

Supporting Information of

New Dimeric and Trimeric *Erythrina* Alkaloids from *Erythrina variegata*

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China

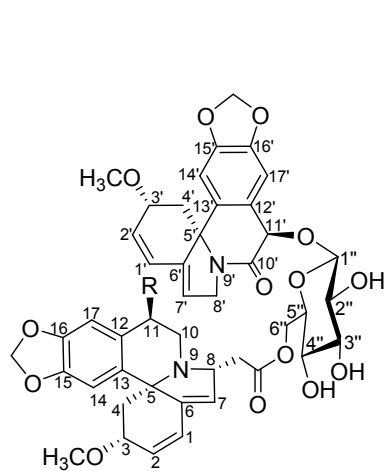
Correspondence

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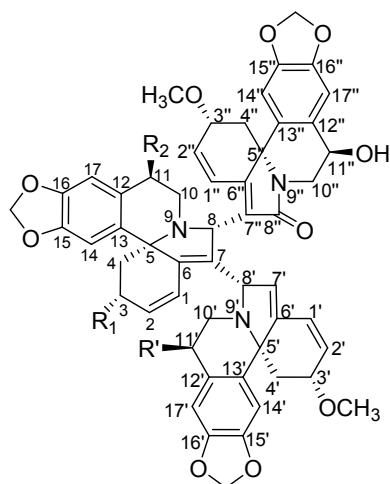
Contents

1、 Structures of erythrivarines C–G (1-5) and their units, erythrinine (6) and 8-oxo-erythrinine (7).	
2、 NMR spectroscopic data of dimeric erythrivarines C-D (1-2)	
Figure S1: ¹ H NMR spectrum of erythrivarine C (1)	P04
Figure S2: ¹³ C NMR spectrum of erythrivarine C (1)	P06
Figure S3: HSQC spectrum of erythrivarine C (1)	P07
Figure S4: HMBC spectrum of erythrivarine C (1)	P09
Figure S5: ¹ H- ¹ H COSY spectrum of erythrivarine C (1)	P10
Figure S6: ROESY spectrum of erythrivarine C (1)	P11
Figure S7: ¹ H NMR spectrum of erythrivarine D (2)	P12
Figure S8: ¹³ C NMR spectrum of erythrivarine D (2)	P13
Figure S9: HSQC spectrum of erythrivarine D (2)	P14
Figure S10: HMBC spectrum of erythrivarine D (2)	P15
Figure S11: ¹ H- ¹ H COSY spectrum of erythrivarine D (2)	P16
Figure S12: ROESY spectrum of erythrivarine D (2)	P17
3、 NMR spectroscopic data of trimeric erythrivarines F-G (3-5)	
Figure S13: ¹ H NMR spectrum of erythrivarine E (3)	P18
Figure S14: ¹³ C NMR spectrum of erythrivarine E (3)	P20
Figure S15: HSQC spectrum of erythrivarine E (3)	P21
Figure S16: HMBC spectrum of erythrivarine E (3)	P23
Figure S17: ROESY spectrum of erythrivarine E (3)	P24
Figure S18: ¹ H NMR spectrum of erythrivarine F (4)	P25
Figure S19: ¹³ C NMR spectrum of erythrivarine F (4)	P27
Figure S20: HSQC spectrum of erythrivarine F (4)	P28
Figure S21: HMBC spectrum of erythrivarine F (4)	P30
Figure S22: ¹ H- ¹ H COSY spectrum of erythrivarine F (4)	P31
Figure S23: ROESY spectrum of erythrivarine F (4)	P32
Figure S24: ¹ H NMR spectrum of erythrivarine G (5)	P33
Figure S25: ¹³ C NMR spectrum of erythrivarine G (5)	P35
Figure S26: HSQC spectrum of erythrivarine G (5)	P36
Figure S27: HMBC spectrum of erythrivarine G (5)	P38
Figure S28: ¹ H- ¹ H COSY spectrum of erythrivarine G (5)	P39
Figure S29: ROESY spectrum of erythrivarine G (5)	P40
4、 NMR spectroscopic data of erythrinine (6) and 8-oxo-erythrinine (7)	
Figure S30: ¹ H NMR spectrum of 8-oxo-erythrinine (6)	P41
Figure S31: ¹³ C NMR spectrum of 8-oxo-erythrinine (6)	P42
Figure S32: ¹ H NMR spectrum of 8-oxo-erythrinine (7)	P43
Figure S33: ¹³ C NMR spectrum of 8-oxo-erythrinine (7)	P44
5、 UPLC-MS-MS chromatograms of 1-5	
Figure S34. The characteristic peak obtained by UPLC-MS-MS of erythrivarine C (1)	P46
Figure S35. The characteristic peak obtained by UPLC-MS-MS of erythrivarine D (2)	P48
Figure S36. The characteristic peak obtained by UPLC-MS-MS of erythrivarine E (3)	P50
Figure S37. The characteristic peak obtained by UPLC-MS-MS of erythrivarine F (4)	P52
Figure S38. The characteristic peak obtained by UPLC-MS-MS of erythrivarine G (5)	P54
6、 The CD and UV chromatography of the unit of erythrivarine C (1)	

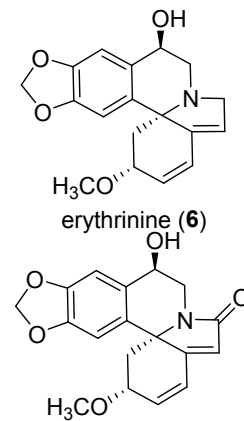
1、 Structures of erythrivarines C–G (1-5) and their units, erythrinine (6) and 8-oxo-erythrinine (7).



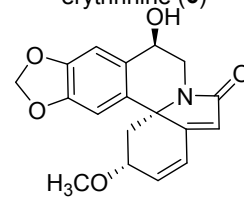
- 1 R=OH
2 R=OCH₃



- 3 R₁=OCH₃ R₂=OH R'=OH
4 R₁=OCH₃ R₂=OCH₃ R'=OH
5 R₁=O R₂=OH R'=OCH₃



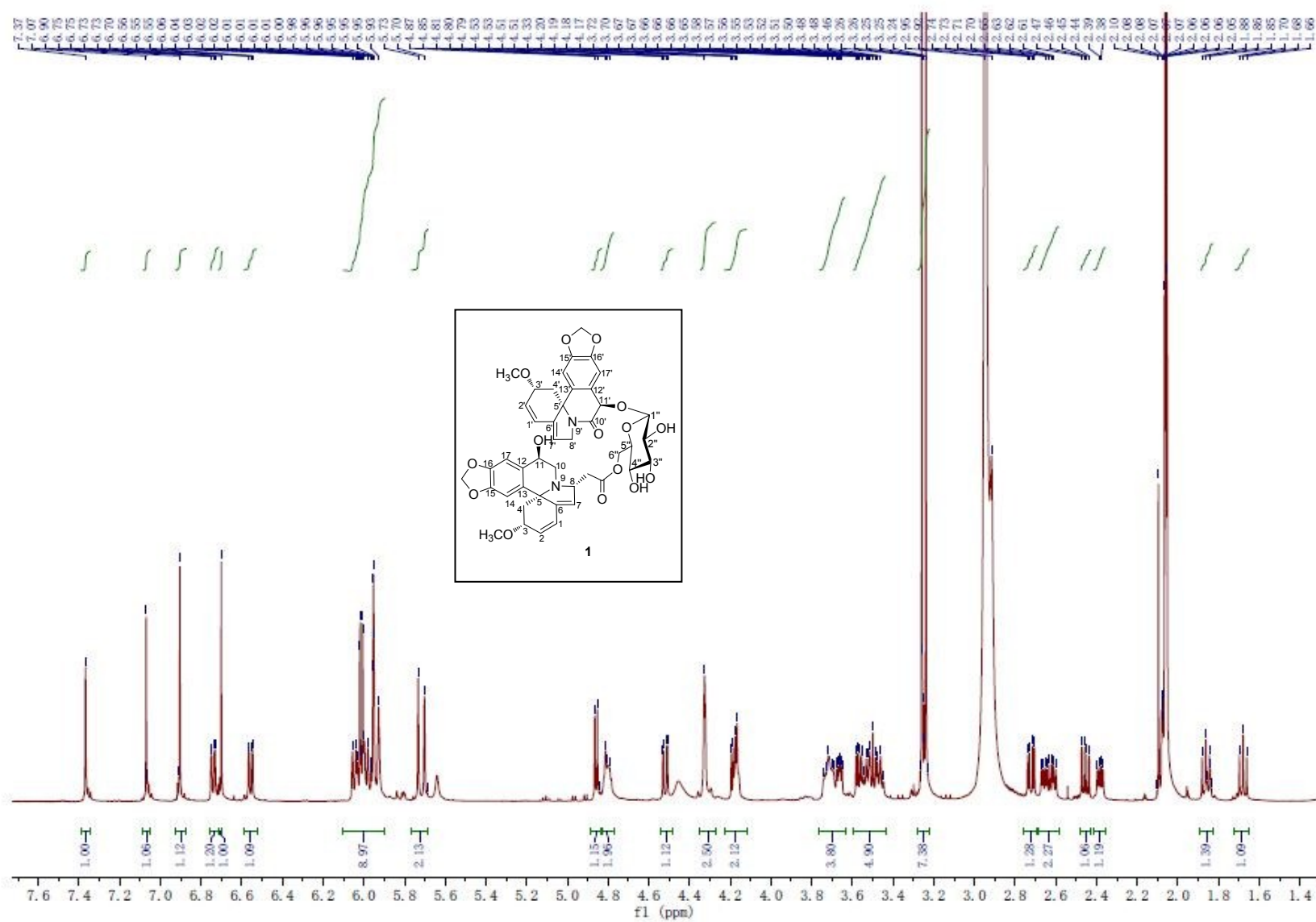
erythrinine (6)



8-oxo-erythrinine (7)

2、NMR spectroscopic data of dimeric erythrivarines C-D (1-2)

Figure S1. ^1H NMR spectrum of Erythrivarine C (1)



Expanded ¹H NMR spectrum of Erythrivarine C (1)

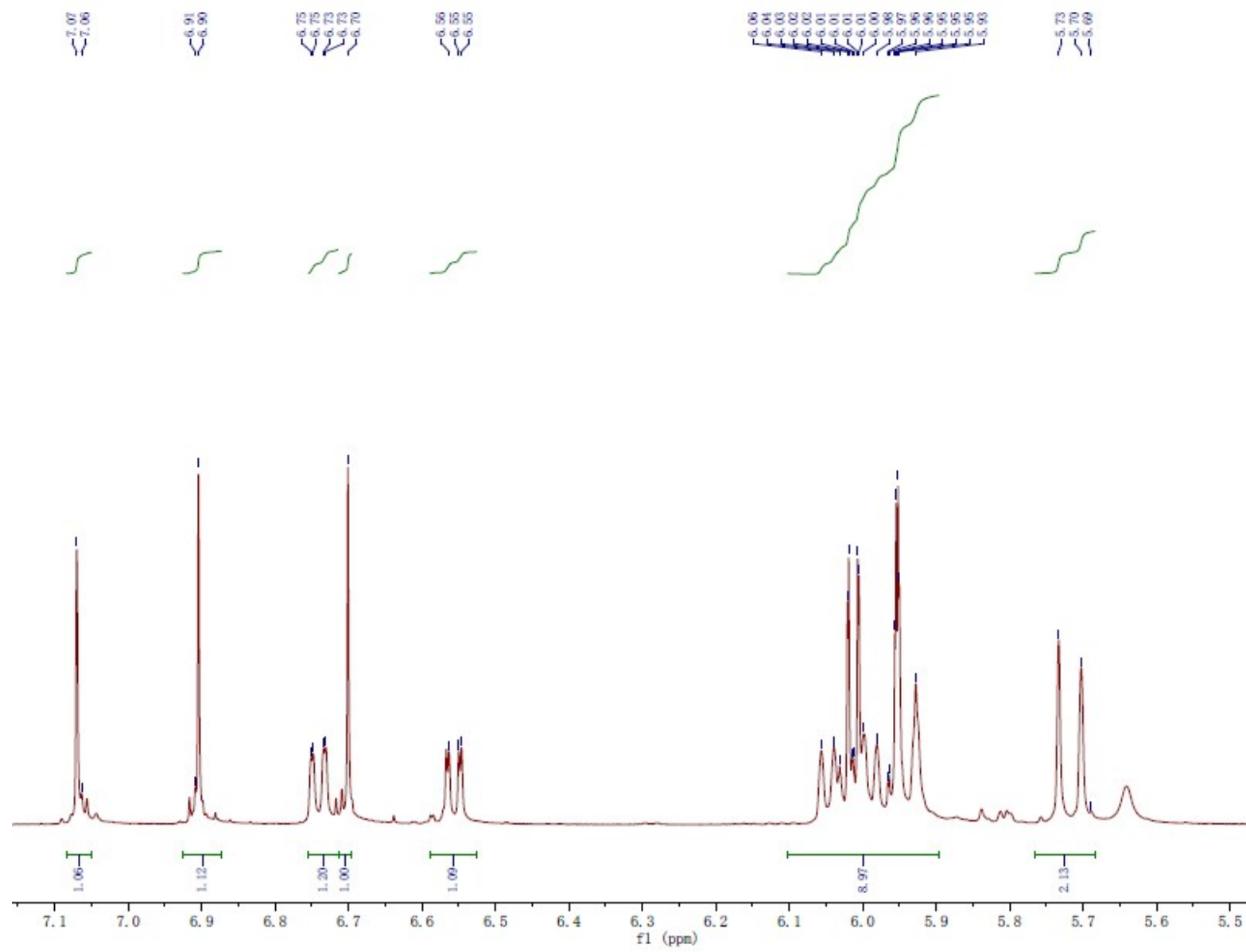


Figure S2. ^{13}C NMR spectrum of erythrivarine C (**1**)

wech49
d135 Acetone F:\ nmr 34

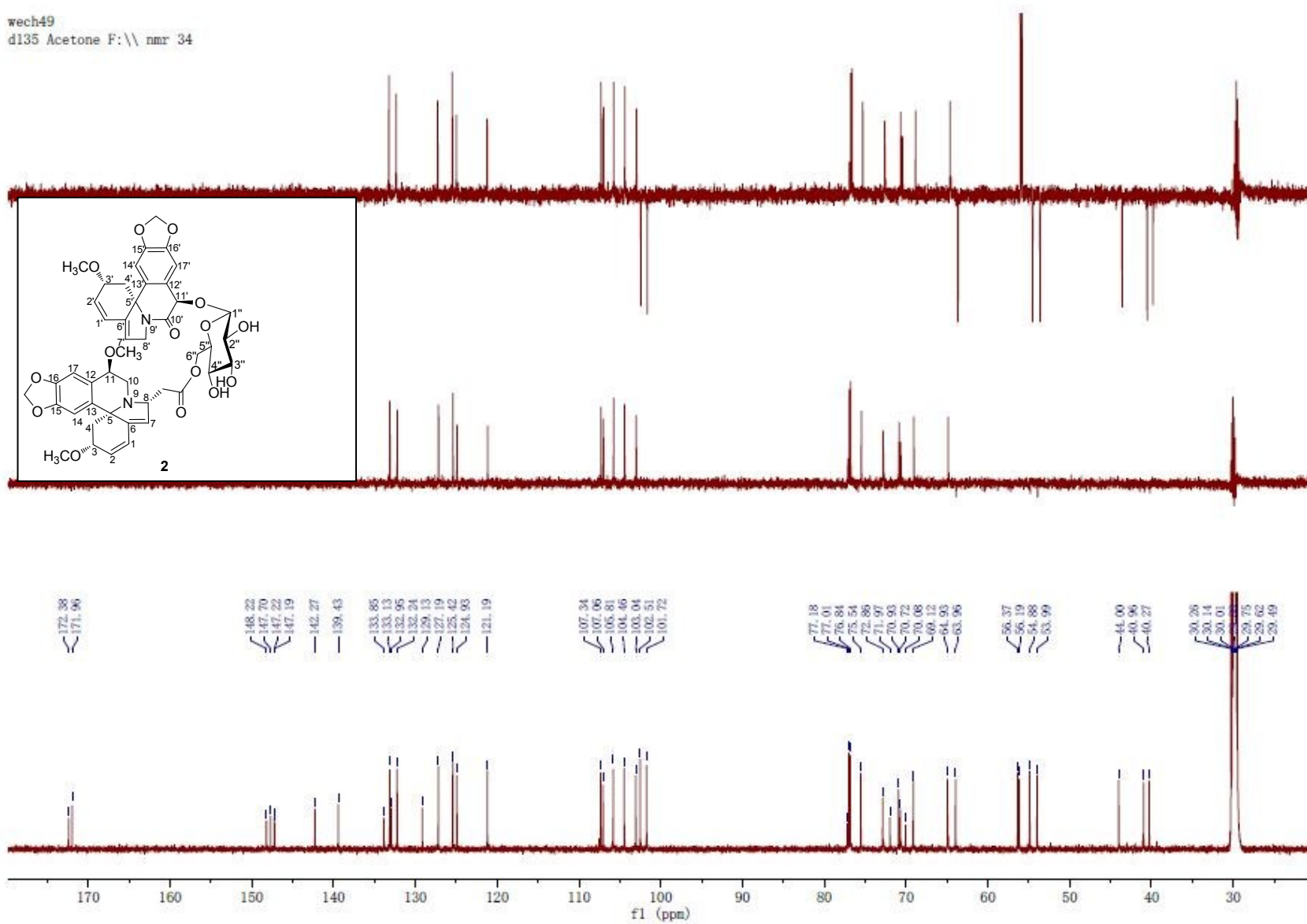
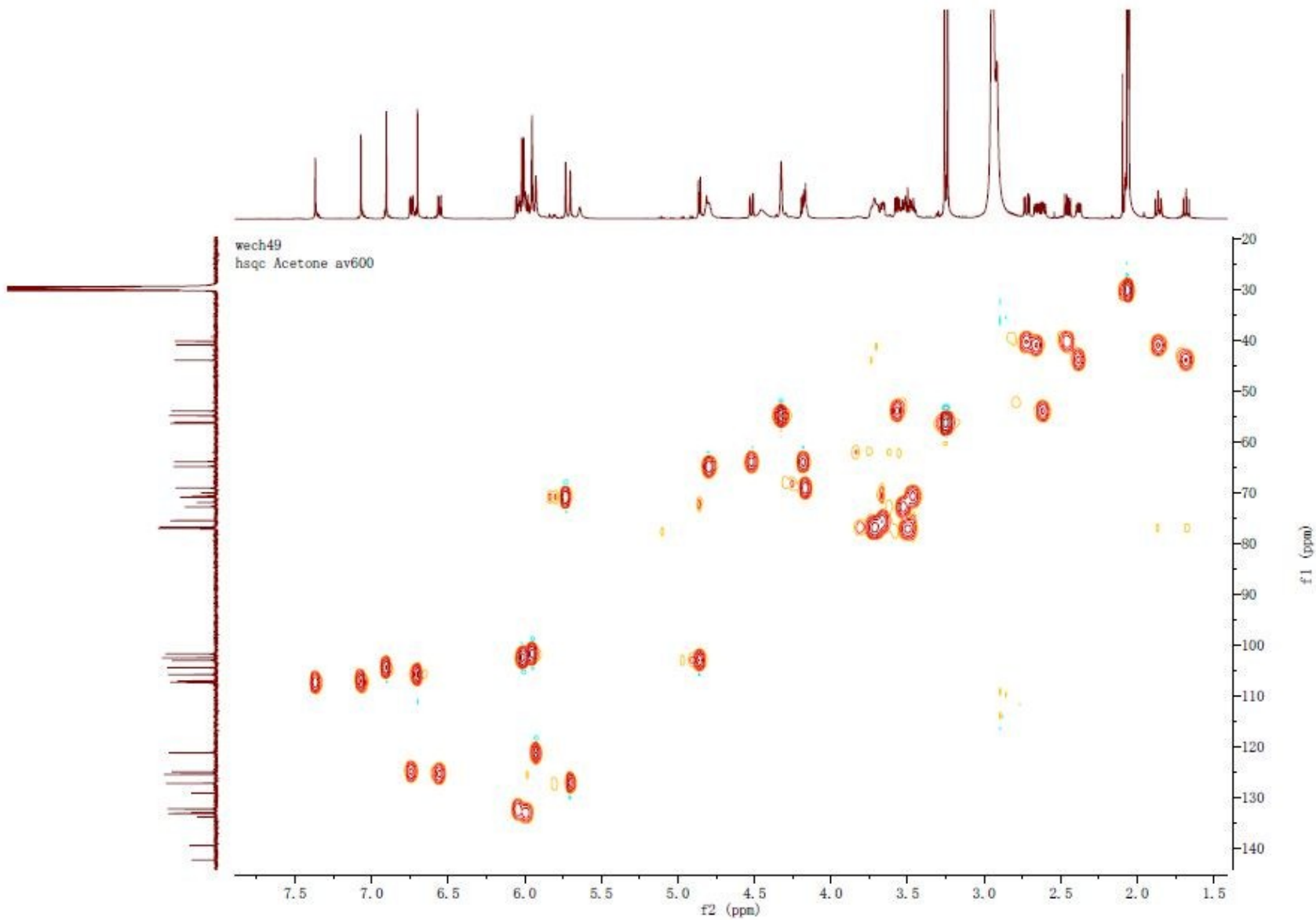


Figure S3. HSQC spectrum of erythrivarine C (**1**)



Expanded HSQC spectrum of erythrivarine C (1)

