

Dimeric *ent*-Kaurane Diterpenoids from *Isodon excisus*

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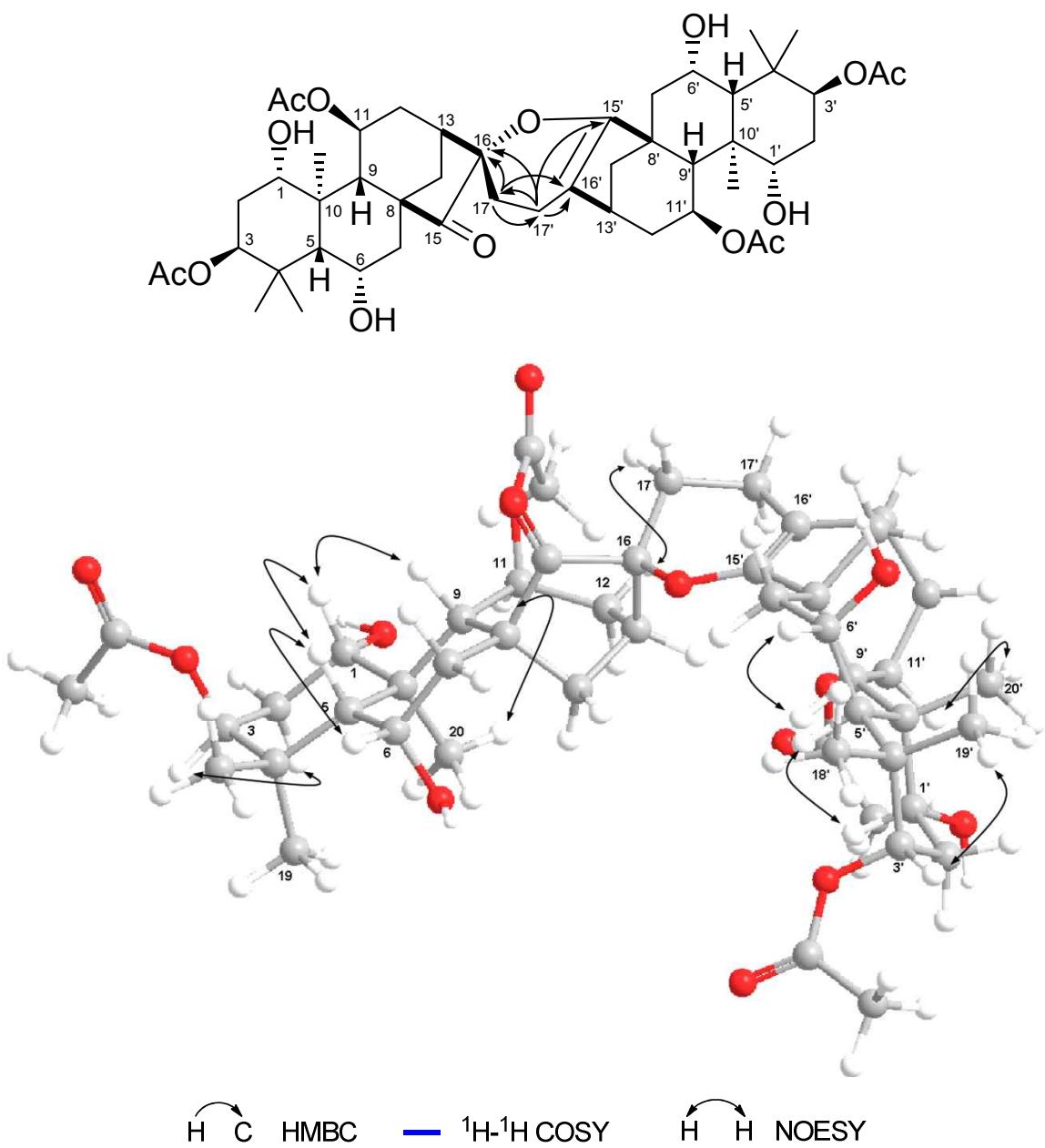


Figure S1. Key HMBC, COSY, and NOESY correlations of biexcisusin B (**2**).

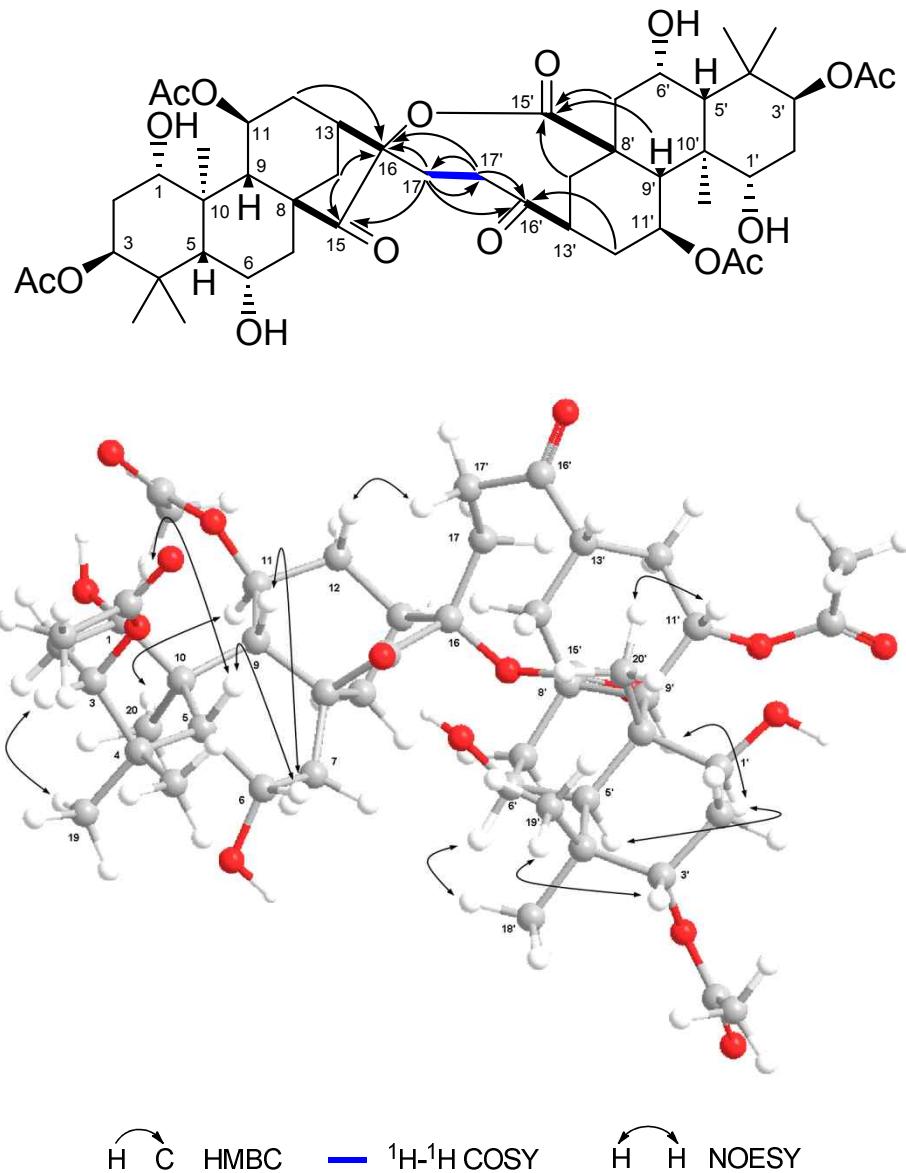


Figure S2. Key HMBC, COSY, and NOESY correlations of biexcisusin C (3).

Figure S1. ^1H NMR spectrum (900 MHz, $\text{C}_5\text{D}_5\text{N}$) of biexcisusin A (**1**)

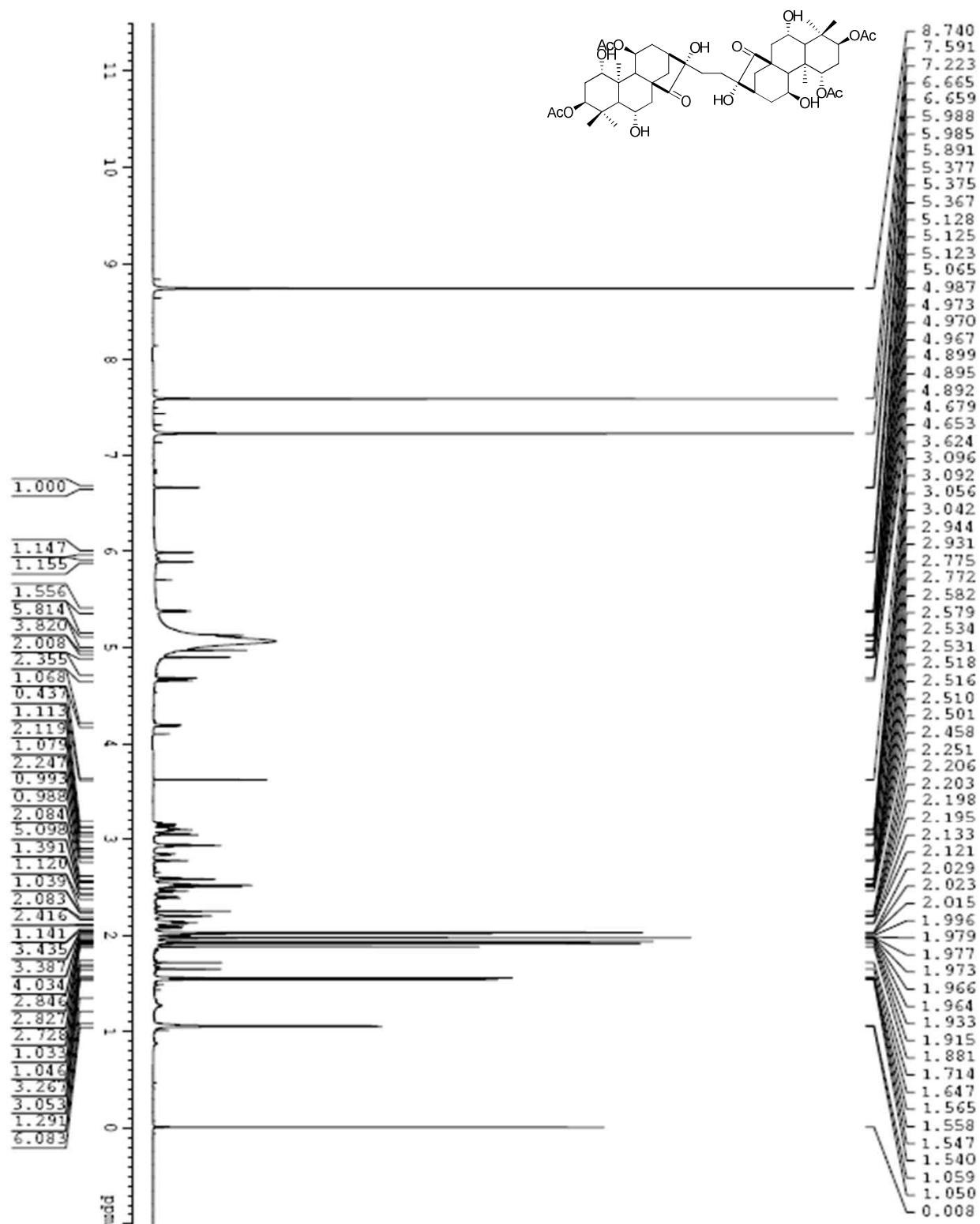


Figure S2. ^{13}C NMR spectrum (225 MHz, $\text{C}_5\text{D}_5\text{N}$) of biexcisusin A (**1**)

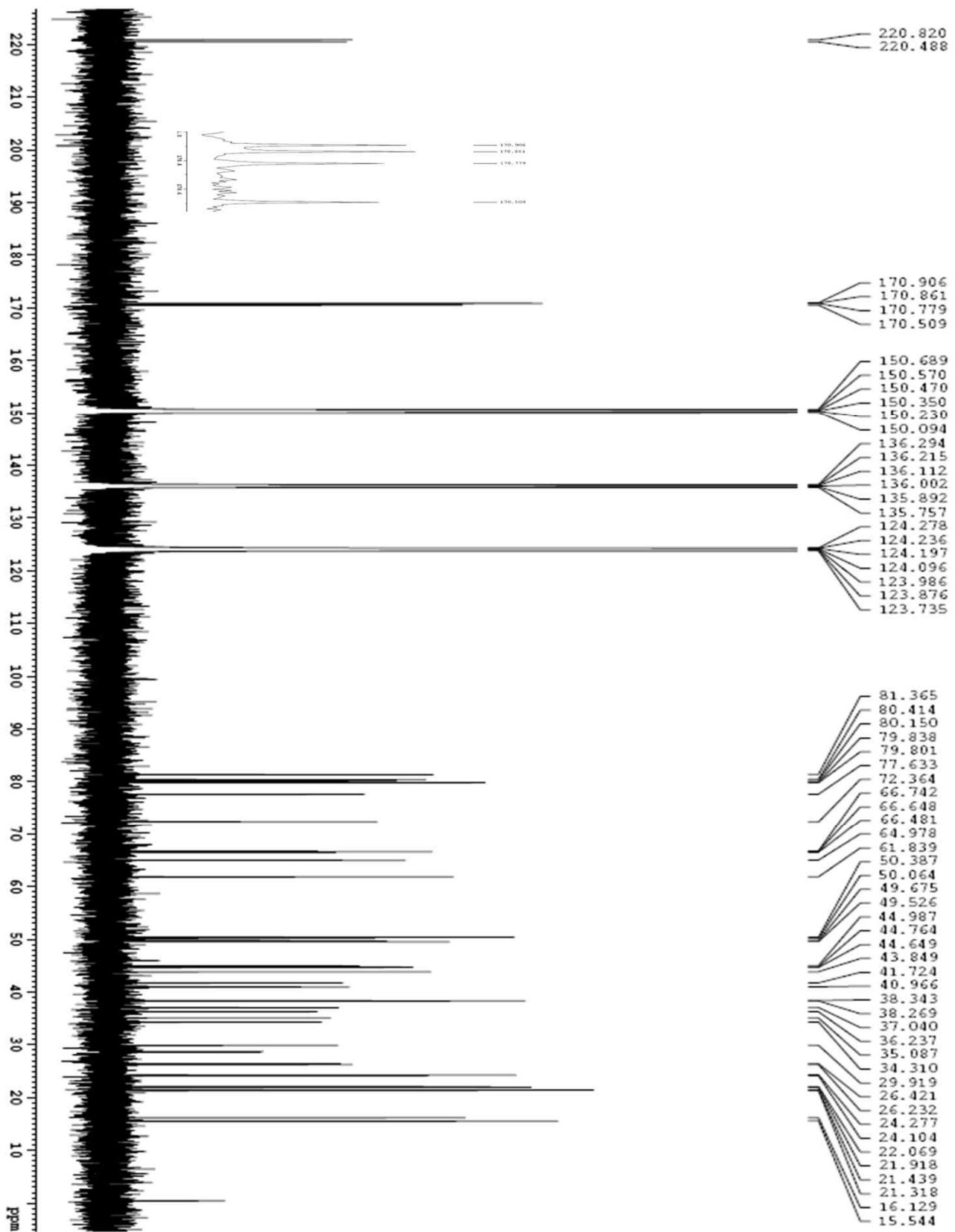


Figure S3. DEPTspectrum (225 MHz, C₅D₅N) of biexcisusin A (**1**)

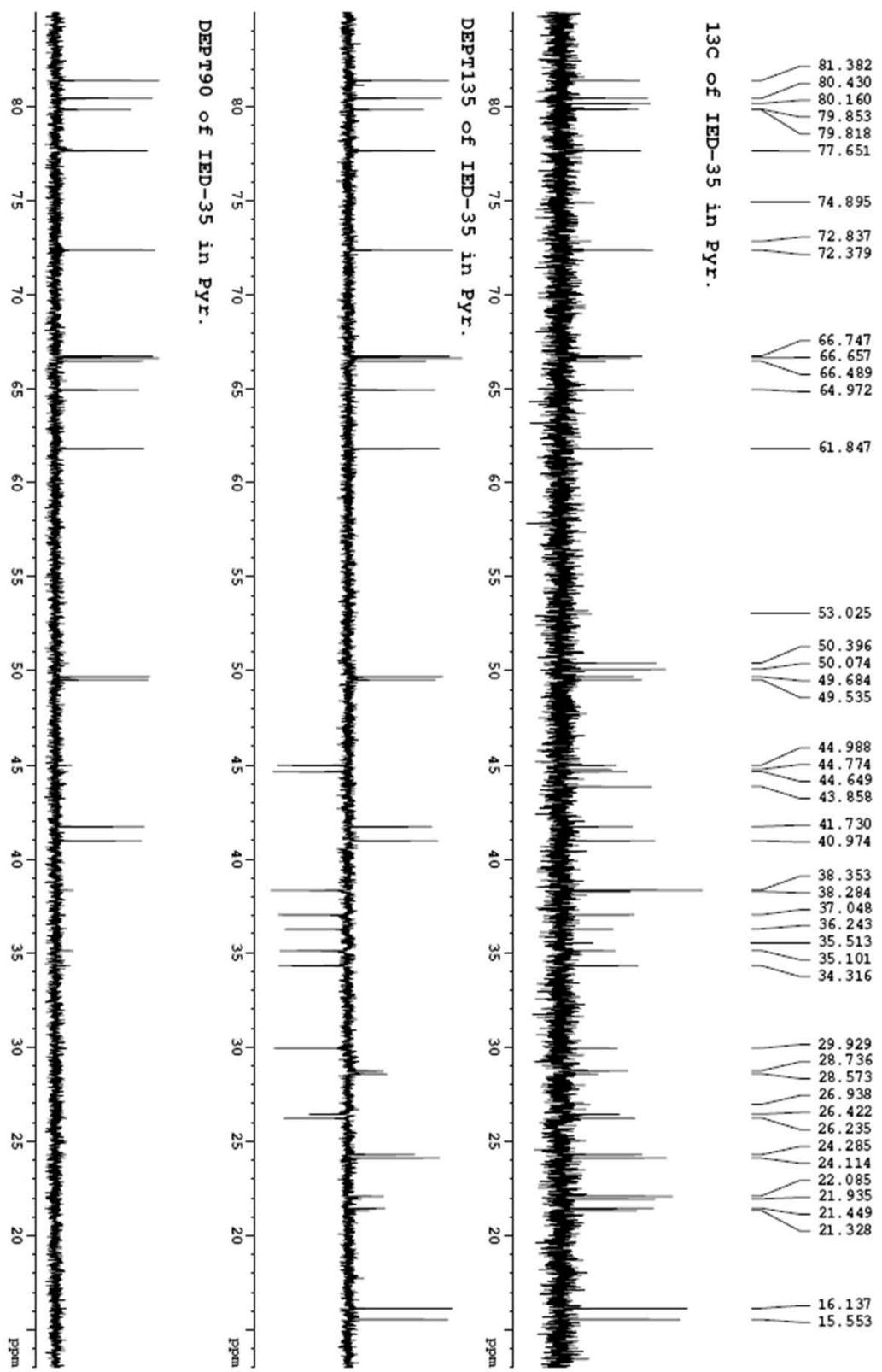


Figure S4. COSY spectrum (900 MHz, C₅D₅N) of biexcisusin A (**1**)

