

Supporting Information

Figure S1. ^1H -NMR spectrum of uncarilic acid (**1**) at 500MHz in CD_3OD .

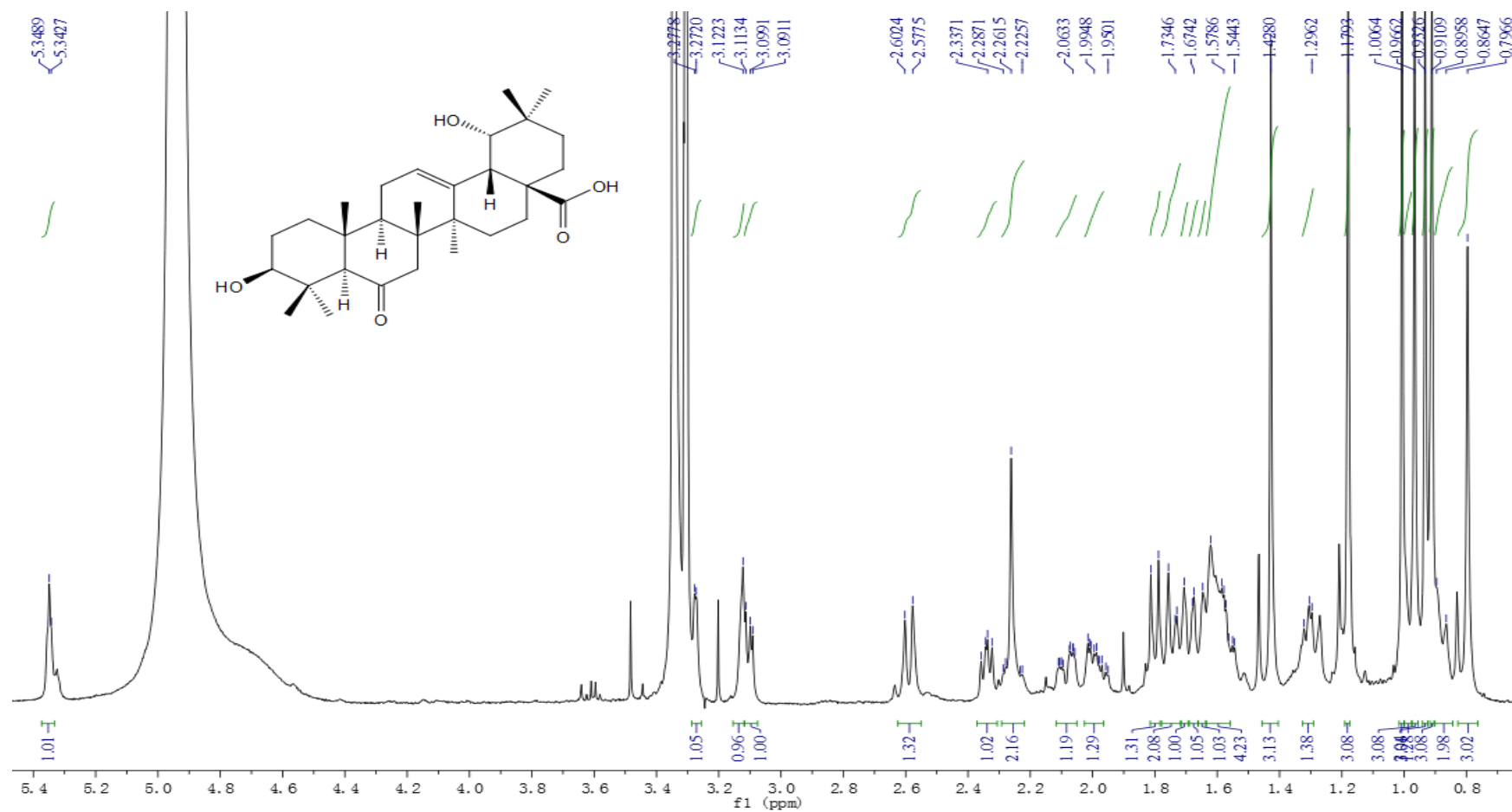


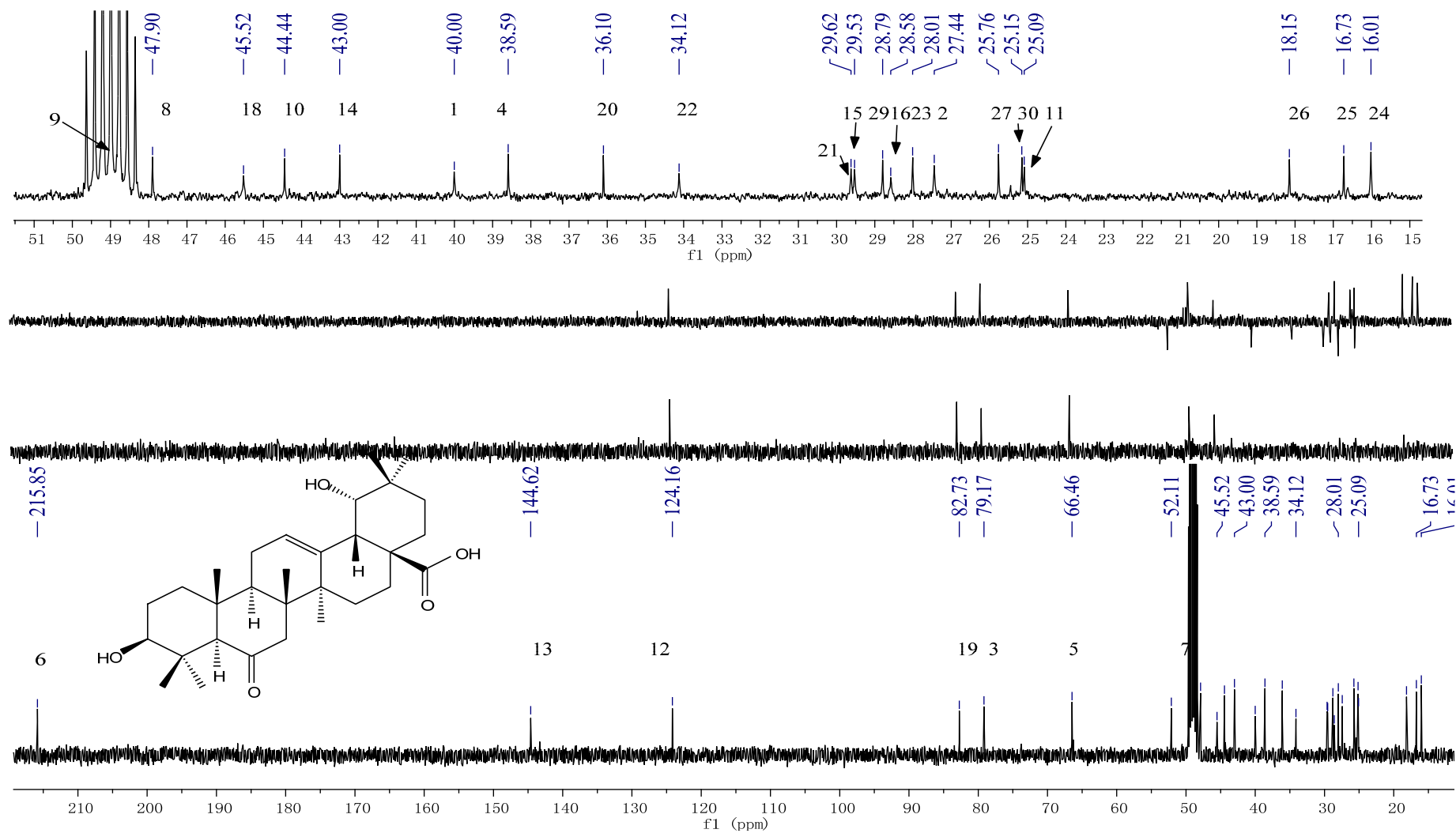
Figure S2. ^{13}C -NMR spectrum of uncarilic acid (1) at 125 MHz in CD_3OD .

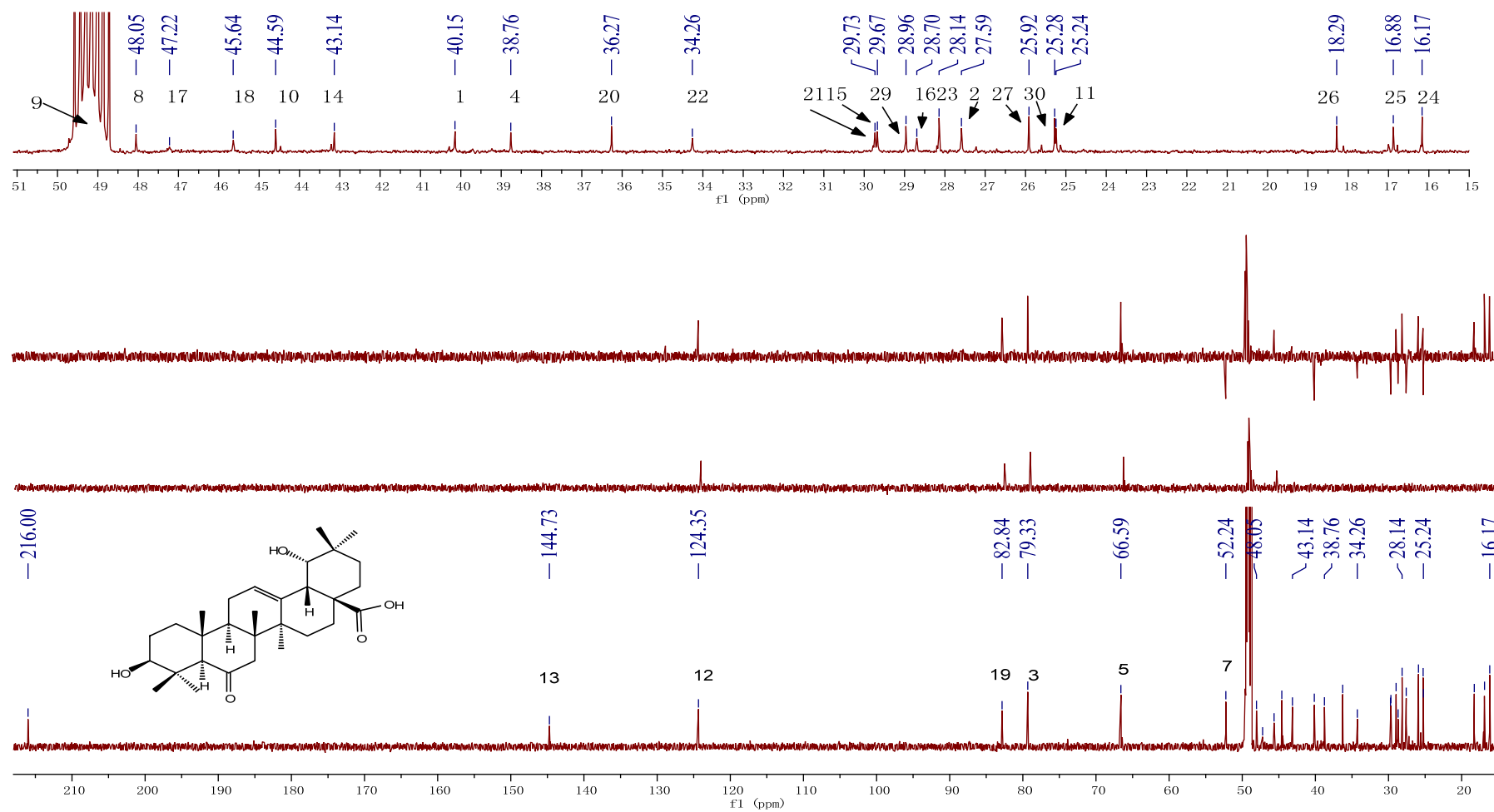
Figure S2-1. ^{13}C -NMR spectrum of uncarilic acid (**1**) at 150 MHz in CD_3OD .

