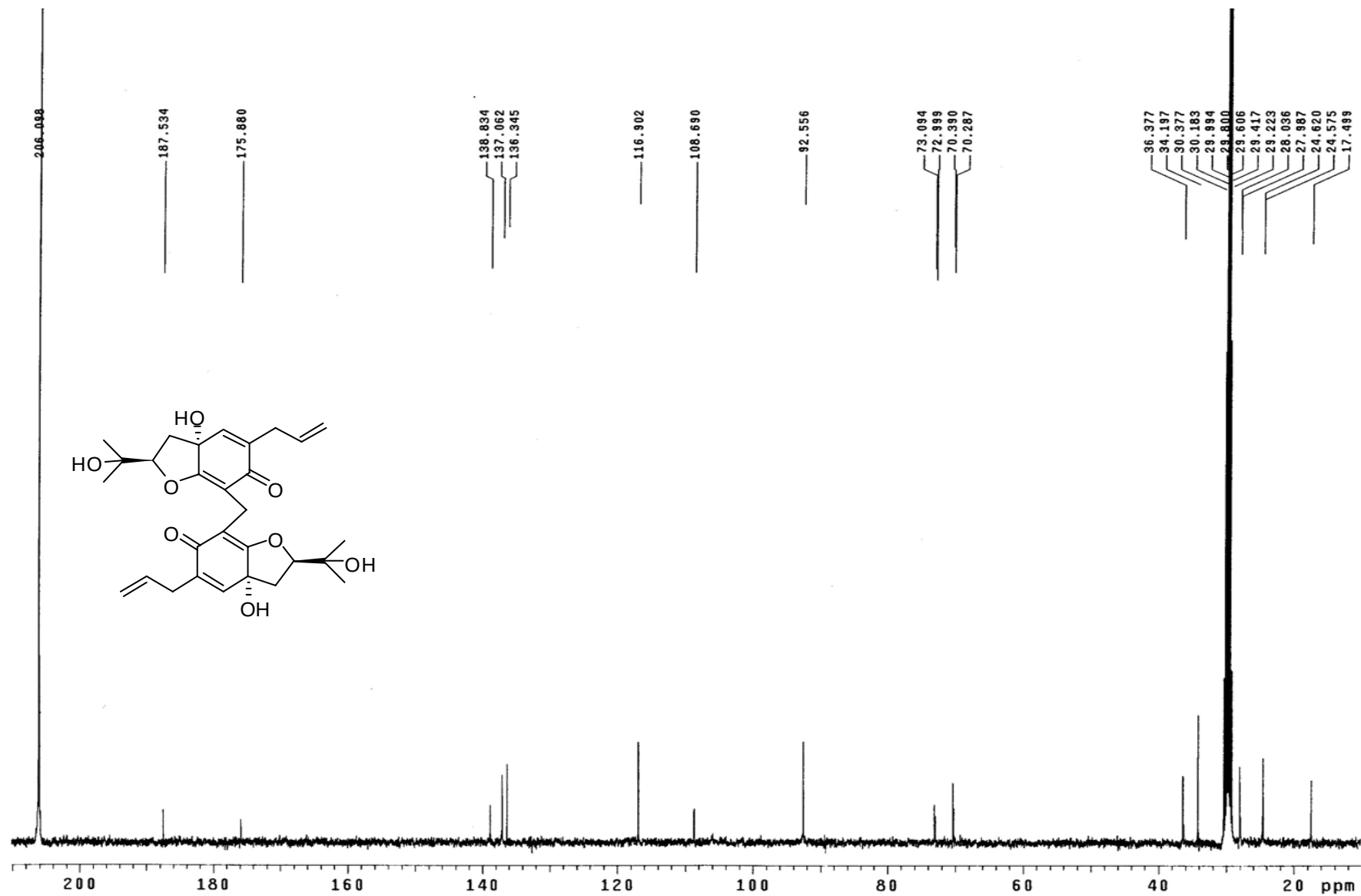
Mass Range Mode	Std/Normal	Trap Drive	80.1	Scan Begin	100 m/z
Ion Polarity	Positive	Octopole RF Amplitude	153.2 Vpp	Scan End	1000 m/z
Ion Source Type	ESI	Capillary Exit	128.5 Volt	Averages	5 Spectra
Dry Temp (Set)	325 °C	Skimmer	40.0 Volt	Max. Accu Time	300000 µs
Nebulizer (Set)	15.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	6.00 l/min	Oct 2 DC	2.70 Volt	Charge Control	on



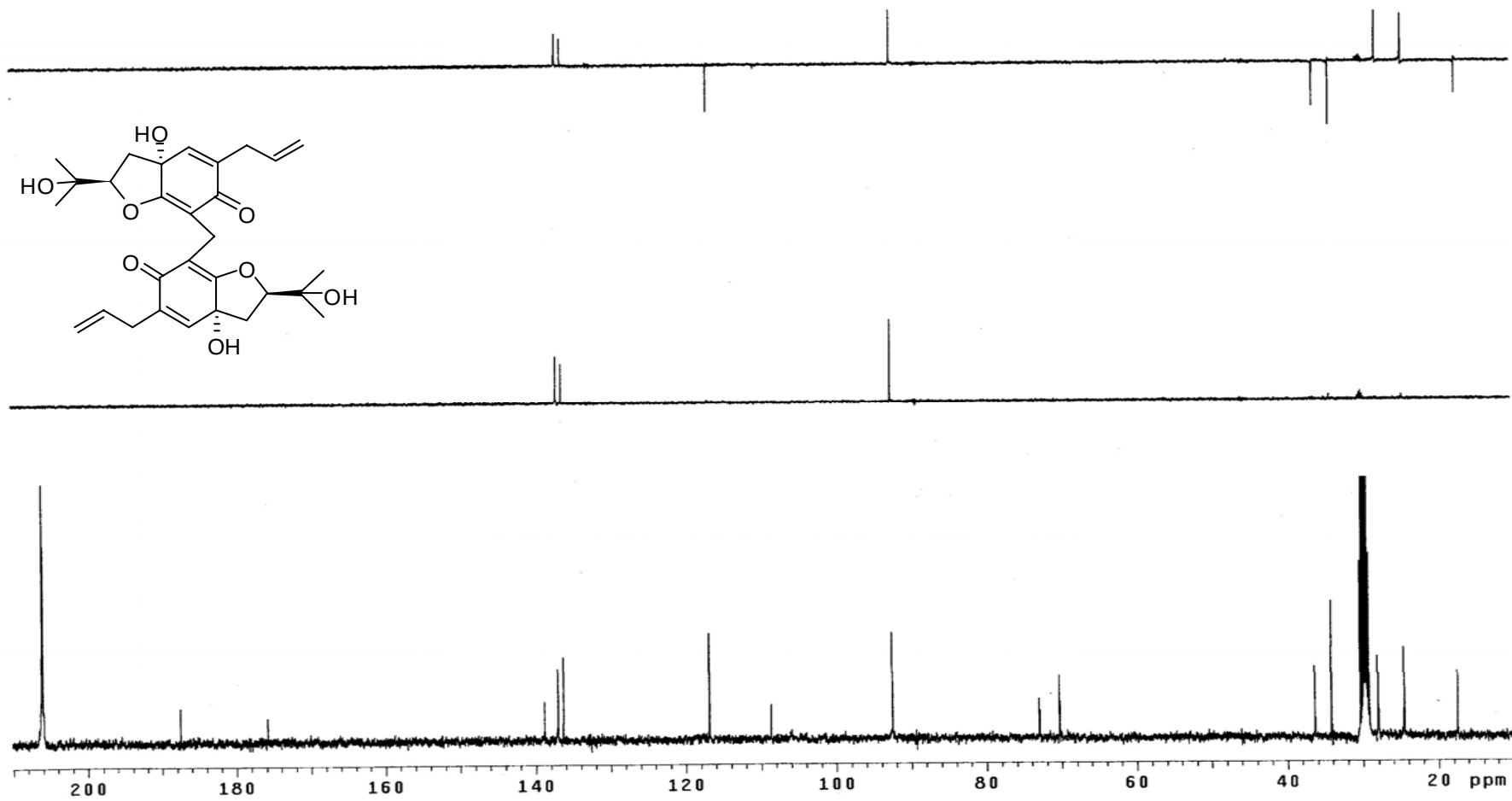
S18 ^1H NMR spectrum (400 MHz) of compound **2** in acetone d_6