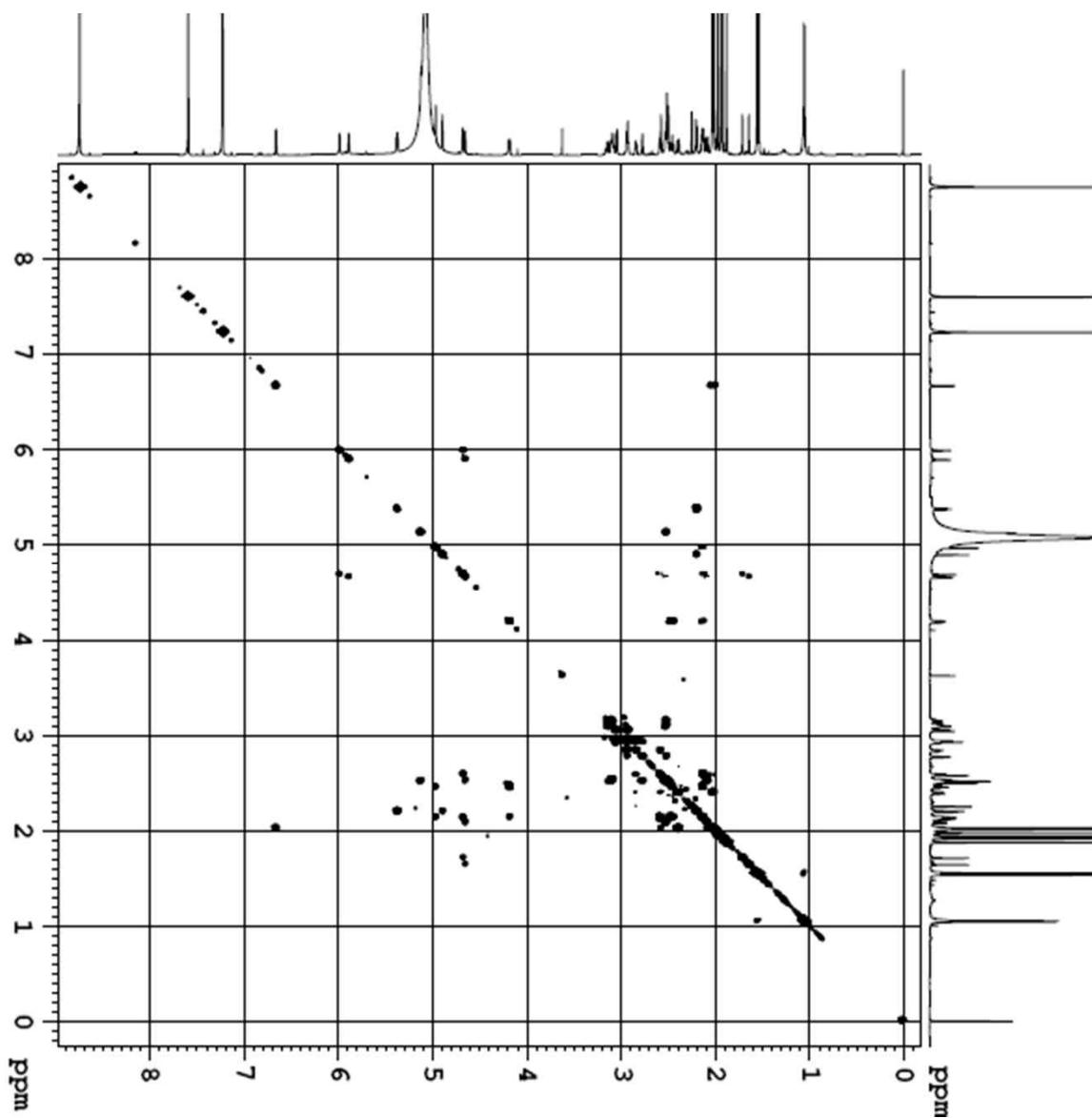


Figure S5. HMQC spectrum (900 MHz, C₅D₅N) of biexcisusin A (**1**)

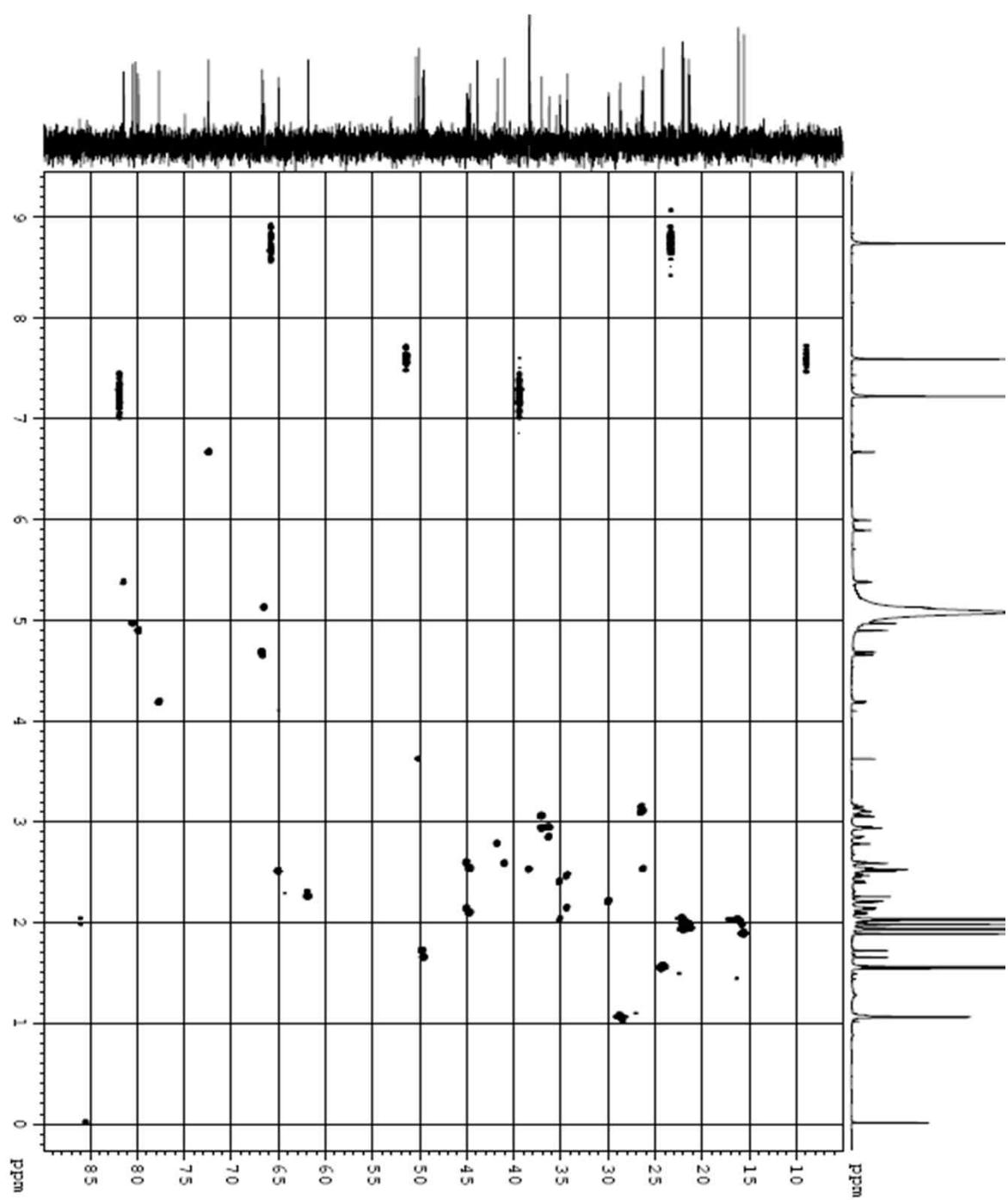


Figure S6. HMBC spectrum (900 MHz, C₅D₅N) of biexcisusin A (**1**)

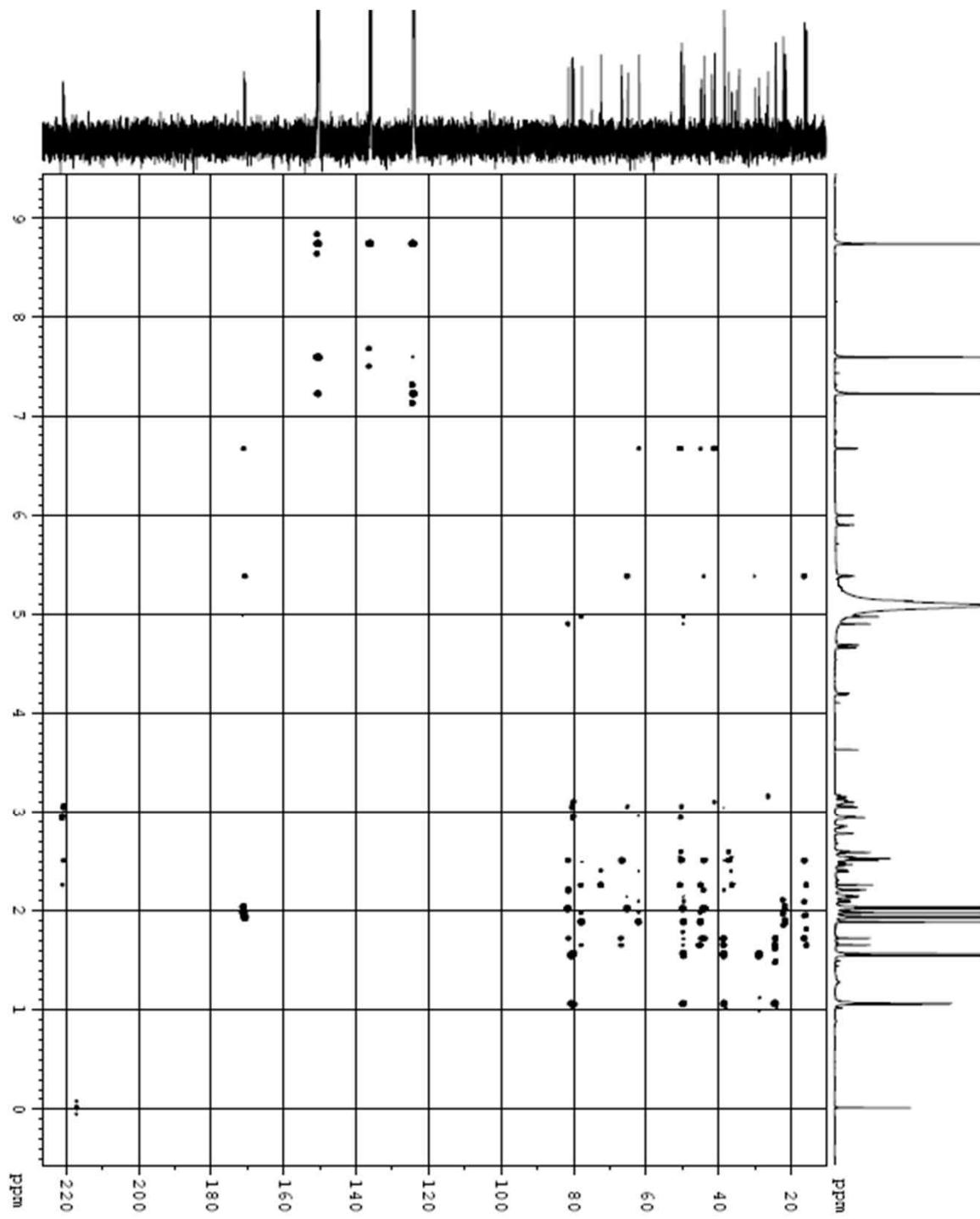


Figure S7. ROESY spectrum (900 MHz, C₅D₅N) of biexcisusin A (**1**)

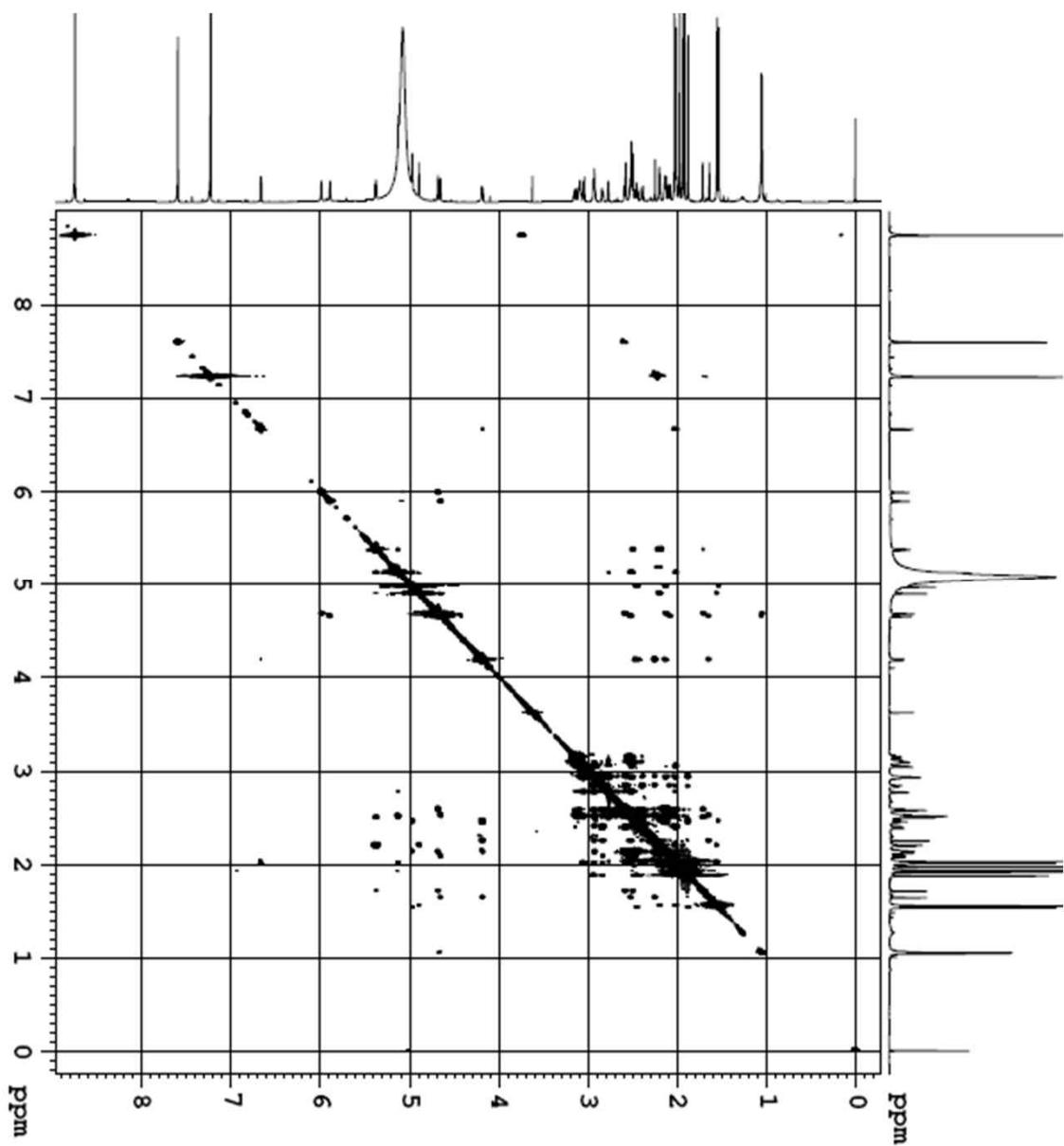
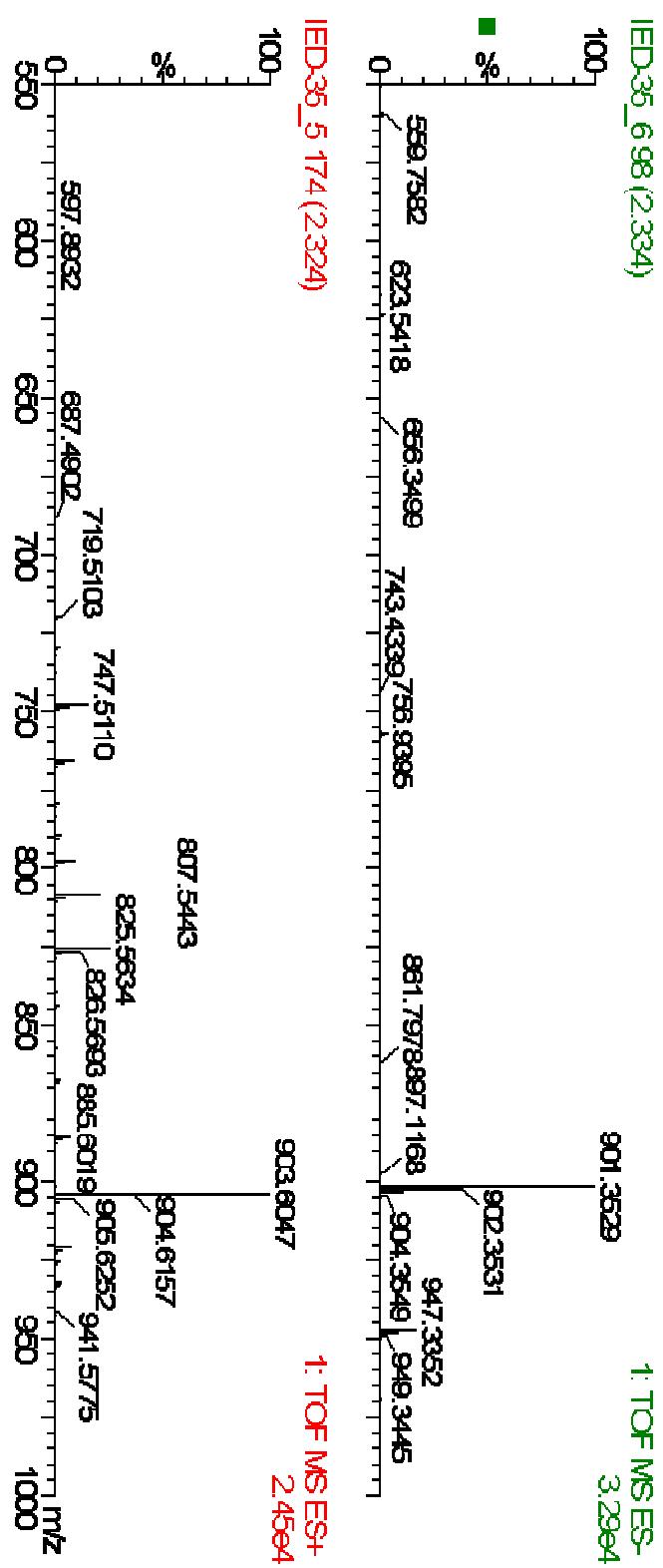


Figure S8. ESIMS spectrum of biexcisusin A (**1**)



Single Mass Analysis (displaying only valid results)

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

122 formula[e] evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	C	H	O
901.4561	901.4492	6.9	7.7	1.5	C ₃₇ H ₇₃ O ₂₄	60.8	37	73	24
	901.4644	-8.3	-9.2	5.5	C ₄₁ H ₇₃ O ₂₁	150.5	41	73	21
	901.4586	-2.5	-2.8	14.5	C ₄₈ H ₆₉ O ₁₆	426.2	48	69	16

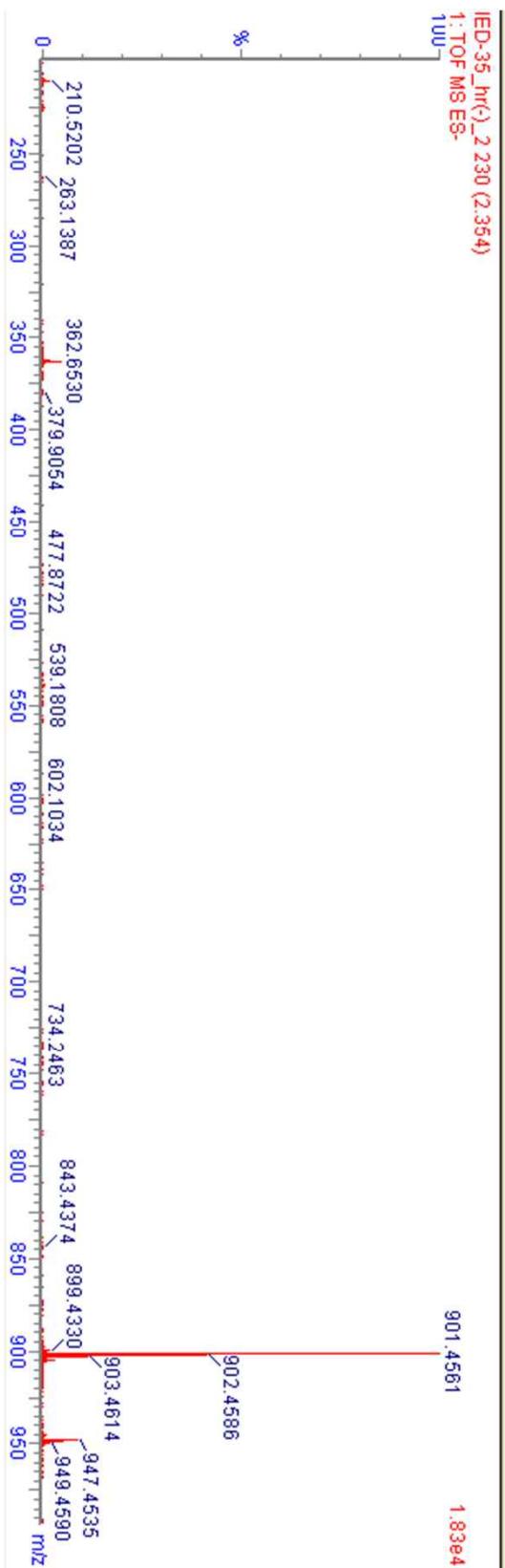


Figure S10. ^1H NMR spectrum (900 MHz, $\text{C}_5\text{D}_5\text{N}$) of biexcisin B (**2**)

