

Electronic Supplementary Information

New Diterpene Alkaloids from the Marine Sponge *Agelas mauritiana*

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Figure S1. ^1H NMR (600 MHz, CDCl_3) spectrum of (–)-8'-oxo-agelasine B (**1**)

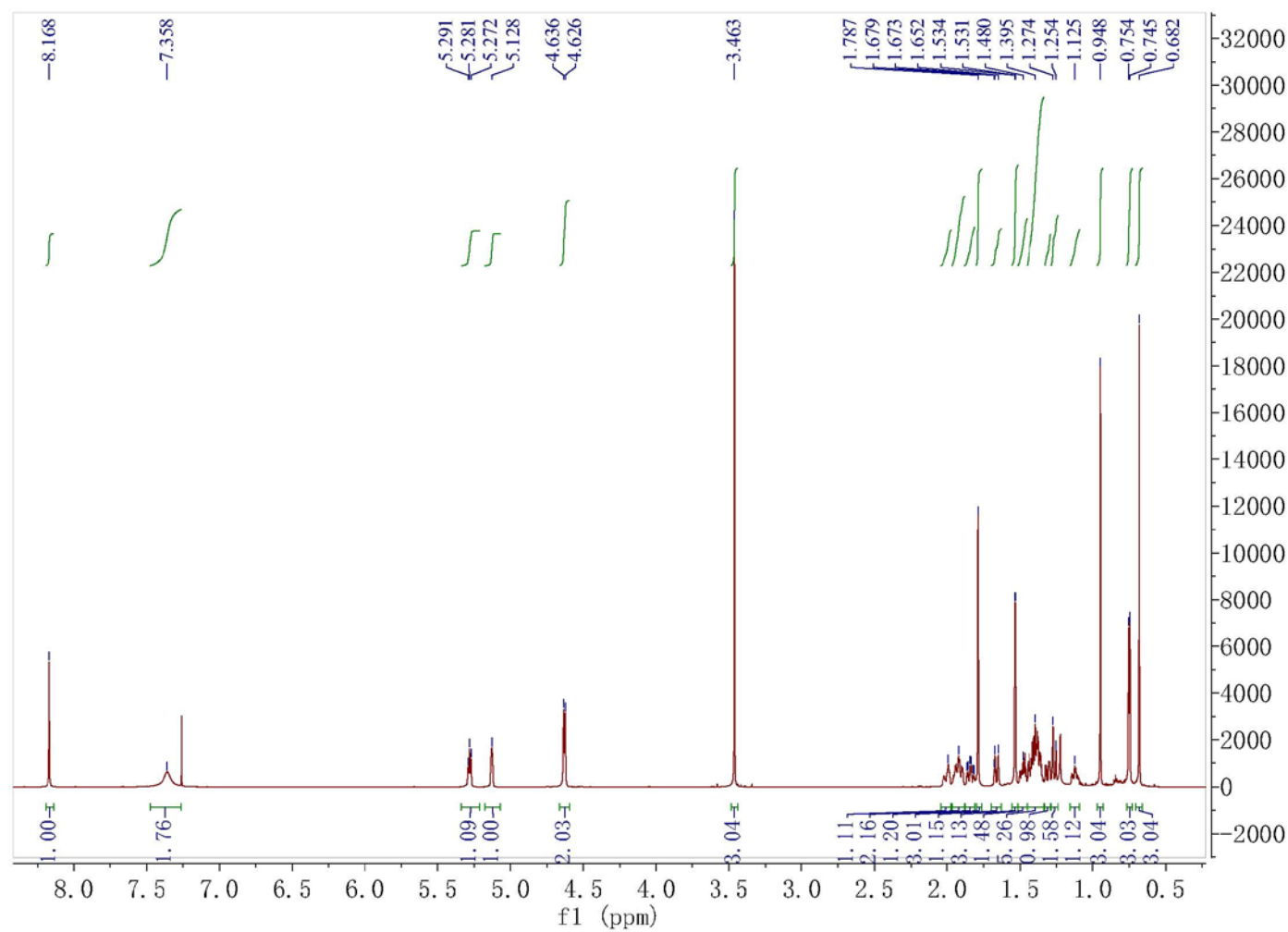


Figure S2. ^{13}C NMR (150 MHz, CDCl_3) spectrum of (–)-8'-oxo-agelasine B (**1**)

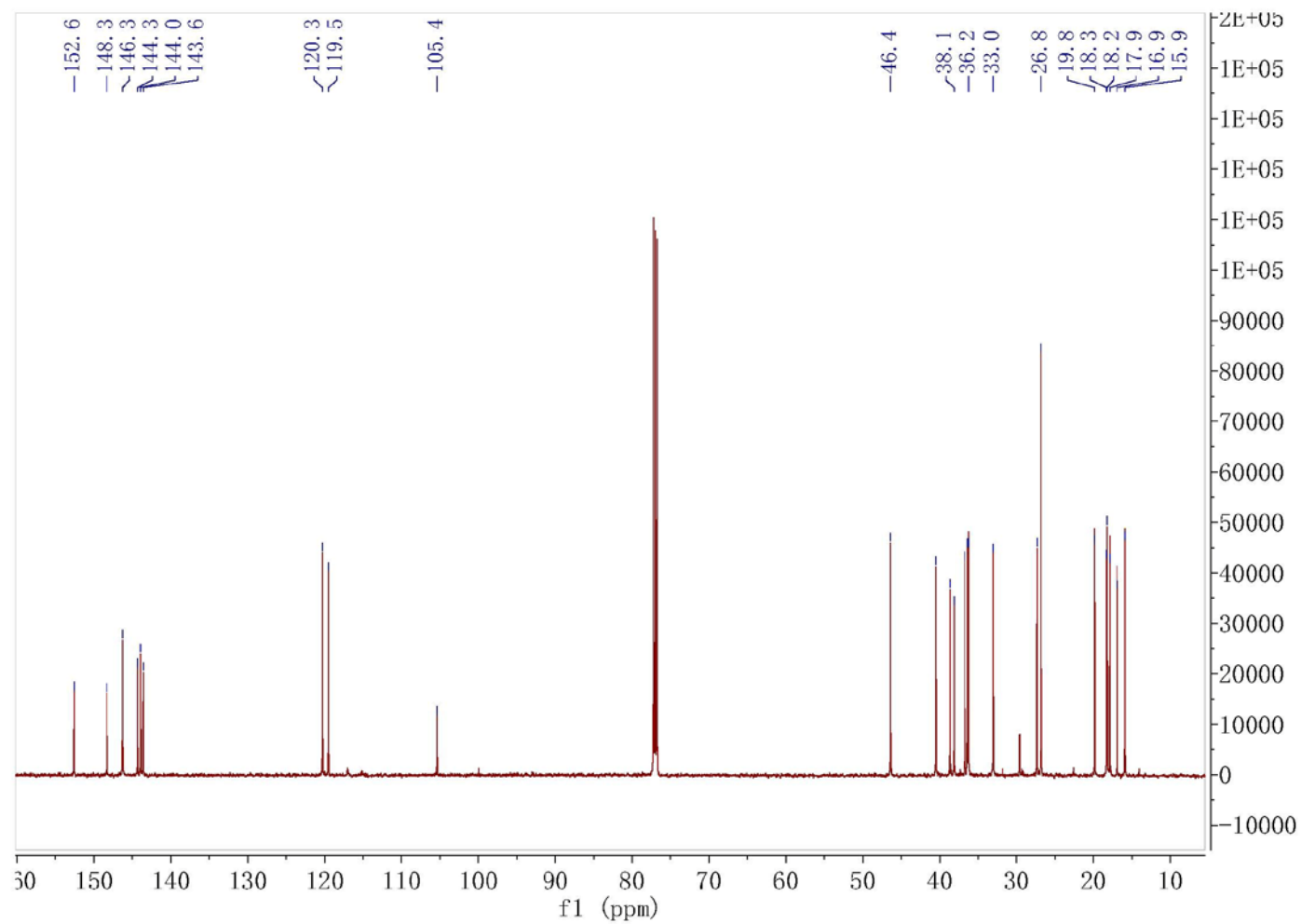


Figure S3. DEPT135 spectrum of (–)-8^l-oxo-agelasine B (**1**) in CDCl₃

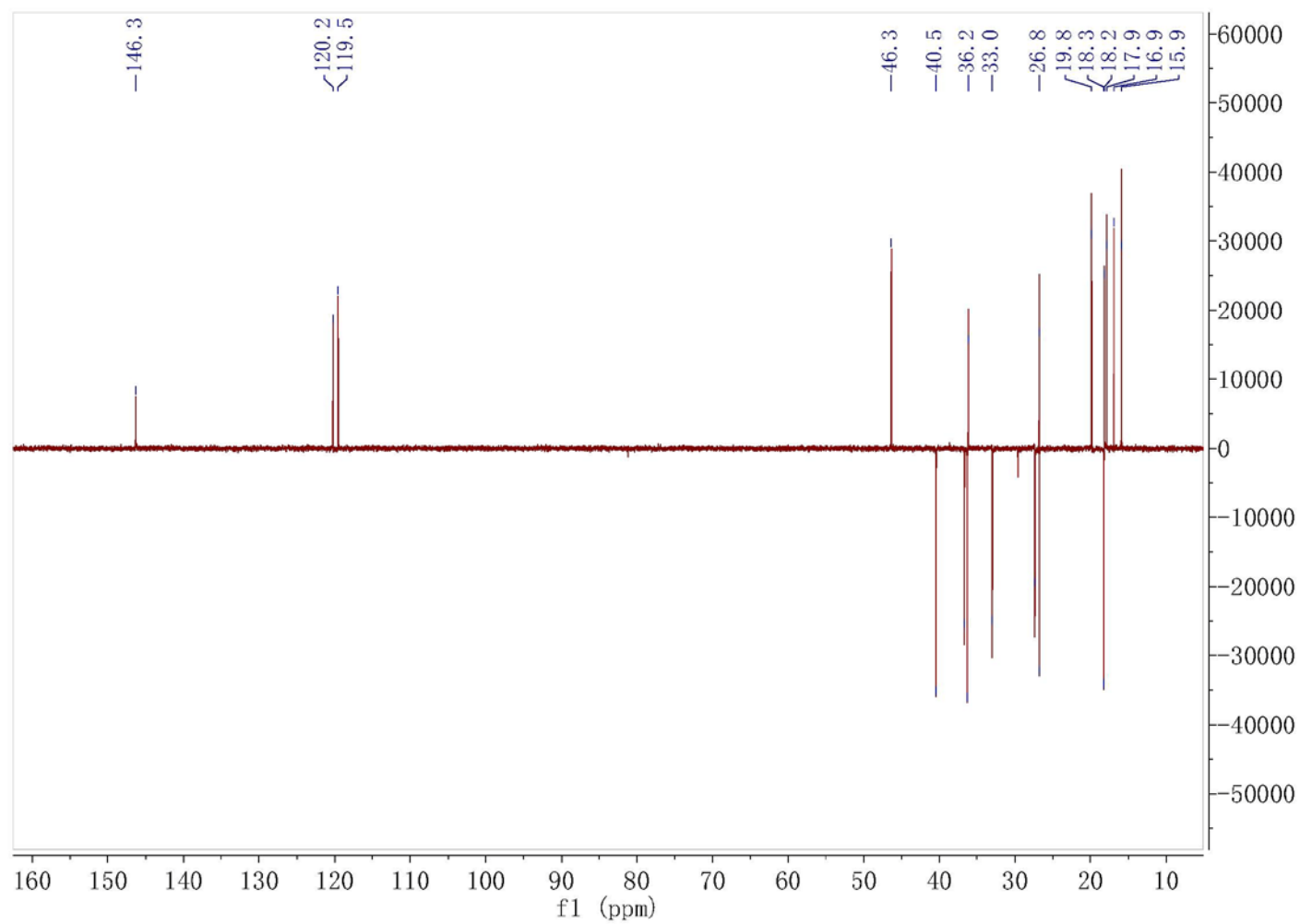


Figure S4. HSQC spectrum of (–)-8'-oxo-agelasine B (**1**) in CDCl₃

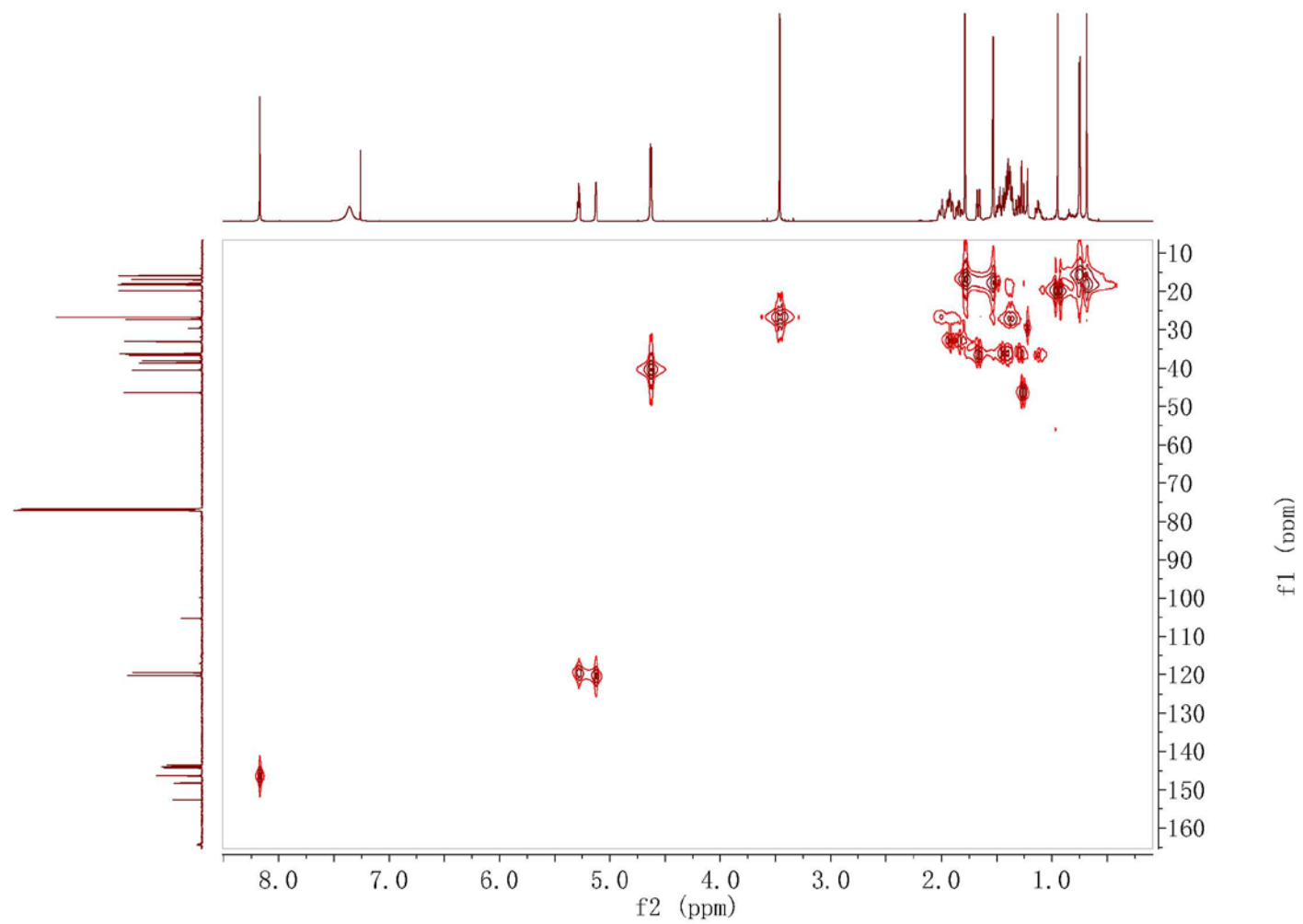


Figure S5. COSY spectrum of (–)-8'-oxo-agelasine B (**1**) in CDCl₃

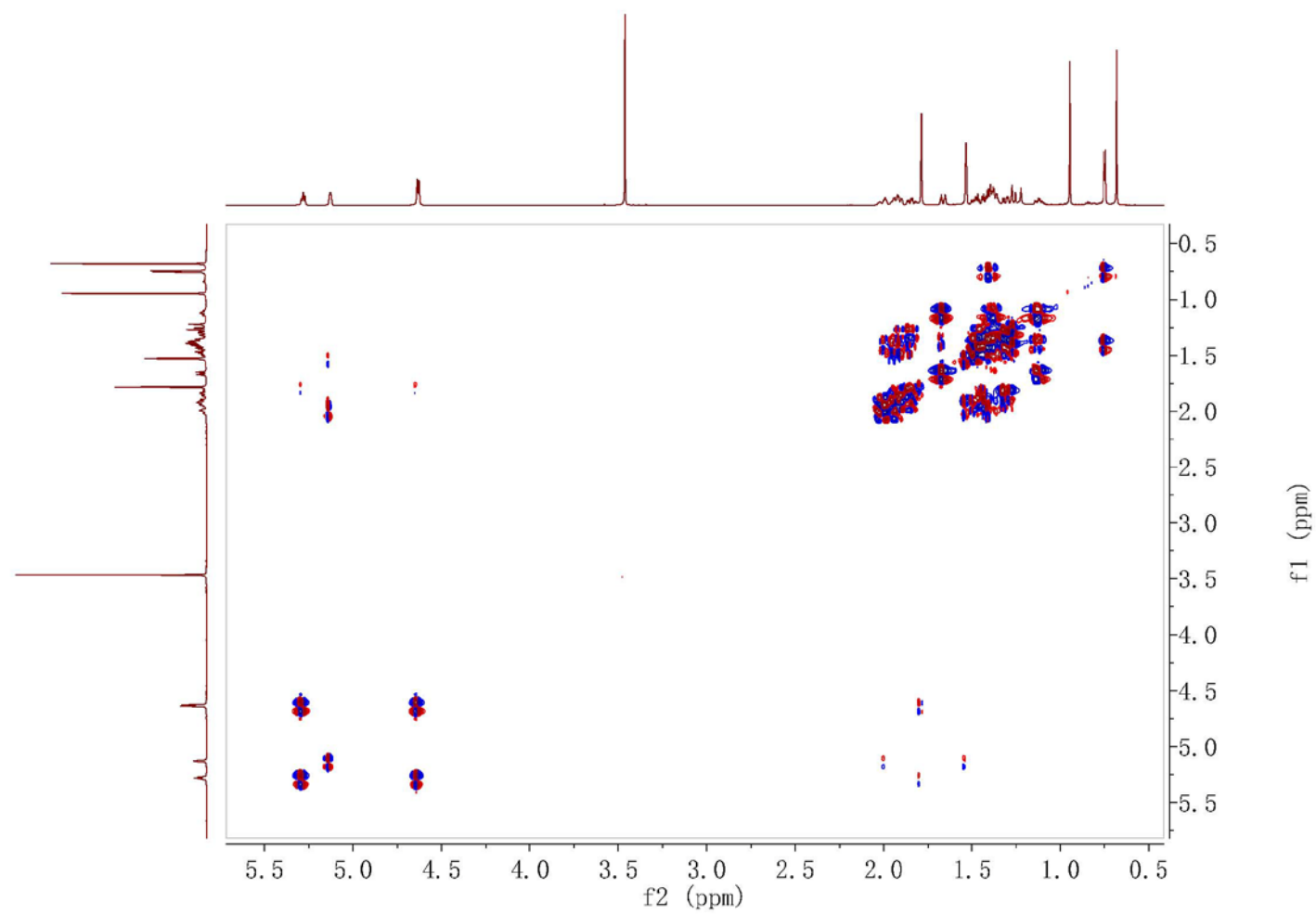


Figure S6. HMBC spectrum of (–)-8'-oxo-agelasine B (**1**) in CDCl₃

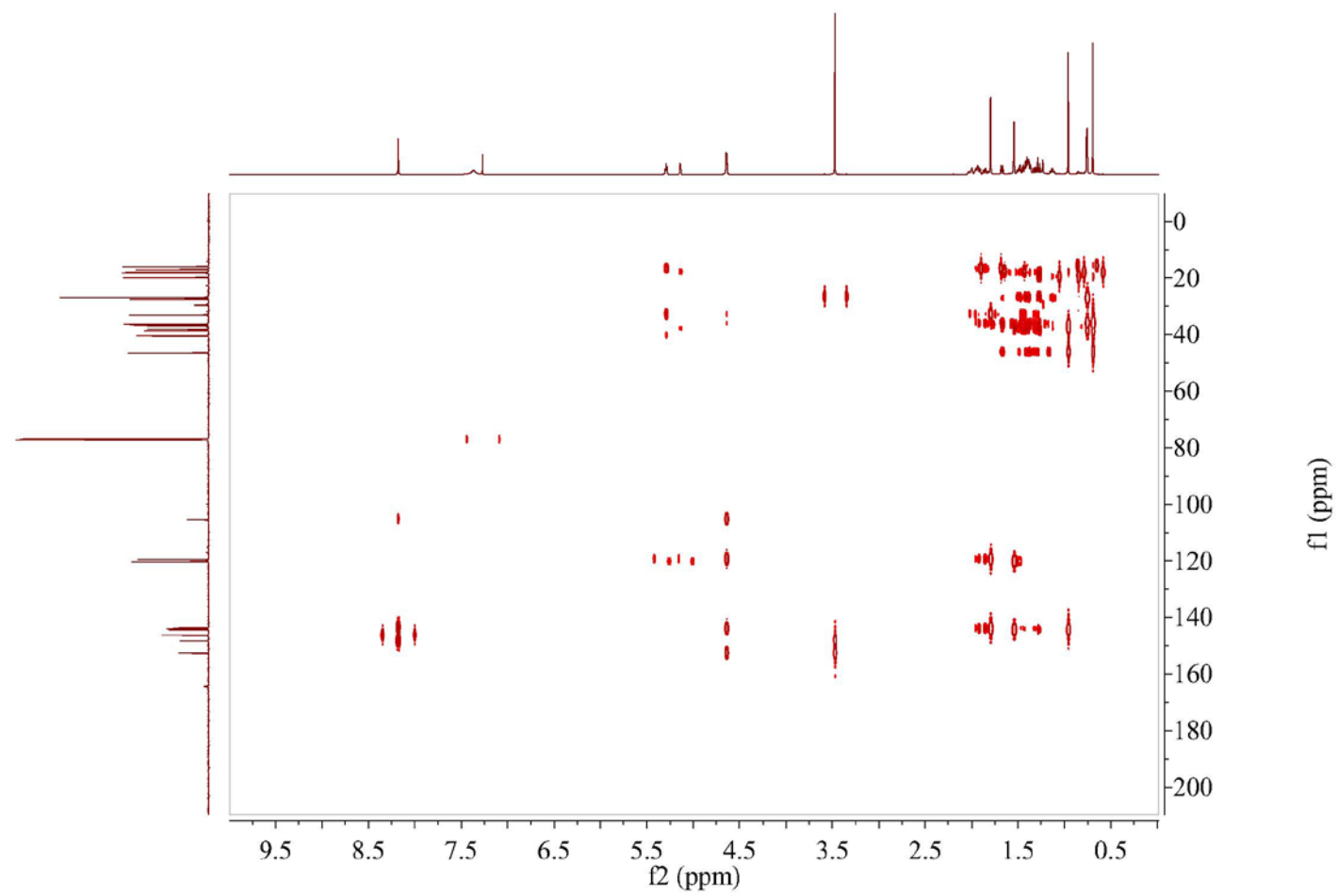


Figure S7. ^1H - ^{15}N HMBC spectrum of (–)-8'-oxo-agelasine B (**1**) in CDCl_3

