

Supporting Information

for

Cycloartane Triterpenoids from *Kleinhovia hospita*

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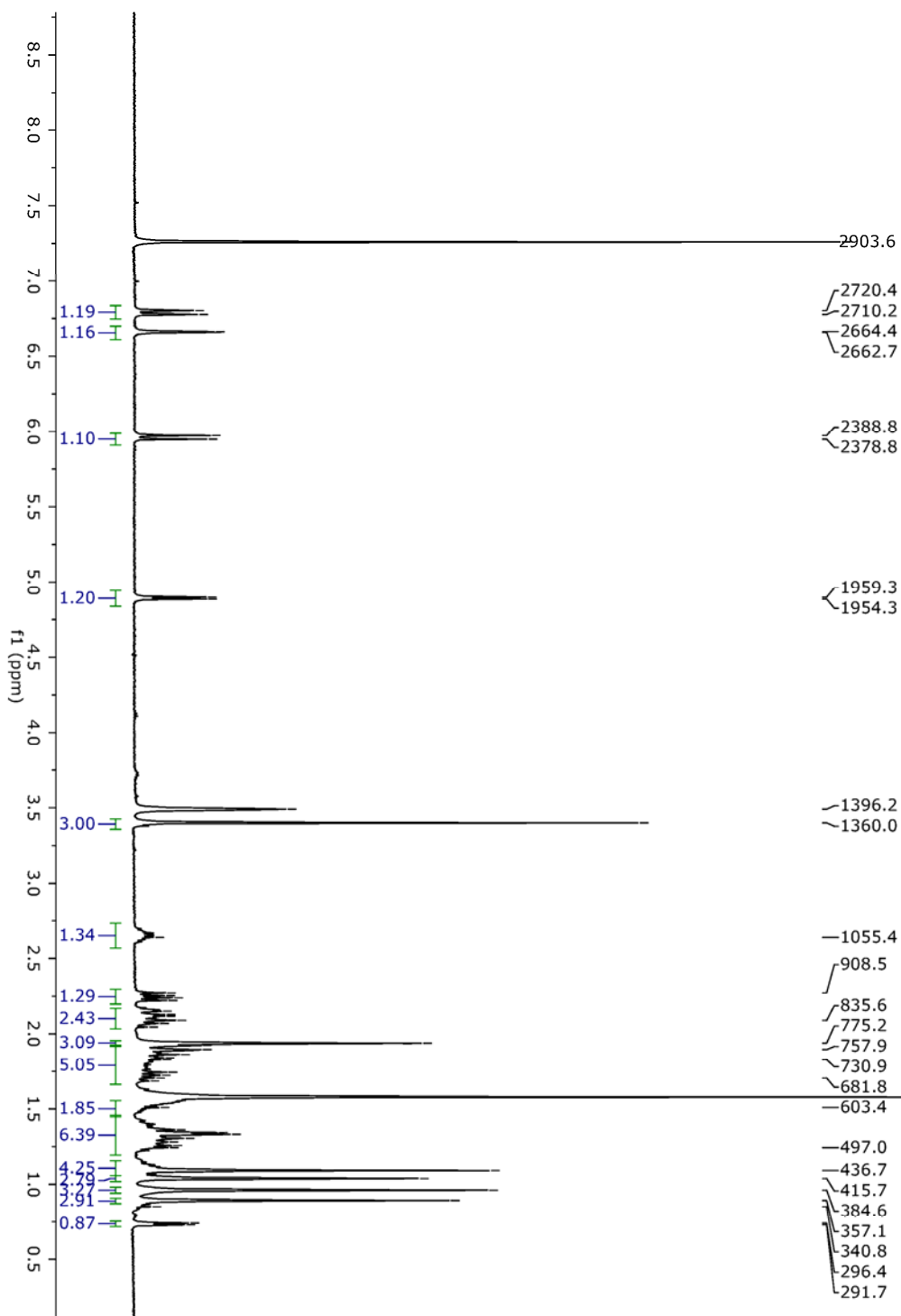
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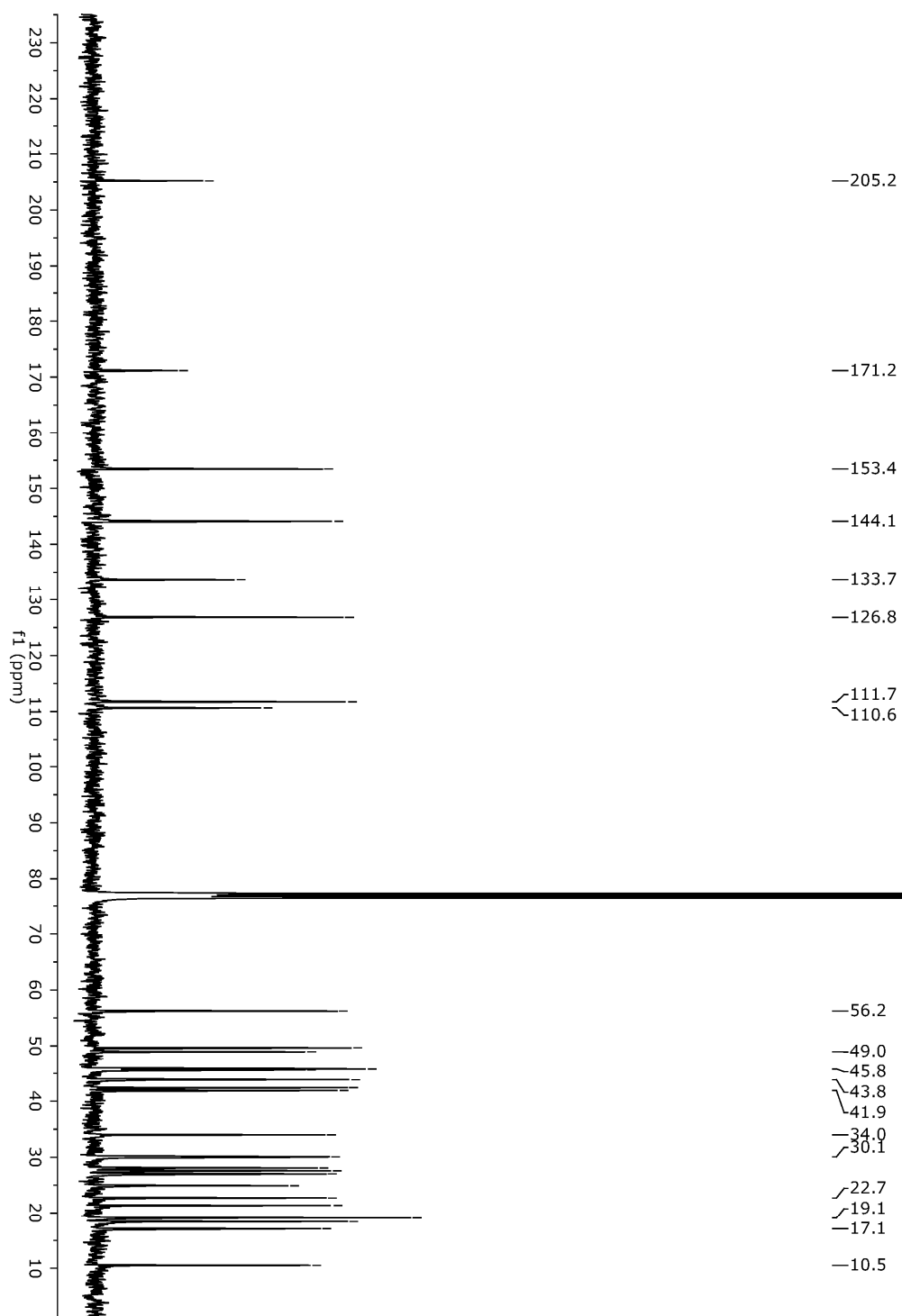
- S1. ¹H NMR spectrum of compound **1** at 400 MHz in CDCl₃.
- S2. ¹³C NMR spectrum of compound **1** at 100 MHz in CDCl₃.
- S3. ¹³C NMR spectrum (high field expanded) of compound **1** at 100 MHz in CDCl₃.
- S4. DEPT (135) spectrum of compound **1** at 100 MHz in CDCl₃.
- S5. ESI MS (positive mode) spectrum of **1**.
- S6. HSQC spectrum of compound **1** at 400 MHz in CDCl₃.
- S7. ¹H-¹H COSY spectrum of compound **1** at 400 MHz in CDCl₃.
- S8. HMBC spectrum of compound **1** at 400 MHz in CDCl₃.
- S9. NOESY spectrum of compound **1** at 400 MHz in CDCl₃.
- S10. IR (KBr disc) spectrum of compound **1**.
- S11. ¹H NMR spectrum of compound **2** and **3** in a mixture at 400 MHz in CDCl₃.
- S12. ¹H NMR spectrum (high field, expanded) of compound **2** and **3** in a mixture at 400 MHz in CDCl₃.
- S13. ¹³C NMR spectrum of compound **2** and **3** in a mixture at 100 MHz in CDCl₃.
- S14. ¹³C NMR spectrum (high field, expanded) of compound **2** and **3** in a mixture at 100 MHz in CDCl₃.
- S15. DEPT (135) spectrum of compound **2** and **3** in a mixture at 100 MHz in CDCl₃.

- S16. HSQC (undecoupling) spectrum of compound **2** and **3** in a mixture at 400 MHz in CDCl₃.
- S17. HMBC spectrum of compound **2** and **3** in a mixture at 400 MHz in CDCl₃.
- S18. NOESY spectrum of compound **2** and **3** in a mixture at 400 MHz in CDCl₃.
- S19. IR (KBr disc) spectrum of compound **2** and **3** in a mixture.
- S20. ¹H NMR spectrum of compound **4** at 400 MHz in CDCl₃.
- S21. ¹³C NMR spectrum of compound **4** at 100 MHz in CDCl₃.
- S22. ¹³C NMR spectrum (high field, expanded) of compound **4** at 100 MHz in CDCl₃.
- S23. DEPT (135) spectrum of compound **4** at 100 MHz in CDCl₃.
- S24. HSQC (undecoupling) spectrum of compound **4** at 400 MHz in CDCl₃.
- S25. HMBC spectrum of compound **4** at 400 MHz in CDCl₃.
- S26. NOESY spectrum of compound **4** at 400 MHz in CDCl₃.
- S27. IR (KBr disc) spectrum of compound **4**.
- S28. ESI MS spectra of compound **4** and a mixture of compounds **2** and **3**.

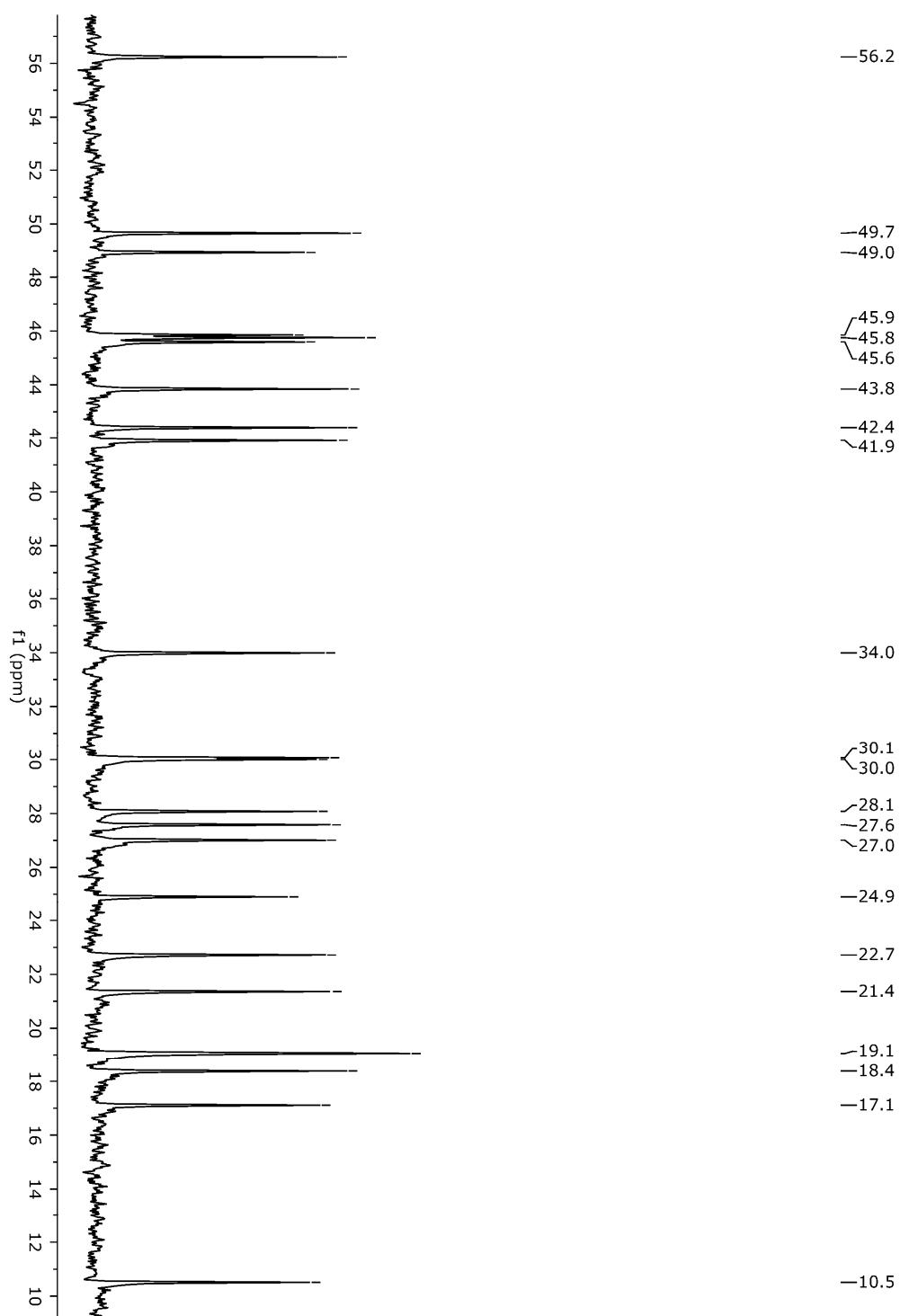
S1. ^1H NMR spectrum of compound **1** at 400 MHz in CDCl_3 .