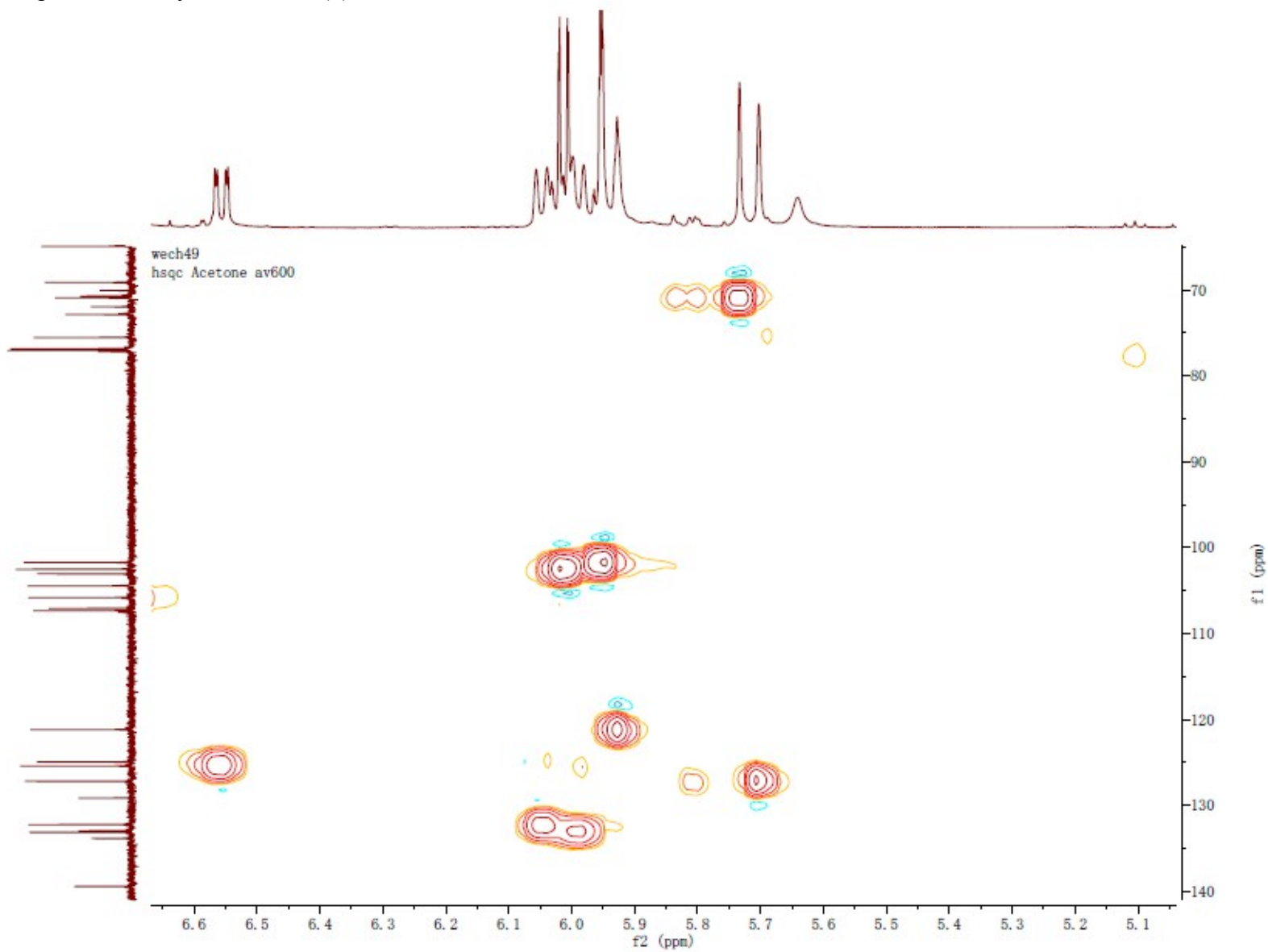


Figure S4. HMBC spectrum of erythrivarine C (**1**)

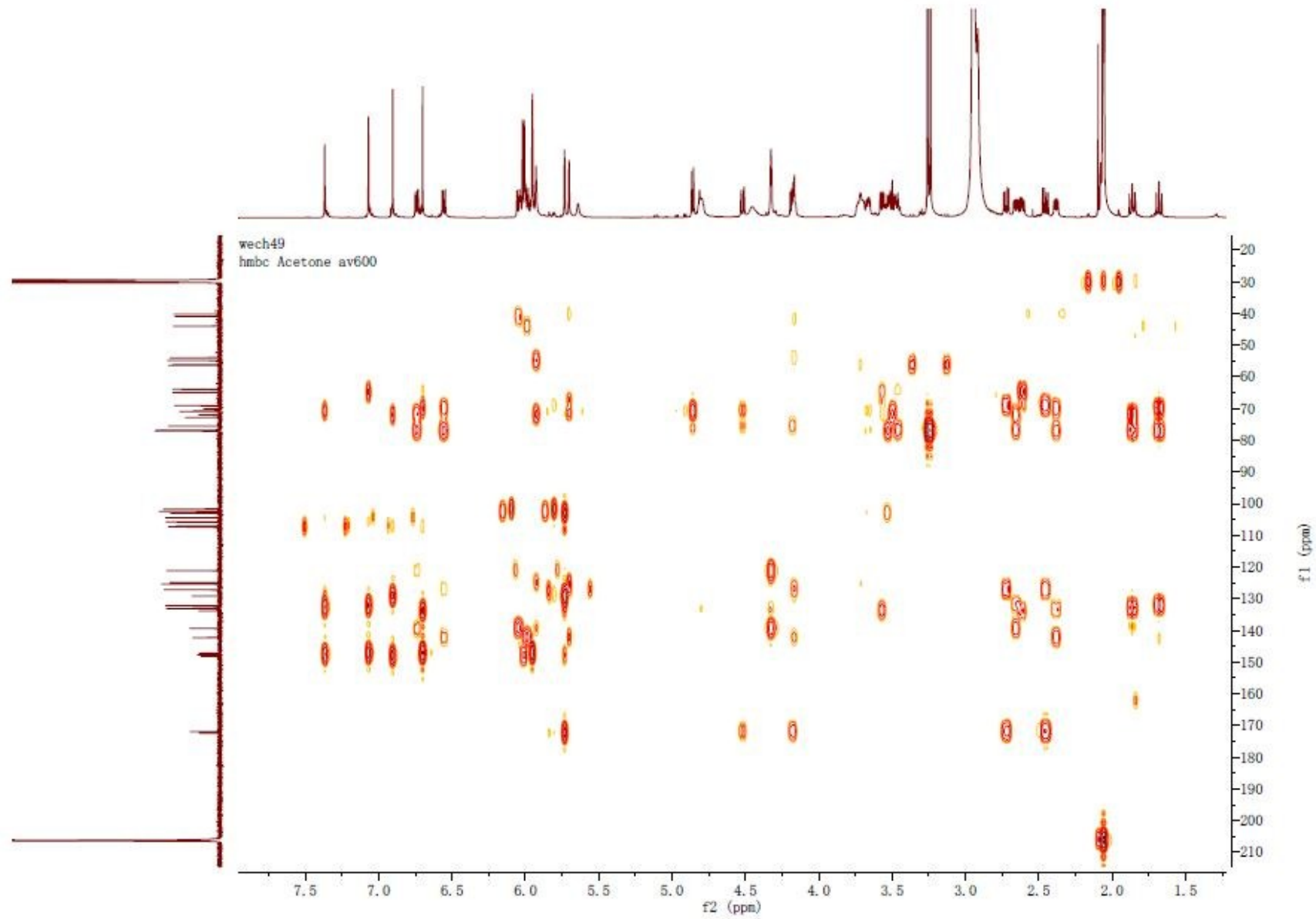


Figure S5. ^1H - ^1H COSY spectrum of erythrivarine C (**1**)

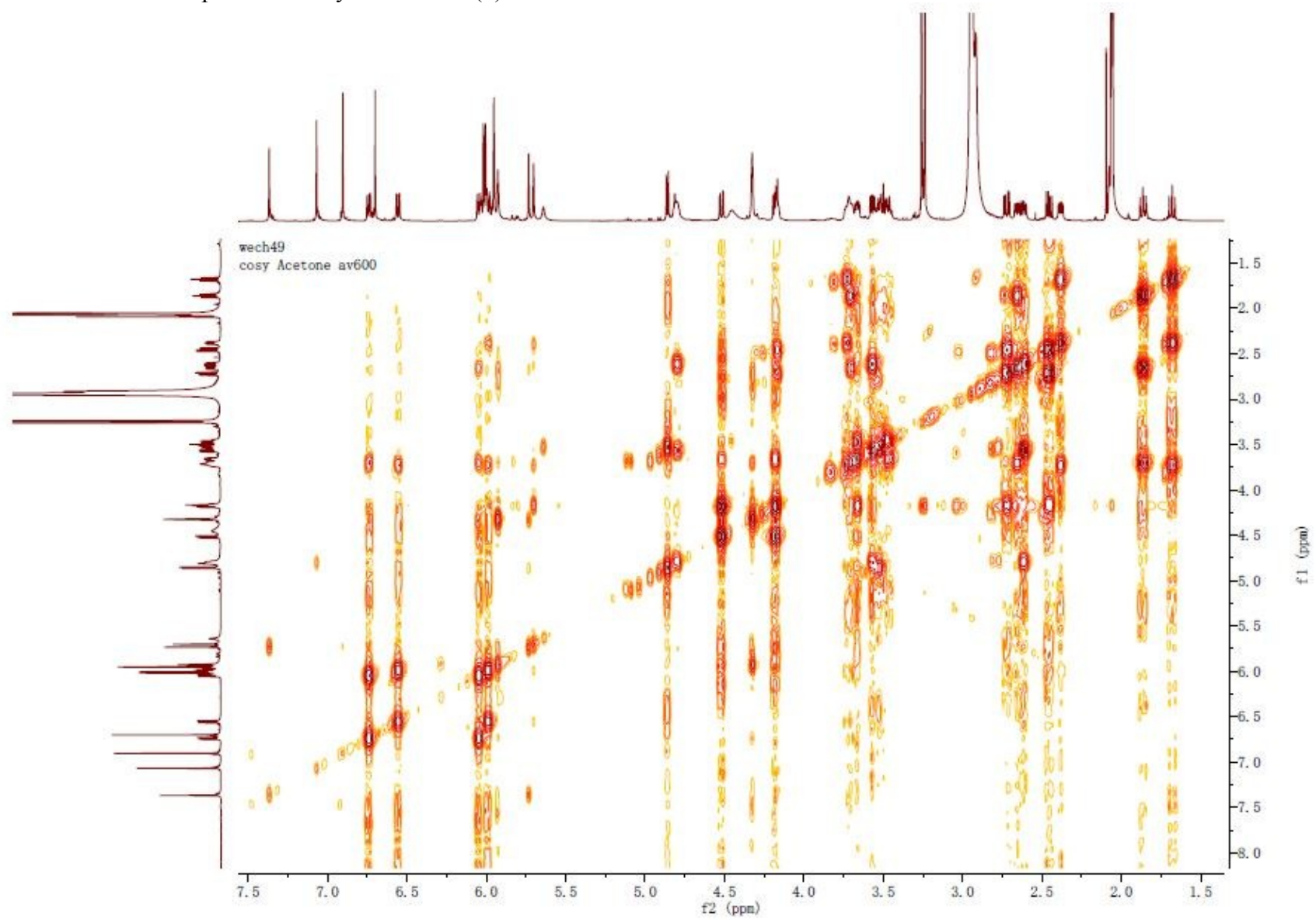


Figure S6. ROESY spectrum of erythrivarine C (**1**)

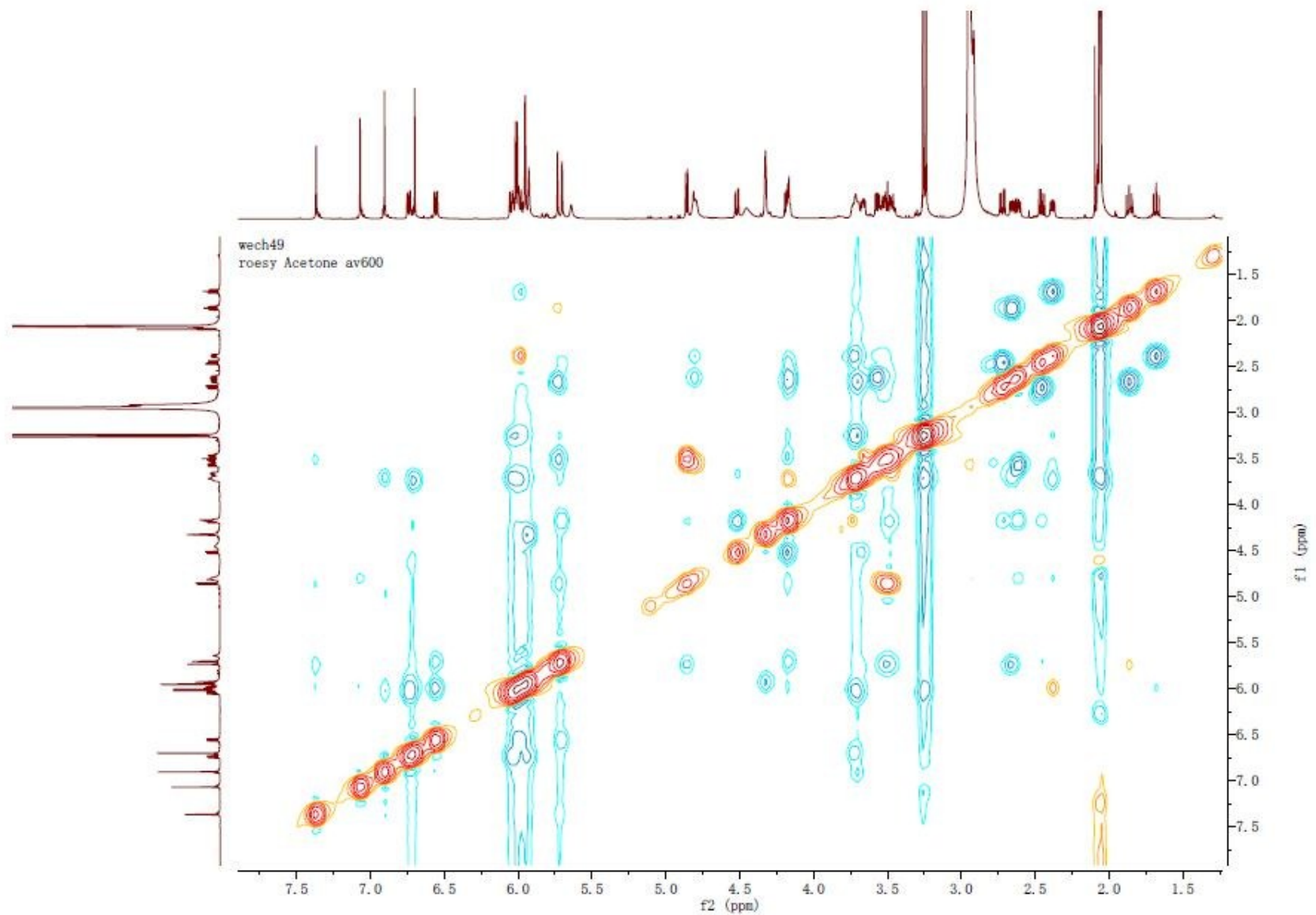


Figure S7. ¹H NMR spectrum of erythrivarine D (2)

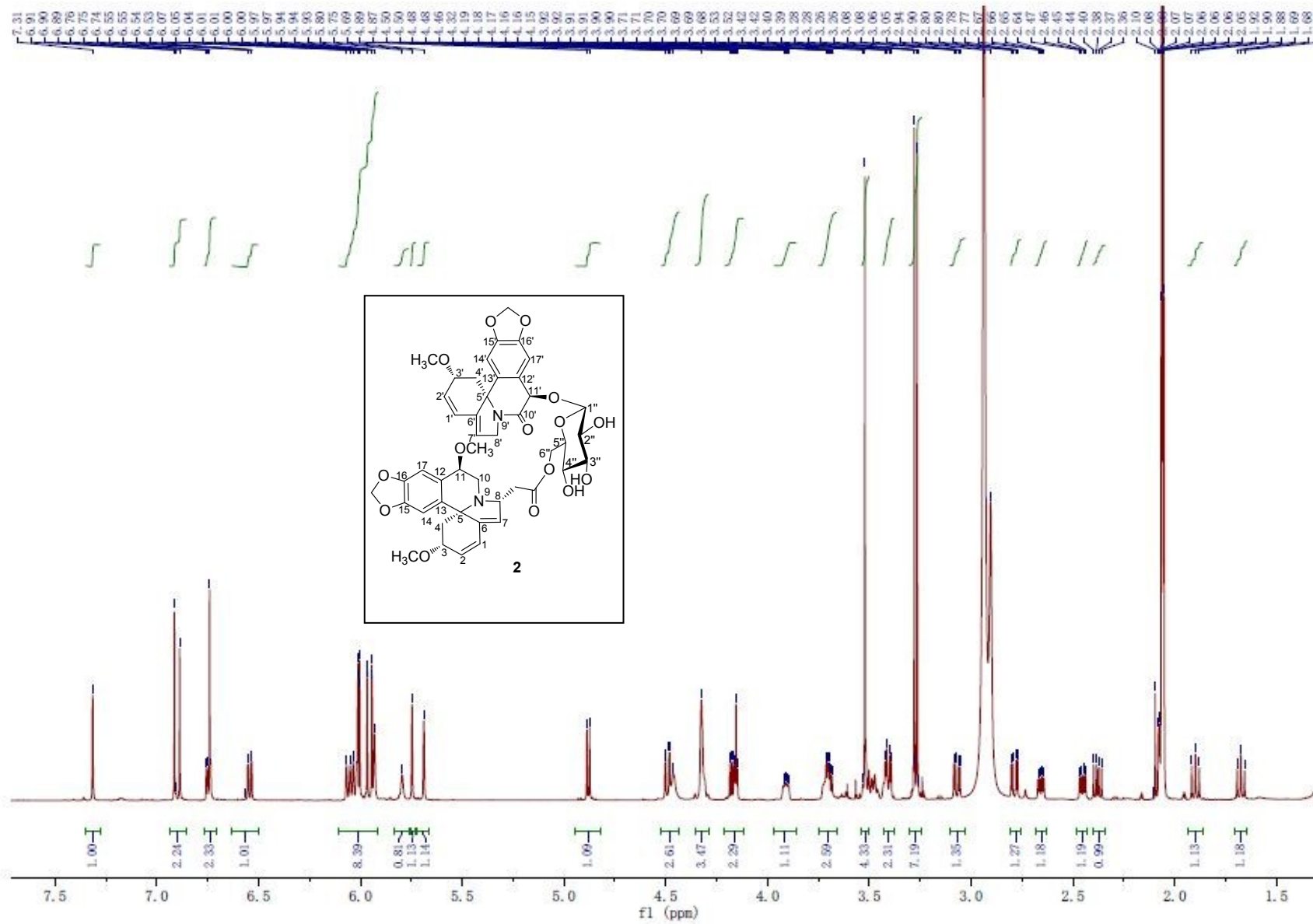


Figure S8. ^{13}C NMR spectrum of erythrivarine D (**2**)

wech51

d135 Acetone F:\ nmr 57

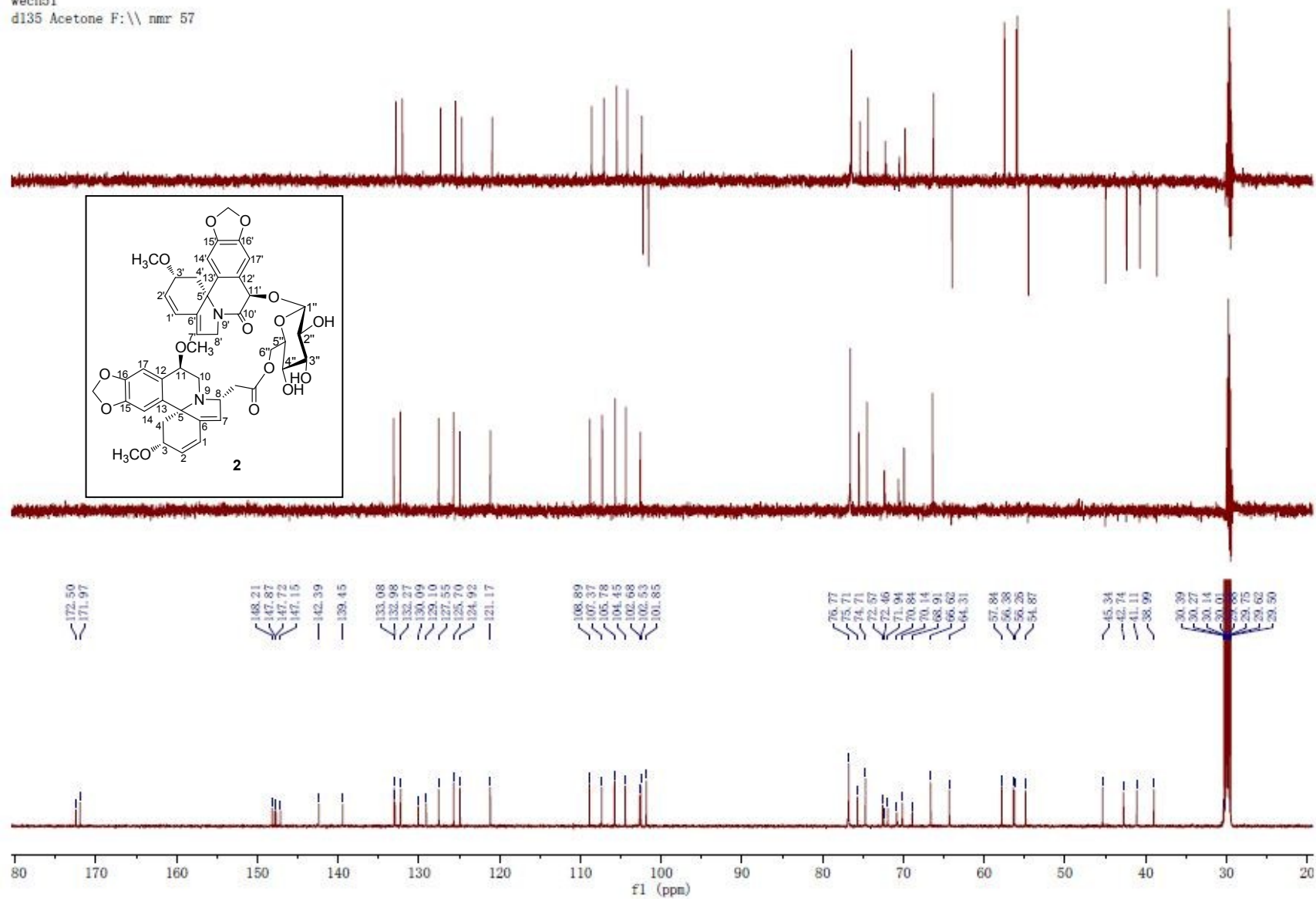


Figure S9. HSQC spectrum of erythrivarine D (2)

