

Steroid and α -Tocopherylhydroquinone Glycosides from two Soft Corals *Cladiella hirsuta* and *Sinularia nanolobata*

Chih-Hua Chao,^{‡ab} Tzu-Zin Huang,^{‡c} Chia-Yun Wu,^c Bo-Wei Chen,^c Chiung-Yao Huang,^c Tsong-Long Hwang,^d
Chang-Feng Dai,^e and Jyh-Horng Sheu^{*c†g}

^a School of Pharmacy, China Medical University, Taichung 404, Taiwan

^b Chinese Medicine Research and Development Center, China Medical University Hospital, Taichung 404, Taiwan

^c Department of Marine Biotechnology and Resources, National Sun Yat-sen University, Kaohsiung 804, Taiwan

^d Graduate Institute of Natural Products, Chang Gung University, Taoyuan 333, Taiwan

^e Institute of Oceanography, National Taiwan University, Taipei 112, Taiwan

^f Graduate Institute of Natural Products, Kaohsiung Medical University, Kaohsiung 807, Taiwan

^g Department of Medical Research, China Medical University Hospital, China Medical University, Taichung 404, Taiwan

‡ These authors contributed equally to this work.

*Corresponding author. Tel: +886-7-5252000 ext.5030; fax: +886-7-5255020; e-mail: sheu@mail.nsysu.edu.tw

For compound 1:

Figure S1-1. ^1H NMR spectrum (400 MHz) of compound **1** in CDCl_3 .
Figure S1-2. ^{13}C NMR spectrum (100 MHz) of compound **1** in CDCl_3 .
Figure S1-3. DEPT135 spectrum (100 MHz) of compound **1** in CDCl_3 .
Figure S1-4. COSY spectrum (400 MHz) of compound **1** in CDCl_3 .
Figure S1-5. HSQC spectrum (400 MHz) of compound **1** in CDCl_3 .
Figure S1-6. HMBC spectrum (400 MHz) of compound **1** in CDCl_3 .
Figure S1-7. NOESY spectrum (400 MHz) of compound **1** in CDCl_3 .

For compound 2:

Figure S2-1. ^1H NMR spectrum (500 MHz) of compound **2** in CDCl_3 .
Figure S2-2. ^{13}C NMR spectrum (125 MHz) of compound **2** in CDCl_3 .
Figure S2-3. DEPT135 spectrum (125 MHz) of compound **2** in CDCl_3 .
Figure S2-4. COSY spectrum (500 MHz) of compound **2** in CDCl_3 .
Figure S2-5. HSQC spectrum (500 MHz) of compound **2** in CDCl_3 .
Figure S2-6. HMBC spectrum (500 MHz) of compound **2** in CDCl_3 .
Figure S2-7. NOESY spectrum (500 MHz) of compound **2** in CDCl_3 .

For compound 3:

Figure S3-1. ^1H NMR spectrum (500 MHz) of compound **3** in CDCl_3 .
Figure S3-2. ^{13}C NMR spectrum (125 MHz) of compound **3** in CDCl_3 .
Figure S3-3. DEPT135 spectrum (125 MHz) of compound **3** in CDCl_3 .
Figure S3-4. COSY spectrum (500 MHz) of compound **3** in CDCl_3 .
Figure S3-5. HSQC spectrum (500 MHz) of compound **3** in CDCl_3 .
Figure S3-6. HMBC spectrum (500 MHz) of compound **3** in CDCl_3 .
Figure S3-7. NOESY spectrum (500 MHz) of compound **3** in CDCl_3 .

For compound 4:

Figure S4-1. ^1H NMR spectrum (400 MHz) of compound **4** in CDCl_3 .
Figure S4-2. ^{13}C NMR spectrum (100 MHz) of compound **4** in CDCl_3 .
Figure S4-3. DEPT135 spectrum (125 MHz) of compound **4** in CDCl_3 .
Figure S4-4. COSY spectrum (500 MHz) of compound **4** in CDCl_3 .
Figure S4-5. HSQC spectrum (500 MHz) of compound **4** in CDCl_3 .
Figure S4-6. HMBC spectrum (500 MHz) of compound **4** in CDCl_3 .
Figure S4-7. NOESY spectrum (500 MHz) of compound **4** in CDCl_3 .

For compound 5:

Figure S5-1. ^1H NMR spectrum (400 MHz) of compound **5** in CDCl_3 .
Figure S5-2. ^{13}C and DEPT NMR spectra (100 MHz) of compound **5** in CDCl_3 .
Figure S5-3. COSY spectrum (400 MHz) of compound **5** in CDCl_3 .
Figure S5-4. HSQC spectrum (400 MHz) of compound **5** in CDCl_3 .
Figure S5-5. HMBC spectrum (400 MHz) of compound **5** in CDCl_3 .
Figure S5-6. NOESY spectrum (400 MHz) of compound **5** in CDCl_3 .

P17-F19-9-3-4
Probe: dual
Pulse Sequence: s2pu1

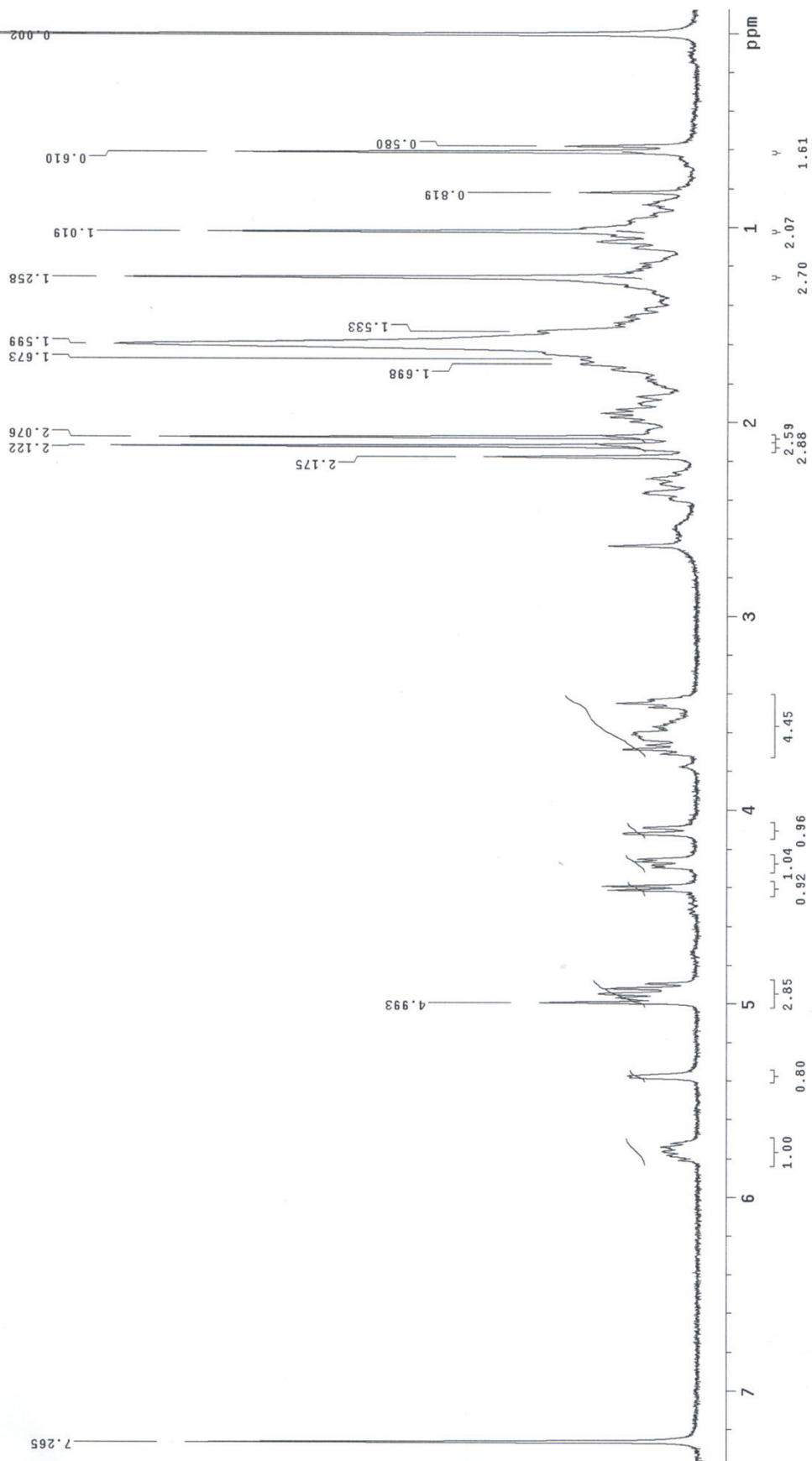


Figure S1-1. ¹H NMR spectrum (400 MHz) of compound **1** in CDCl₃.

P17-F19-9-3-4
Probe: dual
Pulse Sequence: s2pu1

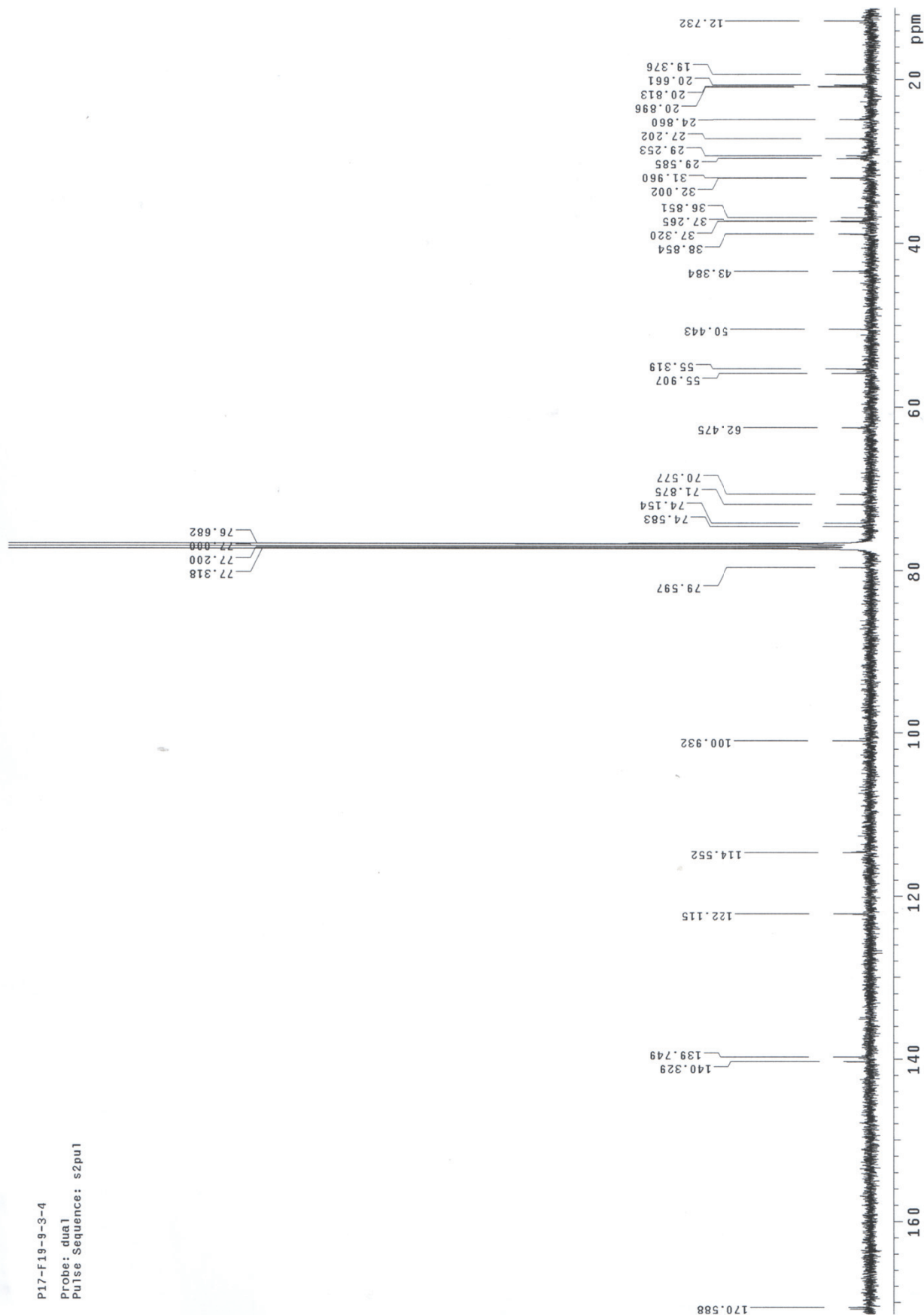


Figure S1-2. ¹³C NMR spectrum (100 MHz) of compound **1** in CDCl₃

P17-F19-9-3-4

Probe: dual

Pulse Sequence: DEPT

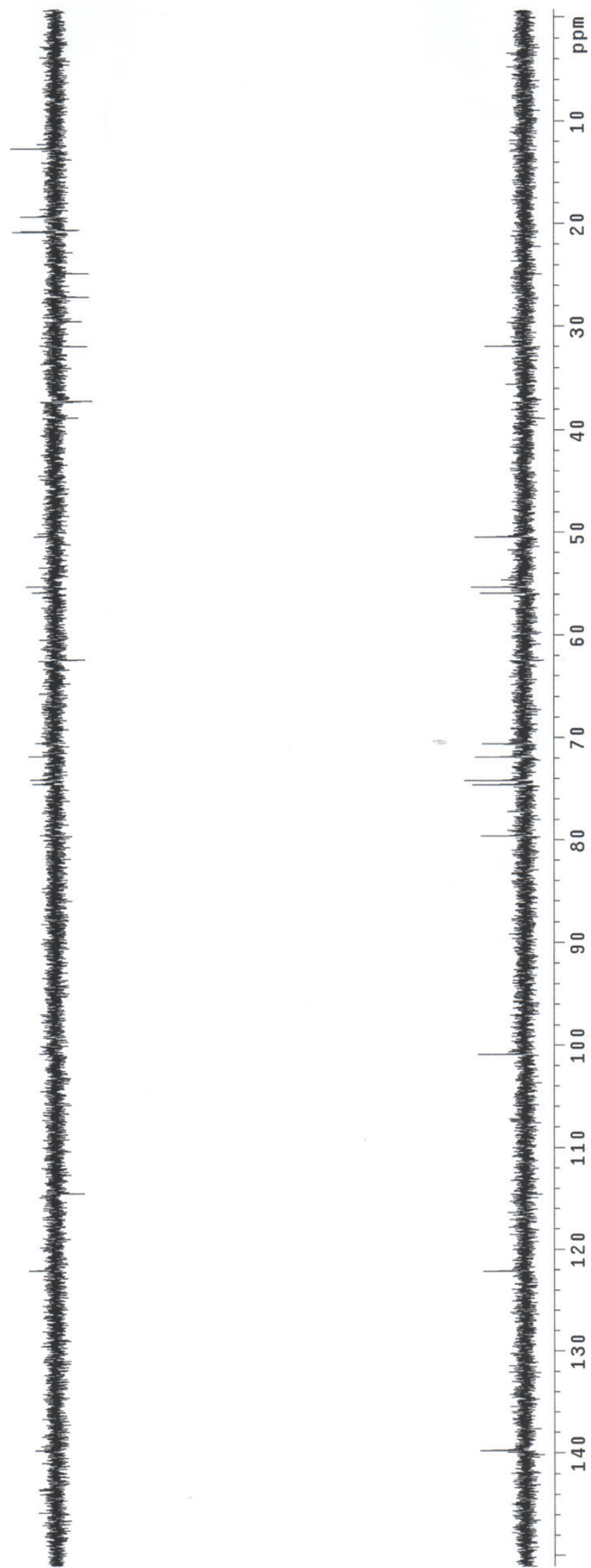


Figure S1-3. DEPT135 spectrum (100 MHz) of compound **1** in CDCl_3 .

