

Supporting Information

Simplexolides A–E and Plakorfuran A, Six Butyrate Derived Polyketides from the Marine Sponge *Plakortis simplex*

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Figure S1. High resolution ESI mass spectrum of simplexolide A (1).

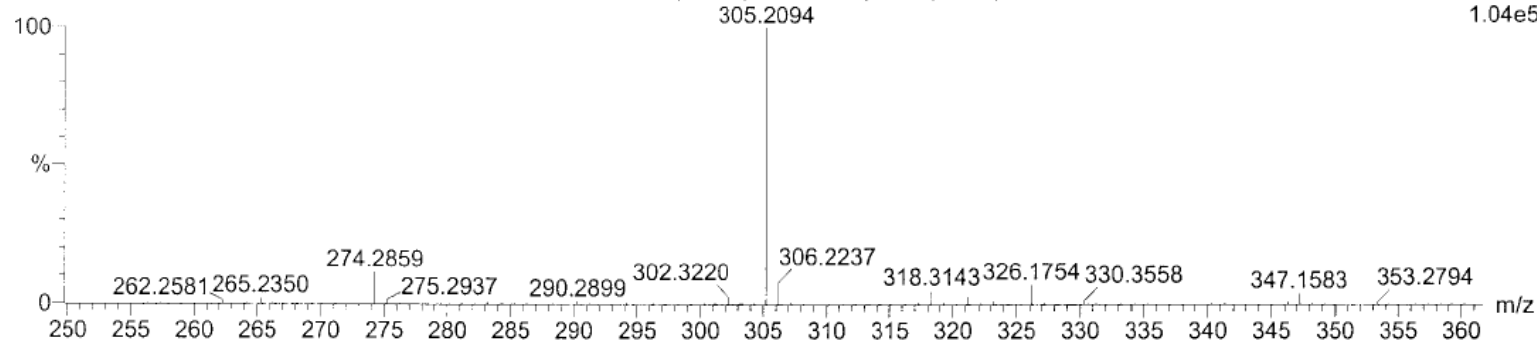
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 Selected filters: None

Monoisotopic Mass, Even Electron Ions
 17 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 5-30 H: 5-50 O: 1-5 Na: 1-1

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 XF-16 M.W=282
 WQ10190H 48 (1.658) AM (Cen,6, 80.00, Ar,5000.0,325.16,0.70); Sm (SG, 2x3.00); Cm (36:50)

21-May-2010,14:24:18
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 TOF MS ES+
 1.04e5



Minimum: 35.00 -1.5
 Maximum: 100.00 5.0 10.0 50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
305.2094	100.00	305.2093	0.1	0.3	2.5	7692.5	C17 H30 O3 Na

Figure S2. IR spectrum of simplexolide A (**1**).

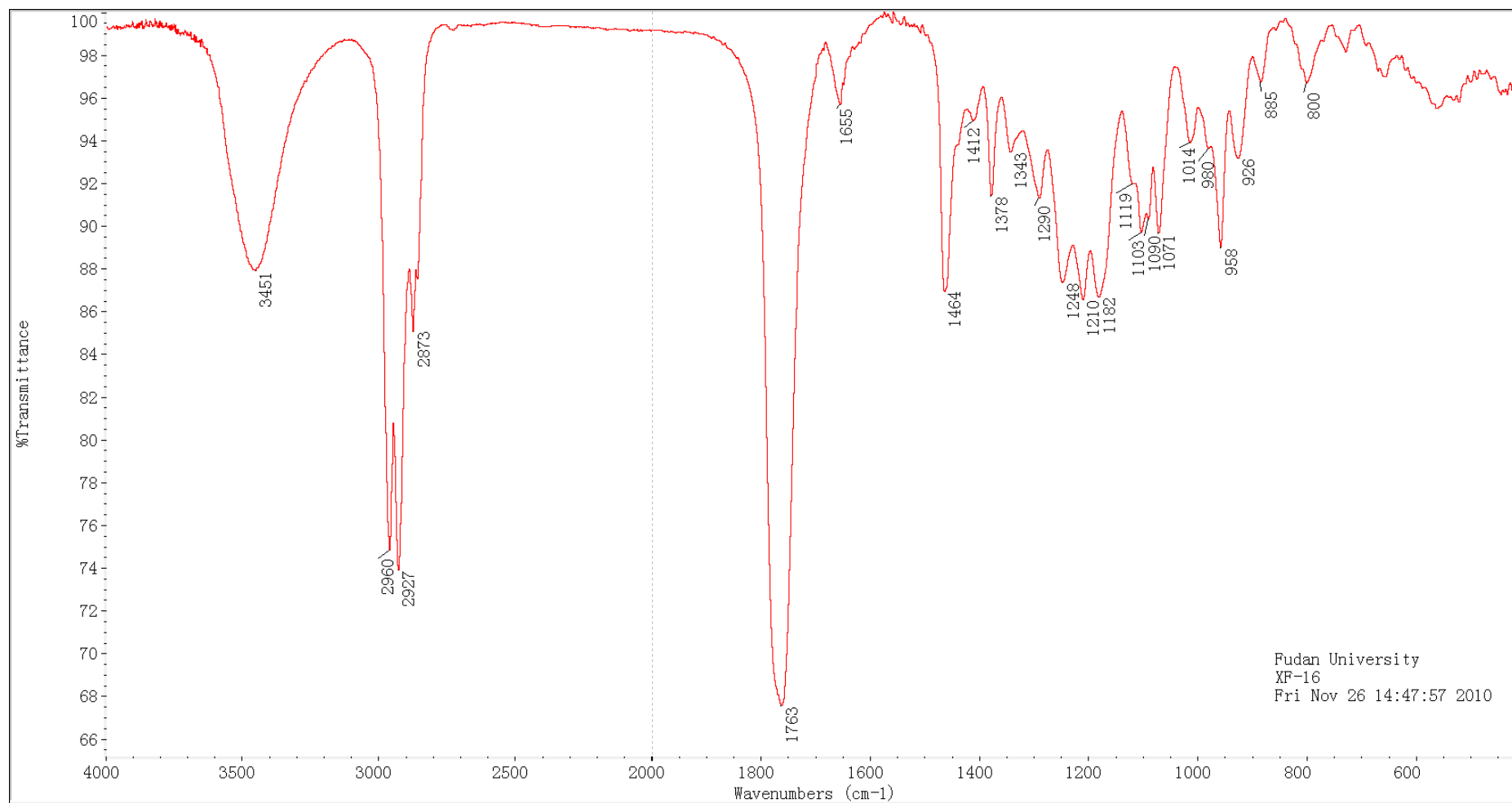


Figure S3. ^1H NMR spectrum of simplexolide A (**1**) in CDCl_3 .

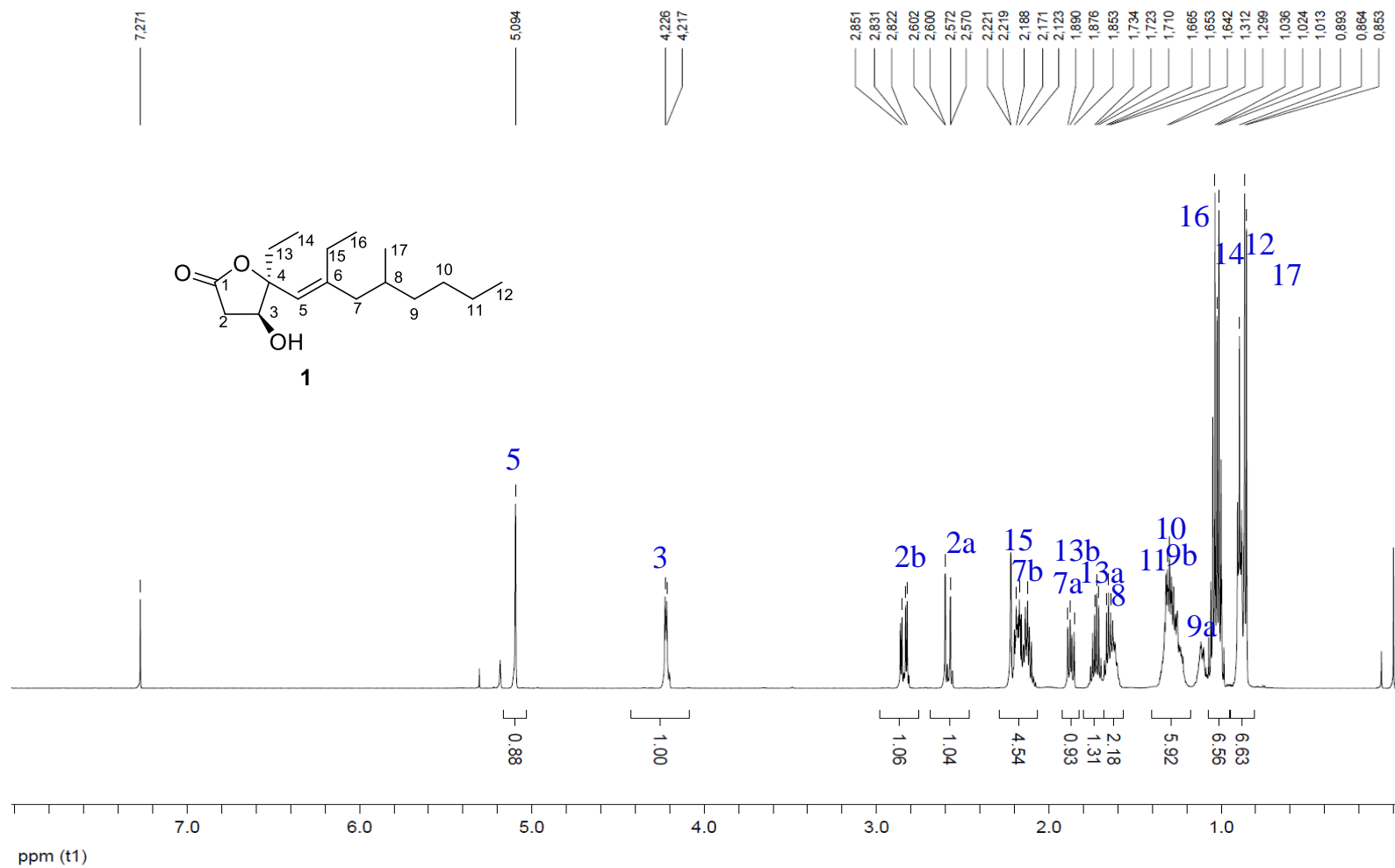


Figure S4. ^{13}C NMR spectrum of simplexolide A (**1**) in CDCl_3 .