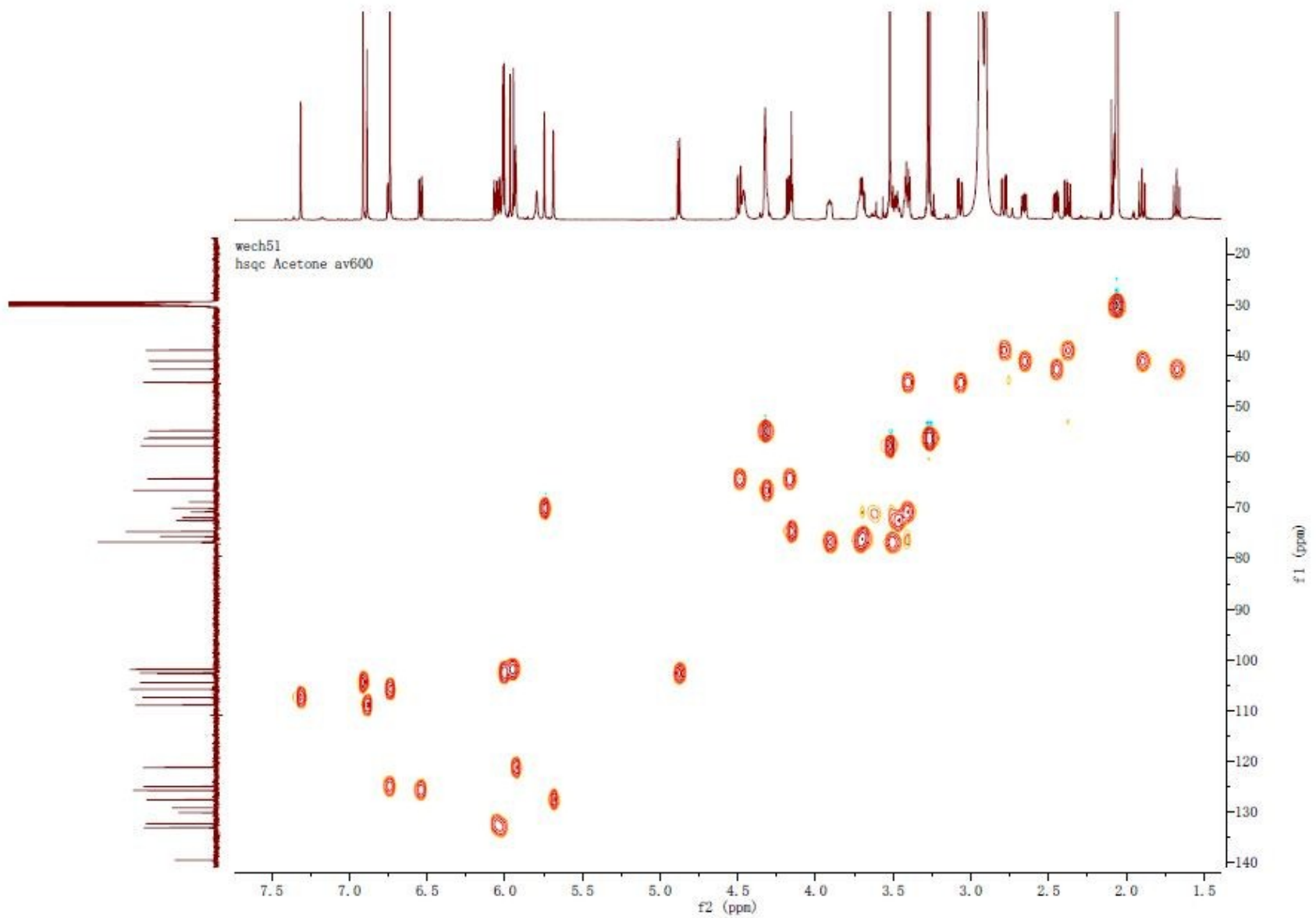


Figure S10. HMBC spectrum of erythrivarine D (2)

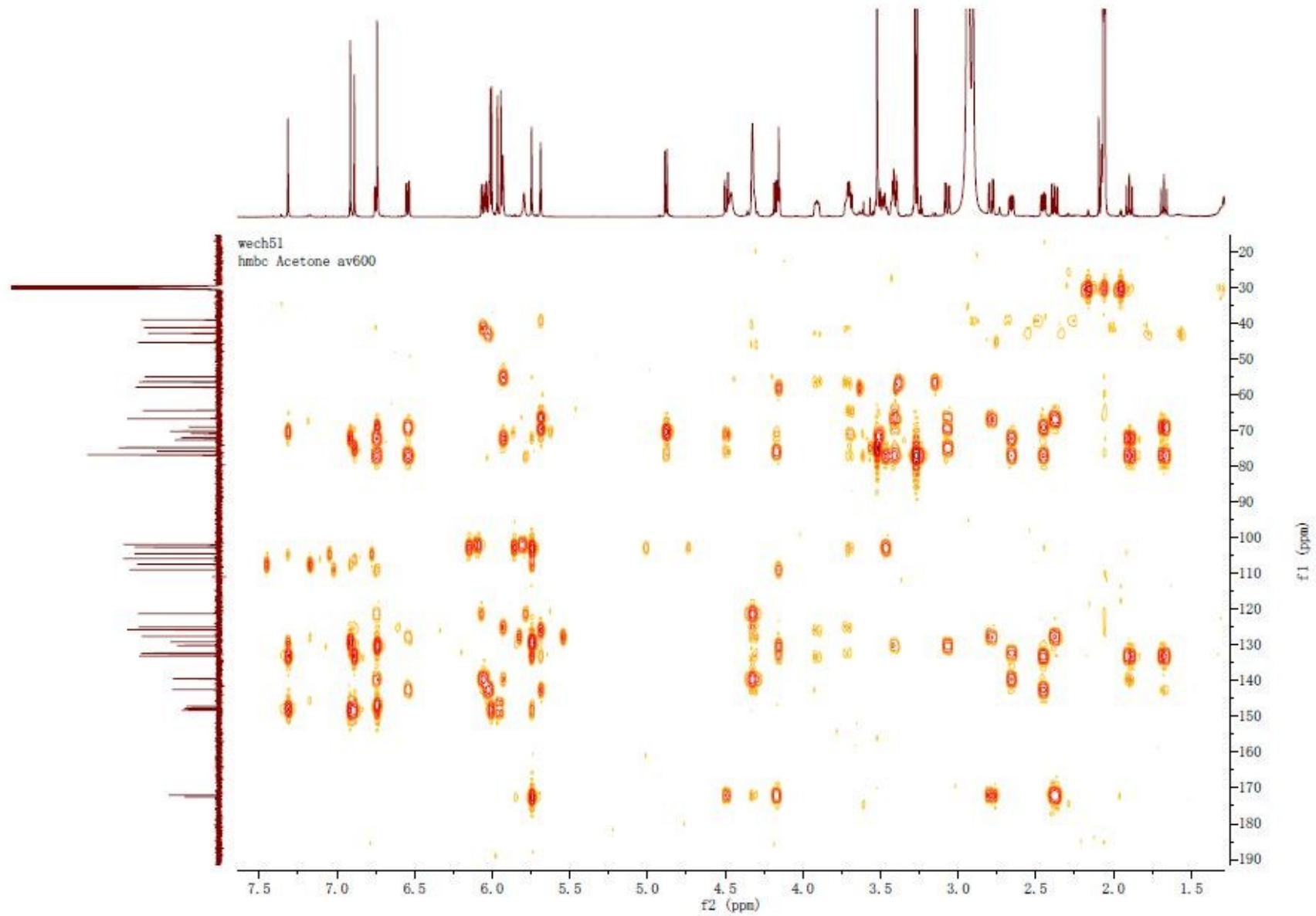


Figure S11. ^1H - ^1H COSY spectrum of erythrivarine D (2)

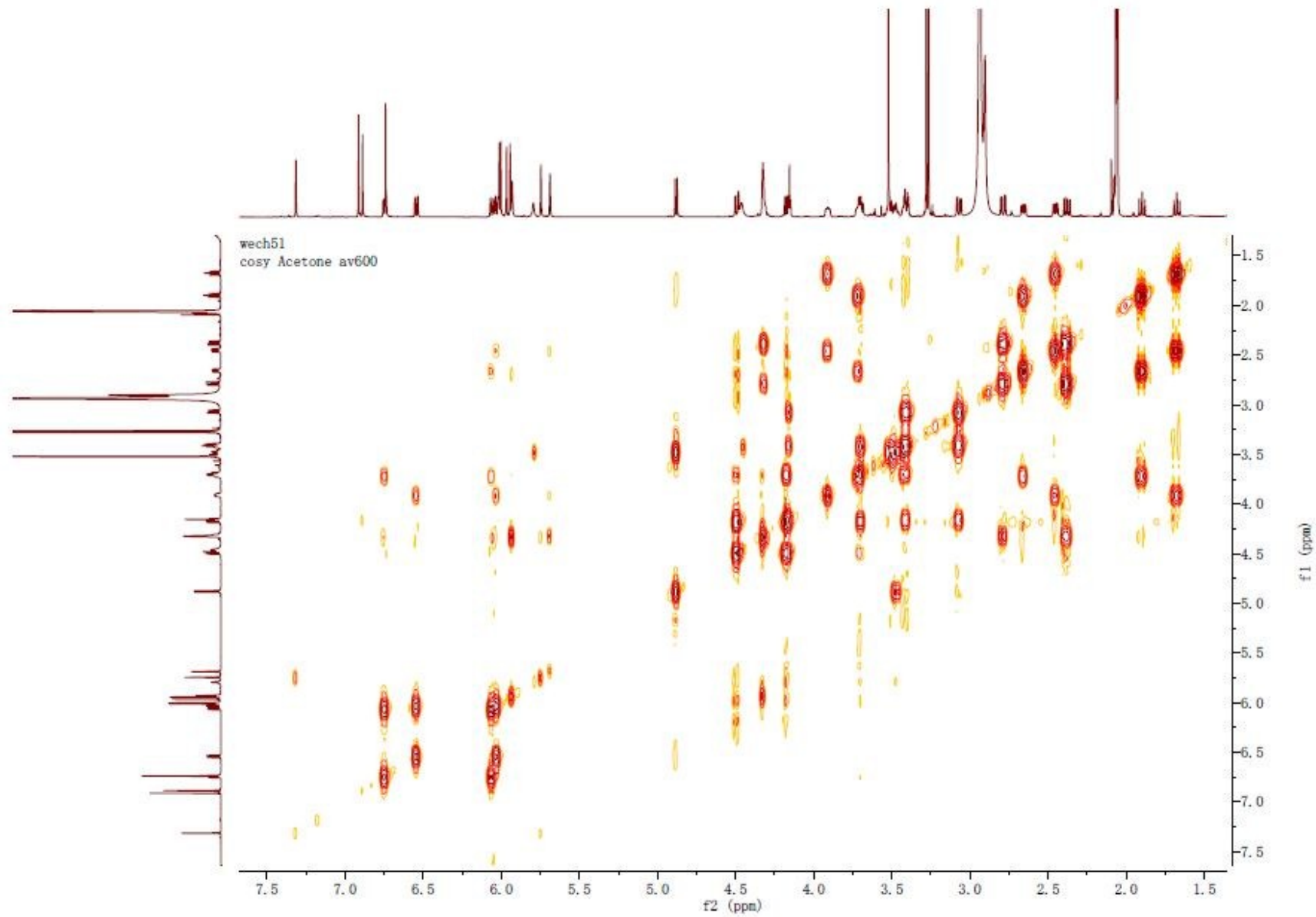
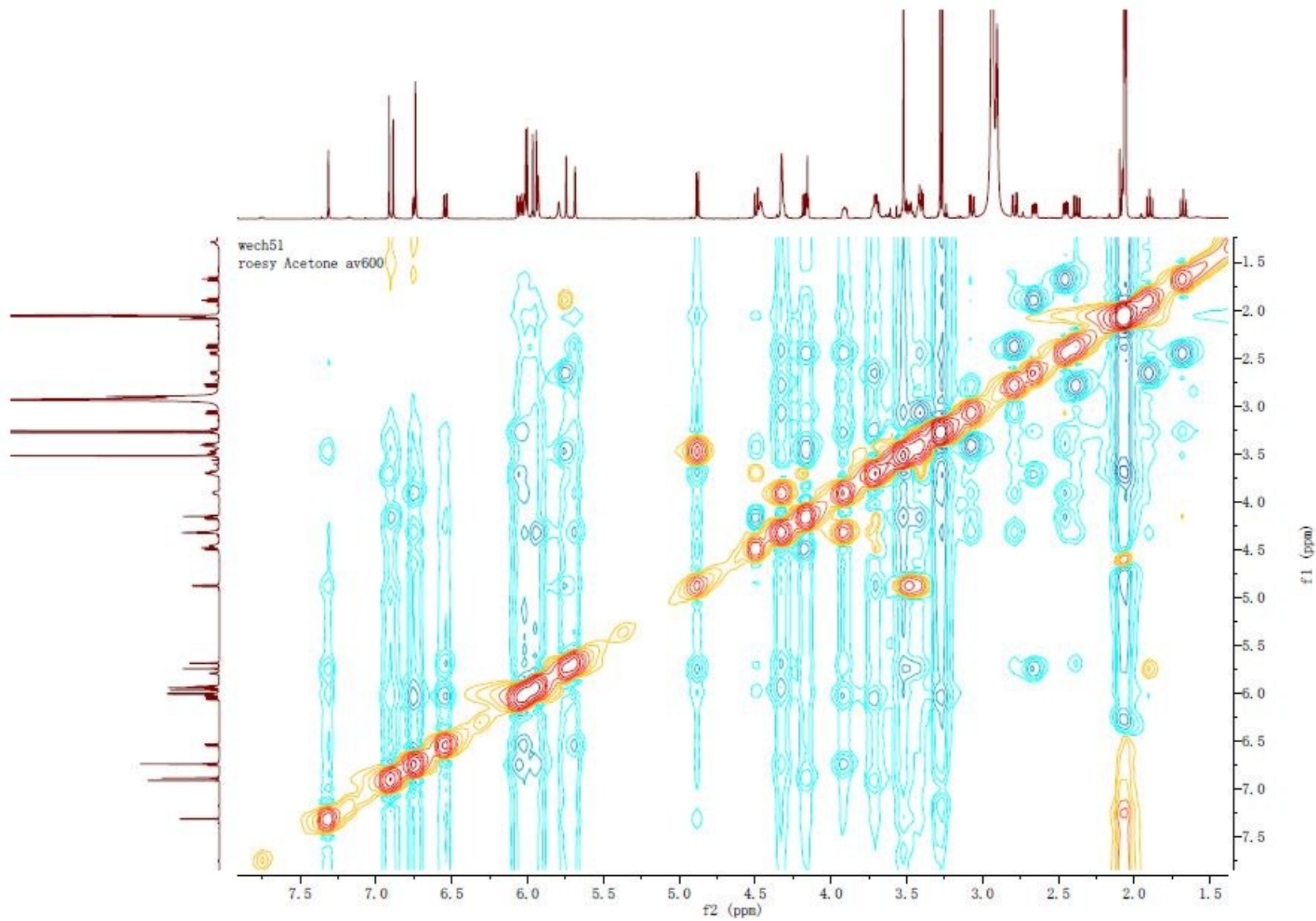
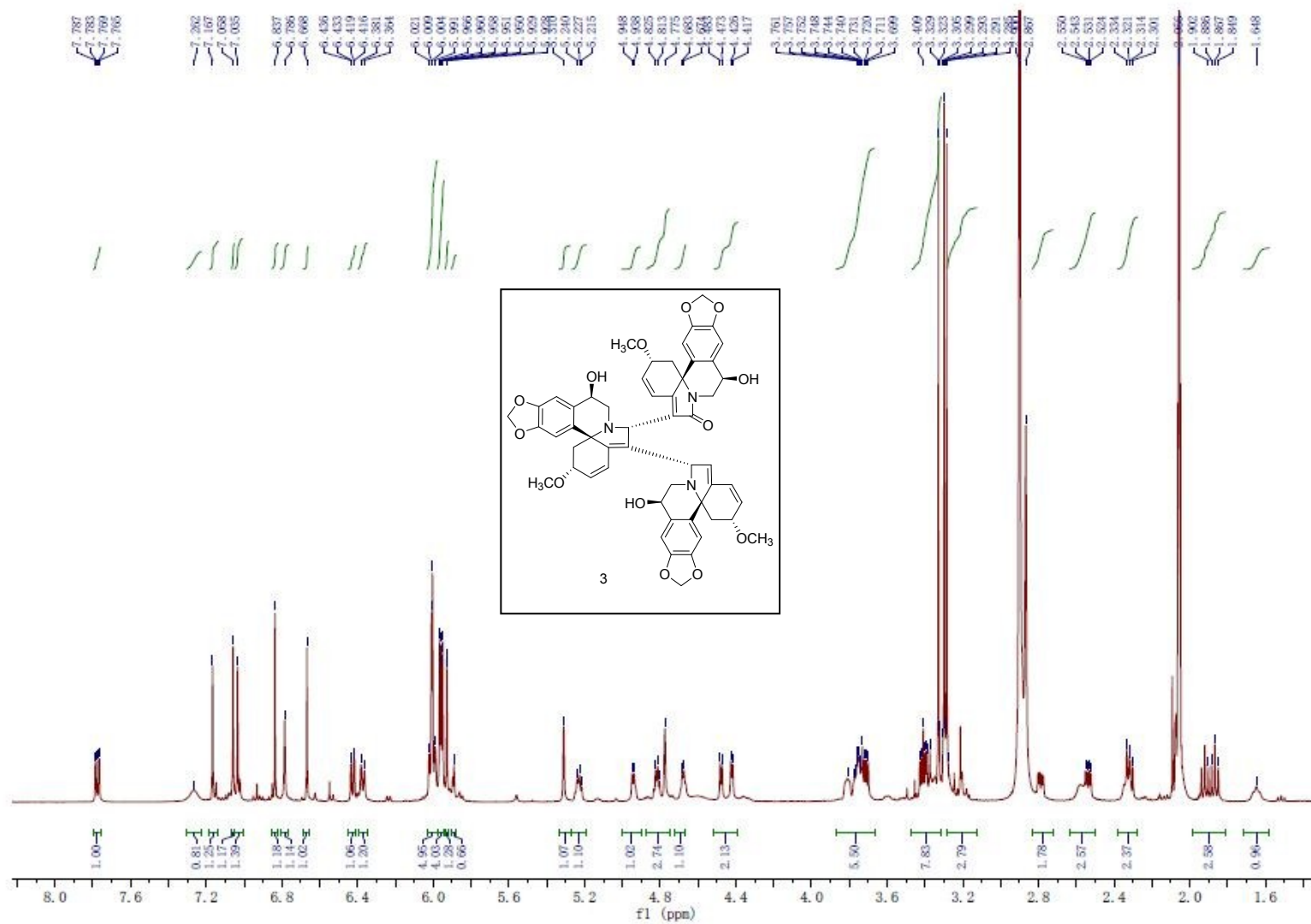


Figure S12. ROESY spectrum of erythrivarine D (2)



3、NMR spectroscopic data of trimeric erythrivarines F-G (3-5)

Figure S13. ¹H NMR spectrum of erythrivarine E (3)



Expanded ^1H NMR spectrum of erythrivarine E (3)

