Supplementary data

New Ophiobolin Derivatives from the Marine Fungus *Aspergillus flocculosus* and Their Cytotoxicities against Cancer Cells

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[5] Laboratory Animal Resource Center, Korea Research Institute of Bioscience and Biotechnology, 30 Yeongudanjiro, Cheongju 28116, Korea; kanjon@kribb.re.kr

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Contents

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
41 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-30 H: 1-50 O: 1-5 Na: 0-1

Minimum:				-1.5				
Maximum:		500.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
405.2405	405.2406	-0.1	-0.2	8.5	953.0	n/a	n/a	C25 H34 O3 Na

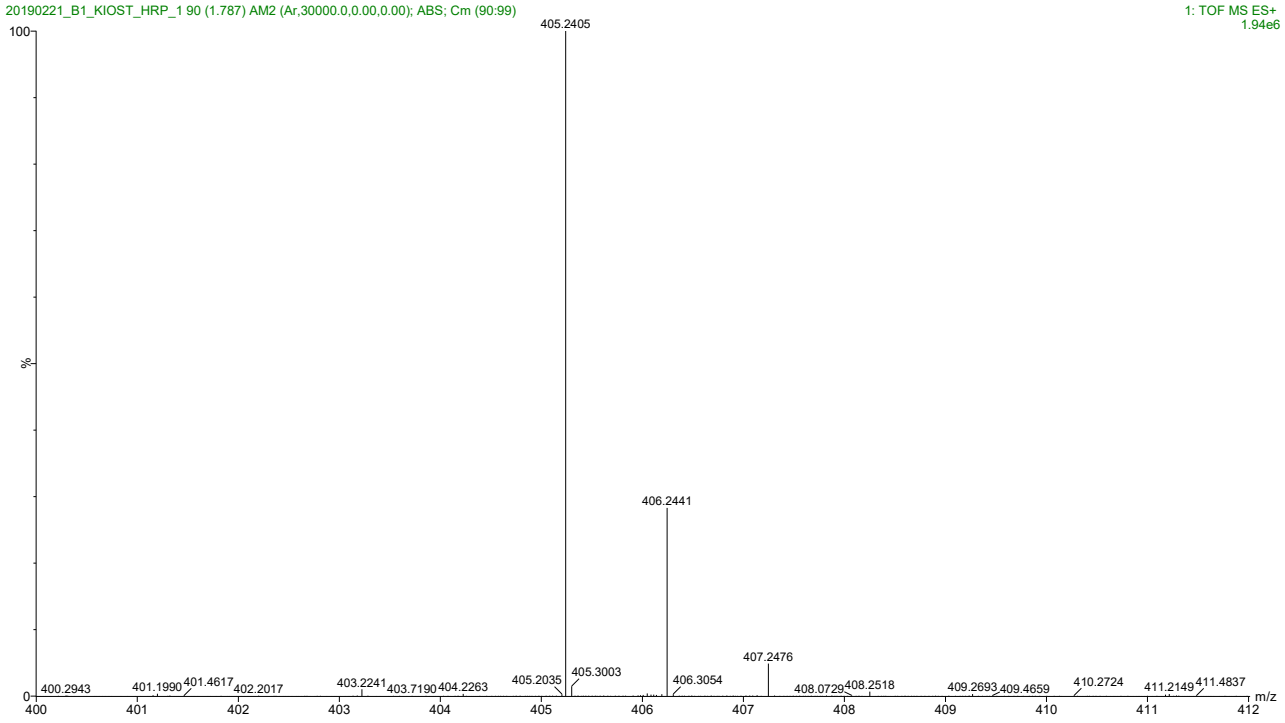

Figure S1. HRESIMS data of 14,15-dehydro-6-*epi*-ophiobolin K (**1**).

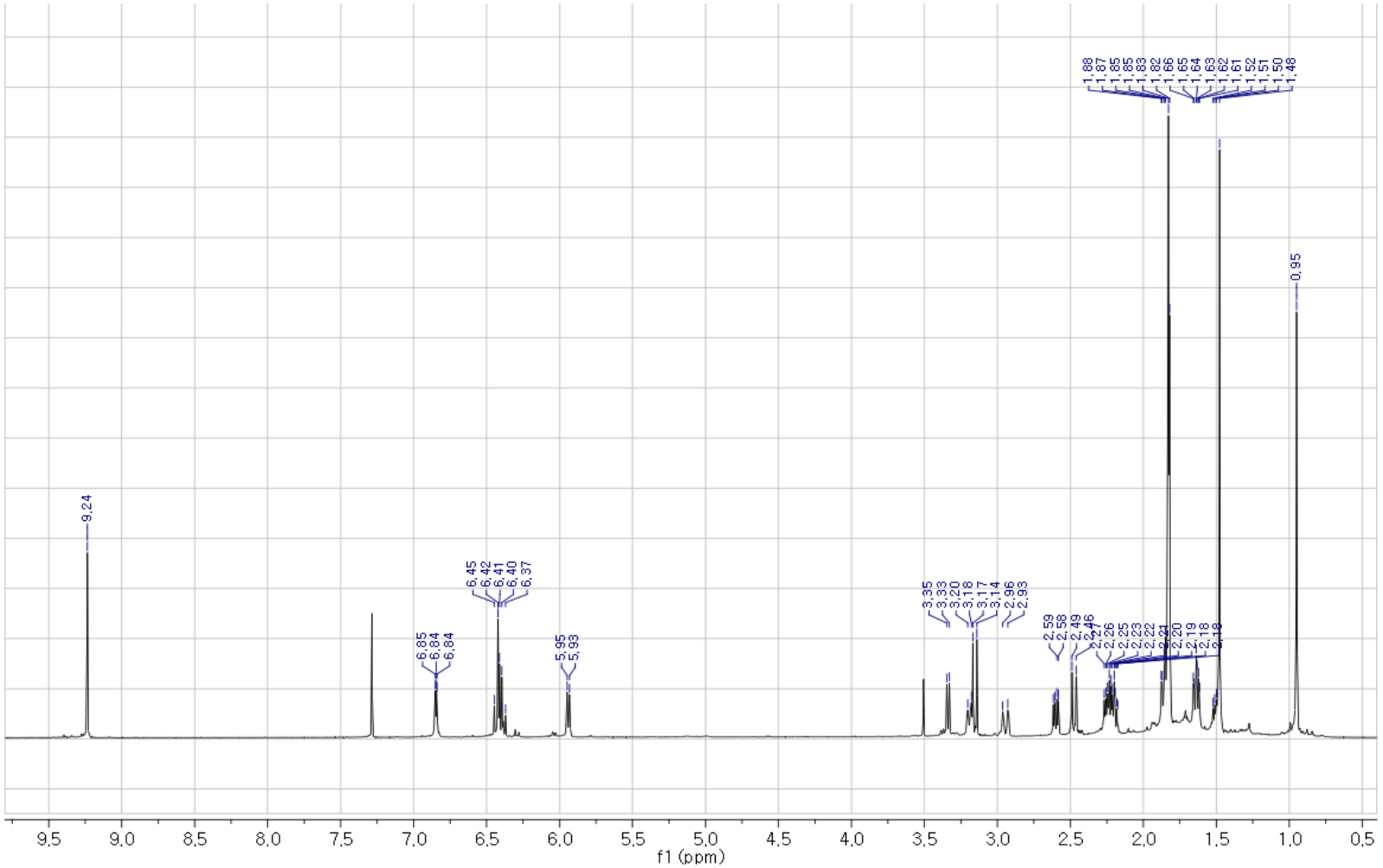

Figure S2. ^{1}H NMR spectrum of 14,15-dehydro-6-*epi*-ophiobolin K (**1**).

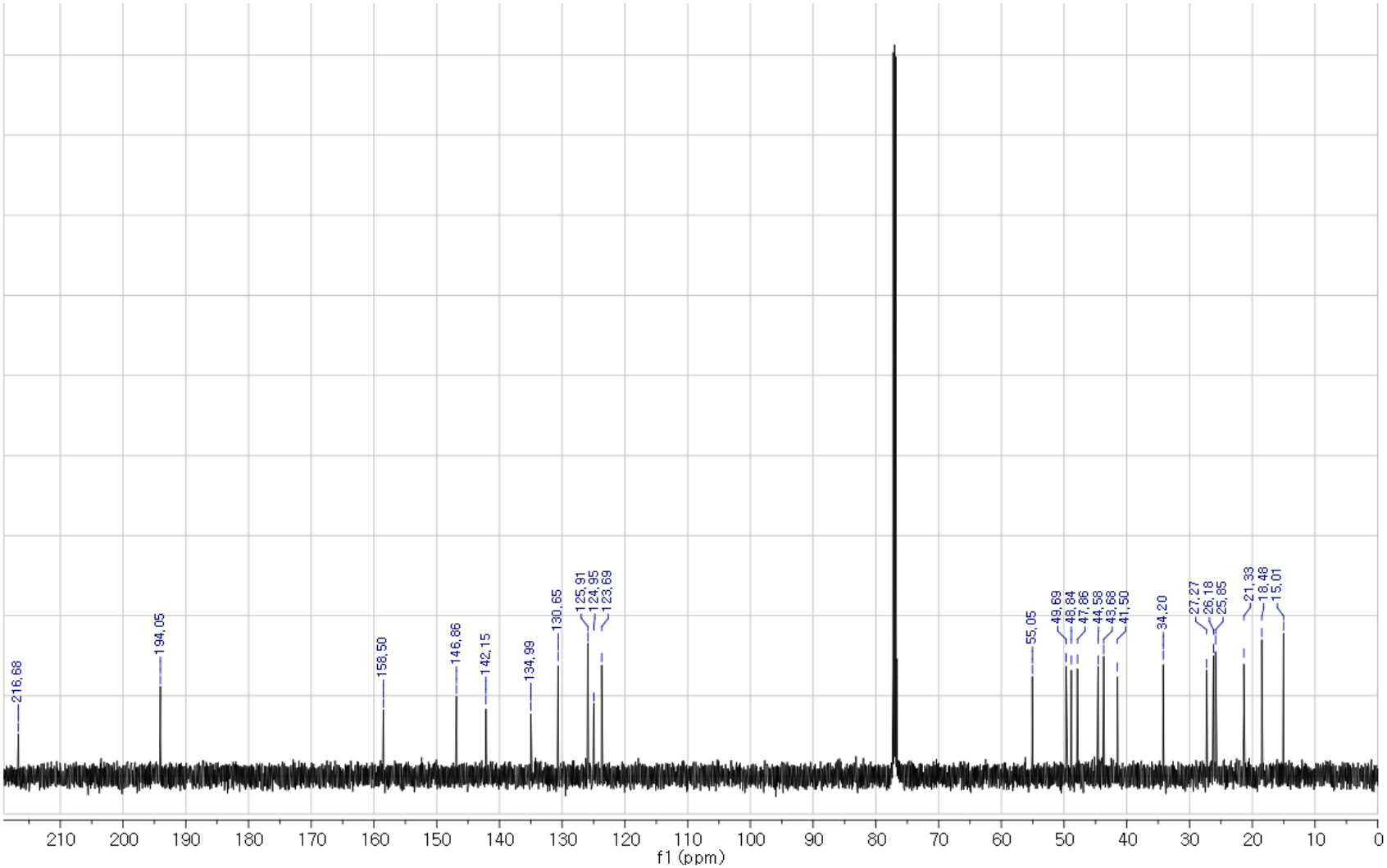

Figure S3. ^{13}C NMR spectrum of 14,15-dehydro-6-*epi*-ophiobolin K (**1**).

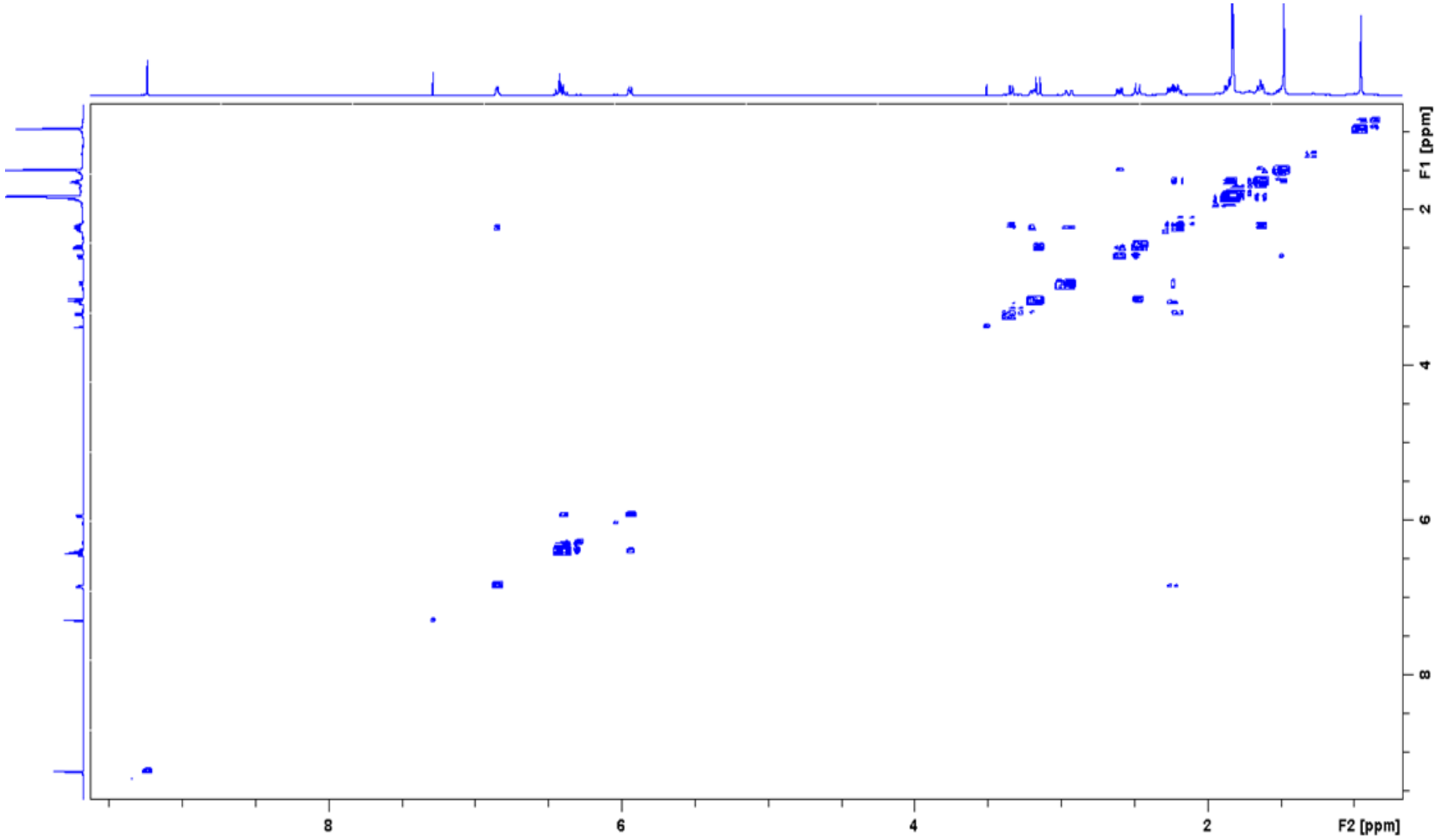

Figure S4. ^{1}H-^{1}H COSY spectrum of 14,15-dehydro-6-*epi*-ophiobolin K (**1**).

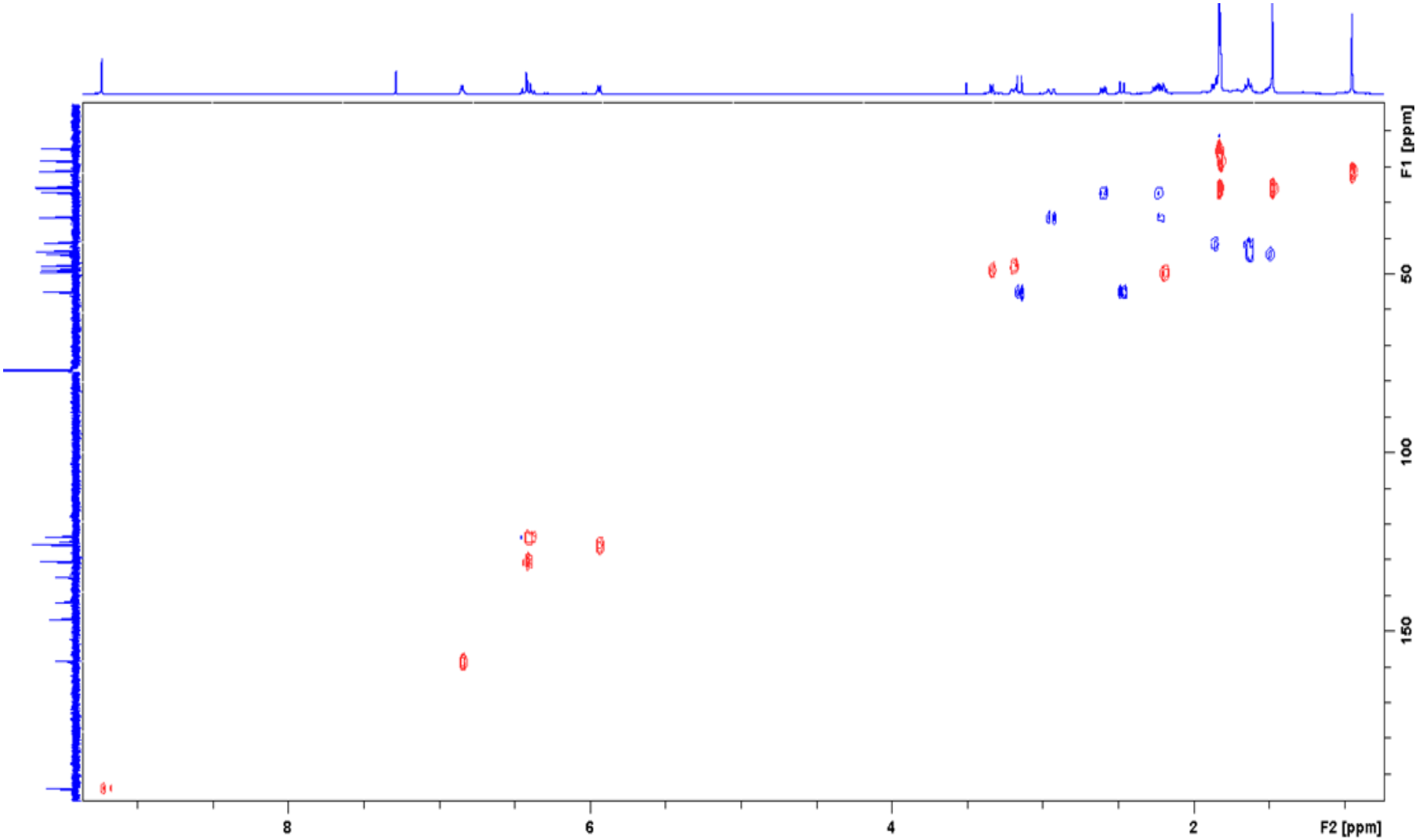

Figure S5. HSQC spectrum of 14,15-dehydro-6-*epi*-ophiobolin K (**1**).

