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

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[‡]*Gyeonggi Pharmaceutical Research Center, Gyeonggi Institute of Science & Technology Promotion, Suwon 443-759, Korea*
[§]*School of Life Sciences and Biotechnology, Korea University, Seoul 136-713, Korea*

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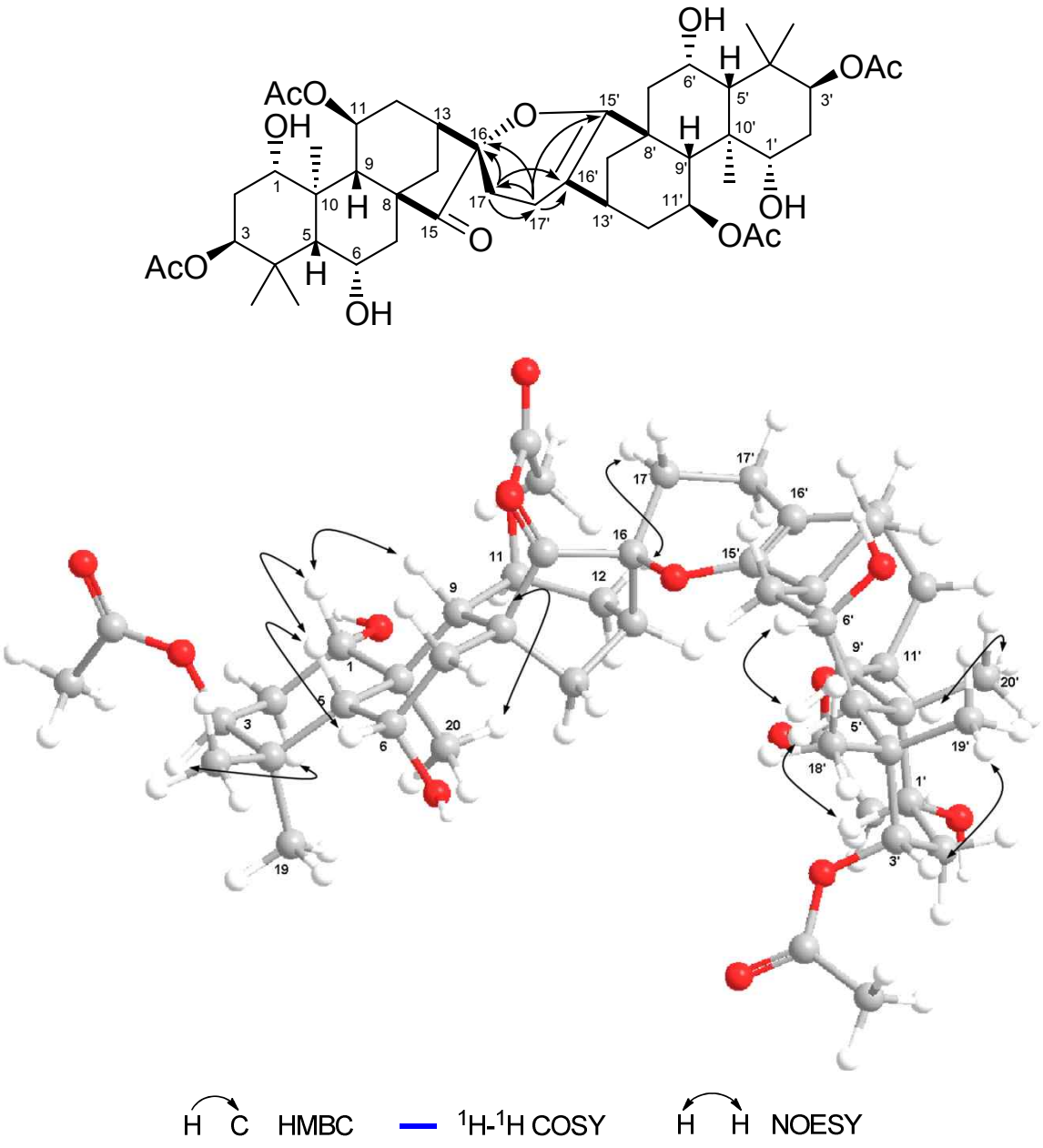


Figure S1. Key HMBC, COSY, and NOESY correlations of biexcisusin B (**2**).

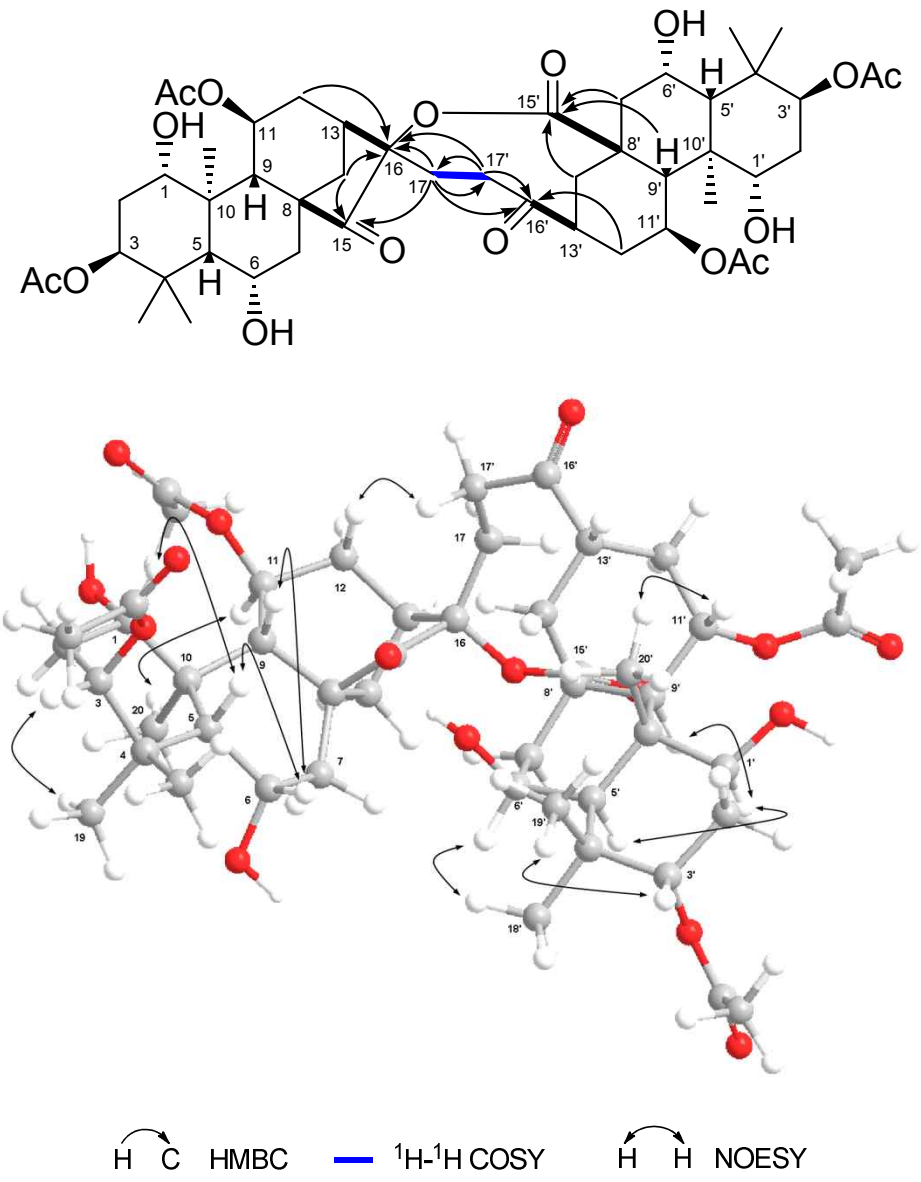


Figure S2. Key HMBC, COSY, and NOESY correlations of biexcisusin C (**3**).

Figure S1. ^{1}H NMR spectrum (900 MHz, C_5D_5N) of biexcisusin A (**1**)

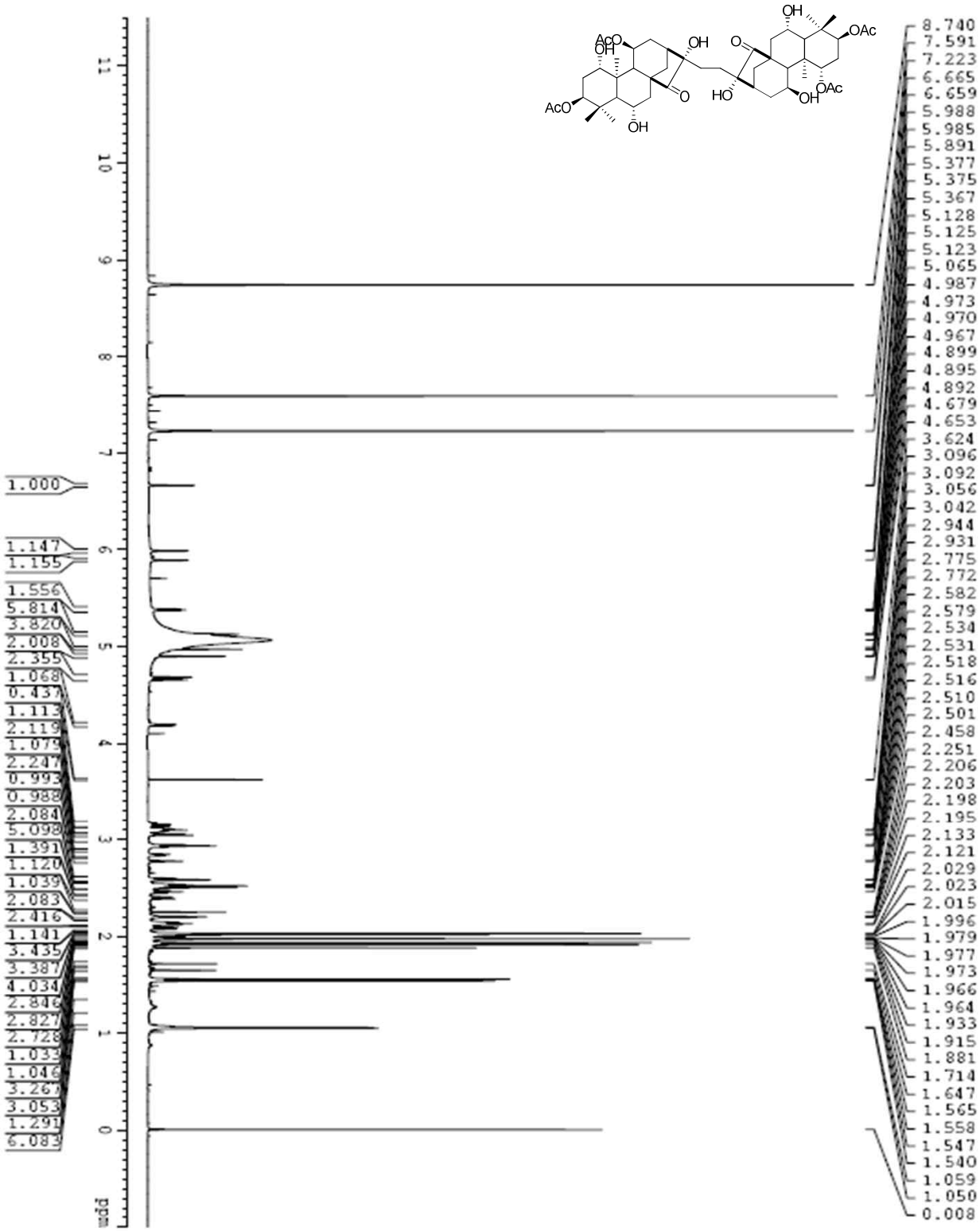


Figure S2. ^{13}C NMR spectrum (225 MHz, C_5D_5N) of biexcisusin A (**1**)

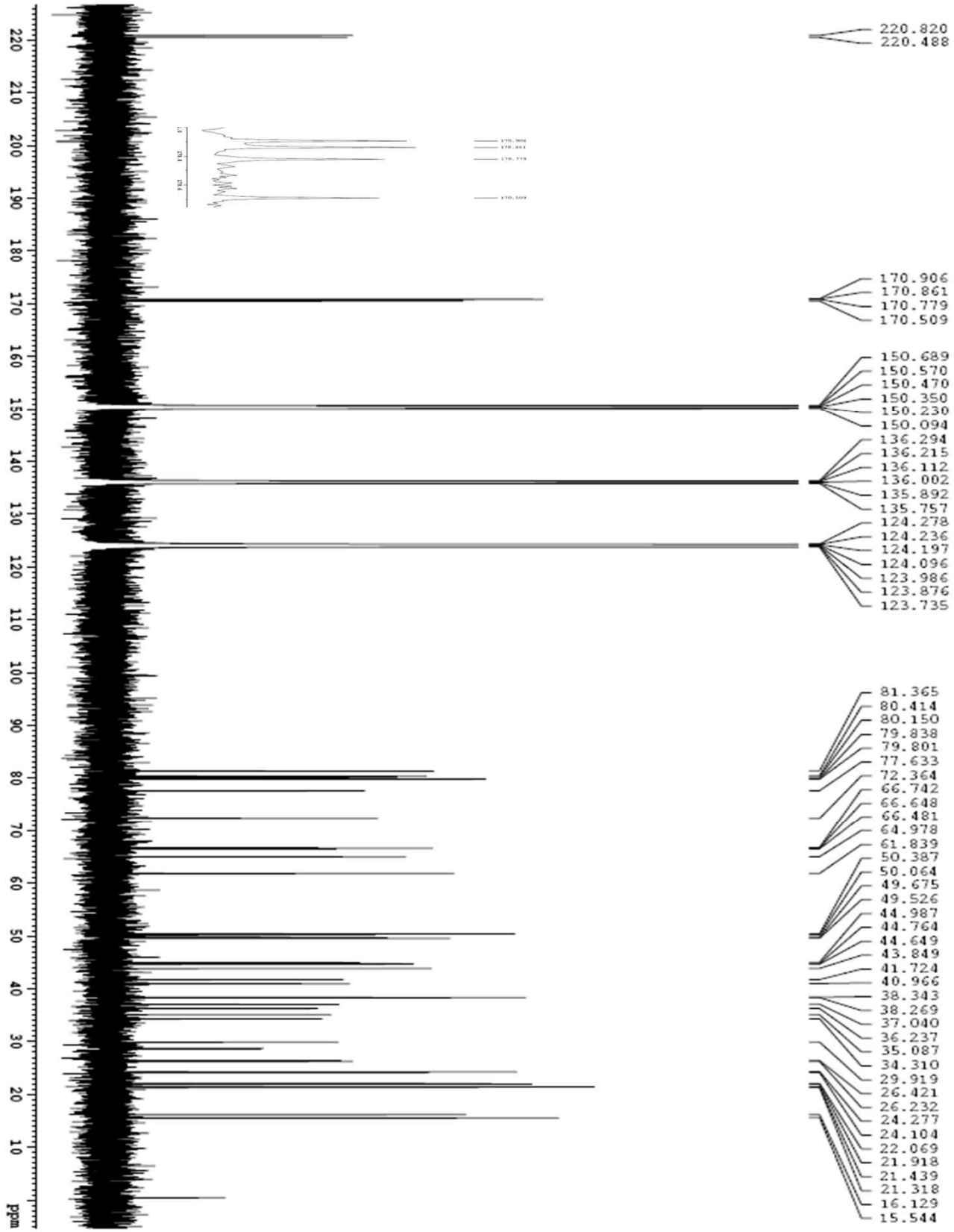


Figure S3. DEPTspectrum (225 MHz, C_5D_5N) of biexcisusin A (**1**)

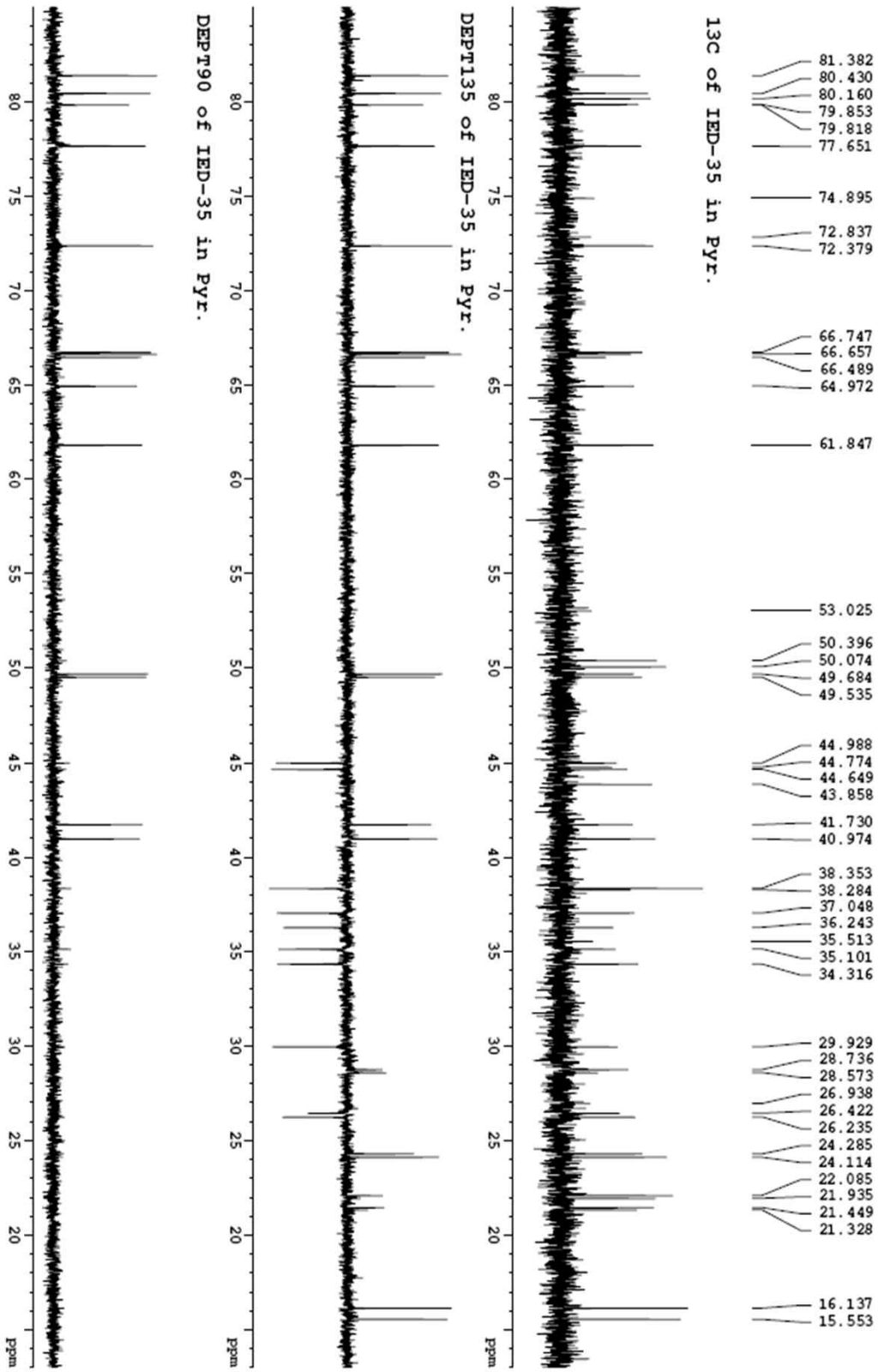


Figure S4. COSY spectrum (900 MHz, C_5D_5N) of biexcisusin A (**1**)

