Supplementary Materials: Five New Cytotoxic Metabolites from the Marine Fungus *Neosartorya pseudofischeri*

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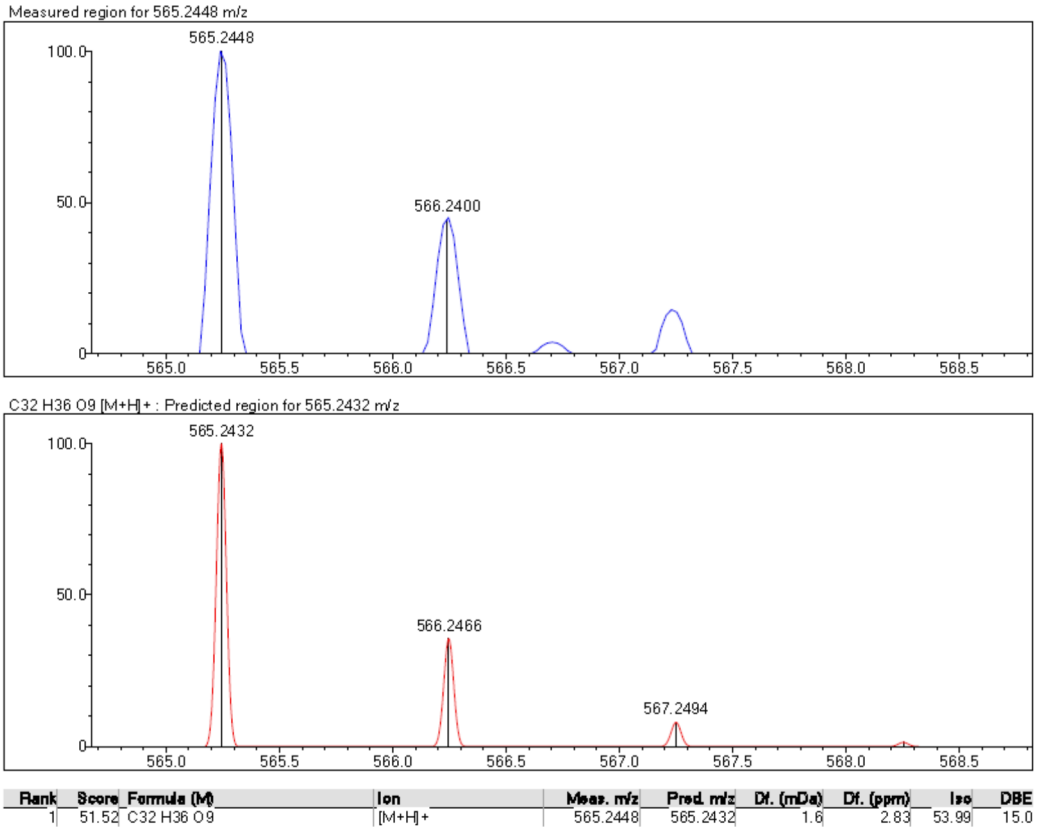


Figure S1. HR(+)ESIMS spectrum of 5-olefin phenylpyropene A (**1**).

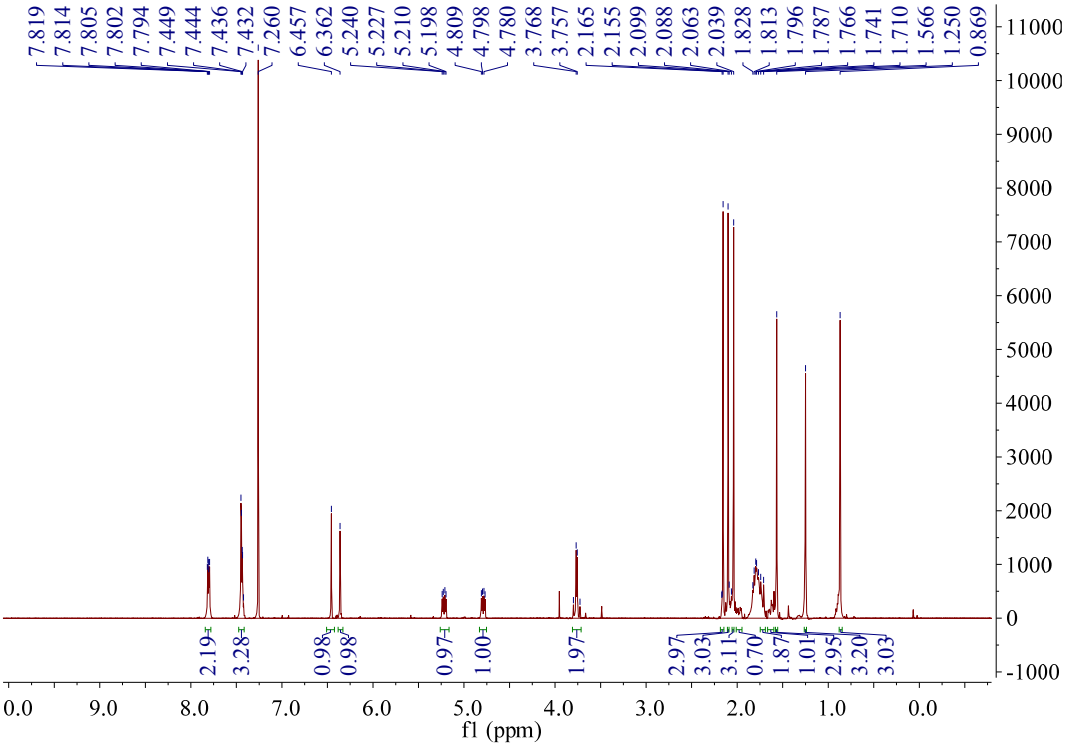


Figure S2. ^{1}H NMR spectrum of 5-olefin phenylpyropene A (**1**) in $CDCl_3$, 400 MHz.

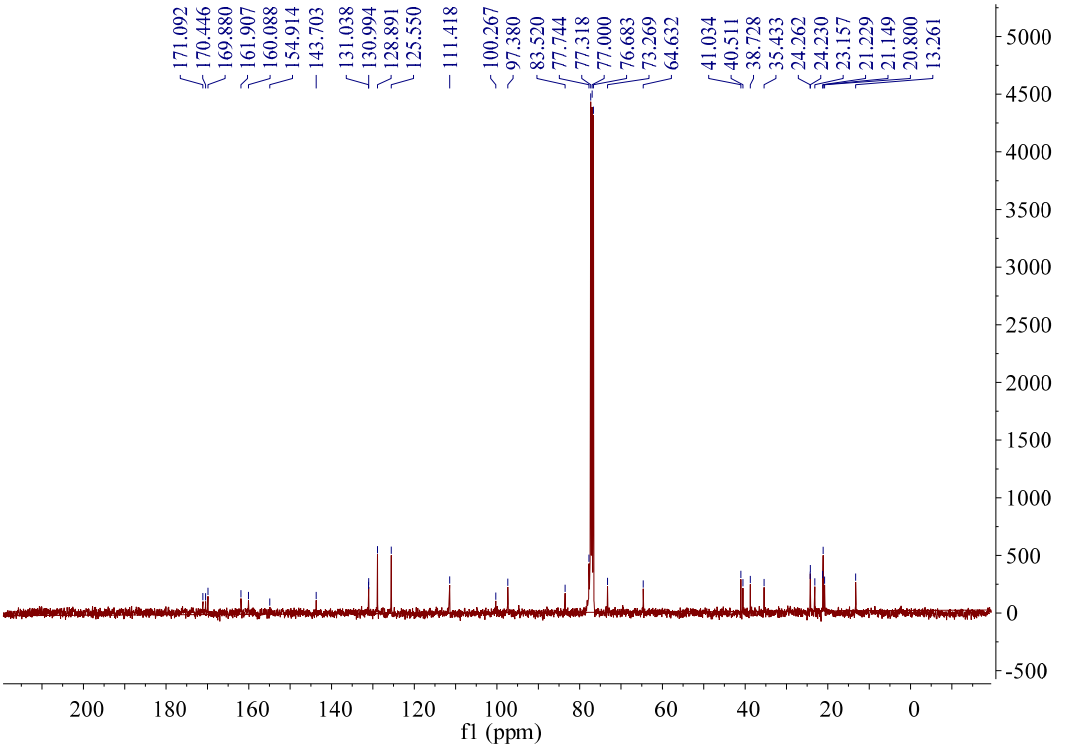


Figure S3. ^{13}C NMR spectrum of 5-olefin phenylpyropene A (**1**) in $CDCl_3$, 100 MHz.

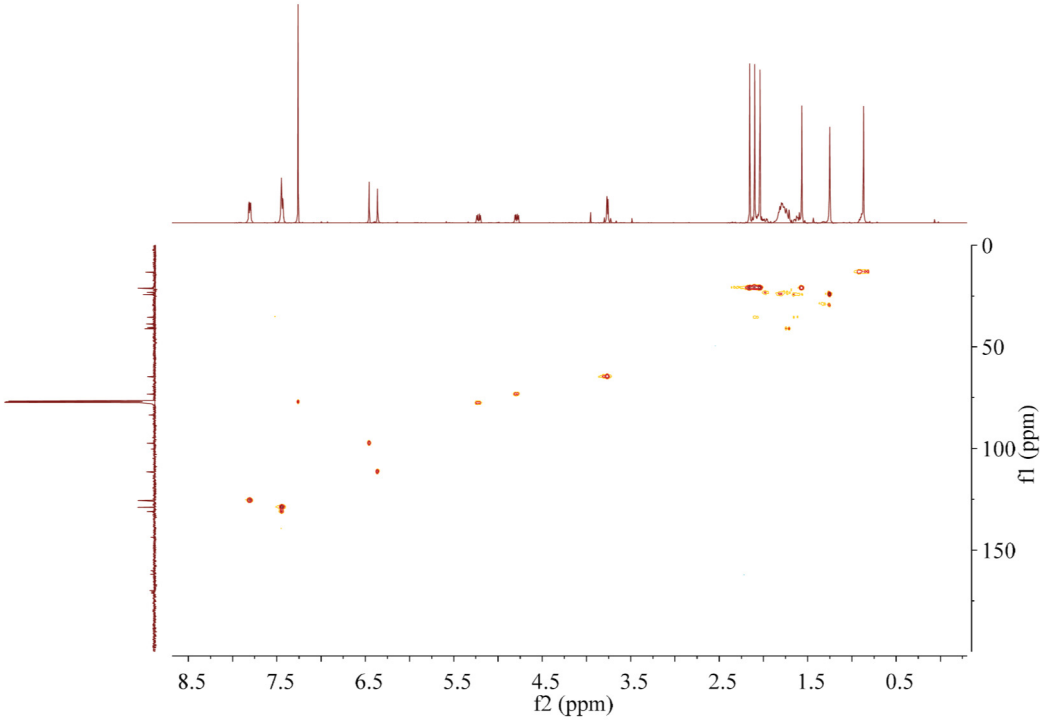


Figure S4. HSQC spectrum of 5-olefin phenylpyropene A (**1**).

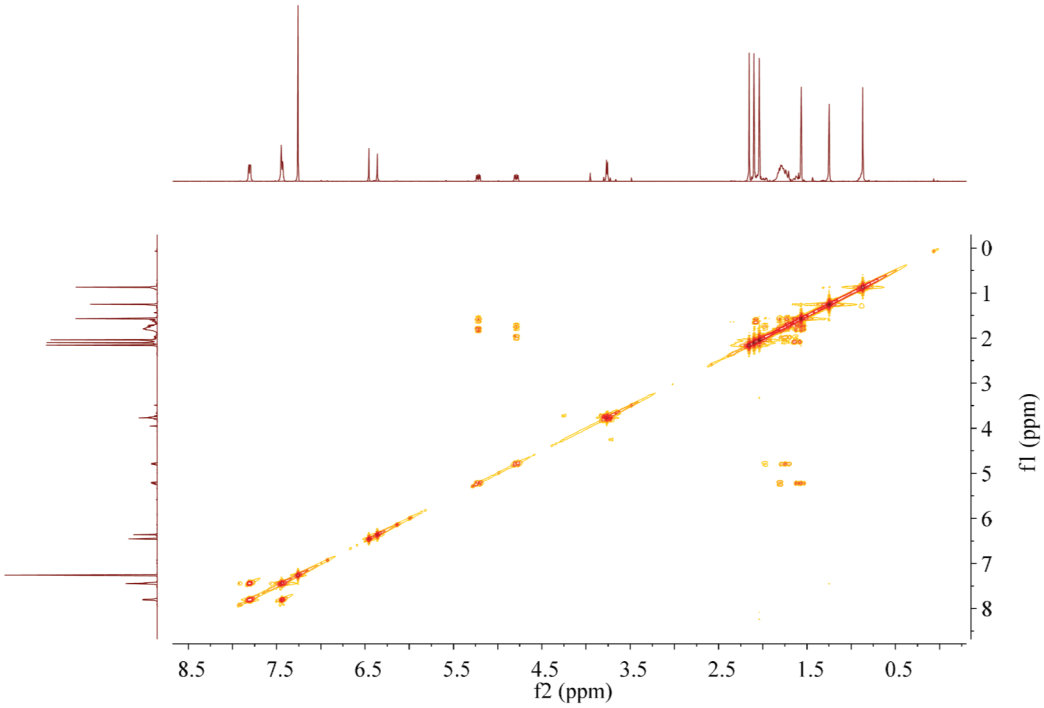


Figure S5. ^{1}H-^{1}H COSY spectrum of 5-olefin phenylpyropene A (**1**).

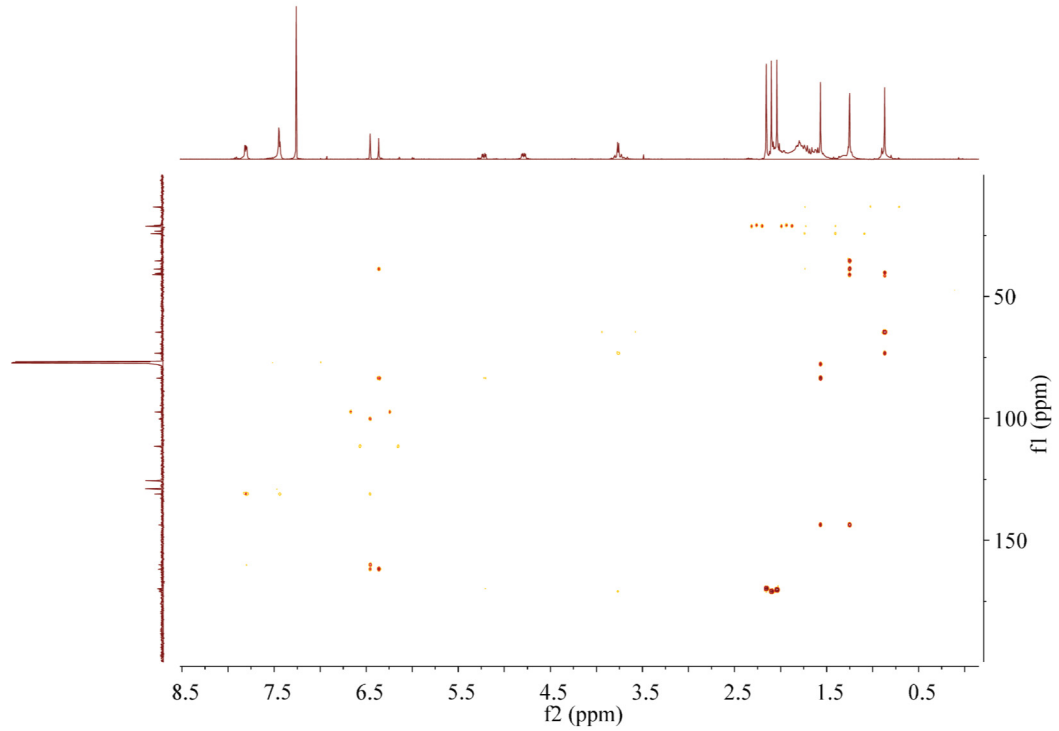


Figure S6. HMBC spectrum of 5-olefin phenylpyropene A (**1**).

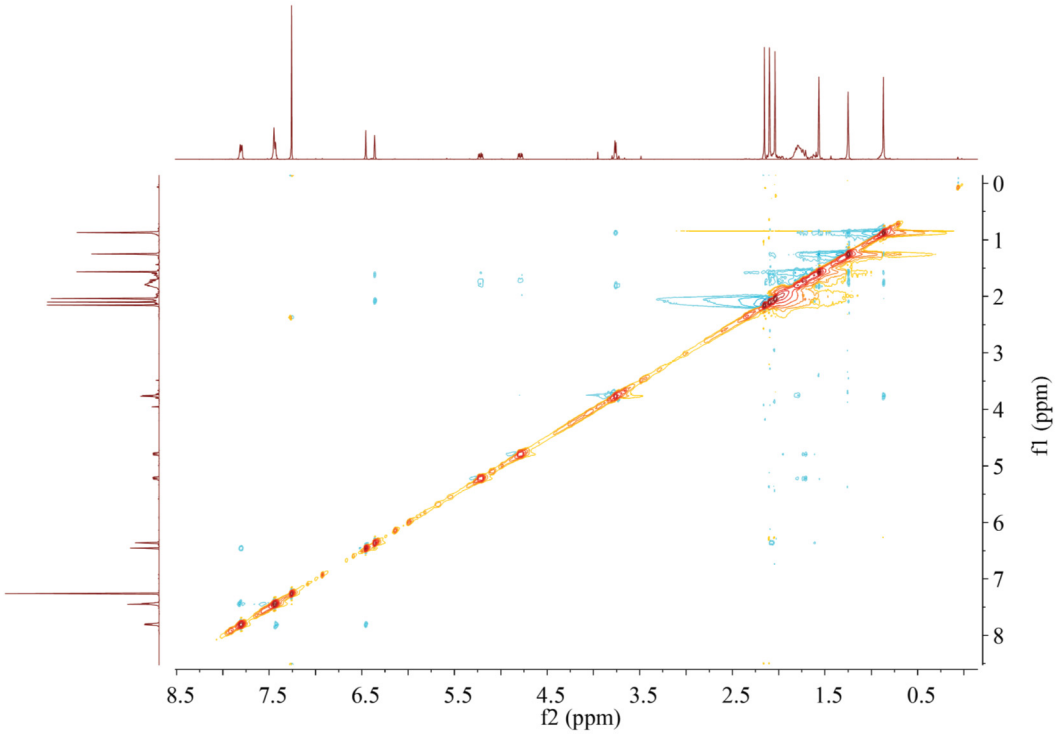


Figure S7. NOESY spectrum of 5-olefin phenylpyropene A (**1**).