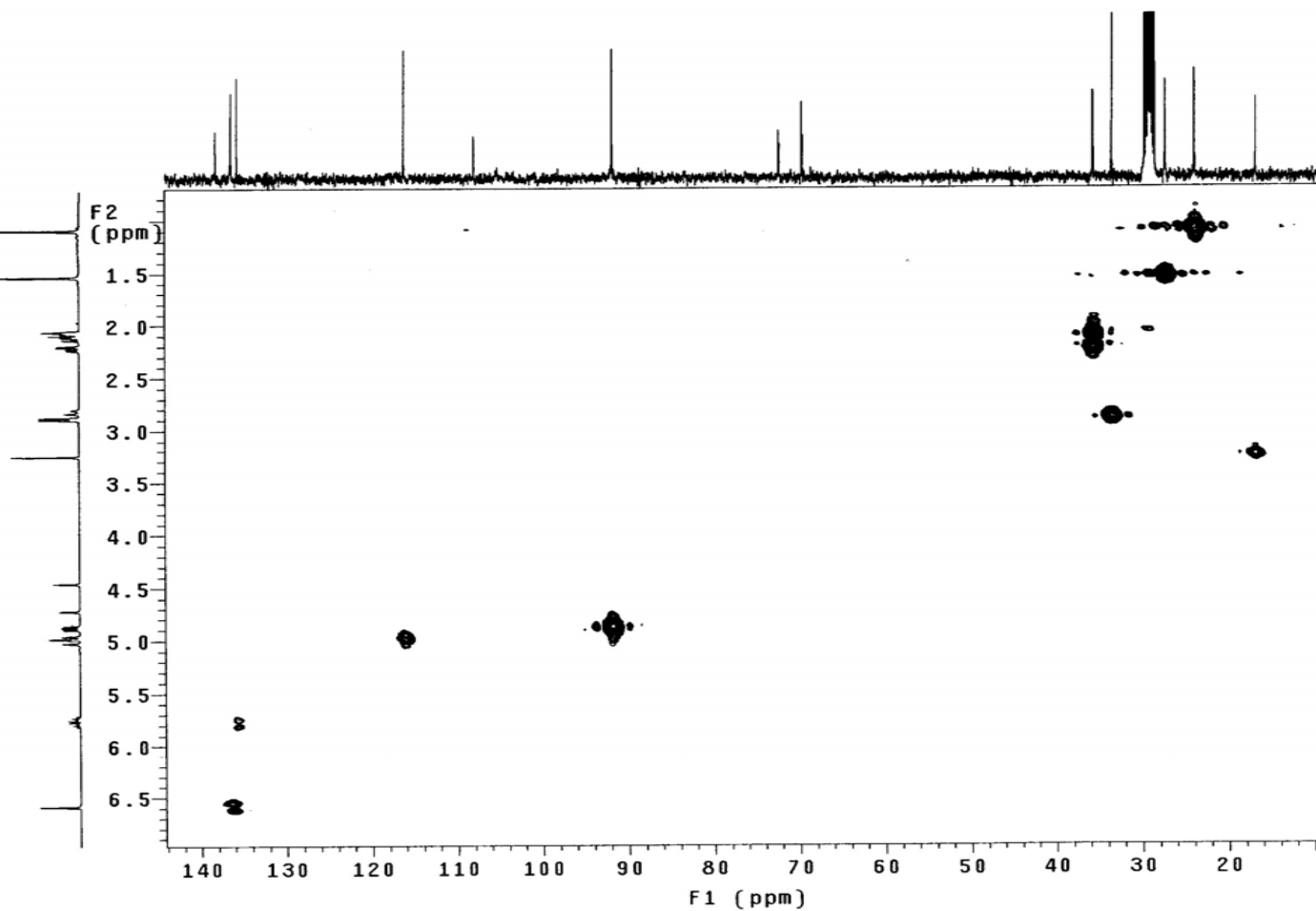
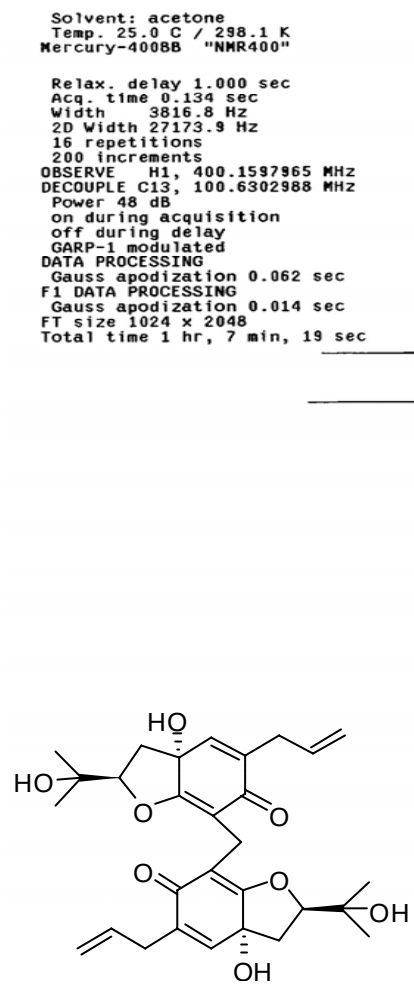
S19 ^{13}C NMR spectrum (100 MHz) of compound **2** in acetone d_6