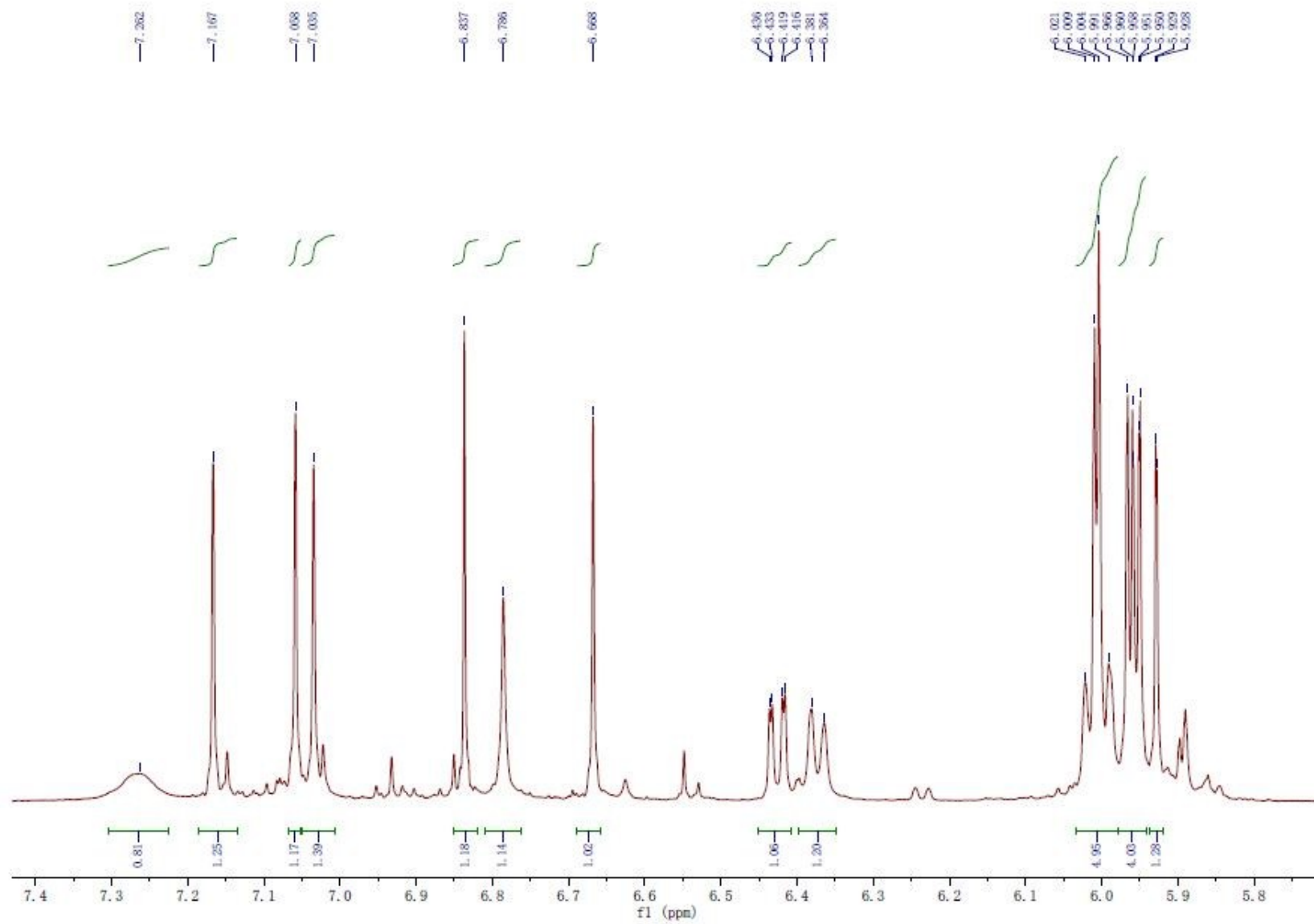


Figure S14. ^{13}C NMR spectrum of erythrivarine E (3)

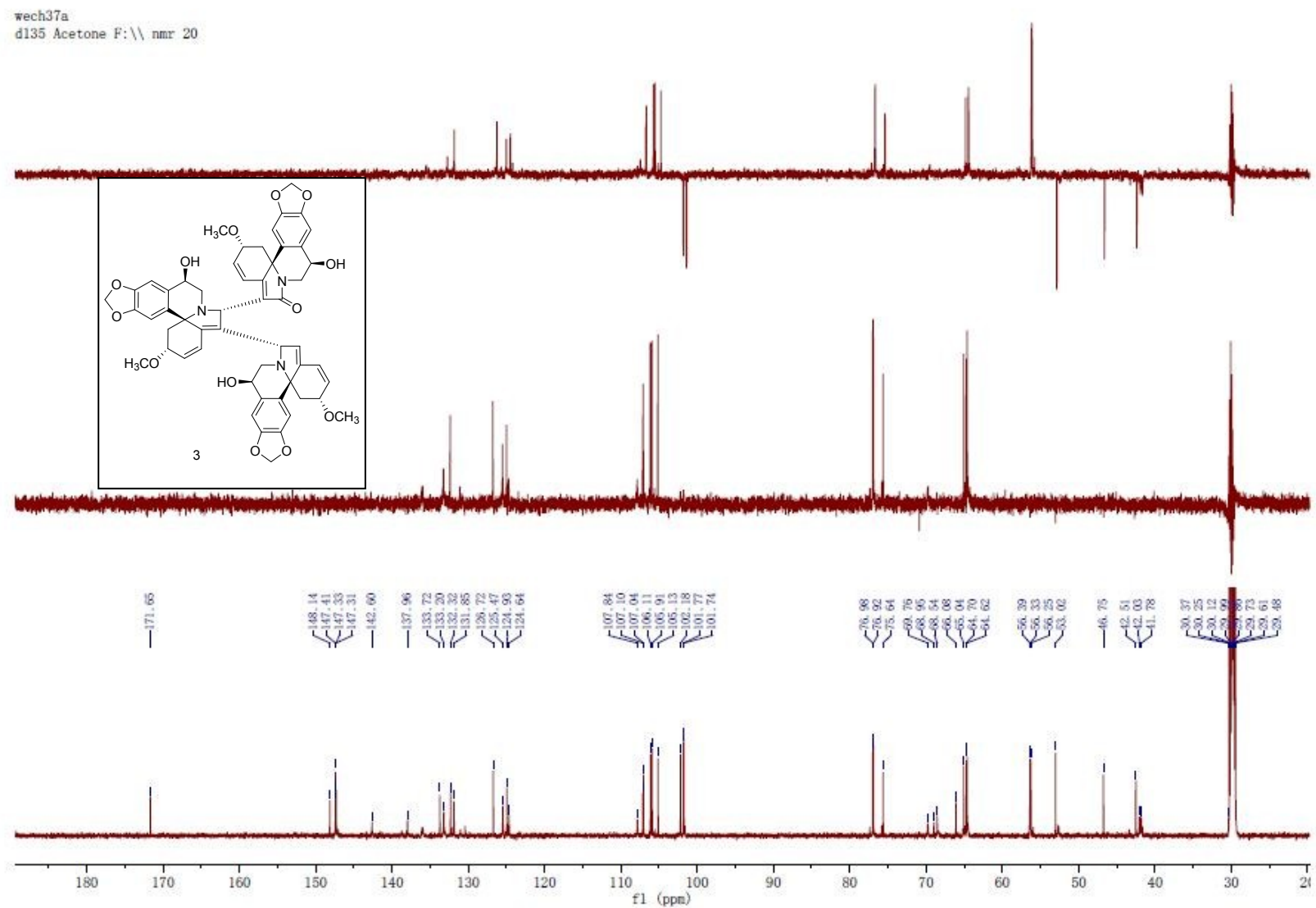
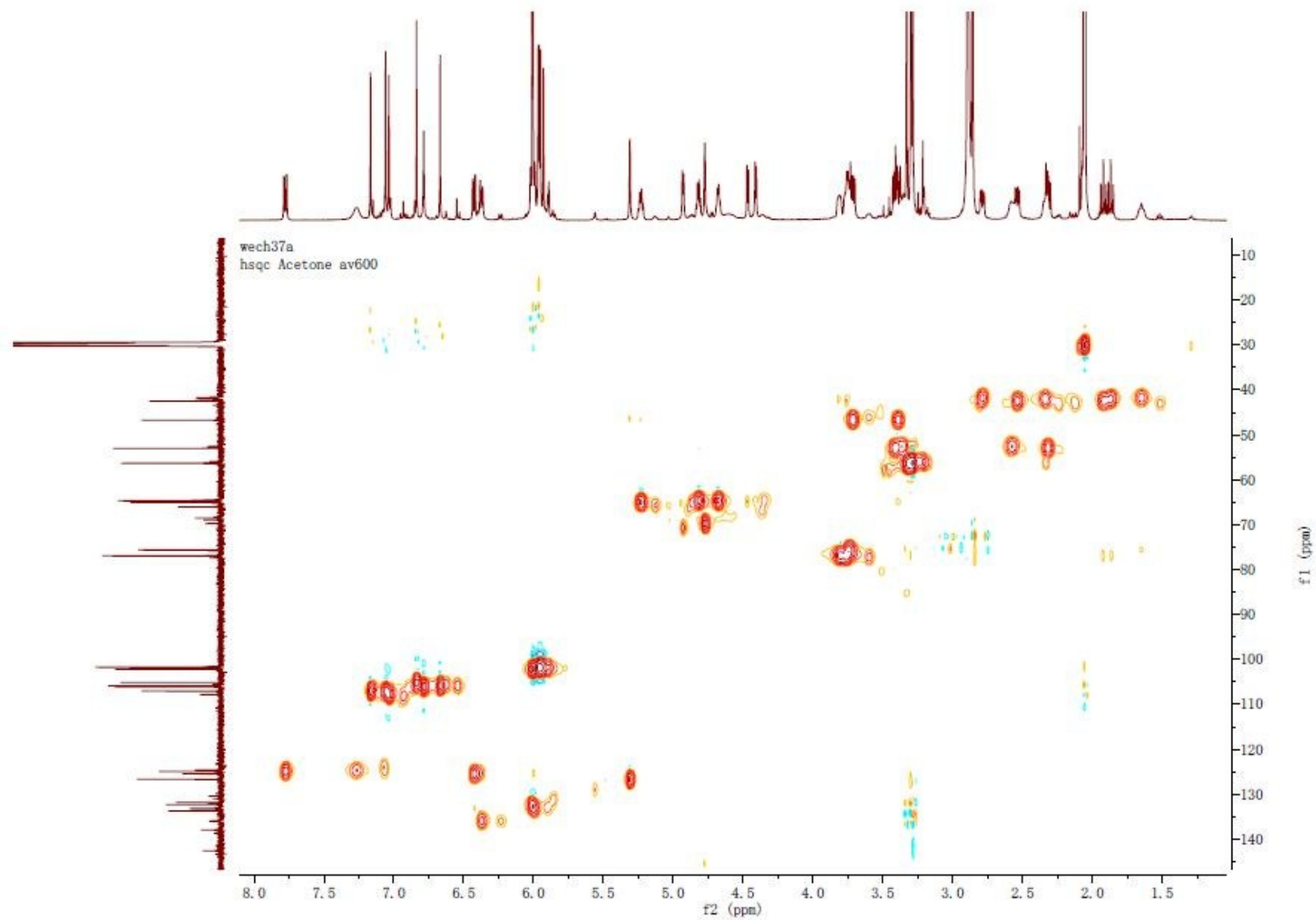


Figure S15. HSQC spectrum of erythrivarine E (**3**)



Expanded HSQC spectrum of erythrivarine E (3)

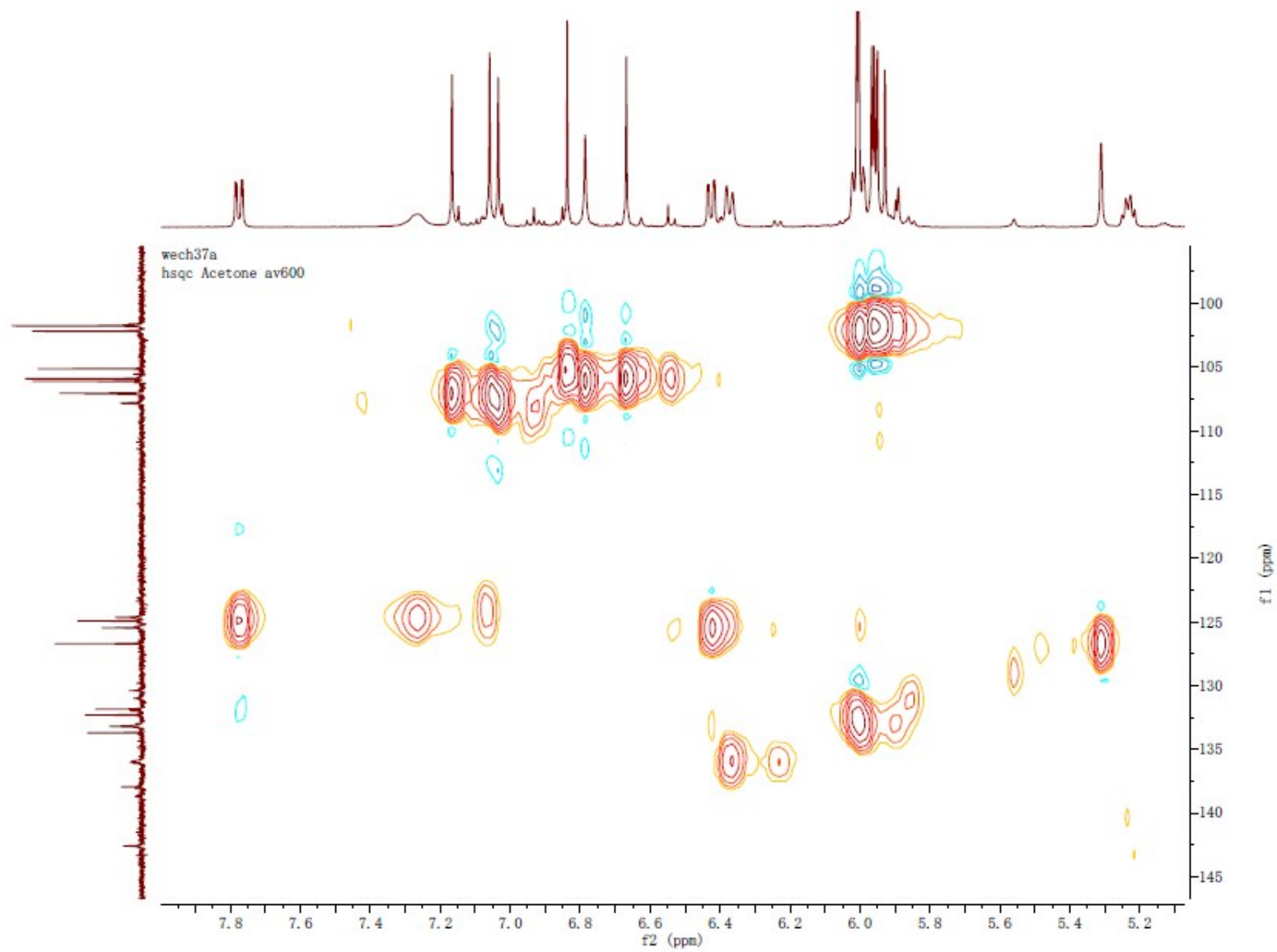


Figure S16. HMBC spectrum of erythrivarine E (**3**)

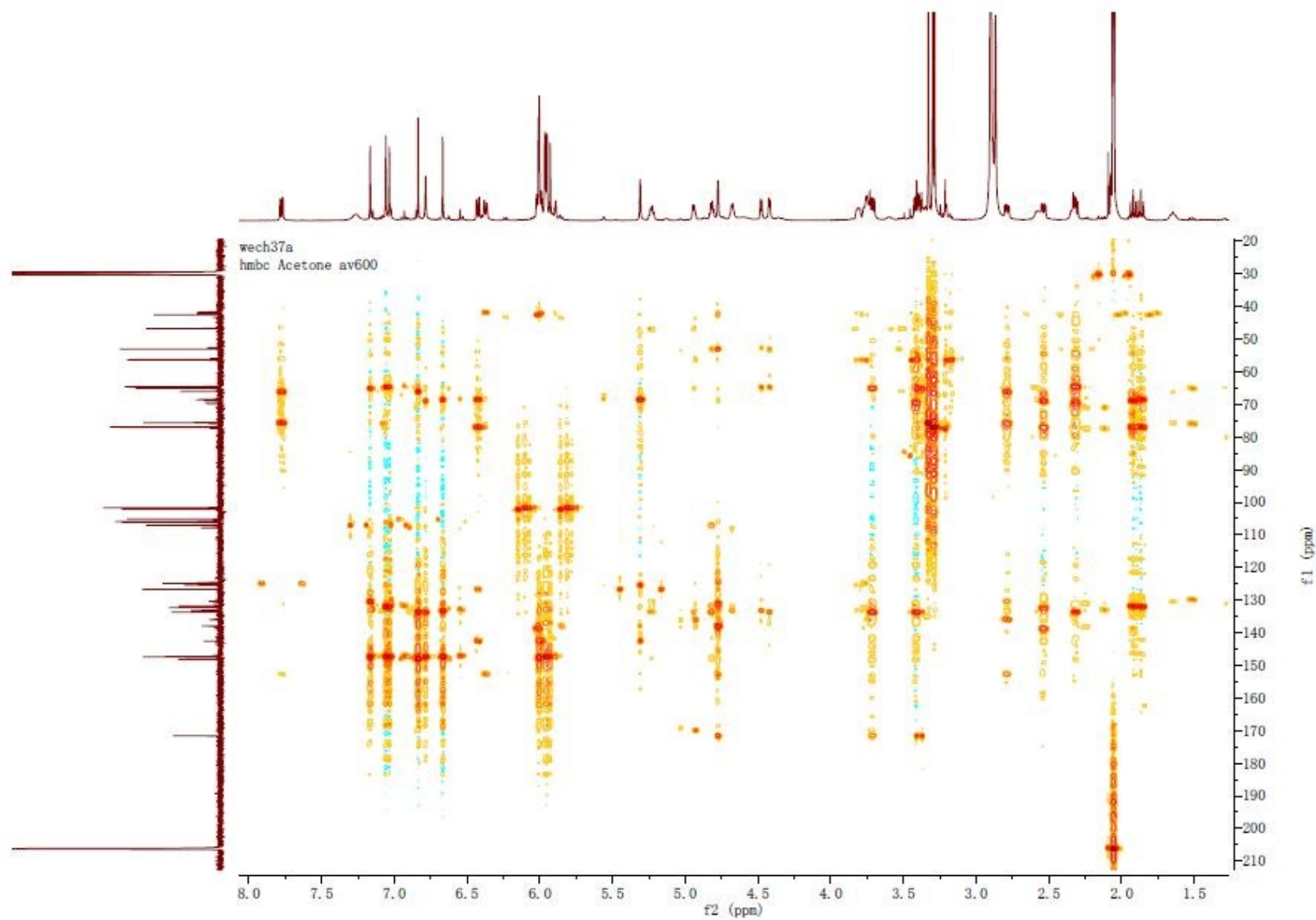


Figure S17. ROESY spectrum of erythrivarine E (**3**)

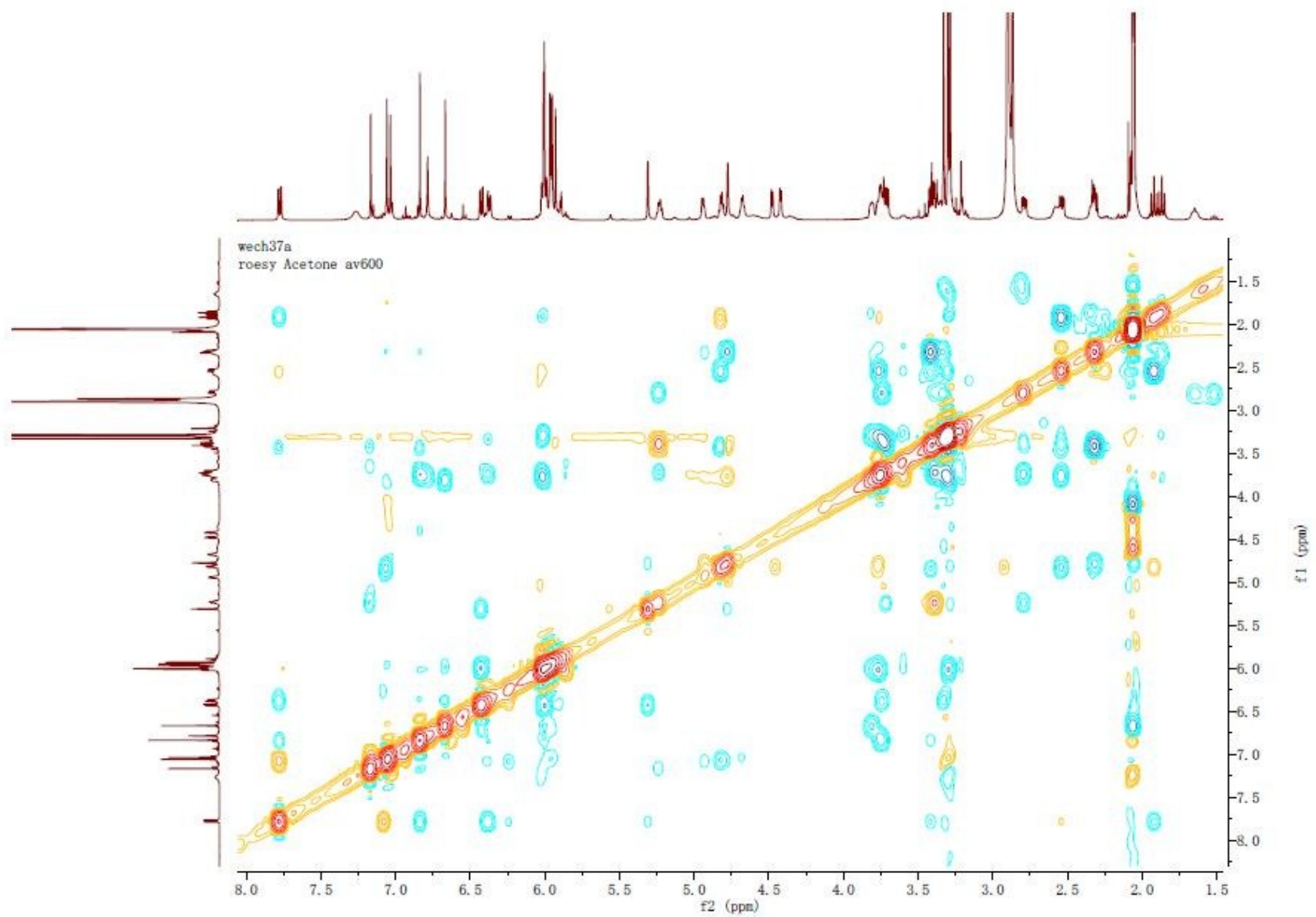
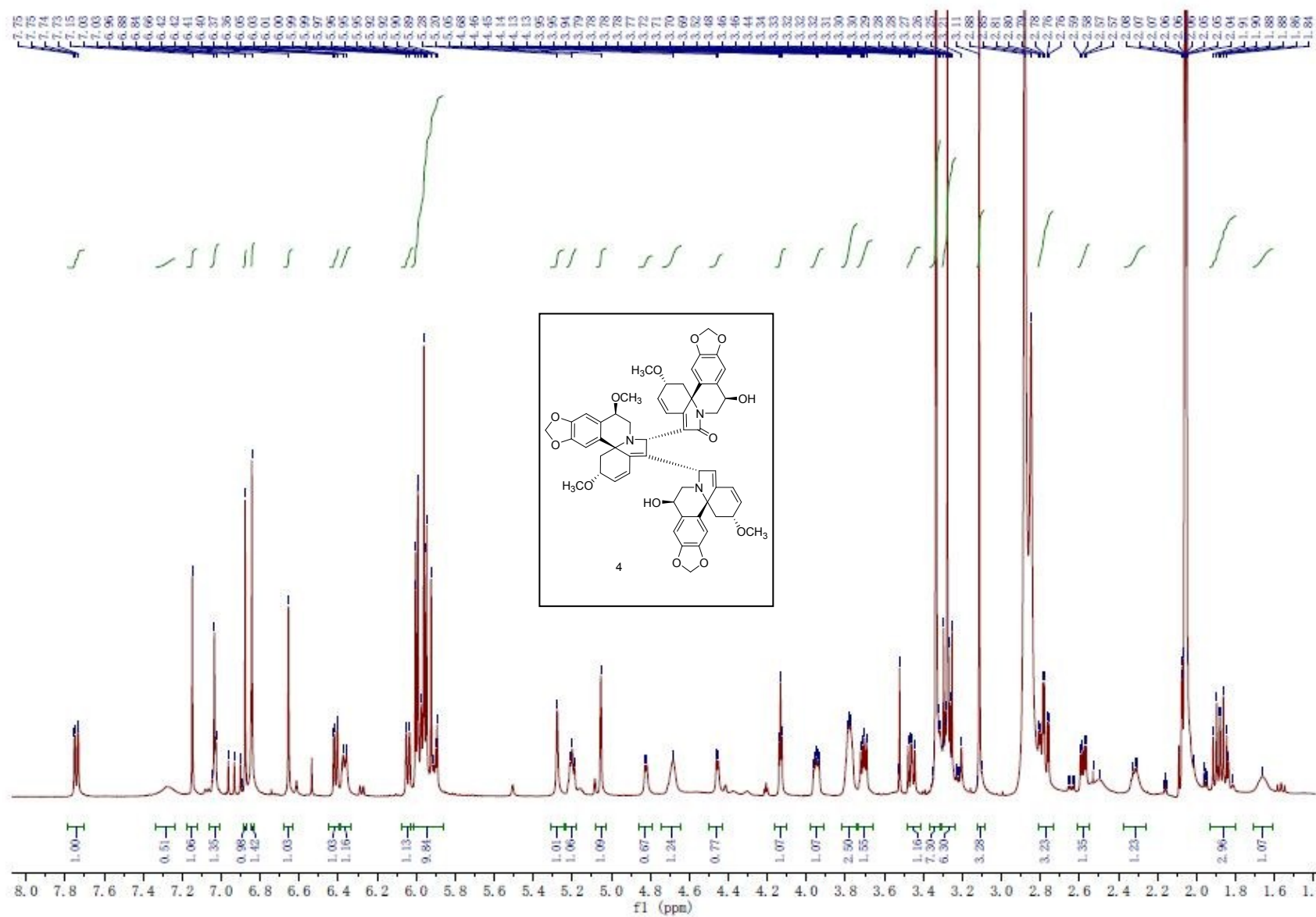


