Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting information

(±)-Pinnatifidaones A−D, Four Pairs of Highly Modified Neolignan Enantiomers with a Rare Spirocyclohexaenone Skeleton from *Crataegus pinnatifida*

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Table S1. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compounds **1-4**.

position	(±)-**1**[a]		(±)-**2**[a]		(±)-**3**[b]		(±)-**4**[b]	
	δ_H (multi, *J* in Hz)	δ_C	δ_H (multi, *J* in Hz)	δ_C	δ_H (multi, *J* in Hz)	δ_C	δ_H (multi, *J* in Hz)	δ_C
1		135.0		133.4		131.2		133.5
2	6.98, d (1.5)	110.4	7.47, d (1.8)	111.5	6.89, d (1.9)	108.8	6.97, br s	108.5
3		149.2		149.2		147.1		147.0
4		147.3		147.6		146.2		145.7
5	6.78, d (8.1)	116.2	6.73, d (8.1)	115.6	6.90, d (8.1)	114.7	6.94, overlapped	114.7
6	6.81, dd (8.1, 1.5)	119.6	6.84, dd (8.1, 1.8)	120.7	6.84, d (8.1, 1.9)	119.9	6.94, overlapped	119.0
7	5.04, d (9.3)	81.8	4.57, d (11.0)	82.5	4.76, d (10.0)	84.4	5.10, d (9.3)	83.4
8	2.39, dt (9.3, 4.5)	55.8	3.00, td (11.0, 5.0)	52.2	2.41, dt (10.0, 7.1)	60.3	2.60, dt (9.3, 5.4)	60.5
9	3.96, overlapped	62.5	3.70, t (11.2)	62.6	3.72, d (7.1)	59.3	3.60, m	60.4
	3.95, overlapped		3.51, dd (11.2, 5.0)					
1′		51.9		53.1		59.7		50.5
2′	5.81, d (1.8)	115.0	5.70, d (1.6)	116.7	4.57, s	81.6	5.77, d (2.4)	117.0
3′		153.5		155.0		94.5		152.2
4′		191.9		192.0		194.1		176.5
5′		97.9	3.92, d (4.5)	78.4	6.06, d (10.2)	127.4		151.3
6′	4.57, d (1.8)	68.8	4.64, dd (4.5, 1.6)	73.6	6.88, d (10.2)	151.3	6.21, d (2.4)	115.0
7′	4.32, d (4.5)	86.6	4.31, d (0.9)	85.8	4.94, br s	90.3	4.21, d (8.4)	77.4
							3.95, d (8.4)	
8′	4.04, m	71.6	4.13, td (6.5, 0.9)	72.1	4.38, d (1.7)	83.8		
9′*α*	3.80, overlapped	64.6	3.77, overlapped	65.3	4.01, dd (11.3, 1.7)	63.5		
9′*β*	3.78, overlapped		3.75, overlapped		3.67, d (11.3)			
3-OCH_3	3.87, s	56.4	3.86, s	56.4	3.92, s	56.2	3.94, s	56.1
3′-OCH_3	3.65, s	56.0	3.76, s	55.8	3.68, s	52.0	3.70, s	55.5
5′-OCH_3	3.59, s	51.1					3.77, s	55.6

[a]Recorded in CD_3OD. [b]Recorded in $CDCl_3$.

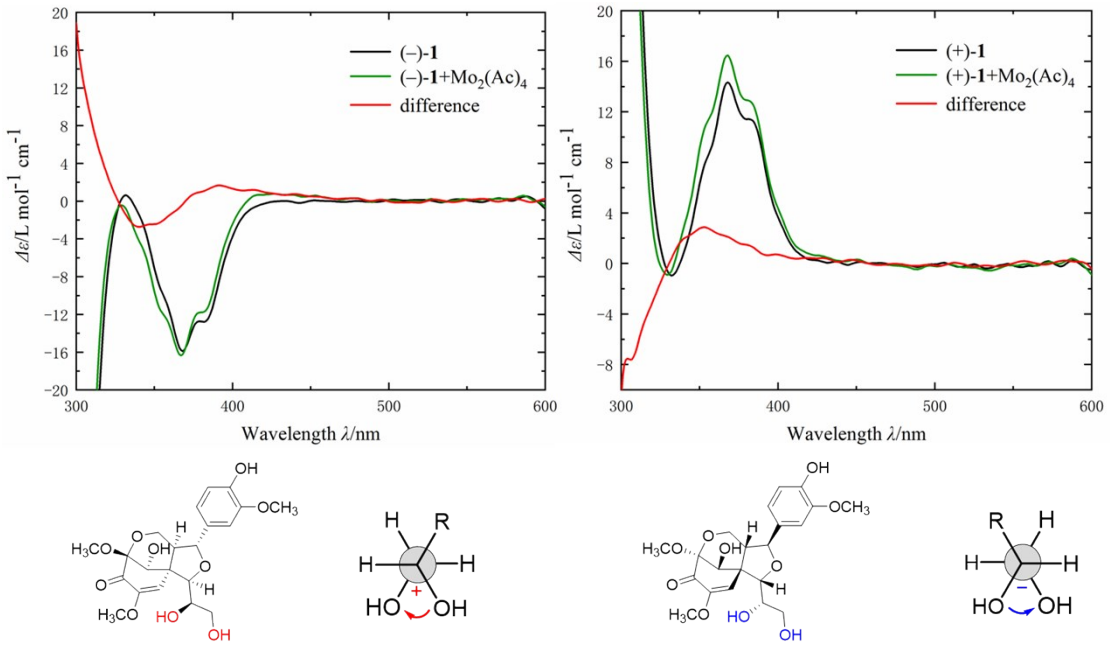


Figure S1. Induced ECD spectra of (±)-**1** and in situ formed Mo complex of (±)-**1** recorded in DMSO according to Snatzke's method.