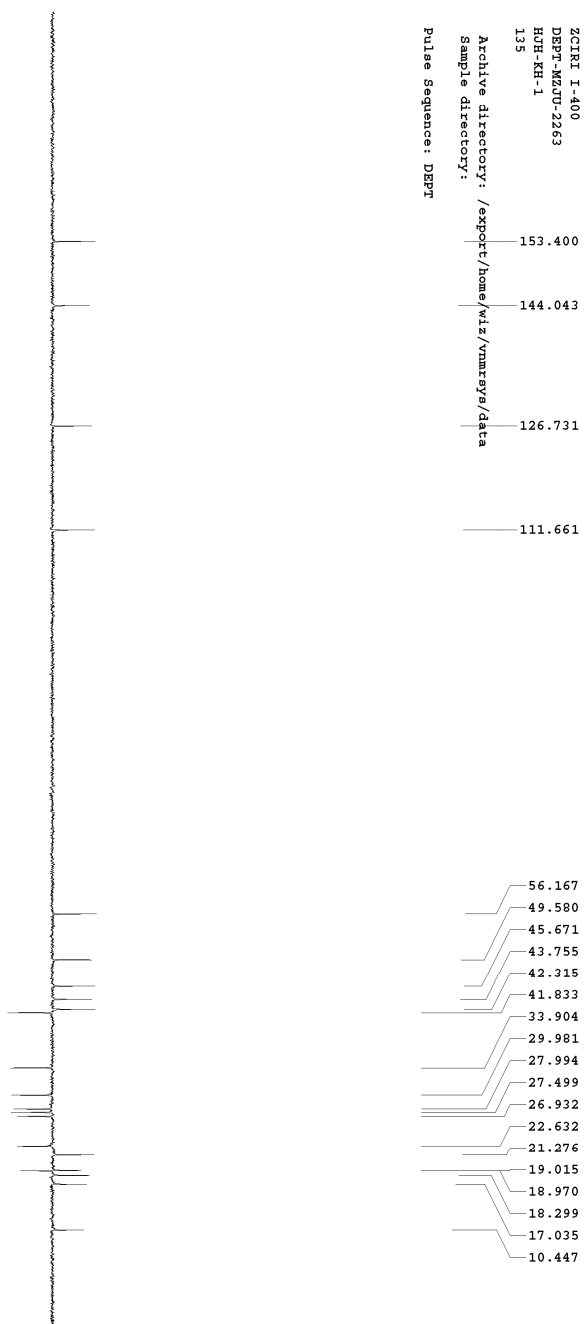
S2. ^{13}C NMR spectrum of compound **1** at 100 MHz in CDCl_3 .



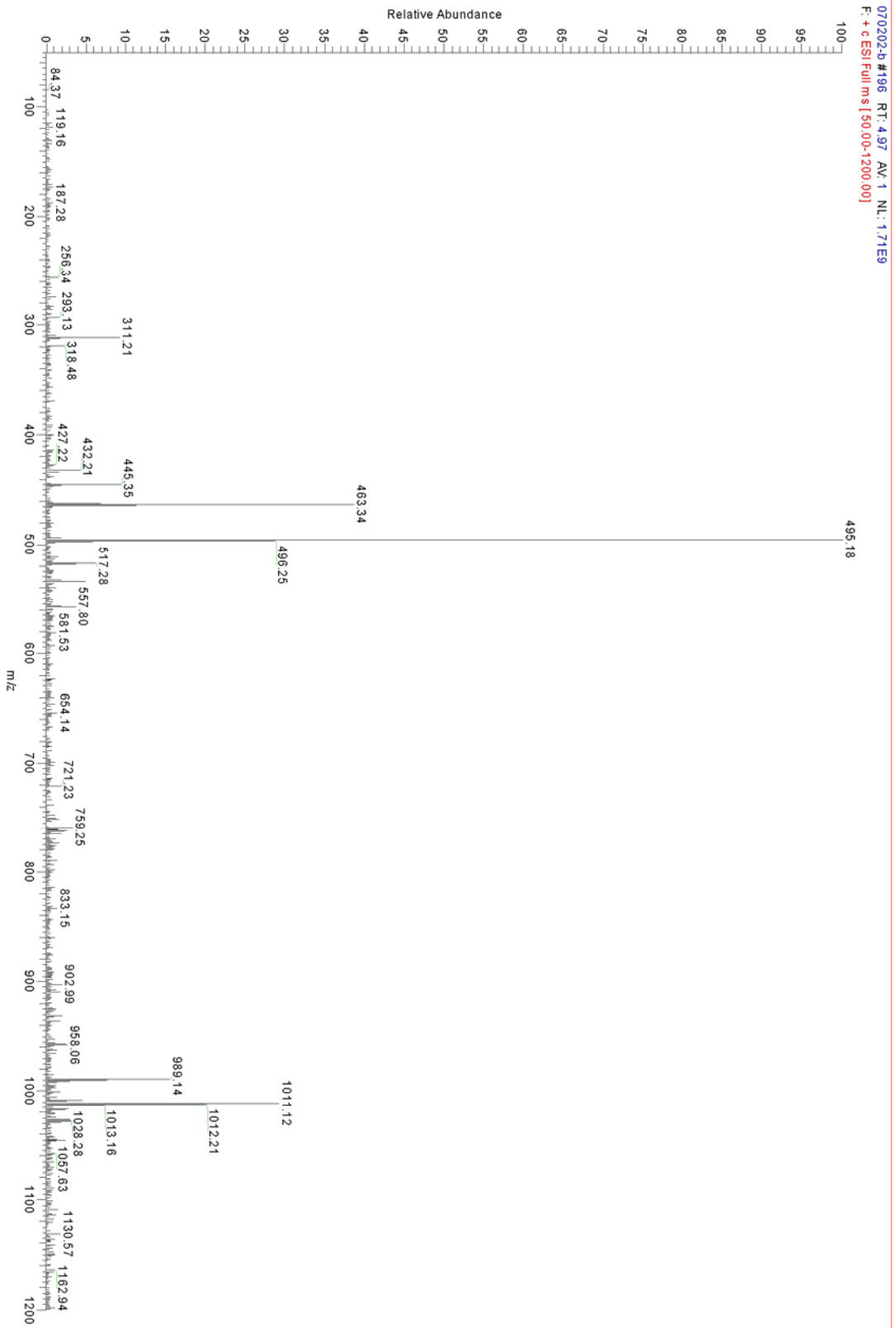
S3. ^{13}C NMR spectrum (high field expanded) of compound **1** at 100 MHz in CDCl_3 .



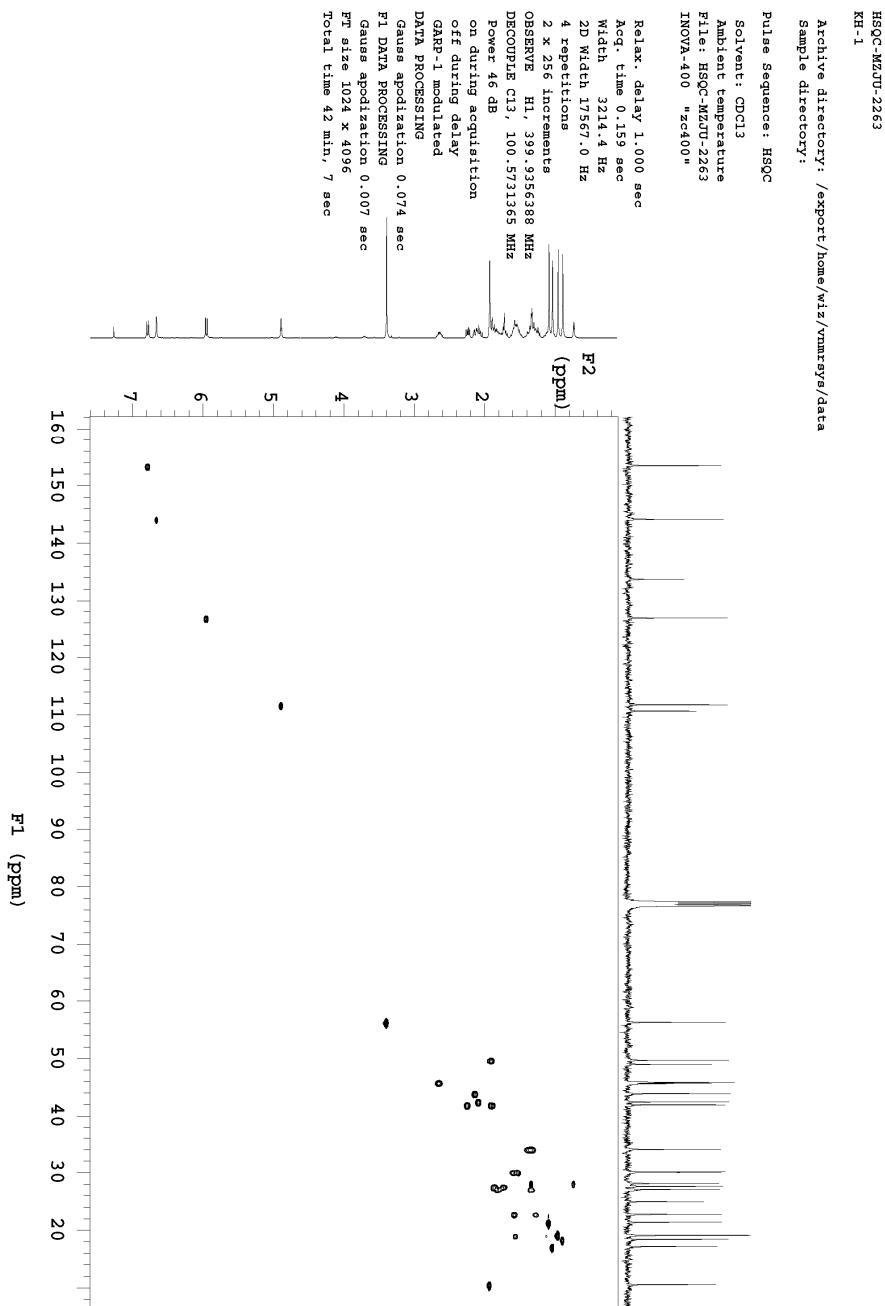
S4. DEPT (135) spectrum of compound **1** at 100 MHz in CDCl₃.