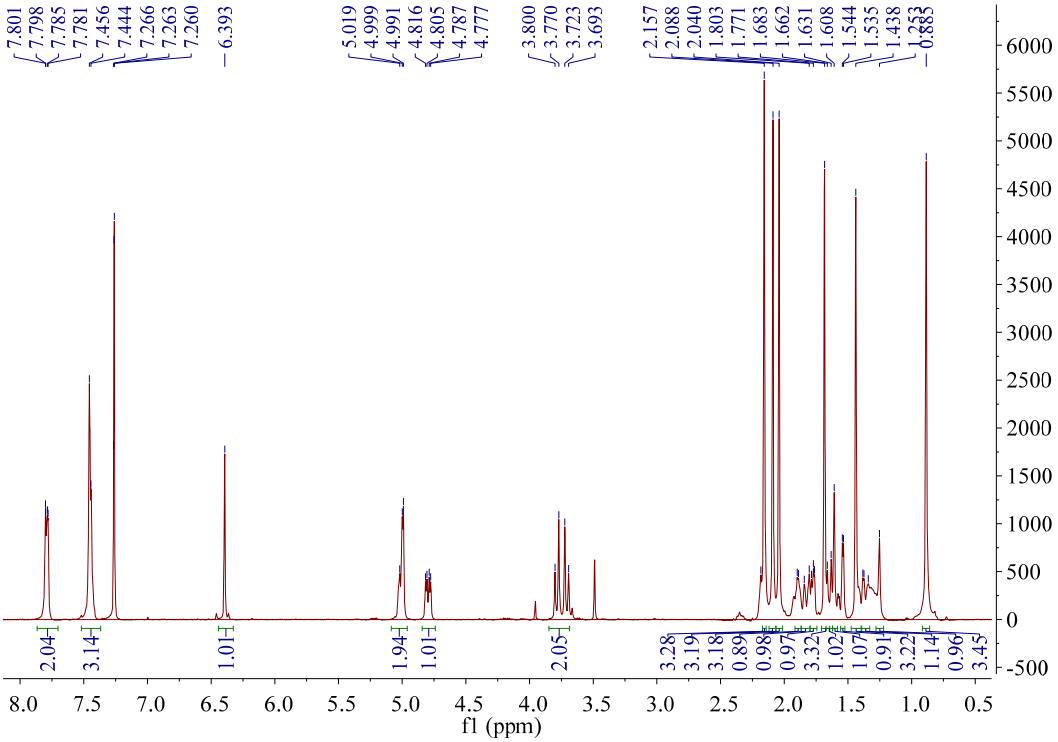


Figure S8. ^{1}H NMR spectrum of phenylpyropene A (**2**) in $CDCl_3$, 400 MHz.

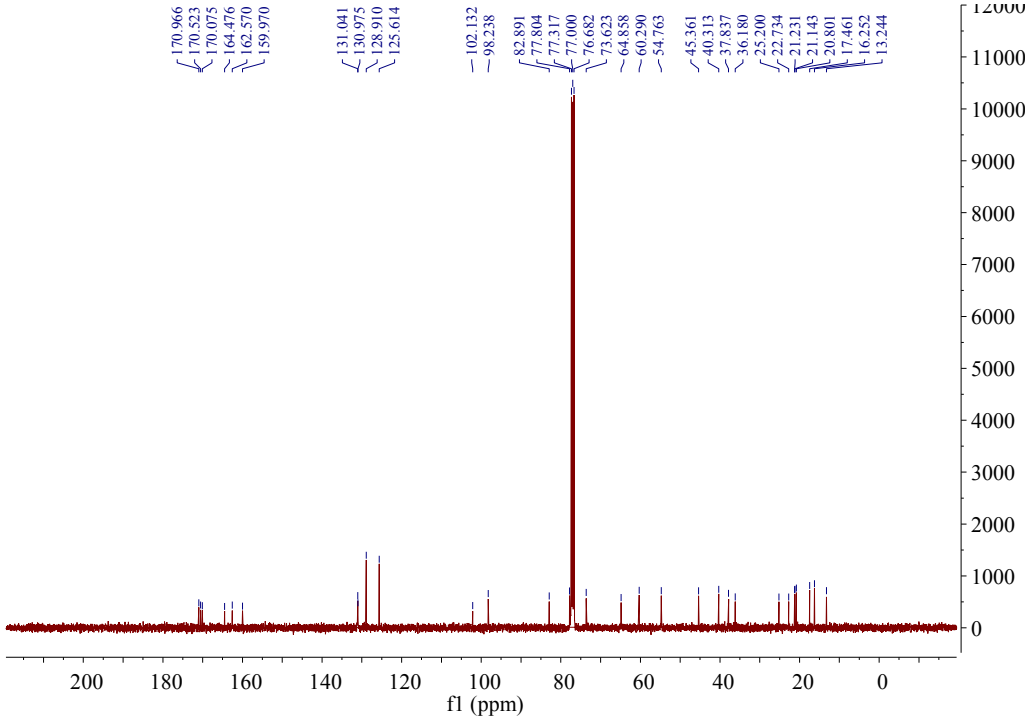


Figure S9. ^{13}C NMR spectrum of phenylpyropene A (**2**) in $CDCl_3$, 100 MHz.

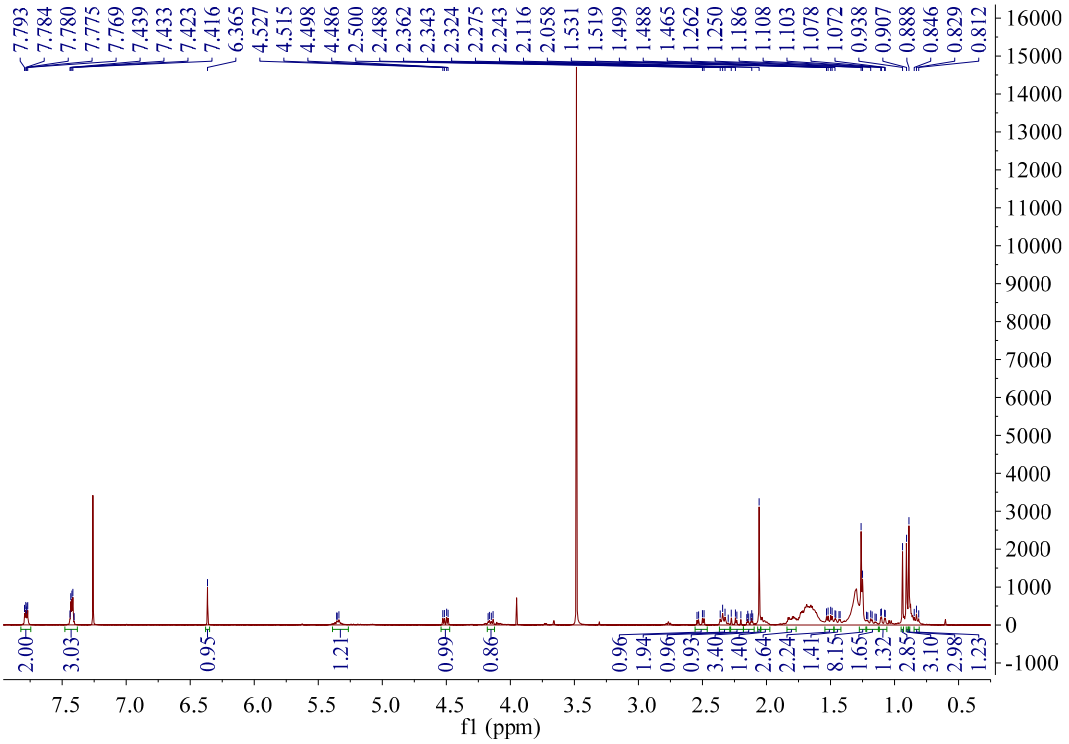


Figure S10. ^{1}H NMR spectrum of phenylpyropene C (**3**) in $CDCl_3$, 400 MHz.

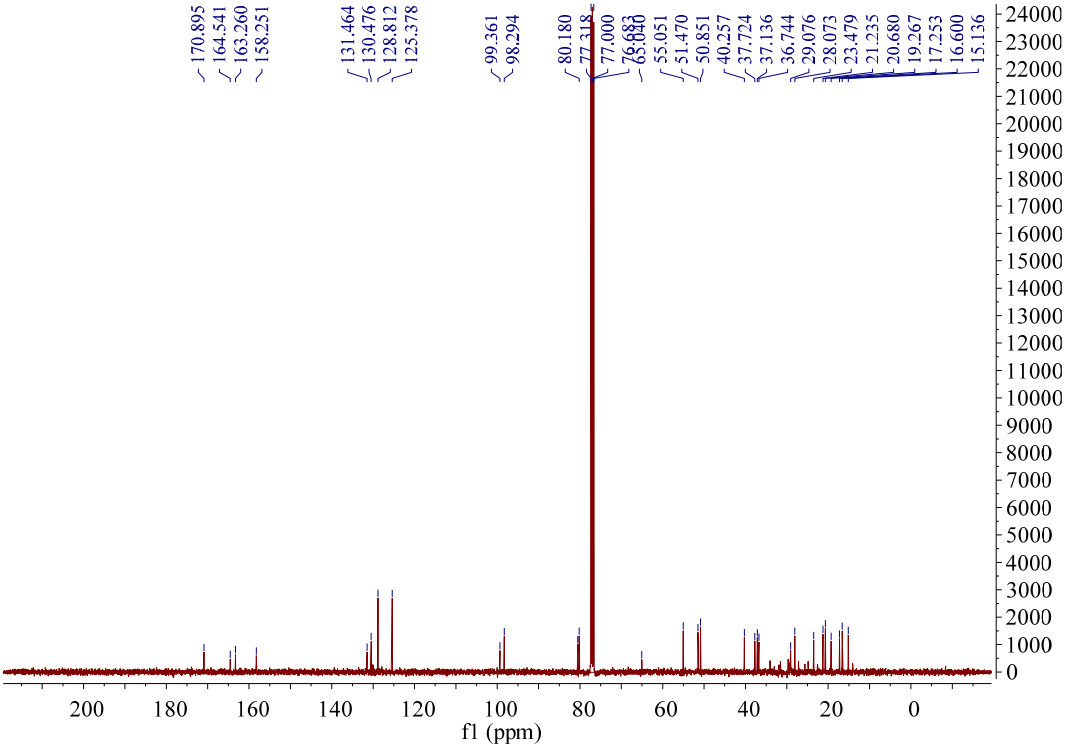
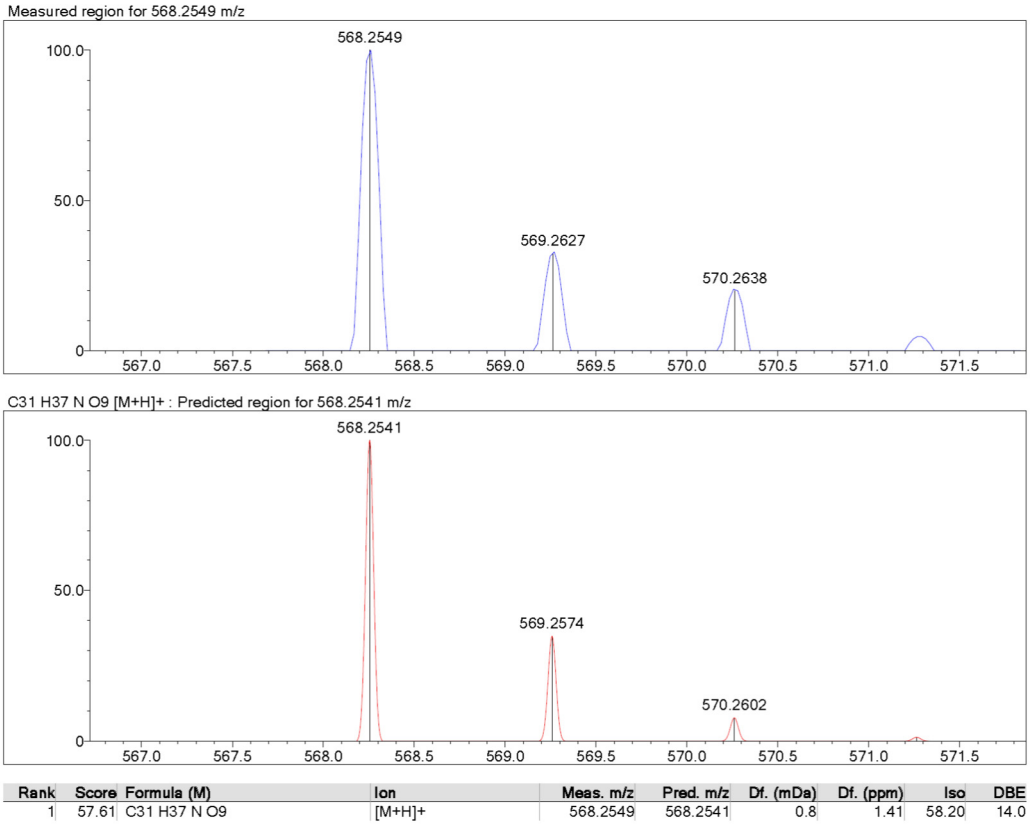


Figure S11. ^{13}C NMR spectrum of phenylpyropene C (**3**) in $CDCl_3$, 100 MHz.



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	57.61	C31 H37 N O9	[M+H]+	568.2549	568.2541	0.8	1.41	58.20	14.0

Figure S12. HR(+)ESIMS spectrum of 13-dehydroxylpyripyropene A (**4**).

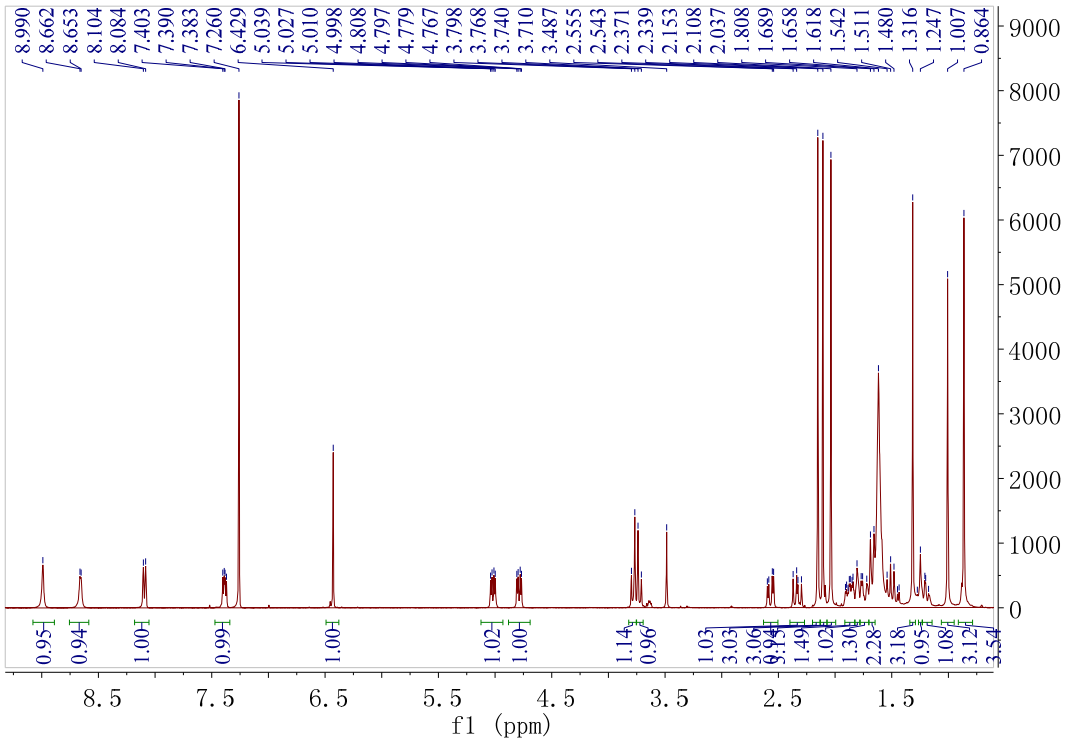


Figure S13. ^{1}H NMR spectrum of 13-dehydroxylpyripyropene A (**4**) in $CDCl_3$, 400 MHz.

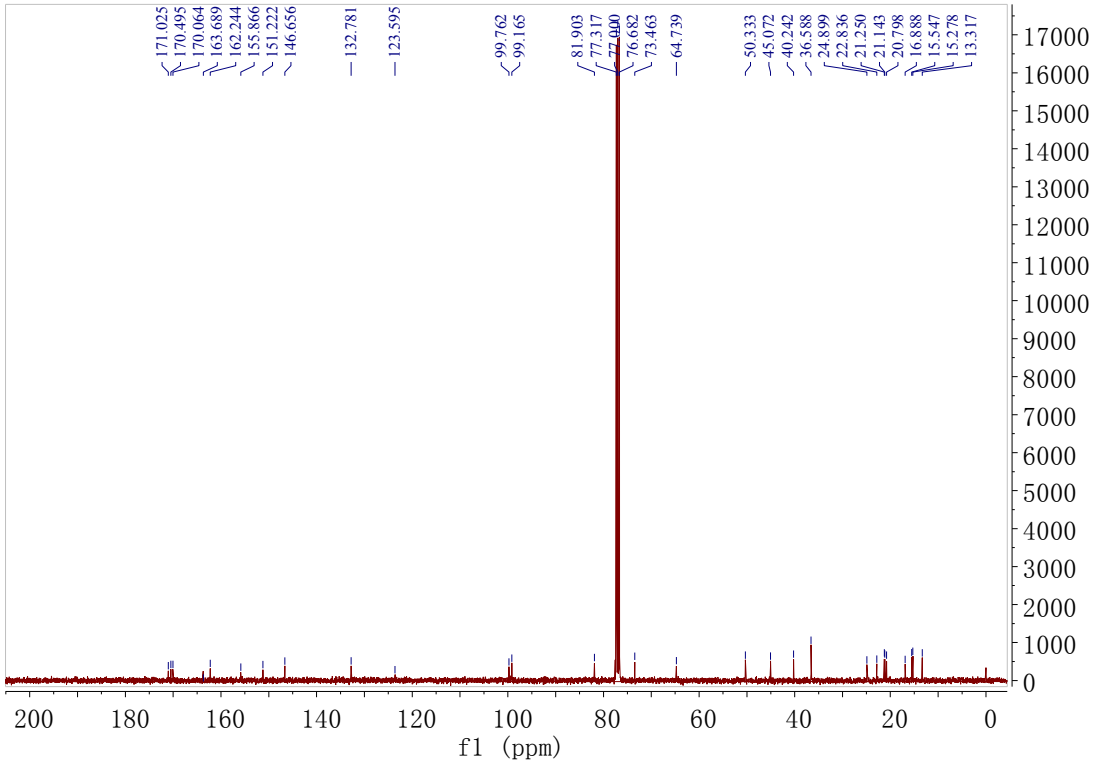


Figure S14. ^{13}C NMR spectrum of 13-dehydroxylpyripyropene A (**4**) in $CDCl_3$, 100 MHz.