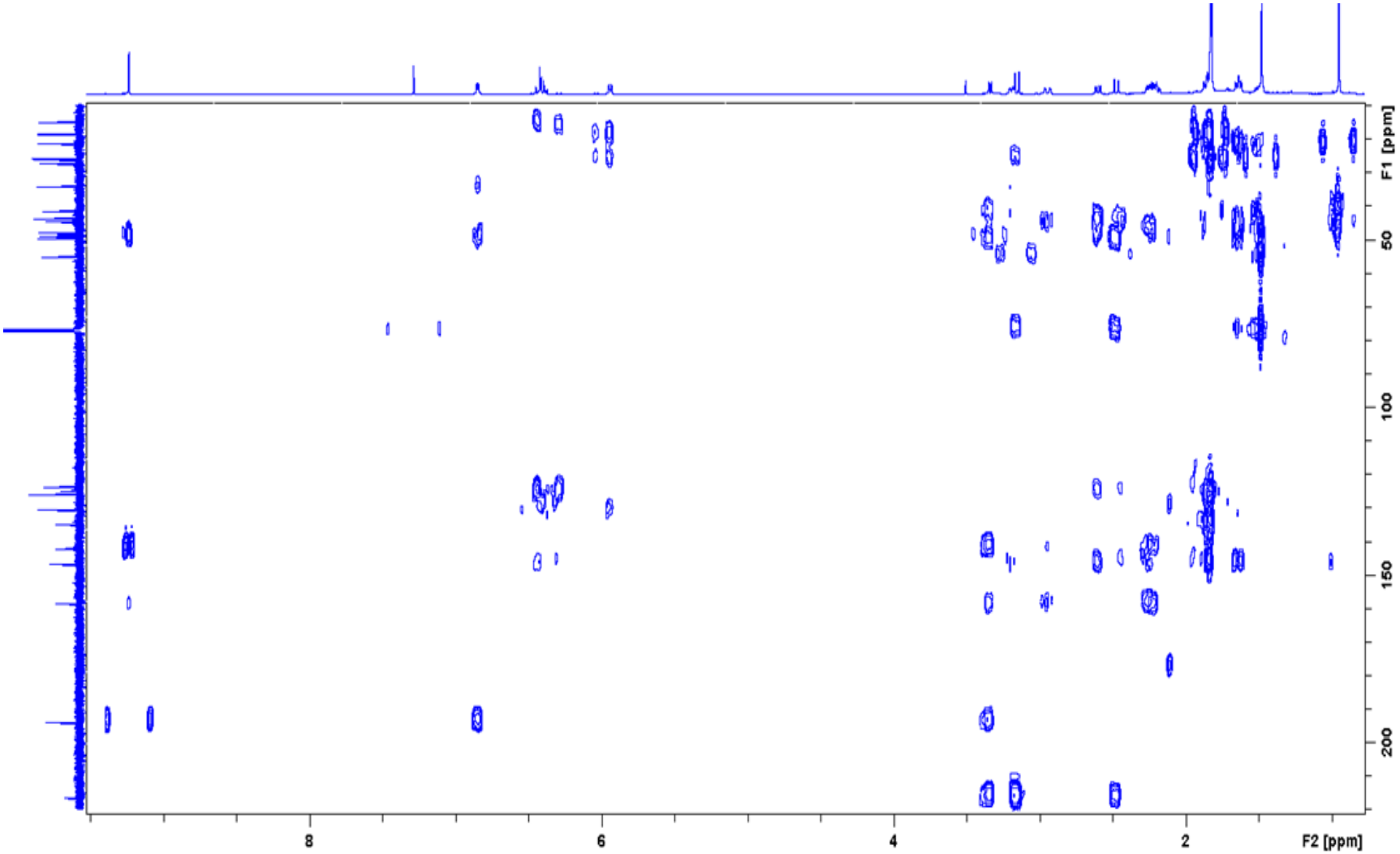

Figure S6. HMBC spectrum of 14,15-dehydro-6-*epi*-ophiobolin K (**1**).

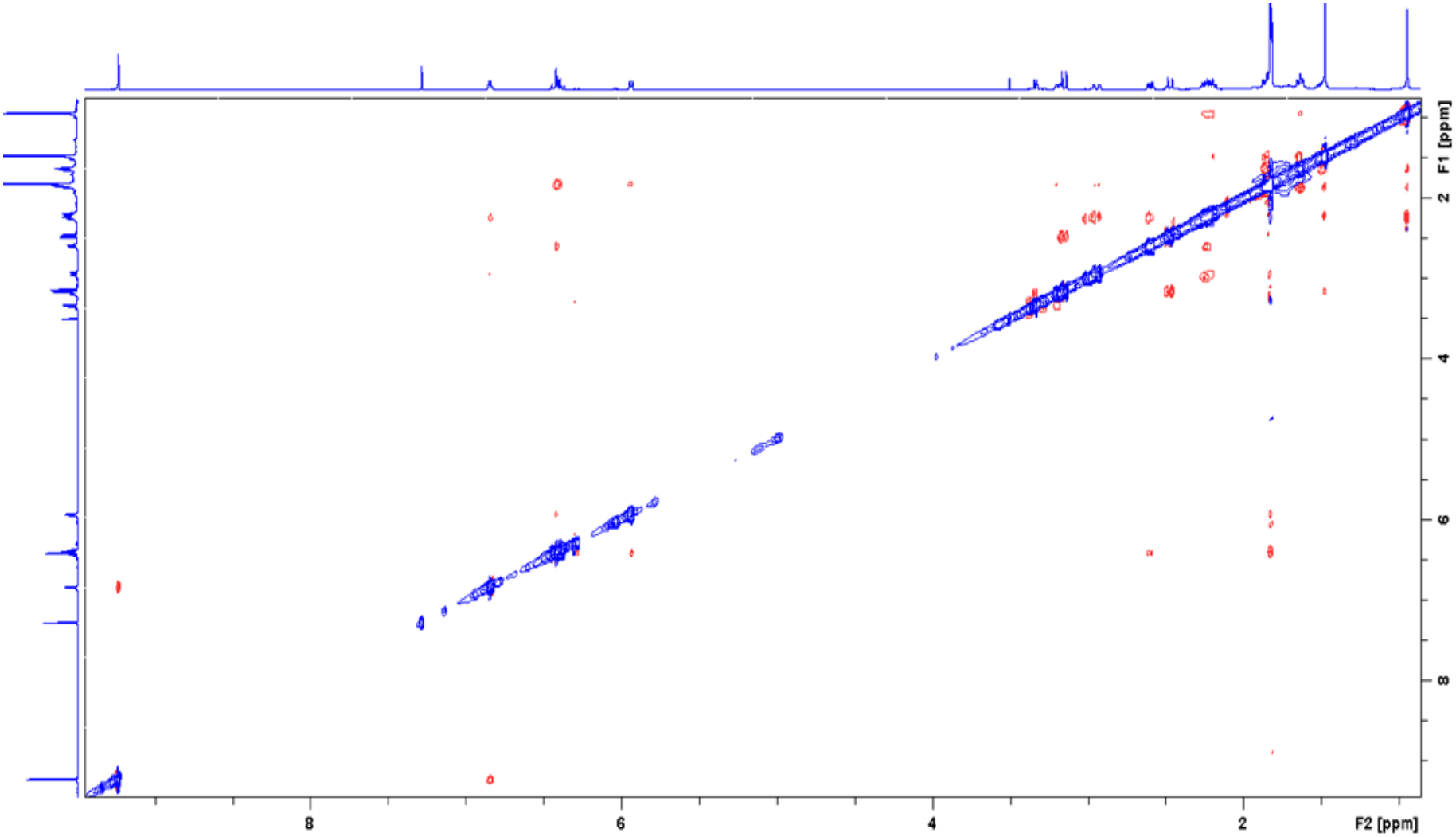

Figure S7. NOESY spectrum of 14,15-dehydro-6-*epi*-ophiobolin K (**1**).

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
41 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-30 H: 1-50 O: 1-5 Na: 0-1

Minimum:				-1.5				
Maximum:		500.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
405.2404	405.2406	-0.2	-0.5	8.5	1146.9	n/a	n/a	C25 H34 O3 Na

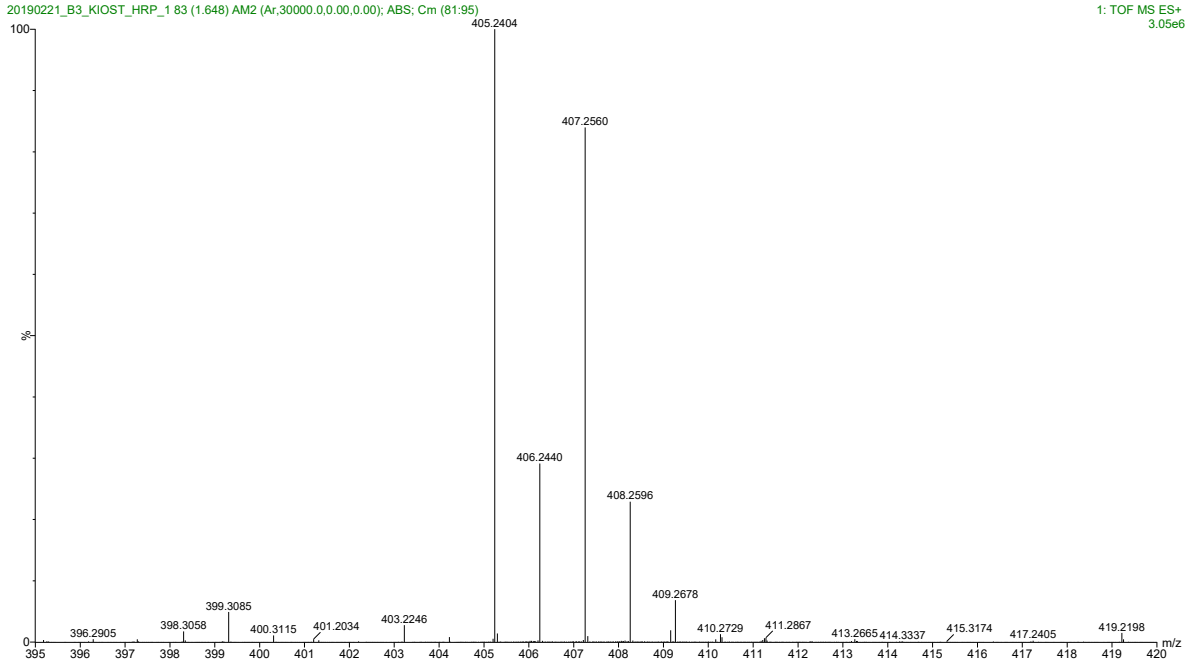

Figure S8. HRESIMS data of 14,15-dehydro-ophiobolin K (**2**).

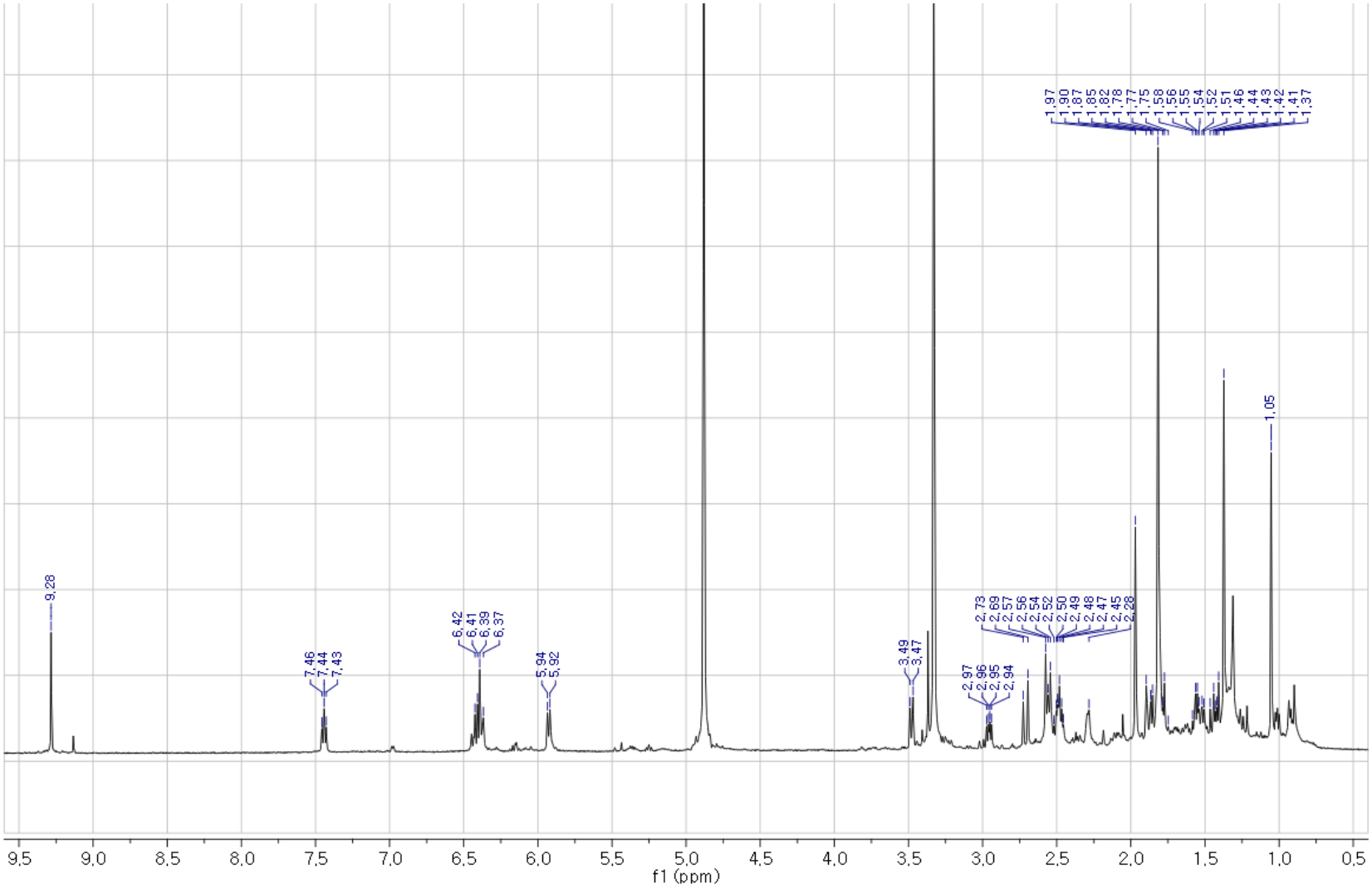

Figure S9. ^{1}H NMR spectrum of 14,15-dehydro-ophiobolin K (**2**).

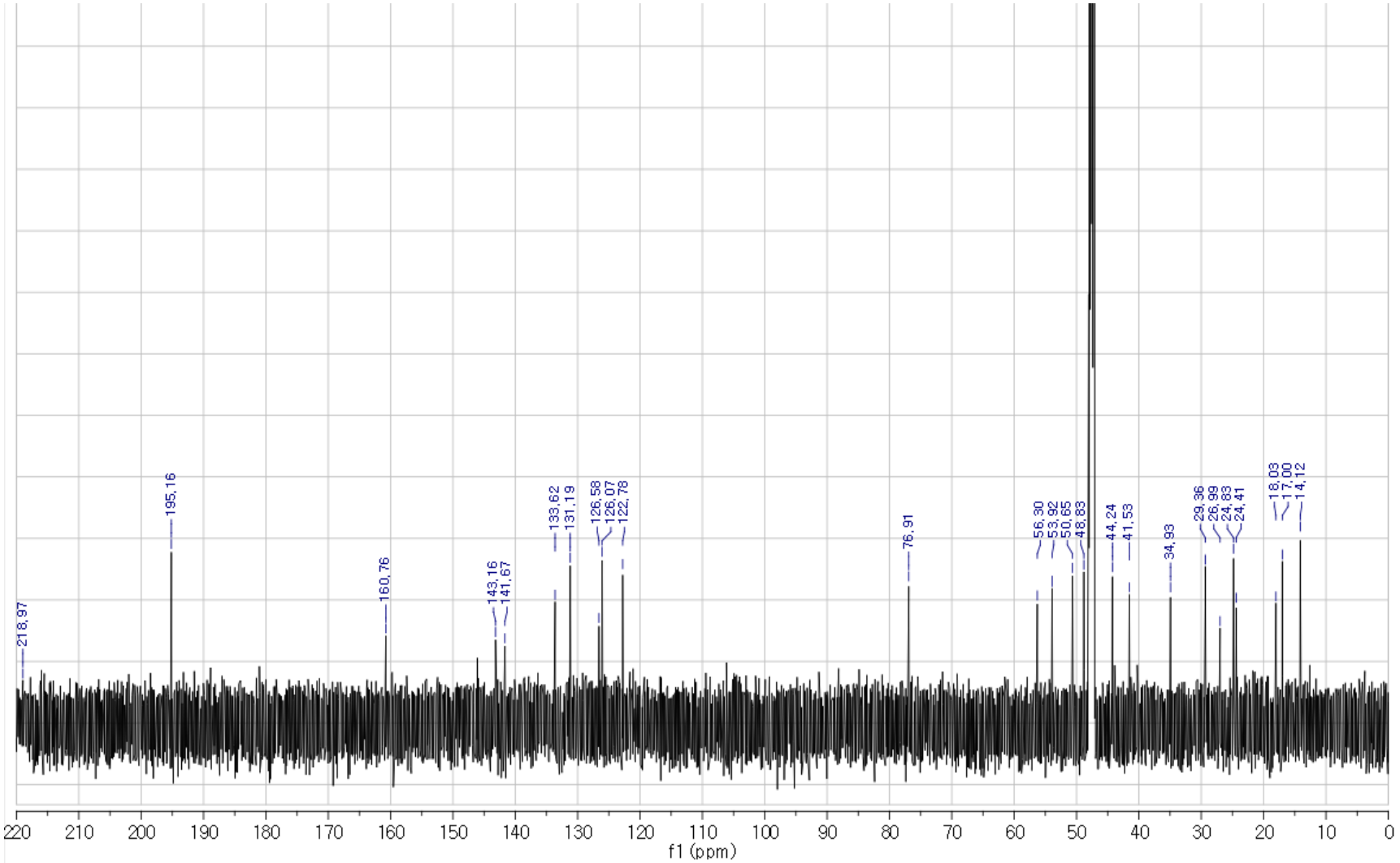

Figure S10. ^{13}C NMR spectrum of 14,15-dehydro-ophiobolin K (**2**).