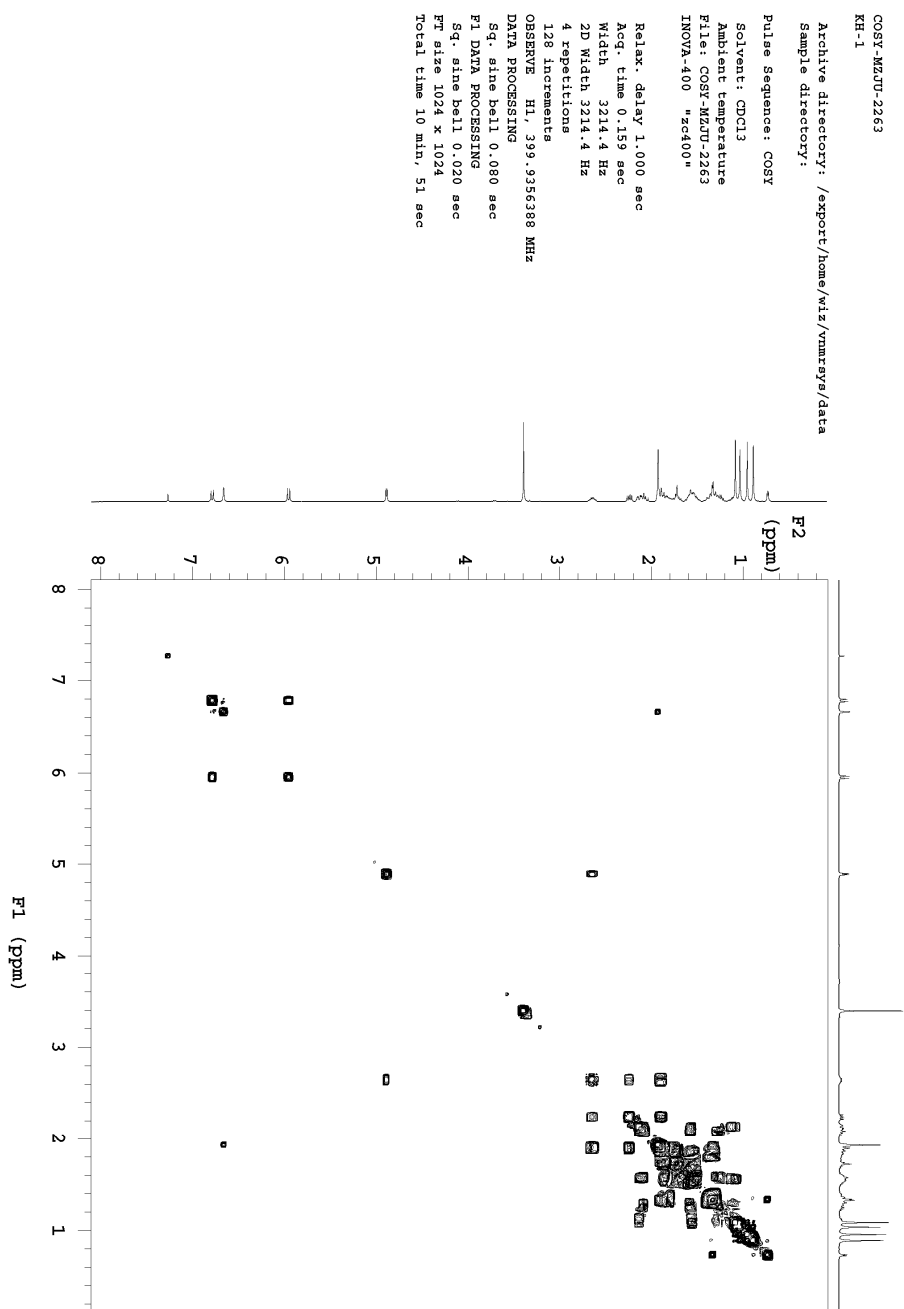
S5. ESI MS (positive mode) spectrum of 1.



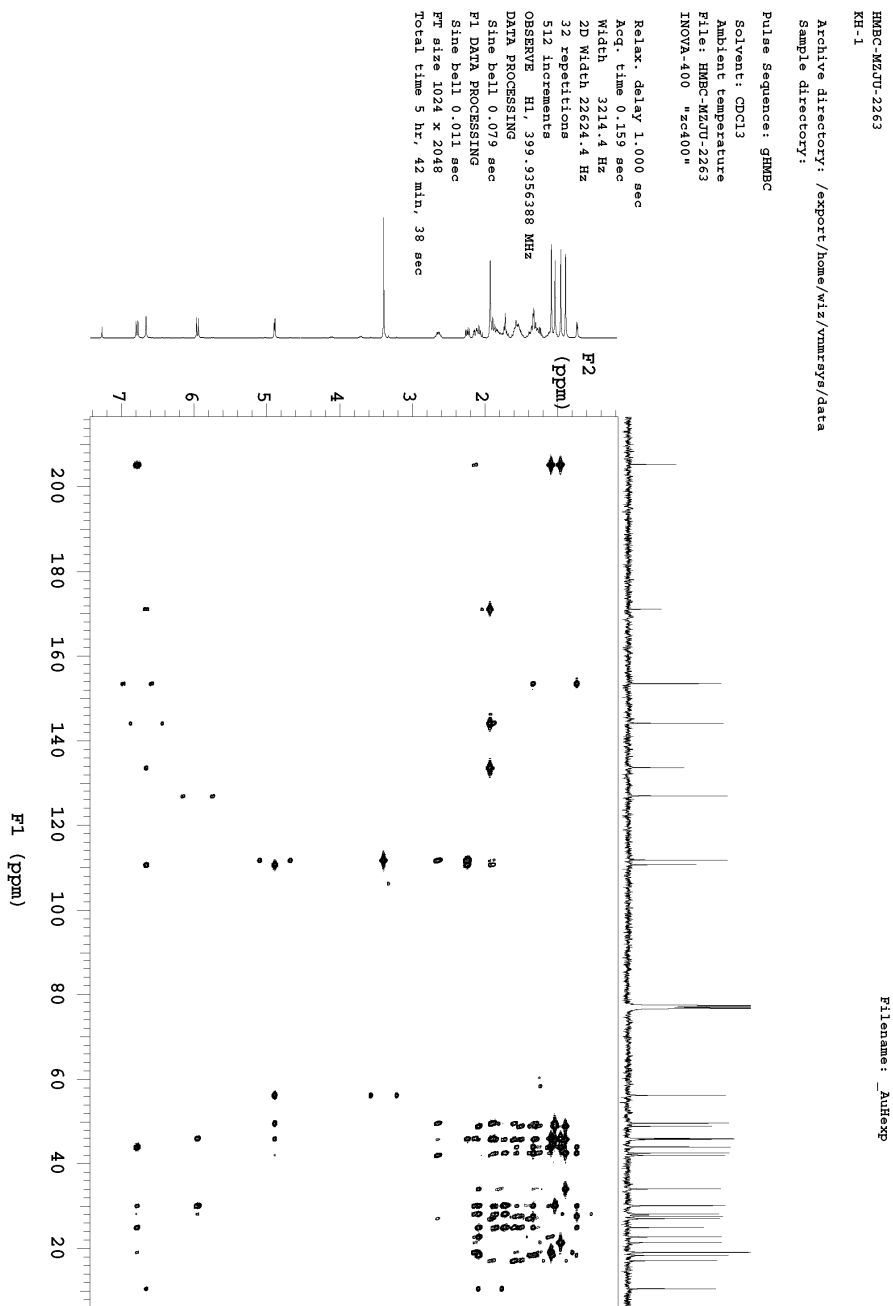
S6. HSQC spectrum of compound **1** at 400 MHz in CDCl₃.



S7. ^1H - ^1H COSY spectrum of compound **1** at 400 MHz in CDCl_3 .



S8. HMBC spectrum of compound 1 at 400 MHz in CDCl₃.



S9. NOESY spectrum of compound **1** at 400 MHz in CDCl₃.

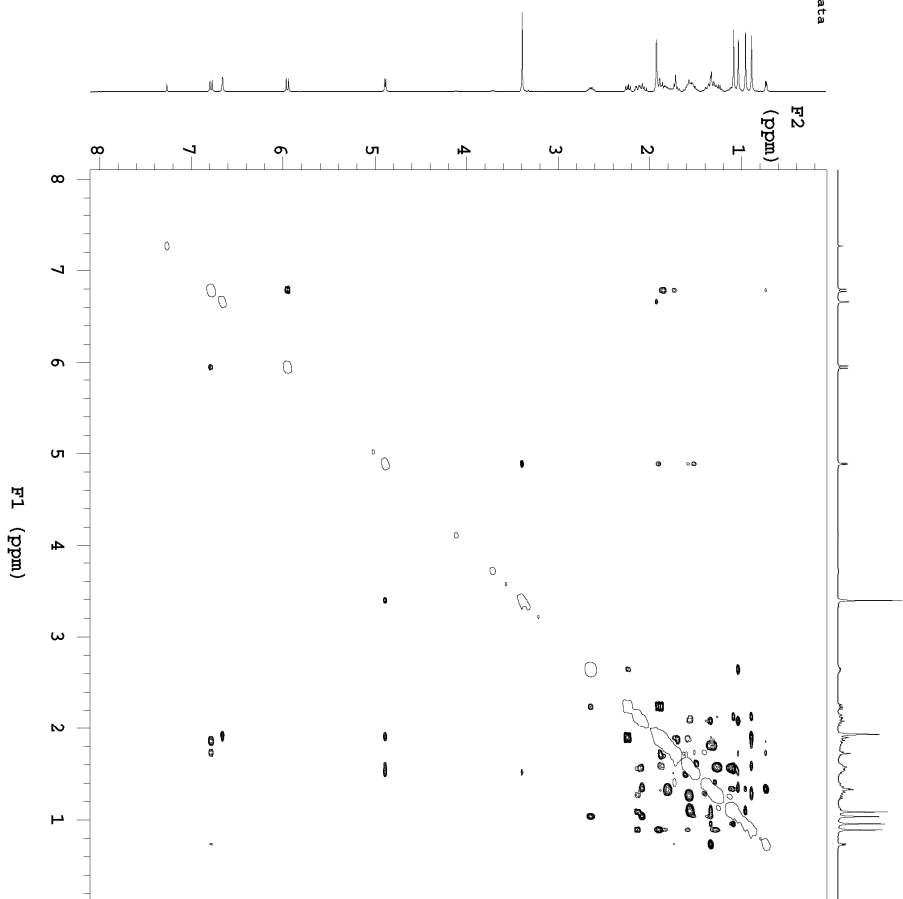
NOESY-MZTU-2263
KH-1

Archive directory: /export/home/wiz/vnmrsys/data
Sample directory:

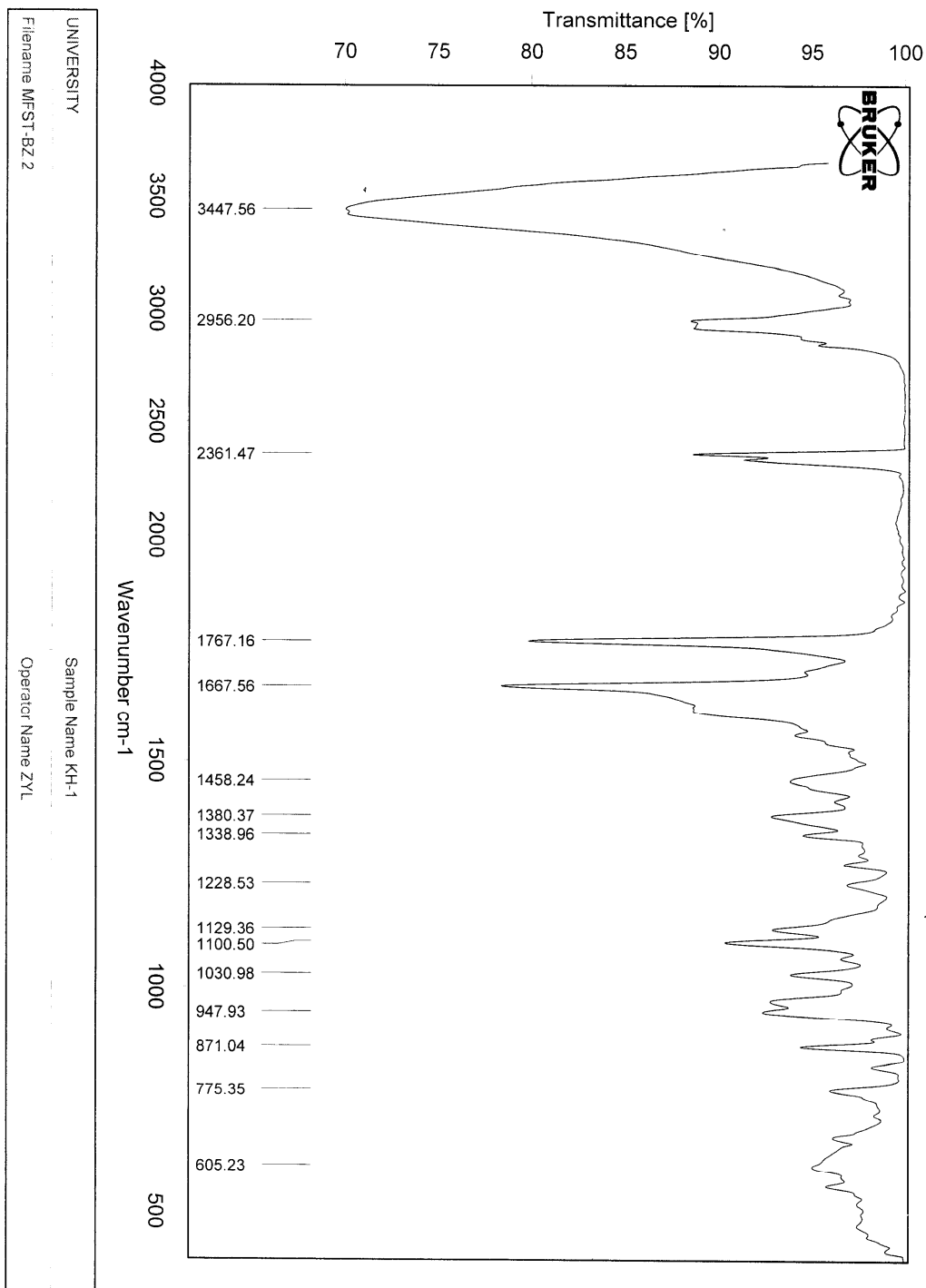
Pulse Sequence: NOESY

Solvent: CDCl₃
Ambient temperature
File: NOESY-MZTU-2263
INOVA-400 "sc400"

