Supplementary Information for

Neoadenoloside A, a Highly Functionalized Diterpene *C*-glycoside, from *Isodon adenolomus*

Wei Zhao,[a] Wei-Guang Wang,[a,b] Xiao-Nian Li,[a] Xue Du,[a] Rui Zhan,[a,b] Juan Zou,[a,b] Yan Li,[a] Hai-Bo Zhang,[a] Fei He,[a] Jian-Xin Pu,*[a] and Han-Dong Sun*[a]

[a] *State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650204, P. R.. China*

[b] *Graduate School of the Chinese Academy of Sciences; Beijing 100039, P. R. China*

[*] Corresponding author Tel.: +86-871-5223251; fax: +86-871-5216343;
E-mail: pujianxin@mail.kib.ac.cn, hdsun@mail.kib.ac.cn

Contents of Supporting Information

Table S1. ^{1}H NMR assignments of **1** and **2** (pyridine-d_5, δ in ppm, J in Hz, 600 MHz)

No.	**1**	**2**	No.	**1**	**2**
1	4.88 (dd, 11.5, 5.4)	4.90 (dd, 11.4, 5.0)	14	5.01 (br. s)	5.27 (br. s)
2	1.85(m)	1.86 (m)	17	2.41 (d, 13.0)	2.71 (dd, 13.4, 2.5)
	1.51 (m)	1.61 (m)		2.20 (dd, 13.0, 2.0)	2.00 (d, 13.4)
3	1.32 (m)	1.35 (overlap)	18	1.18 (s)	1.01 (s)
5	1.64 (d, 5.4)	1.37 (overlap)	19	1.11 (s)	1.08 (s)
6	4.09 (d, 5.4)	4.06 (br. s)	20	4.47 (d, 9.8)	4.16 (d, 10.2)
8		2.31 (d, 12.2)		4.32 (dd, 9.8, 2.2)	4.12 (d, 10.2)
9	2.90 (dd, 11.3, 6.5)	2.08 (br. t, 12.2)	1’	4.65 (s)	4.49 (d, 1.8)
11	1.90 (m)	1.61 (m)	4’	4.62 (d, 1.0)	5.05 (d, 1.4)
	1.18 (m)	1.45 (m)	5’	3.93 (br. s)	4.04 (br. s)
12	1.91 (m)	2.48 (m)	6’	4.31 (dd, 9.6, 1.3)	4.39 (dd, 10.0, 2.3)
	1.62 (m)	2.00 (m)		4.03 (br. d, 9.6)	4.20 (d, 10.0)
13	2.92 (br. d, 9,7)	2.38 (dd, 11.6, 1.5)	OAc	2.03 (s)	1.96 (s)
OH-6	6.48 (br. s)		OH-15	6.74 (s)	

Table S2. ^{1}H- and ^{13}C-NMR assignments of **3** (pyridine-d_5, δ in ppm, J in Hz)[a]

No.	^{1}H	^{13}C	No.	^{1}H	^{13}C
1	4.81 (dd, 11.3, 5.4)	75.8 d	12	2.38 (m)	30.5 t
2	1.84 (m)	25.6 t		1.50 (m)	
	1.50 (m)		13	3.20 (br. d, 9.7)	43.8 d
3	1.35 (m)	38.5 t	14	5.25 (br. s)	73.4 d
4		33.9 s	15	5.01 (br. s)	209.2 s
5	1.51 (overlapped)	60.7 d	16		152.9 s
6	4.22 (br. t, 7.5)	74.4 d	17	6.27 (br. s)	119.6 t
				5.52 (br. s)	
7		98.2 s	18	1.25 (s)	33.0 q
8		62.4 s	19	1.11 (s)	22.0 q
9	1.91 (dd, 12.9, 6.0)	52.7 d	20	4.52 (d, 10.2)	63.5 t
10		40.1 s		4.33 (d, 10.2)	
11	2.11 (m)	18.4 t	OAc	2.06 (s)	21.5 q
	1.25 (m)				170.1 s

[a] ^{1}H in 500 MHz, ^{13}C in 125 MHz.

Figure S1. ^{1}H NMR spectrum of neoadenoloside A (**1**) (pyridine-d_5)

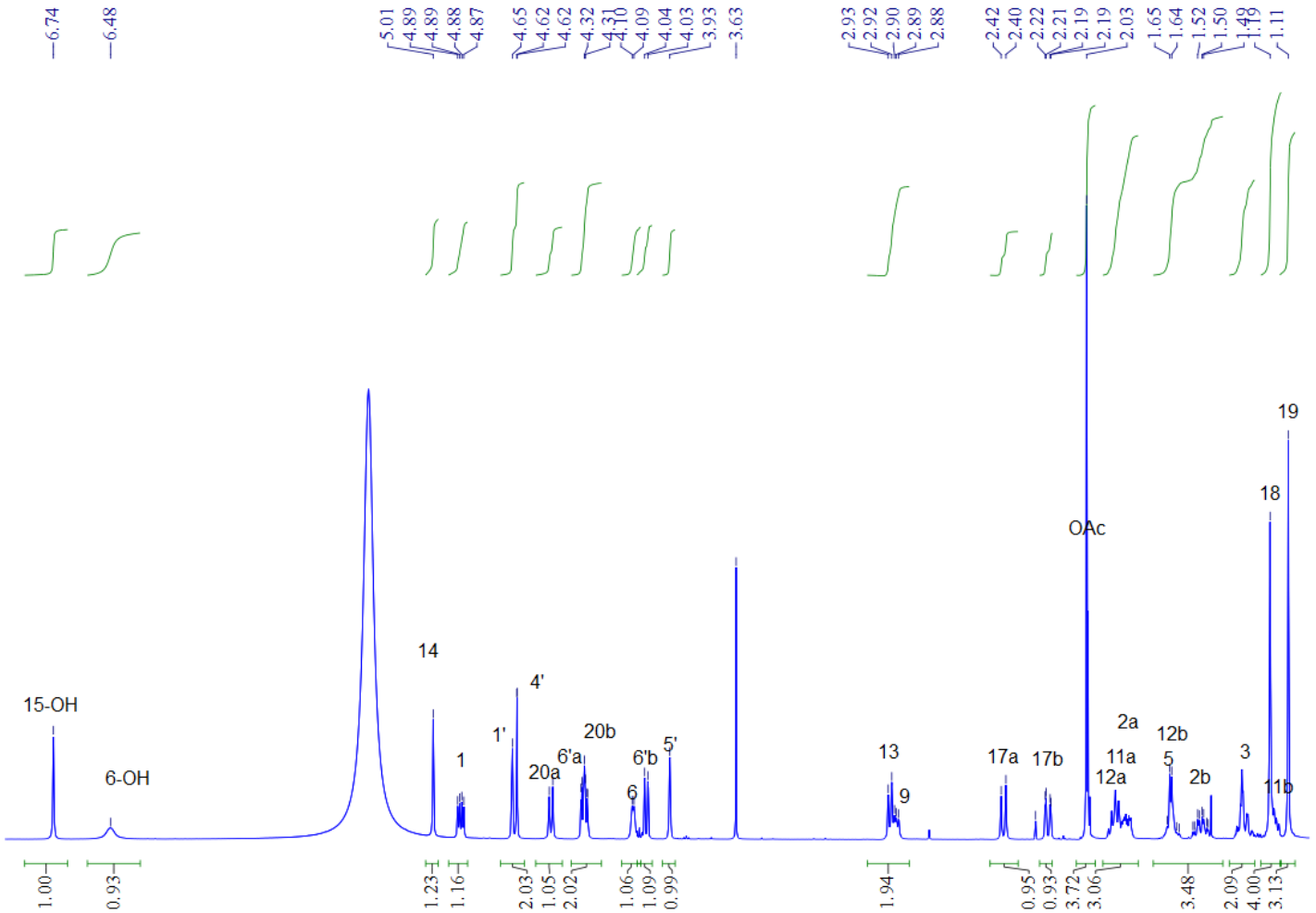


Figure S2. ^{13}C NMR spectrum of neoadenoloside A (**1**) (pyridine-d_5)

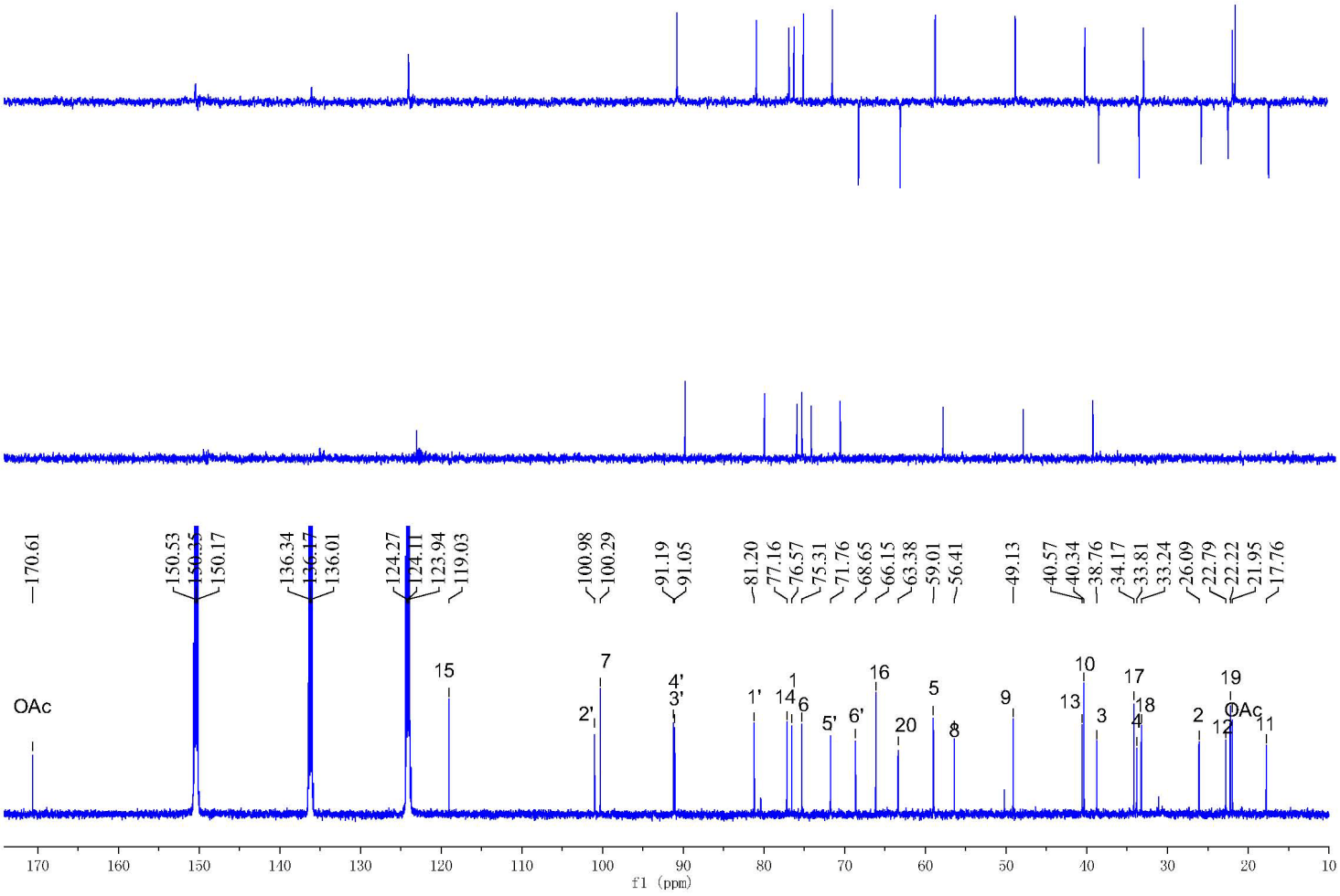
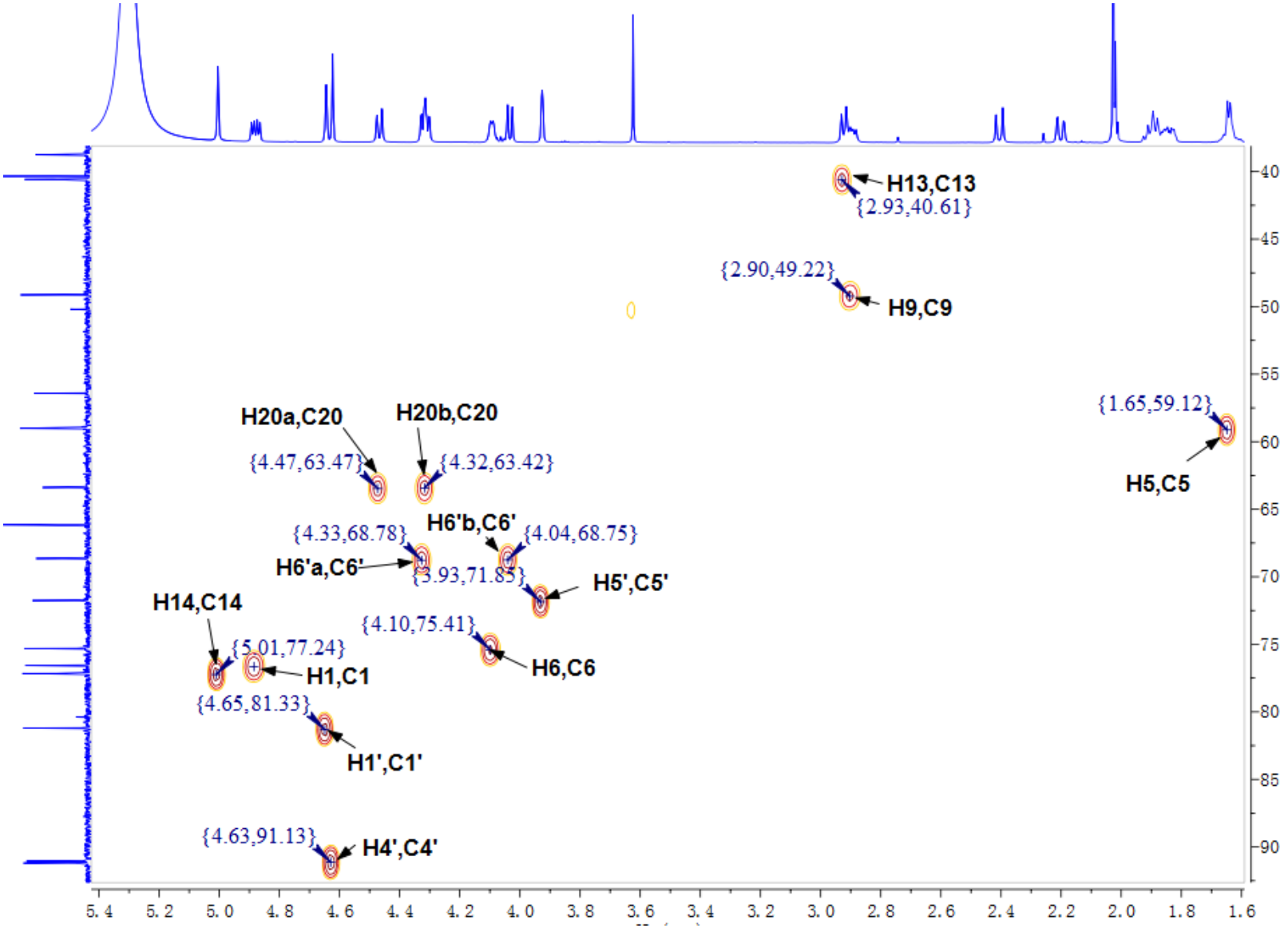


Figure S3. HSQC spectrum of neoadenoloside A (**1**) (pyridine-d_5)