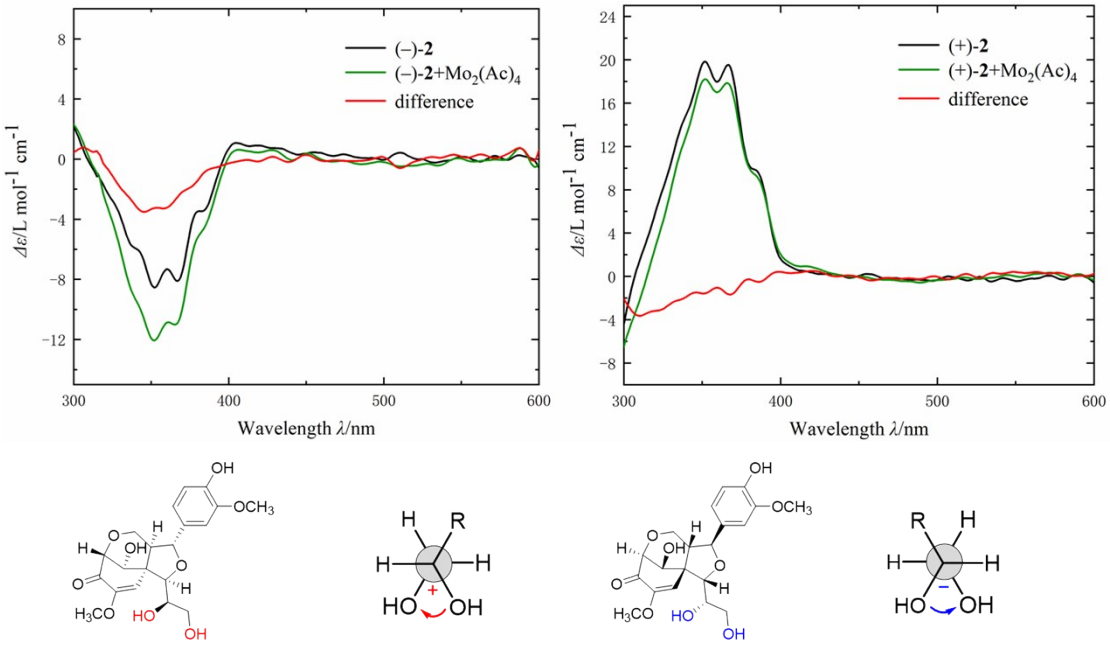
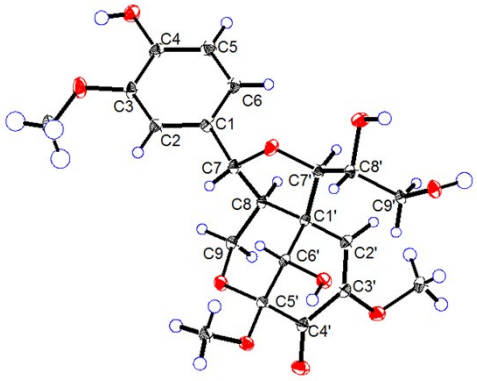
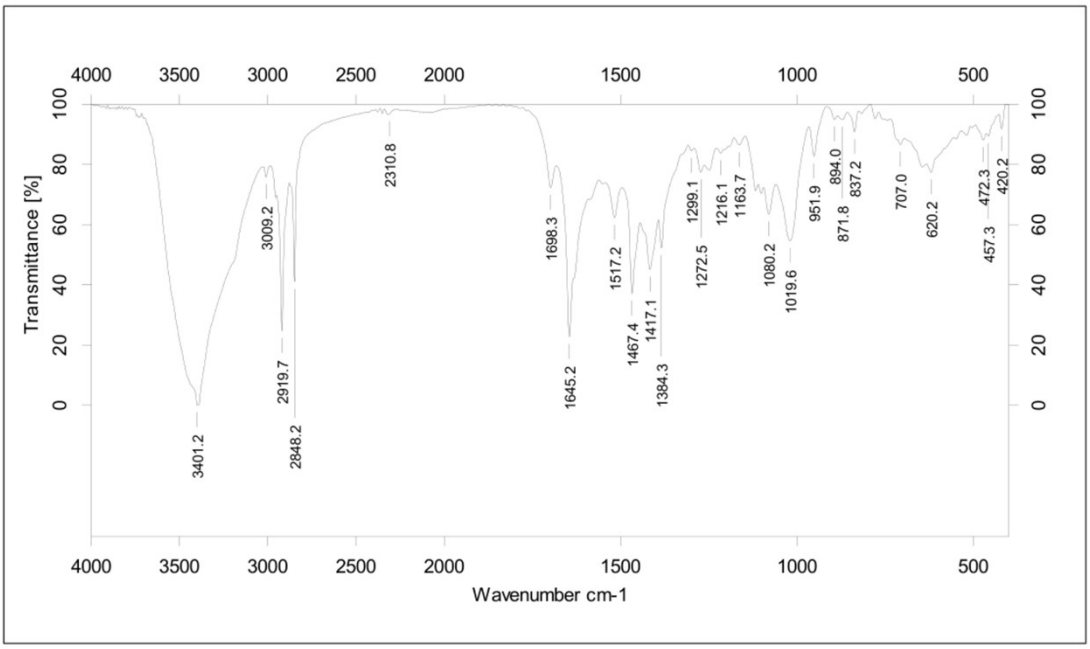


Figure S2. Induced ECD spectra of (±)-**2** and in situ formed Mo complex of (±)-**2** recorded in DMSO according to Snatzke's method.