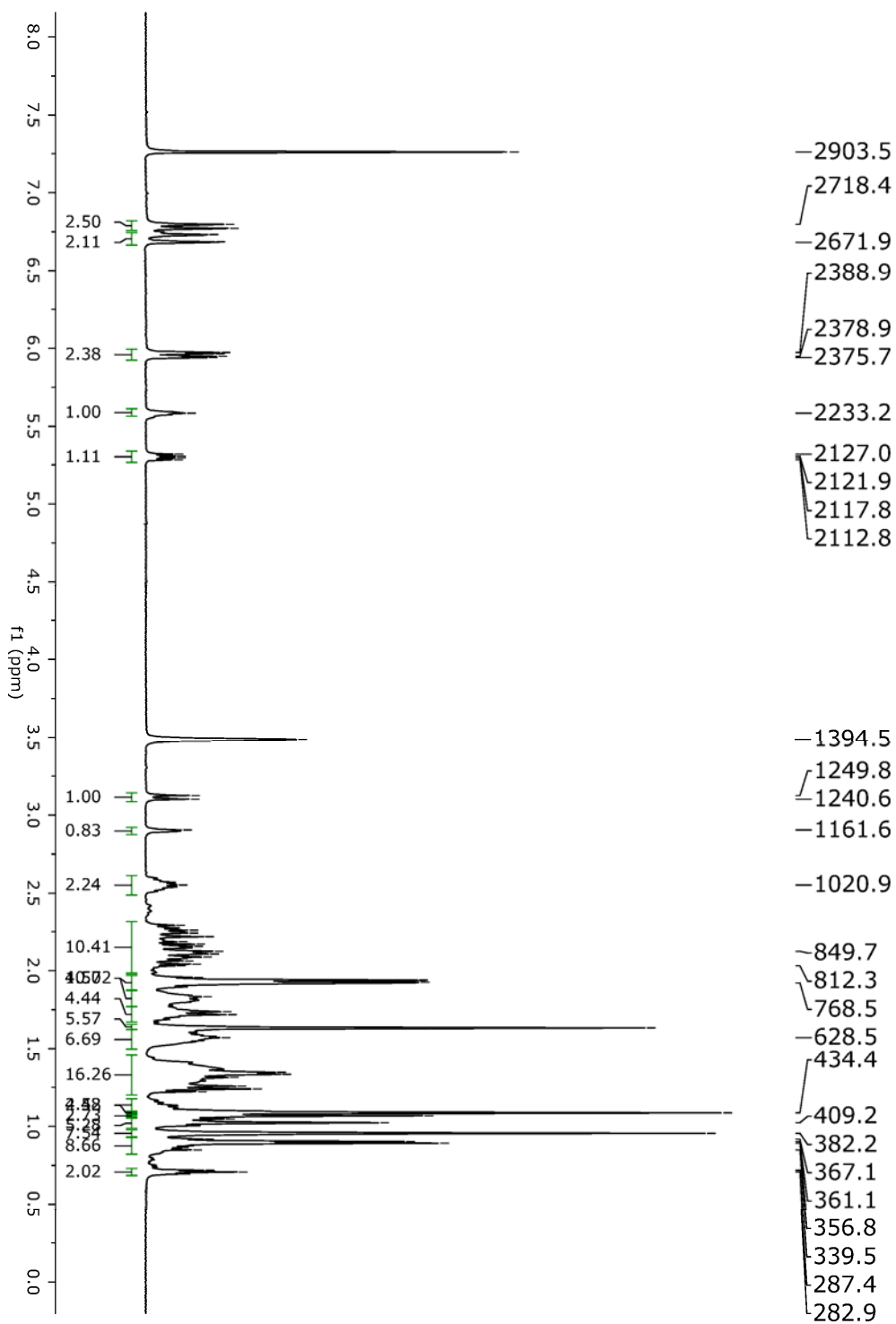
Relax. delay 1.000 sec
Mixing 0.700 sec
Acq. time 0.159 sec
Width 3214.4 Hz
2D Width 3214.4 Hz
32 repetitions
2 x 200 increments
OBSERVE H1, 399.9356388 MHz
DATA PROCESSING
Gauss apodization 0.067 sec
F1 DATA PROCESSING
Gauss apodization 0.029 sec
F2 size 2048 x 2048
Total time 6 hr, 47 min, 10 sec



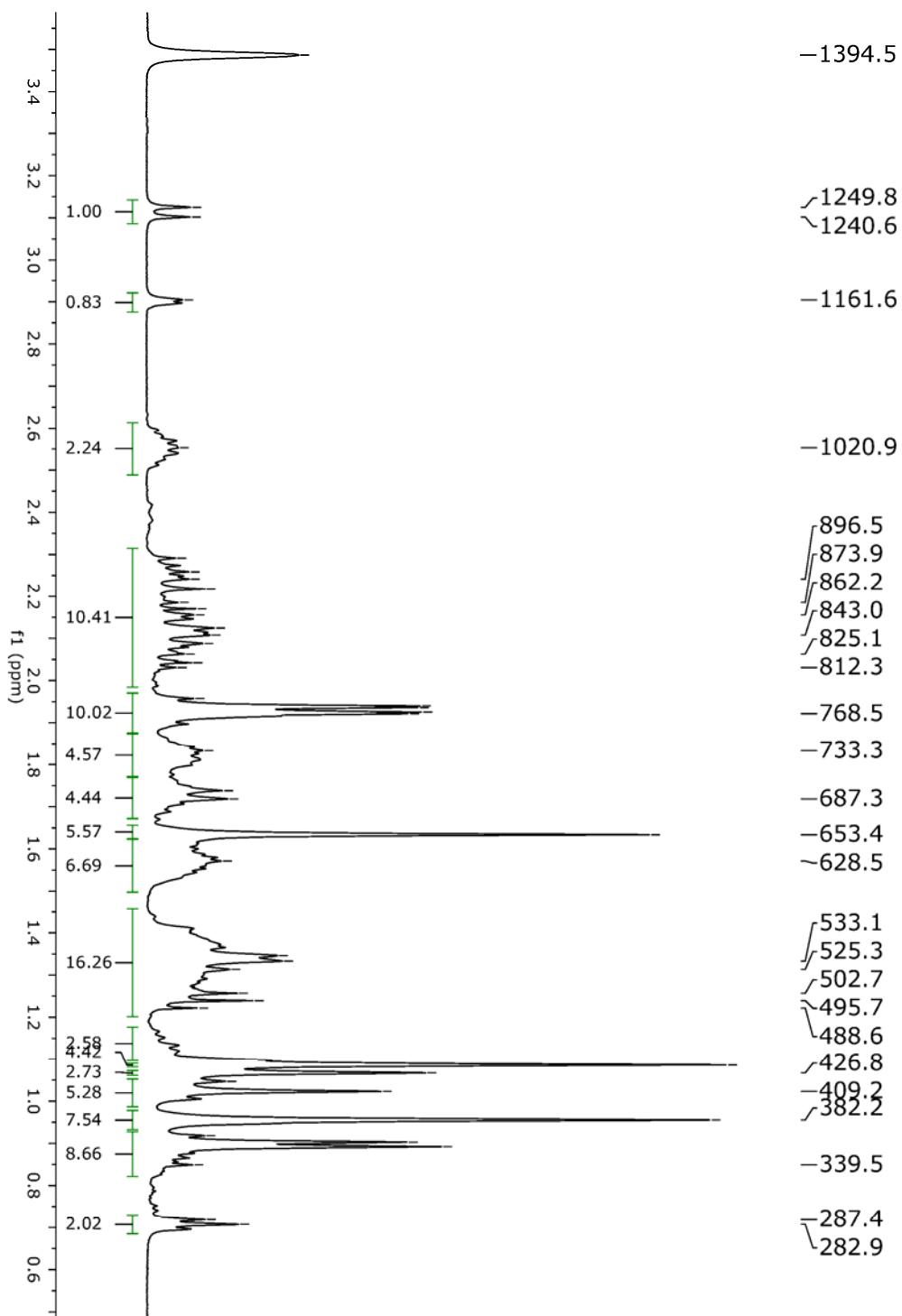
S10. IR (KBr disc) spectrum of compound 1.



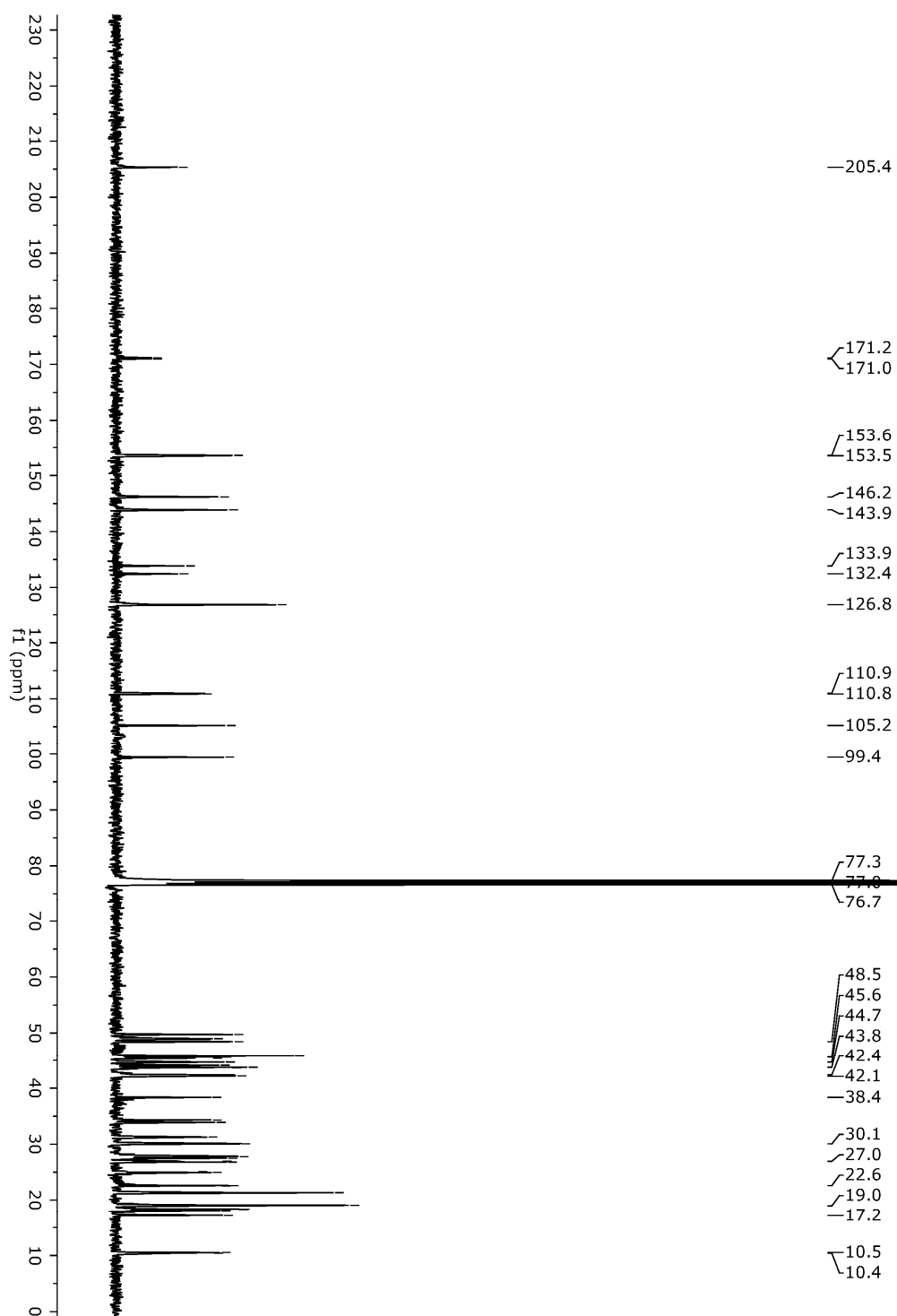
S11. ^1H NMR spectrum of compound **2** and **3** in a mixture at 400 MHz in CDCl_3 .