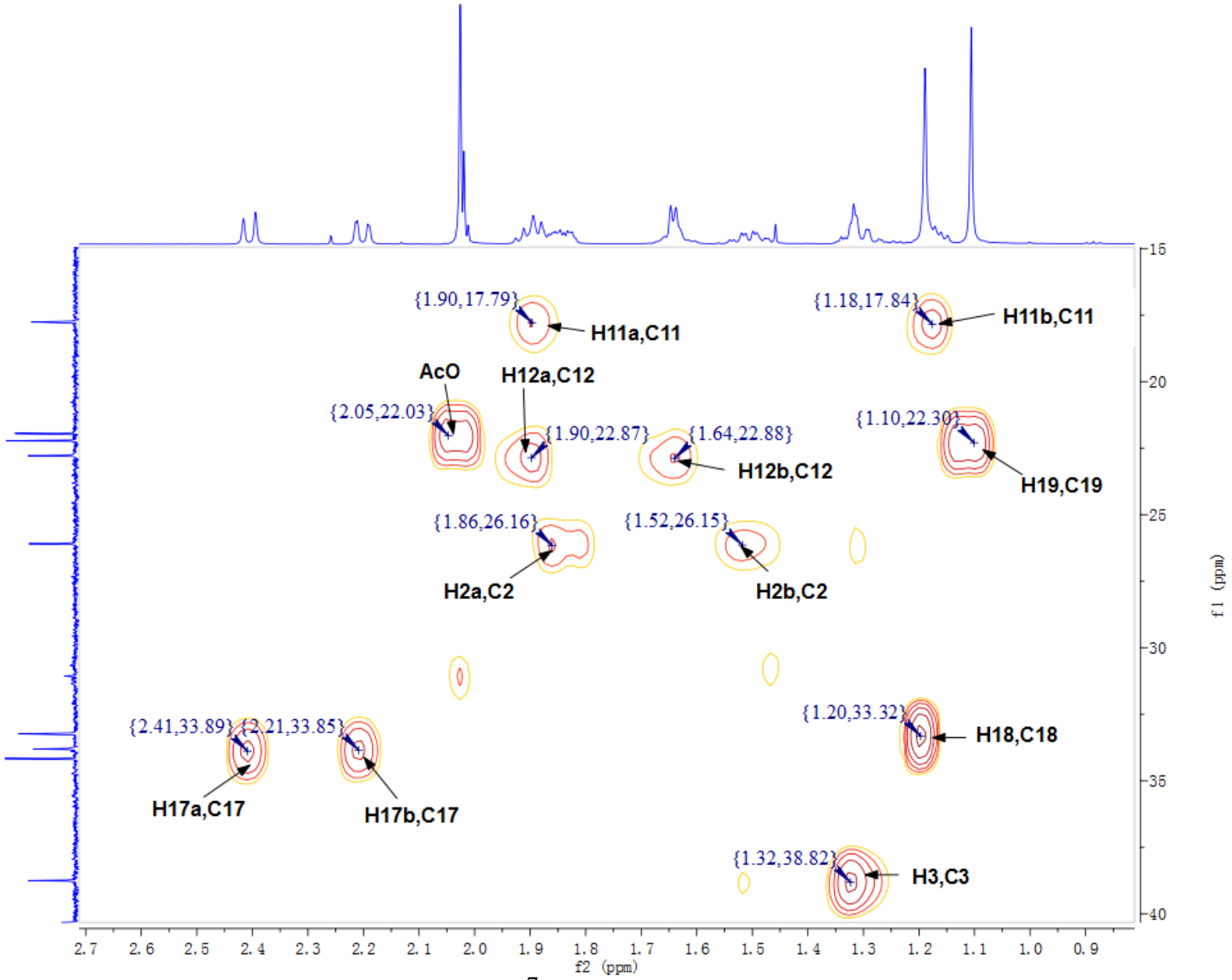
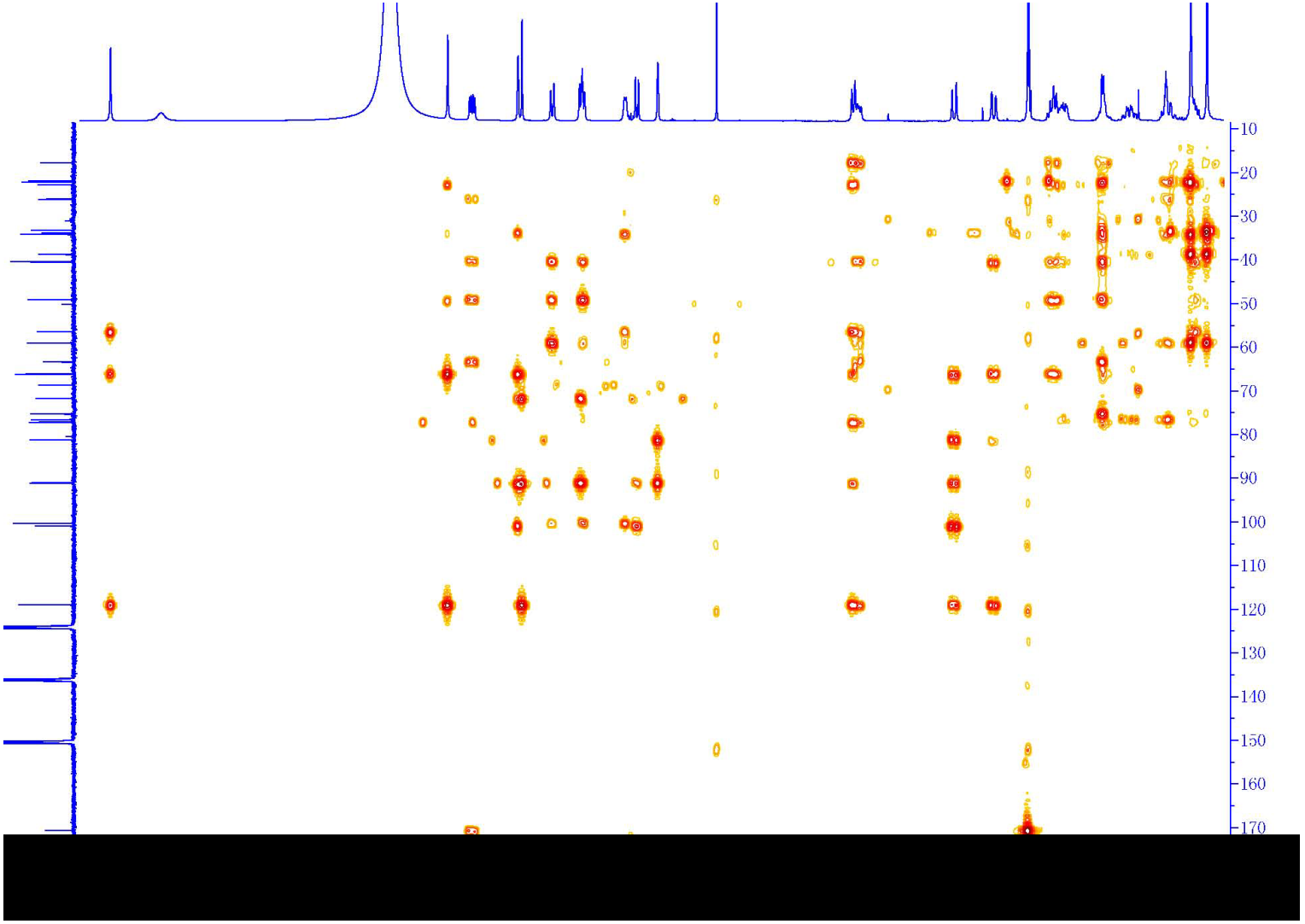
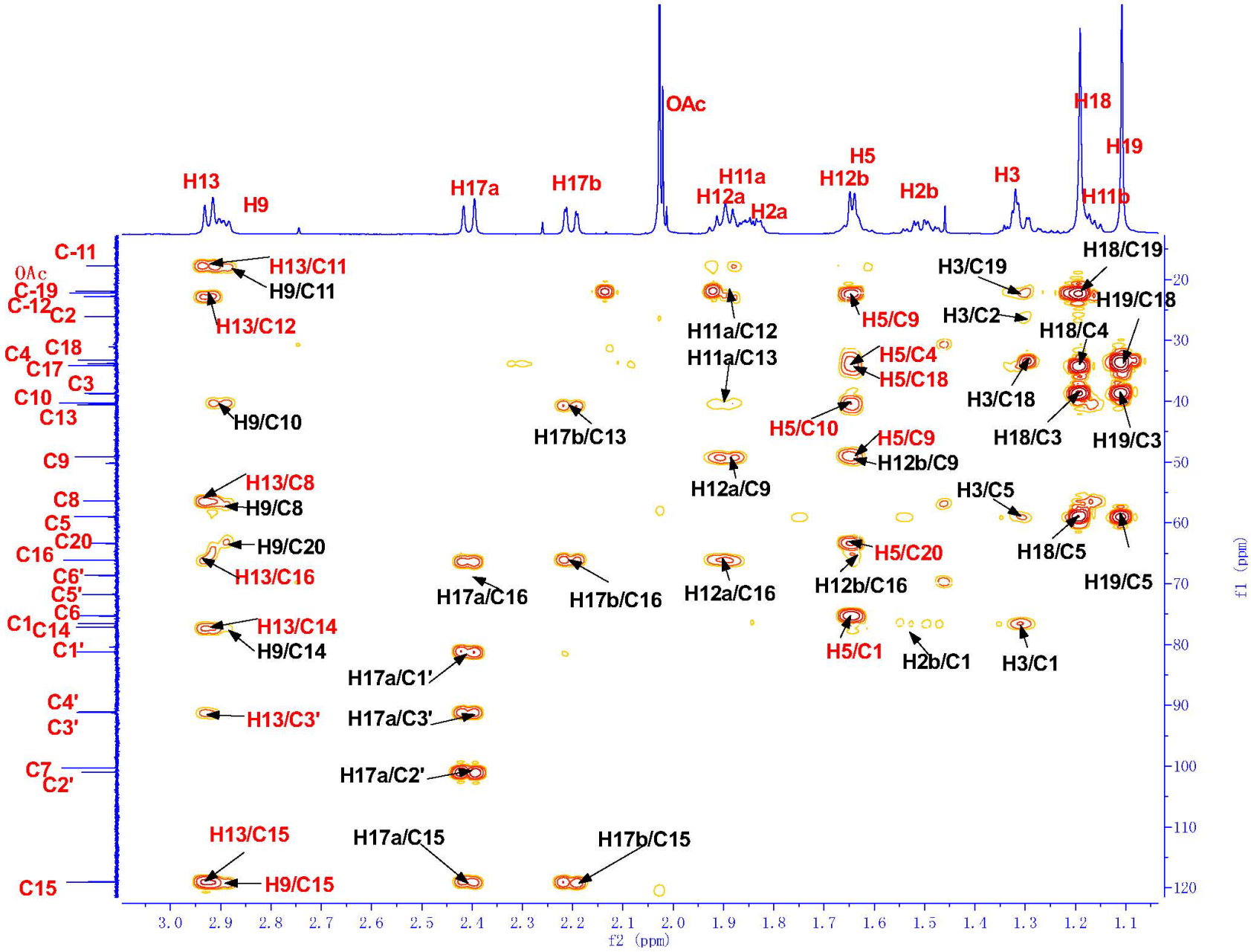
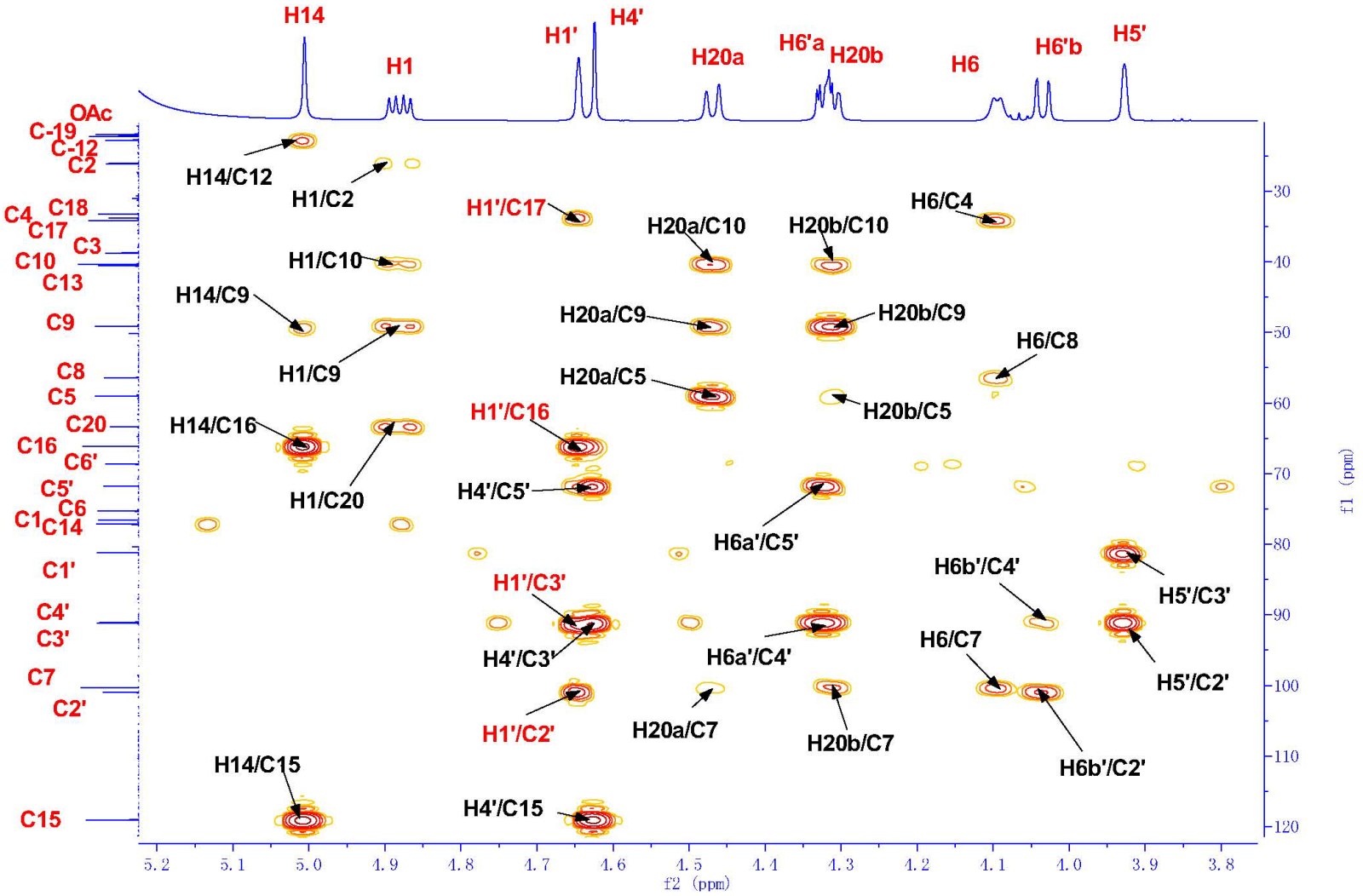


Figure S4. HMBC spectrum of neoadenoloside A (**1**) (pyridine-d_5)







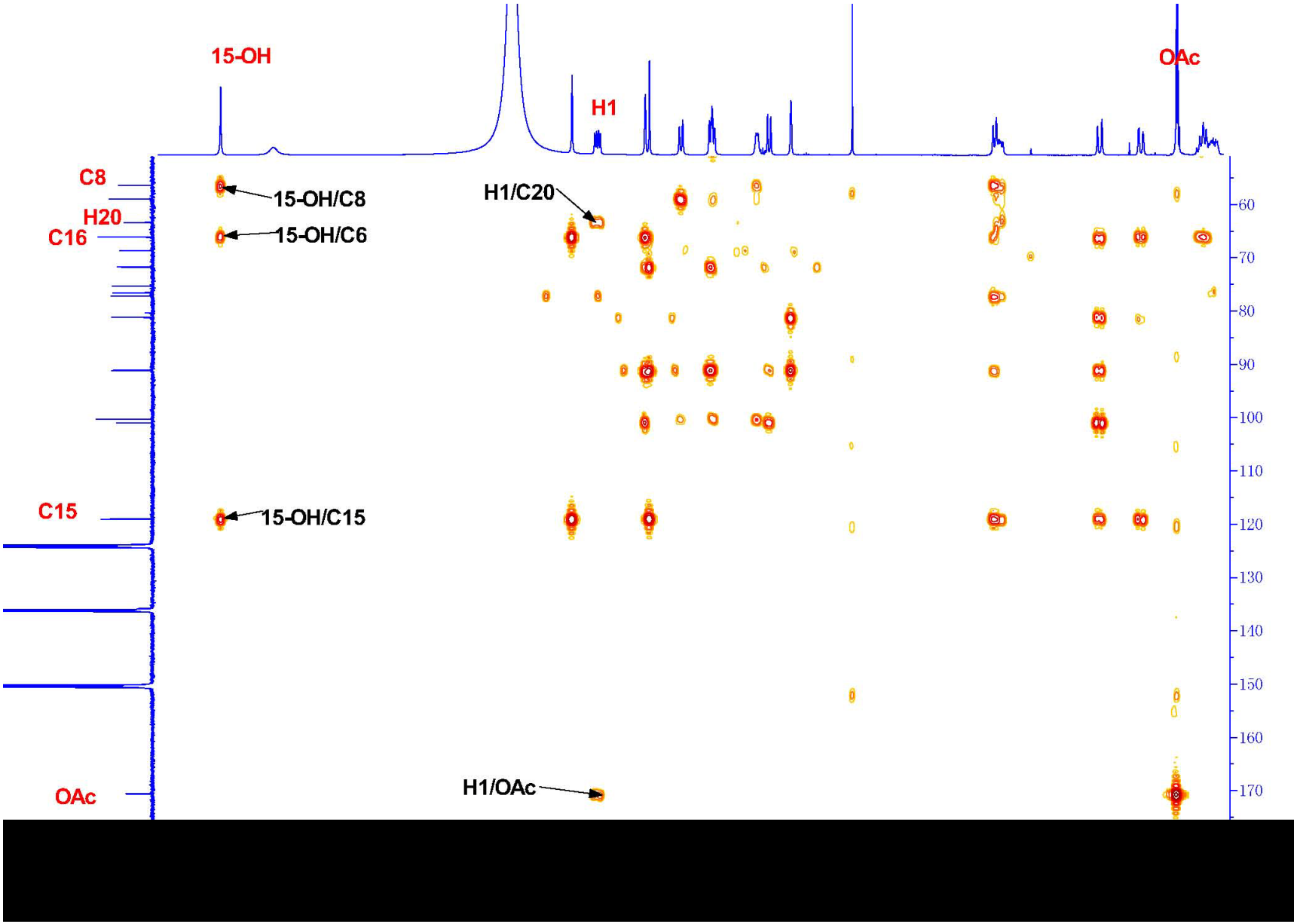
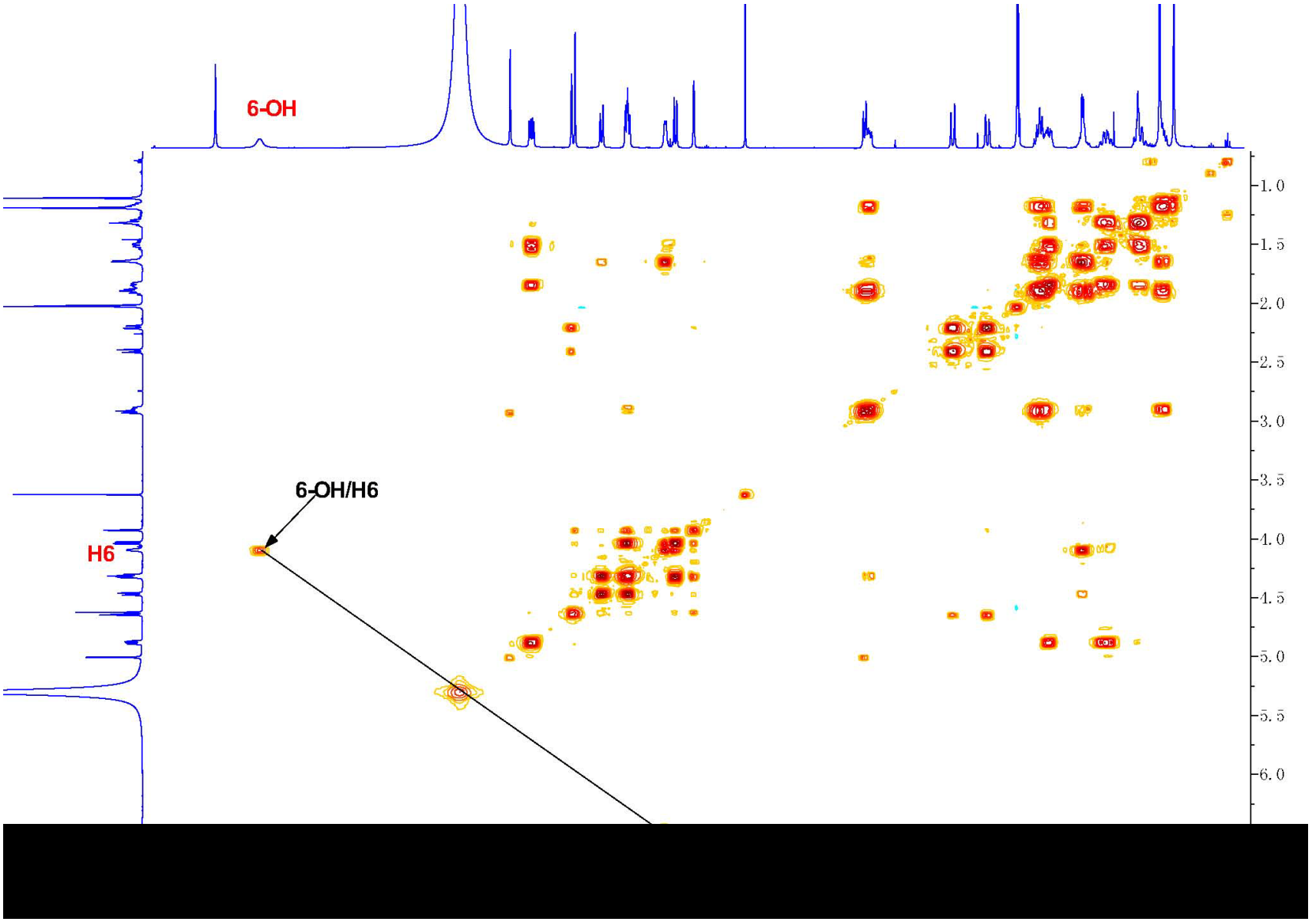
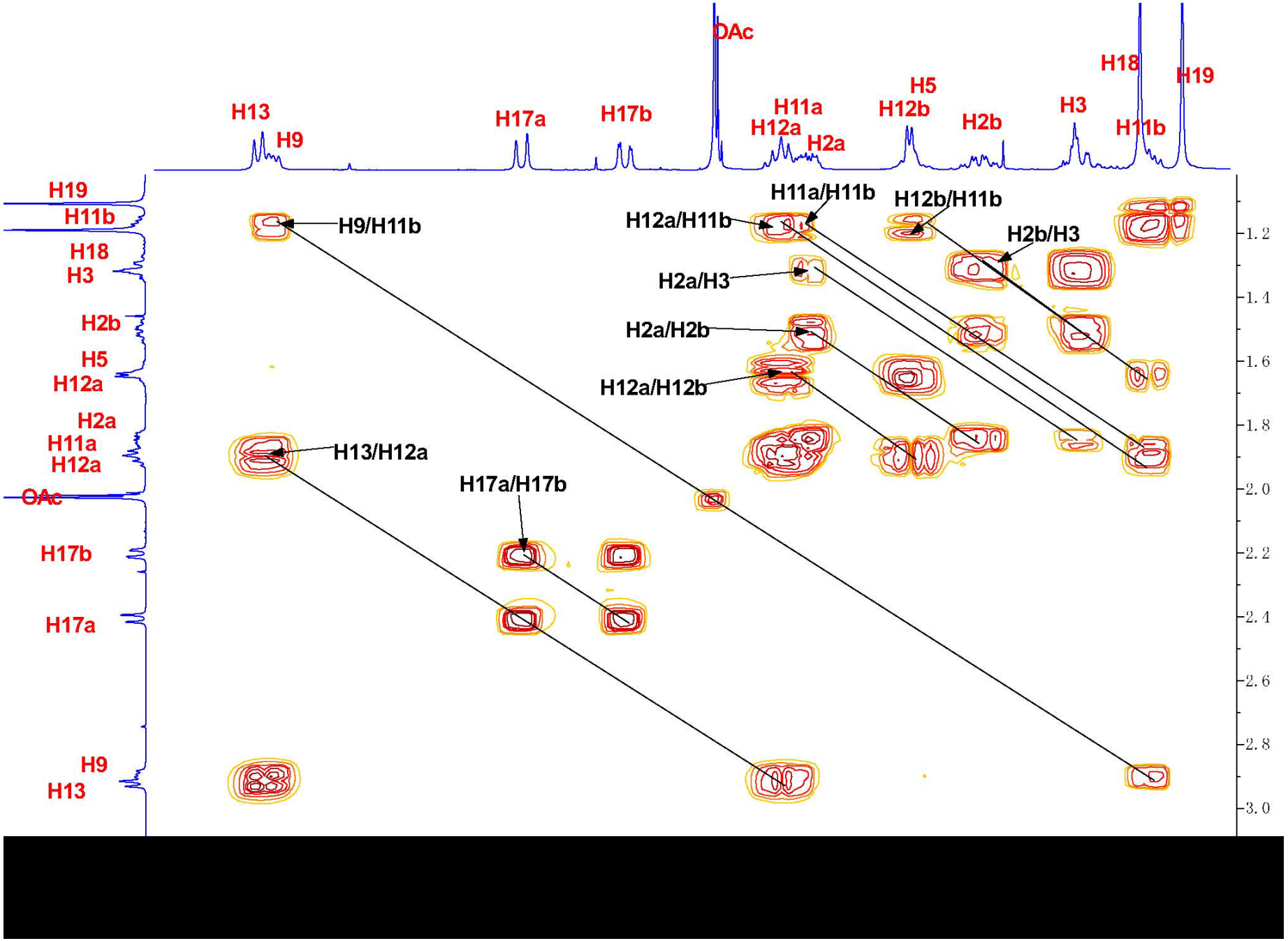


Figure S5. ^{1}H-^{1}H COSY spectrum of neoadenoloside A (**1**) (pyridine-d_5)