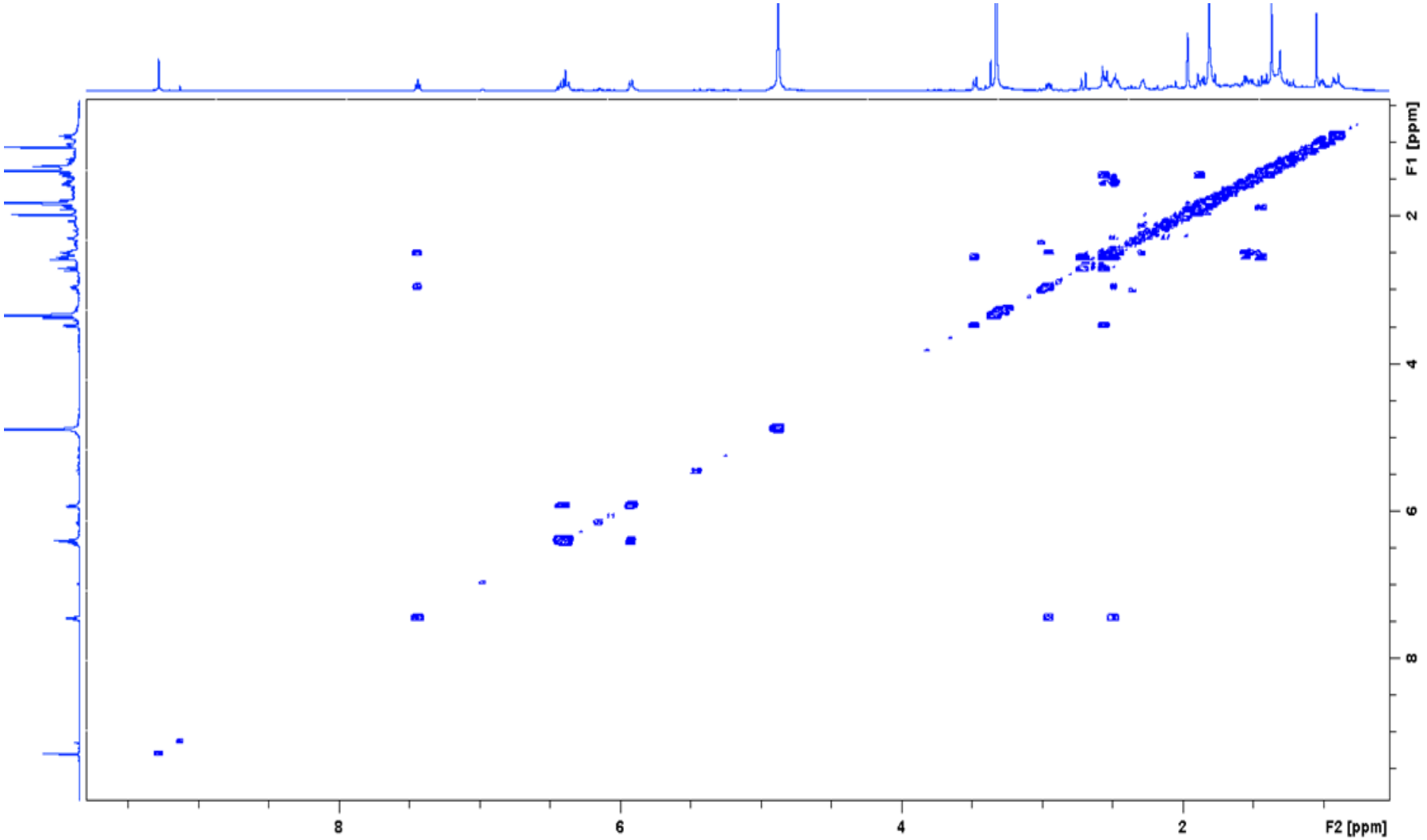

Figure S11. ^{1}H-^{1}H COSY spectrum of 14,15-dehydro-ophiobolin K (**2**).

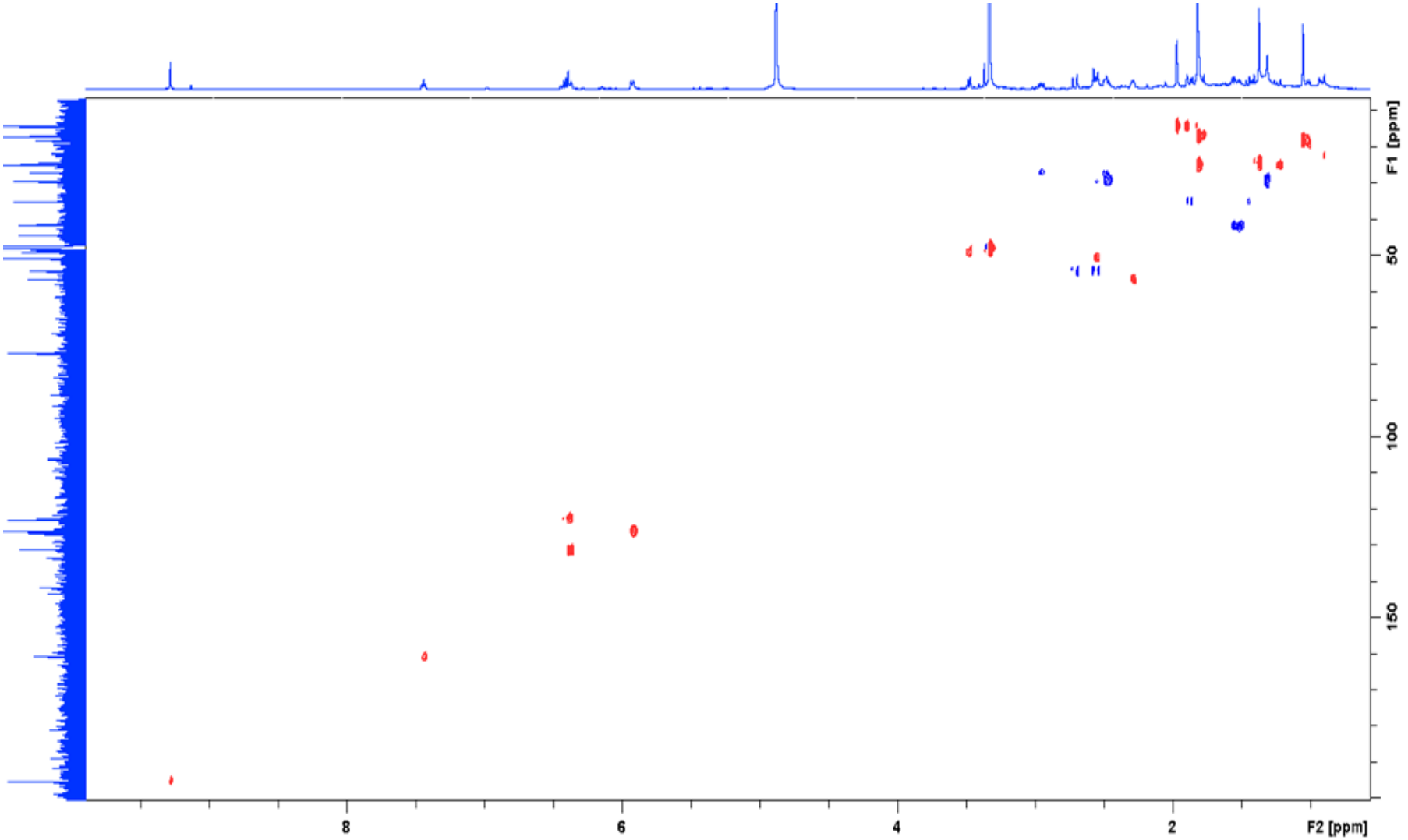

Figure S12. HSQC spectrum of 14,15-dehydro-ophiobolin K (**2**).

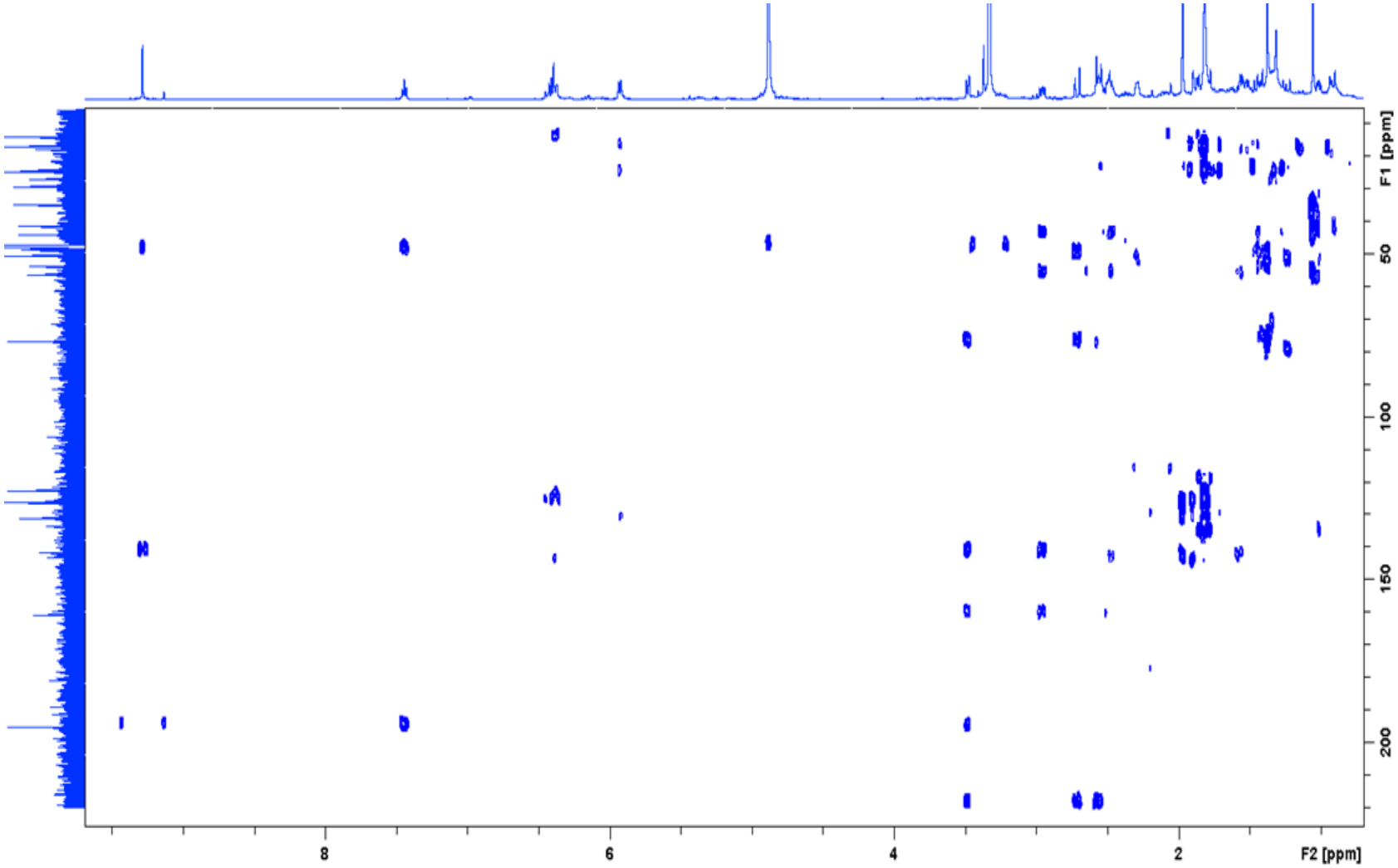

Figure S13. HMBC spectrum of 14,15-dehydro-ophiobolin K (**2**).

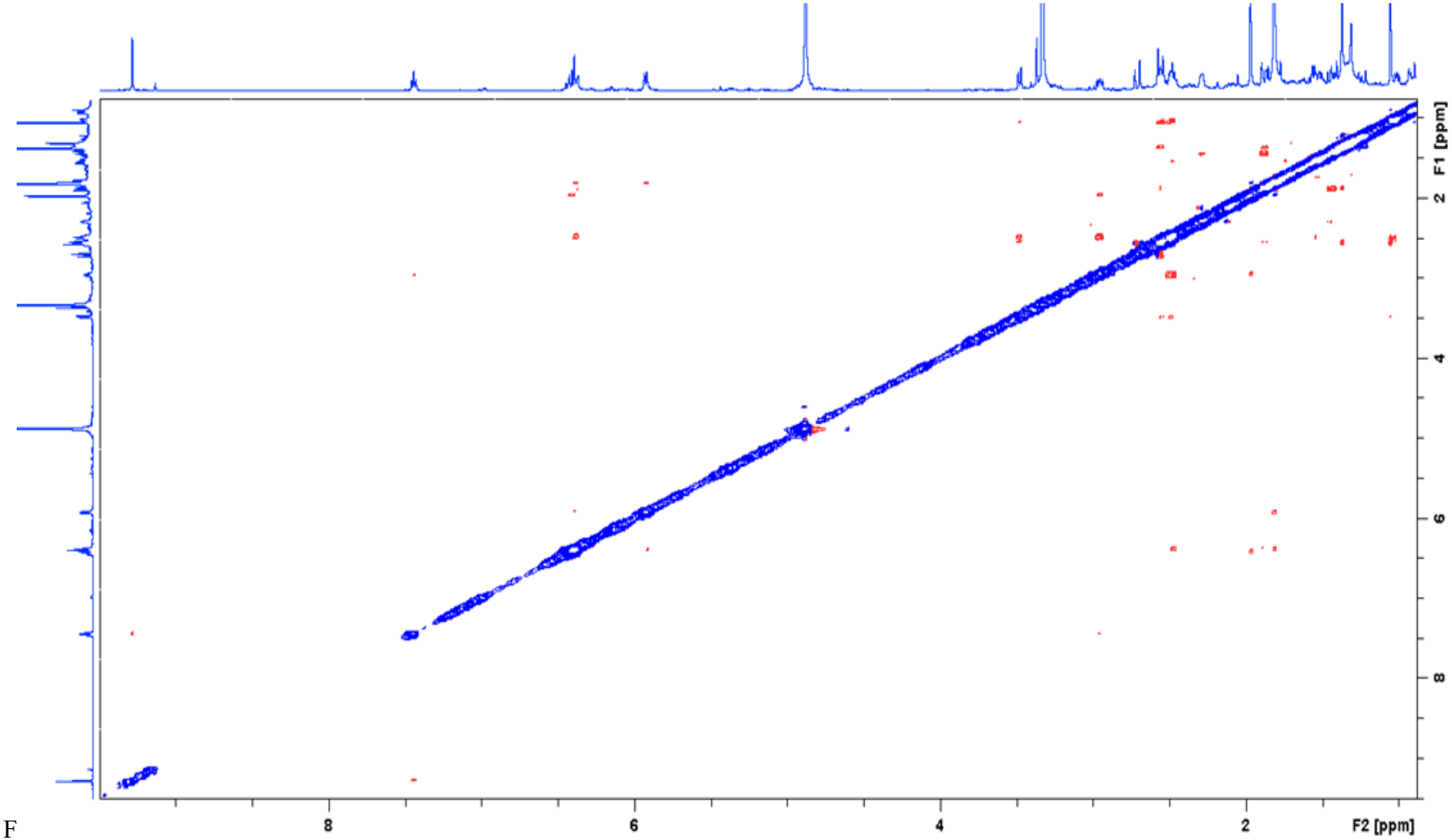

Figure S14. NOESY spectrum of 14,15-dehydro-ophiobolin K (**2**).

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
82 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-55 H: 1-80 O: 1-10 Na: 0-1

Minimum:				-1.5				
Maximum:		500.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
387.2301	387.2300	0.1	0.3	9.5	1107.4	n/a	n/a	C25 H32 O2 Na

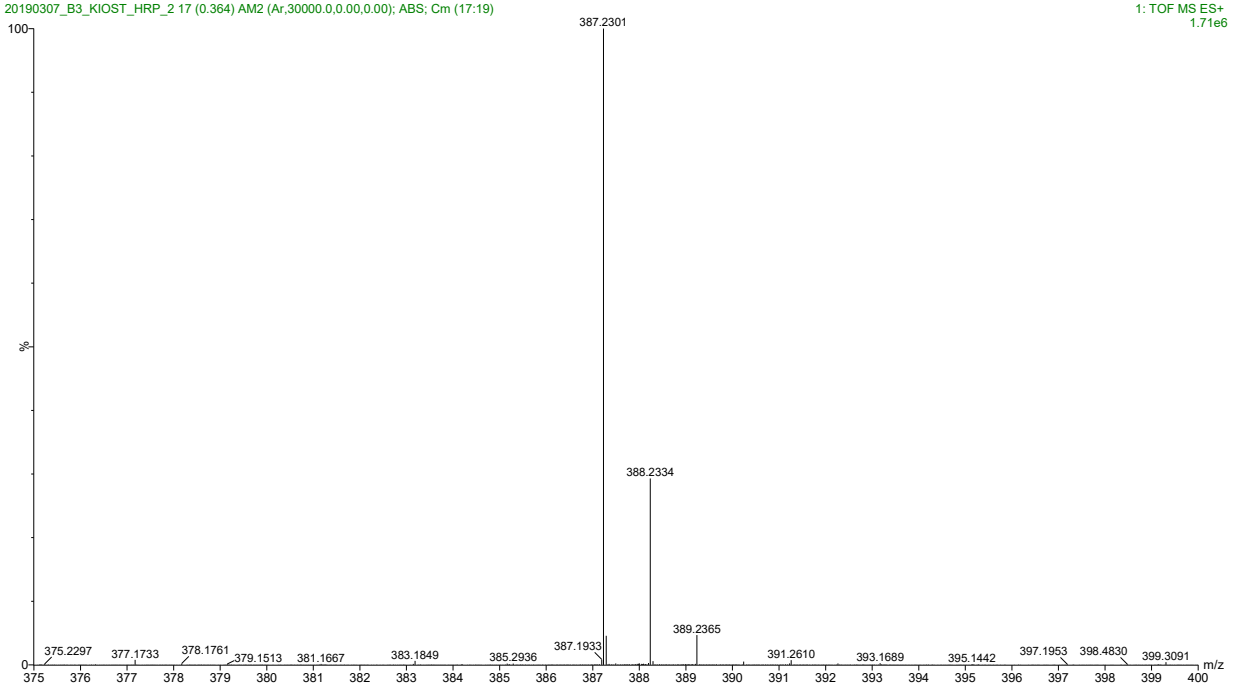

Figure S15. HRESIMS data of 14,15-dehydro-6-*epi*-ophiobolin G (**3**).

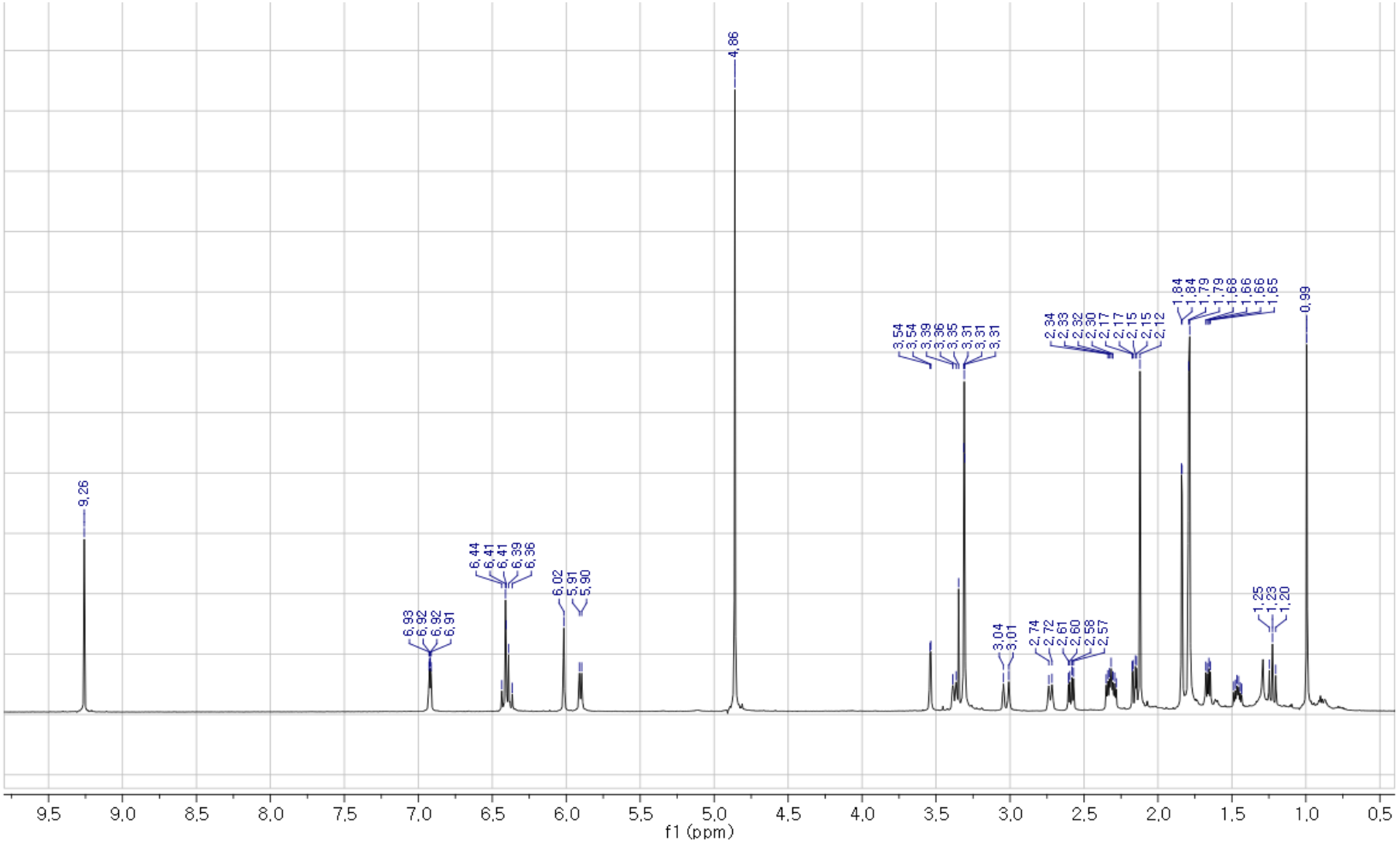

Figure S16. ^{1}H NMR spectrum of 14,15-dehydro-6-*epi*-ophiobolin G (**3**).