P17-F19-9-3-4
Probe: dual
Pulse Sequence: gCOSY

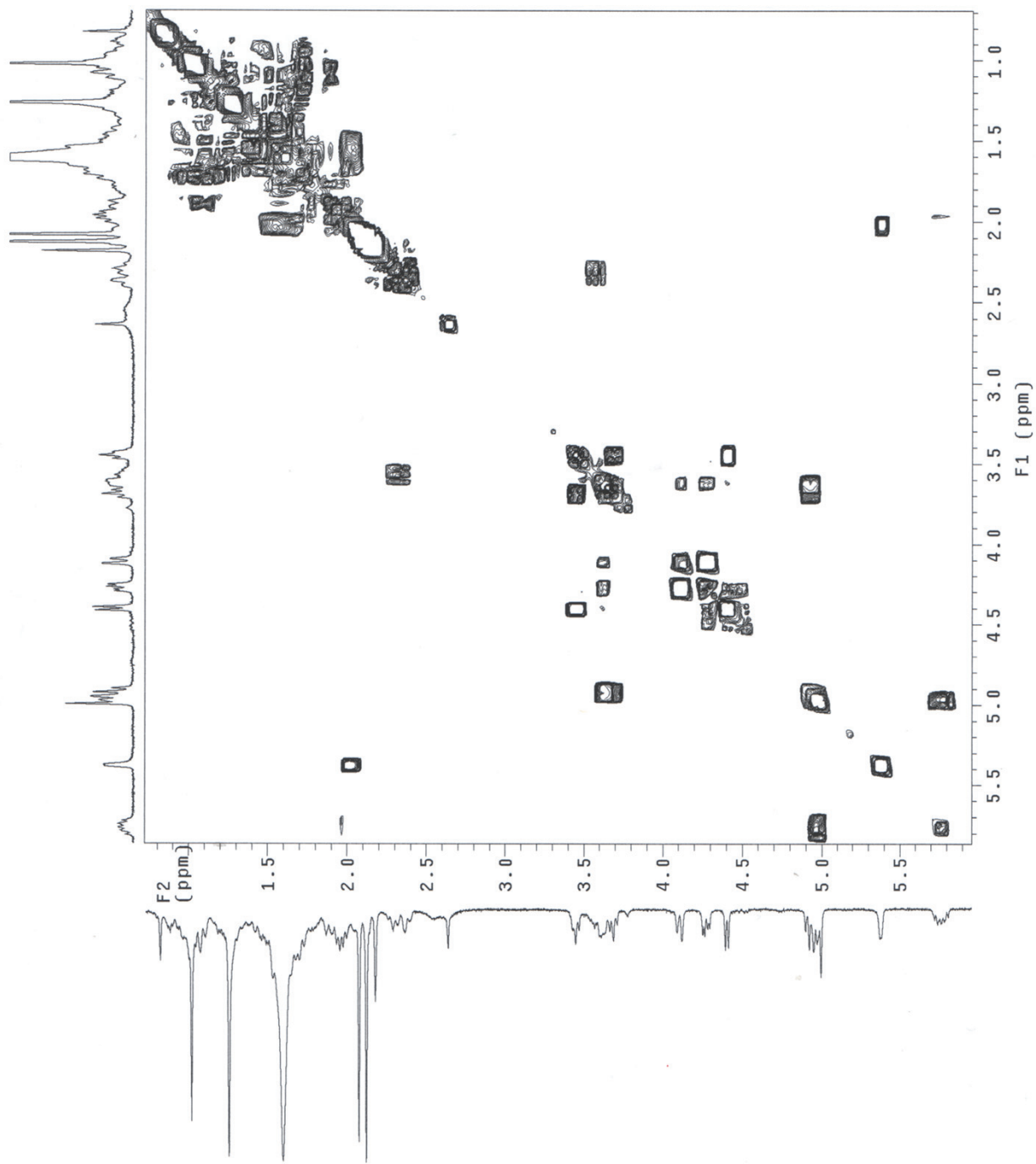


Figure S1-4. COSY spectrum (400 MHz) of compound **1** in CDCl_3 .

P17-F19-9-3-4
Probe: dual
Pulse Sequence: HSQCAD

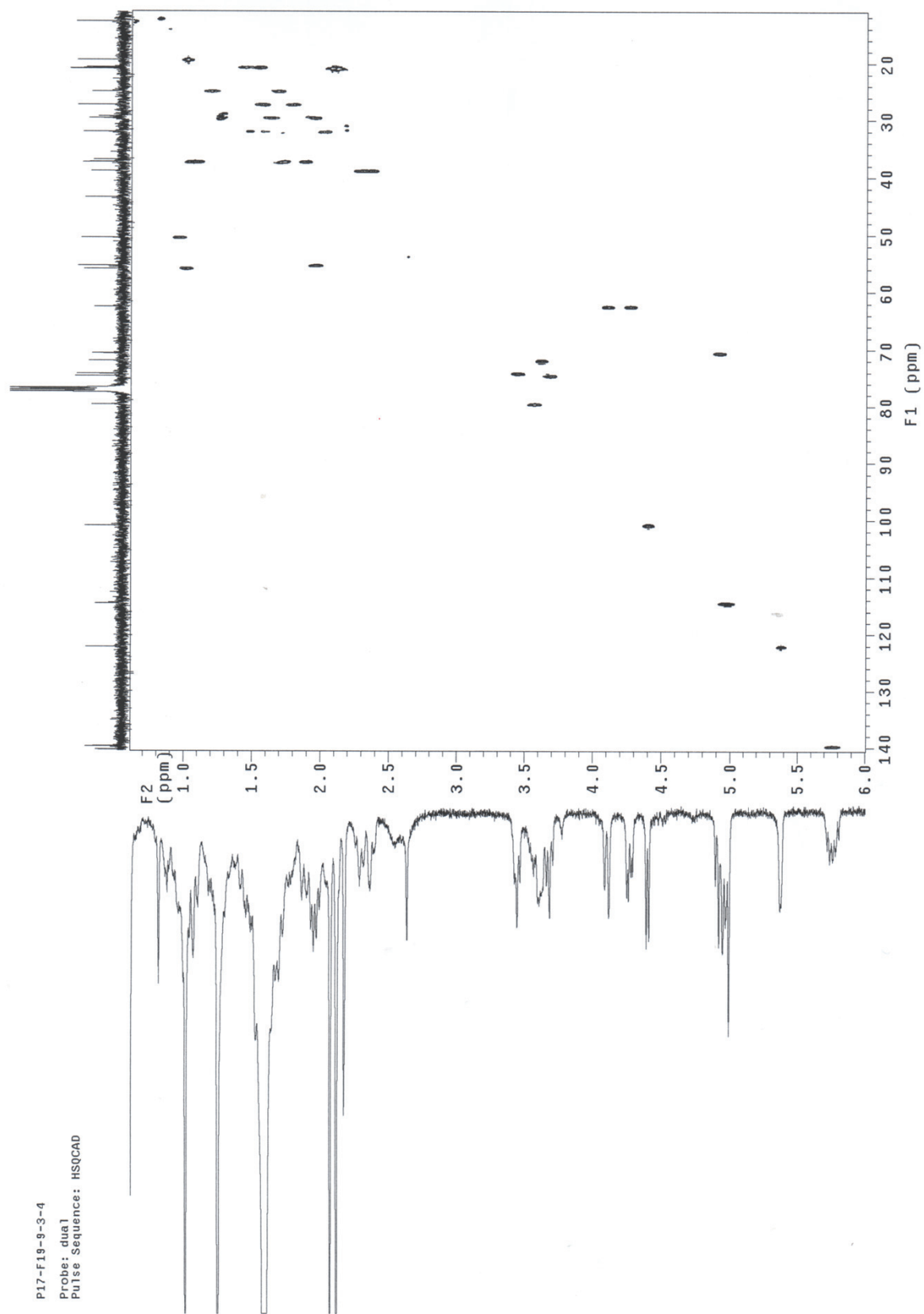


Figure S1-5. HSQC spectrum (400 MHz) of compound **1** in CDCl₃.

P17-F19-9-3-4
Probe: dua
Pulse Sequence: gHMBCAD

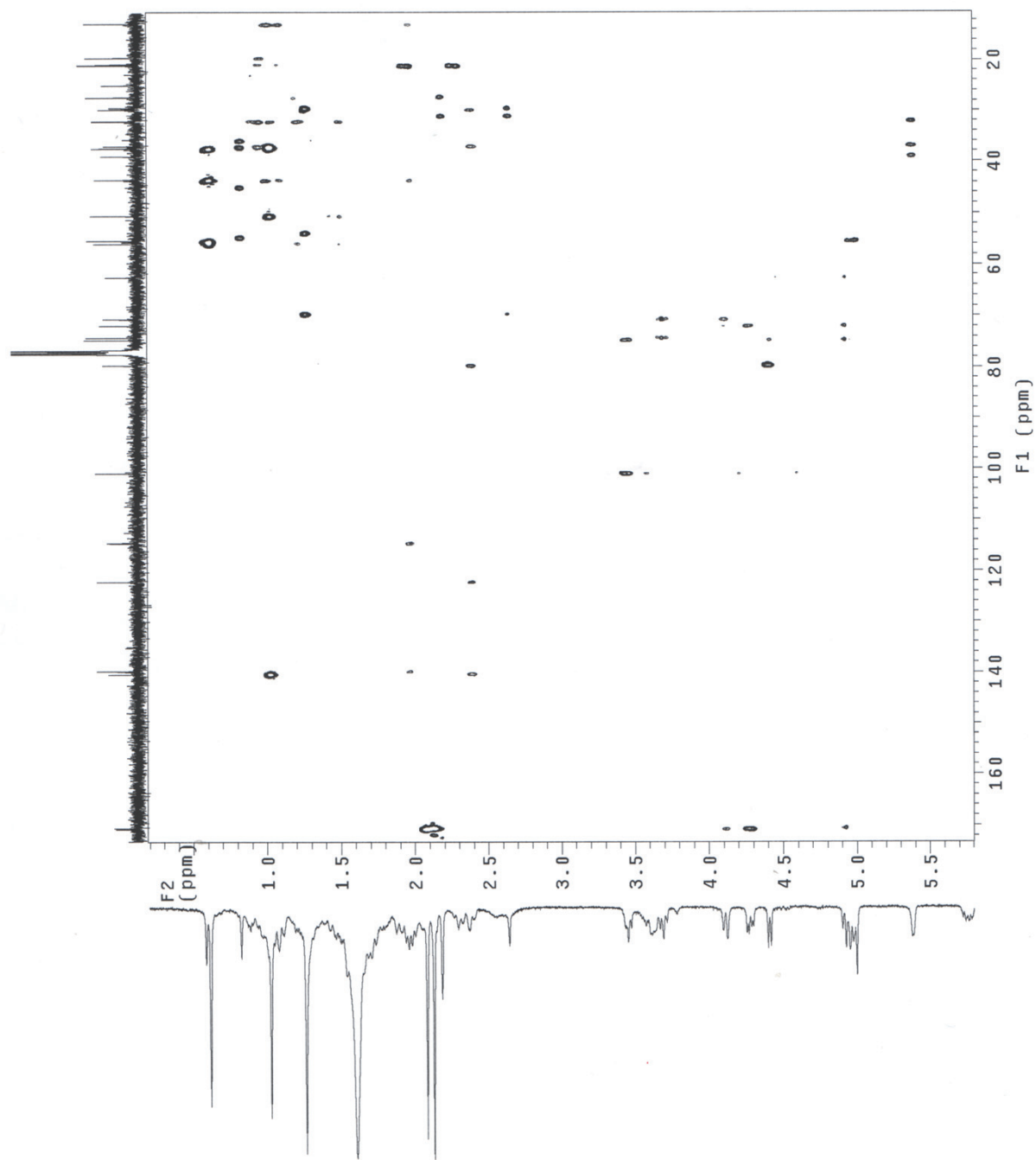


Figure S1-6. HMBC spectrum (400 MHz) of compound **1** in CDCl₃.