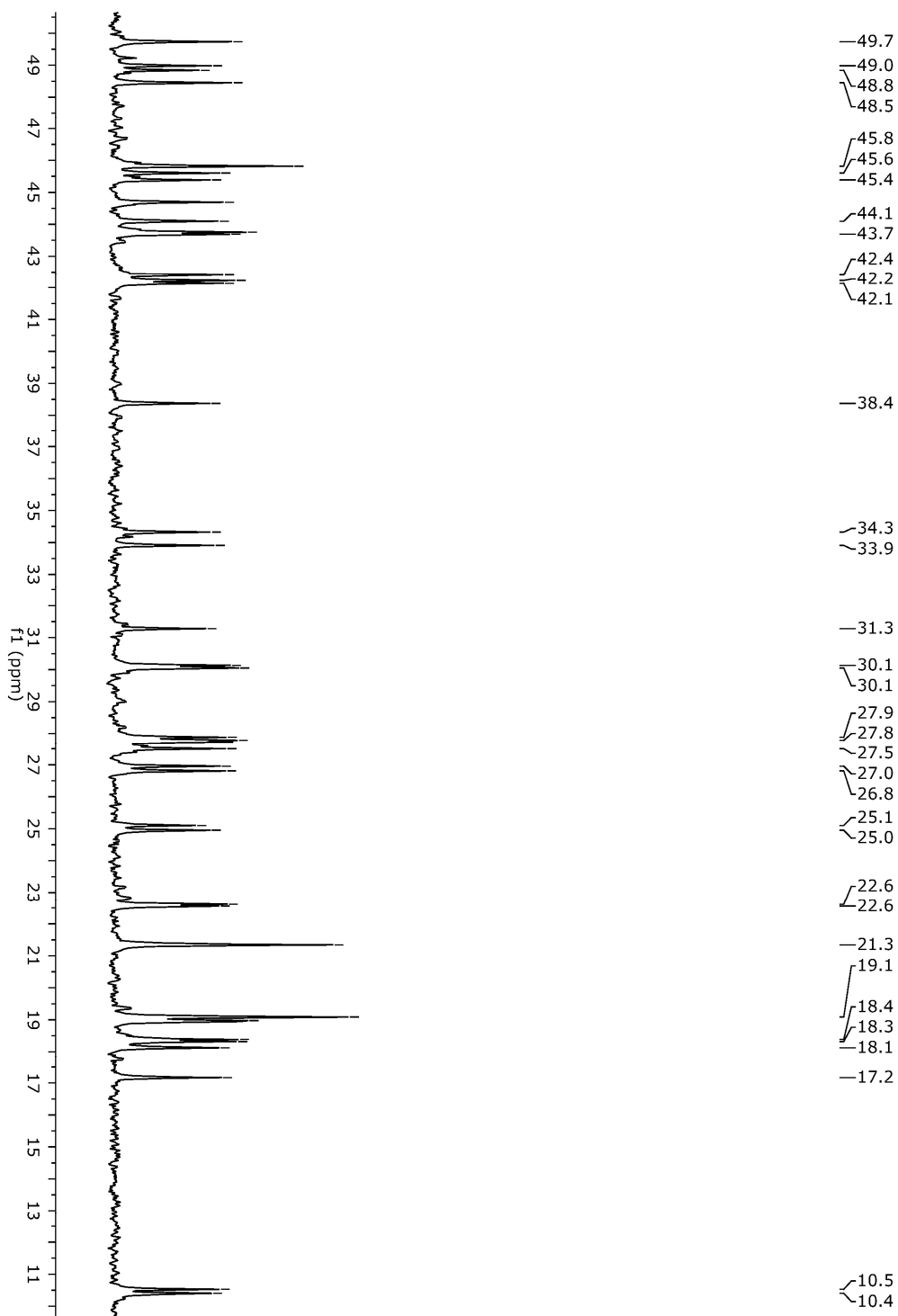
S12. ^1H NMR spectrum (high field, expanded) of compound **2** and **3** in a mixture at 400 MHz in CDCl_3 .



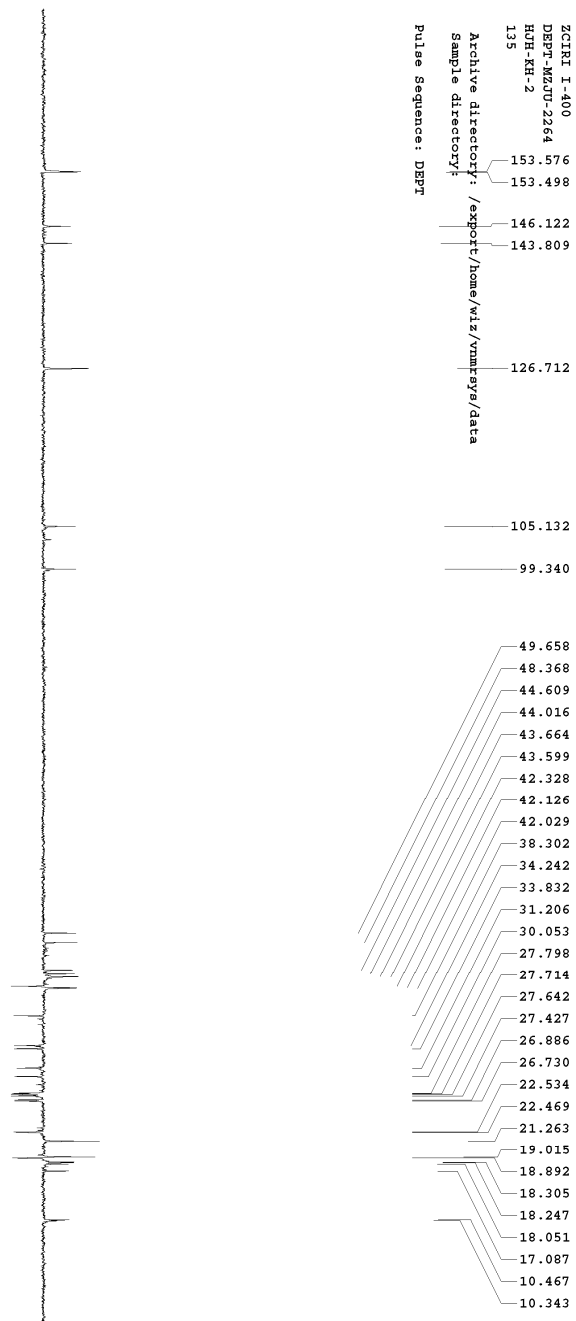
S13. ^{13}C NMR spectrum of compound **2** and **3** in a mixture at 100 MHz in CDCl_3 .



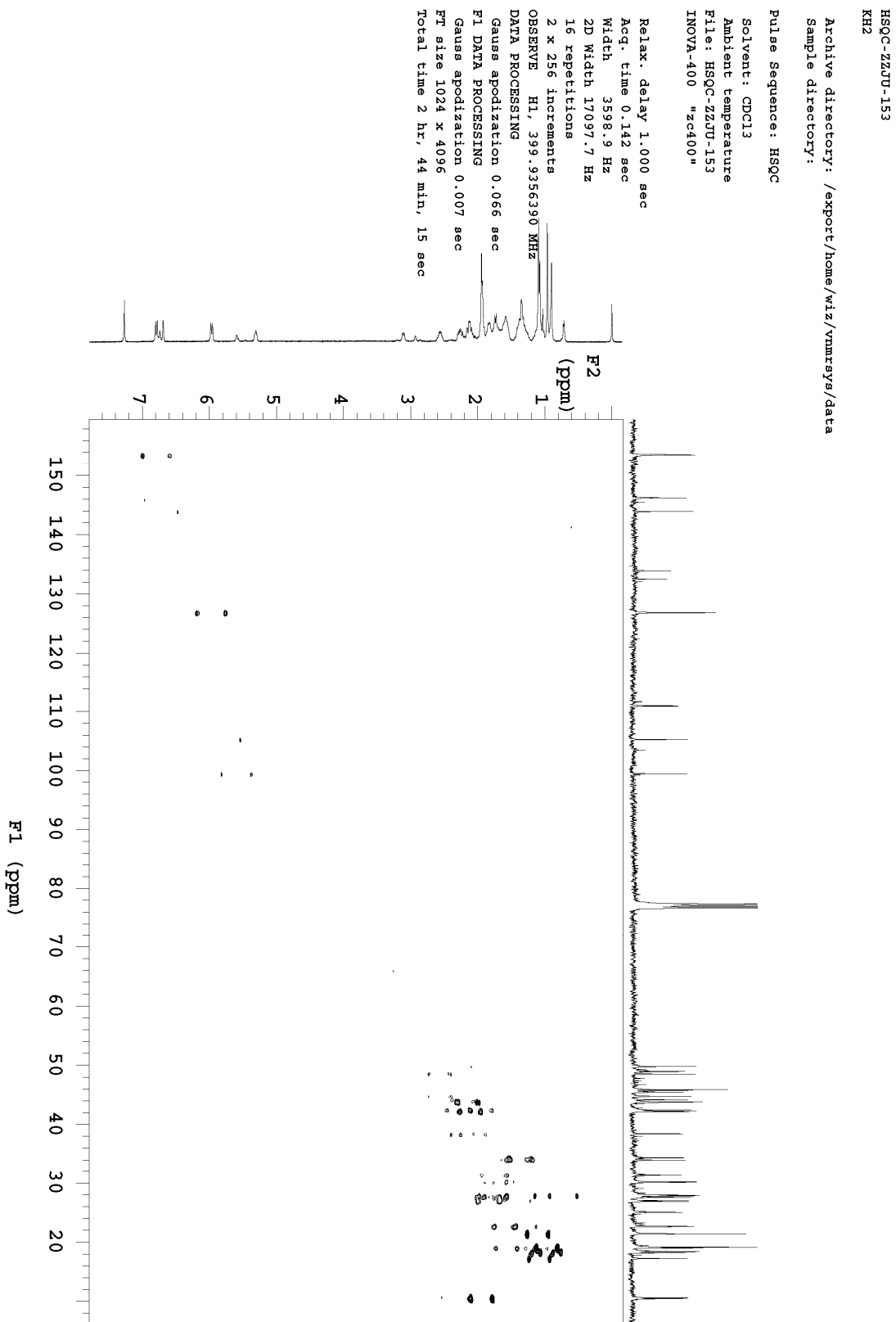
S14. ^{13}C NMR spectrum (high field, expanded) of compound **2** and **3** in a mixture at 100 MHz in CDCl_3 .



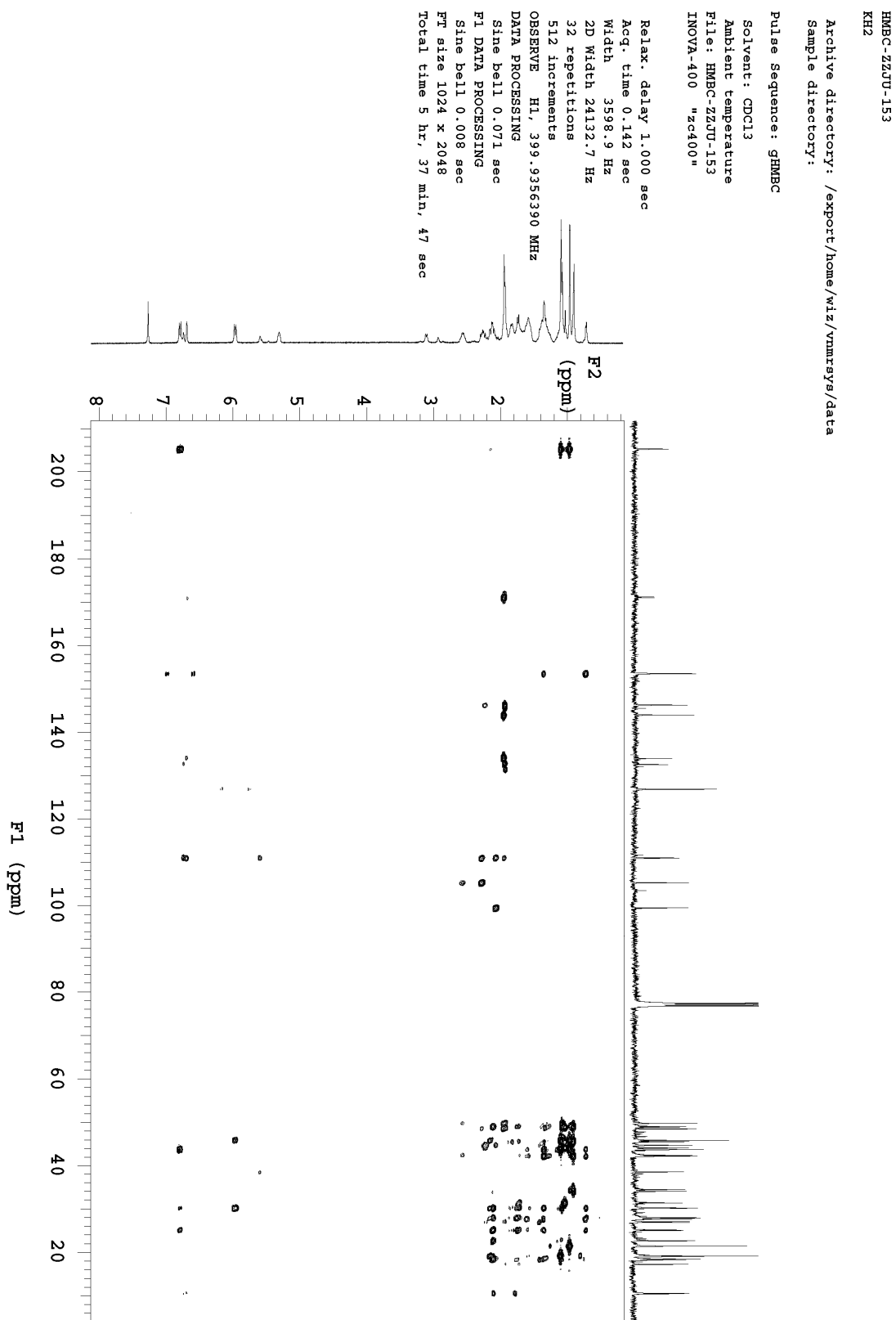
S15. DEPT (135) spectrum of compound **2** and **3** in a mixture at 100 MHz in CDCl₃.