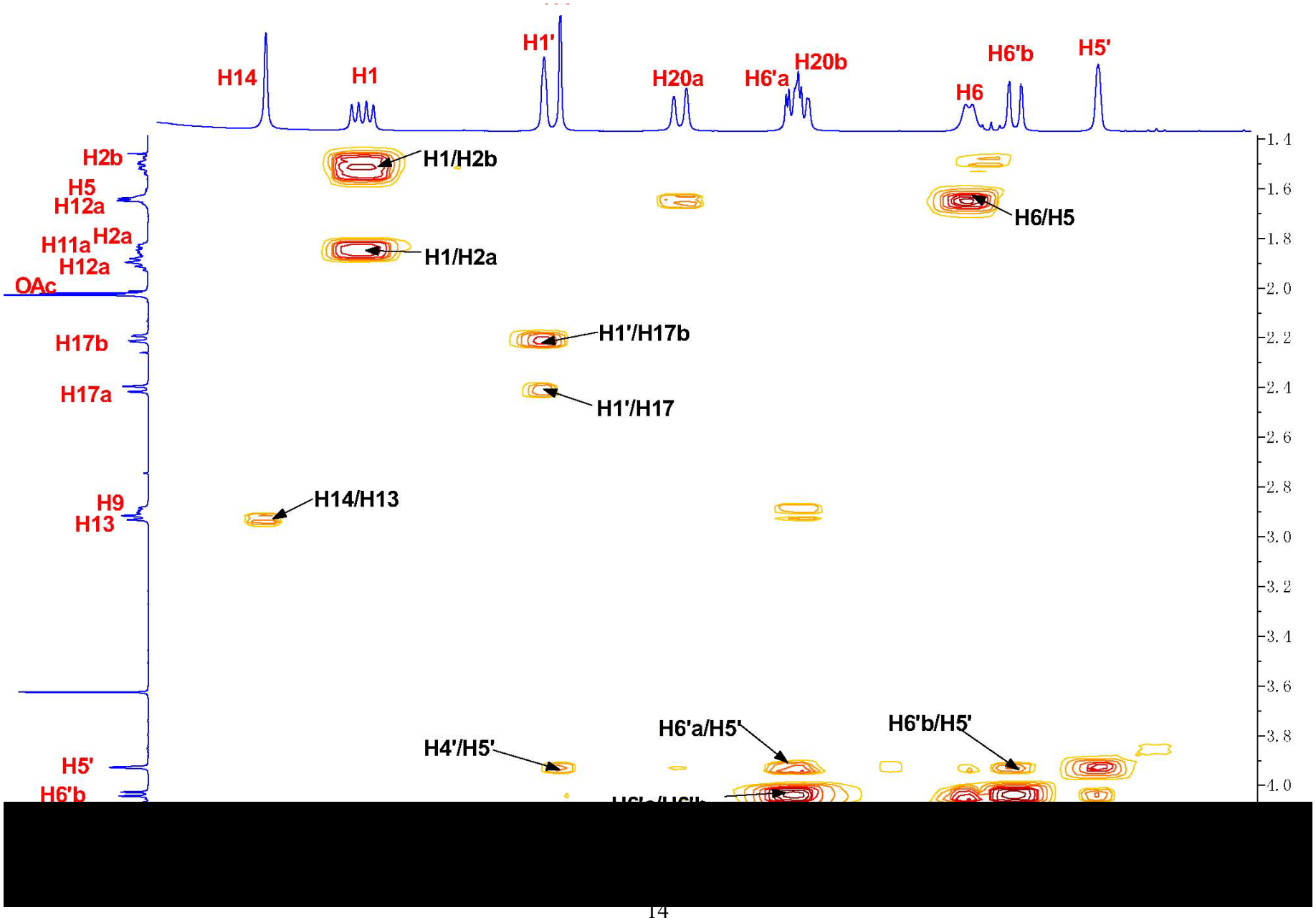
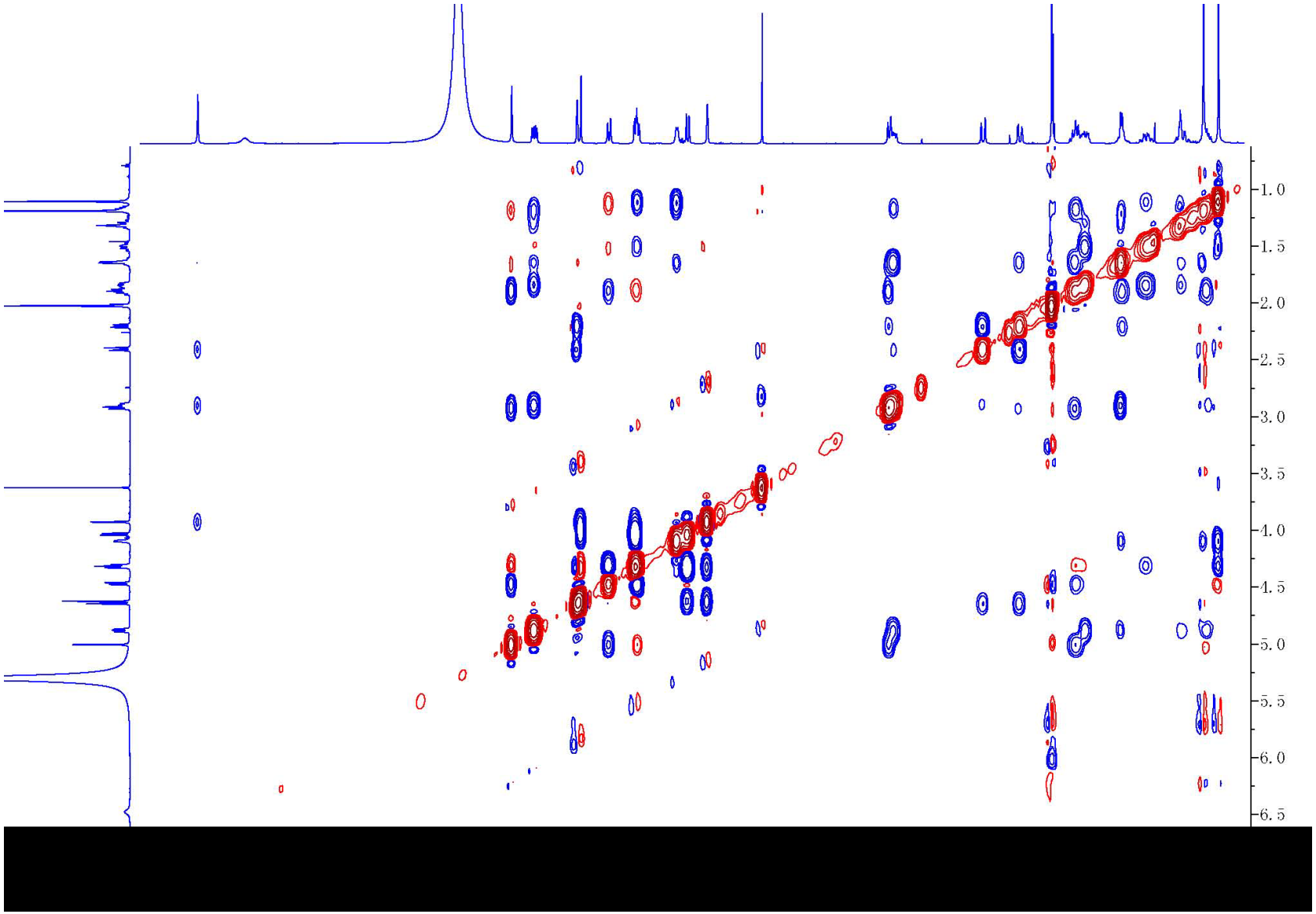
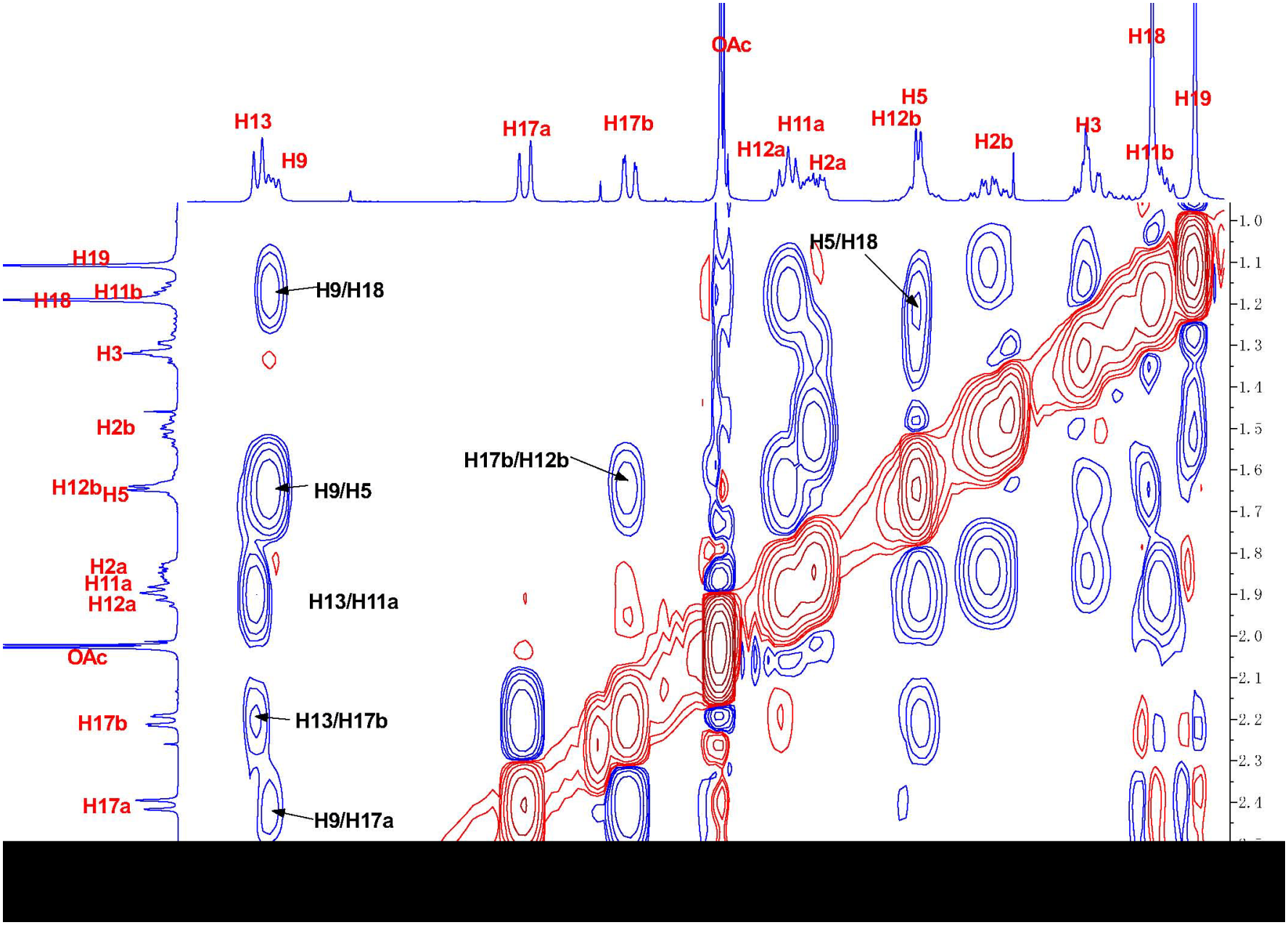


Figure S6. ROESY spectrum of neoadenoloside A (**1**) (pyridine-d_5)





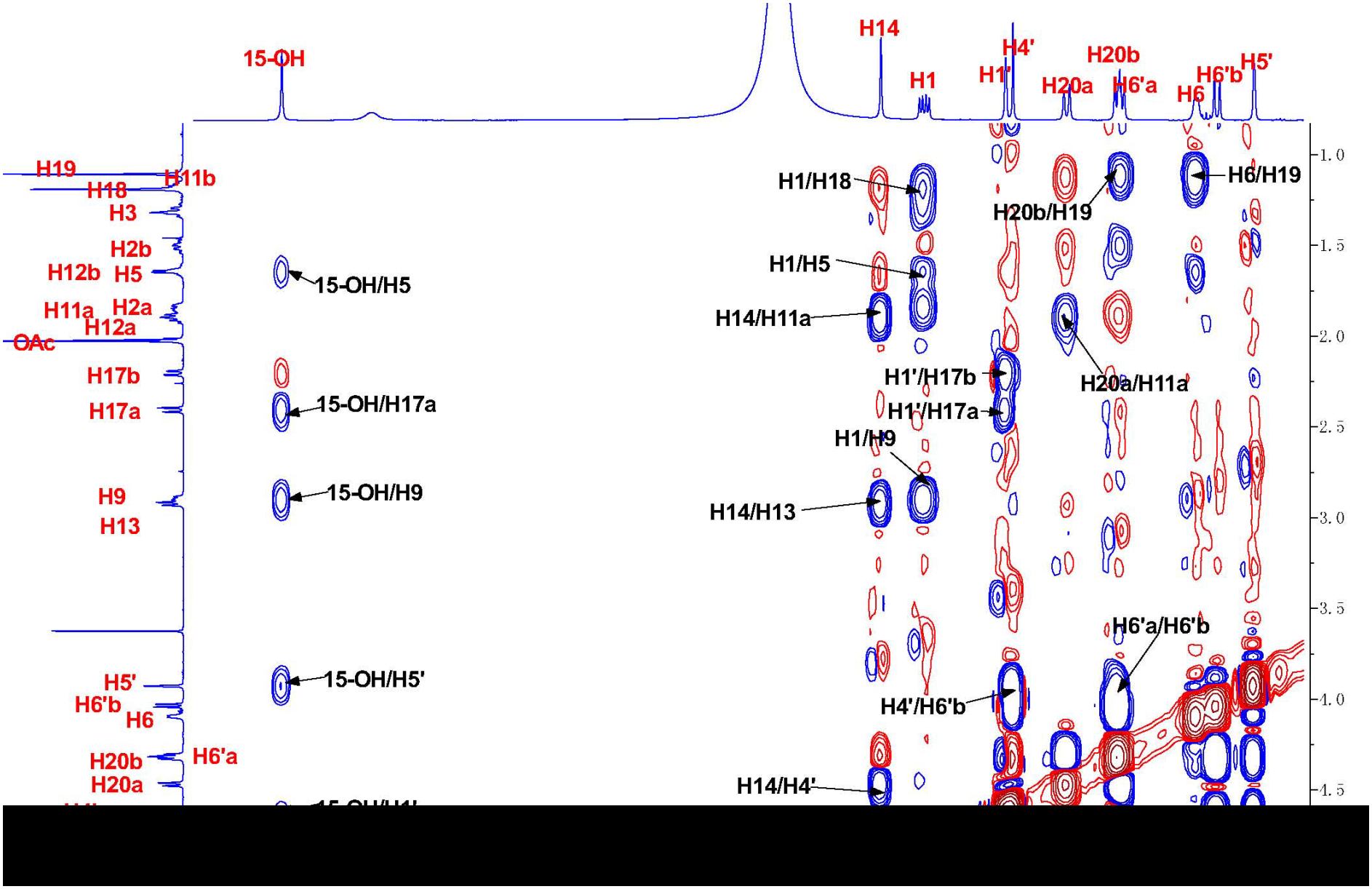


Figure S7. MS and HRESIMS data of neoadenoloside A (**1**)

Mass Spectrum List Report

Analysis Info

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Sample Name	Szia-104e	Instrument	HCT
Comment	balance method		

Acquisition Parameter

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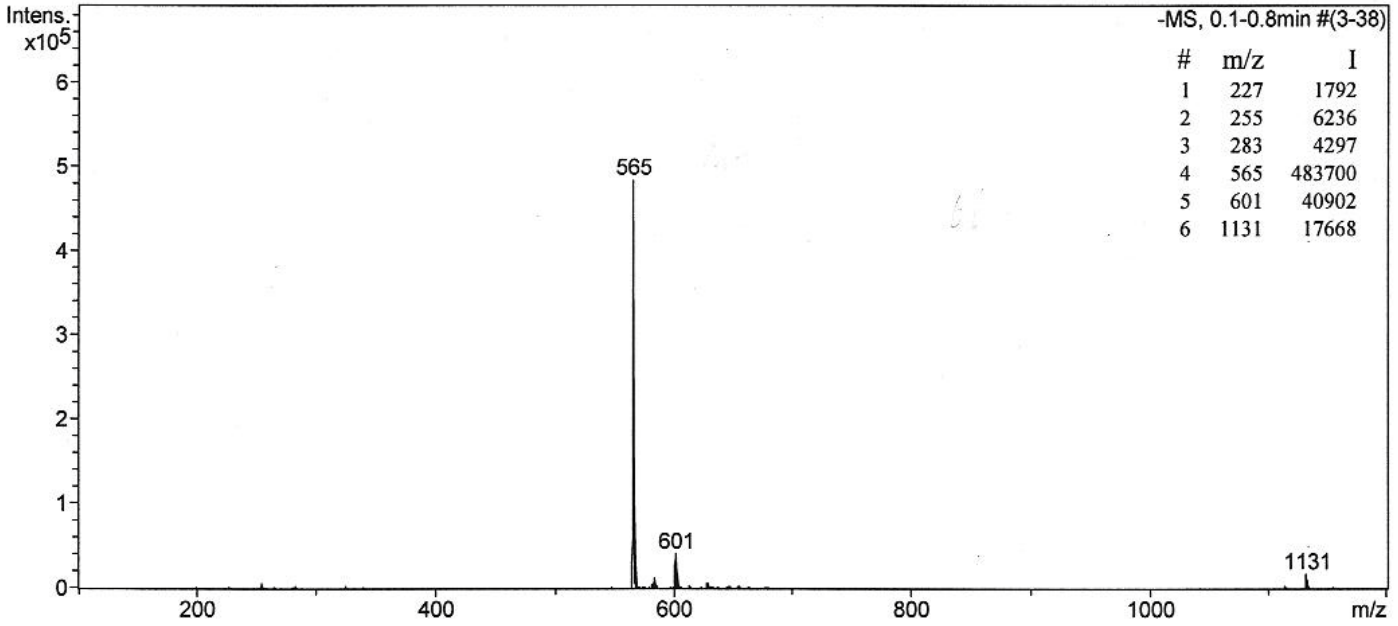
Mass Range Mode	Std/Enhanced	Scan Begin	100 m/z	Scan End	1200 m/z
Capillary Exit	-128.5 Volt	Skimmer	-40.0 Volt	Trap Drive	58.8
Accumulation Time	1000 µs	Averages	7 Spectra	Auto MS/MS	off



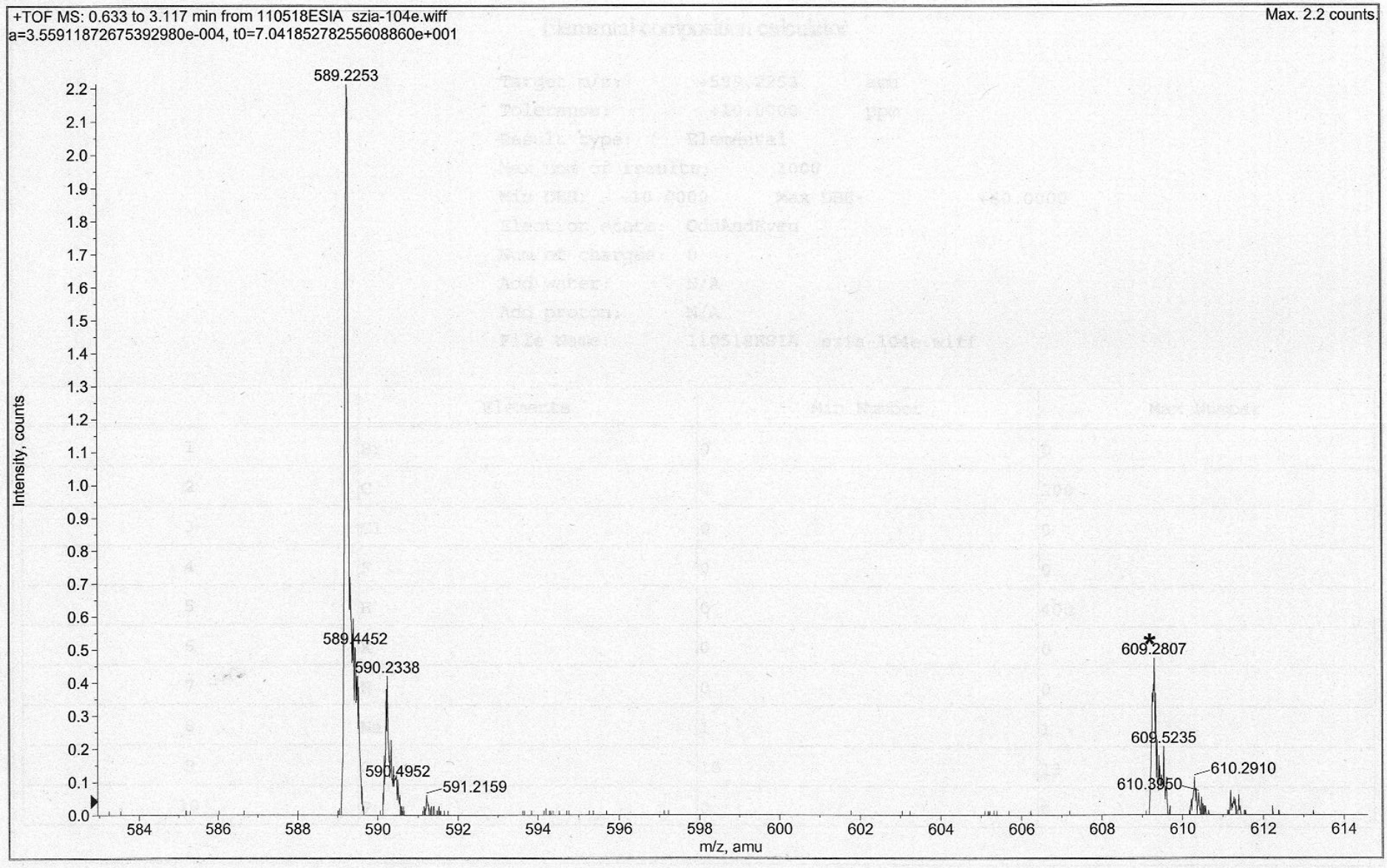


Figure S8. IR spectrum of neoadenoloside A (**1**)

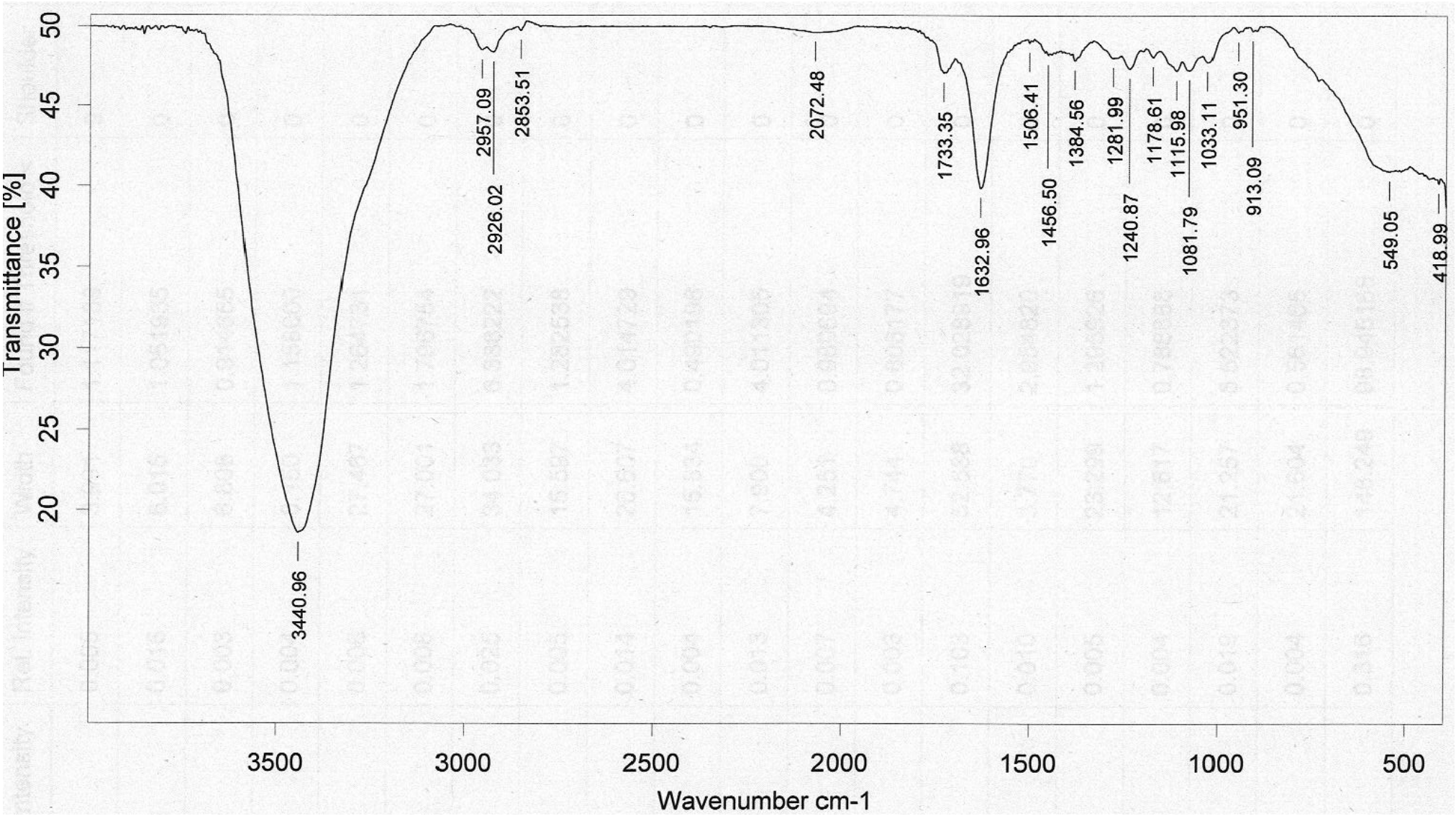


Figure S9. UV spectrum of neoadenoloside A (**1**)