S20 DEPT spectrum (400 MHz) of compound **2** in acetone d_6



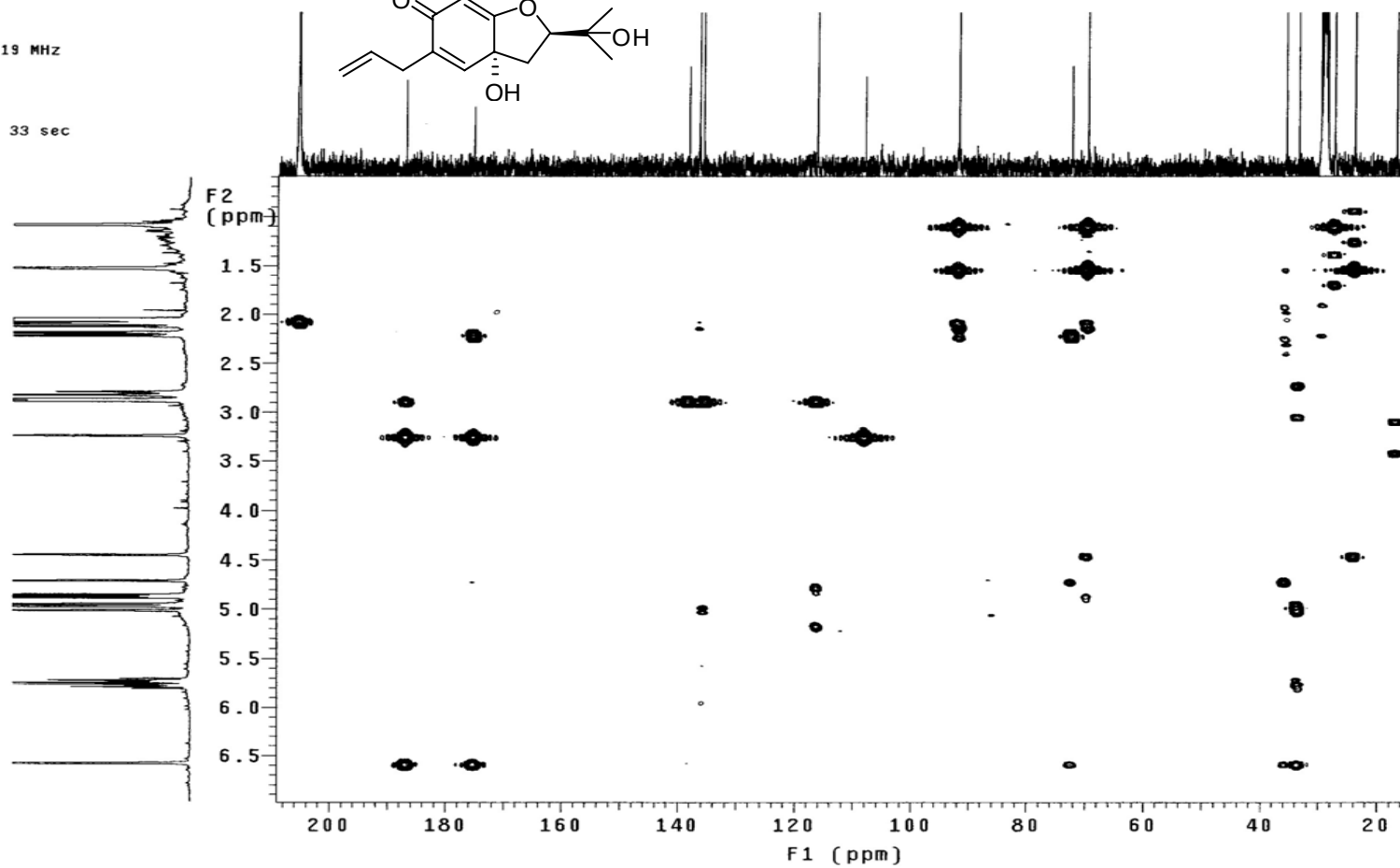
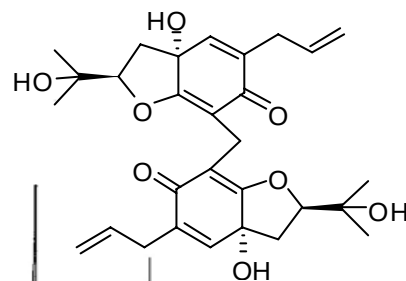
S21 HSQC spectrum (400 MHz) of compound 2 in acetone- d_6



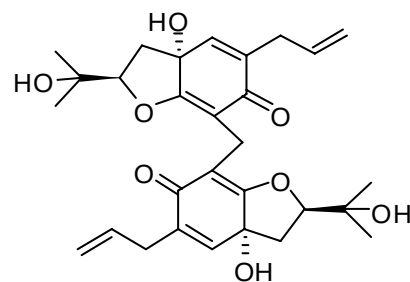
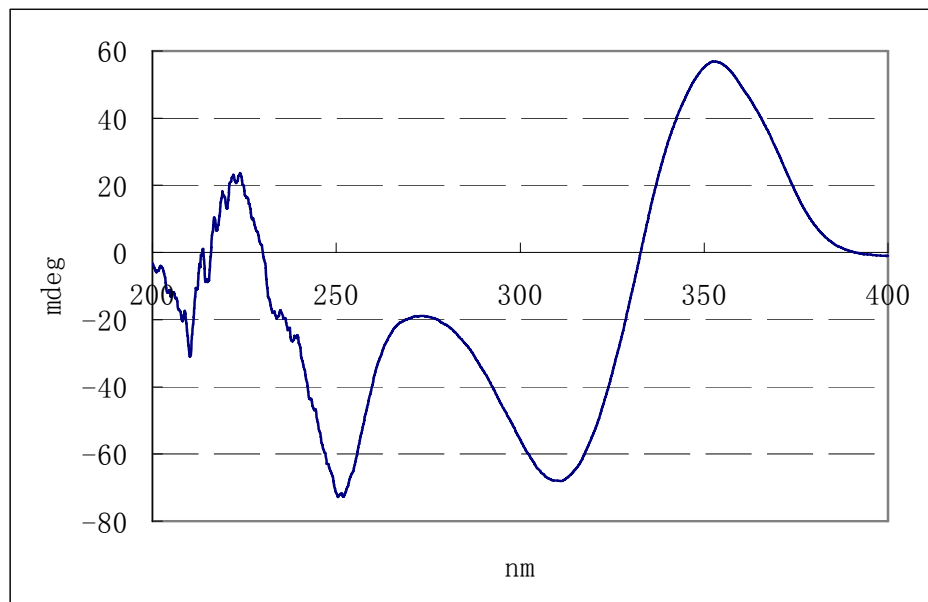
S22 HMBC spectrum (400 MHz) of compound 2 in acetone- d_6

Solvent: acetone
 Temp. 25.0 C / 298.1 K
 File: 0102
 Mercury-400BB "NMR400"