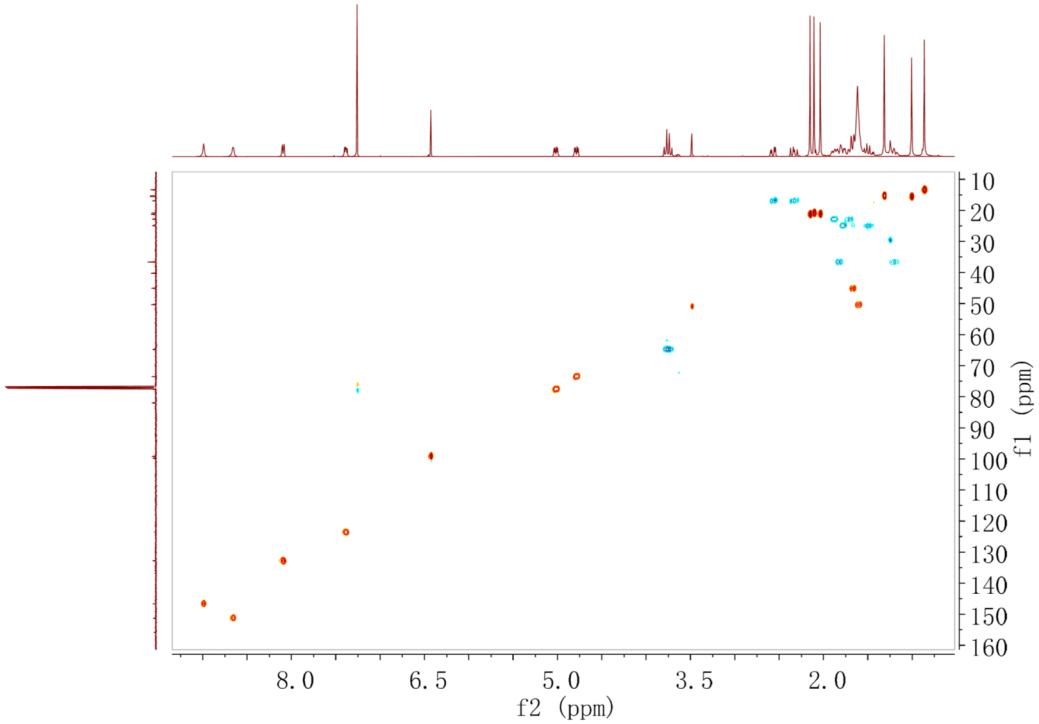


Figure S15. HSQC spectrum of 13-dehydroxylpyripyropene A (**4**).

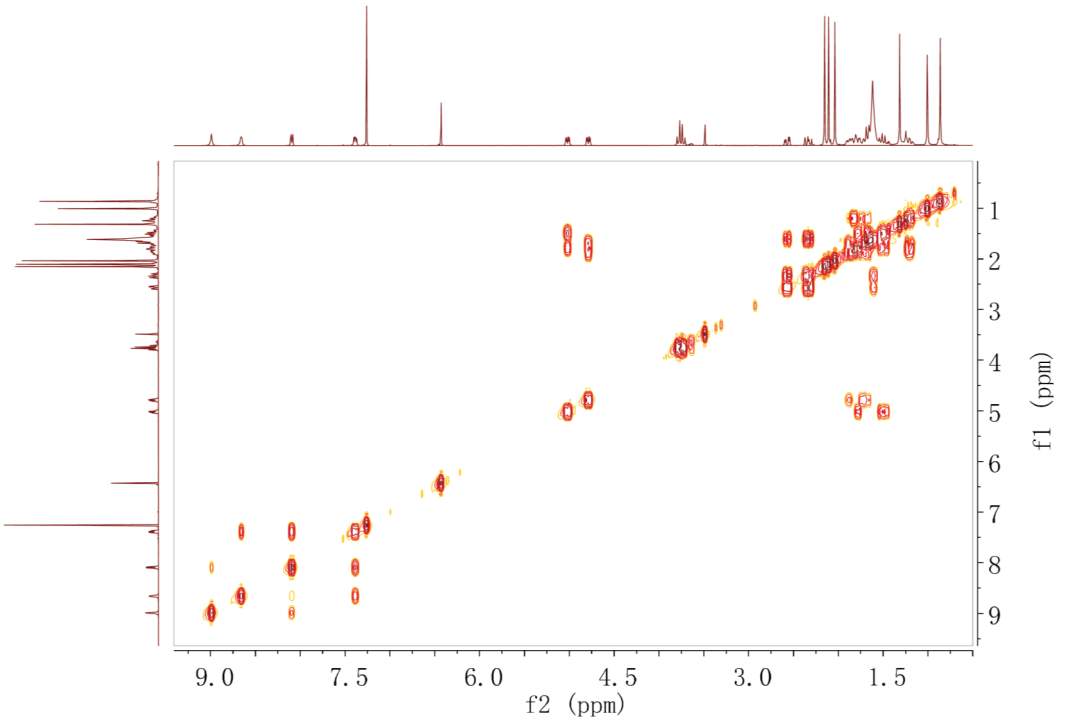


Figure S16. ^{1}H-^{1}H COSY spectrum of13-dehydroxylpyripyropene A (**4**).

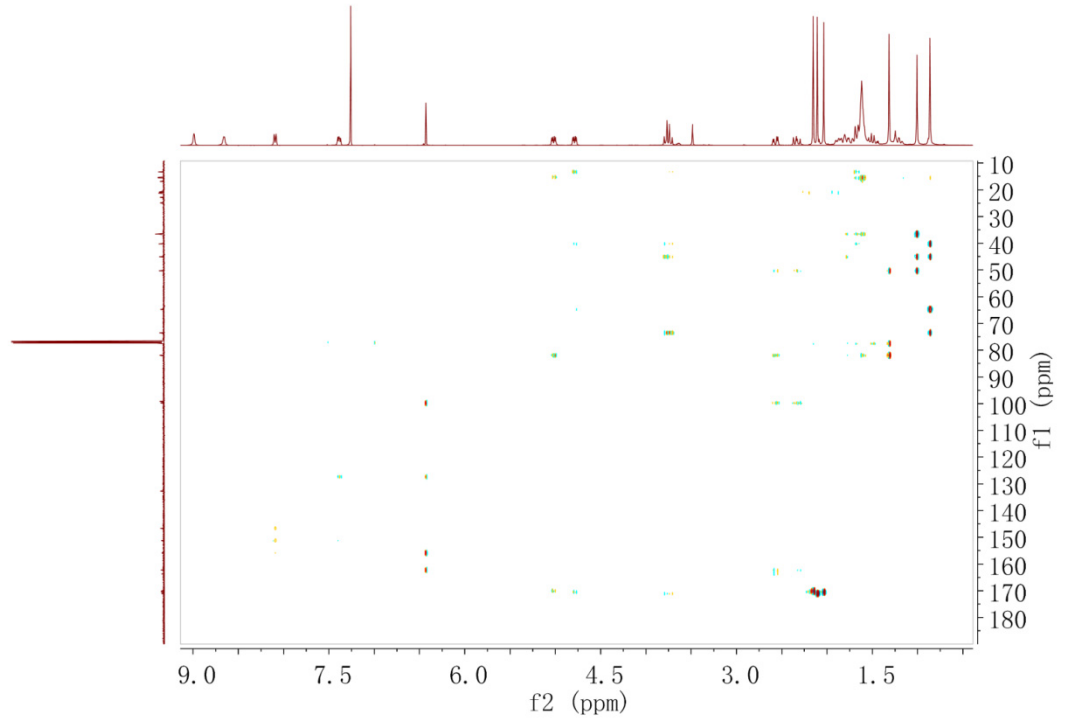


Figure S17. HMBC spectrum of 13-dehydroxylpyripyropene A (**4**).

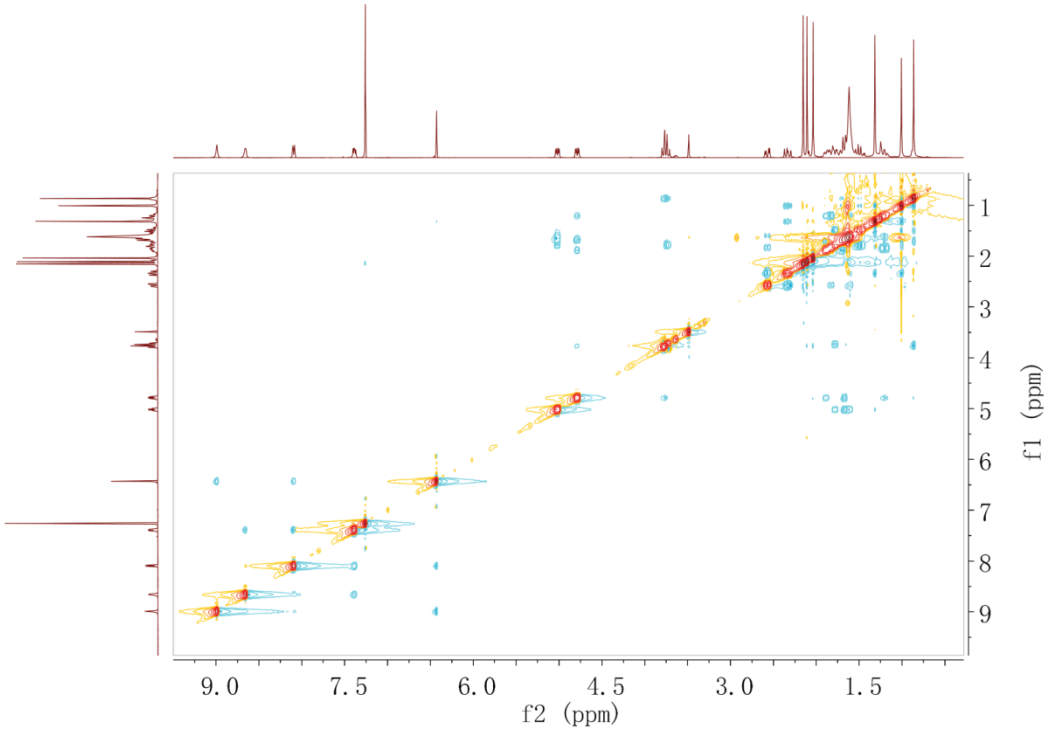


Figure S18. NOESY spectrum of 13-dehydroxylpyripyropene A (**4**).

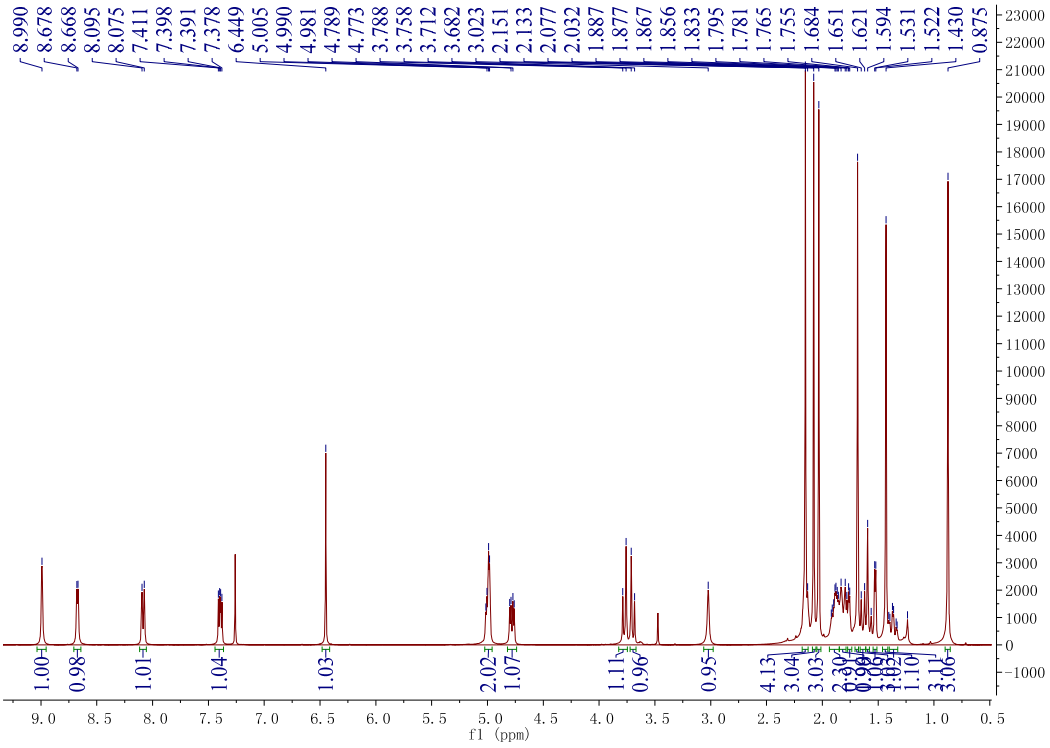


Figure S19. ^{1}H NMR spectrum of pyripyropene A (**5**) in $CDCl_3$, 400 MHz.

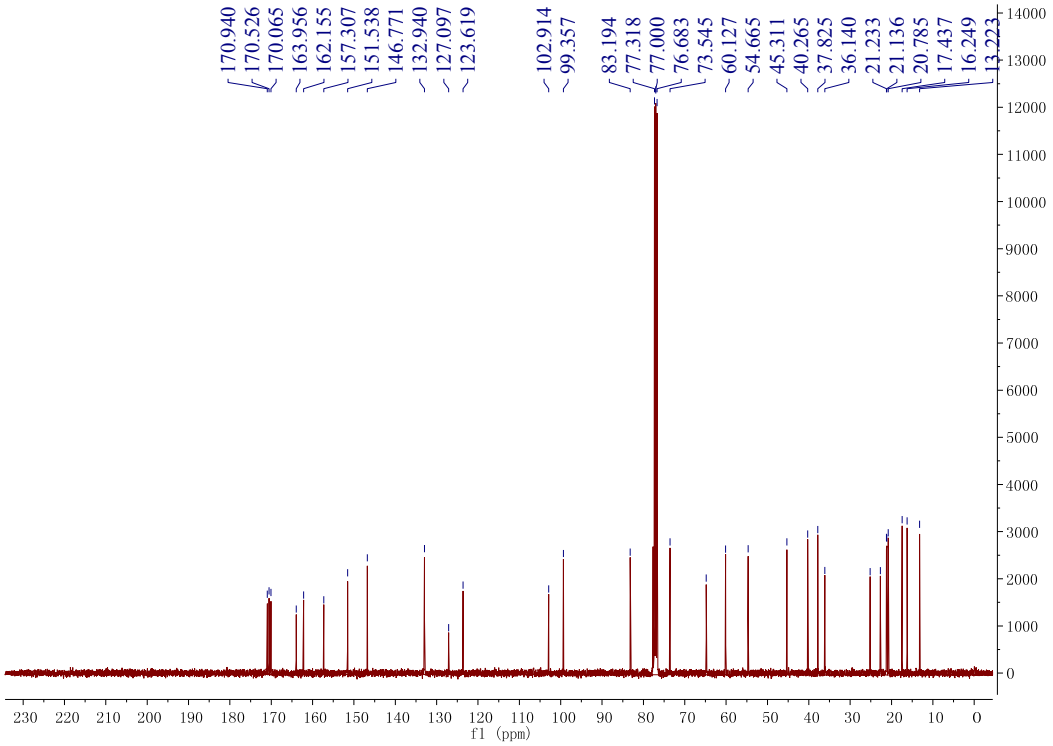


Figure S20. ^{13}C NMR spectrum of pyripyropene A (**5**) in $CDCl_3$, 100 MHz.

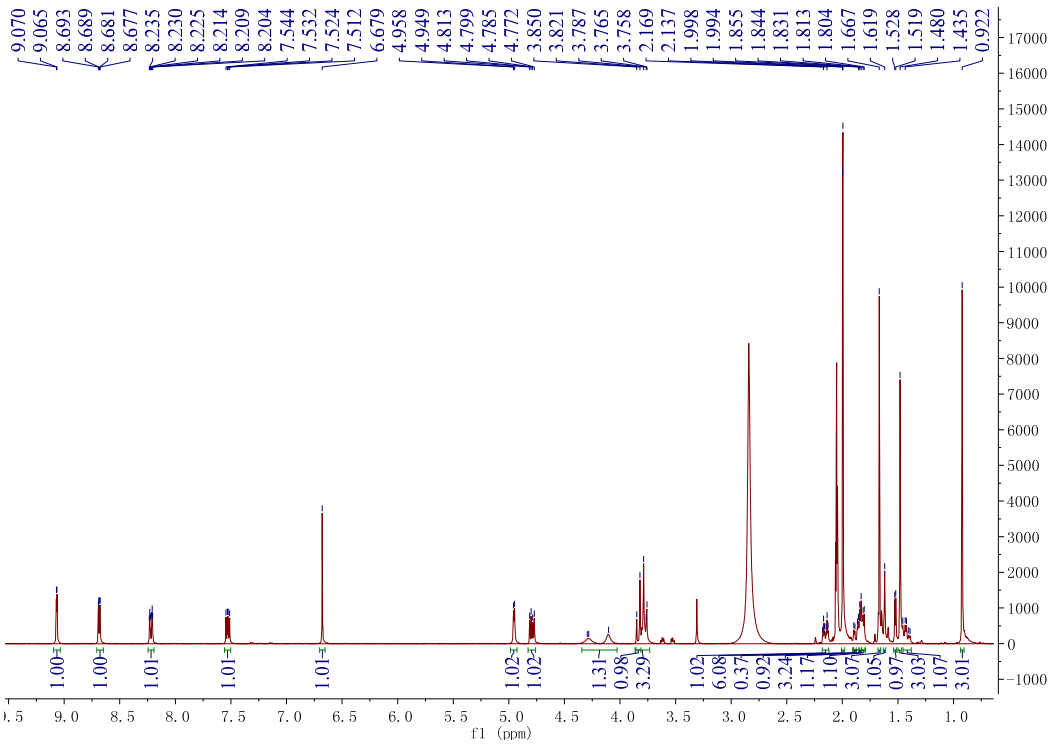


Figure S21. ^{1}H NMR spectrum of 7-deacetylpyripyropene A (**6**) in acetone-d_6, 400 MHz.