P17-F19-9-3-4
Probe: dual
Pulse Sequence: NOESY

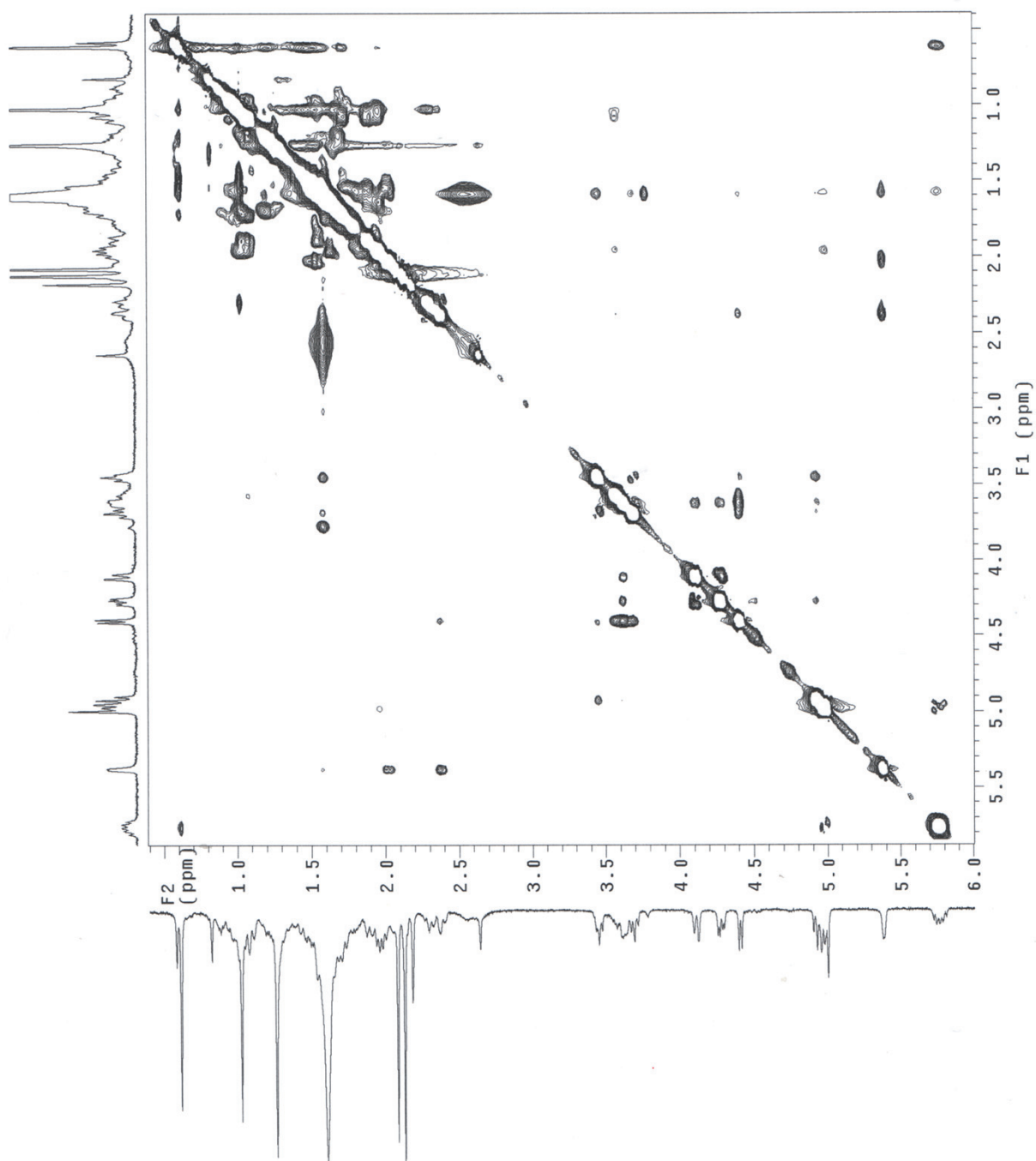


Figure S1-7. NOESY spectrum (100 MHz) of compound **1** in CDCl_3

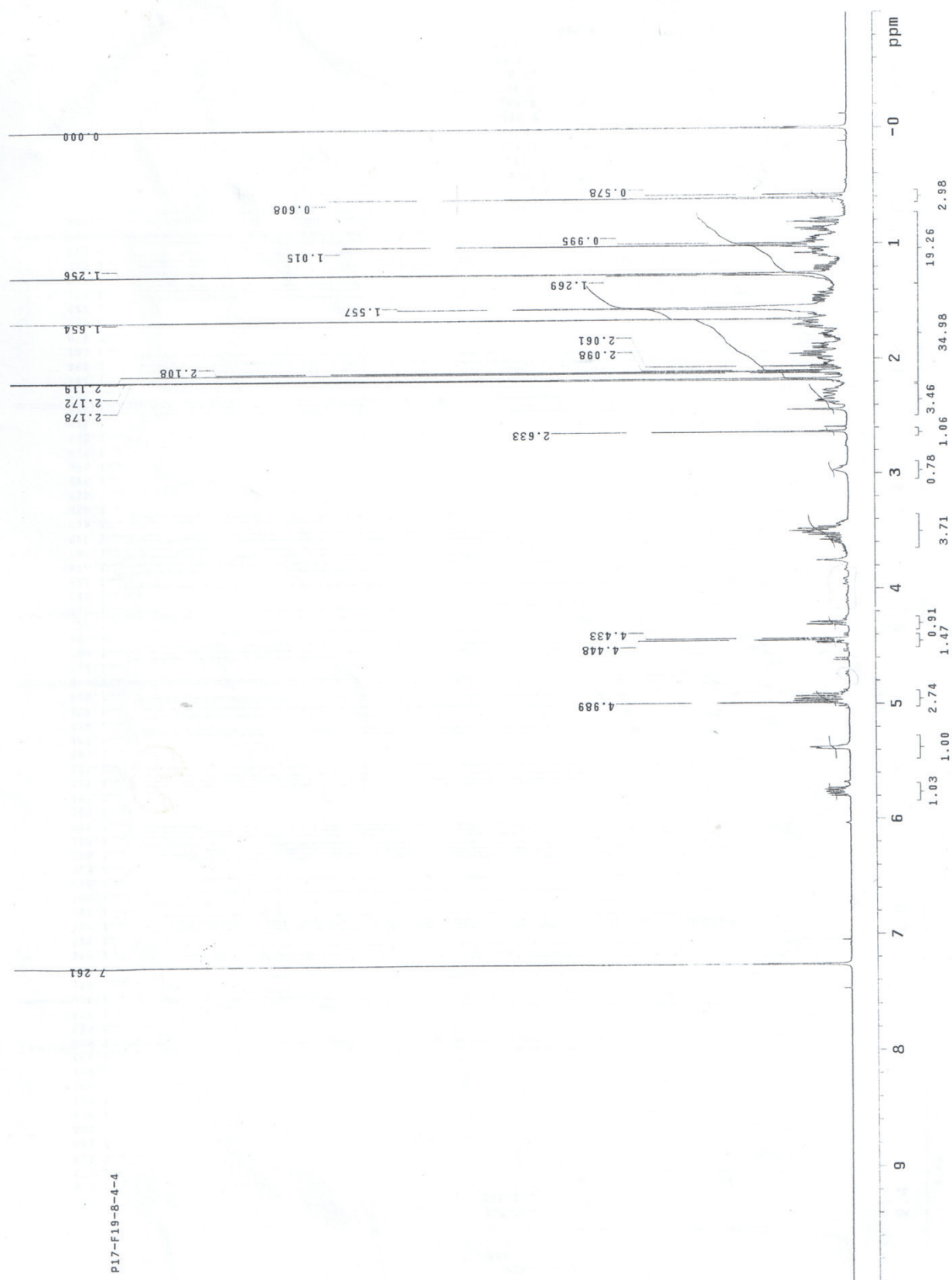


Figure S2-1. ^1H NMR spectrum (500 MHz) of compound **2** in CDCl_3 .

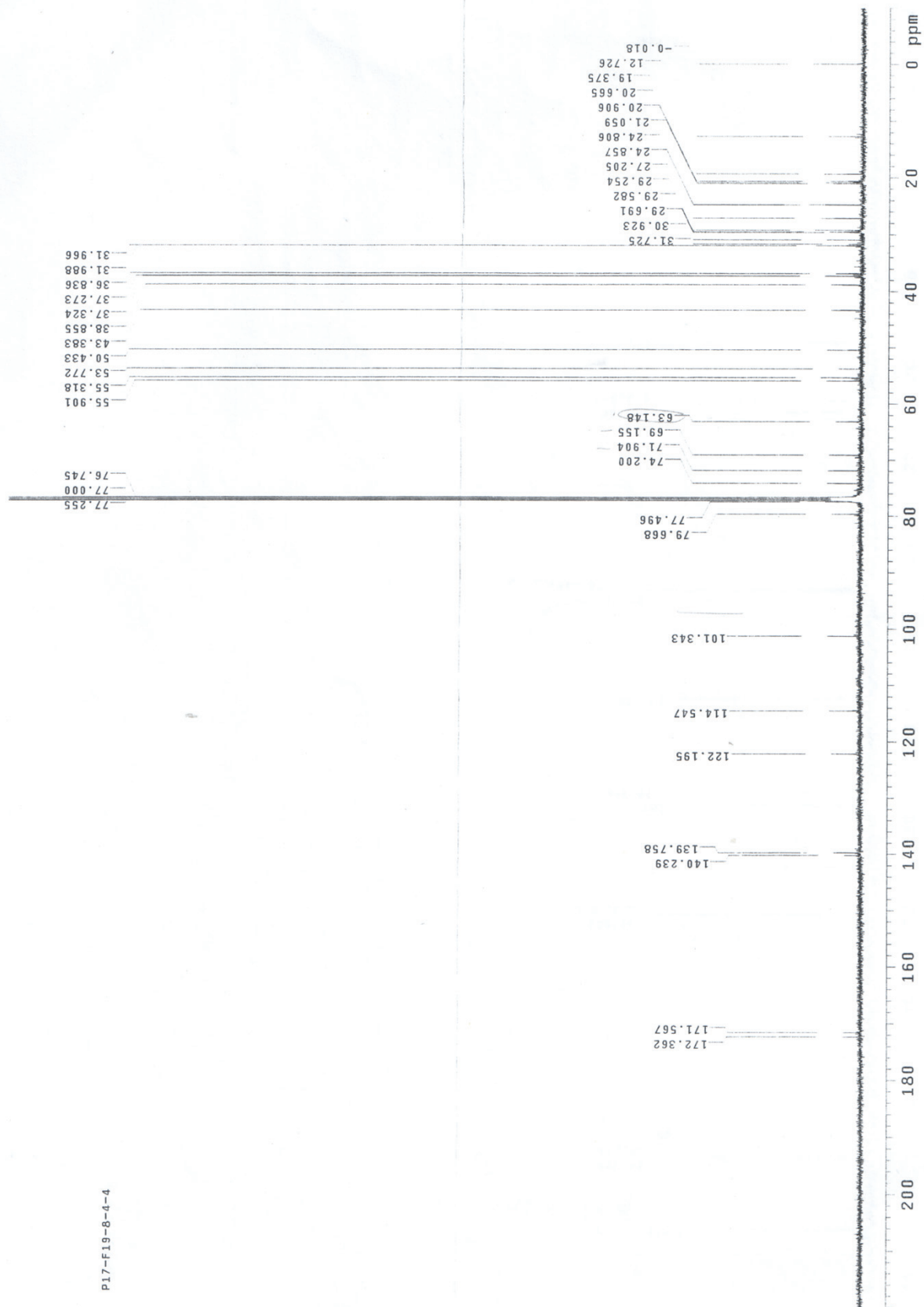


Figure S2-2. ¹³C NMR spectrum (125 MHz) of compound 2 in CDCl₃

CH/CH3 up , CH2 down



CH carbons

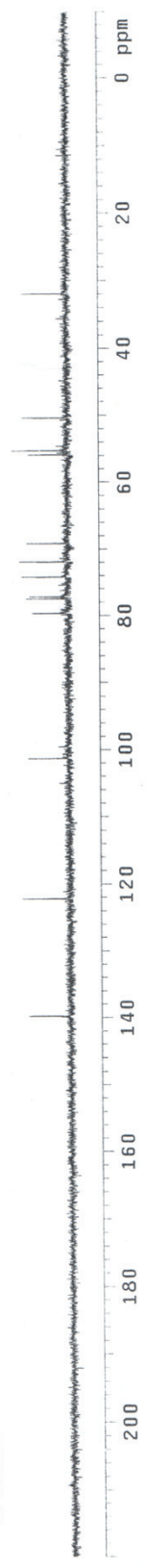


Figure S2-3. DEPT135 spectrum (125 MHz) of compound **2** in CDCl_3 .

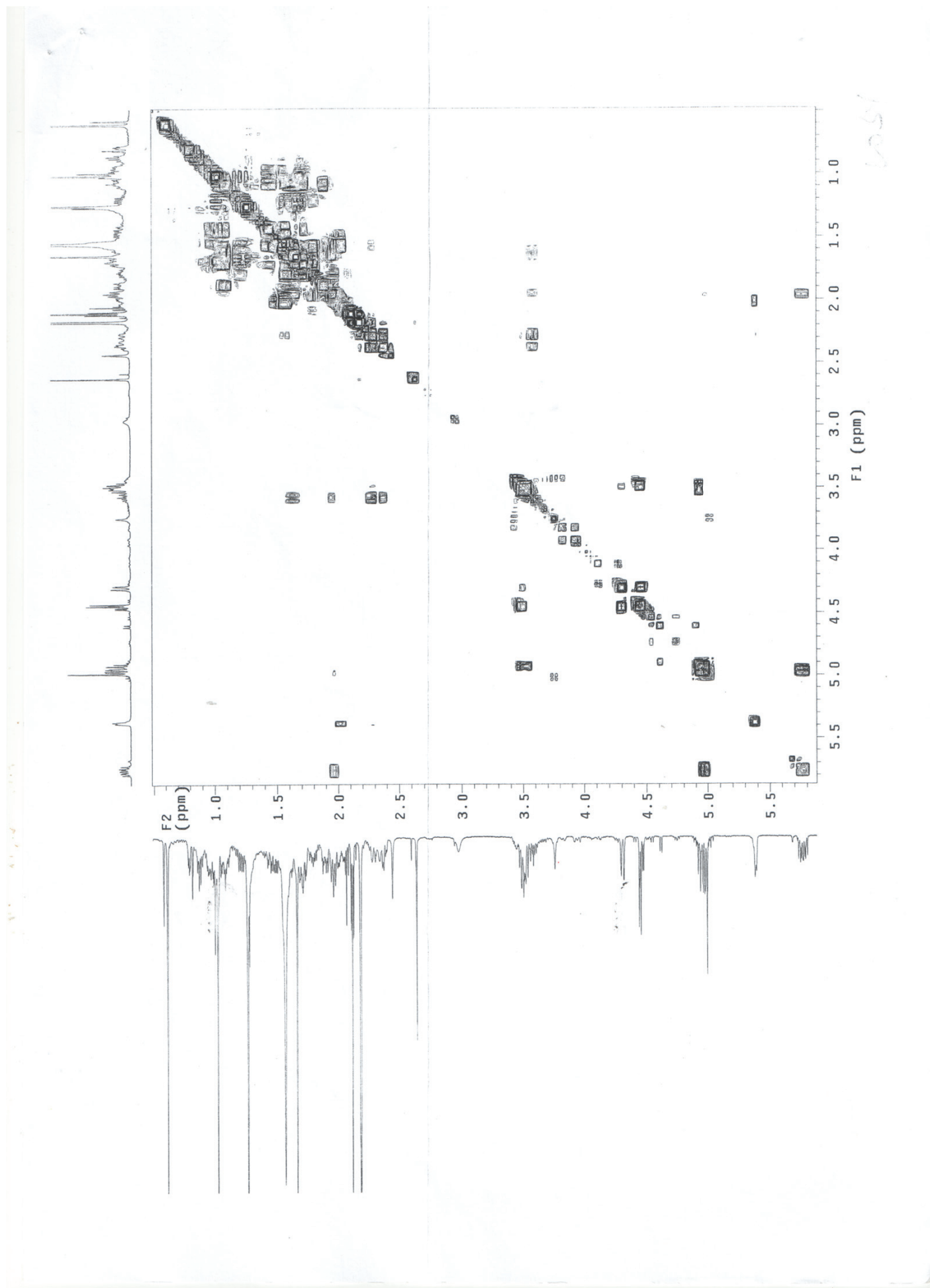


Figure S2-4. COSY spectrum (500 MHz) of compound **2** in CDCl_3 .

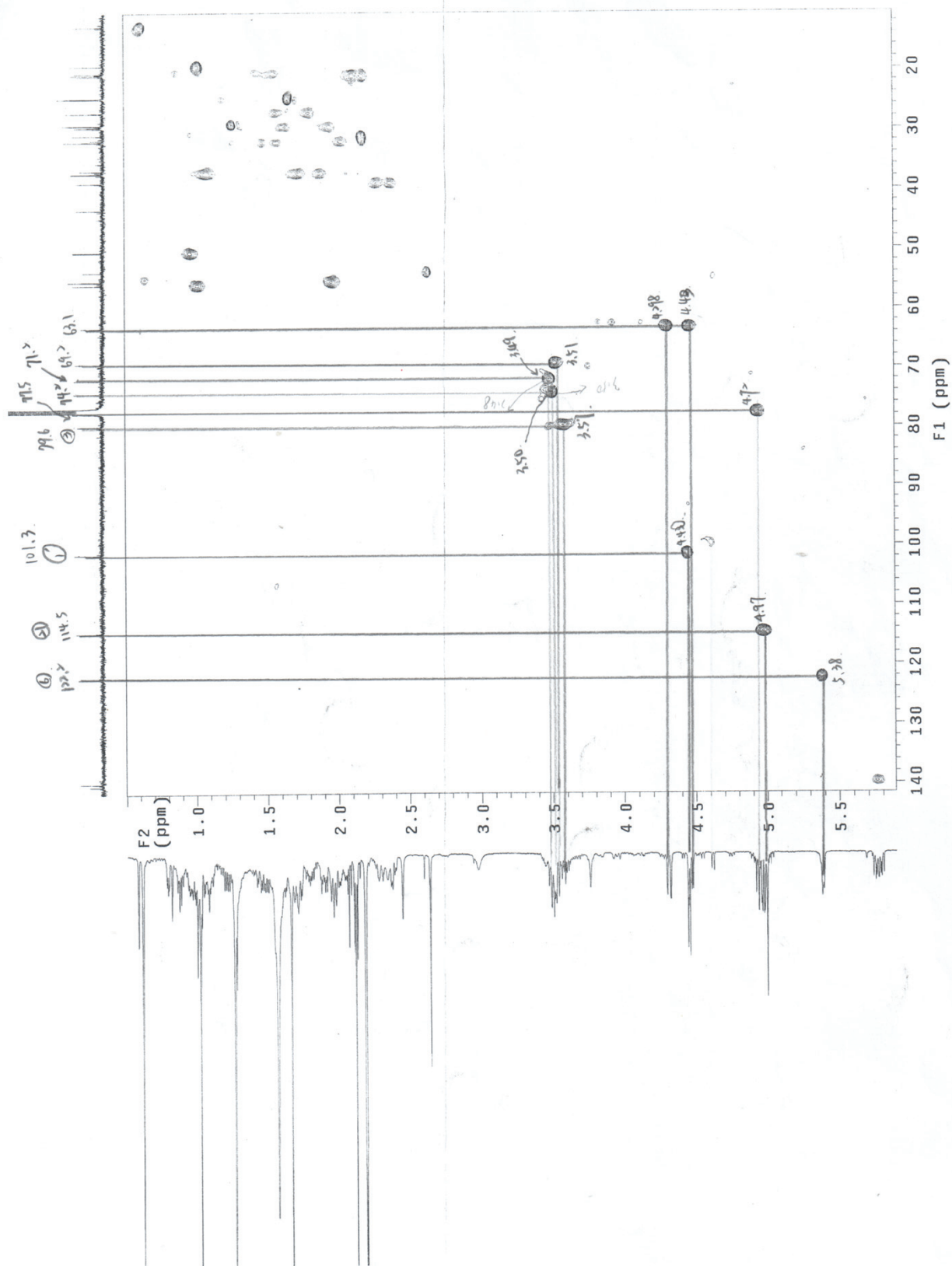


Figure S2-5. HSQC spectrum (500 MHz) of compound 2 in CDCl_3 .