Figure S18. ¹H NMR spectrum of erythrivarine F (4)



Expanded ^1H NMR spectrum of erythrivarine F (4)

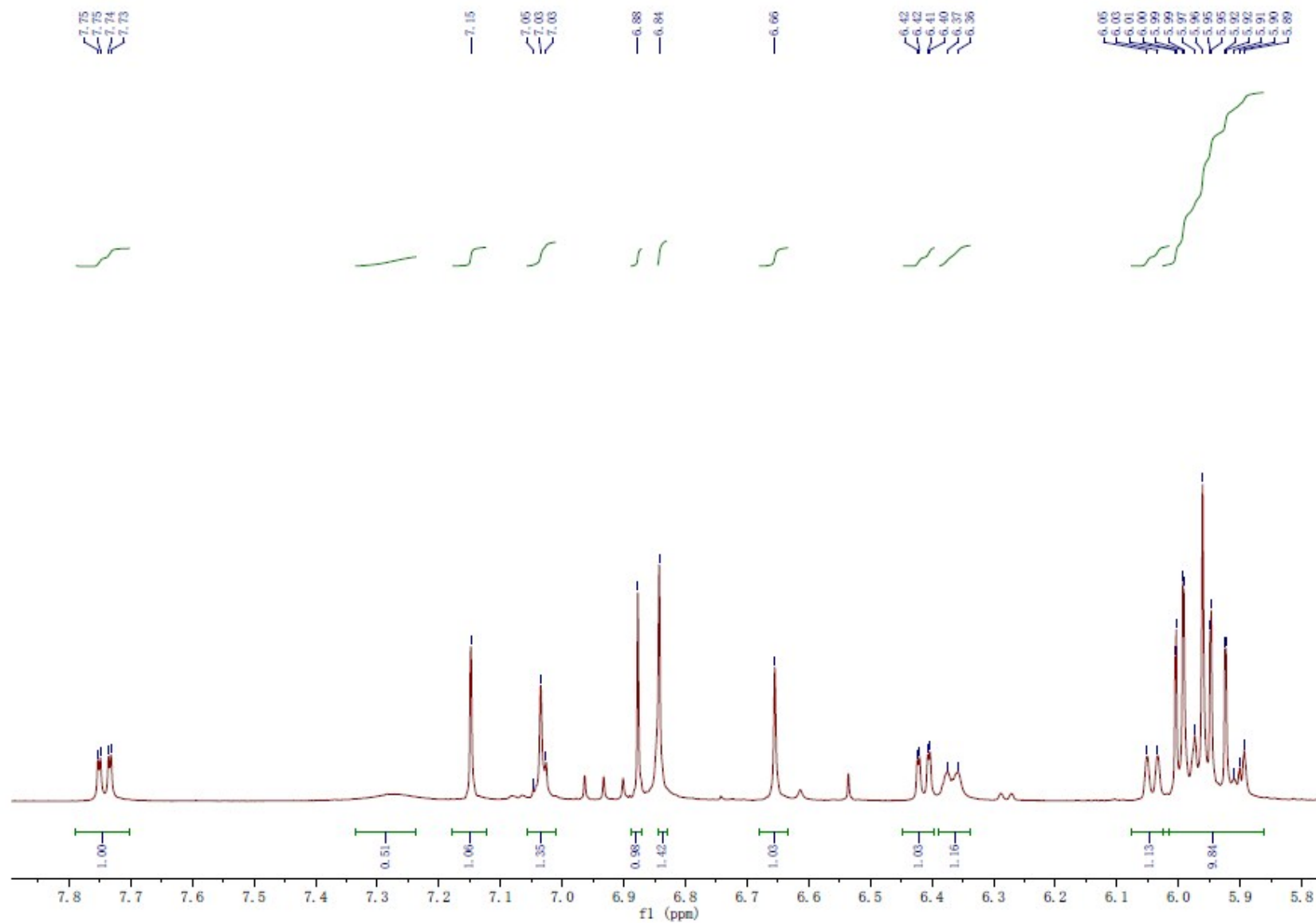


Figure S19. ¹³C NMR spectrum of erythrivarine F (4)

wech43

d135 Acetone F:\ nmr 25

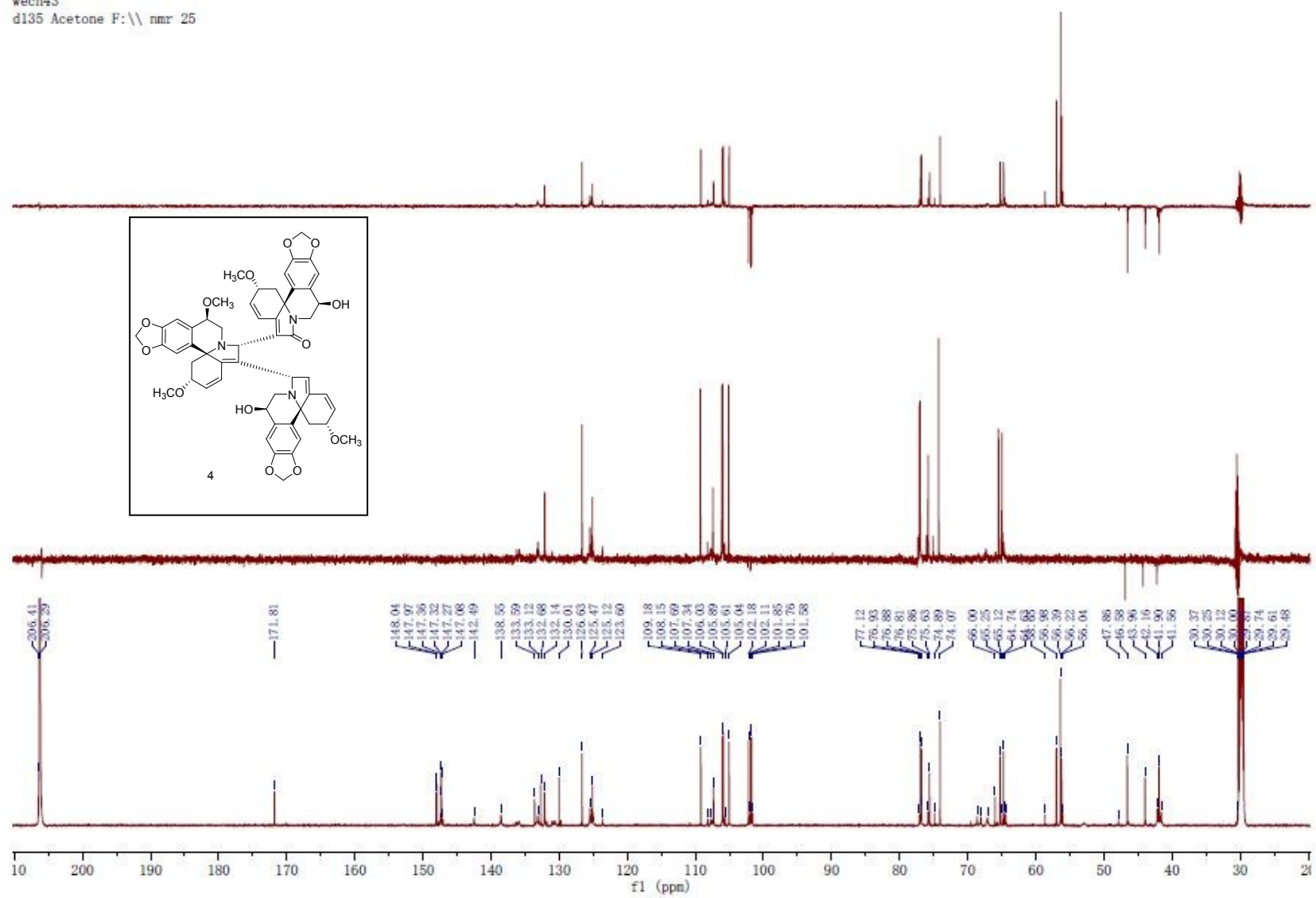
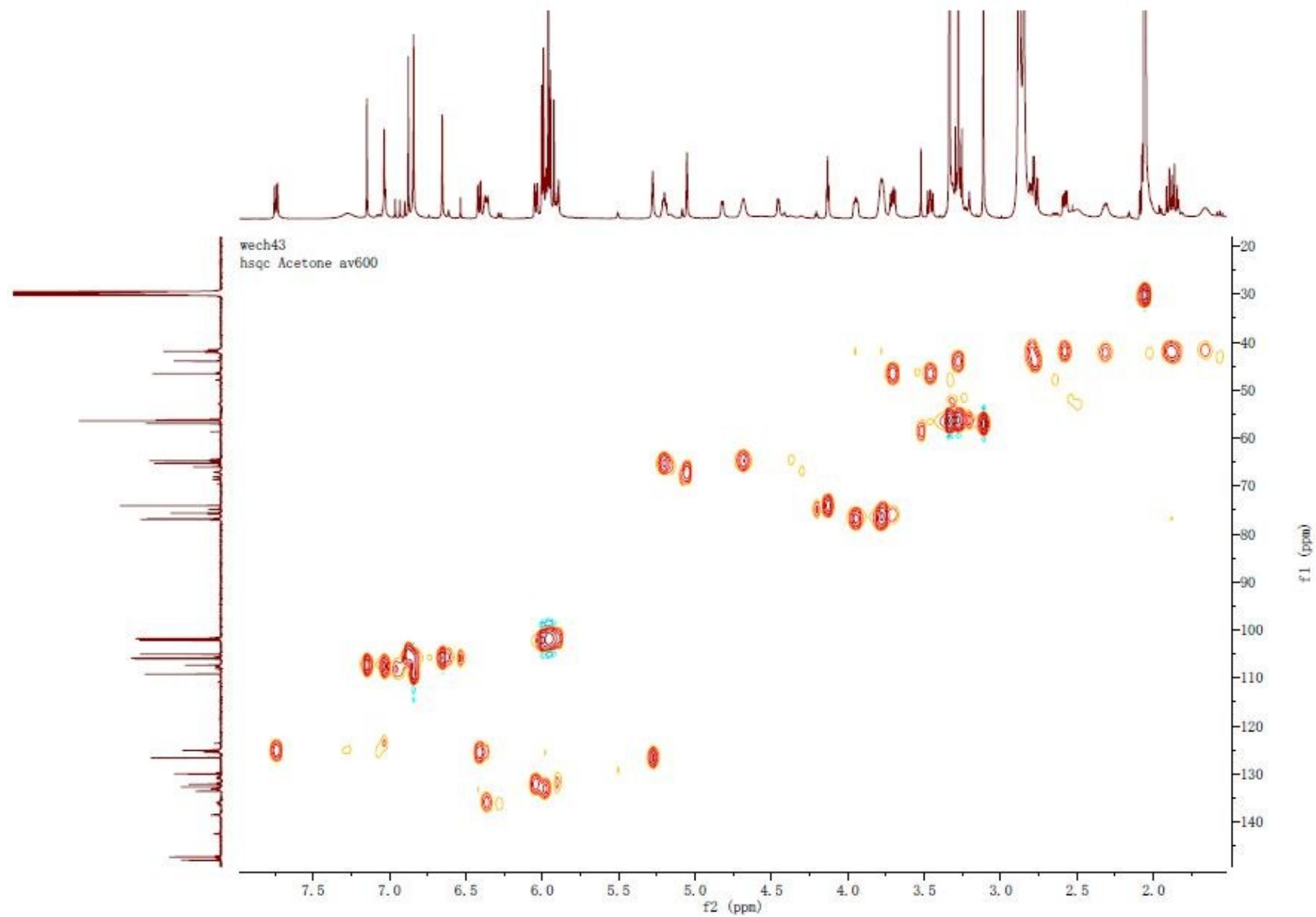


Figure S20. HSQC spectrum of erythrivarine F (4)



Expanded HSQC spectrum of erythrivarine F (4)

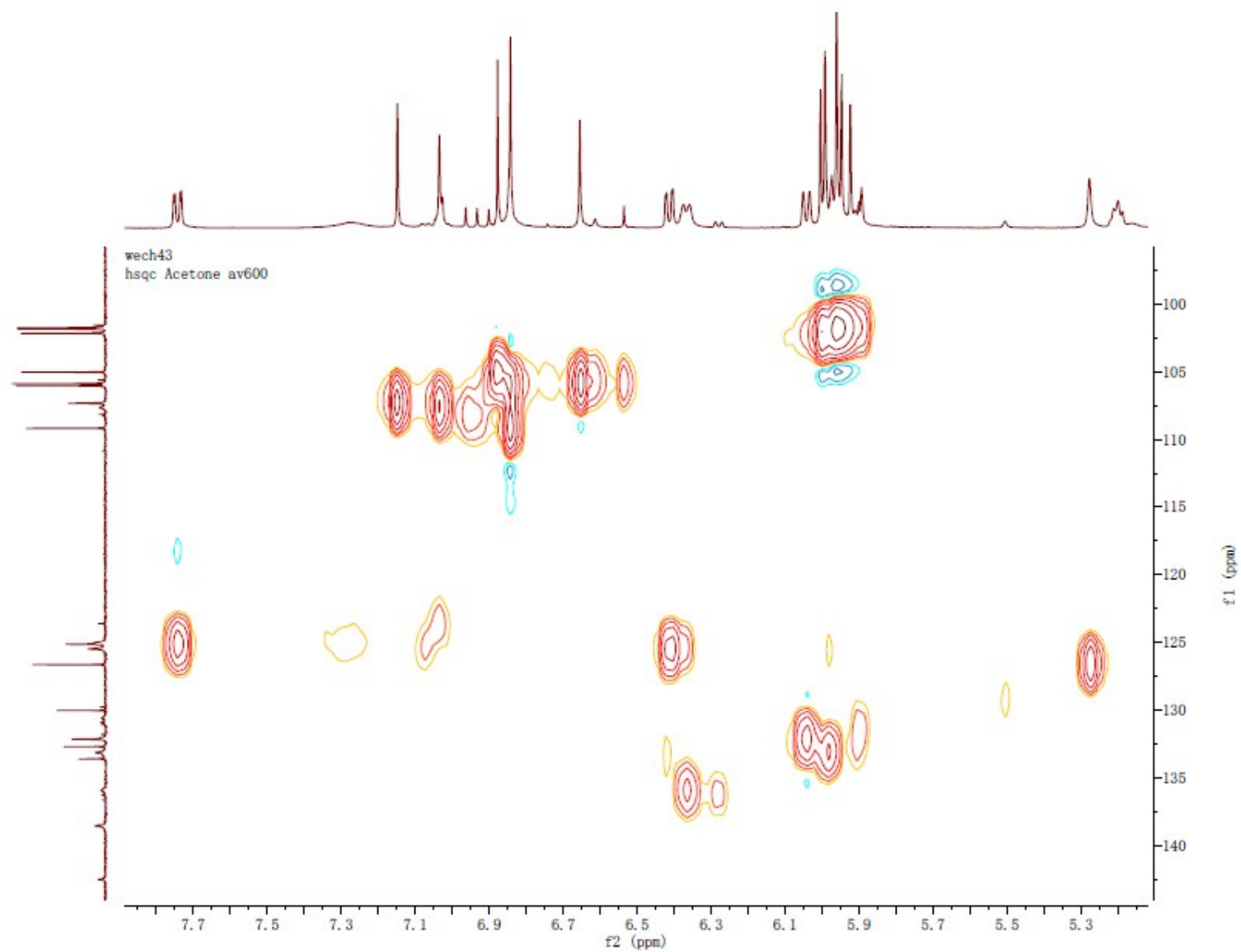


Figure S21. HMBC spectrum of erythrivarine F (4)

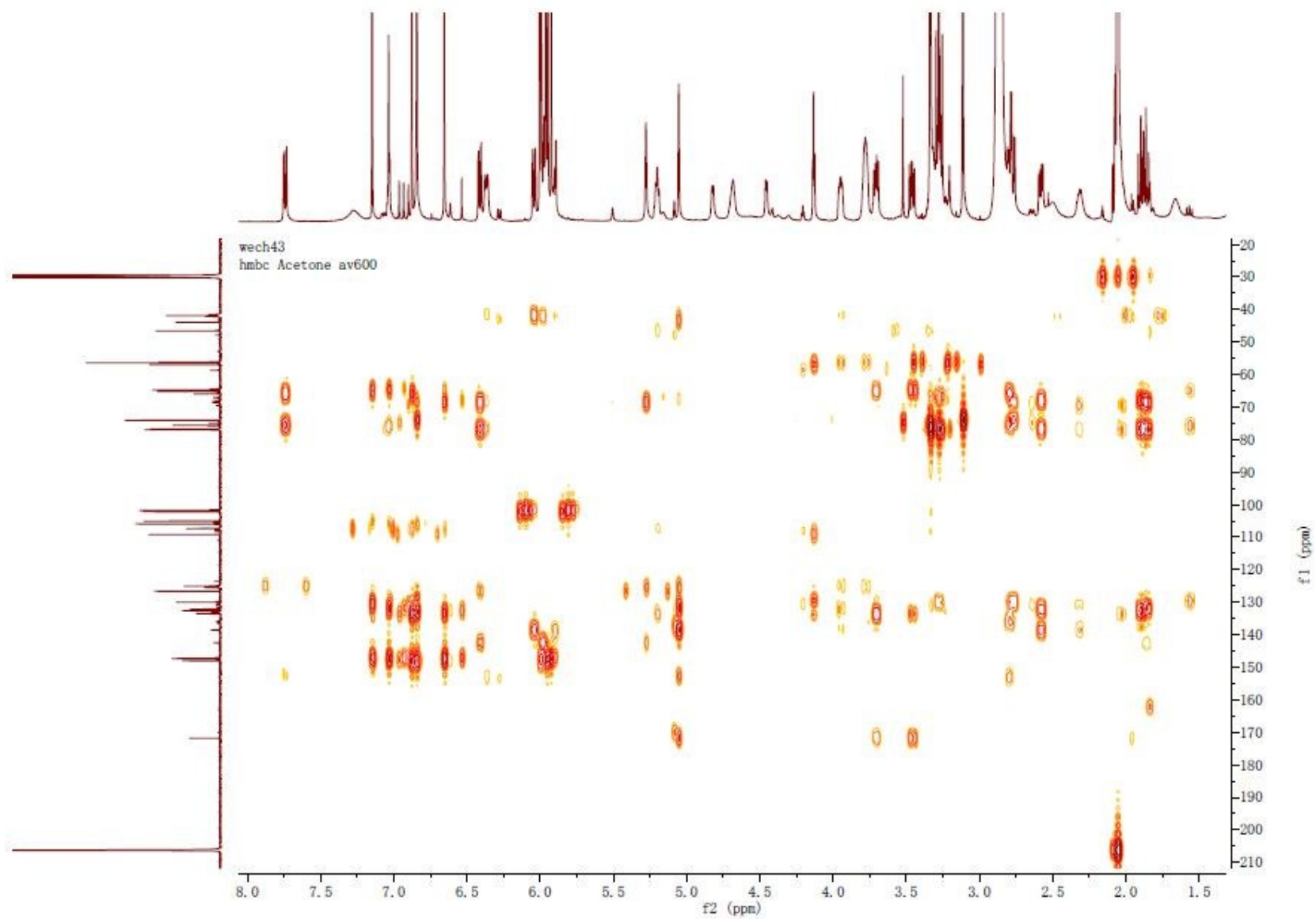


Figure S22. ^1H - ^1H COSY spectrum of erythrivarine F (4)