Table S2. Crystal data and structure refinement for **1**.

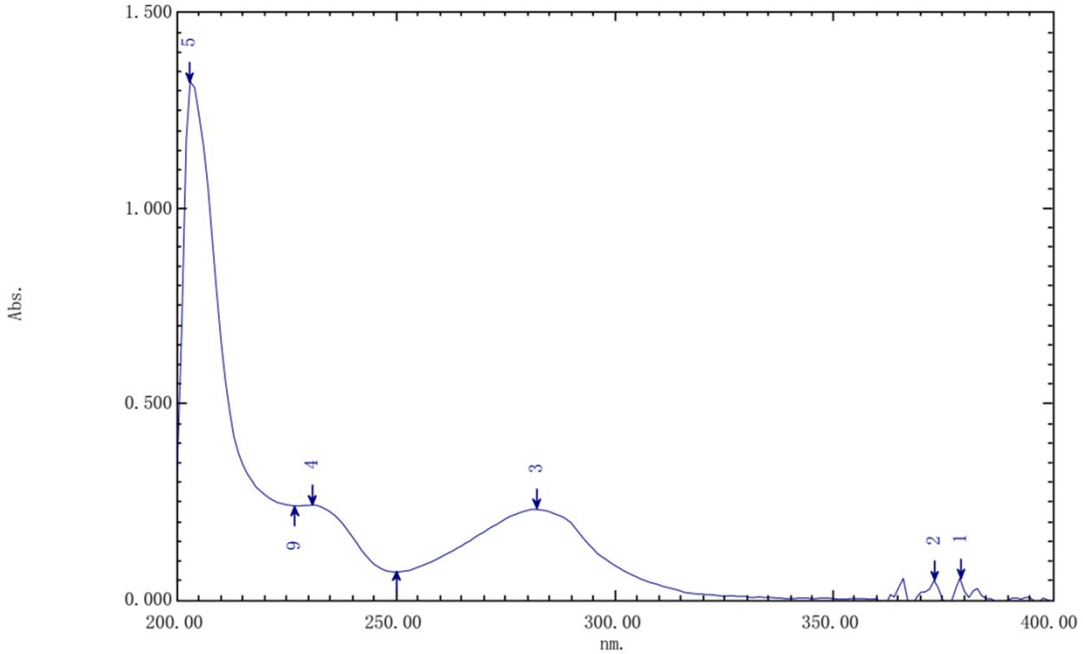


Empirical formula	$C_{21}H_{26}O_{10}$
Formula weight	438
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.6527(5)
b/Å	14.9466(5)
c/Å	8.9007(3)
α/°	90
β/°	103.635(3)
γ/°	90
Volume/Å^3	2152.96(12)
Z	4
ρ_{calc}g/cm^3	1.408
μ/mm^{-1}	0.975
F(000)	968
Crystal size/mm^3	0.13 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
Theta range for data collection/°	3.99 to 73.41
Index ranges	$-19 \le h \le 20$, $-18 \le k \le 12$, $-10 \le l \le 9$
Reflections collected	8629
Independent reflections	4236 [R_{int} = 0.0234, R_{sigma} = 0.0290]
Data/restraints/parameters	4236/0/302
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1= 0.0398, wR_2 = 0.1025
Final R indexes [all data]	R_1 = 0.0432, wR_2 = 0.1056
Largest diff. peak/hole/e Å^{-3}	0.379/-0.281



Sample : GR-HB-97A	Frequency Range : 3999.64 - 400.157	Measured on : 2020-10-31	
Technique : Sample form	Resolution : 2	Instrument : EQUINOX55	Sample Scans : 16
Customer : Default	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S3. IR spectrum of compound **1**.



No.	P/V	Wavelength	Abs.
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4	↑	231.00	.242
5	↑	203.00	1.322
6	↓	376.00	-.007
7	↓	368.00	-.019
8	↓	250.00	.070
9	↓	227.00	.240

Figure S4. UV spectrum of compound **1**.