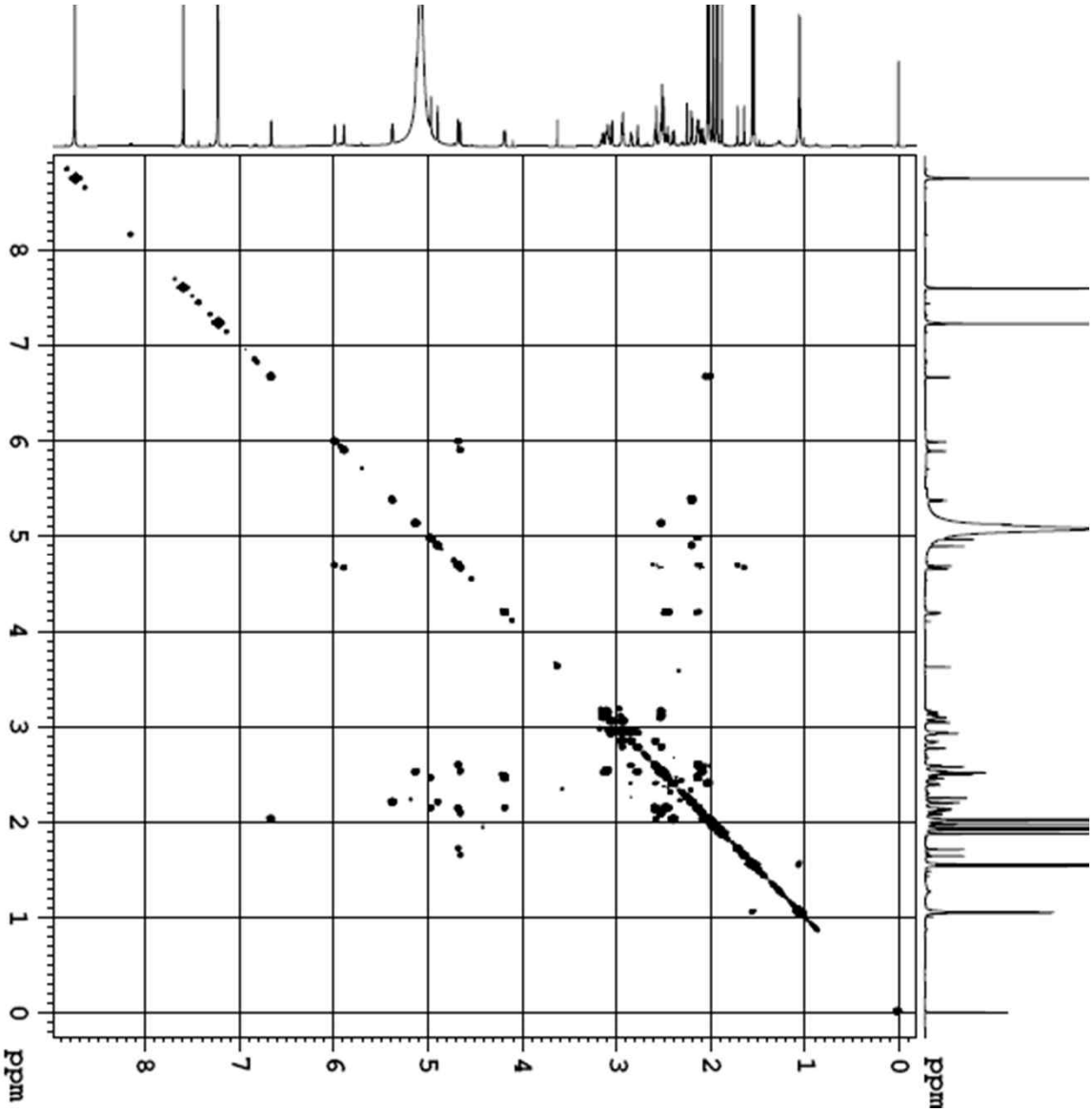


Figure S5. HMQC spectrum (900 MHz, C_5D_5N) of biexcisusin A (**1**)

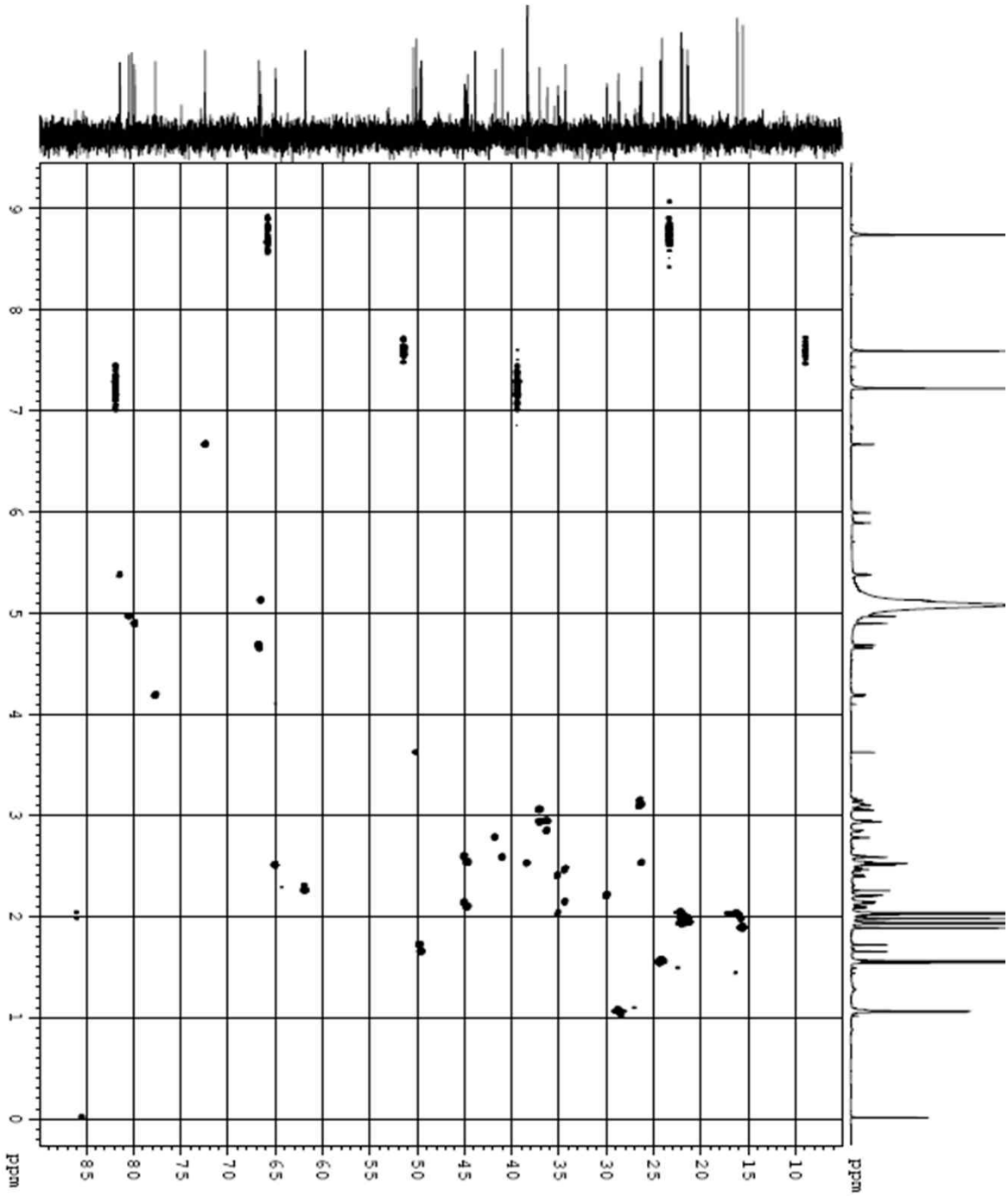


Figure S6. HMBC spectrum (900 MHz, C_5D_5N) of biexcisusin A (**1**)

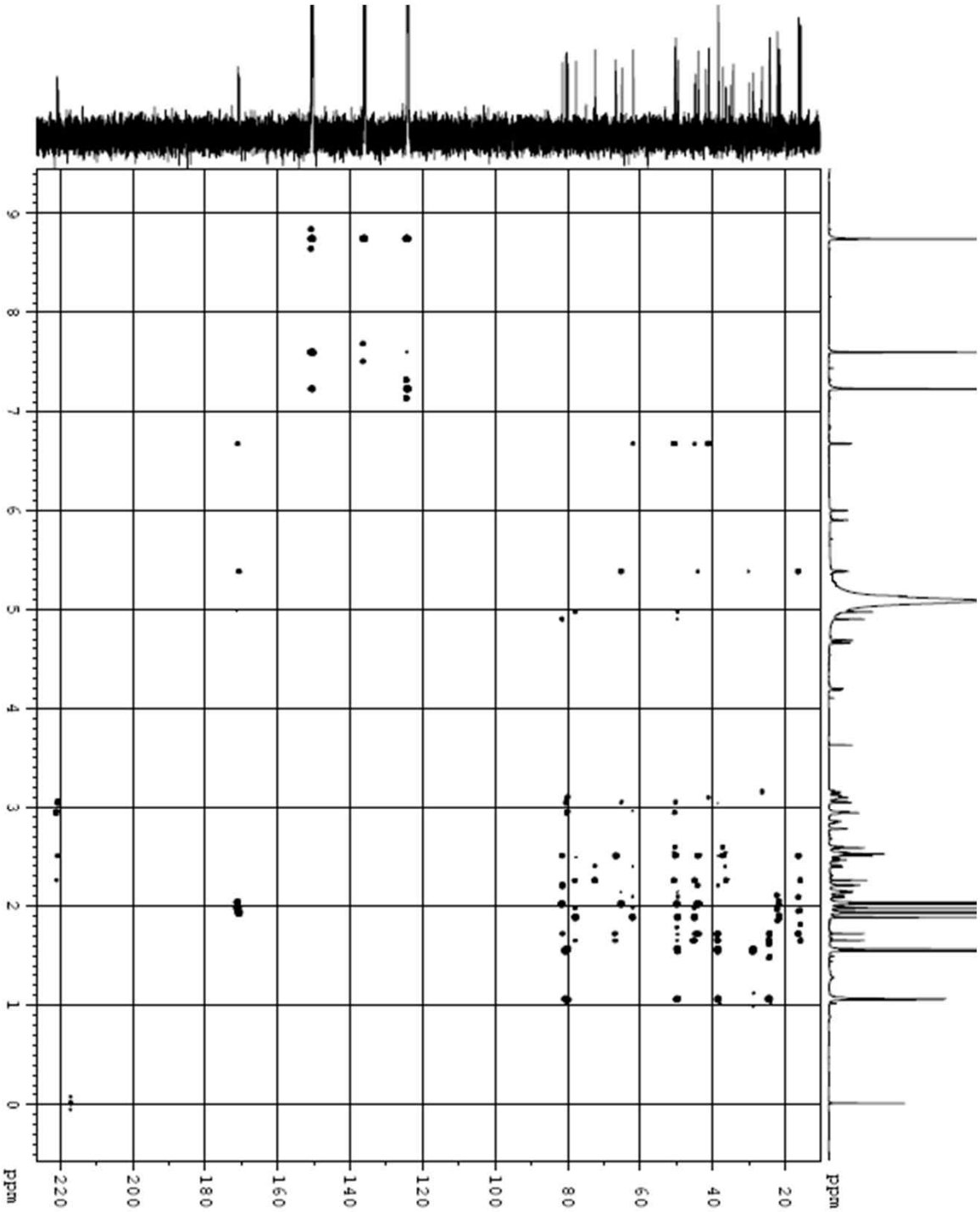


Figure S7. ROESY spectrum (900 MHz, C_5D_5N) of biexcisusin A (**1**)

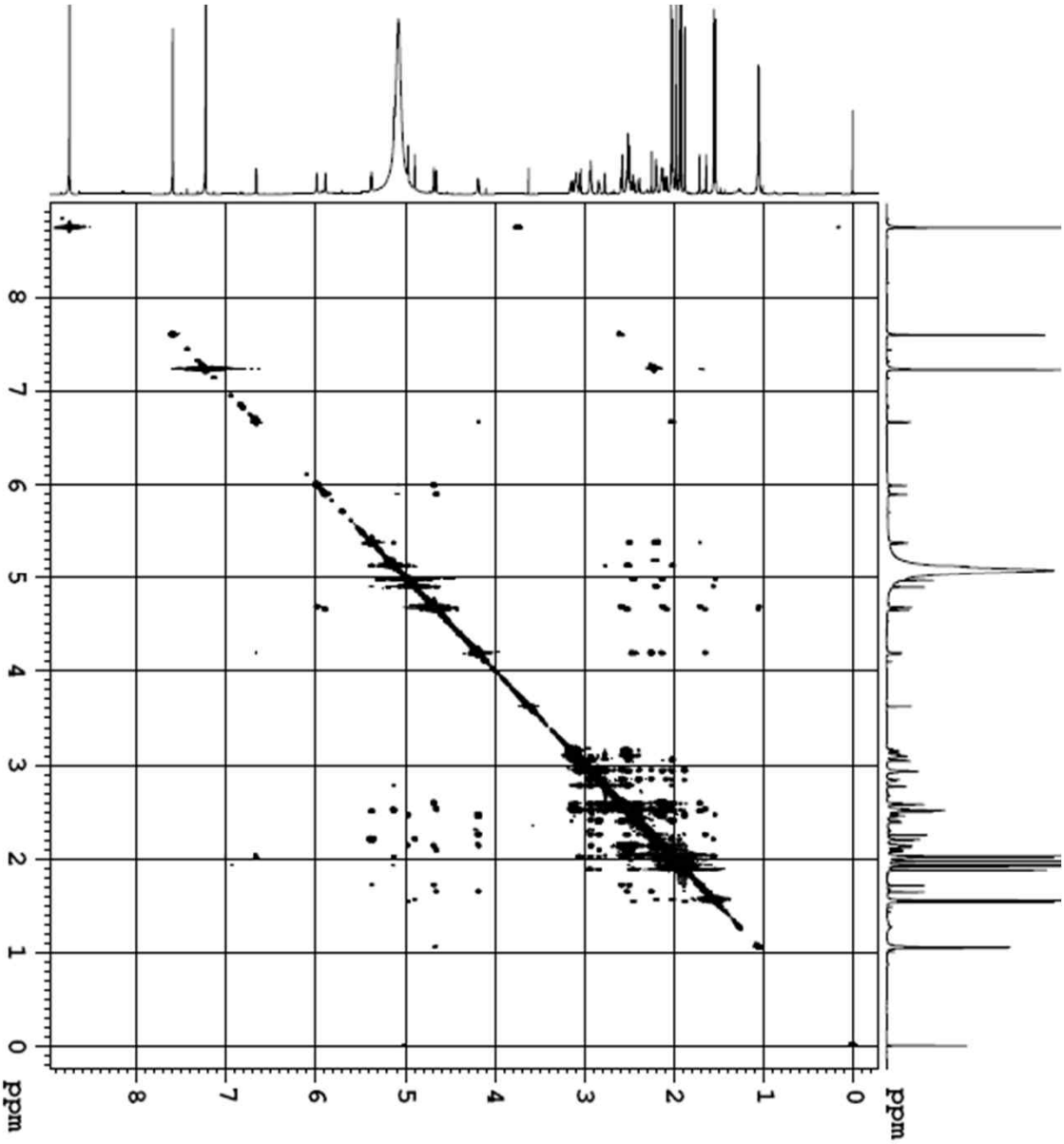


Figure S8. ESIMS spectrum of biexcisusin A (**1**)

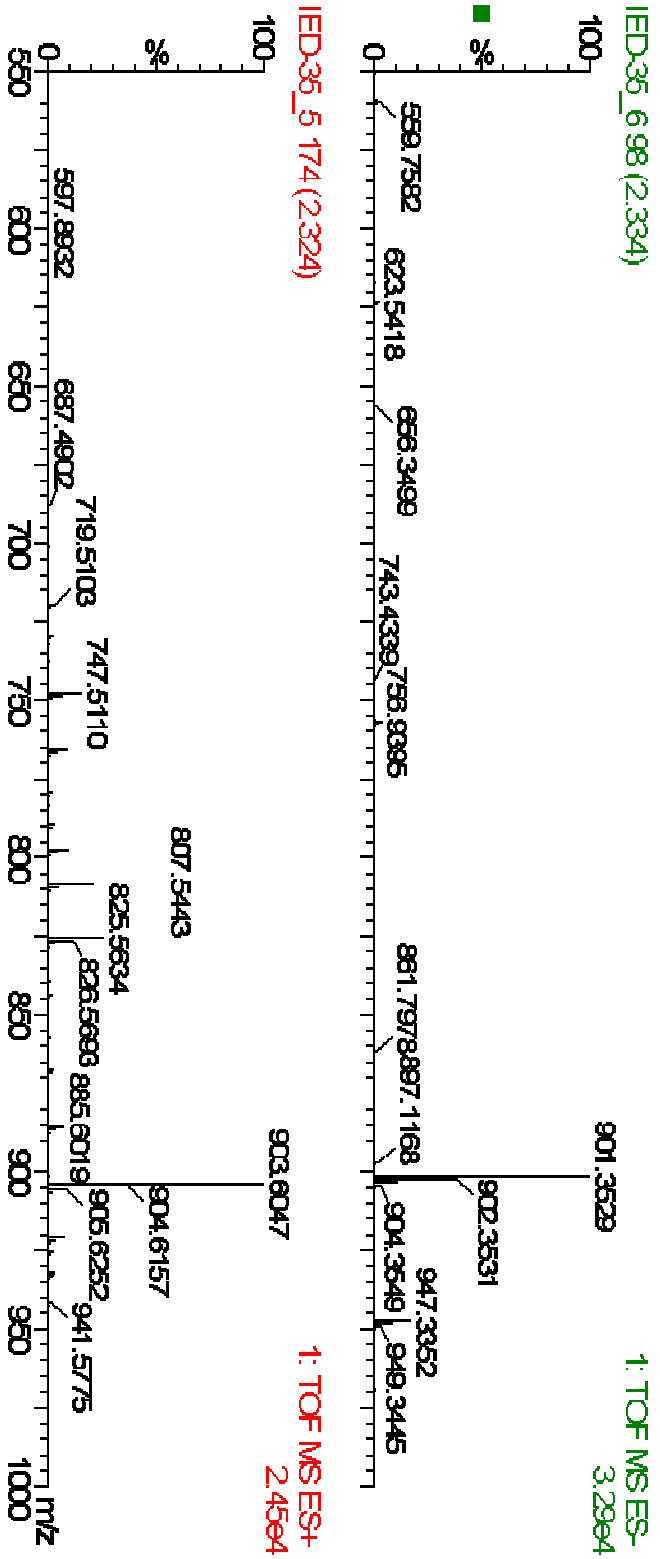
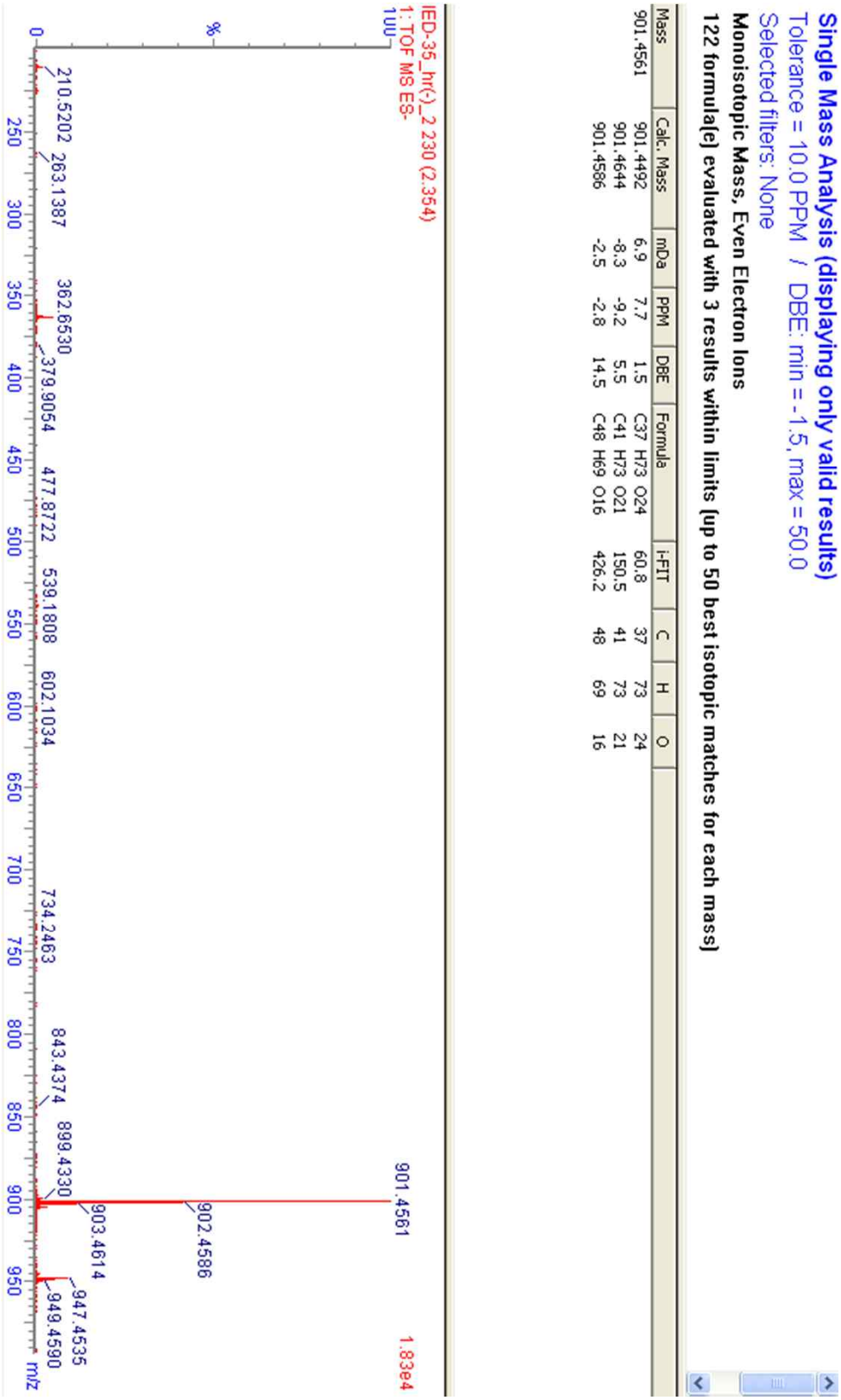