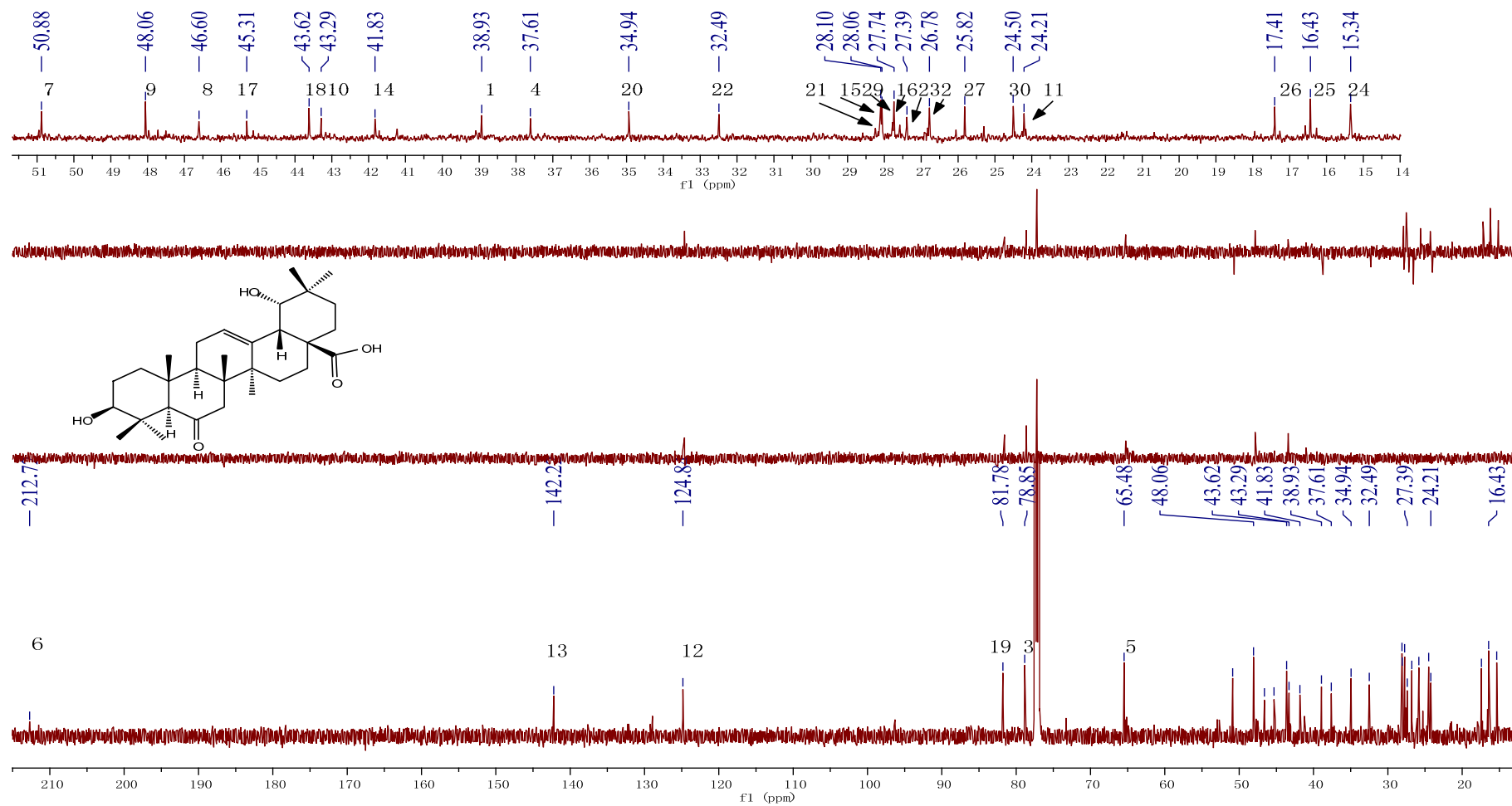
Figure S2-2. ^{13}C -NMR spectrum of uncarilic acid (**1**) at 150 MHz in CDCl_3 .

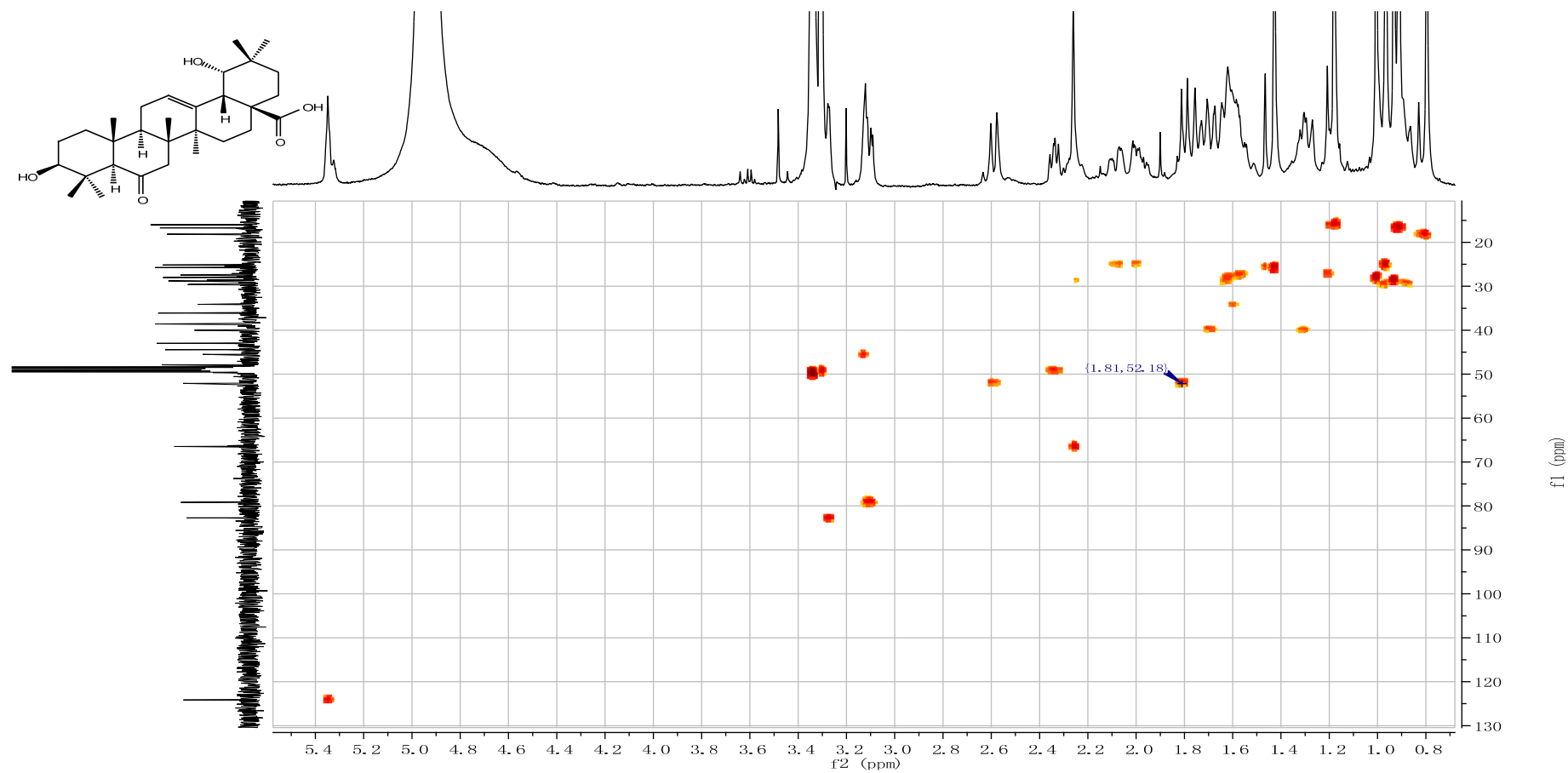
Figure S3. HSQC spectrum of uncarilic acid (1) at 500/125 MHz in CD₃OD.