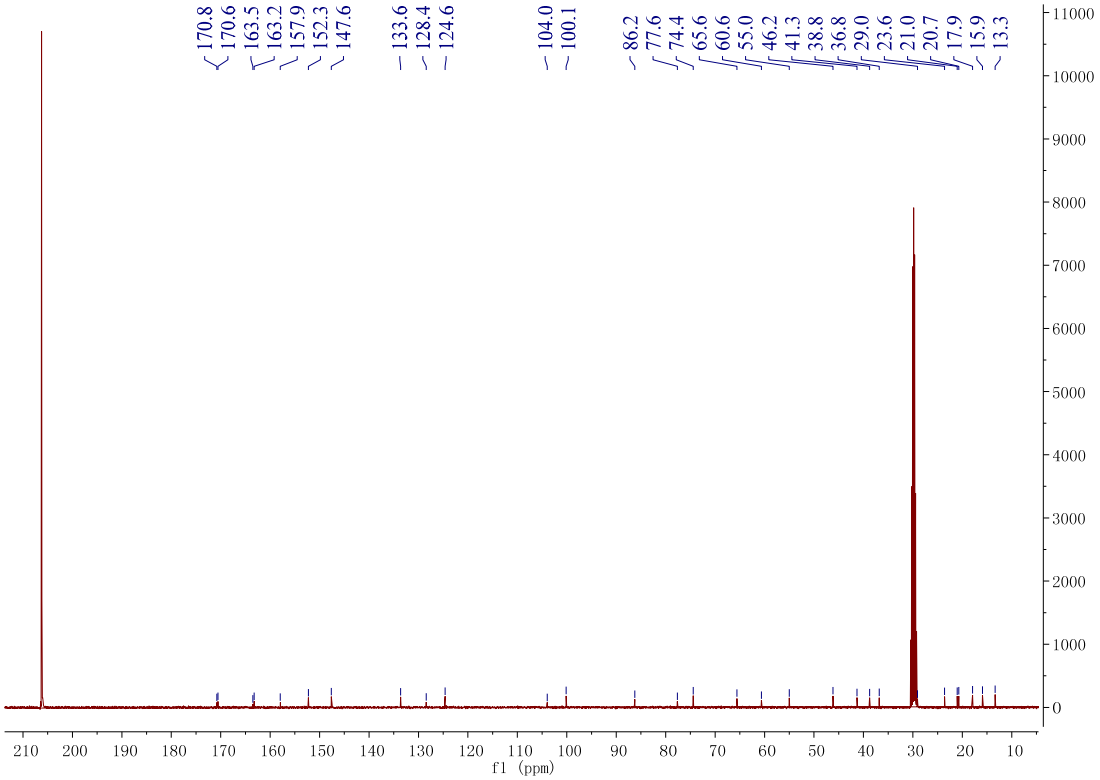
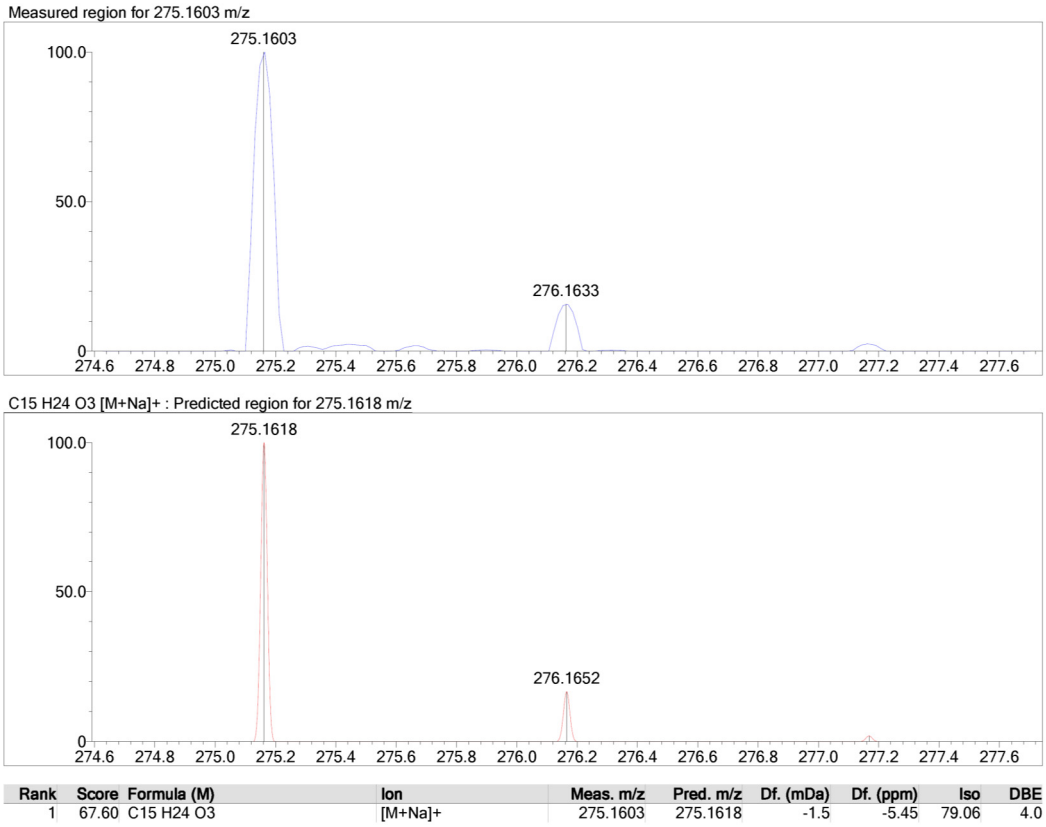


Figure S22. ^{13}C NMR spectrum of 7-deacetylpyripyropene A (**6**) in acetone-d_6, 100 MHz.



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	67.60	C15 H24 O3	[M+Na]+	275.1603	275.1618	-1.5	-5.45	79.06	4.0

Figure S23. HR(+)ESIMS spectrum of deacetylsequiterpene (**7**).

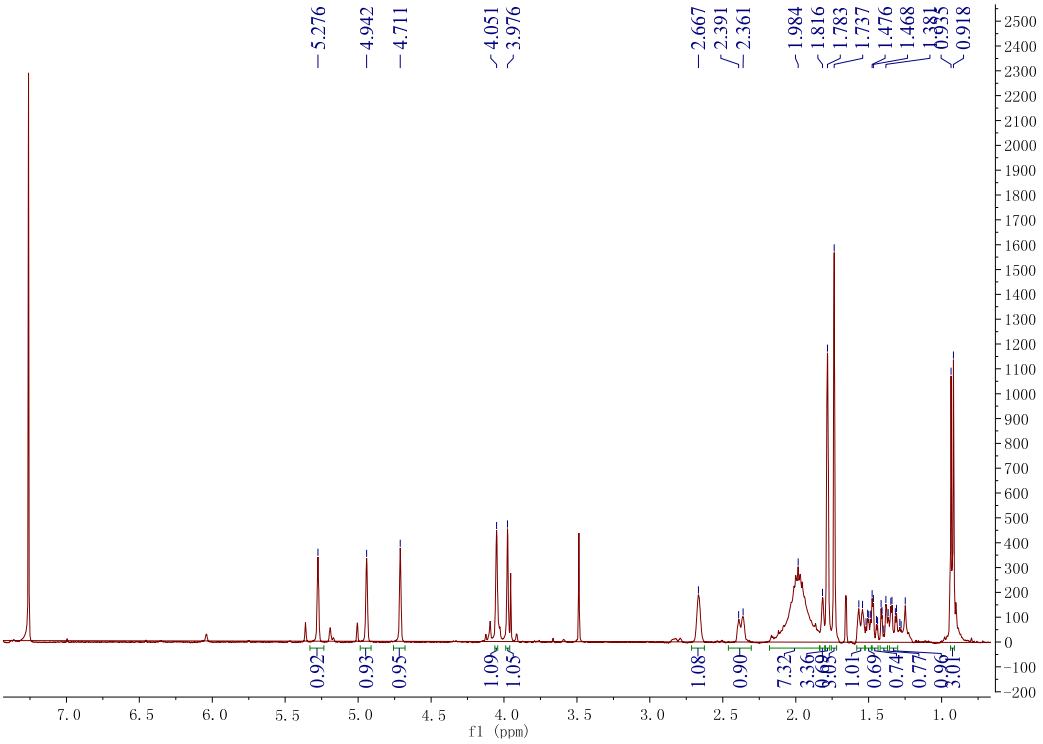


Figure S24. ^{1}H NMR spectrum of deacetylsequiterpene (**7**) in $CDCl_3$, 400 MHz.

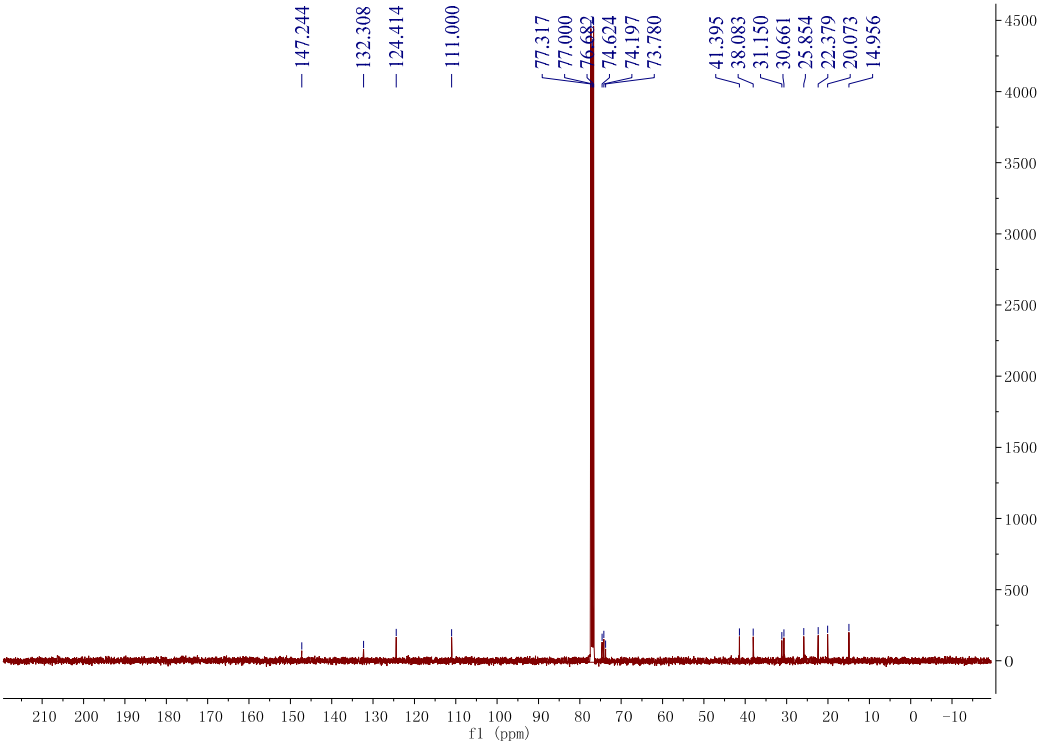


Figure S25. ^{13}C NMR spectrum of deacetylsequiterpene (**7**) in $CDCl_3$, 100 MHz.

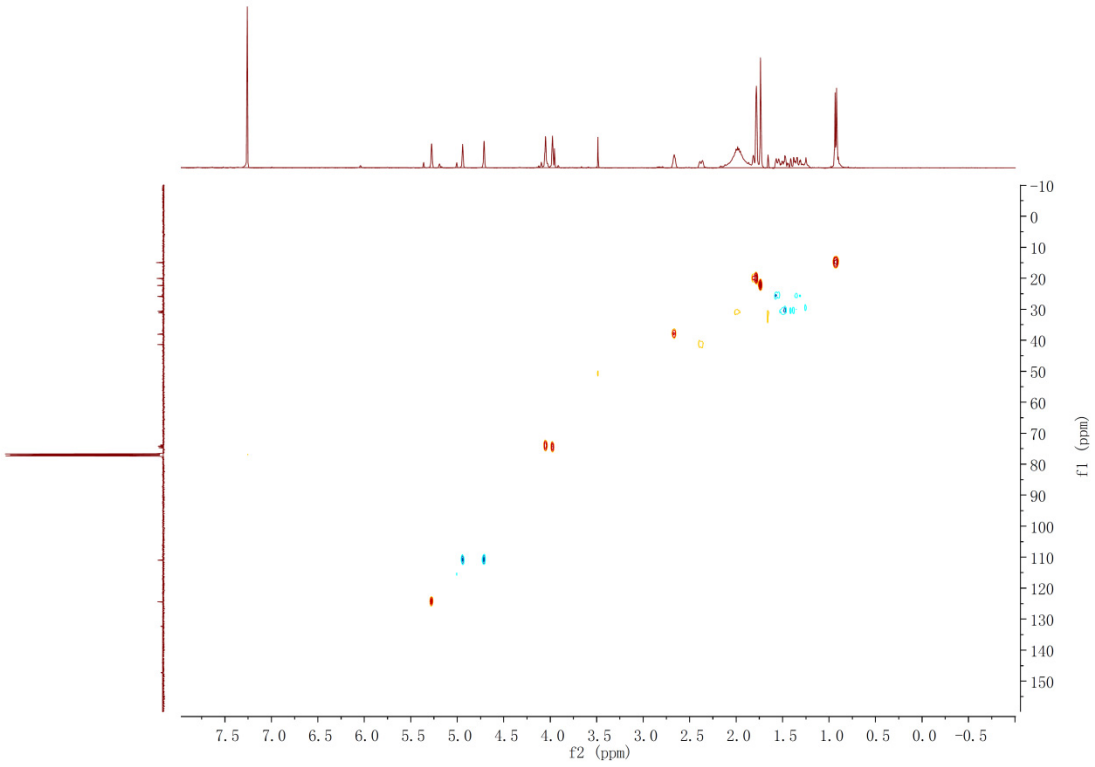


Figure S26. HSQC spectrum of deacetylsequiterpene (**7**).

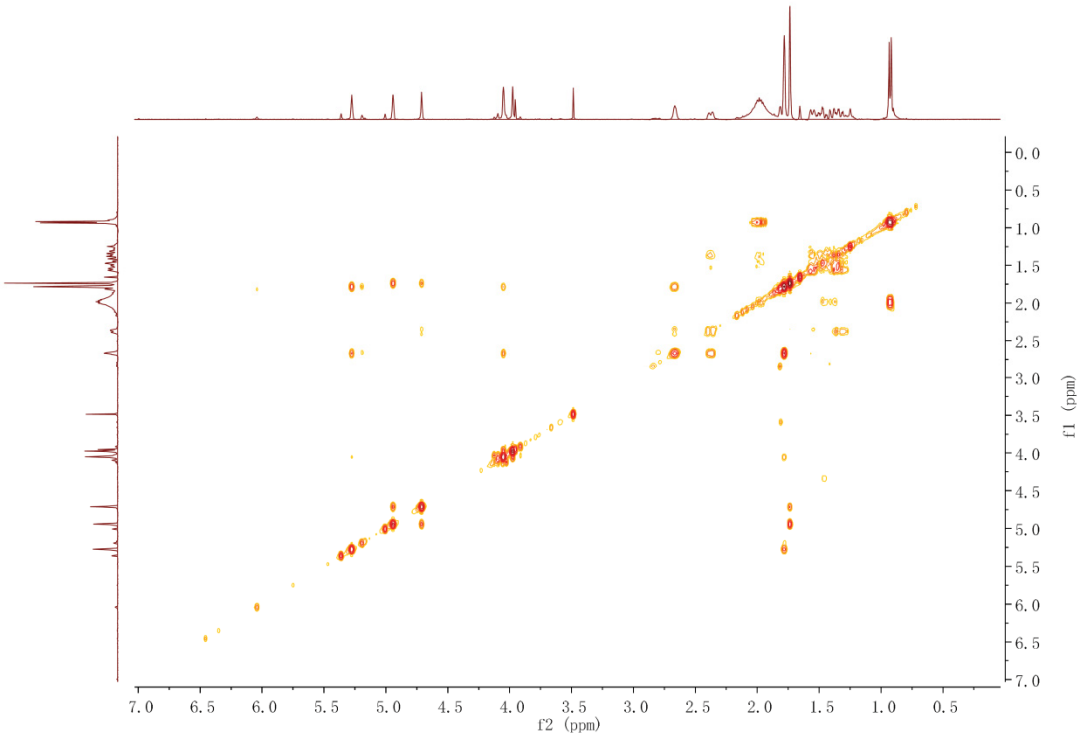


Figure S27. ^{1}H-^{1}H COSY spectrum of deacetylsequiterpene (**7**).

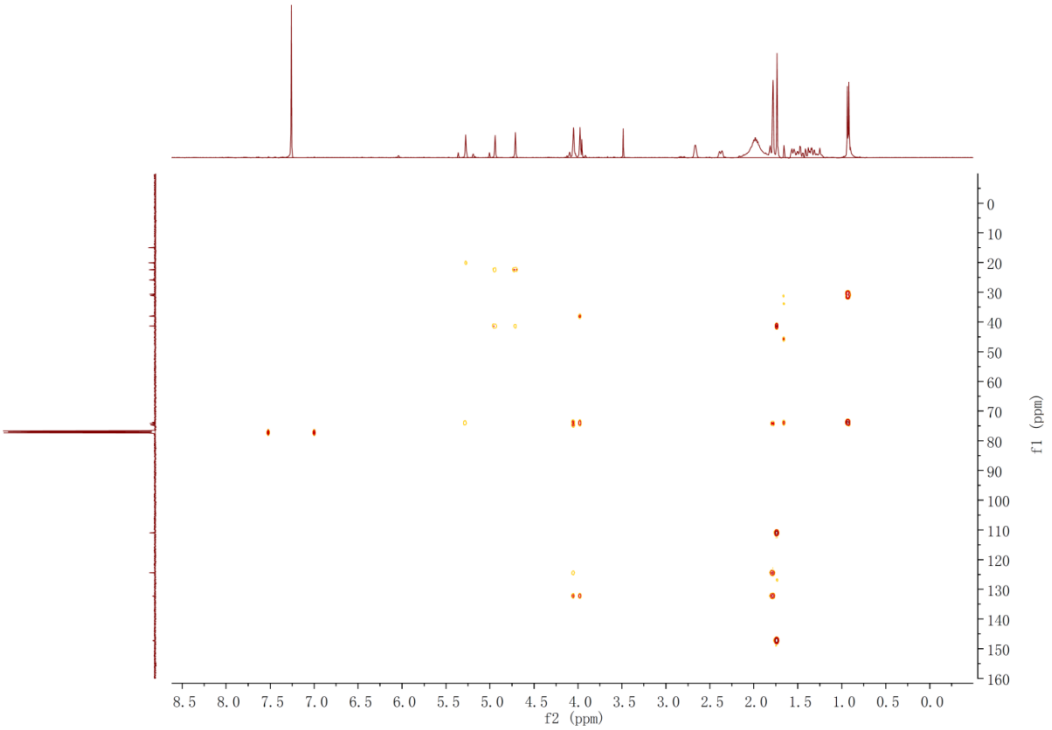


Figure S28. HMBC spectrum of deacetylsequiterpene (**7**).