Figure S9. HRESIMS spectrum of biexcisusin A (**1**)



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	C37 H73 O24	60.8	37	73	24
	901.4644	-8.3	-9.2	5.5	C41 H73 O21	150.5	41	73	21
	901.4586	-2.5	-2.8	14.5	C48 H69 O16	426.2	48	69	16

Figure S10. ^{1}H NMR spectrum (900 MHz, C_5D_5N) of biexcisusin B (**2**)

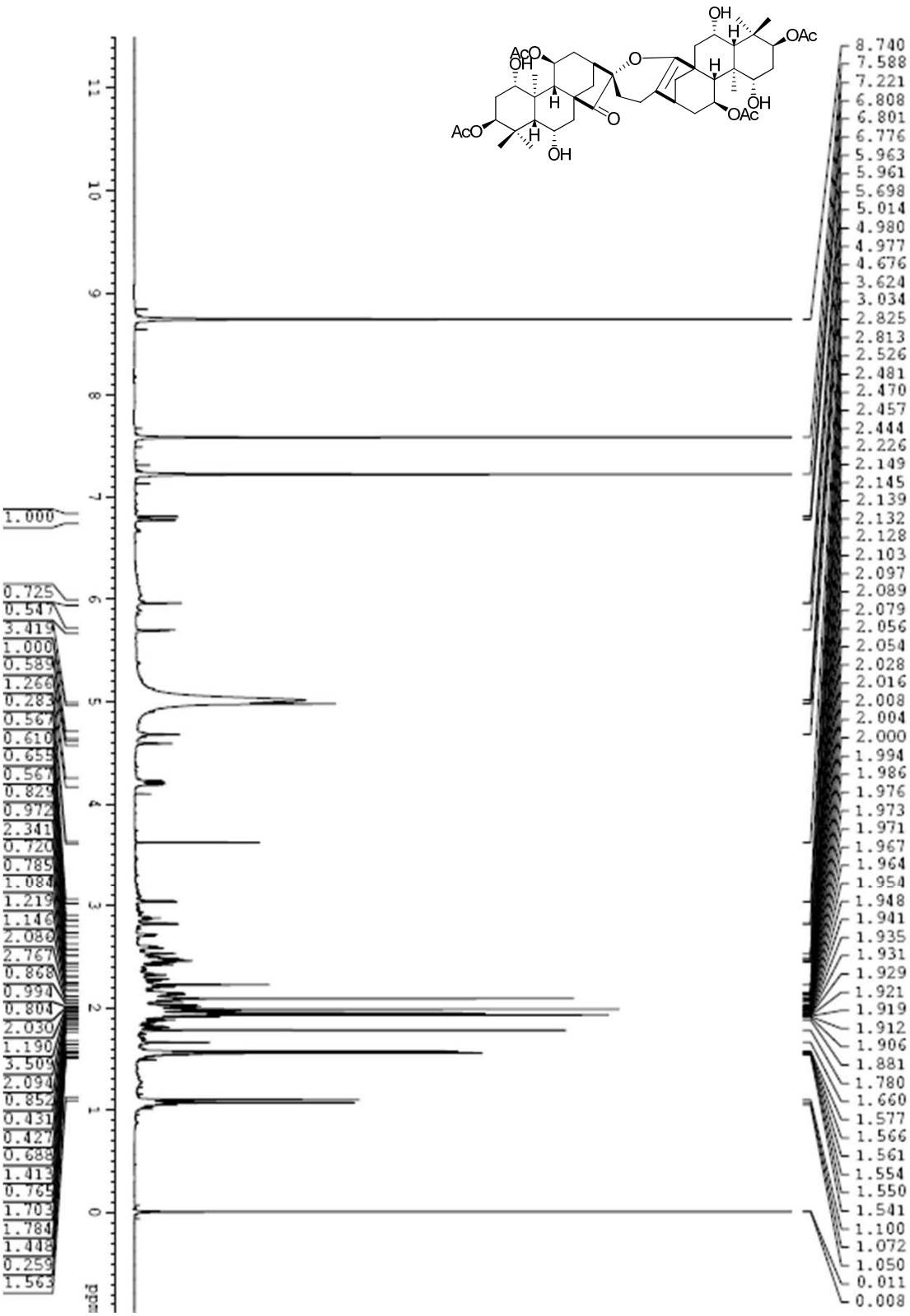


Figure S11. ^{13}C NMR spectrum (225 MHz, C_5D_5N) of biexcisusin B (**2**)

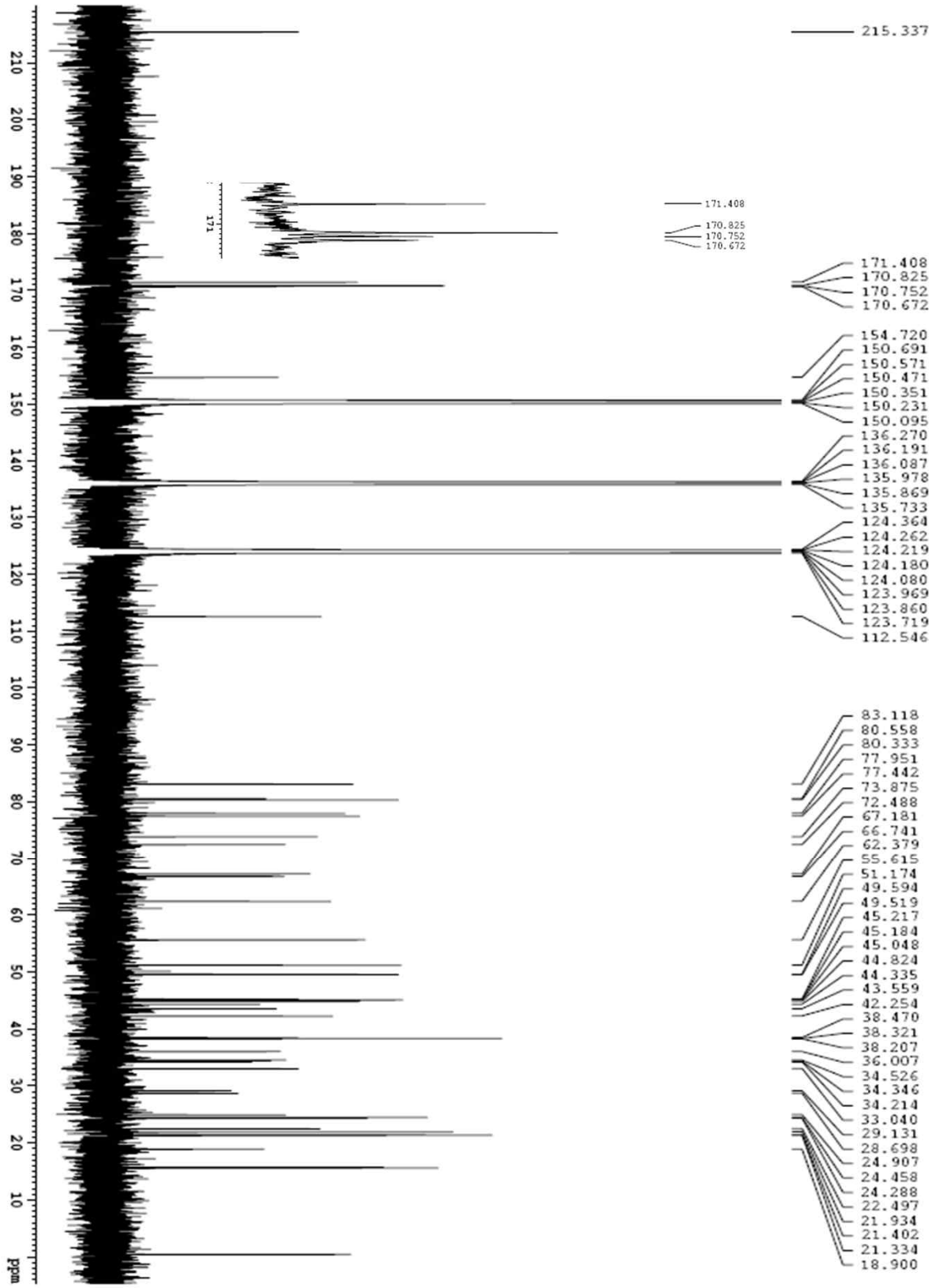


Figure S12. DEPT spectrum (225 MHz, C_5D_5N) of biexcisusin B (**2**)

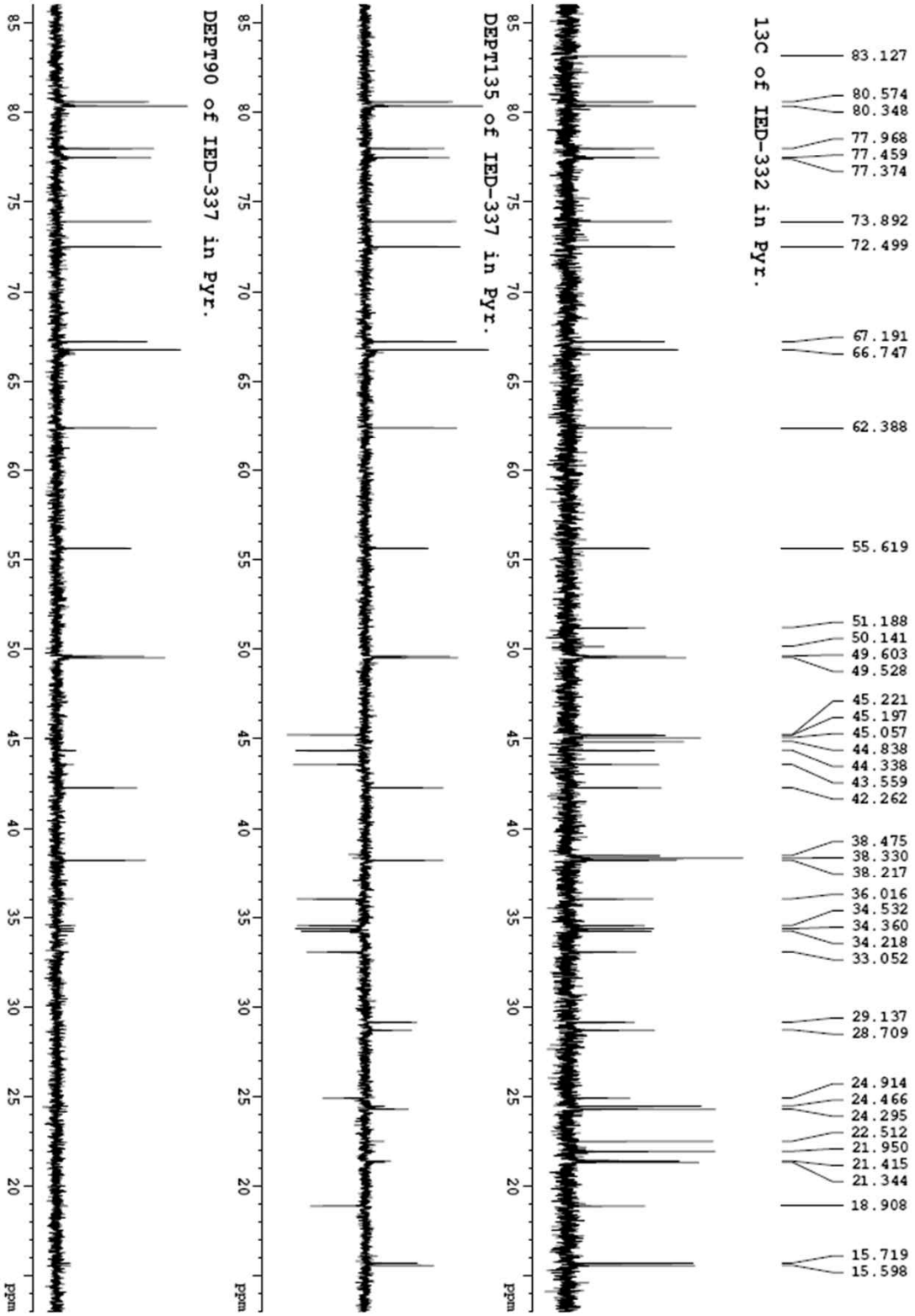


Figure S13. COSY spectrum (900 MHz, C_5D_5N) of biexcisusin B (**2**)

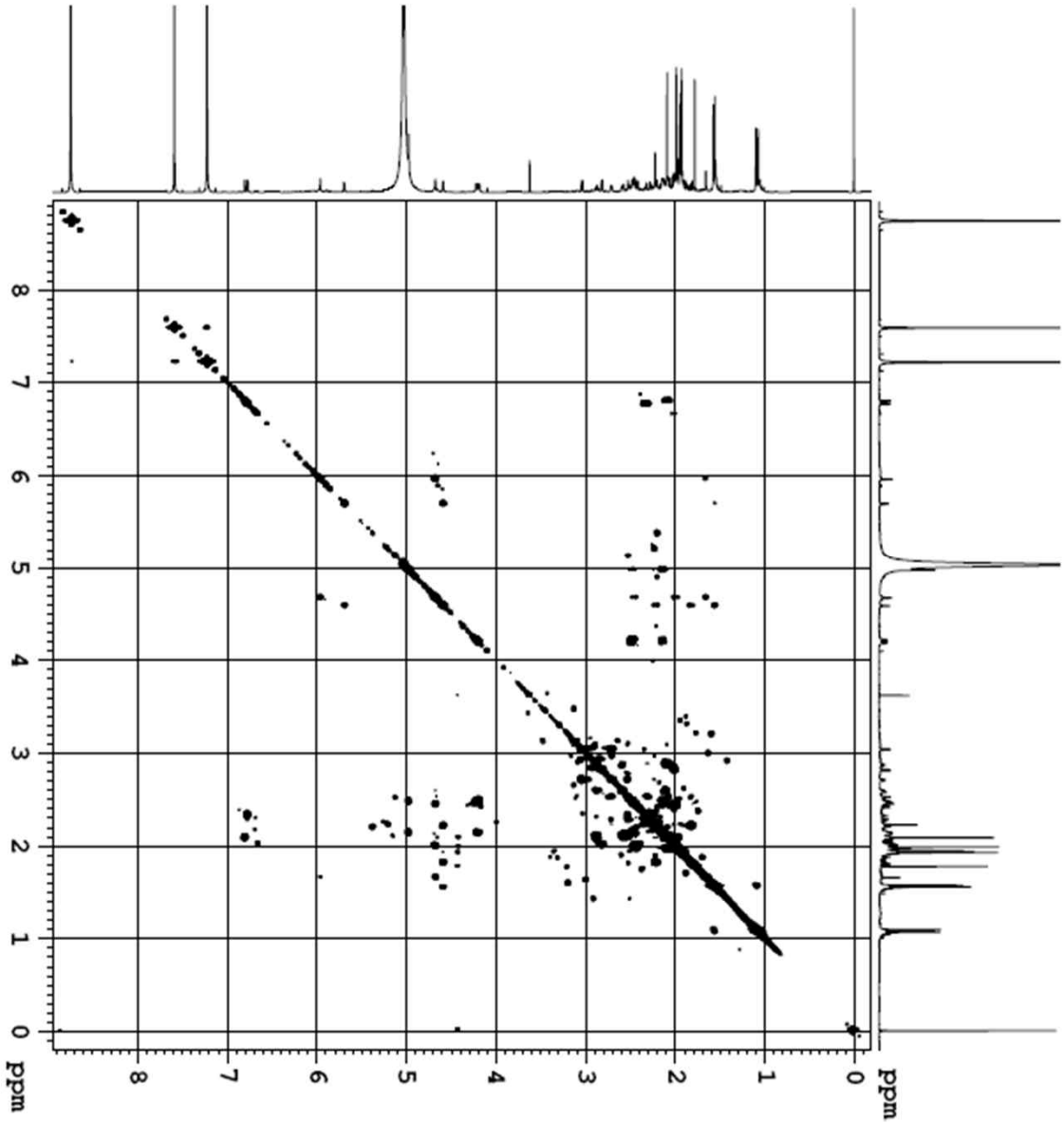


Figure S14. HMQC spectrum (900 MHz, C_5D_5N) of biexcisusin B (**2**)

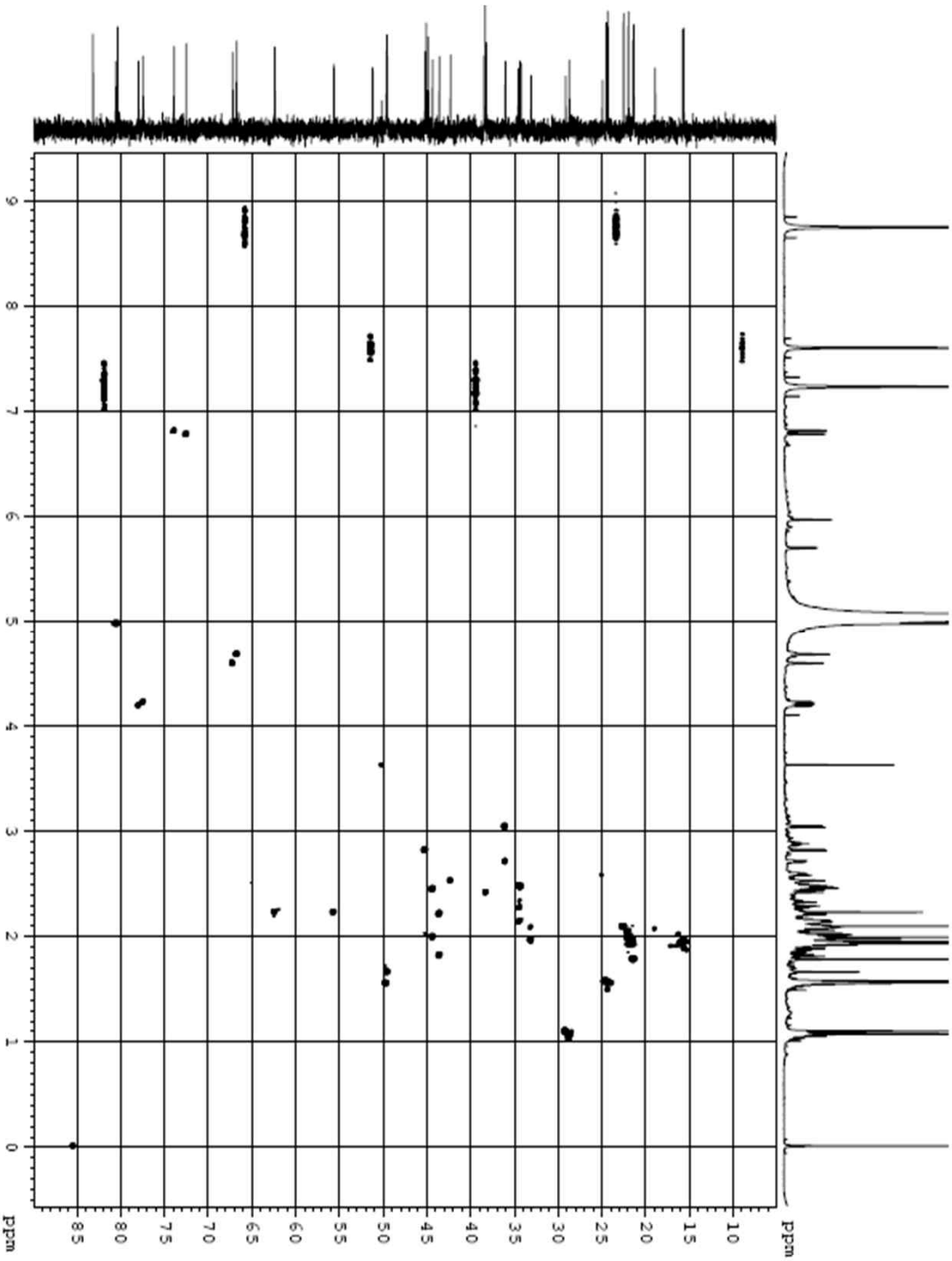


Figure S15. HMBC spectrum (900 MHz, C_5D_5N) of biexcisusin B (**2**)