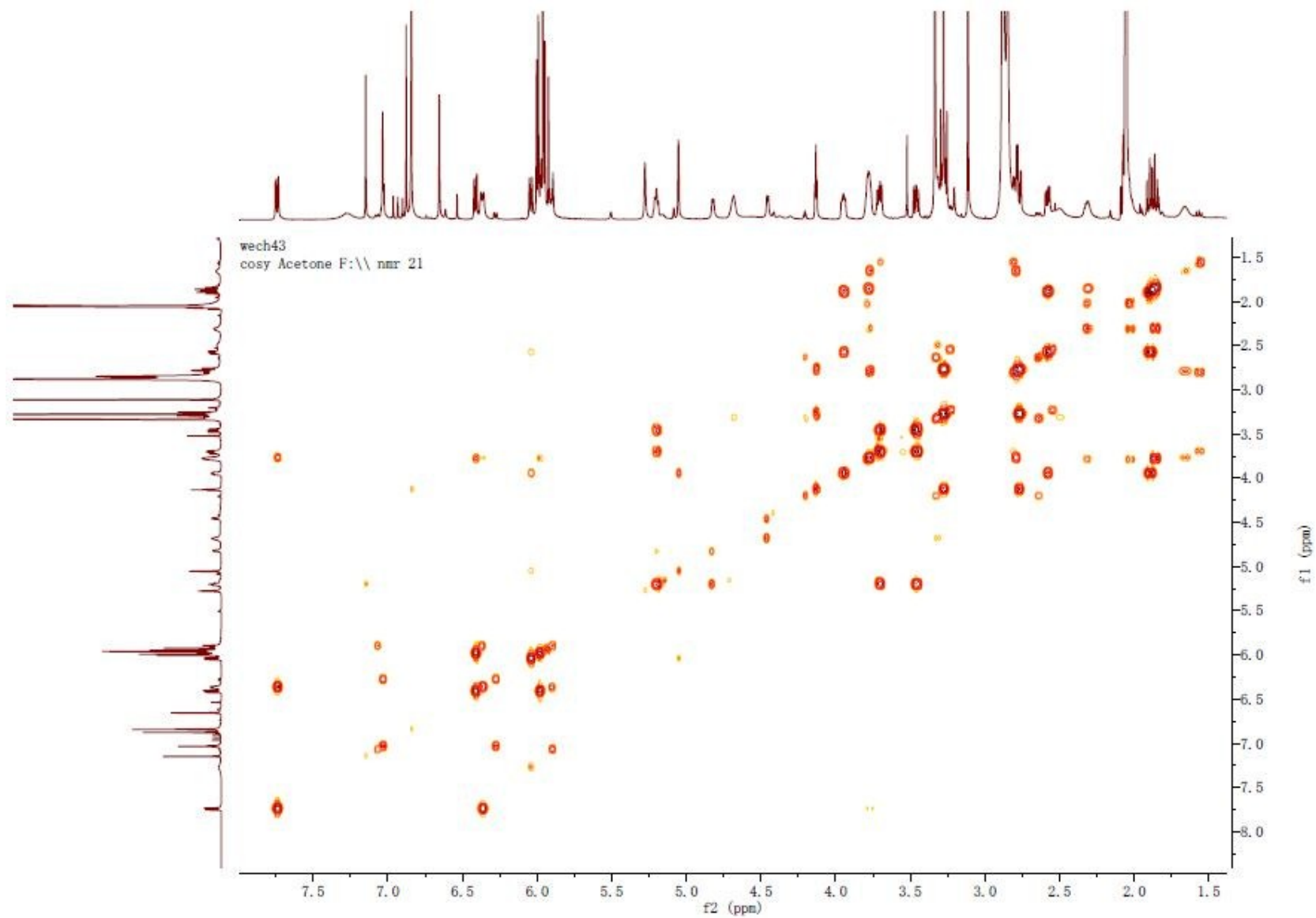


Figure S23. ROESY spectrum of erythrivarine F (4)

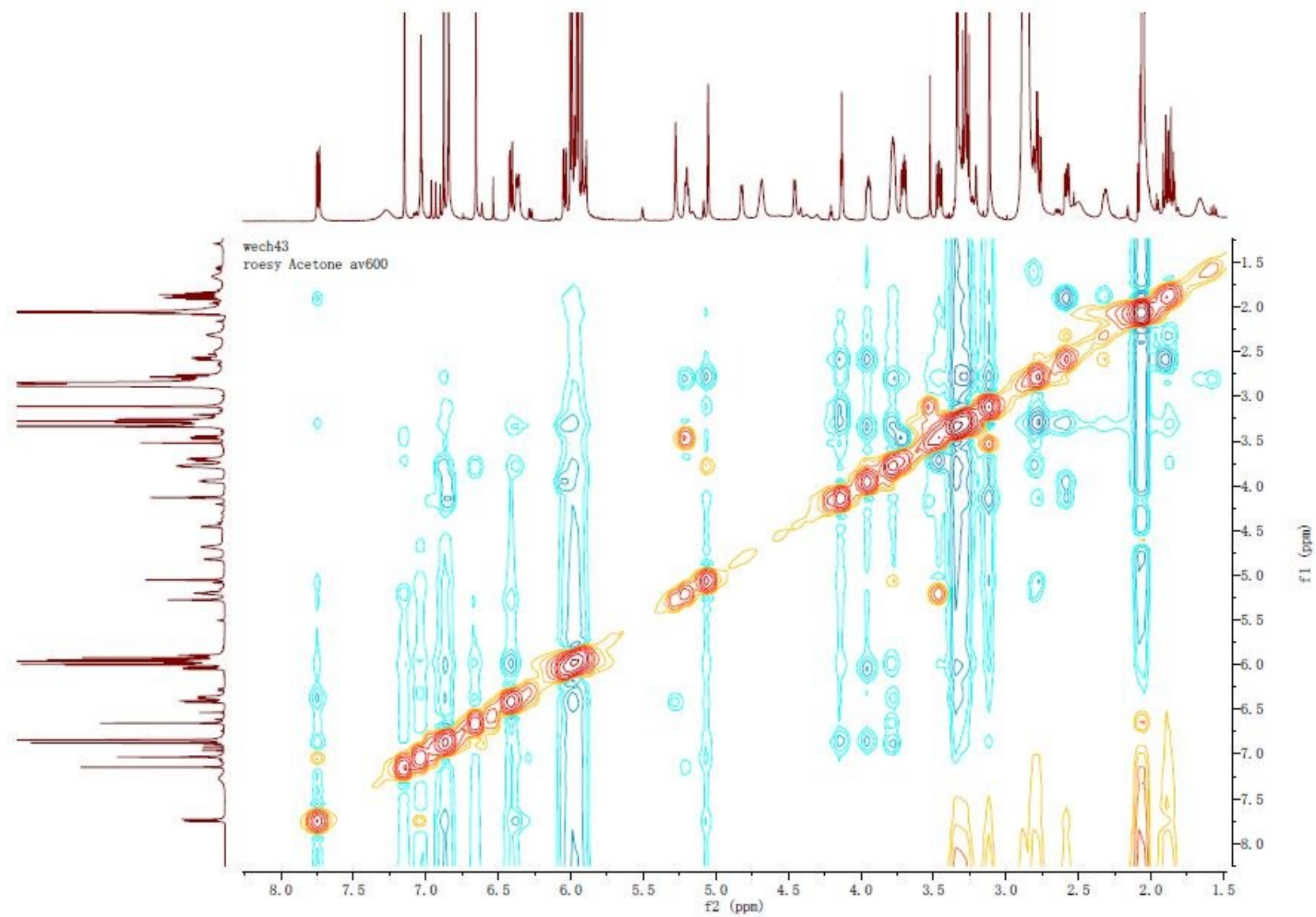
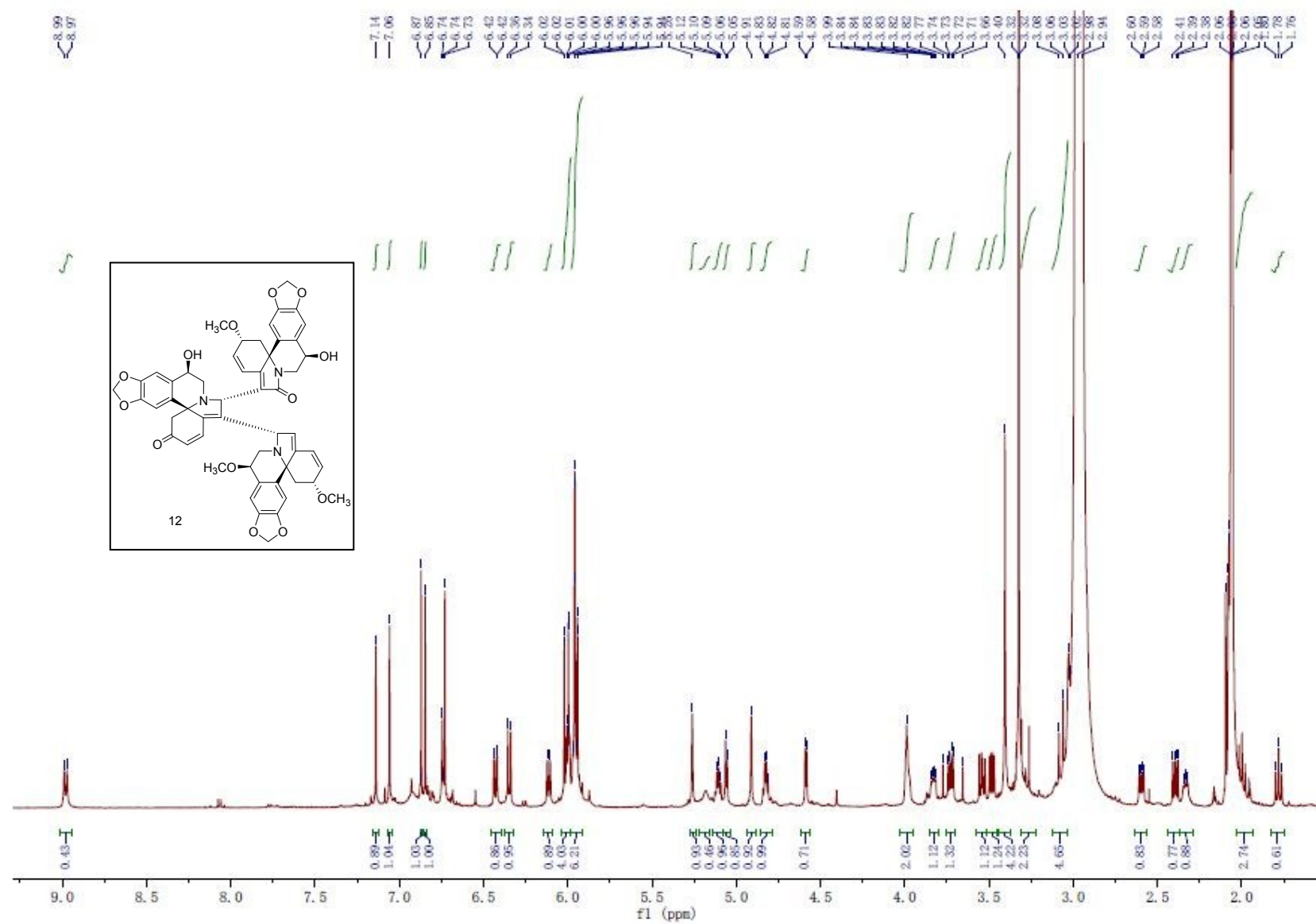


Figure S24. ¹H NMR spectrum of erythrivarine G (5)



Expanded ^1H NMR spectrum of erythrivarine G (5)

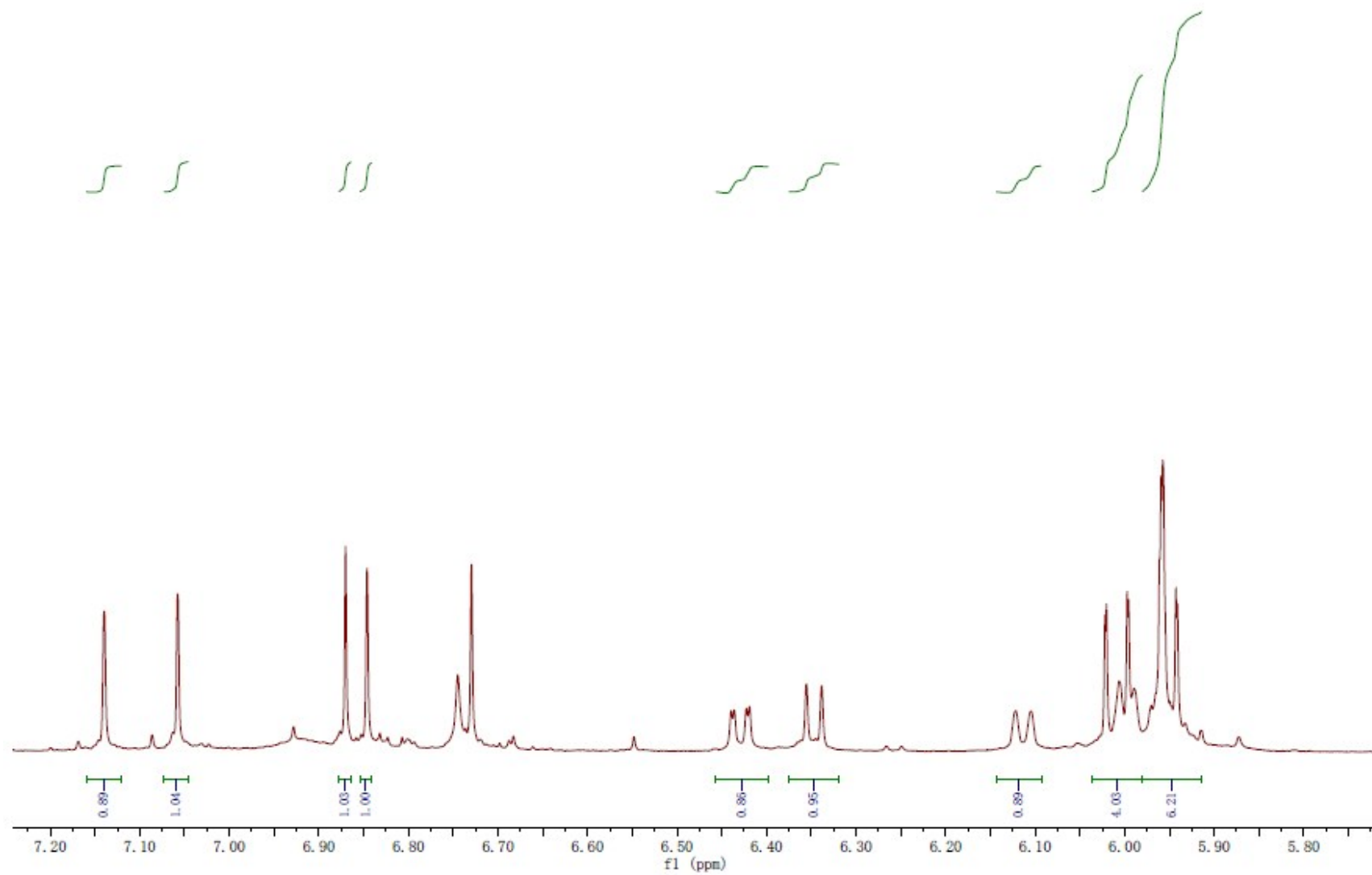


Figure S25. ^{13}C NMR spectrum of erythrivarine G (5)

wech41
d135 Acetone F:\ nmr 58

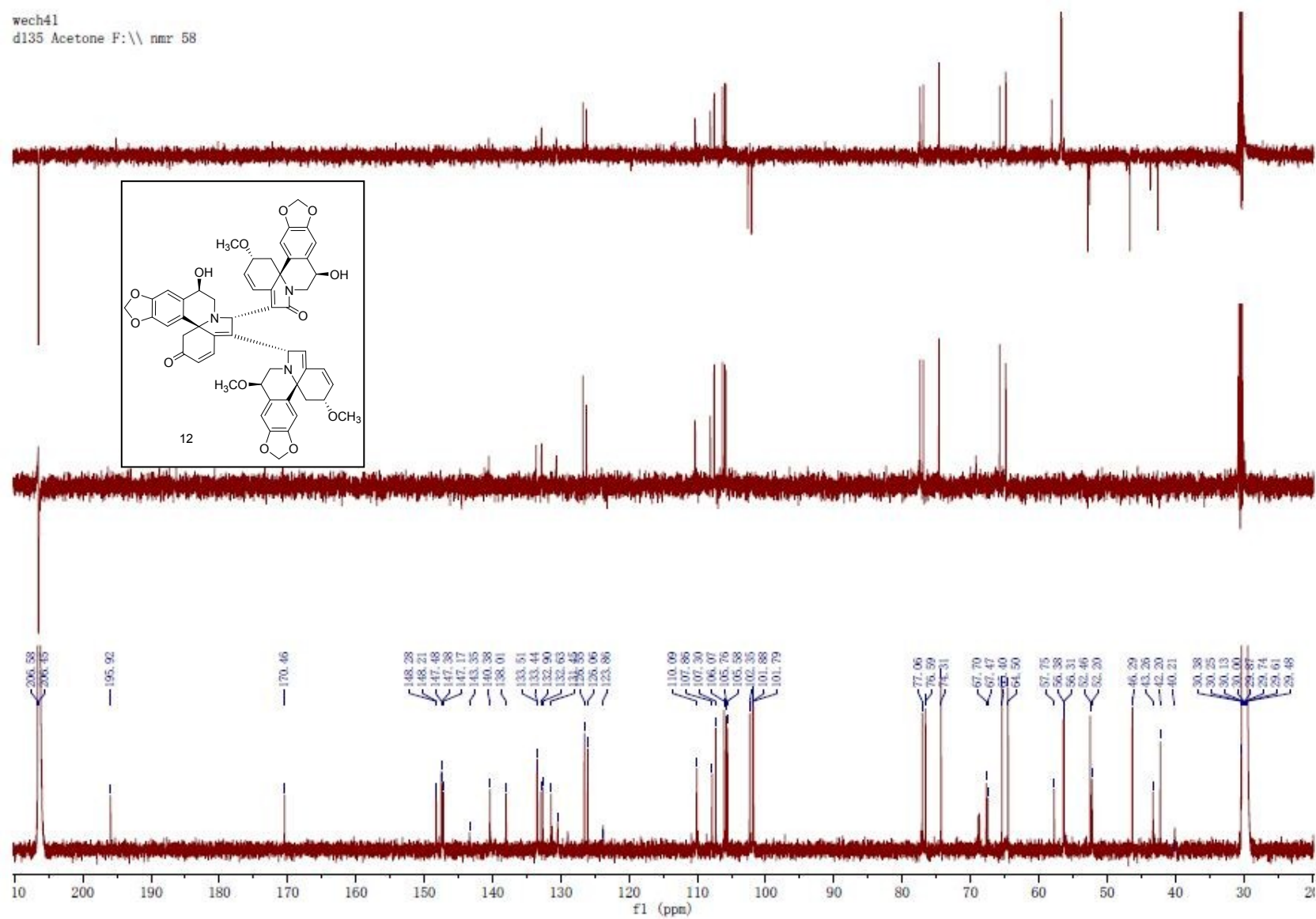
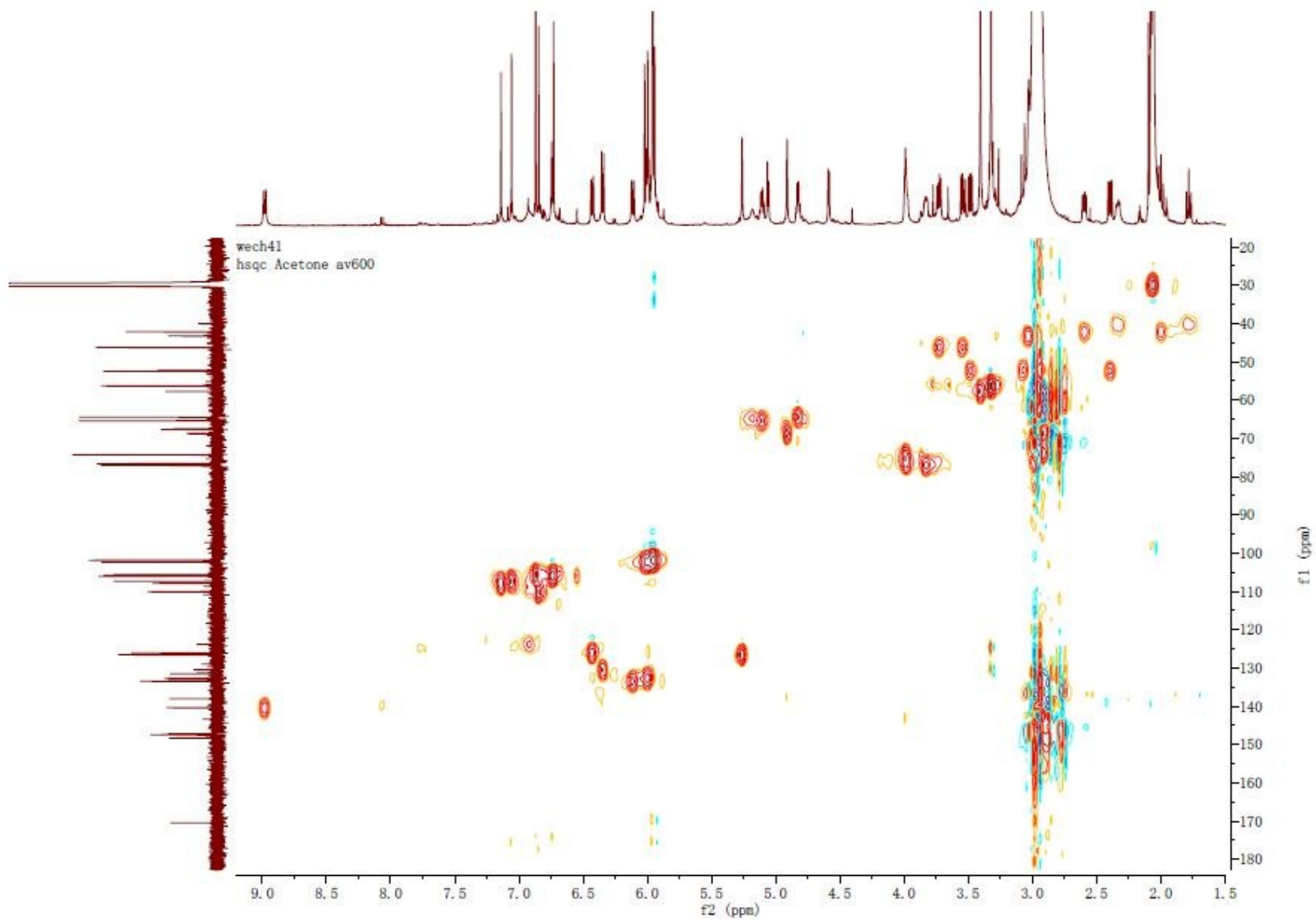