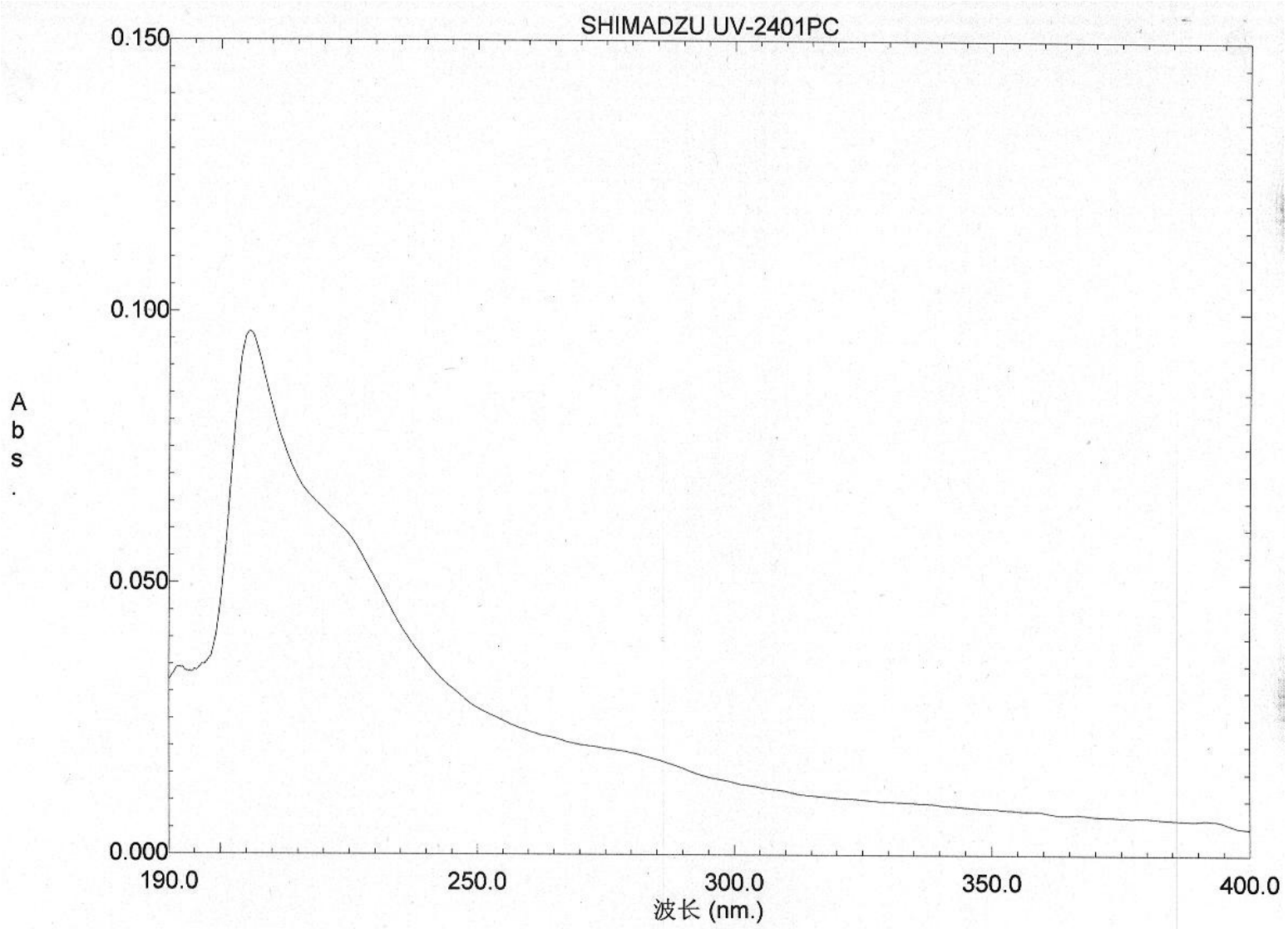


Figure S10. ^{1}H NMR spectrum of neoadenoloside B (**2**) (pyridine-d_5)

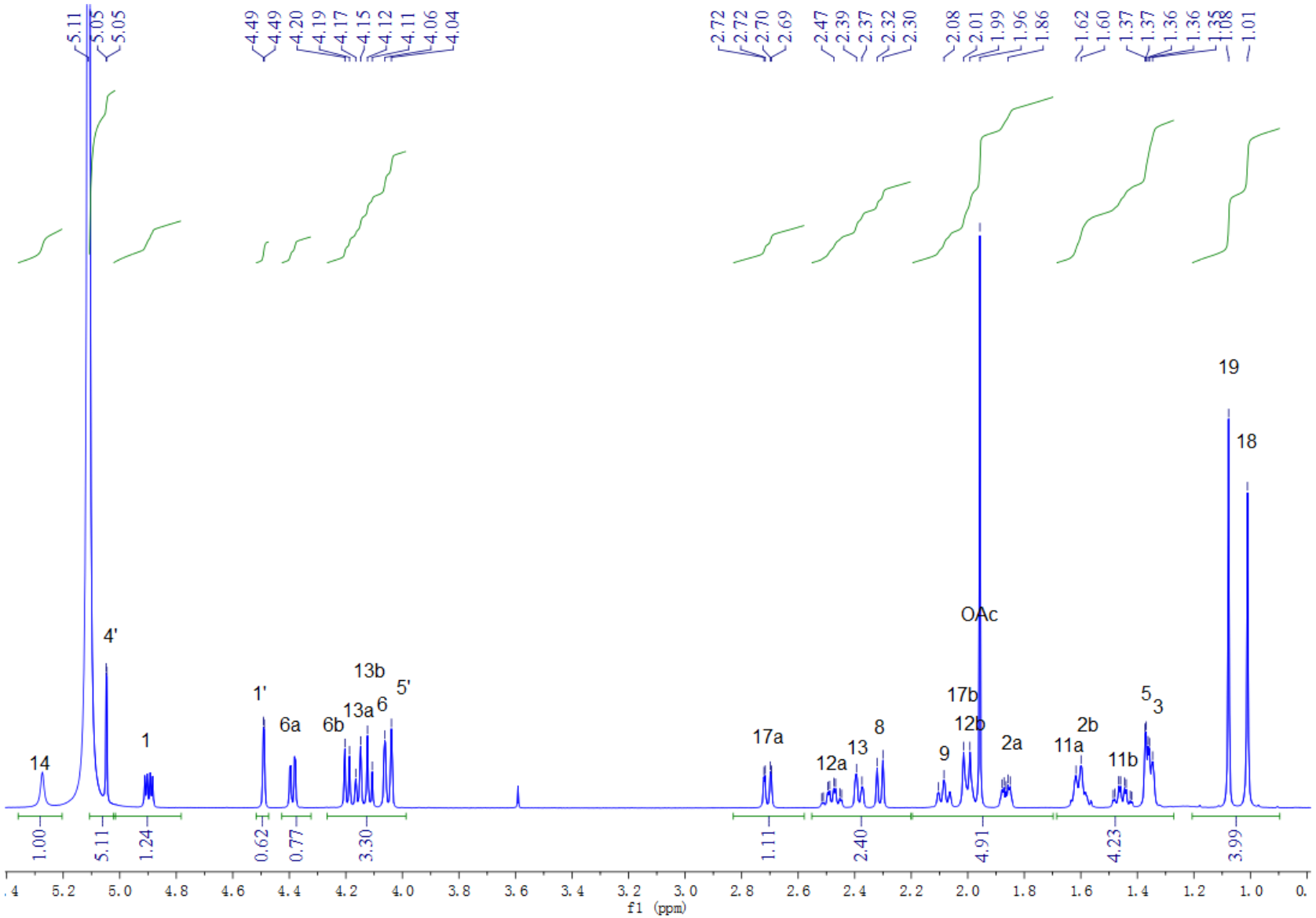


Figure S11. ^{13}C NMR and DEPT spectra of neoadenoloside B (**2**) (pyridine-d_5)

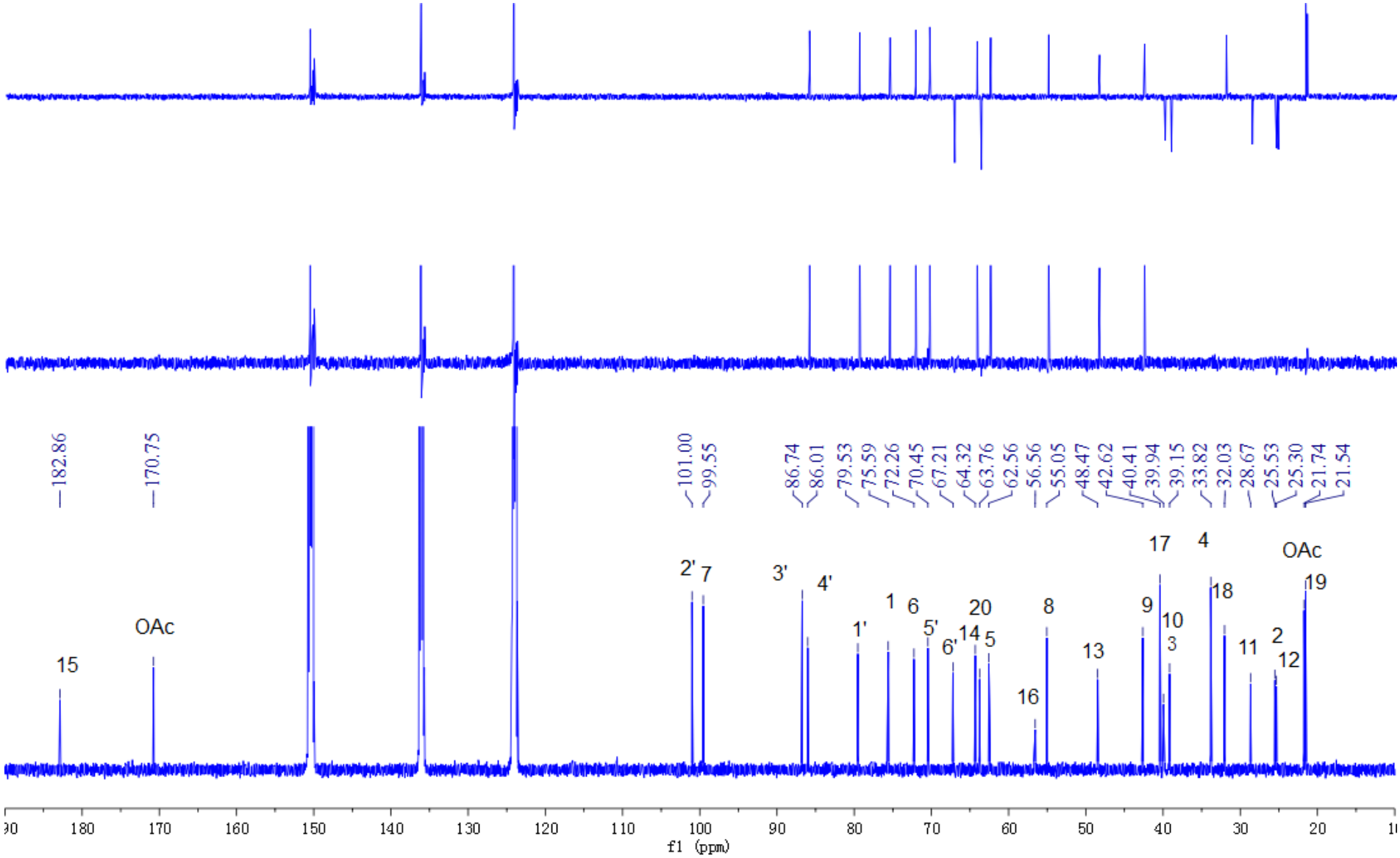


Figure S12. HMQC spectra of neoadenoloside B (**2**) (pyridine-d_5)

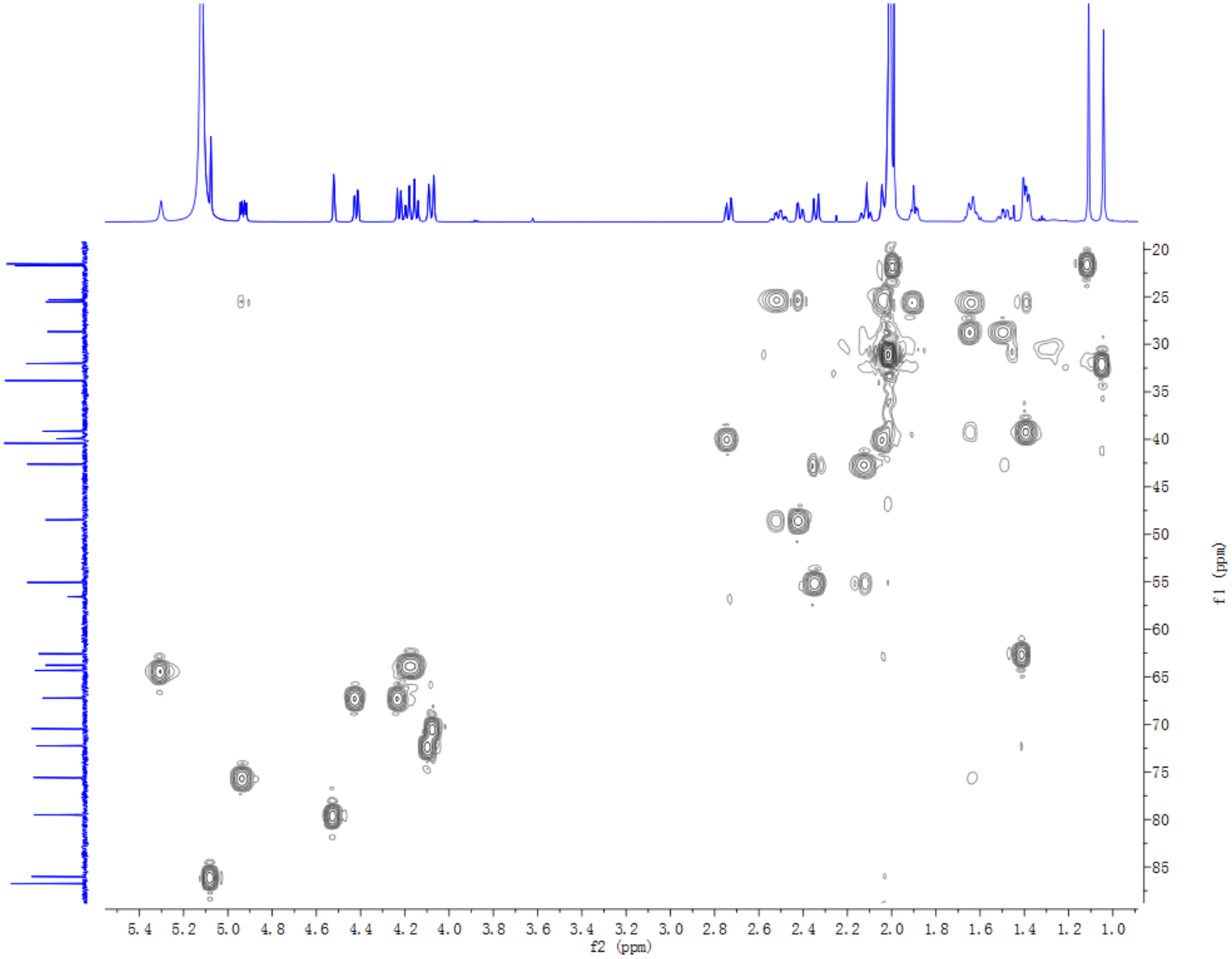


Figure S13. HMBC spectrum of neoadenoloside B (**2**) (pyridine-d_5)

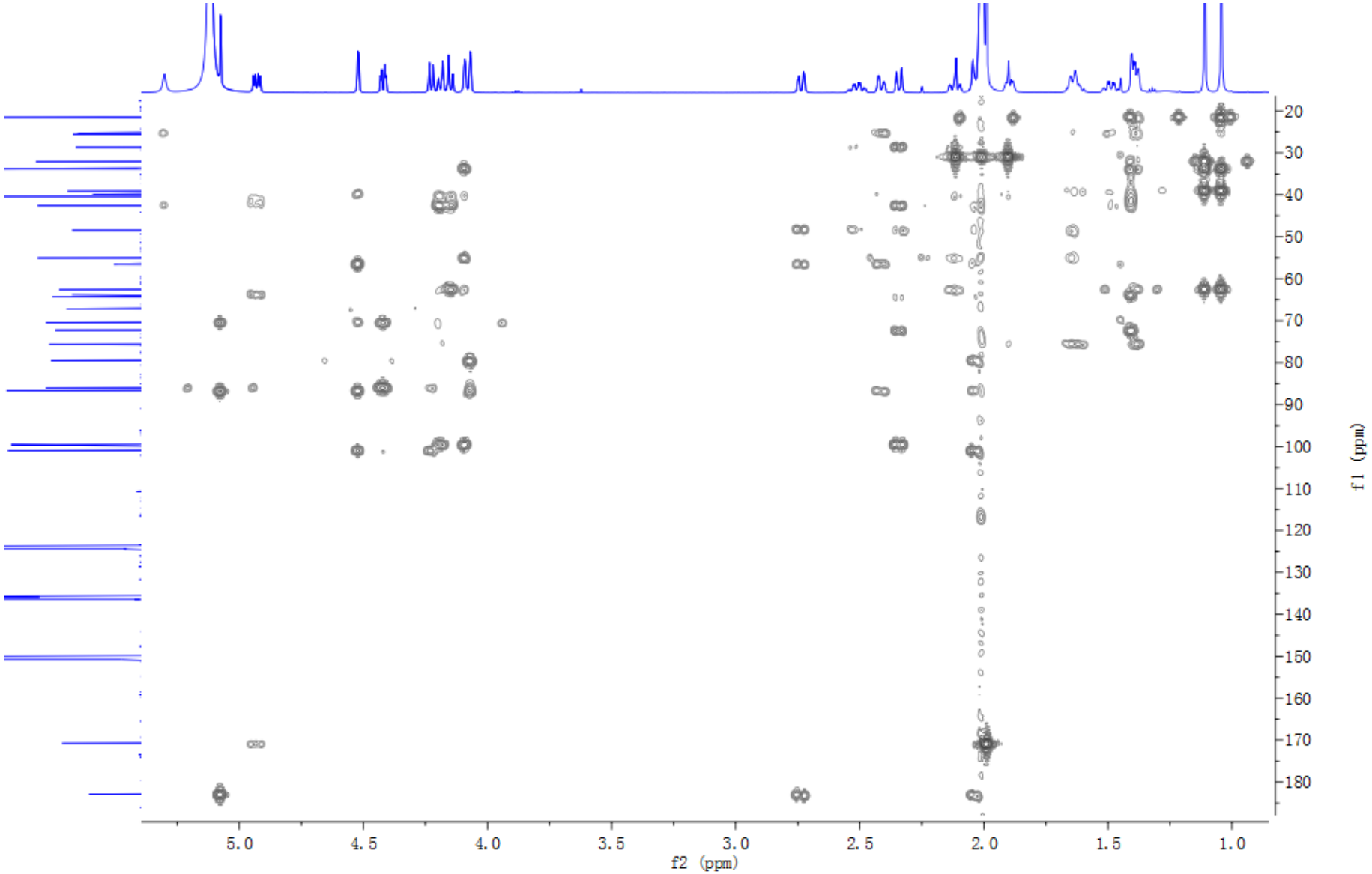


Figure S14. COSY spectrum of neoadenoloside B (**2**) (pyridine-d_5)

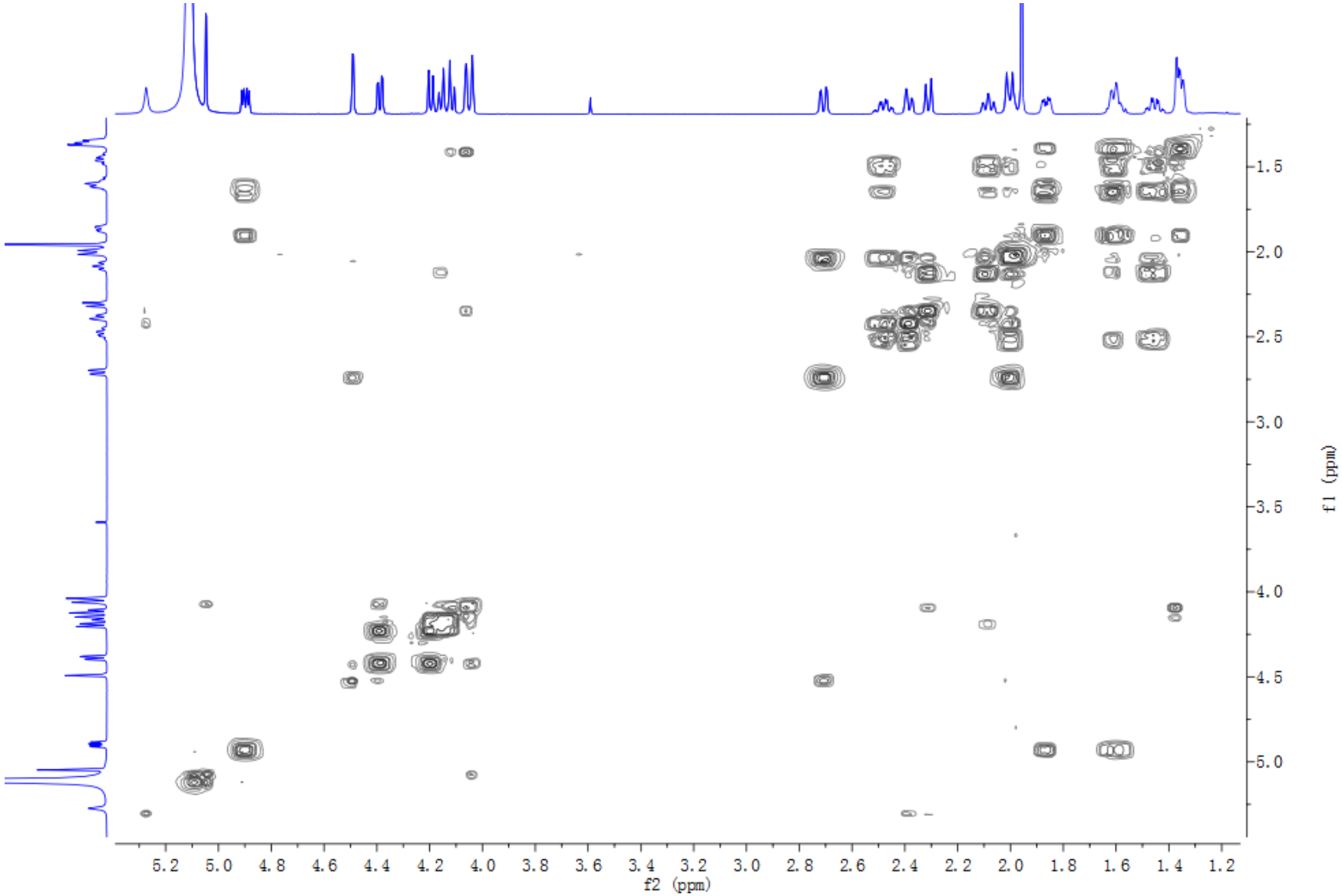


Figure S15. ROESY spectrum of neoadenoloside B (**2**) (pyridine-d_5)