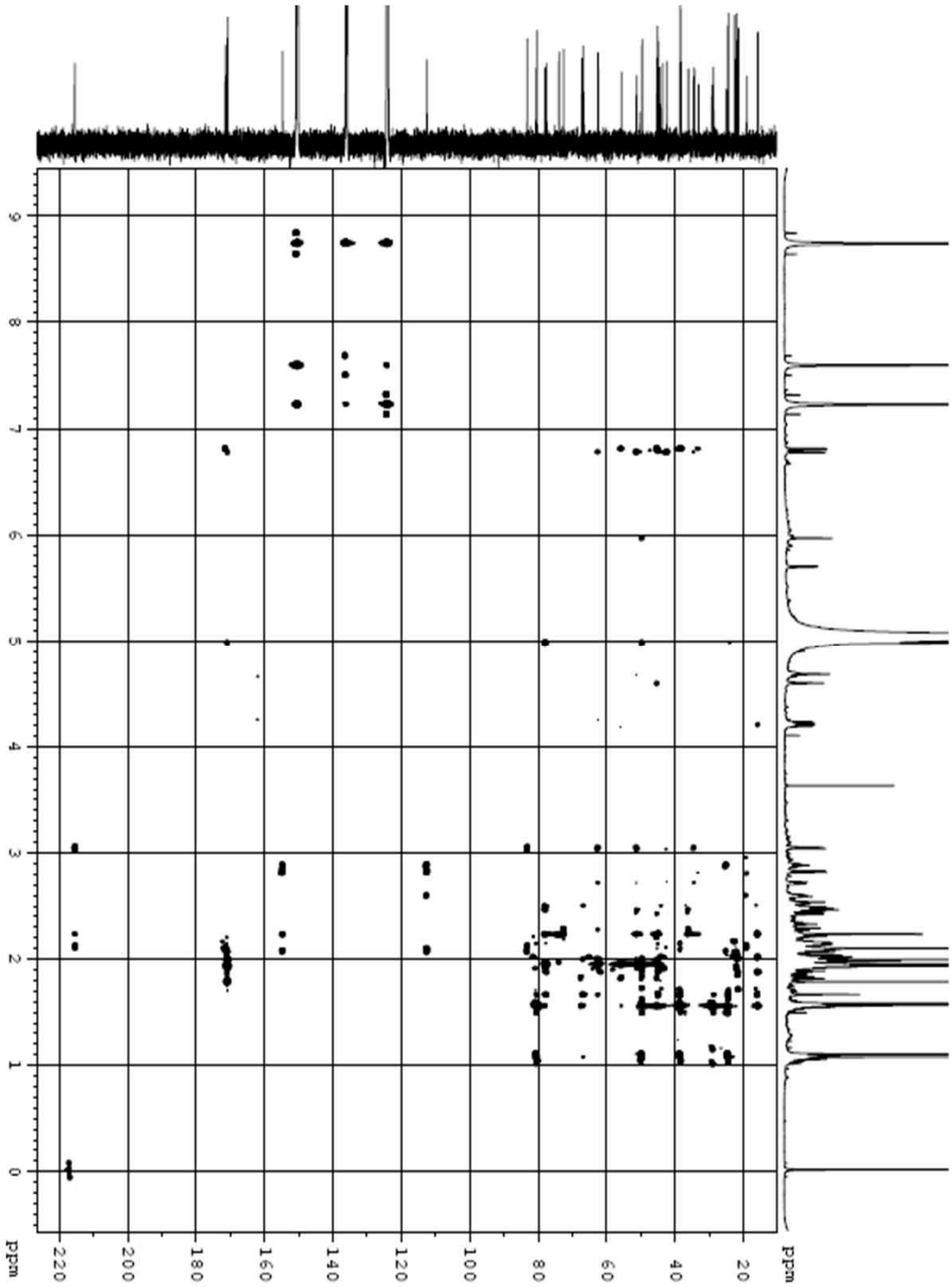


Figure S16. NOESY spectrum (900 MHz, C_5D_5N) of biexcisusin B (**2**)

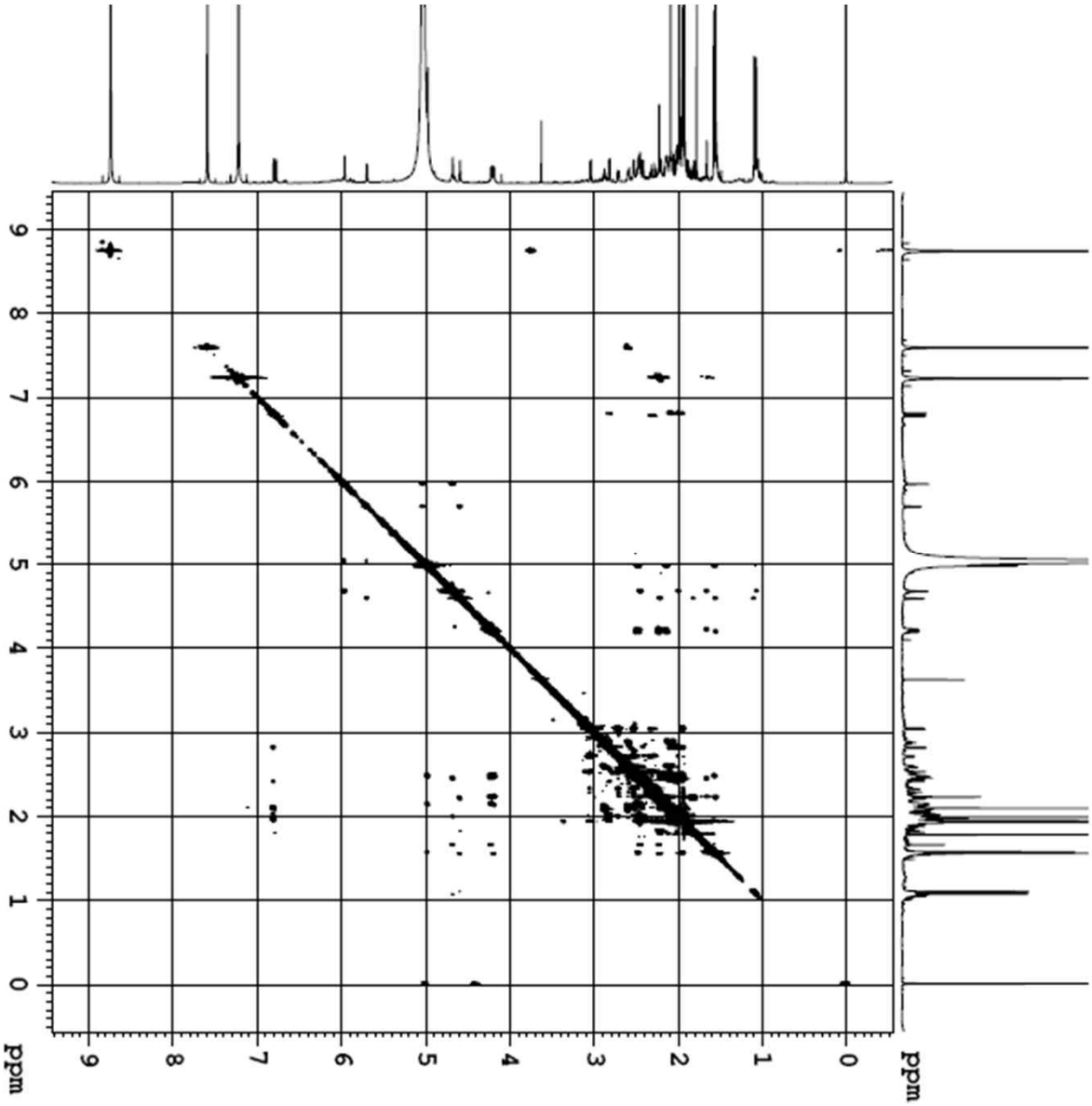


Figure S17. ESIMS spectrum of biexcisusin B (**2**)

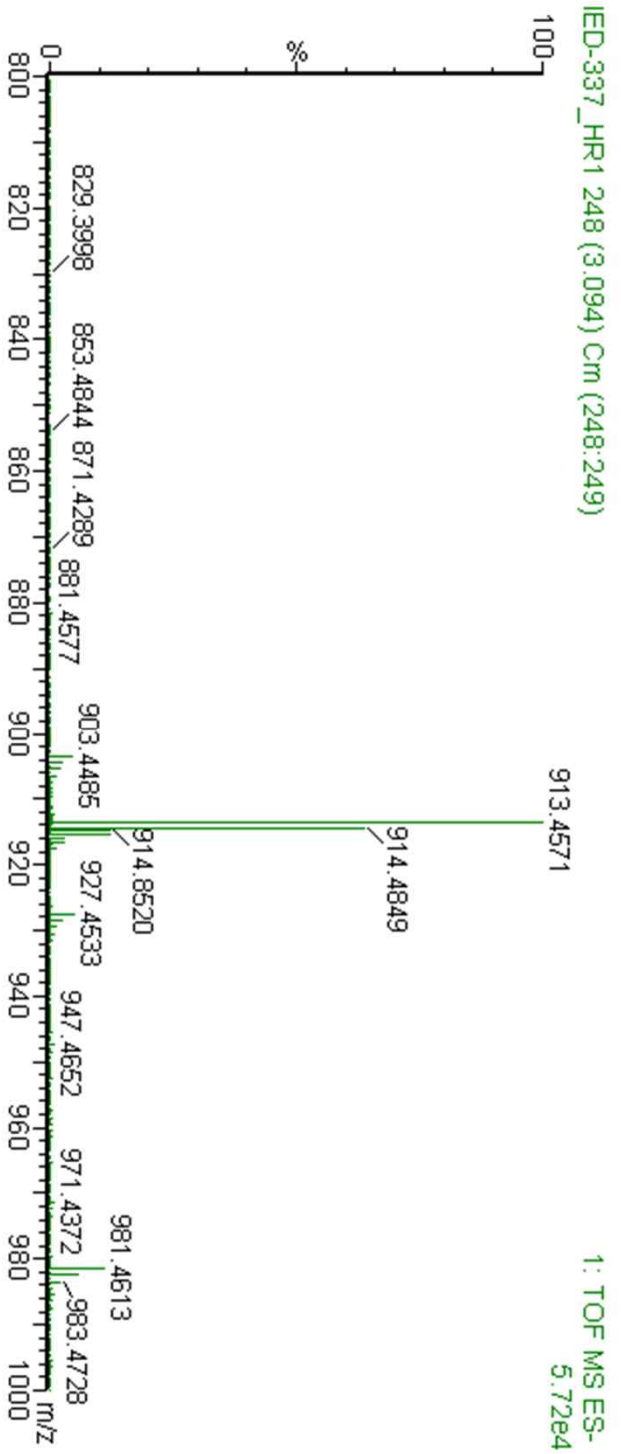


Figure S18. HRESIMS spectrum of biexcisusin B (**2**)

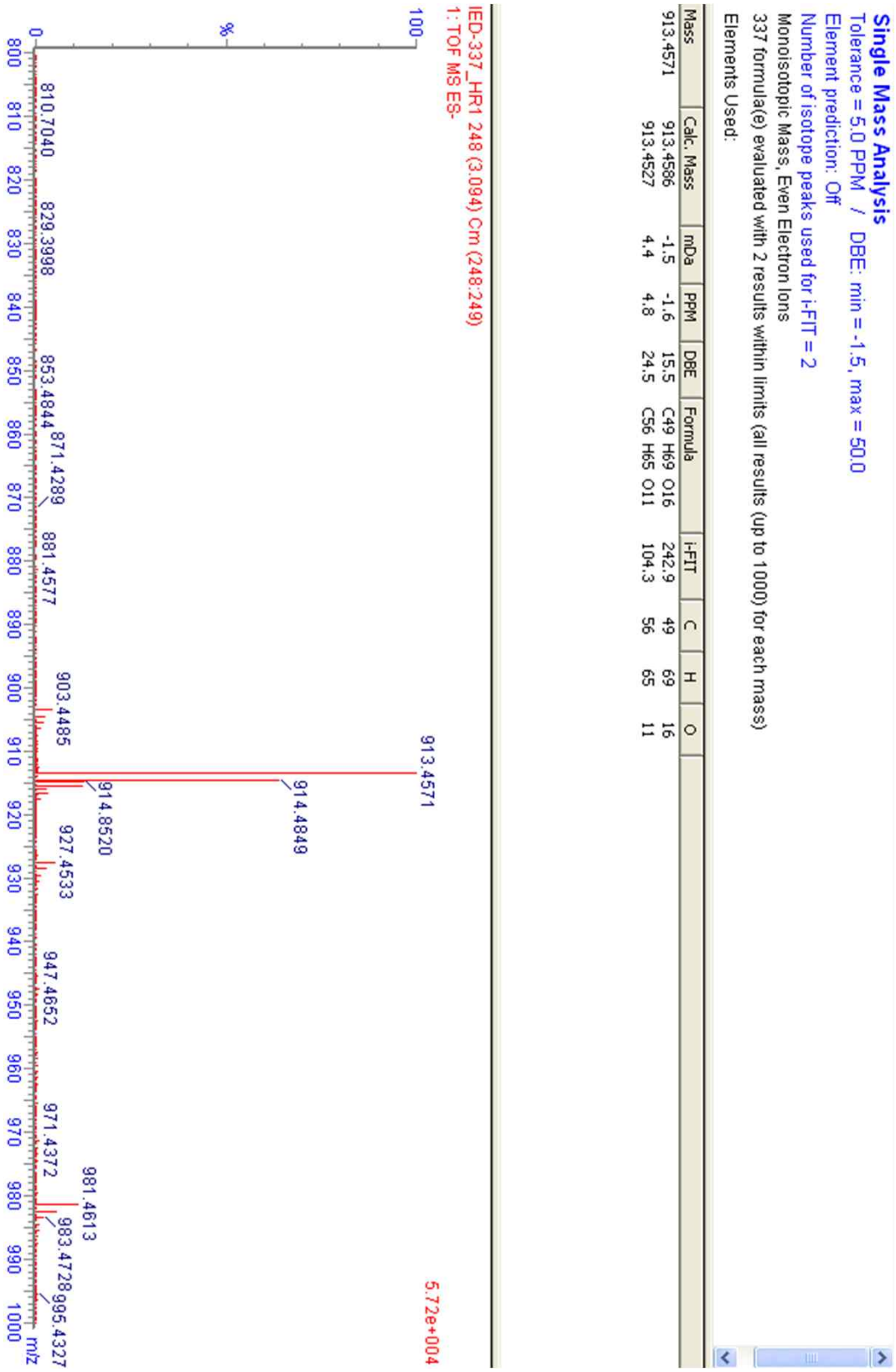


Figure S19. ^{1}H NMR spectrum (900 MHz, C_5D_5N) of bisexcisusin C (**3**)

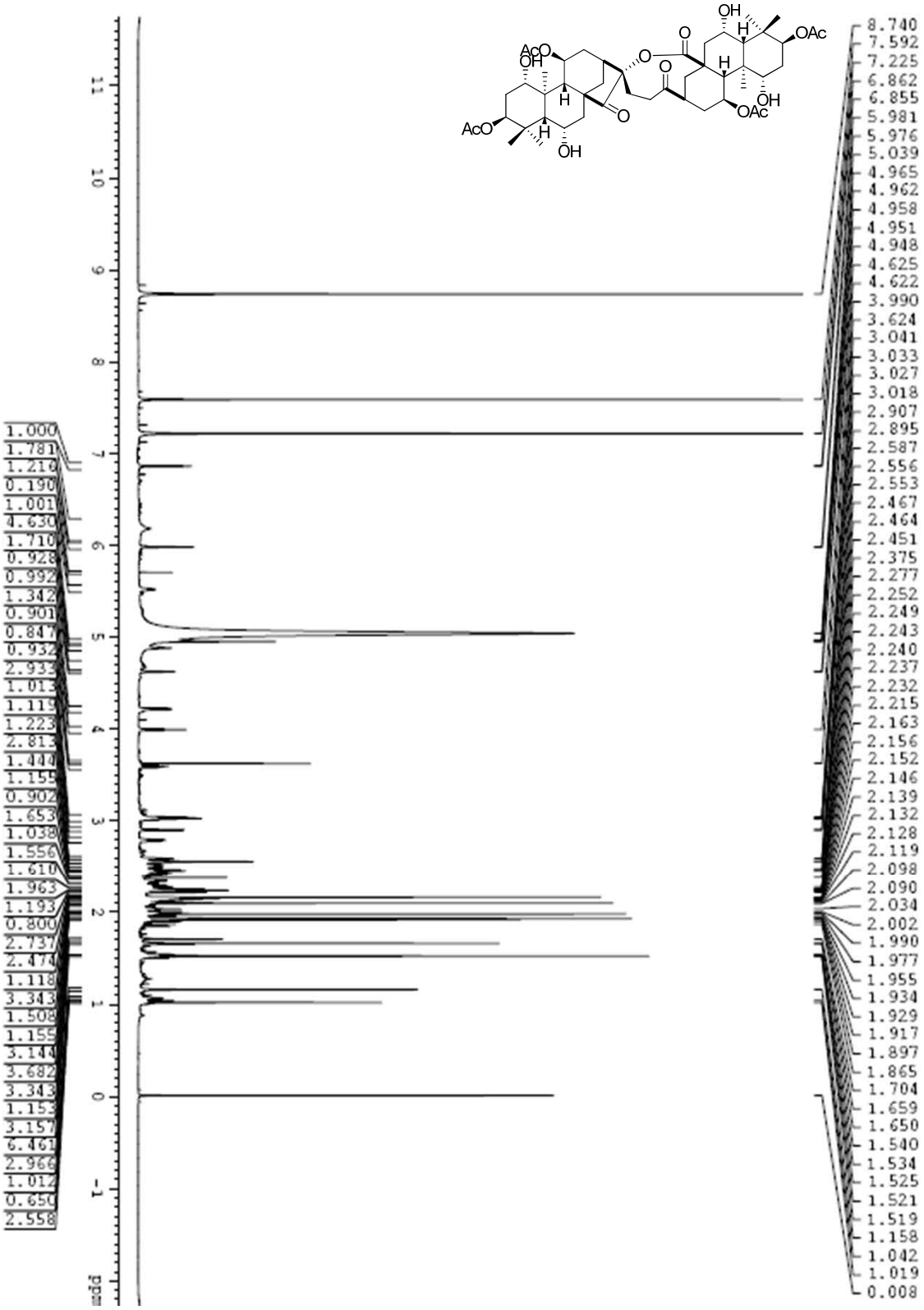


Figure S20. ^{13}C NMR spectrum (225 MHz, C_5D_5N) of biexcisusin C (**3**)

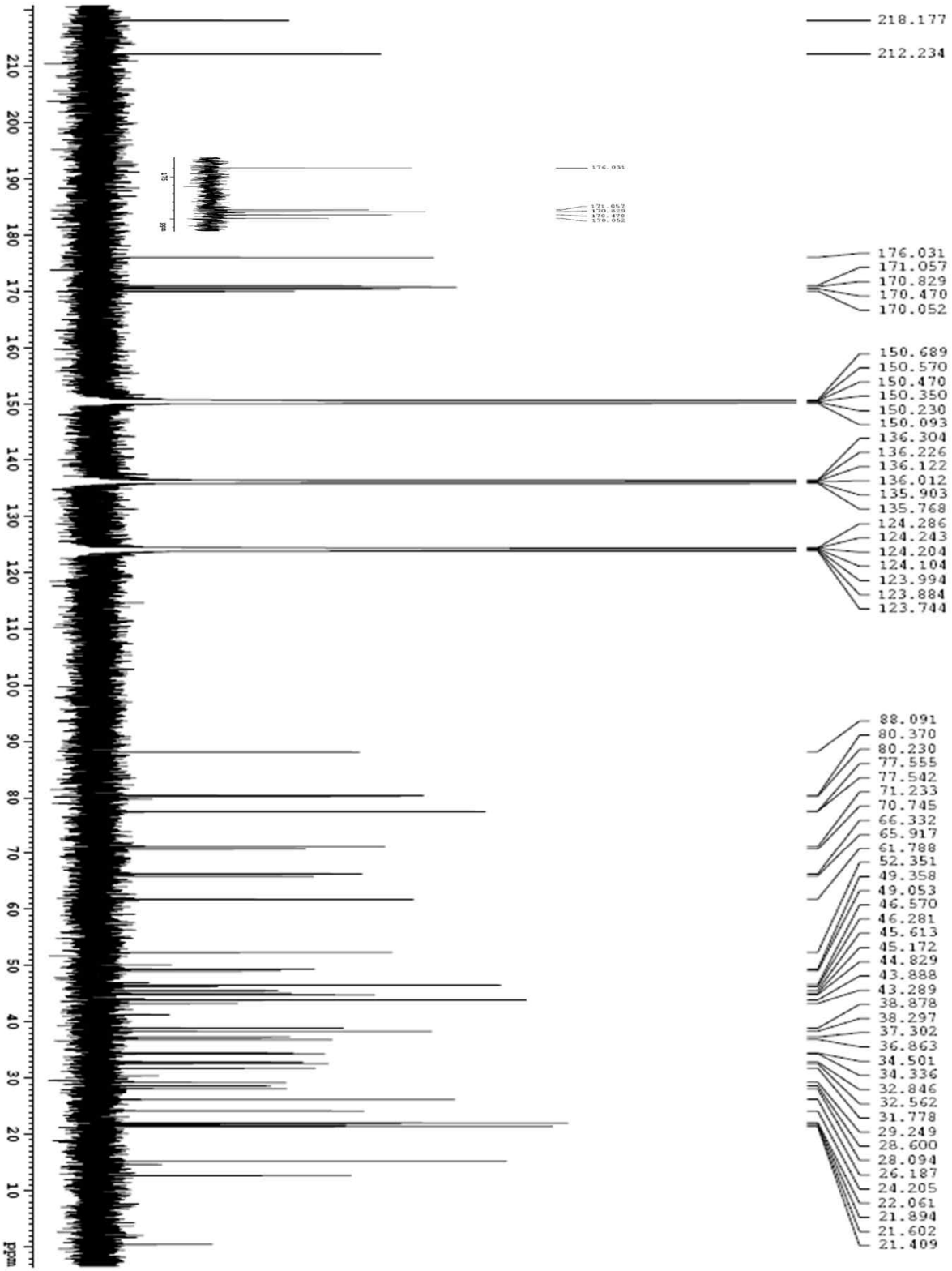


Figure S21. DEPT spectrum (225 MHz, C_5D_5N) of biexcisusin C (**3**)