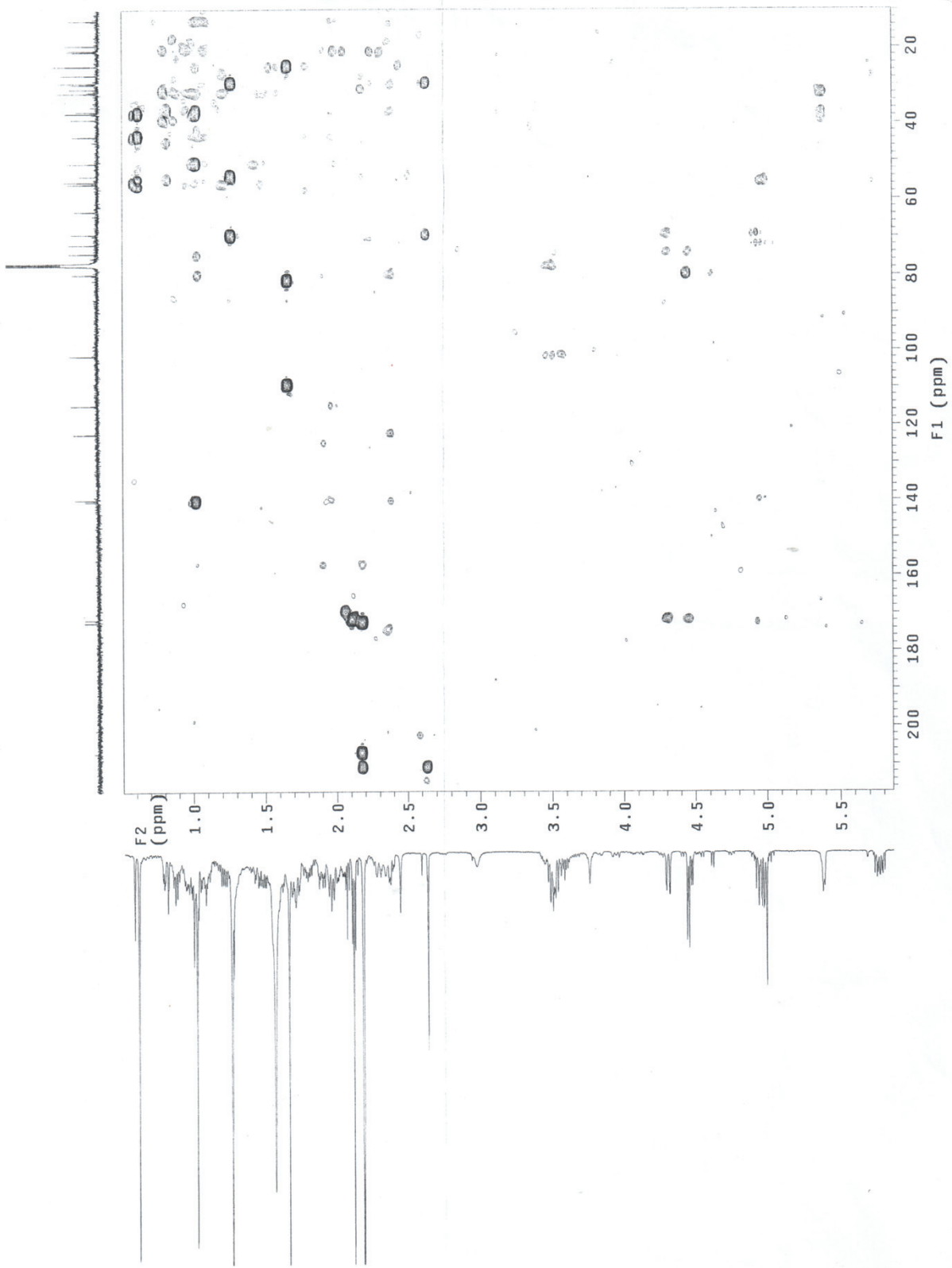


Figure S2-6. HMBC spectrum (500 MHz) of compound 2 in CDCl₃.

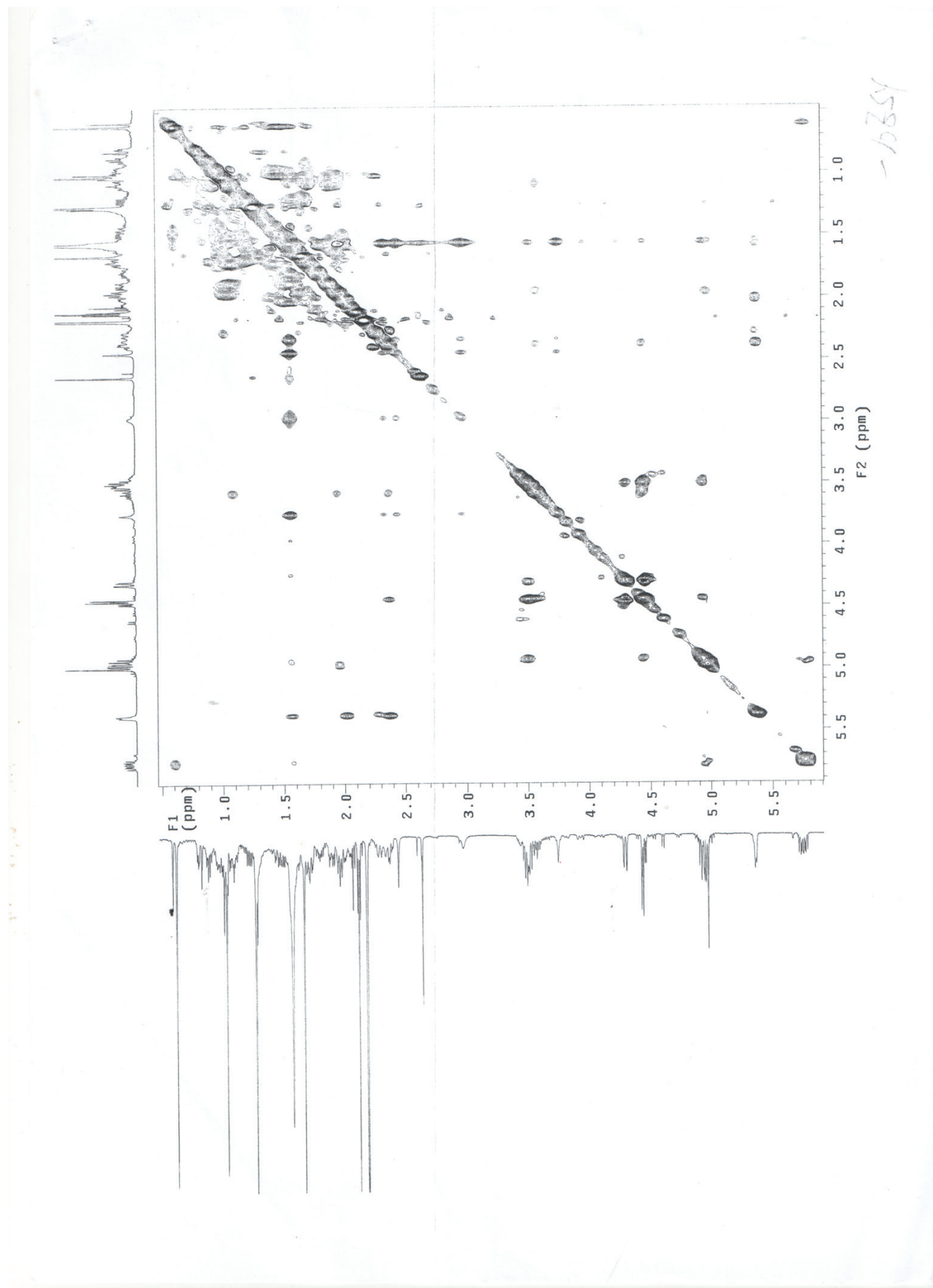


Figure S2-7. NOESY spectrum (500 MHz) of compound **2** in CDCl₃.

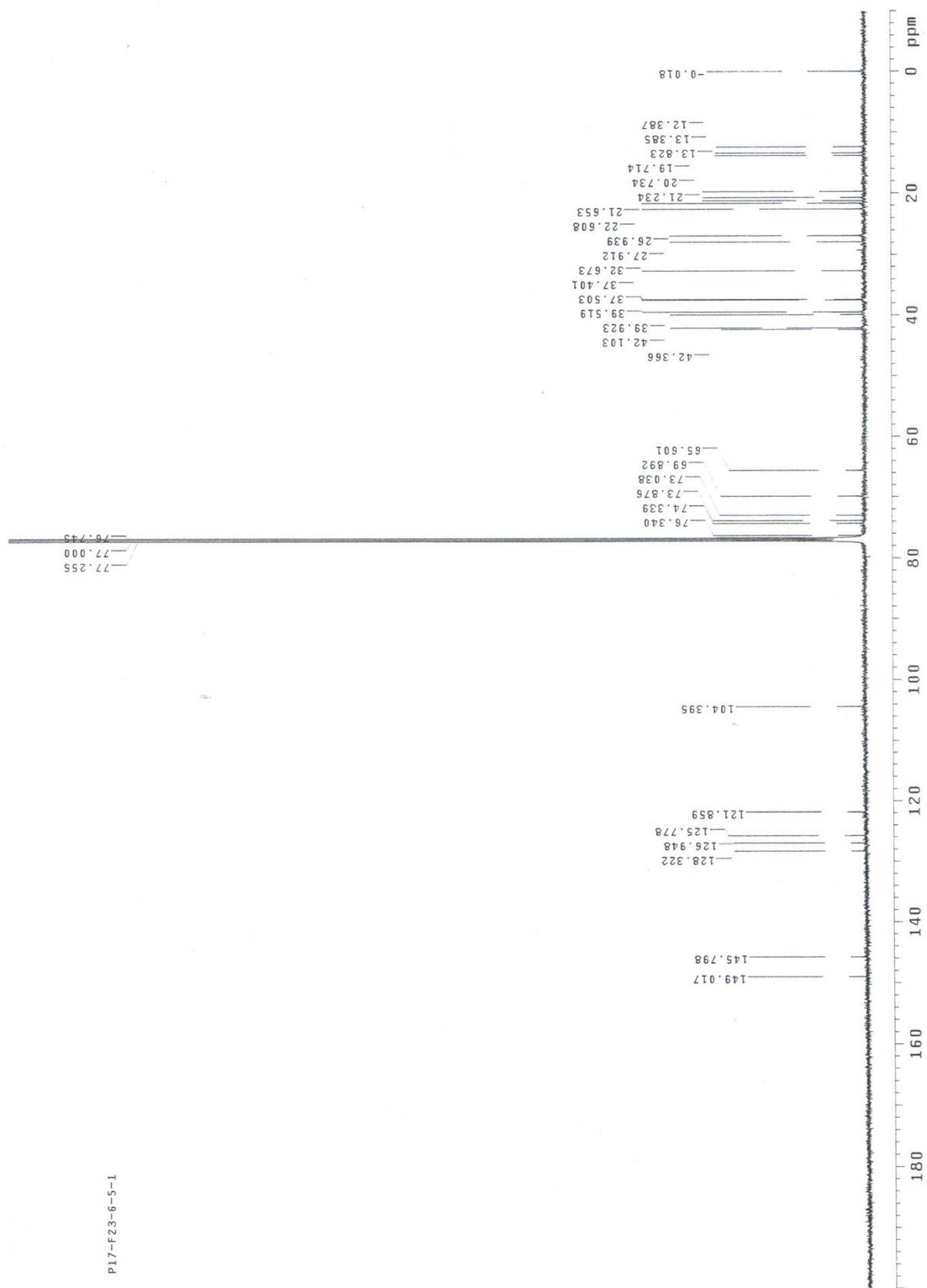


Figure S3-2. ^{13}C NMR spectrum (125 MHz) of compound **3** in CDCl_3 .

CH/CH3 up , CH2 down



CH carbons

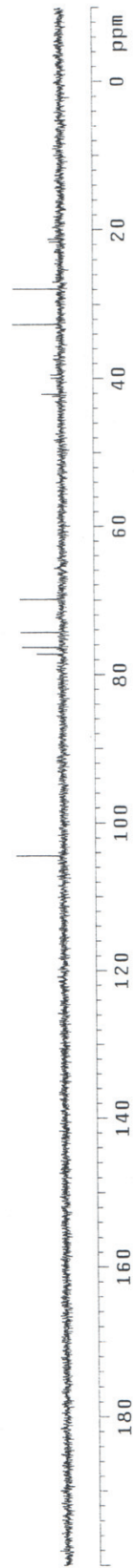
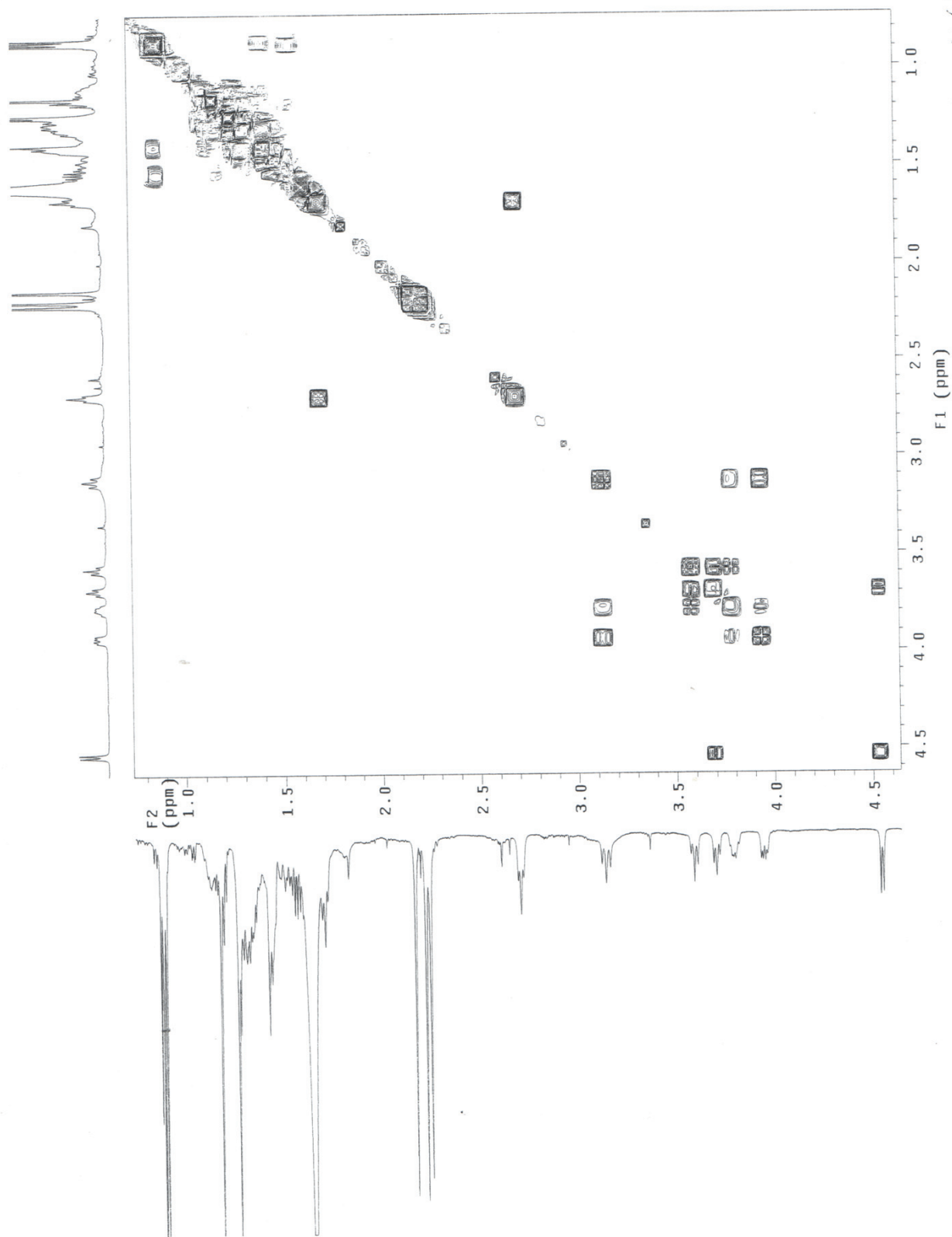


Figure S3-3. DEPT135 spectrum (125 MHz) of compound **3** in CDCl₃.