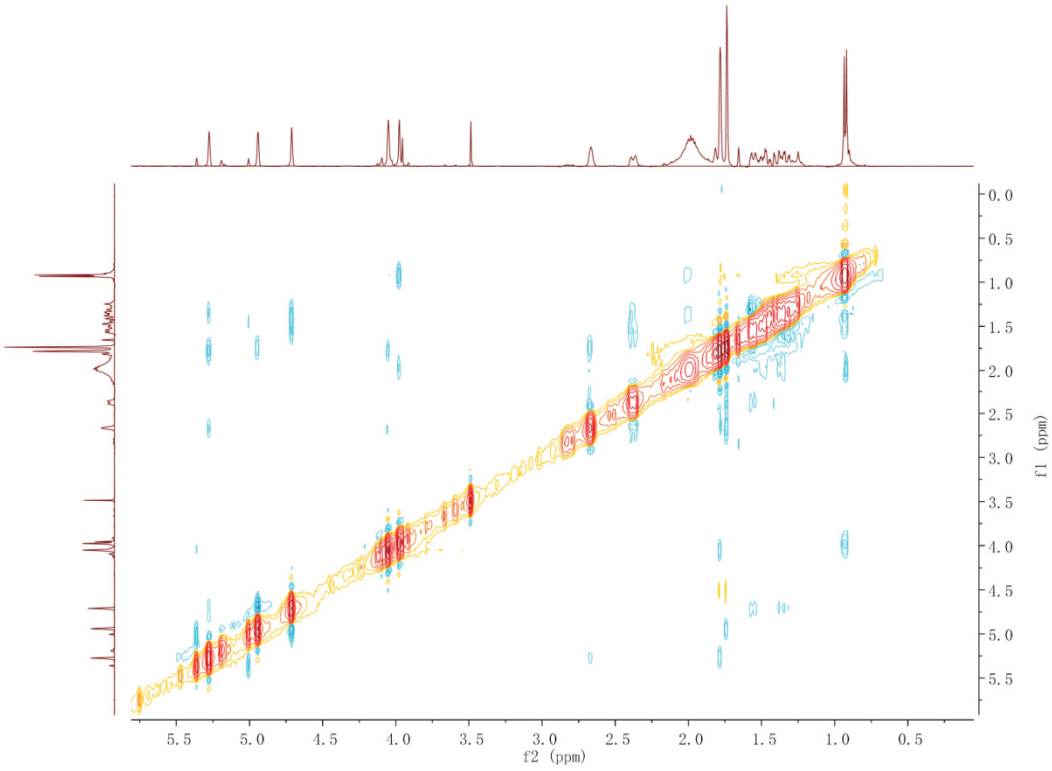


Figure S29. NOESY spectrum of deacetylsequiterpene (**7**).

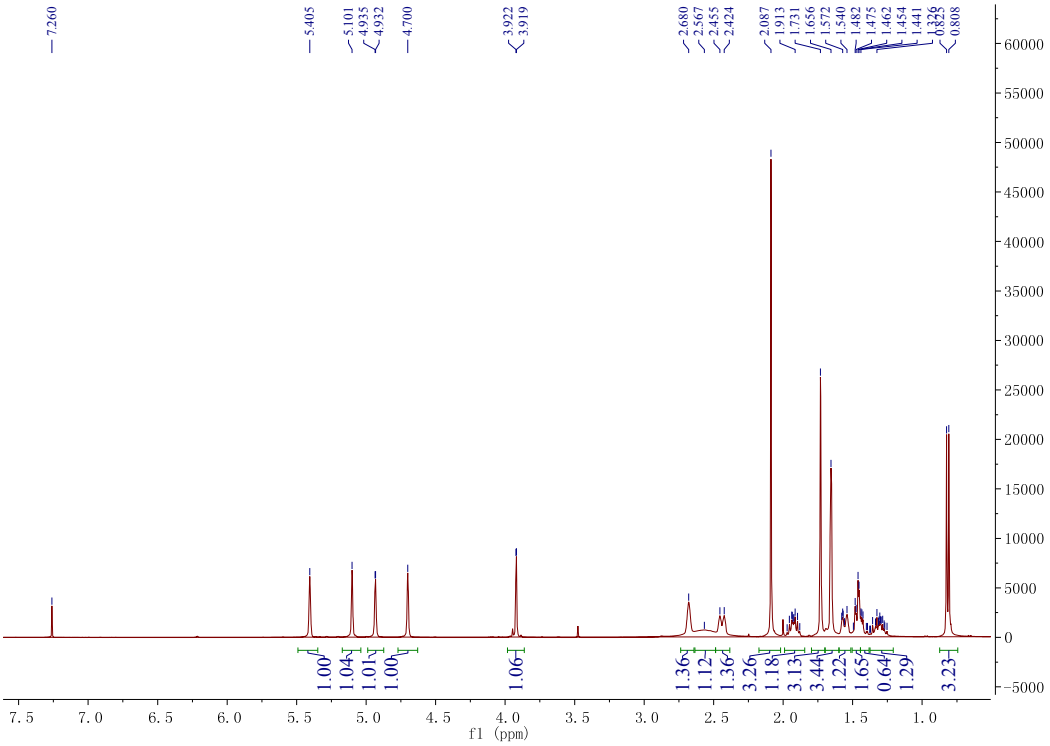


Figure S30. ^{1}H NMR spectrum of sesquiterpene (**8**) in $CDCl_3$, 400 MHz.

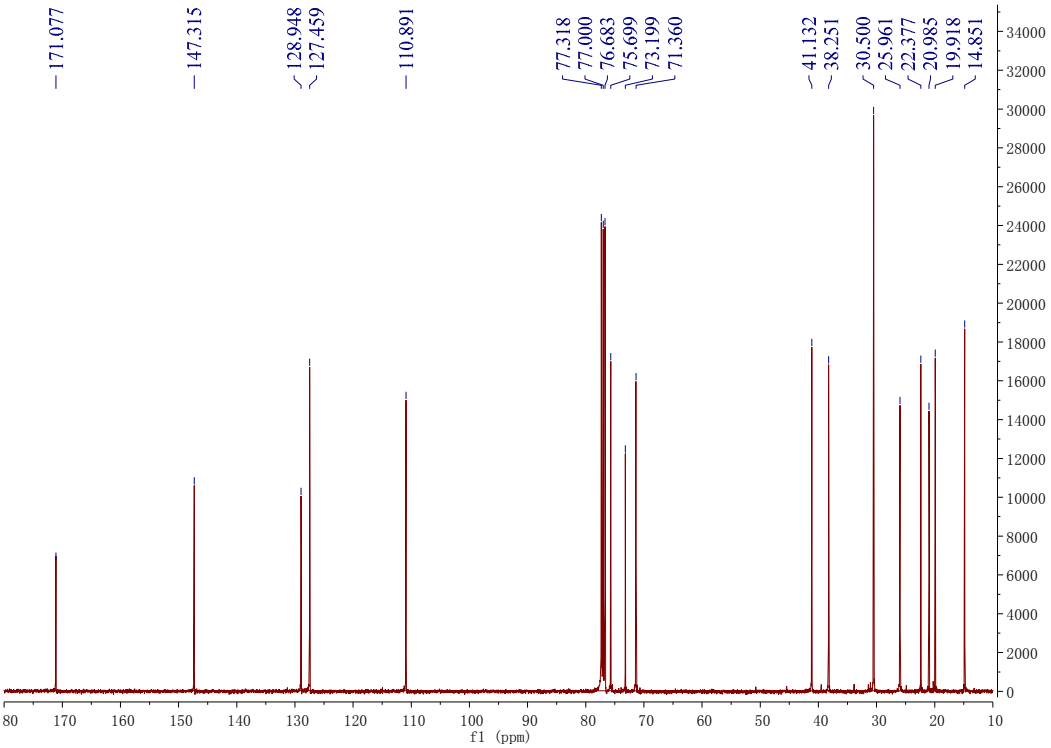
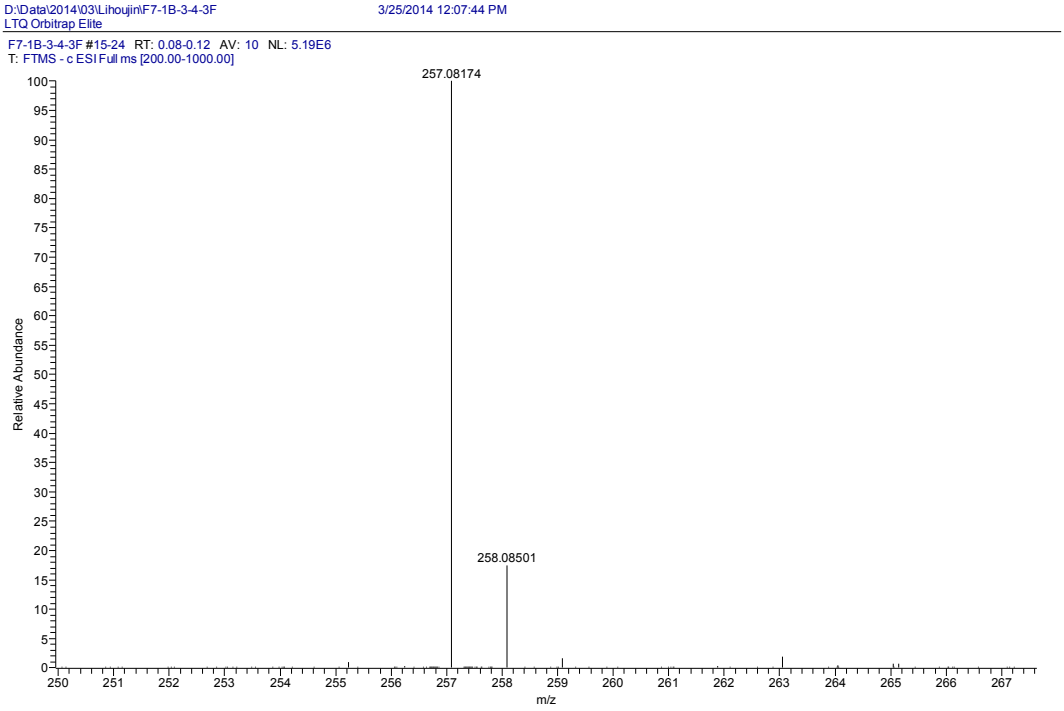


Figure S31. ^{13}C NMR spectrum of sesquiterpene (**8**) in $CDCl_3$, 100 MHz.



SPECTRUM-Simulation				
m/z	**Theo. Mass**	**Delta (ppm)**	**RDB Equiv.**	**Composition**
257.08174	257.08193	−0.75	9.5	C15 H13 O4

Figure S32. HR(-)ESIMS spectrum of 5-formly-6-hydroxy-8-isopro-pyl-2-naphthoic acid (**9**).

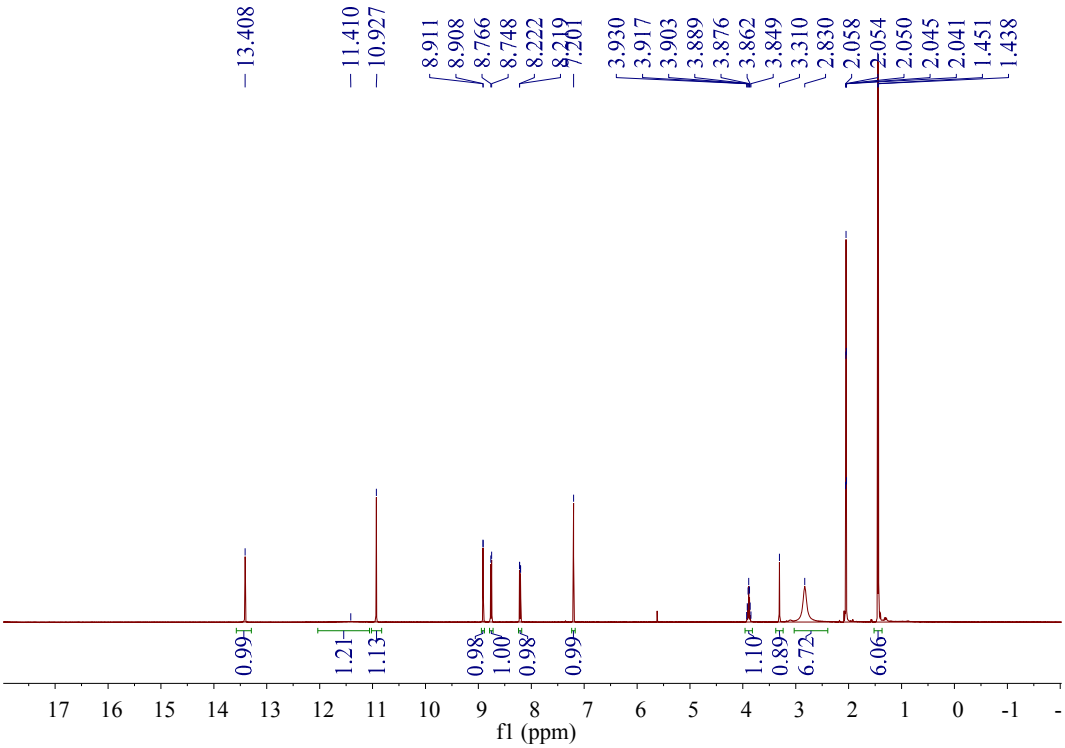


Figure S33. ^{1}H NMR spectrum of 5-formly-6-hydroxy-8-isopro-pyl-2-naphthoic acid (**9**) in Acetone-d_6, 500MHz.

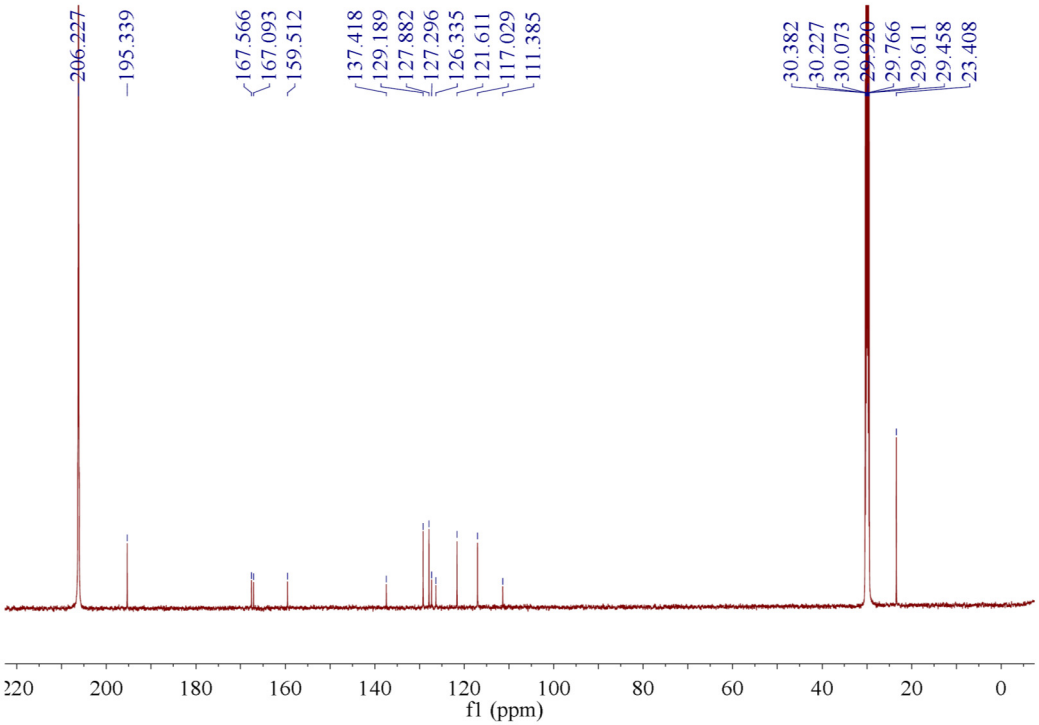


Figure S34. ^{13}C NMR spectrum of 5-formly-6-hydroxy-8-isopro-pyl-2-naphthoic acid (**9**) in Acetone-d_6, 125 MHz.

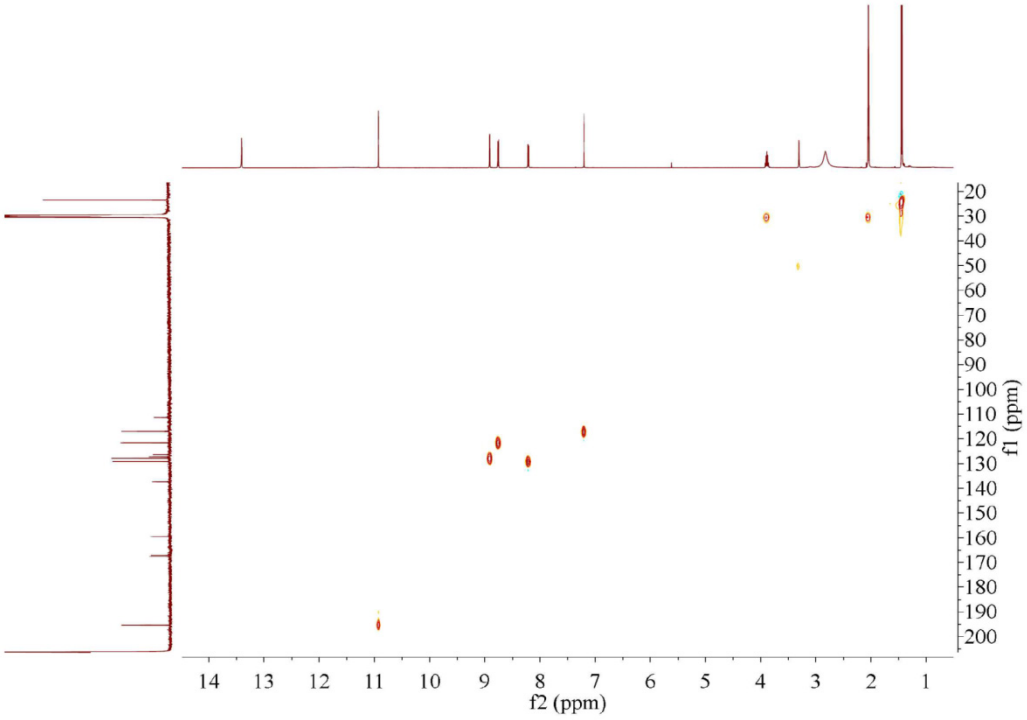


Figure S35. HSQC spectrum of 5-formly-6-hydroxy-8-isopro-pyl-2-naphthoic acid (**9**).