Figure S26. HSQC spectrum of erythrivarine G (**5**)



Expanded HSQC spectrum of erythrivarine G (5)

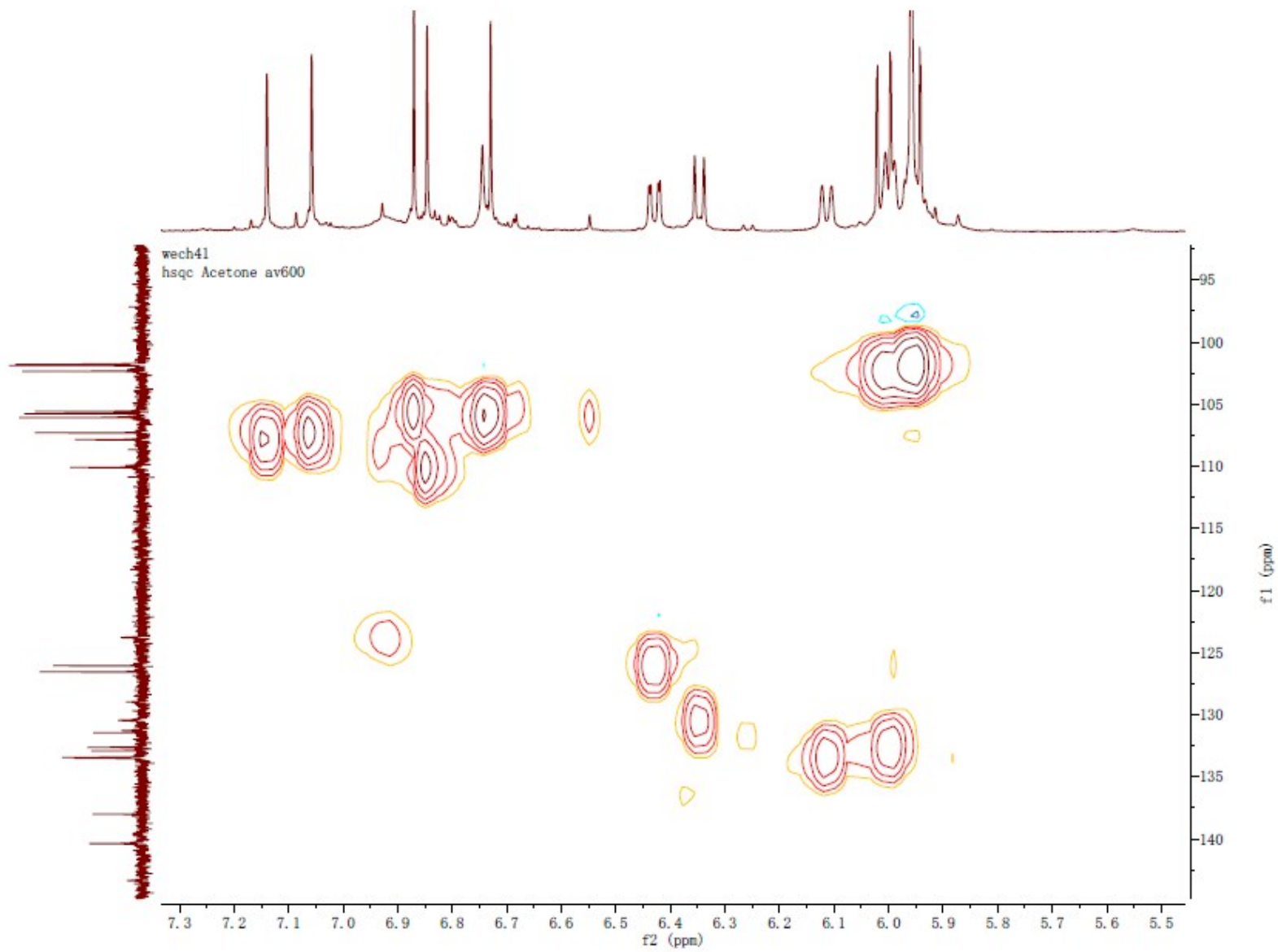


Figure S27. HMBC spectrum of erythrivarine G (**5**)

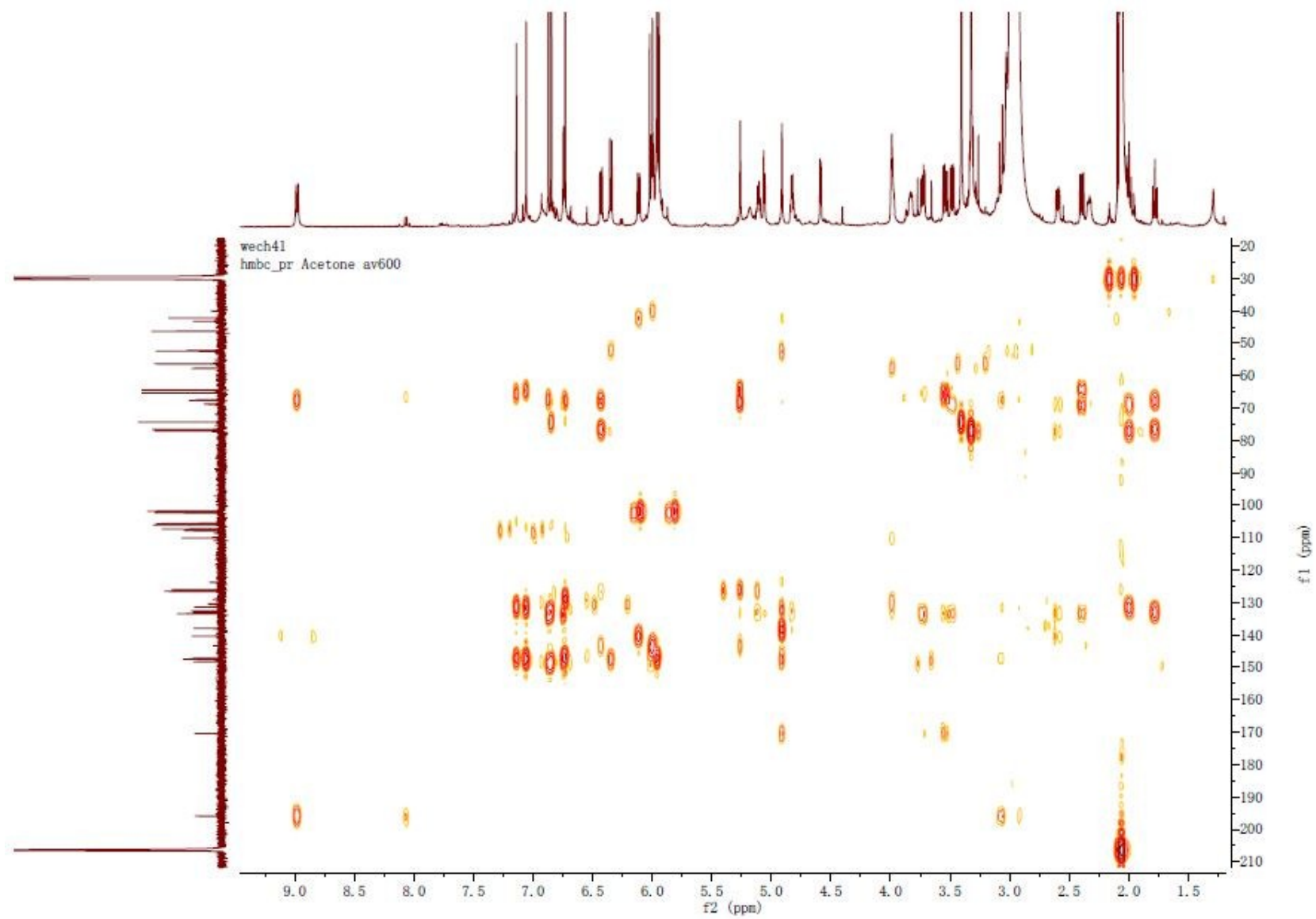


Figure S28. ^1H - ^1H COSY spectrum of erythrivarine G (**5**)

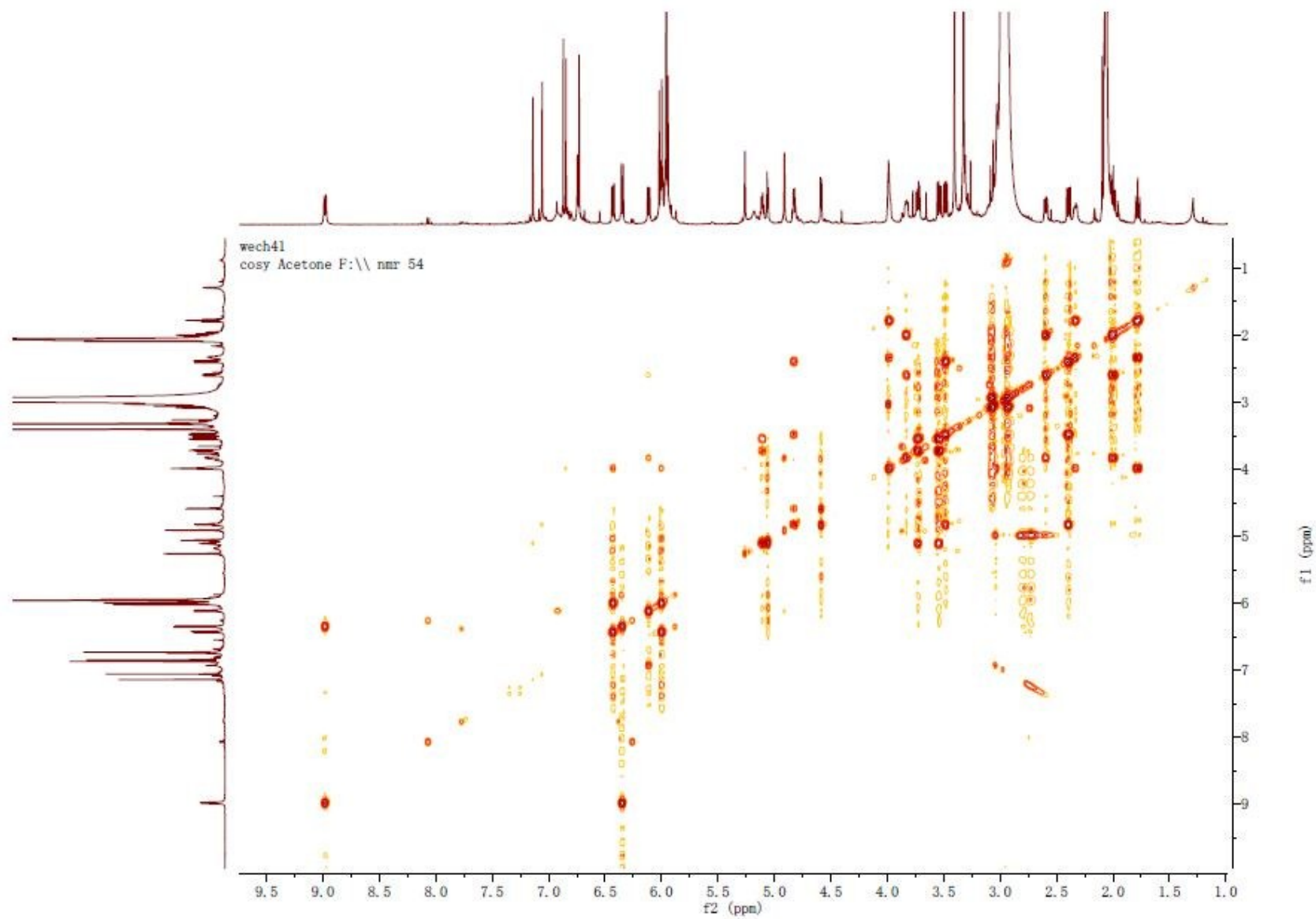
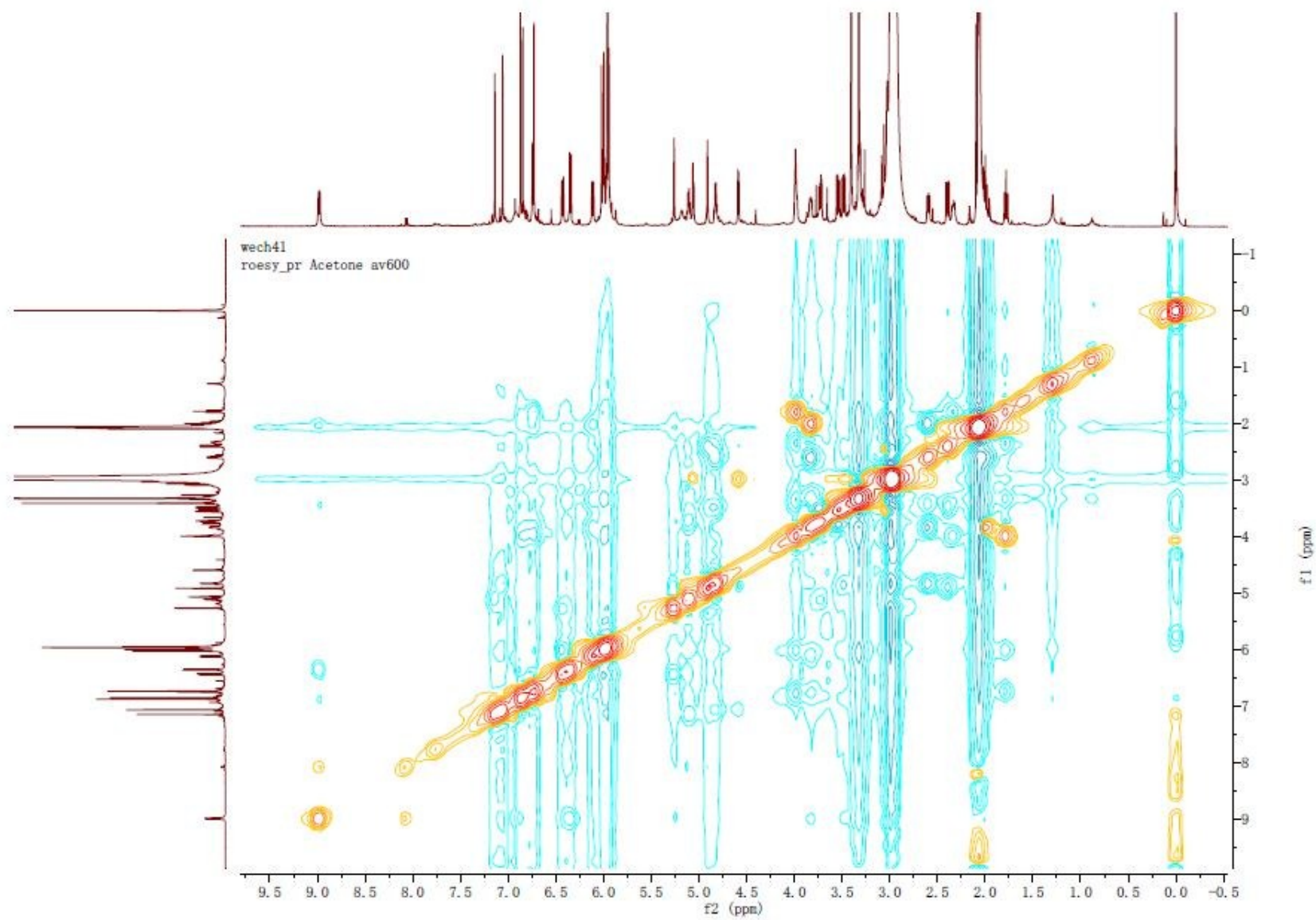


Figure S29. ROESY spectrum of erythrivarine G (**5**)



4、NMR spectroscopic data of erythrinine (6) and 8-oxo-erythrinine (7)

Figure S30: ¹H NMR spectrum of erythrinine (6)

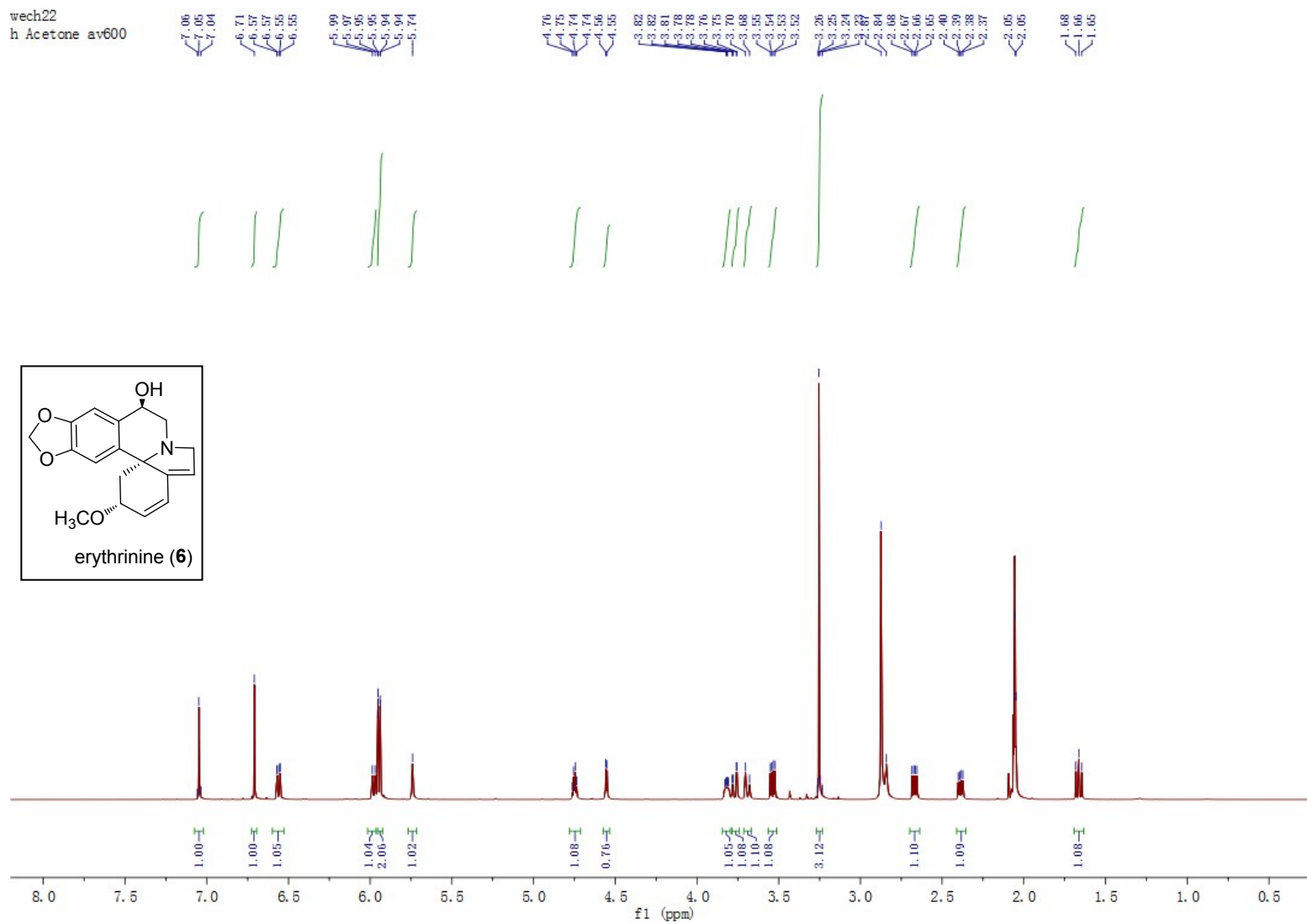


Figure S31: ^{13}C NMR spectrum of erythrine (6)