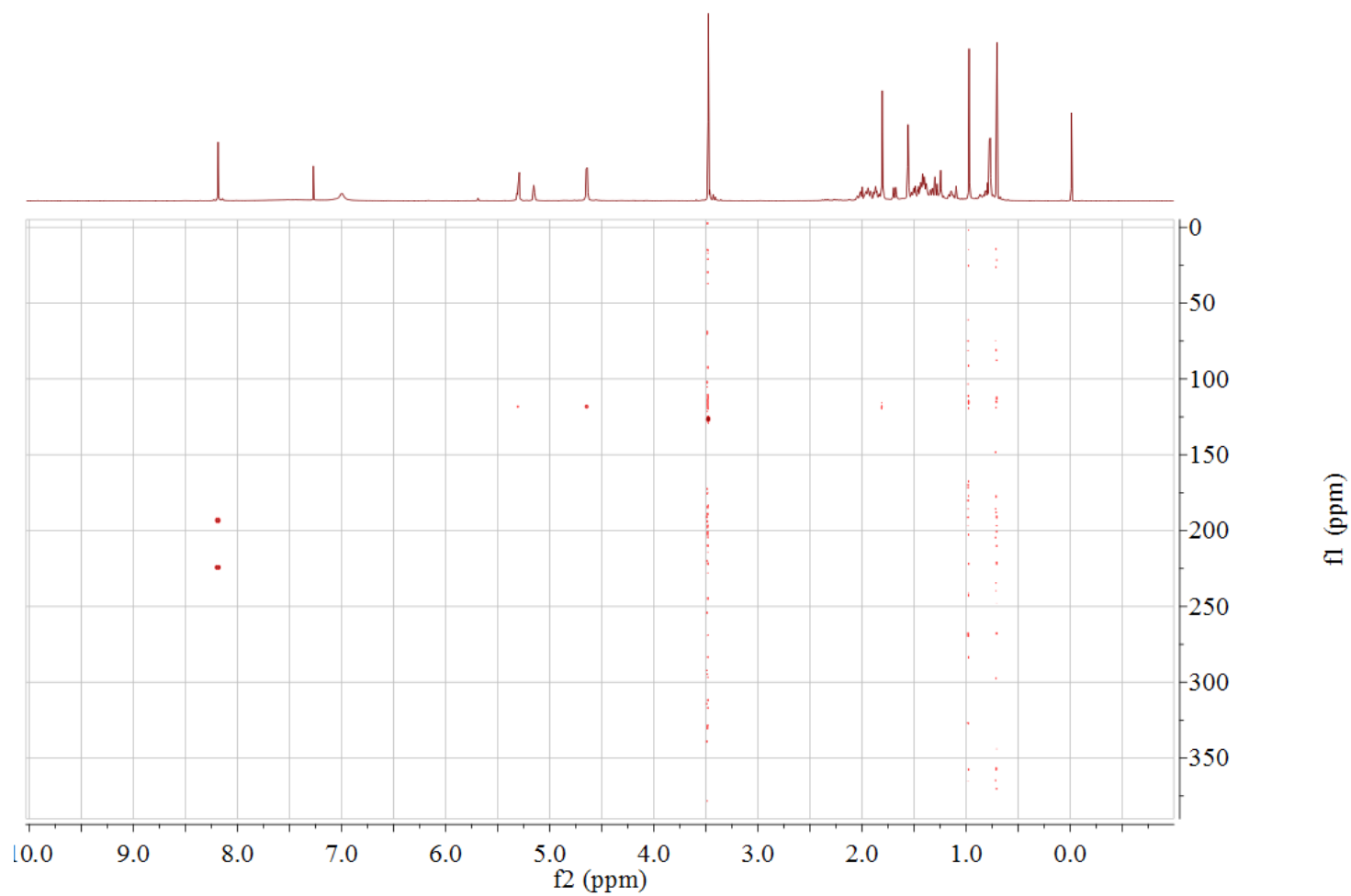


Figure S8. NOESY spectrum of (–)-8'-oxo-agelasine B (**1**) in CDCl₃

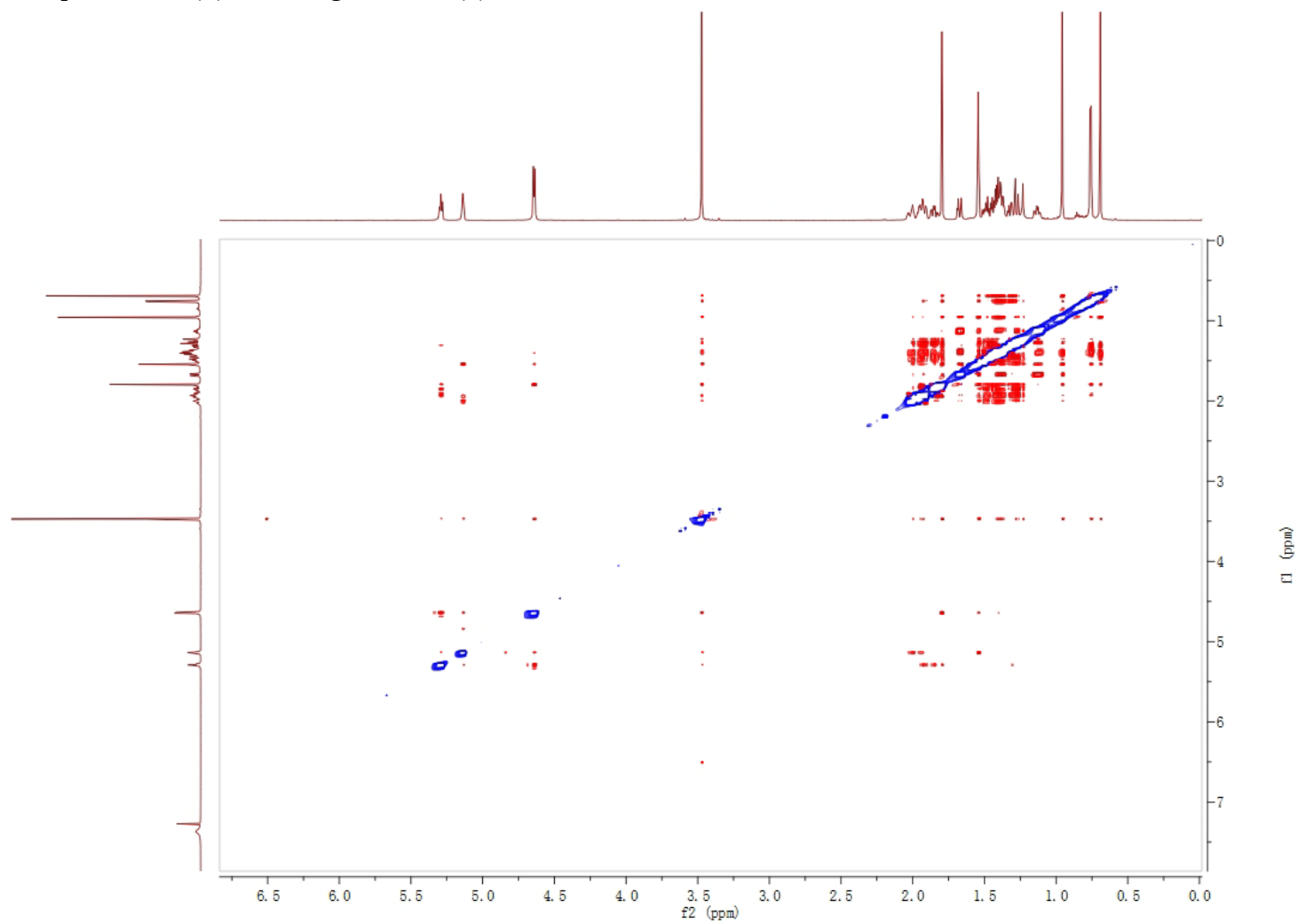


Figure S9. HRESIMS of (–)-8'-oxo-agelasine B (1)

Elemental Composition Report

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

39 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 5-27 H: 5-50 N: 1-6 O: 1-3

SIP1

hi-8

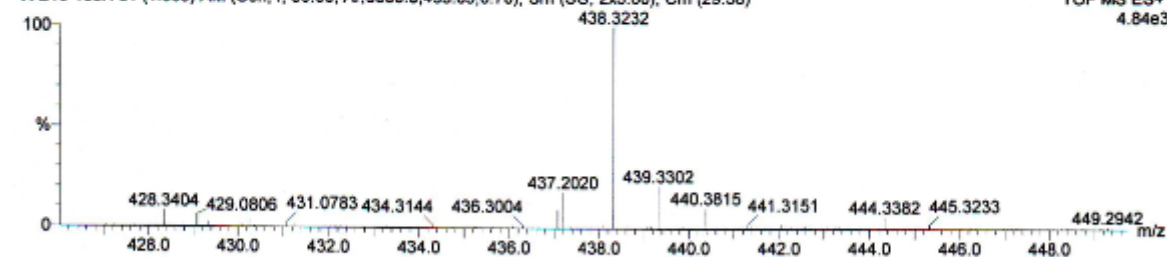
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Q-ToF micro

YA019

TOF MS ES+

4.84e3



Minimum: 40.00

Maximum: 100.00

5.0 10.0 -1.5 50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
438.3232	100.00	438.3233	-0.1	-0.2	9.5	179.4	C26 H40 N5 O

Figure S10. UV spectrum of (–)-8'-oxo-agelasine B (**1**) in MeOH

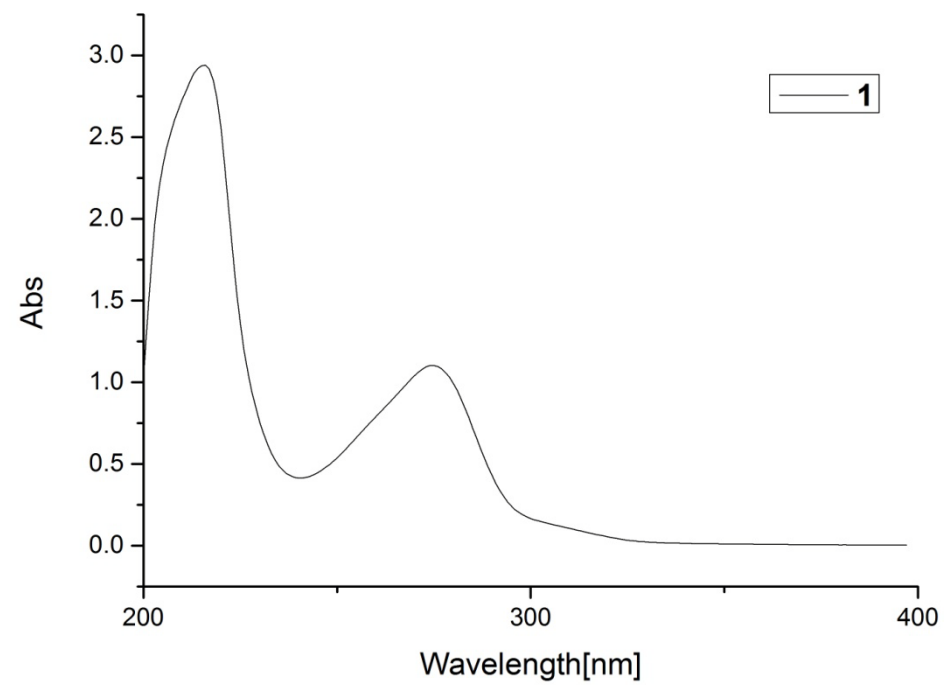


Figure S11. IR spectrum of (–)-8'-oxo-agelasine B (**1**)

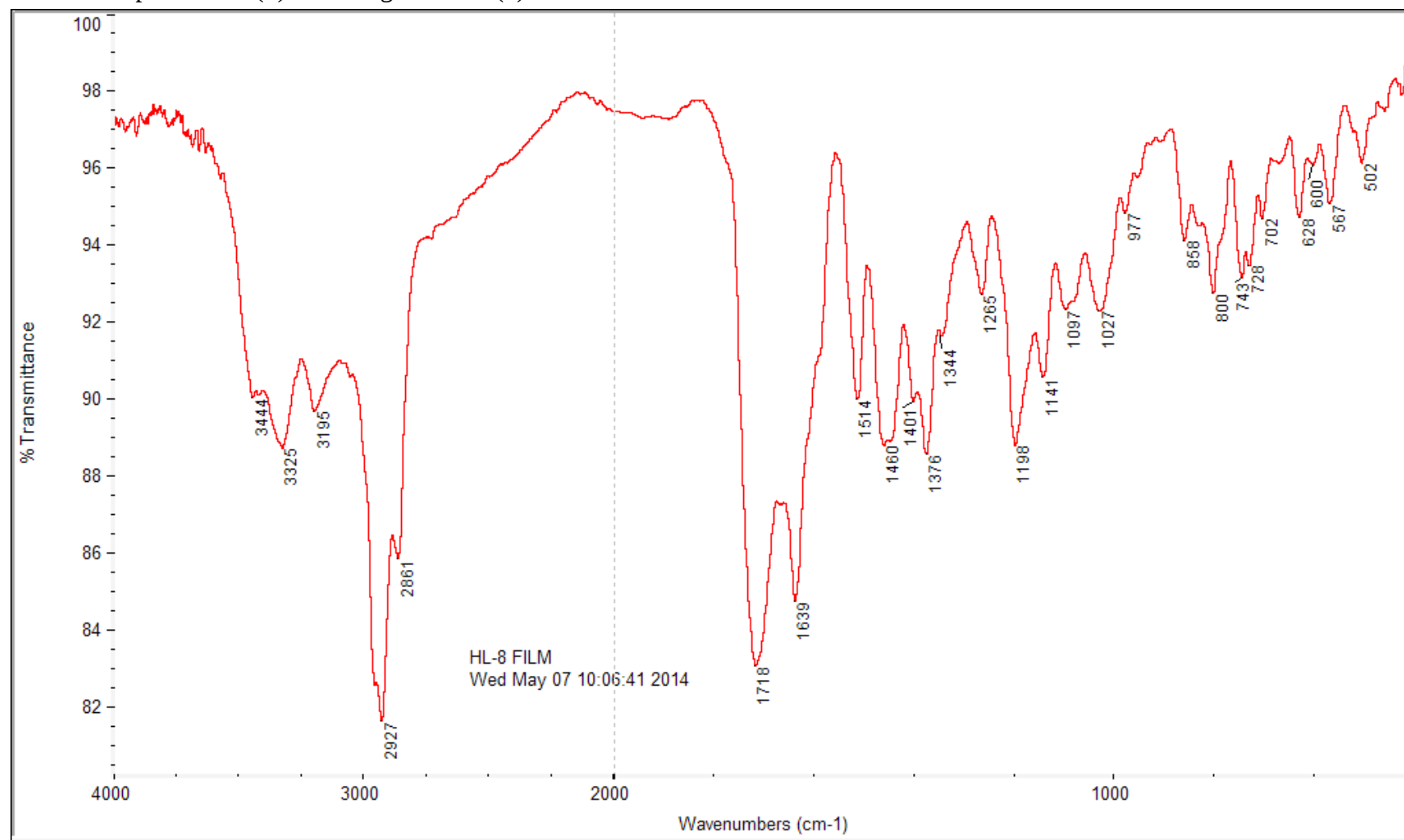


Figure S12. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) spectrum of (+)-agelasine B (2)

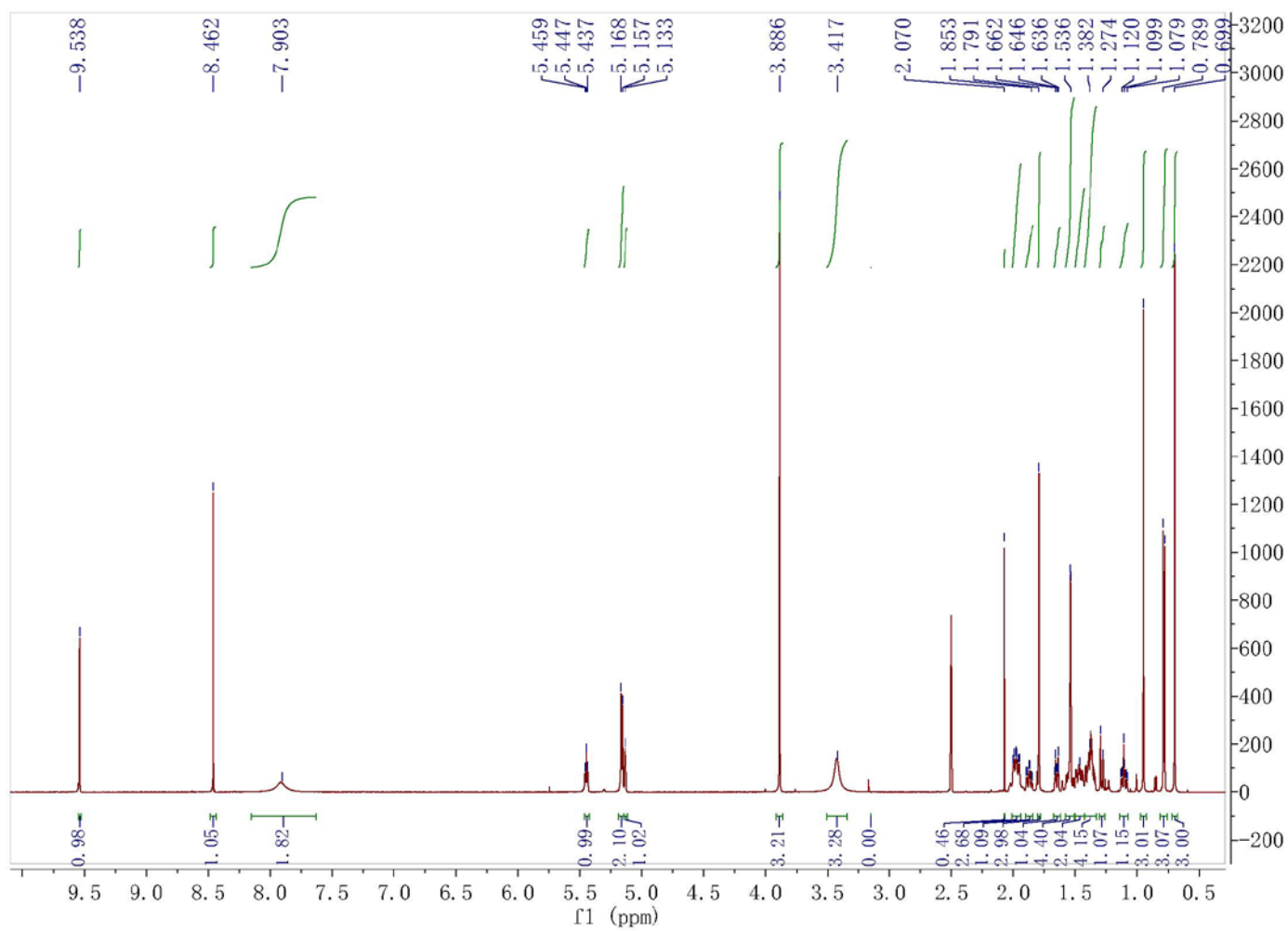


Figure S13. ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of (+)-agelasine B (**2**)