054

Figure S3-4. COSY spectrum (500 MHz) of compound **3** in CDCl_3 .

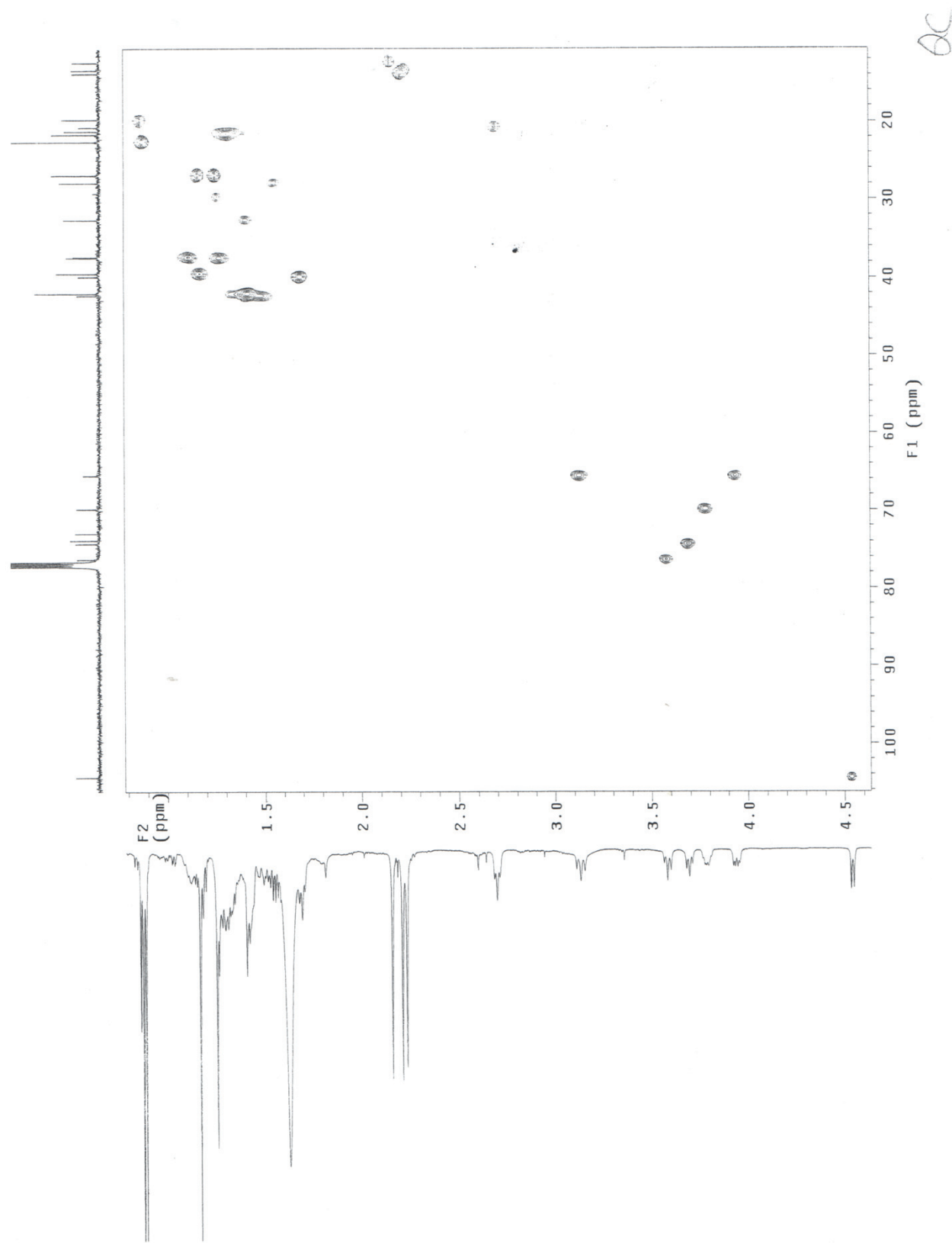


Figure S3-5. HSQC spectrum (500 MHz) of compound **3** in CDCl_3 .

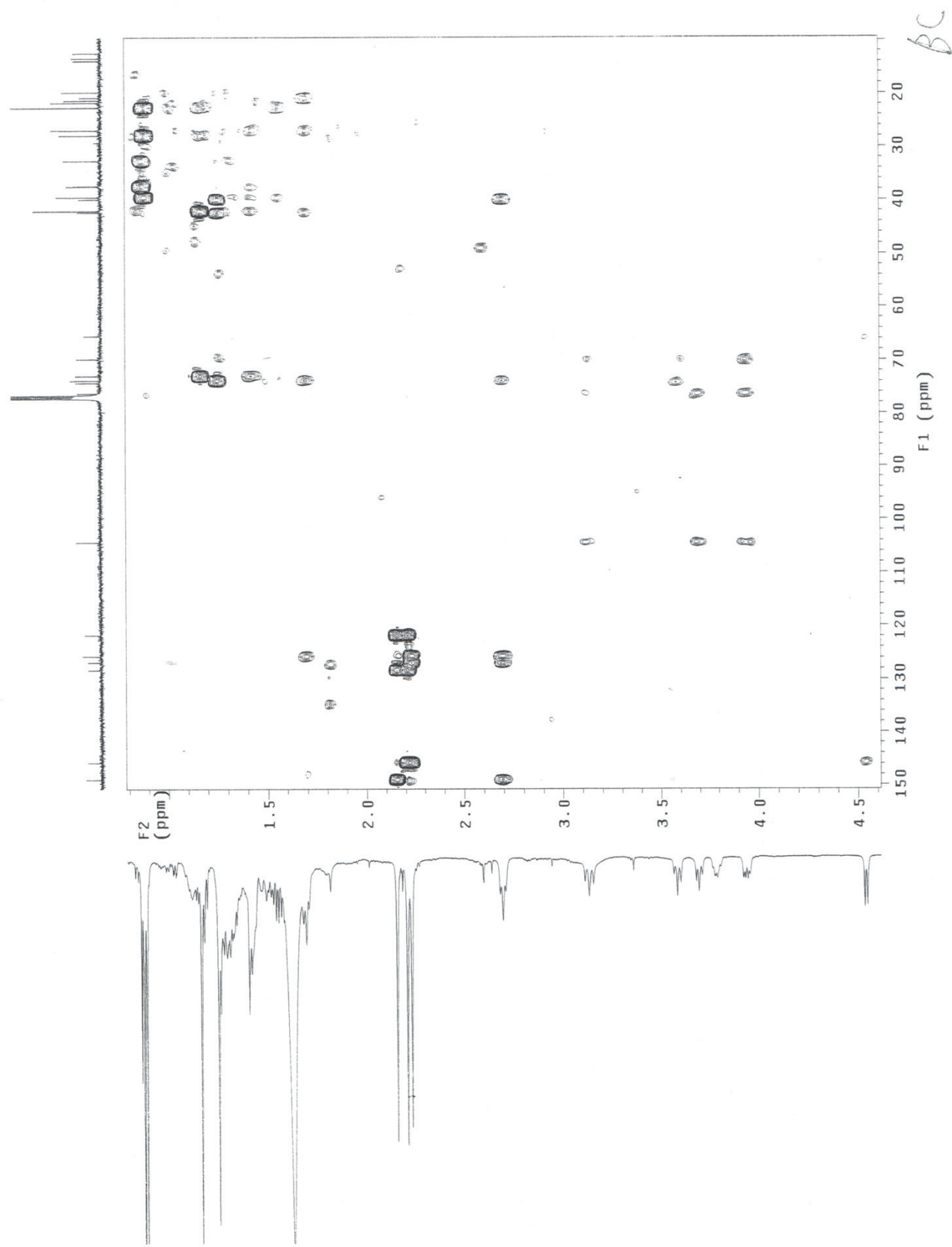
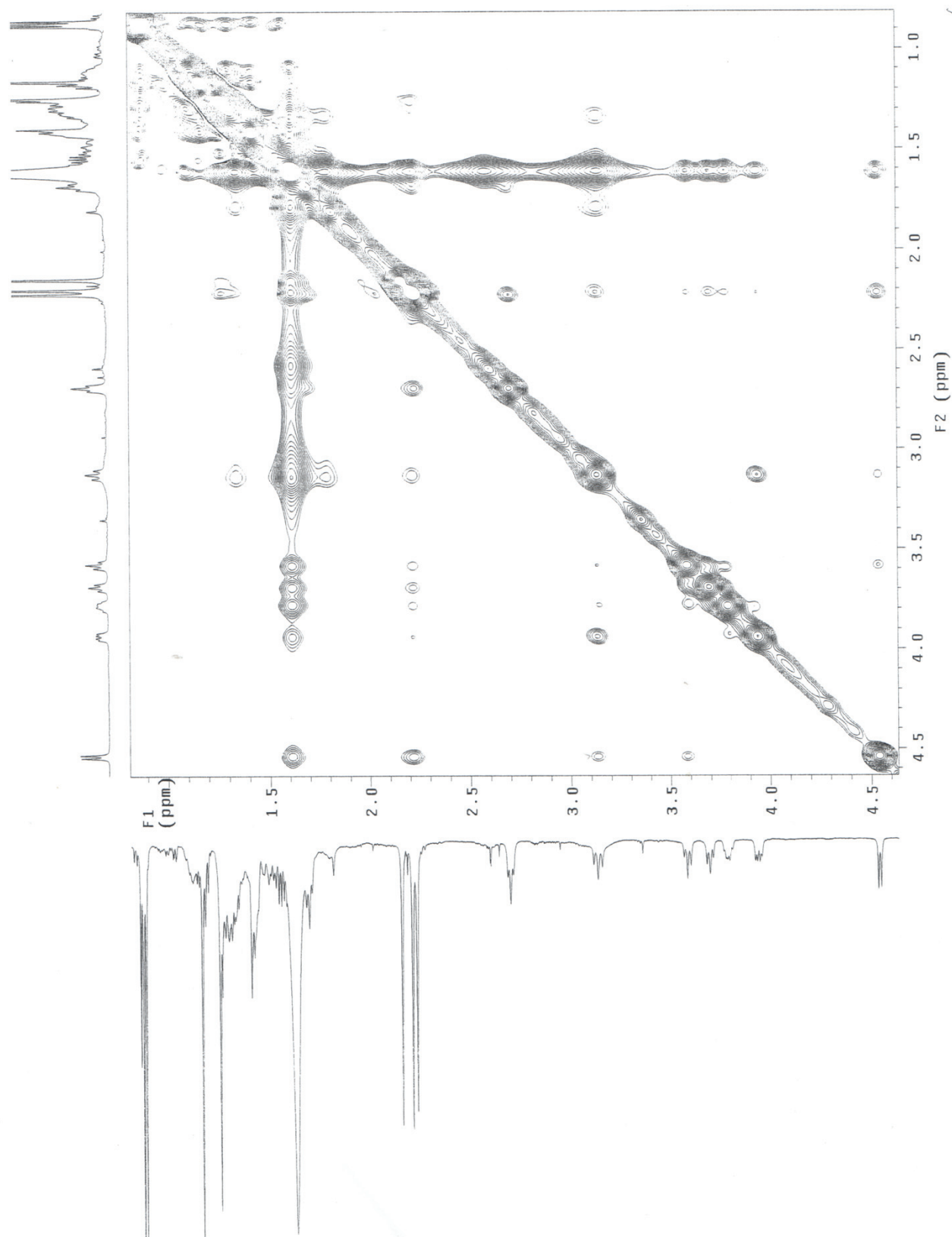


Figure S3-6. HMBC spectrum (500 MHz) of compound **3** in CDCl₃.



abcsy

Figure S3-7. NOESY spectrum (500 MHz) of compound **3** in CDCl₃.

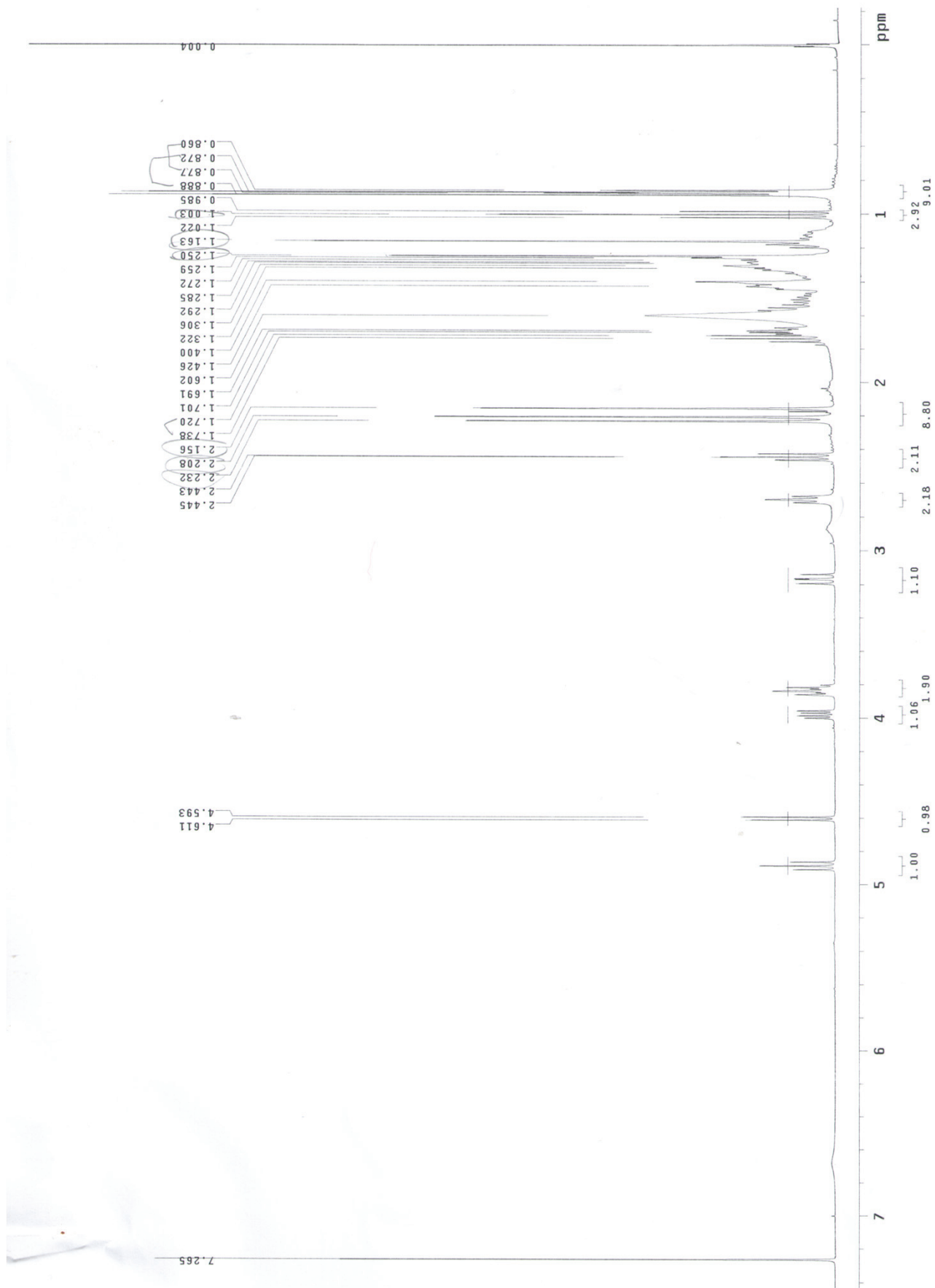


Figure S4-1. ¹H NMR spectrum (400 MHz) of compound **4** in CDCl₃.