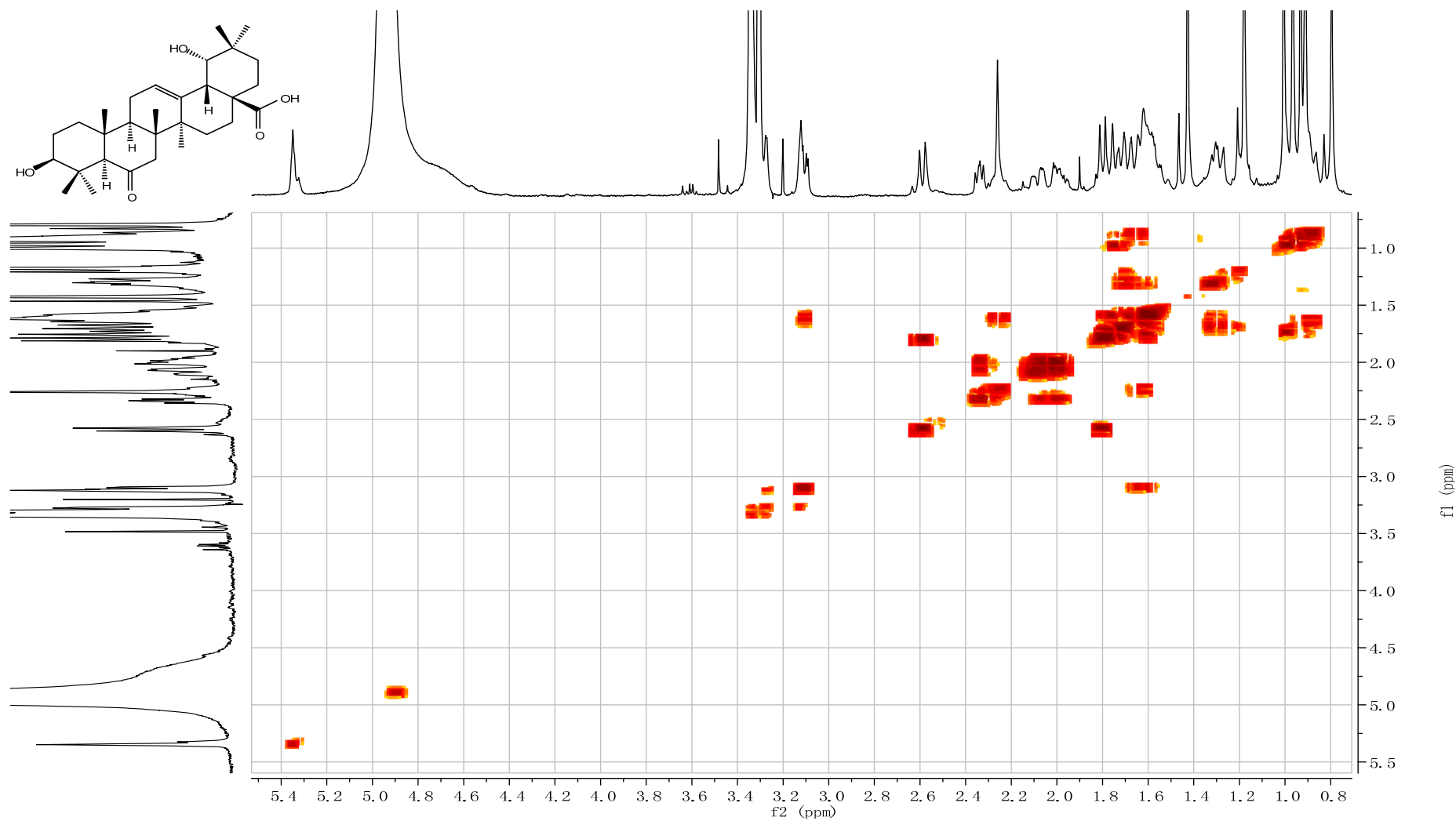
Figure S4. COSY spectrum of uncarilic acid (**1**) at 500 MHz in CD₃OD.

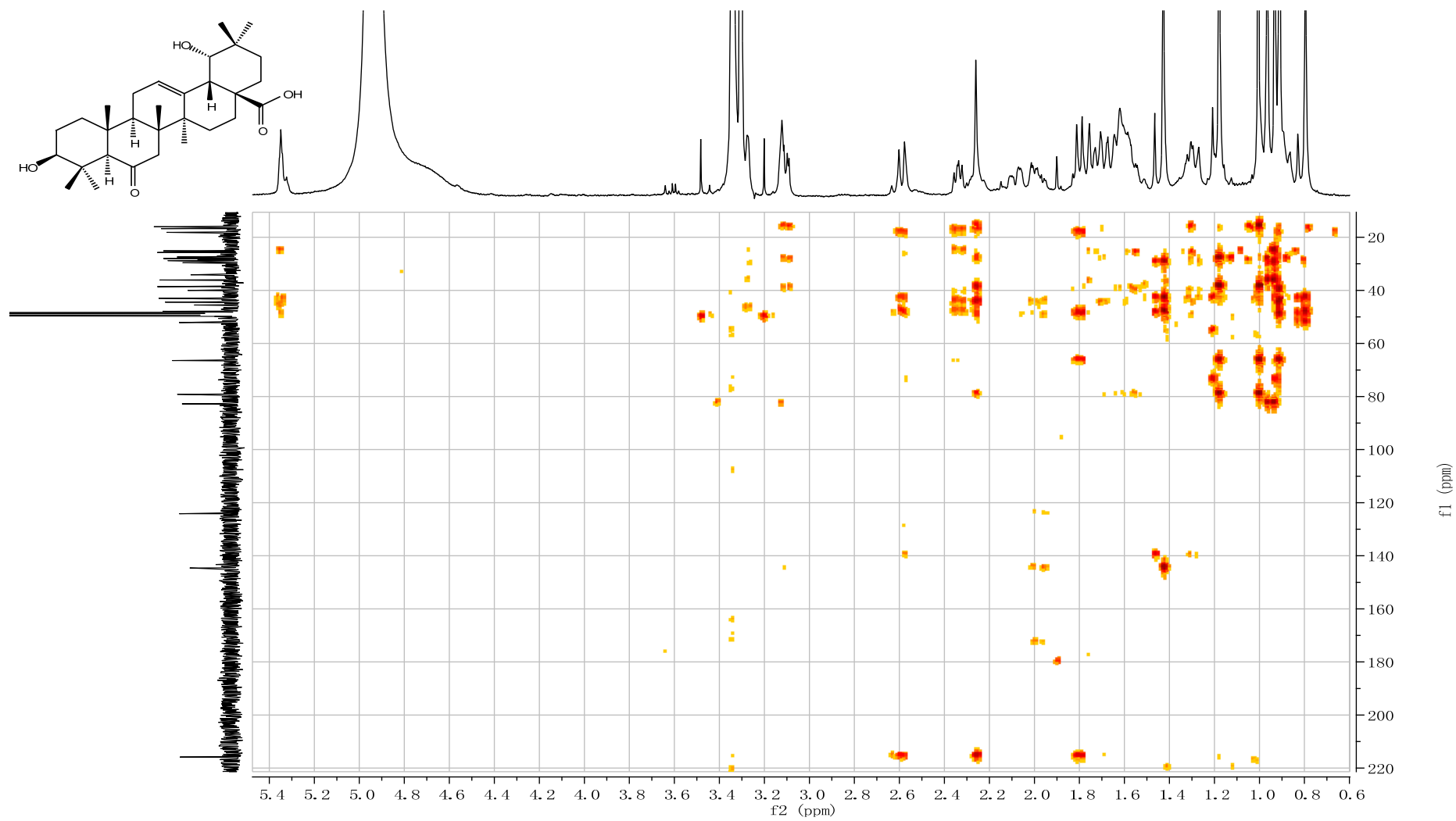
Figure S5. HMBC spectrum of uncarilic acid (**1**) at 500/125MHz in CD₃OD.

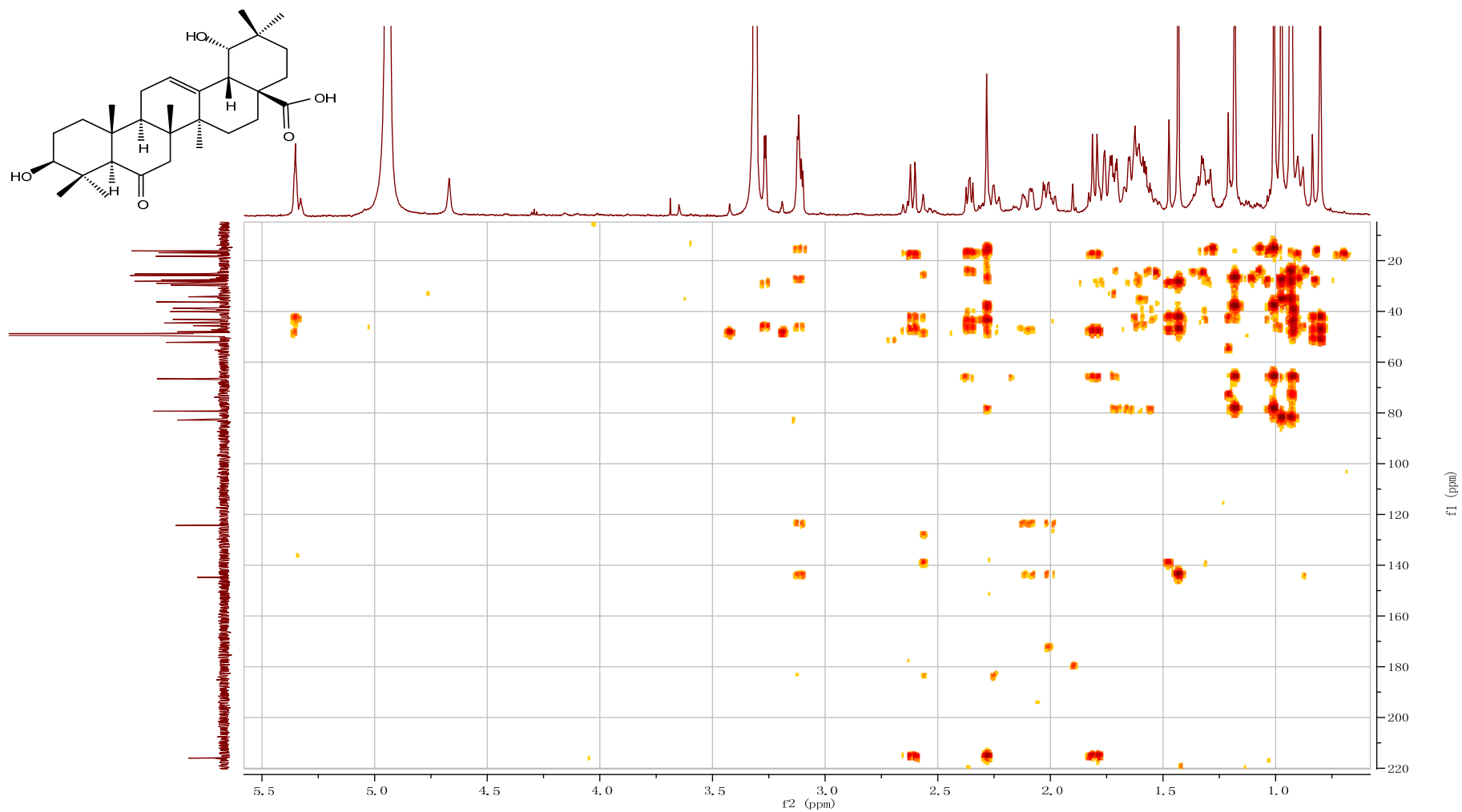
Figure S5-1. HMBC spectrum of uncarilic acid (**1**) at 600/150 MHz in CD₃OD.