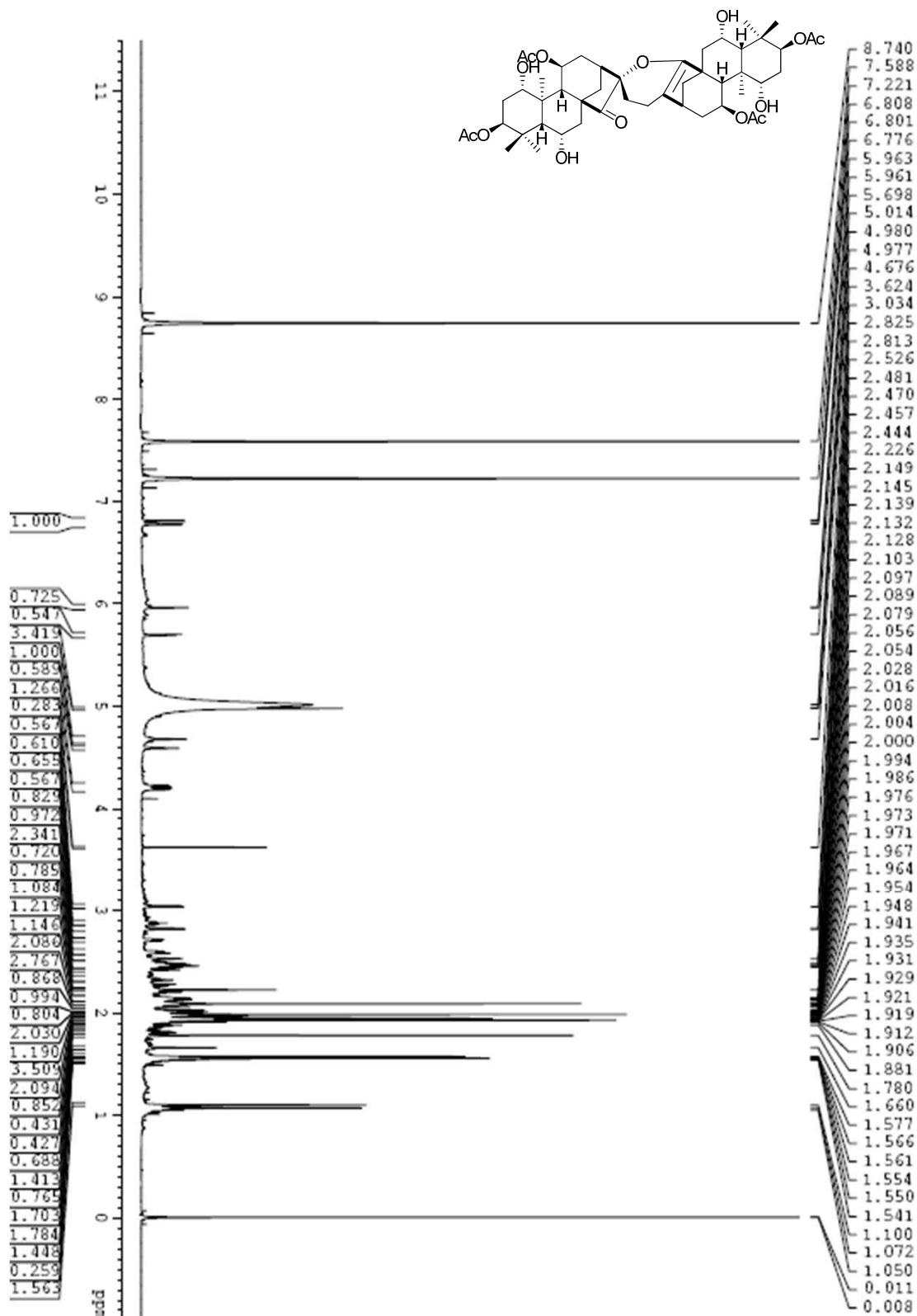


Figure S11. ^{13}C NMR spectrum (225 MHz, $\text{C}_5\text{D}_5\text{N}$) of biexcisusin B (**2**)

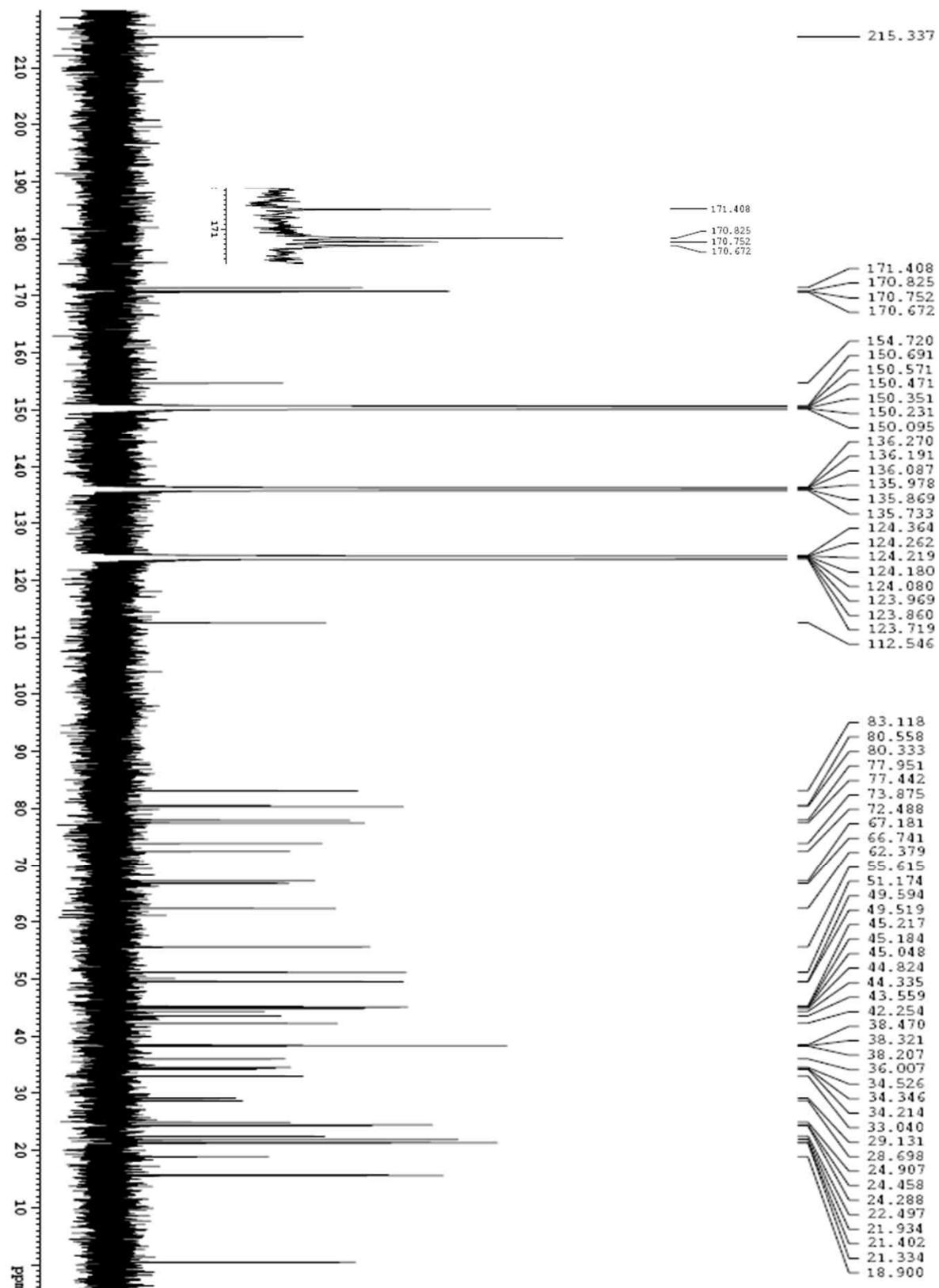


Figure S12. DEPT spectrum (225 MHz, C₅D₅N) of biexcisusin B (**2**)

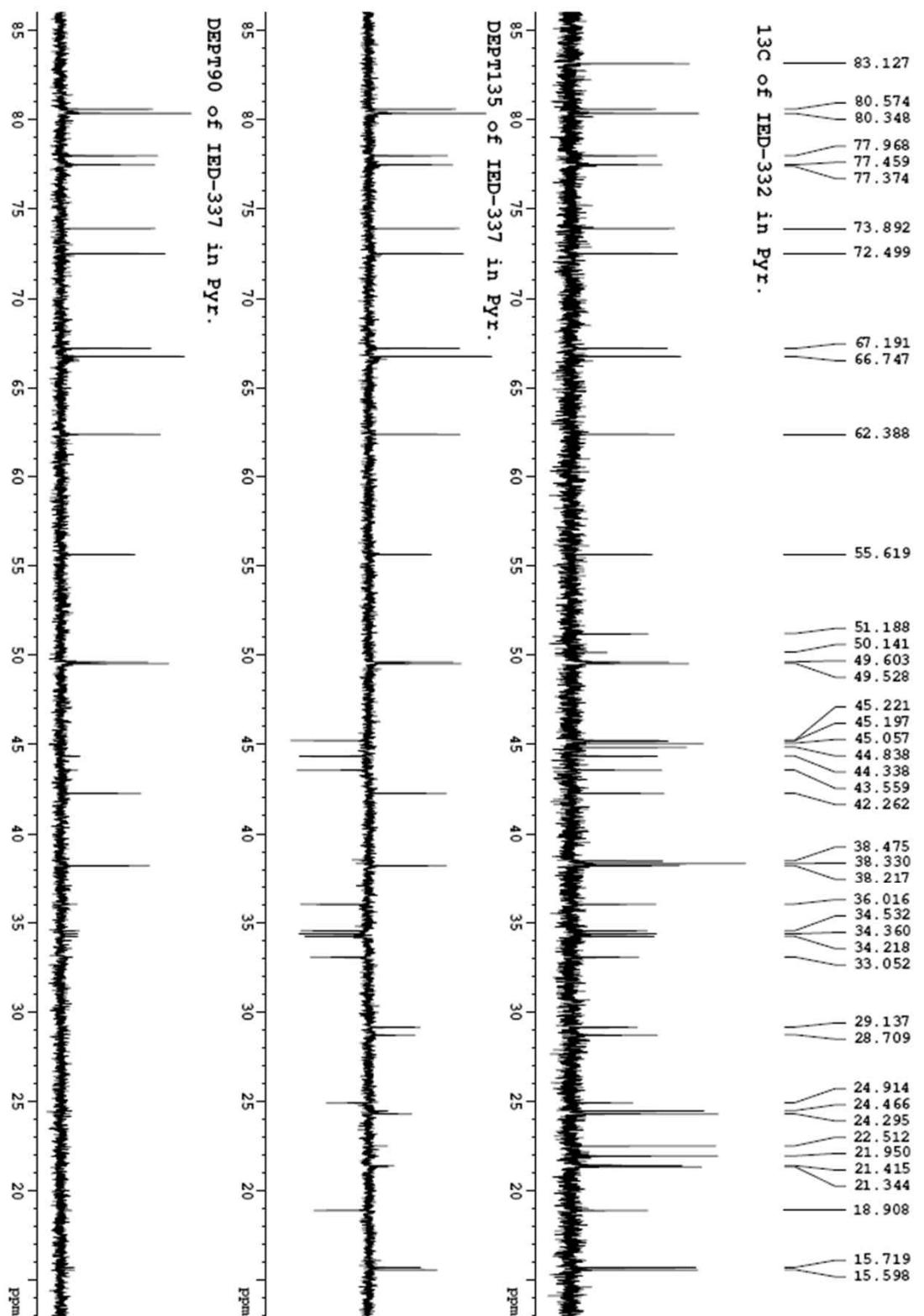


Figure S13. COSY spectrum (900 MHz, C₅D₅N) of biexcisusin B (**2**)

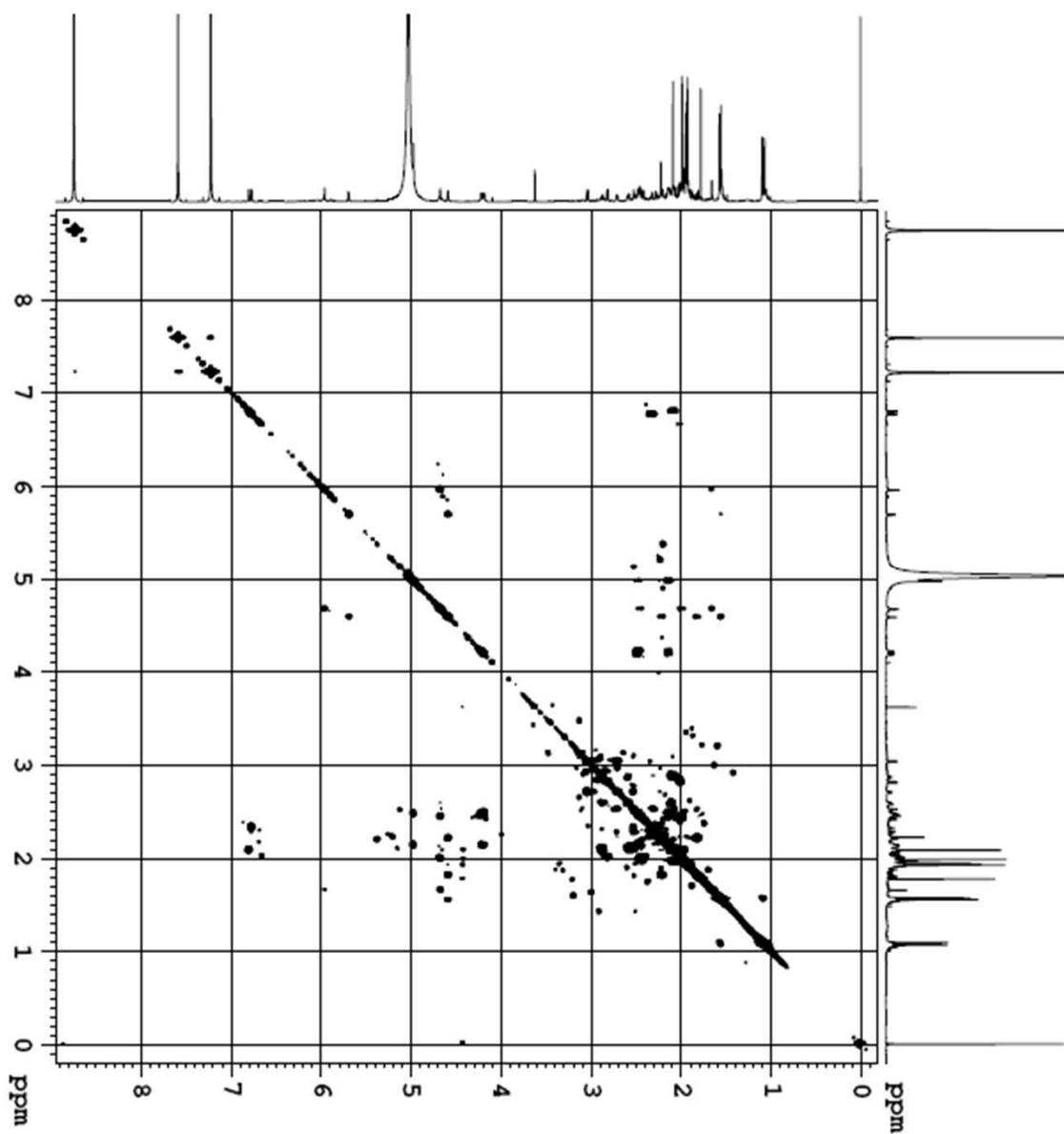


Figure S14. HMQC spectrum (900 MHz, C₅D₅N) of biexcusin B (**2**)

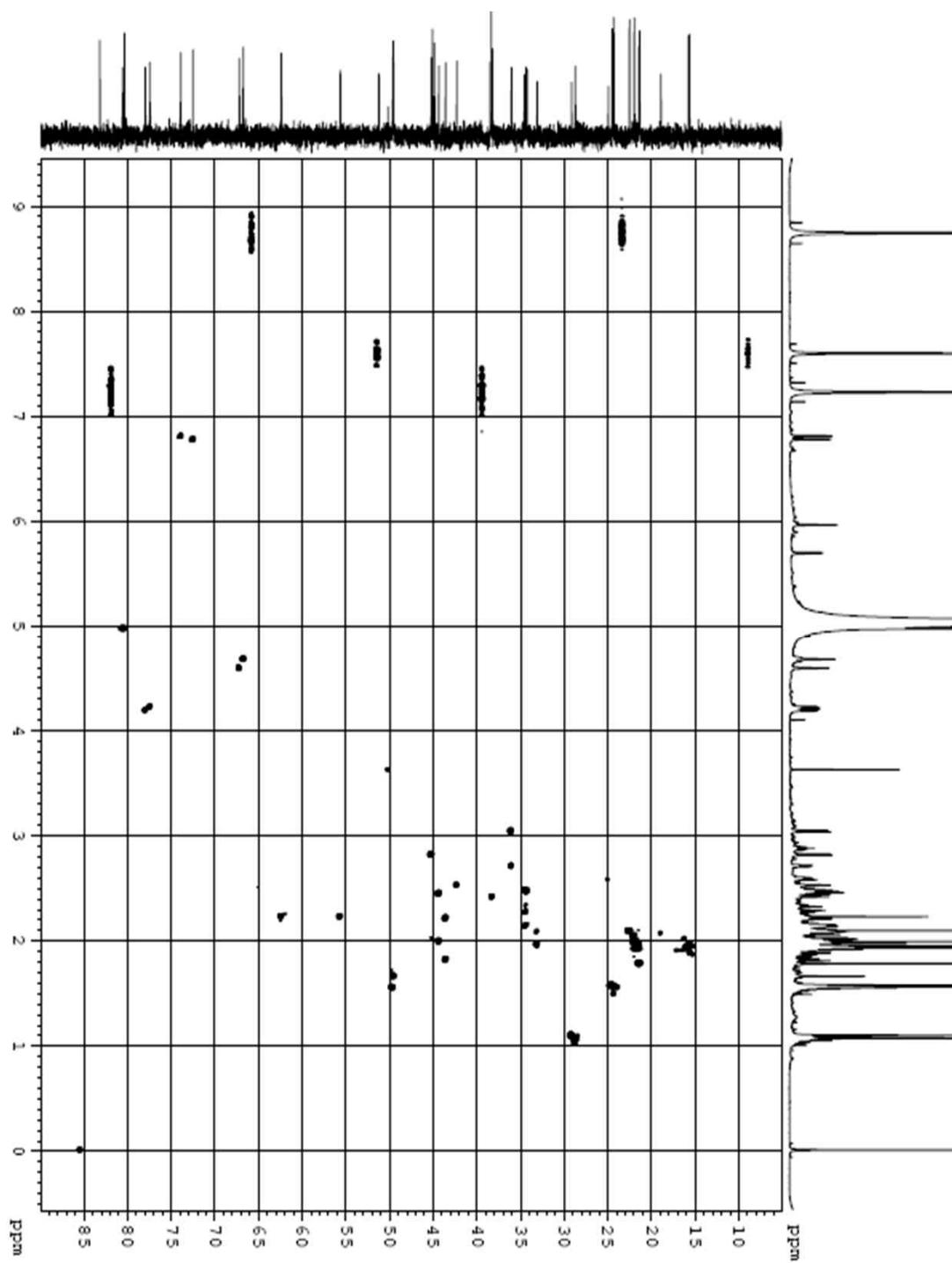


Figure S15. HMBC spectrum (900 MHz, C₅D₅N) of biexcisin B (**2**)