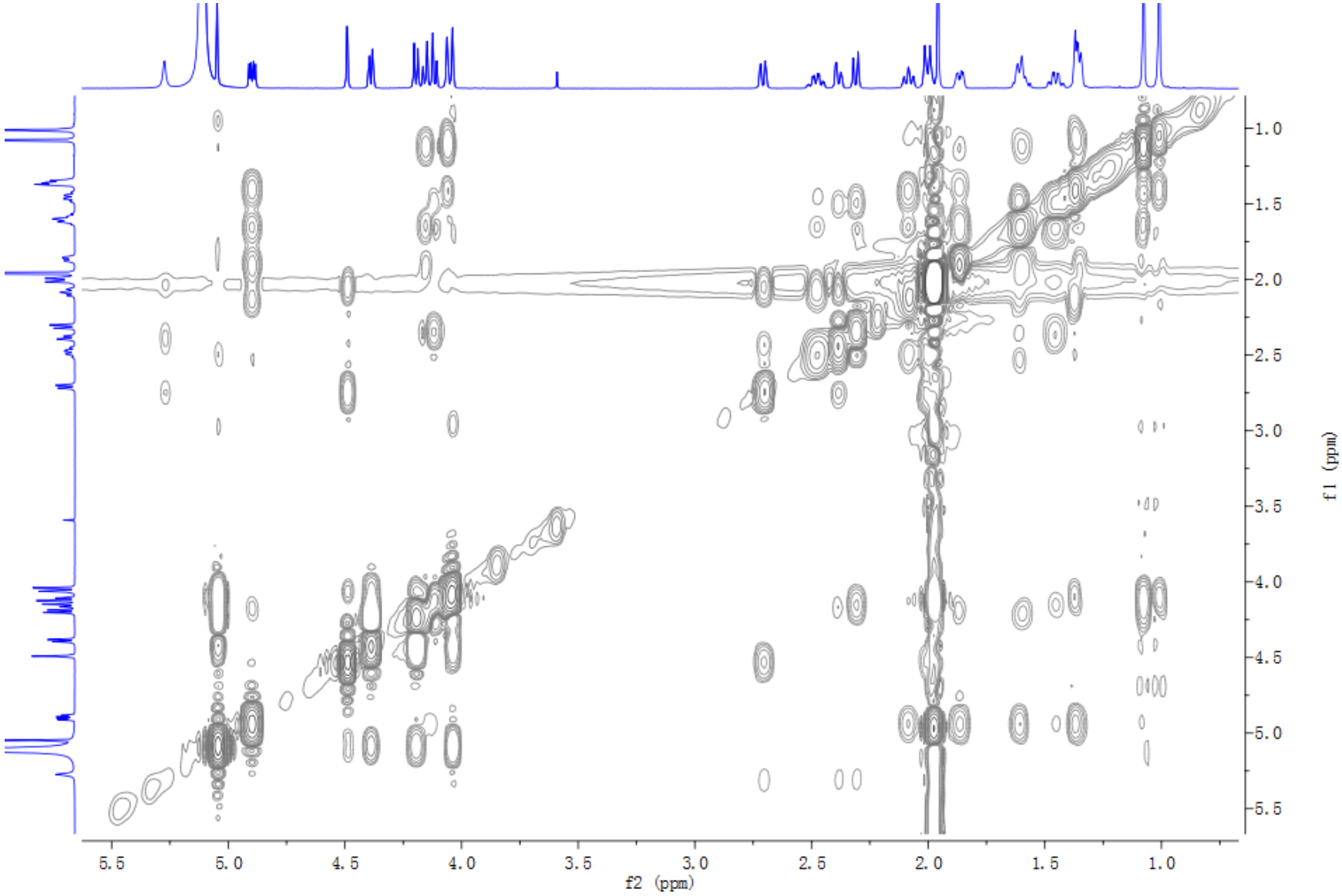
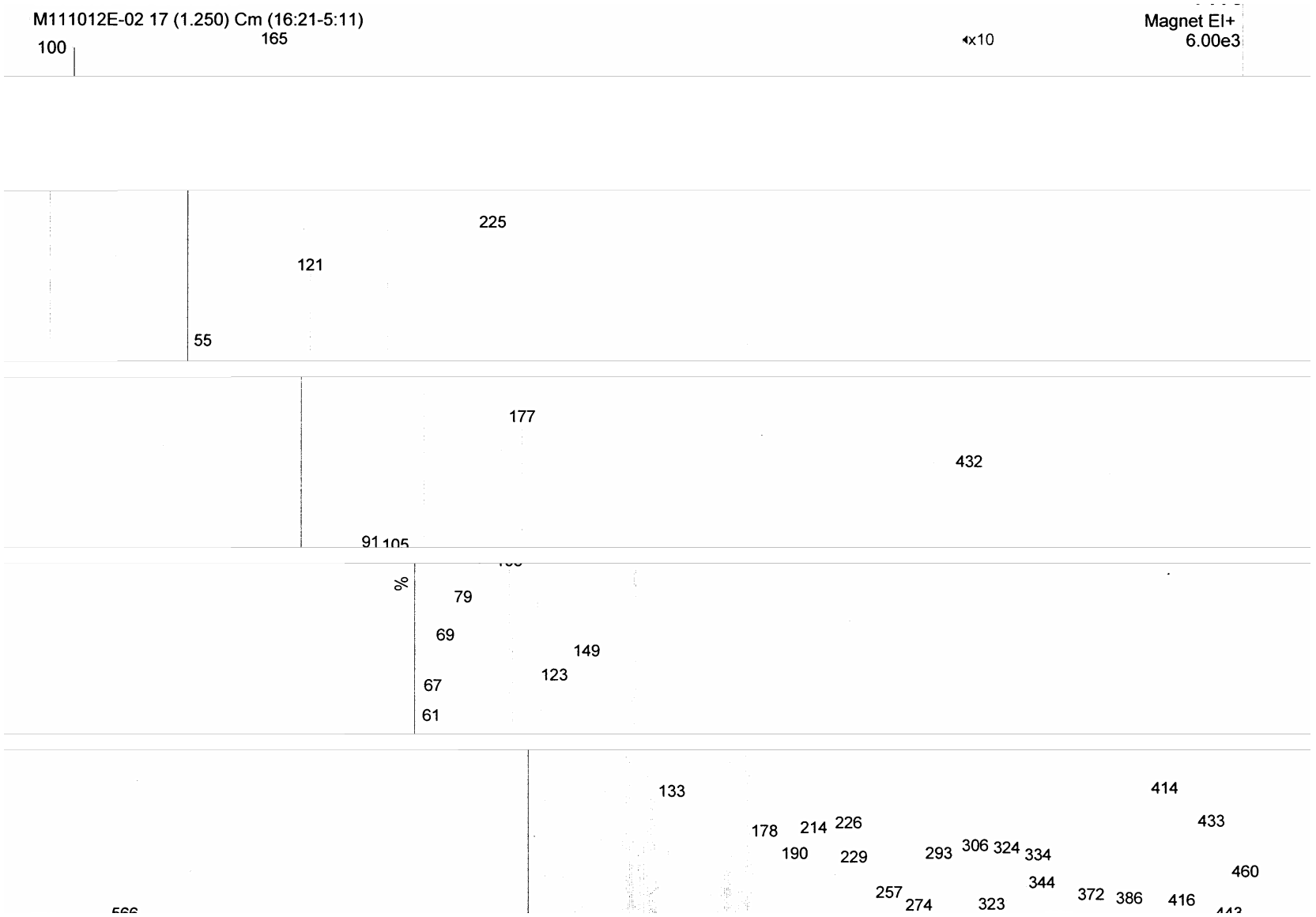


Figure S16. MS and HRESIMS data of neoadenoloside B (**2**)



Elemental Composition Report

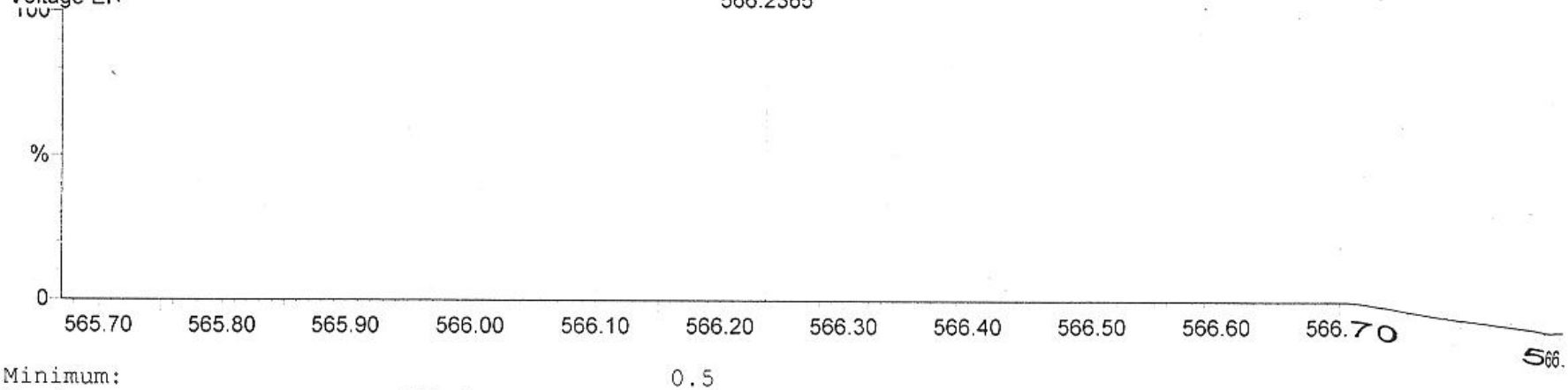
Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 40.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
15 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 O: 10-12

szia104e2
11:10:39 12-Oct-2011
Voltage EI+

KIB
M111012EA-01AFAMMA 18 (1.652)
566.2365



Minimum:				0.5		
Maximum:		100.0	10.0	40.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
566.2365	566.2363	0.2	0.4	10.0	5546054.5	C28 H38 O12

Figure S17. IR spectrum of neoadenoloside B (**2**)

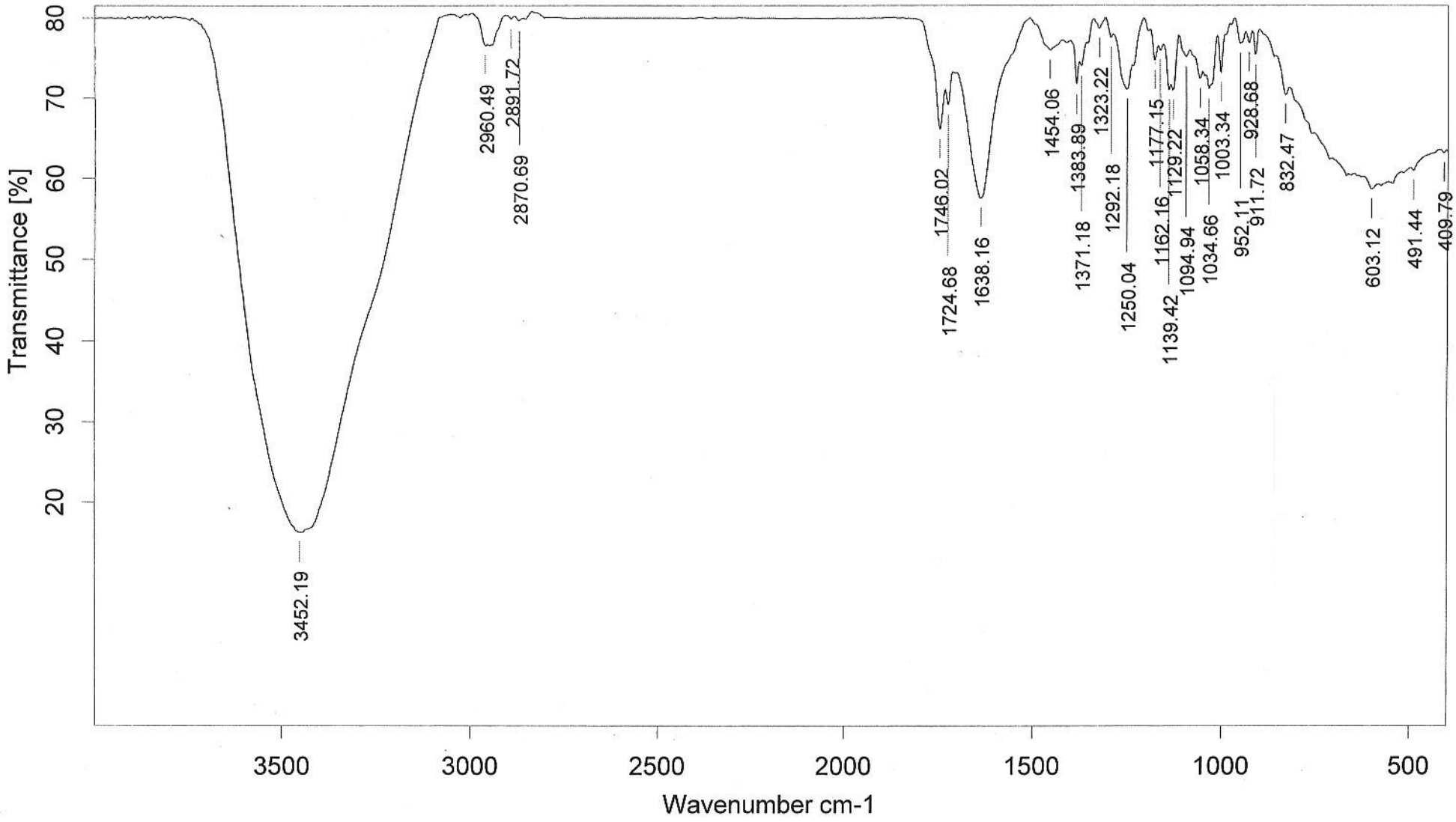


Figure S18. UV spectrum of neoadenoloside B (**2**)

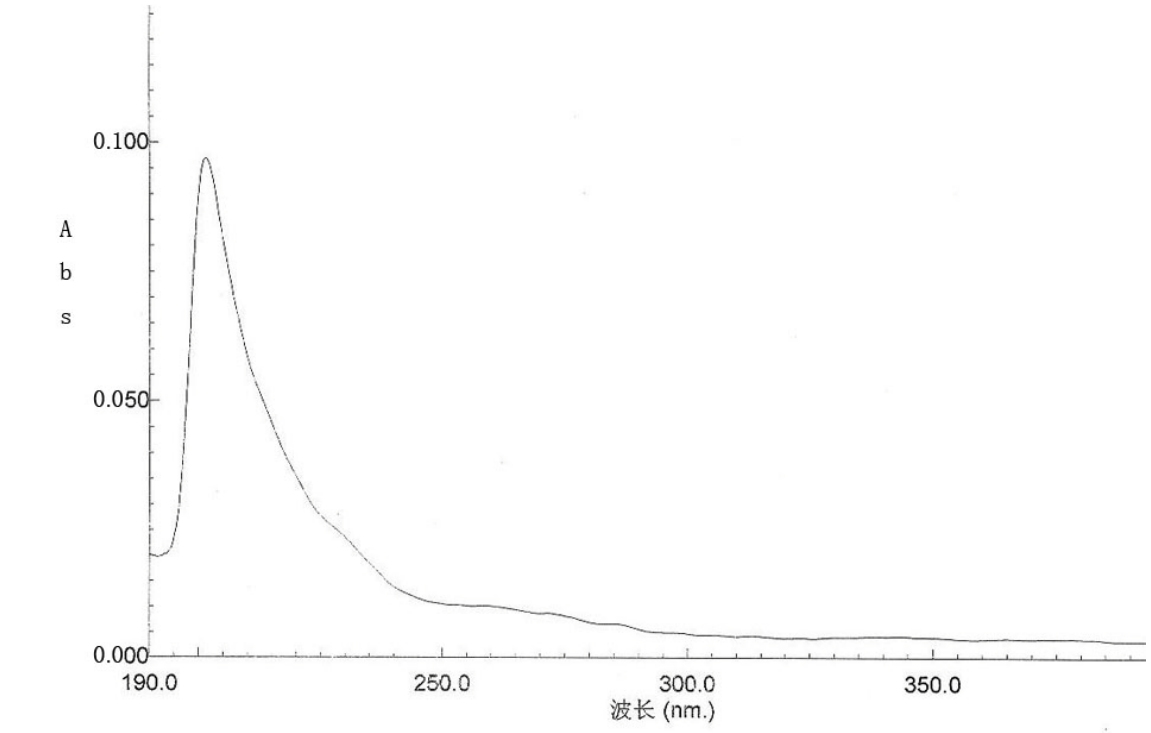
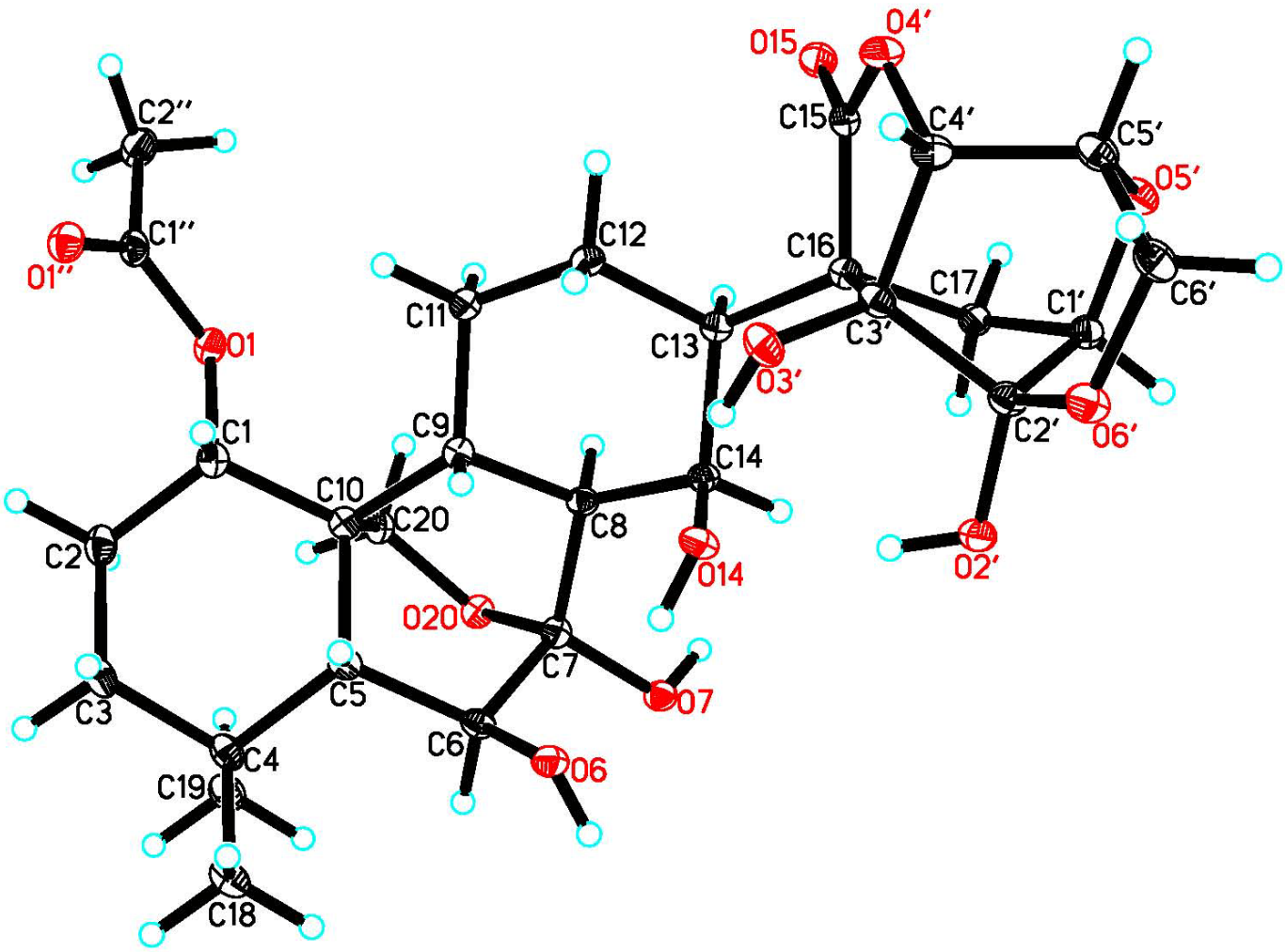


Figure S19. X-ray structure of neoadenoloside B (**2**)



Displacement ellipsoids are drawn at the 30% probability level.