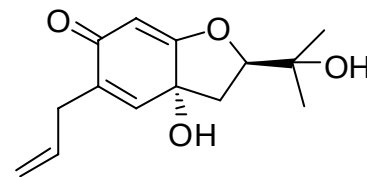
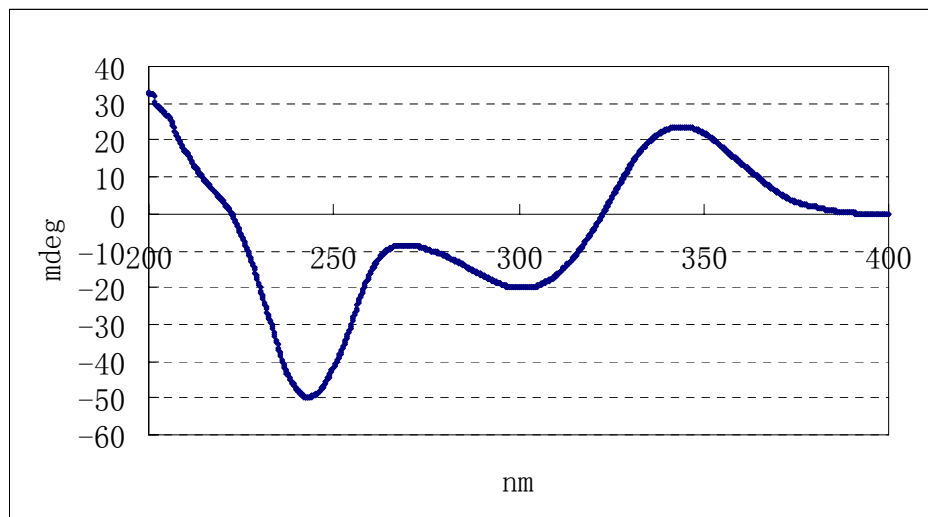
 Relax. delay 1.000 sec
 Acq. time 0.213 sec
 Width 9615.4 Hz
 2D Width 24154.6 Hz
 32 repetitions
 256 increments
 OBSERVE H1, 400.1597919 MHz
 DATA PROCESSING
 Sine bell 0.054 sec
 F1 DATA PROCESSING
 Sine bell 0.005 sec
 FT size 2048 x 4096
 Total time 3 hr, 5 min, 33 sec