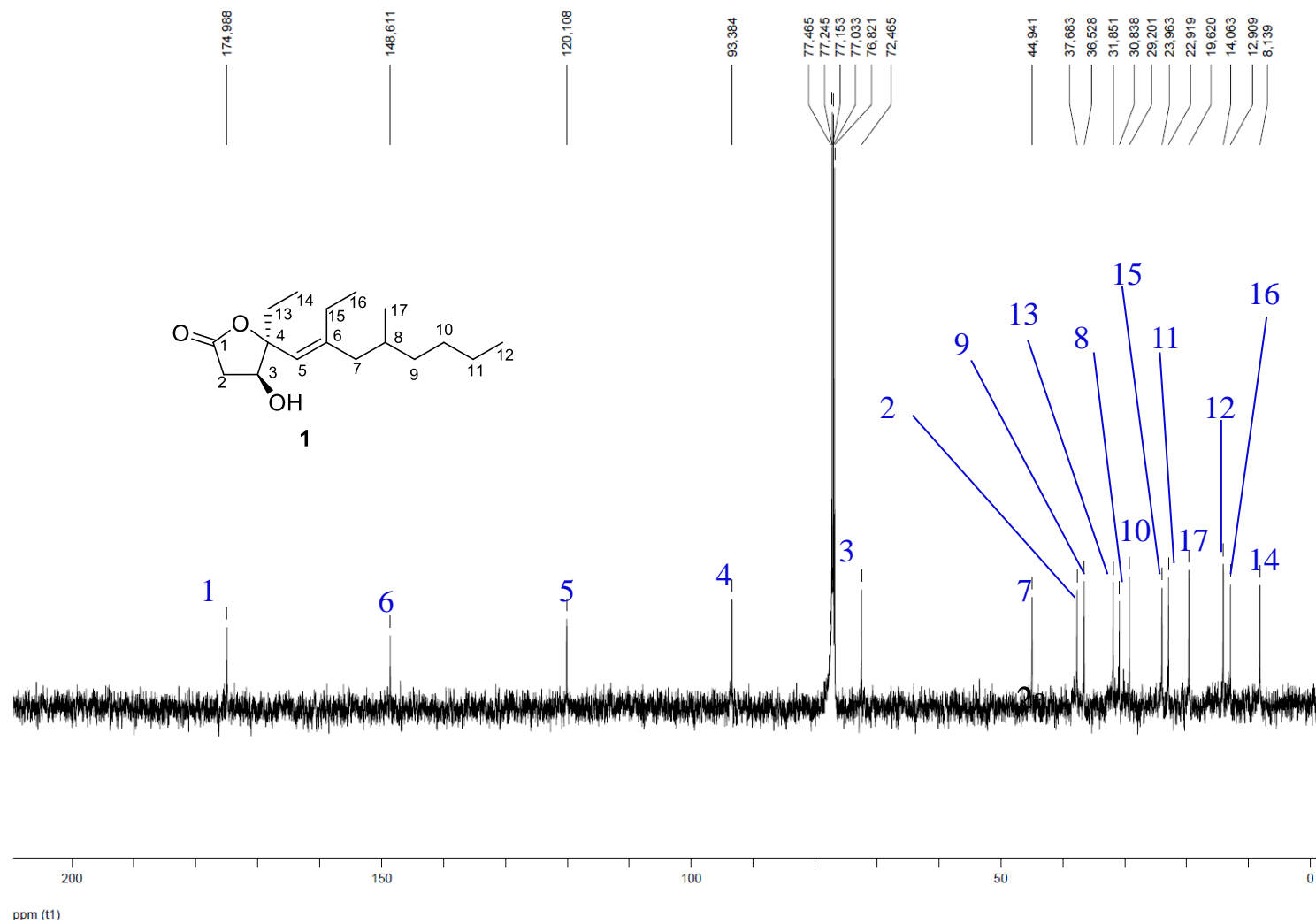


Figure S5. ^1H - ^1H COSY spectrum of simplexolide A (**1**) CDCl_3

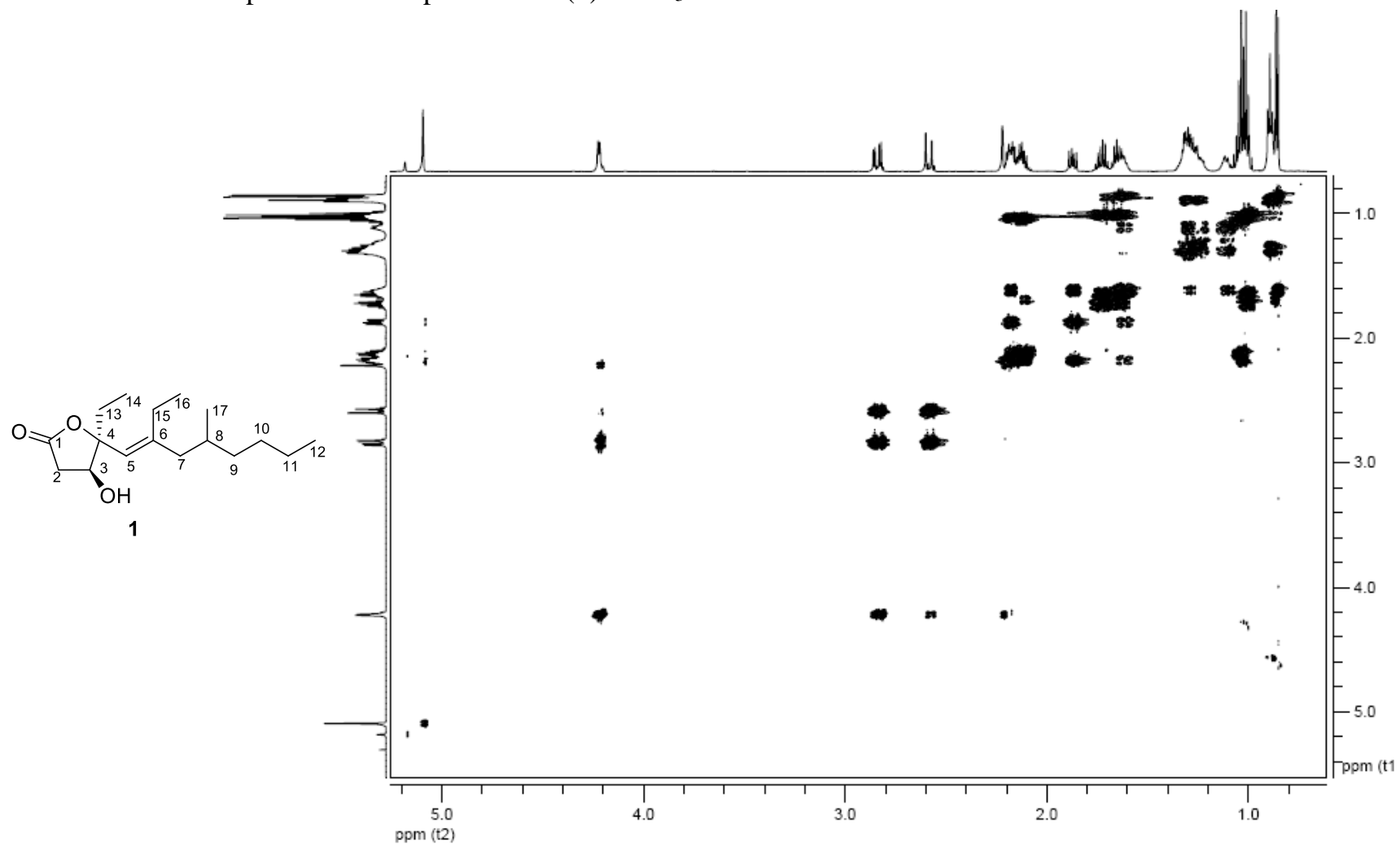


Figure S6. HSQC spectrum of simplexolide A (**1**) CDCl₃

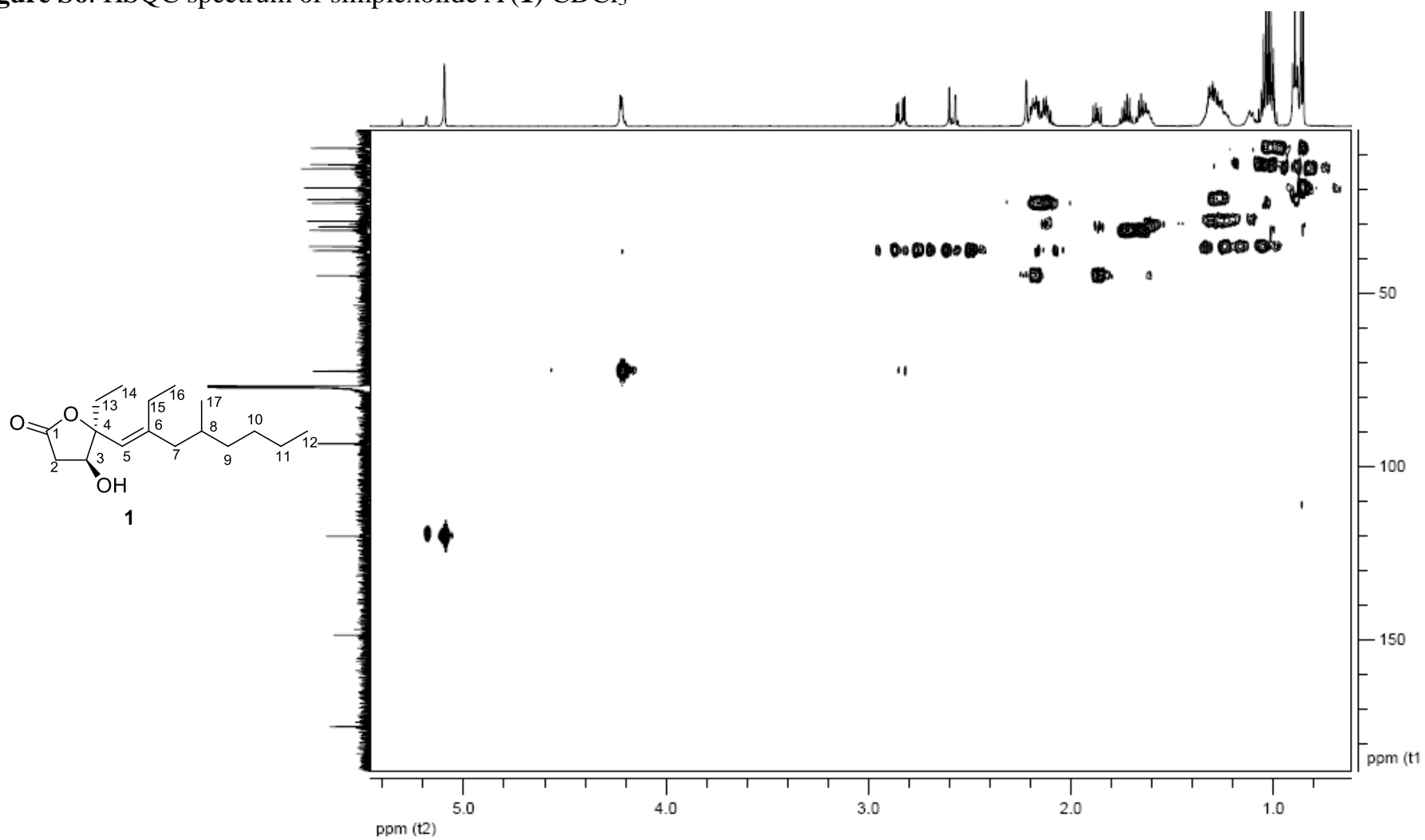


Figure S7. HMBC spectrum of simplexolide A (1) CDCl₃

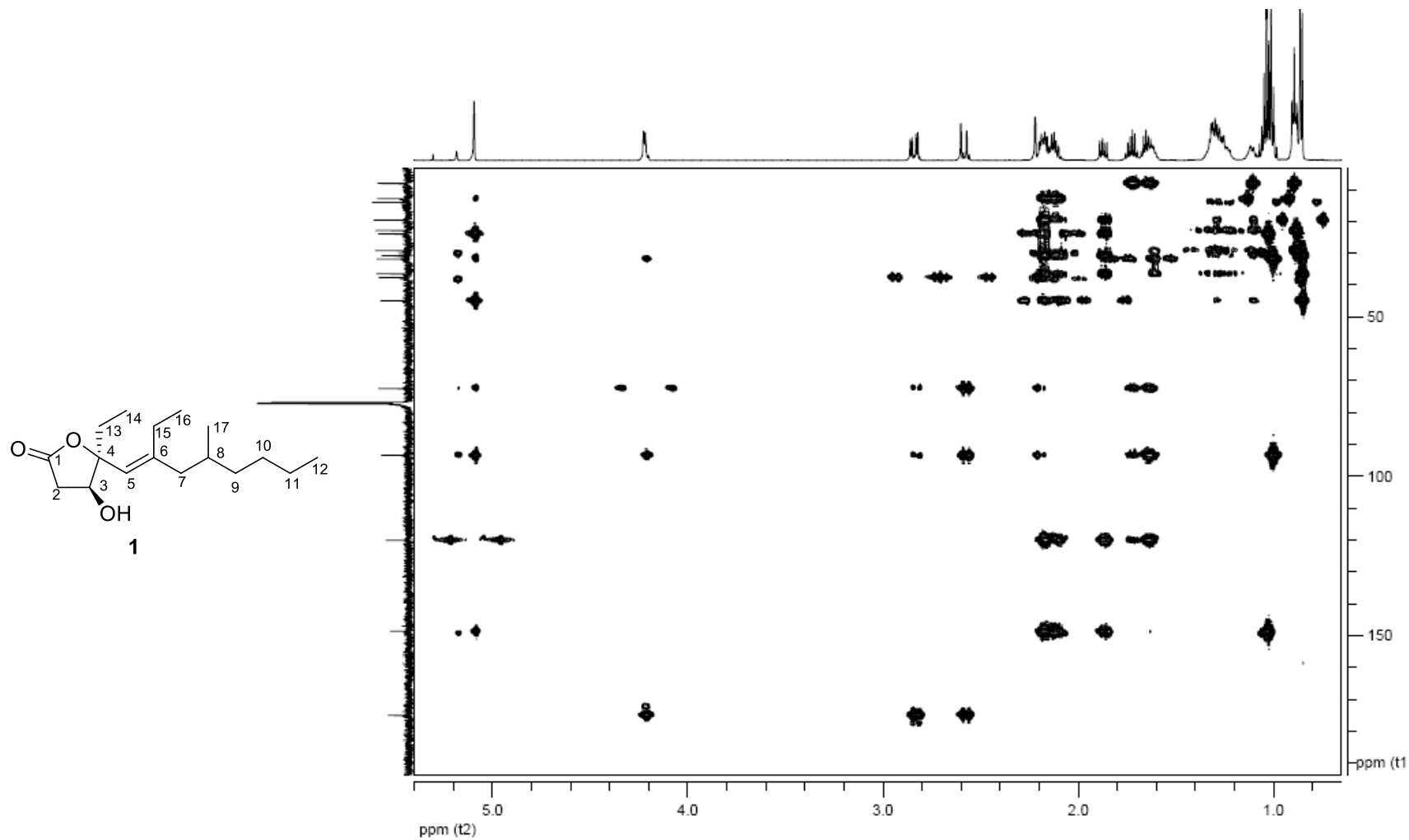


Figure S8. NOESY spectrum of simplexolide A (**1**) CDCl₃

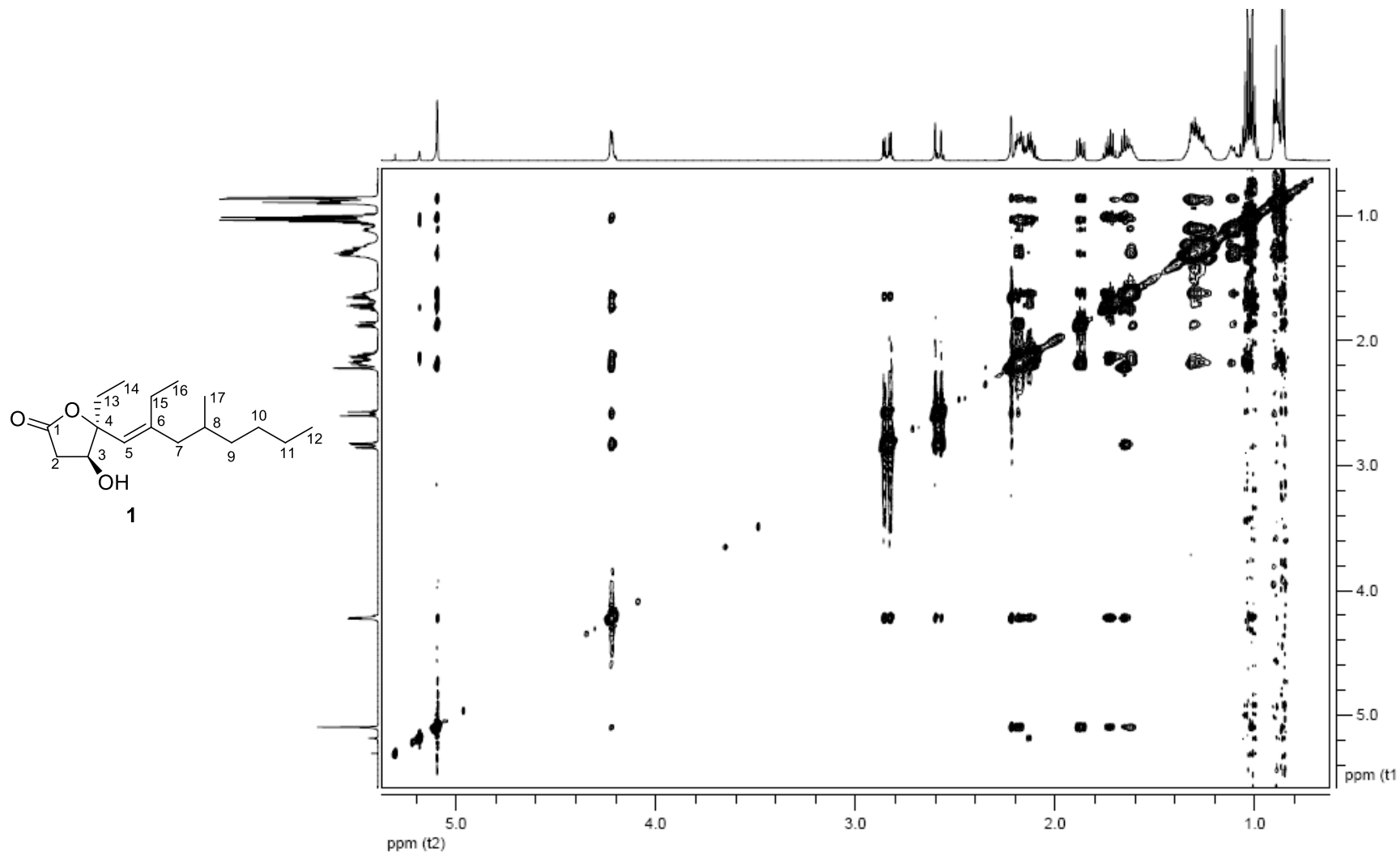


Figure S9. High resolution ESI mass spectrum of simplexolide B (2).

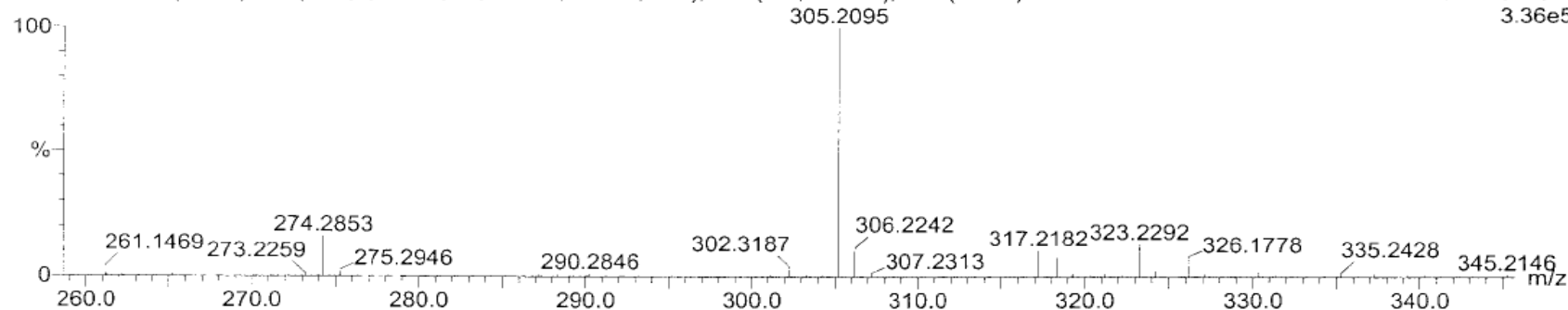
Elemental Composition Report

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

Monoisotopic Mass, Even Electron Ions
 17 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 5-30 H: 5-50 O: 1-5 Na: 1-1

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 XF-22a M.W=282
 WQ10196H 29 (1.002) AM (Cen,6, 80.00, Ar,5000.0,325.16,0.70); Sm (SG, 2x3.00); Cm (16:39)

24-May-2010,11:01:02
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 TOF MS ES+
 3.36e5



Minimum: 35.00
 Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
305.2095	100.00	305.2093	0.2	0.7	2.5	9415.2	C17 H30 O3 Na

Figure S10. IR spectrum of simplexolide B (2).

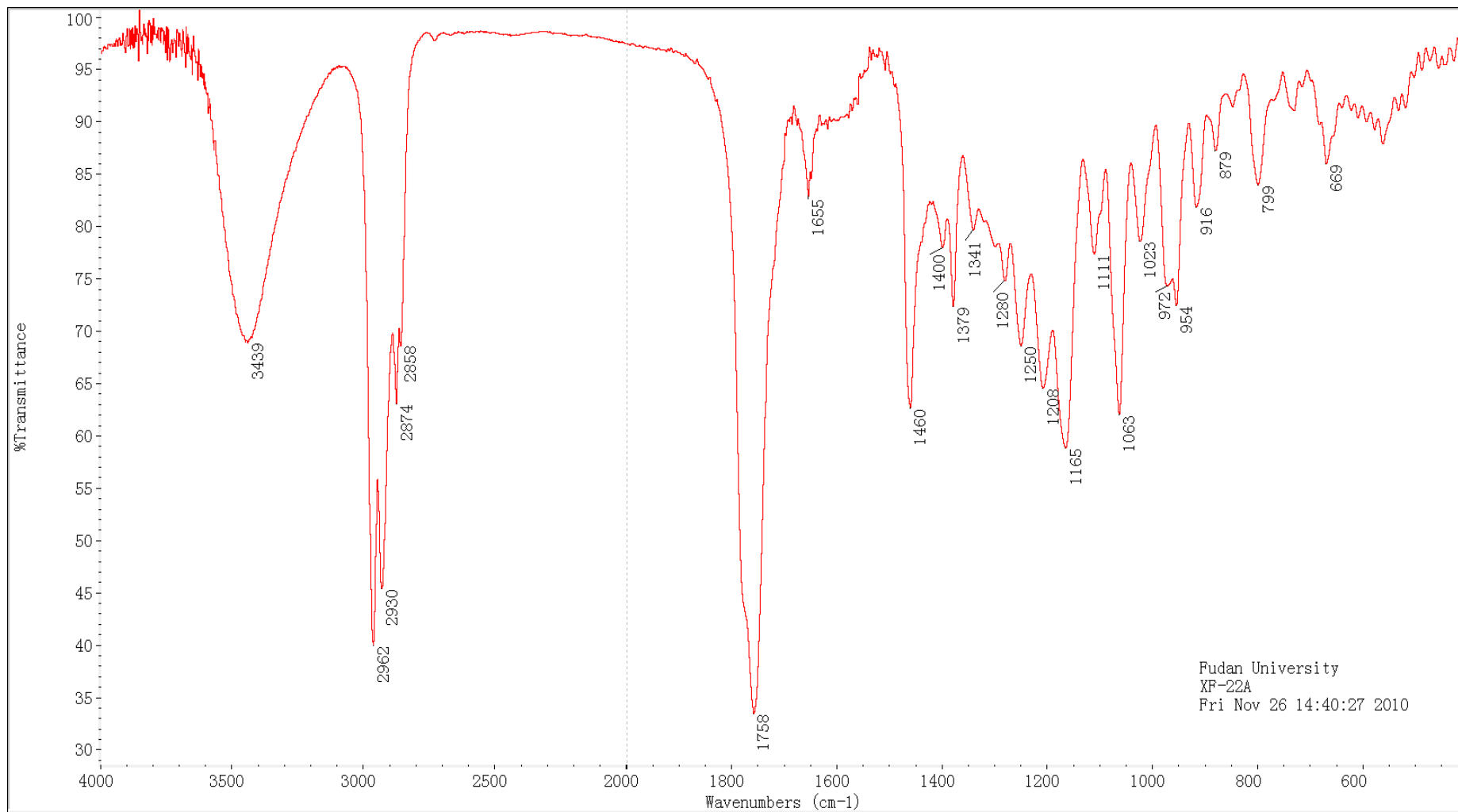


Figure S11. ^1H NMR spectrum of simplexolide B (**2**) in CDCl_3 .

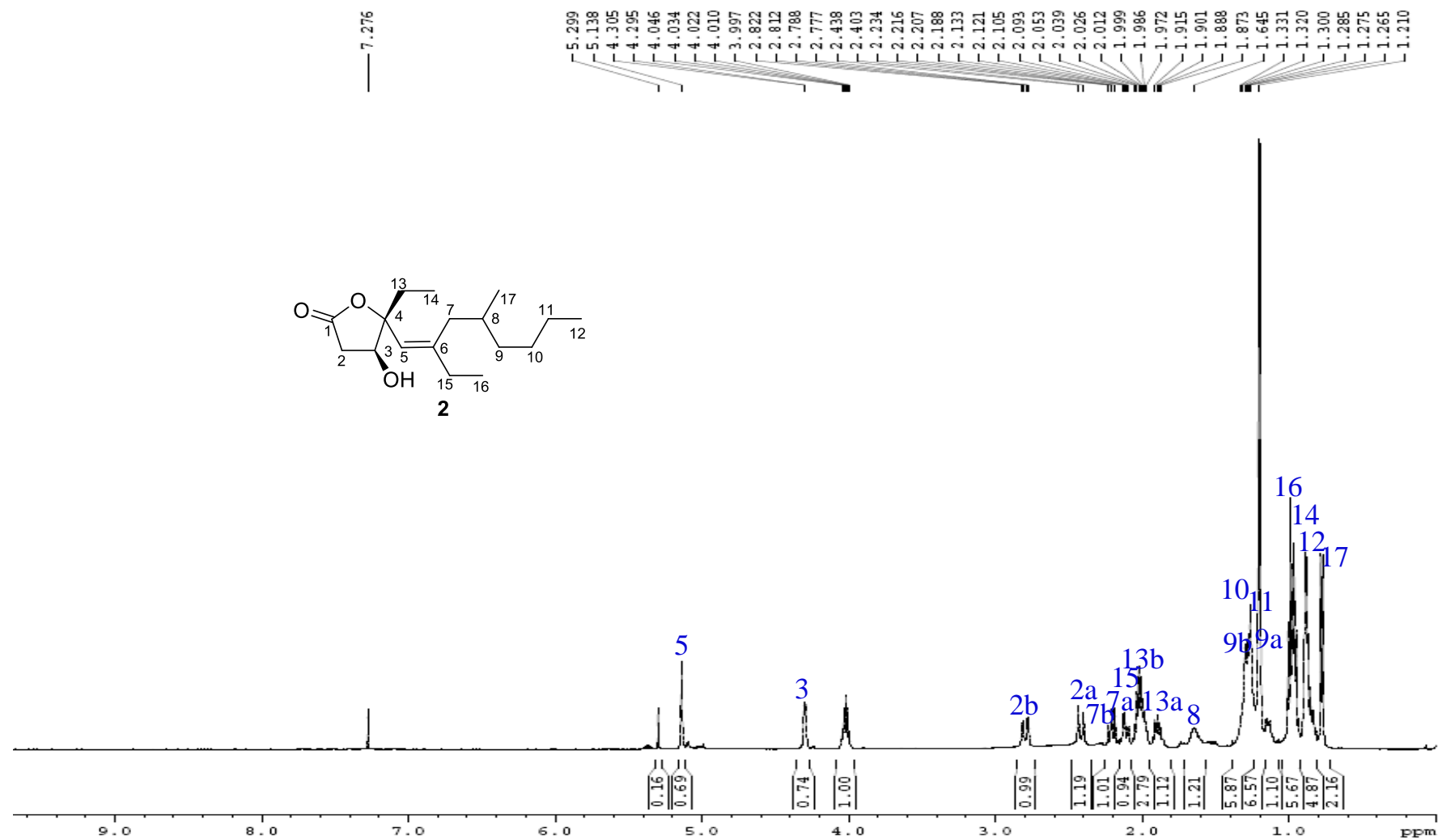


Figure S12. ^{13}C NMR spectrum of simplexolide B (**2**) in CDCl_3 .