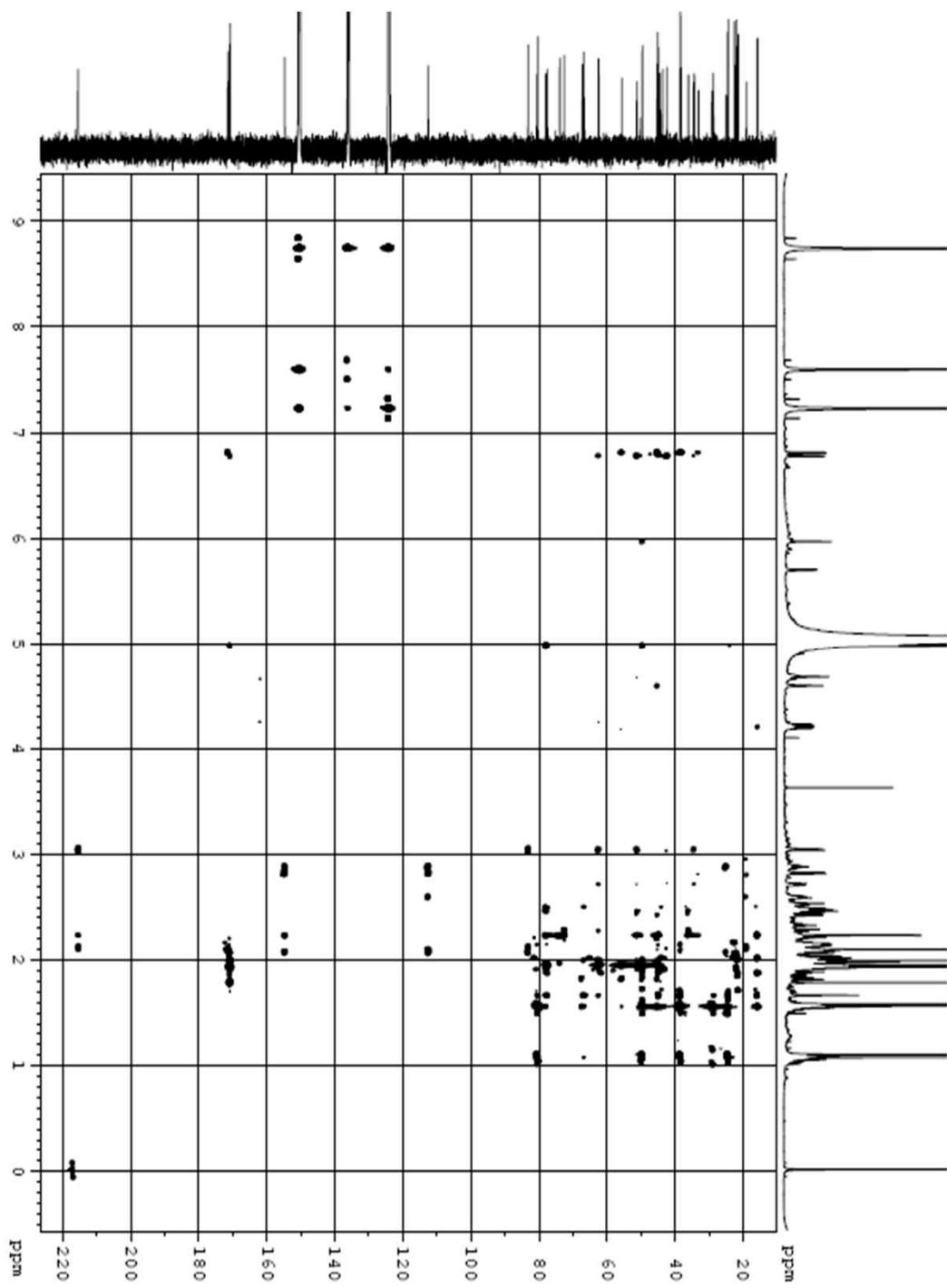


Figure S16. NOESY spectrum (900 MHz, C₅D₅N) of biexcisusin B (**2**)

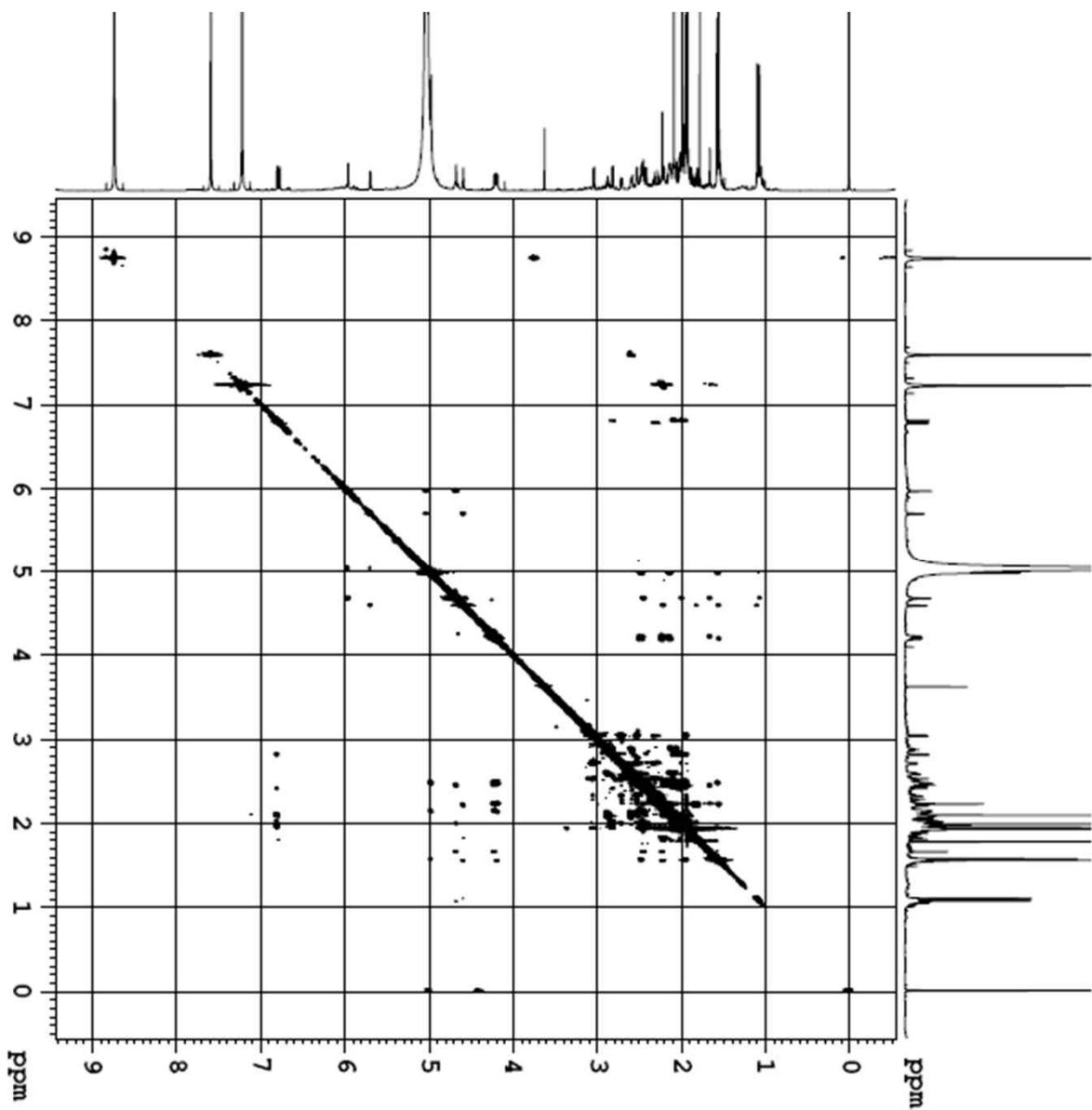


Figure S17. ESIMS spectrum of biexcisusin B (2)

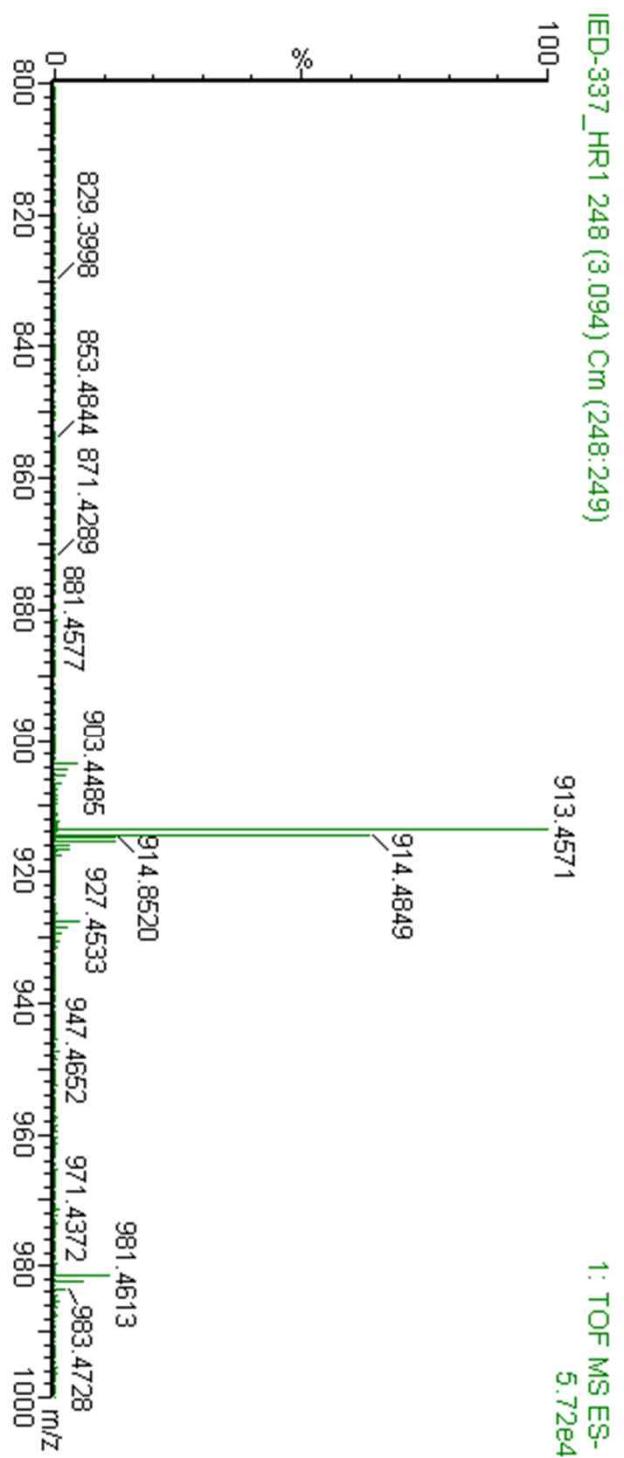


Figure S18. HRESIMS spectrum of biexcisin B (2)

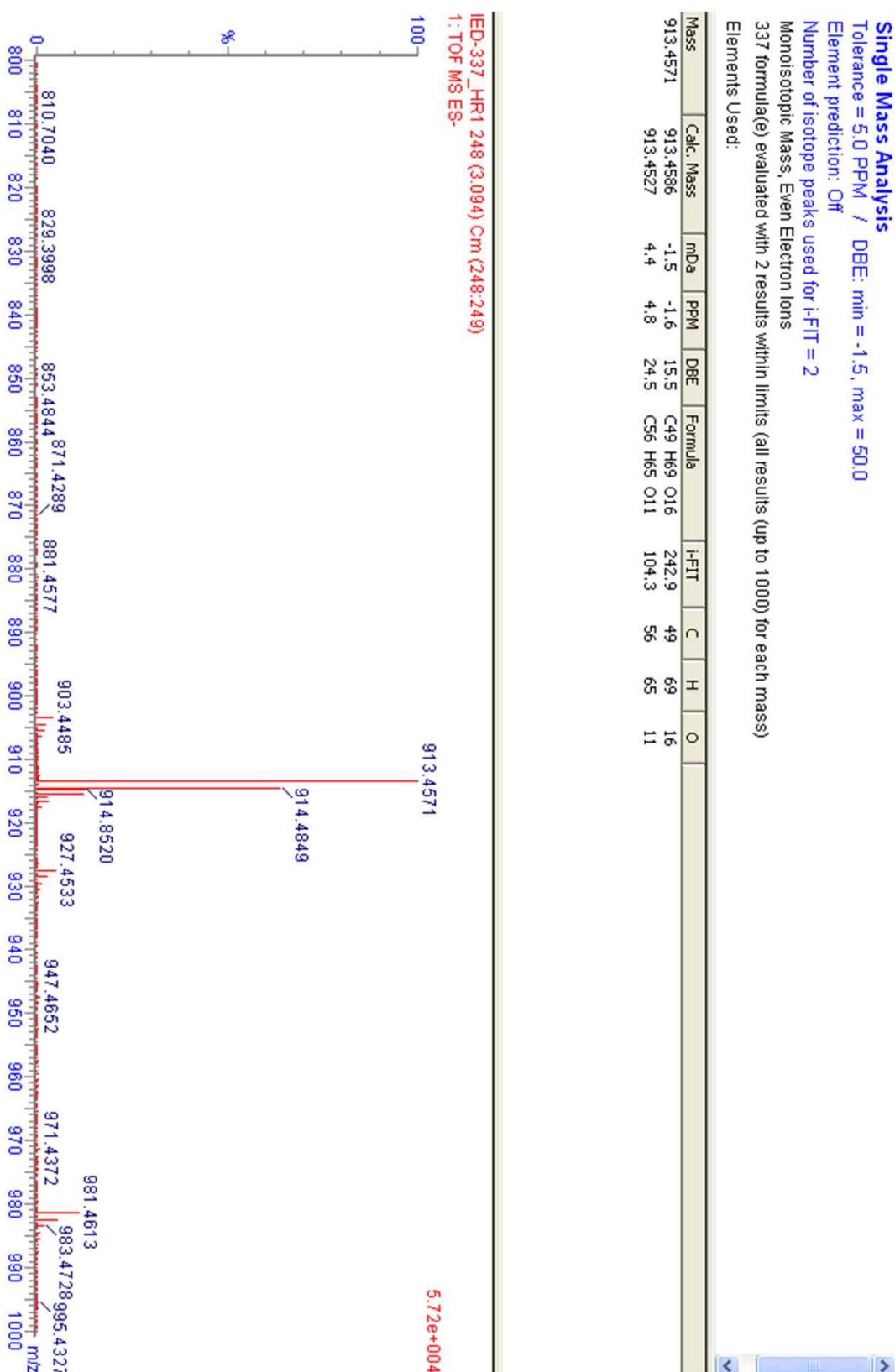


Figure S19. ^1H NMR spectrum (900 MHz, $\text{C}_5\text{D}_5\text{N}$) of bisexcisusin C (3)

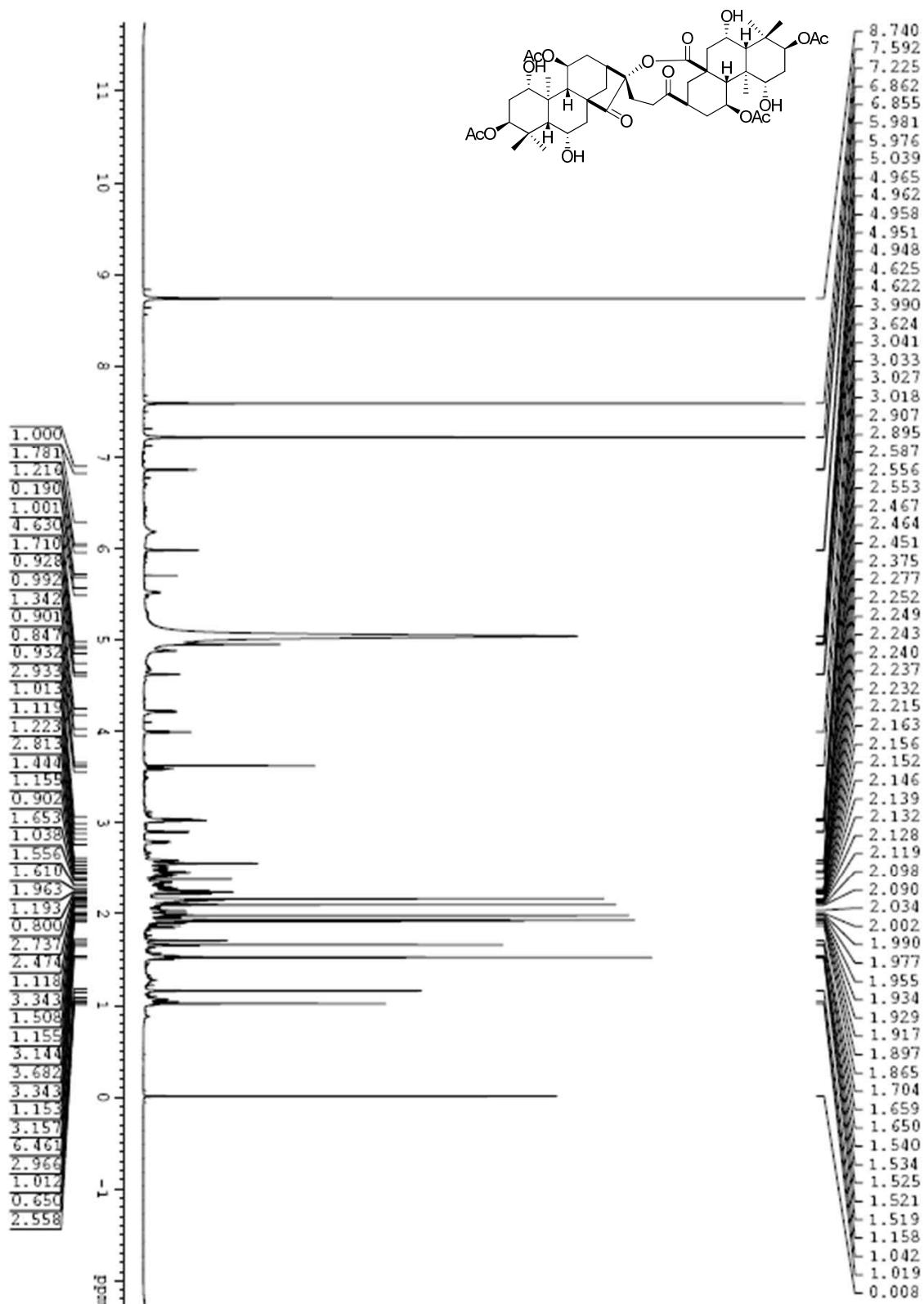


Figure S20. ^{13}C NMR spectrum (225 MHz, $\text{C}_5\text{D}_5\text{N}$) of biexcisusin C (**3**)

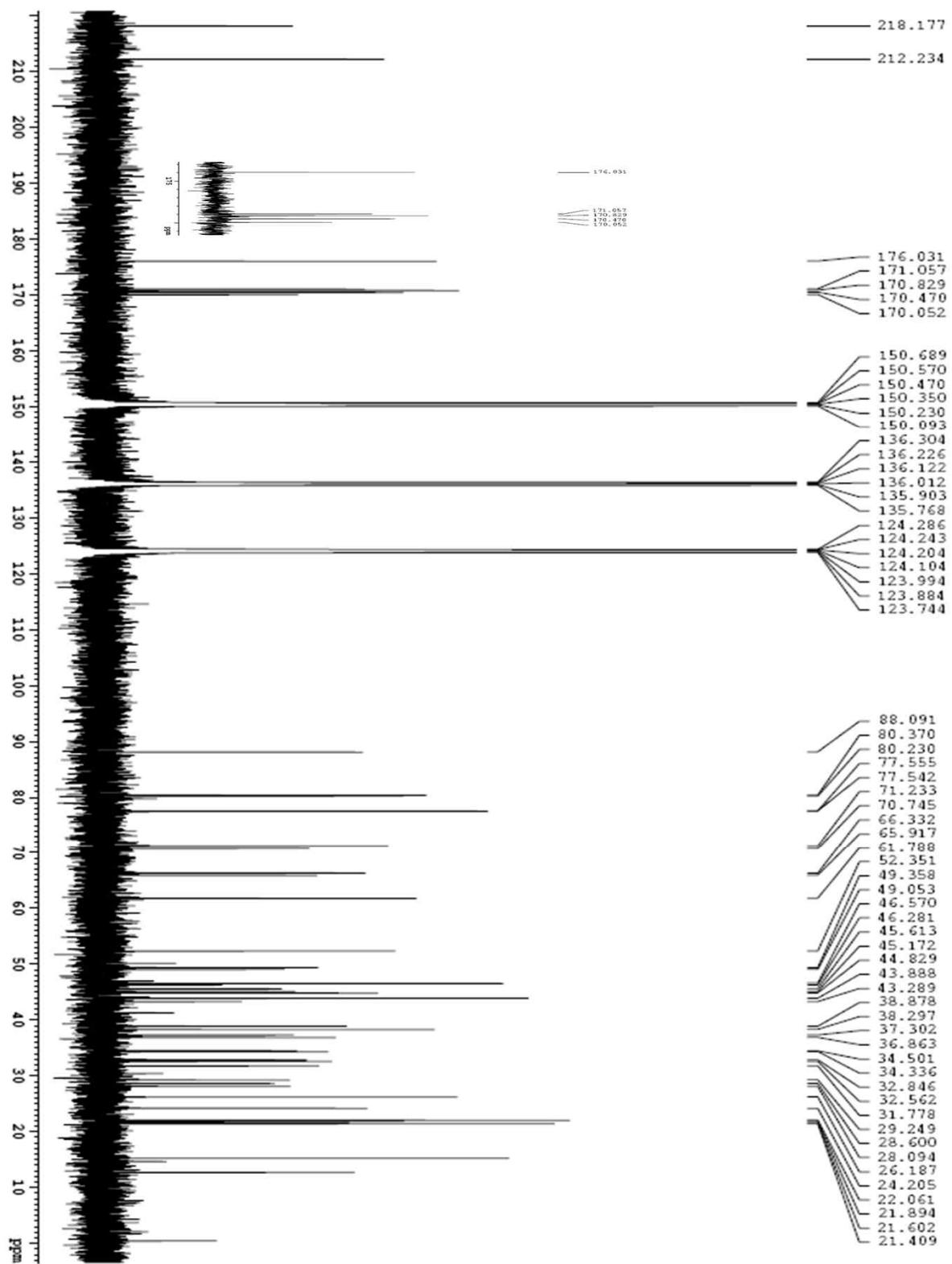


Figure S21. DEPT spectrum (225 MHz, C₅D₅N) of biexcusin C (**3**)