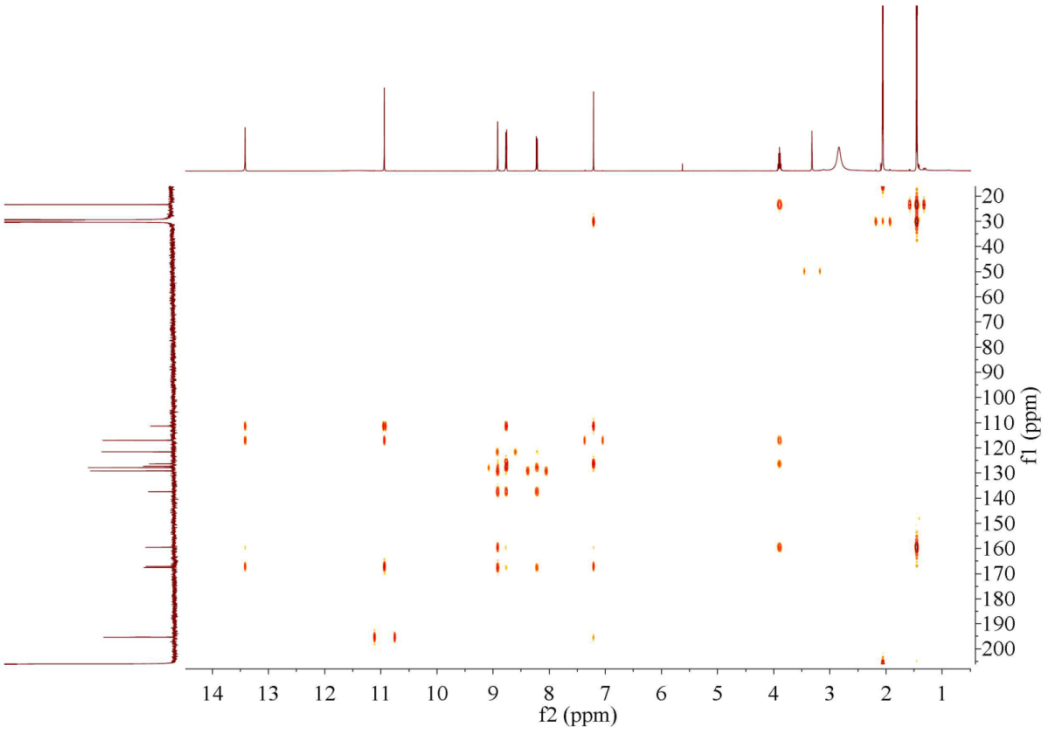
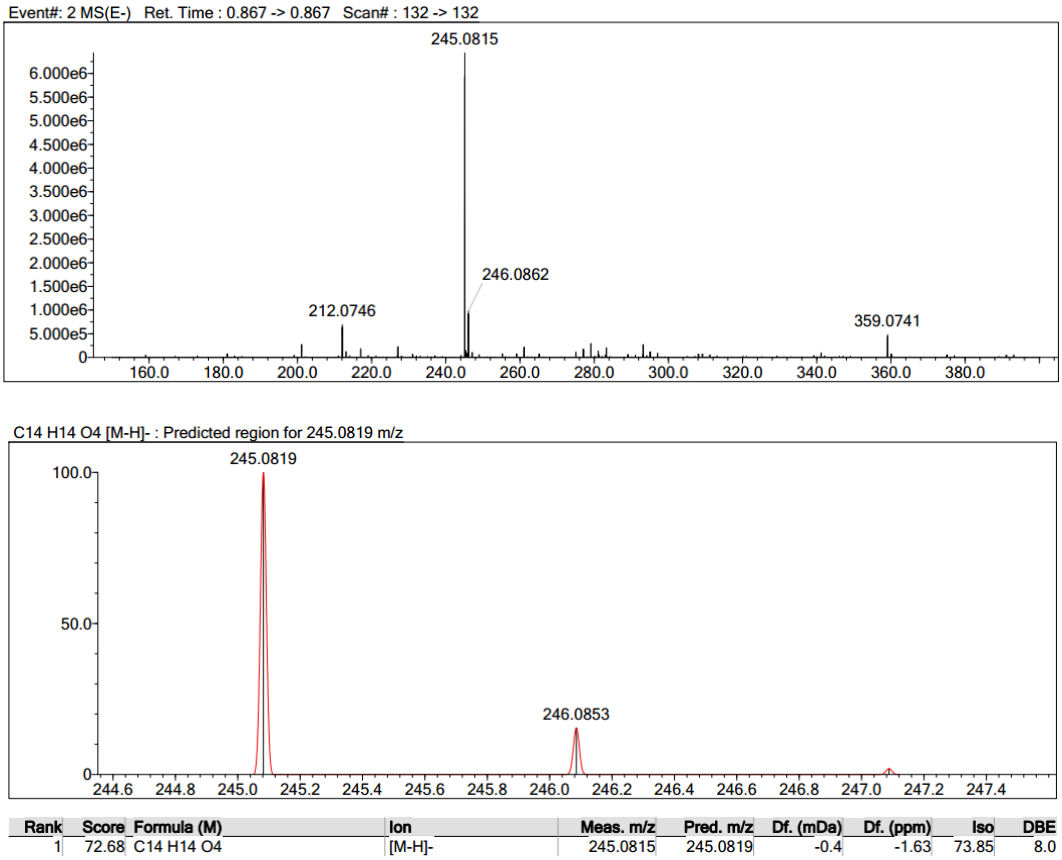


Figure S36. HMBC spectrum of 5-formly-6-hydroxy-8-isopro-pyl-2-naphthoic acid (**9**).



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	72.68	C14 H14 O4	[M-H]-	245.0815	245.0819	-0.4	-1.63	73.85	8.0

Figure S37. HRESIMS spectrum of **10**.

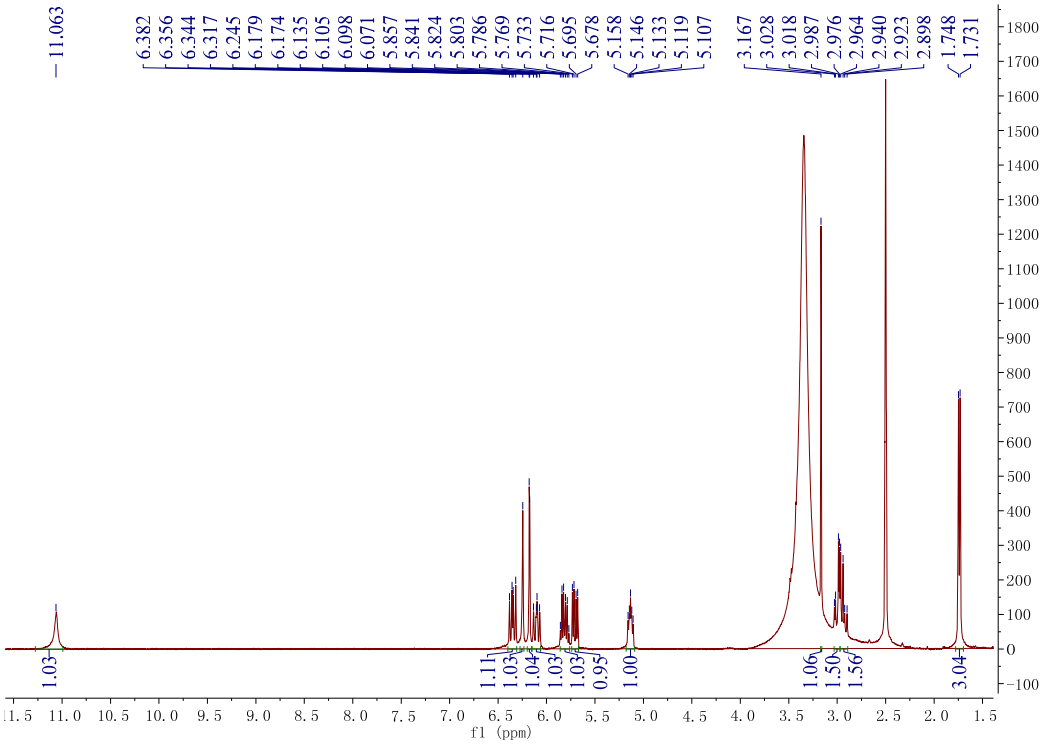


Figure S38. [1]H NMR spectrum of **10** in DMSO-d_6, 400 MHz.

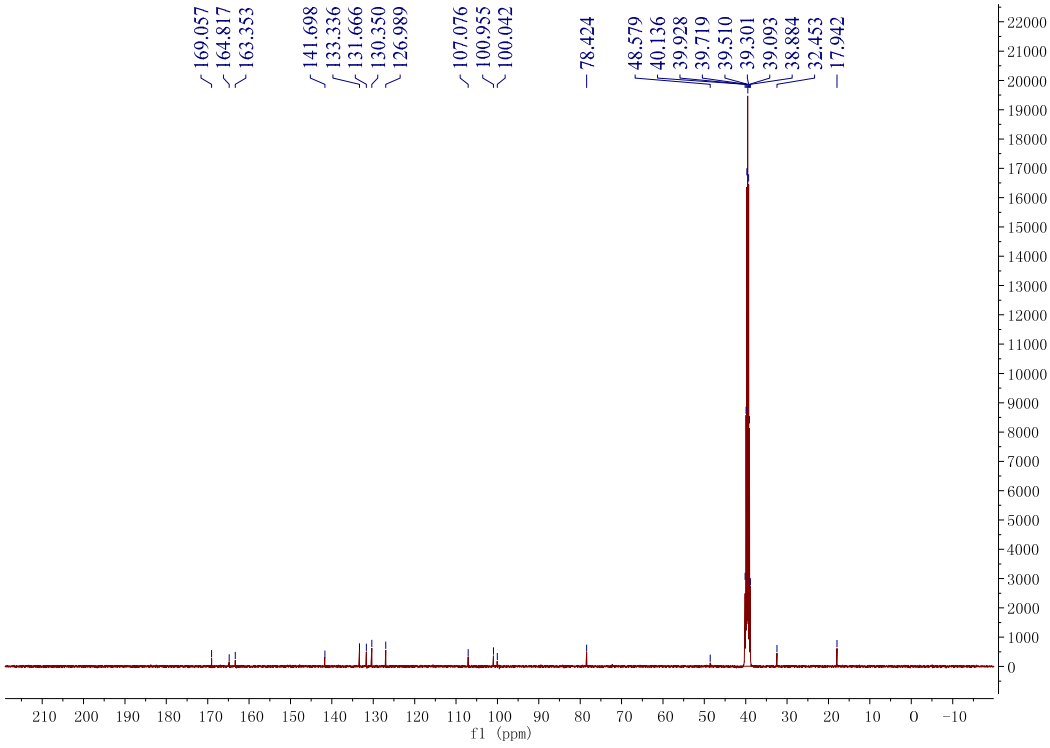


Figure S39. [13]C NMR spectrum of **10** in DMSO-d_6, 100 MHz.

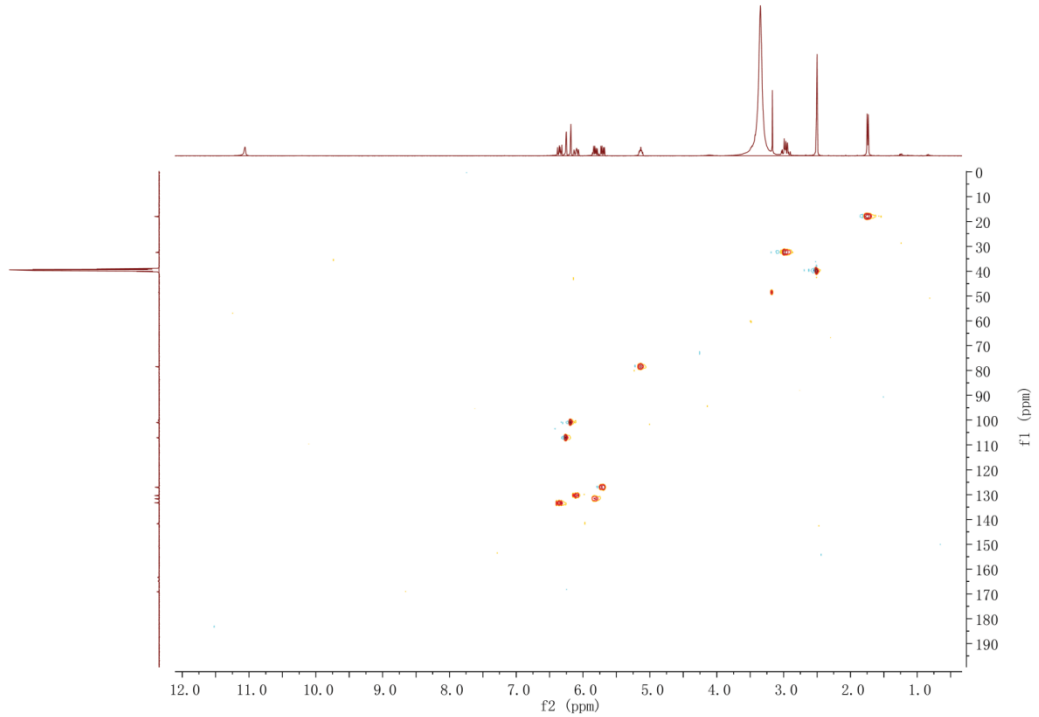


Figure S40. HSQC spectrum of 6,8-dihydroxy-3-((1*E*,3*E*)-penta-1,3-dien-1-yl)isochroman-1-one (**10**).

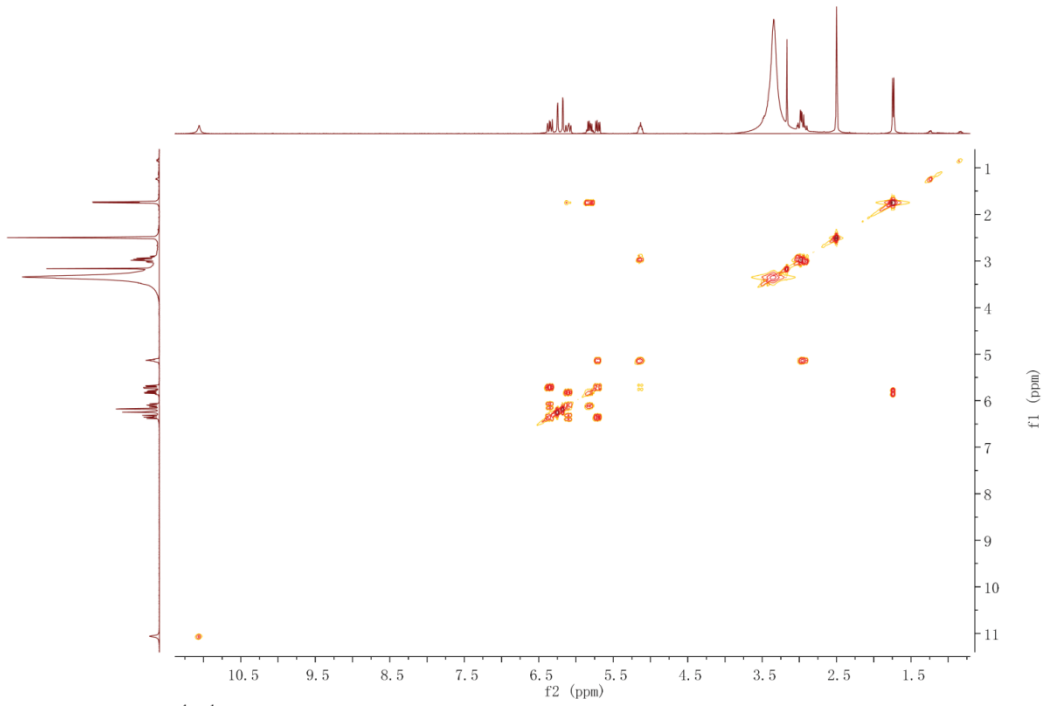


Figure S41. ^{1}H-^{1}H COSY spectrum of 6,8-dihydroxy-3-((1*E*,3*E*)-penta-1,3-dien-1-yl)isochroman-1-one (**10**).

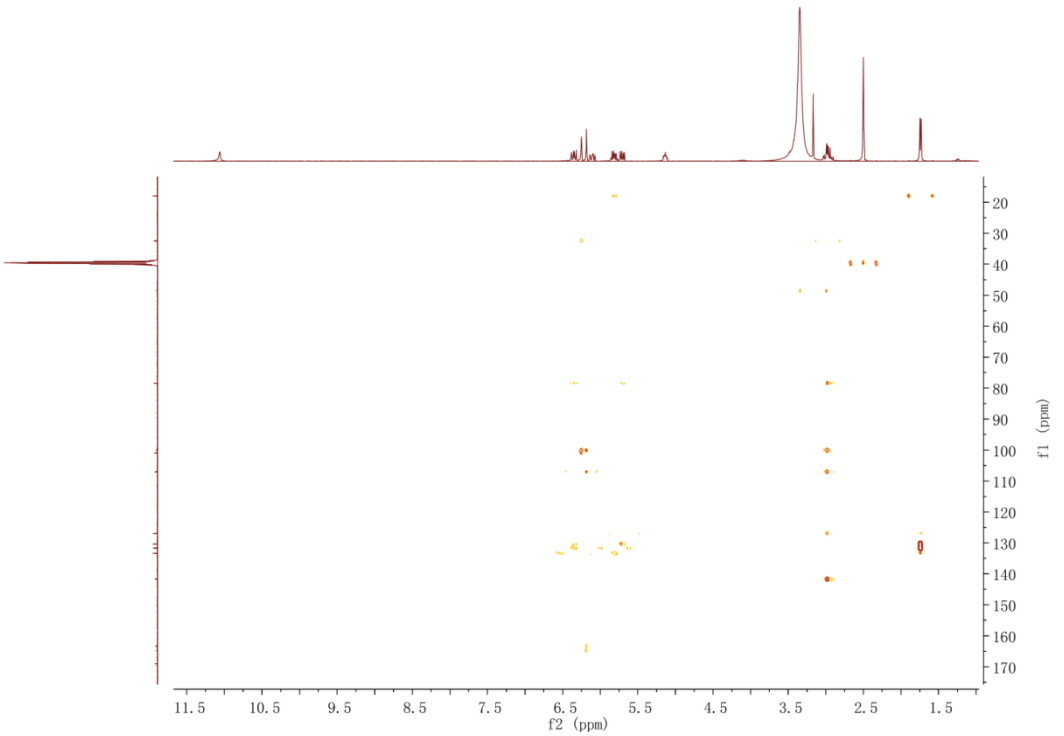


Figure S42. HMBC spectrum of 6,8-dihydroxy-3-((1*E*,3*E*)-penta-1,3-dien-1-yl)isochroman-1-one (**10**).

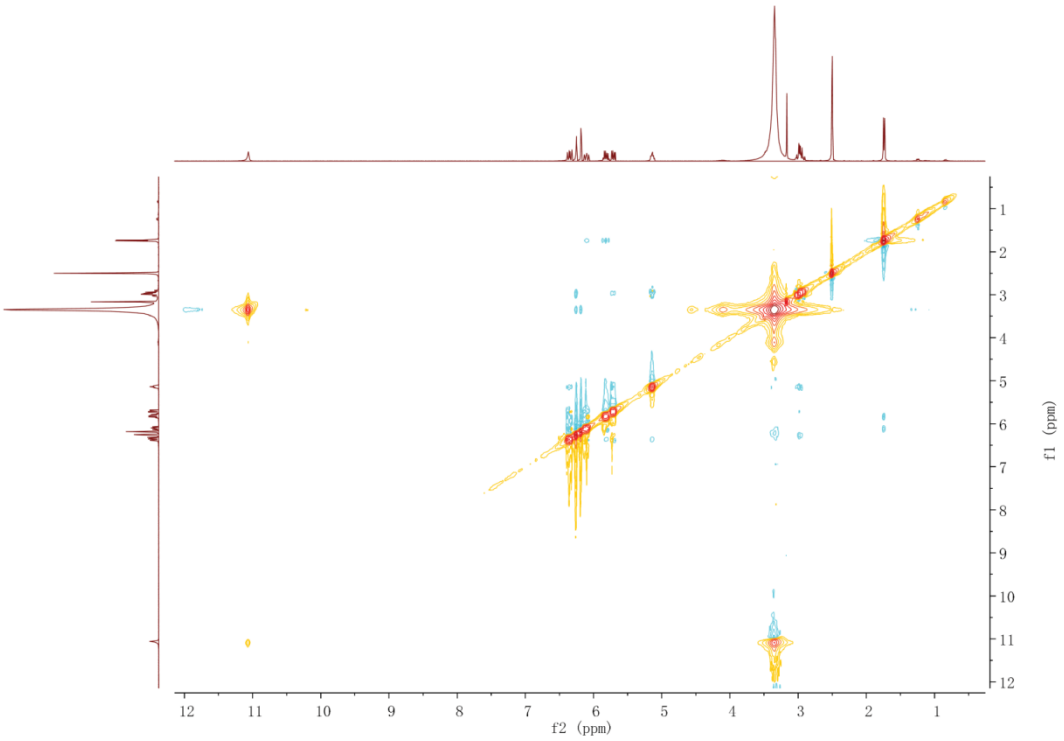


Figure S43. NOESY spectrum of 6,8-dihydroxy-3-((1*E*,3*E*)-penta-1,3-dien-1-yl)isochroman-1-one (**10**).