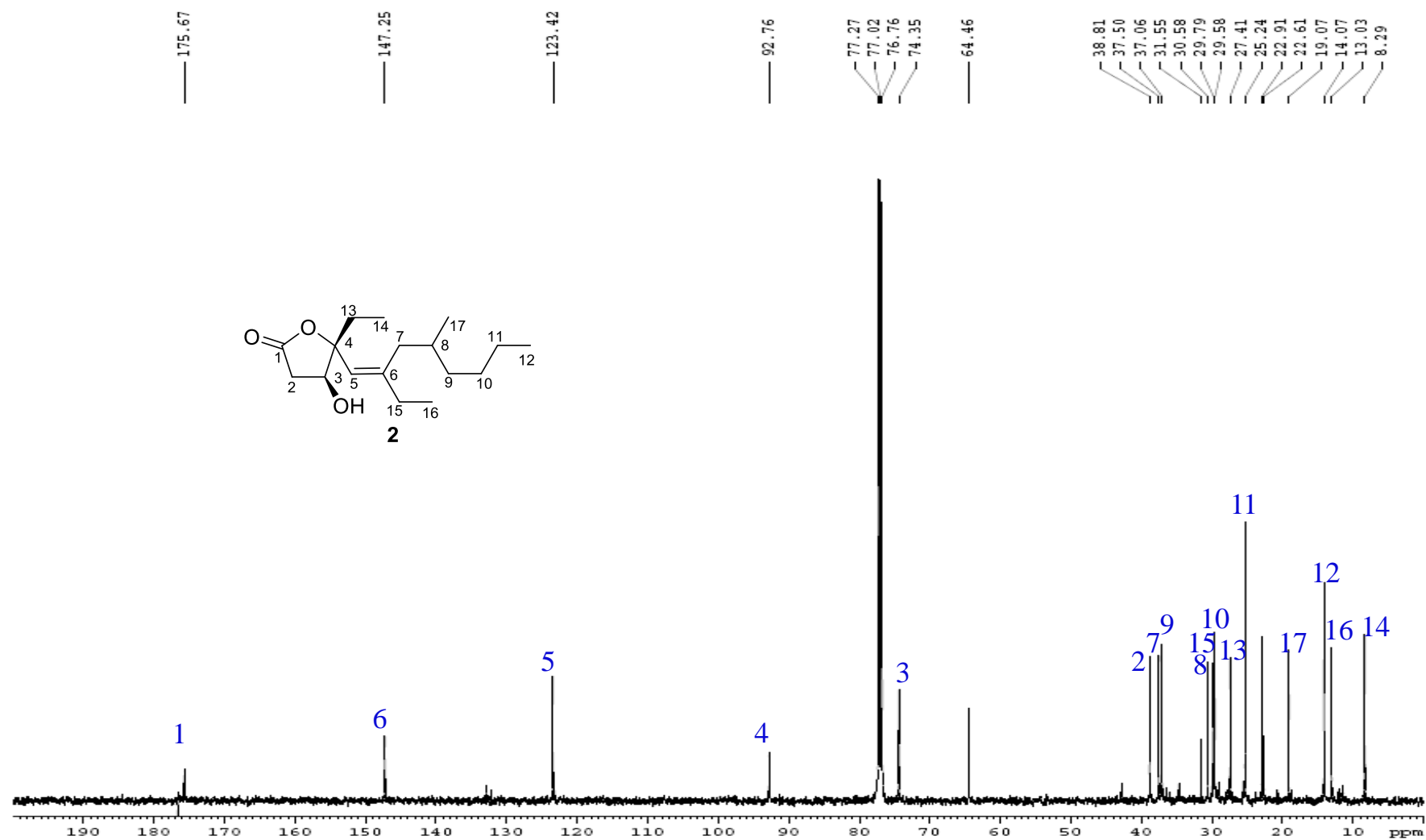


Figure S13. ^1H - ^1H COSY spectrum of simplexolide B (**2**) in CDCl_3

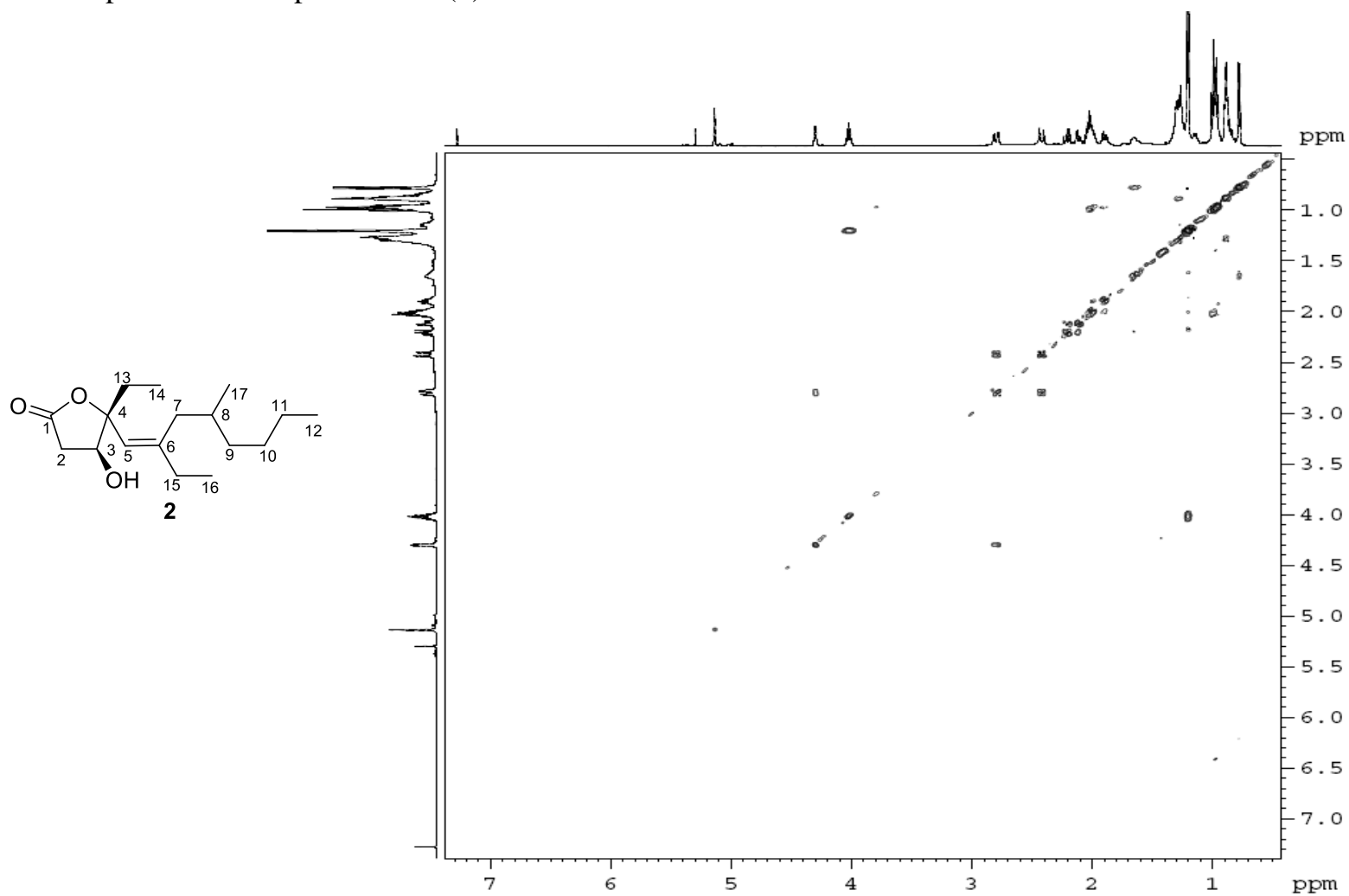


Figure S15. HMBC spectrum of simplexolide B (**2**) in CDCl₃.

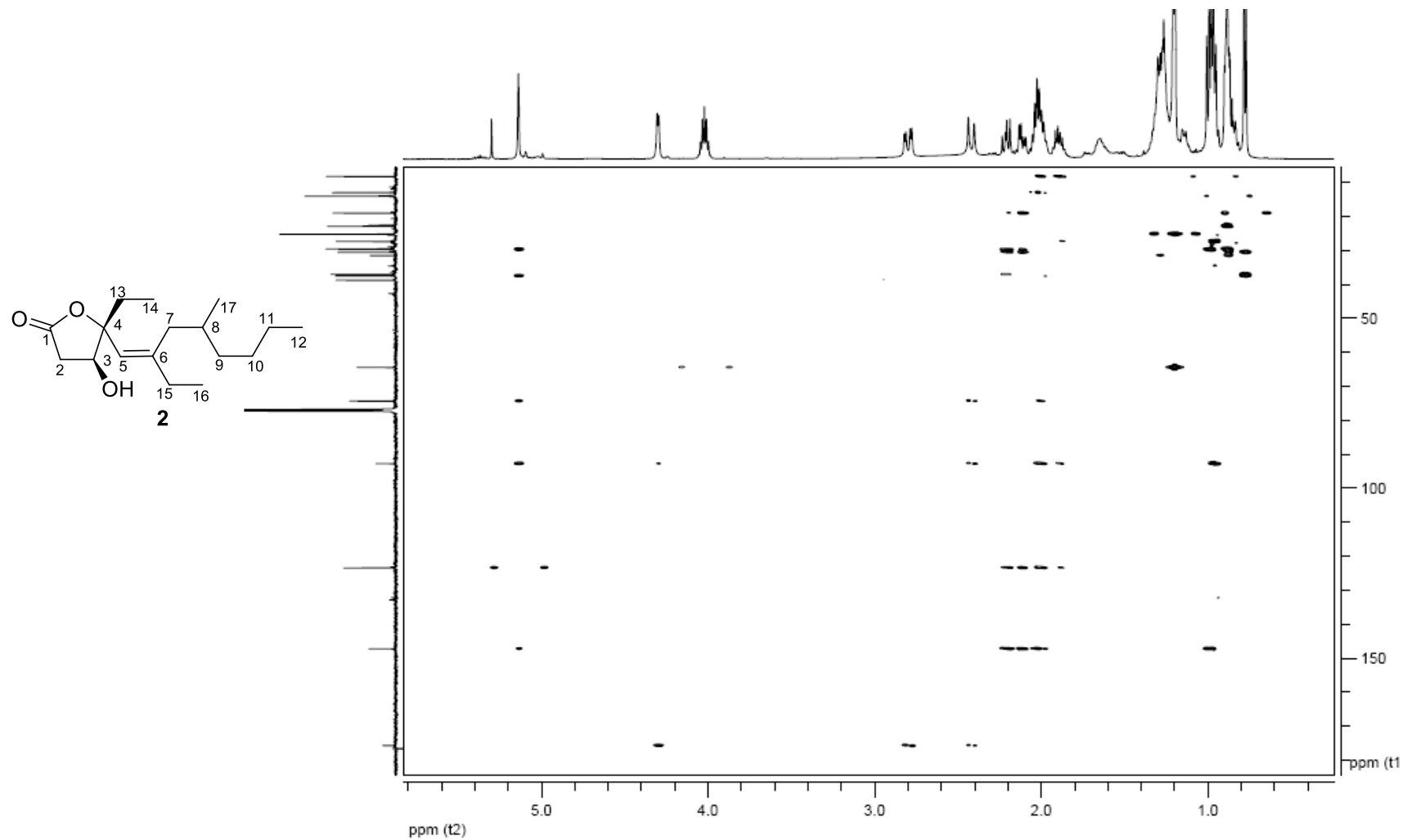


Figure S16. NOESY spectrum of simplexolide B (**2**) in CDCl₃.

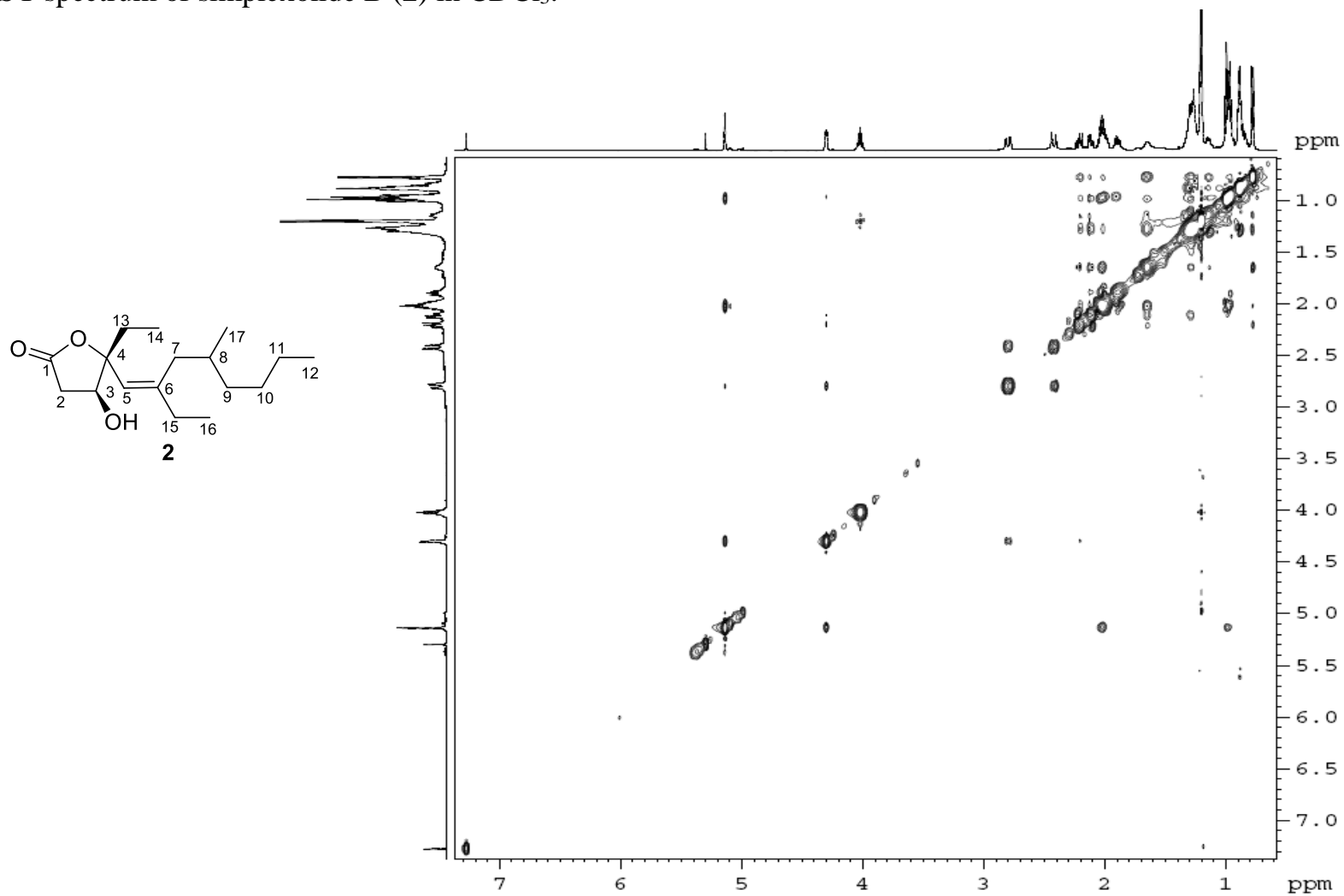


Figure S17. High resolution ESI mass spectrum of simplexolide C (**3**).

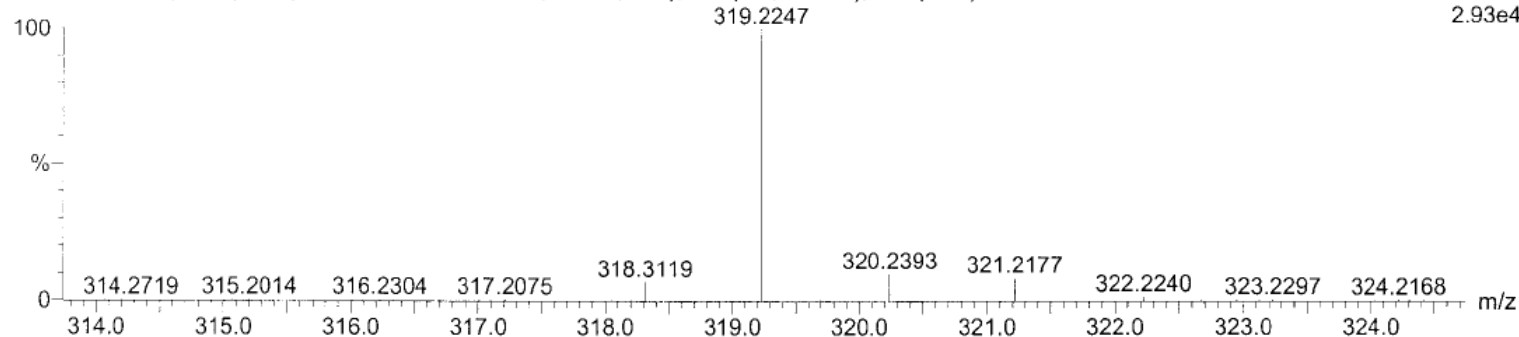
Elemental Composition Report

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

Monoisotopic Mass, Even Electron Ions
 17 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 5-30 H: 5-50 O: 1-5 Na: 1-1

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 XF-23b M.W=296
 WQ10194H1 9 (0.311) AM (Cen,6, 80.00, Ar,5000.0,325.16,0.70); Sm (SG, 2x3.00); Cm (1:15)

21-May-2010,15:33:54
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 TOF MS ES+
 2.93e4



Minimum: 35.00 -1.5
 Maximum: 100.00 5.0 10.0 50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
319.2247	100.00	319.2249	-0.2	-0.6	2.5	1893.8	C18 H32 O3 Na

Figure S18. IR spectrum of simplexolide C (**3**).

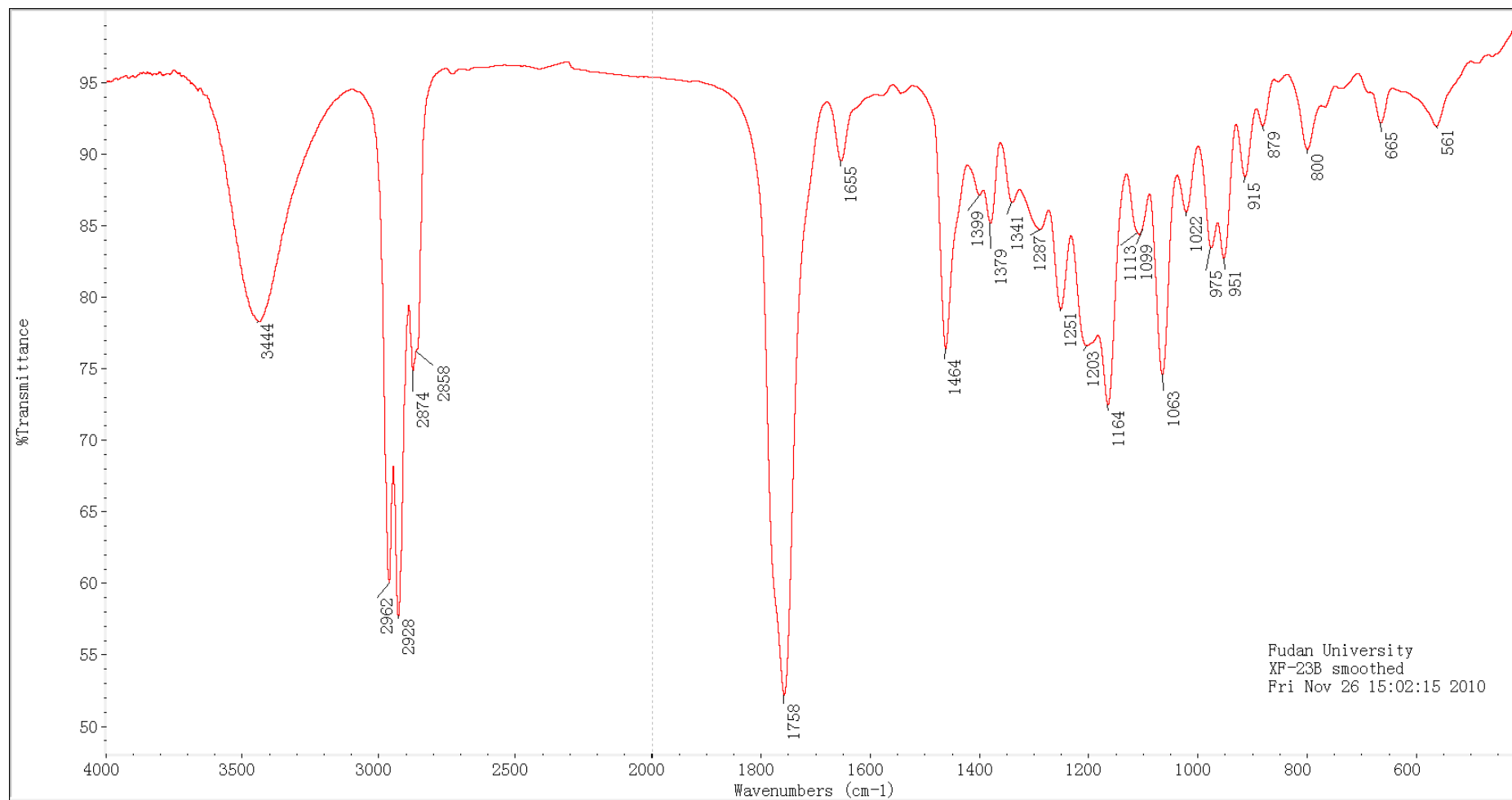


Figure S19. ^1H NMR spectrum of simplexolide C (**3**) in CDCl_3 .