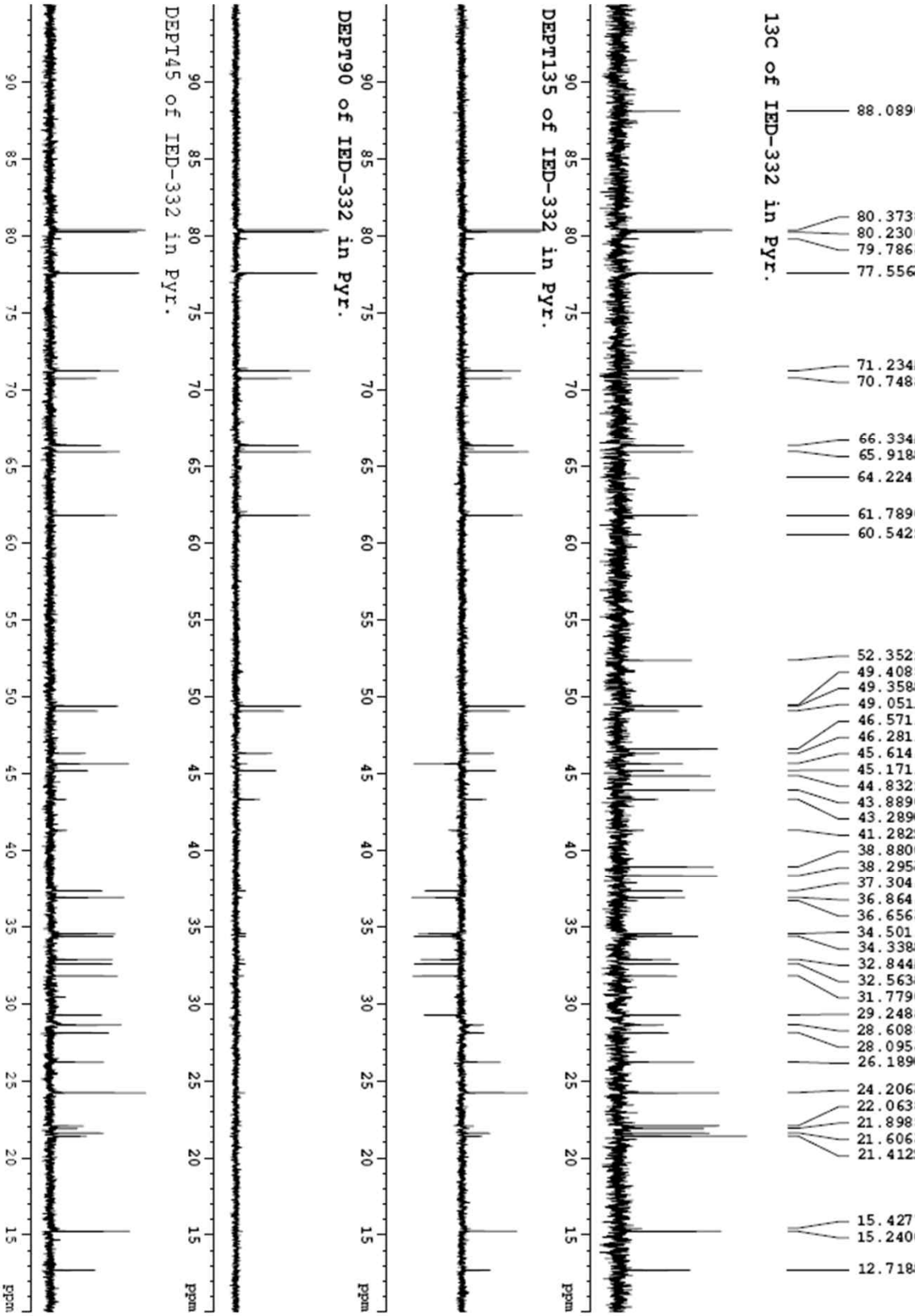


Figure S22. COSY spectrum (900 MHz, C_5D_5N) of biexcisusin C (**3**)

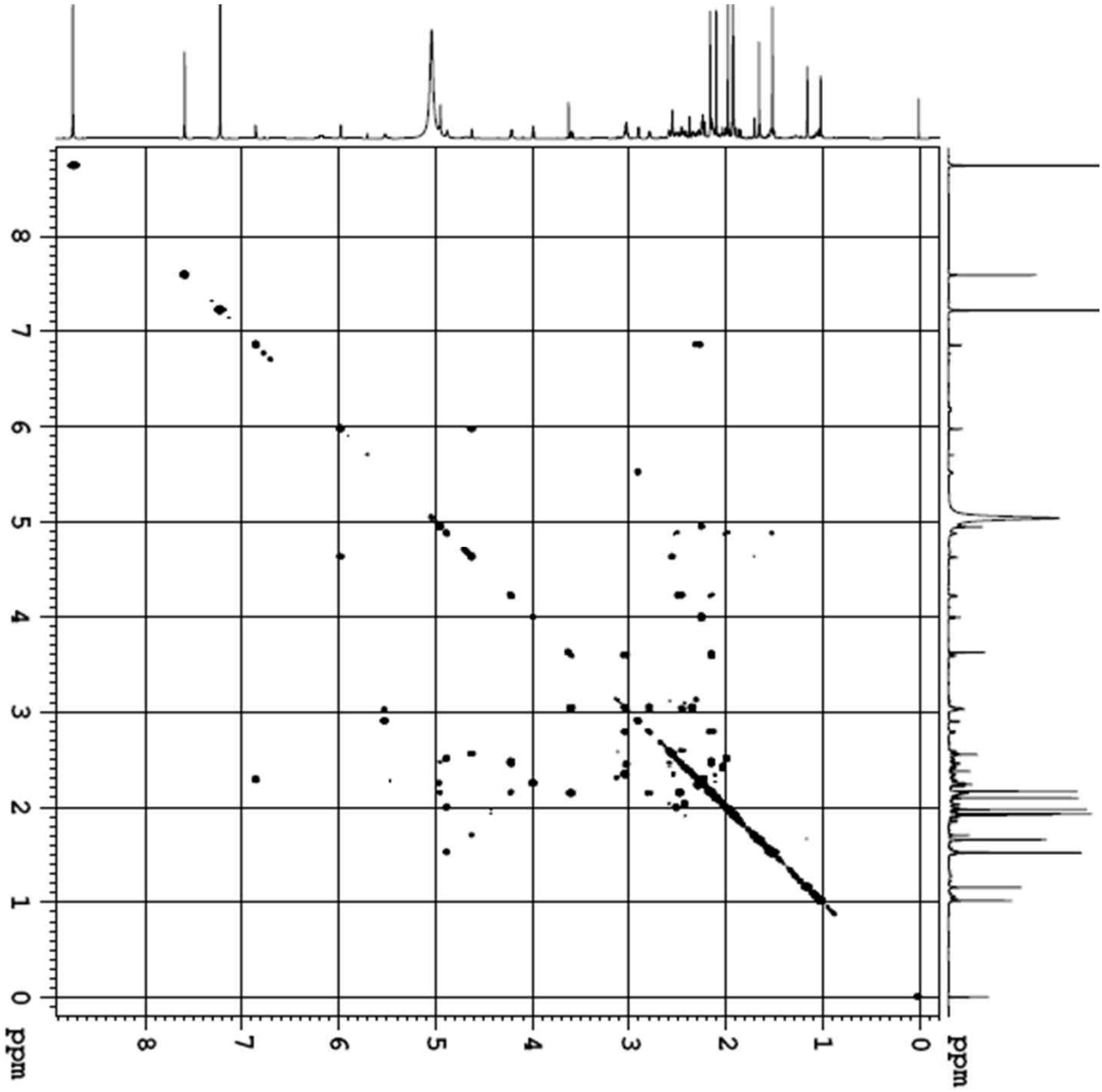


Figure S23. HMQC spectrum (900 MHz, C_5D_5N) of biexcisusin C (**3**)

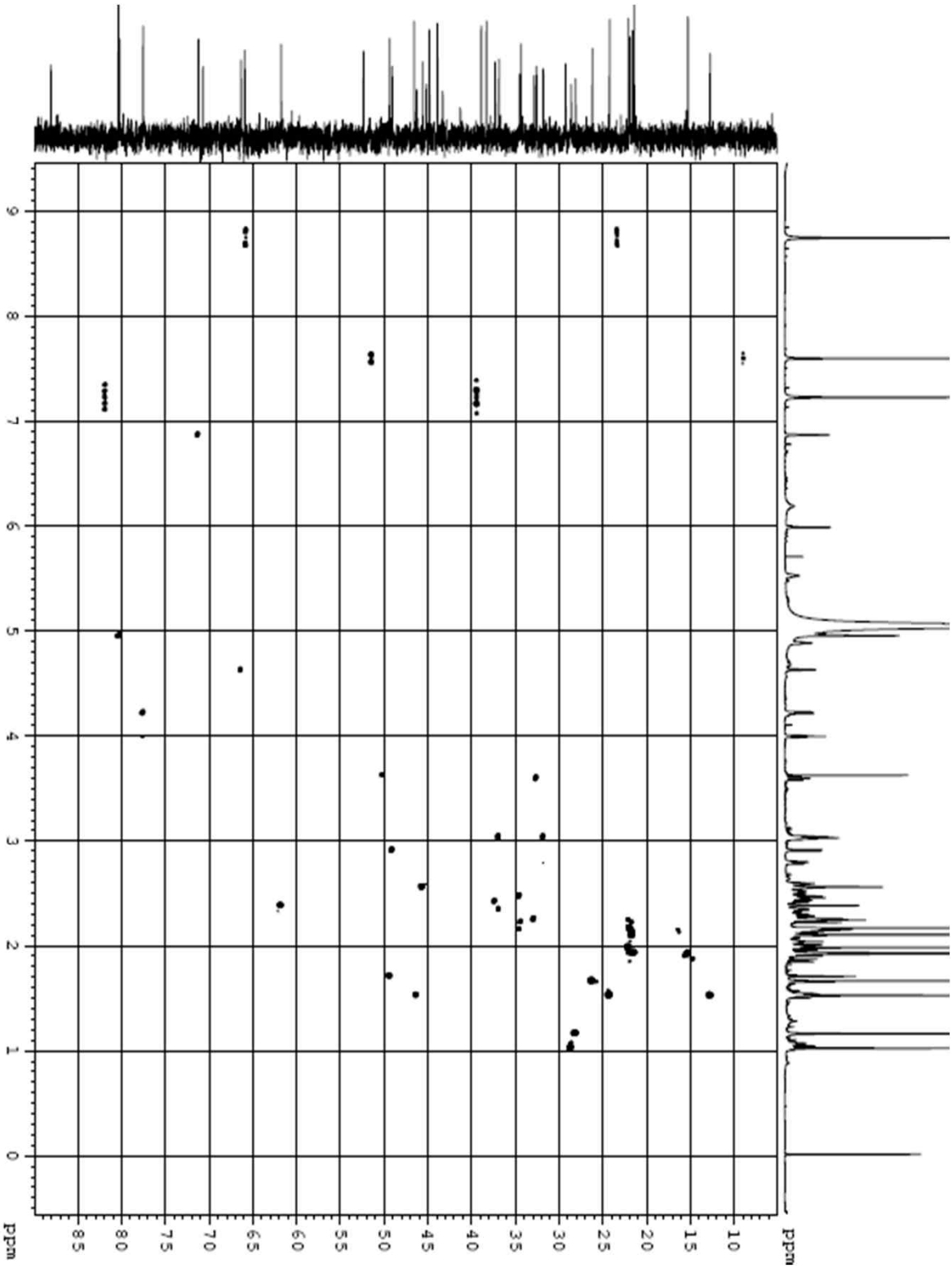


Figure S24. HMBC spectrum (900 MHz, C_5D_5N) of biexcisusin C (**3**)

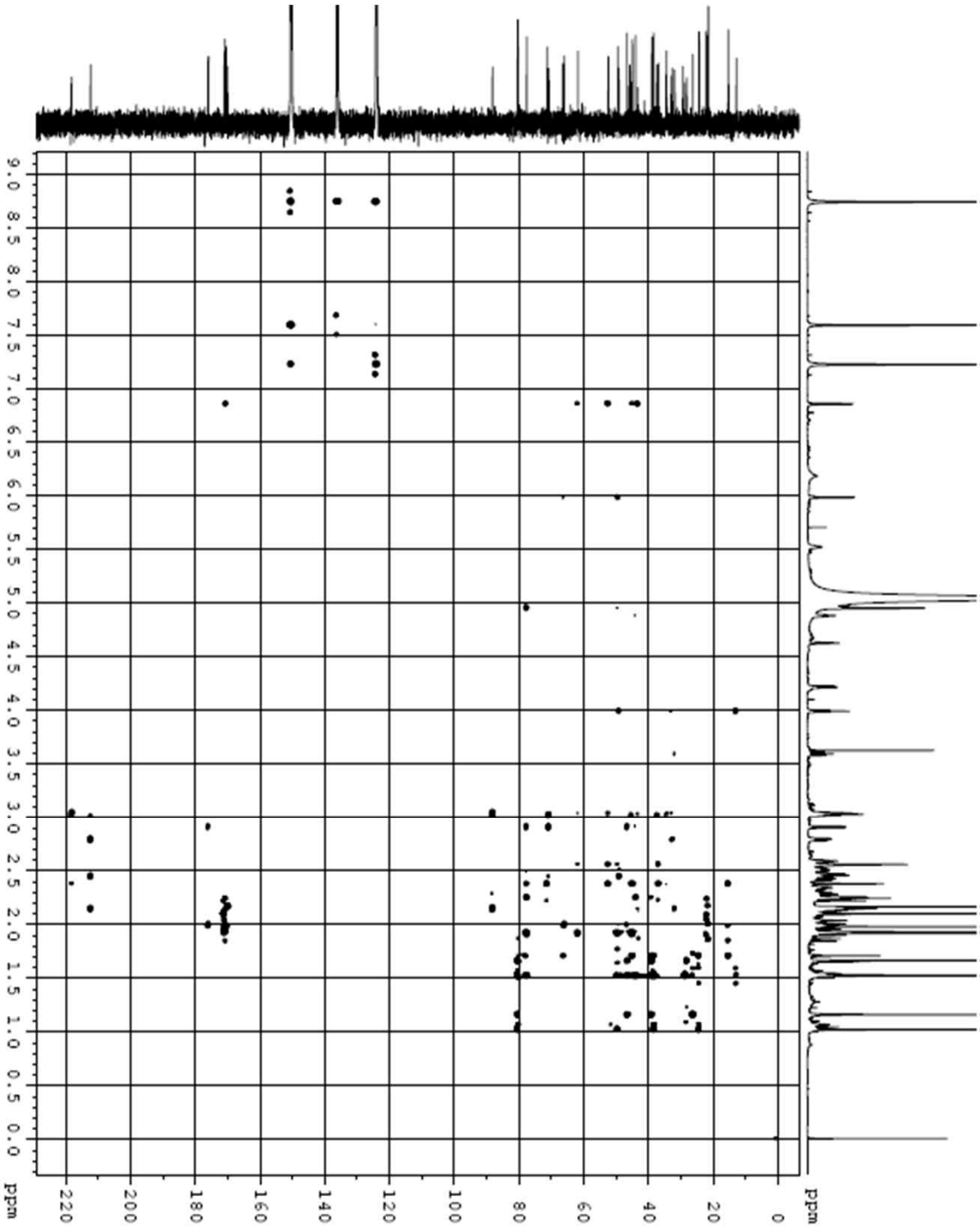


Figure S25. NOESY spectrum (900 MHz, C_5D_5N) of biexcisusin C (**3**)

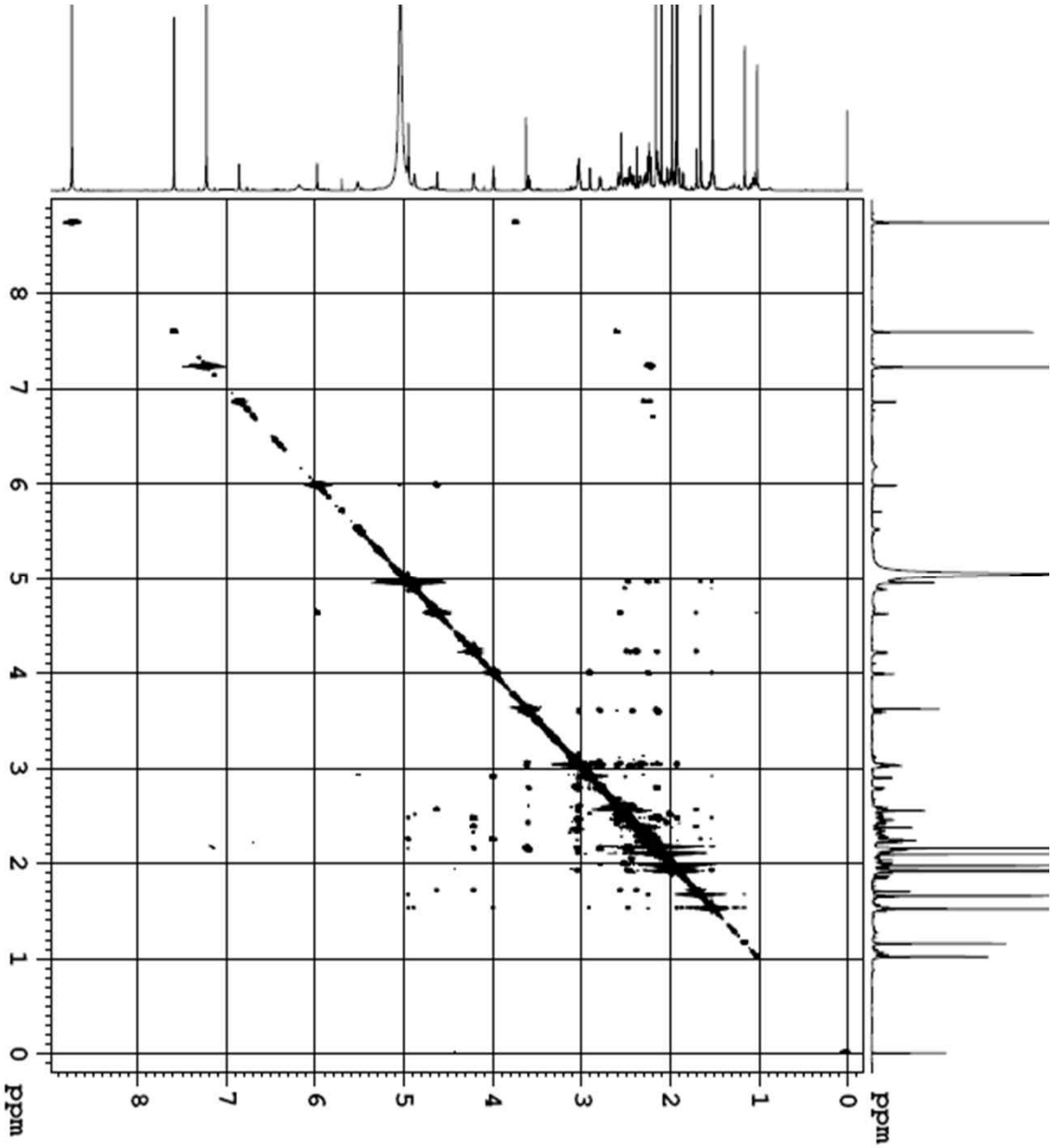


Figure S26. ESIMS spectrum of biexcisusin C (**3**)