Figure S5-2. Key correlations H-9/C-25 and H-7/C-9, H₃-26/C-9 of HMBC (**1**) at 600/150MHz in CD₃OD.

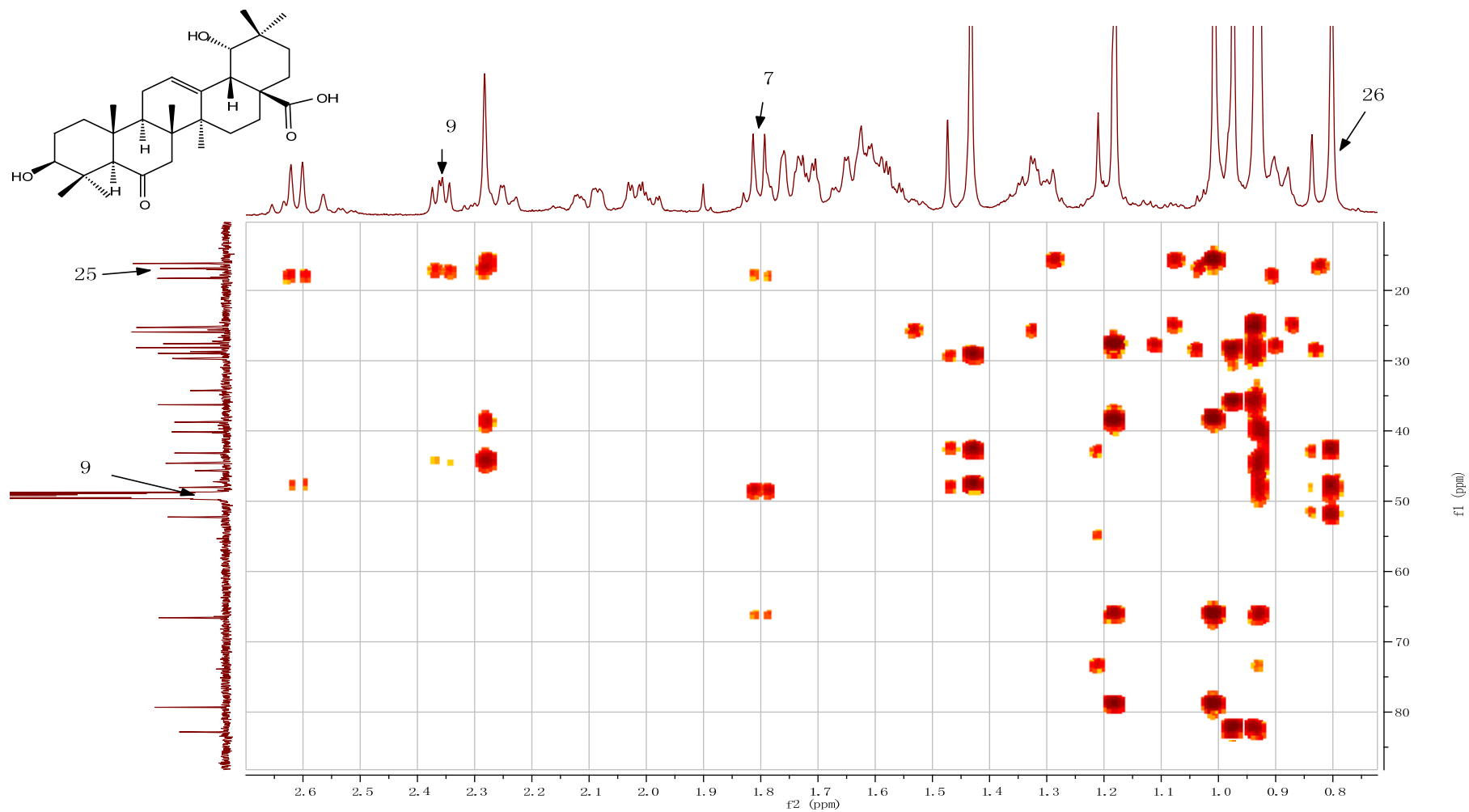


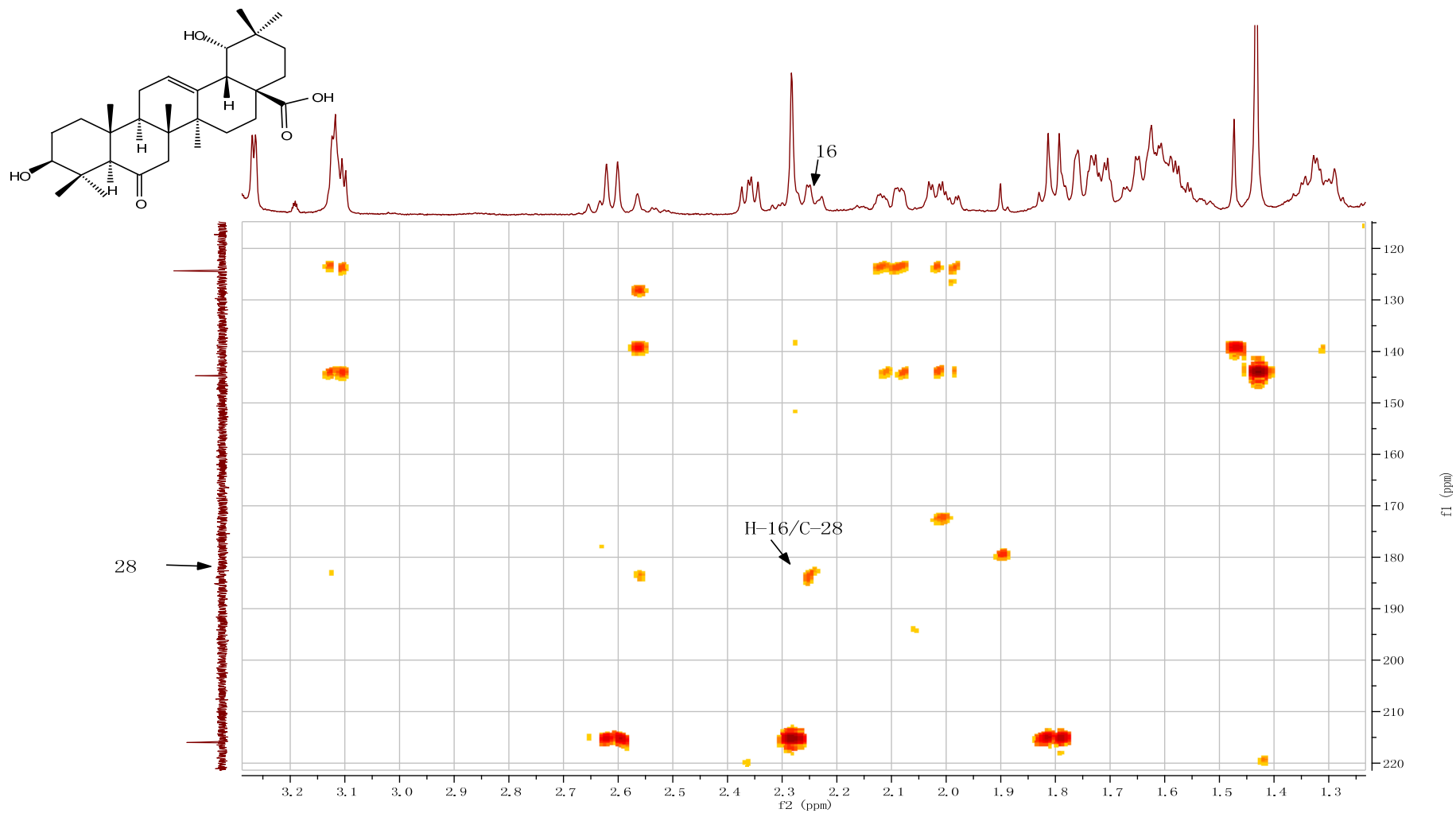
Figure S5-3. Key correlations H-16/C-28 of HMBC(1) at 600/150 MHz in CD₃OD.