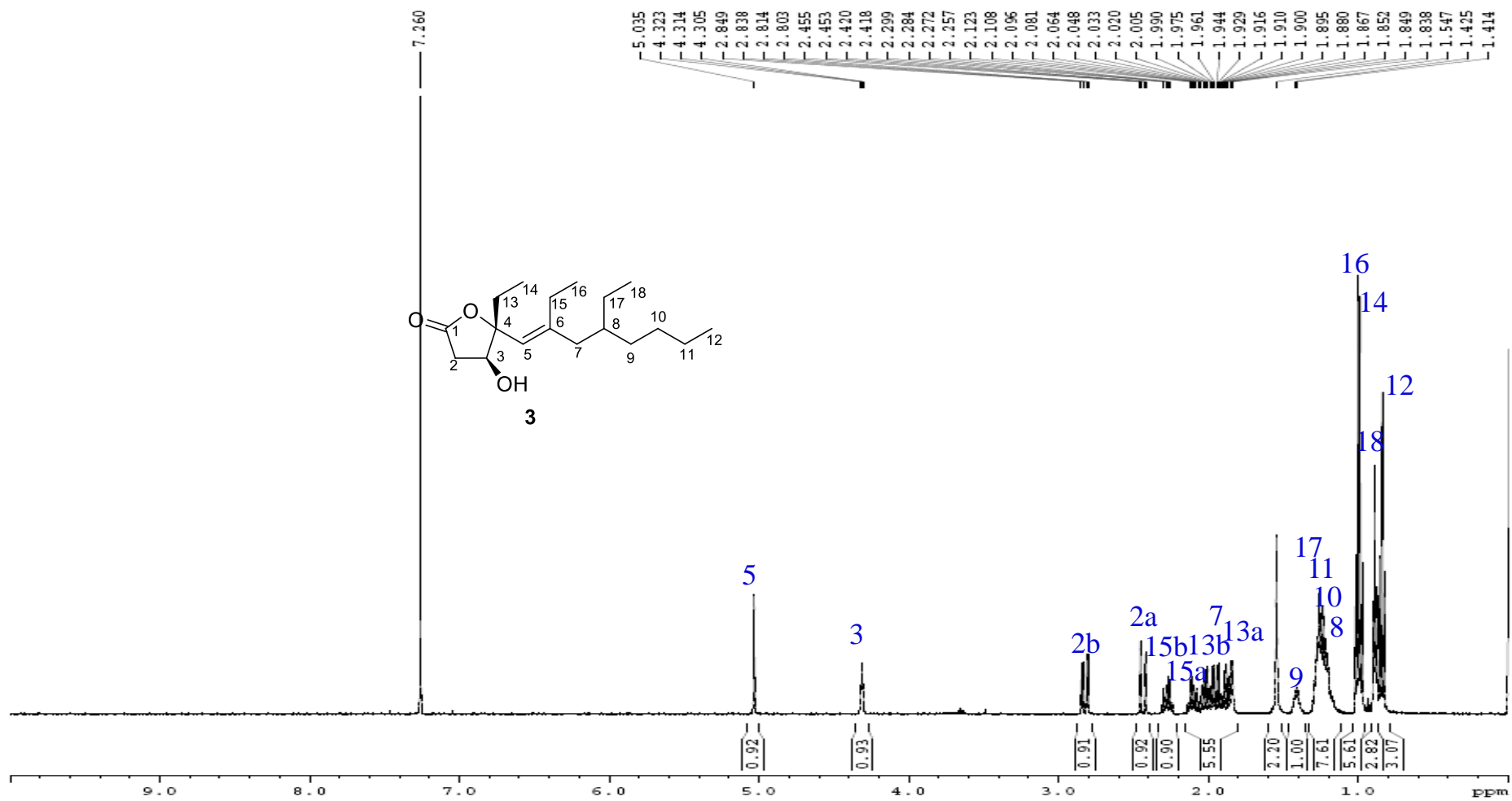


Figure S20. ^{13}C NMR spectrum of simplexolide C (**3**) in CDCl_3

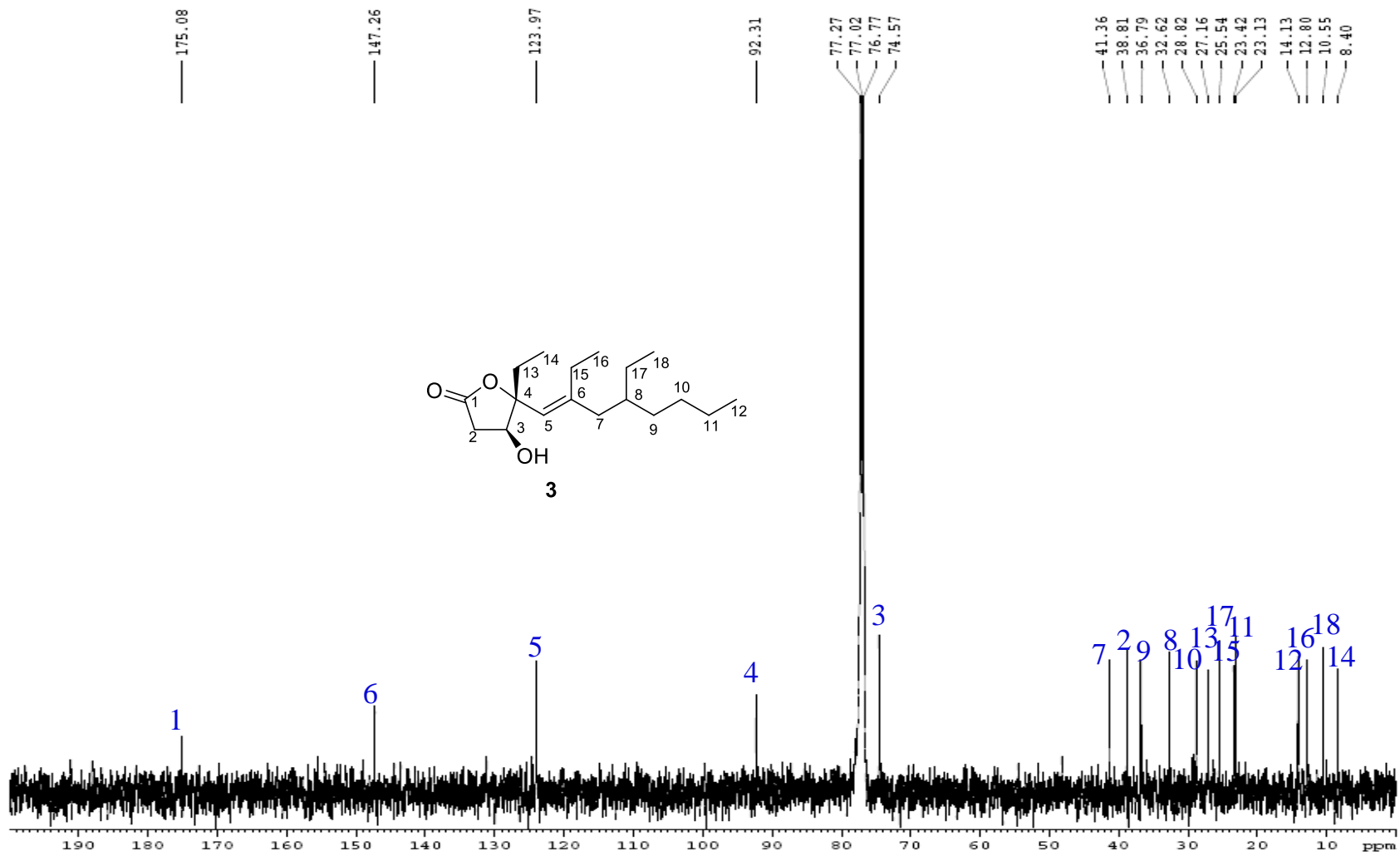


Figure S21. ^1H - ^1H COSY spectrum of simplexolide C (**3**) in CDCl_3 .

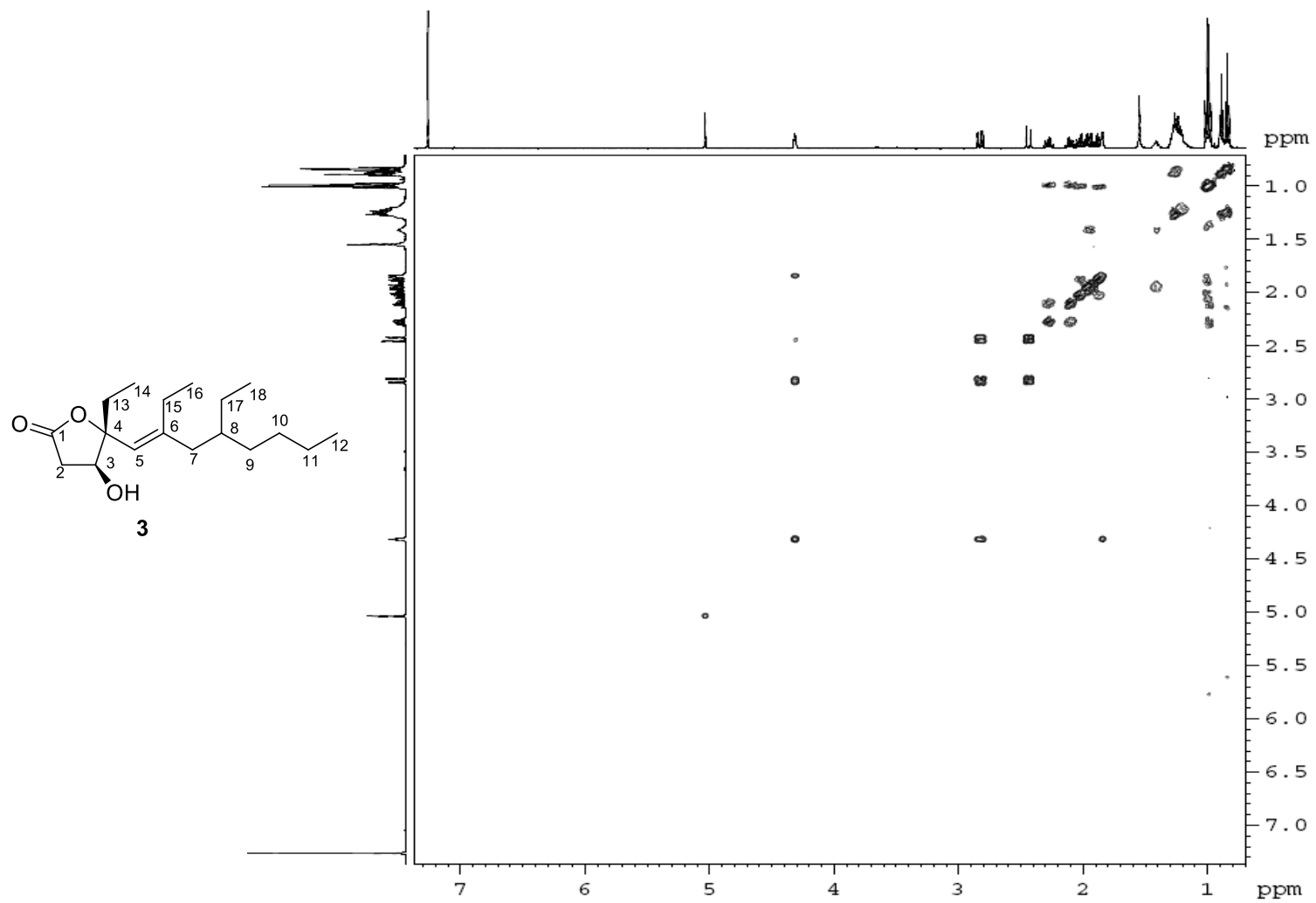


Figure S22. HSQC spectrum of simplexolide C (**3**) in CDCl₃.

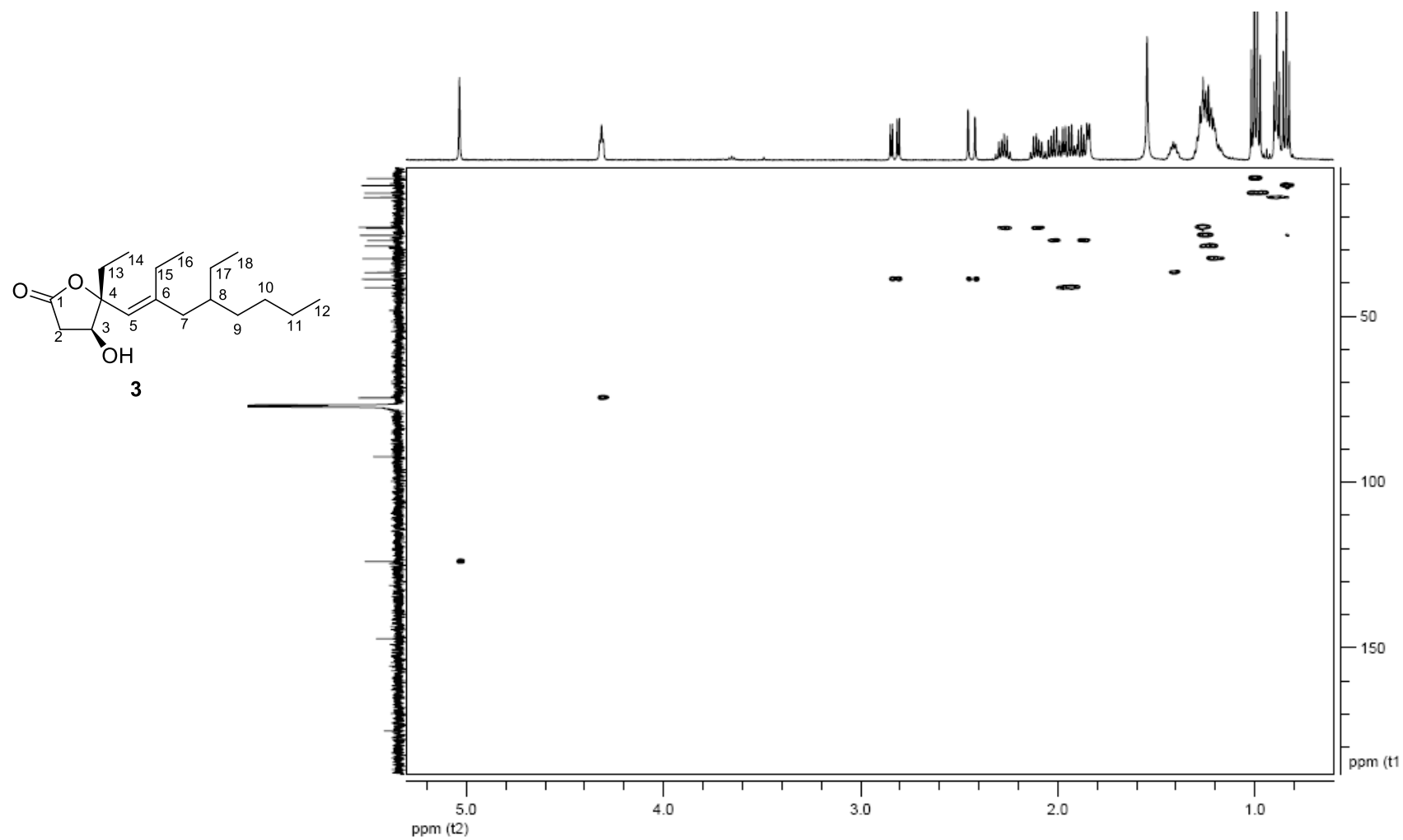


Figure S23. HMBC spectrum of simplexolide C (**3**) in CDCl₃.

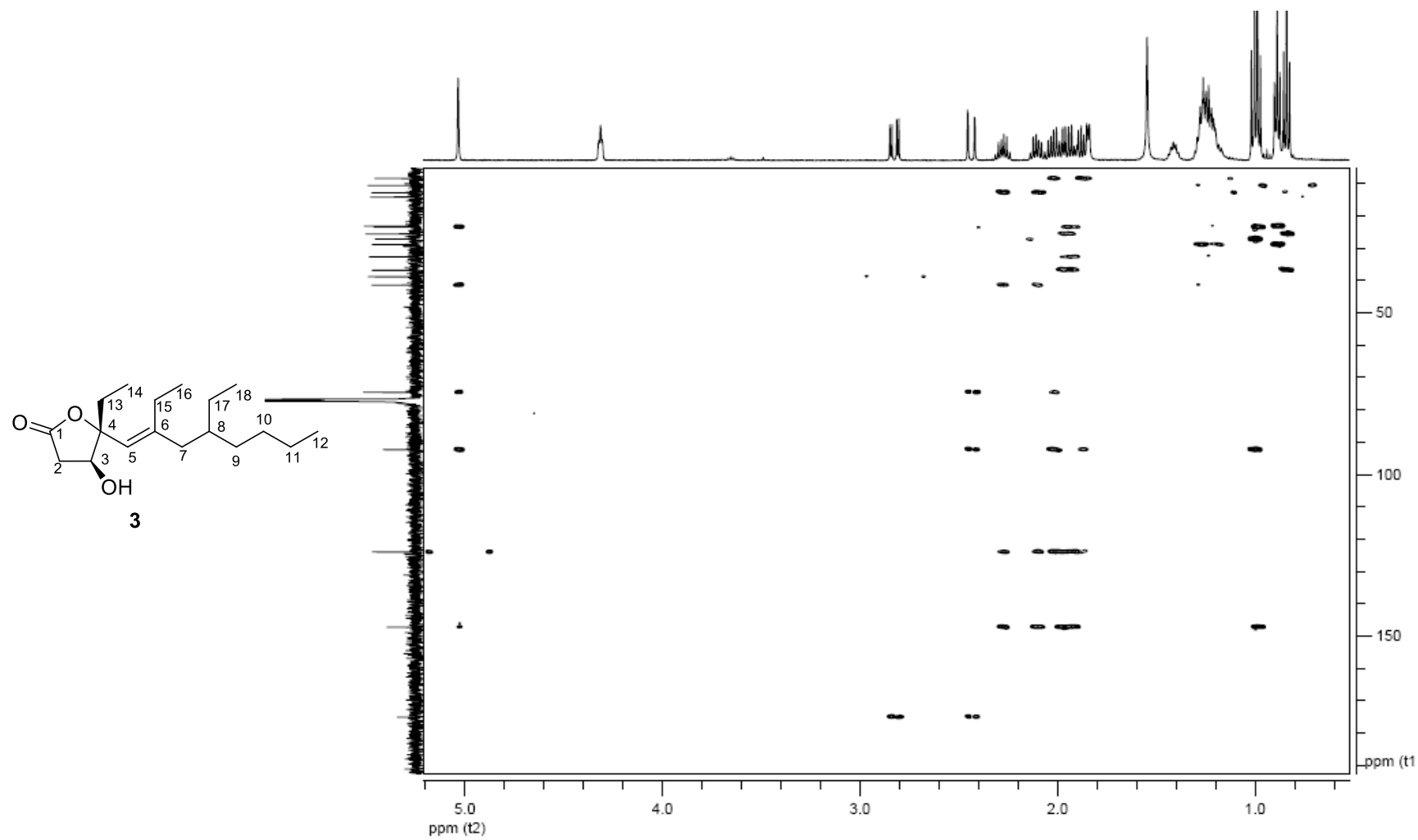


Figure S24. NOESY spectrum of simplexolide C (**3**) in CDCl₃.