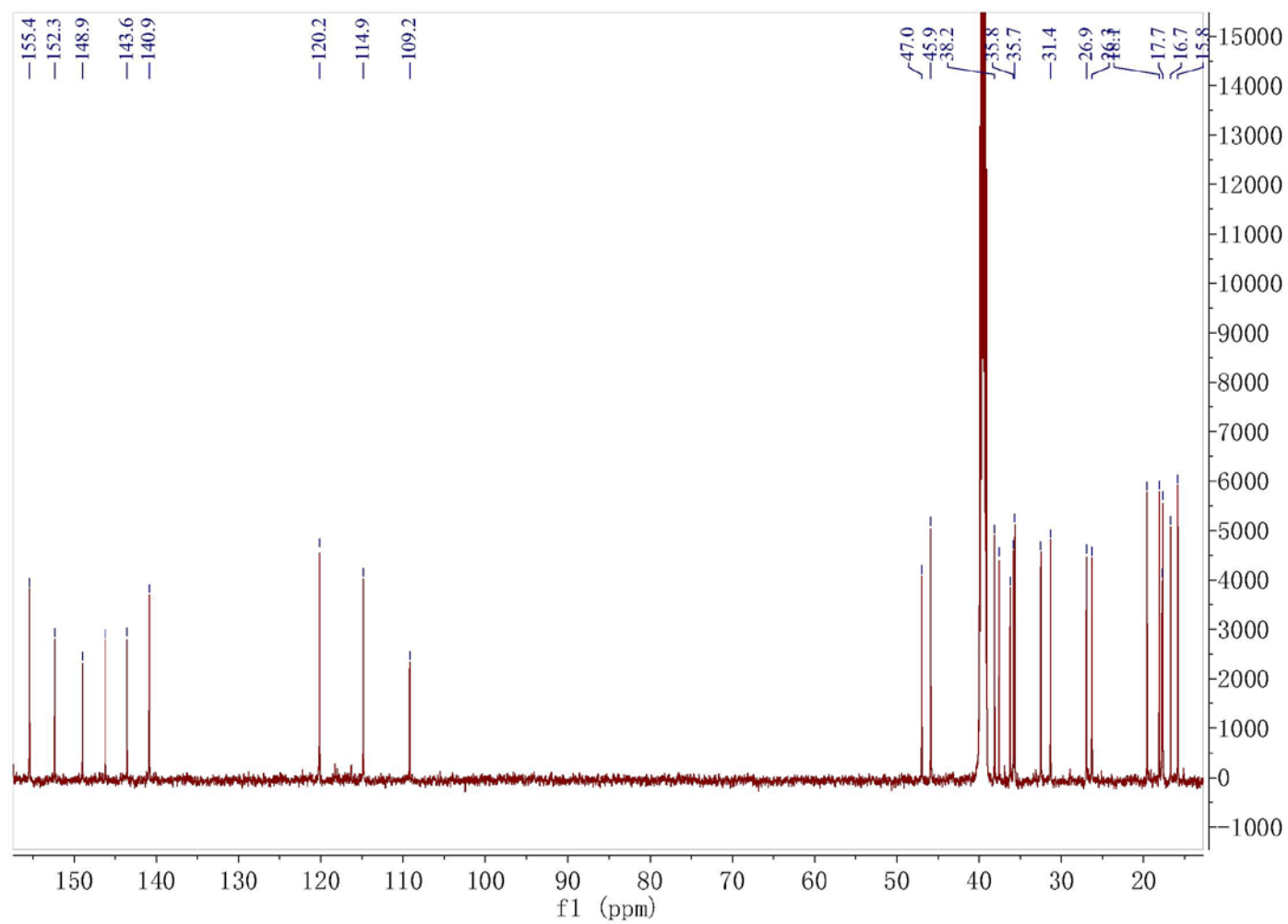


Figure S14. DEPT135 spectrum of (+)-agelasine B (**2**) in DMSO-*d*₆

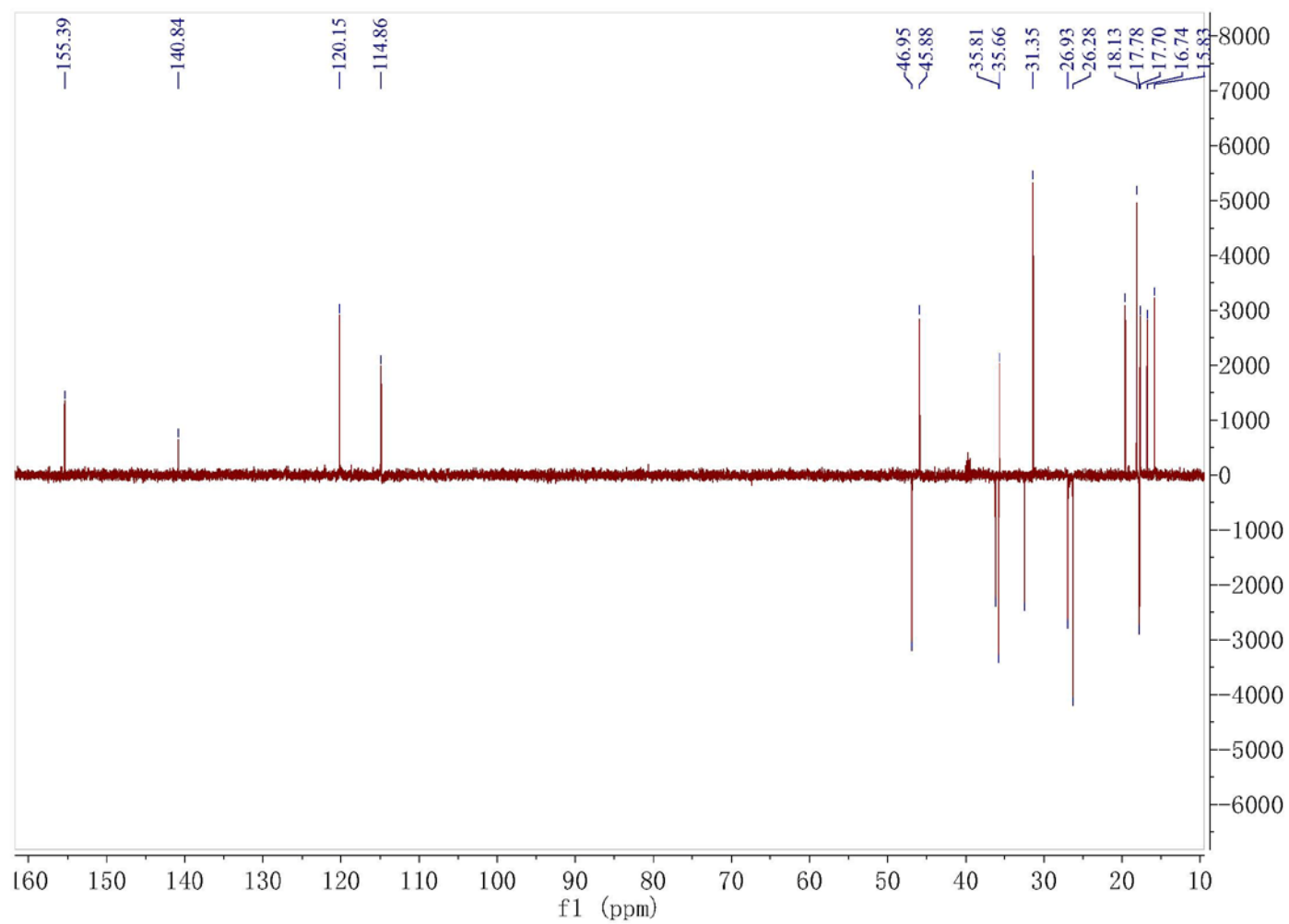


Figure S15. HSQC spectrum of (+)-agelasine B (**2**) in DMSO- d_6

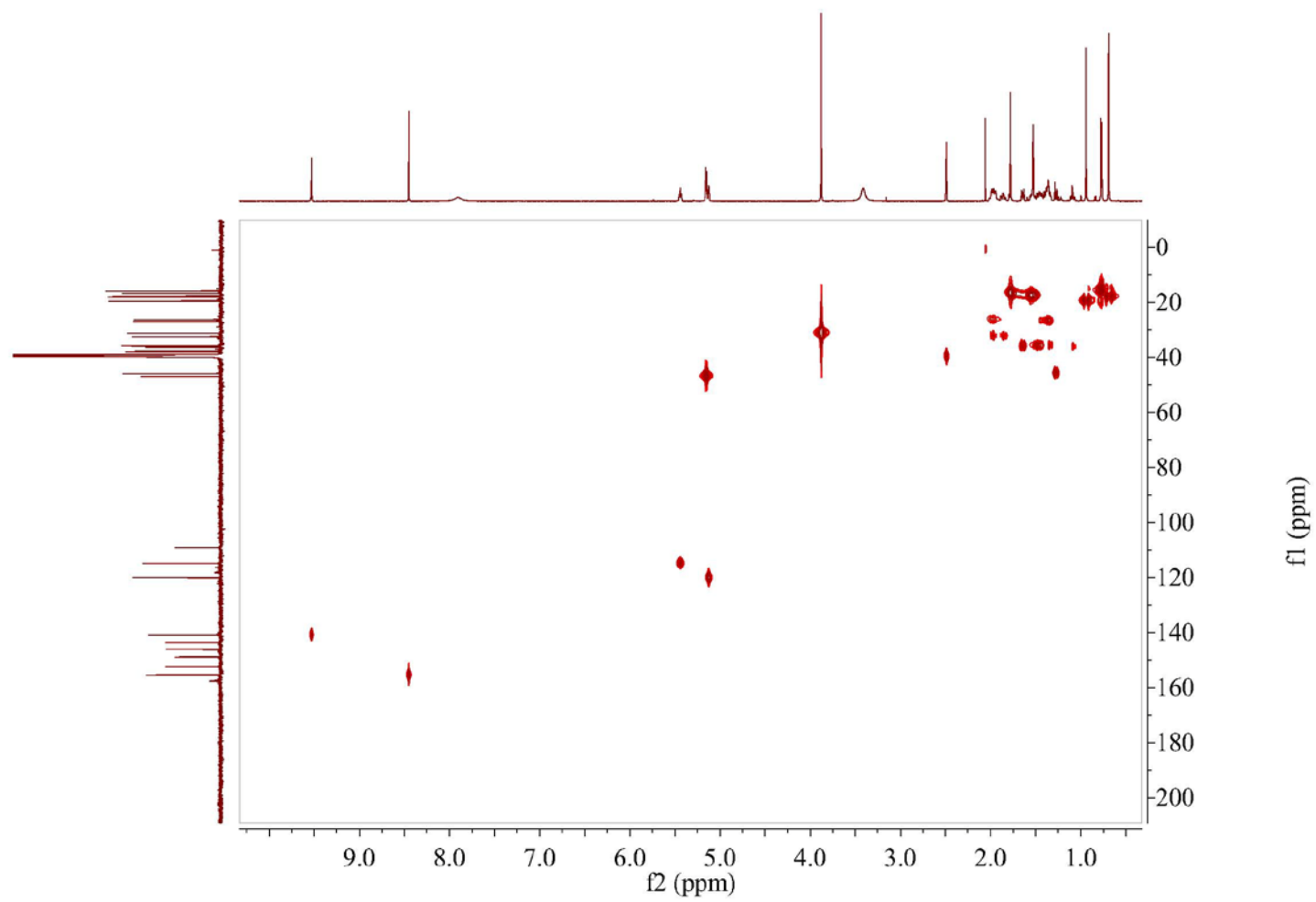


Figure S16. COSY spectrum of (+)-agelasine B (**2**) in DMSO- d_6

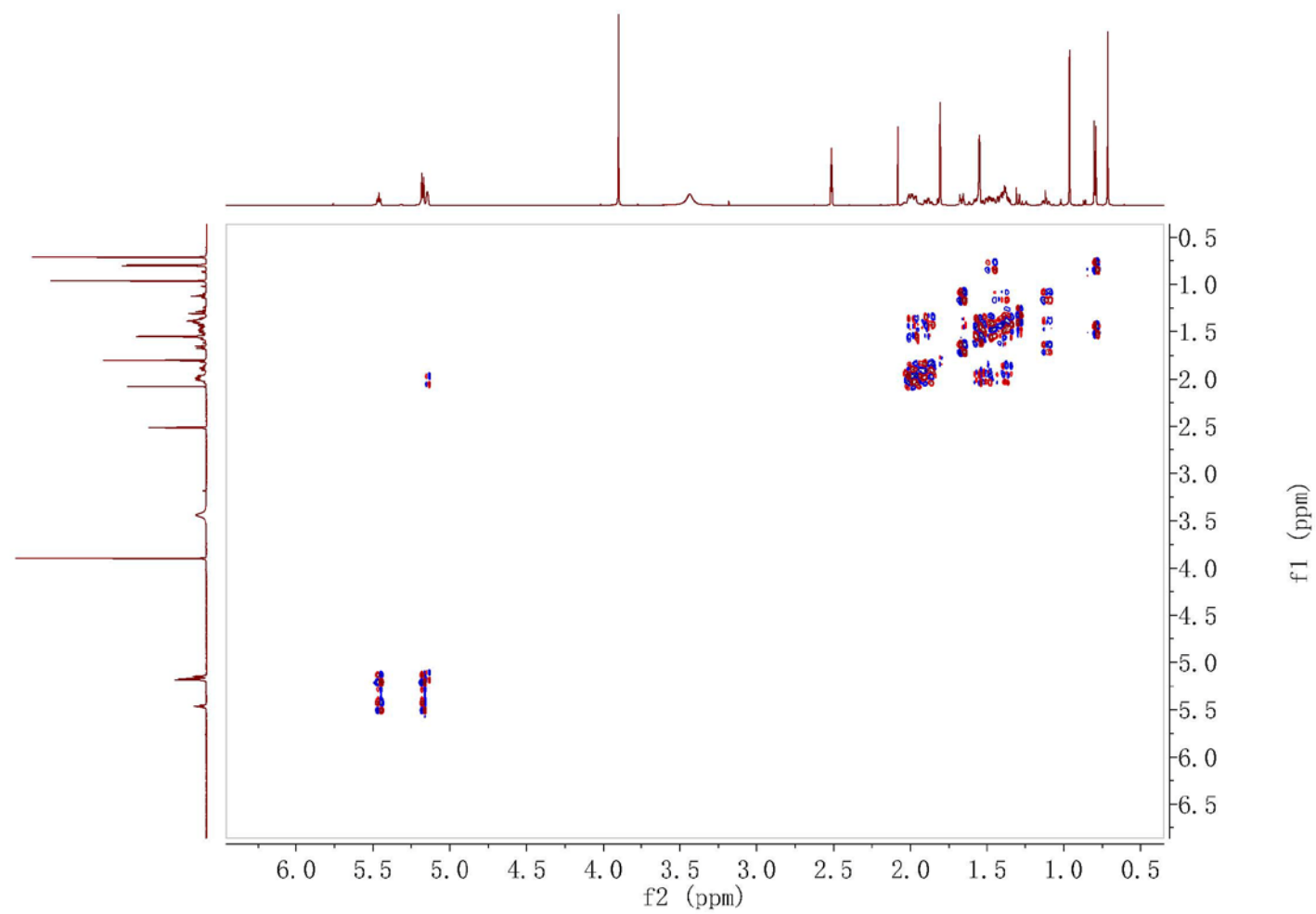


Figure S17. HMBC spectrum of (+)-agelasine B (**2**) in DMSO- d_6

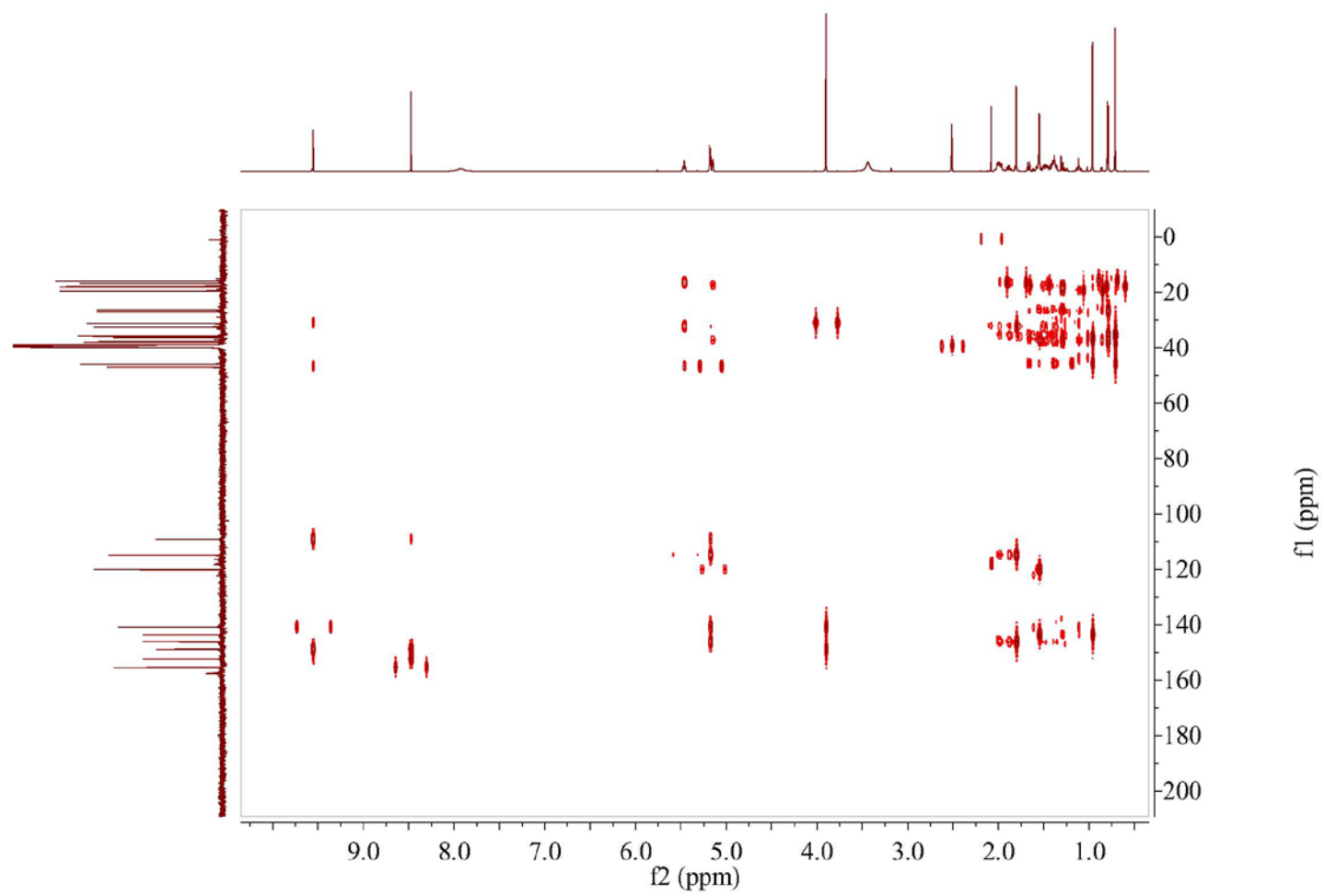


Figure S18. NOESY spectrum of (+)-agelasine B (**2**) in DMSO- d_6

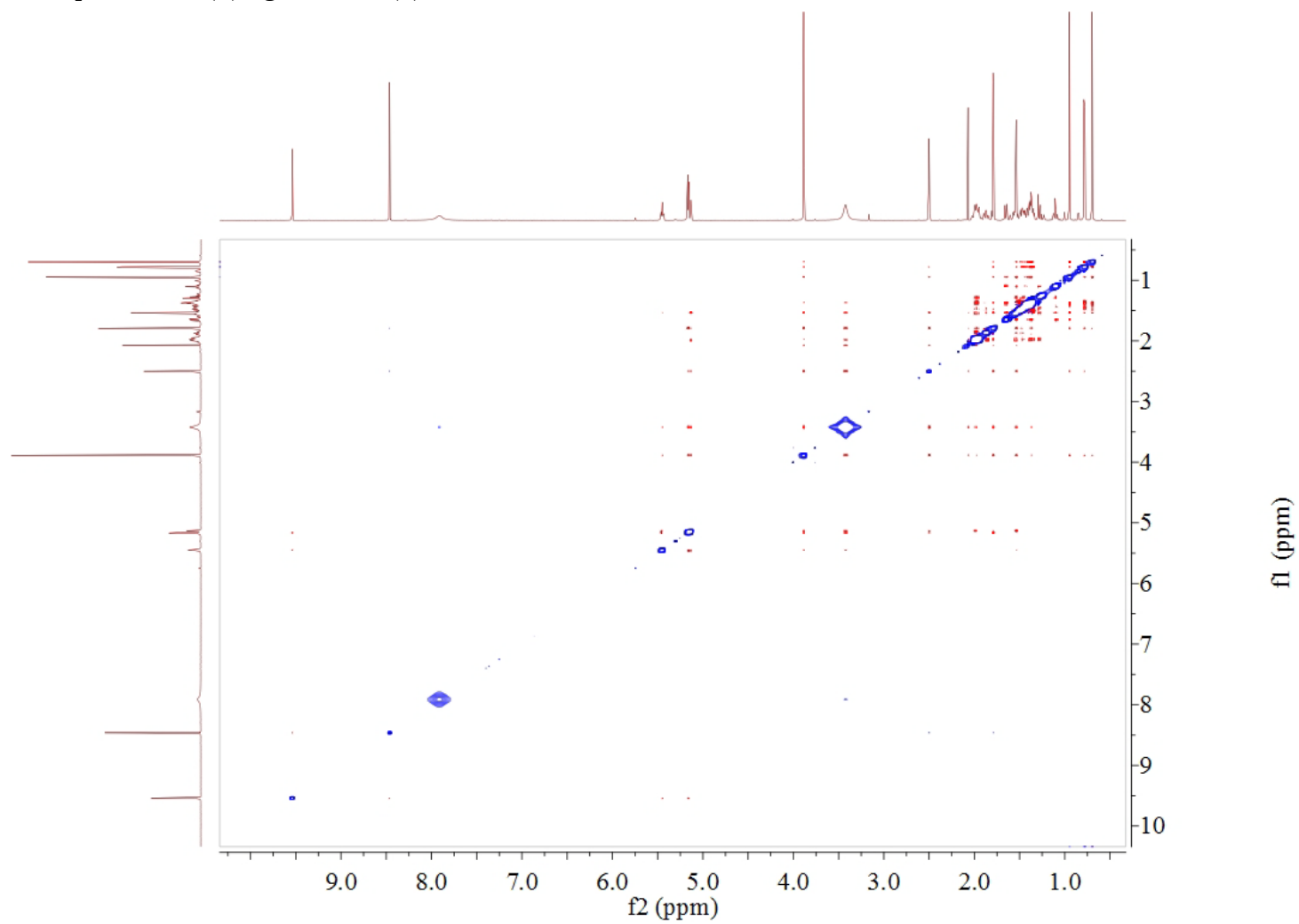


Figure S19. HRESIMS of (+)-agelasine B (2)