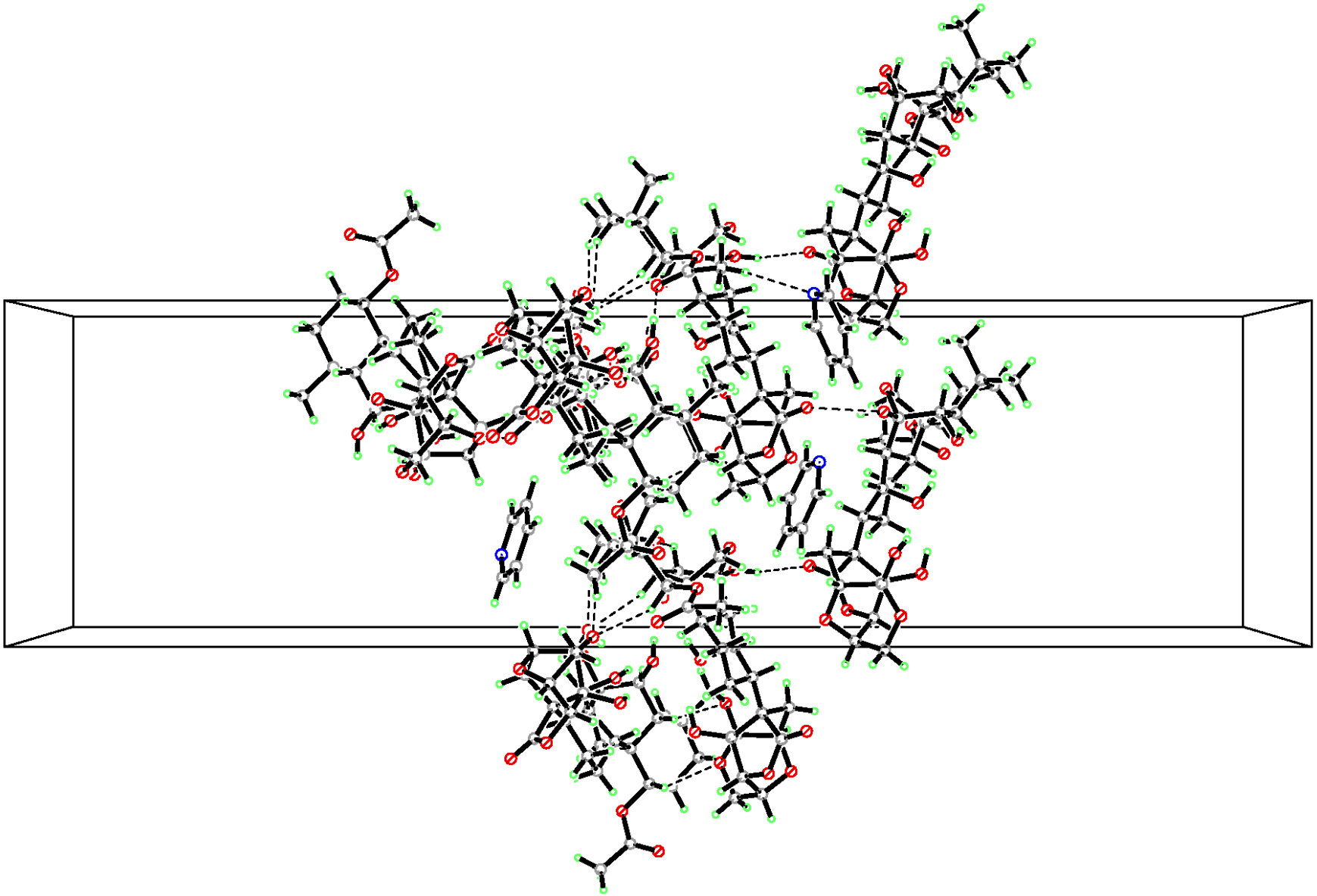


Figure S20. ^{1}H NMR spectrum of lasiokaurin (**3**) (pyridine-d_5)

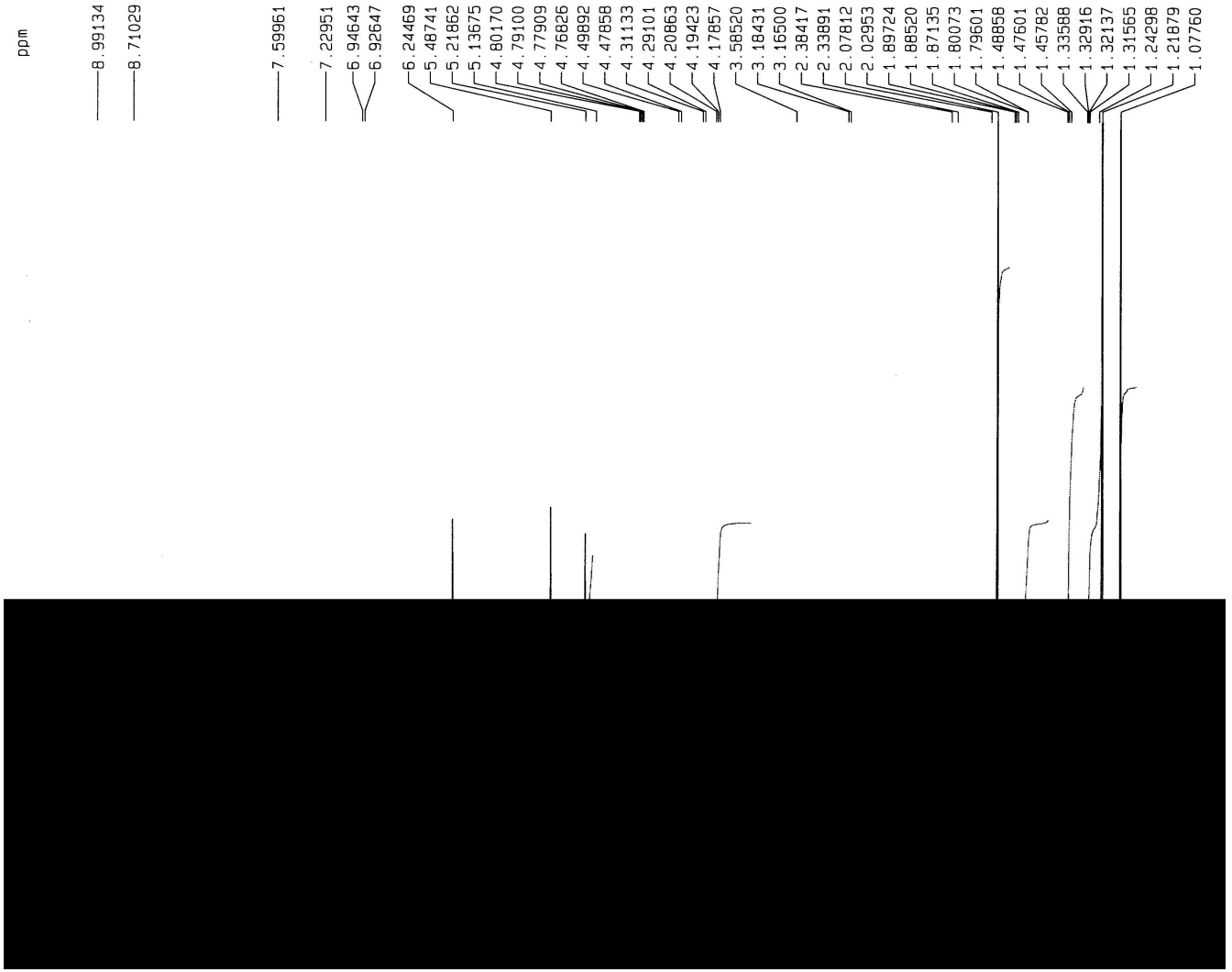


Figure S21. ^{13}C NMR spectrum of lasiokaurin (**3**) (pyridine-d_5)

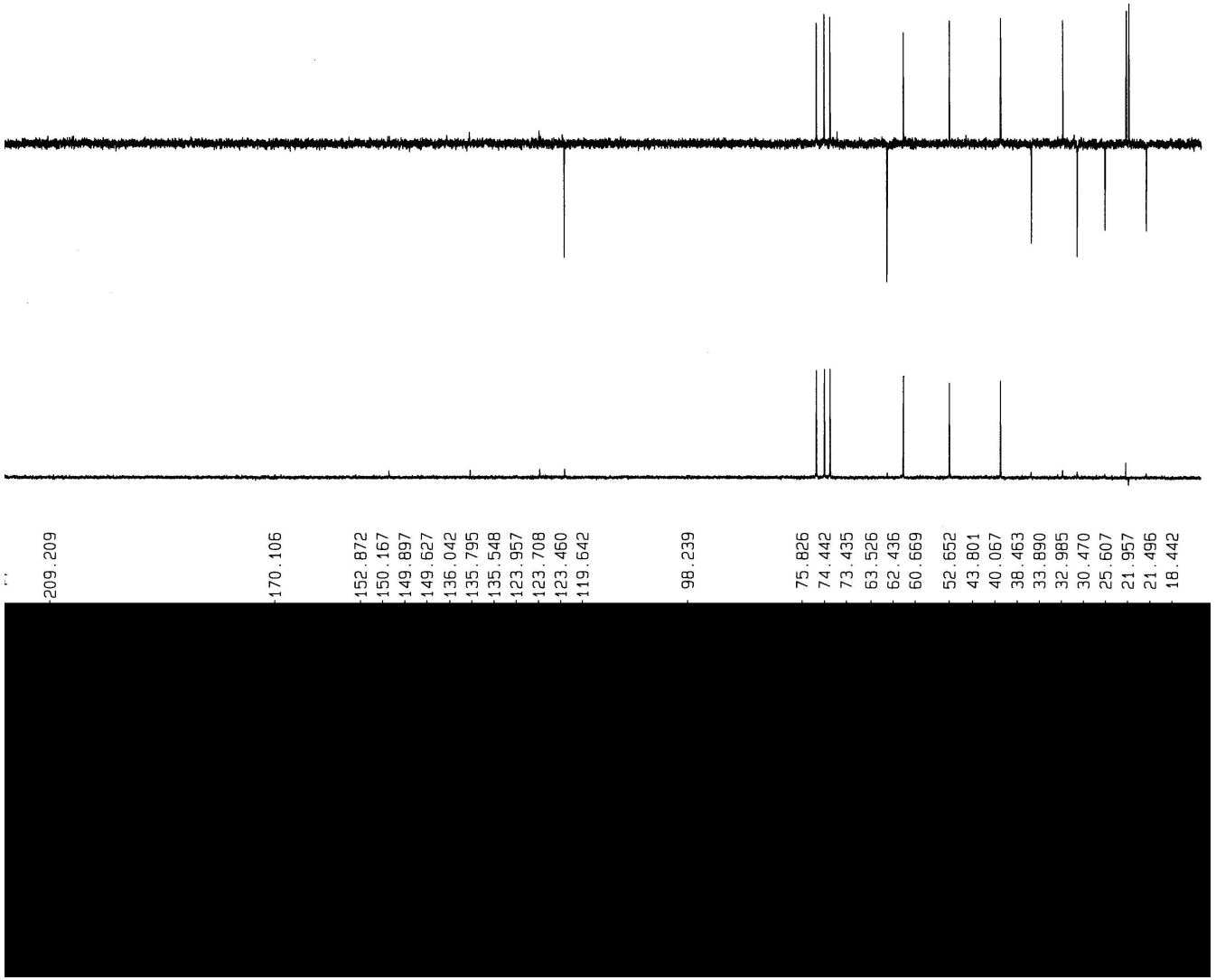


Figure S22. HSQC spectrum of lasiokaurin (**3**) (pyridine-d_5)

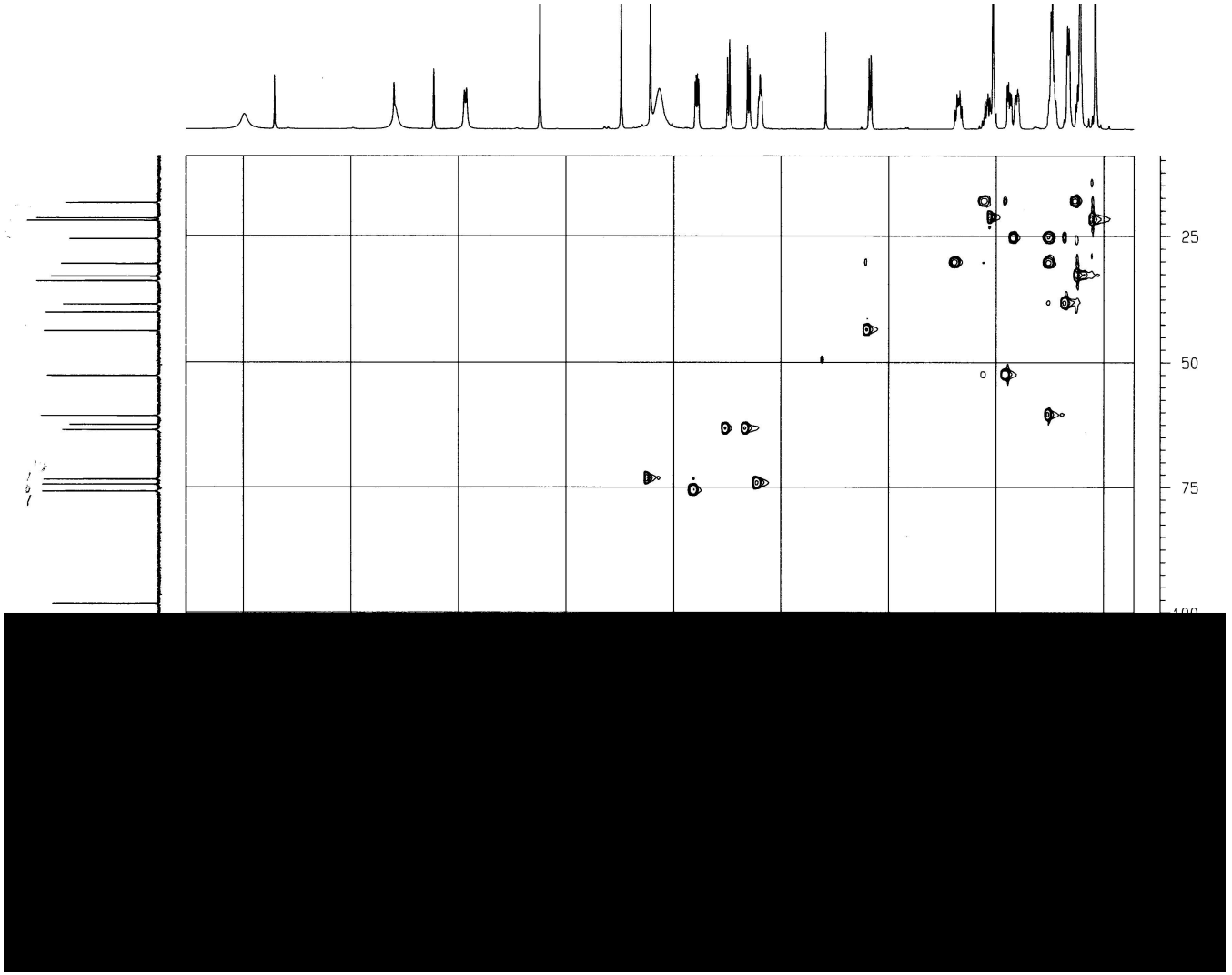


Figure S23. HMBC spectrum of lasiokaurin (**3**) (pyridine-d_5)

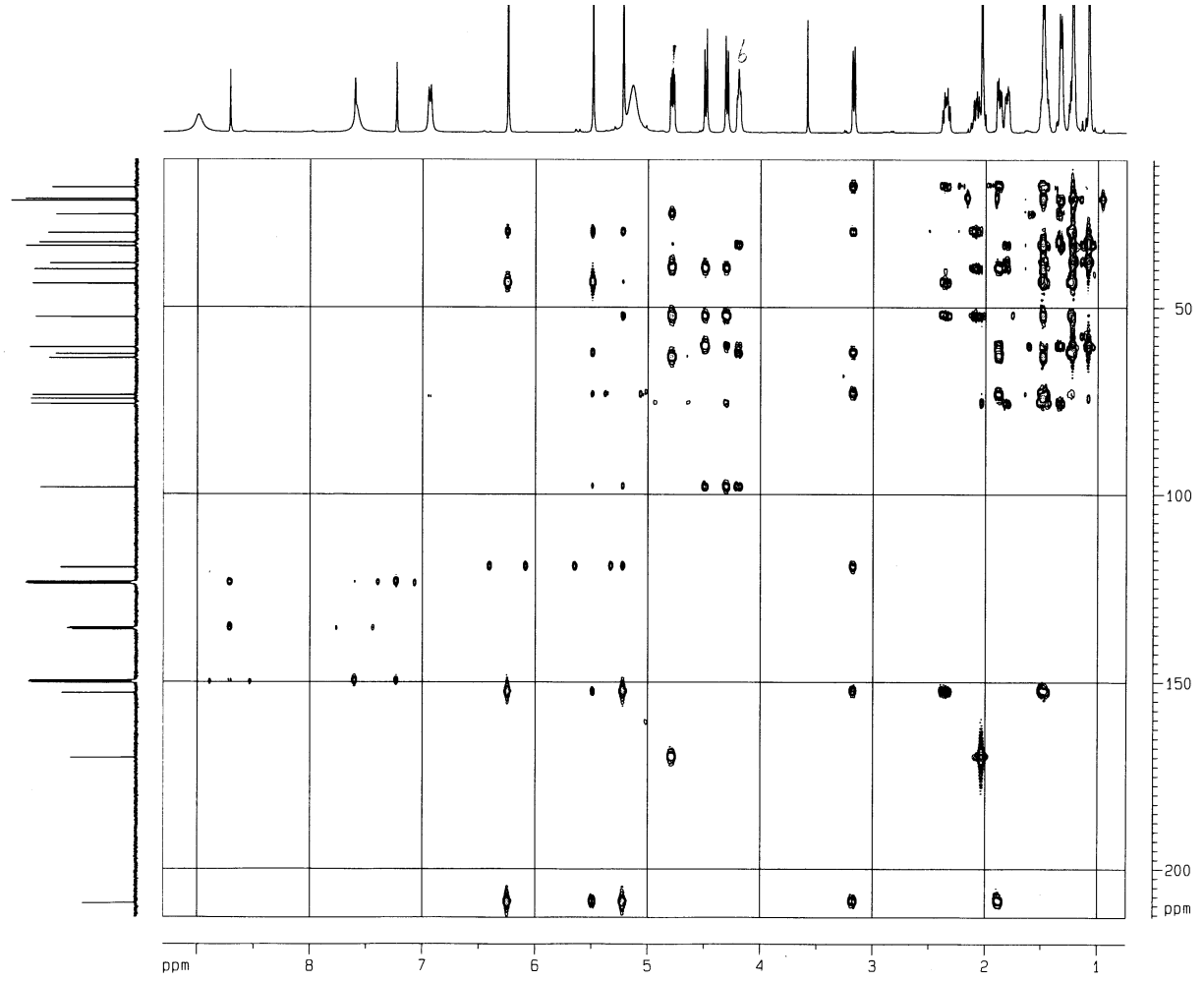


Figure S23. ^{1}H-^{1}H COSY spectrum of lasiokaurin (**3**) (pyridine-d_5)

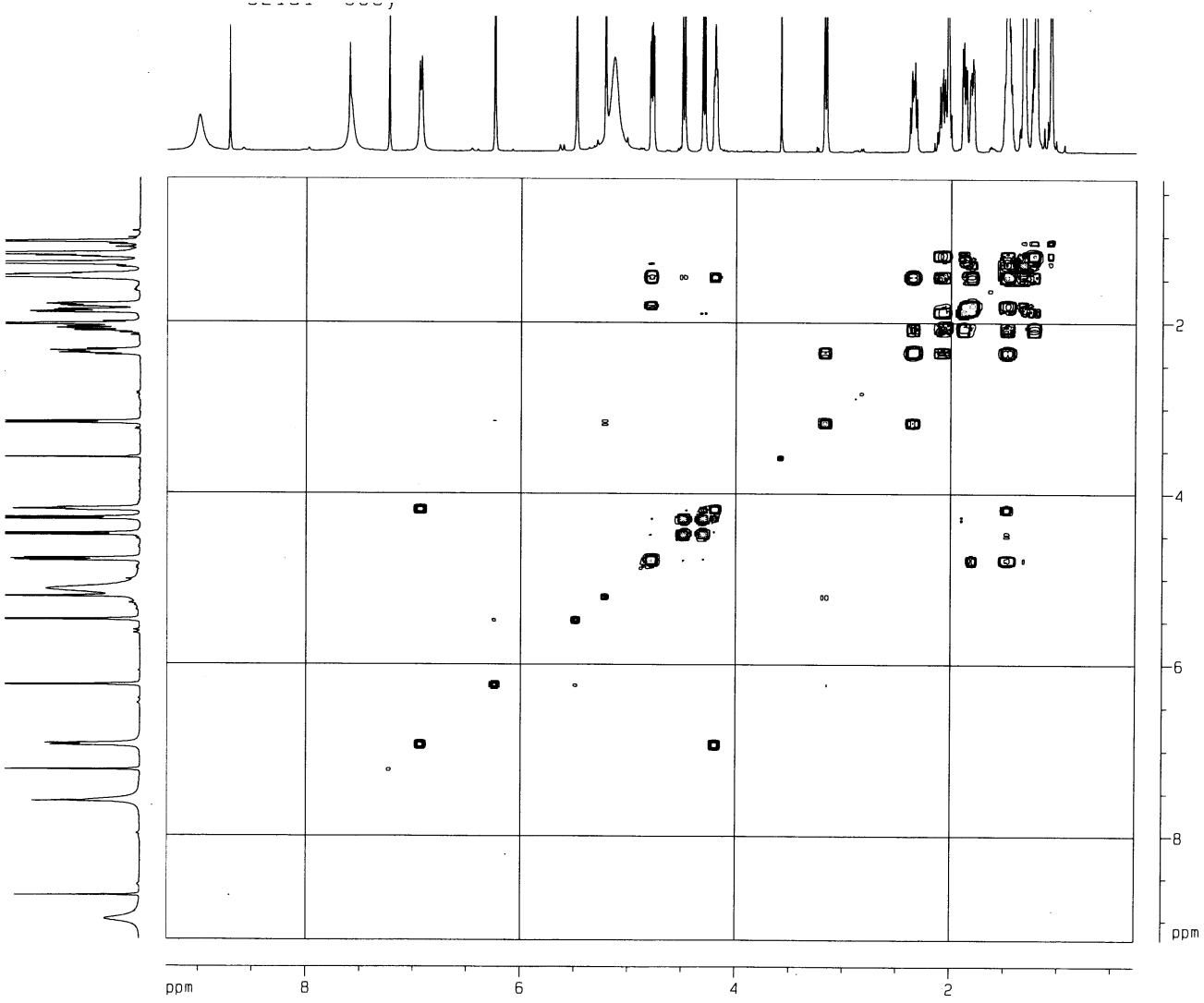


Figure S24. ROESY spectrum of lasiokaurin (**3**) (pyridine-d_5)