S23 CD spectra of compound **2** and 2,3-dehydroillifunone in MeOH

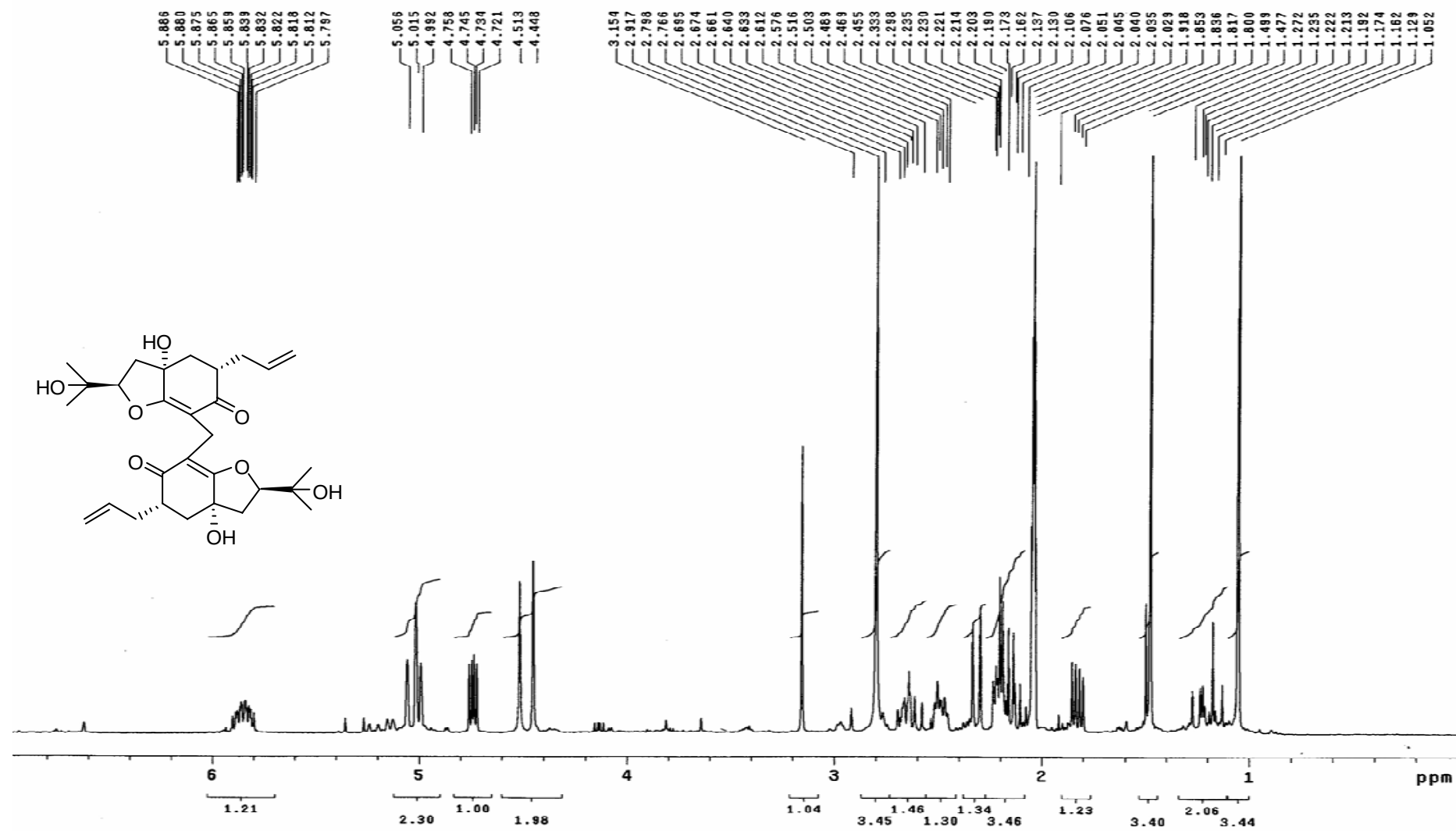


2



2,3-dehydroillifunone

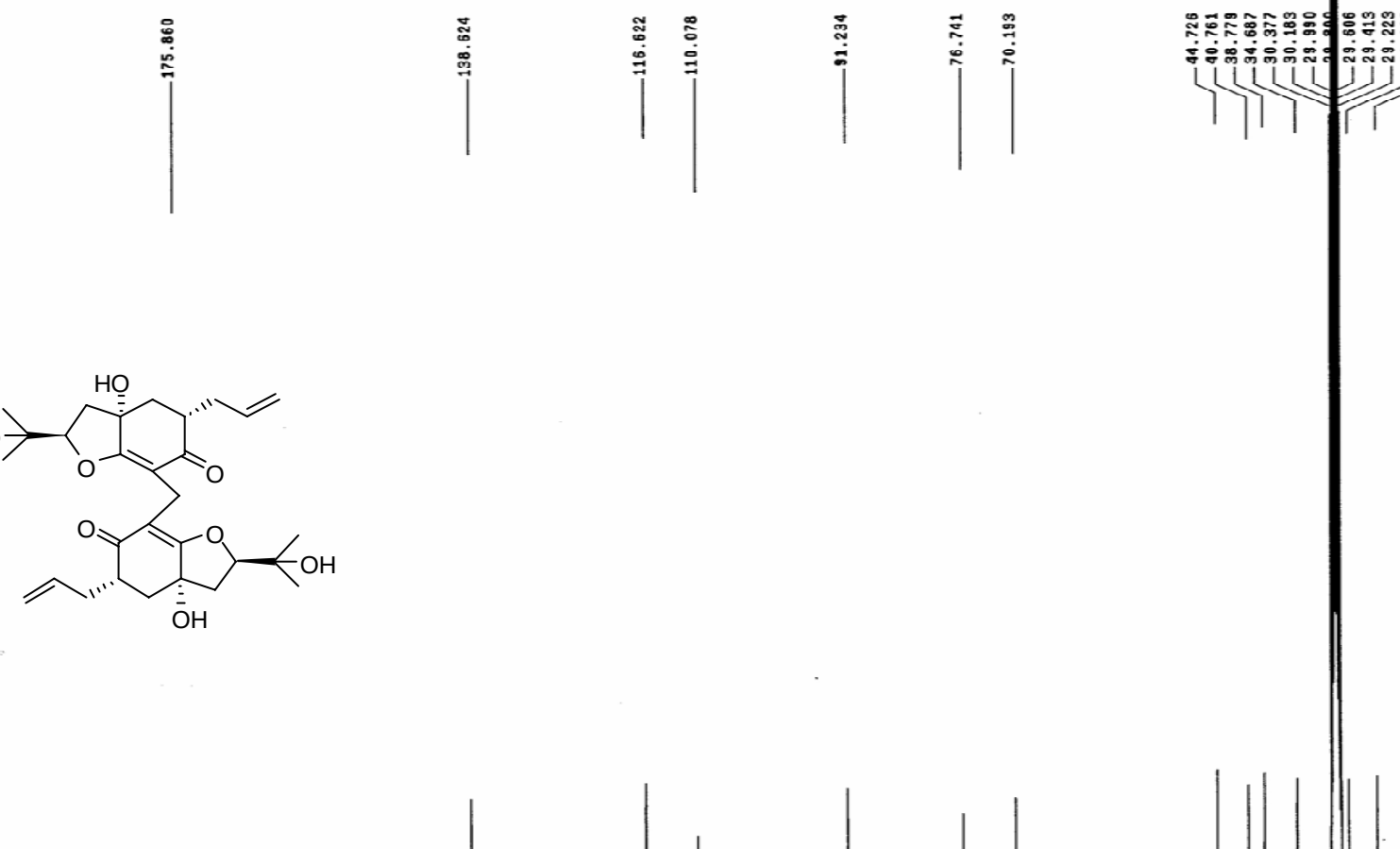
S24 ^1H NMR spectrum (400 MHz) of compound **3** acetone- d_6



Chemical structure of the compound is shown above the spectrum. The structure is a complex polycyclic molecule with multiple hydroxyl groups and a vinyl group.