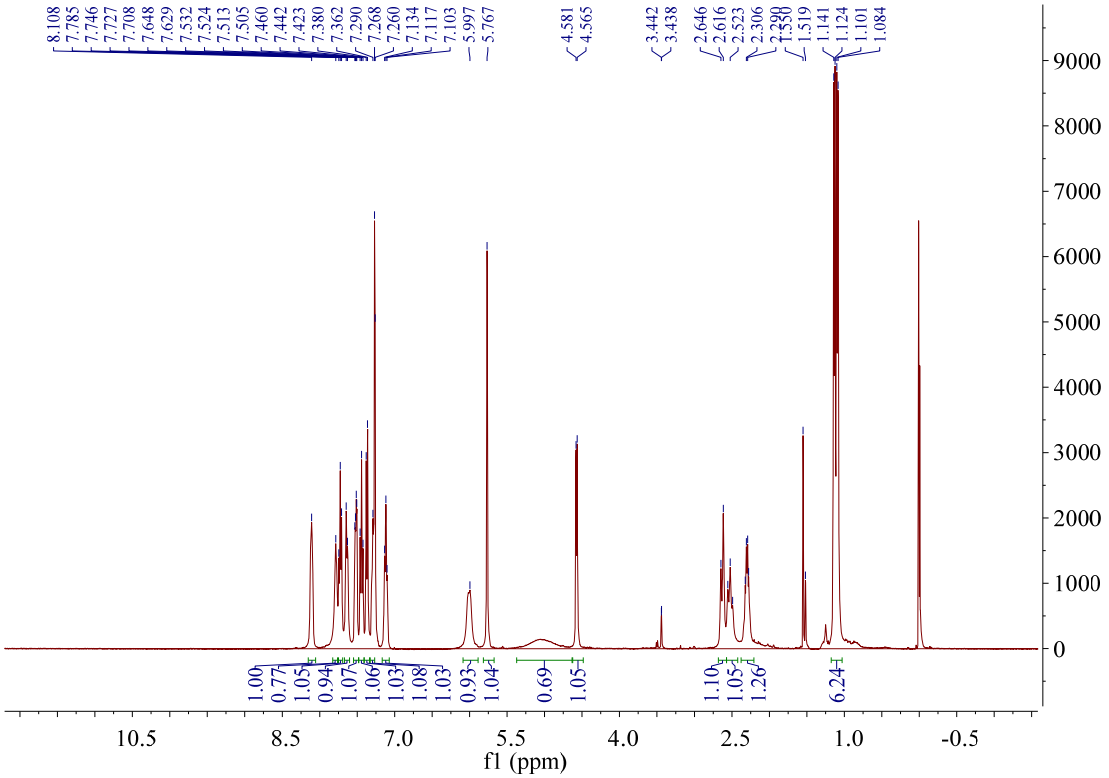


Figure S44. ^{1}H NMR spectrum of isochaetominine C (**11**) in $CDCl_3$, 400 MHz.

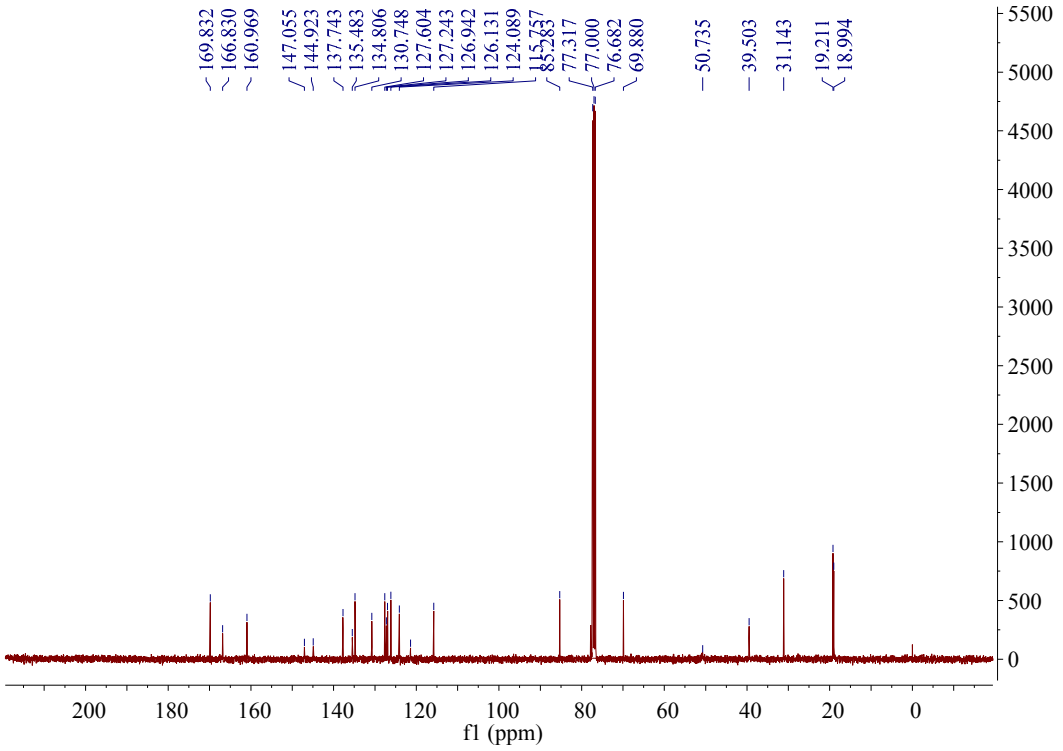


Figure S45. ^{13}C NMR spectrum of isochaetominine C (**11**) in $CDCl_3$, 100 MHz.

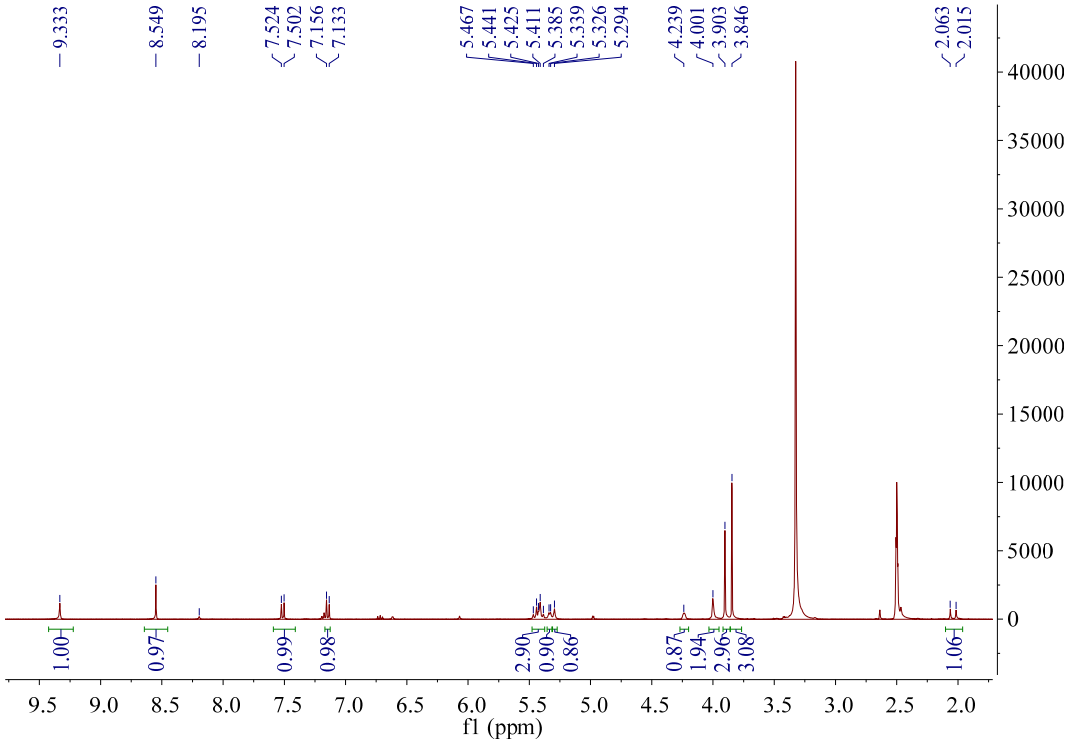


Figure S46. [1]H NMR spectrum of trichodermamide A (**12**) in DMSO-d_6, 400 MHz.

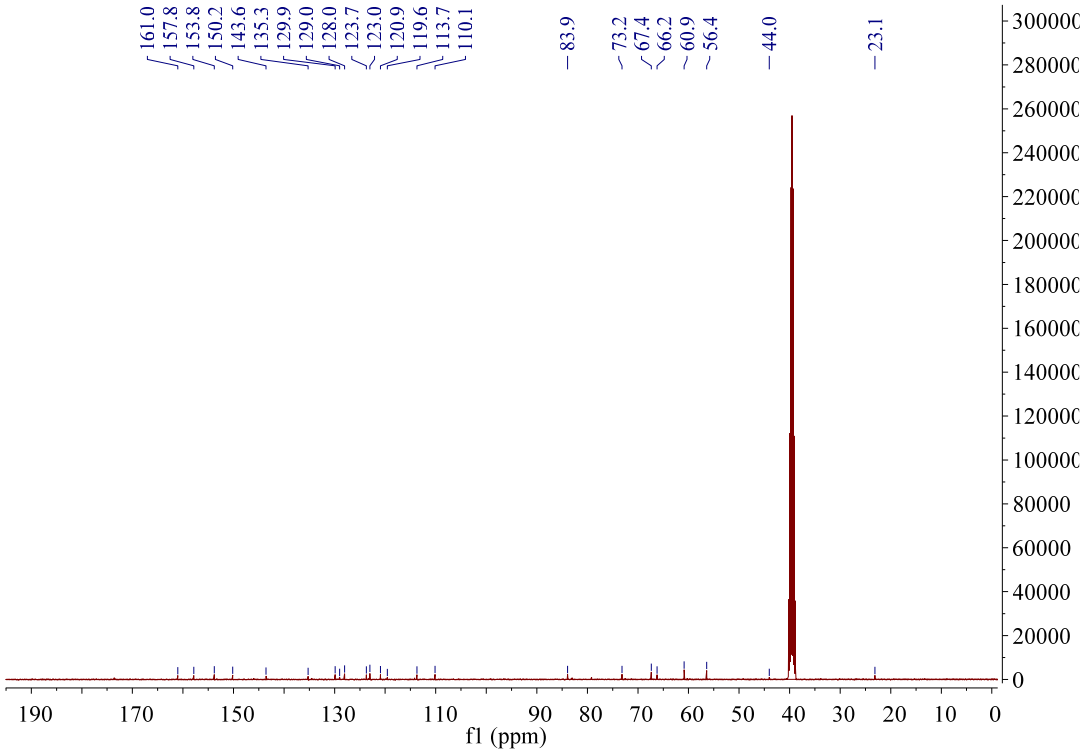


Figure S47. [13]C NMR spectrum of trichodermamide A (**12**) in DMSO-d_6, 100 MHz.

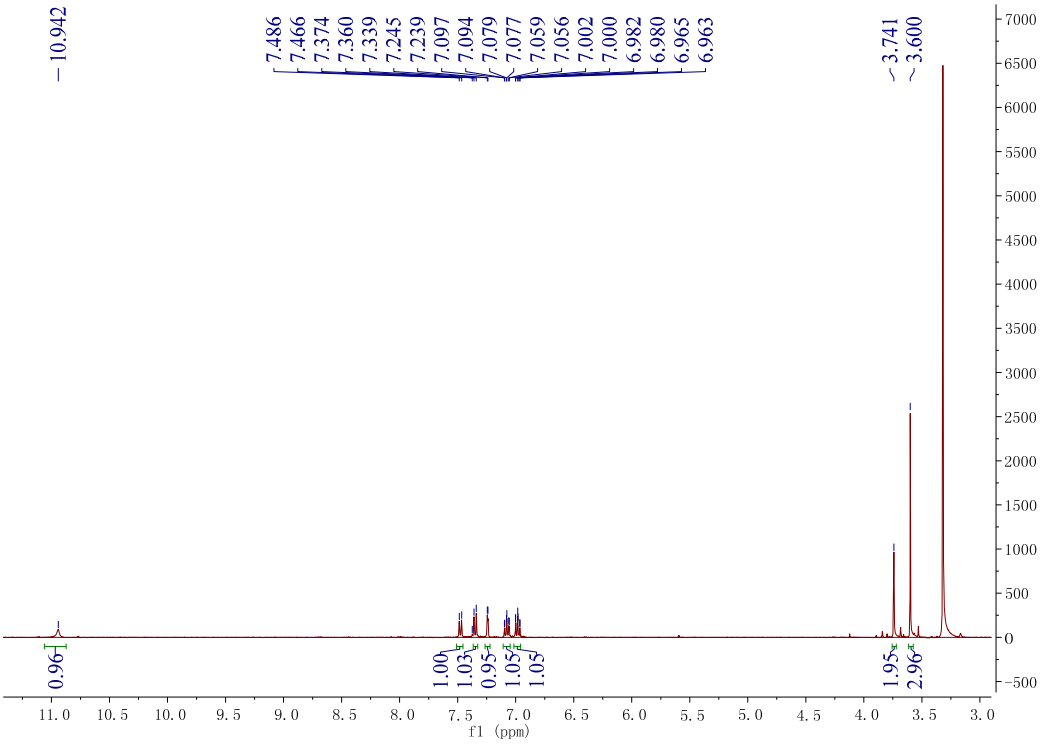


Figure S48. [1]H NMR spectrum of indolyl-3-acetic acid methyl ester (**13**) in DMSO-d_6, 400 MHz.

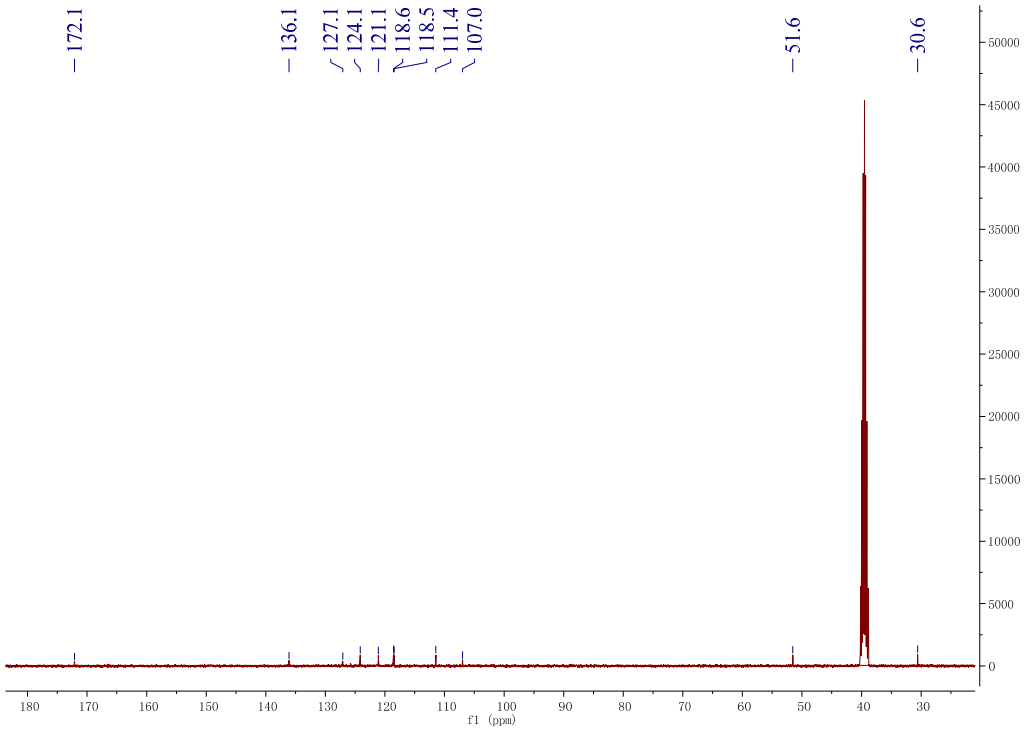


Figure S49. [13]C NMR spectrum of indolyl-3-acetic acid methyl ester (**13**) in DMSO-d_6, 100 MHz.

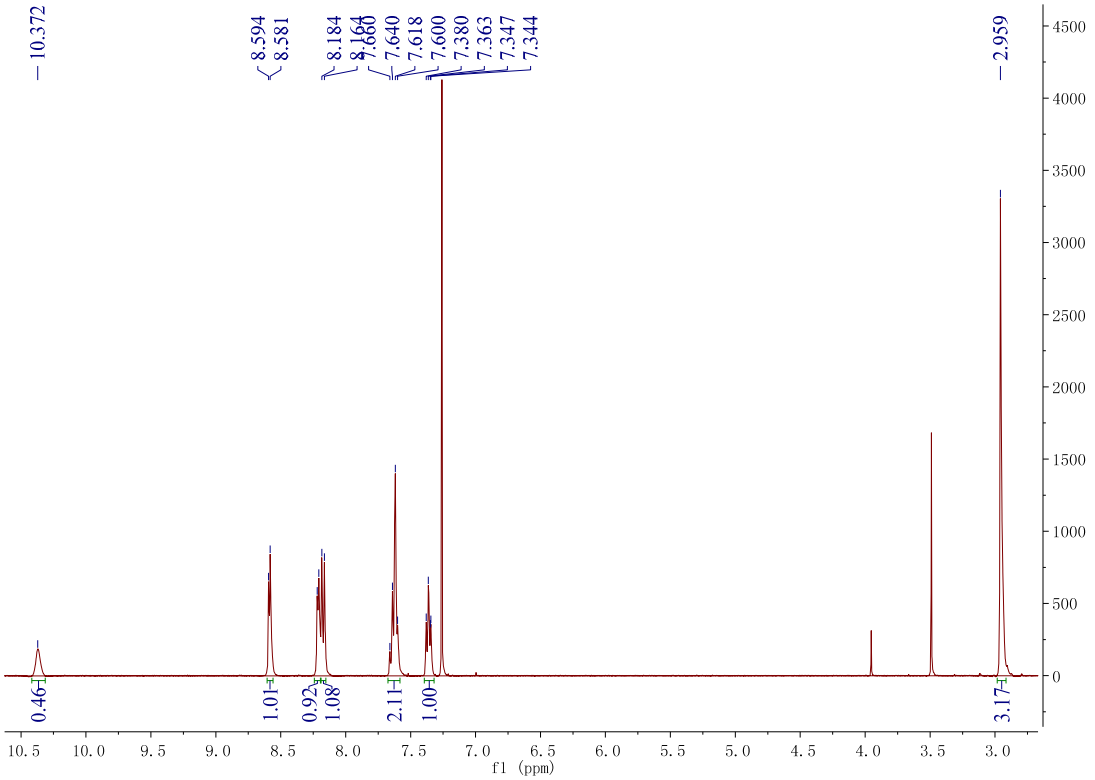


Figure S50. [1]H NMR spectrum of 1-(9*H*-β-carbolin-1-yl)-ethanone (**14**) in $CDCl_3$, 400 MHz.