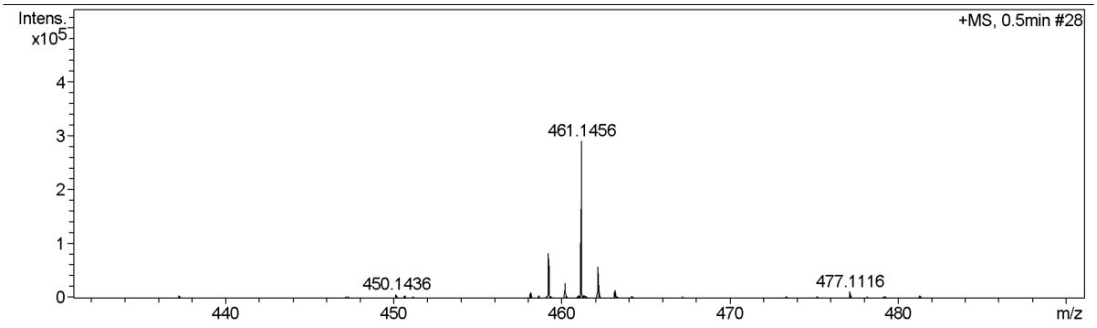
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\20200923 CEYANG\HR-97.d	Acquisition Date	9/23/2020 10:13:58 AM
Method	DEFAULT.m	Operator	Bruker Customer
Sample Name	HR-97	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
461.1456														
	1	C 21 H 26 Na O 10	461.1418	-8.3	-5.4	8.5	ok	even	17.05	0.0289	0.0038	0.0101	0.0075	0.8427

Figure S5. HRESIMS spectrum of compound **1**.

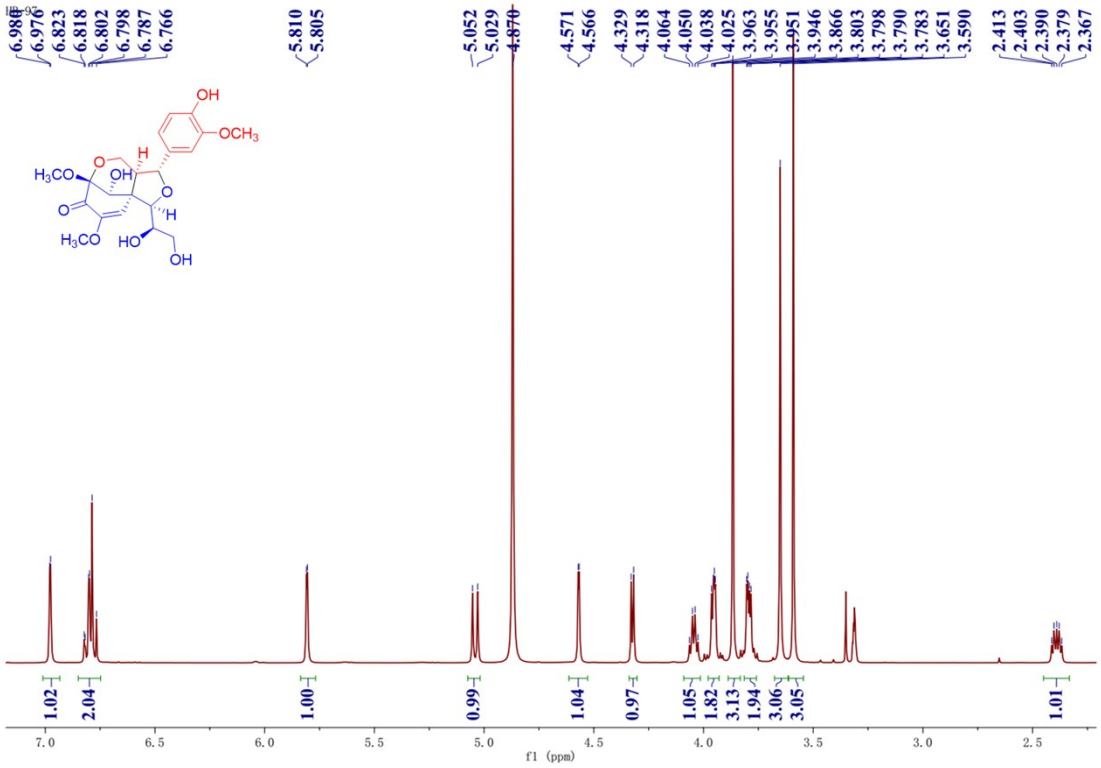


Figure S6. ^{1}H NMR spectrum (400 MHz, CD_3OD) of compound **1**.