wech22

d135 Acetone D:\ nmr 2

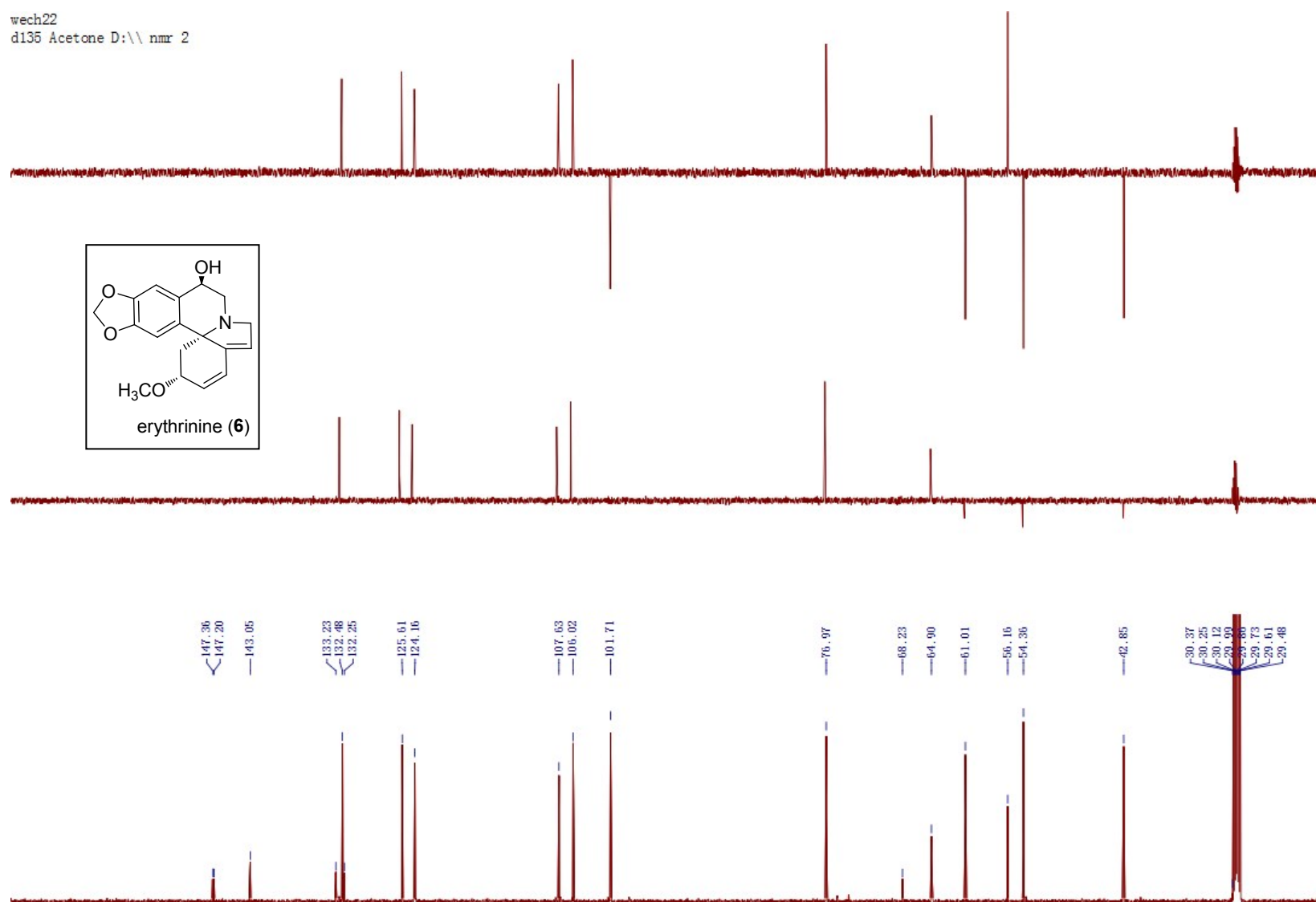


Figure S32: ^1H NMR spectrum of 8-oxo-erythrinine (7)

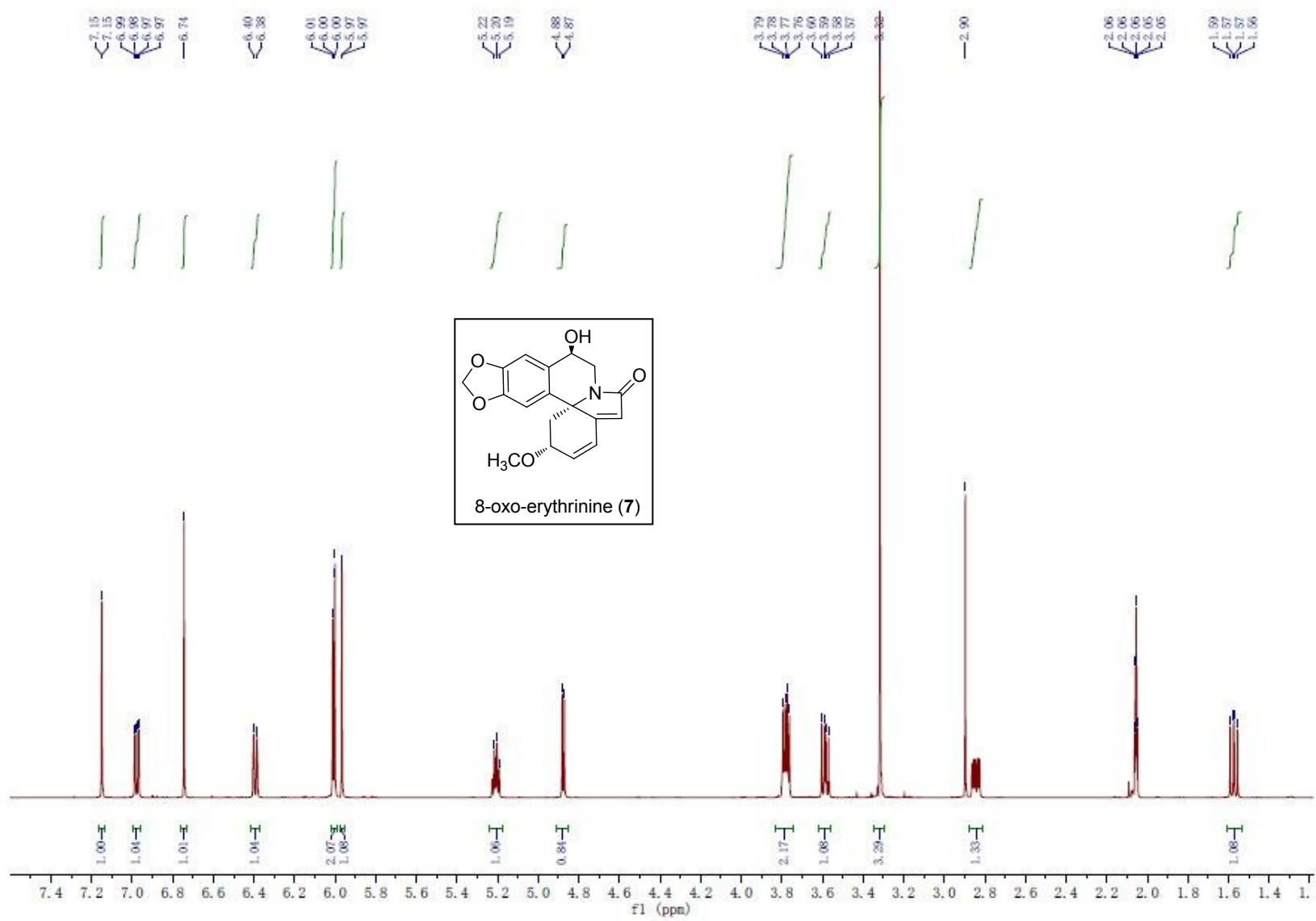
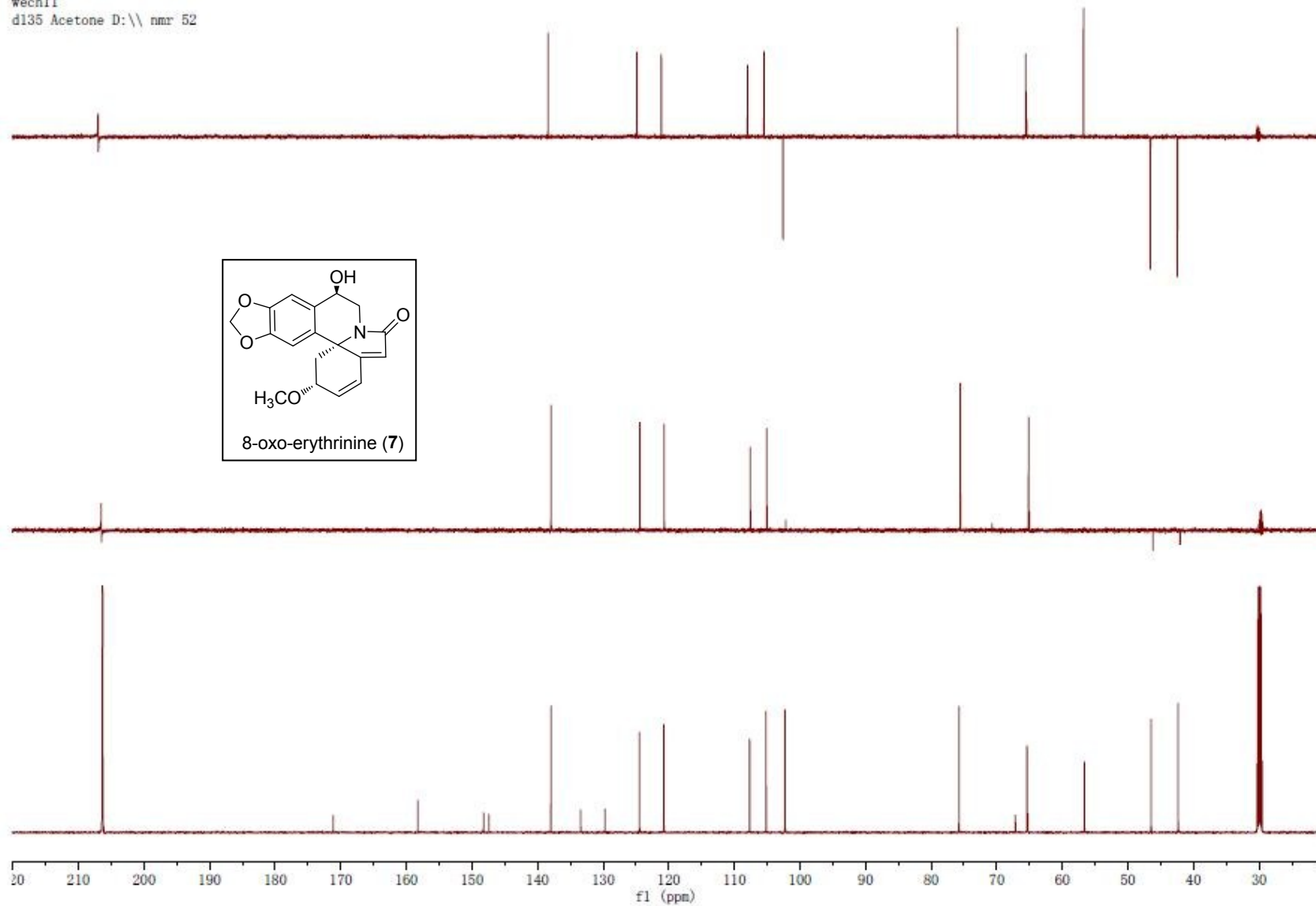


Figure S33. ^{13}C NMR spectrum of 8-oxo-erythrinine (7)

wechl1
d135 Acetone D:\ nmr 52



5、 UPLC-MS-MS analysis of the polymeric alkaloids

Preparation of reference solution

The purified compounds were accurately weighed and further dissolved in methanol respectively to yield the stock solutions at the concentration of 5000 ng/mL, the equal volumes of stock solutions were then mixed well to yield the reference solution containing the compounds at the concentration of 1000 ng/mL.

Preparation of sample solution

The total alkaloid extract was accurately weighed and dissolved in methanol to yield the sample solution at the concentration of 1000 $\mu\text{g/mL}$.

UPLC conditions

UPLC analyses were performed on a Waters Acquity H CLASS system; the compounds were analyzed by an Acquity UPLC BEH C18 column (2.1 \times 50 mm, 1.7 μm , Serial NO. 021132332157 96) using ACN-H₂O (10 % ACN – 100 % ACN in 1.5 mins, linear mode) as eluent.

MS conditions

MS analyses were performed on a Waters Xevo TQD ESI-MS instrument. The compounds were analyzed using the MRM mode. The parameters (Cone voltage and collision energy) were tuned respectively for each compound (Table S1).

Table S1: The parameters for MS/MS analysis

	Compound	Parent (m/z)	Daughter (m/z)	Dwell (s)	Cone (V)	Collision (V)
1	Erythrivarine C	843.3856	262.0836	0.063	42	66
2	Erythrivarine D	857.3374	466.0262	0.063	42	36
3	Erythrivarine E	949.7628	311.9421	0.063	60	30
4	Erythrivarine F	964.5174	280.0855	0.063	56	44
5	Erythrivarine G	948.4223	262.0193	0.063	50	50

Figure S34. The characteristic peak obtained by ESI-MS-MS of erythrivarine C (1)

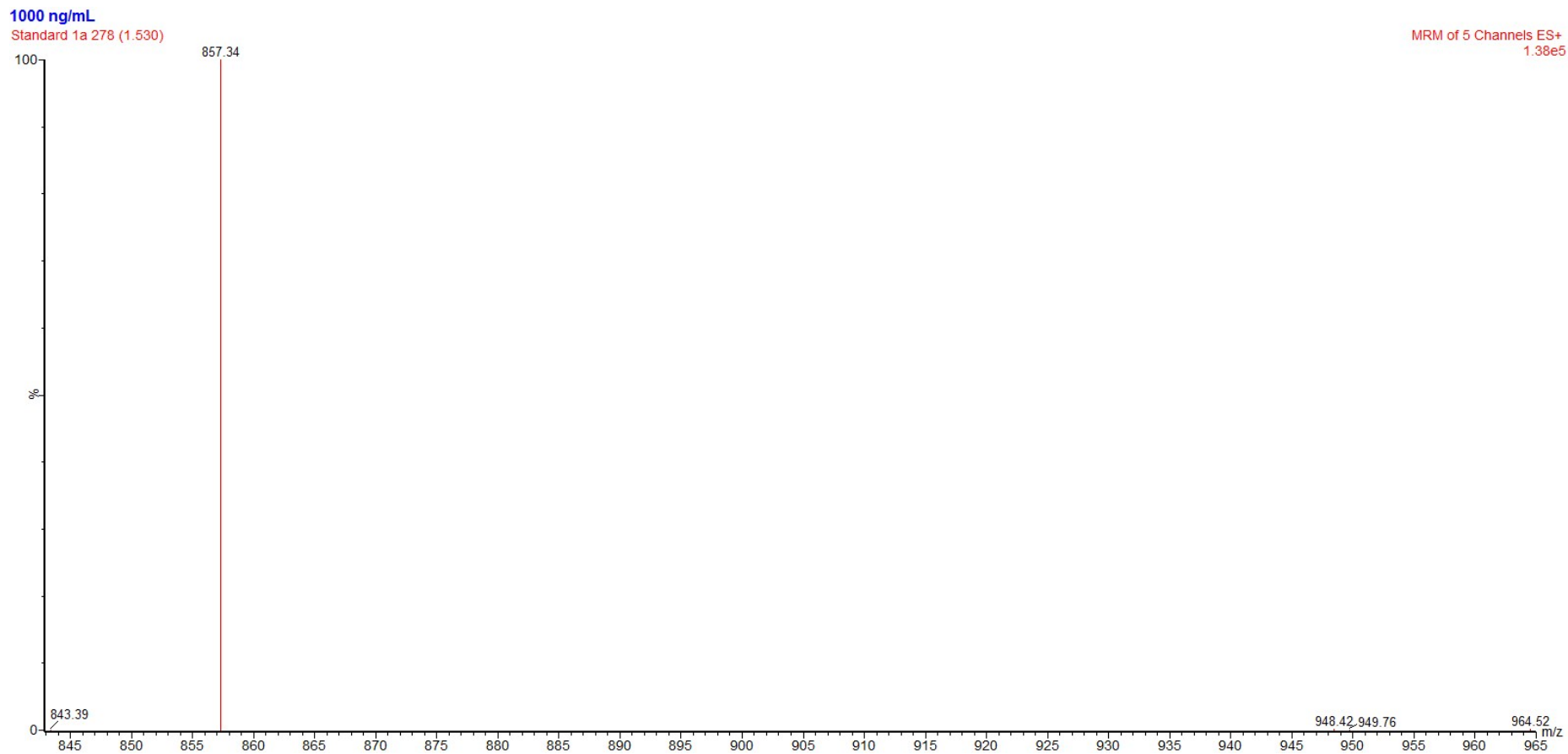


Sample 1 265 (1.458)

MRM of 5 Channels ES+
3.83e3



Figure S35. The characteristic peak obtained by ESI-MS-MS of erythrivarine D (2)



Sample 1 277 (1.524)

MRM of 5 Channels ES+
3.02e3



Figure S36 The characteristic peak obtained by ESI-MS-MS of erythrivarine E (3)

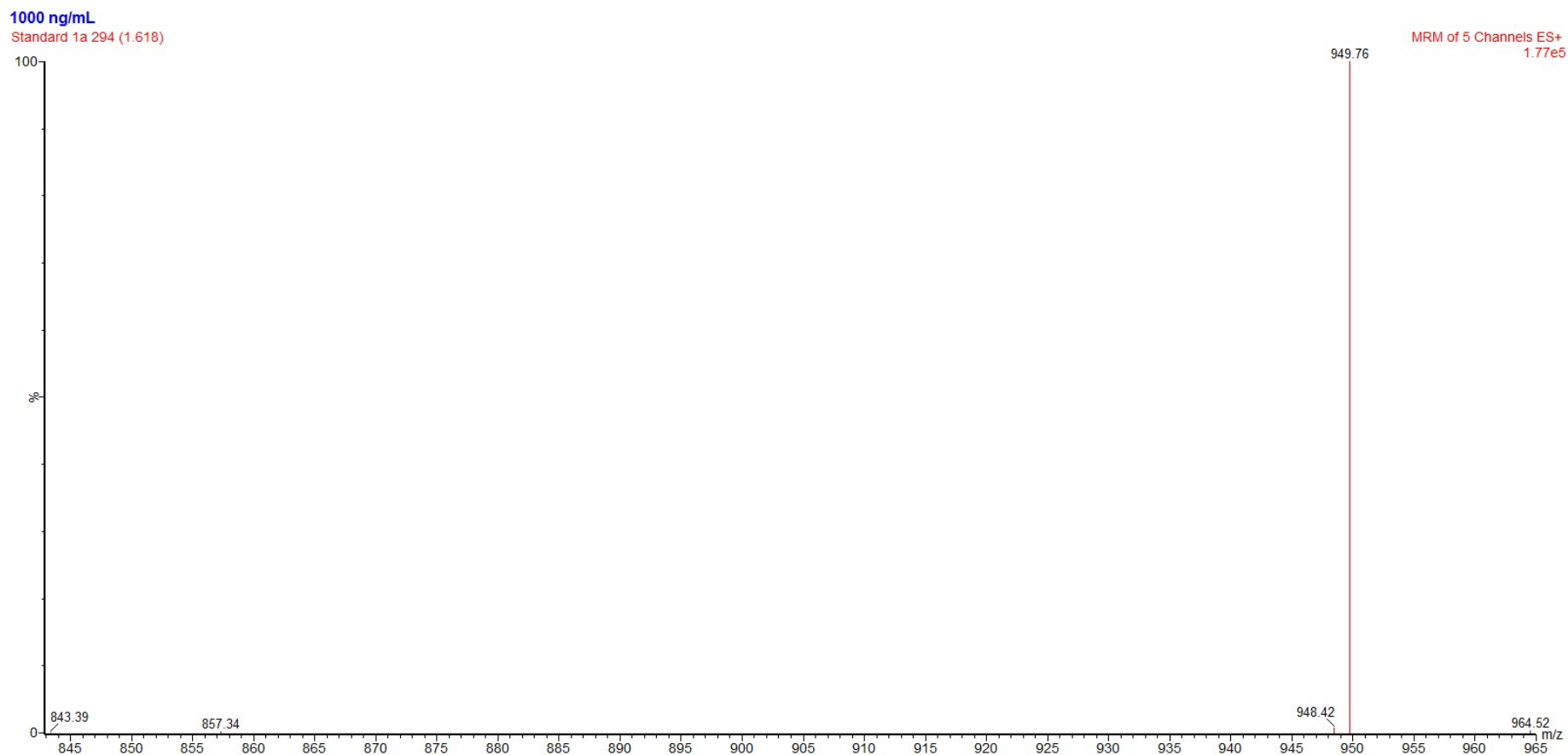




Figure S37. The characteristic peak obtained by ESI-MS-MS of erythrivarine F (4)



Sample 1 308 (1.695)

MRM of 5 Channels ES+
964.521.03e4



Figure S38. The characteristic peak obtained by ESI-MS-MS of erythrivarine G (5)



Sample 1 331 (1.821)

MRM of 5 Channels ES+
2.09e3



6、The CD and UV chromatography of the unit of erythrivarine C (1)