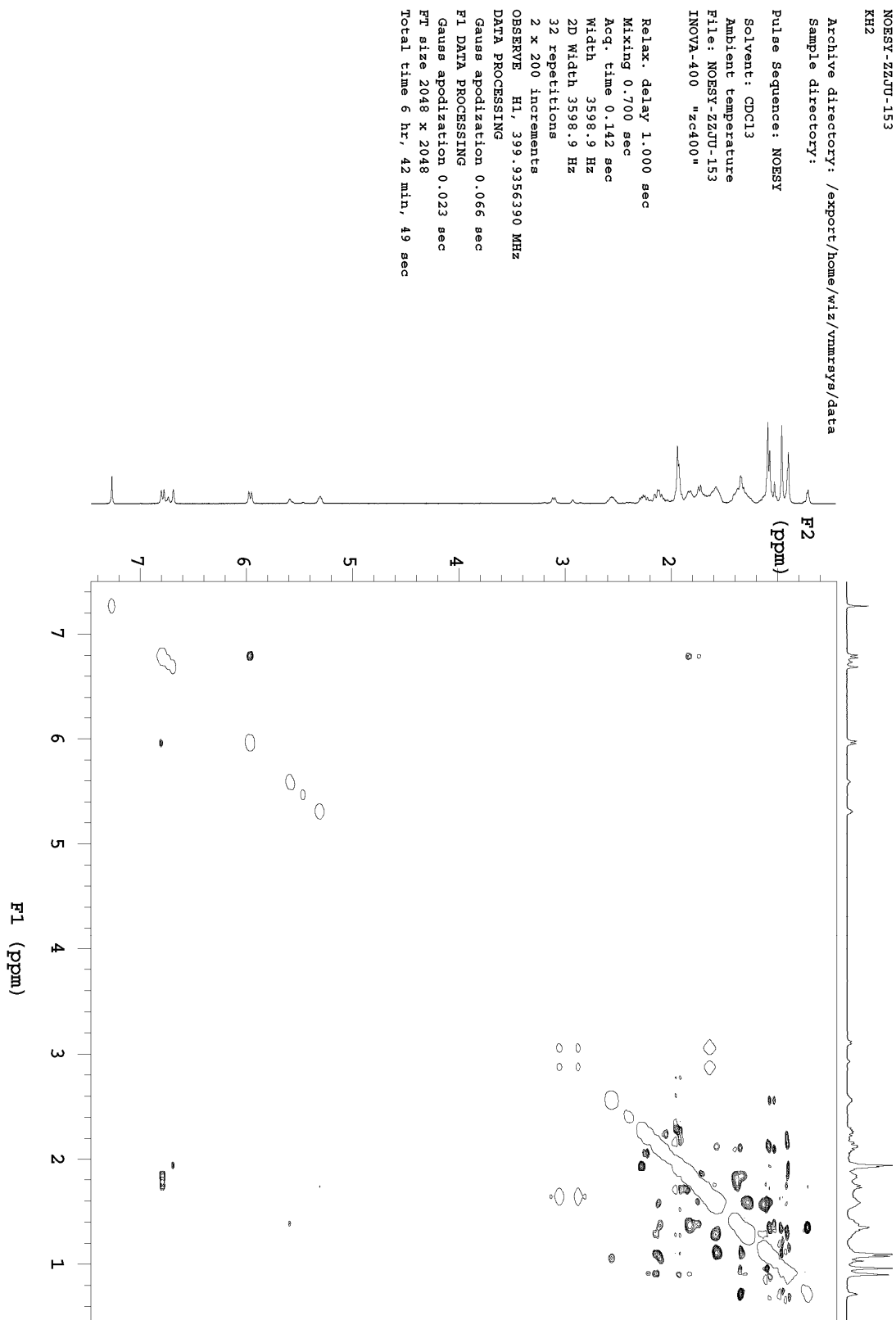
S16. HSQC (undecoupling) spectrum of compound **2** and **3** in a mixture at 400 MHz in CDCl₃.



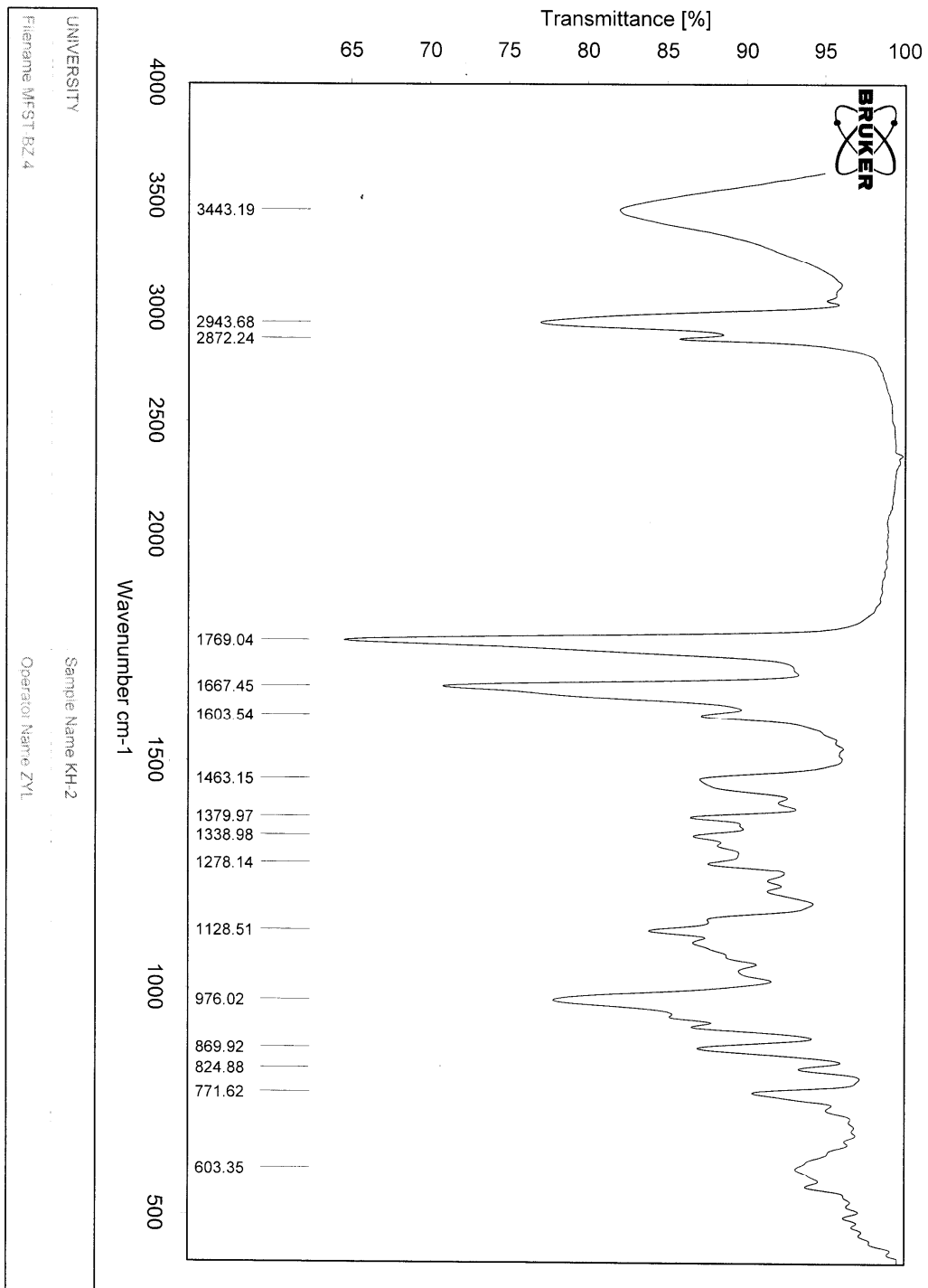
S17. HMBC spectrum of compound **2** and **3** in a mixture at 400 MHz in CDCl₃.



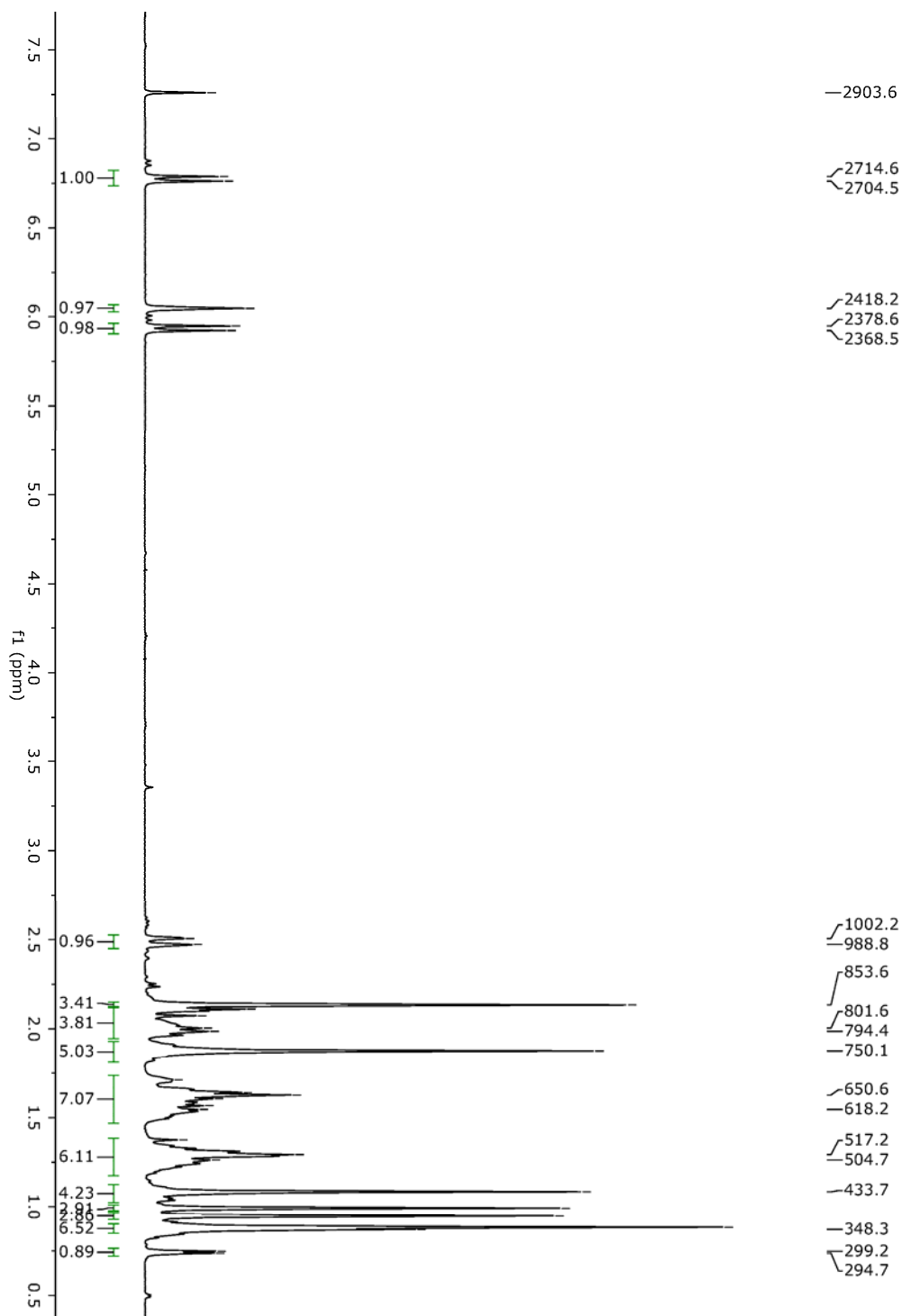
S18. NOESY spectrum of compound **2** and **3** in a mixture at 400 MHz in CDCl₃.