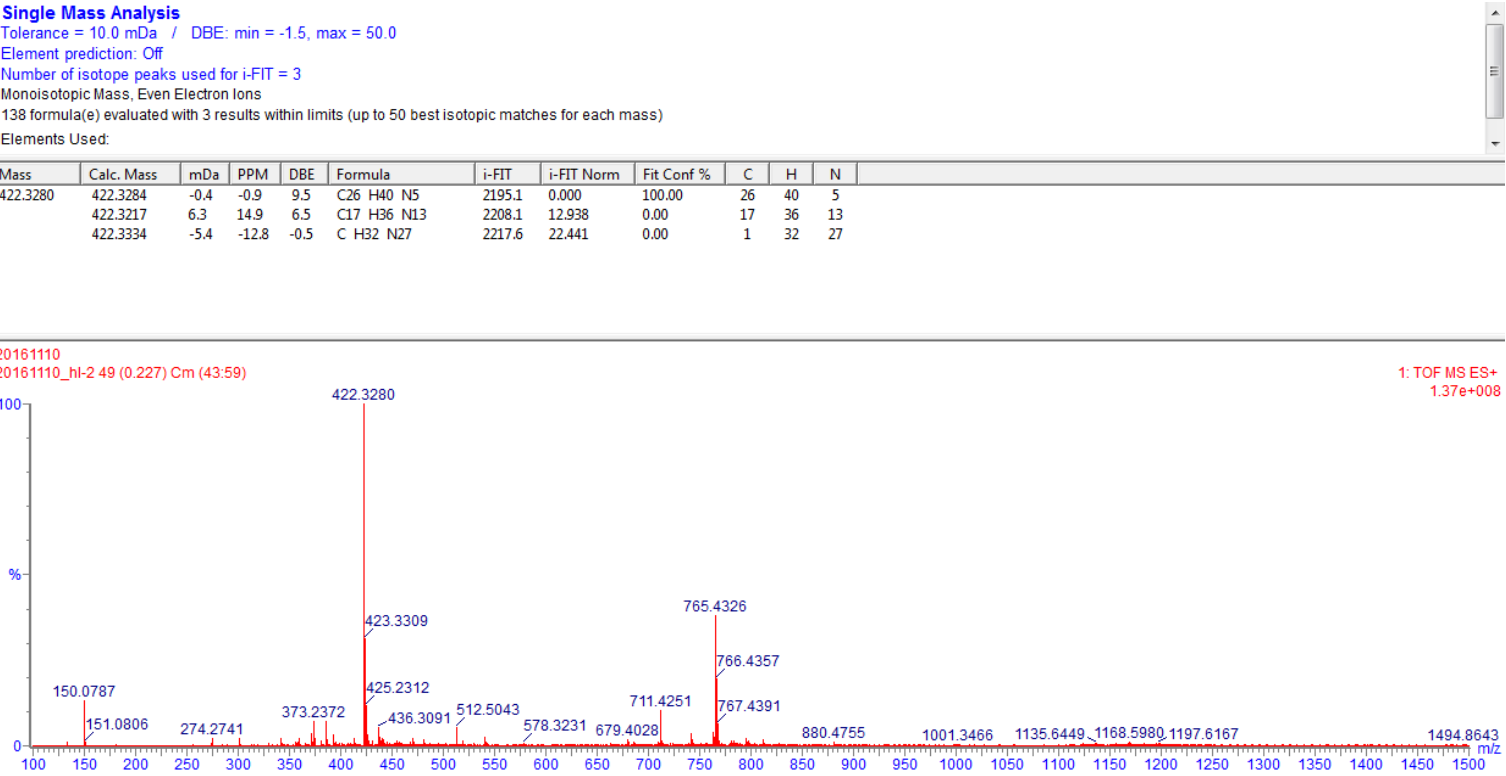


Figure S20. UV spectrum of (+)-agelasine B (**2**) in MeOH

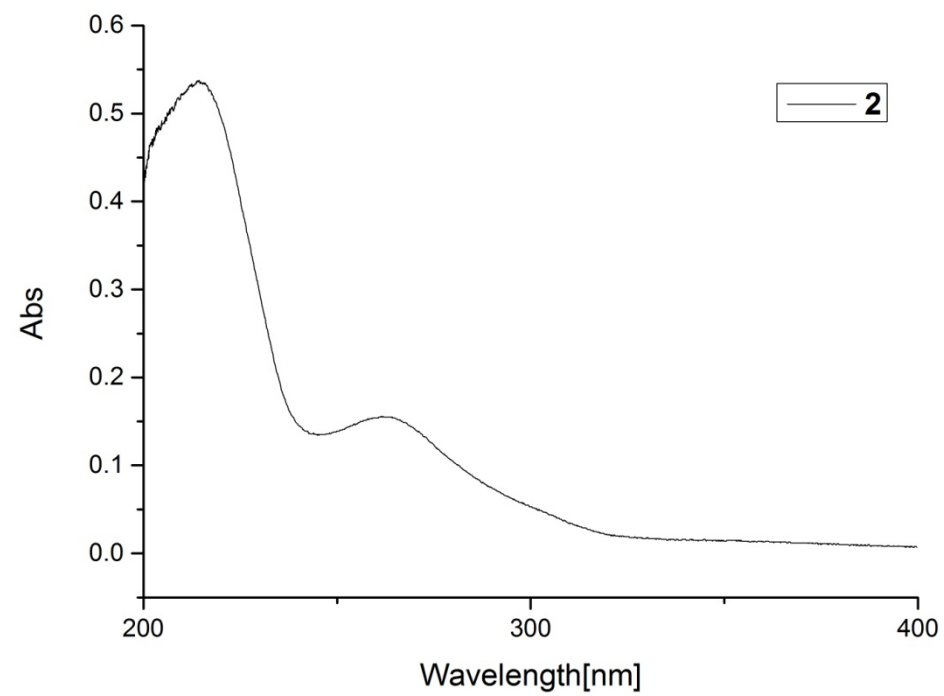


Figure S21. IR spectrum of (+)-agelasine B (2)

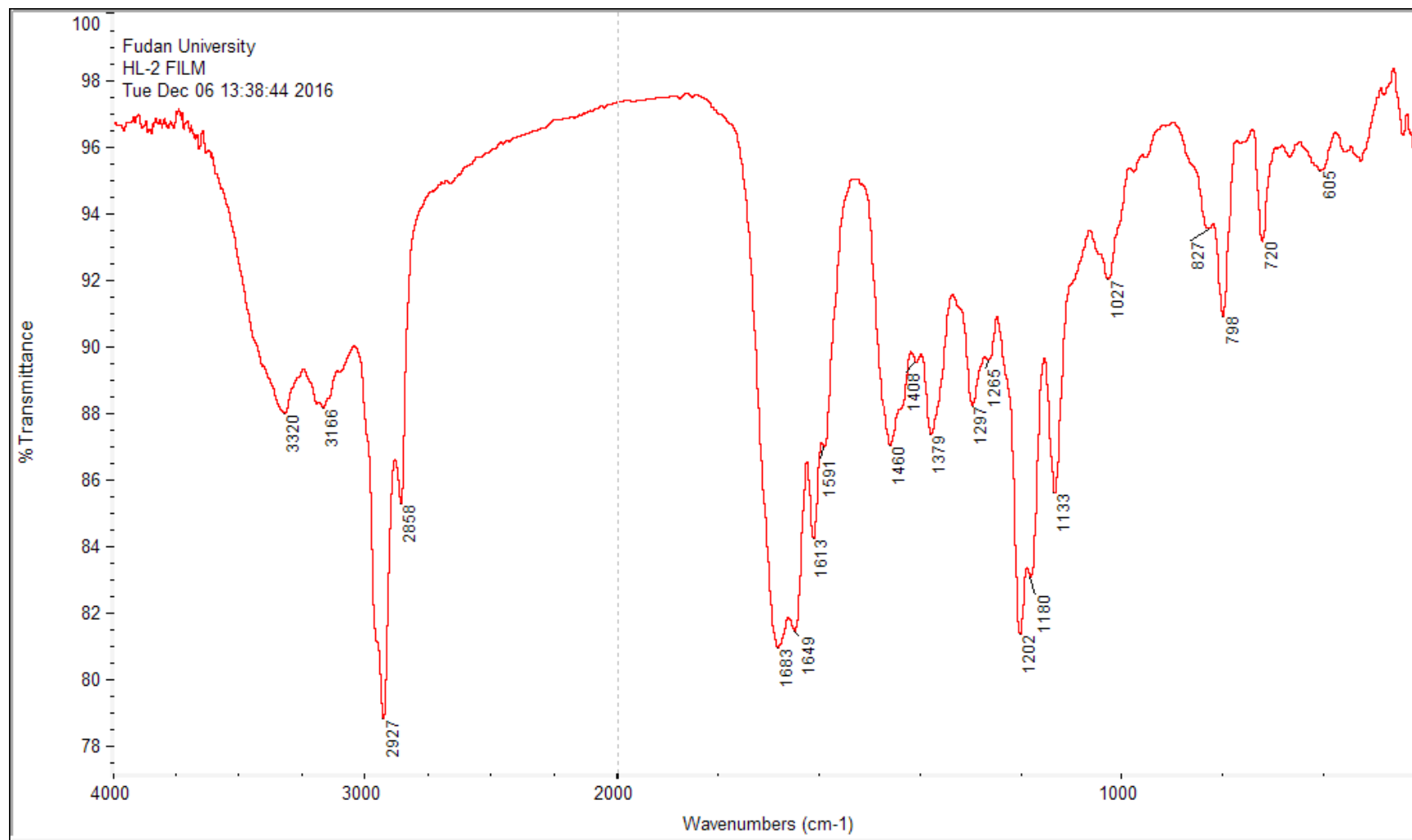


Figure S22. ^1H NMR (600 MHz, CDCl_3) spectrum of (+)-8'-oxo-*epi*-agelasine C (**3**)

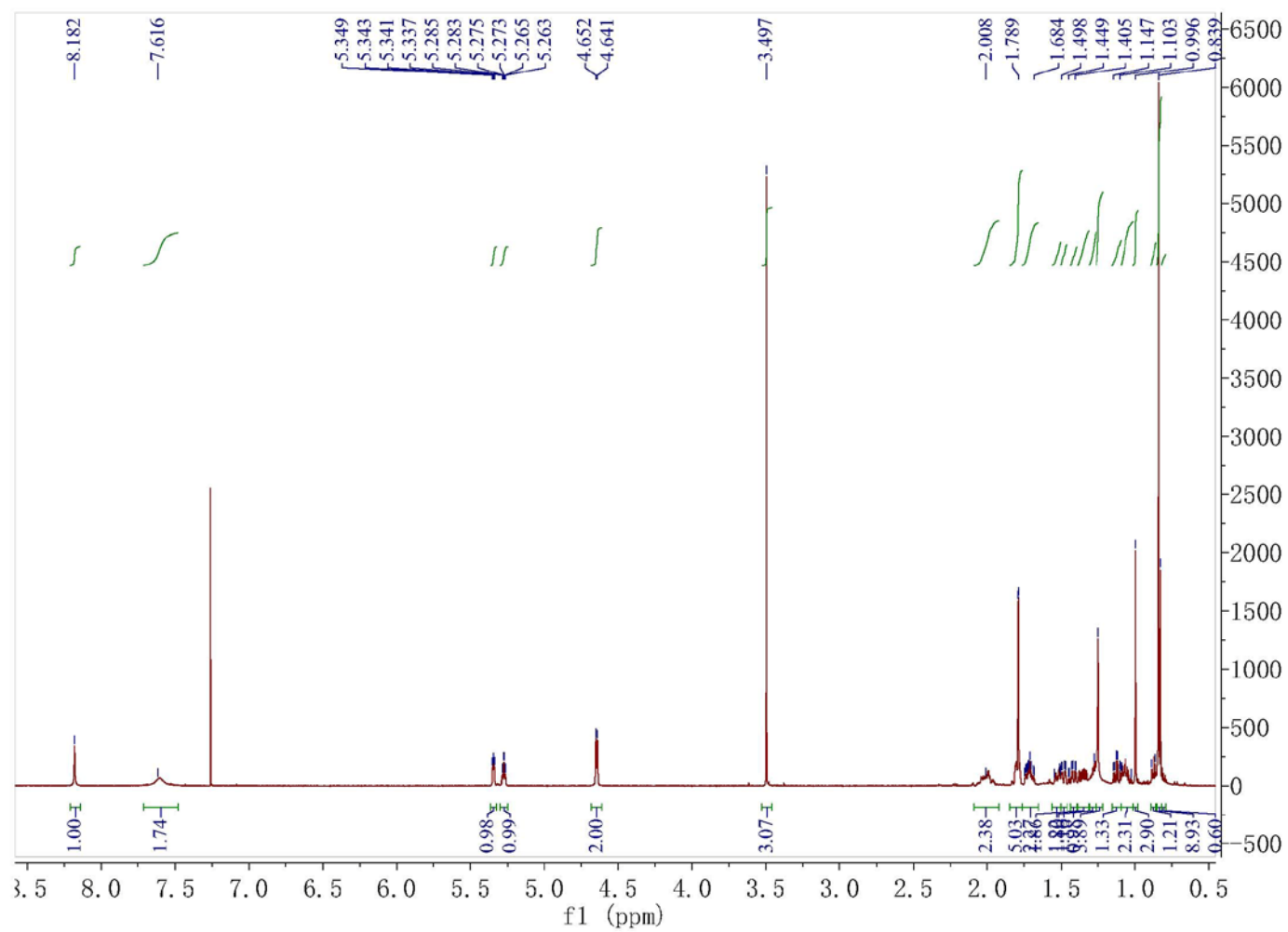


Figure S23. ^{13}C NMR (150 MHz, CDCl_3) spectrum of (+)-8'-oxo-*epi*-agelasine C (**3**)