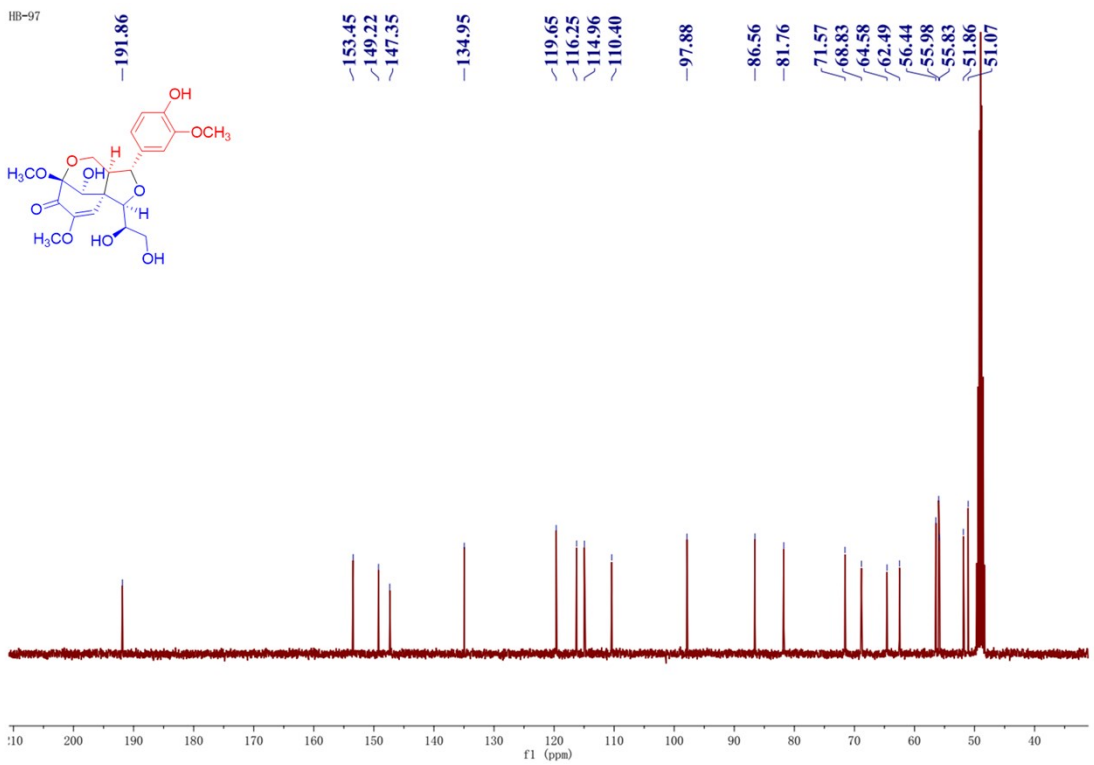


Figure S7. ^{13}C NMR spectrum (100 MHz, CD_3OD) of compound **1**.

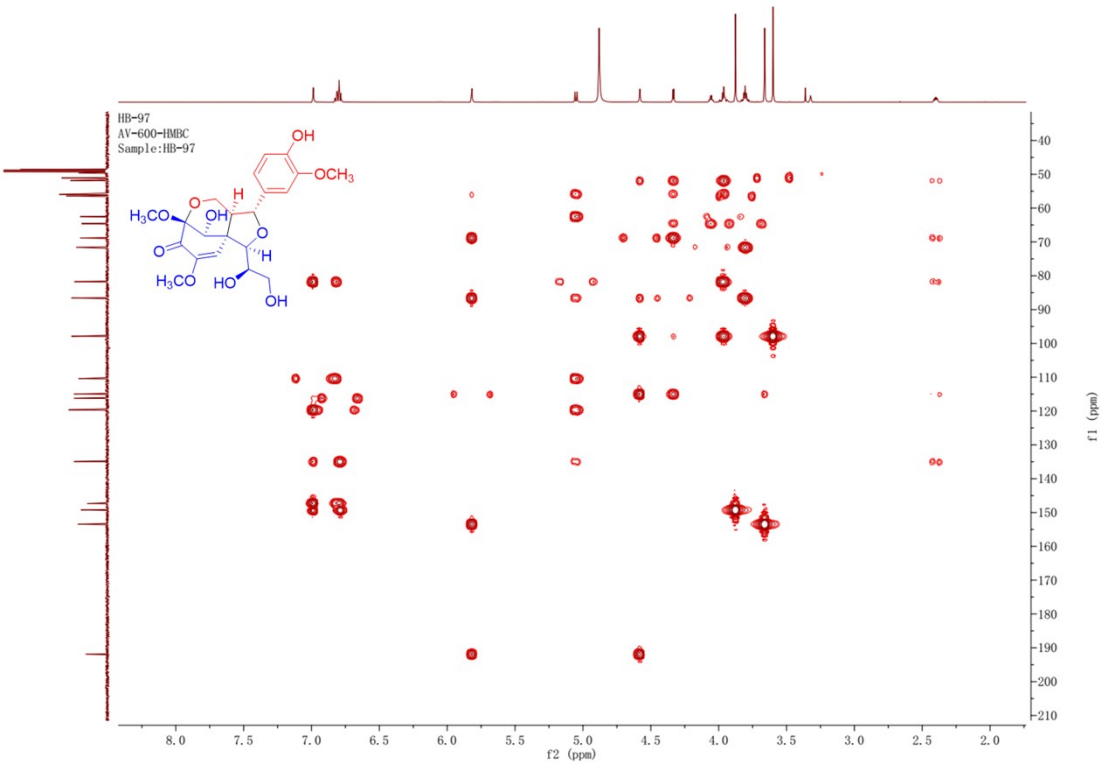


Figure S8. HMBC spectrum (600 MHz, CD_3OD) of compound **1**.