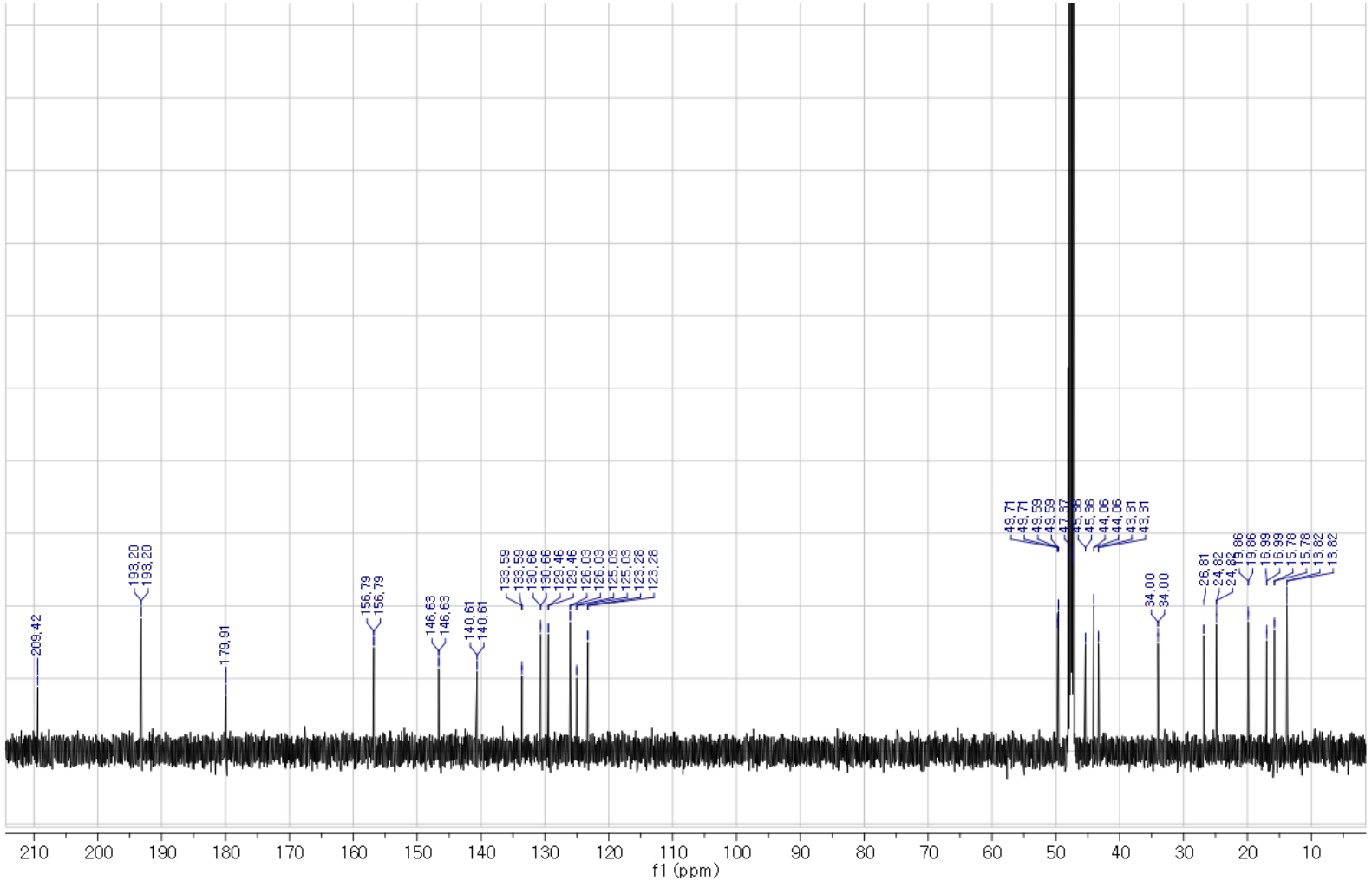

Figure S17. ^{13}C NMR spectrum of 14,15-dehydro-6-*epi*-ophiobolin G (**3**).

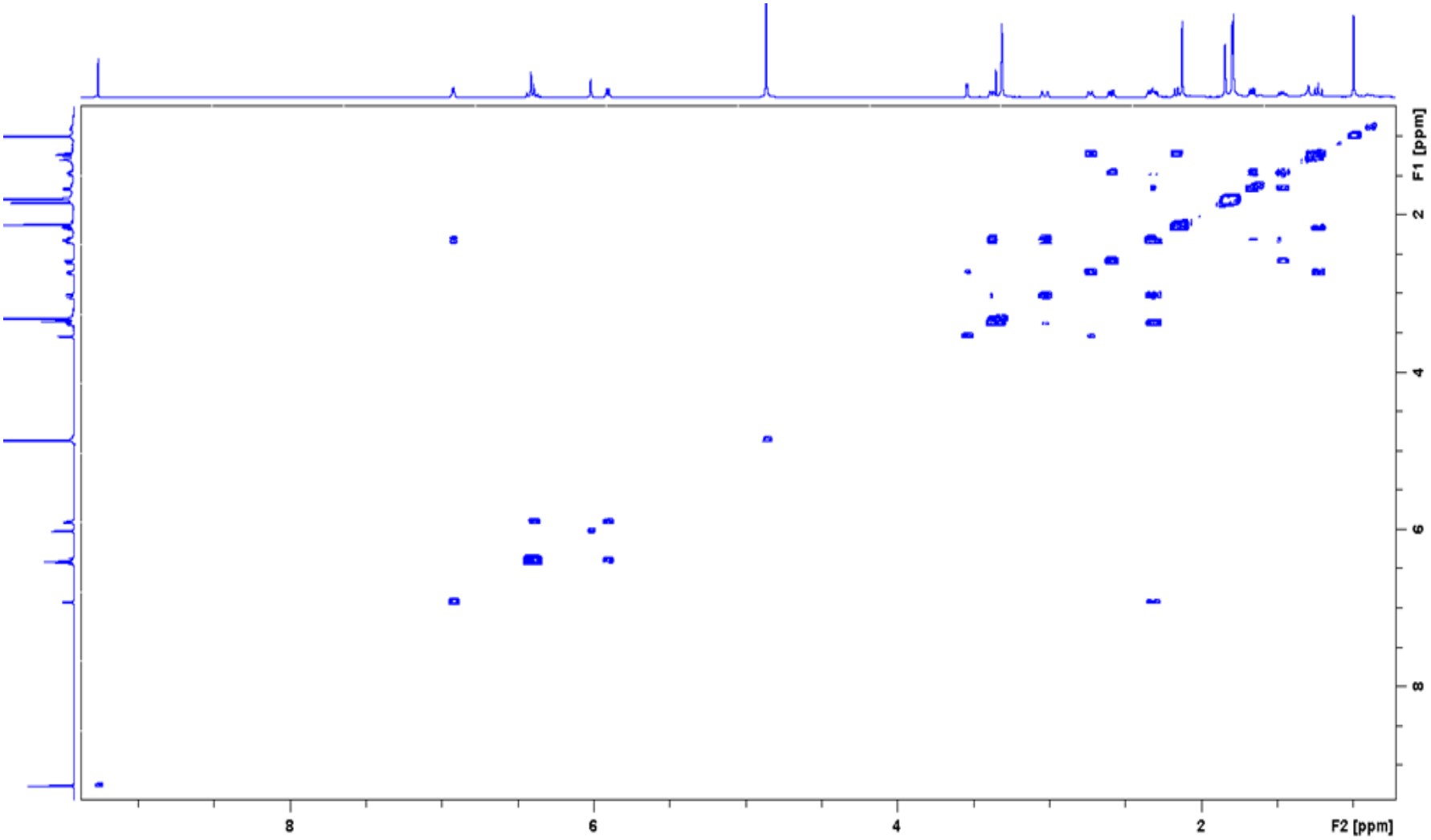

Figure S18. ^{1}H-^{1}H COSY spectrum of 14,15-dehydro-6-*epi*-ophiobolin G (**3**).

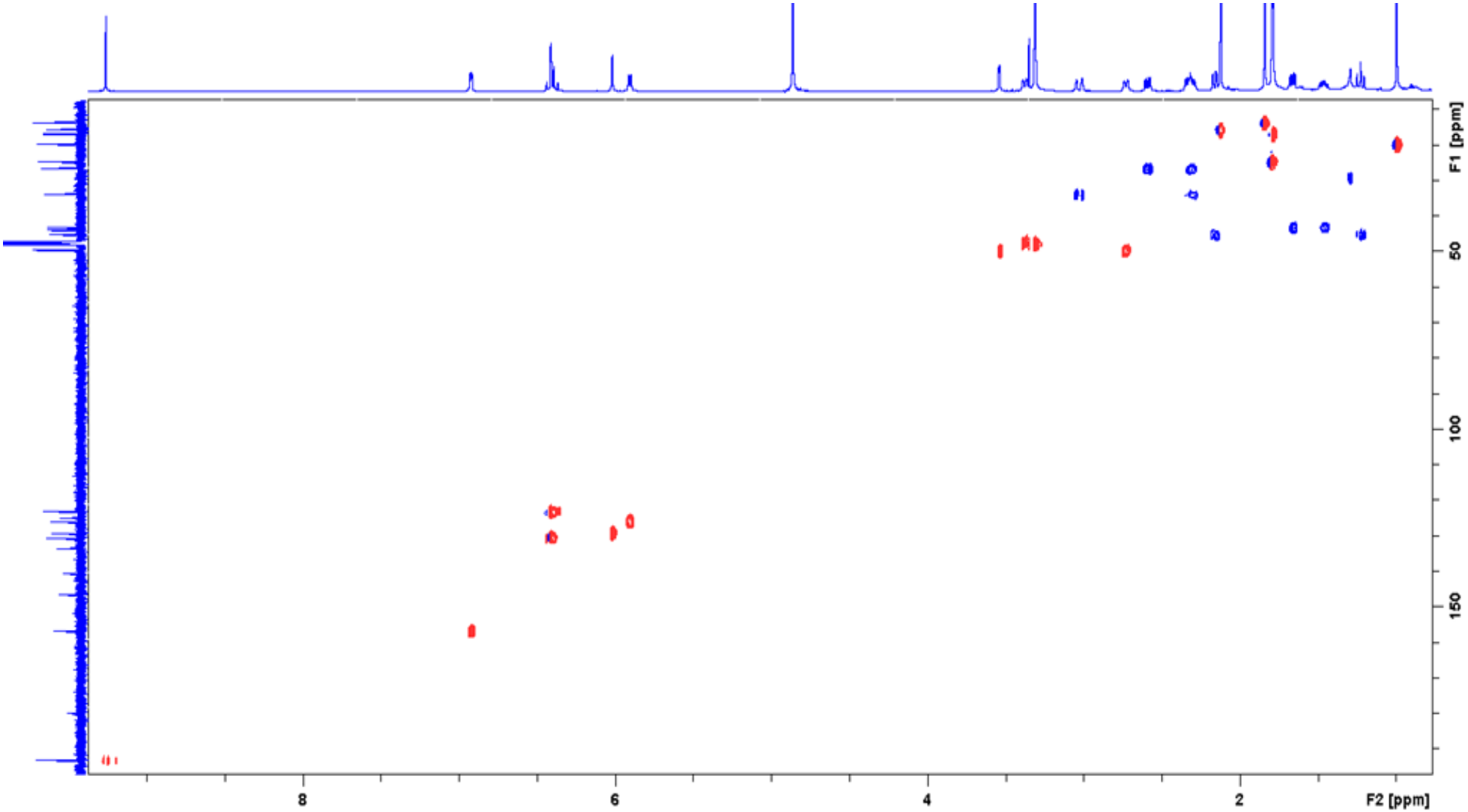

Figure S19. HSQC spectrum of 14,15-dehydro-6-*epi*-ophiobolin G (**3**).

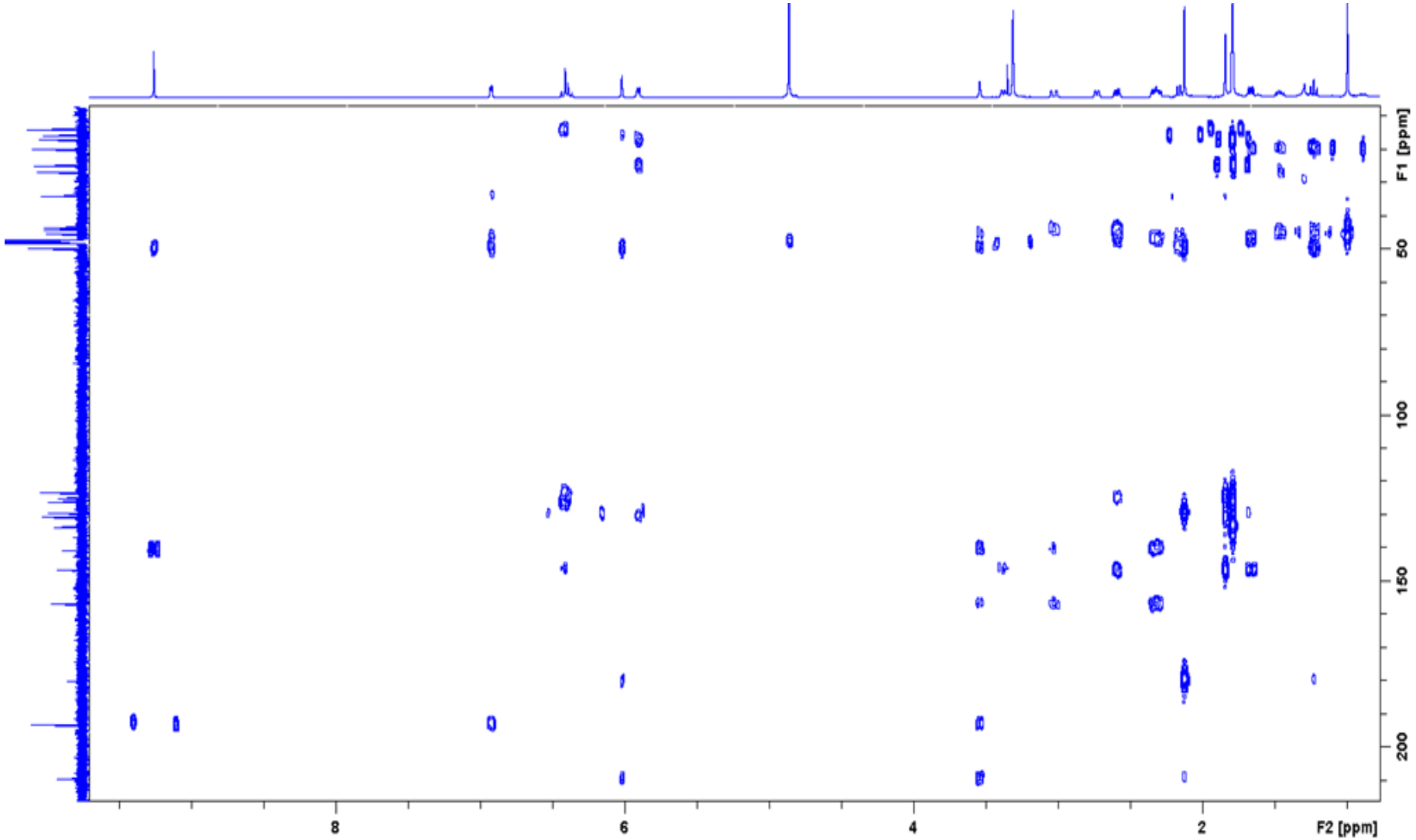

Figure S20. HMBC spectrum of 14,15-dehydro-6-*epi*-ophiobolin G (**3**).

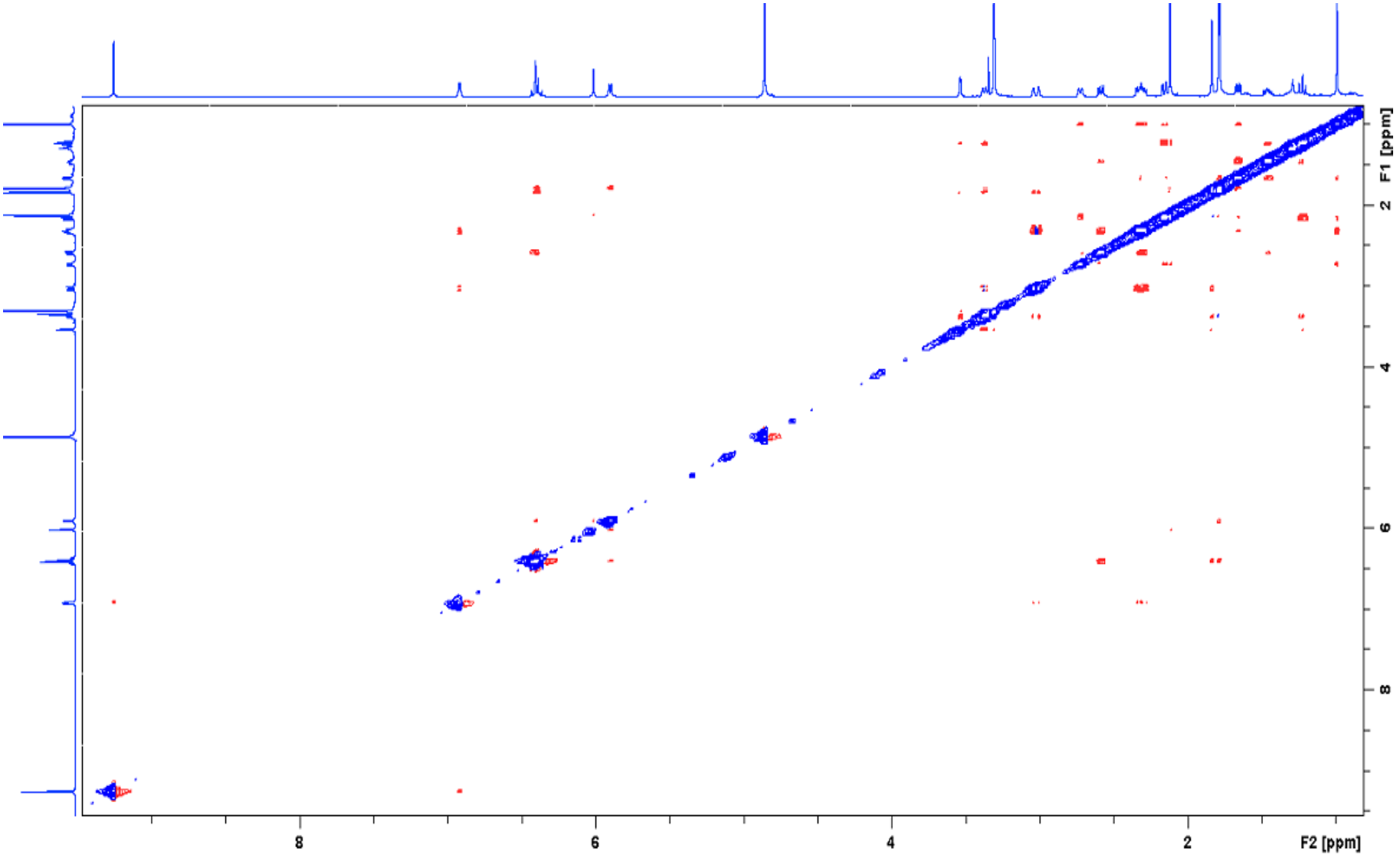

Figure S21.NOESY spectrum of 14,15-dehydro-6-*epi*-ophiobolin G (**3**).