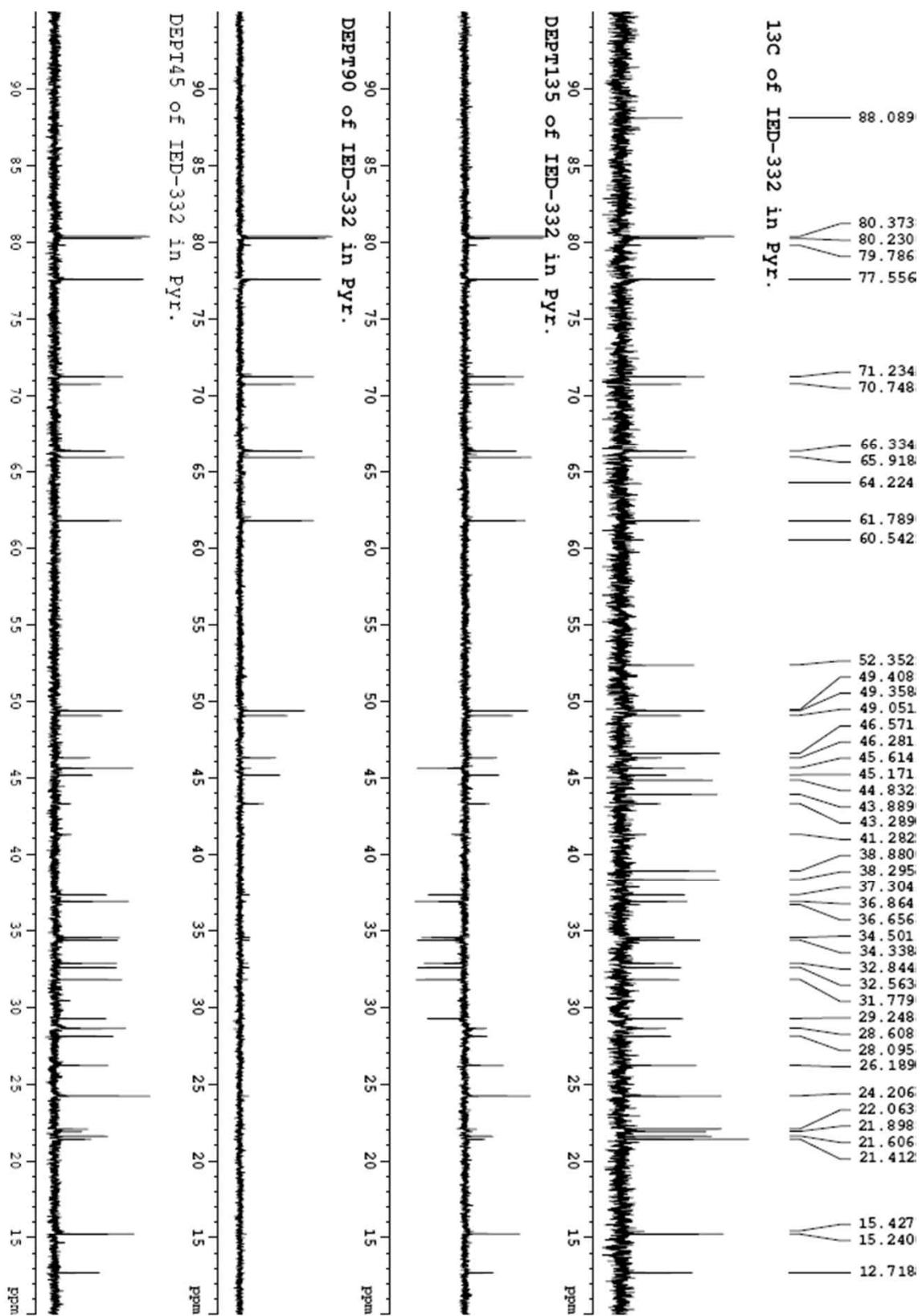


Figure S22. COSY spectrum (900 MHz, C₅D₅N) of biexcisusin C (**3**)

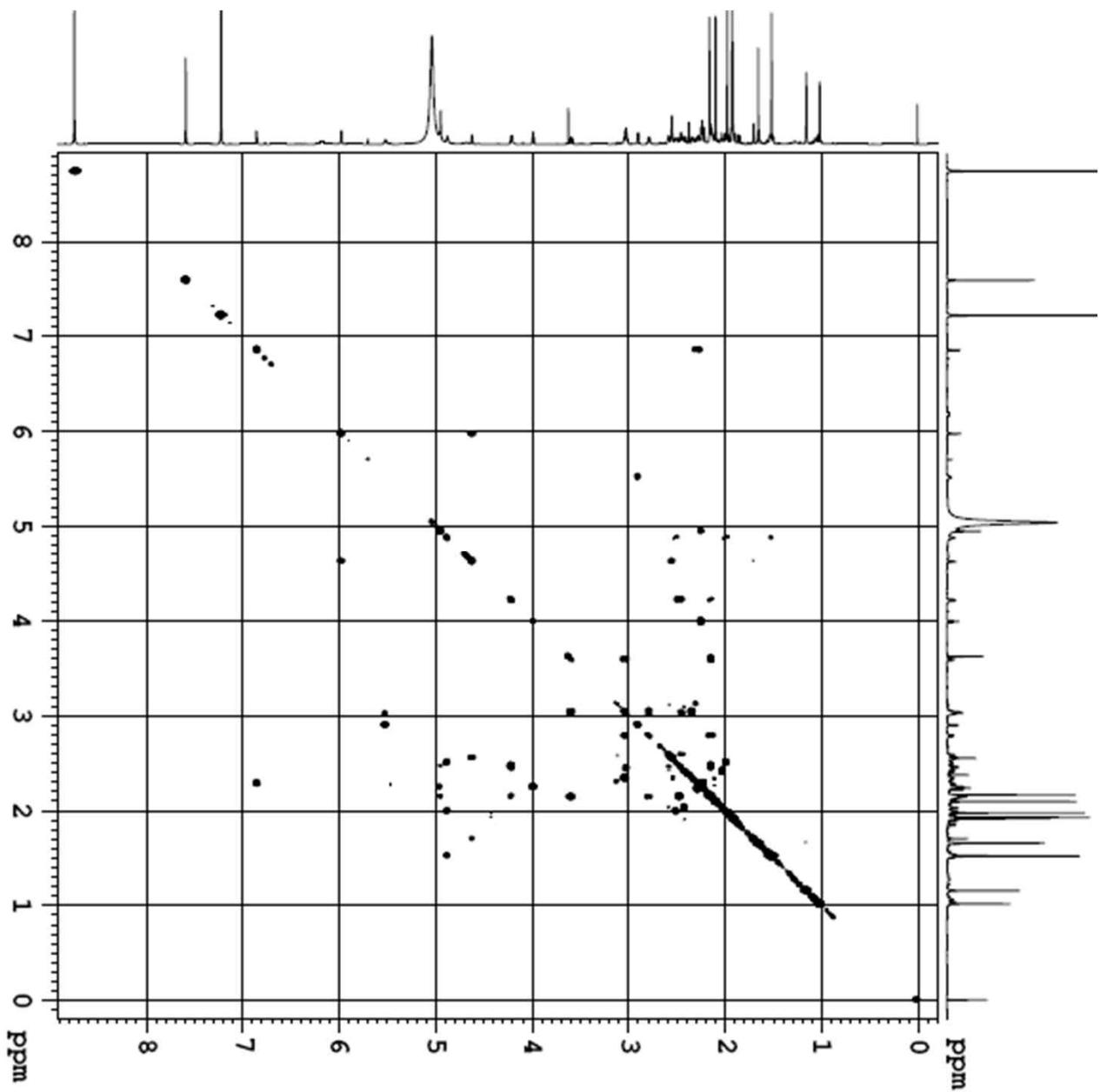


Figure S23. HMQC spectrum (900 MHz, C₅D₅N) of biexcisin C (**3**)

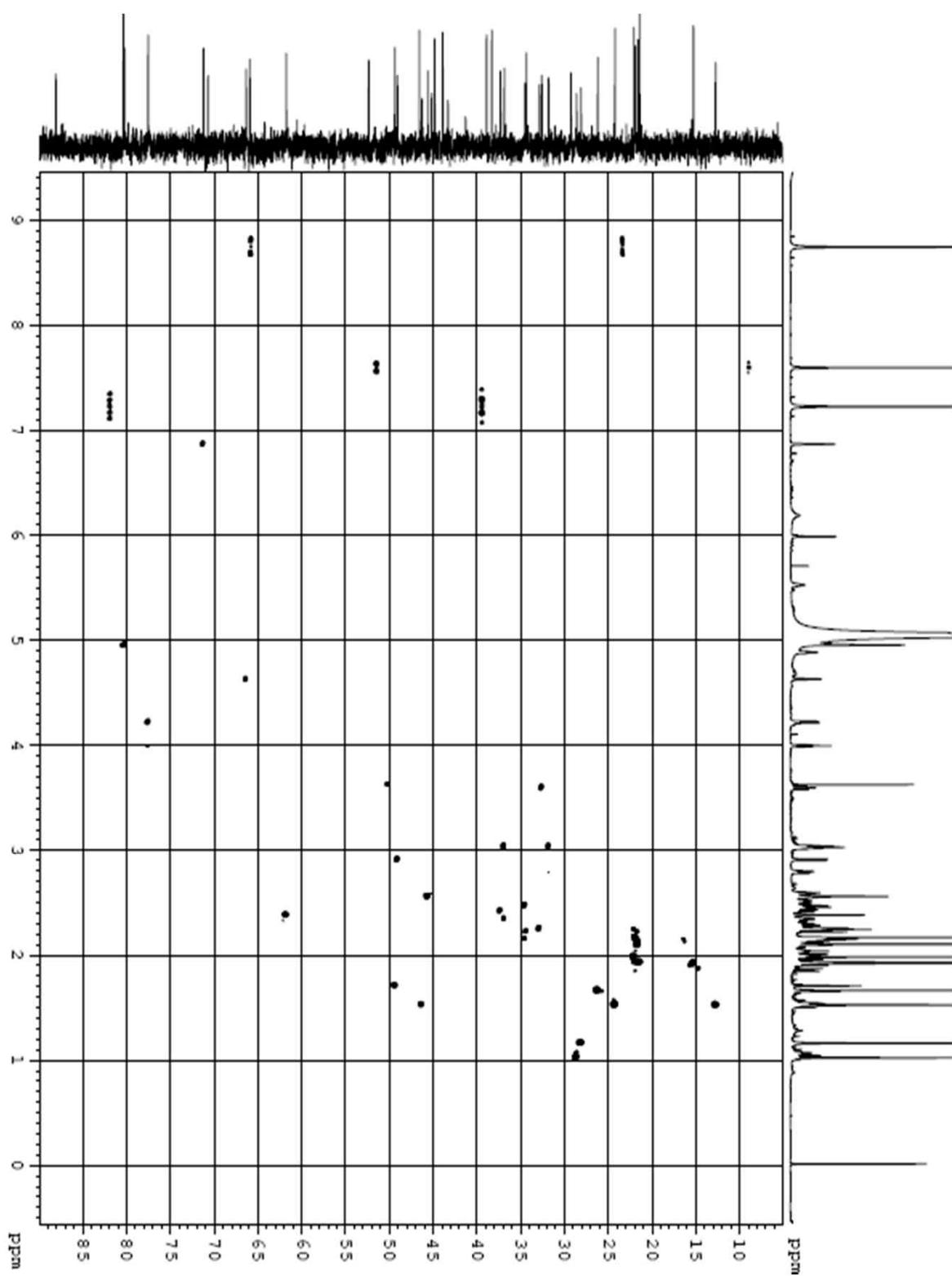


Figure S24. HMBC spectrum (900 MHz, C₅D₅N) of biexcisin C (**3**)

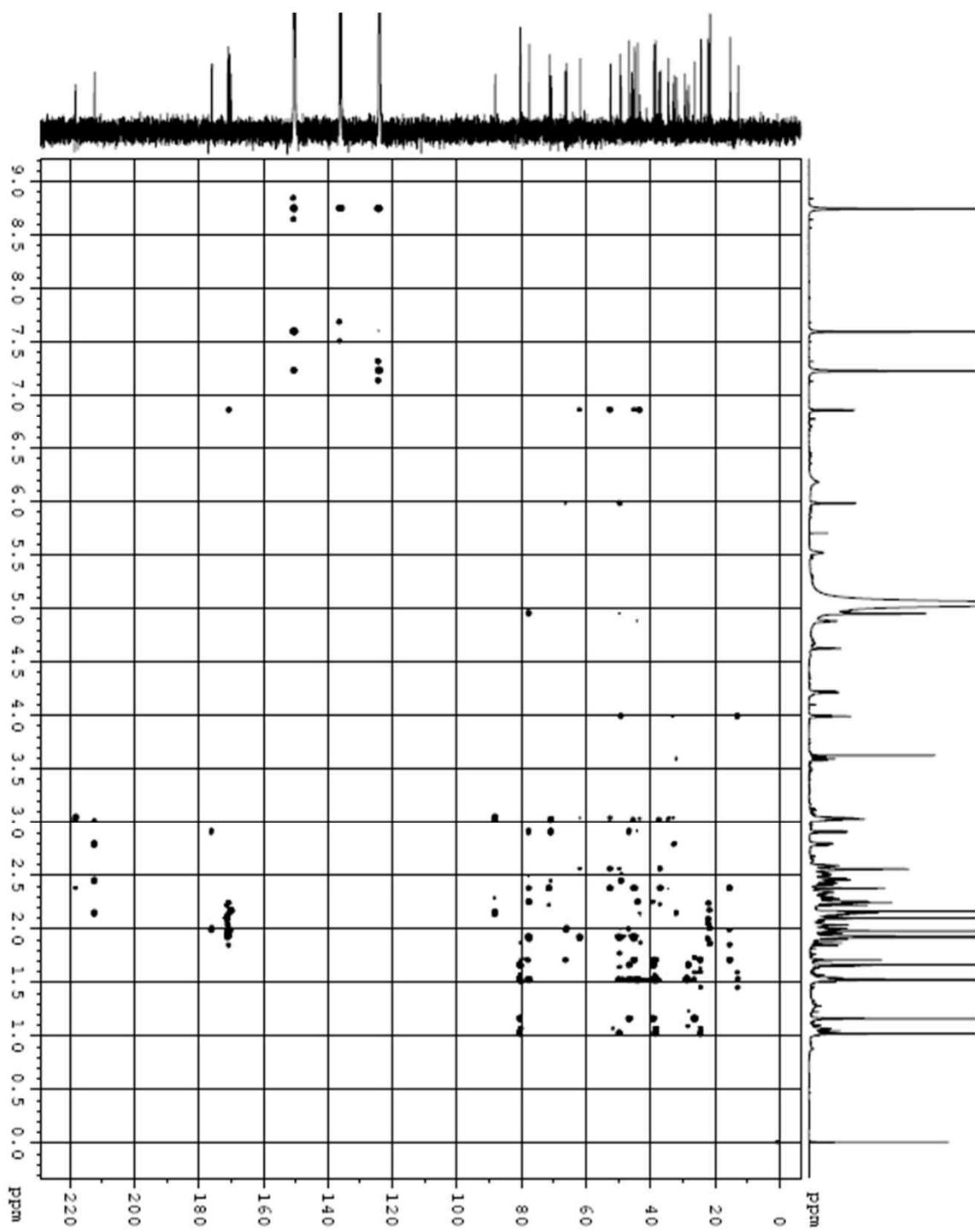


Figure S25. NOESY spectrum (900 MHz, C₅D₅N) of biexcisusin C (**3**)

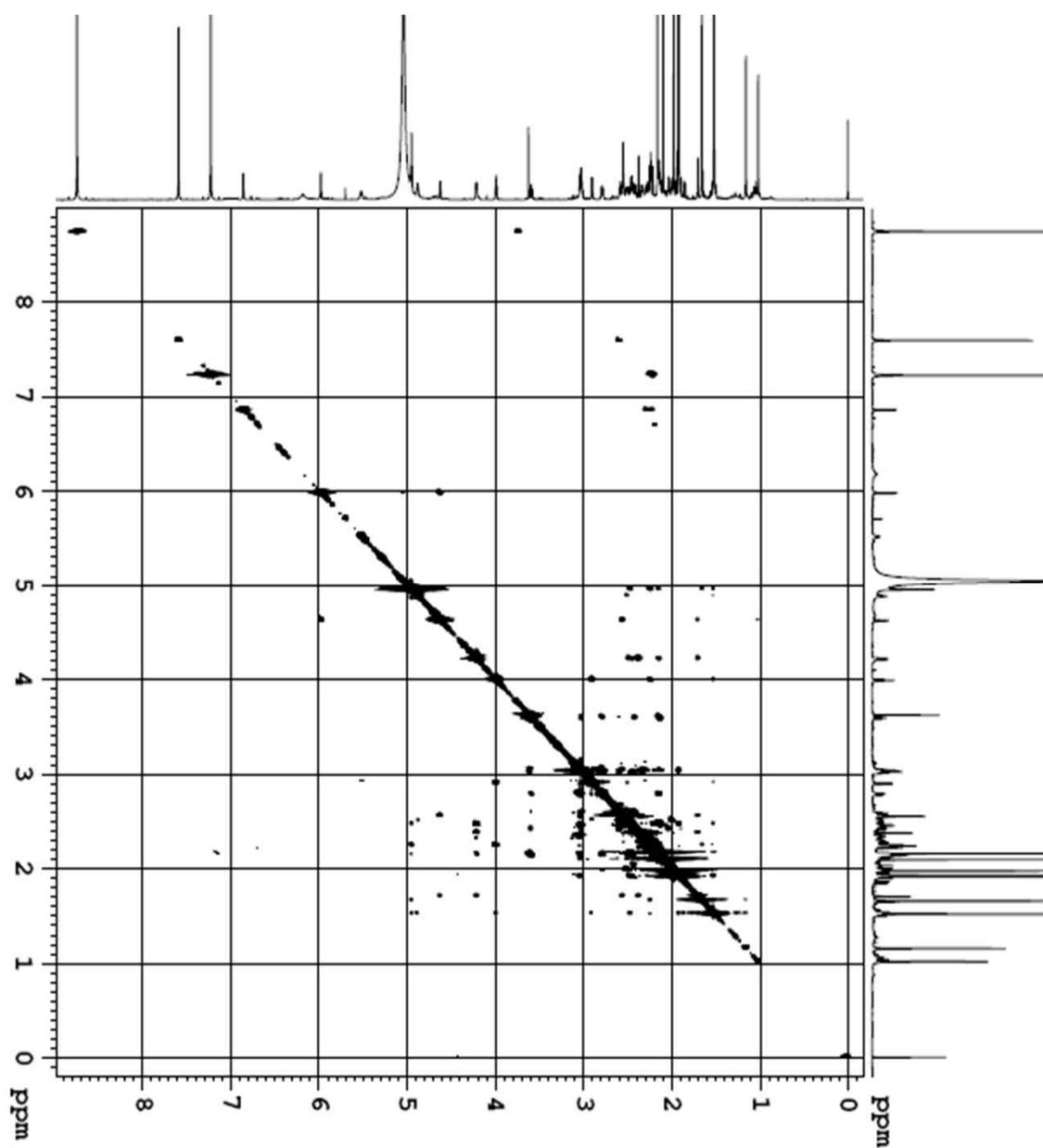
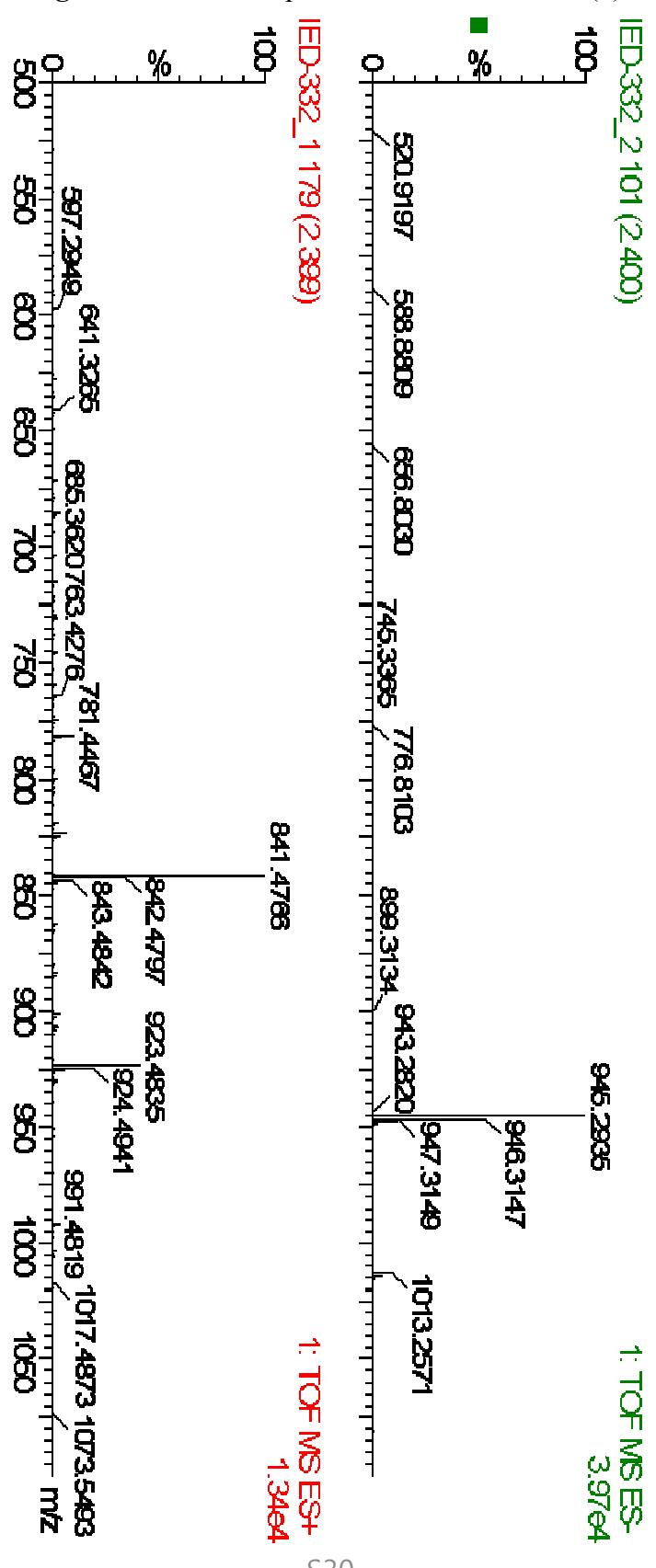