The spectrum displays the following chemical shifts (ppm):

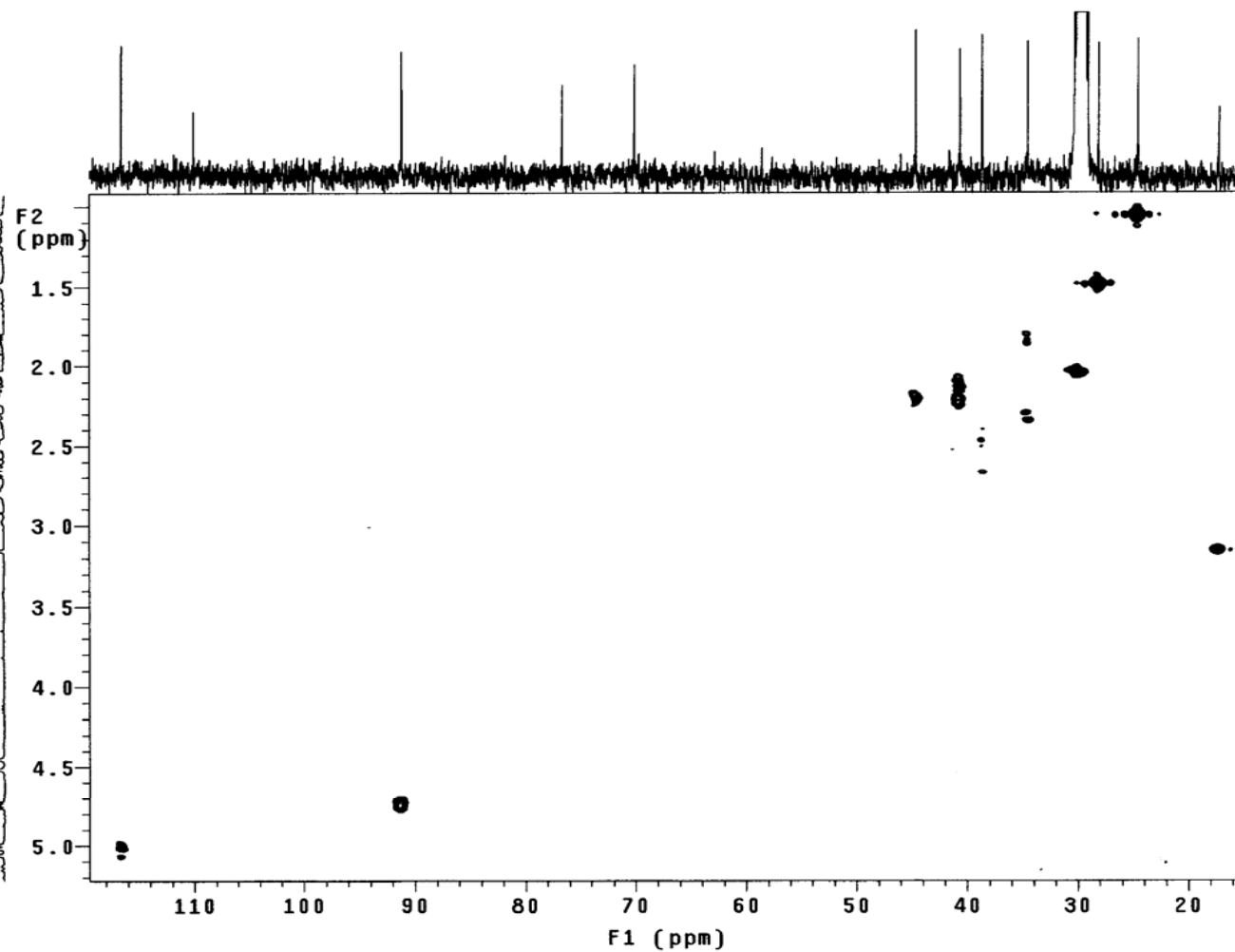
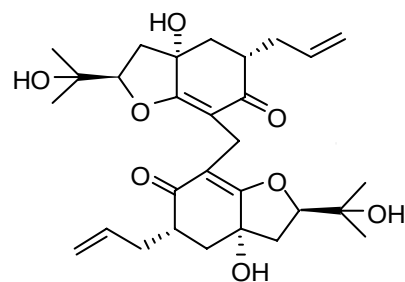
- 206.078
- 200.428
- 175.860
- 138.624
- 116.622
- 110.078
- 91.234
- 76.741
- 70.193
- 44.726
- 40.761
- 38.779
- 34.687
- 30.377
- 30.183
- 29.990
- 29.900
- 29.806
- 29.413
- 29.223
- 28.238
- 24.698
- 17.380