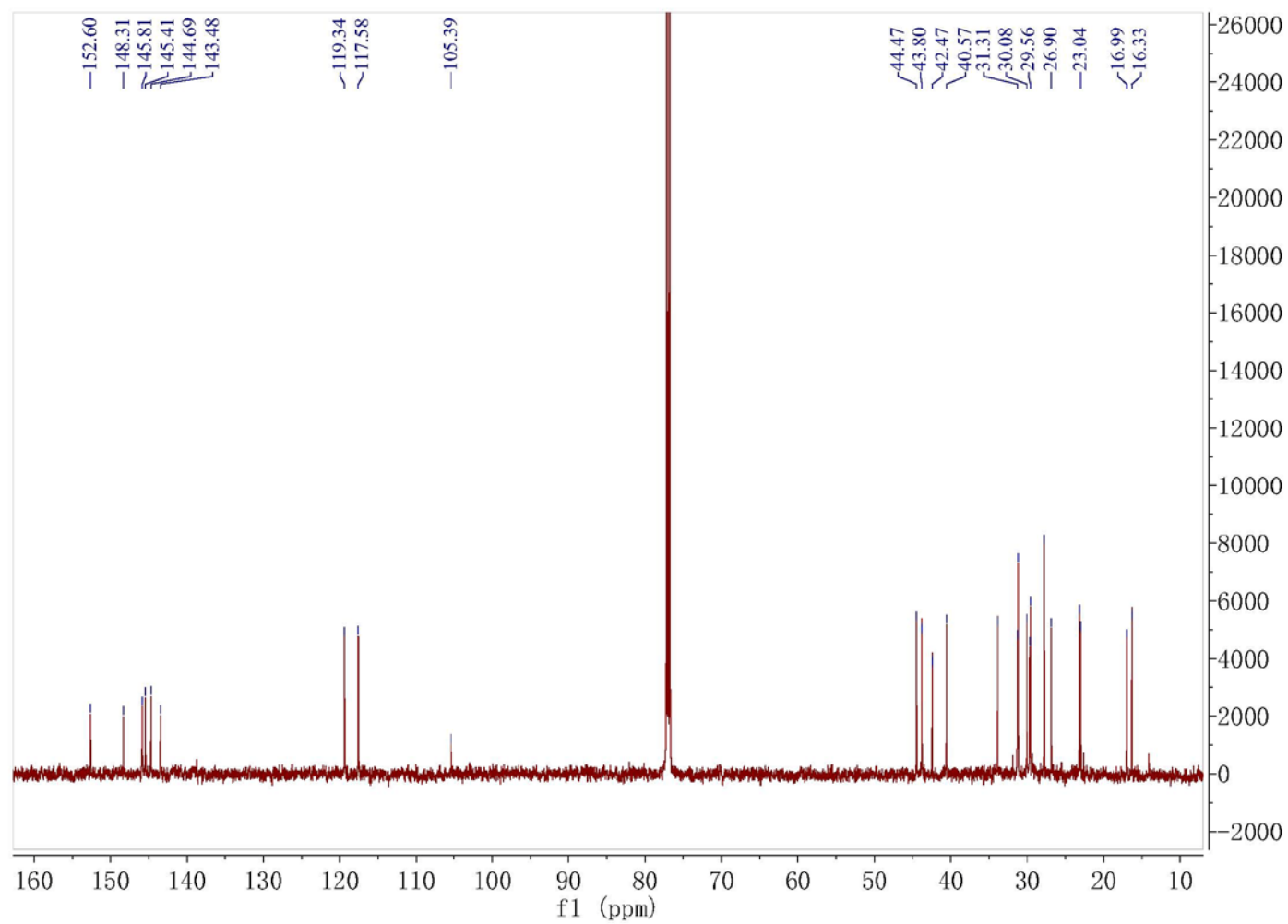


Figure S24. DEPT135 spectrum of (+)-8'-oxo-*epi*-agelasine C (**3**) in CDCl₃

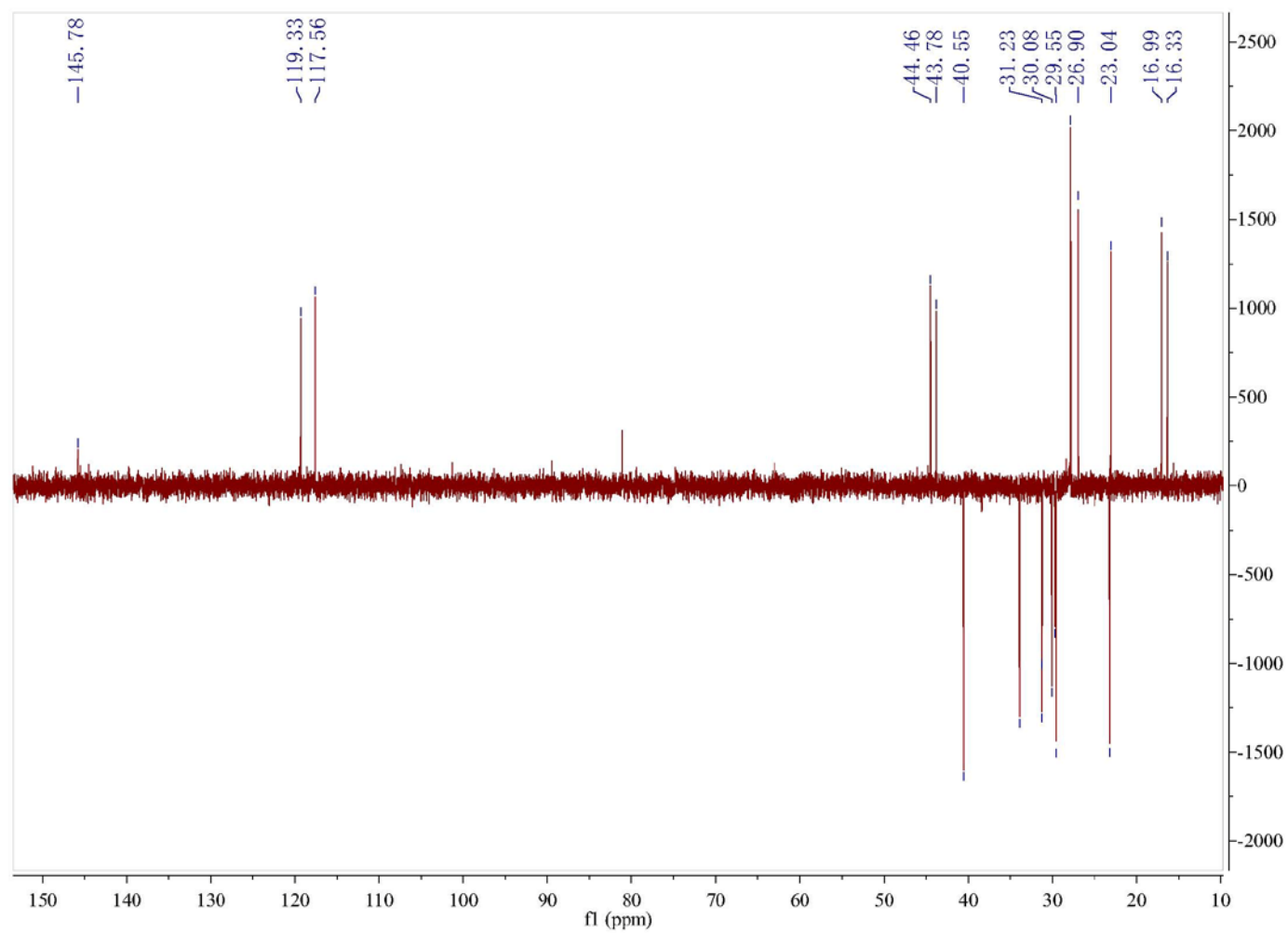


Figure S25. HSQC spectrum of (+)-8'-oxo-*epi*-agelasine C (**3**) in CDCl₃

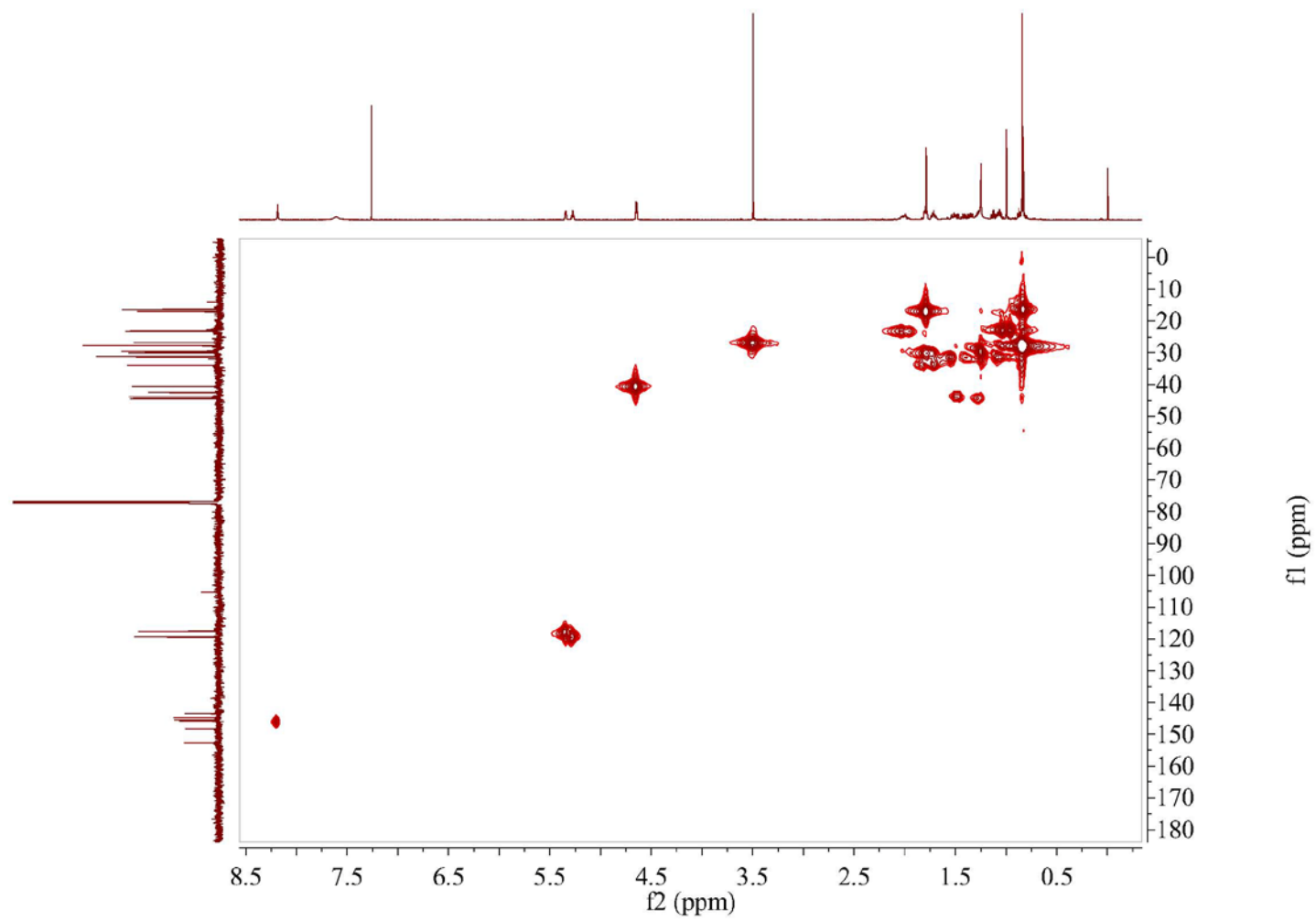


Figure S26. COSY spectrum of (+)-8'-oxo-*epi*-agelasine C (**3**) in CDCl₃

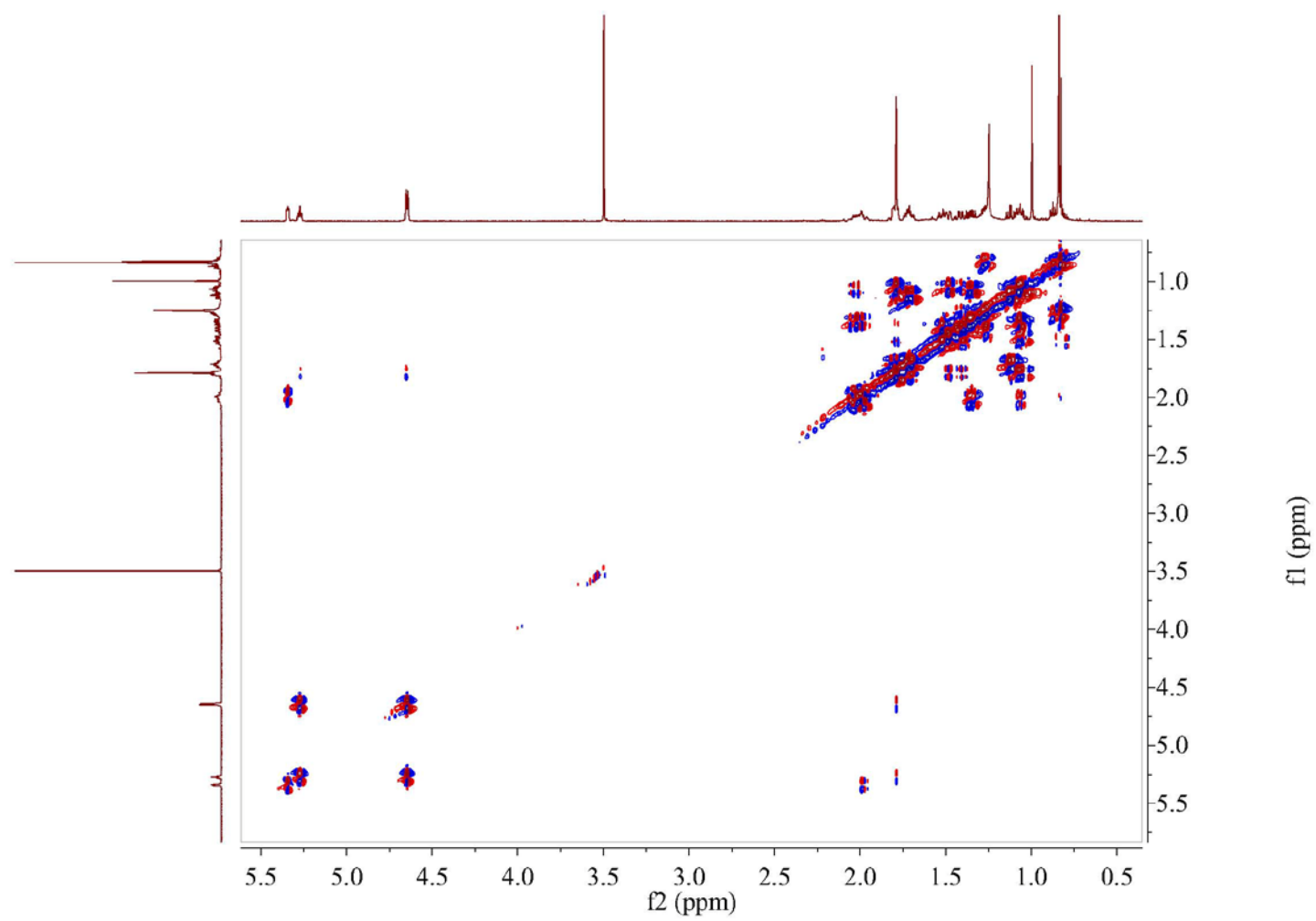


Figure S27. HMBC spectrum of (+)-8'-oxo-*epi*-agelasine C (**3**) in CDCl₃

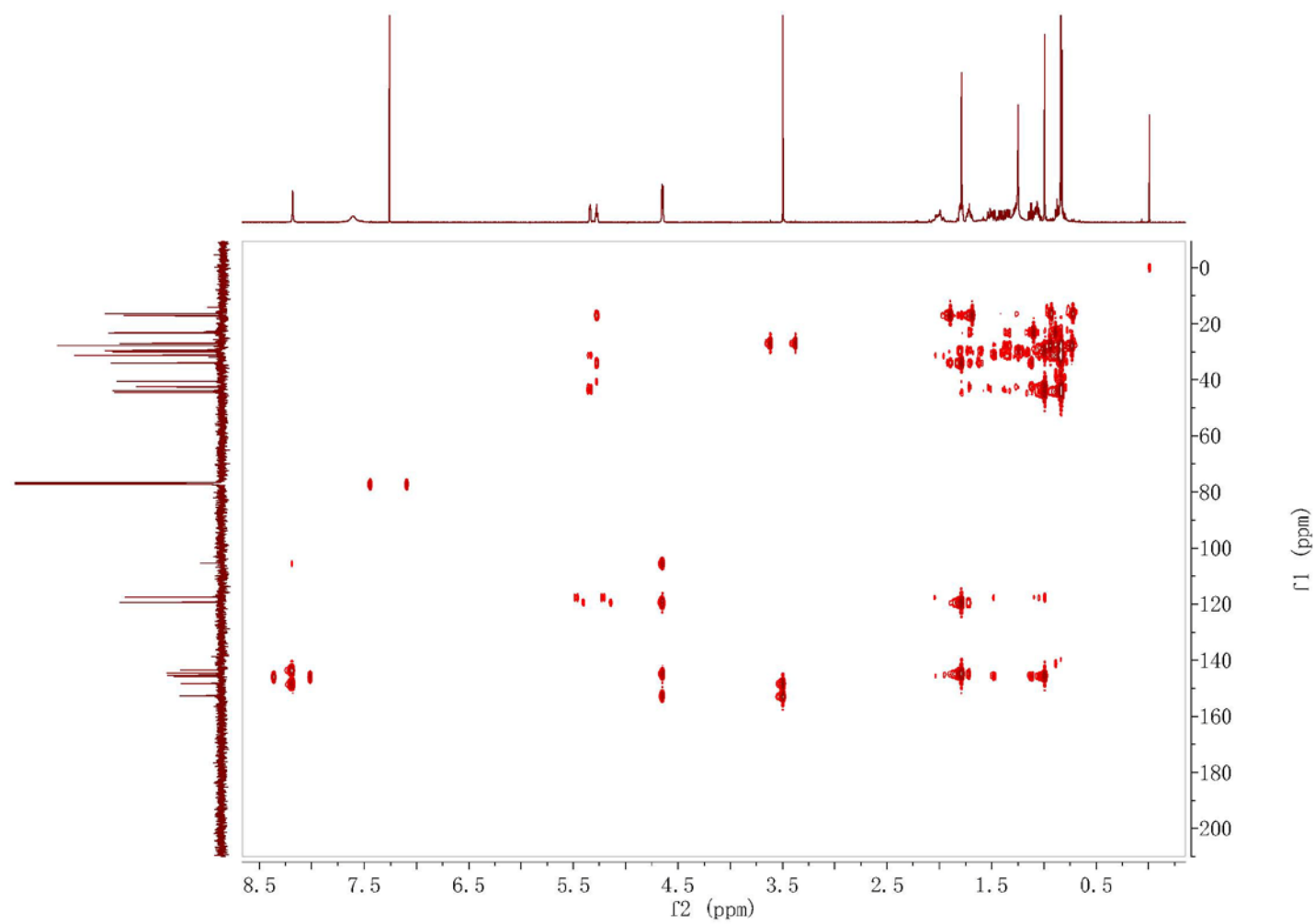


Figure S28. NOESY spectrum of (+)-8'-oxo-*epi*-agelasine C (**3**) in CDCl₃

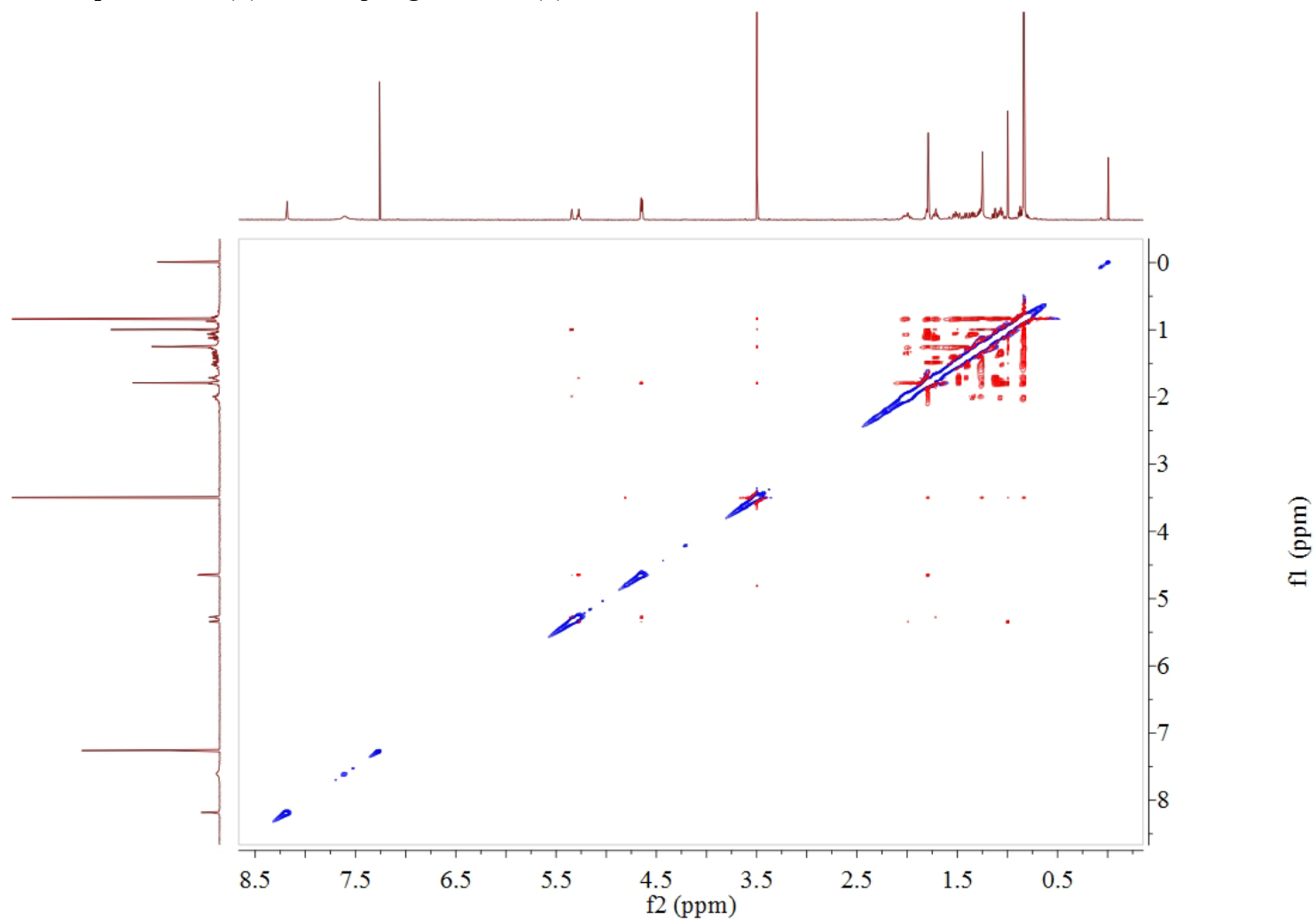


Figure S29. HRESIMS of (+)-8'-oxo-*epi*-agelasine C (3)

Elemental Composition Report

Page 1

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

39 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 5-27 H: 5-50 N: 1-6 O: 1-3

SIPI

hi-6

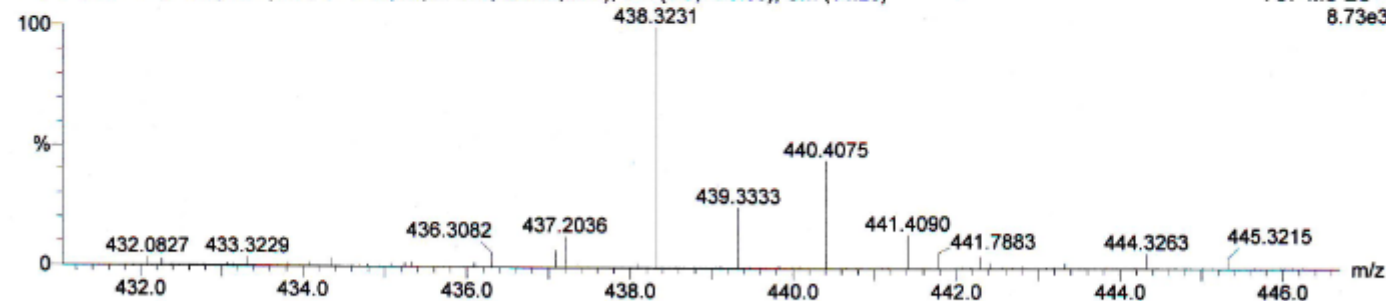
WQ13-135H 19 (0.656) AM (Cen,4, 80.00, Ar,5000.0,453.05,0.70); Sm (SG, 2x3.00); Cm (14:23)

Q-ToF micro

YA019

TOF MS ES+

8.73e3



Minimum:	50.00				-1.5		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
438.3231	100.00	438.3233	-0.2	-0.5	9.5	1955.2	C26 H40 N5 O

Figure S30. UV spectrum of (+)-8'-oxo-*epi*-agelasine C (**3**) in MeOH

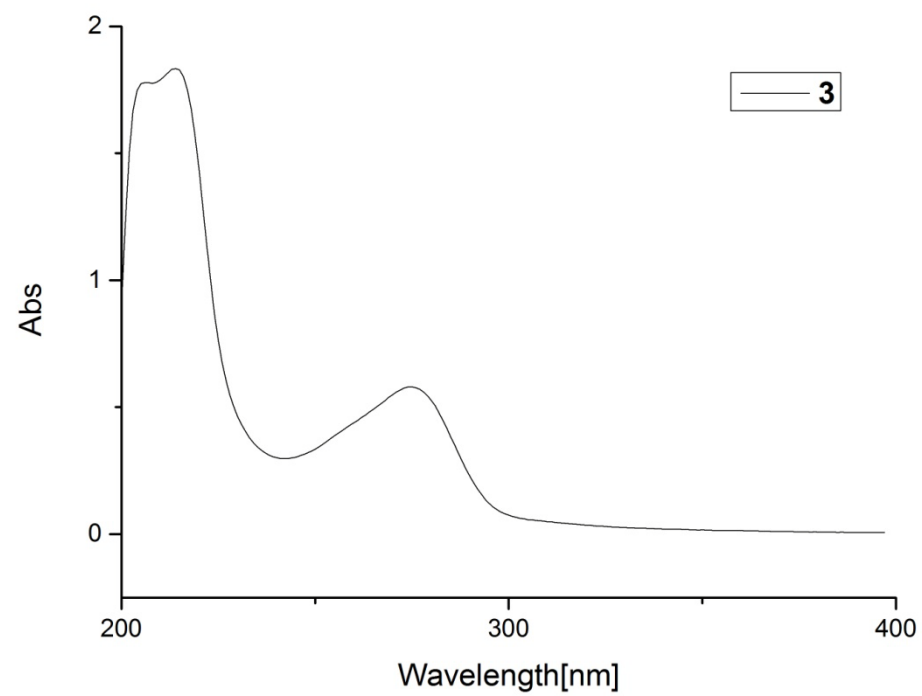


Figure S31. IR spectrum of (+)-8'-oxo-*epi*-agelasine C (**3**)

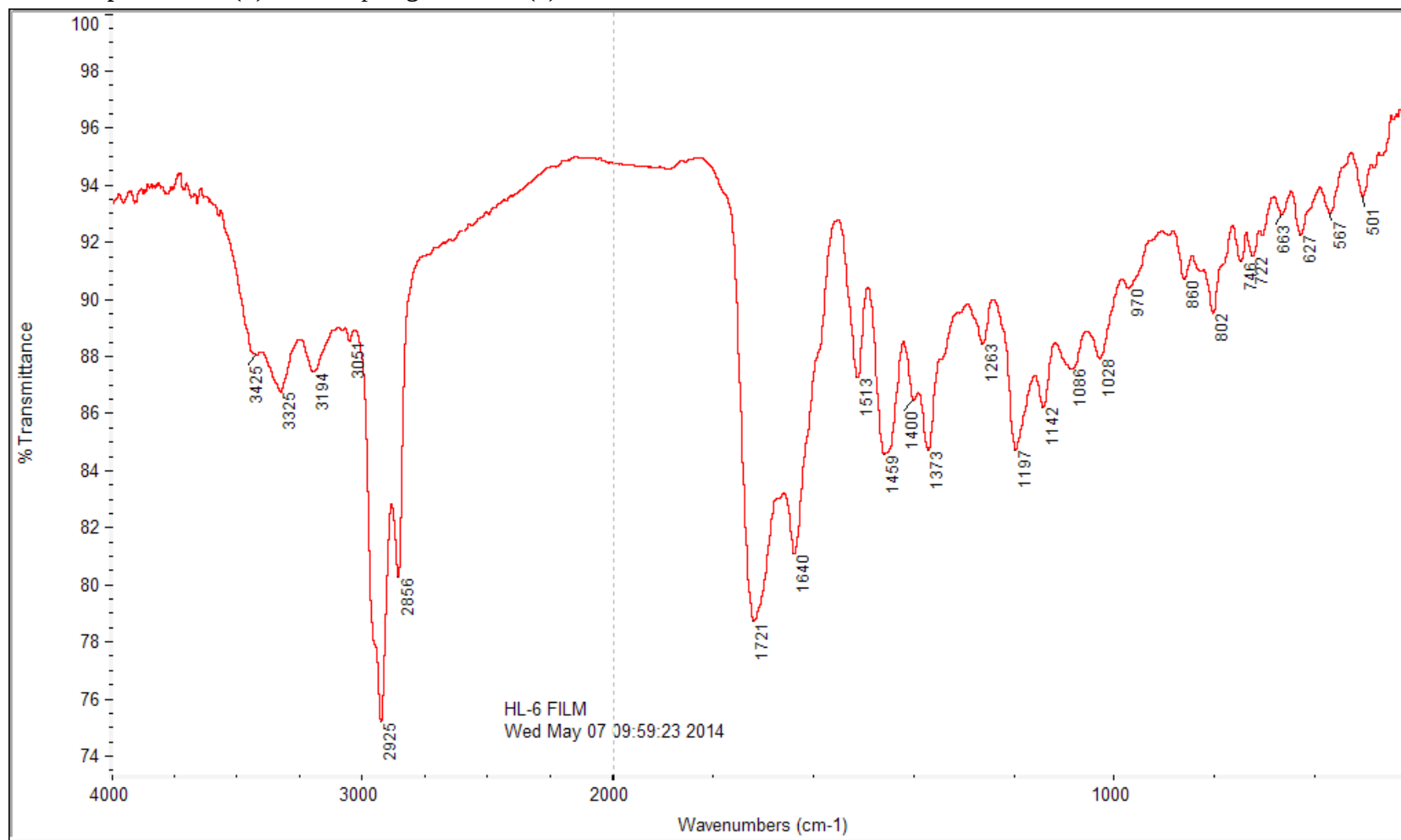


Figure S32. ^1H NMR (400 MHz, CDCl_3) spectrum of agelasine V (**4**)