Figure S26. ESIMS spectrum of biexcisin C (3)



Single Mass Analysis (displaying only valid results)

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

108 formula[e] evaluated with 3 results within limits [up to 50 best isotopic matches for each mass]

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	C	H	O
945.4449	945.4390	5.9	6.2	2.5	C ₃₈ H ₇₃ O ₂₆	72.3	38	73	26
945.4543	-	-9.4	-9.9	6.5	C ₄₂ H ₇₃ O ₂₃	183.9	42	73	23
945.4484	-3.5	-3.7	15.5	C ₄₉ H ₆₉ O ₁₈	486.0	49	69	18	

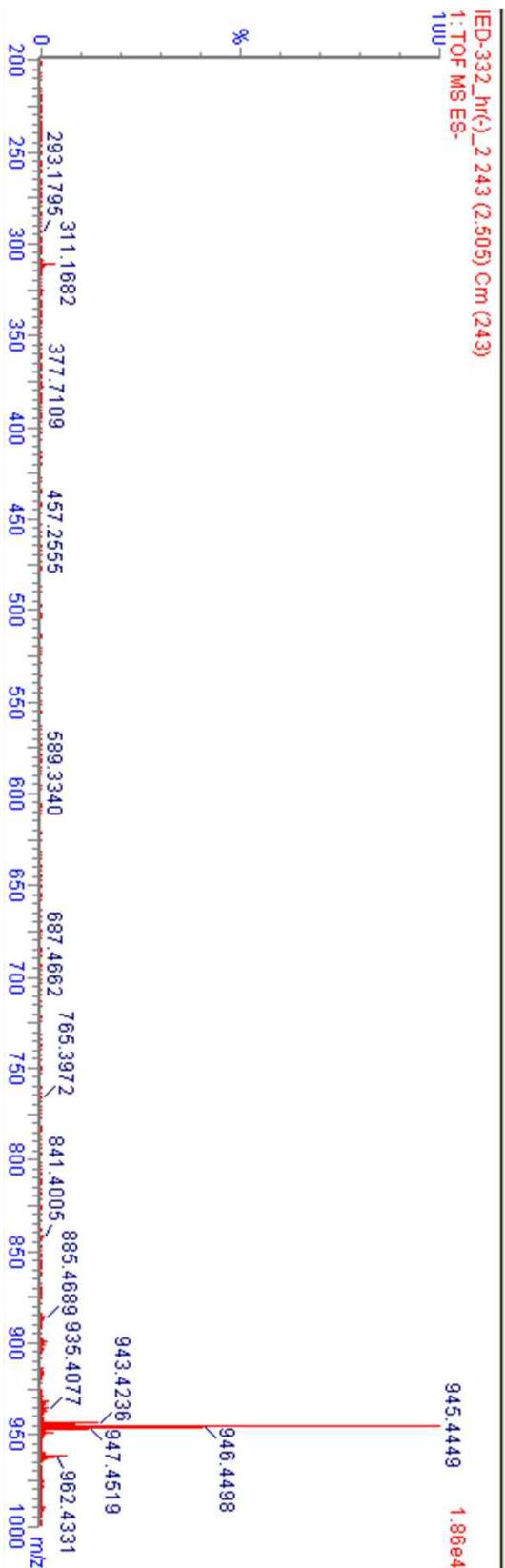


Figure S28. ^1H NMR spectrum (500 MHz, CDCl_3) of biexcisusin D (**4**)

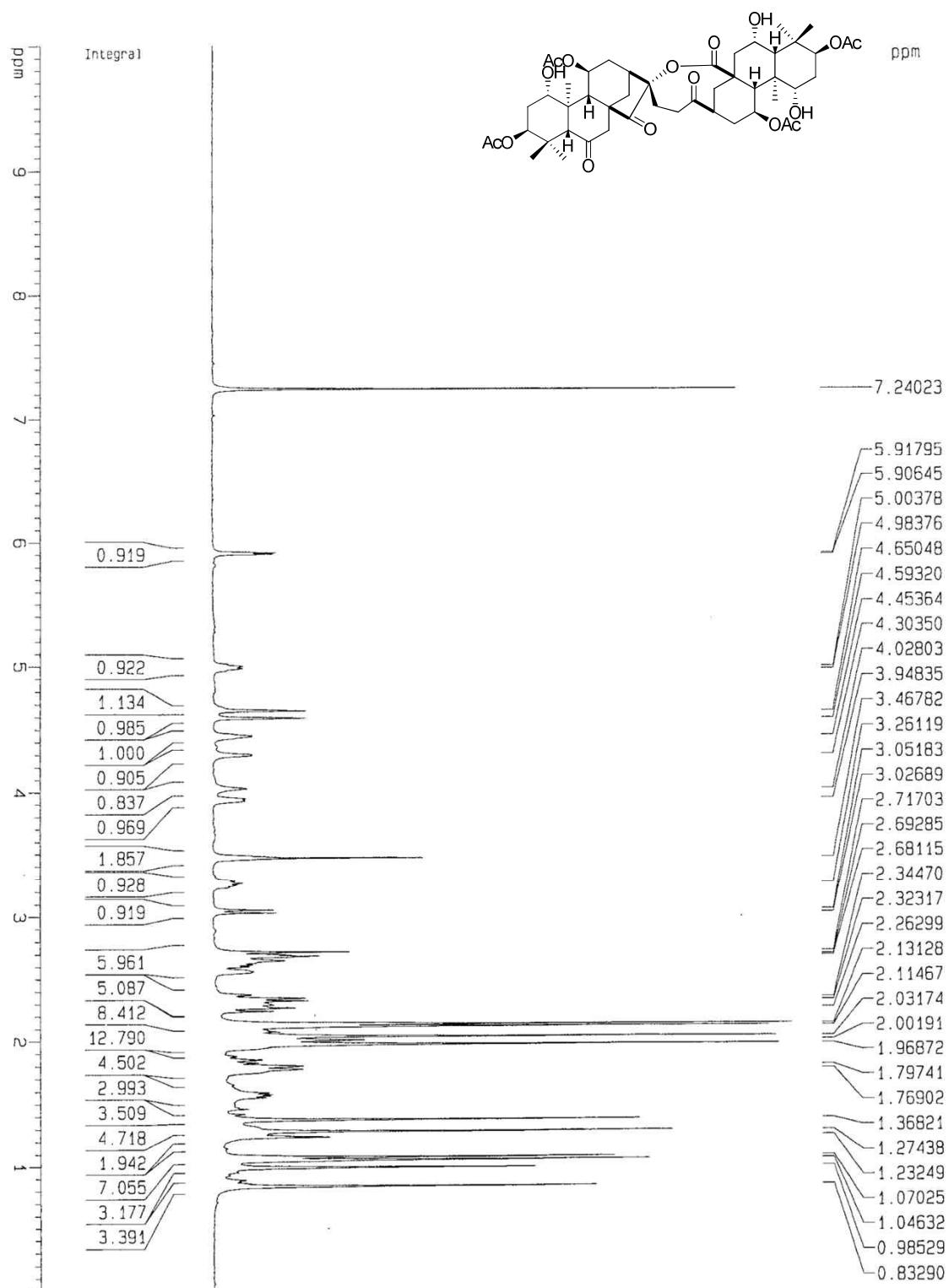


Figure S29. ^{13}C NMR spectrum (125 MHz, CDCl_3) of biexcisusin D (**4**)

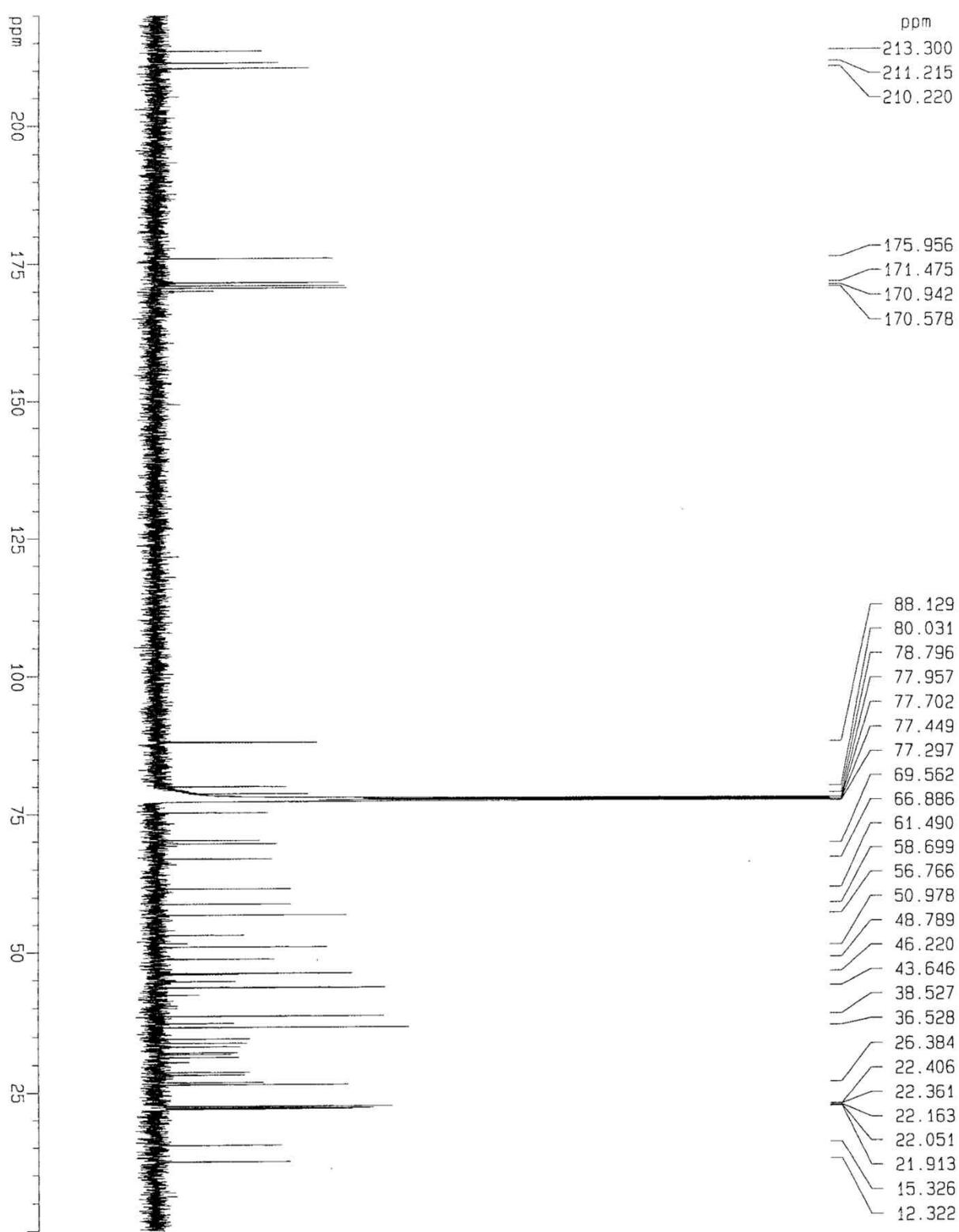


Figure S30. DEPT spectrum (500 MHz, CDCl_3) of biexcisin D (**4**)

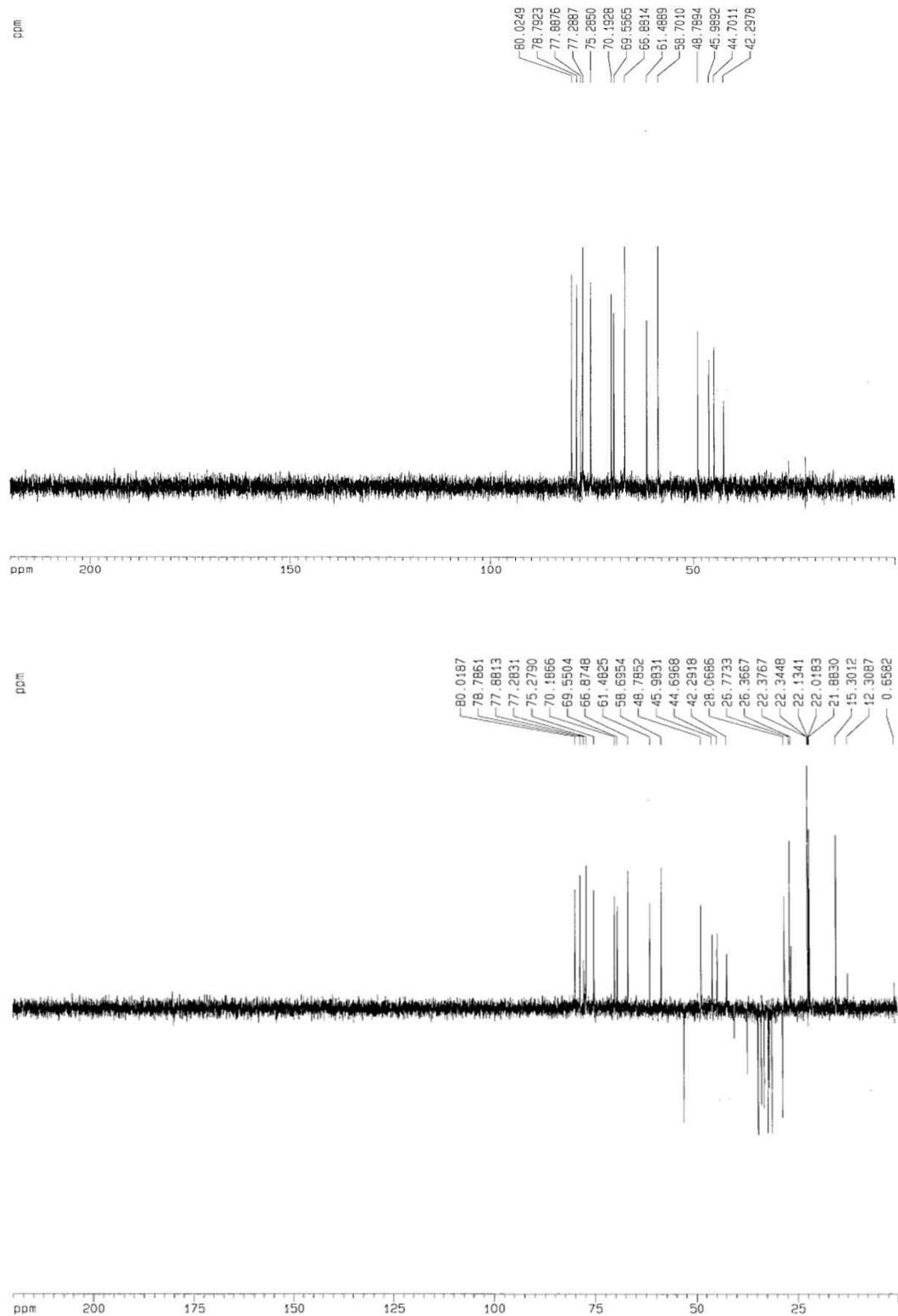


Figure S31. HMQC spectrum (500 MHz, CDCl_3) of biexcisusin D (**4**)

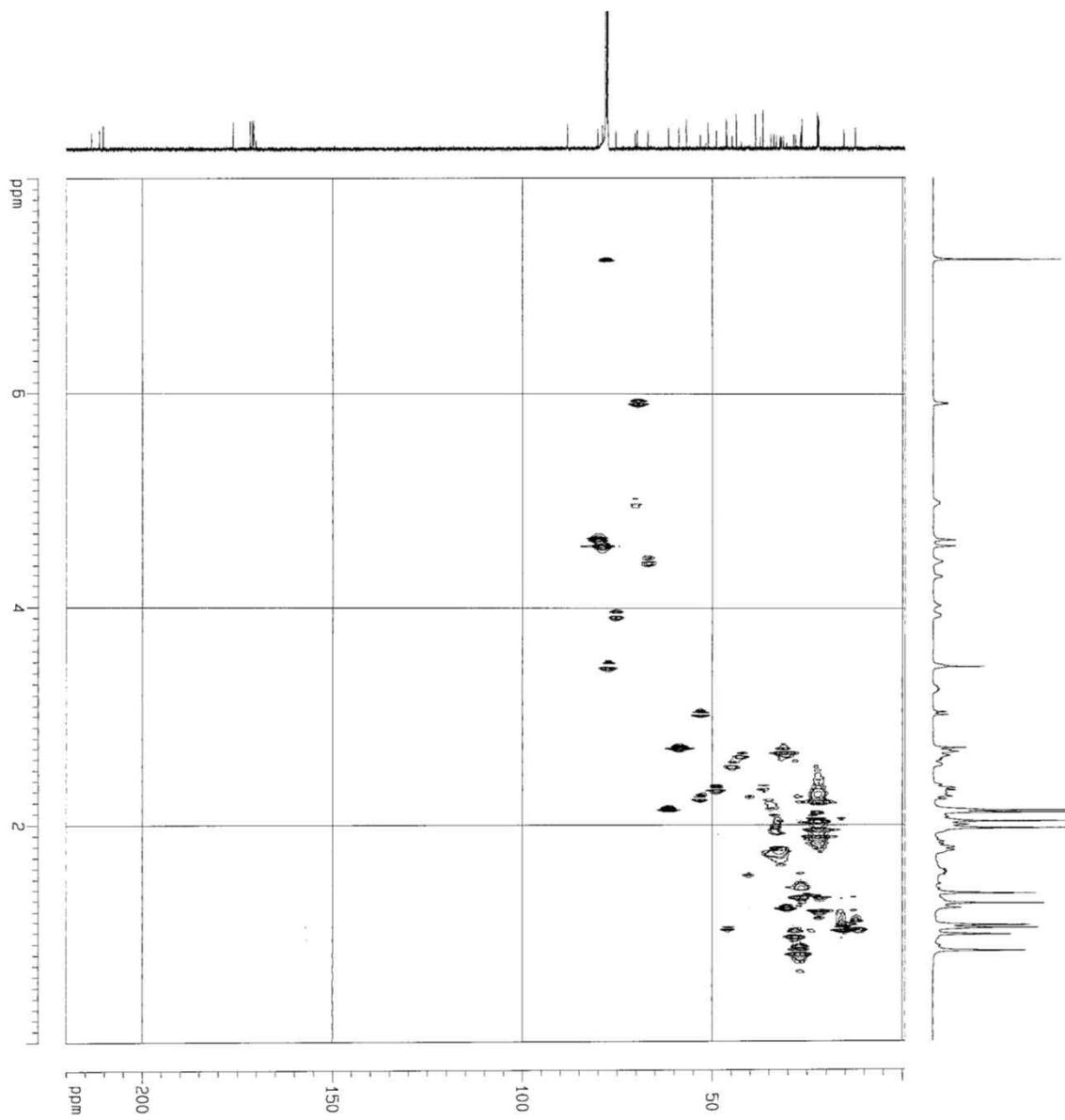


Figure S32. HMBC spectrum (500 MHz, CDCl₃) of biexcisin D (**4**)