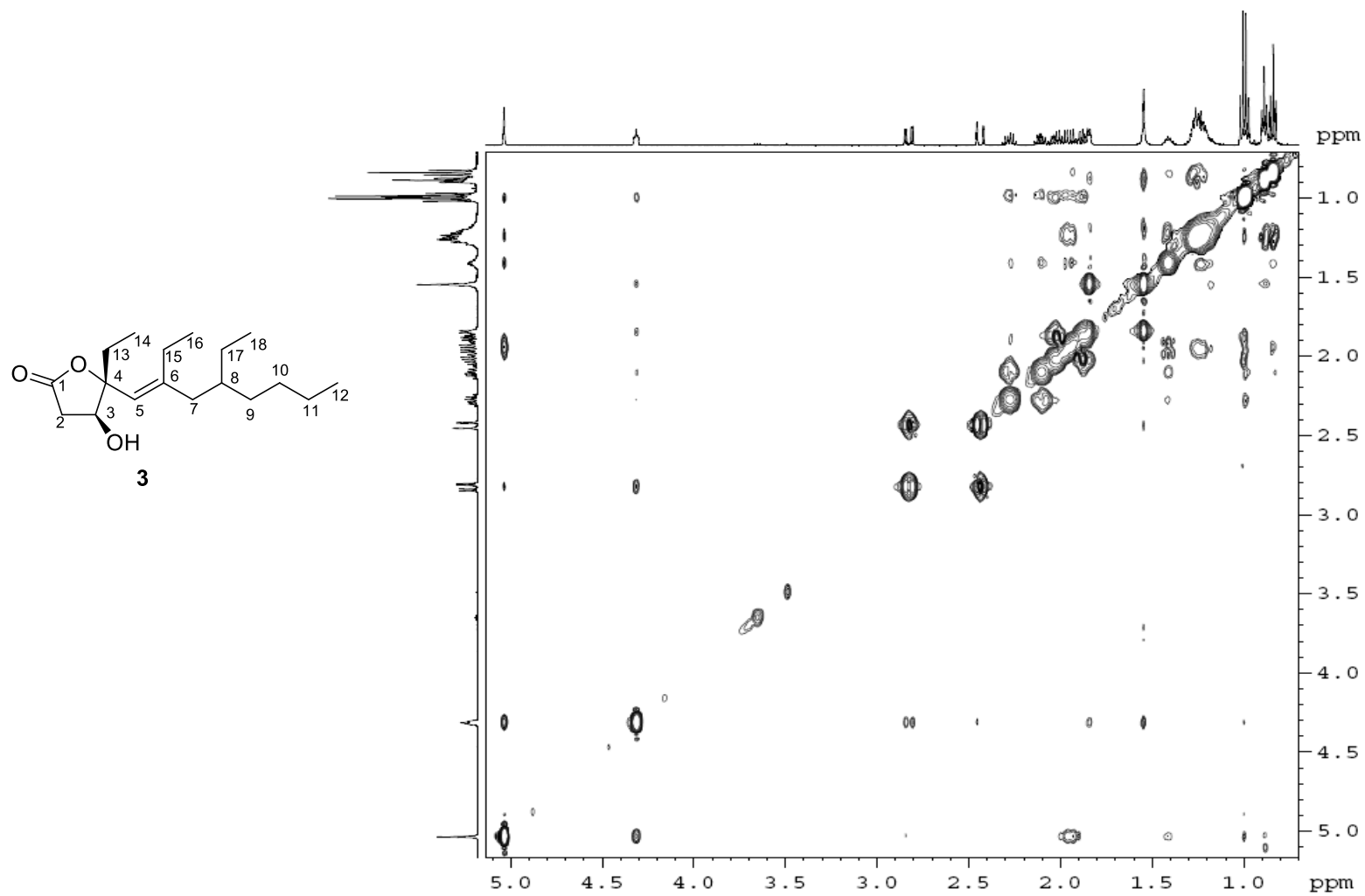


Figure S25. High resolution ESI mass spectrum of simplexolide D (4).

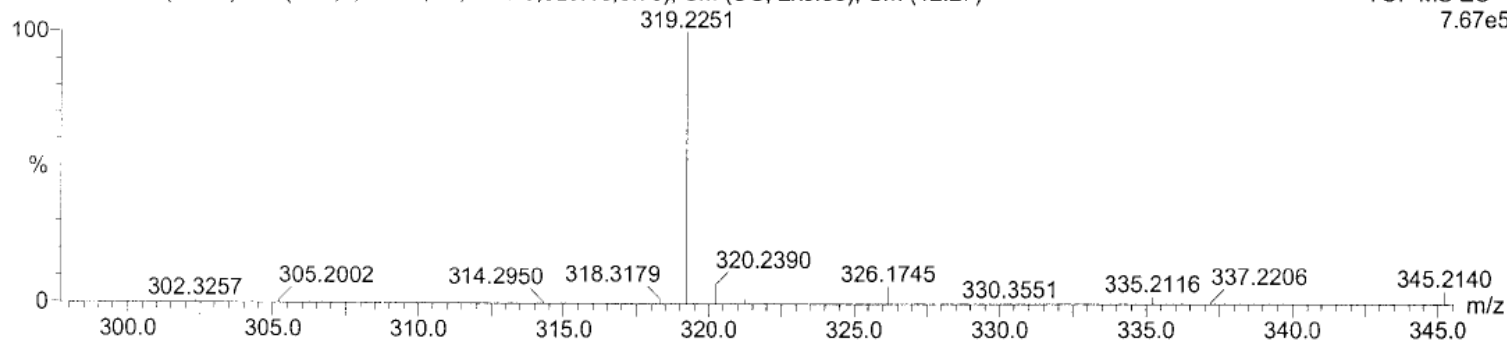
Elemental Composition Report

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

Monoisotopic Mass, Even Electron Ions
 17 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 5-30 H: 5-50 O: 1-5 Na: 1-1

SIP1
 XF-23a M.W=296
 WQ10195H 20 (0.691) AM (Cen,6, 80.00, Ar,5000.0,325.16,0.70); Sm (SG, 2x3.00); Cm (12:27)

21-May-2010,15:44:18
 0.00000000
 TOF MS ES+
 7.67e5



Minimum: 35.00
 Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
319.2251	100.00	319.2249	0.2	0.6	2.5	73541.7	C18 H32 O3 Na

Figure S26. IR spectrum of simplexolide D (4).

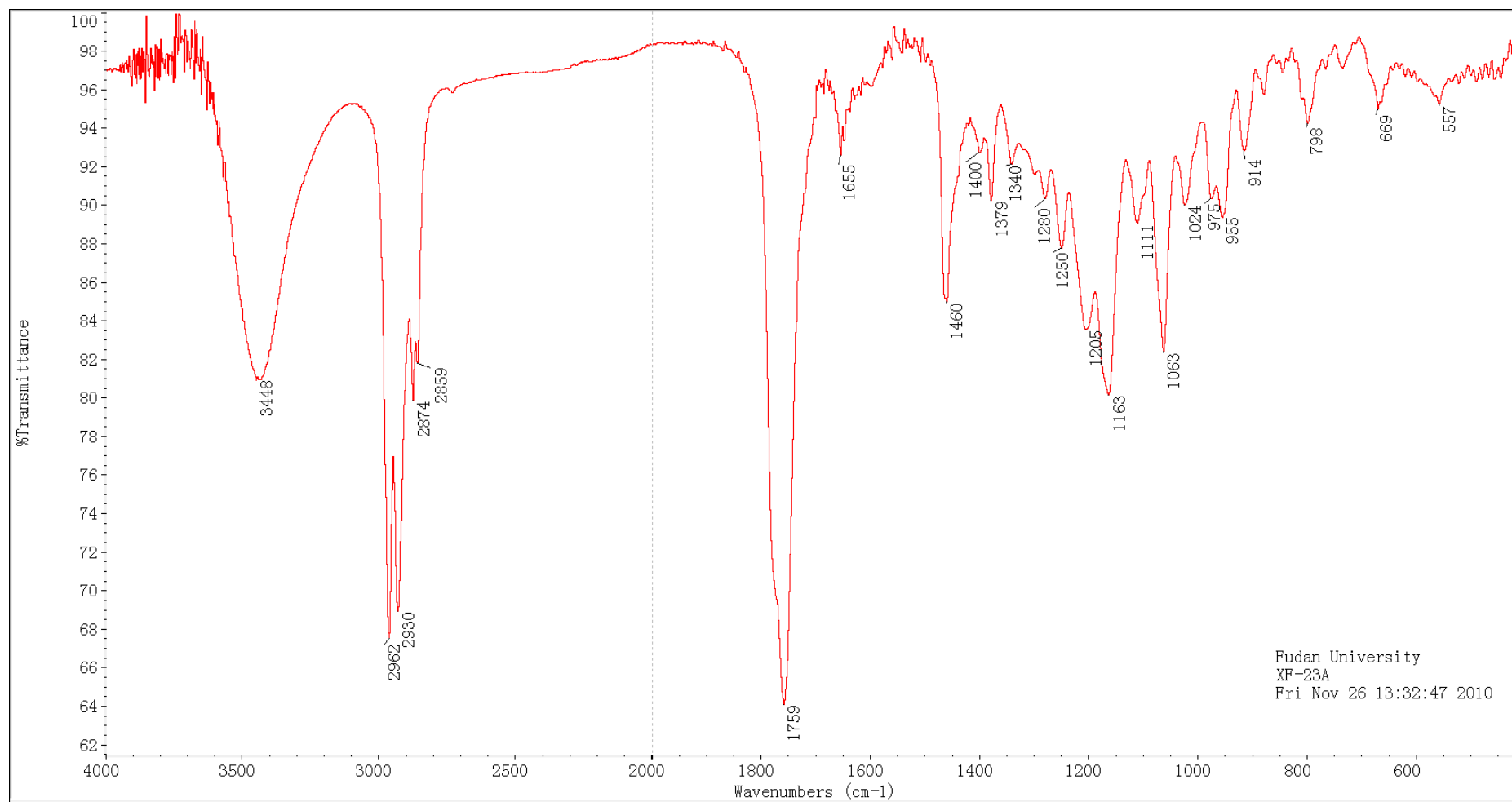


Figure S27. ^1H NMR spectrum of simplexolide D (**4**) in CDCl_3 .

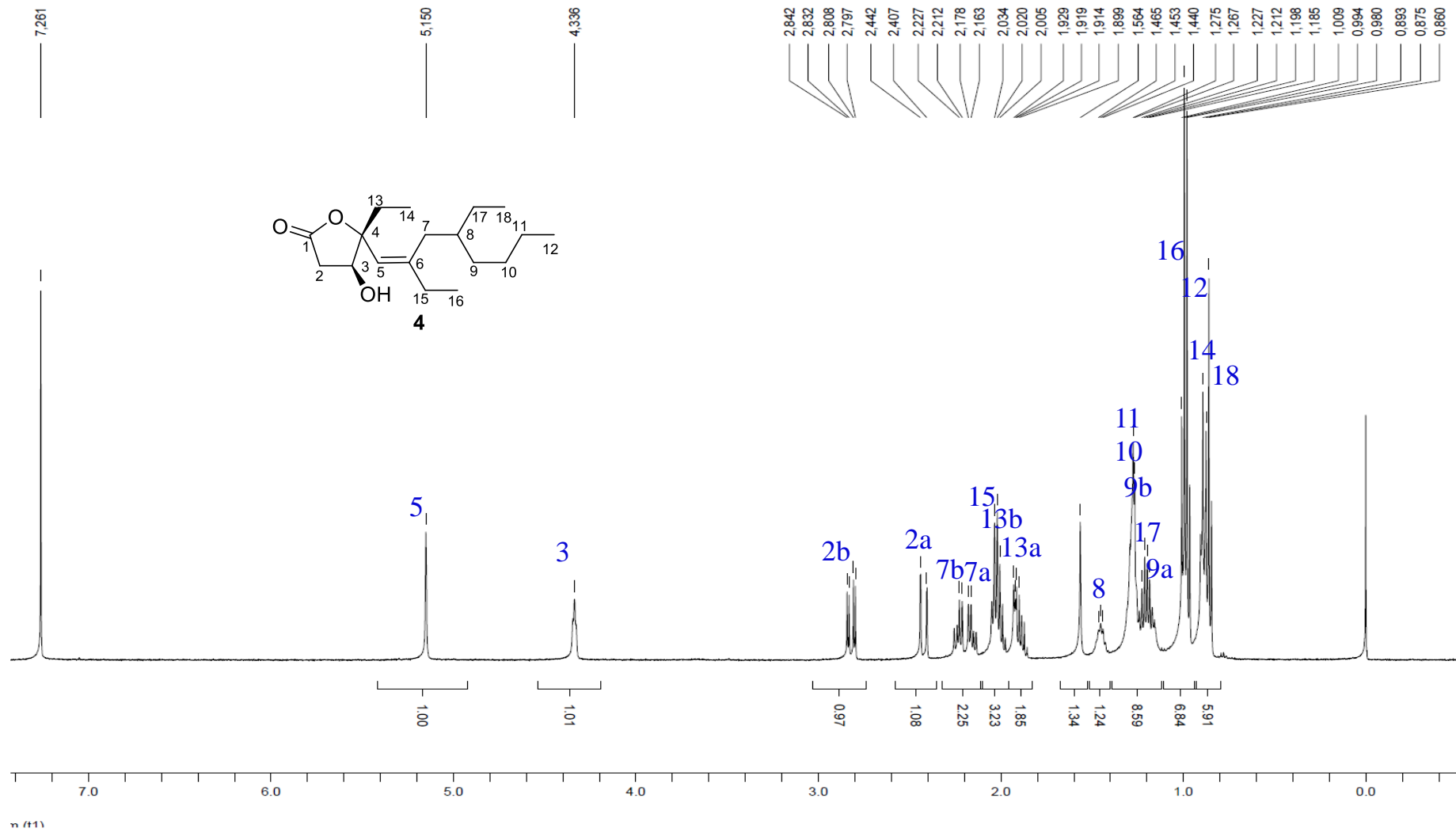


Figure S28. ^{13}C NMR spectrum of simplexolide D (**4**) in CDCl_3 .

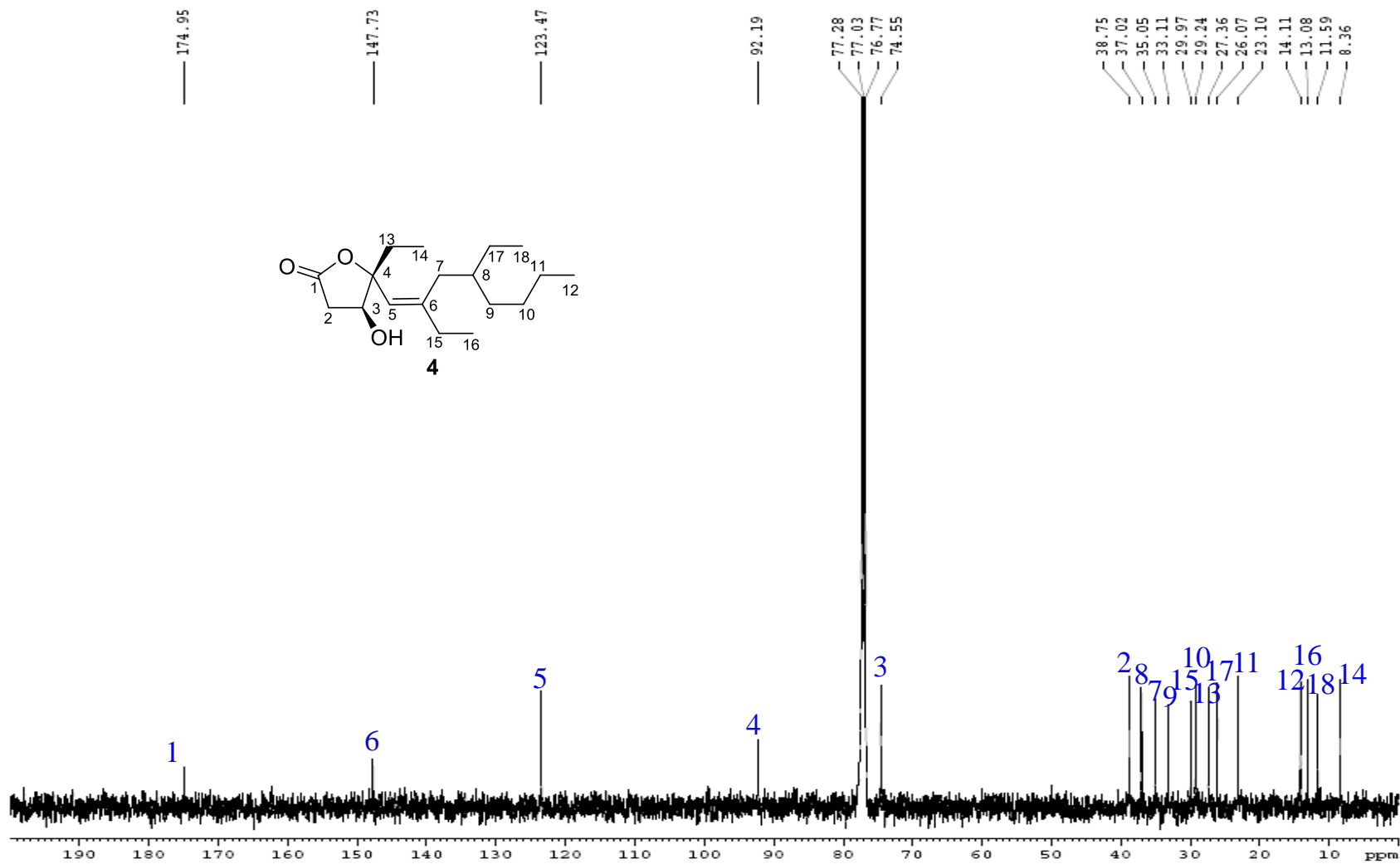


Figure S29. ^1H - ^1H COSY spectrum of simplexolide D (**4**) in CDCl_3 .

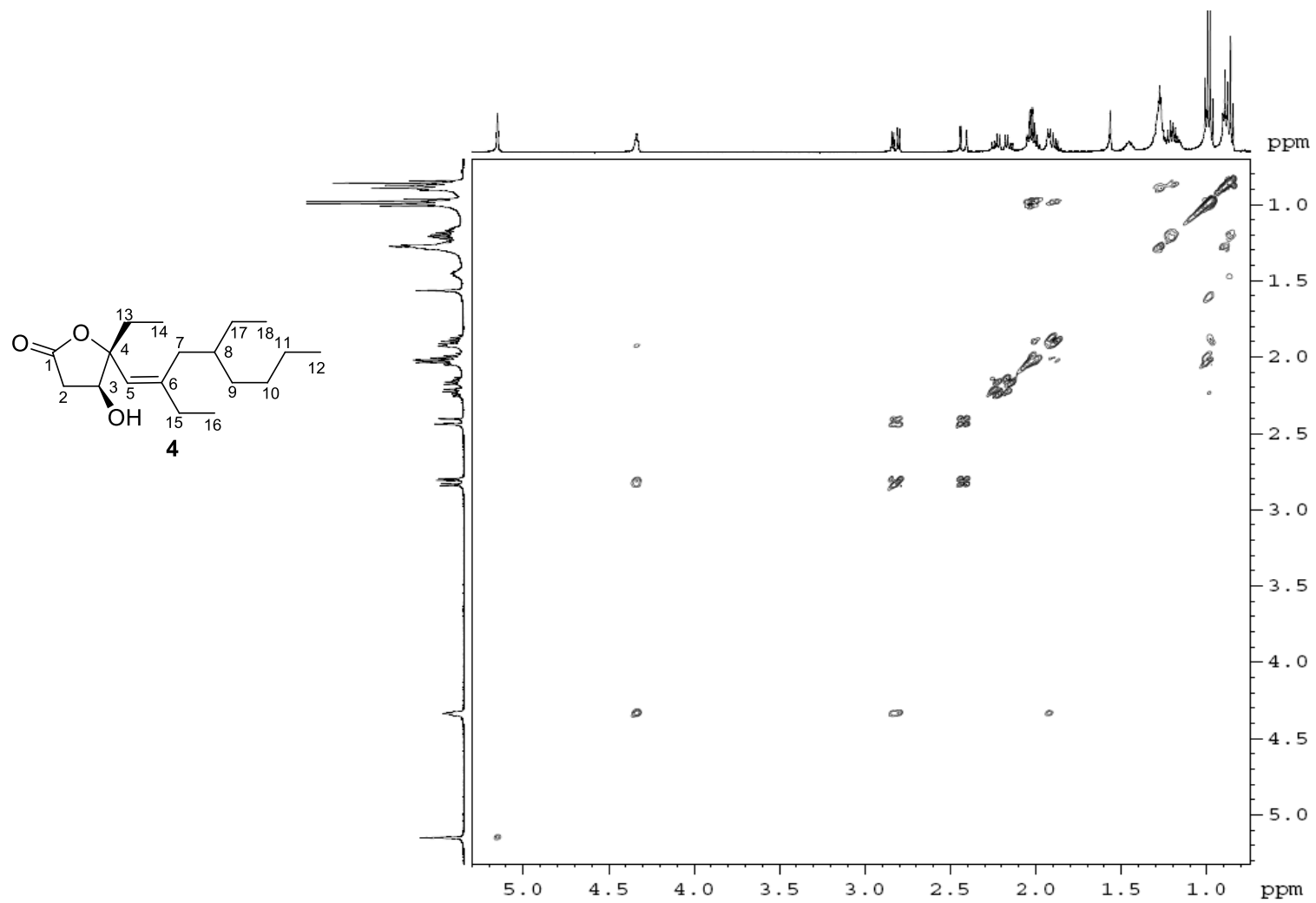


Figure S30. HSQC spectrum of simplexolide D (**4**) in CDCl₃.