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-30 H: 1-50 O: 1-5 Na: 0-1

Minimum:				-1.5				
Maximum:		500.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
387.2299	387.2300	-0.1	-0.3	9.5	1248.9	n/a	n/a	C25 H32 O2 Na

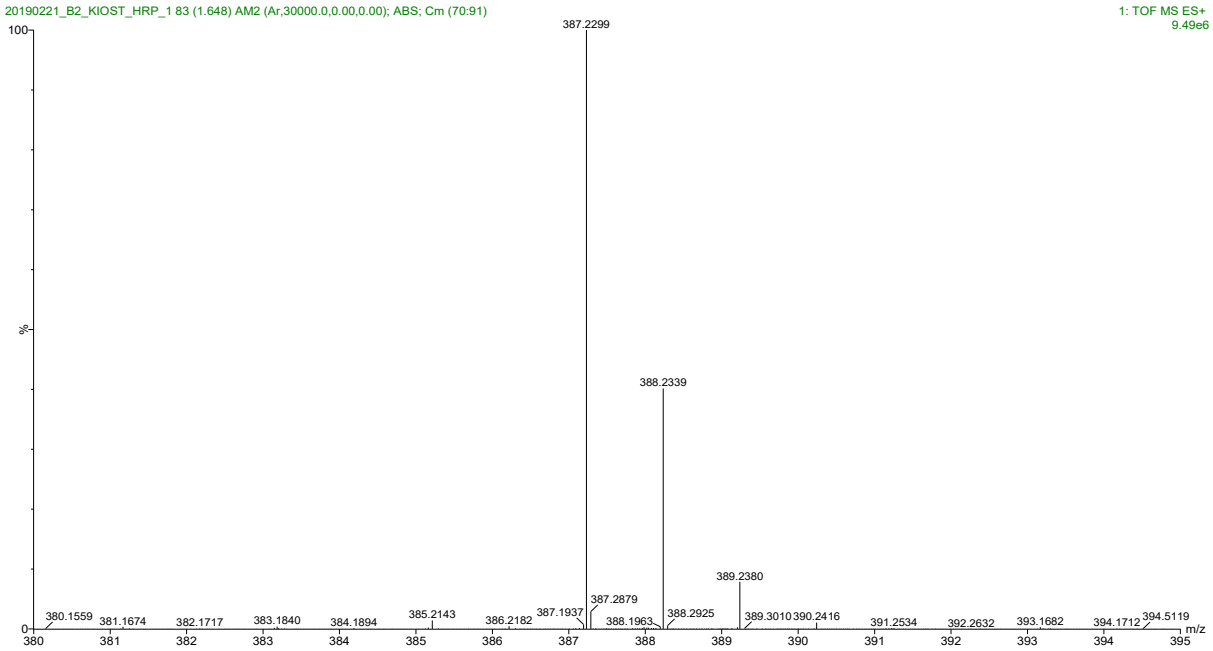

Figure S22. HRESIMS data of 14,15-dehydro-ophiobolin G (**4**).

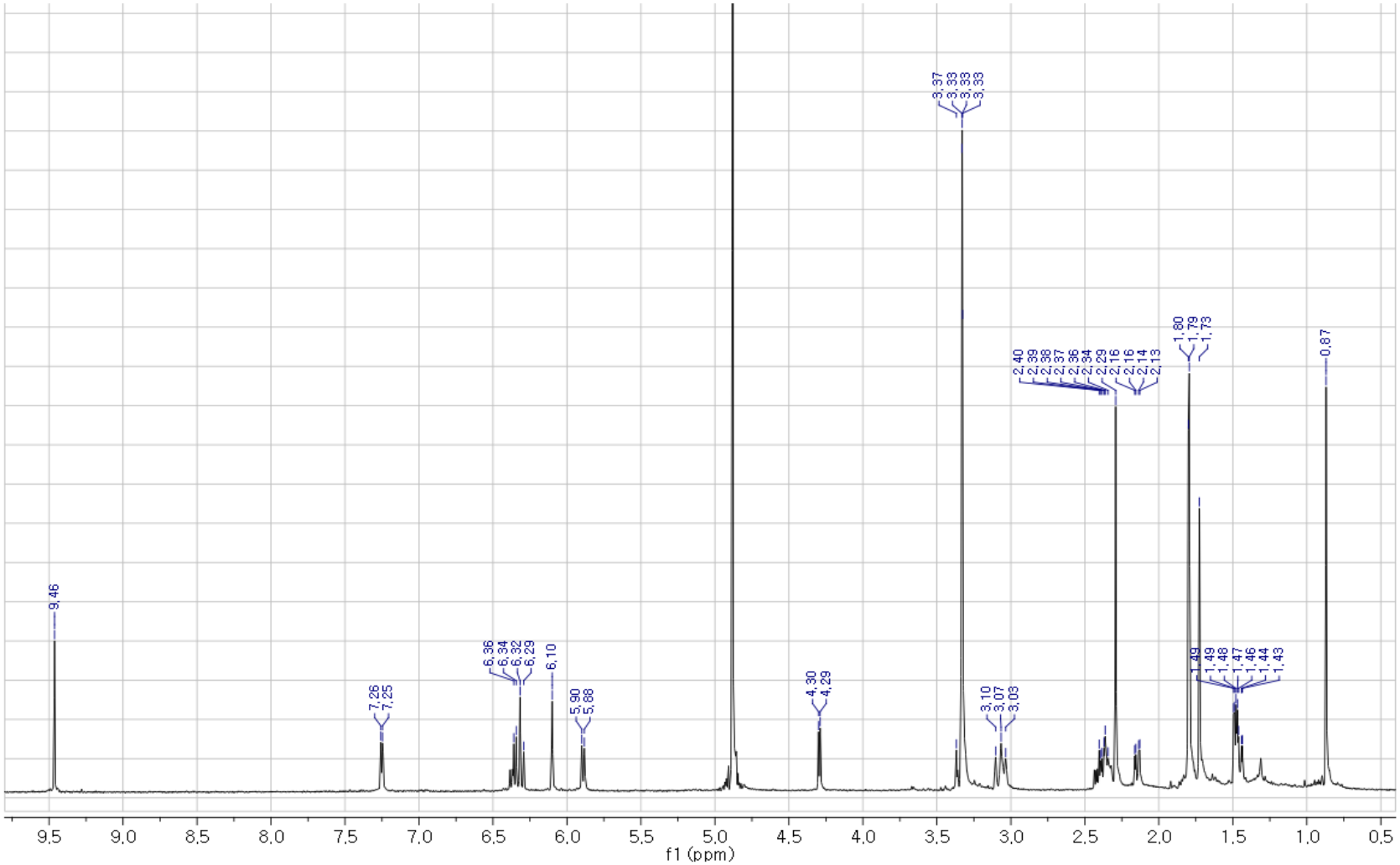

Figure S23. ^{1}H NMR spectrum of 14,15-dehydro-ophiobolin G (**4**).

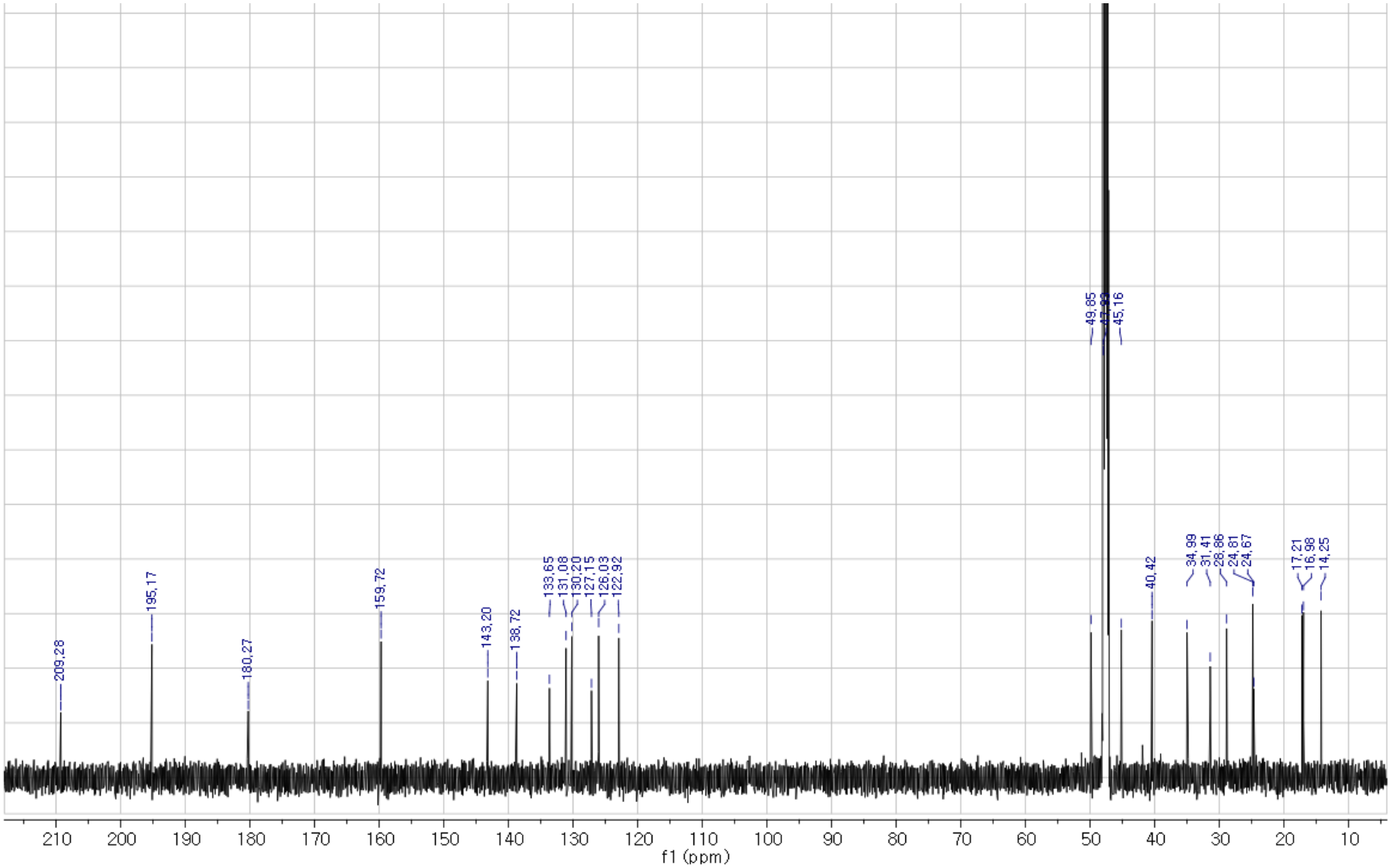

Figure S24. ^{13}C NMR spectrum of 14,15-dehydro-ophiobolin G (**4**).

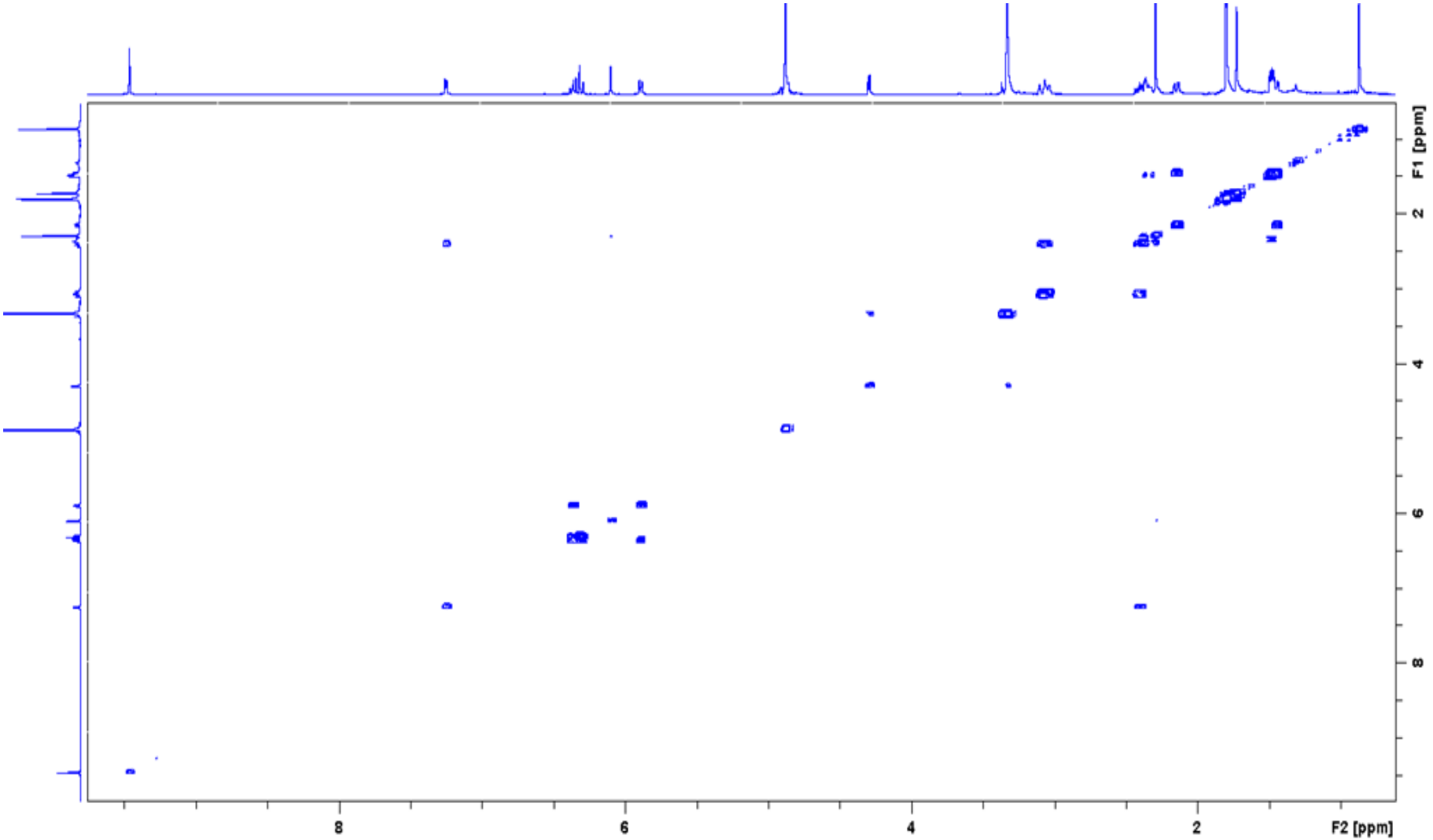

Figure S25. ^{1}H-^{1}H COSY spectrum of 14,15-dehydro-ophiobolin G (**4**).

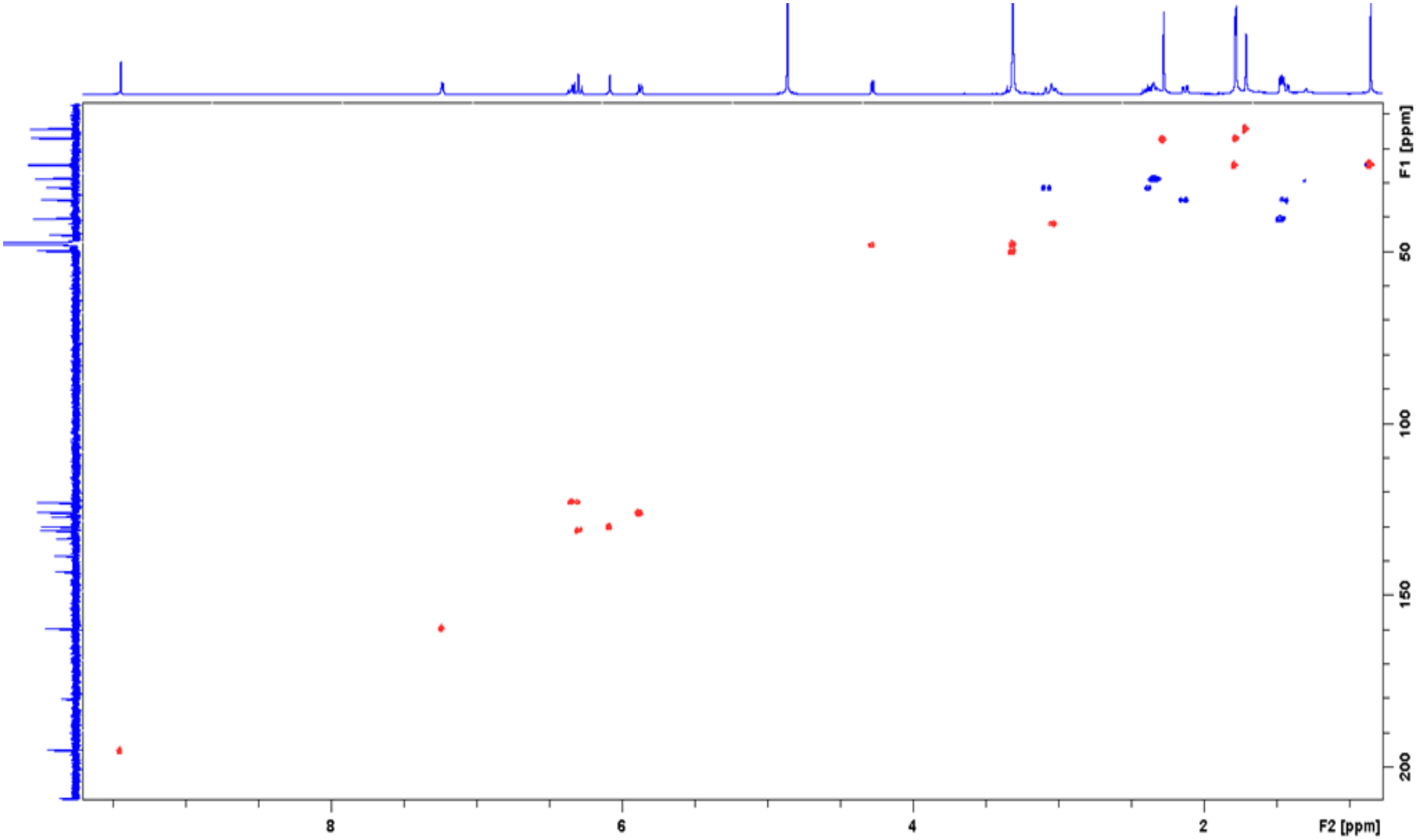

Figure S26. HSQC spectrum of 14,15-dehydro-ophiobolin G (**4**).