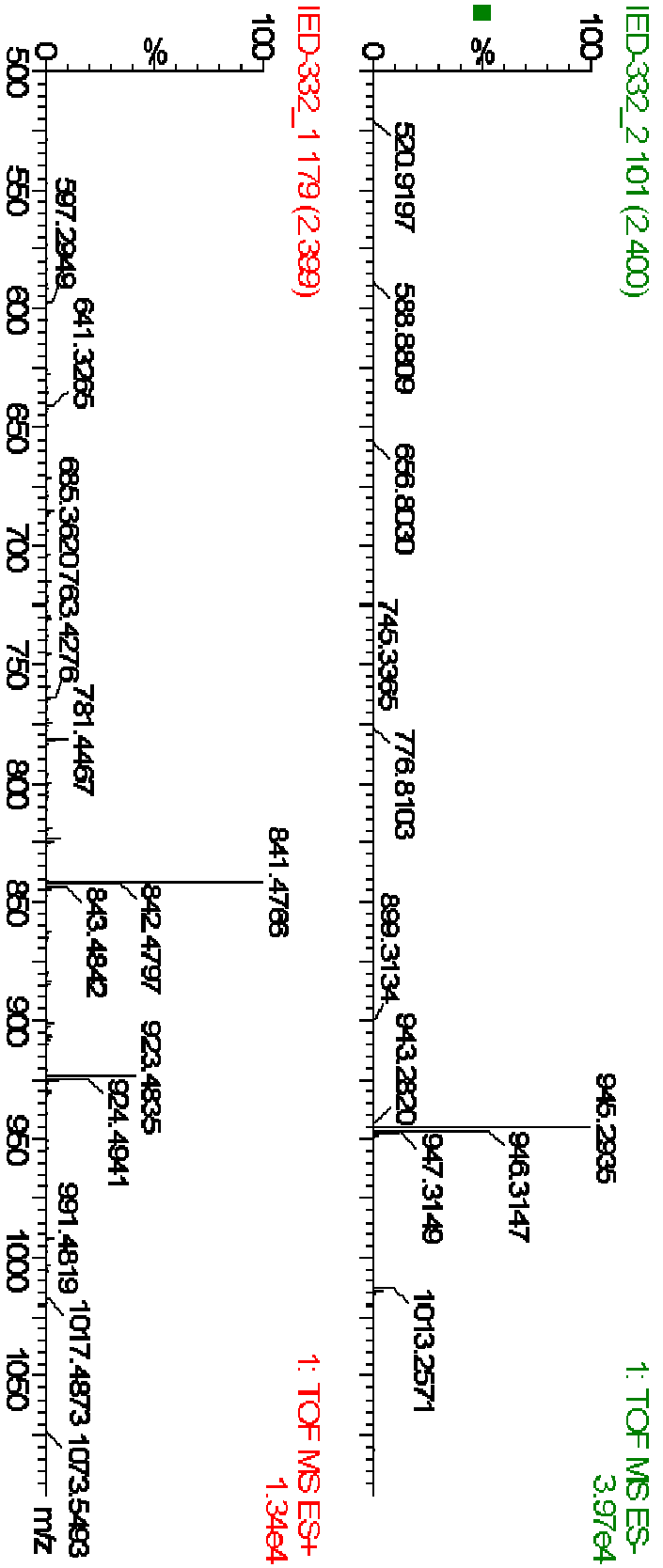
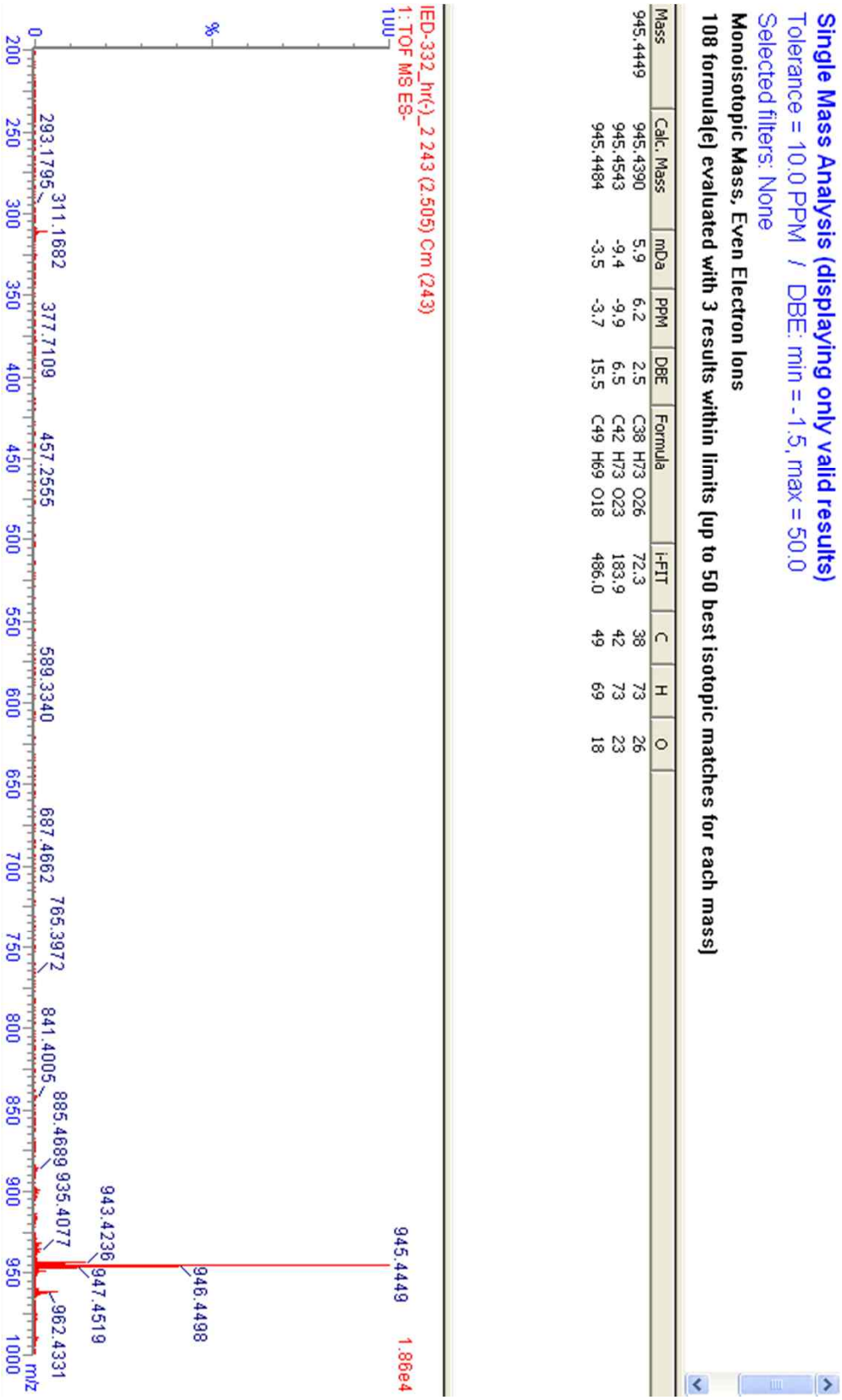


Figure S27. HRESIMS spectrum of biexcisusin C (**3**)



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	C38 H73 O26	72.3	38	73	26
	945.4543	-9.4	-9.9	6.5	C42 H73 O23	183.9	42	73	23
	945.4484	-3.5	-3.7	15.5	C49 H69 O18	486.0	49	69	18

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

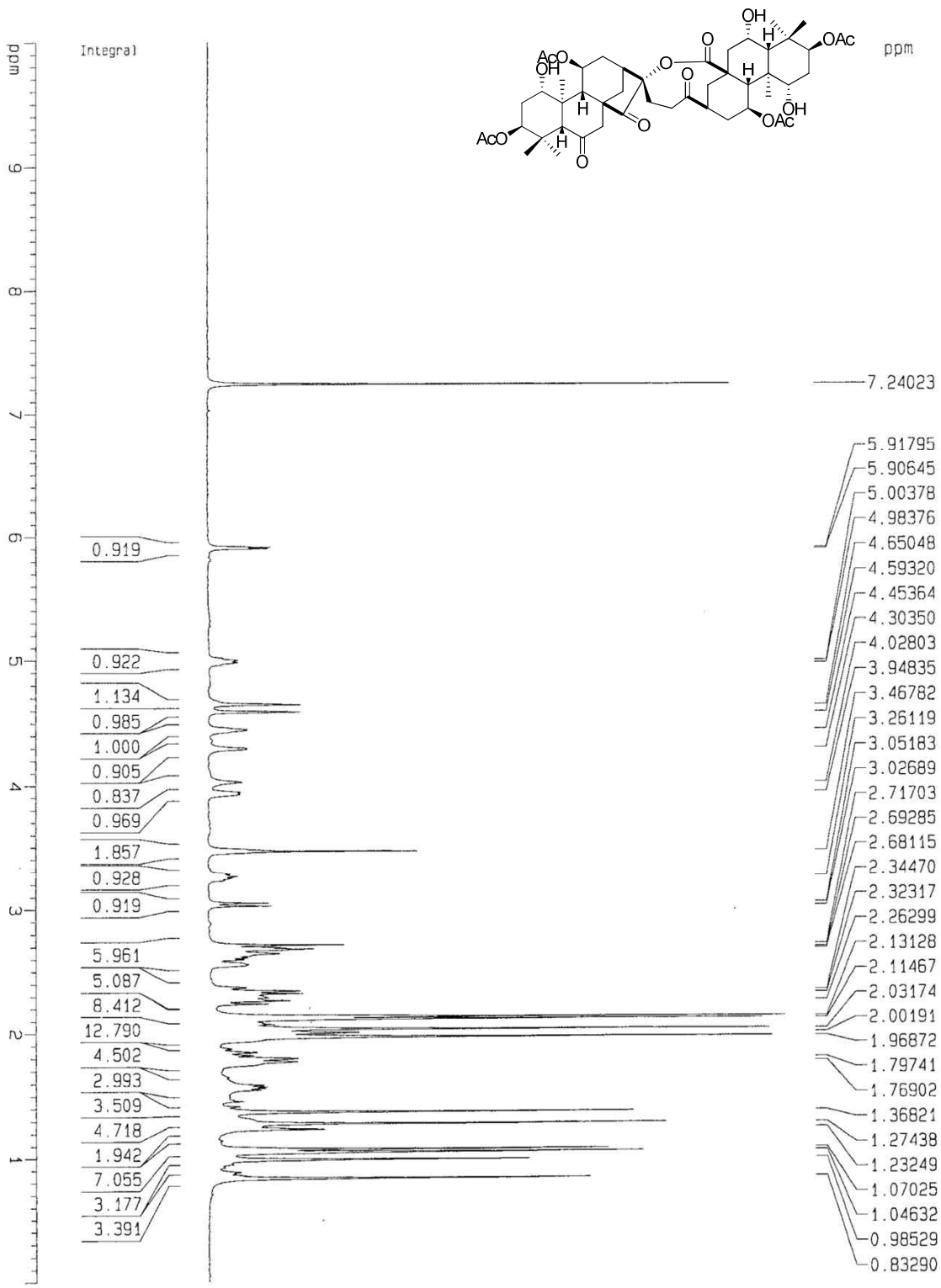


Figure S29. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of biexcisusin D (**4**)

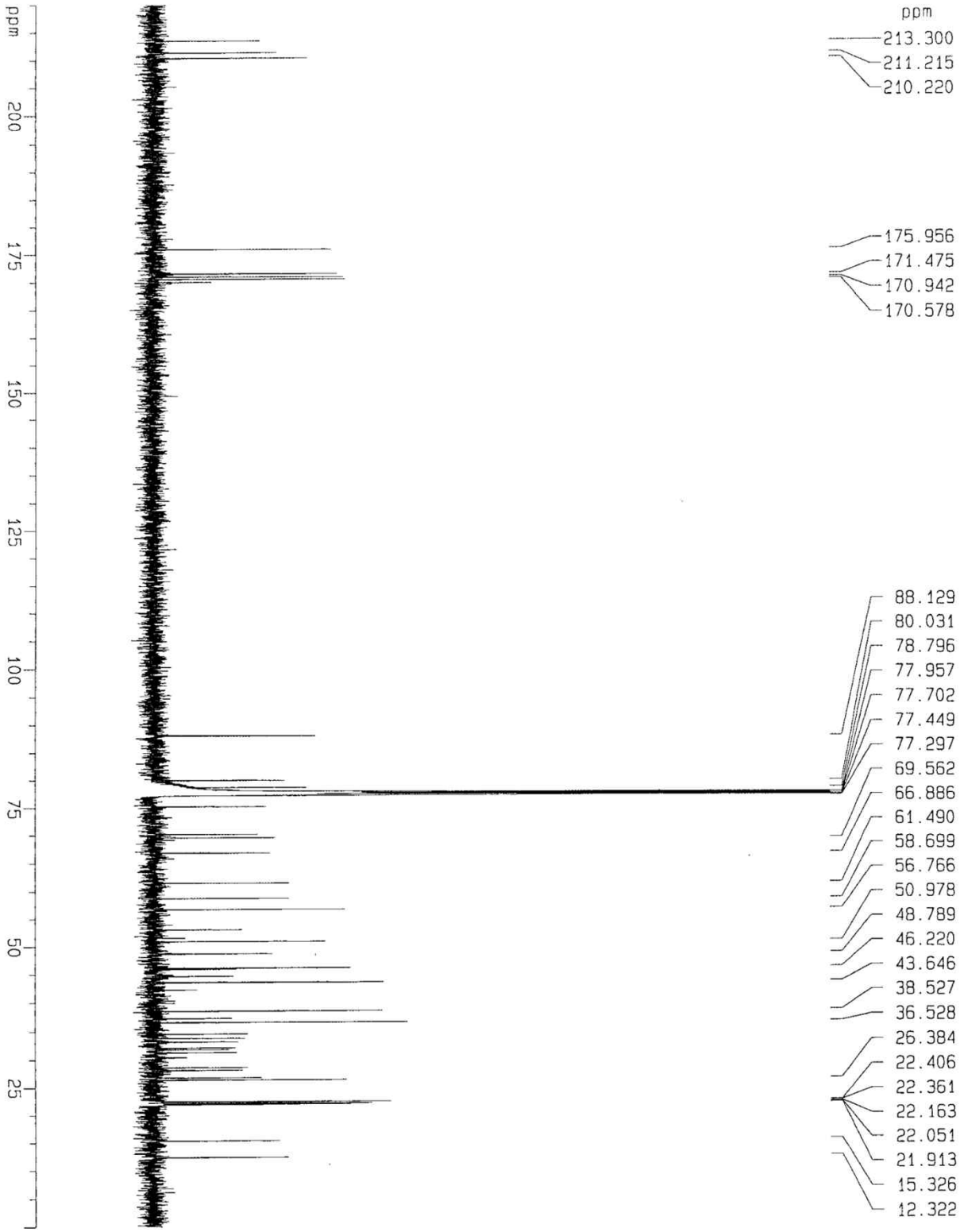


Figure S30. DEPT spectrum (500 MHz, $CDCl_3$) of biexcisusin D (**4**)

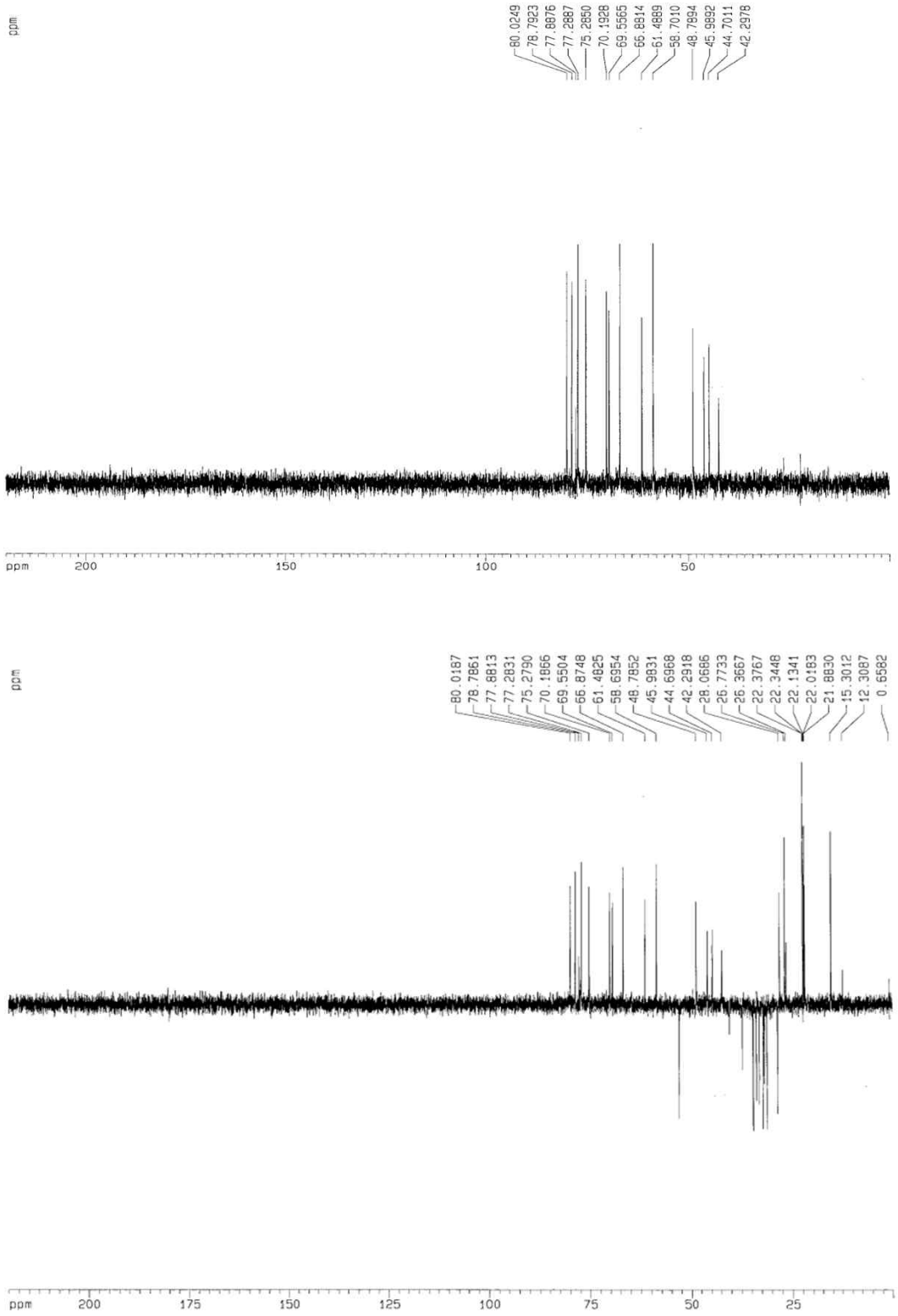


Figure S31. HMQC spectrum (500 MHz, $CDCl_3$) of biexcisusin D (**4**)

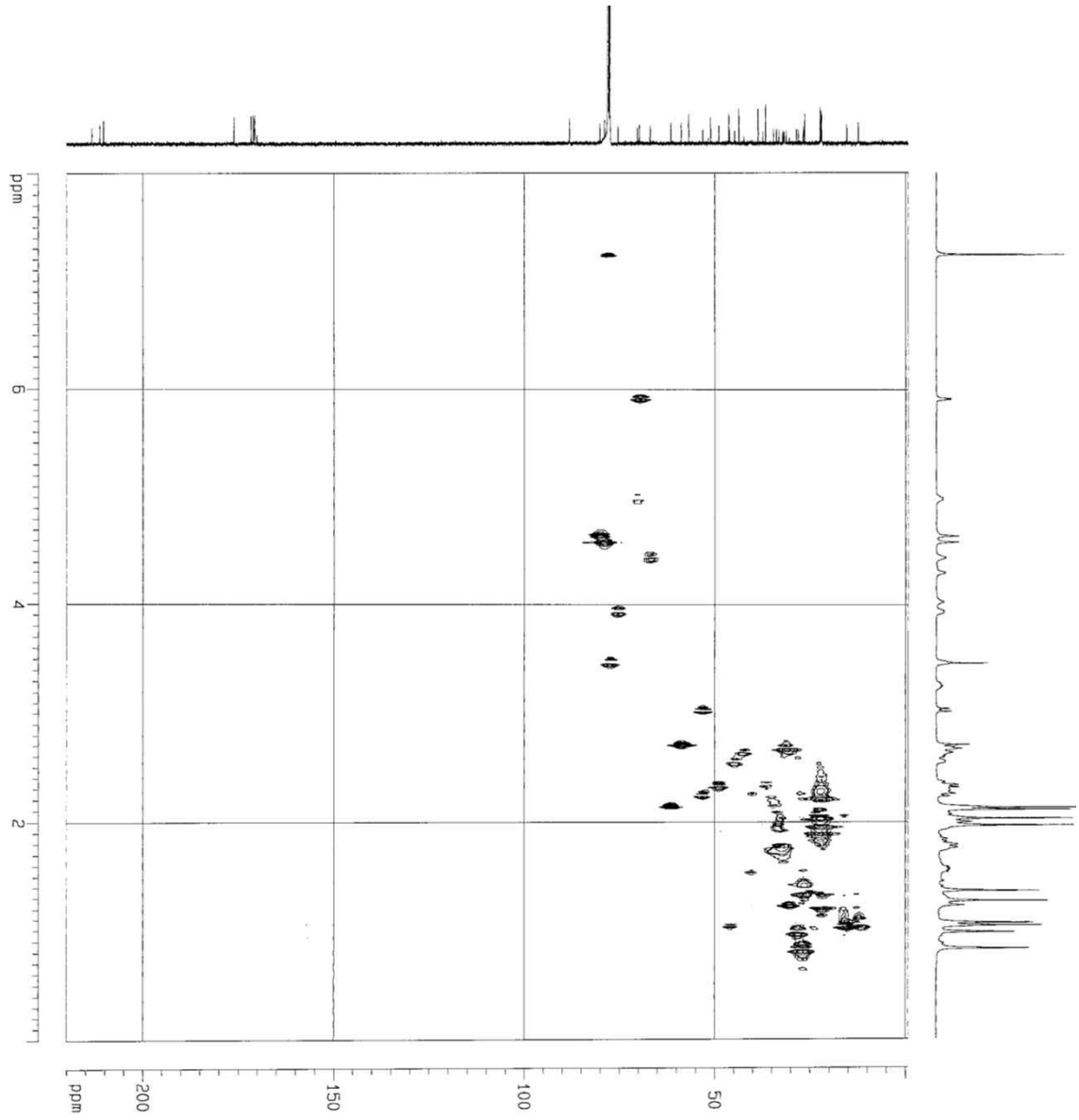


Figure S32. HMBC spectrum (500 MHz, $CDCl_3$) of biexcisusin D (**4**)