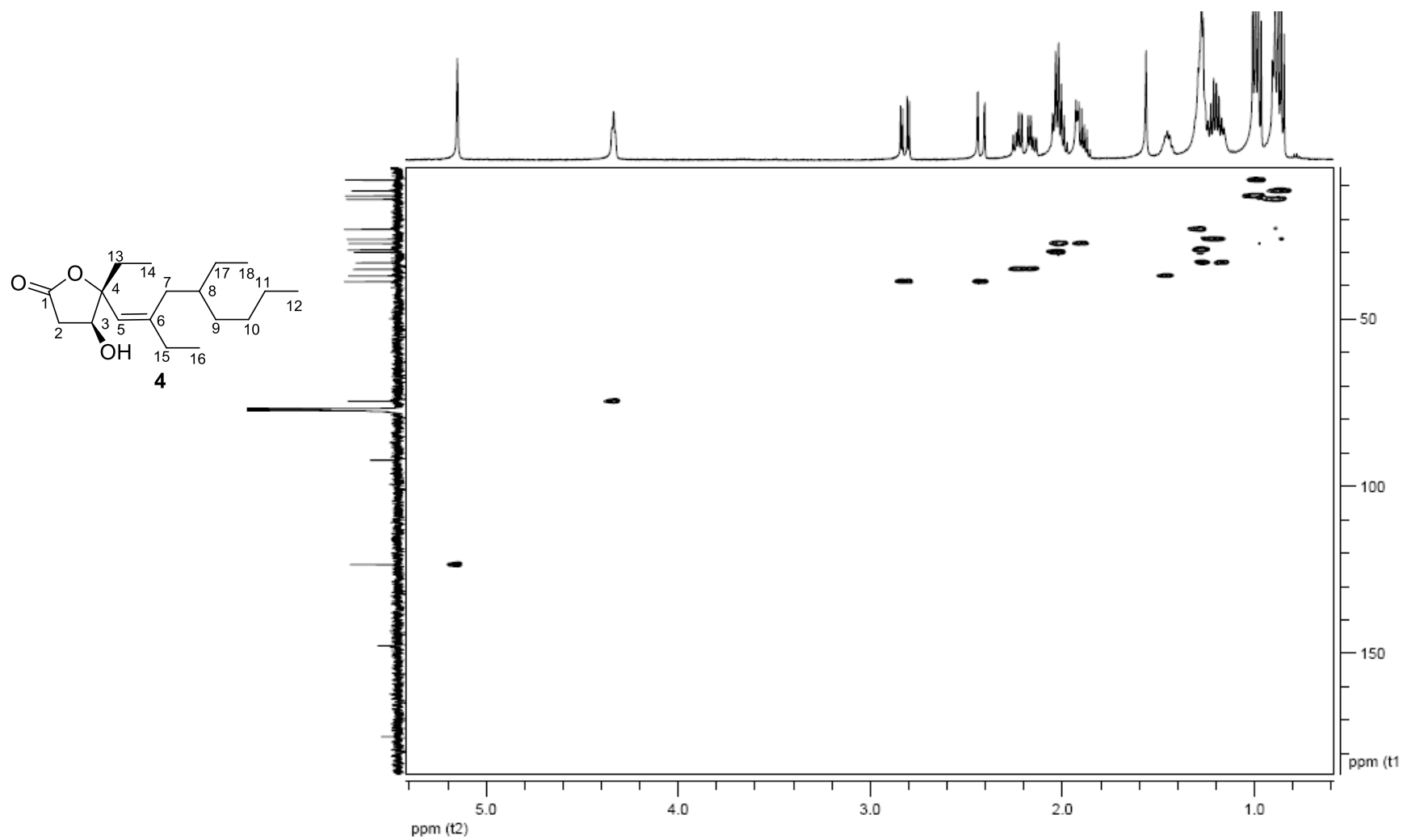


Figure S31. HMBC spectrum of simplexolide D (**4**) in CDCl₃.

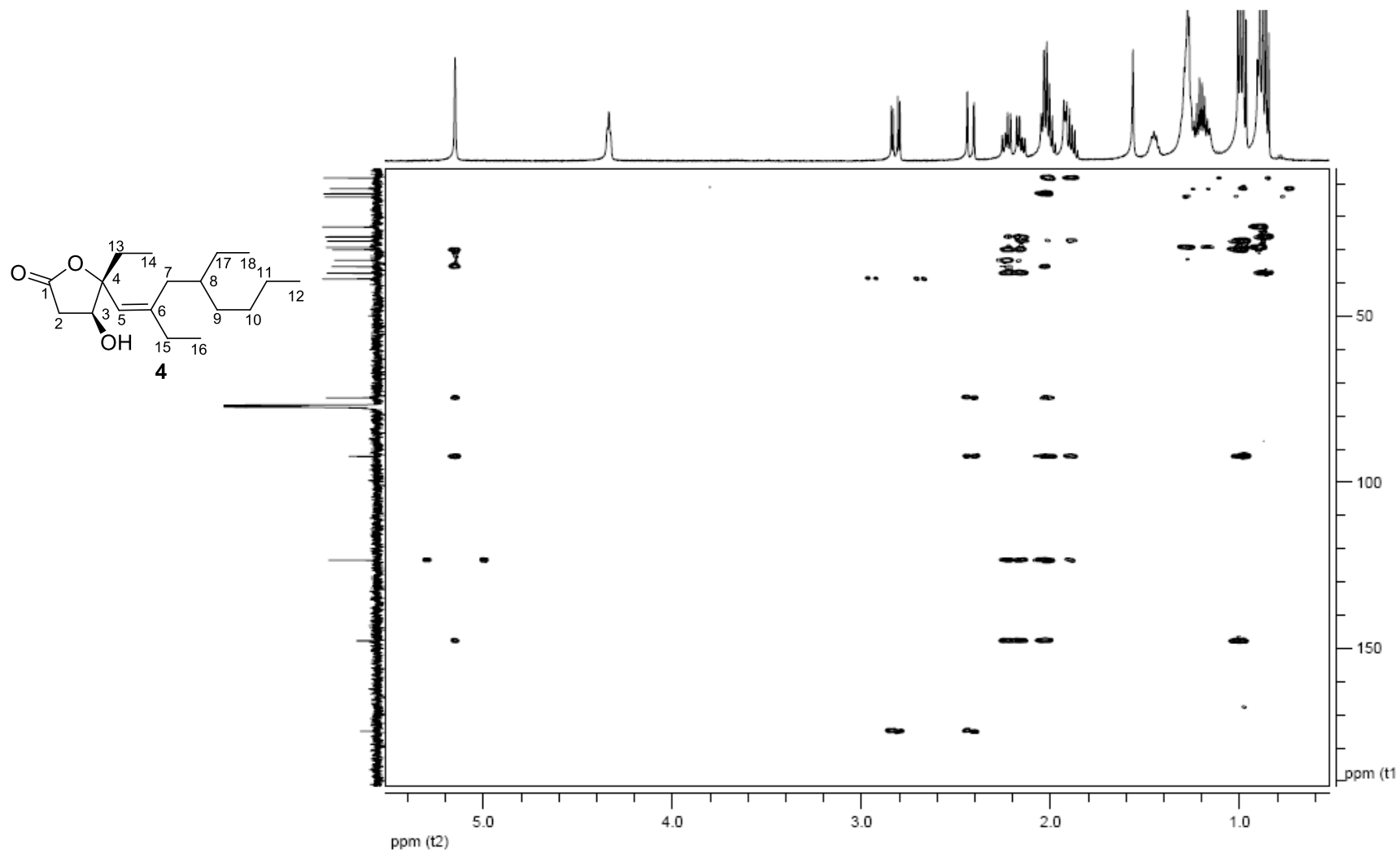


Figure S32. NOESY spectrum of simplexolide D (**4**) in CDCl₃.

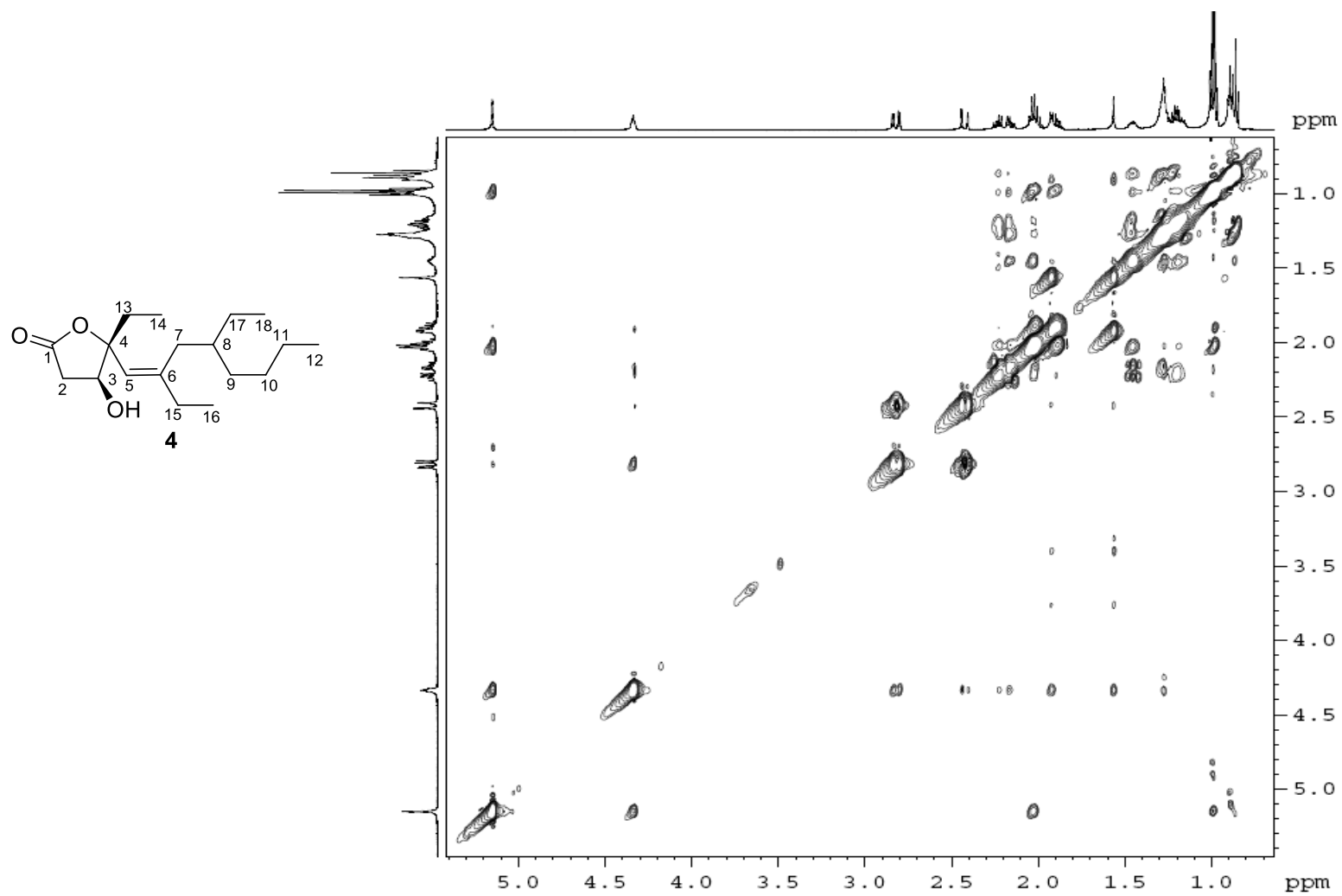


Figure S33. High resolution ESI mass spectrum of simplexolide E (**5**).

Elemental Composition Report

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

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 5-30 H: 5-50 O: 1-5 Na: 1-1

SIPI

XF-22b M.W=282

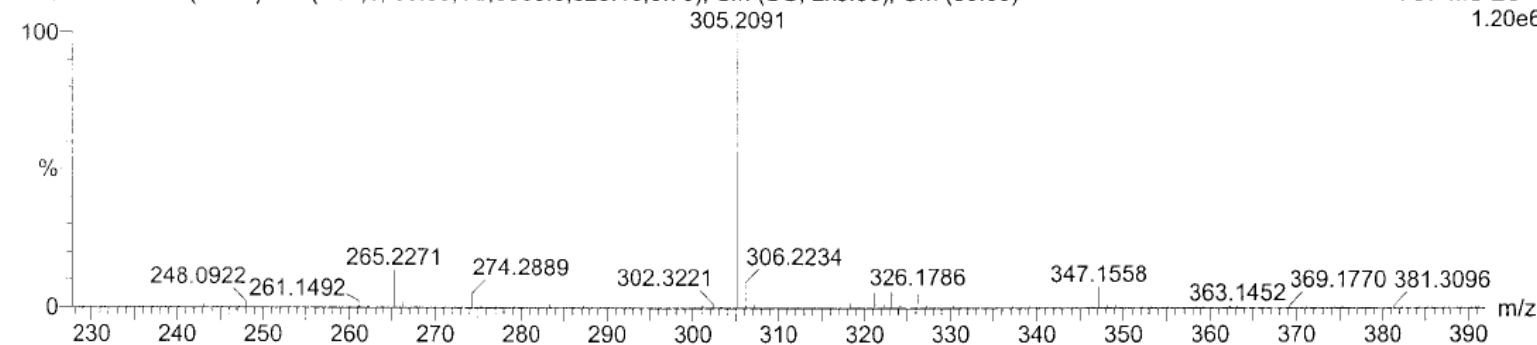
WQ10197H1 50 (1.728) AM (Cen,6, 80.00, Ar,5000.0,325.16,0.70); Sm (SG, 2x3.00); Cm (30:60)

24-May-2010,11:20:57

0.00000000

TOF MS ES+

1.20e6



Minimum: 35.00 -1.5
 Maximum: 100.00 5.0 10.0 50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
305.2091	100.00	305.2093	-0.2	-0.7	2.5	58921.2	C17 H30 O3 Na

Figure S34. IR spectrum of simplexolide E (5).

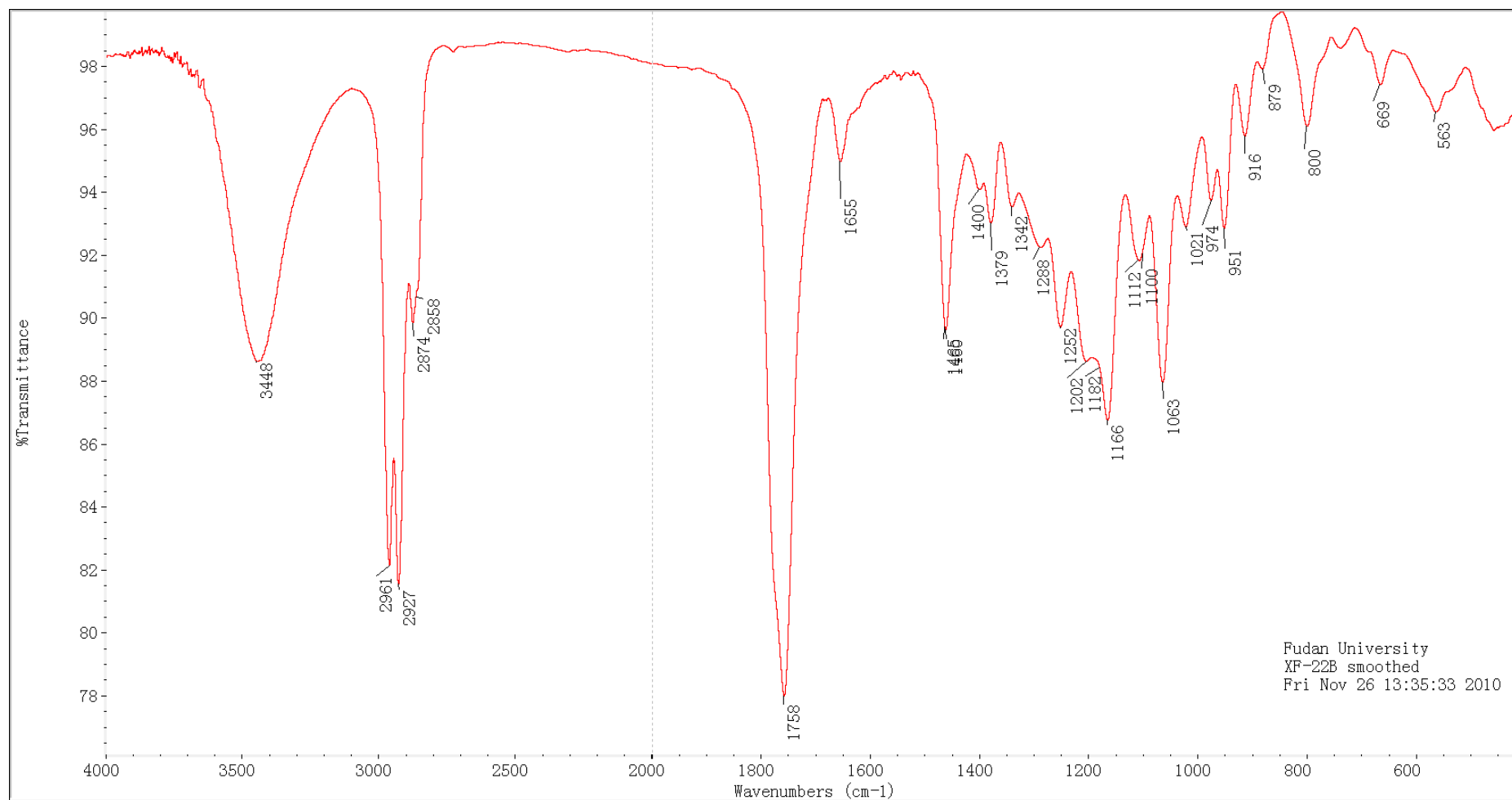


Figure S35. ^1H NMR spectrum of simplexolide E (**5**) in CDCl_3 .

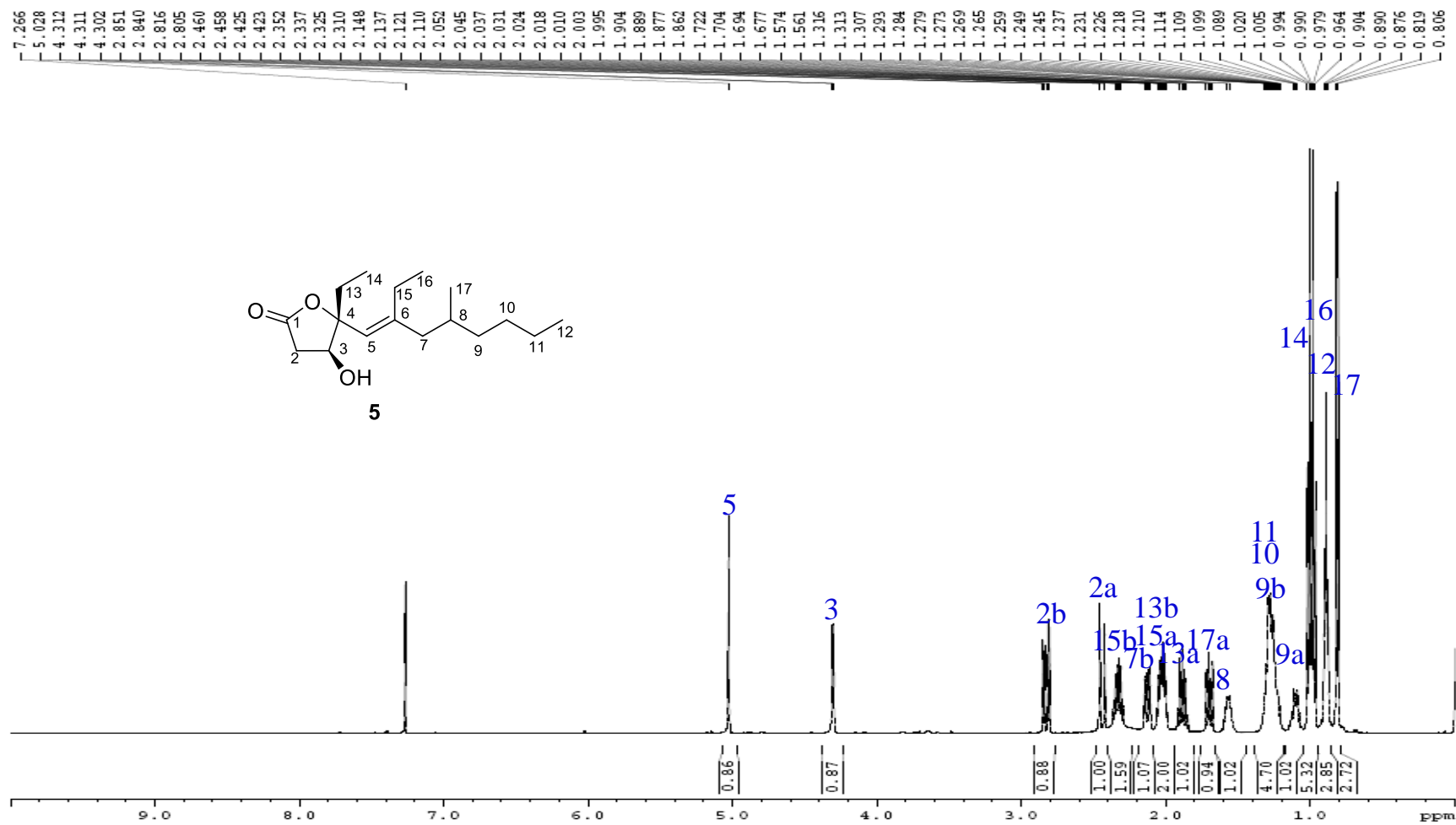


Figure S36. ^{13}C NMR spectrum of simplexolide E (**5**) in CDCl_3 .