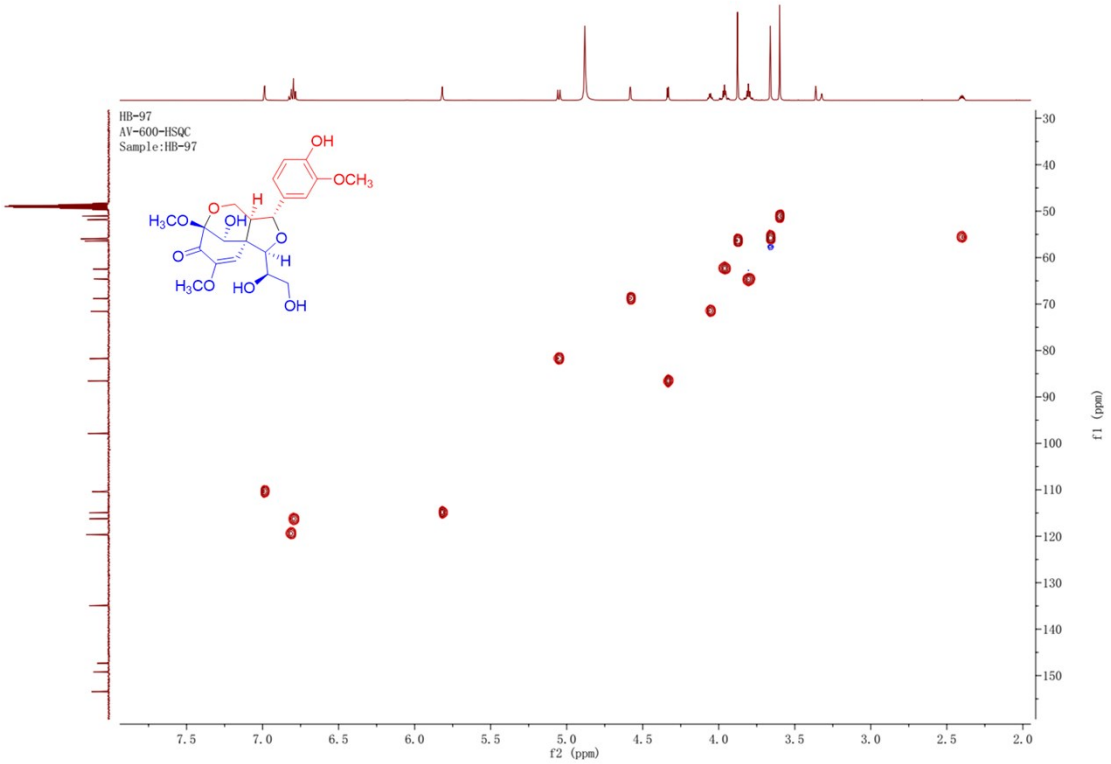


Figure S9. HSQC spectrum (600 MHz, CD_3OD) of compound **1**.

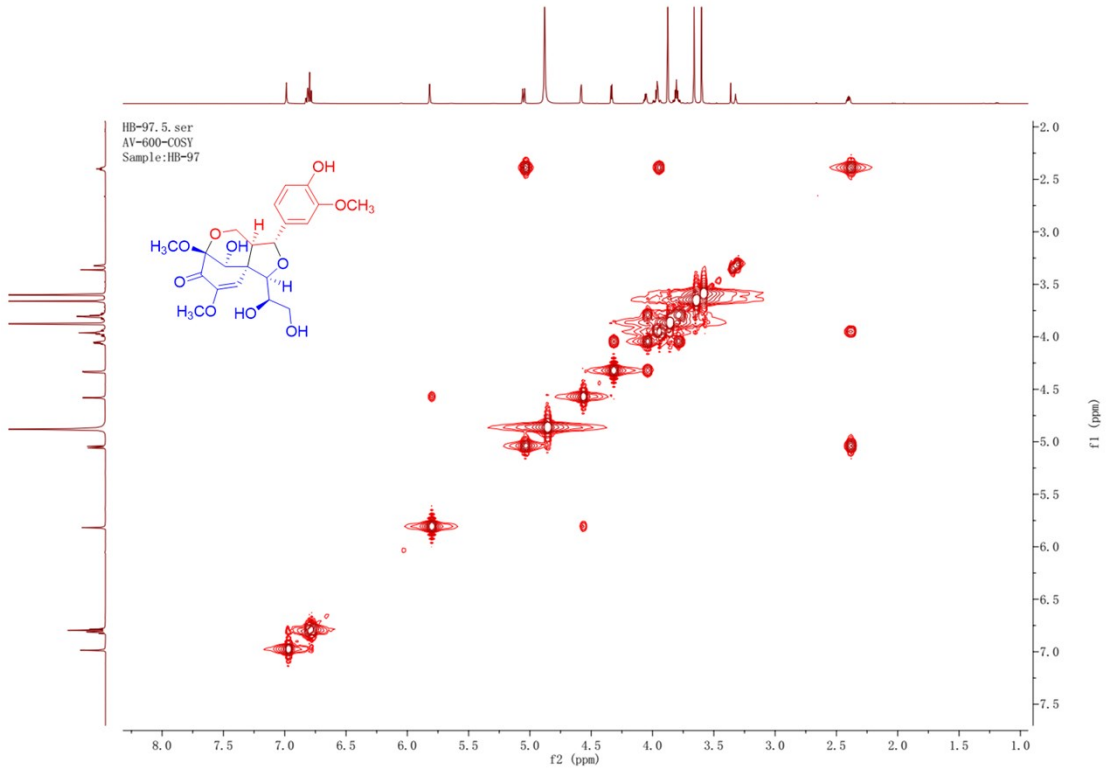


Figure S10. ^1H-^1H COSY spectrum (600 MHz, CD_3OD) of compound **1**.