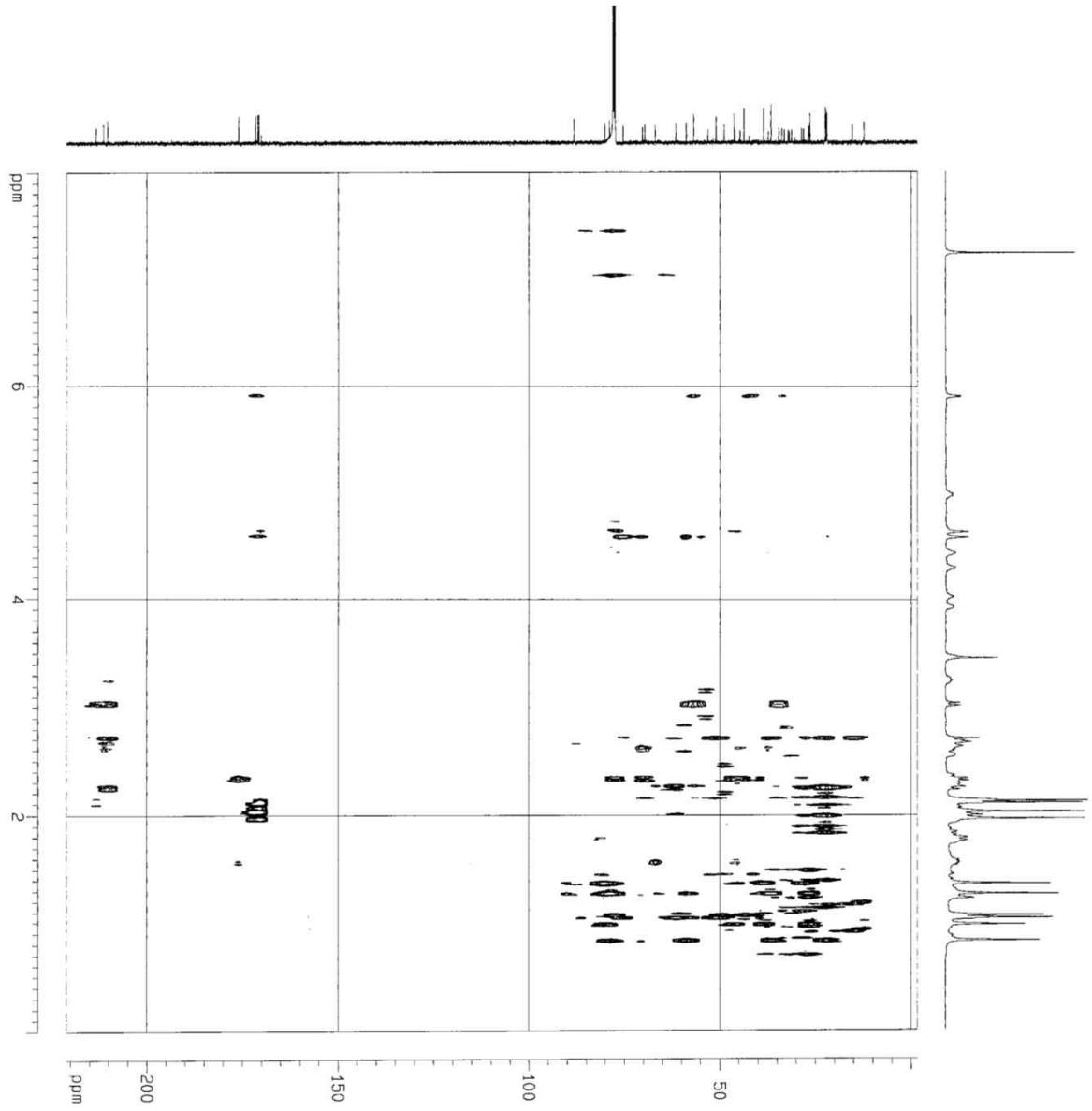


Figure S33. ESIMS spectrum of bi7excisusin D (**4**)

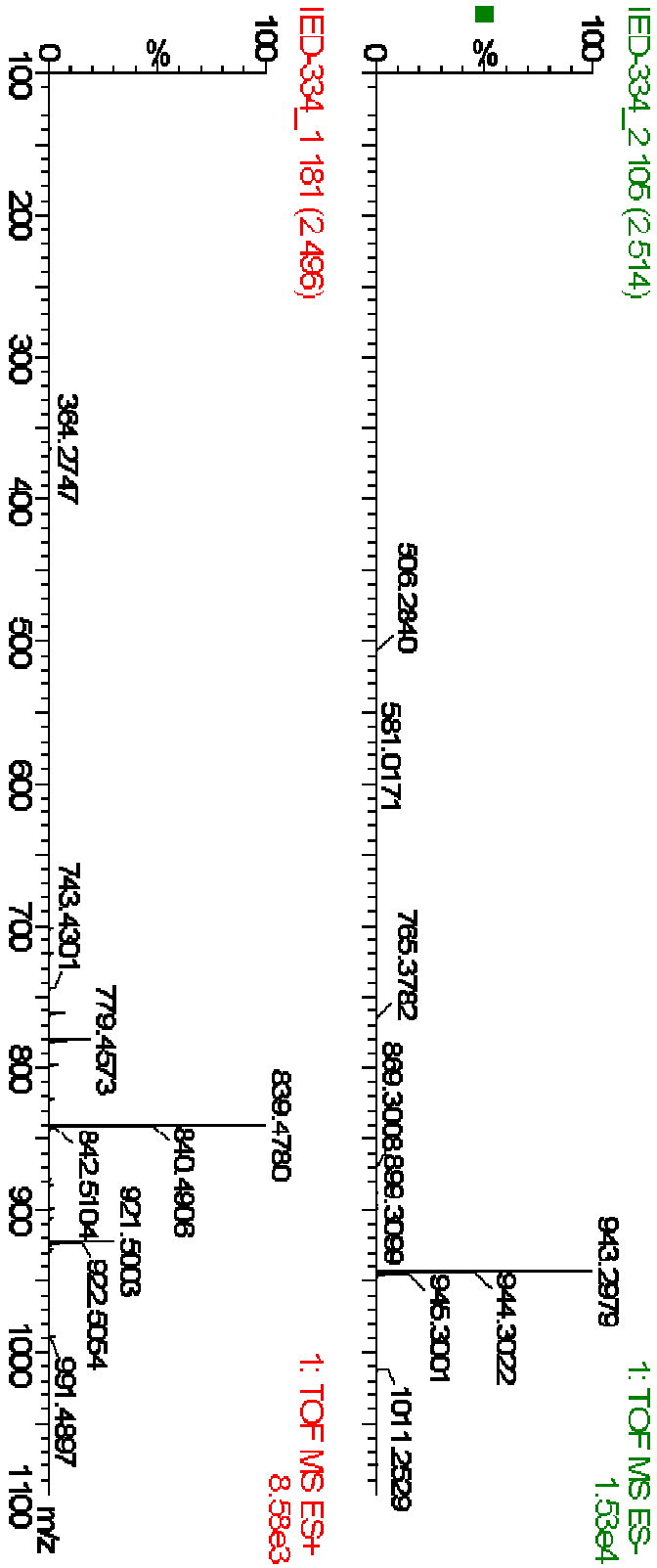


Figure S34. HRESIMS spectrum of biexcisusin D (**4**)

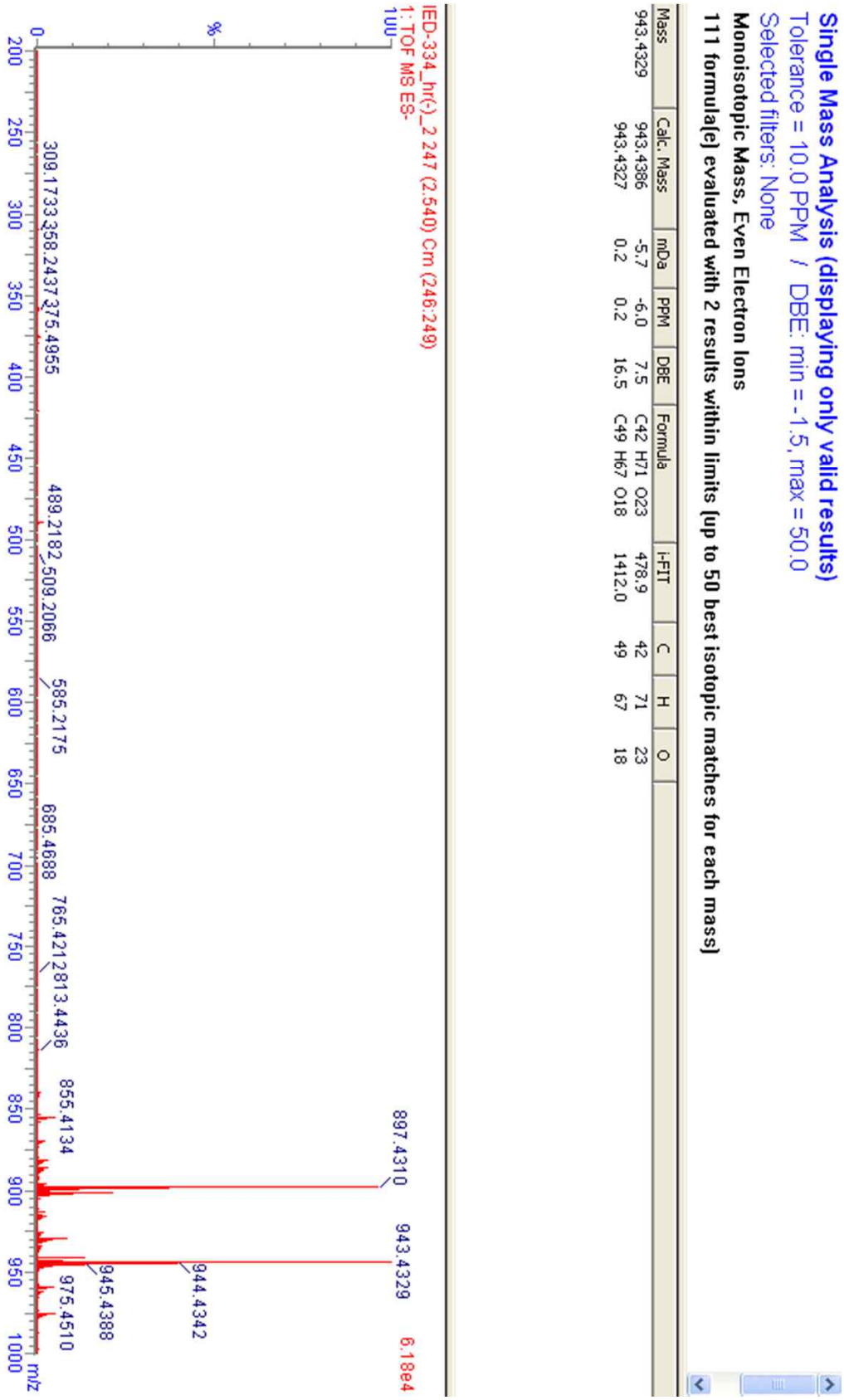


Figure S35. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of biexcisusin E (**5**)

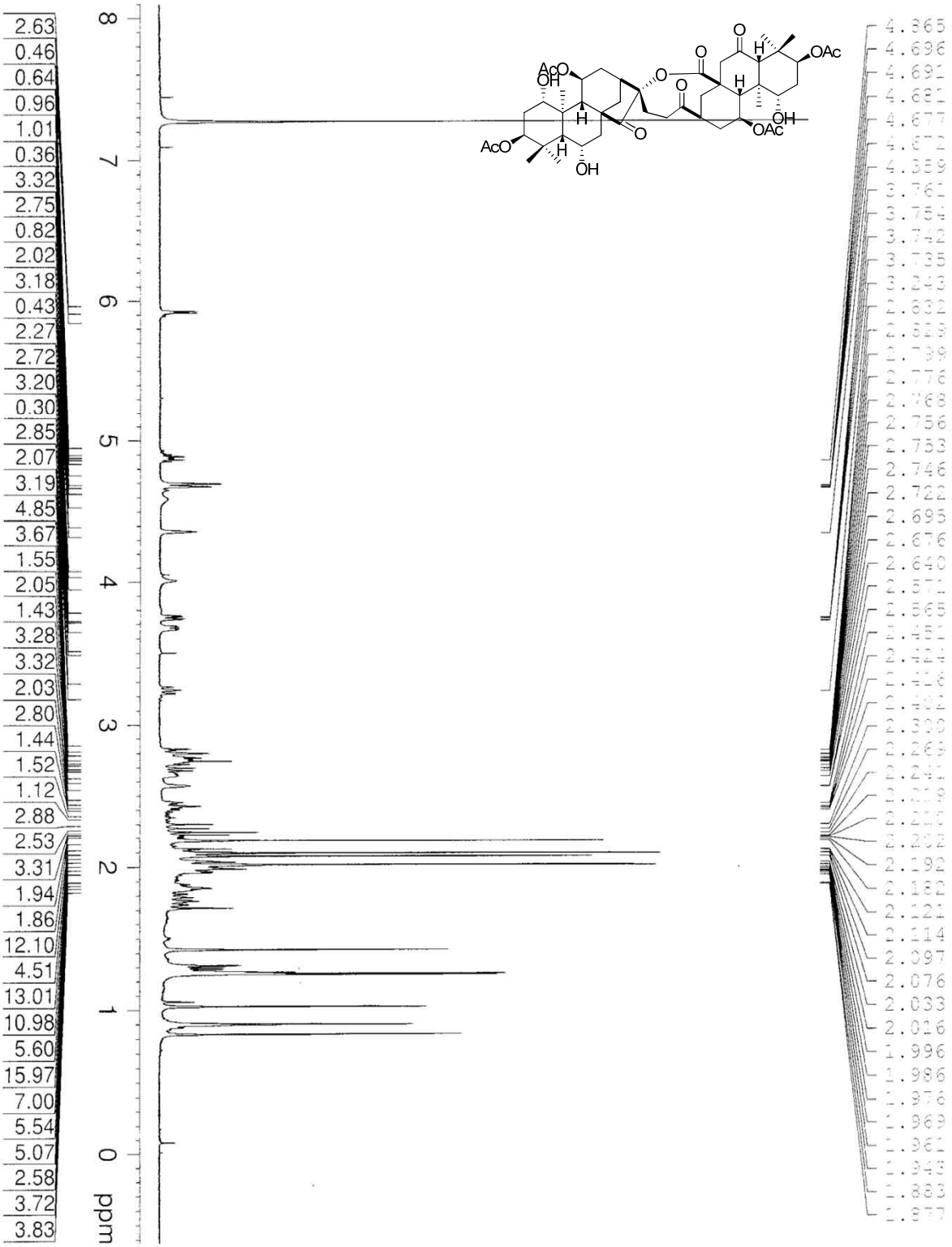


Figure S36. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of biexcisusin E (**5**)

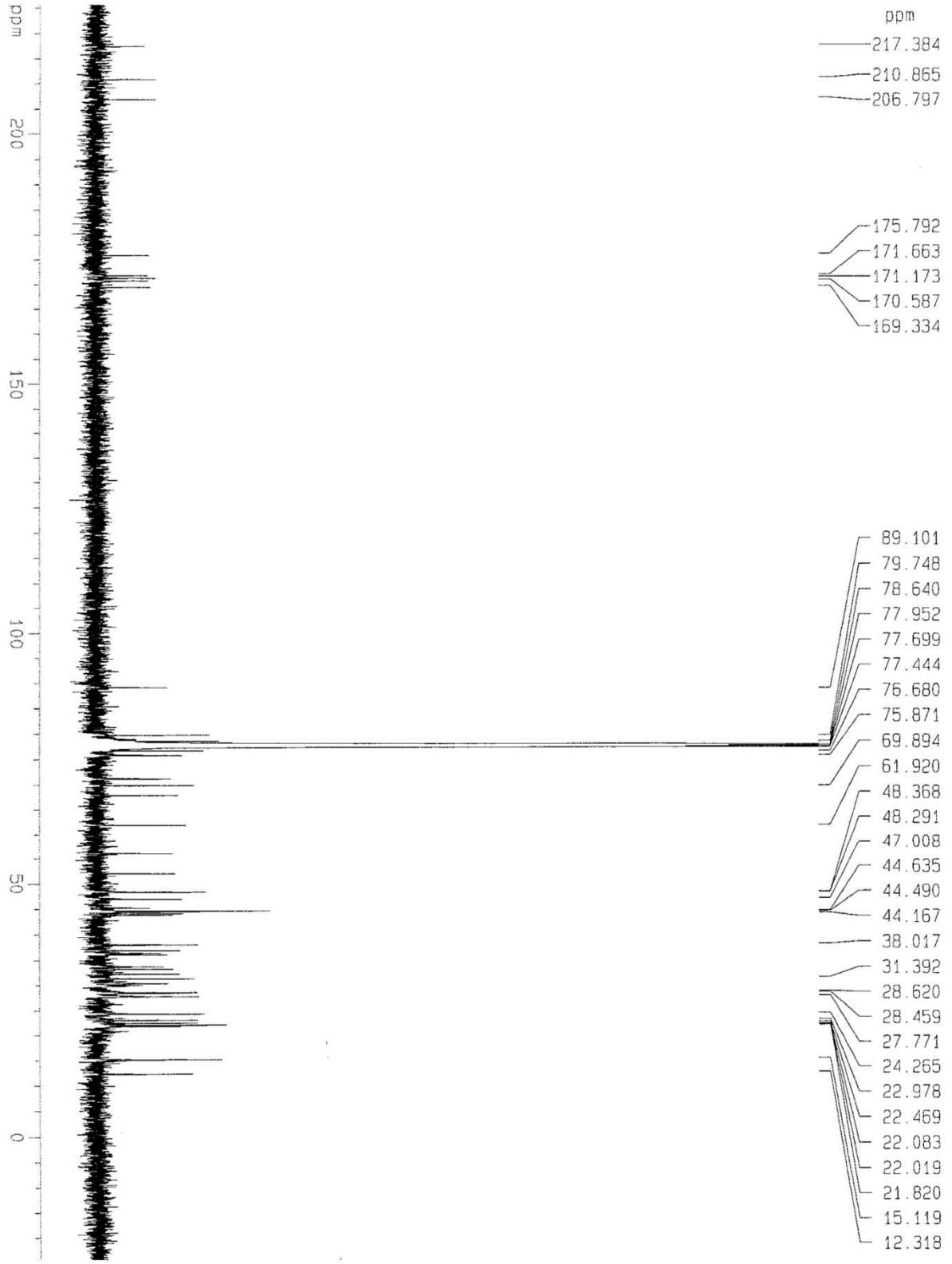


Figure S37. DEPT spectrum (125 MHz, $CDCl_3$) of biexcisusin E (**5**)