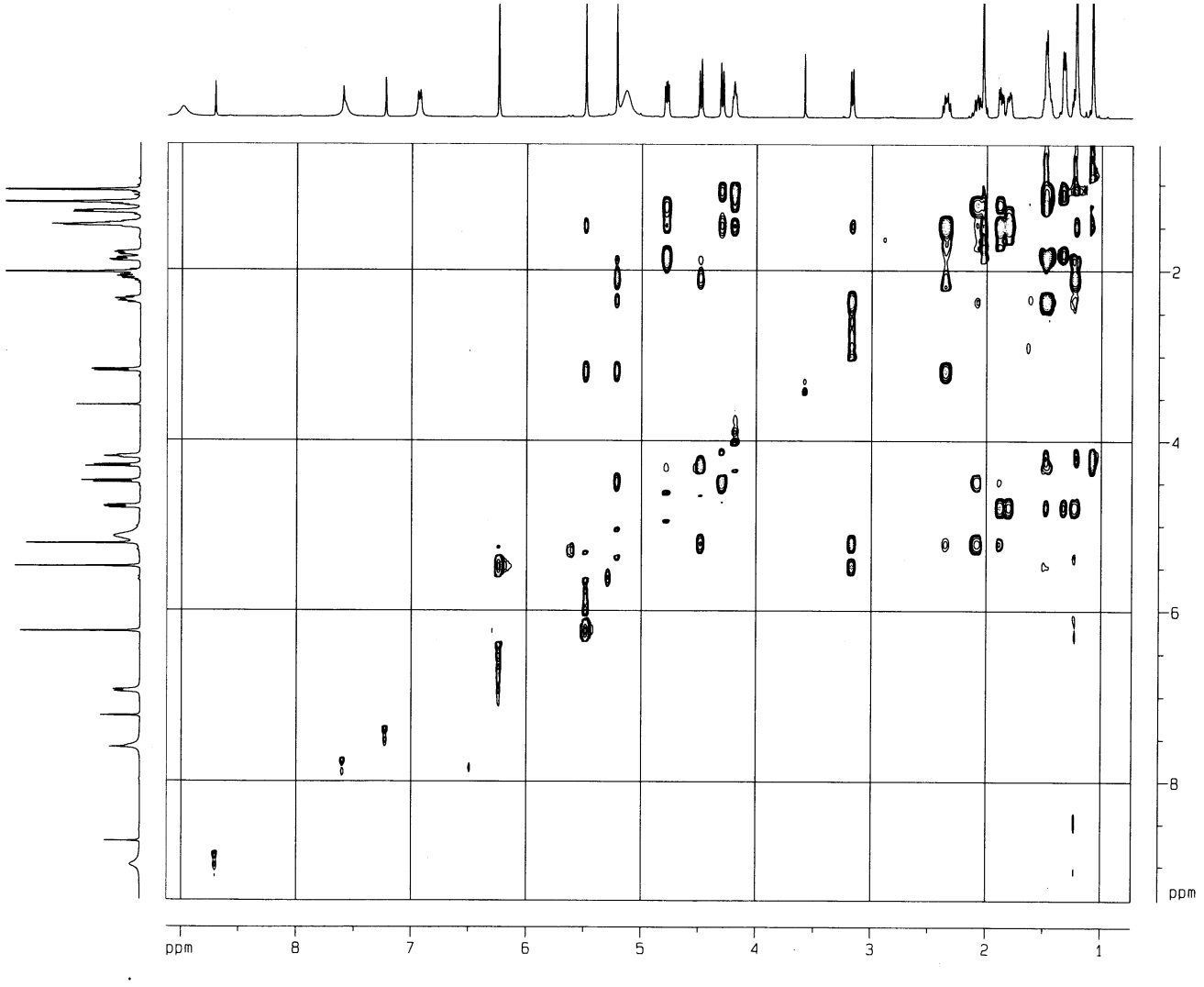


Figure S24. MS spectrum of lasiokaurin (**3**) (pyridine-d_5)

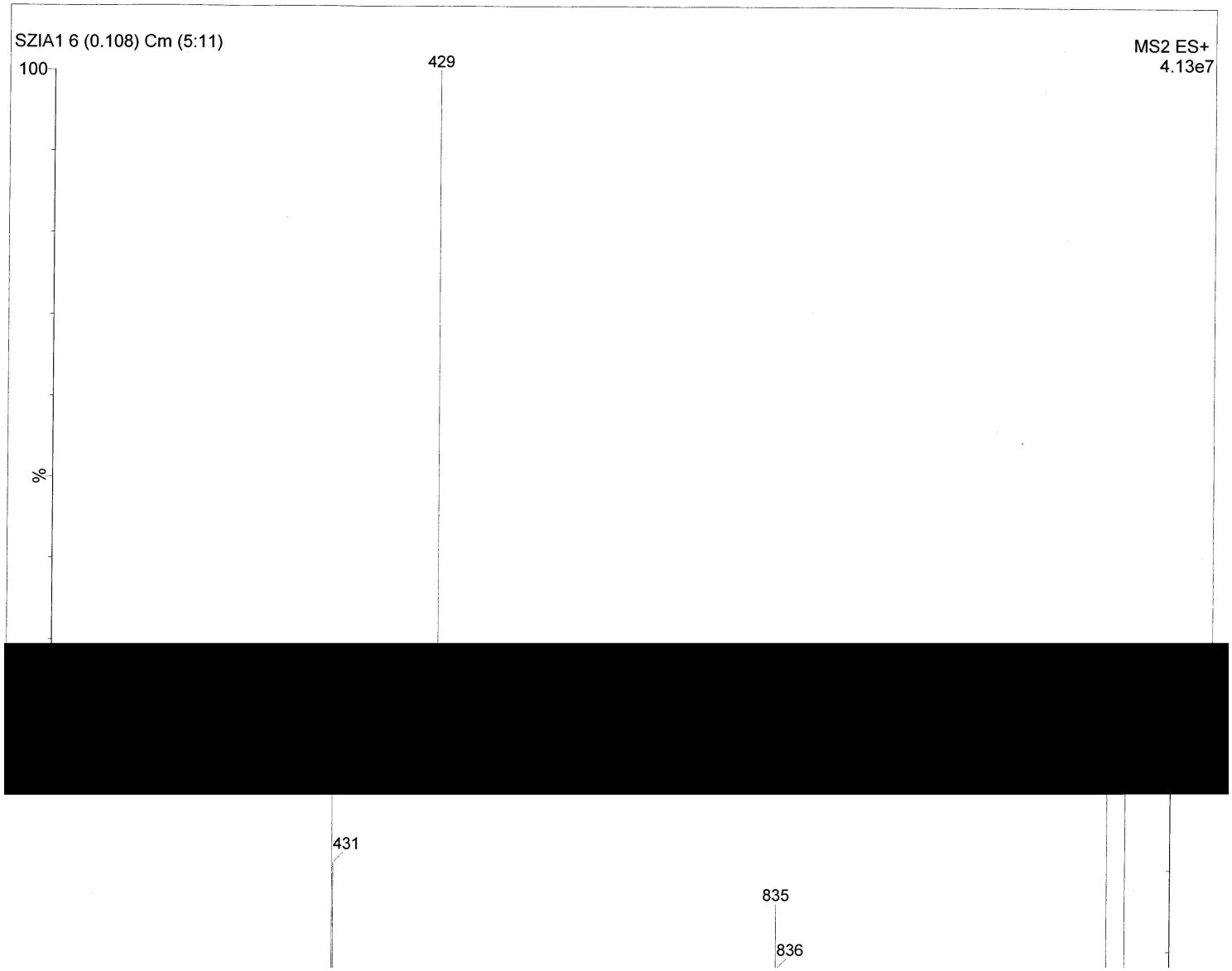


Table S3. Crystal data and structure refinement for neoadenoloside B (**2**).

Identification code	Neoadenoloside B (2)
Empirical formula	C33 H43 N O12
Formula weight	645.68
Temperature	100(2) K
Wavelength	1.54178 A
Crystal system, space group	Tetragonal, P 41 21 2
Unit cell dimensions	a = 11.6541(2) A alpha = 90 deg. b = 11.6541(2) A beta = 90 deg. c = 43.9234(8) A gamma = 90 deg.
Volume	5965.59(18) A^3
Z, Calculated density	8, 1.438 Mg/m^3
Absorption coefficient	0.914 mm^-1
F(000)	2752
Crystal size	0.25 x 0.25 x 0.25 mm
Theta range for data collection	3.92 to 69.69 deg.
Limiting indices	-13<=h<=12, -14<=k<=13, -52<=l<=50
Reflections collected / unique	44905 / 5504 [R(int) = 0.0336]
Completeness to theta = 69.69	98.5 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5504 / 0 / 424

Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0279, wR2 = 0.0715
R indices (all data)	R1 = 0.0279, wR2 = 0.0715
Absolute structure parameter	0.07(11)
Extinction coefficient	0.00022(4)
Largest diff. peak and hole	0.220 and -0.159 e.A^-3

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for neoadenoloside B (**2**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	3876(1)	11519(1)	311(1)	21(1)
O(1'')	2688(1)	10577(1)	-5(1)	25(1)
O(6)	8816(1)	11005(1)	43(1)	20(1)
O(20)	7136(1)	12635(1)	595(1)	19(1)
O(14)	8423(1)	9054(1)	360(1)	21(1)
O(15)	6060(1)	7004(1)	1218(1)	23(1)
O(4')	6692(1)	5631(1)	911(1)	24(1)
O(6')	9949(1)	5620(1)	532(1)	24(1)
O(2')	10033(1)	7538(1)	580(1)	23(1)
O(5')	8979(1)	5455(1)	1127(1)	21(1)
O(3')	7816(1)	6817(1)	312(1)	23(1)
O(7)	8938(1)	11869(1)	648(1)	20(1)
N(1S)	2519(2)	10324(2)	1229(1)	44(1)
C(1S)	3179(2)	9392(2)	1253(1)	40(1)
C(2S)	2800(2)	8368(2)	1371(1)	43(1)
C(3S)	1678(2)	8284(2)	1470(1)	40(1)
C(4S)	984(2)	9226(2)	1443(1)	35(1)
C(5S)	1432(2)	10215(2)	1322(1)	41(1)
C(6')	9554(1)	4545(1)	656(1)	24(1)
C(5')	8581(1)	4773(1)	876(1)	22(1)
C(4')	7654(1)	5433(1)	710(1)	21(1)
C(3')	8127(1)	6622(1)	617(1)	18(1)
C(16)	7643(1)	7429(1)	869(1)	17(1)
C(13)	7114(1)	8604(1)	782(1)	17(1)
C(14)	7951(1)	9490(1)	641(1)	18(1)
C(8)	7269(1)	10585(1)	593(1)	17(1)
C(9)	6282(1)	10389(1)	364(1)	17(1)
C(10)	5930(1)	11579(1)	237(1)	18(1)
C(1)	4772(1)	11552(1)	75(1)	20(1)
C(1'')	2878(1)	11020(1)	239(1)	21(1)
C(2'')	2032(1)	11076(2)	495(1)	29(1)
C(2)	4565(1)	12596(1)	-124(1)	24(1)
C(3)	5512(1)	12759(1)	-359(1)	24(1)
C(4)	6695(1)	12915(1)	-214(1)	21(1)

C(5)	6892(1)	11866(1)	1(1)	18(1)
C(6)	8059(1)	11870(1)	165(1)	18(1)
C(7)	7890(1)	11700(1)	507(1)	18(1)
C(20)	5964(1)	12423(1)	507(1)	19(1)
C(15)	6716(1)	6703(1)	1020(1)	18(1)
C(2')	9435(1)	6580(1)	675(1)	20(1)
C(1')	9452(1)	6537(1)	1023(1)	19(1)
C(17)	8645(1)	7516(1)	1106(1)	18(1)
C(12)	6001(1)	8471(1)	593(1)	20(1)
C(11)	5407(1)	9610(1)	520(1)	20(1)
C(18)	7600(1)	12865(1)	-467(1)	25(1)
C(19)	6784(1)	14098(1)	-61(1)	25(1)

Table S5. Bond lengths [A] and angles [deg] for neoadenoloside B (**2**).

O(1)-C(1")	1.3373(19)
O(1)-C(1)	1.4728(17)
O(1")-C(1")	1.2112(18)
O(6)-C(6)	1.4418(17)
O(6)-H(6)	0.8400
O(20)-C(20)	1.4410(17)
O(20)-C(7)	1.4523(17)
O(14)-C(14)	1.4459(17)
O(14)-H(14)	0.8400
O(15)-C(15)	1.2091(18)
O(4')-C(15)	1.3386(17)
O(4')-C(4')	1.4450(18)
O(6')-C(2')	1.4160(17)
O(6')-C(6')	1.4431(18)
O(2')-C(2')	1.3810(18)
O(2')-H(2')	0.8400
O(5')-C(5')	1.4354(18)
O(5')-C(1')	1.4488(17)
O(3')-C(3')	1.4059(16)
O(3')-H(3')	0.8400
O(7)-C(7)	1.3853(17)
O(7)-H(7)	0.8400
N(1S)-C(1S)	1.336(3)
N(1S)-C(5S)	1.337(3)
C(1S)-C(2S)	1.375(3)
C(1S)-H(1S)	0.9500
C(2S)-C(3S)	1.382(3)
C(2S)-H(2S)	0.9500
C(3S)-C(4S)	1.368(3)
C(3S)-H(3S)	0.9500
C(4S)-C(5S)	1.373(3)
C(4S)-H(4S)	0.9500
C(5S)-H(5S)	0.9500
C(6')-C(5')	1.513(2)
C(6')-H(6'1)	0.9900
C(6')-H(6'2)	0.9900
C(5')-C(4')	1.514(2)
C(5')-H(5')	1.0000
C(4')-C(3')	1.546(2)
C(4')-H(4')	1.0000
C(3')-C(2')	1.546(2)

C(3')-C(16)	1.5604(19)
C(16)-C(15)	1.5228(19)
C(16)-C(13)	1.5501(19)
C(16)-C(17)	1.5654(18)
C(13)-C(12)	1.5489(19)
C(13)-C(14)	1.5492(19)
C(13)-H(13)	1.0000
C(14)-C(8)	1.519(2)
C(14)-H(14A)	1.0000
C(8)-C(7)	1.5343(19)
C(8)-C(9)	1.5433(18)
C(8)-H(8)	1.0000
C(9)-C(11)	1.5261(19)
C(9)-C(10)	1.5499(19)
C(9)-H(9)	1.0000
C(10)-C(1)	1.5269(19)
C(10)-C(20)	1.5396(19)
C(10)-C(5)	1.5650(19)
C(1)-C(2)	1.517(2)
C(1)-H(1)	1.0000
C(1")-C(2")	1.496(2)
C(2")-H(2'1)	0.9800
C(2")-H(2'2)	0.9800
C(2")-H(2'3)	0.9800
C(2)-C(3)	1.523(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.530(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(18)	1.534(2)
C(4)-C(19)	1.536(2)
C(4)-C(5)	1.5607(19)
C(5)-C(6)	1.539(2)
C(5)-H(5)	1.0000
C(6)-C(7)	1.5267(19)
C(6)-H(6A)	1.0000
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(2')-C(1')	1.5314(19)
C(1')-C(17)	1.522(2)
C(1')-H(1')	1.0000
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(12)-C(11)	1.531(2)

C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(1")-O(1)-C(1)	117.53(11)
C(6)-O(6)-H(6)	109.5
C(20)-O(20)-C(7)	111.95(10)
C(14)-O(14)-H(14)	109.5
C(15)-O(4')-C(4')	110.56(11)
C(2')-O(6')-C(6')	112.45(11)
C(2')-O(2')-H(2')	109.5
C(5')-O(5')-C(1')	111.35(10)
C(3')-O(3')-H(3')	109.5
C(7)-O(7)-H(7)	109.5
C(1S)-N(1S)-C(5S)	116.35(18)
N(1S)-C(1S)-C(2S)	123.44(18)
N(1S)-C(1S)-H(1S)	118.3
C(2S)-C(1S)-H(1S)	118.3
C(1S)-C(2S)-C(3S)	119.00(19)
C(1S)-C(2S)-H(2S)	120.5
C(3S)-C(2S)-H(2S)	120.5
C(4S)-C(3S)-C(2S)	118.37(18)
C(4S)-C(3S)-H(3S)	120.8
C(2S)-C(3S)-H(3S)	120.8
C(3S)-C(4S)-C(5S)	118.85(18)
C(3S)-C(4S)-H(4S)	120.6
C(5S)-C(4S)-H(4S)	120.6
N(1S)-C(5S)-C(4S)	123.98(19)
N(1S)-C(5S)-H(5S)	118.0
C(4S)-C(5S)-H(5S)	118.0
O(6')-C(6')-C(5')	109.23(12)
O(6')-C(6')-H(6'1)	109.8
C(5')-C(6')-H(6'1)	109.8
O(6')-C(6')-H(6'2)	109.8
C(5')-C(6')-H(6'2)	109.8
H(6'1)-C(6')-H(6'2)	108.3
O(5')-C(5')-C(6')	110.16(13)
O(5')-C(5')-C(4')	108.62(11)

C(6')-C(5')-C(4')	108.36(12)
O(5')-C(5')-H(5')	109.9
C(6')-C(5')-H(5')	109.9
C(4')-C(5')-H(5')	109.9
O(4')-C(4')-C(5')	109.91(12)
O(4')-C(4')-C(3')	107.17(11)
C(5')-C(4')-C(3')	109.20(12)
O(4')-C(4')-H(4')	110.2
C(5')-C(4')-H(4')	110.2
C(3')-C(4')-H(4')	110.2
O(3')-C(3')-C(2')	114.65(12)
O(3')-C(3')-C(4')	107.80(11)
C(2')-C(3')-C(4')	106.21(11)
O(3')-C(3')-C(16)	119.10(12)
C(2')-C(3')-C(16)	104.94(11)
C(4')-C(3')-C(16)	102.87(11)
C(15)-C(16)-C(13)	108.42(11)
C(15)-C(16)-C(3')	103.32(11)
C(13)-C(16)-C(3')	120.05(11)
C(15)-C(16)-C(17)	106.12(11)
C(13)-C(16)-C(17)	113.80(11)
C(3')-C(16)-C(17)	103.89(11)
C(12)-C(13)-C(14)	112.32(11)
C(12)-C(13)-C(16)	112.17(11)
C(14)-C(13)-C(16)	115.91(11)
C(12)-C(13)-H(13)	105.1
C(14)-C(13)-H(13)	105.1
C(16)-C(13)-H(13)	105.1
O(14)-C(14)-C(8)	112.04(11)
O(14)-C(14)-C(13)	110.31(11)
C(8)-C(14)-C(13)	106.64(11)
O(14)-C(14)-H(14A)	109.3
C(8)-C(14)-H(14A)	109.3
C(13)-C(14)-H(14A)	109.3
C(14)-C(8)-C(7)	119.95(11)
C(14)-C(8)-C(9)	110.88(11)
C(7)-C(8)-C(9)	108.45(11)
C(14)-C(8)-H(8)	105.5
C(7)-C(8)-H(8)	105.5
C(9)-C(8)-H(8)	105.5
C(11)-C(9)-C(8)	107.22(11)
C(11)-C(9)-C(10)	121.07(12)
C(8)-C(9)-C(10)	107.36(11)
C(11)-C(9)-H(9)	106.8
C(8)-C(9)-H(9)	106.8

C(10)-C(9)-H(9)	106.8
C(1)-C(10)-C(20)	113.25(12)
C(1)-C(10)-C(9)	112.55(11)
C(20)-C(10)-C(9)	106.78(11)
C(1)-C(10)-C(5)	109.08(11)
C(20)-C(10)-C(5)	110.85(11)
C(9)-C(10)-C(5)	103.94(11)
O(1)-C(1)-C(2)	108.24(12)
O(1)-C(1)-C(10)	107.38(11)
C(2)-C(1)-C(10)	113.16(12)
O(1)-C(1)-H(1)	109.3
C(2)-C(1)-H(1)	109.3
C(10)-C(1)-H(1)	109.3
O(1")-C(1")-O(1)	123.61(14)
O(1")-C(1")-C(2")	124.27(14)
O(1)-C(1")-C(2")	112.12(12)
C(1")-C(2")-H(2'1)	109.5
C(1")-C(2")-H(2'2)	109.5
H(2'1)-C(2")-H(2'2)	109.5
C(1")-C(2")-H(2'3)	109.5
H(2'1)-C(2")-H(2'3)	109.5
H(2'2)-C(2")-H(2'3)	109.5
C(1)-C(2)-C(3)	112.01(12)
C(1)-C(2)-H(2A)	109.2
C(3)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2B)	109.2
C(3)-C(2)-H(2B)	109.2
H(2A)-C(2)-H(2B)	107.9
C(2)-C(3)-C(4)	112.67(12)
C(2)-C(3)-H(3A)	109.1
C(4)-C(3)-H(3A)	109.1
C(2)-C(3)-H(3B)	109.1
C(4)-C(3)-H(3B)	109.1
H(3A)-C(3)-H(3B)	107.8
C(3)-C(4)-C(18)	108.23(12)
C(3)-C(4)-C(19)	110.46(13)
C(18)-C(4)-C(19)	107.76(12)
C(3)-C(4)-C(5)	106.89(12)
C(18)-C(4)-C(5)	107.85(12)
C(19)-C(4)-C(5)	115.44(12)
C(6)-C(5)-C(4)	114.23(11)
C(6)-C(5)-C(10)	108.79(11)
C(4)-C(5)-C(10)	117.59(12)
C(6)-C(5)-H(5)	105.0
C(4)-C(5)-H(5)	105.0

C(10)-C(5)-H(5)	105.0
O(6)-C(6)-C(7)	110.67(11)
O(6)-C(6)-C(5)	111.37(11)
C(7)-C(6)-C(5)	110.25(11)
O(6)-C(6)-H(6A)	108.1
C(7)-C(6)-H(6A)	108.1
C(5)-C(6)-H(6A)	108.1
O(7)-C(7)-O(20)	107.90(10)
O(7)-C(7)-C(6)	107.96(11)
O(20)-C(7)-C(6)	104.03(11)
O(7)-C(7)-C(8)	115.24(11)
O(20)-C(7)-C(8)	106.52(11)
C(6)-C(7)-C(8)	114.42(11)
O(20)-C(20)-C(10)	109.82(11)
O(20)-C(20)-H(20A)	109.7
C(10)-C(20)-H(20A)	109.7
O(20)-C(20)-H(20B)	109.7
C(10)-C(20)-H(20B)	109.7
H(20A)-C(20)-H(20B)	108.2
O(15)-C(15)-O(4')	121.00(13)
O(15)-C(15)-C(16)	126.79(13)
O(4')-C(15)-C(16)	112.20(12)
O(2')-C(2')-O(6')	106.91(11)
O(2')-C(2')-C(1')	108.70(12)
O(6')-C(2')-C(1')	114.40(12)
O(2')-C(2')-C(3')	115.01(12)
O(6')-C(2')-C(3')	111.61(12)
C(1')-C(2')-C(3')	100.33(11)
O(5')-C(1')-C(17)	110.06(11)
O(5')-C(1')-C(2')	109.72(11)
C(17)-C(1')-C(2')	101.77(11)
O(5')-C(1')-H(1')	111.6
C(17)-C(1')-H(1')	111.6
C(2')-C(1')-H(1')	111.6
C(1')-C(17)-C(16)	104.82(11)
C(1')-C(17)-H(17A)	110.8
C(16)-C(17)-H(17A)	110.8
C(1')-C(17)-H(17B)	110.8
C(16)-C(17)-H(17B)	110.8
H(17A)-C(17)-H(17B)	108.9
C(11)-C(12)-C(13)	113.84(12)
C(11)-C(12)-H(12A)	108.8
C(13)-C(12)-H(12A)	108.8
C(11)-C(12)-H(12B)	108.8
C(13)-C(12)-H(12B)	108.8