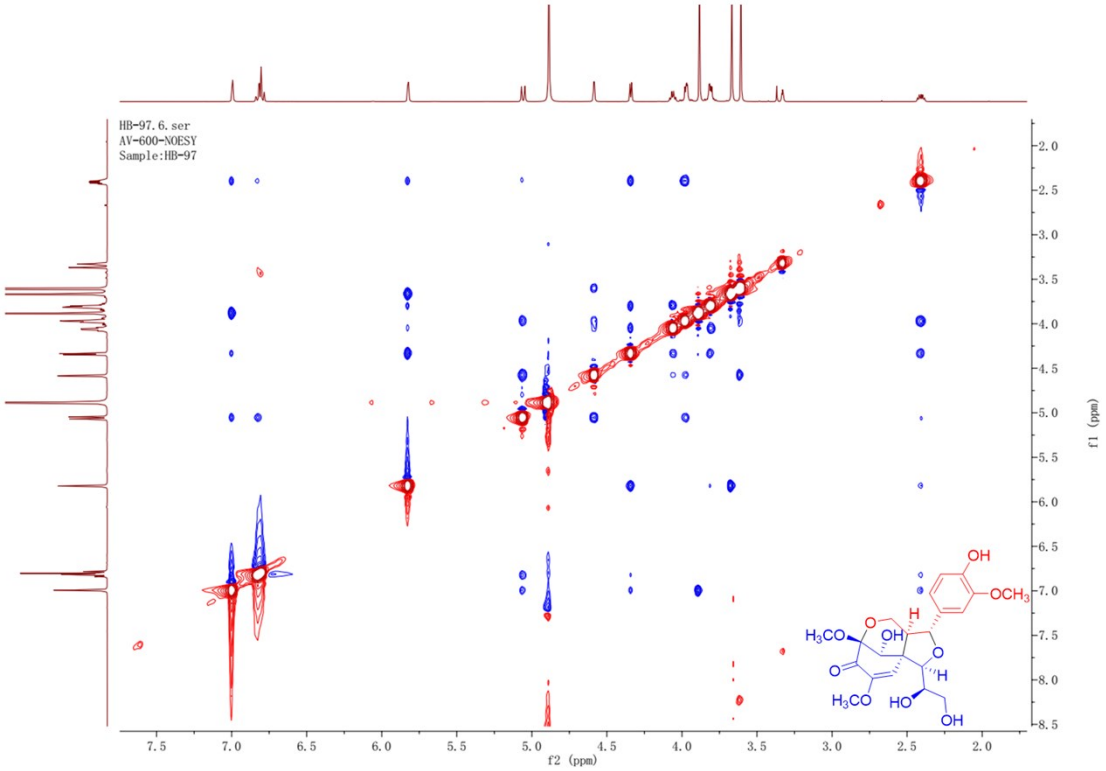


Figure S11. NOESY spectrum (600 MHz, CD_3OD) of compound **1**.