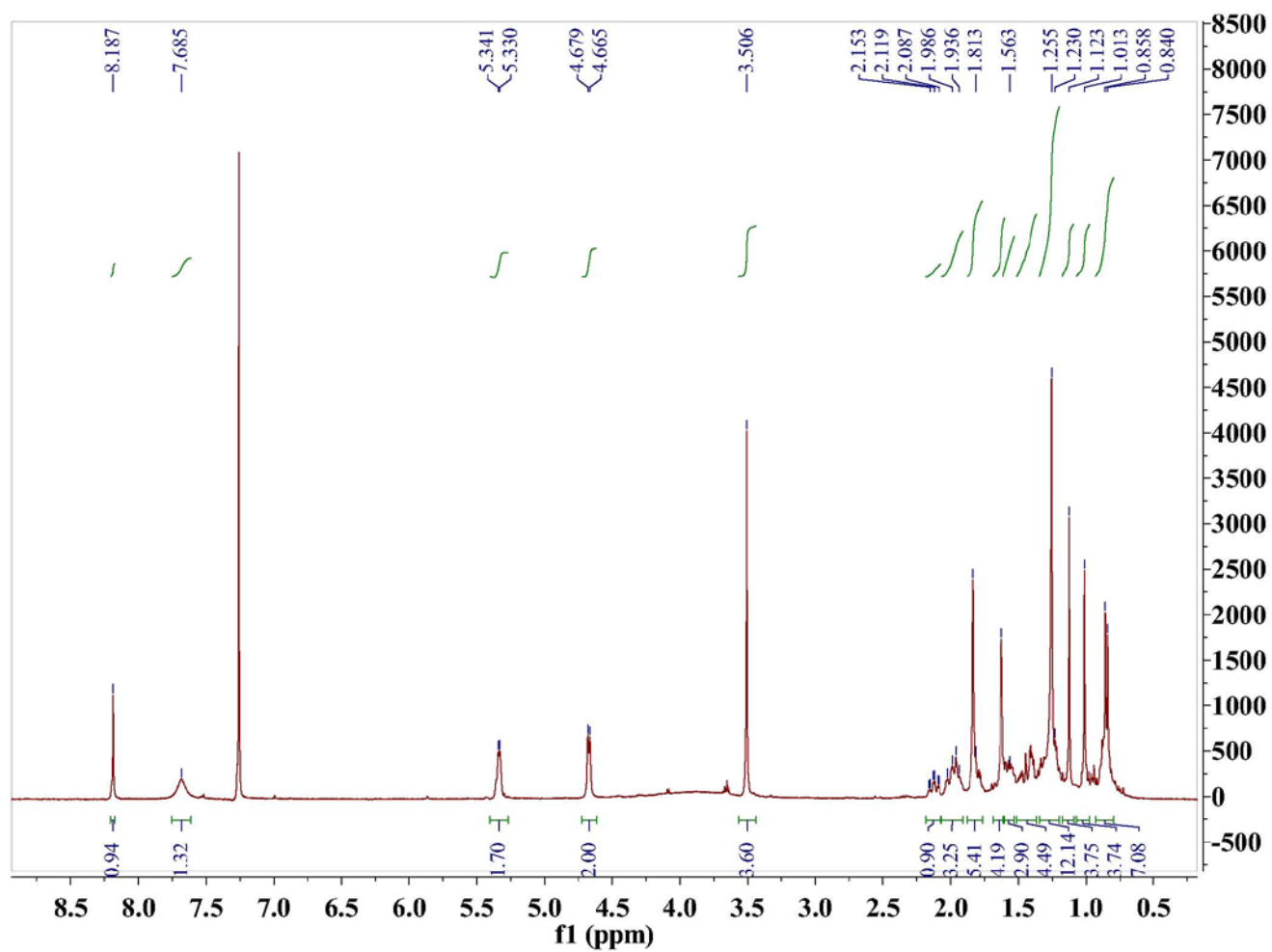


Figure S33. ^{13}C NMR (100 MHz, CDCl_3) spectrum of agelasine V (**4**)