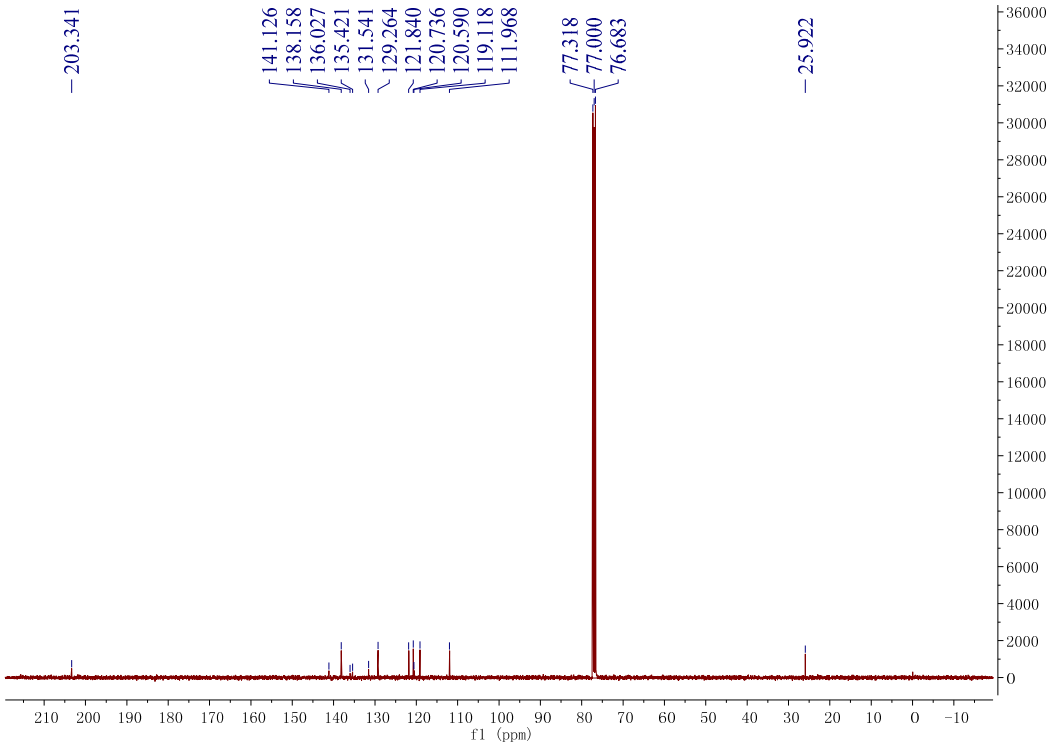


Figure S51. [13]C NMR spectrum of 1-(9*H*-β-carbolin-1-yl)-ethanone (**14**) in $CDCl_3$, 100 MHz.

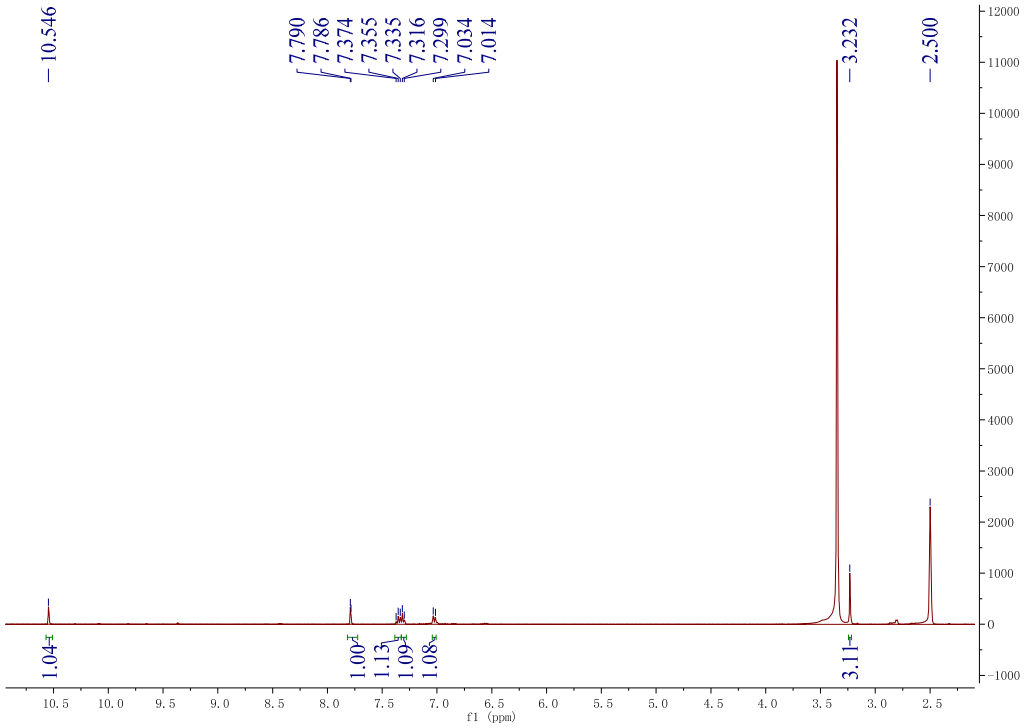


Figure S52. [1]H NMR spectrum of 1,2,3,4-tetrahydro-6-hydroxyl-2-methyl-l,3,4-trioxopyrazino [l,2-a]-indole (**15**) in DMSO-d_6, 400 MHz.

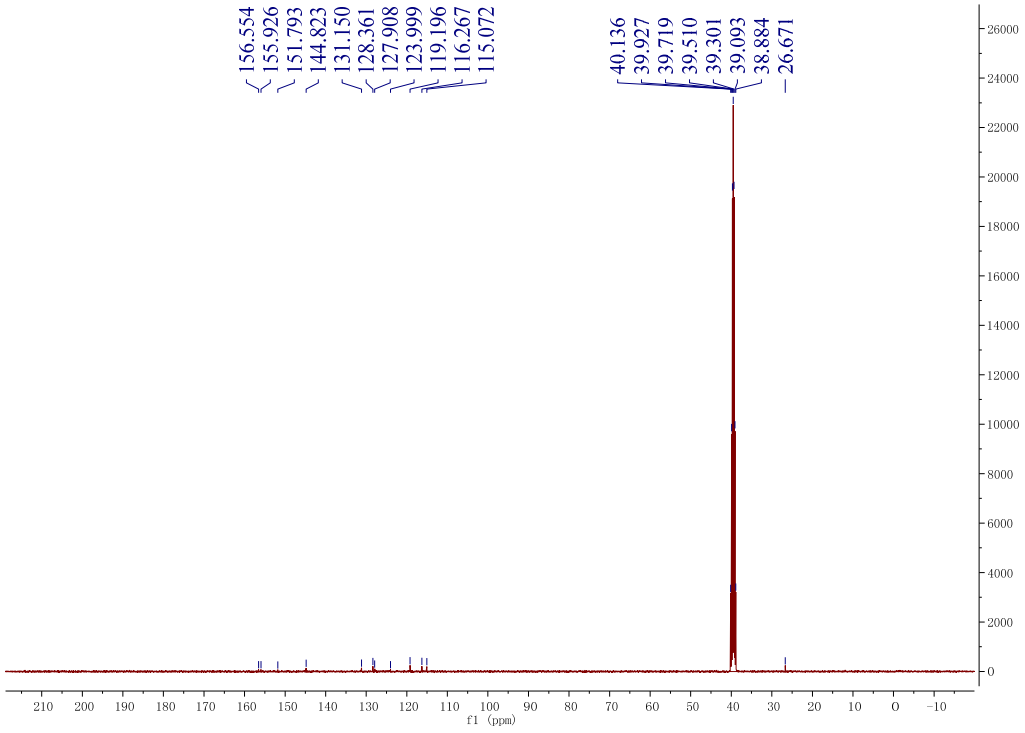


Figure S53. [13]C NMR spectrum of 1,2,3,4-tetrahydro-6-hydroxyl-2-methyl-l,3,4-trioxopyrazino[l,2-a]-indole (**15**) in DMSO-d_6, 100 MHz.

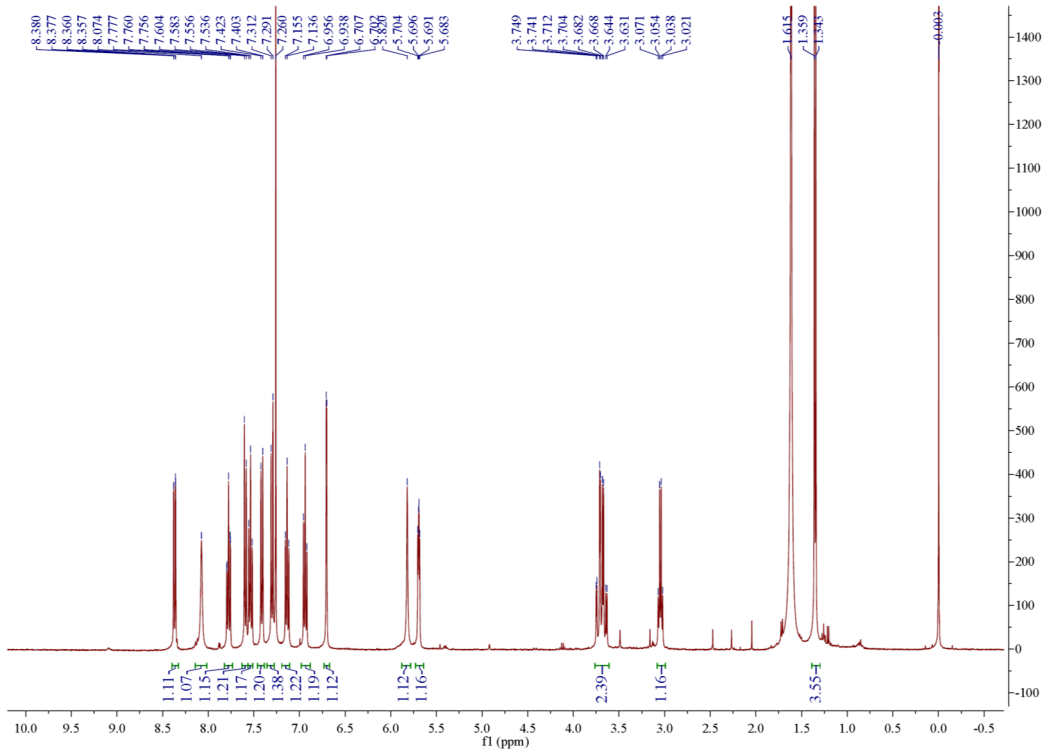


Figure S54. ^{1}H NMR spectrum of fumiquinazoline F (**16**) in $CDCl_3$, 400MHz.

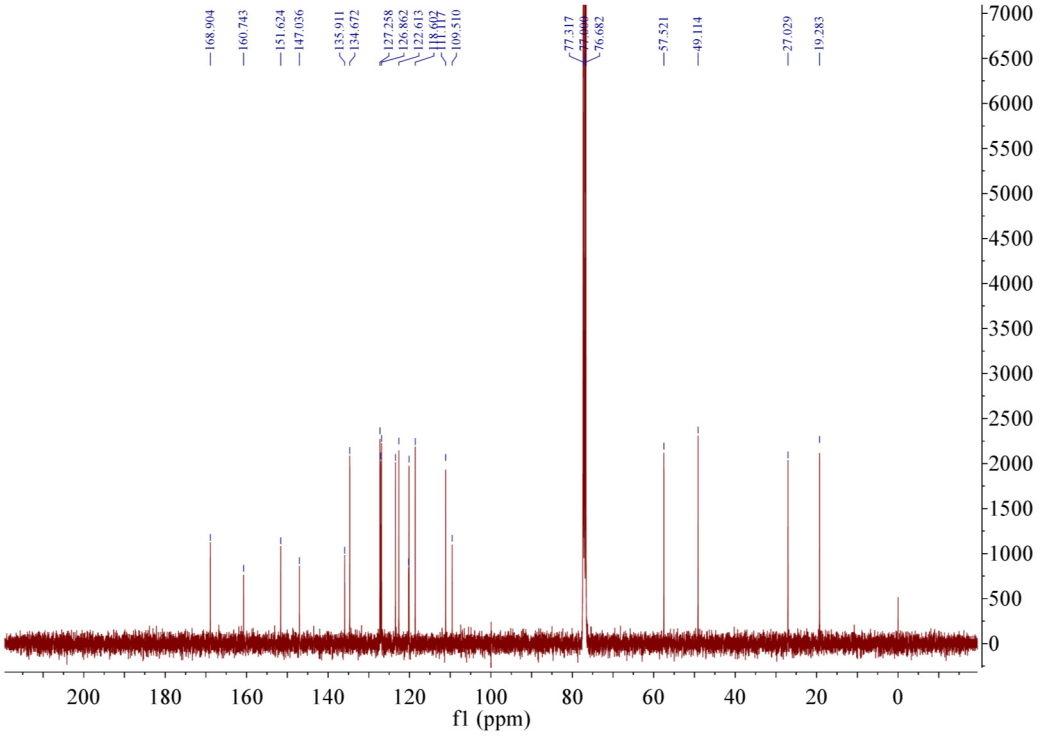


Figure S55. ^{13}C NMR spectrum of fumiquinazoline F (**16**) in $CDCl_3$, 100 MHz.

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H8A C8 H8B 108.2 . . ?
C8 C9 C10 112.44(12) . . ?
C8 C9 H9A 109.1 . . ?
C10 C9 H9A 109.1 . . ?
C8 C9 H9B 109.1 . . ?
C10 C9 H9B 109.1 . . ?
H9A C9 H9B 107.8 . . ?
C11 C10 C9 109.91(12) . . ?
C11 C10 C1 112.96(13) . . ?
C9 C10 C1 111.15(12) . . ?
C11 C10 H10A 107.5 . . ?
C9 C10 H10A 107.5 . . ?
C1 C10 H10A 107.5 . . ?
C10 C11 H11A 109.5 . . ?
C10 C11 H11B 109.5 . . ?
H11A C11 H11B 109.5 . . ?
C10 C11 H11C 109.5 . . ?
H11A C11 H11C 109.5 . . ?
H11B C11 H11C 109.5 . . ?
C14 C12 C13 121.19(17) . . ?
C14 C12 C17 124.19(17) . . ?
C13 C12 C17 114.60(15) . . ?
C12 C13 H13A 109.5 . . ?
C12 C13 H13B 109.5 . . ?
H13A C13 H13B 109.5 . . ?
C12 C13 H13C 109.5 . . ?
H13A C13 H13C 109.5 . . ?
H13B C13 H13C 109.5 . . ?
C12 C14 H14A 120.0 . . ?
C12 C14 H14B 120.0 . . ?
H14A C14 H14B 120.0 . . ?
O4 C15 O3 124.09(14) . . ?
O4 C15 C16 124.47(15) . . ?
O3 C15 C16 111.44(13) . . ?
C15 C16 H16A 109.5 . . ?
C15 C16 H16B 109.5 . . ?
H16A C16 H16B 109.5 . . ?

C15 C16 H16C 109.5 . . ?
H16A C16 H16C 109.5 . . ?
H16B C16 H16C 109.5 . . ?

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O1 C1 C2 O2 56.97(14) . . . . ?
C6 C1 C2 O2 -60.56(14) . . . . ?
C10 C1 C2 O2 175.23(11) . . . . ?
O1 C1 C2 C3 176.12(11) . . . . ?
C6 C1 C2 C3 58.59(15) . . . . ?
C10 C1 C2 C3 -65.62(16) . . . . ?
C15 O3 C3 C4 -160.20(12) . . . . ?
C15 O3 C3 C2 74.41(15) . . . . ?
O2 C2 C3 O3 -156.28(11) . . . . ?
C1 C2 C3 O3 86.26(14) . . . . ?
O2 C2 C3 C4 82.90(15) . . . . ?
C1 C2 C3 C4 -34.56(18) . . . . ?
O3 C3 C4 C5 -119.42(15) . . . . ?
C2 C3 C4 C5 3.6(2) . . . . ?
O3 C3 C4 C7 63.97(16) . . . . ?
C2 C3 C4 C7 -173.04(13) . . . . ?
C3 C4 C5 C6 1.3(2) . . . . ?
C7 C4 C5 C6 177.60(14) . . . . ?
C4 C5 C6 C1 24.3(2) . . . . ?
C4 C5 C6 C17 150.37(14) . . . . ?
O1 C1 C6 C5 -166.99(11) . . . . ?
C2 C1 C6 C5 -51.74(15) . . . . ?
C10 C1 C6 C5 73.31(15) . . . . ?
O1 C1 C6 C17 65.72(14) . . . . ?
C2 C1 C6 C17 -179.04(11) . . . . ?
C10 C1 C6 C17 -53.99(15) . . . . ?
C5 C6 C17 C12 61.91(16) . . . . ?
C1 C6 C17 C12 -172.17(12) . . . . ?
C5 C6 C17 C8 -67.73(15) . . . . ?

C1 C6 C17 C8 58.19(15) . . . . ?
C12 C17 C8 C9 172.87(13) . . . . ?
C6 C17 C8 C9 -59.84(15) . . . . ?
C17 C8 C9 C10 58.82(16) . . . . ?
C8 C9 C10 C11 -179.79(13) . . . . ?
C8 C9 C10 C1 -53.98(16) . . . . ?
O1 C1 C10 C11 54.48(15) . . . . ?
C2 C1 C10 C11 -62.83(16) . . . . ?
C6 C1 C10 C11 175.28(12) . . . . ?
O1 C1 C10 C9 -69.61(14) . . . . ?
C2 C1 C10 C9 173.08(12) . . . . ?
C6 C1 C10 C9 51.19(15) . . . . ?
C8 C17 C12 C14 14.2(2) . . . . ?
C6 C17 C12 C14 -111.93(19) . . . . ?
C8 C17 C12 C13 -164.11(18) . . . . ?
C6 C17 C12 C13 69.8(2) . . . . ?
C3 O3 C15 O4 1.1(2) . . . . ?
C3 O3 C15 C16 -178.88(13) . . . . ?

loop_
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O2 H2A O1 0.84 1.89 2.7080(14) 164.5 4_645
C2 H2B O4 1.00 2.57 3.0718(18) 110.8 .
C10 H10A O3 1.00 2.54 3.1737(18) 121.2 .

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