P17-F18-11-3-1

Sample Name:

P17-F18-11-3-1

Data Collected on:

Varian-NMR-vnmr400

Archive directory:

/home/shen/vnmr400/data

Sample name:

P17-F18-11-3-1_20120912_02

Fidfile: CARBON_01

Pulse Sequence: CARBON (szpul)

Solvent: cdcl3

Data collected on: Sep 12 2012

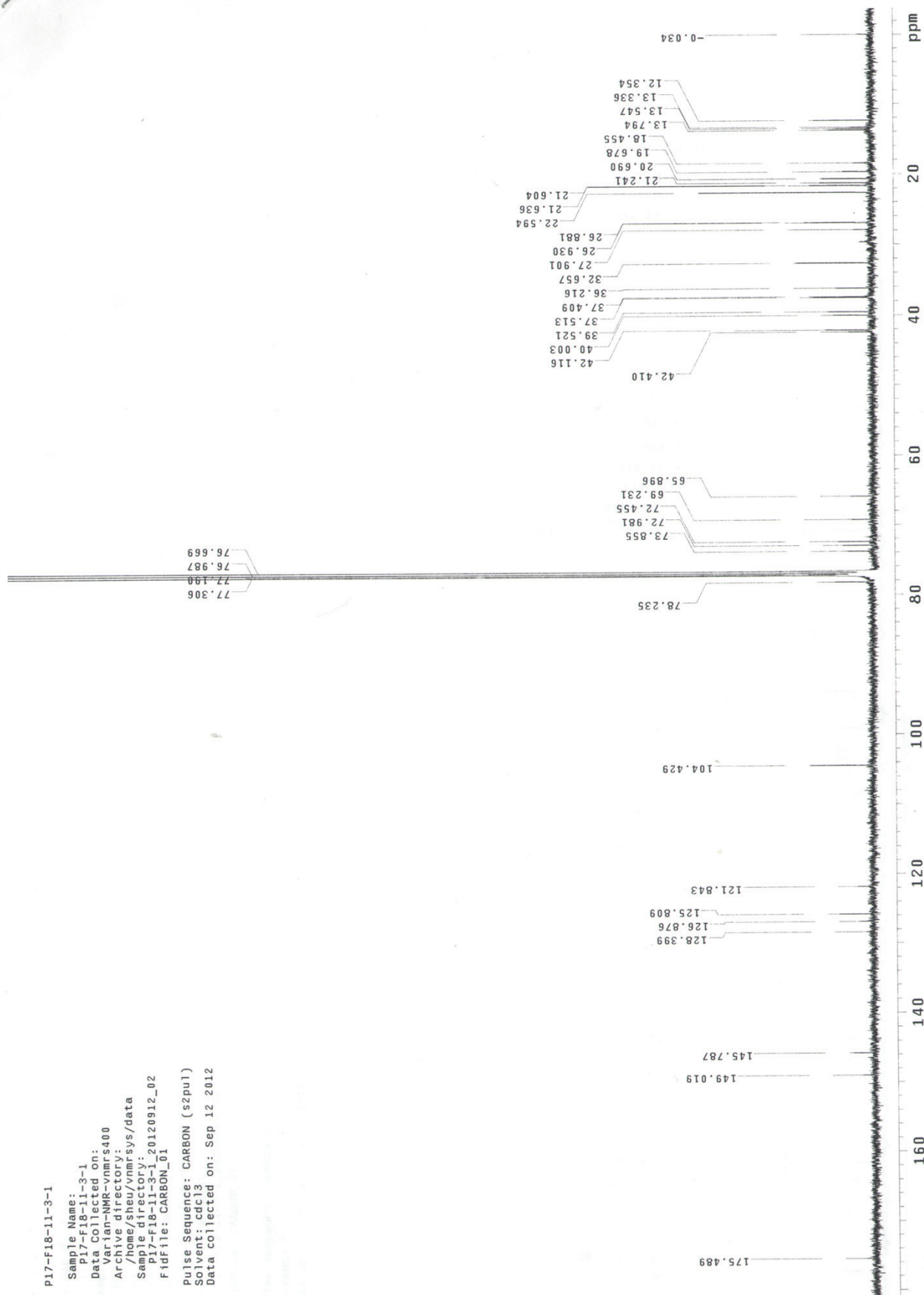


Figure S4-2. ^{13}C NMR spectrum (100 MHz) of compound **4** in CDCl_3 .

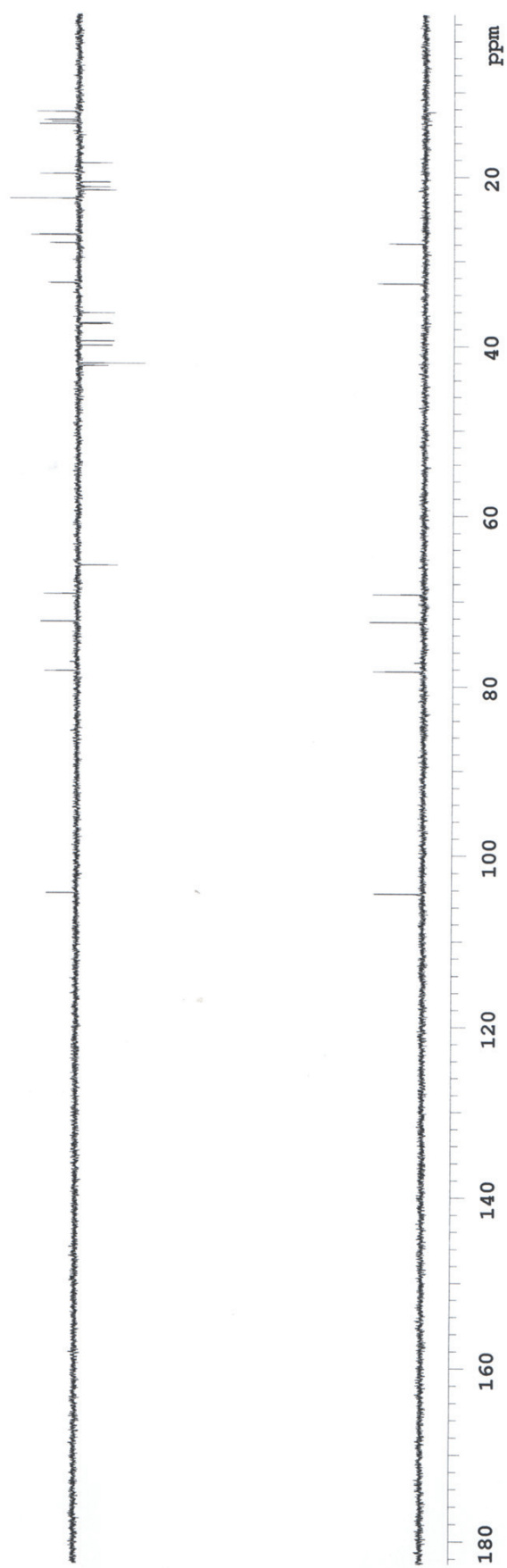


Figure S4-3. DEPT135 spectrum (125 MHz) of compound **4** in CDCl₃.

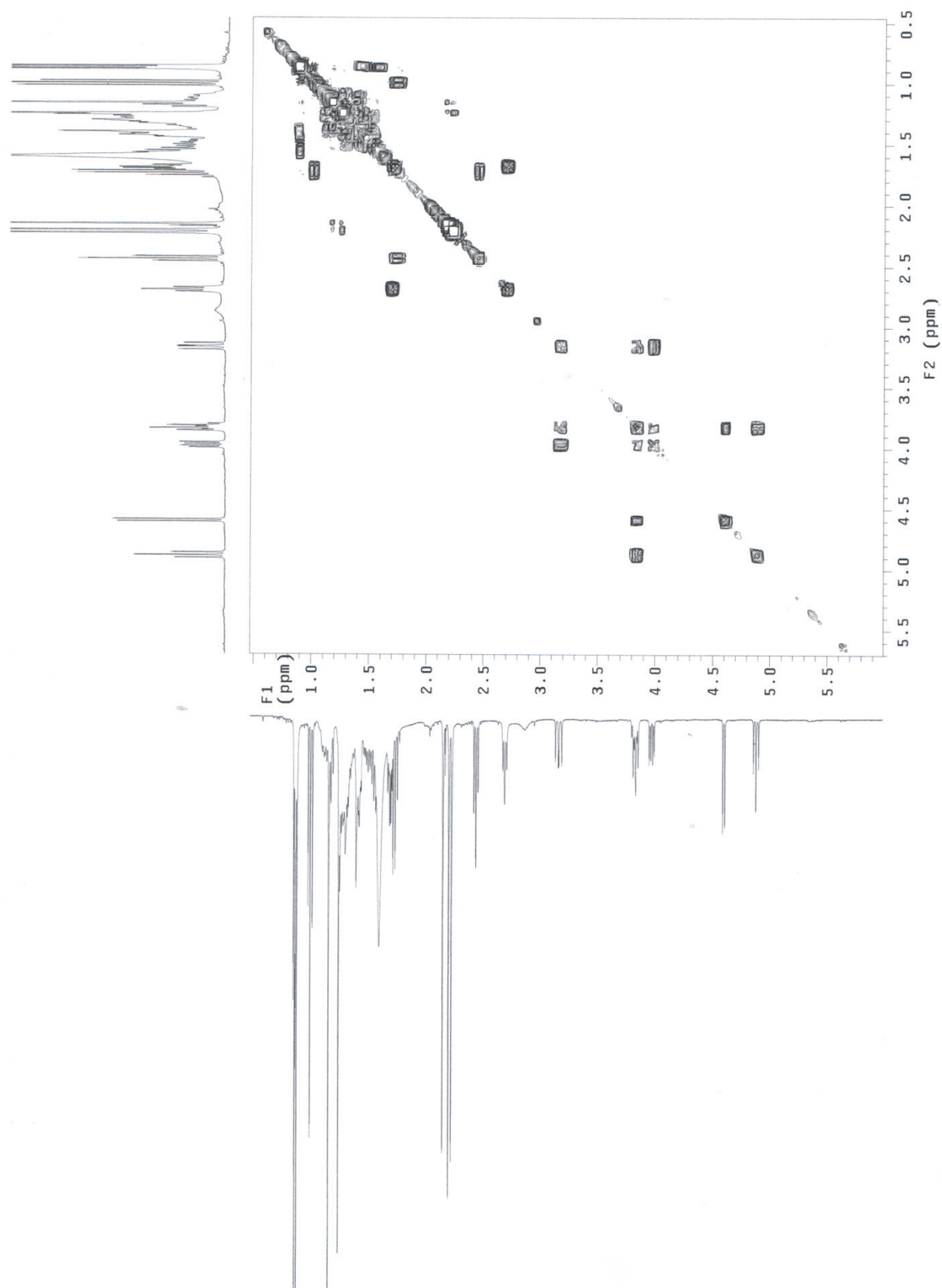


Figure S4-4. COSY spectrum (500 MHz) of compound **4** in CDCl₃.

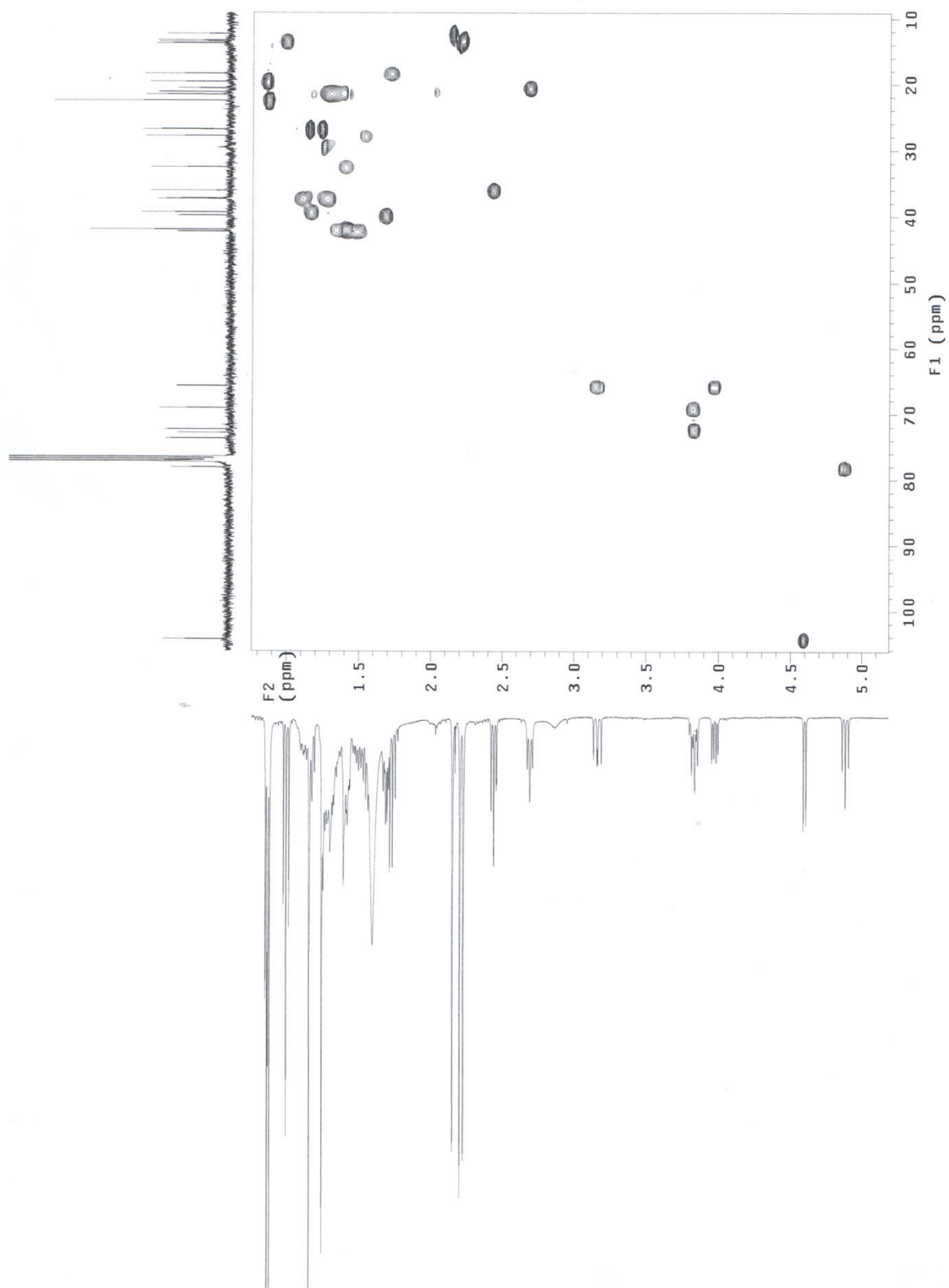


Figure S4-5. HSQC spectrum (500 MHz) of compound 4 in CDCl₃.