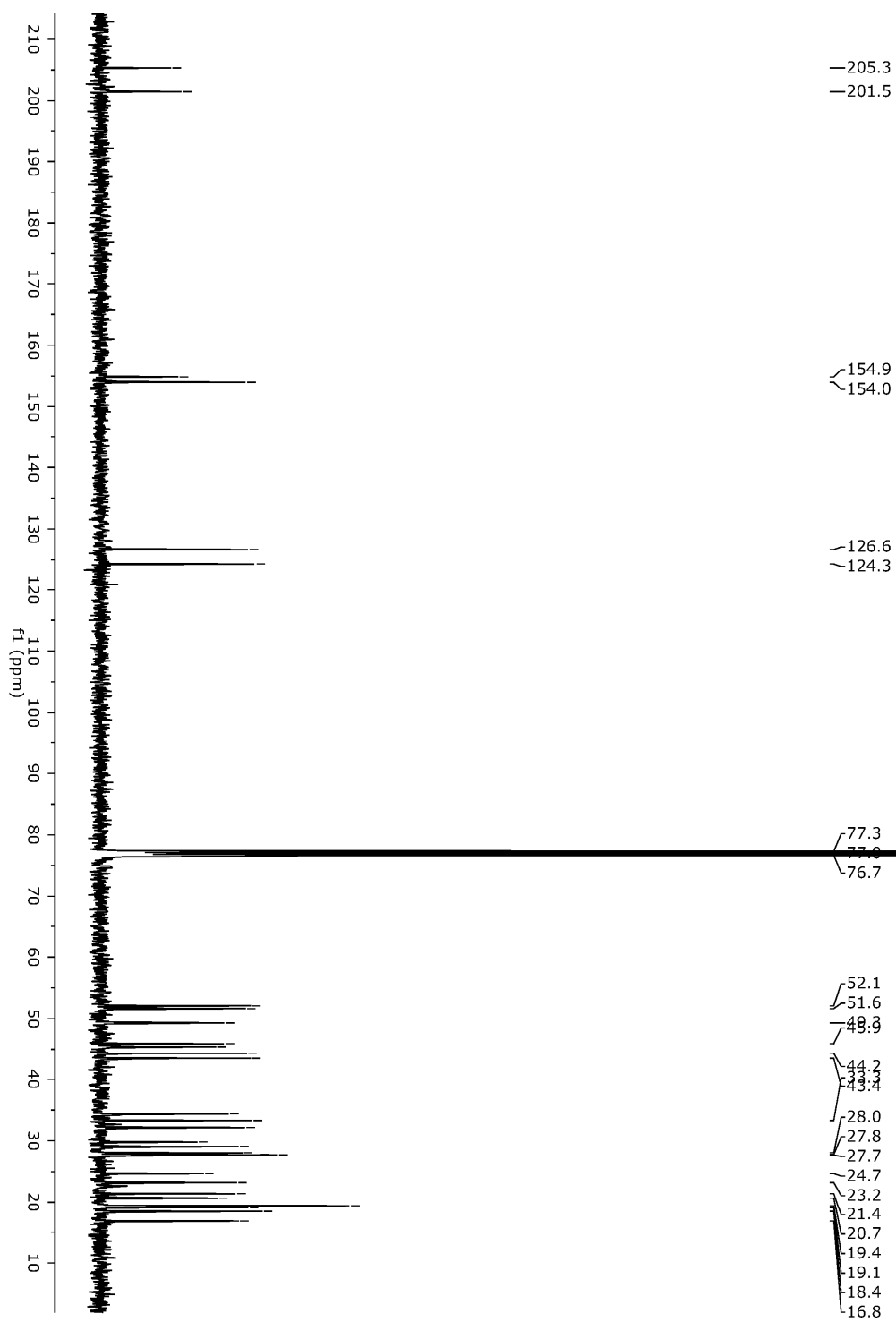
S19. IR (KBr disc) spectrum of compound **2** and **3** in a mixture.



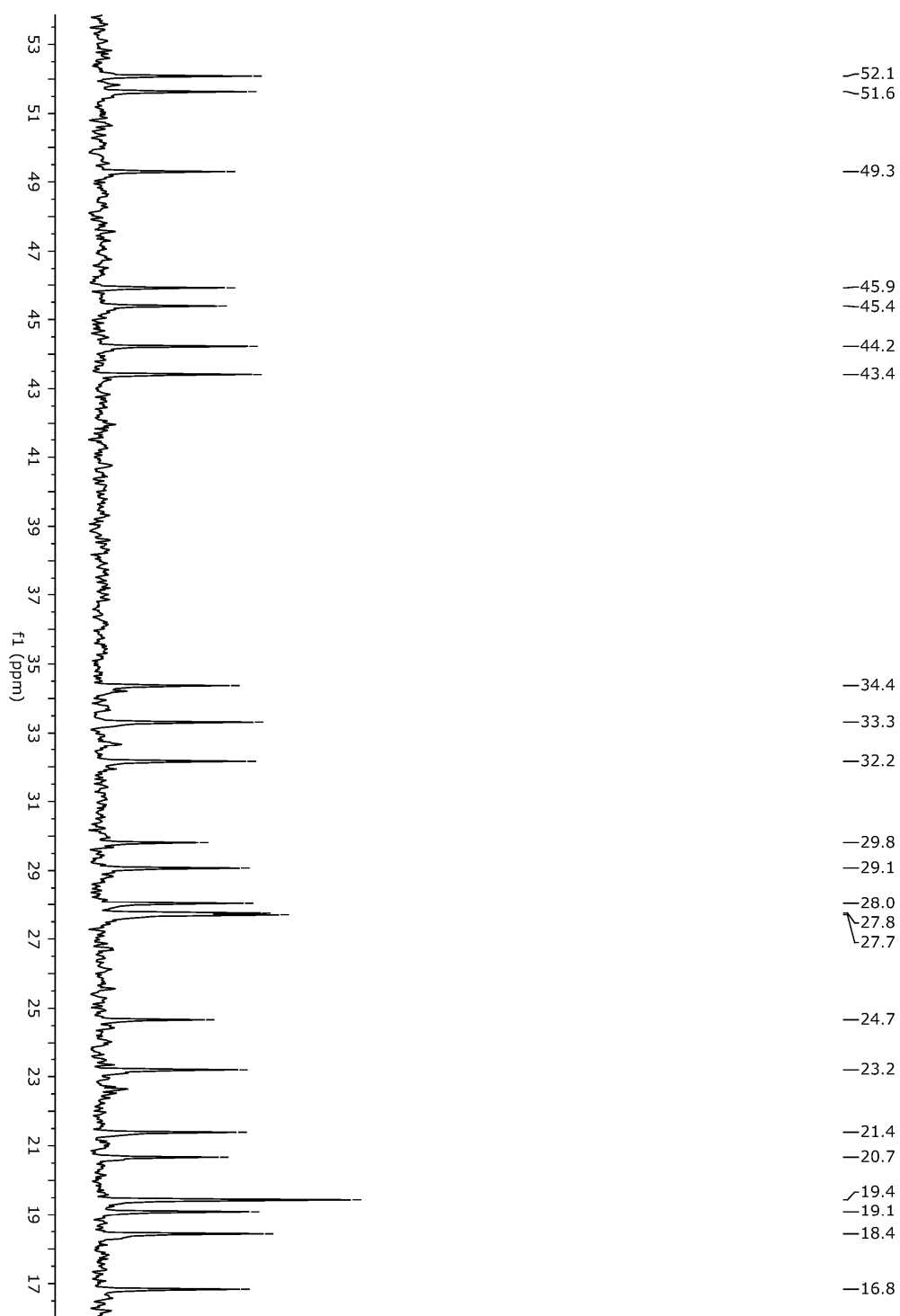
S20. ^1H NMR spectrum of compound **4** at 400 MHz in CDCl_3 .



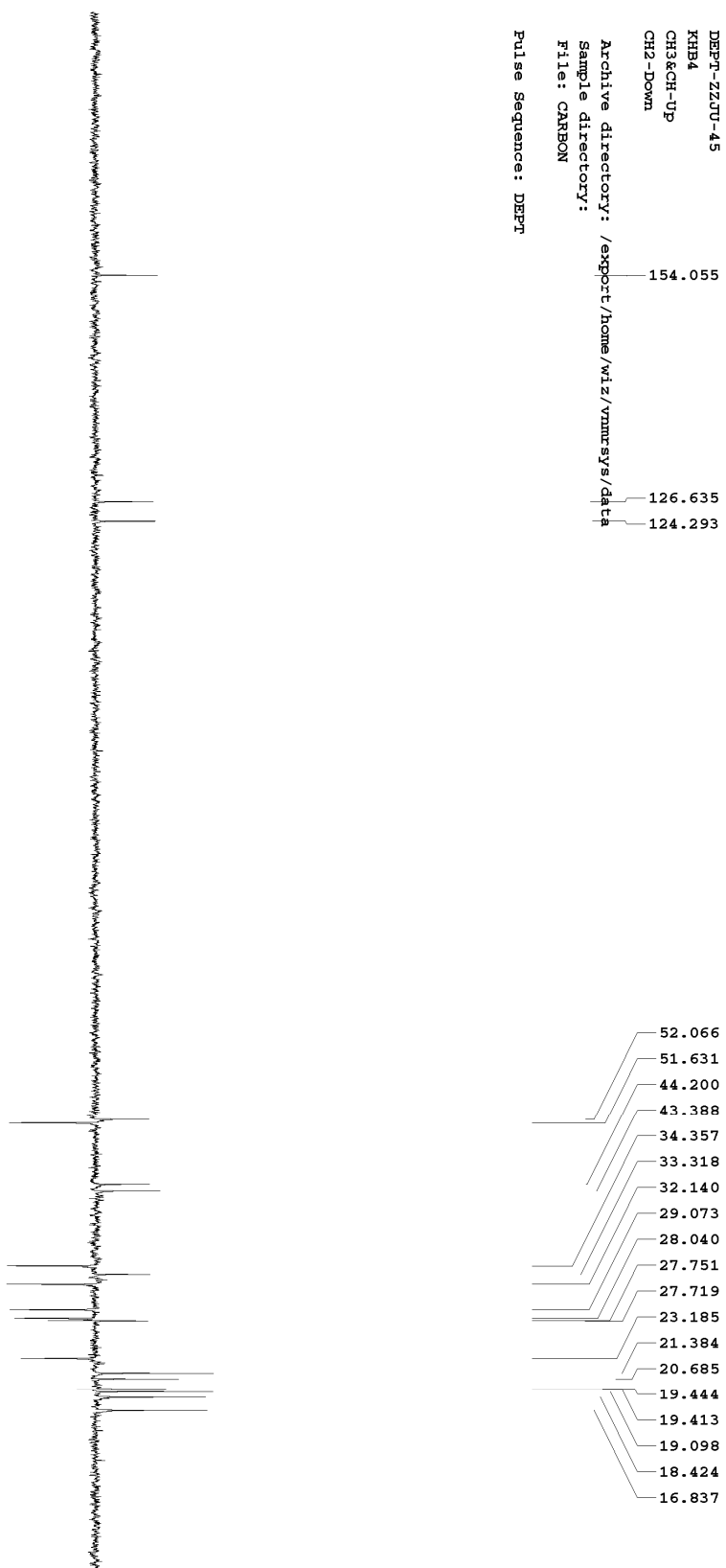
S21. ^{13}C NMR spectrum of compound **4** at 100 MHz in CDCl_3 .



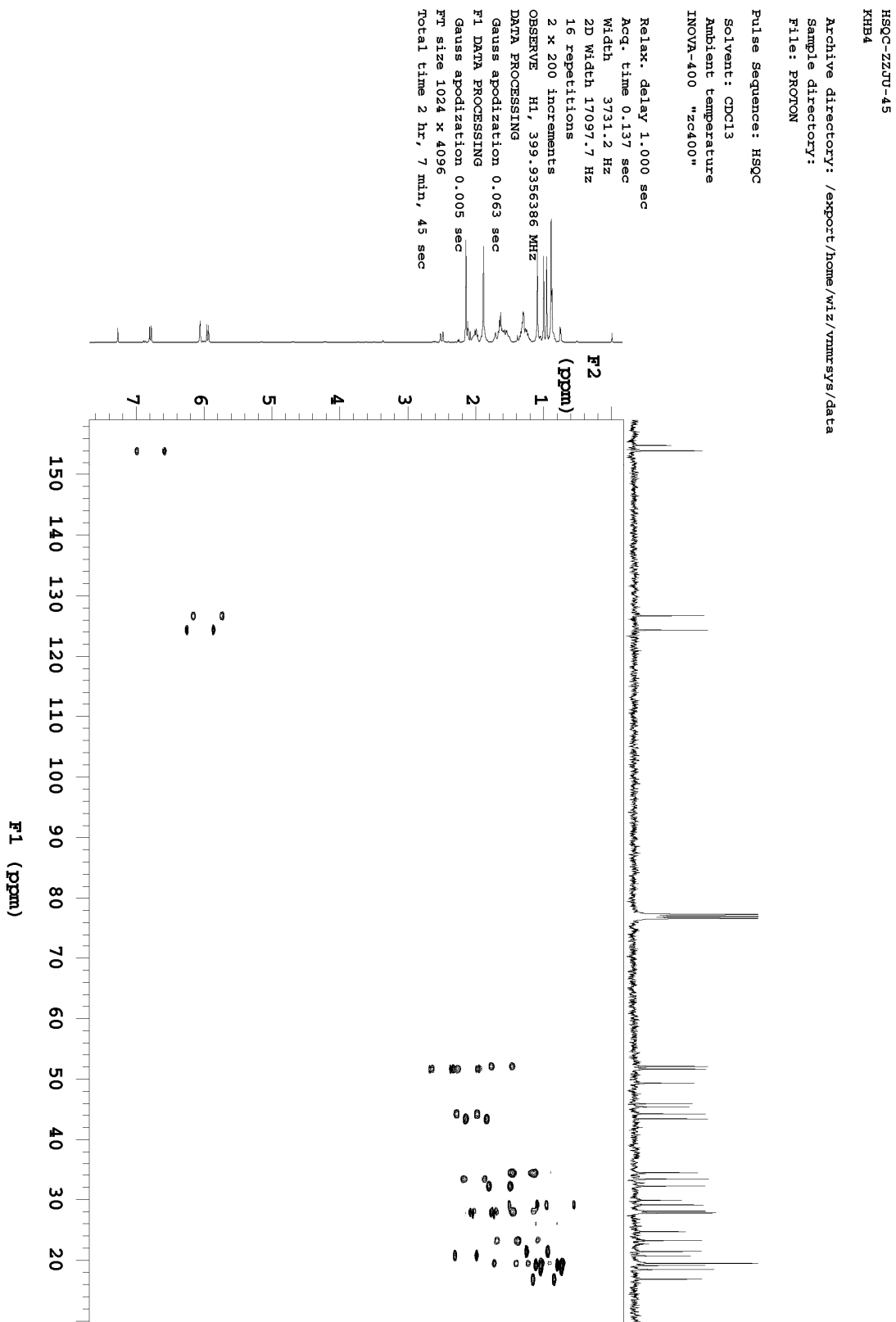
S22. ^{13}C NMR spectrum (high field, expanded) of compound **4** at 100 MHz in CDCl_3 .