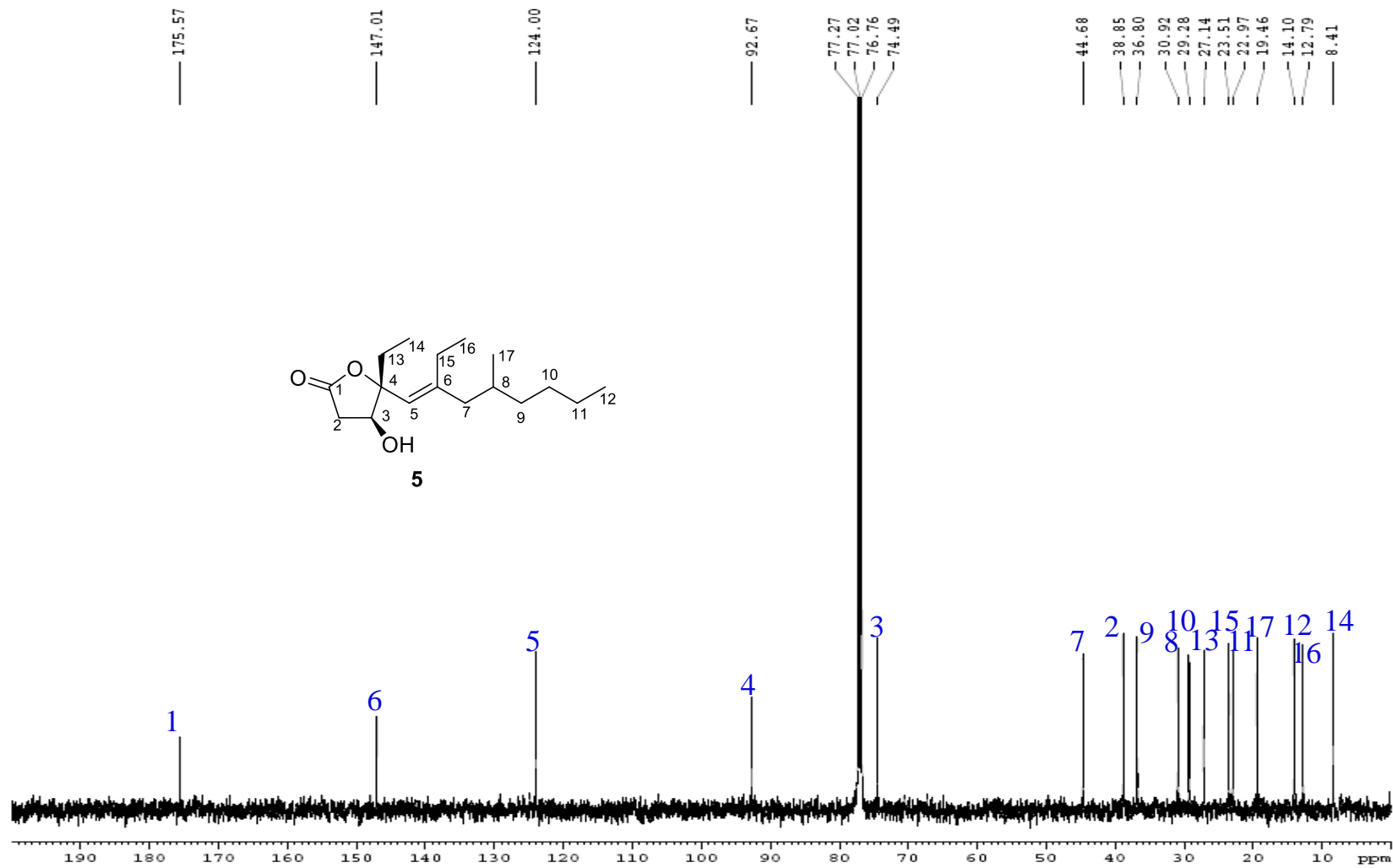


Figure S37. ^1H - ^1H COSY spectrum of simplexolide E (**5**) in CDCl_3 .

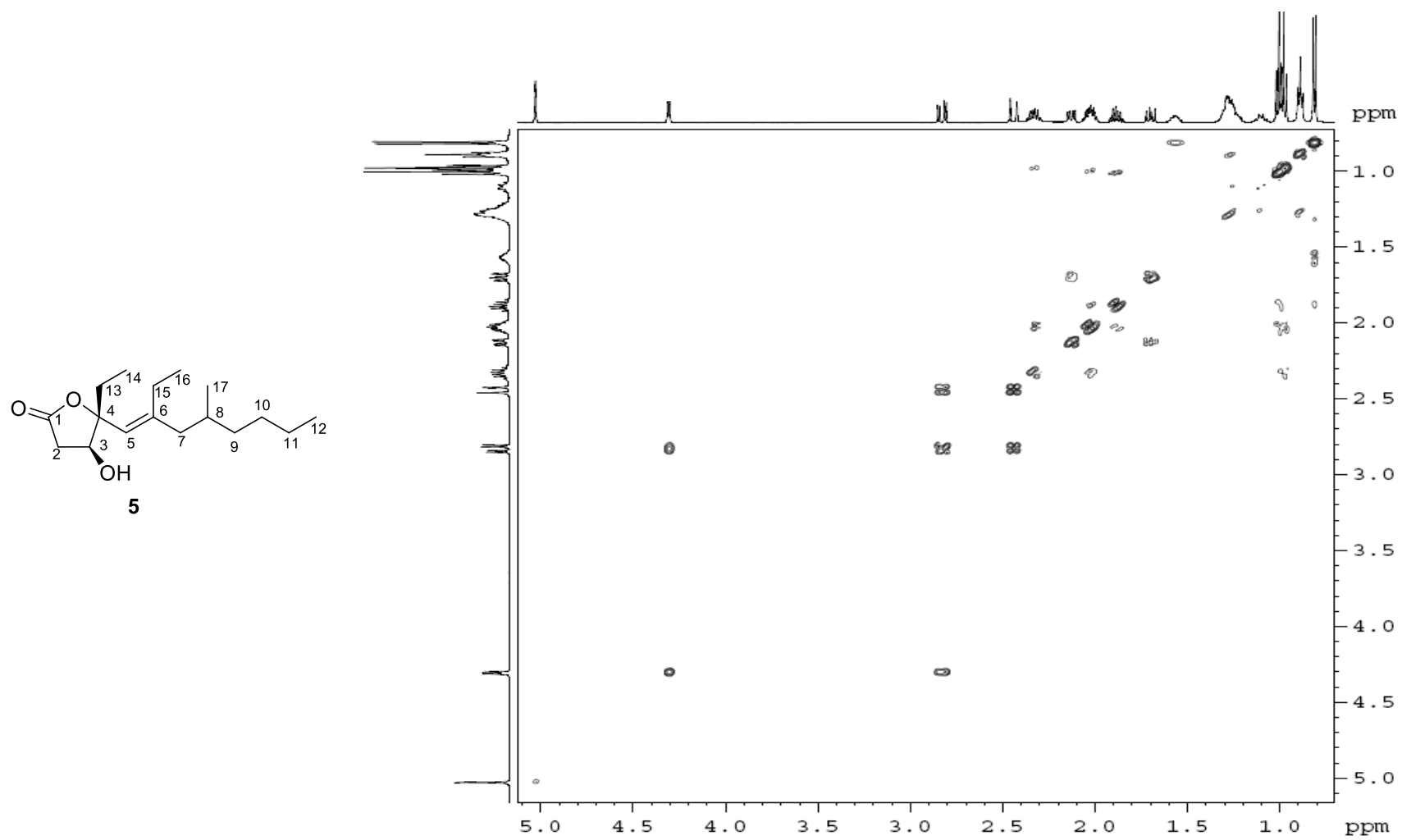


Figure S38. HSQC spectrum of simplexolide E (**5**) in CDCl₃.

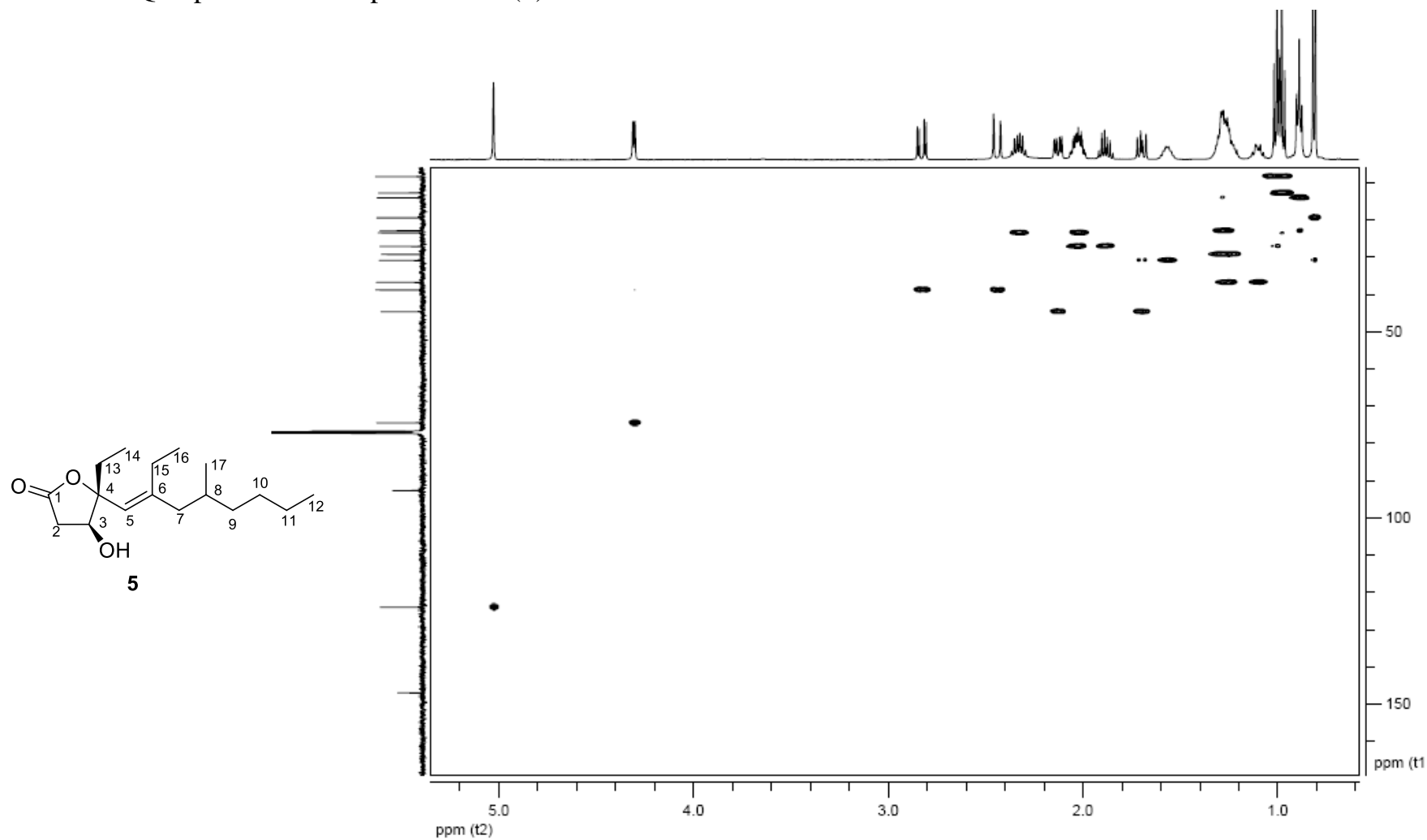


Figure S39. HMBC spectrum of simplexolide E (**5**) in CDCl₃.

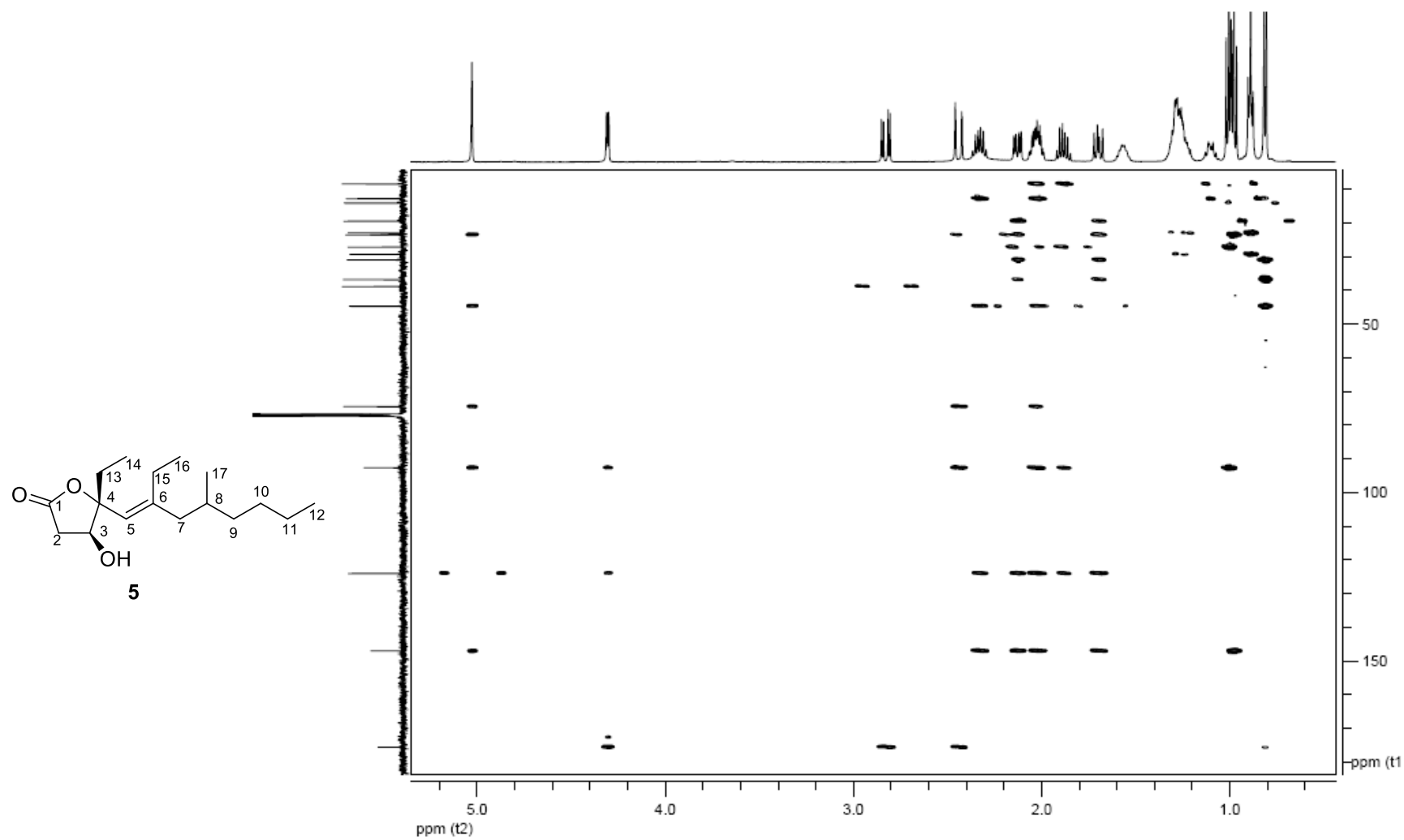


Figure S40. NOESY spectrum of simplexolide E (**5**) in CDCl₃.

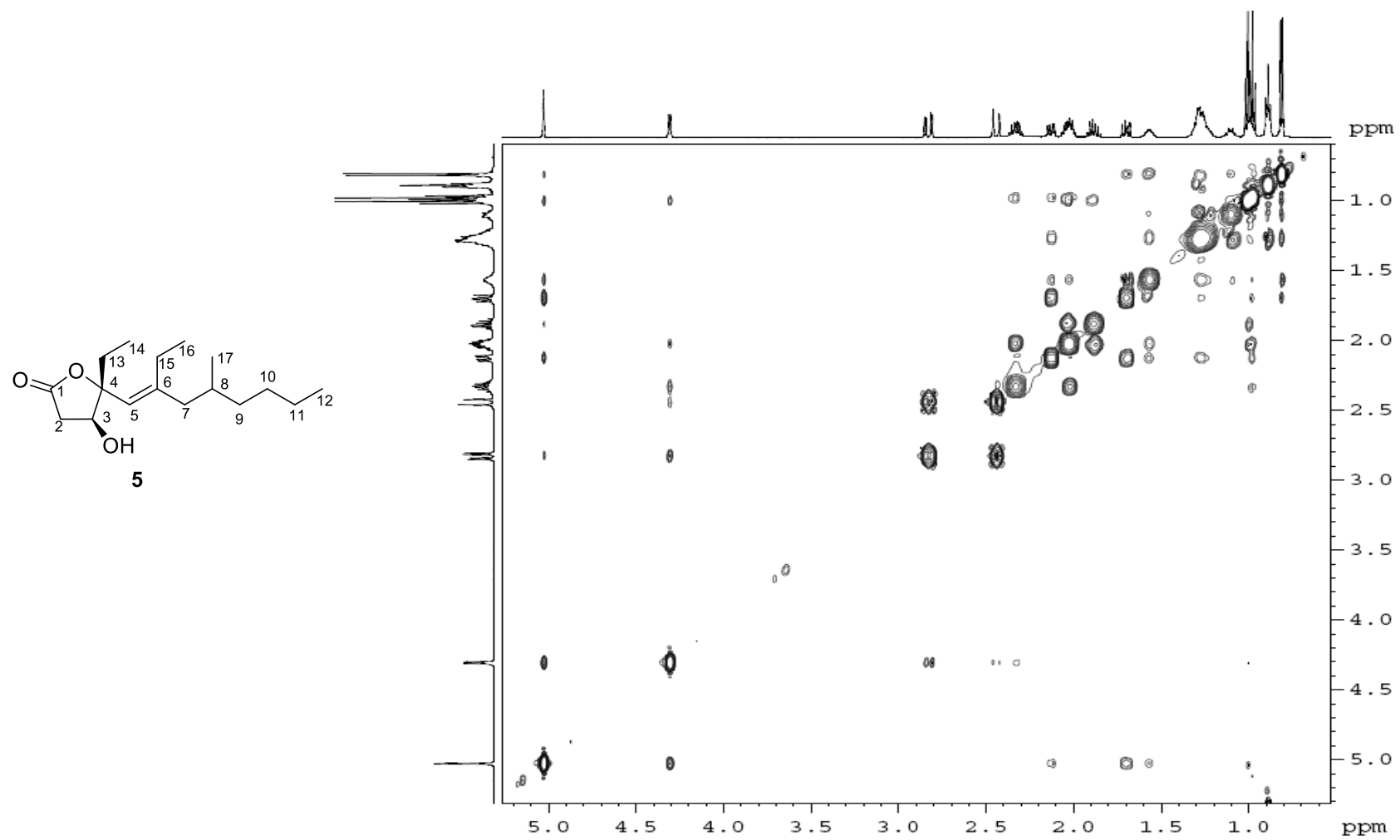


Figure S41. High resolution ESI mass spectrum of plakorfan A (6).