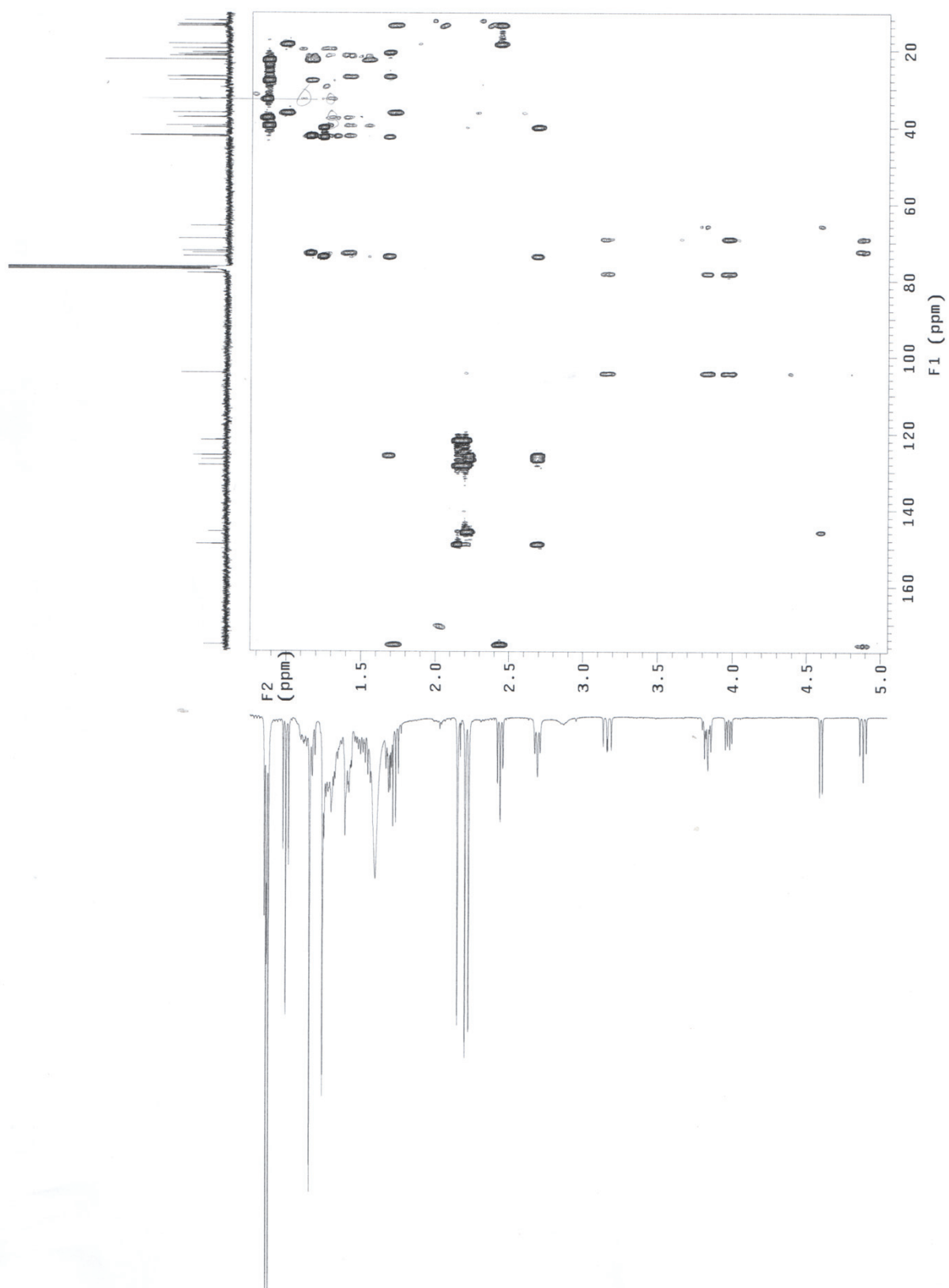


Figure S4-6. HMBC spectrum (500 MHz) of compound **4** in CDCl_3 .

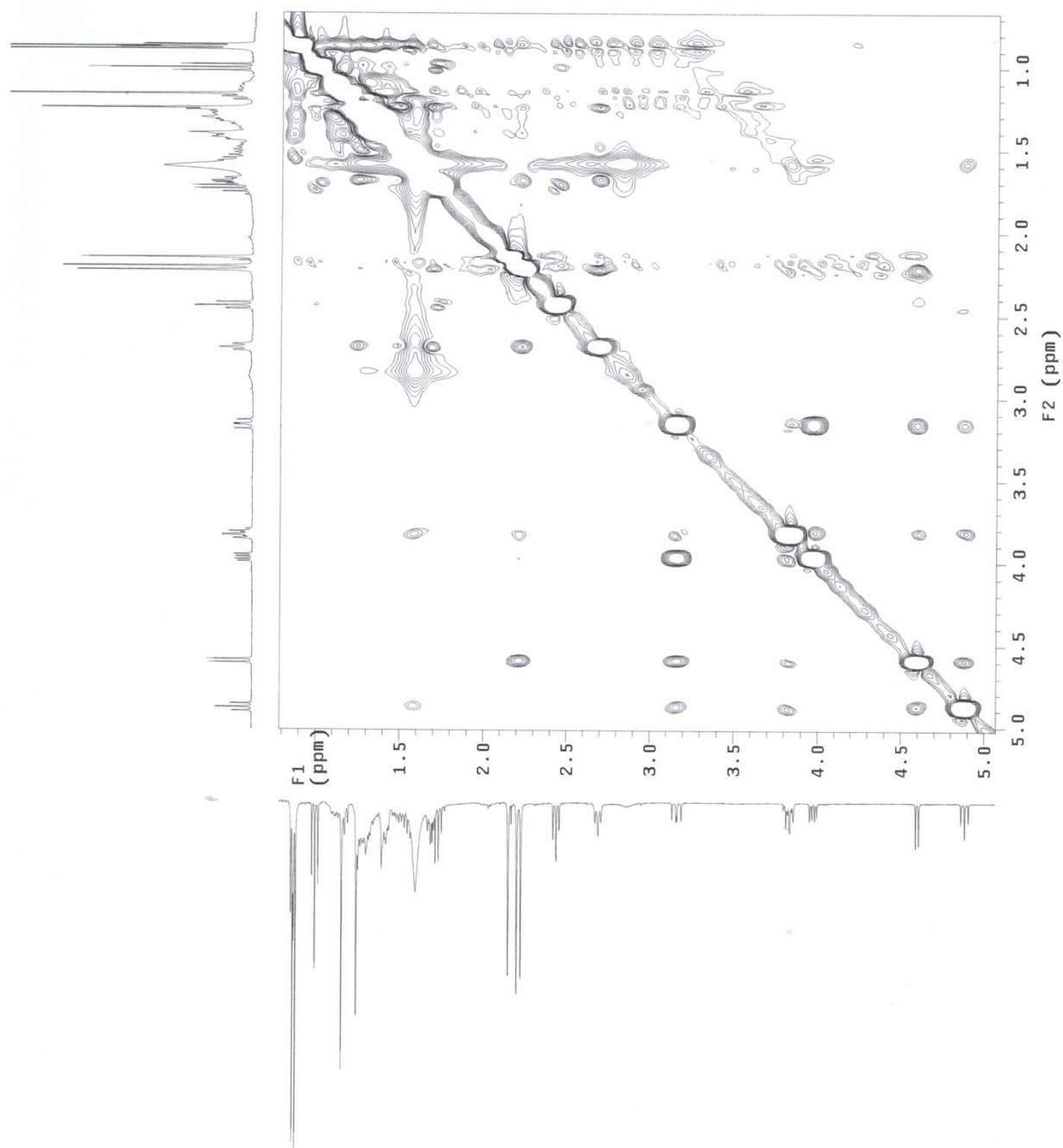


Figure S4-7. NOESY spectrum (500 MHz) of compound **4** in CDCl₃.

Sample Name:
 3H6-18n-4-2-1
 Data Collected on:
 Varian-NMR-vnmrs400
 Archive directory:
 /home/sheu/vnmrsys/data
 Sample directory:
 3H6-18n-4-2-1.20140206_01
 FID file: PROTON_02
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Feb 6 2014

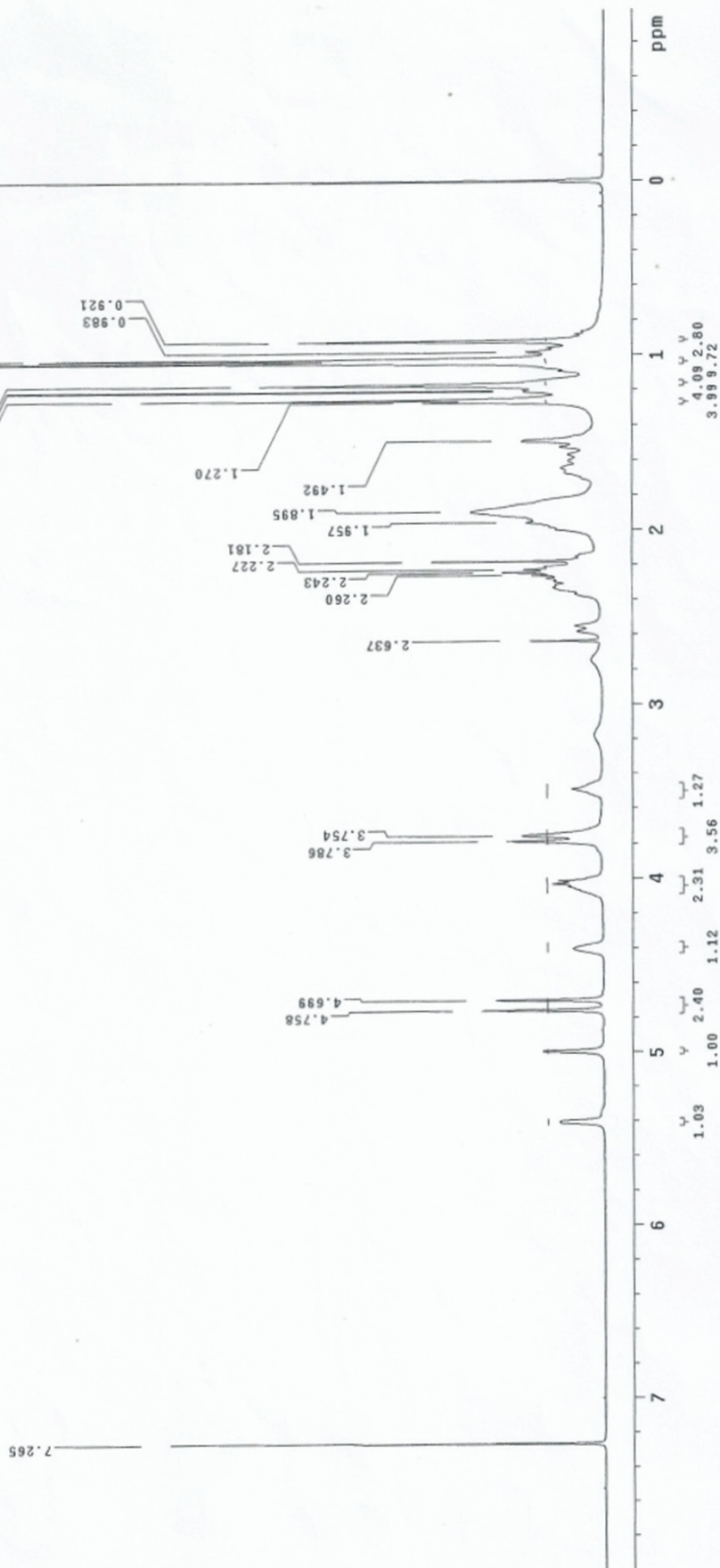


Figure S5-1. ¹H NMR spectrum (400 MHz) of compound 5 in CDCl₃.

JiH6-18n-4-2-1

Sample Name:

JiH6-18n-4-2-1

Data Collected on:

Varian-NMR-vnmrs400

Archive directory:

/home/sheu/vnmrsys/data

Sample directory:

JiH6-18n-4-2-1_20140206_01

FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Feb 7 2014

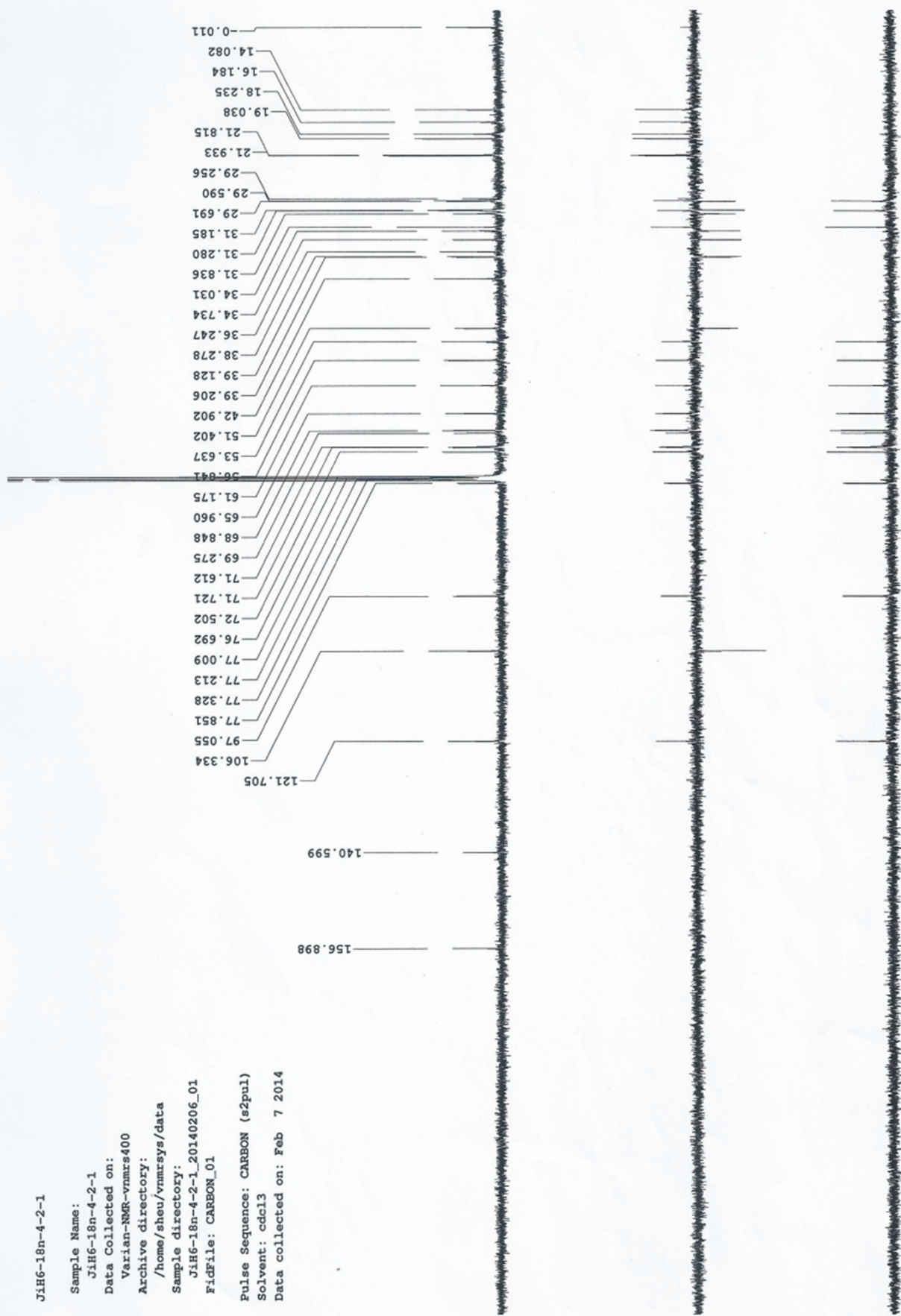


Figure S5-2. ^{13}C and DEPT NMR spectra (100 MHz) of compound **5** in CDCl_3

JiH6-18n-4-2-1

Sample Name:
JiH6-18n-4-2-1
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
JiH6-18n-4-2-1.20140206_01
FidFile: gCOSY_01
Pulse Sequence: gCOSY
Solvent: cdcl3
Data collected on: Feb 7 2014