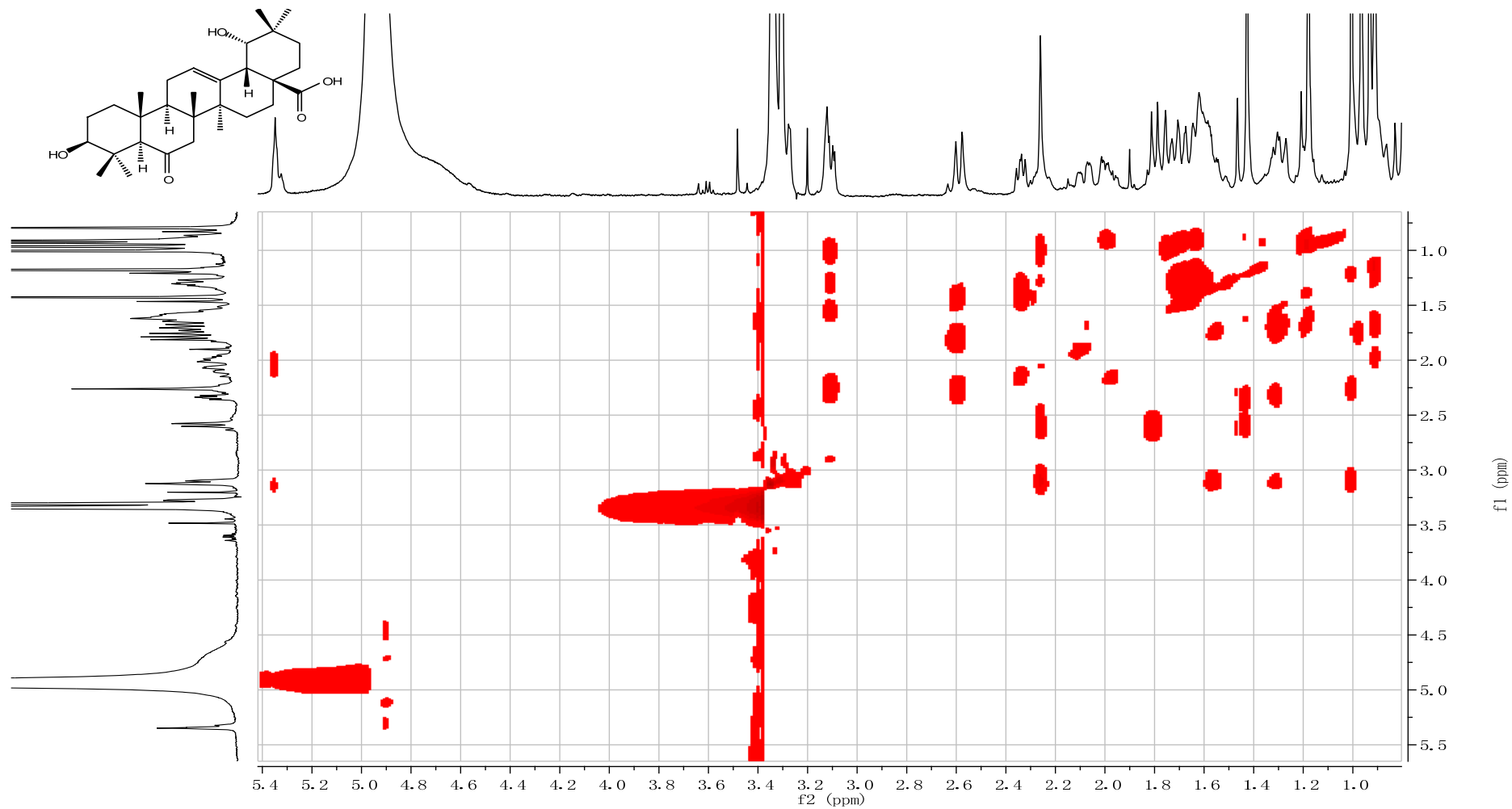
Figure S6. ROESY spectrum of uncarilic acid (**1**) at 500 MHz in CD₃OD.

Figure S7. HREI-MS spectrum of uncarilic acid (**1**).**Elemental Composition Report**

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

21 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 4-6

Moa-14

09:22:45 13-Mar-2013

Voltage El+

100

%

0

485.900

486.000

486.100

486.200

486.300

486.400

486.500

486.600

486.700

486.800

Minimum:

Maximum:

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

486.3356

486.3345

1.1

2.3

8.0

5546031.5

C30

H46

O5

KIB
M130313EA-03AFAMM 30 (2.754)
486.3356Autospec Premier
P776
23.3

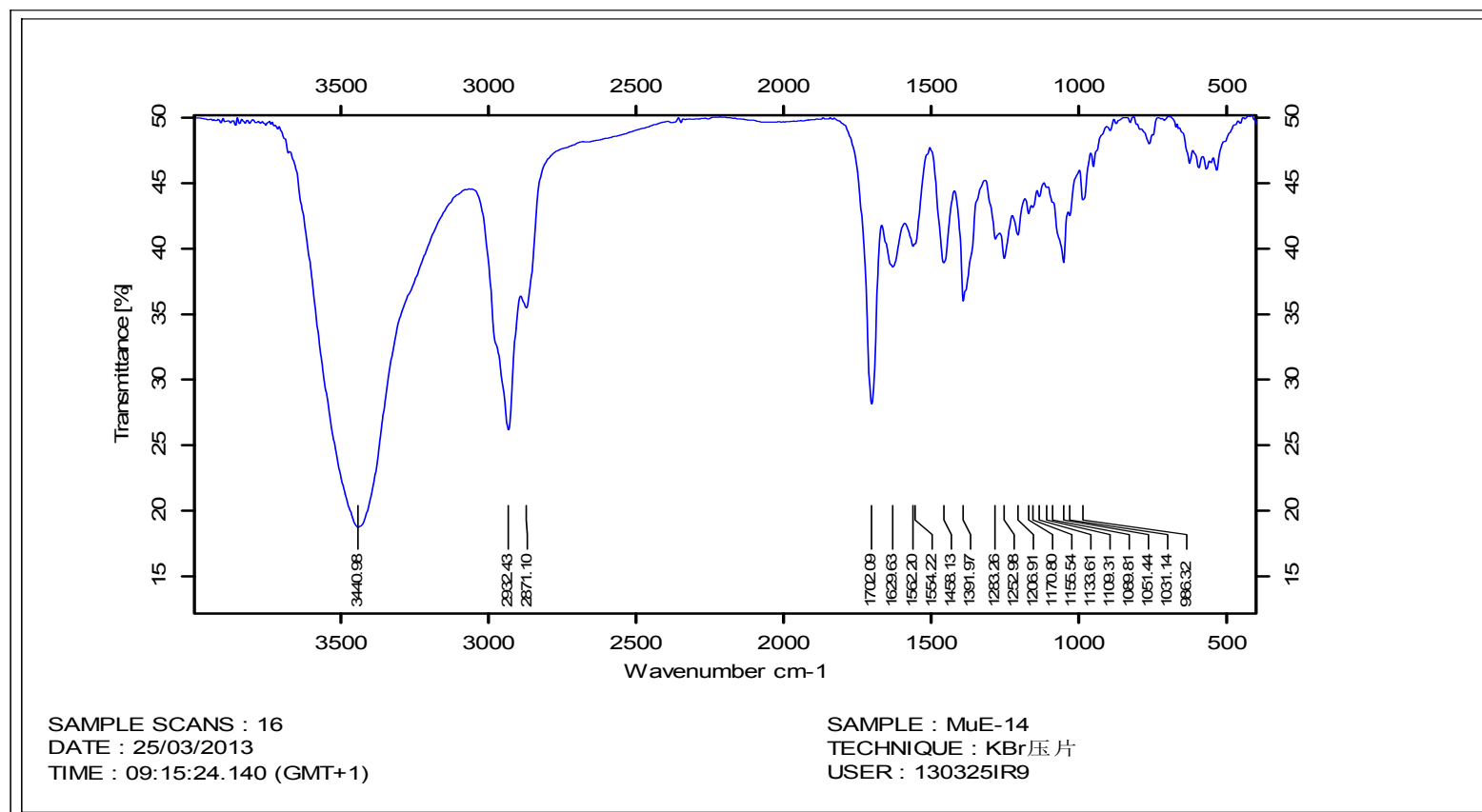
Figure S8. IR spectrum of uncarilic acid; (1).

Figure S9. Optical rotation measurement of uncarilic acid (**1**)

5 (1/3)	Specific O.R.	19.000	20.4	0	Mon Mar 25 13:06:46 2013	0.00180g/mlMeOH	MUE-14
5 (2/3)	Specific O.R.	20.556	20.4	0	Mon Mar 25 13:07:00 2013	0.00180g/mlMeOH	MUE-14
5 (3/3)	Specific O.R.	19.444	20.4	0	Mon Mar 25 13:07:13 2013	0.00180g/mlMeOH	MUE-14

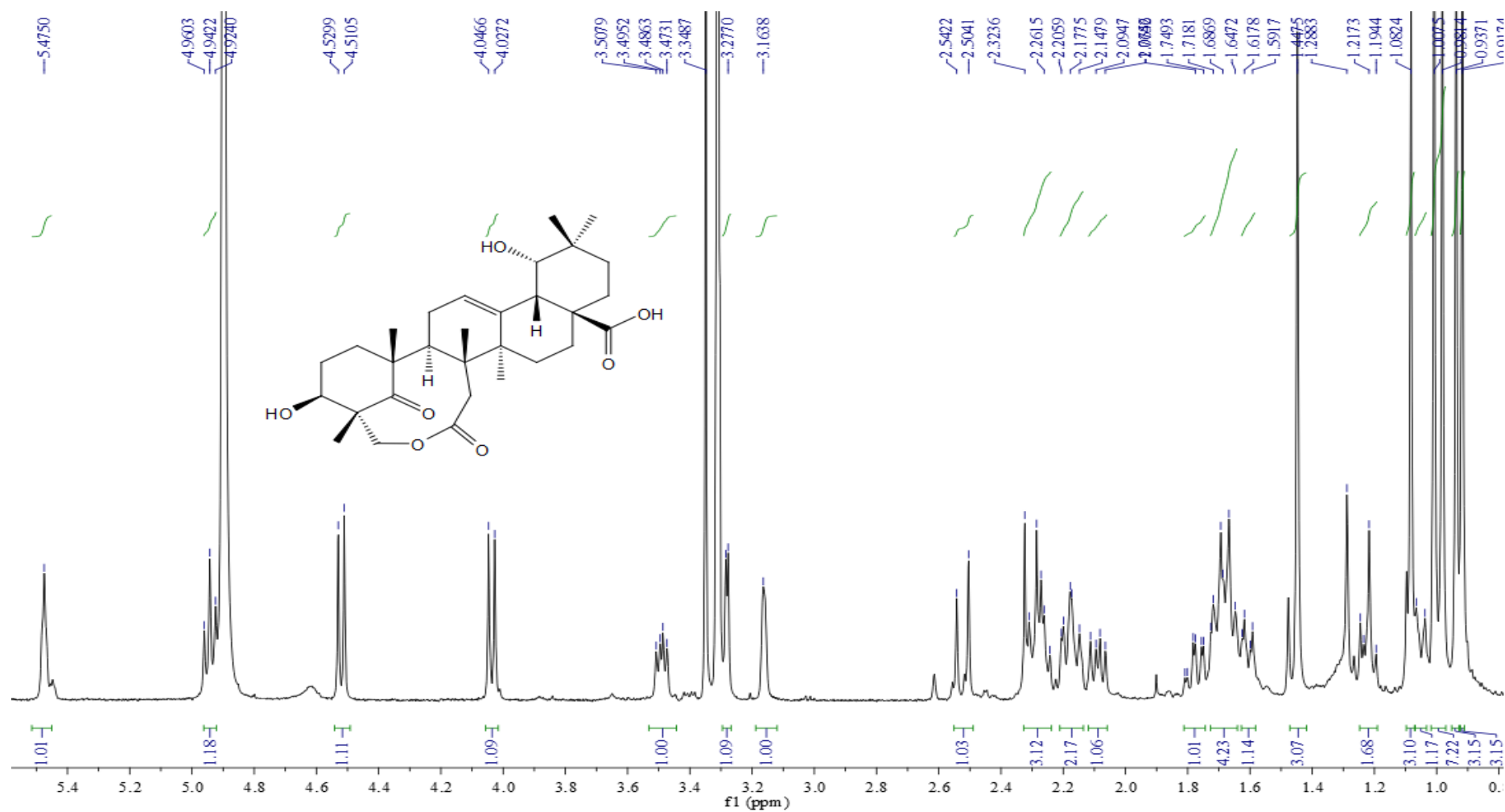
Figure S10. ^1H -NMR spectrum of secuncarilic acid (**2**) at 500 MHz in CD_3OD .