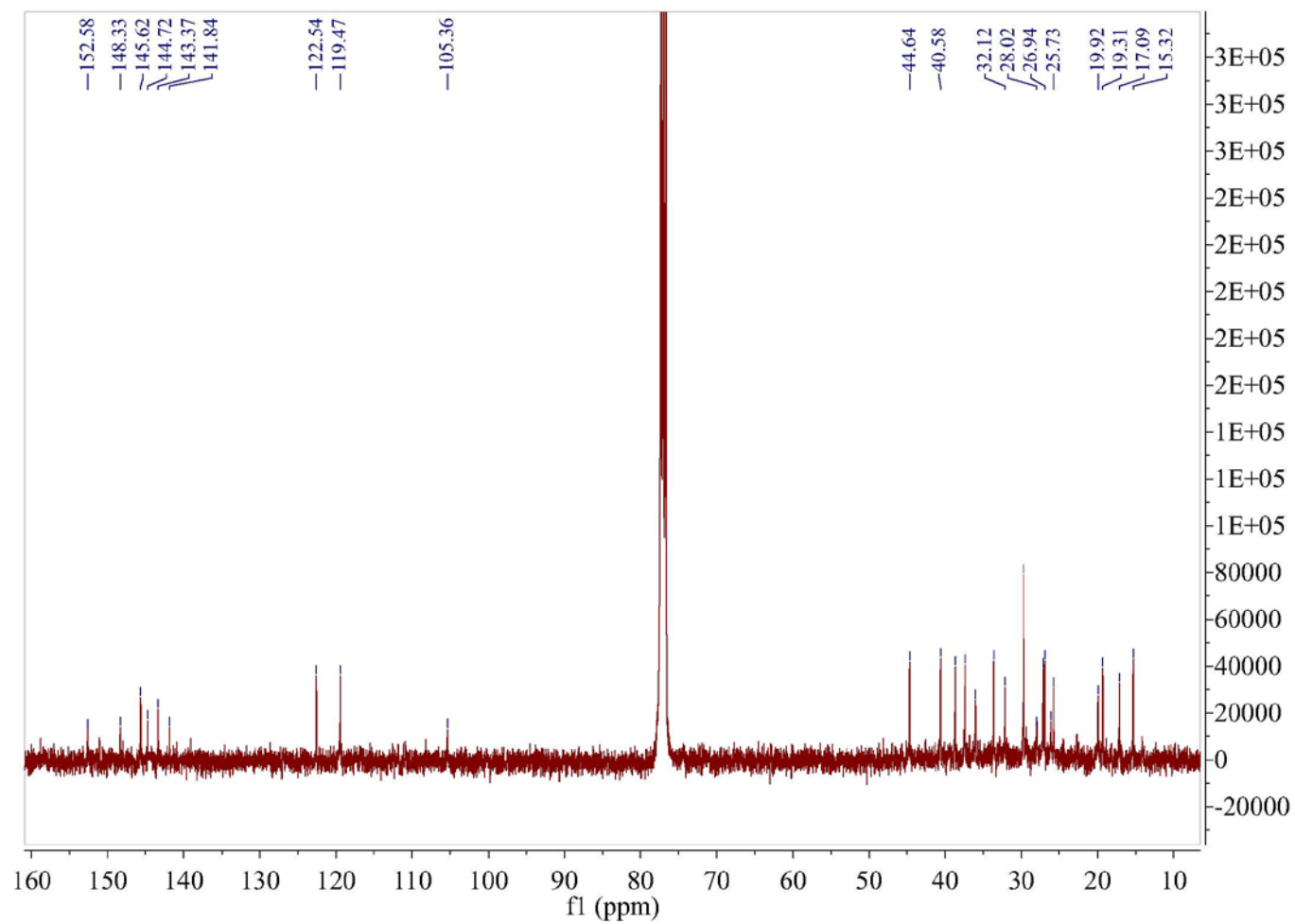


Figure S34. DEPT135 spectrum of agelasine V (**4**) in CDCl₃

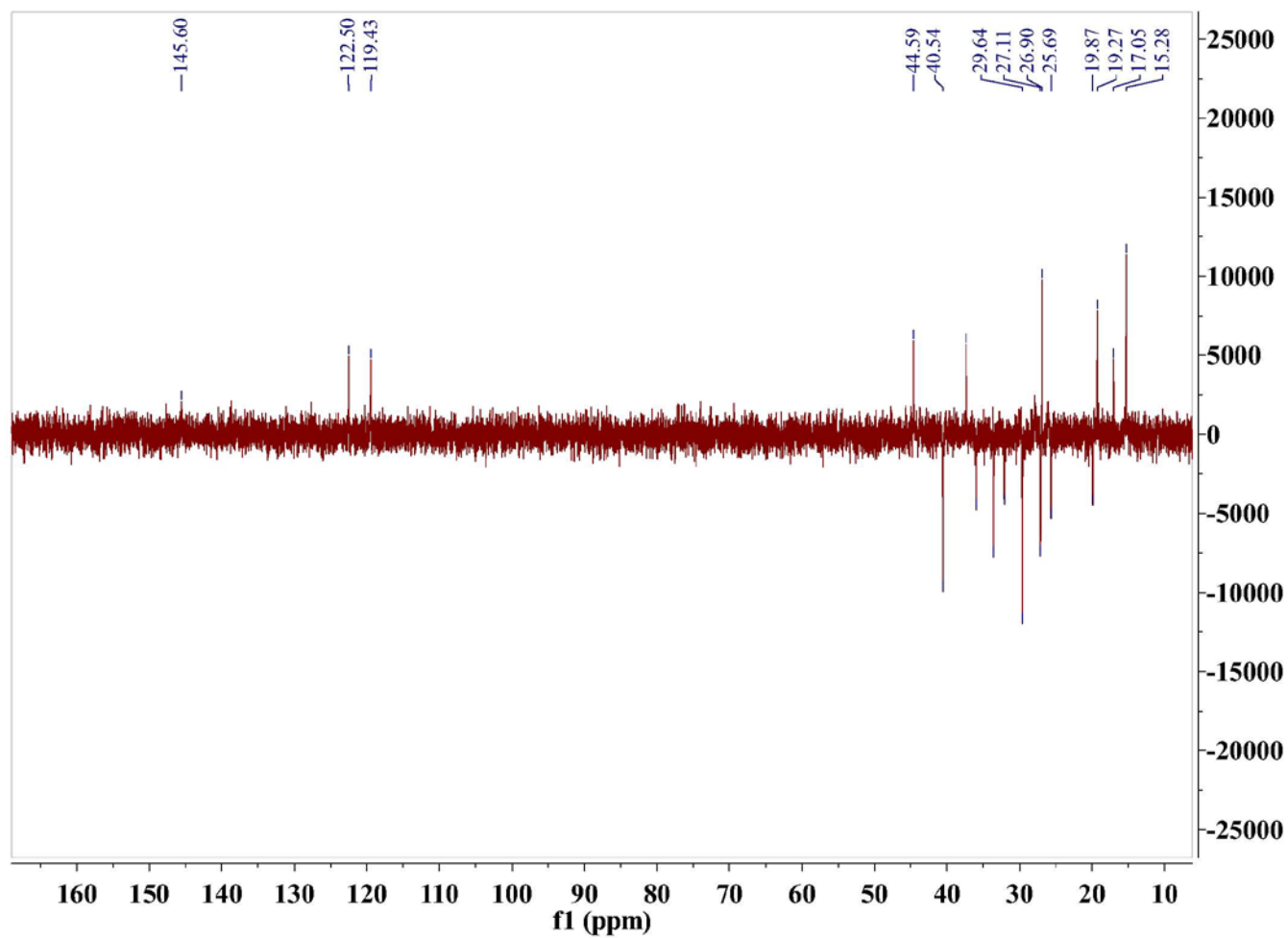


Figure S35. HSQC spectrum of agelasine V (**4**) in CDCl₃

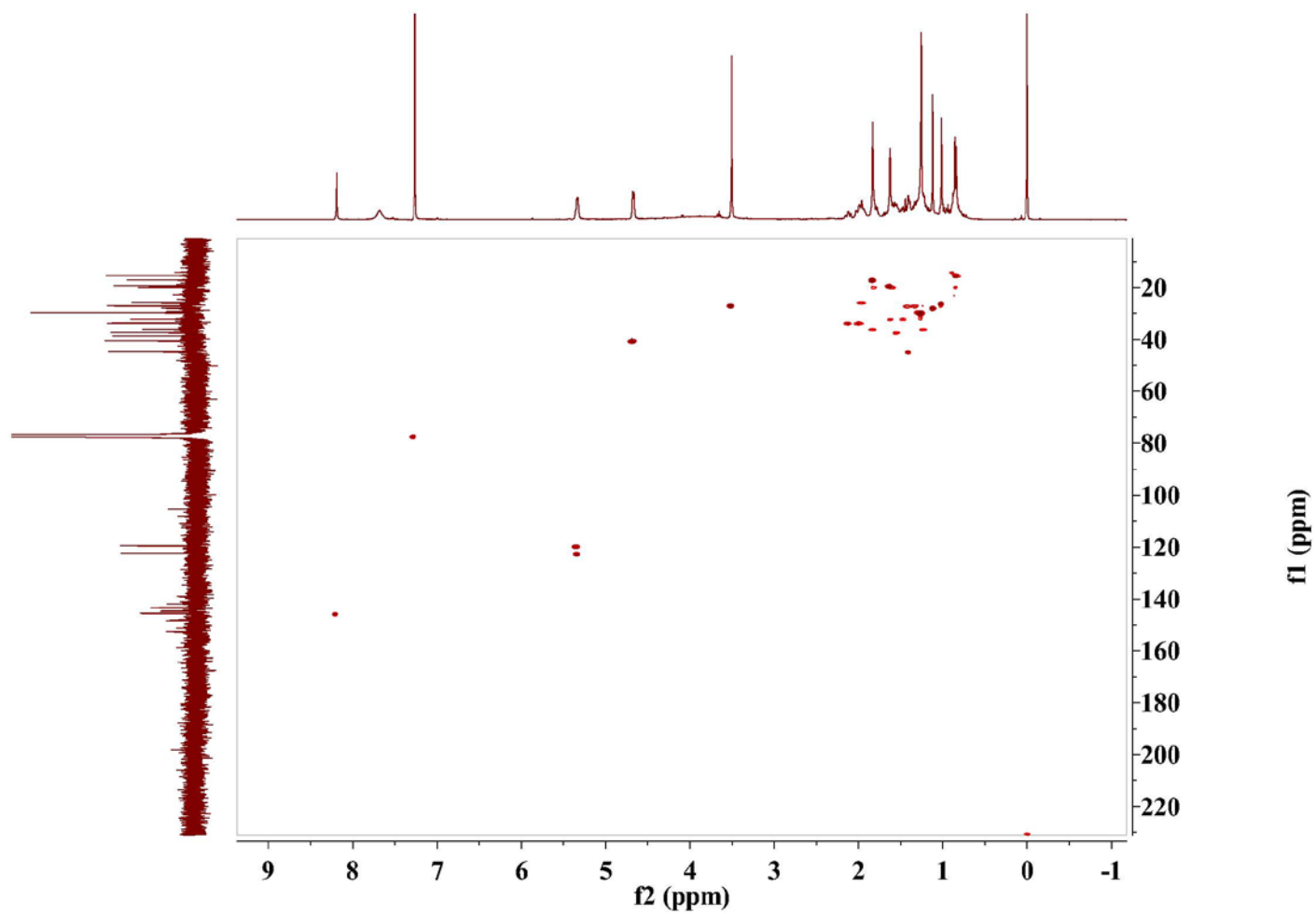


Figure S36. COSY spectrum of agelasine V (**4**) in CDCl₃

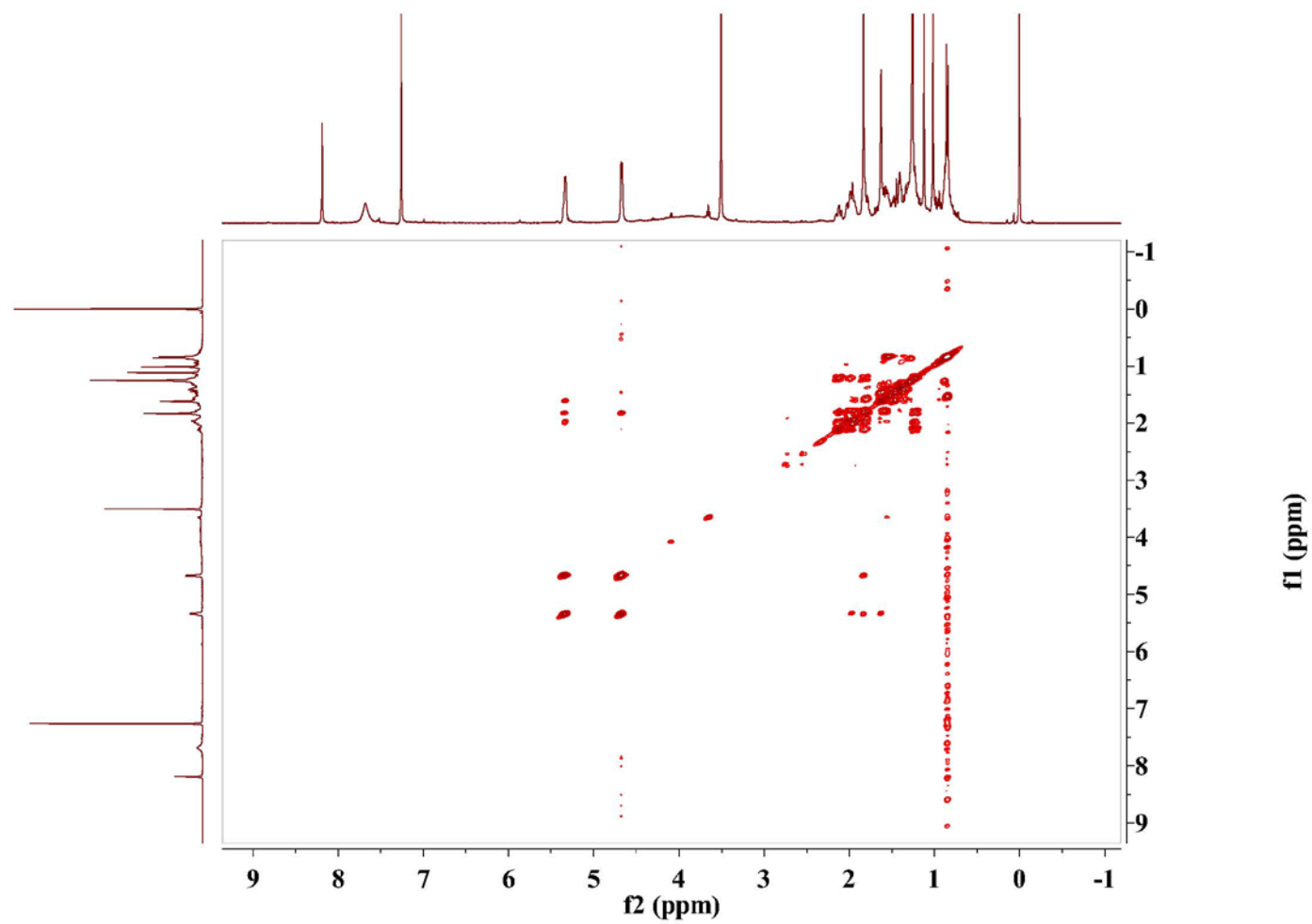


Figure S37. HMBC spectrum of agelasine V (**4**) in CDCl₃

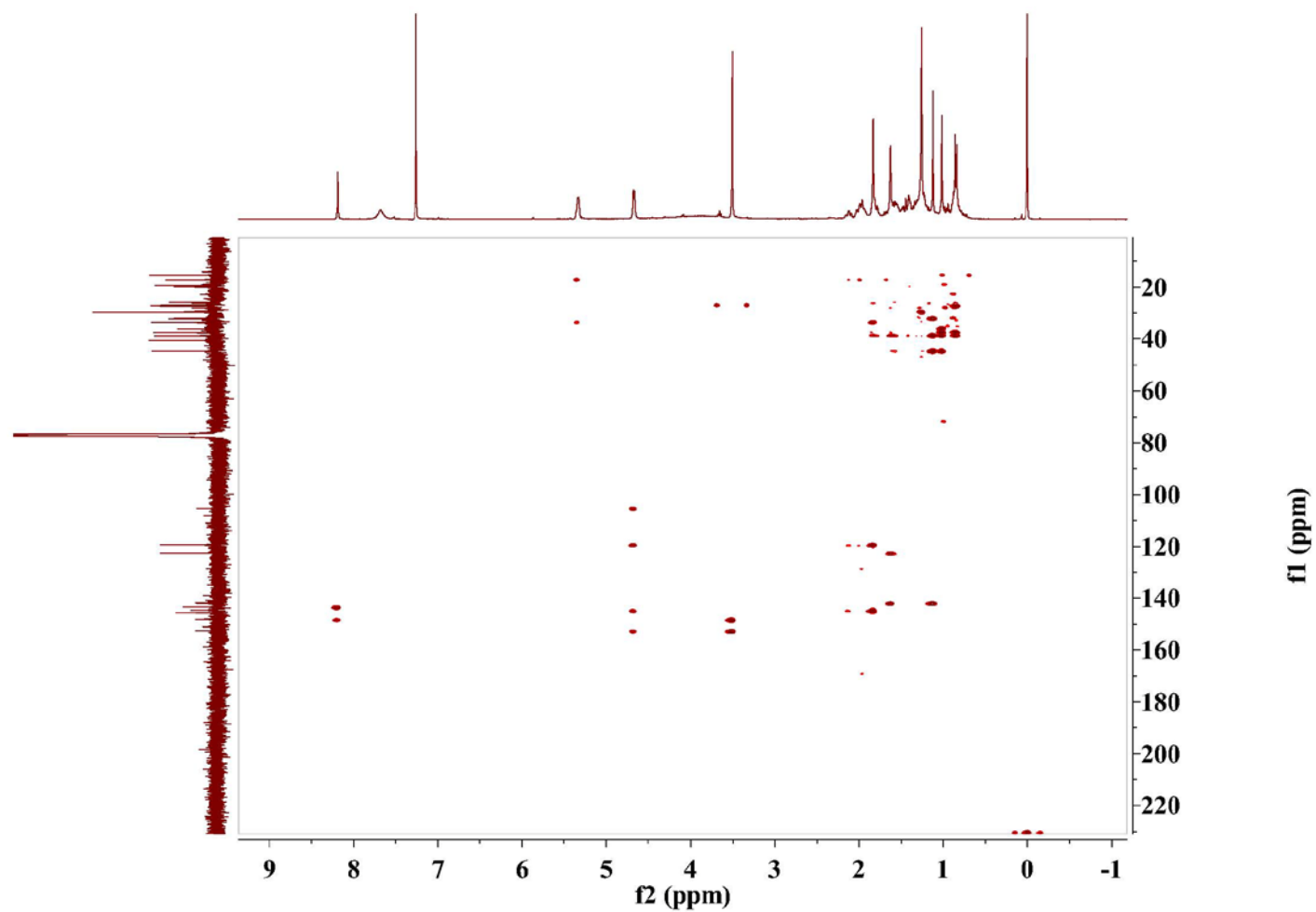


Figure S38. NOESY spectrum of agelasine V (**4**) in CDCl₃

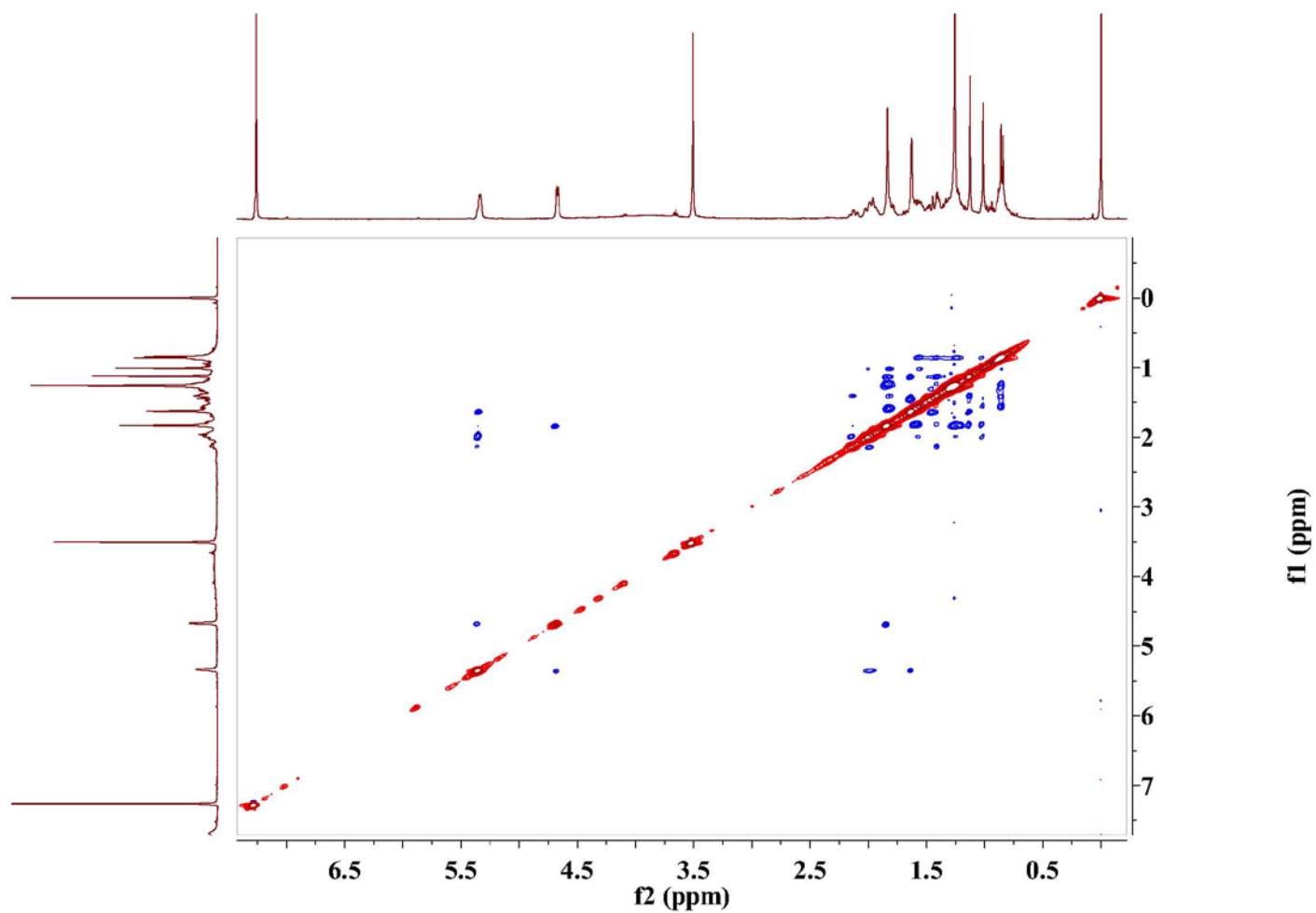


Figure S39. HRESIMS of agelasine V (4)

Elemental Composition Report

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions

57 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

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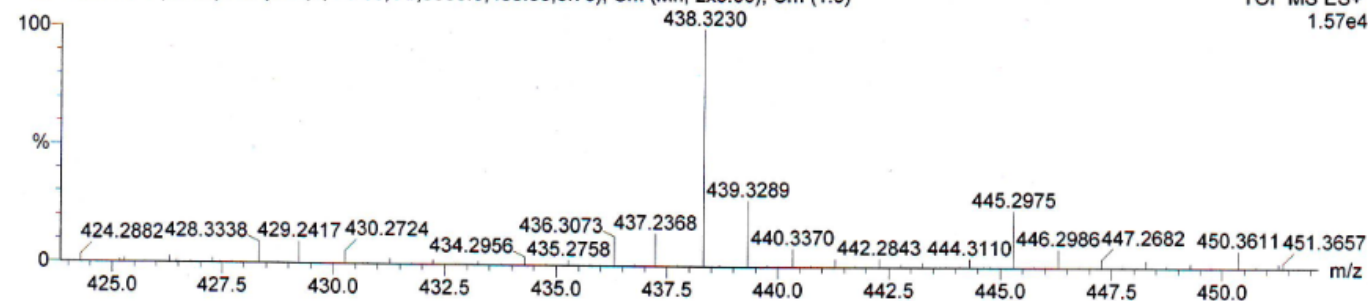
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SIPI

hj-9

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TOF MS ES+
1.57e4



Minimum: 80.00

Maximum: 100.00

-1.5

50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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438.3230	100.00	438.3233	-0.3	-0.7	9.5	96.0	C26 H40 N5 O
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Figure S40. UV spectrum of agelasine V (**4**) in MeOH

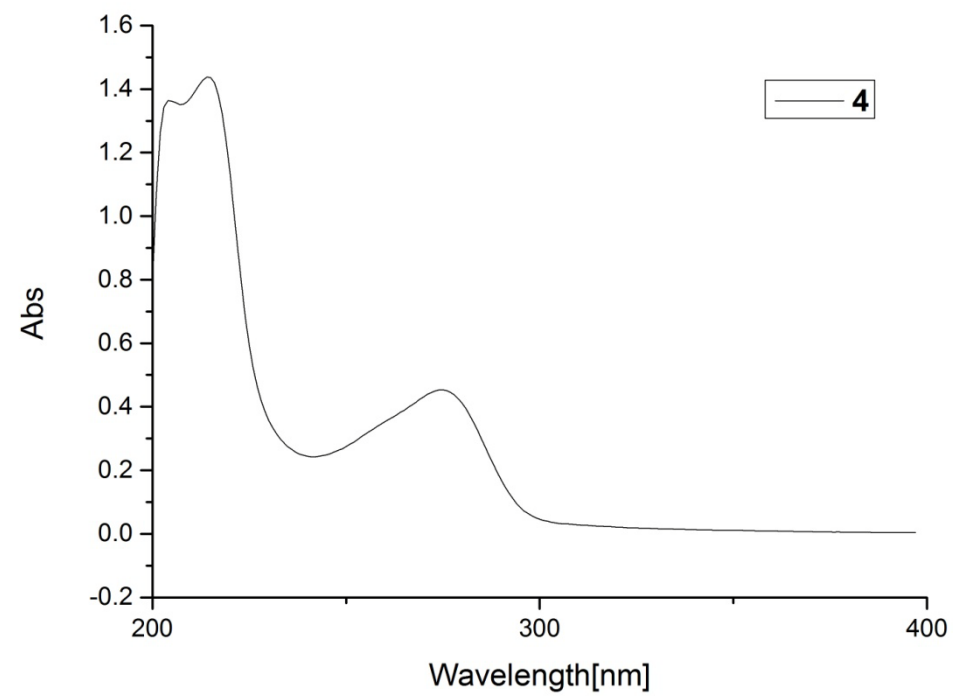


Figure S41. IR spectrum of agelasine V (**4**)

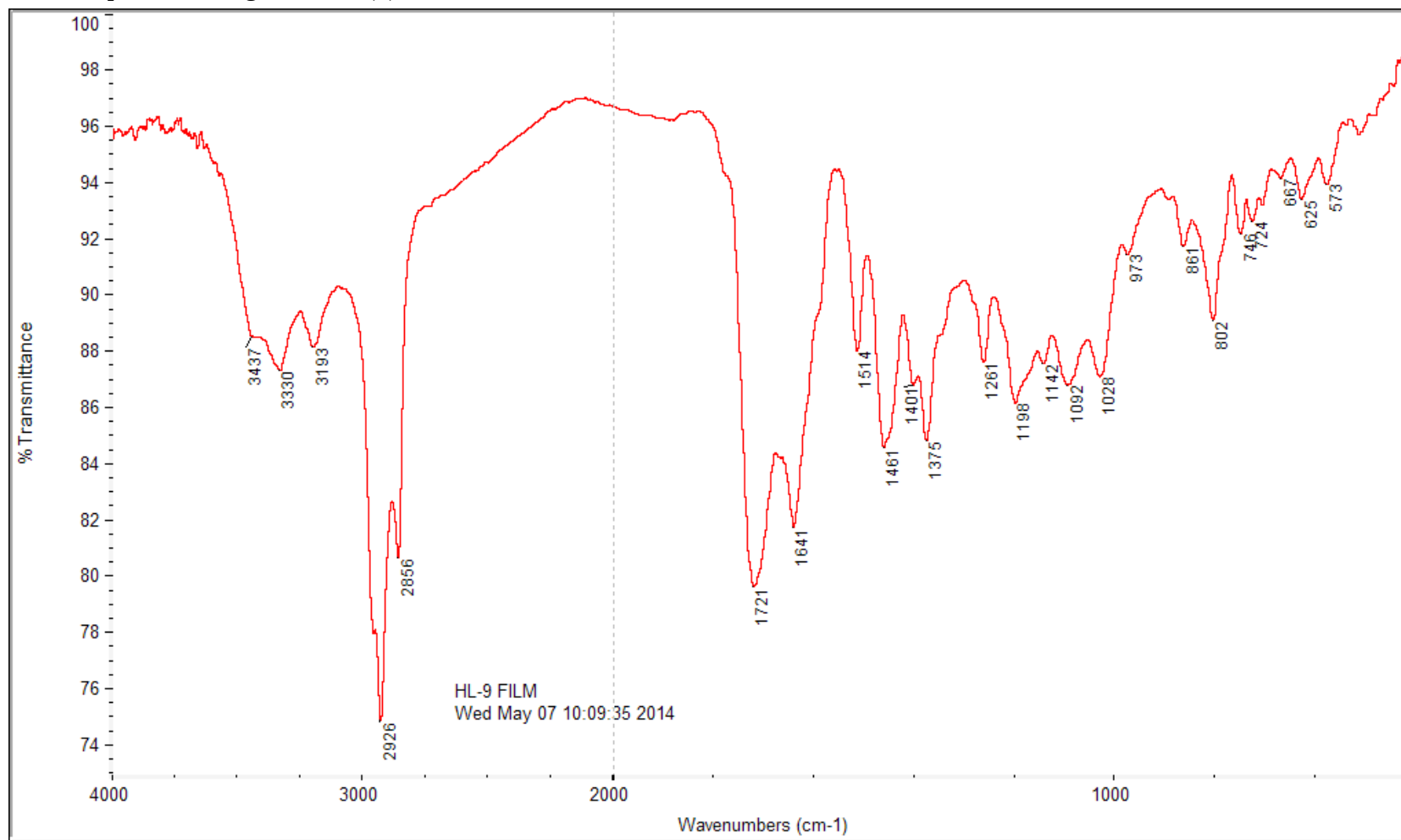


Figure S42. ^1H NMR (400 MHz, CDCl_3) spectrum of (+)-8'-oxo-agelasine E (5)

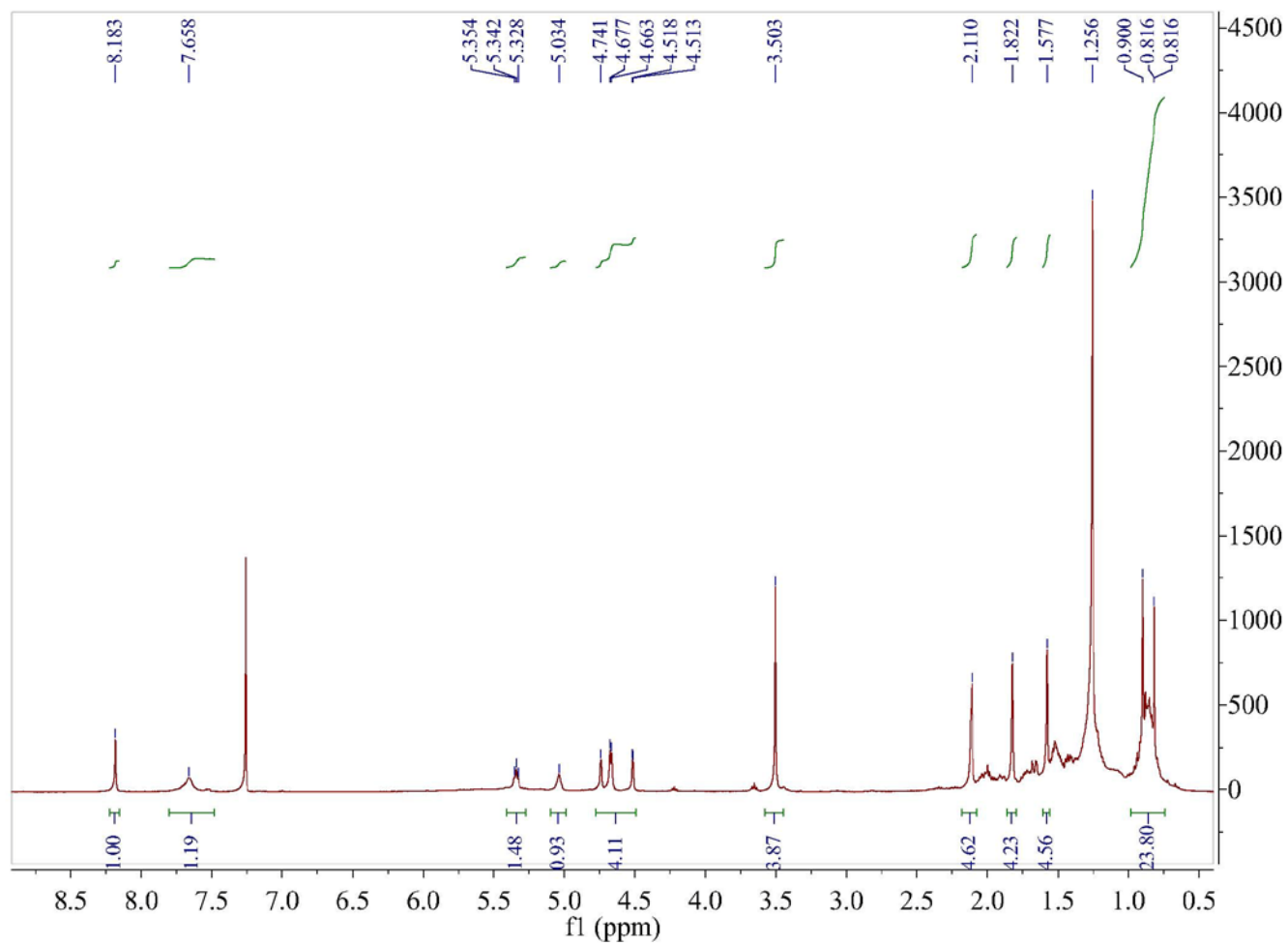


Figure S43. ^{13}C NMR (100 MHz, CDCl_3) spectrum of (+)-8'-oxo-agelasine E (5)