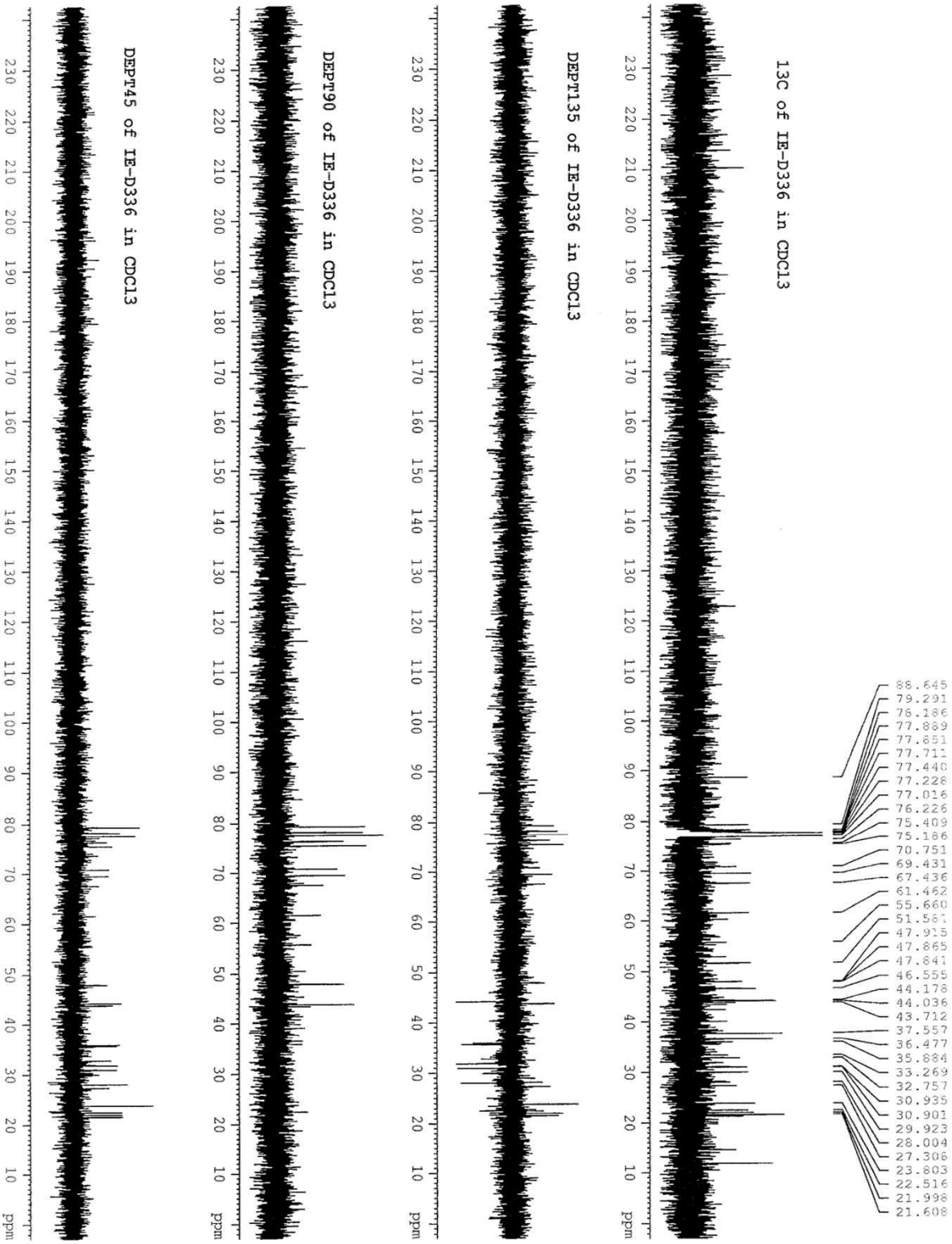


Figure S38. HMQC spectrum (500 MHz, $CDCl_3$) of biexcisusin E (**5**)

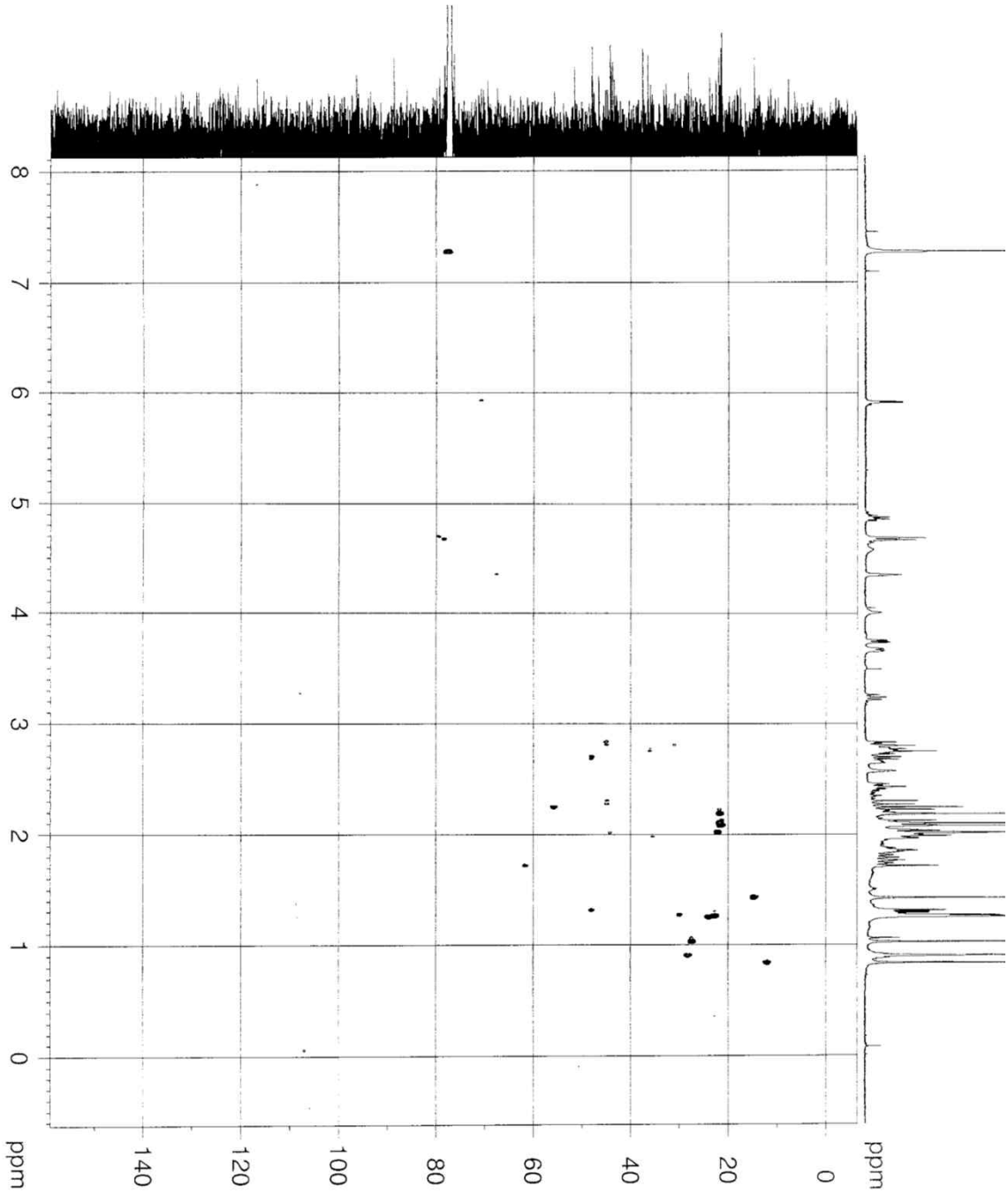


Figure S39. HMBC spectrum (500 MHz, $CDCl_3$) of biexcisusin E (**5**)

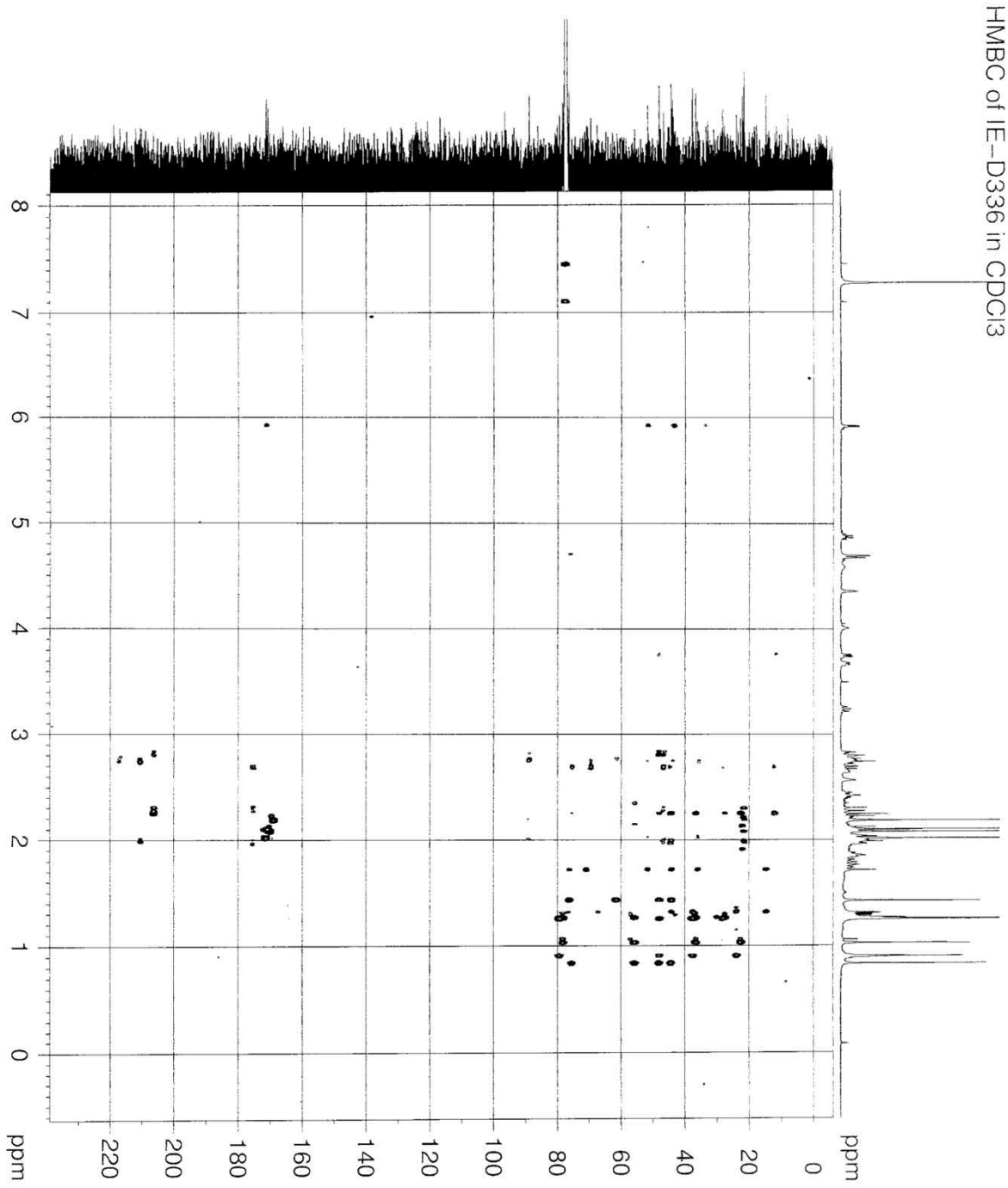


Figure S40. ESIMS spectrum of biexcisusin E (**5**)

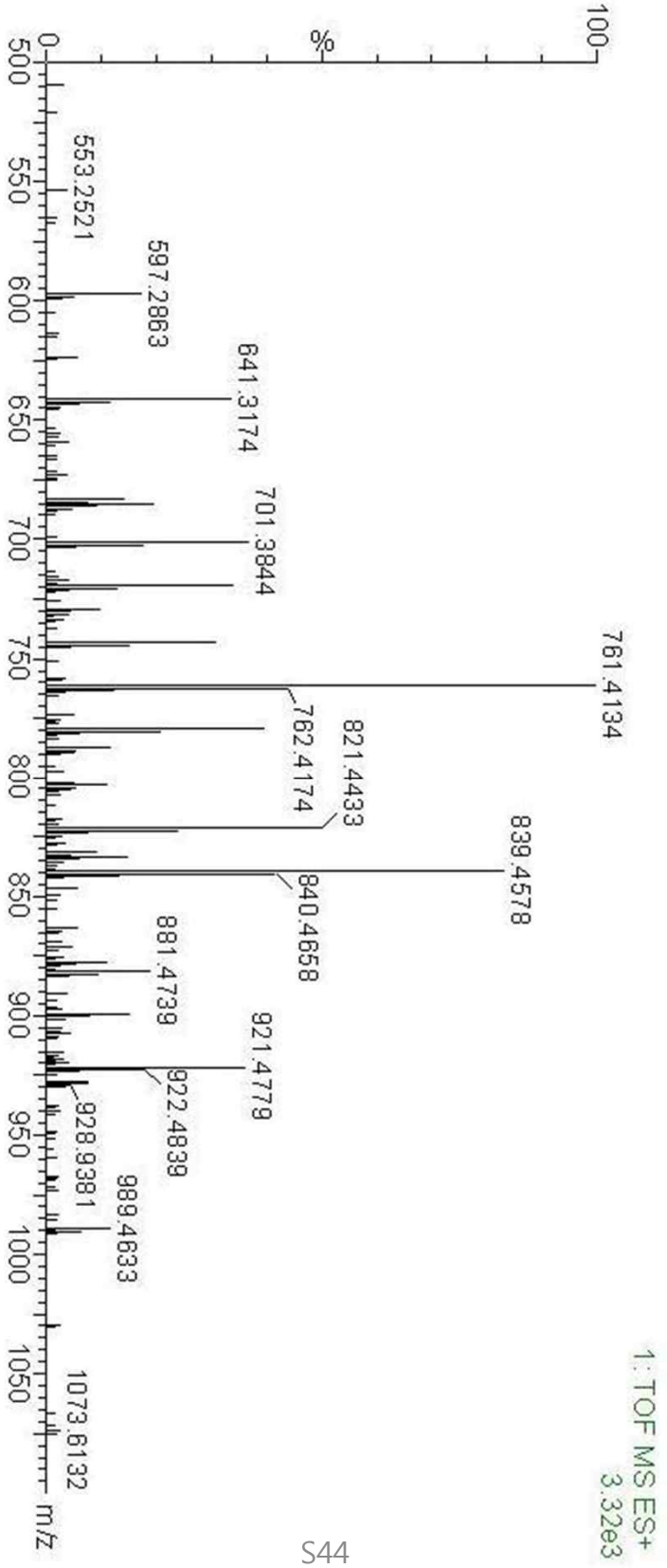
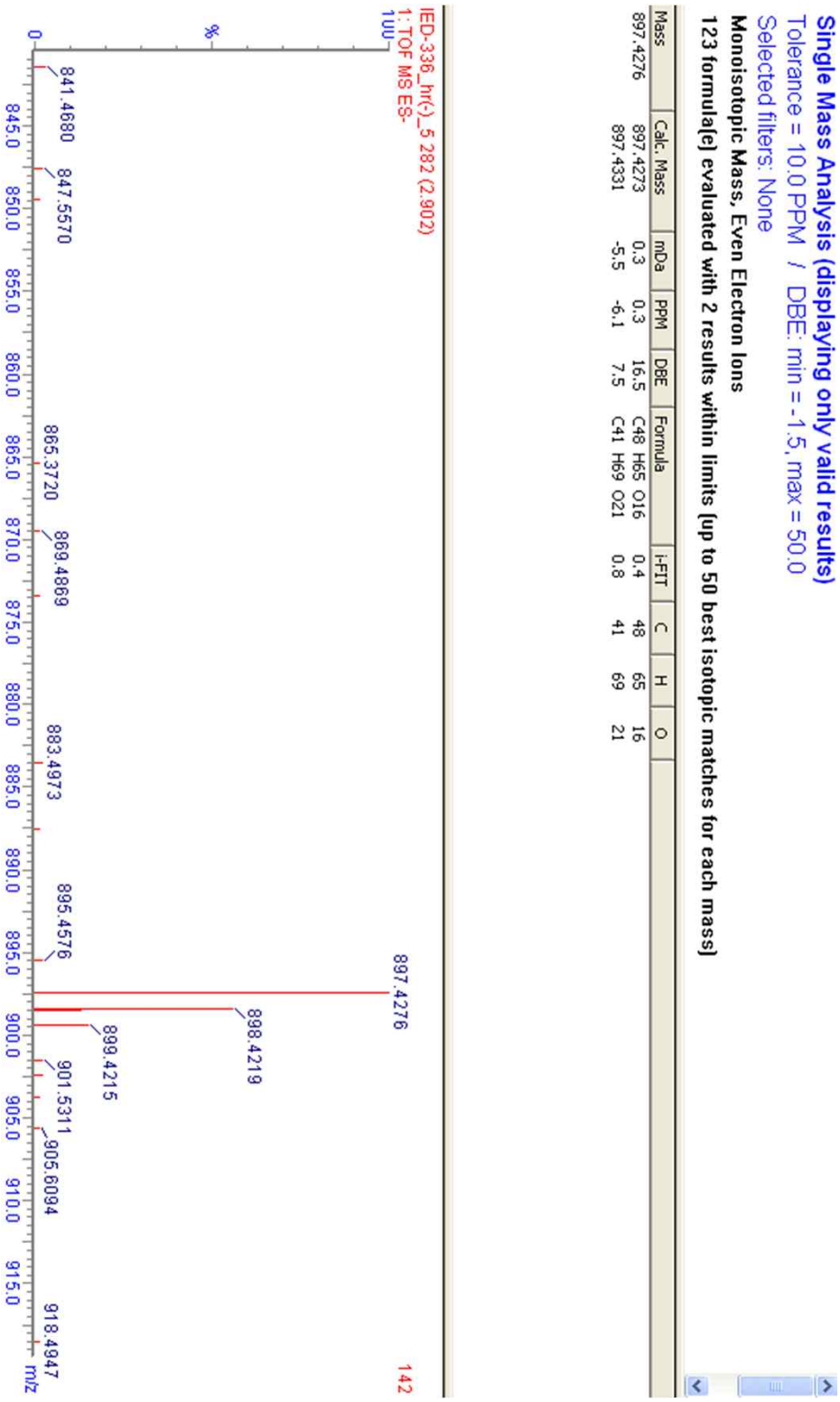
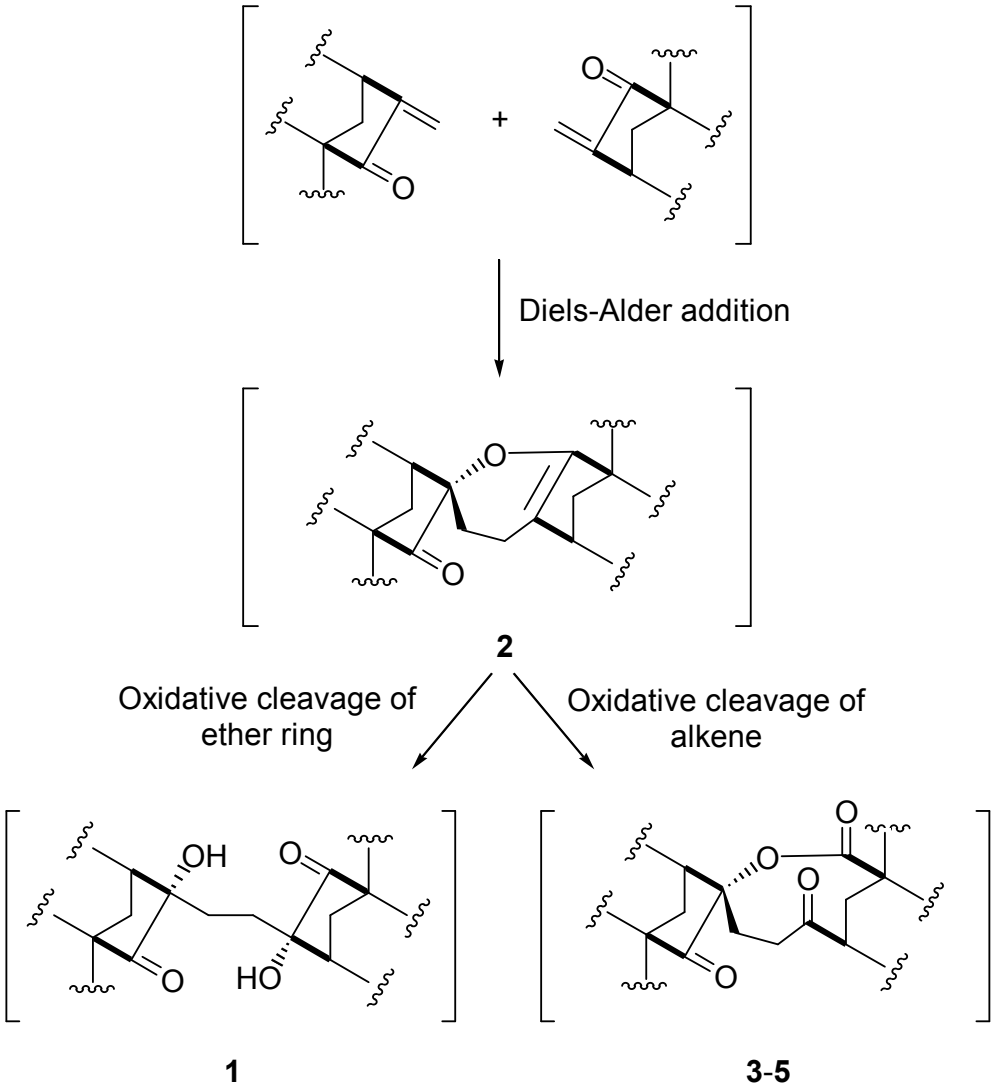


Figure S41. HRESIMS spectrum of biexcisusin E (**5**)



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
123 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	C	H	O
897.4276	897.4273	0.3	0.3	16.5	C48 H65 O16	0.4	48	65	16
	897.4331	-5.5	-6.1	7.5	C41 H69 O21	0.8	41	69	21



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