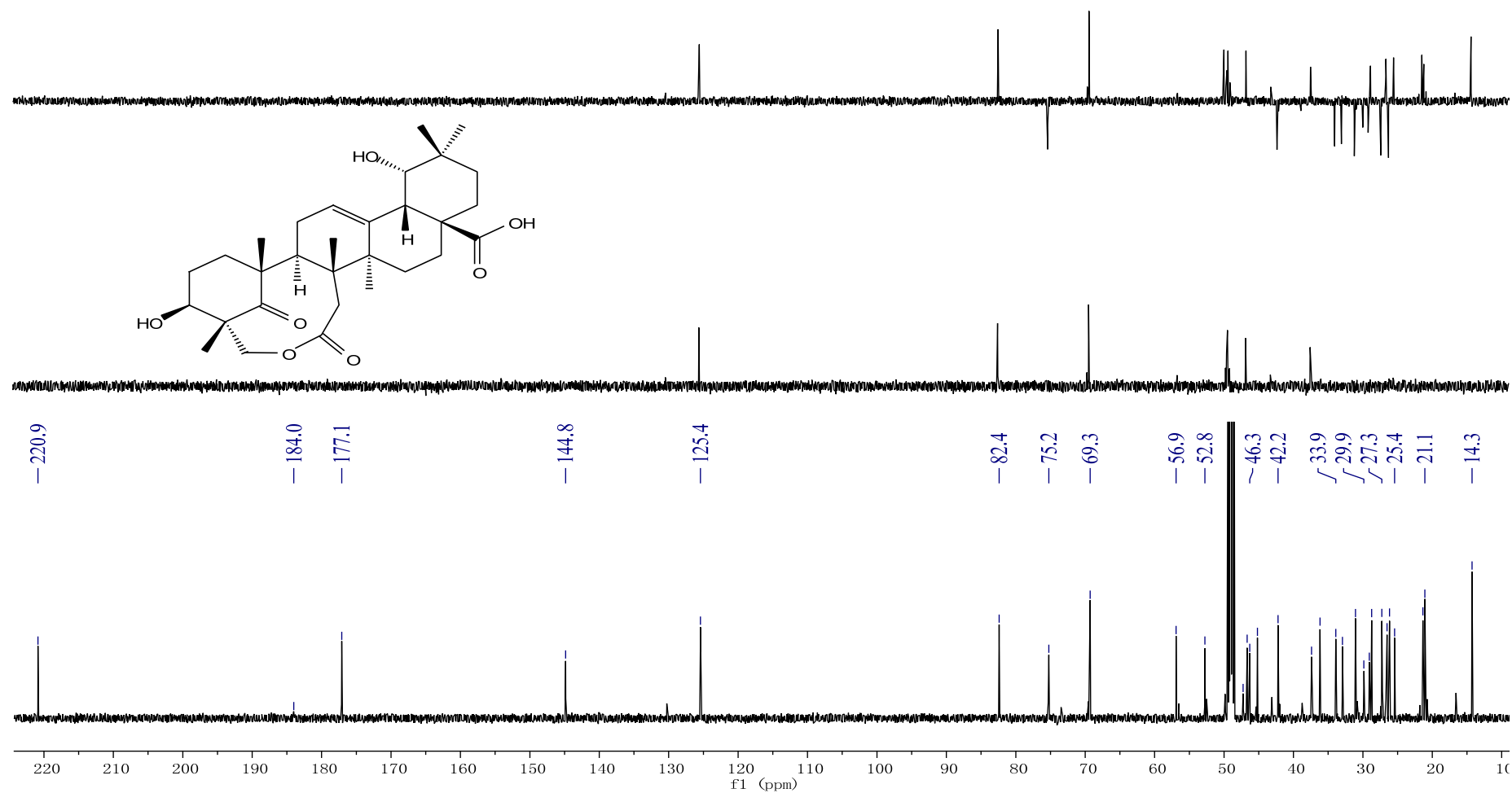
Figure S11. ^{13}C -NMR of spectrum of secuncarilic acid (**2**) at 125 MHz in CD_3OD .

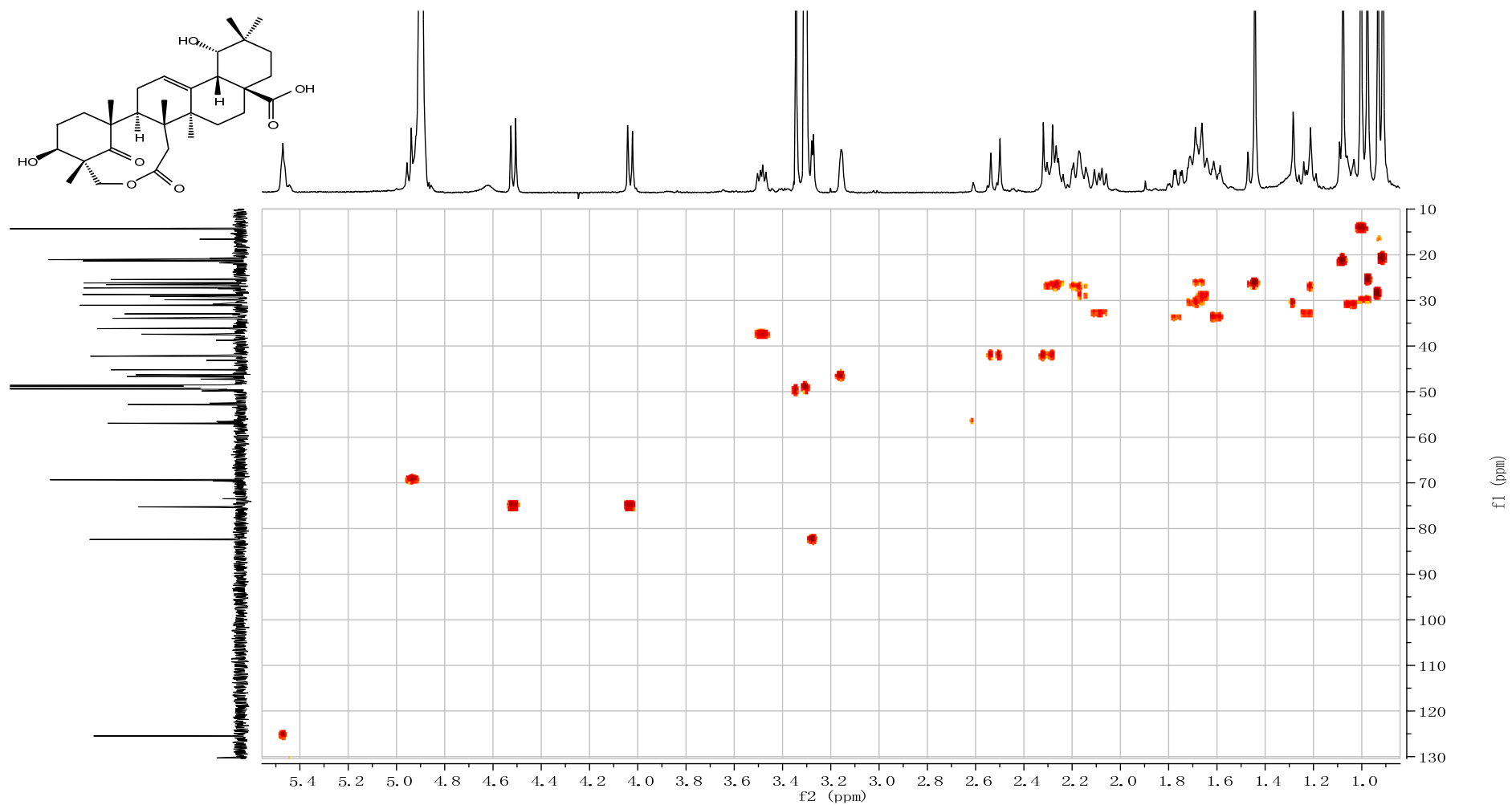
Figure S12. HSQC spectrum of secuncarilic acid (**2**) at 500/125 MHz in CD₃OD.

Figure S13. COSY spectrum of secuncarilic acid (**2**) at 500 MHz in CD₃OD.