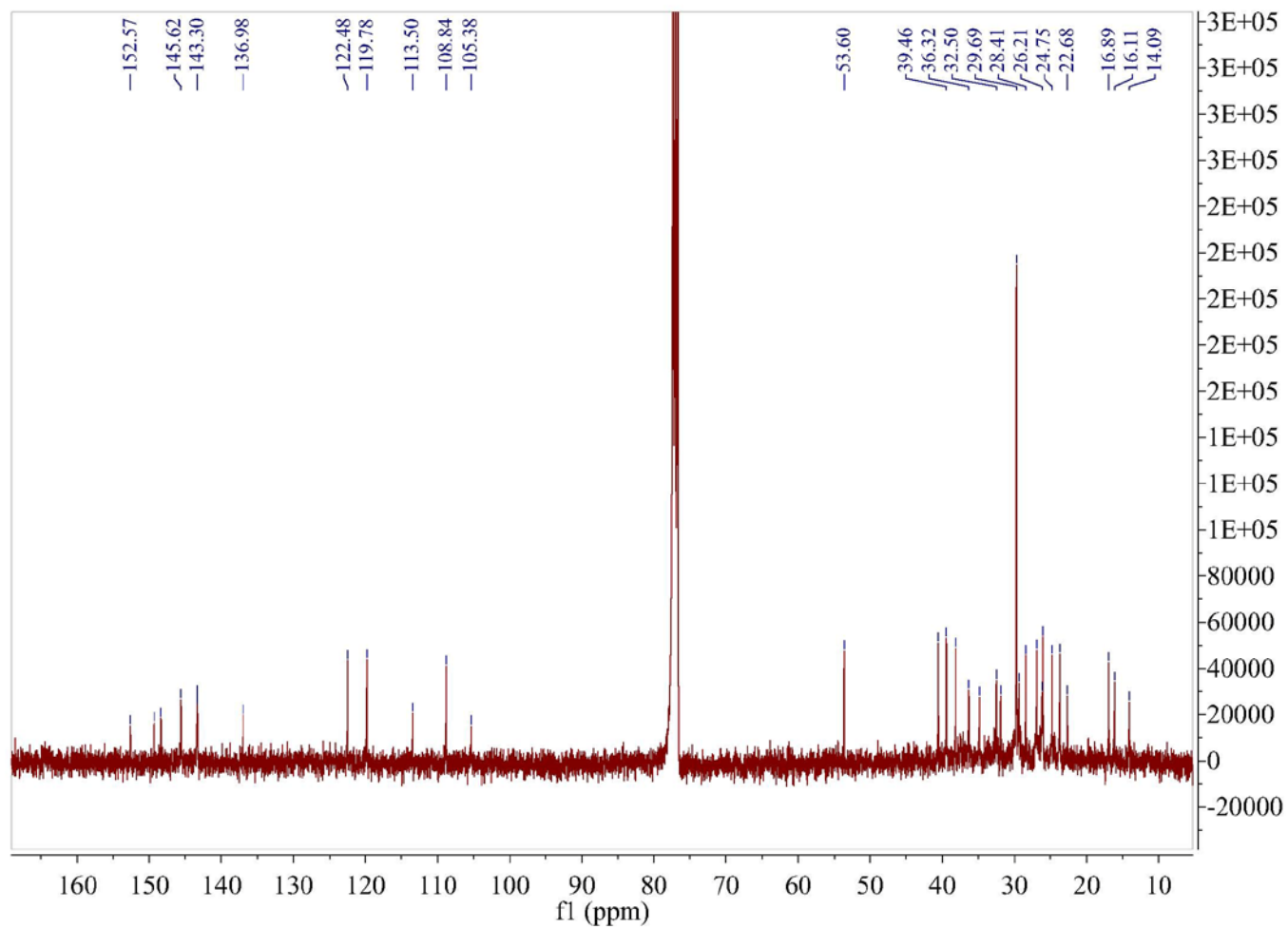


Figure S44. DEPT135 spectrum of (+)-8'-oxo-agelasine E (**5**) in CDCl₃

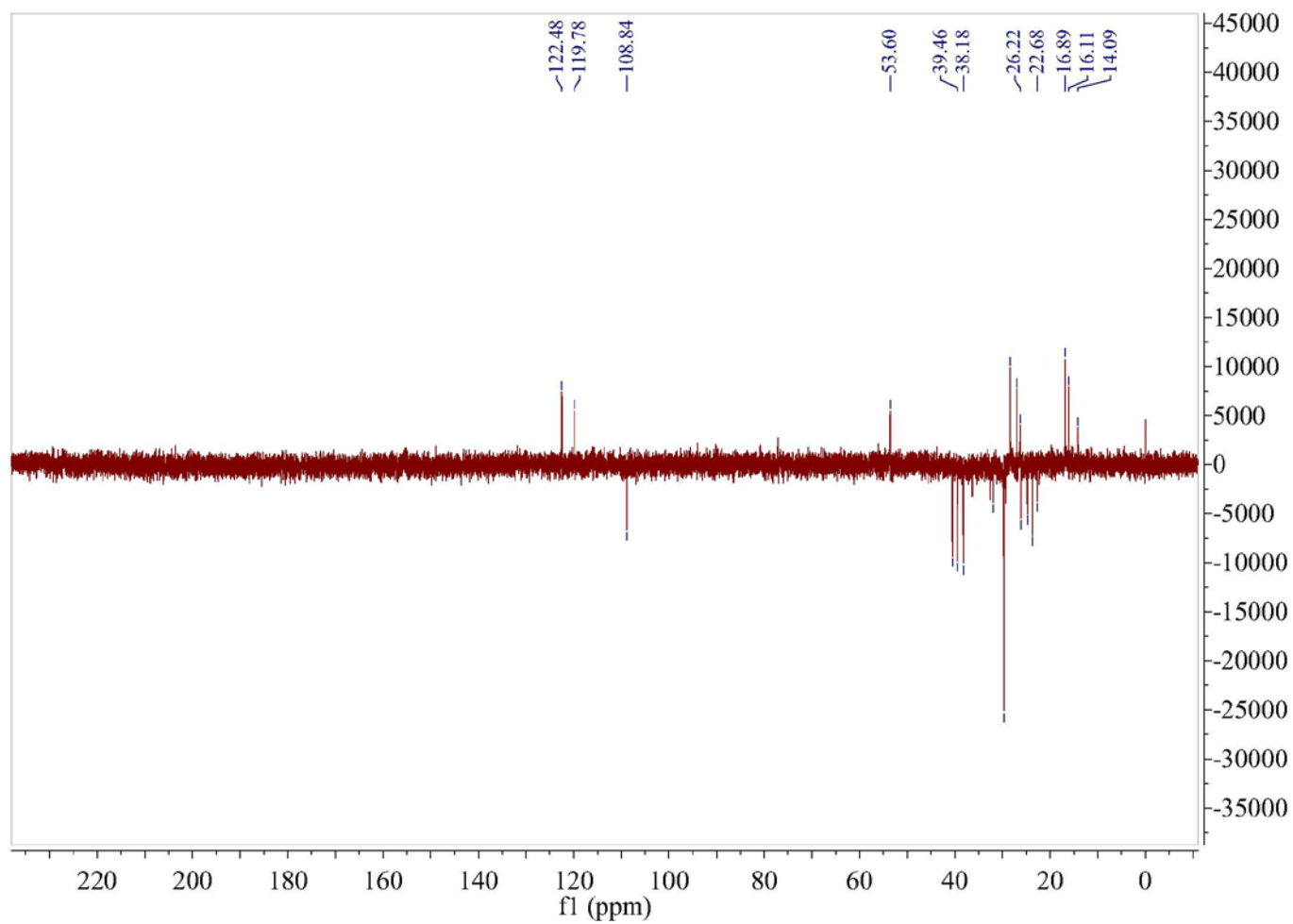


Figure S45. HSQC spectrum of (+)-8'-oxo-agelasine E (**5**) in CDCl₃

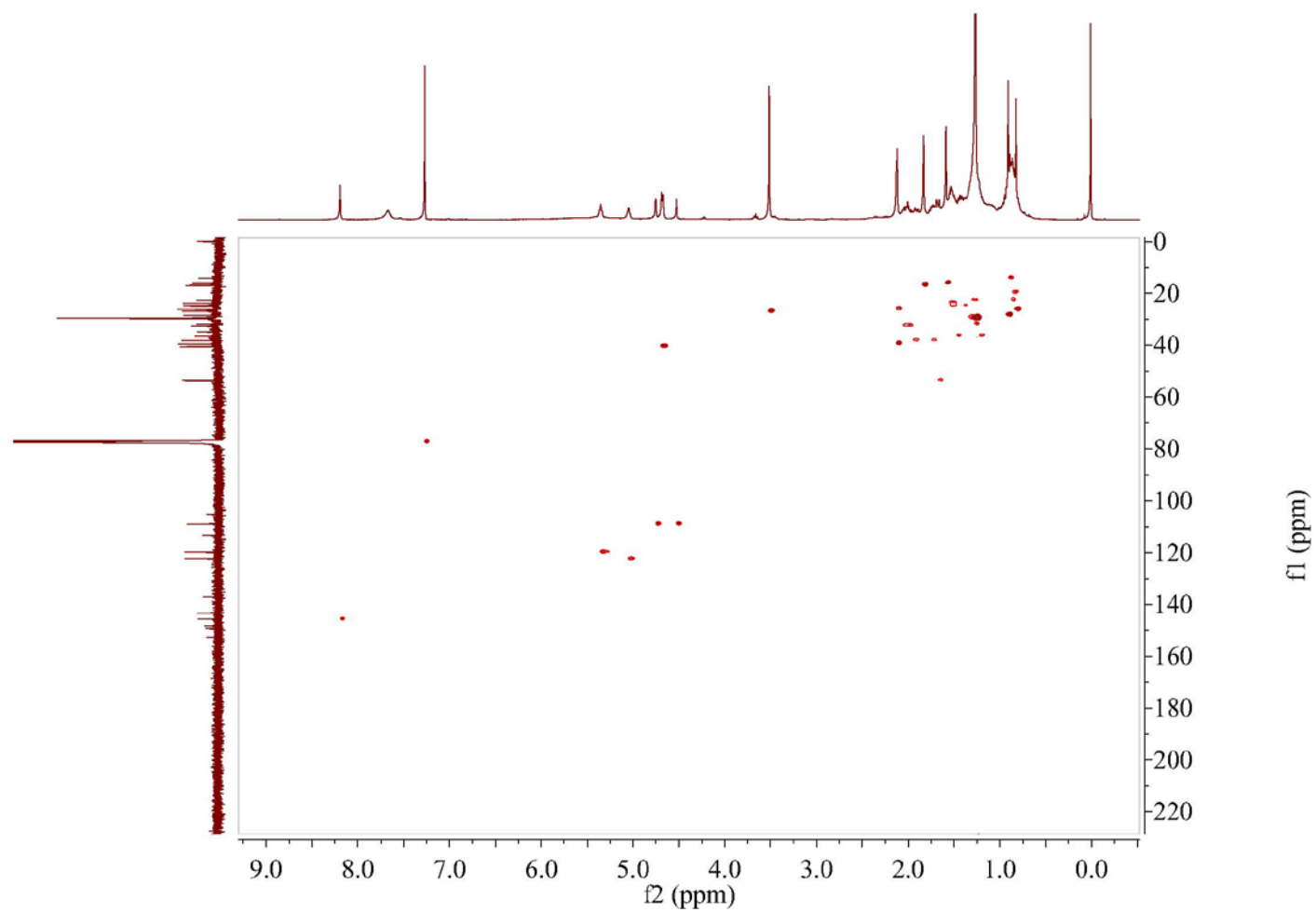


Figure S46. COSY spectrum of (+)-8'-oxo-agelasine E (**5**) in CDCl₃

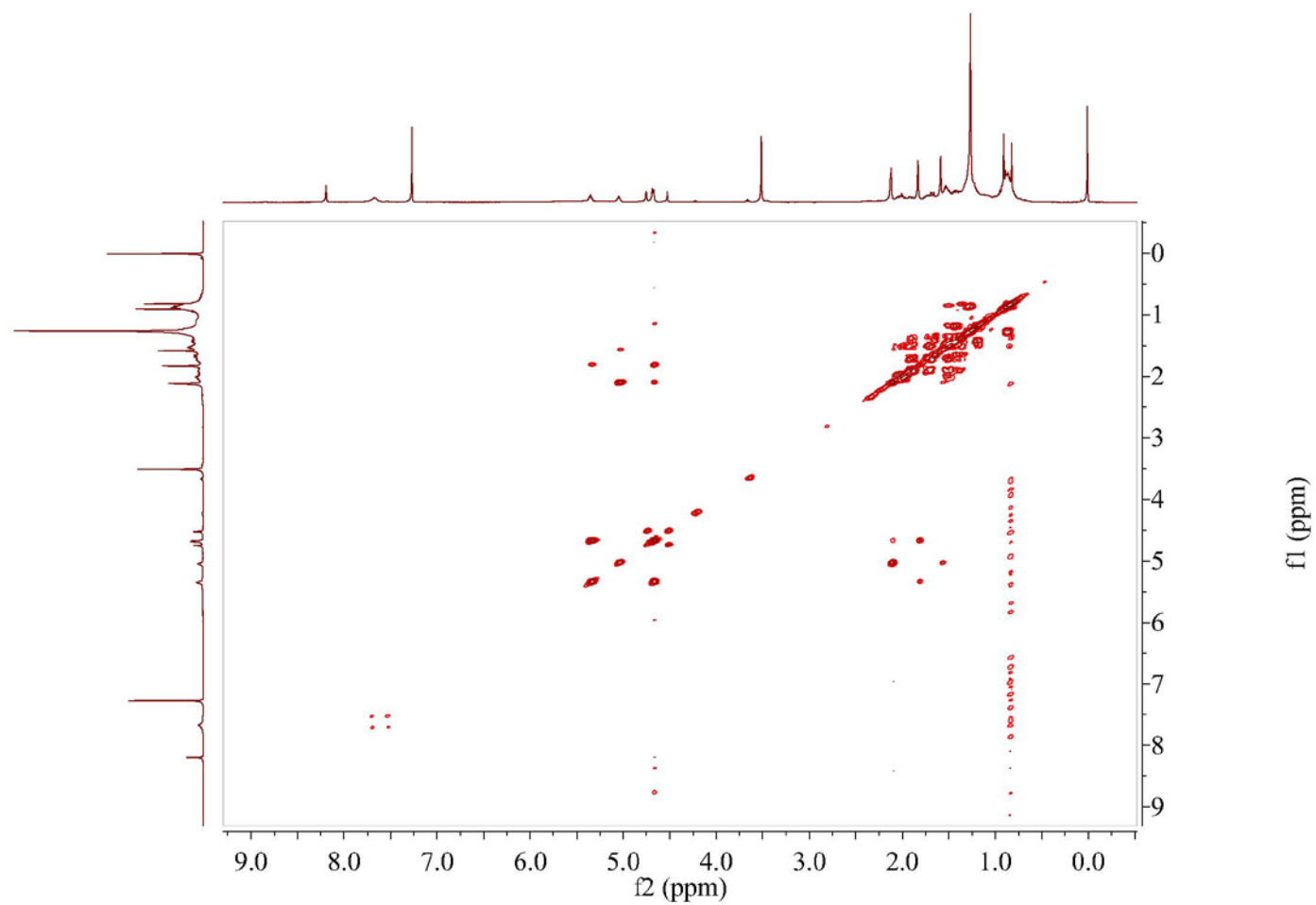


Figure S47. HMBC spectrum of (+)-8'-oxo-agelasine E (**5**) in CDCl₃

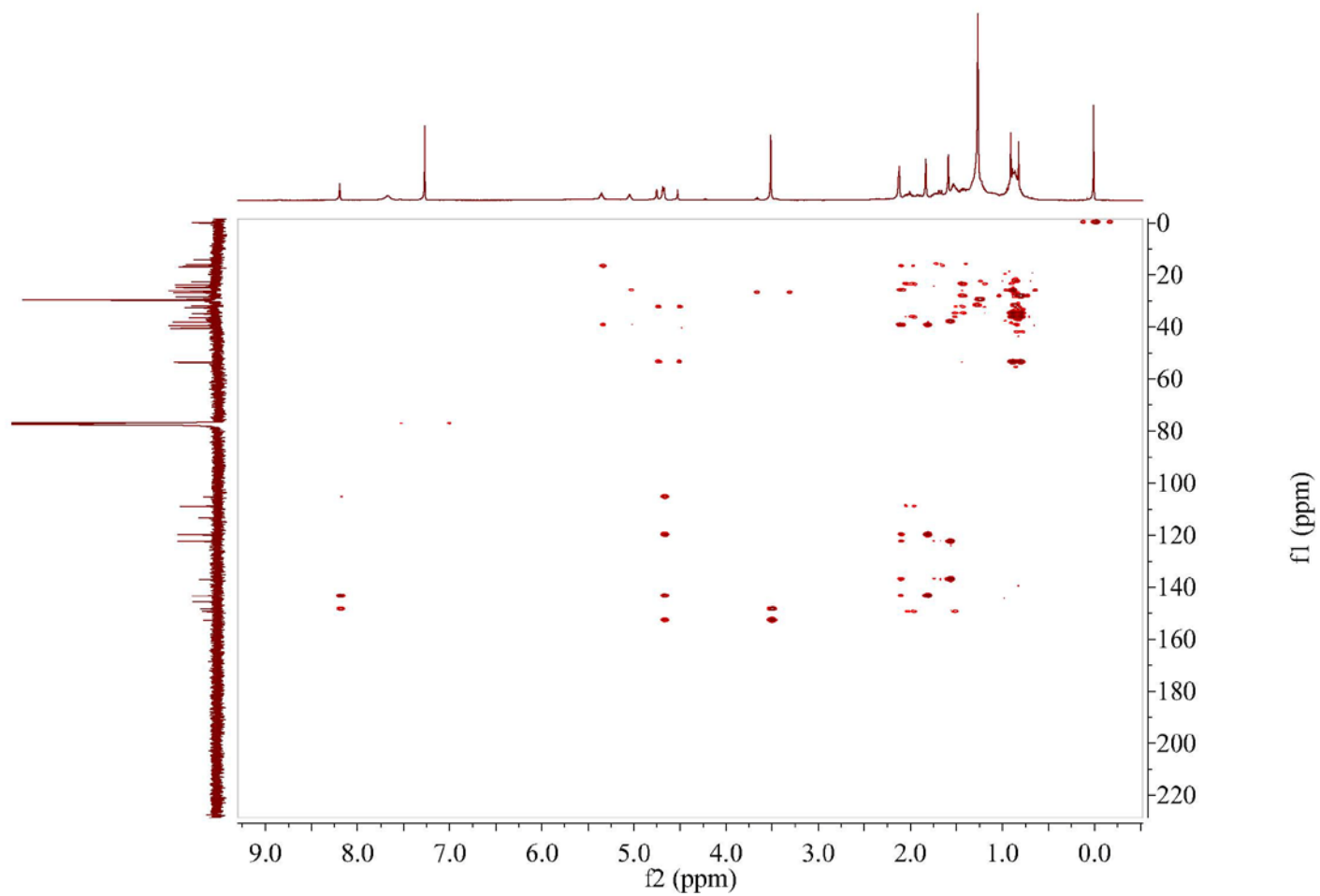


Figure S48. NOESY spectrum of (+)-8'-oxo-agelasine E (**5**) in CDCl₃

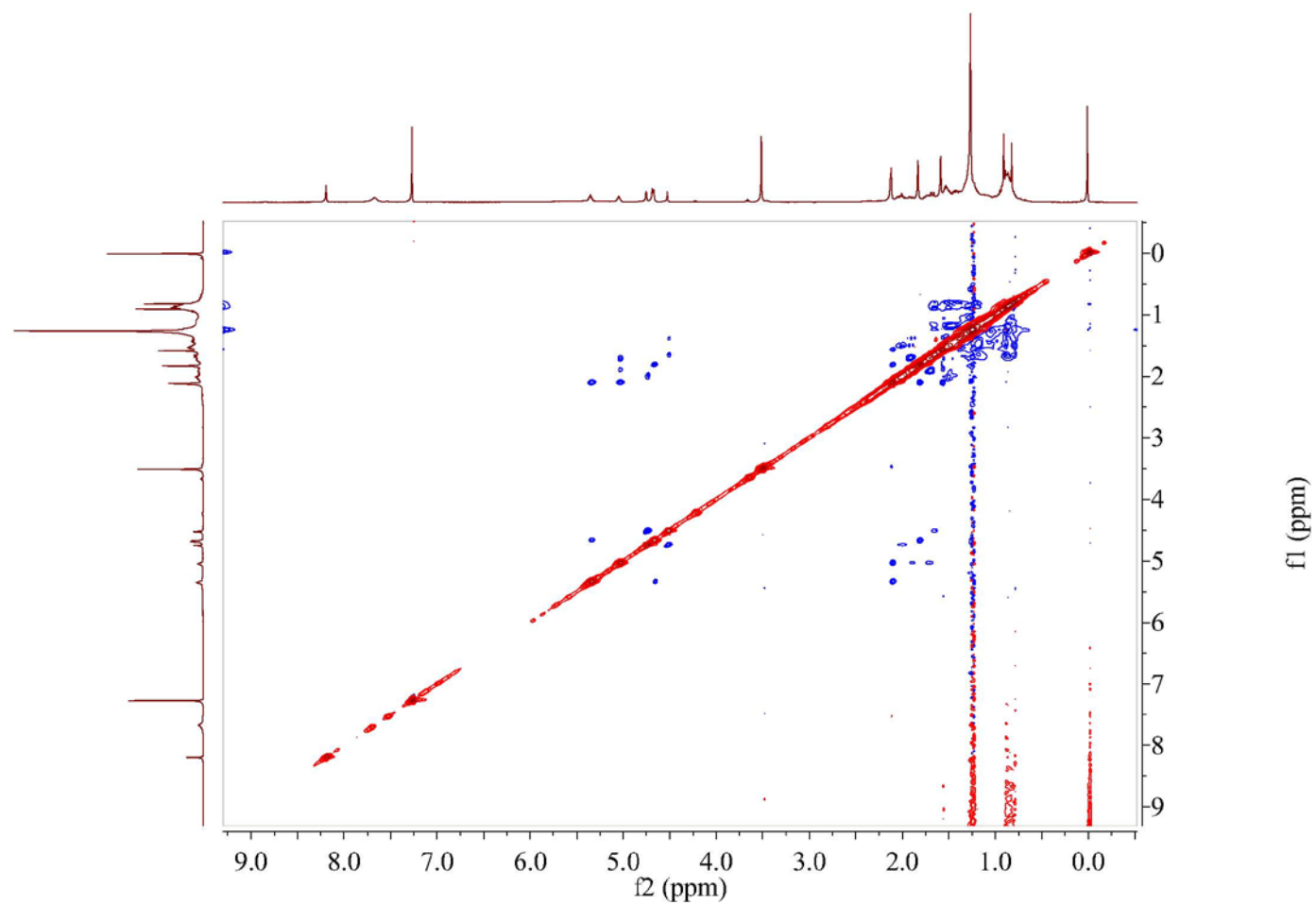


Figure S49. HRESIMS of (+)-8'-oxo-agelasine E (5)

Elemental Composition Report

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions

48 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 5-30 H: 5-50 N: 1-5 O: 1-3

SIPI

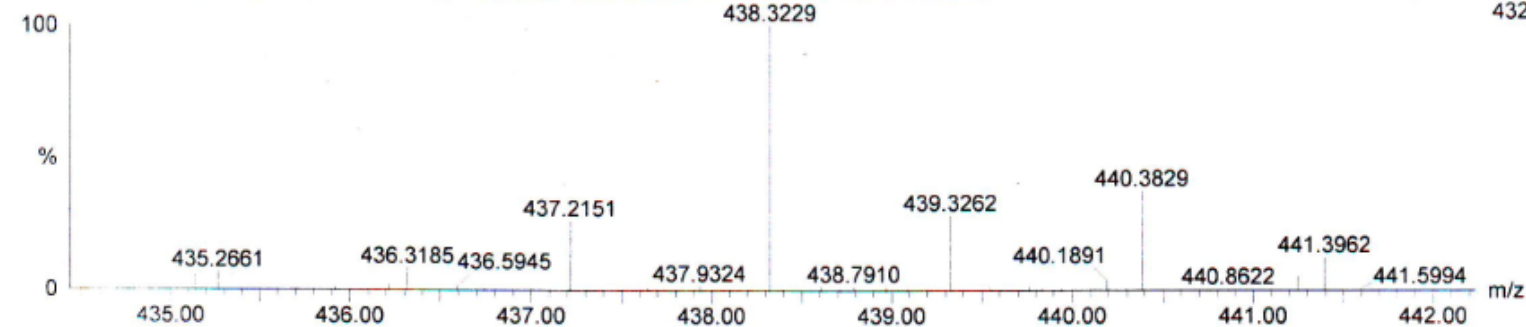
hl-7

WQ14-077HH 44 (1.522) AM (Cen,4, 80.00, Ar,5000.0,432.14,0.70); Sm (Mn, 2x3.00); Cm (38:55)

Q-ToF micro

YA019

TOF MS ES+
432



Minimum: 80.00
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
438.3229	100.00	438.3233	-0.4	-0.9	9.5	68.1	C26 H40 N5 O

Figure S50. UV spectrum of (+)-8'-oxo-agelasine E (**5**) in MeOH

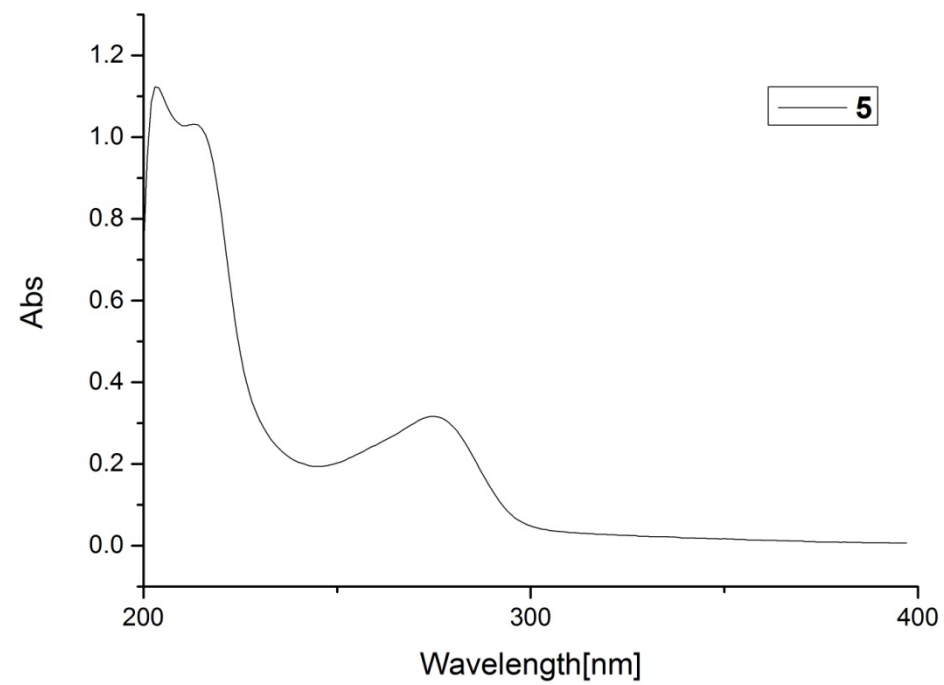


Figure S51. IR spectrum of (+)-8'-oxo-agelasine E (5)