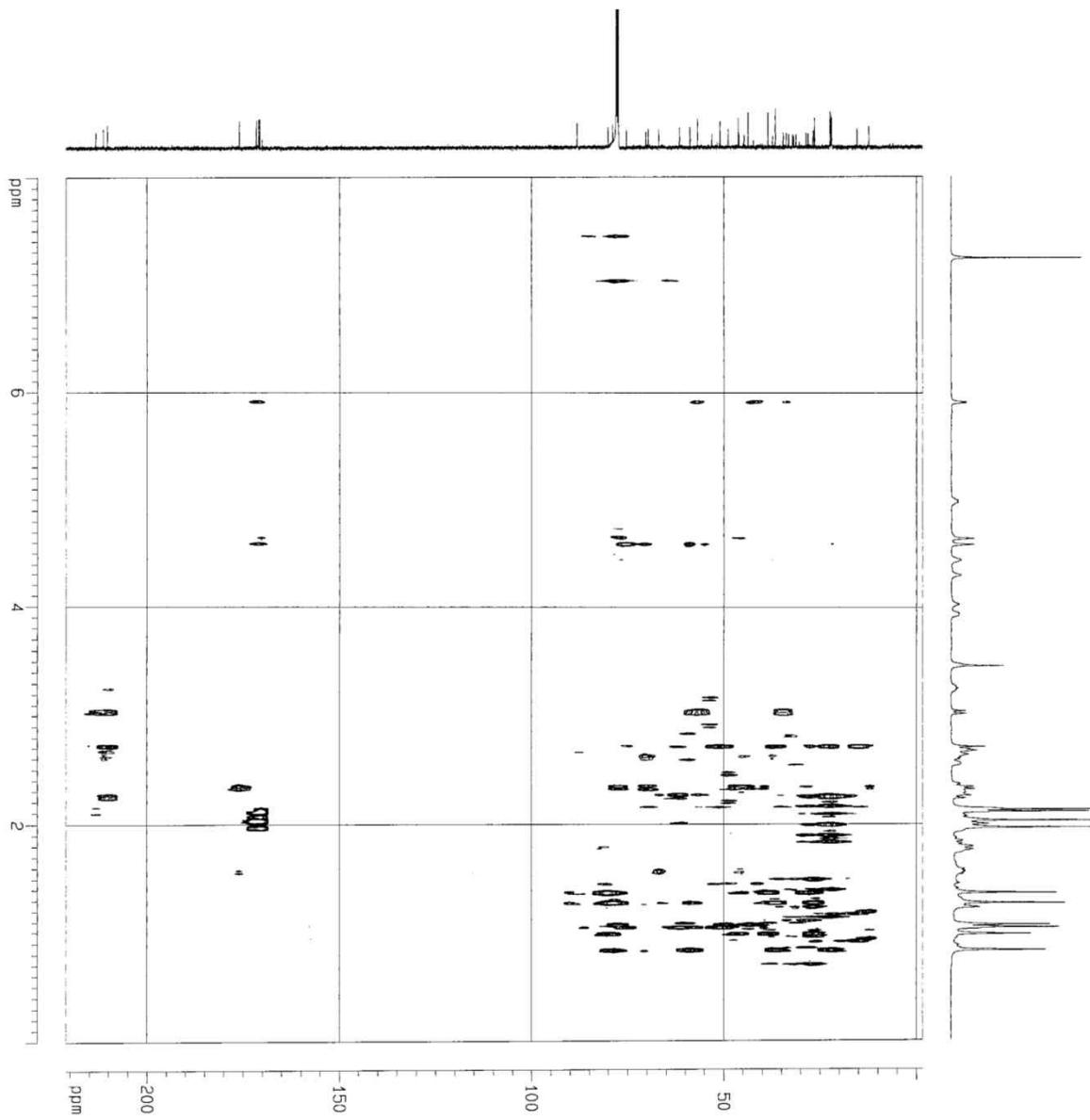


Figure S33. ESIMS spectrum of bi7excisusin D (**4**)

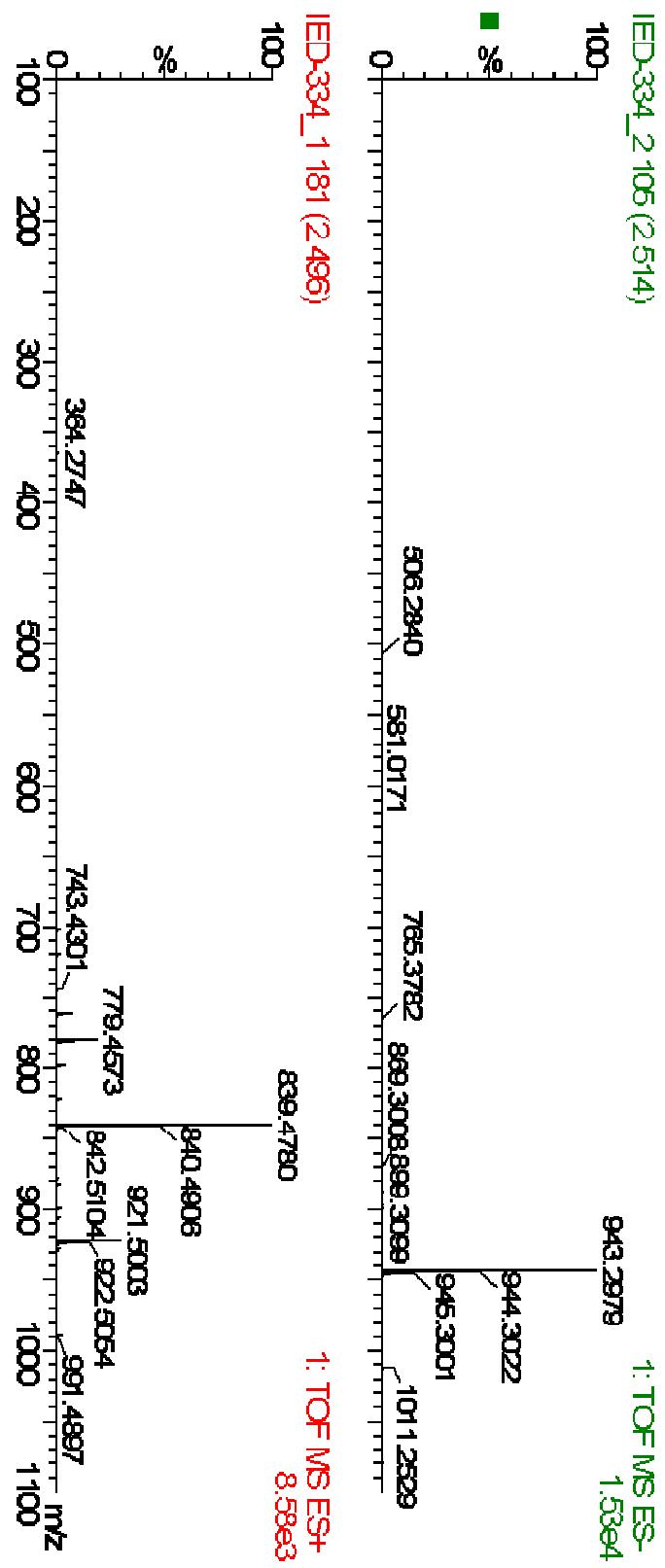


Figure S34. HRESIMS spectrum of biexcisin D (4)

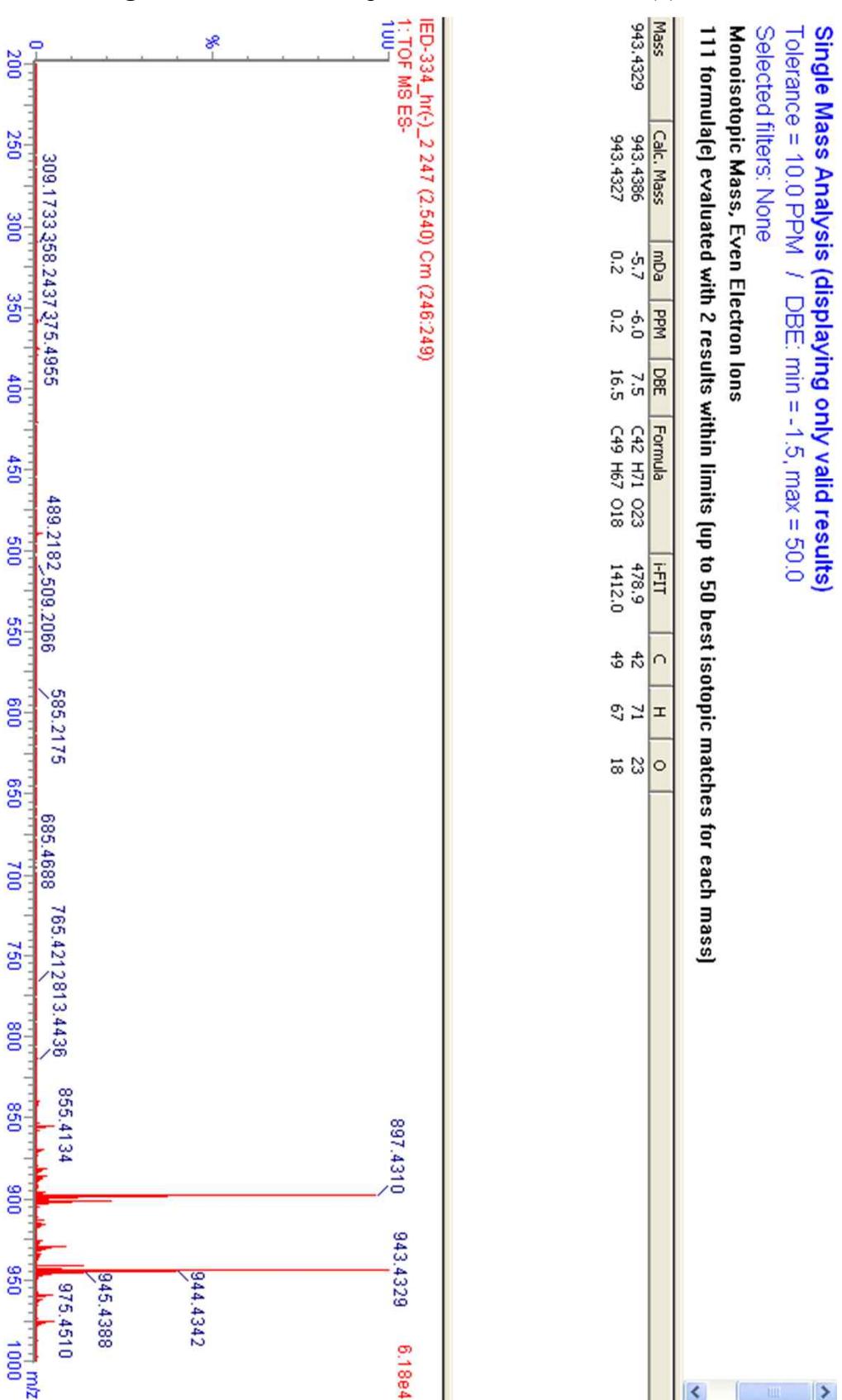


Figure S35. ^1H NMR spectrum (500 MHz, CDCl_3) of biexcisin E (**5**)

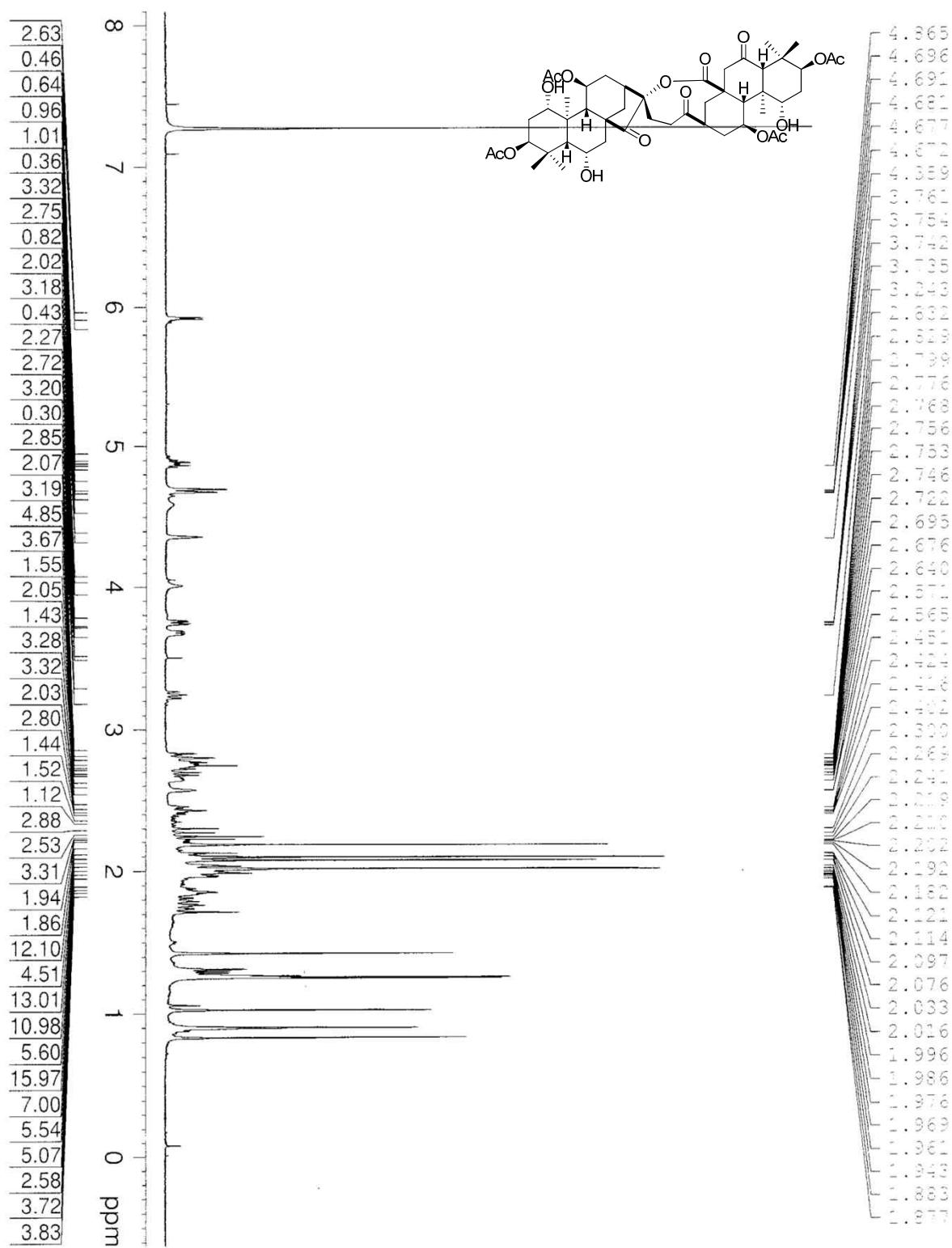


Figure S36. ^{13}C NMR spectrum (125 MHz, CDCl_3) of biexcisusin E (**5**)

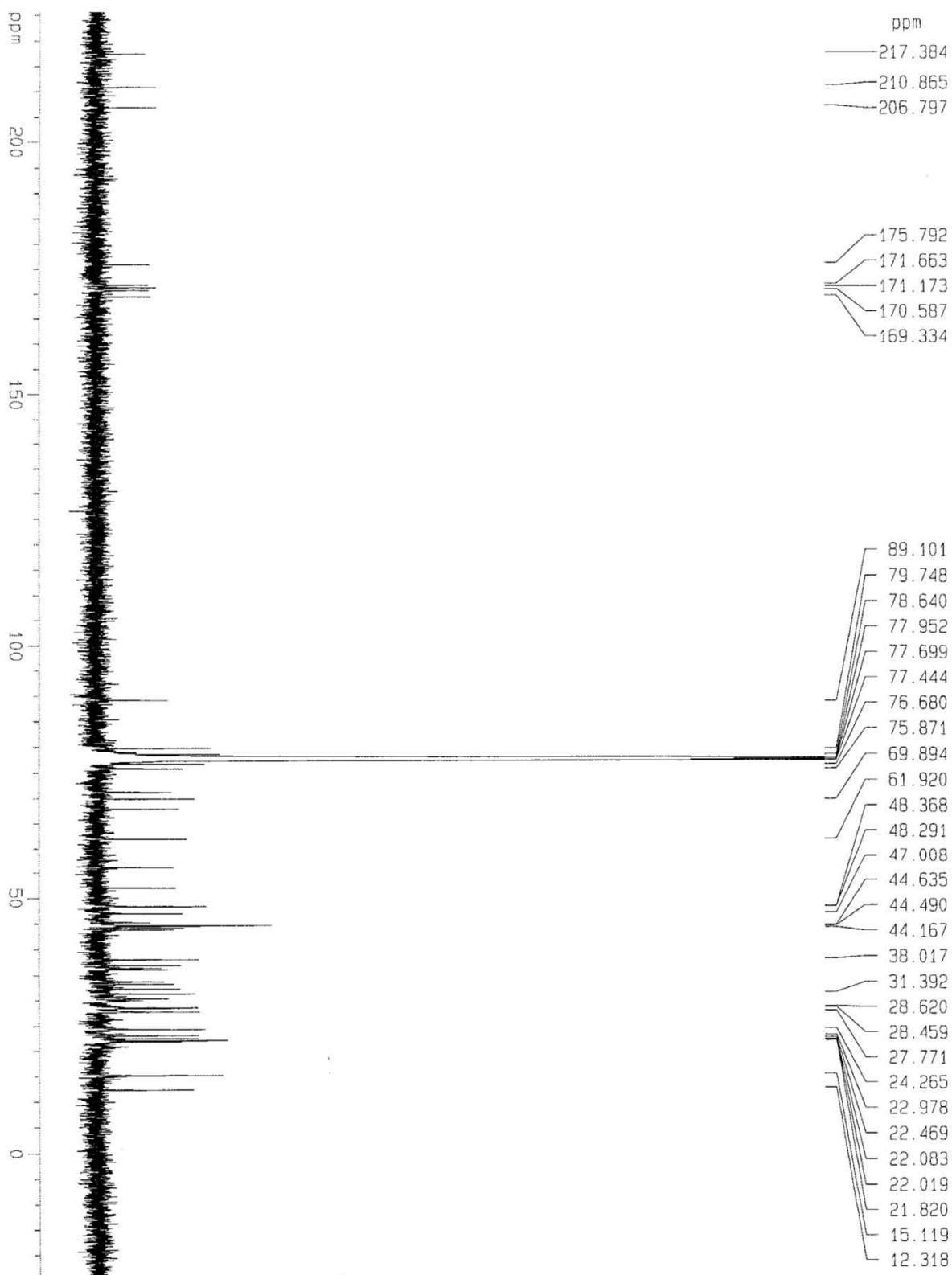


Figure S37. DEPT spectrum (125 MHz, CDCl₃) of biexcisusin E (**5**)