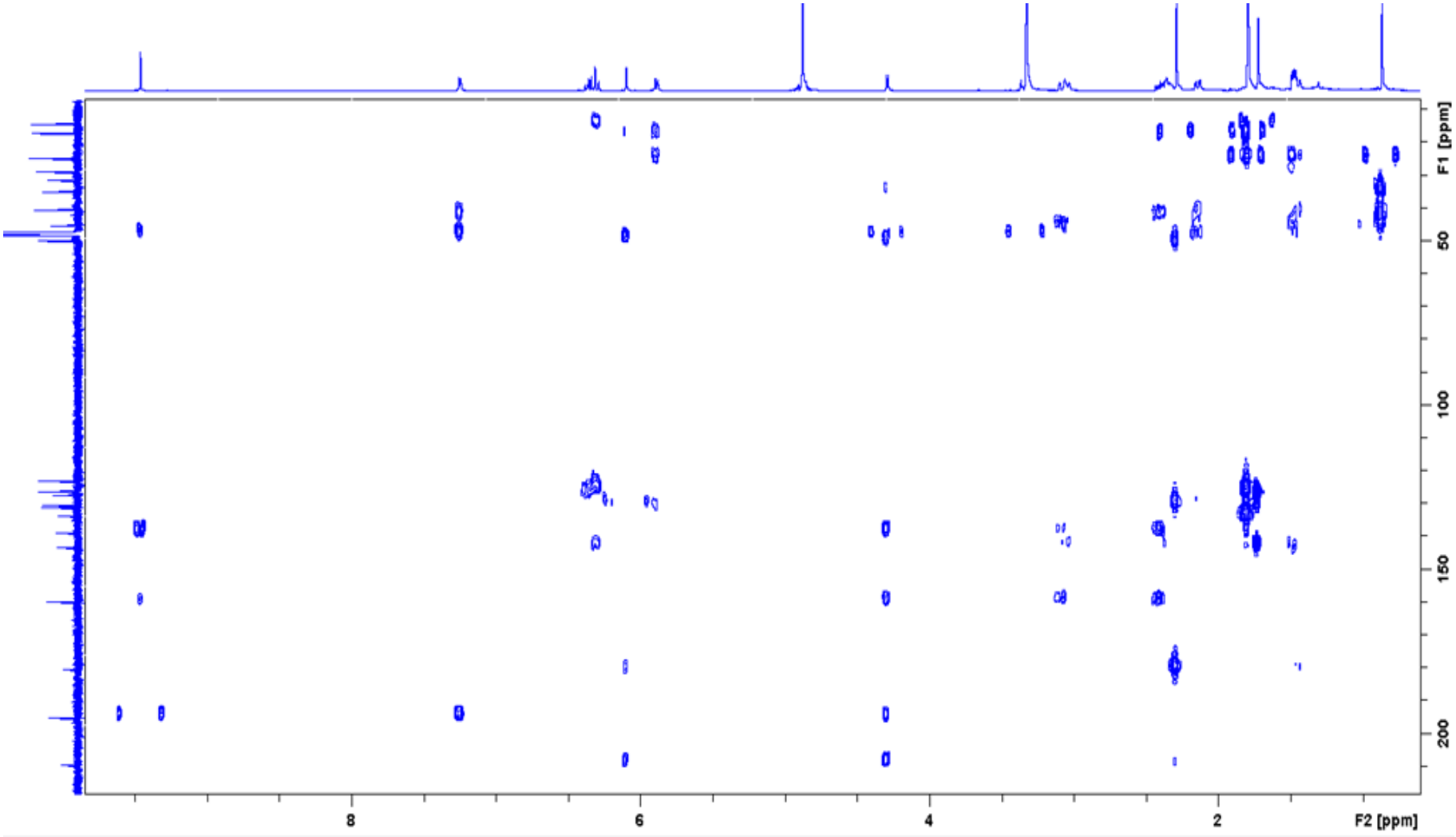

Figure S27. HMBC spectrum of 14,15-dehydro-ophiobolin G (**4**).

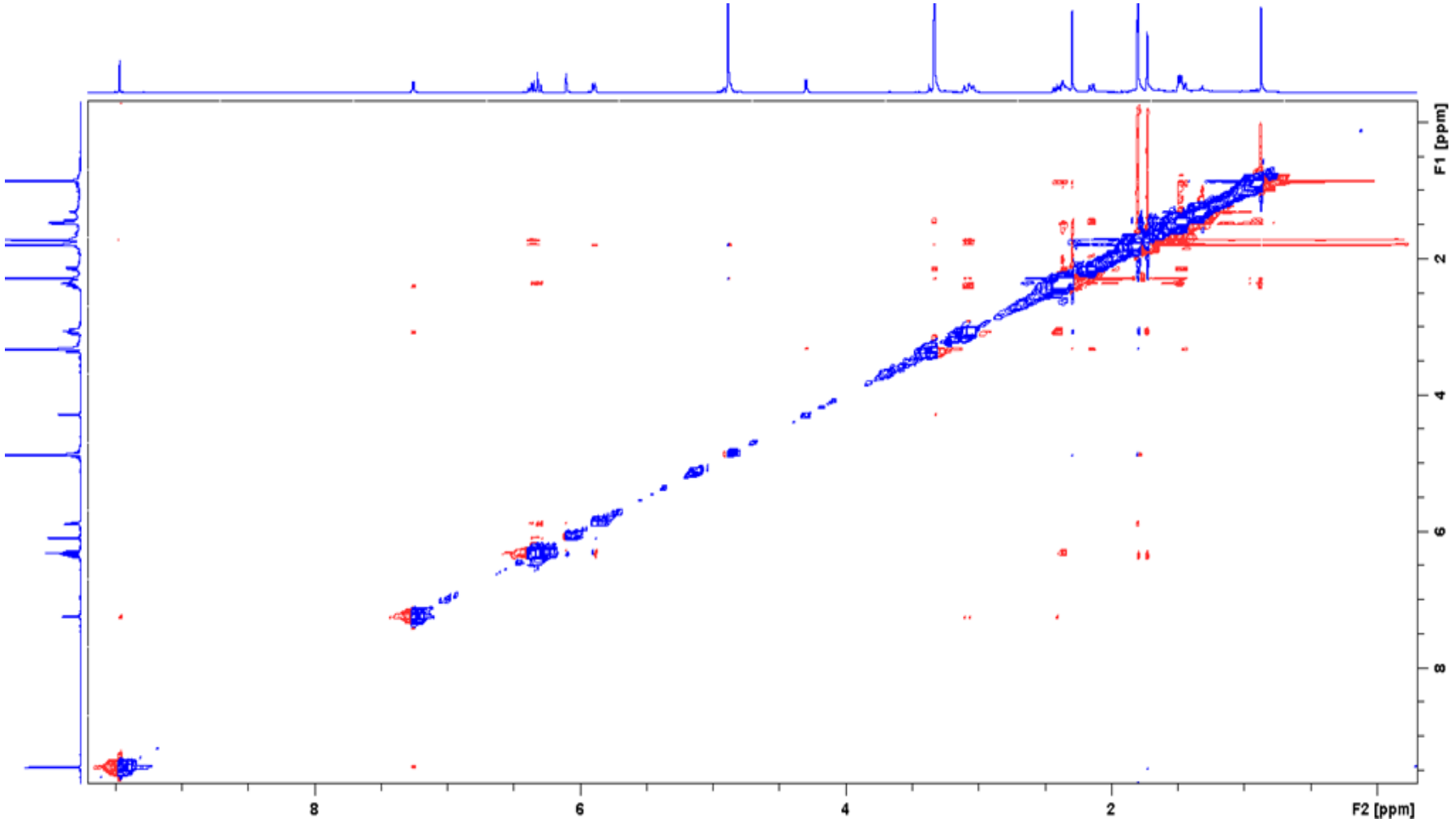

Figure S28. NOESY spectrum of 14,15-dehydro-ophiobolin G (**4**).

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
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82 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
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Minimum:				-1.5				
Maximum:		500.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
387.2299	387.2300	-0.1	-0.3	9.5	1135.1	n/a	n/a	C25 H32 O2 Na

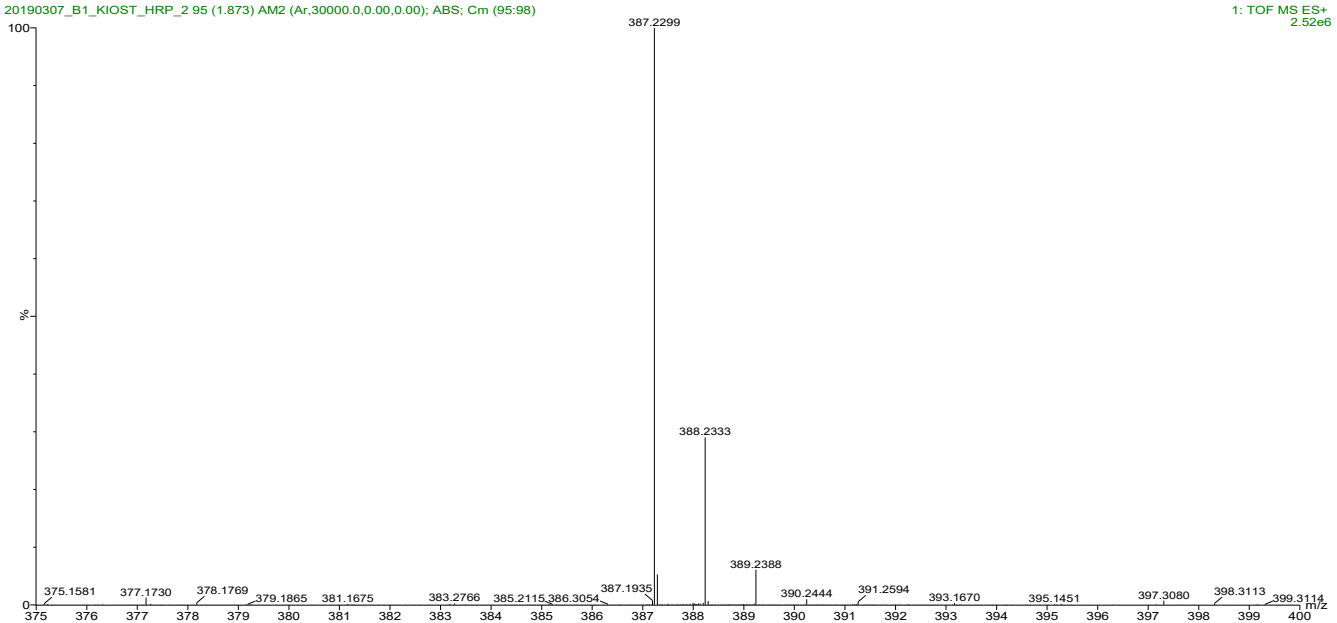

Figure S29. HRESIMS data of 14,15-dehydro-(*Z*)-14-ophiobolin G (**5**).

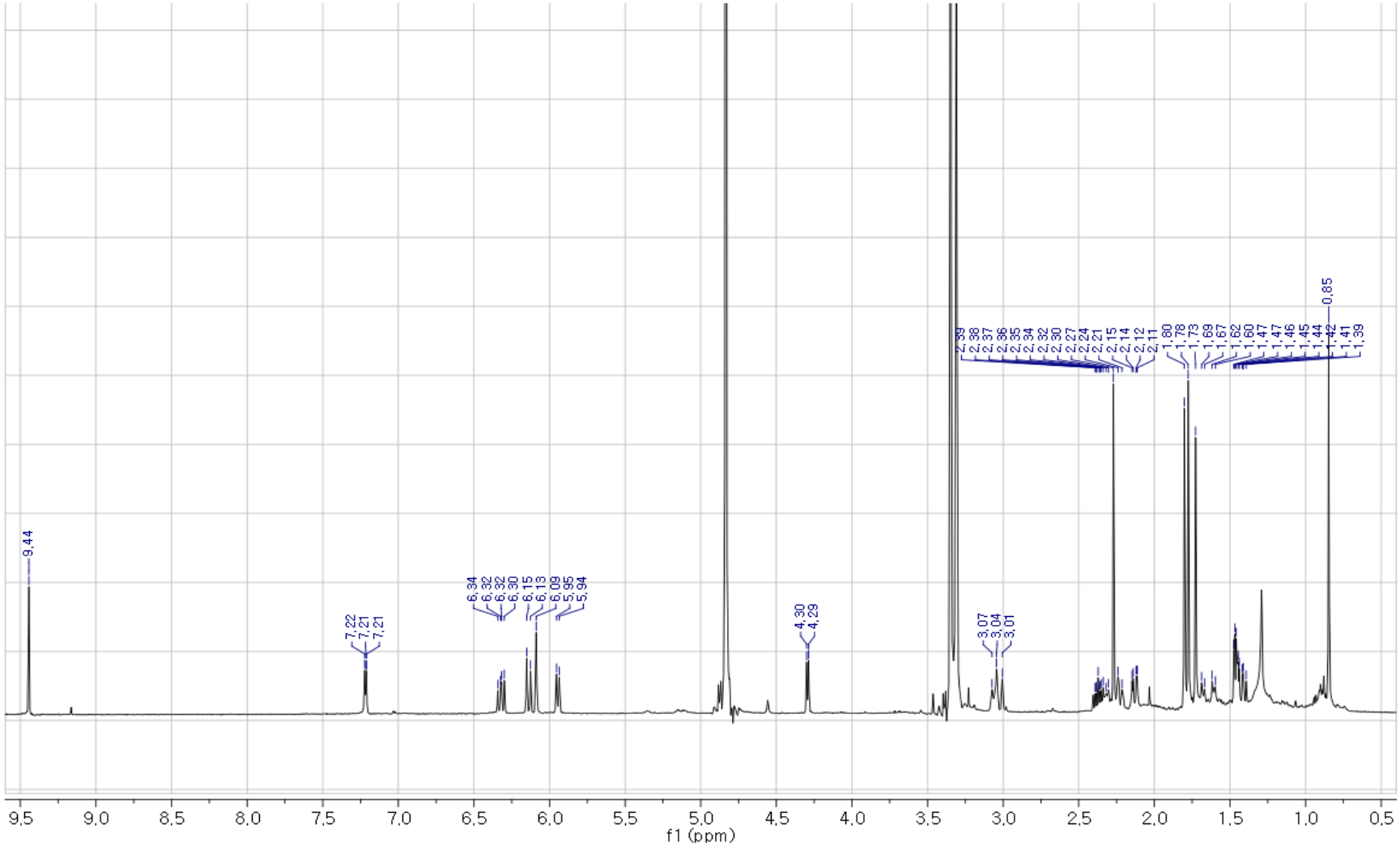

Figure S30. ^{1}H NMR spectrum of 14,15-dehydro-(*Z*)-14-ophiobolin G (**5**).

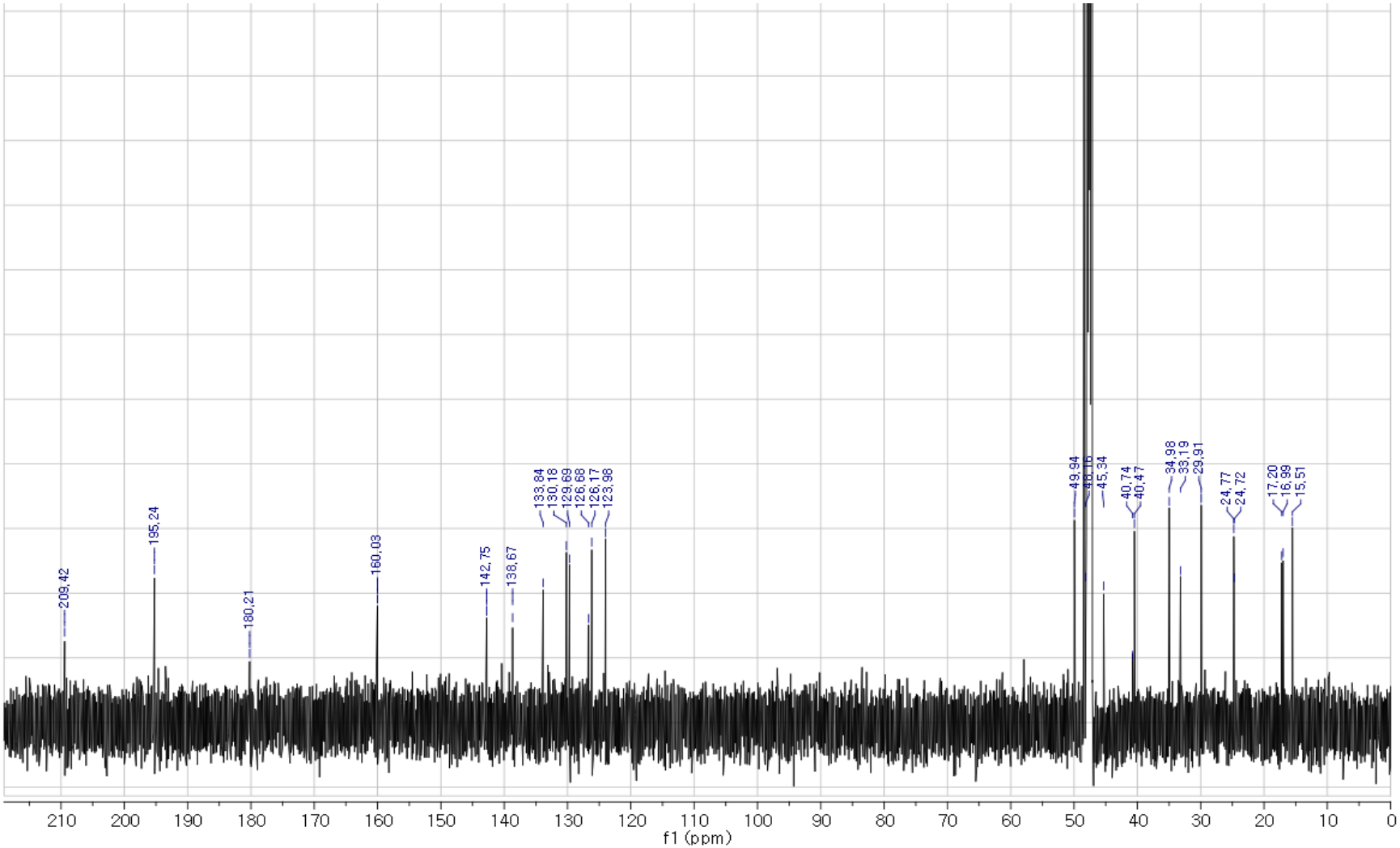

Figure S31. ^{13}C NMR spectrum of 14,15-dehydro-(*Z*)-14-ophiobolin G (**5**).