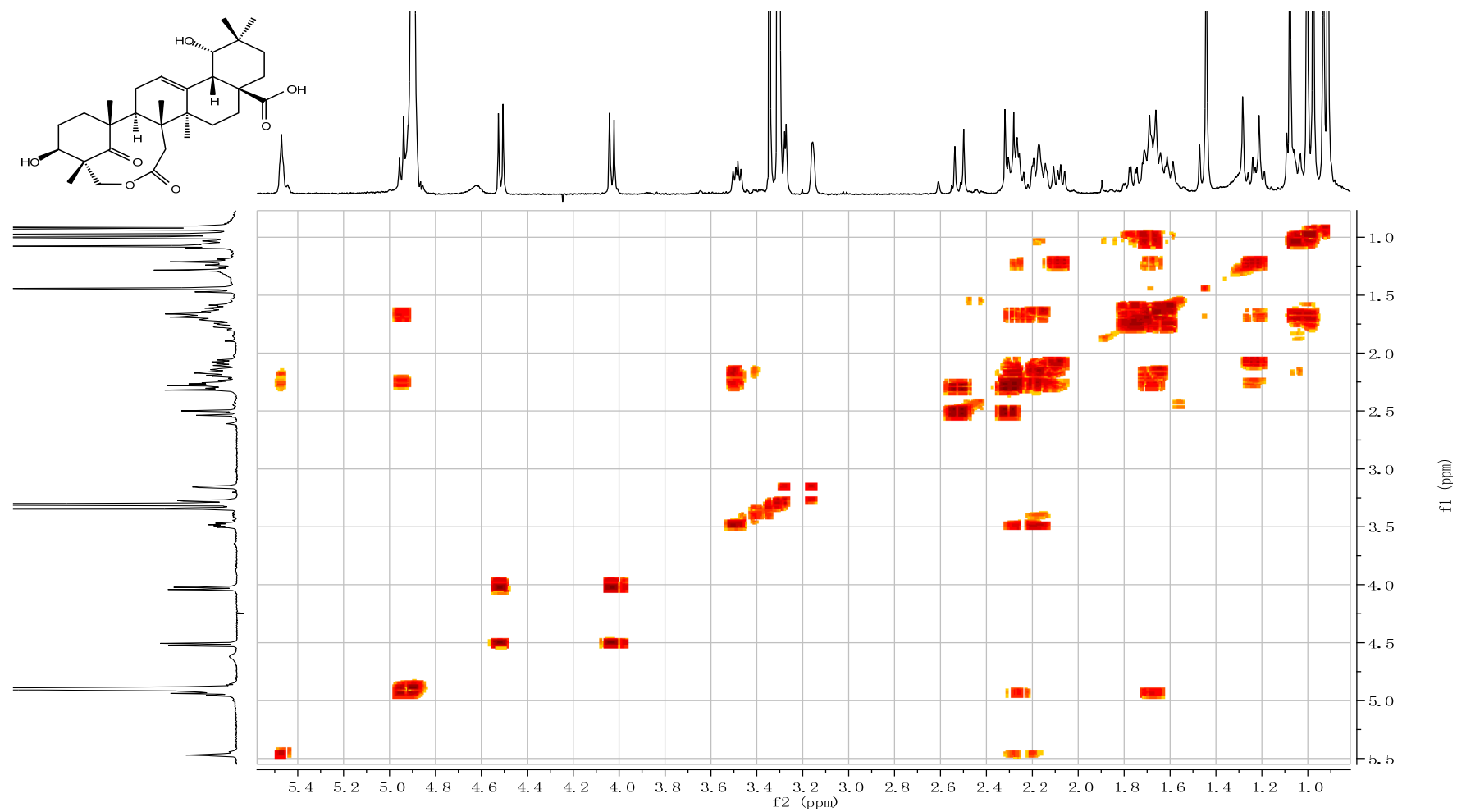


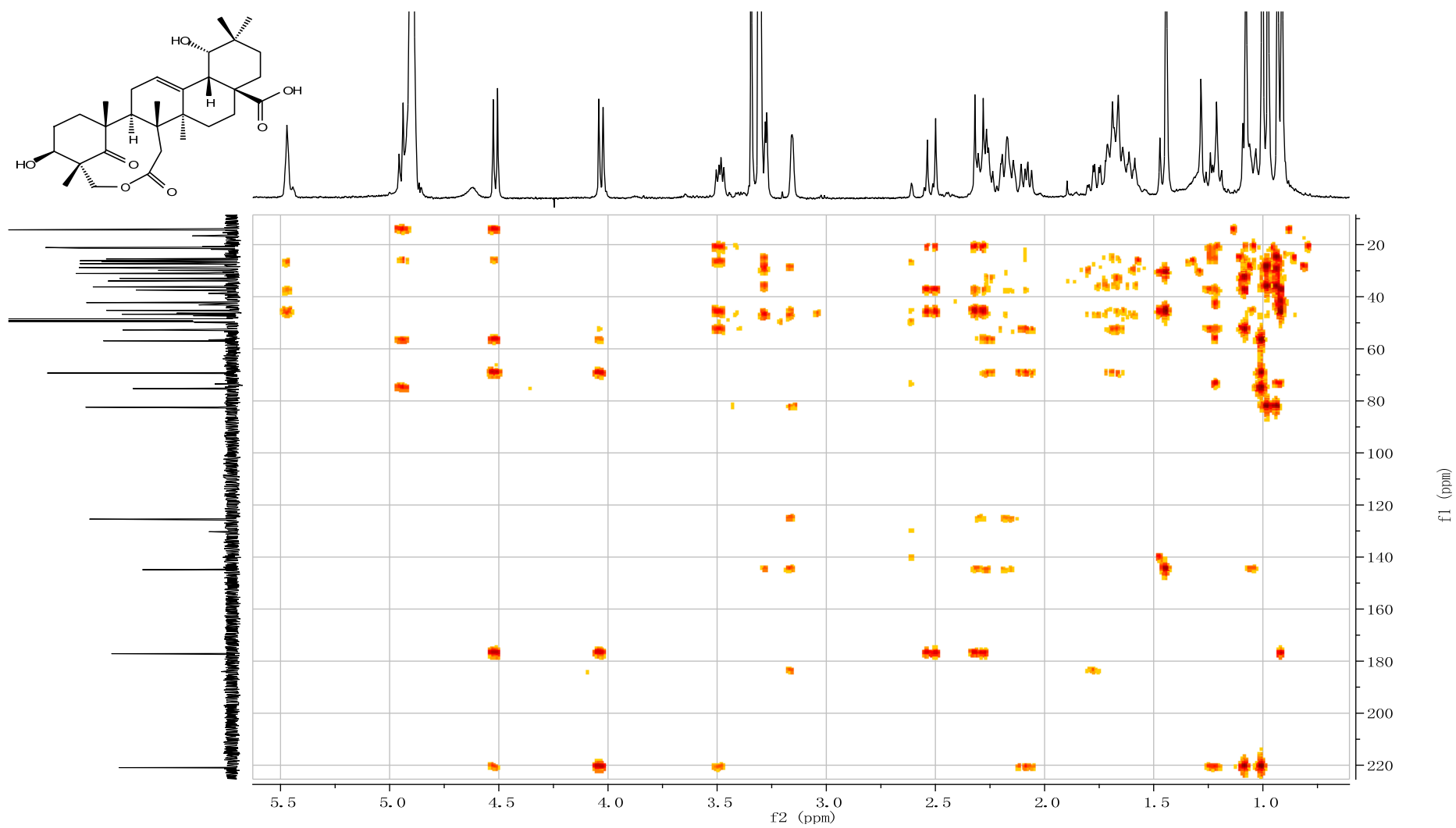
Figure S14. HMBC spectrum of secuncarilic acid (2) at 500/125 MHz in CD₃OD.

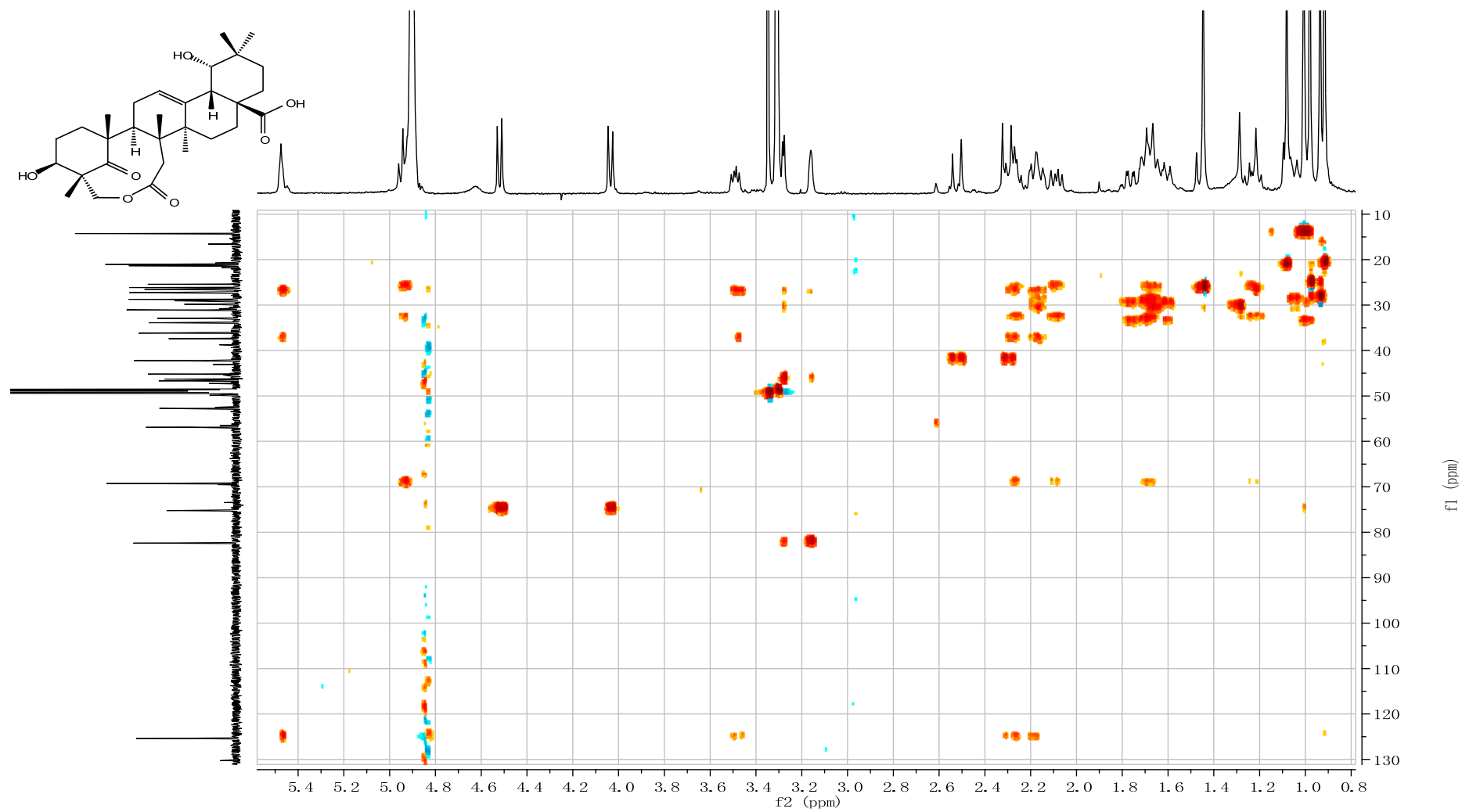
Figure S15. HSQC-TOCSY spectrum of secuncarilic acid (**2**) at 500/125 MHz in CD₃OD.