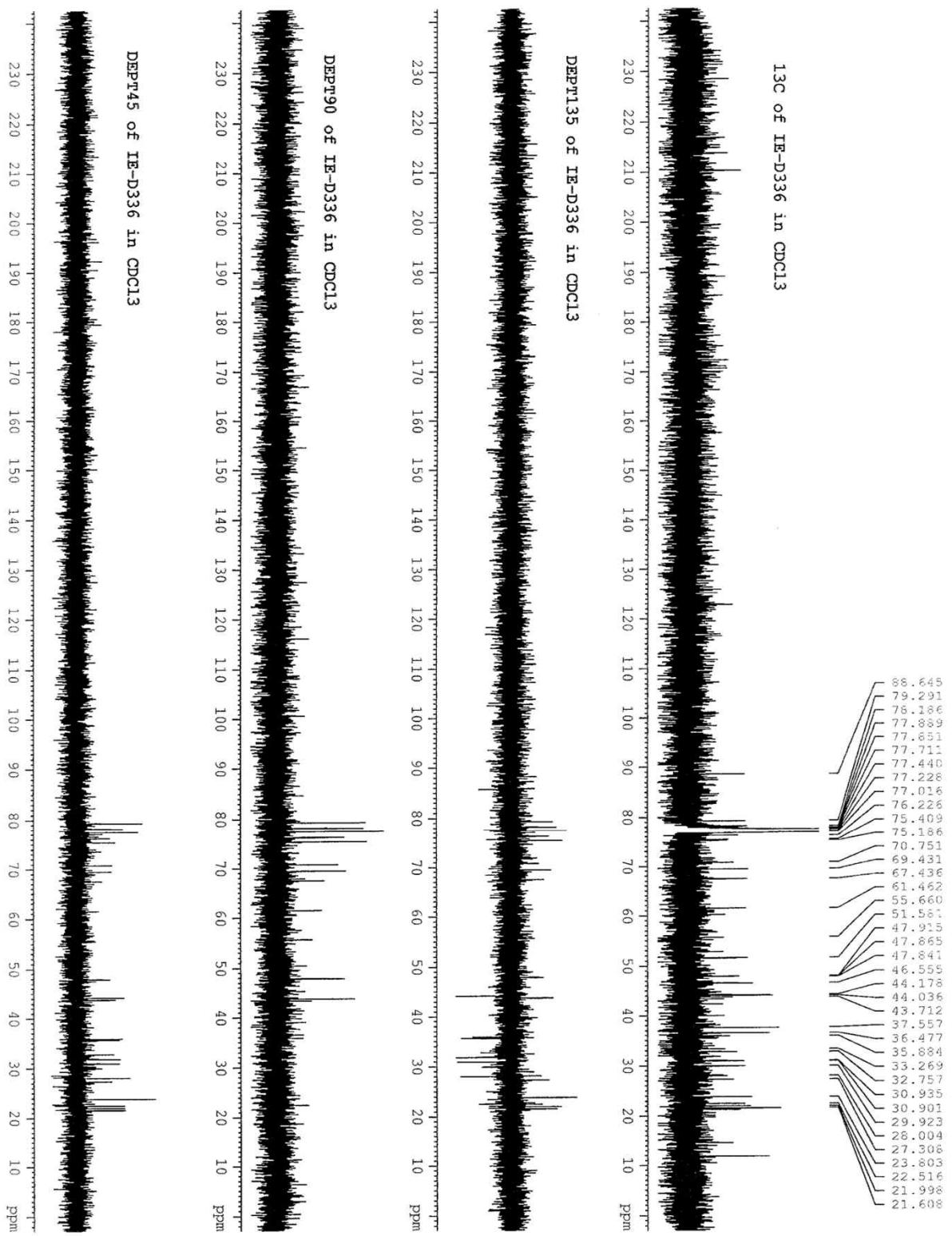
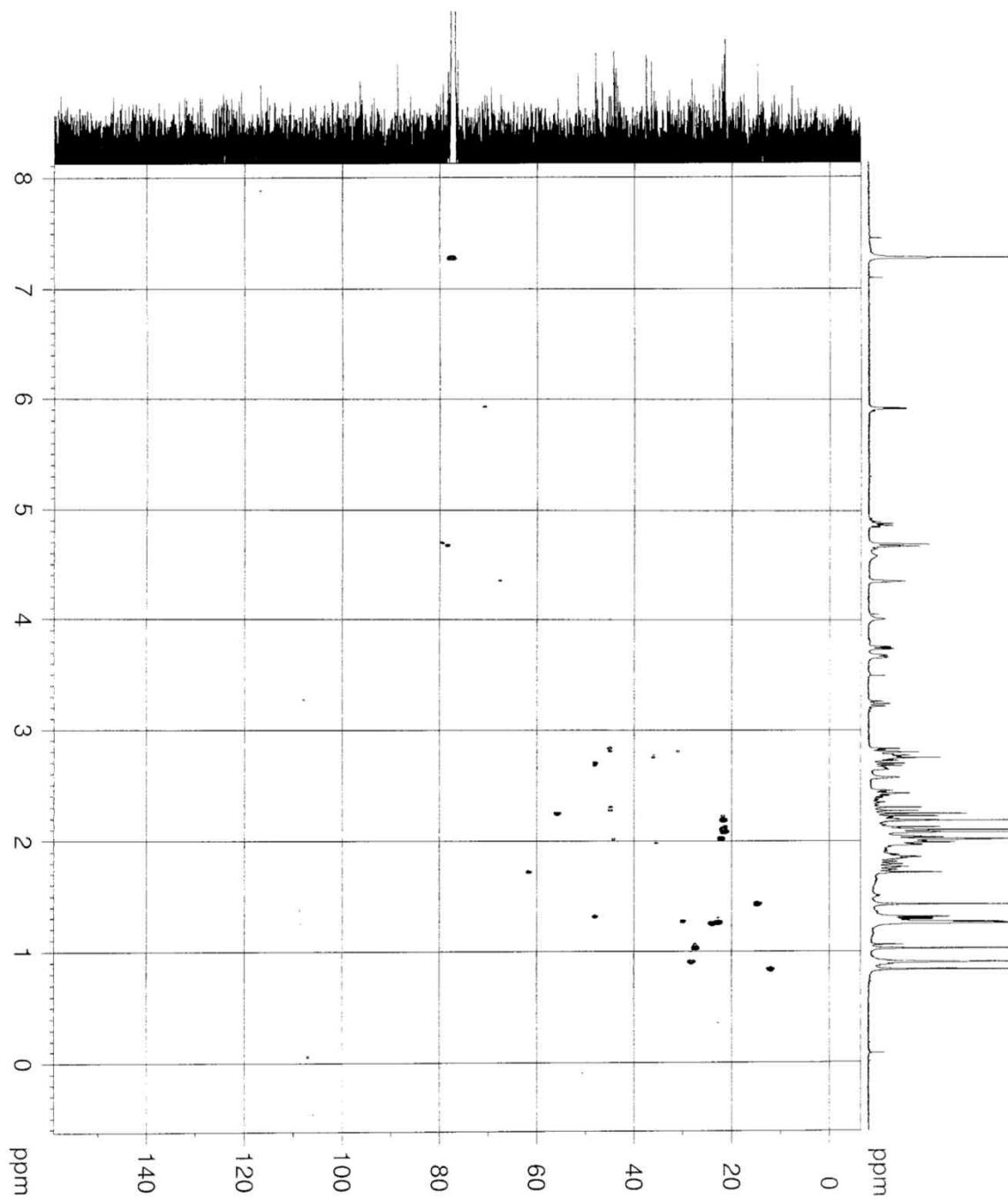


Figure S38. HMQC spectrum (500 MHz, CDCl_3) of biexcisin E (**5**)



HMBC of 1E-D336 in CDCl₃

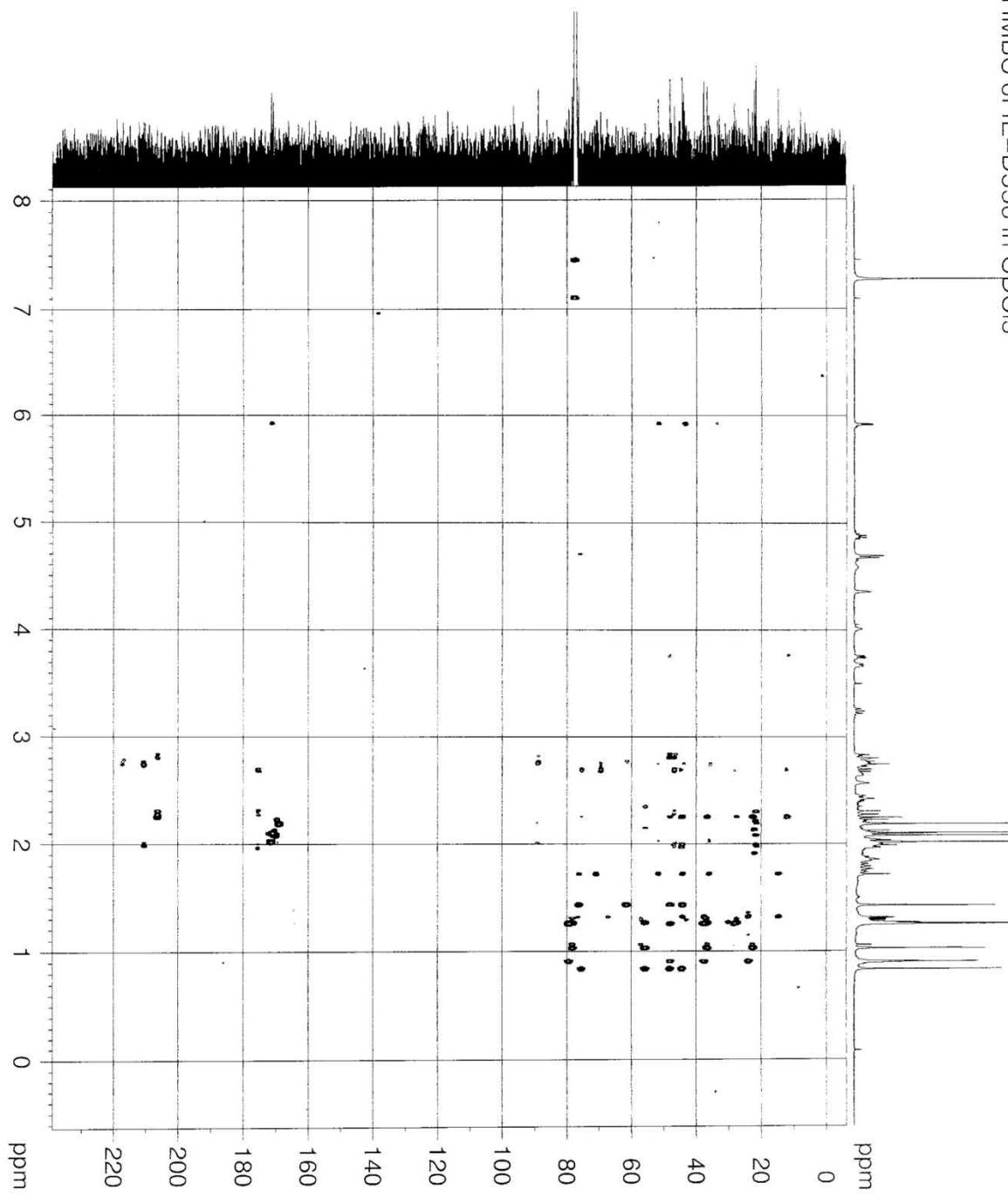


Figure S40. ESIMS spectrum of biexcisusin E (**5**)

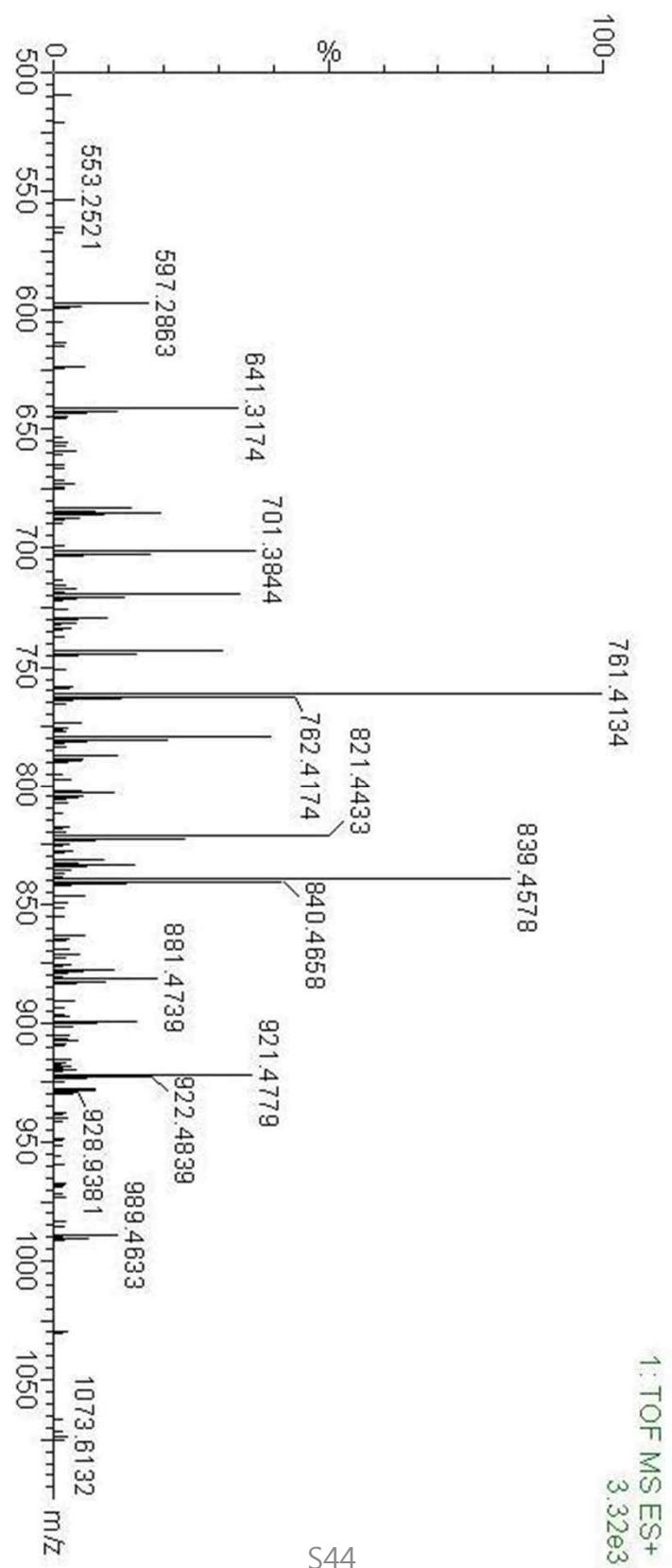
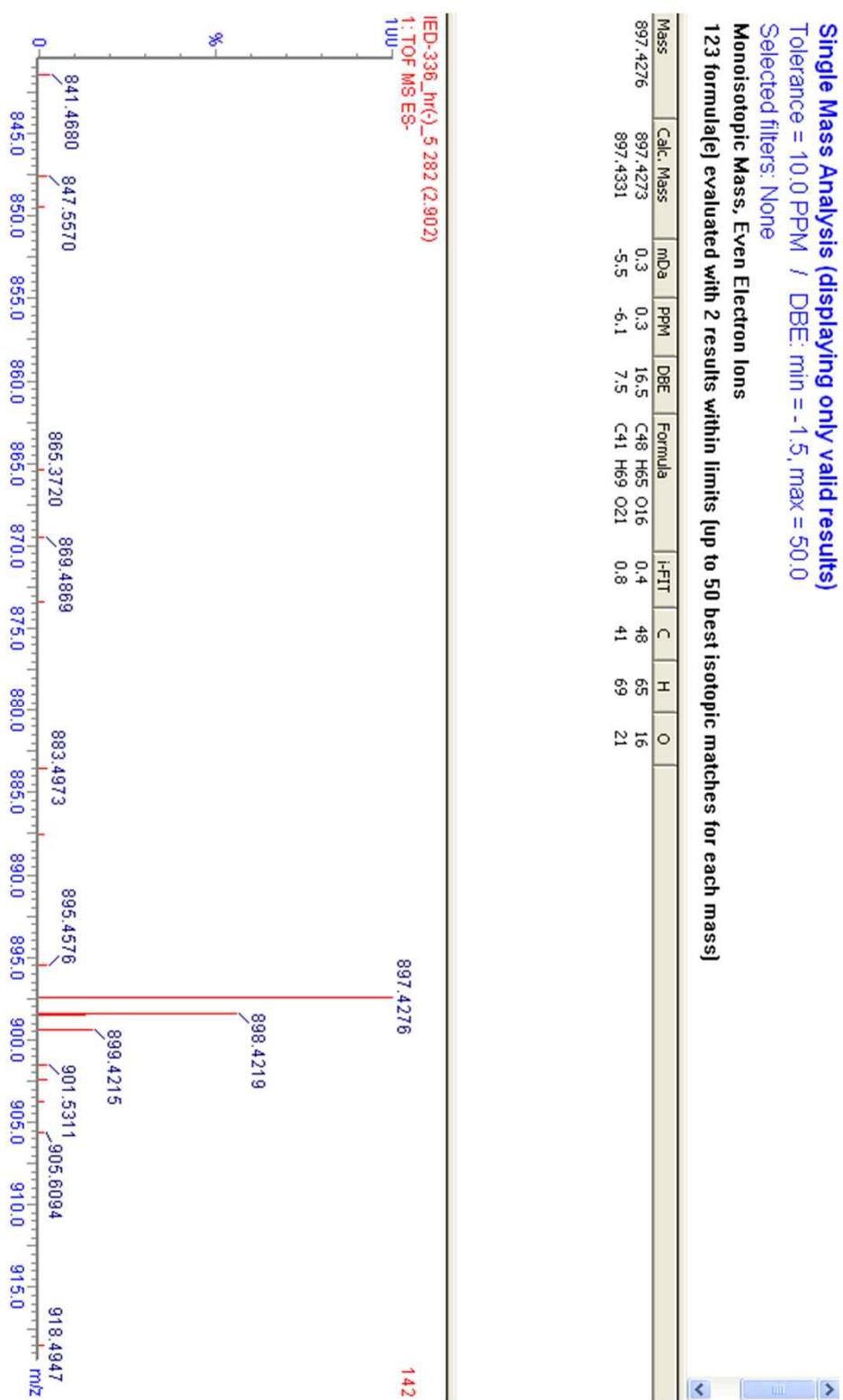
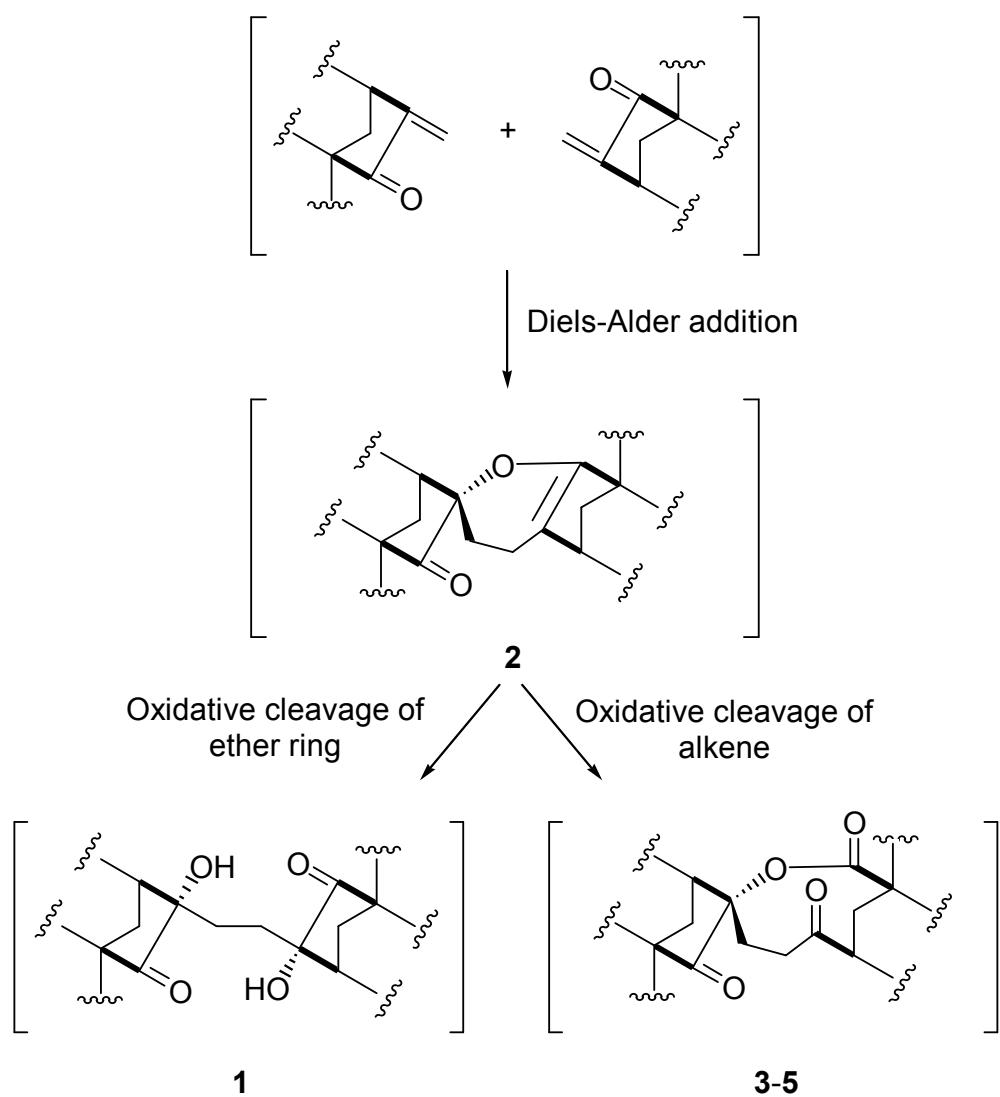


Figure S41. HRESIMS spectrum of biexcisusin E (**5**)





Scheme S1. Hypothetical biogenetic pathway of **1-5**