Elemental Composition Report

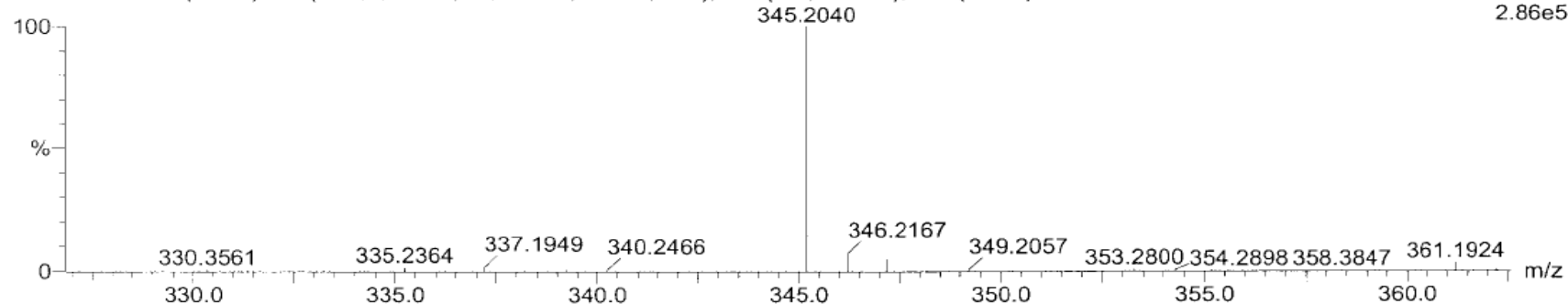
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 Selected filters: None

Monoisotopic Mass, Even Electron Ions
 19 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:

C: 5-30 H: 5-50 O: 1-5 Na: 1-1

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 XF-26 M.W=322
 WQ10193H1 42 (1.453) AM (Cen,6, 80.00, Ar,5000.0,325.16,0.70); Sm (SG, 2x3.00); Cm (35:55)

21-May-2010,15:13:53
 0.00000000
 TOF MS ES+
 2.86e5



Minimum: 35.00
 Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
345.2040	100.00	345.2042	-0.2	-0.6	4.5	28493.4	C19 H30 O4 Na

Figure S42. IR spectrum of plakorfuran A (6).

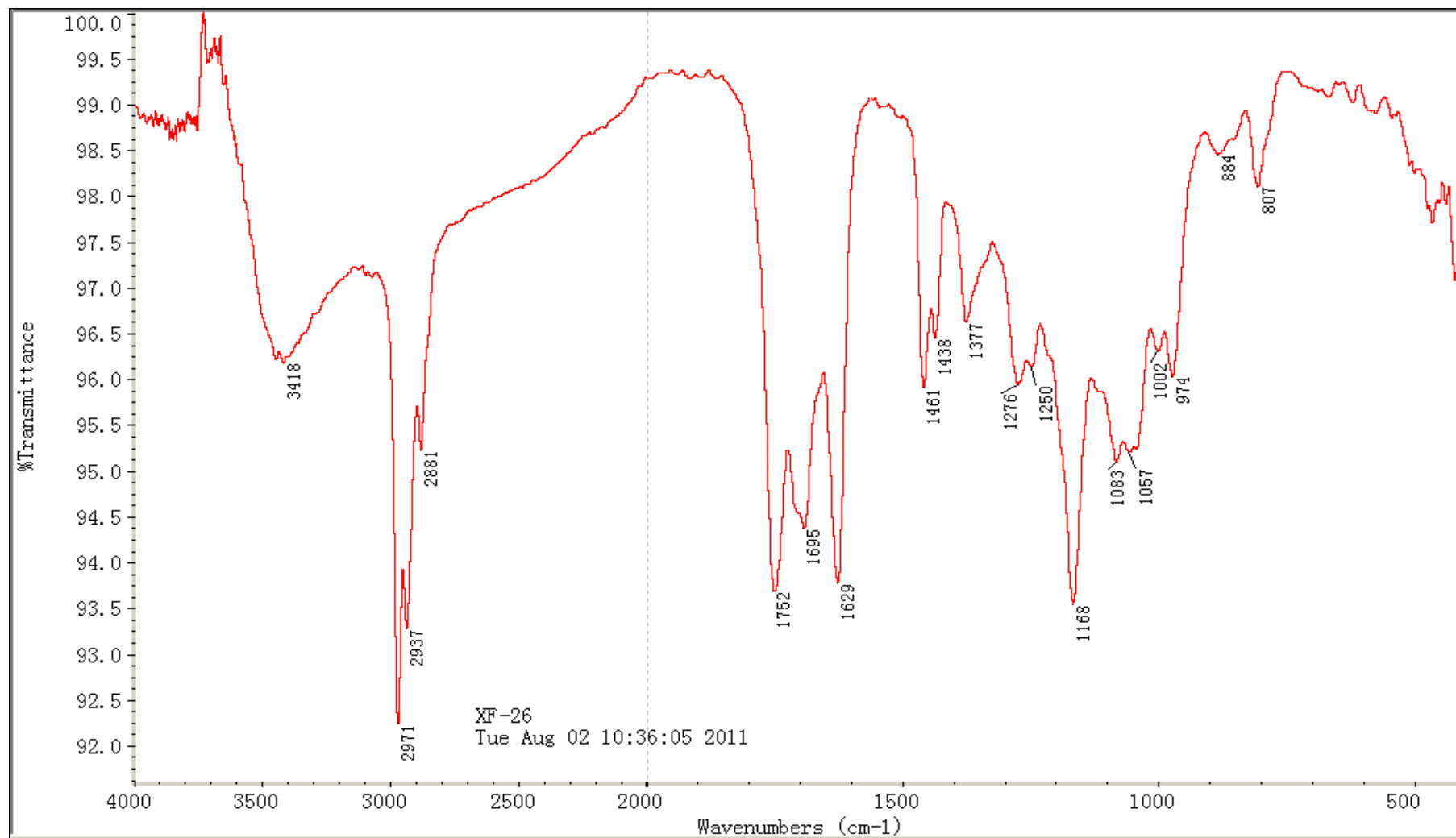


Figure S43. ^1H NMR spectrum of plakorfuran A (**6**) in CDCl_3 .

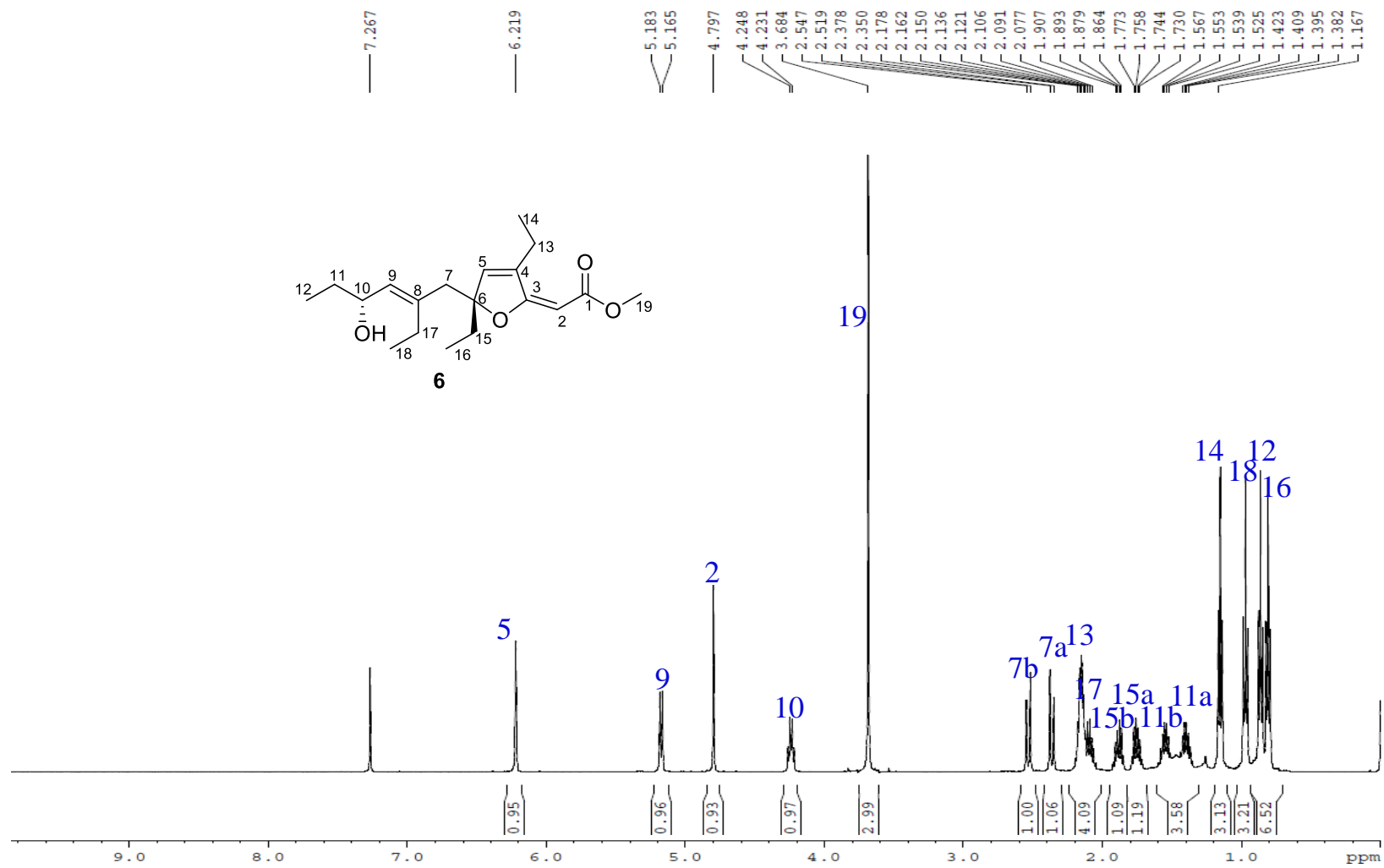


Figure S44. ^{13}C NMR spectrum of plakorfuran A (**6**) in CDCl_3 .

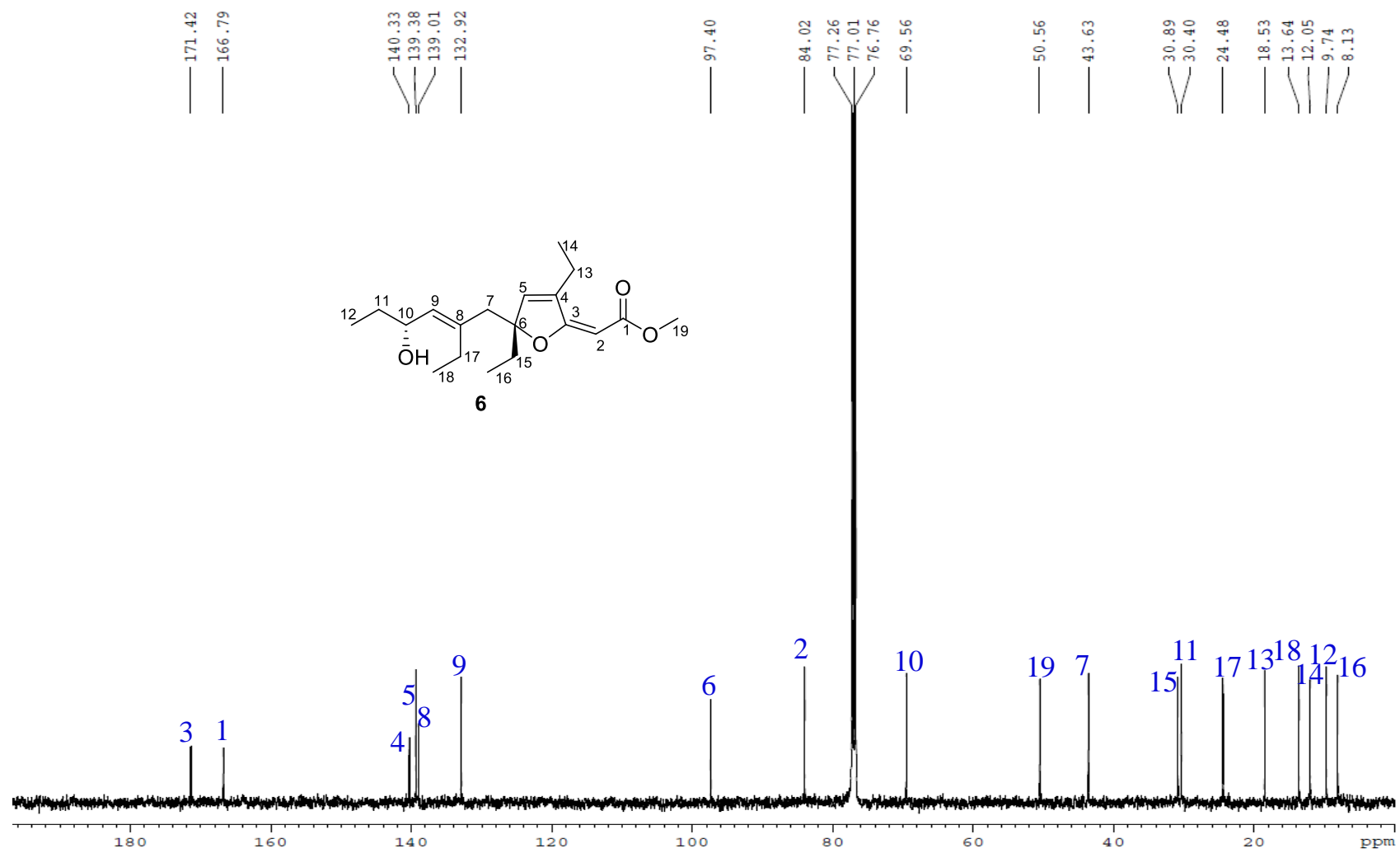


Figure S45. ^1H - ^1H COSY spectrum of plakorfulran A (**6**) in CDCl_3 .

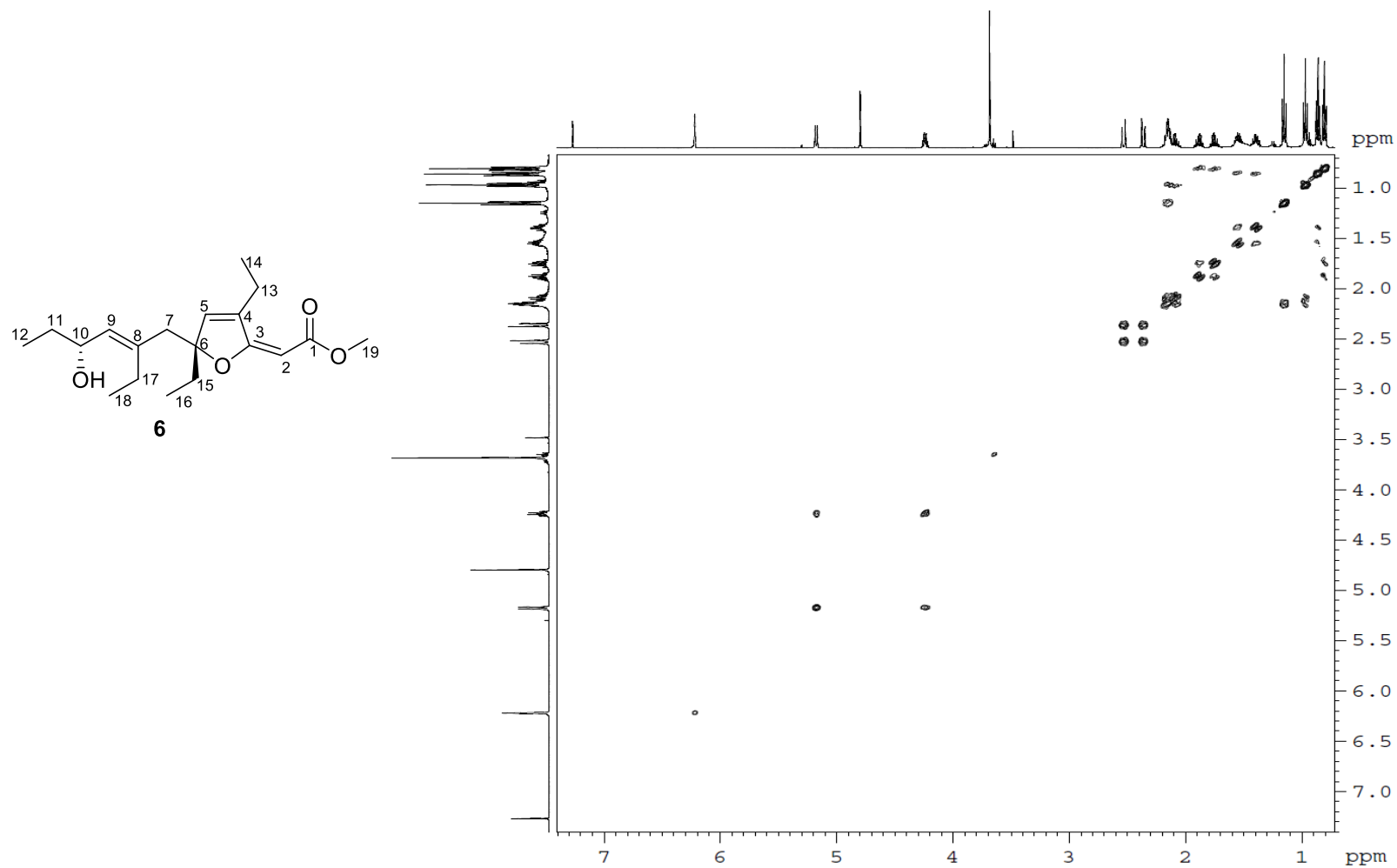


Figure S46. HSQC spectrum of plakorfuran A (**6**) in CDCl₃.

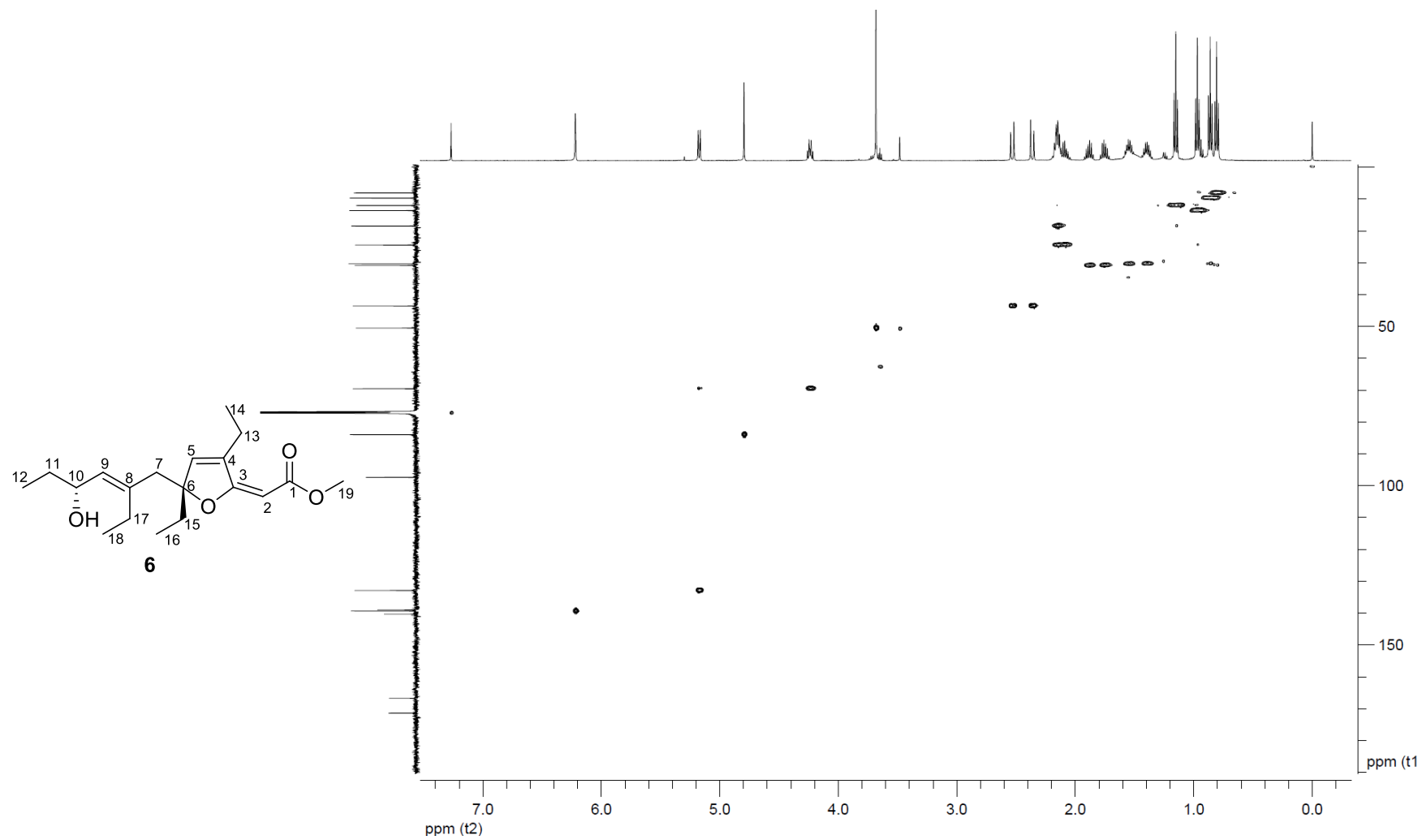


Figure S48. NOESY spectrum of plakorfulran A (**6**) in CDCl₃.