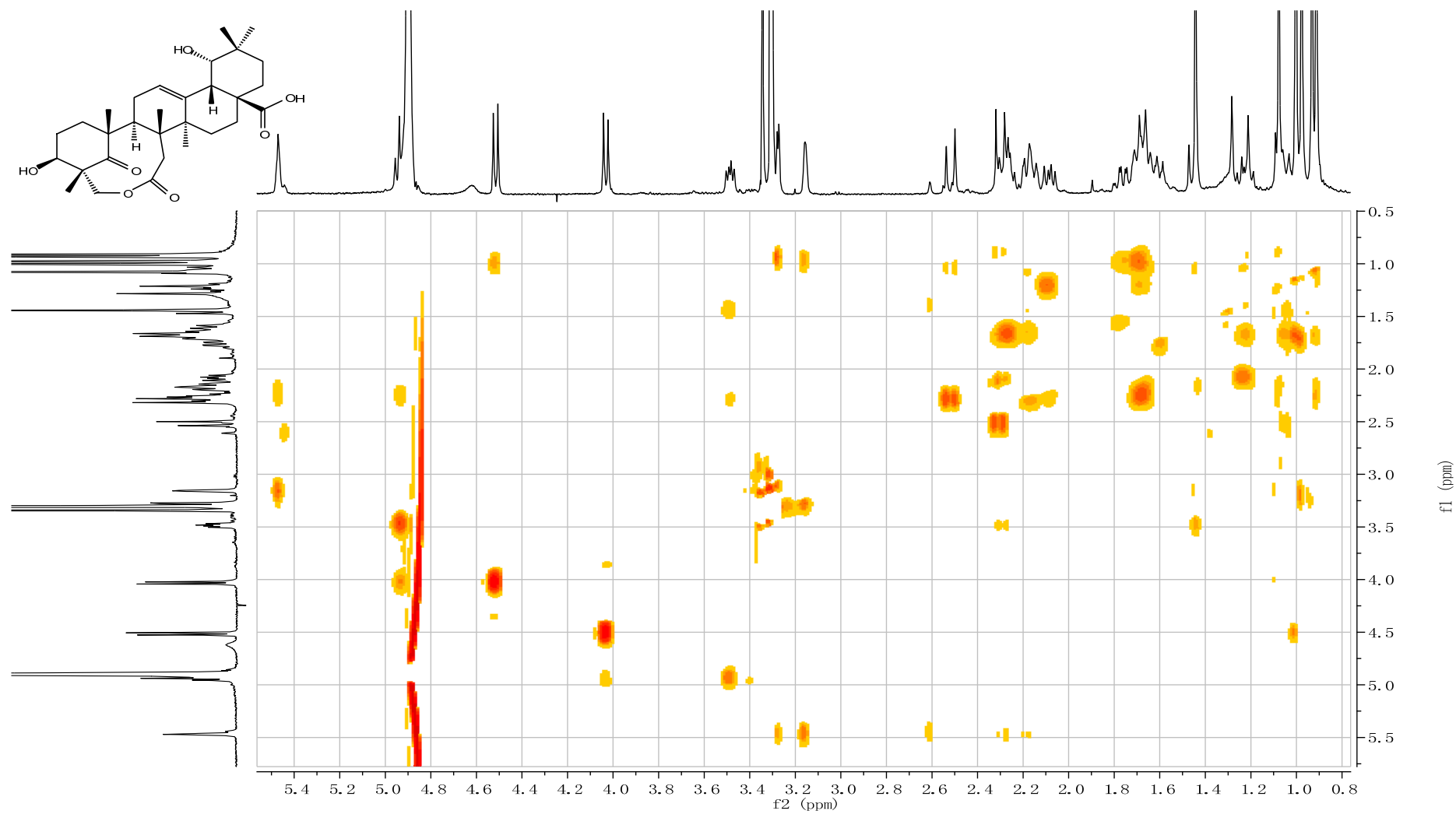
Figure S16. ROESY spectrum of secuncarilic acid (**2**) at 500 MHz in CD₃OD.

Figure S17. HREI-MS spectrum of secoungarilic acid (2).**Elemental Composition Report**

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 6-8

Mua-7

09:32:34 13-Mar-2013

Voltage El+

100%

%

0

515.80

515.90

516.00

516.10

516.20

516.30

516.40

516.50

516.60

516.70

516.80

m/z

Minimum:

Maximum:

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

516.3096

516.3087

0.9

1.7

9.0

5546118.5

C30

H44

O7

KIB
M130313EA-04AFAMM 21 (1.928) Cm (20:21)
516.3096Autospec Premier
P776
201

Figure S18. IR spectrum of secoumaric acid (2).

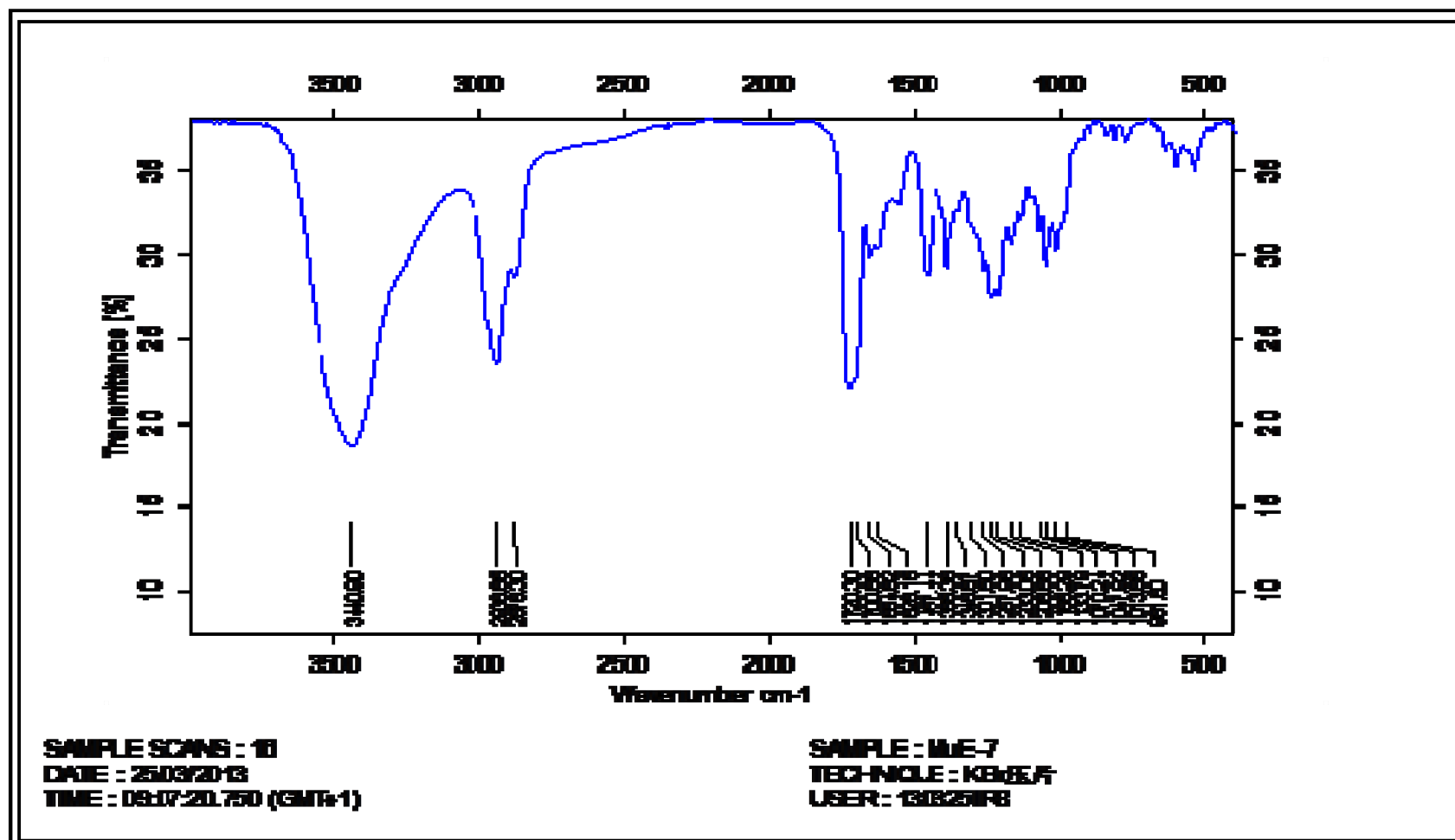


Figure S19. Optical rotation measurement of secouncarilic acid (**2**).

3 (1/3)	Specific O.R.	34.211	20.4	0	Mon Mar 25 12:56:20 2013	0.00190g/mlMeOH	MUE-7
3 (2/3)	Specific O.R.	35.053	20.4	0	Mon Mar 25 12:56:33 2013	0.00190g/mlMeOH	MUE-7
3 (3/3)	Specific O.R.	35.263	20.4	0	Mon Mar 25 12:56:46 2013	0.00190g/mlMeOH	MUE-7