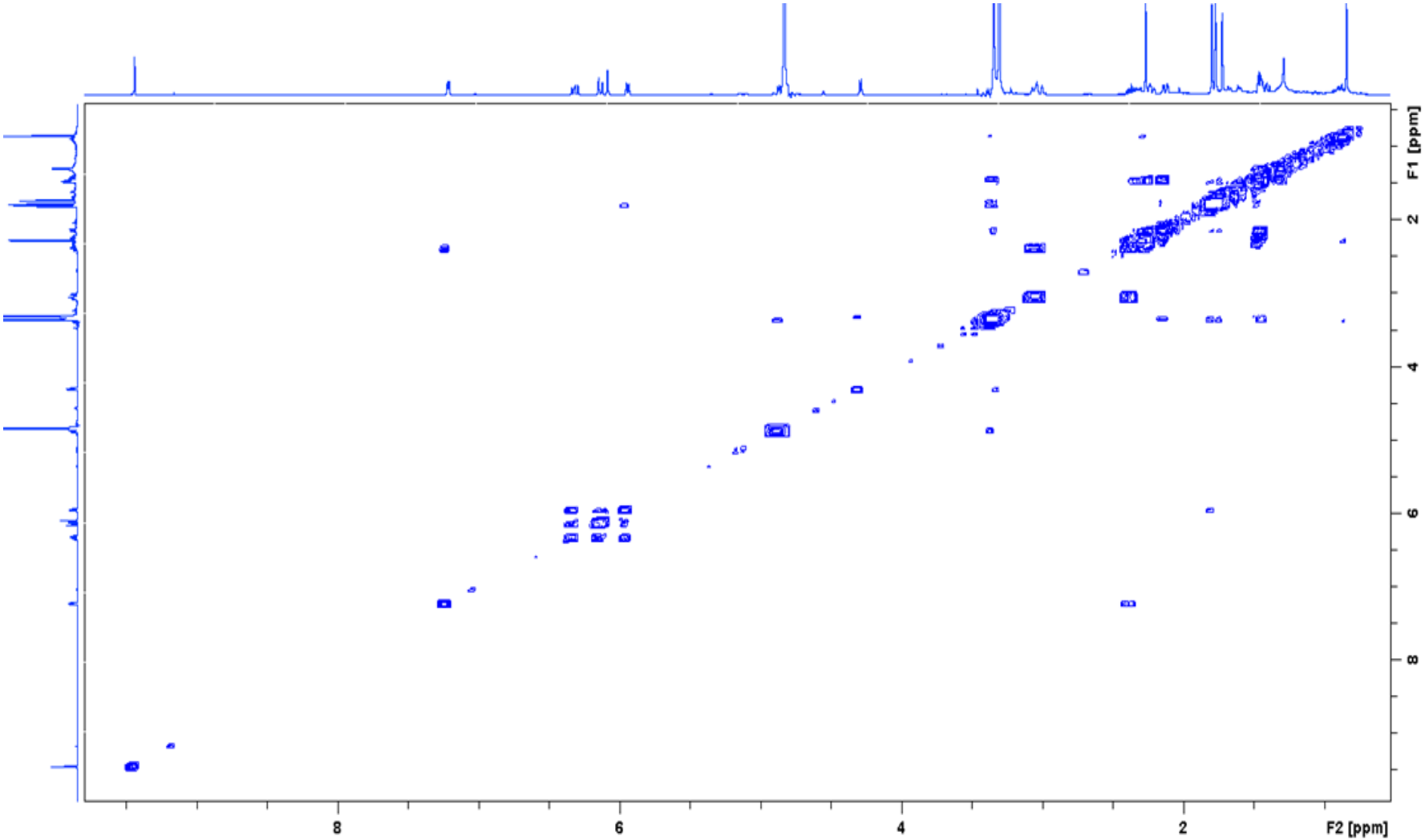

Figure S32. ^{1}H-^{1}H COSY spectrum of 14,15-dehydro-(*Z*)-14-ophiobolin G (**5**).

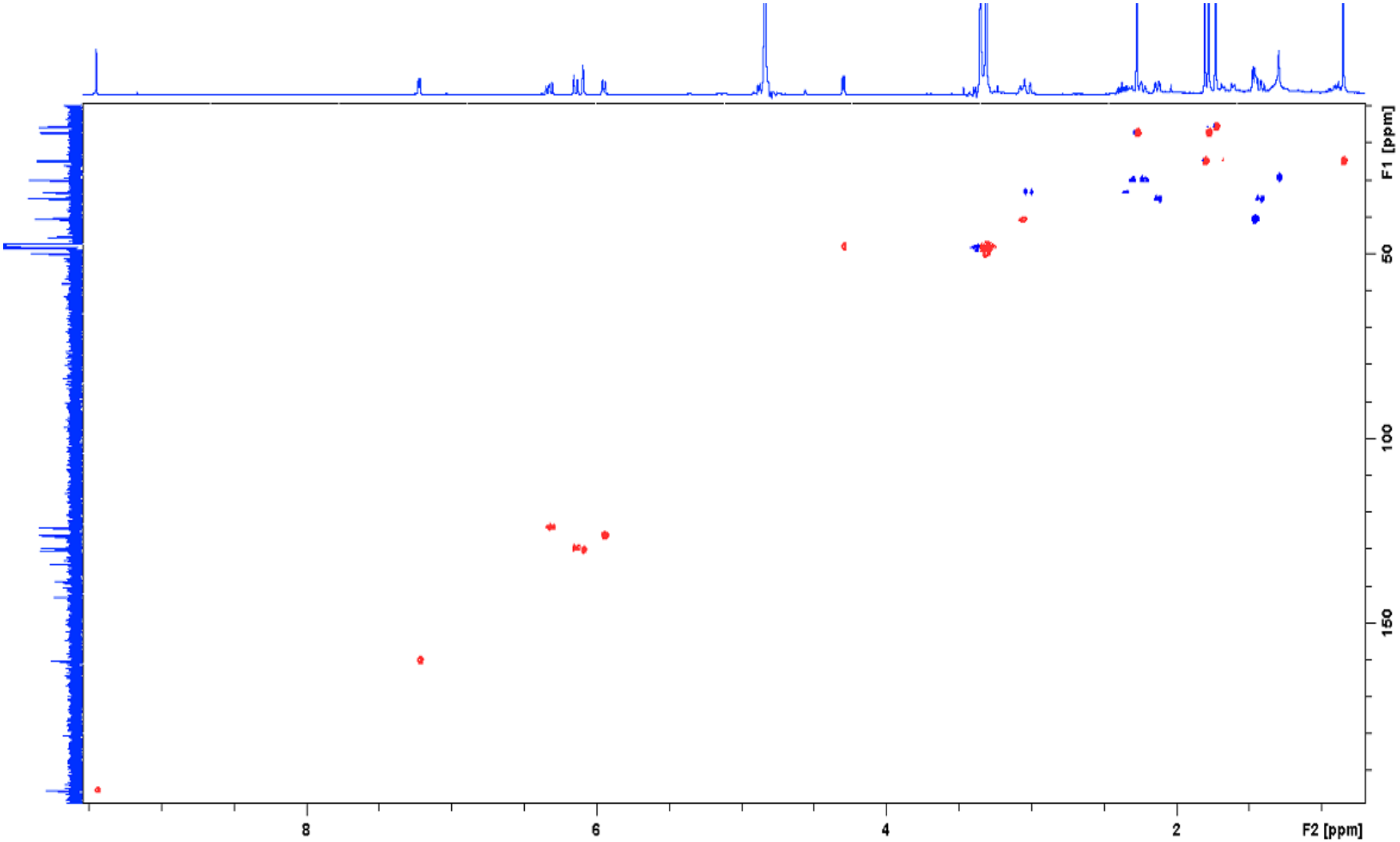

Figure S33. HSQC spectrum of 14,15-dehydro-(*Z*)-14-ophiobolin G (**5**).

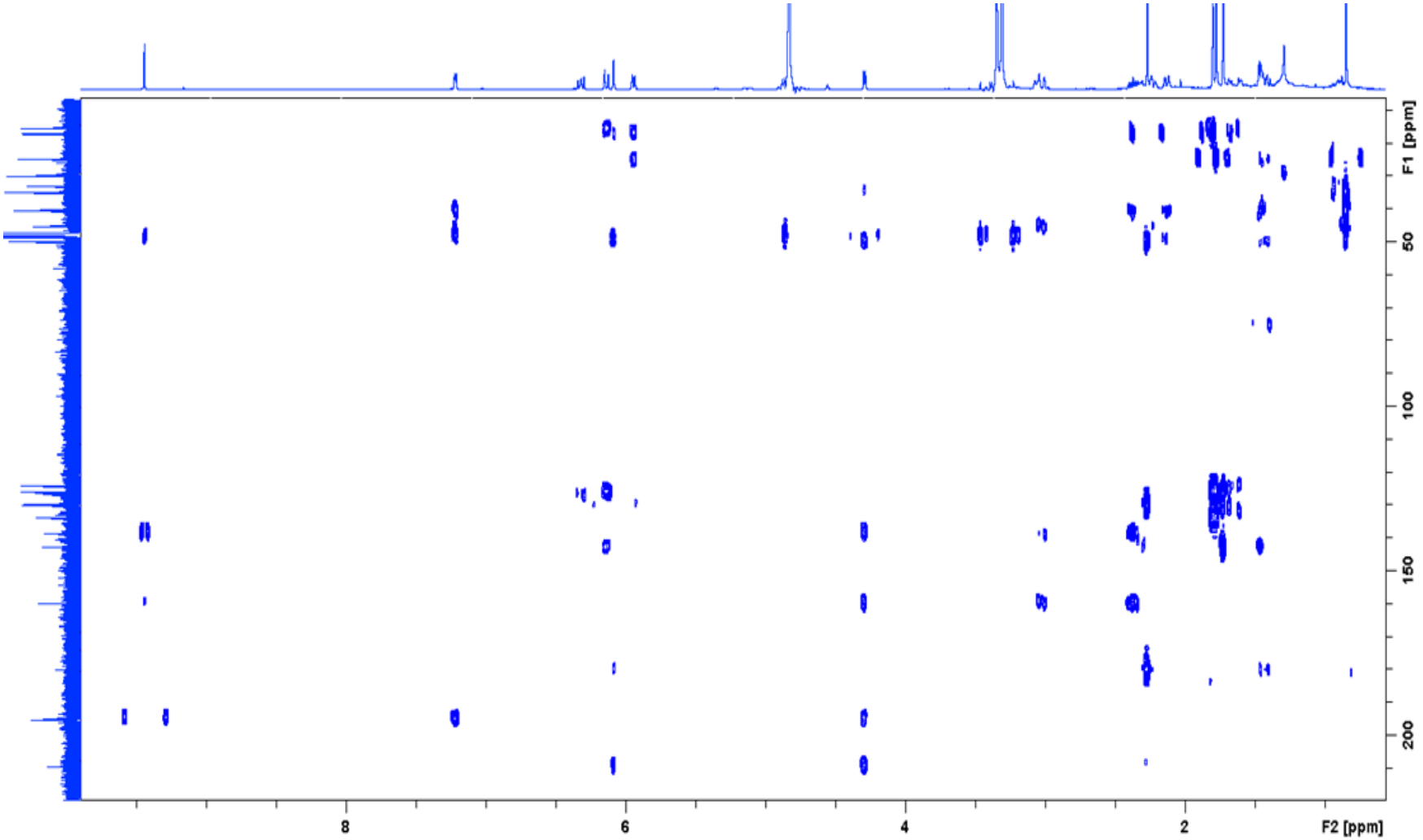

Figure S34. HMBC spectrum of 14,15-dehydro-(*Z*)-14-ophiobolin G (**5**).

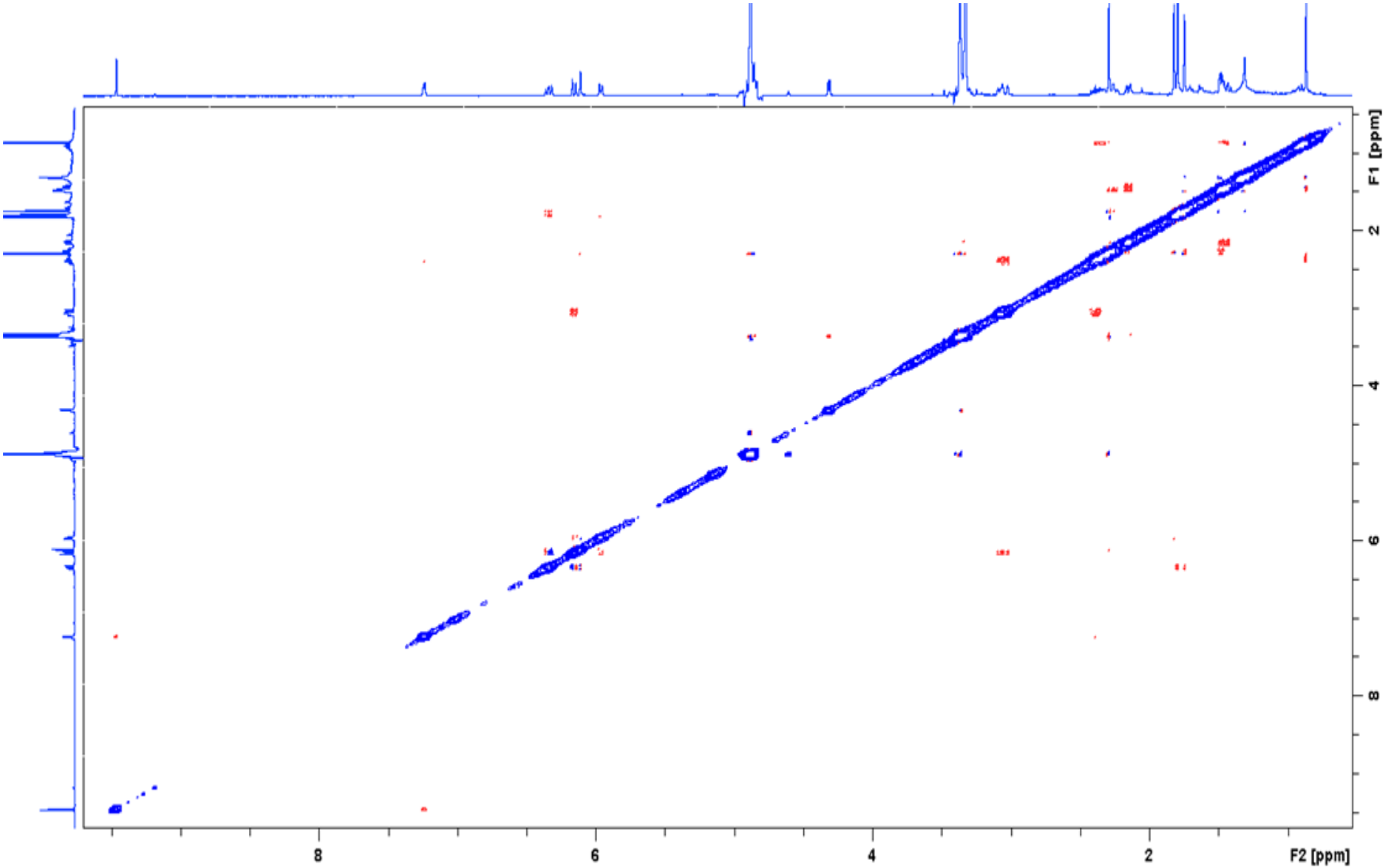

Figure S35. NOESY spectrum of 14,15-dehydro-(*Z*)-14-ophiobolin G (**5**).

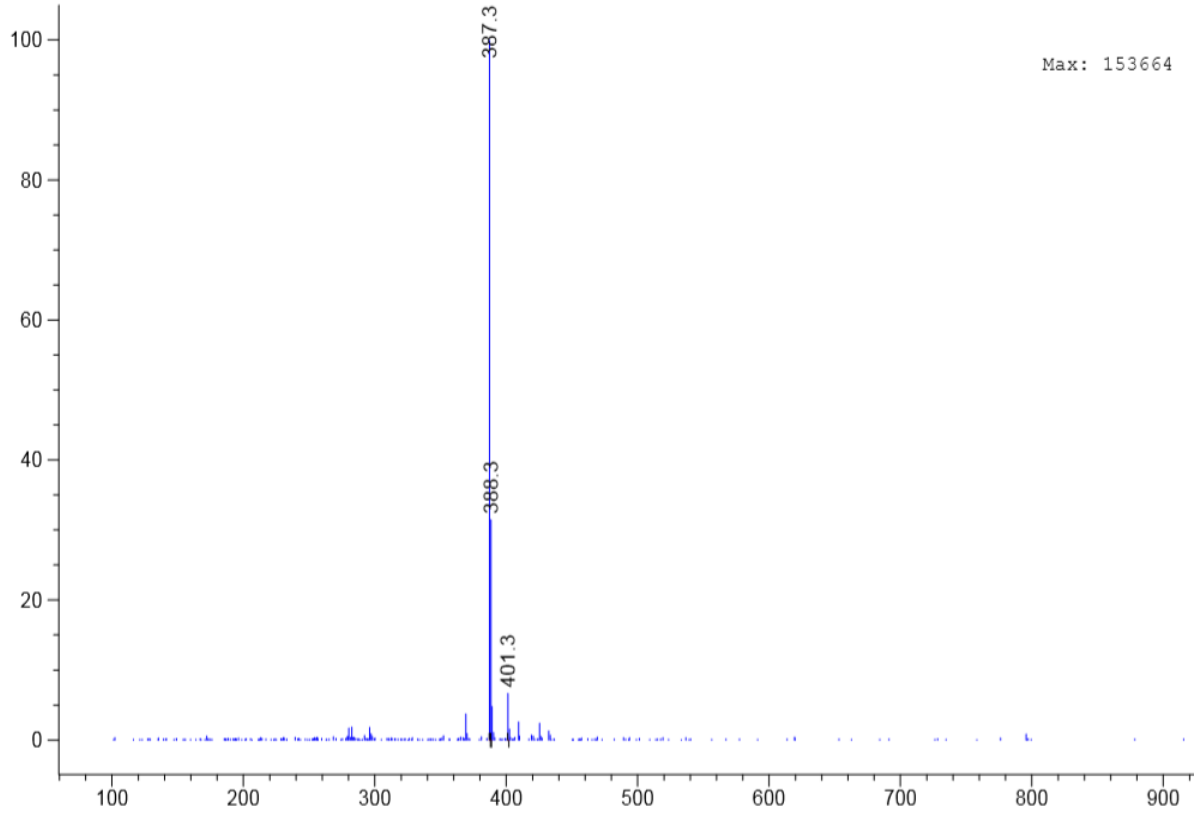

Figure S36. LRMS data of 6-*epi*-ophiobolin C (**6**).

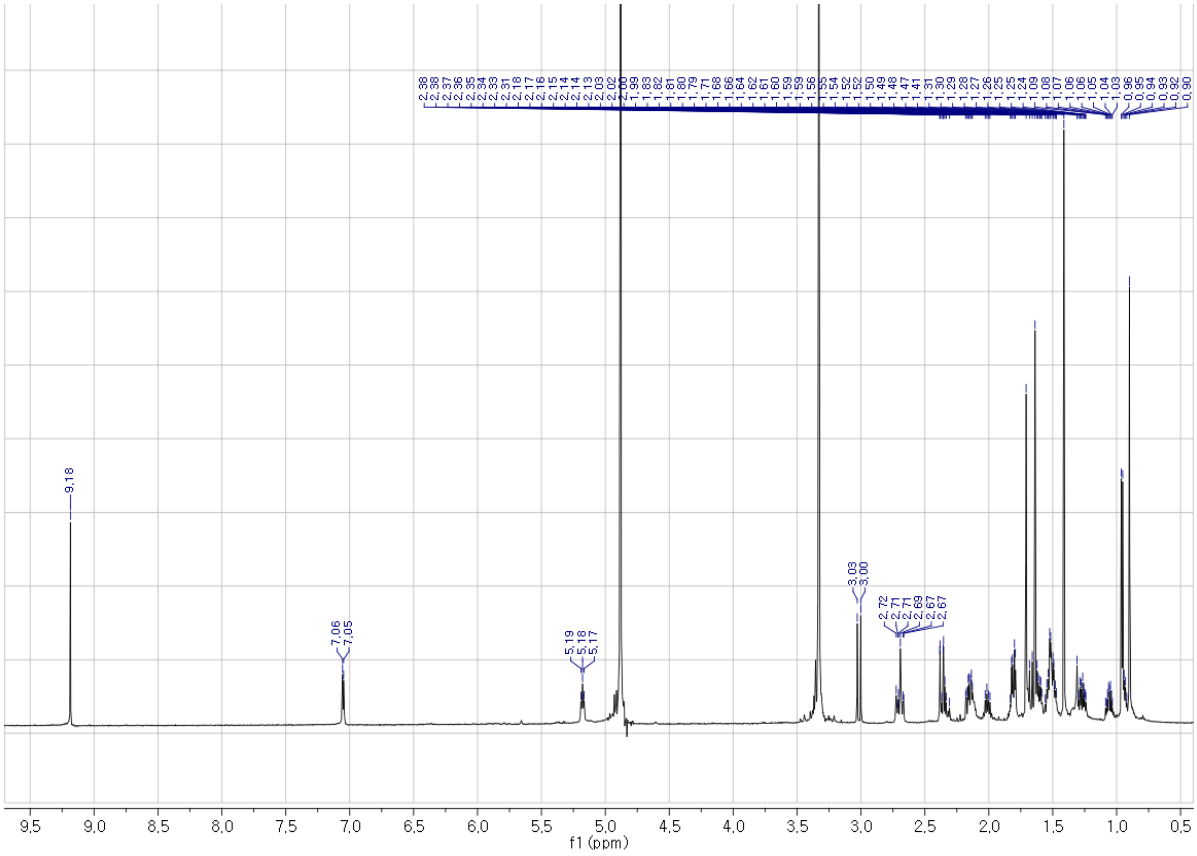

Figure S37. ^{1}H NMR spectrum of 6-*epi*-ophiobolin C (**6**).