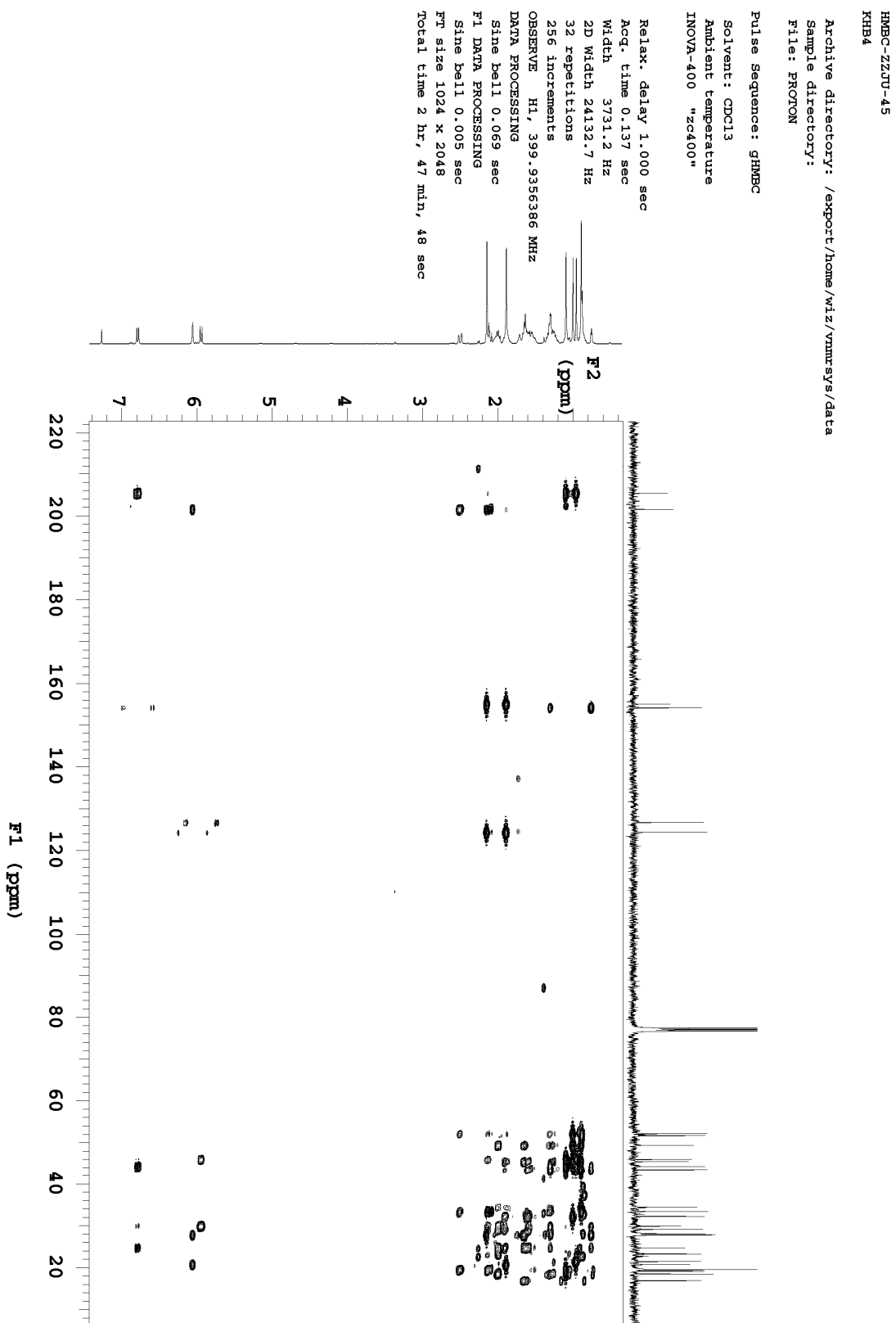
S23. DEPT (135) spectrum of compound **4** at 100 MHz in CDCl₃.



S24. HSQC (undecoupling) spectrum of compound **4** at 400 MHz in CDCl₃.



S25. HMBC spectrum of compound **4** at 400 MHz in CDCl₃.



S26. NOESY spectrum of compound **4** at 400 MHz in CDCl₃.

noesy-zzju-45
KHB4

Archive directory: /export/home/wiz/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: NOESY

Solvent: CDCl₃
Ambient temperature
INOVA-400 "zc400"

Relax. delay 1.000 sec

Mixing 0.700 sec

Acq. time 0.137 sec

Width 3731.2 Hz

2D Width 3731.2 Hz

16 repetitions

2 x 200 increments

OBSERVE H1, 399.9356386 MHz

DATA PROCESSING

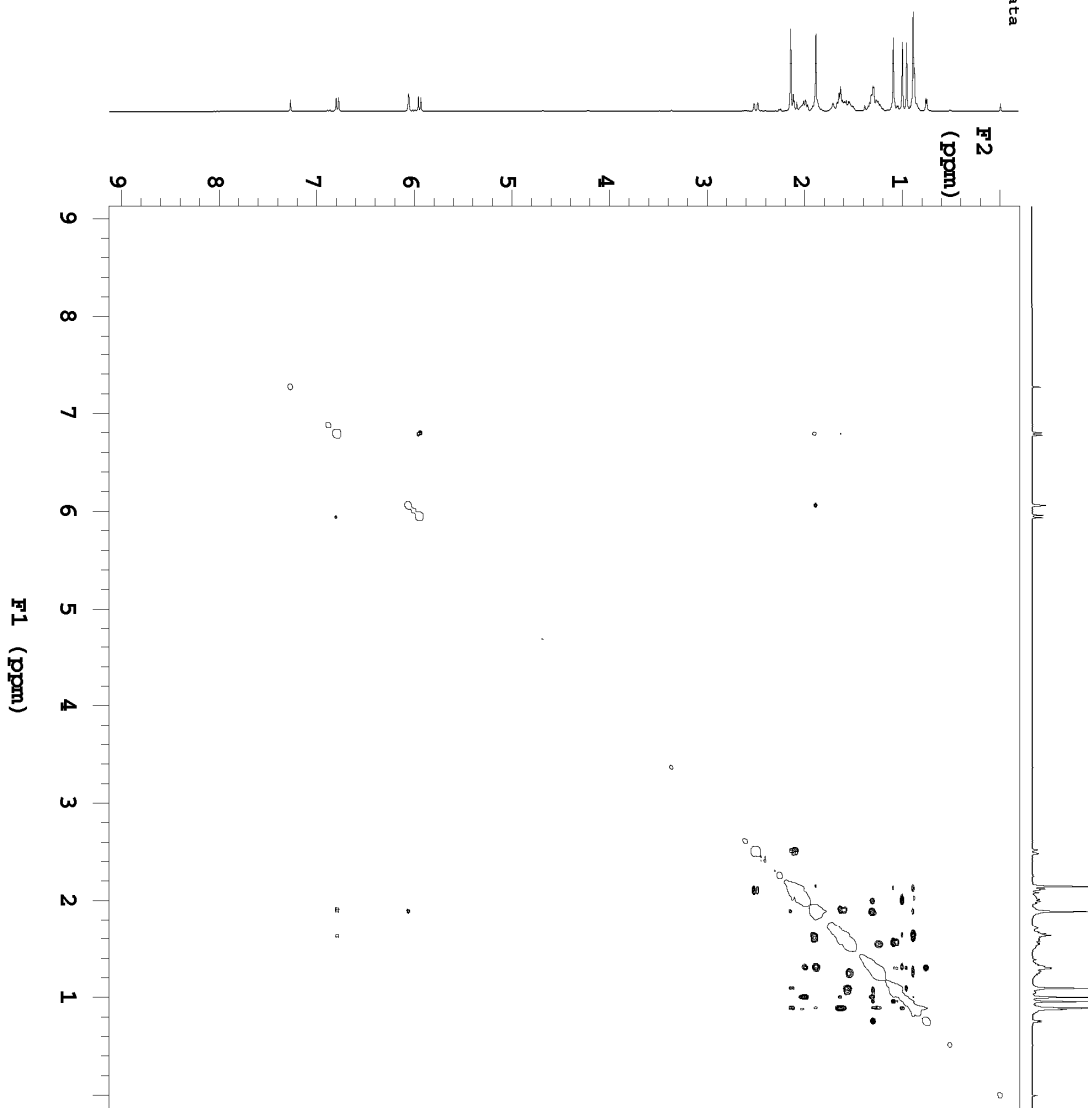
Gauss apodization 0.063 sec

F1 DATA PROCESSING

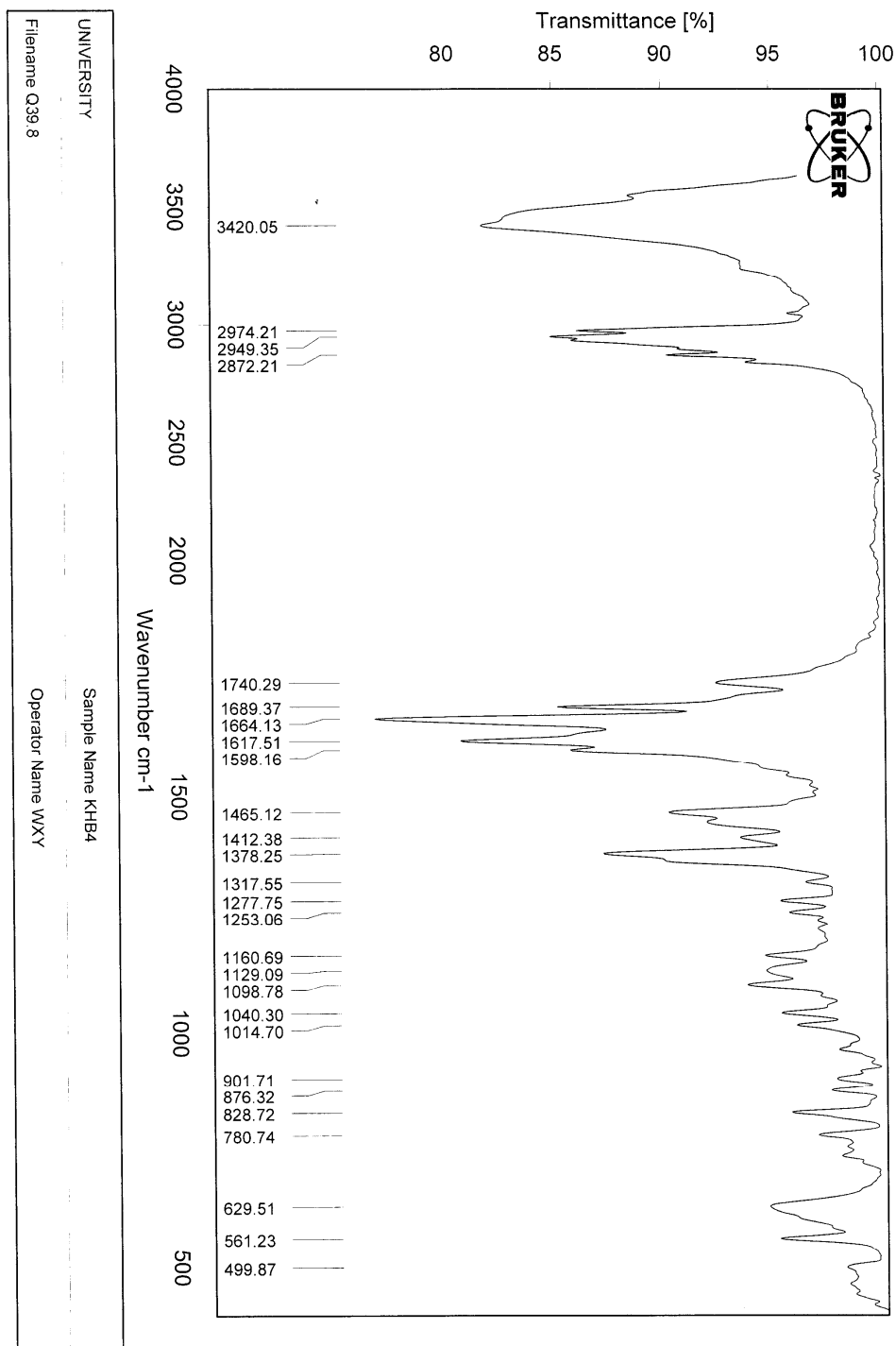
Gauss apodization 0.049 sec

FF size 2048 x 2048

Total time 3 hr, 21 min, 15 sec



S27. IR (KBr disc) spectrum of compound 4.



S28. ESI MS spectra of compound 4 and a mixture of compounds 2 and 3 (1:1).