CC(=C)[C@H]1CC[C@@H]2[C@@H](O)[C@H](C(C)(C)O)O[C@H]2C(=O)C=C[C@H]1C(=O)C=C[C@H]3[C@@H](O)[C@H](C(C)(C)O)O[C@H]3C(=O)C=C[C@H]4[C@@H](O)[C@H](C(C)(C)O)O[C@H]4C(=O)C=C[C@H]5[C@@H](O)[C@H](C(C)(C)O)O[C@H]5C(=O)C=C[C@H]6[C@@H](O)[C@H](C(C)(C)O)O[C@H]6C(=O)C=C[C@H]7[C@@H](O)[C@H](C(C)(C)O)O[C@H]7C(=O)C=C[C@H]8[C@@H](O)[C@H](C(C)(C)O)O[C@H]8C(=O)C=C[C@H]9[C@@H](O)[C@H](C(C)(C)O)O[C@H]9C(=O)C=C[C@H]10[C@@H](O)[C@H](C(C)(C)O)O[C@H]10C(=O)C=C[C@H]11[C@@H](O)[C@H](C(C)(C)O)O[C@H]11C(=O)C=C[C@H]12[C@@H](O)[C@H](C(C)(C)O)O[C@H]12C(=O)C=C[C@H]13[C@@H](O)[C@H](C(C)(C)O)O[C@H]13C(=O)C=C[C@H]14[C@@H](O)[C@H](C(C)(C)O)O[C@H]14C(=O)C=C[C@H]15[C@@H](O)[C@H](C(C)(C)O)O[C@H]15C(=O)C=C[C@H]16[C@@H](O)[C@H](C(C)(C)O)O[C@H]16C(=O)C=C[C@H]17[C@@H](O)[C@H](C(C)(C)O)O[C@H]17C(=O)C=C[C@H]18[C@@H](O)[C@H](C(C)(C)O)O[C@H]18C(=O)C=C[C@H]19[C@@H](O)[C@H](C(C)(C)O)O[C@H]19C(=O)C=C[C@H]20[C@@H](O)[C@H](C(C)(C)O)O[C@H]20C(=O)C=C[C@H]21[C@@H](O)[C@H](C(C)(C)O)O[C@H]21C(=O)C=C[C@H]22[C@@H](O)[C@H](C(C)(C)O)O[C@H]22C(=O)C=C[C@H]23[C@@H](O)[C@H](C(C)(C)O)O[C@H]23C(=O)C=C[C@H]24[C@@H](O)[C@H](C(C)(C)O)O[C@H]24C(=O)C=C[C@H]25[C@@H](O)[C@H](C(C)(C)O)O[C@H]25C(=O)C=C[C@H]26[C@@H](O)[C@H](C(C)(C)O)O[C@H]26C(=O)C=C[C@H]27[C@@H](O)[C@H](C(C)(C)O)O[C@H]27C(=O)C=C[C@H]28[C@@H](O)[C@H](C(C)(C)O)O[C@H]28C(=O)C=C[C@H]29[C@@H](O)[C@H](C(C)(C)O)O[C@H]29C(=O)C=C[C@H]30[C@@H](O)[C@H](C(C)(C)O)O[C@H]30C(=O)C=C[C@H]31[C@@H](O)[C@H](C(C)(C)O)O[C@H]31C(=O)C=C[C@H]32[C@@H](O)[C@H](C(C)(C)O)O[C@H]32C(=O)C=C[C@H]33[C@@H](O)[C@H](C(C)(C)O)O[C@H]33C(=O)C=C[C@H]34[C@@H](O)[C@H](C(C)(C)O)O[C@H]34C(=O)C=C[C@H]35[C@@H](O)[C@H](C(C)(C)O)O[C@H]35C(=O)C=C[C@H]36[C@@H](O)[C@H](C(C)(C)O)O[C@H]36C(=O)C=C[C@H]37[C@@H](O)[C@H](C(C)(C)O)O[C@H]37C(=O)C=C[C@H]38[C@@H](O)[C@H](C(C)(C)O)O[C@H]38C(=O)C=C[C@H]39[C@@H](O)[C@H](C(C)(C)O)O[C@H]39C(=O)C=C[C@H]40[C@@H](O)[C@H](C(C)(C)O)O[C@H]40C(=O)C=C[C@H]41[C@@H](O)[C@H](C(C)(C)O)O[C@H]41C(=O)C=C[C@H]42[C@@H](O)[C@H](C(C)(C)O)O[C@H]42C(=O)C=C[C@H]43[C@@H](O)[C@H](C(C)(C)O)O[C@H]43C(=O)C=C[C@H]44[C@@H](O)[C@H](C(C)(C)O)O[C@H]44C(=O)C=C[C@H]45[C@@H](O)[C@H](C(C)(C)O)O[C@H]45C(=O)C=C[C@H]46[C@@H](O)[C@H](C(C)(C)O)O[C@H]46C(=O)C=C[C@H]47[C@@H](O)[C@H](C(C)(C)O)O[C@H]47C(=O)C=C[C@H]48[C@@H](O)[C@H](C(C)(C)O)O[C@H]48C(=O)C=C[C@H]49[C@@H](O)[C@H](C(C)(C)O)O[C@H]49C(=O)C=C[C@H]50[C@@H](O)[C@H](C(C)(C)O)O[C@H]50C(=O)C=C[C@H]51[C@@H](O)[C@H](C(C)(C)O)O[C@H]51C(=O)C=C[C@H]52[C@@H](O)[C@H](C(C)(C)O)O[C@H]52C(=O)C=C[C@H]53[C@@H](O)[C@H](C(C)(C)O)O[C@H]53C(=O)C=C[C@H]54[C@@H](O)[C@H](C(C)(C)O)O[C@H]54C(=O)C=C[C@H]55[C@@H](O)[C@H](C(C)(C)O)O[C@H]55C(=O)C=C[C@H]56[C@@H](O)[C@H](C(C)(C)O)O[C@H]56C(=O)C=C[C@H]57[C@@H](O)[C@H](C(C)(C)O)O[C@H]57C(=O)C=C[C@H]58[C@@H](O)[C@H](C(C)(C)O)O[C@H]58C(=O)C=C[C@H]59[C@@H](O)[C@H](C(C)(C)O)O[C@H]59C(=O)C=C[C@H]60[C@@H](O)[C@H](C(C)(C)O)O[C@H]60C(=O)C=C[C@H]61[C@@H](O)[C@H](C(C)(C)O)O[C@H]61C(=O)C=C[C@H]62[C@@H](O)[C@H](C(C)(C)O)O[C@H]62C(=O)C=C[C@H]63[C@@H](O)[C@H](C(C)(C)O)O[C@H]63C(=O)C=C[C@H]64[C@@H](O)[C@H](C(C)(C)O)O[C@H]64C(=O)C=C[C@H]65[C@@H](O)[C@H](C(C)(C)O)O[C@H]65C(=O)C=C[C@H]66[C@@H](O)[C@H](C(C)(C)O)O[C@H]66C(=O)C=C[C@H]67[C@@H](O)[C@H](C(C)(C)O)O[C@H]67C(=O)C=C[C@H]68[C@@H](O)[C@H](C(C)(C)O)O[C@H]68C(=O)C=C[C@H]69[C@@H](O)[C@H](C(C)(C)O)O[C@H]69C(=O)C=C[C@H]70[C@@H](O)[C@H](C(C)(C)O)O[C@H]70C(=O)C=C[C@H]71[C@@H](O)[C@H](C(C)(C)O)O[C@H]71C(=O)C=C[C@H]72[C@@H](O)[C@H](C(C)(C)O)O[C@H]72C(=O)C=C[C@H]73[C@@H](O)[C@H](C(C)(C)O)O[C@H]73C(=O)C=C[C@H]74[C@@H](O)[C@H](C(C)(C)O)O[C@H]74C(=O)C=C[C@H]75[C@@H](O)[C@H](C(C)(C)O)O[C@H]75C(=O)C=C[C@H]76[C@@H](O)[C@H](C(C)(C)O)O[C@H]76C(=O)C=C[C@H]77[C@@H](O)[C@H](C(C)(C)O)O[C@H]77C(=O)C=C[C@H]78[C@@H](O)[C@H](C(C)(C)O)O[C@H]78C(=O)C=C[C@H]79[C@@H](O)[C@H](C(C)(C)O)O[C@H]79C(=O)C=C[C@H]80[C@@H](O)[C@H](C(C)(C)O)O[C@H]80C(=O)C=C[C@H]81[C@@H](O)[C@H](C(C)(C)O)O[C@H]81C(=O)C=C[C@H]82[C@@H](O)[C@H](C(C)(C)O)O[C@H]82C(=O)C=C[C@H]83[C@@H](O)[C@H](C(C)(C)O)O[C@H]83C(=O)C=C[C@H]84[C@@H](O)[C@H](C(C)(C)O)O[C@H]84C(=O)C=C[C@H]85[C@@H](O)[C@H](C(C)(C)O)O[C@H]85C(=O)C=C[C@H]86[C@@H](O)[C@H](C(C)(C)O)O[C@H]86C(=O)C=C[C@H]87[C@@H](O)[C@H](C(C)(C)O)O[C@H]87C(=O)C=C[C@H]88[C@@H](O)[C@H](C(C)(C)O)O[C@H]88C(=O)C=C[C@H]89[C@@H](O)[C@H](C(C)(C)O)O[C@H]89C(=O)C=C[C@H]90[C@@H](O)[C@H](C(C)(C)O)O[C@H]90C(=O)C=C[C@H]91[C@@H](O)[C@H](C(C)(C)O)O[C@H]91C(=O)C=C[C@H]92[C@@H](O)[C@H](C(C)(C)O)O[C@H]92C(=O)C=C[C@H]93[C@@H](O)[C@H](C(C)(C)O)O[C@H]93C(=O)C=C[C@H]94[C@@H](O)[C@H](C(C)(C)O)O[C@H]94C(=O)C=C[C@H]95[C@@H](O)[C@H](C(C)(C)O)O[C@H]95C(=O)C=C[C@H]96[C@@H](O)[C@H](C(C)(C)O)O[C@H]96C(=O)C=C[C@H]97[C@@H](O)[C@H](C(C)(C)O)O[C@H]97C(=O)C=C[C@H]98[C@@H](O)[C@H](C(C)(C)O)O[C@H]98C(=O)C=C[C@H]99[C@@H](O)[C@H](C(C)(C)O)O[C@H]99C(=O)C=C[C@H]100[C@@H](O)[C@H](C(C)(C)O)O[C@H]100C(=O)C=C[C@H]101[C@@H](O