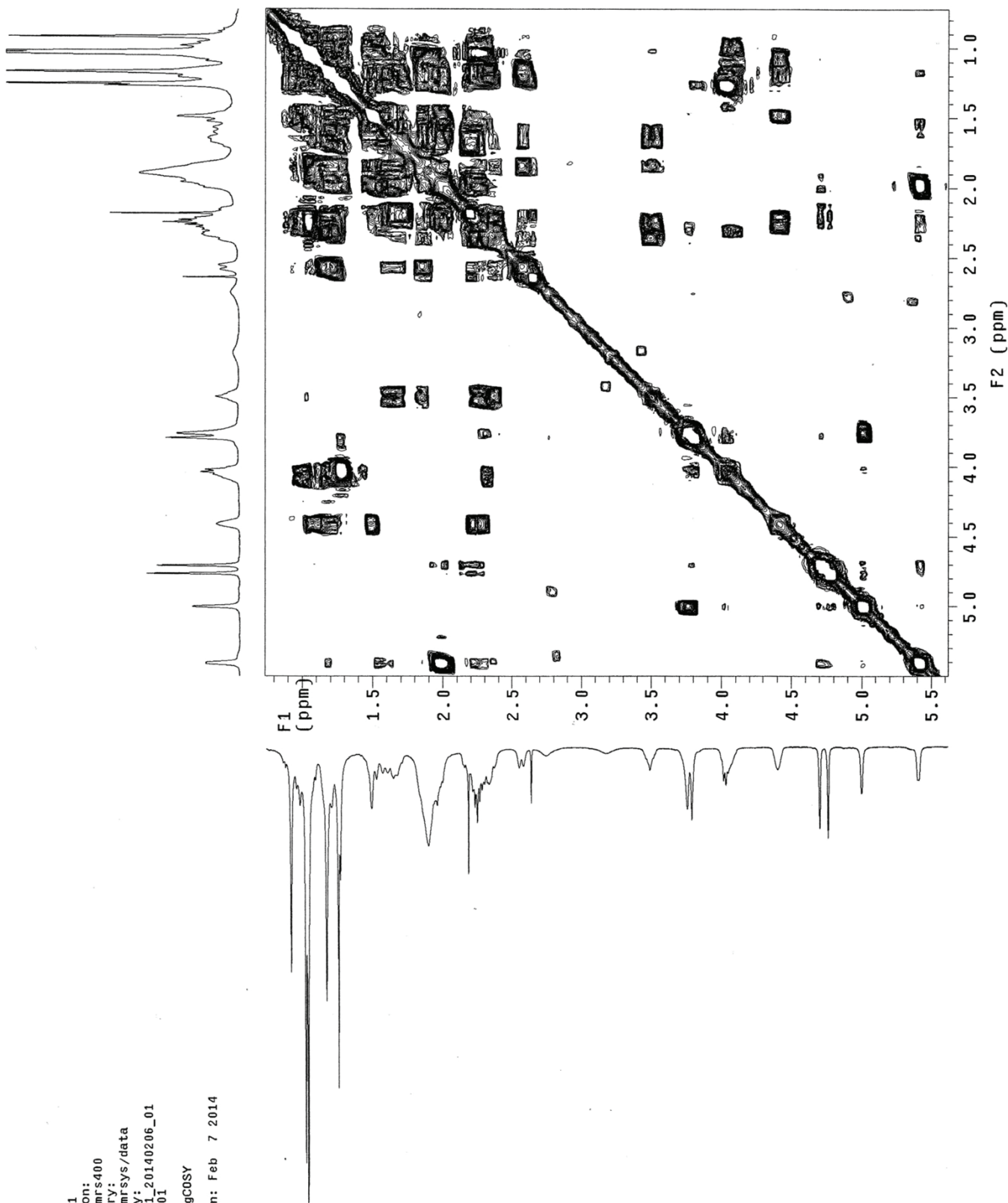


Figure S5-3. COSY spectrum (400 MHz) of compound **5** in CDCl_3 .

Sample Name: JIH6-18n-4-2-1
Data Collected on: Varian-NMR-vnmrs400
Archive directory: /home/sheu/vnmrsys/data
Sample directory: JIH6-18n-4-2-1_20140206_01
FidFile: gHSQCAD_01
Pulse Sequence: gHSQCAD
Solvent: cdcl3
Data collected on: Feb 6 2014

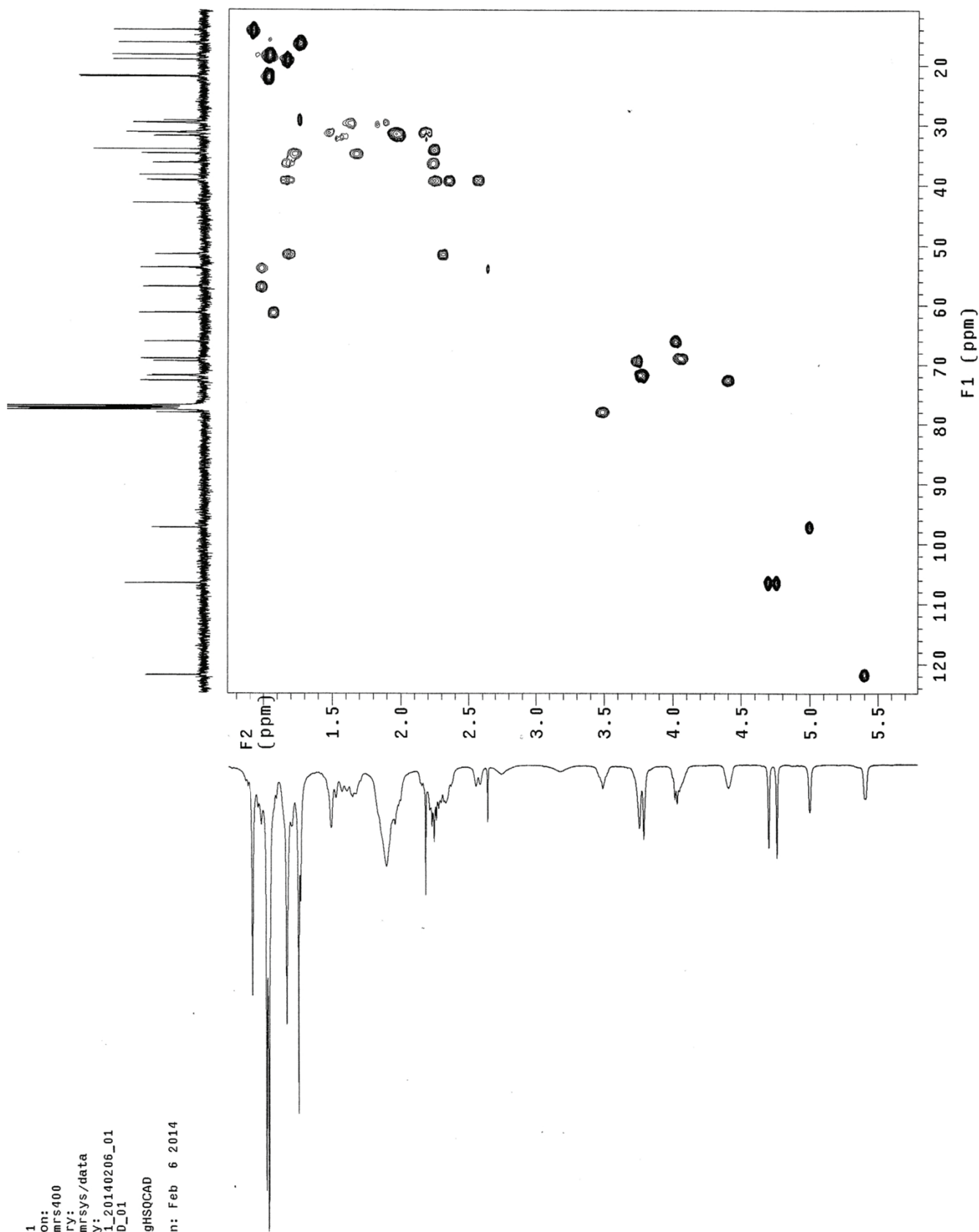


Figure S5-4. HSQC spectrum (400 MHz) of compound **5** in CDCl_3 .

Sample Name:
J1H6-18n-4-2-1
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
J1H6-18n-4-2-1_20140206_01
FidFile: gHMBCAD_01

Pulse Sequence: gHMBCAD
Solvent: cdcl3
Data collected on: Feb 7 2014

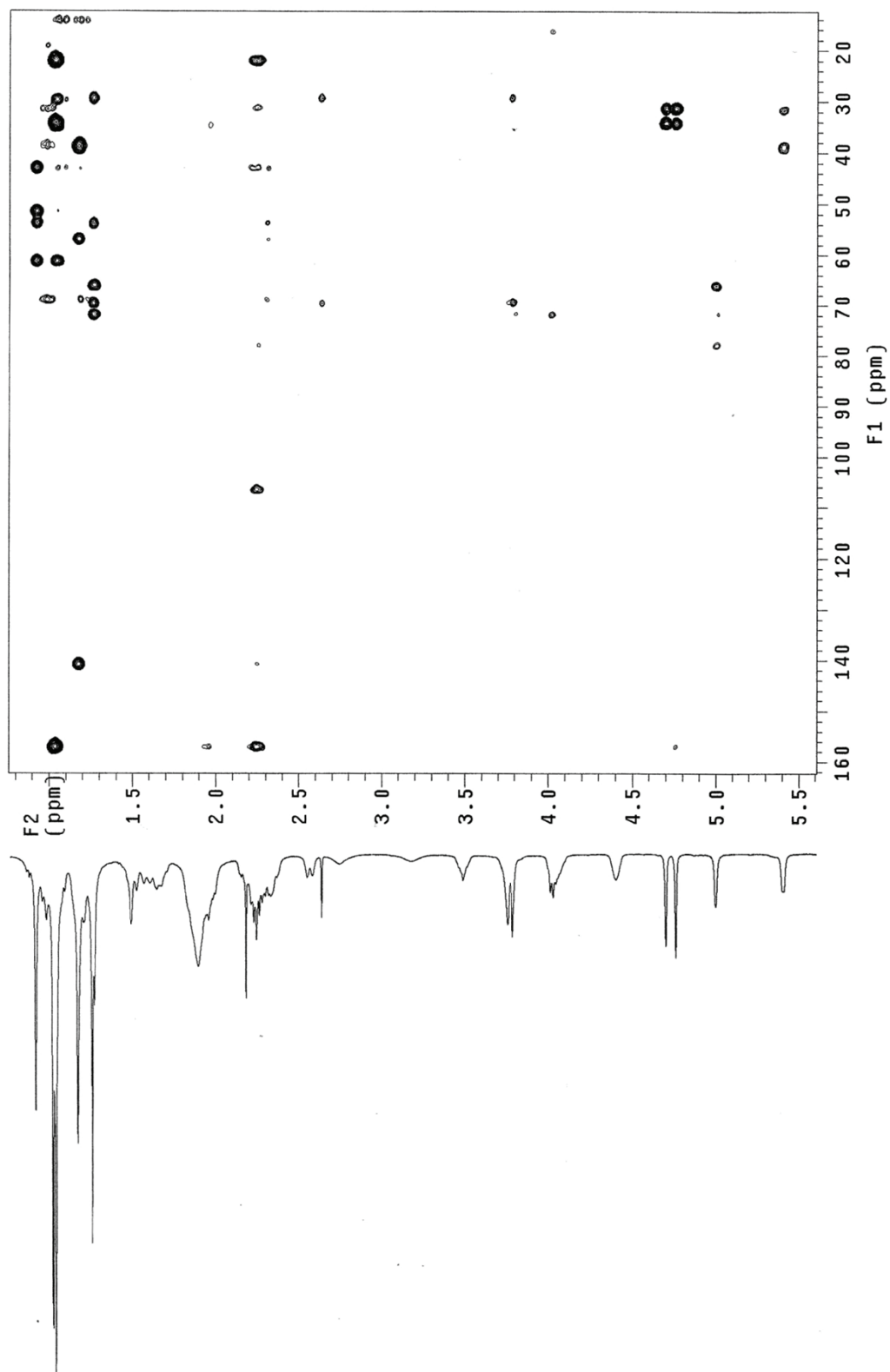


Figure S5-5. HMB spectrum (400 MHz) of compound **5** in CDCl₃.

J1H6-18n-4-2-1

Sample Name:
J1H6-18n-4-2-1
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
J1H6-18n-4-2-1_20140206_01
FidFile: NOESY_01
Pulse Sequence: NOESY
Solvent: cdc13
Data collected on: Feb 6 2014

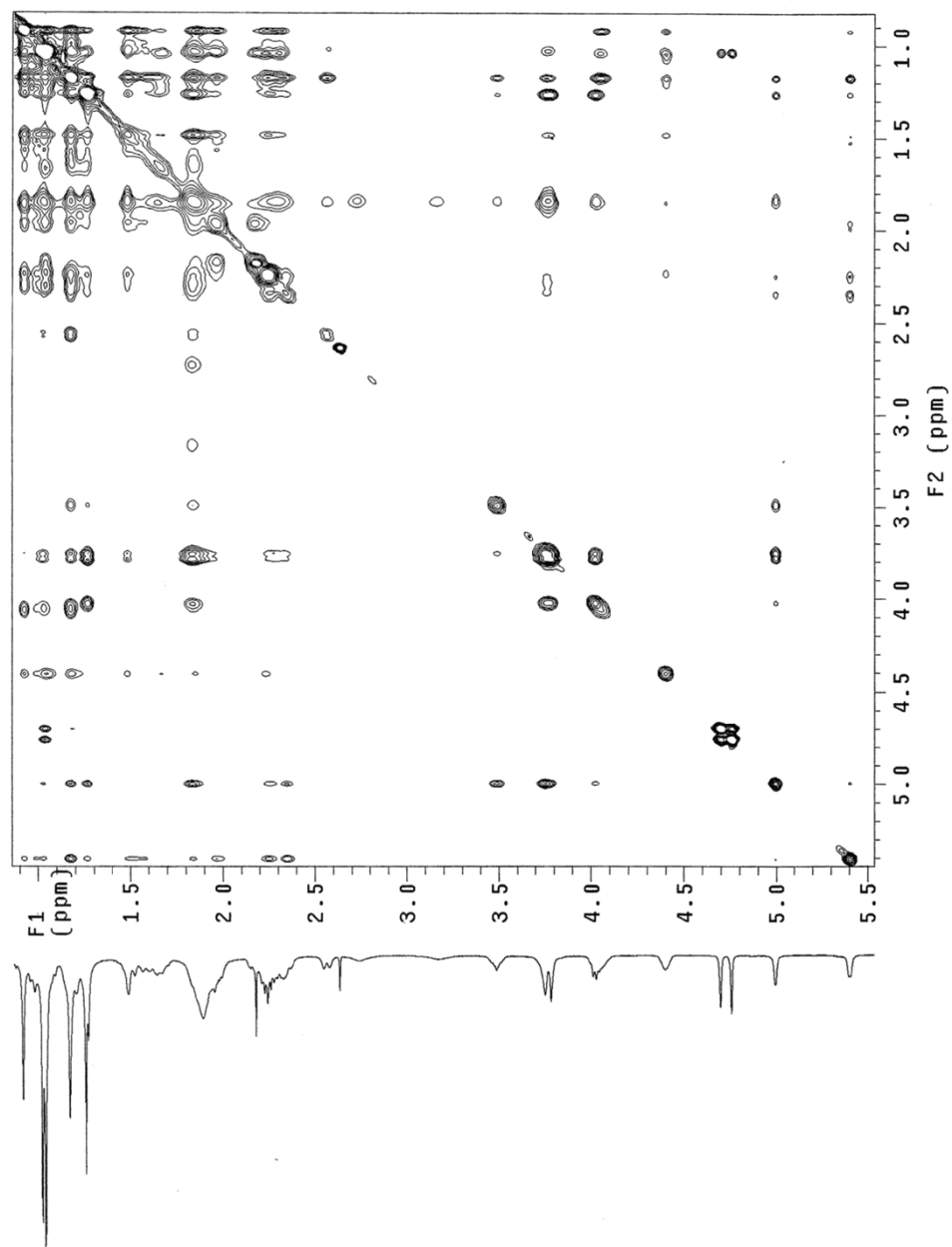


Figure S5-6. NOESY spectrum (400 MHz) of compound **5** in CDCl₃.