H(12A)-C(12)-H(12B)	107.7
C(9)-C(11)-C(12)	107.89(11)
C(9)-C(11)-H(11A)	110.1
C(12)-C(11)-H(11A)	110.1
C(9)-C(11)-H(11B)	110.1
C(12)-C(11)-H(11B)	110.1
H(11A)-C(11)-H(11B)	108.4
C(4)-C(18)-H(18A)	109.5
C(4)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(4)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(4)-C(19)-H(19A)	109.5
C(4)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(4)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters (A^2 x 10^3) for neoadenoloside B (**2**).
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	18(1)	24(1)	20(1)	-2(1)	-1(1)	3(1)
O(1")	25(1)	23(1)	25(1)	-3(1)	-4(1)	0(1)
O(6)	20(1)	19(1)	21(1)	1(1)	4(1)	0(1)
O(20)	20(1)	17(1)	20(1)	-4(1)	0(1)	0(1)
O(14)	25(1)	17(1)	21(1)	2(1)	6(1)	0(1)
O(15)	23(1)	27(1)	20(1)	3(1)	3(1)	0(1)
O(4')	23(1)	20(1)	28(1)	-1(1)	2(1)	-6(1)
O(6')	28(1)	19(1)	27(1)	0(1)	8(1)	2(1)
O(2')	21(1)	20(1)	28(1)	5(1)	4(1)	-1(1)
O(5')	28(1)	16(1)	19(1)	1(1)	0(1)	-2(1)
O(3')	33(1)	22(1)	14(1)	1(1)	-3(1)	0(1)
O(7)	19(1)	22(1)	18(1)	0(1)	-1(1)	-4(1)
N(1S)	49(1)	45(1)	38(1)	14(1)	-3(1)	-4(1)
C(1S)	35(1)	53(1)	31(1)	5(1)	-1(1)	-5(1)
C(2S)	41(1)	36(1)	51(1)	-2(1)	-2(1)	2(1)
C(3S)	40(1)	30(1)	48(1)	0(1)	-3(1)	-11(1)
C(4S)	32(1)	46(1)	28(1)	-4(1)	-5(1)	-4(1)
C(5S)	45(1)	44(1)	35(1)	5(1)	-6(1)	7(1)
C(6')	32(1)	16(1)	24(1)	0(1)	2(1)	2(1)
C(5')	30(1)	15(1)	22(1)	-1(1)	0(1)	-2(1)
C(4')	23(1)	18(1)	21(1)	-3(1)	2(1)	-3(1)
C(3')	24(1)	16(1)	14(1)	0(1)	0(1)	-2(1)
C(16)	19(1)	17(1)	16(1)	0(1)	0(1)	-1(1)
C(13)	18(1)	17(1)	17(1)	0(1)	1(1)	-1(1)
C(14)	17(1)	18(1)	18(1)	1(1)	0(1)	-2(1)
C(8)	17(1)	18(1)	15(1)	-1(1)	2(1)	-1(1)
C(9)	17(1)	17(1)	17(1)	-2(1)	0(1)	0(1)
C(10)	20(1)	17(1)	17(1)	-1(1)	0(1)	0(1)
C(1)	20(1)	20(1)	19(1)	-1(1)	-1(1)	2(1)
C(1")	20(1)	20(1)	24(1)	2(1)	-4(1)	4(1)
C(2")	22(1)	37(1)	26(1)	-1(1)	-1(1)	1(1)
C(2)	24(1)	21(1)	27(1)	0(1)	-6(1)	4(1)
C(3)	32(1)	20(1)	21(1)	4(1)	-5(1)	1(1)
C(4)	29(1)	16(1)	20(1)	2(1)	-2(1)	0(1)
C(5)	23(1)	15(1)	17(1)	-2(1)	1(1)	0(1)

C(6)	22(1)	14(1)	19(1)	1(1)	3(1)	-1(1)
C(7)	18(1)	15(1)	19(1)	-1(1)	-1(1)	1(1)
C(20)	19(1)	19(1)	19(1)	-2(1)	0(1)	3(1)
C(15)	18(1)	19(1)	18(1)	3(1)	-2(1)	0(1)
C(2')	23(1)	17(1)	22(1)	0(1)	3(1)	-1(1)
C(1')	19(1)	17(1)	21(1)	1(1)	-2(1)	-2(1)
C(17)	20(1)	18(1)	18(1)	1(1)	-2(1)	-2(1)
C(12)	19(1)	18(1)	23(1)	1(1)	-2(1)	-3(1)
C(11)	18(1)	21(1)	20(1)	2(1)	-2(1)	-2(1)
C(18)	35(1)	20(1)	20(1)	2(1)	1(1)	-3(1)
C(19)	33(1)	18(1)	25(1)	2(1)	0(1)	1(1)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for neoadenoloside B (**2**).

	x	y	z	U(eq)
H(6)	9487	11266	34	30
H(14)	8644	9605	251	31
H(2')	9605	7952	473	34
H(3')	7930	7509	268	35
H(7)	8859	11804	837	30
H(1S)	3951	9439	1185	48
H(2S)	3302	7727	1385	51
H(3S)	1394	7589	1555	47
H(4S)	206	9196	1508	42
H(5S)	941	10862	1304	50
H(6'1)	10191	4155	764	29
H(6'2)	9286	4038	490	29
H(5')	8265	4030	953	27
H(4')	7400	4998	526	25
H(13)	6862	8952	979	21
H(14A)	8589	9643	788	21
H(8)	6888	10746	792	20
H(9)	6610	9945	190	20
H(1)	4722	10843	-53	24
H(2'1)	1661	11830	496	43
H(2'2)	2431	10957	689	43
H(2'3)	1451	10477	468	43
H(2A)	4520	13287	7	29
H(2B)	3820	12510	-230	29
H(3A)	5334	13441	-485	29
H(3B)	5531	12082	-495	29
H(5)	6920	11186	-138	22
H(6A)	8424	12636	132	22
H(20A)	5592	13154	448	23
H(20B)	5535	12098	681	23
H(1')	10241	6668	1106	23
H(17A)	9041	8265	1088	22
H(17B)	8353	7427	1316	22
H(12A)	6189	8077	399	24
H(12B)	5459	7976	706	24
H(11A)	4744	9477	383	24

H(11B)	5124	9972	709	24
H(18A)	7549	12125	-572	37
H(18B)	8367	12951	-378	37
H(18C)	7463	13487	-613	37
H(19A)	6652	14699	-213	38
H(19B)	7551	14191	27	38
H(19C)	6206	14158	100	38

Table S8. Torsion angles [deg] for neoadenoloside B (**2**).

C(5S)-N(1S)-C(1S)-C(2S)	-1.1(3)
N(1S)-C(1S)-C(2S)-C(3S)	0.2(3)
C(1S)-C(2S)-C(3S)-C(4S)	0.6(3)
C(2S)-C(3S)-C(4S)-C(5S)	-0.6(3)
C(1S)-N(1S)-C(5S)-C(4S)	1.1(3)
C(3S)-C(4S)-C(5S)-N(1S)	-0.3(3)
C(2')-O(6')-C(6')-C(5')	7.57(16)
C(1')-O(5')-C(5')-C(6')	58.36(14)
C(1')-O(5')-C(5')-C(4')	-60.19(15)
O(6')-C(6')-C(5')-O(5')	-62.67(15)
O(6')-C(6')-C(5')-C(4')	56.04(15)
C(15)-O(4')-C(4')-C(5')	100.91(13)
C(15)-O(4')-C(4')-C(3')	-17.65(15)
O(5')-C(5')-C(4')-O(4')	-62.32(15)
C(6')-C(5')-C(4')-O(4')	178.00(11)
O(5')-C(5')-C(4')-C(3')	54.98(15)
C(6')-C(5')-C(4')-C(3')	-64.70(14)
O(4')-C(4')-C(3')-O(3')	-106.90(13)
C(5')-C(4')-C(3')-O(3')	134.09(12)
O(4')-C(4')-C(3')-C(2')	129.76(12)
C(5')-C(4')-C(3')-C(2')	10.75(15)
O(4')-C(4')-C(3')-C(16)	19.77(14)
C(5')-C(4')-C(3')-C(16)	-99.24(13)
O(3')-C(3')-C(16)-C(15)	104.20(14)
C(2')-C(3')-C(16)-C(15)	-125.82(12)
C(4')-C(3')-C(16)-C(15)	-14.88(14)
O(3')-C(3')-C(16)-C(13)	-16.60(19)
C(2')-C(3')-C(16)-C(13)	113.38(13)
C(4')-C(3')-C(16)-C(13)	-135.68(12)
O(3')-C(3')-C(16)-C(17)	-145.16(12)
C(2')-C(3')-C(16)-C(17)	-15.19(14)
C(4')-C(3')-C(16)-C(17)	95.76(12)
C(15)-C(16)-C(13)-C(12)	-52.45(14)
C(3')-C(16)-C(13)-C(12)	65.79(16)
C(17)-C(16)-C(13)-C(12)	-170.27(11)
C(15)-C(16)-C(13)-C(14)	176.73(11)
C(3')-C(16)-C(13)-C(14)	-65.03(16)
C(17)-C(16)-C(13)-C(14)	58.91(15)
C(12)-C(13)-C(14)-O(14)	-69.23(14)
C(16)-C(13)-C(14)-O(14)	61.52(15)
C(12)-C(13)-C(14)-C(8)	52.65(14)

C(16)-C(13)-C(14)-C(8)	-176.60(11)
O(14)-C(14)-C(8)-C(7)	-69.56(16)
C(13)-C(14)-C(8)-C(7)	169.66(11)
O(14)-C(14)-C(8)-C(9)	58.07(15)
C(13)-C(14)-C(8)-C(9)	-62.71(14)
C(14)-C(8)-C(9)-C(11)	69.12(14)
C(7)-C(8)-C(9)-C(11)	-157.22(11)
C(14)-C(8)-C(9)-C(10)	-159.35(11)
C(7)-C(8)-C(9)-C(10)	-25.69(14)
C(11)-C(9)-C(10)-C(1)	-41.51(17)
C(8)-C(9)-C(10)-C(1)	-164.91(11)
C(11)-C(9)-C(10)-C(20)	83.35(15)
C(8)-C(9)-C(10)-C(20)	-40.05(14)
C(11)-C(9)-C(10)-C(5)	-159.40(12)
C(8)-C(9)-C(10)-C(5)	77.20(12)
C(1")-O(1)-C(1)-C(2)	85.25(14)
C(1")-O(1)-C(1)-C(10)	-152.27(12)
C(20)-C(10)-C(1)-O(1)	-44.59(15)
C(9)-C(10)-C(1)-O(1)	76.64(14)
C(5)-C(10)-C(1)-O(1)	-168.55(11)
C(20)-C(10)-C(1)-C(2)	74.79(15)
C(9)-C(10)-C(1)-C(2)	-163.98(12)
C(5)-C(10)-C(1)-C(2)	-49.17(15)
C(1)-O(1)-C(1")-O(1")	1.6(2)
C(1)-O(1)-C(1")-C(2")	-178.22(12)
O(1)-C(1)-C(2)-C(3)	175.15(12)
C(10)-C(1)-C(2)-C(3)	56.26(16)
C(1)-C(2)-C(3)-C(4)	-59.66(17)
C(2)-C(3)-C(4)-C(18)	170.46(12)
C(2)-C(3)-C(4)-C(19)	-71.79(16)
C(2)-C(3)-C(4)-C(5)	54.53(15)
C(3)-C(4)-C(5)-C(6)	179.24(11)
C(18)-C(4)-C(5)-C(6)	63.07(15)
C(19)-C(4)-C(5)-C(6)	-57.47(17)
C(3)-C(4)-C(5)-C(10)	-51.44(15)
C(18)-C(4)-C(5)-C(10)	-167.61(12)
C(19)-C(4)-C(5)-C(10)	71.85(17)
C(1)-C(10)-C(5)-C(6)	-178.96(12)
C(20)-C(10)-C(5)-C(6)	55.68(14)
C(9)-C(10)-C(5)-C(6)	-58.70(13)
C(1)-C(10)-C(5)-C(4)	49.21(15)
C(20)-C(10)-C(5)-C(4)	-76.15(15)
C(9)-C(10)-C(5)-C(4)	169.47(11)
C(4)-C(5)-C(6)-O(6)	-108.14(13)
C(10)-C(5)-C(6)-O(6)	118.27(12)

C(4)-C(5)-C(6)-C(7)	128.60(12)
C(10)-C(5)-C(6)-C(7)	-4.99(15)
C(20)-O(20)-C(7)-O(7)	-168.93(10)
C(20)-O(20)-C(7)-C(6)	76.57(13)
C(20)-O(20)-C(7)-C(8)	-44.66(14)
O(6)-C(6)-C(7)-O(7)	64.56(14)
C(5)-C(6)-C(7)-O(7)	-171.77(11)
O(6)-C(6)-C(7)-O(20)	179.02(10)
C(5)-C(6)-C(7)-O(20)	-57.32(14)
O(6)-C(6)-C(7)-C(8)	-65.18(15)
C(5)-C(6)-C(7)-C(8)	58.49(15)
C(14)-C(8)-C(7)-O(7)	-38.03(17)
C(9)-C(8)-C(7)-O(7)	-166.76(11)
C(14)-C(8)-C(7)-O(20)	-157.64(11)
C(9)-C(8)-C(7)-O(20)	73.62(13)
C(14)-C(8)-C(7)-C(6)	88.01(15)
C(9)-C(8)-C(7)-C(6)	-40.73(15)
C(7)-O(20)-C(20)-C(10)	-24.22(15)
C(1)-C(10)-C(20)-O(20)	-164.47(11)
C(9)-C(10)-C(20)-O(20)	71.10(14)
C(5)-C(10)-C(20)-O(20)	-41.48(15)
C(4')-O(4')-C(15)-O(15)	-171.76(13)
C(4')-O(4')-C(15)-C(16)	7.60(16)
C(13)-C(16)-C(15)-O(15)	-46.88(18)
C(3')-C(16)-C(15)-O(15)	-175.28(13)
C(17)-C(16)-C(15)-O(15)	75.74(17)
C(13)-C(16)-C(15)-O(4')	133.81(12)
C(3')-C(16)-C(15)-O(4')	5.41(15)
C(17)-C(16)-C(15)-O(4')	-103.57(13)
C(6')-O(6')-C(2')-O(2')	168.57(12)
C(6')-O(6')-C(2')-C(1')	48.18(16)
C(6')-O(6')-C(2')-C(3')	-64.87(15)
O(3')-C(3')-C(2')-O(2')	55.74(17)
C(4')-C(3')-C(2')-O(2')	174.67(11)
C(16)-C(3')-C(2')-O(2')	-76.81(14)
O(3')-C(3')-C(2')-O(6')	-66.27(16)
C(4')-C(3')-C(2')-O(6')	52.66(14)
C(16)-C(3')-C(2')-O(6')	161.18(11)
O(3')-C(3')-C(2')-C(1')	172.14(11)
C(4')-C(3')-C(2')-C(1')	-68.93(13)
C(16)-C(3')-C(2')-C(1')	39.59(13)
C(5')-O(5')-C(1')-C(17)	108.14(13)
C(5')-O(5')-C(1')-C(2')	-3.06(15)
O(2')-C(2')-C(1')-O(5')	-171.57(11)
O(6')-C(2')-C(1')-O(5')	-52.18(16)

C(3')-C(2')-C(1')-O(5')	67.41(13)
O(2')-C(2')-C(1')-C(17)	71.89(14)
O(6')-C(2')-C(1')-C(17)	-168.73(12)
C(3')-C(2')-C(1')-C(17)	-49.14(13)
O(5')-C(1')-C(17)-C(16)	-76.01(13)
C(2')-C(1')-C(17)-C(16)	40.29(13)
C(15)-C(16)-C(17)-C(1')	93.30(13)
C(13)-C(16)-C(17)-C(1')	-147.56(11)
C(3')-C(16)-C(17)-C(1')	-15.27(14)
C(14)-C(13)-C(12)-C(11)	-51.20(16)
C(16)-C(13)-C(12)-C(11)	176.17(12)
C(8)-C(9)-C(11)-C(12)	-61.37(14)
C(10)-C(9)-C(11)-C(12)	175.16(11)
C(13)-C(12)-C(11)-C(9)	54.63(15)

Symmetry transformations used to generate equivalent atoms:

Table S9. Hydrogen bonds for neoadenoloside B (**2**) [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(6)-H(6)...O(1")#1	0.84	2.09	2.8438(14)	148.8
O(14)-H(14)...O(6)	0.84	1.88	2.7041(14)	166.2
O(2')-H(2')...O(14)	0.84	1.95	2.7531(15)	160.6
O(3')-H(3')...O(14)	0.84	1.93	2.7092(15)	153.4
O(7)-H(7)...O(15)#2	0.84	1.97	2.7898(13)	165.0

Symmetry transformations used to generate equivalent atoms:
#1 y,x+1,-z #2 -x+3/2,y+1/2,-z+1/4

Isolation procedures:

The roots of *I. adenolomus* were collected in the reigon of Shangrila in Yunnan Province of China, in July, 2008, and were identified by Prof. H. W. Li. The air-dried and powdered sample (10.0 kg) was extracted with 70% aqueous Me_2CO (4 × 100 L, each 3 days) at room temperature, and the solvent was evaporated *in vacuo* and partitioned with EtOAc (4 × 60 L). The EtOAc residue (900g) was subjected to column chromatography over silica gel eluting with $CHCl_3$–Me_2CO (1:0–0:1 gradient system), to give six fractions. Fraction Ⅵ (165 g) was decolorized on MCI gel, eluted with 90% MeOH–H_2O, and separated utilizing a preparative reversed-phase C_{18}–MPLC column with a gradient flow of 60–100% (V/V) aqueous MeOH to yield seven subfractions. The forth subfraction (308 mg) was further separated by MPLC eluted with MeOH–H_2O (85:15) to give neoadenoloside A (**1**, 5.0 mg).

Neoadenoloside A (**1**): White power; $[\alpha]_D^{23}$ – 32.6 (*c* 0.10, MeOH); UV (MeOH) λ_{max} (log ε) 206 (2.5) nm; IR (KBr) v_{max} 3440, 2957, 2926, 1733, 1632, 1456, 1384, 1281, 1240, 1178, 1081 cm^{-1}; For ^1H and ^{13}C NMR data, see Tables 1 and S1; Positive HRESIMS $[M + Na]^+$ *m/z* 589.2253 (calcd for $C_{28}H_{38}O_{12}Na$, 589.2260).

Neoadenoloside B (**2**): Colorless needles; $[\alpha]_D^{25.5}$ – 139 (*c* 0.10, MeOH); UV (MeOH) λ_{max} (log ε) 201 (2.5); IR (KBr) v_{max} 3452, 2960, 2870, 1746, 1724, 1638, 1454, 1383, 1371, 1250, 1177, 1162, 1034 cm^{-1}; For ^1H and ^{13}C NMR data, see Tables 1 and S1; Positive HREIMS $[M]^+$ *m/z* 566.2365 (calcd for $C_{28}H_{38}O_{12}$, 566.2365).

X-ray Crystal Structure Analysis.

The intensity data for neoadenoloside B (**2**) was collected on a Bruker APEX DUO diffractometer using graphite-monochromated Cu Kα radiation. The structures of these compounds were solved by direct methods (SHELXS97), expanded using difference Fourier techniques, and refined by the program and full-matrix least-squares calculations. The non-hydrogen atoms were refined

anisotropically, and hydrogen atoms were fixed at calculated positions. Crystallographic data for the structures of neoadenoloside B (**2**) has been deposited in the Cambridge Crystallographic Data Centre database (deposition number CCDC 882511). Copies of the data can be obtained free of charge from the CCDC at www.ccdc.cam.ac.uk.

*Crystallographic data for neoadenoloside B (**2**):* $C_{28}H_{38}O_{12}•C_5H_5N$, M = 645.68, tetragonal, a = 11.6541(2) Å b = 11.6541(2) Å c = 43.9234(8) Å α = 90.00°, β = 90.00°, γ = 90.00°, V = 5965.59(18) Å ^{3}, T = 100(2) K, space group P41212, Z = 8, 44905 reflections measured, 5504 independent reflections (R_{int} = 0.0336). The final R_1 values were 0.0279 (I > 2σ(I)). The final wR(F^2) values were 0.0715 (I > 2σ(I)). The final R_1 values were 0.0279 (all data). The final wR(F^2) values were 0.0715 (all data). Flack parameter = 0.07(11).

Cytotoxic Activity Assay. Colorimetric assays were performed to evaluate each compound's activity. The following human tumor cell lines were used: the A549 lung cancer cell line, the HL-60 human myeloid leukemia cell line, the MCF-7 breast cancer cell line, the SMMC-7721 human hepatocarcinoma cell line, and the SW-480 human pancreatic carcinoma. All cells were cultured in RPMI-1640 or DMEM medium (Hyclone, Logan, UT) supplemented with 10% fetal bovine serum (Hyclone) at 37 °C in a humidified atmosphere with 5% CO_2. Cell viability was assessed by conducting colorimetric measurements of the amount of insoluble formazan formed in living cells based on the reduction of 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) (Sigma, St. Louis, MO). Briefly, 100 μL of suspended adherent cells were seeded into each well of a 96-well cell culture plate and allowed to adhere for 12 h before drug addition. In addition, suspended cells were seeded just before drug addition, with an initial density of 1 × 10^5 cells/mL in 100 μL of medium. Each tumor cell line was exposed to each test compound at various concentrations in

triplicate for 48 h; cisplatin (Sigma) was used as a positive control. After the incubation, MTT (100 μg) was added to each well, and the incubation was continued for 4 h at 37 °C. The cells were lysed with 100 μL of 20% SDS-50% DMF after removal of 100 μL of the medium. The optical density of the lysate was measured at 595 nm in a 96-well microtiter plate reader (Bio-Rad 680). The IC_{50} value of each compound was calculated by Reed and Muench's method.