S26 HSQC spectrum (400 MHz) of compound 3 in acetone- d_6

Solvent: acetone
Temp. 25.0 C / 298.1 K
Sample #9
Mercury-400BB "NMR400"

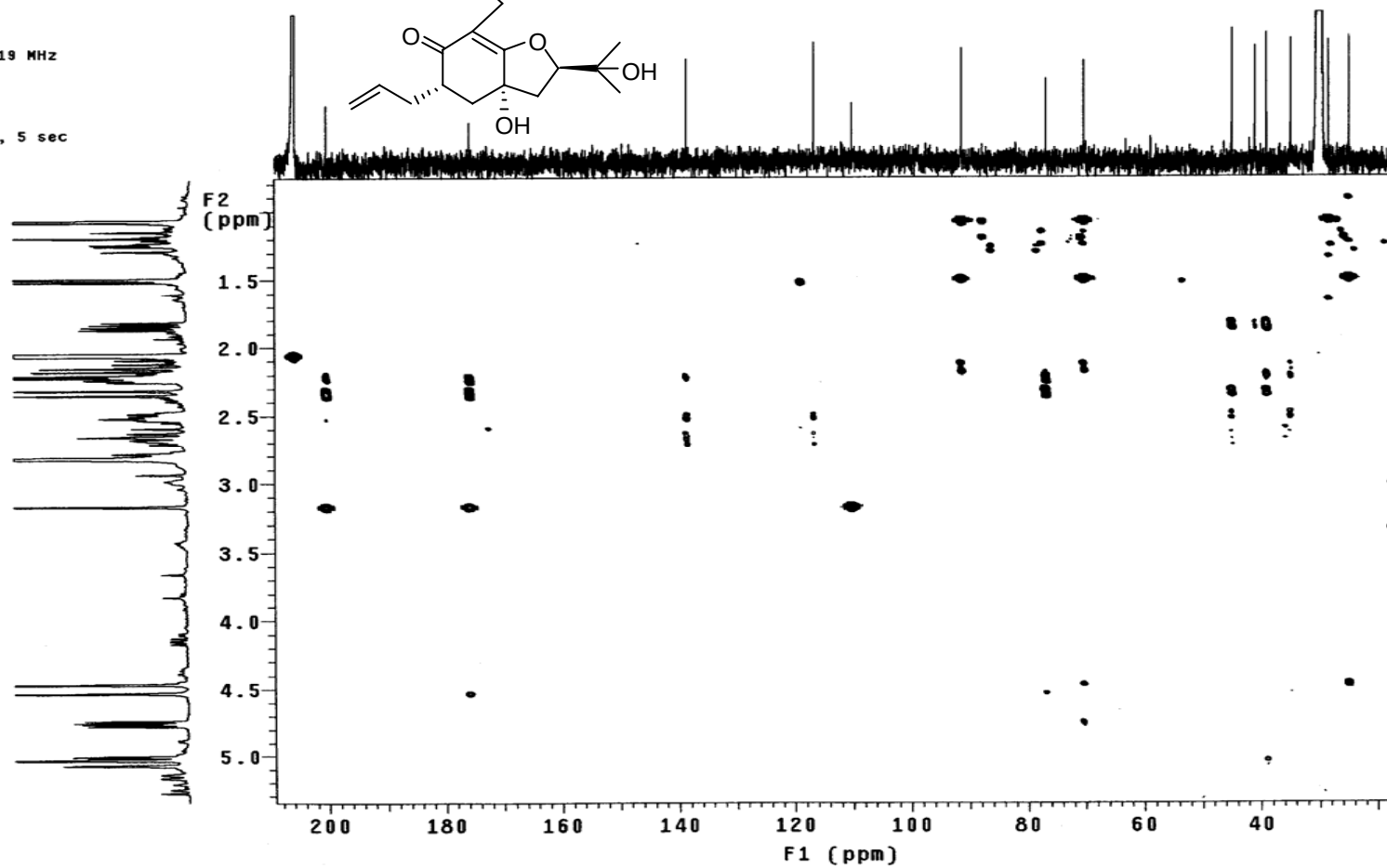
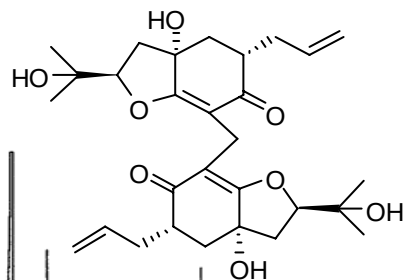
Relax. delay 1.000 sec
Acq. time 0.152 sec
Width 3373.8 Hz
2D Width 16077.2 Hz
16 repetitions
200 increments
OBSERVE H1, 400.1598013 MHz
DECOUPLE C13, 100.6282078 MHz
Power 48 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Gauss apodization 0.070 sec
F1 DATA PROCESSING
Gauss apodization 0.014 sec
FT size 2048 x 4096
Total time 1 hr, 8 min, 24 sec



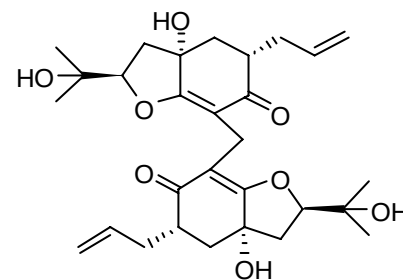
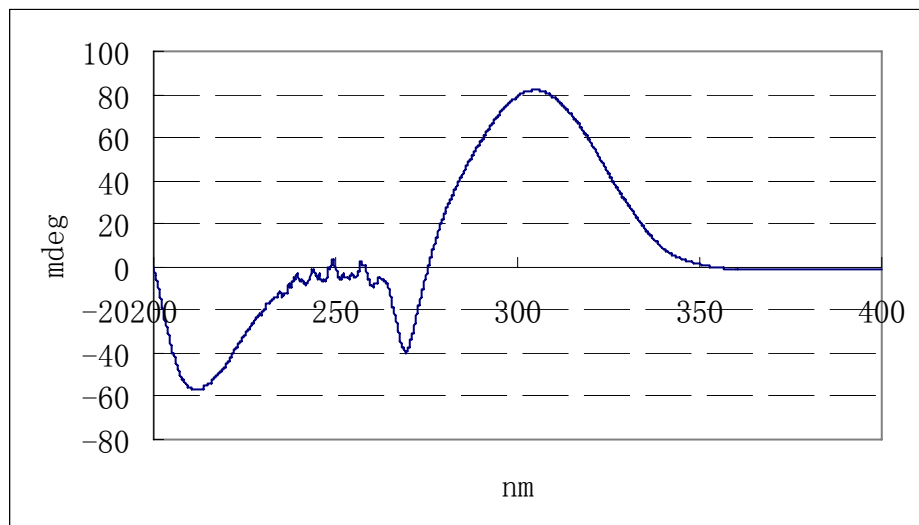
S27 HMBC spectrum (400 MHz) of compound 3 in acetone- d_6

Solvent: acetone
 Temp. 25.0 C / 298.1 K
 File: 0502
 Mercury-400BB "NMR400"

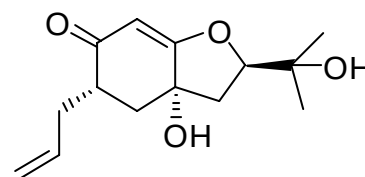
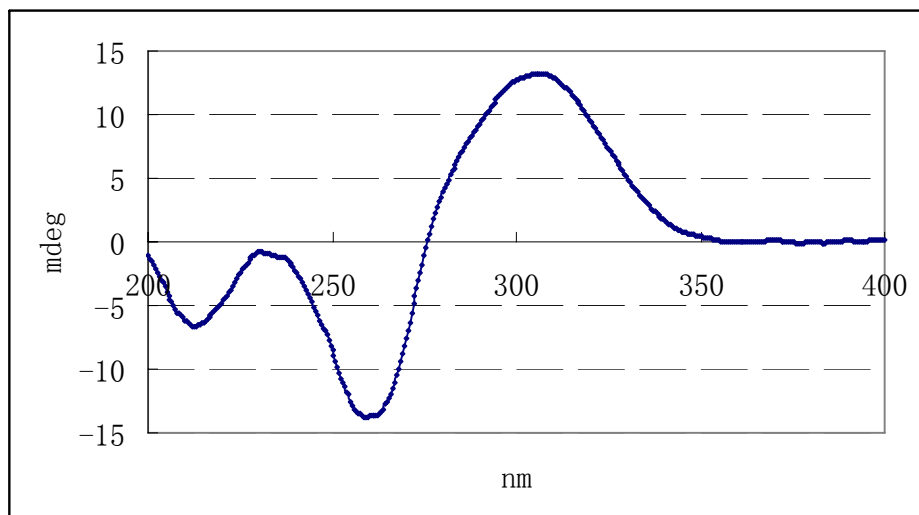
 Relax. delay 1.000 sec
 Acq. time 0.213 sec
 Width 9615.4 Hz
 2D Width 24154.6 Hz
 64 repetitions
 400 increments
 OBSERVE H1, 400.1597919 MHz
 DATA PROCESSING
 Sine bell 0.107 sec
 F1 DATA PROCESSING
 Sine bell 0.008 sec
 FT size 4096 x 2048
 Total time 9 hr, 39 min, 5 sec



S28 CD spectra of compound **3** and illifunone D in MeOH



3



illifunone D