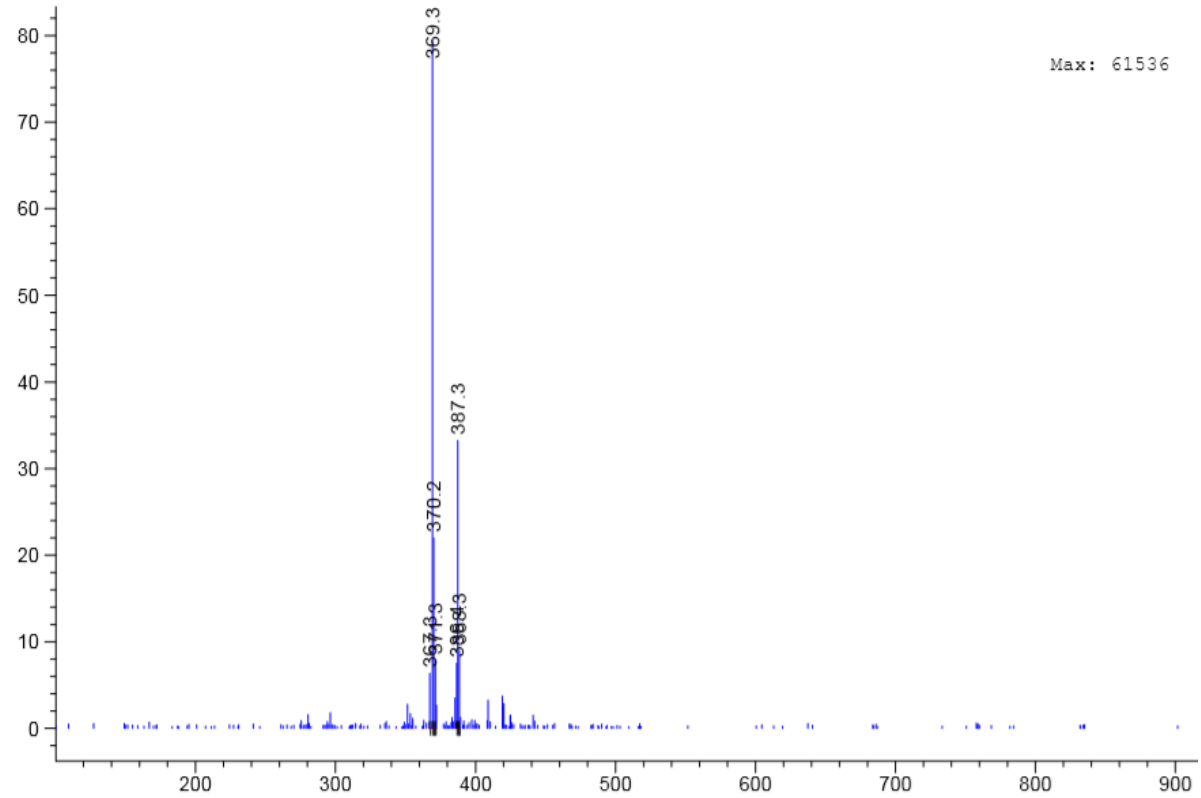

Figure S38. LRMS data of Ophiobolin C (**7**).

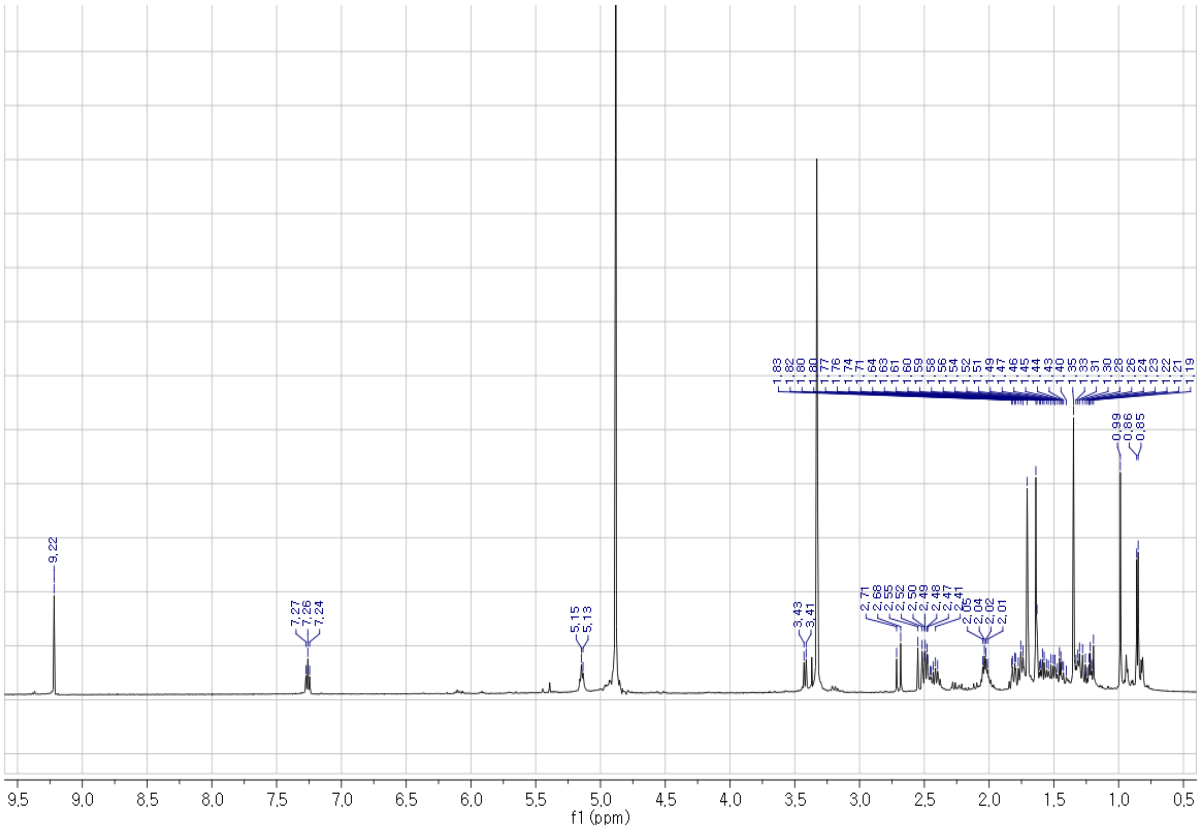

Figure S39. ^{1}H NMR spectrum of Ophiobolin C (**7**).

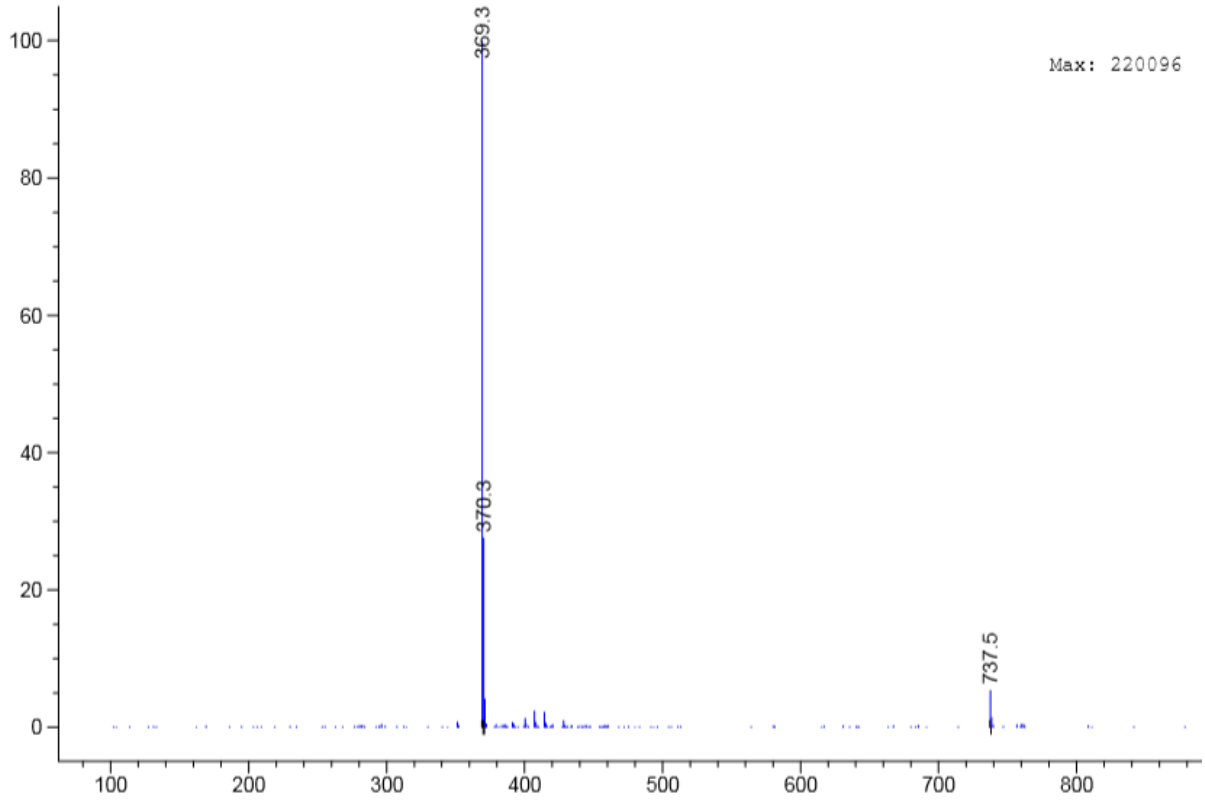

Figure S40. LRMS data of 6-*epi*-ophiobolin N (**8**).

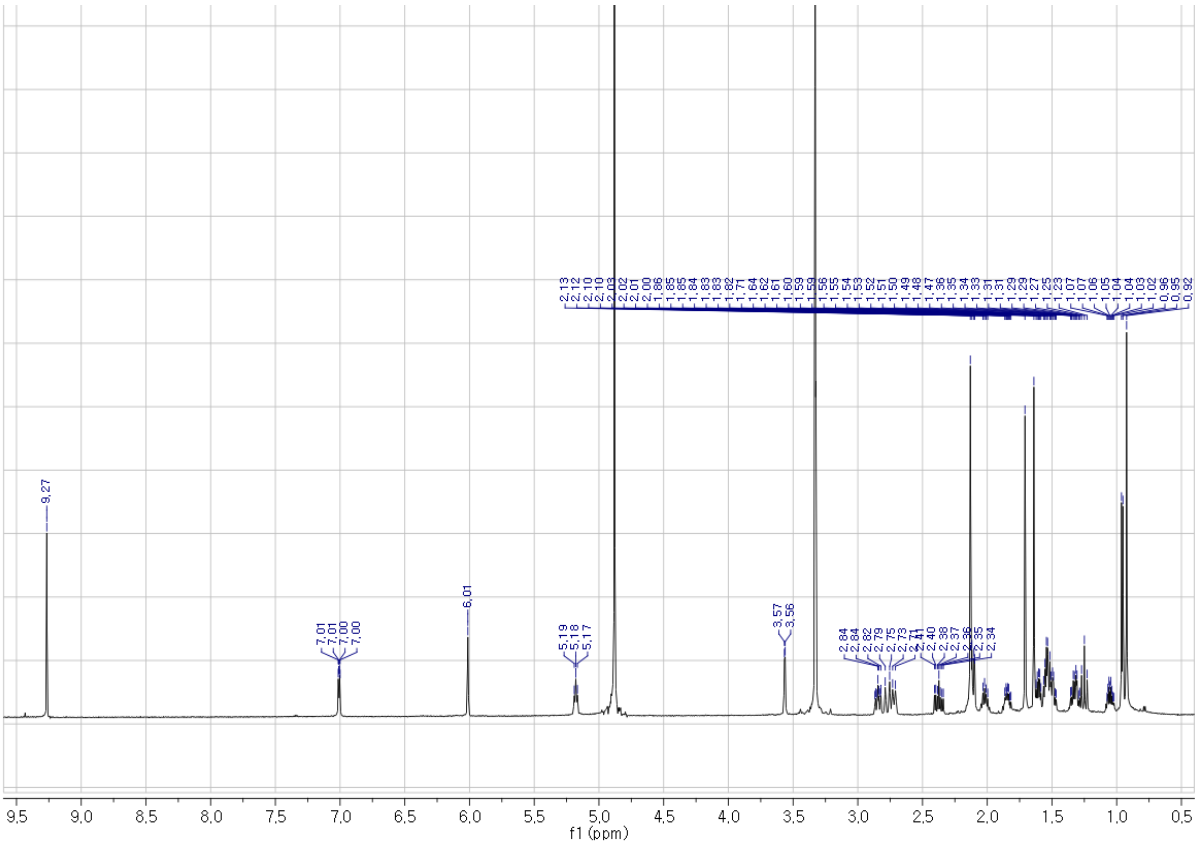

Figure S41. ^{1}H NMR spectrum of 6-*epi*-ophiobolin N (**8**).

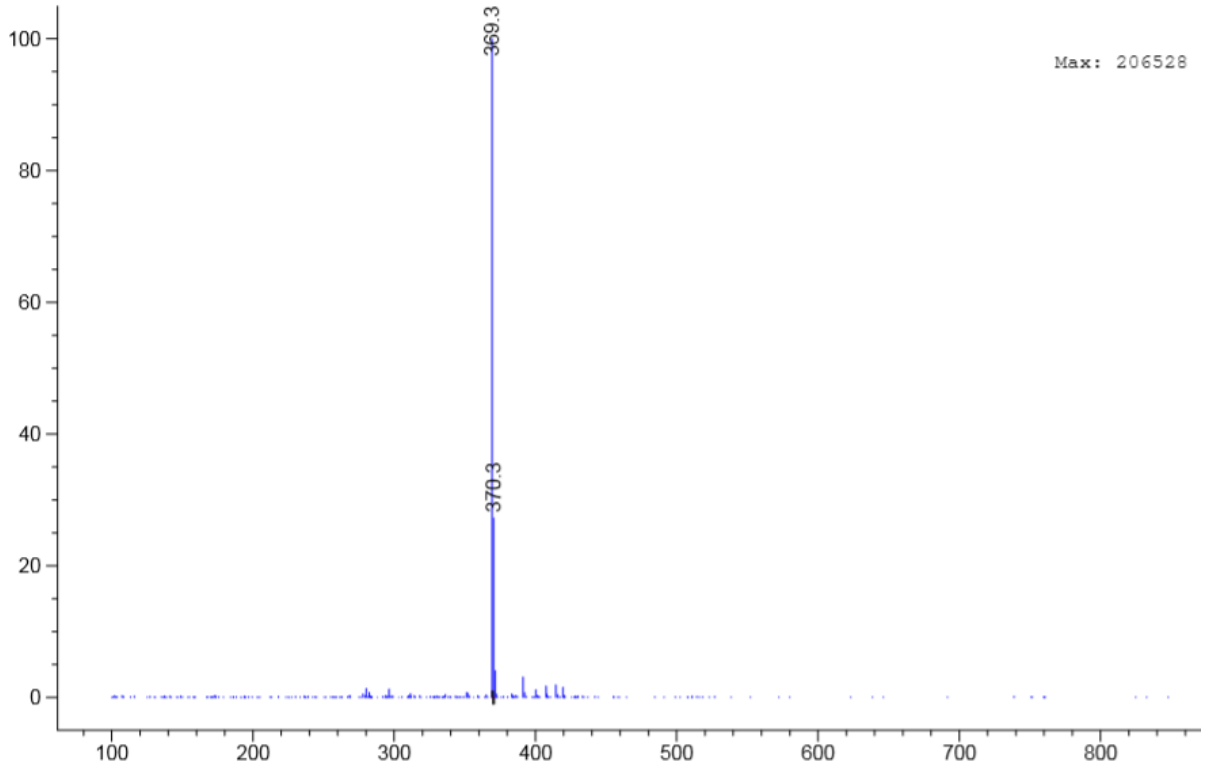

Figure S42. LRMS data of Ophiobolin N (**9**).

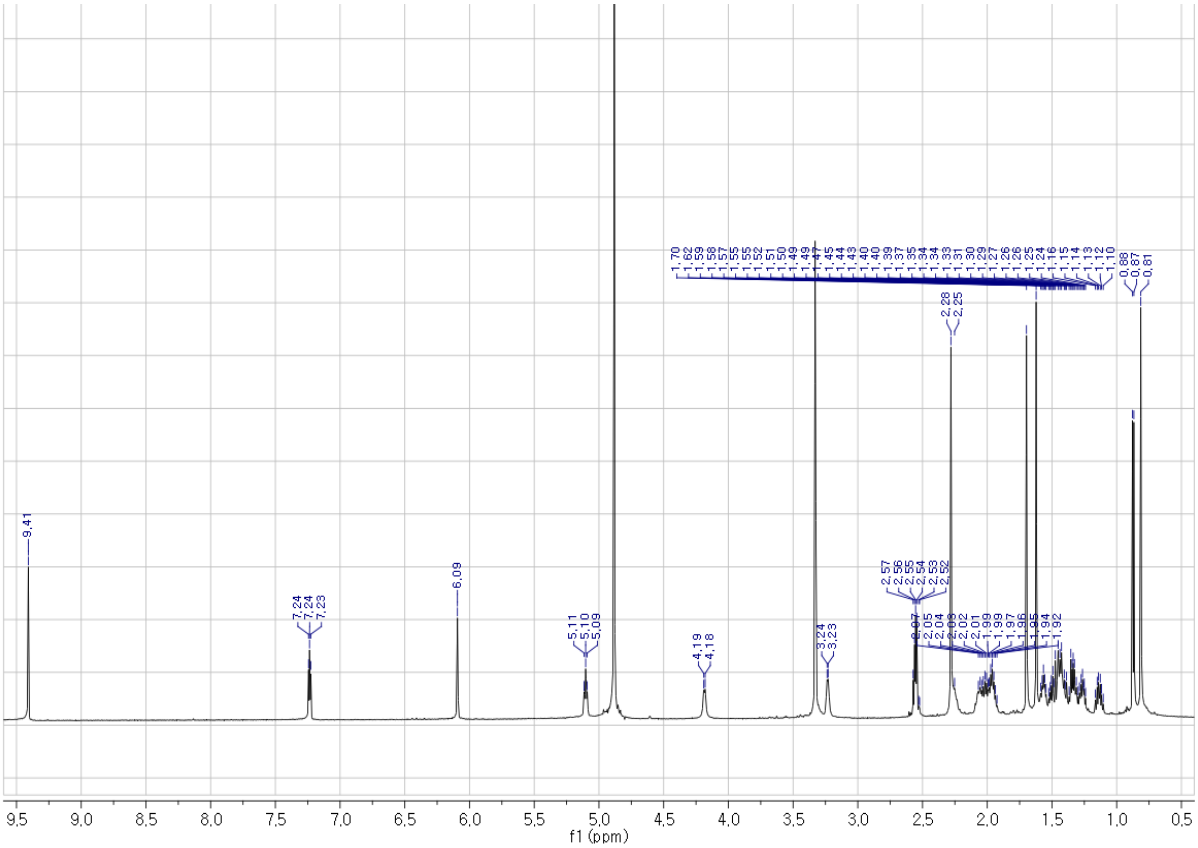

Figure S43. ^{1}H NMR spectrum of Ophiobolin N (**9**).