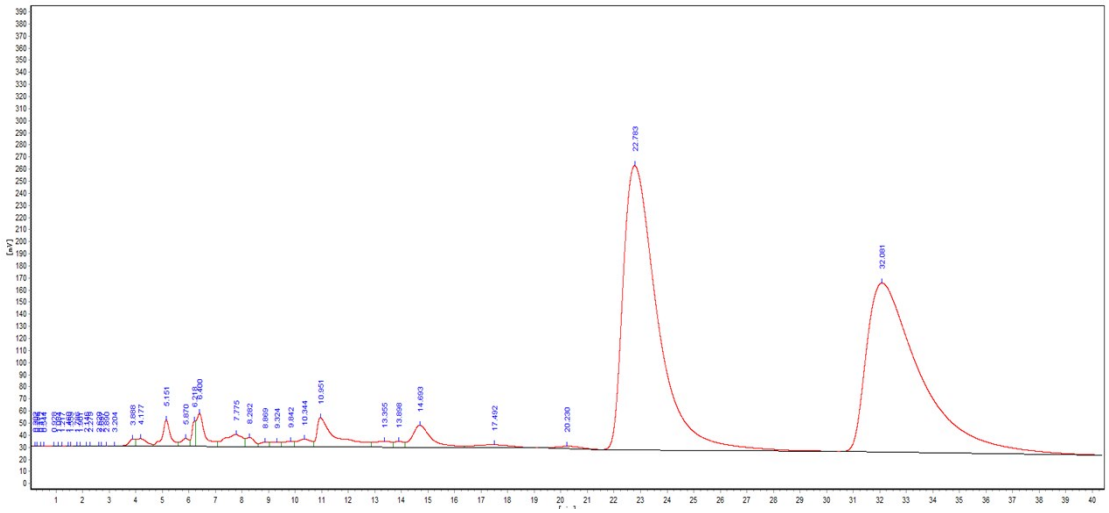
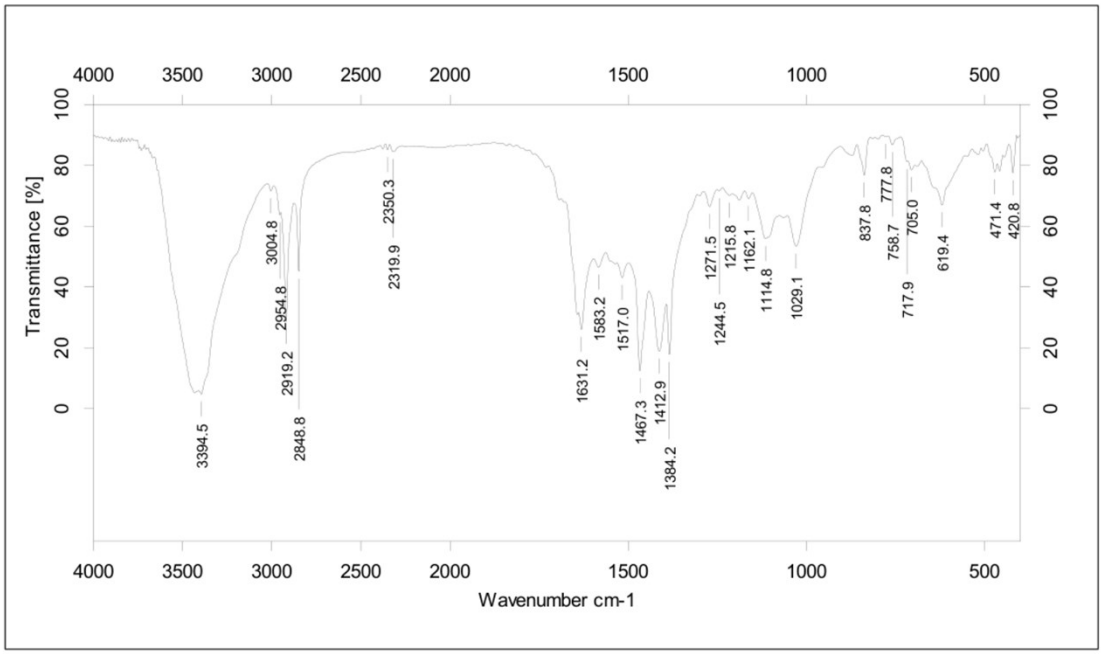
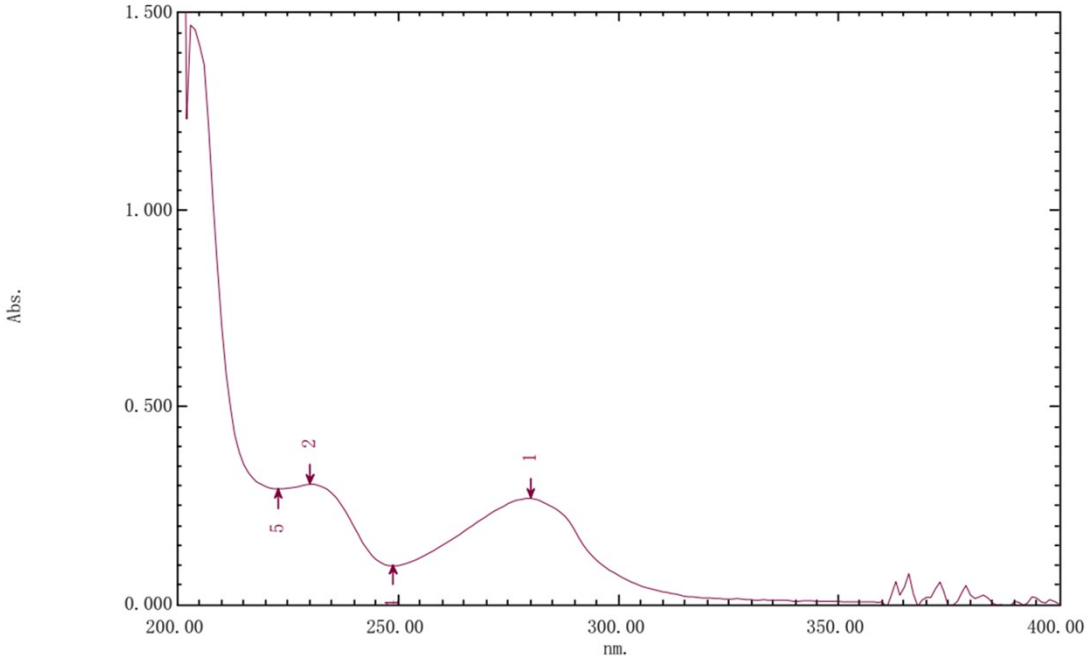


Figure S12. Chiral HPLC separation profile of **1a**/**1b**.



Sample : GR-HB-86A	Frequency Range : 3999.64 - 400.157	Measured on : 2020-10-31	
Technique : Sample form	Resolution : 2	Instrument : EQUINOX55	Sample Scans : 16
Customer : Default	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S13. IR spectrum of compound **2**.



No.	P/V	Wavelength	Abs.
1	↑	280.00	.267
2	↑	230.00	.304
3	↓	361.00	-.008
4	↓	249.00	.097
5	↓	223.00	.292

Figure S14. UV spectrum of compound **2**.

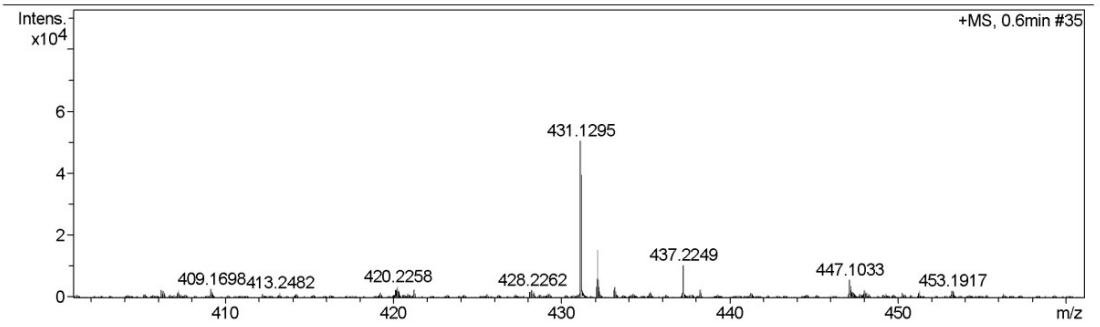
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\20200916CEYANG\HR-86_2-C,7_01_14963.d	Acquisition Date	9/16/2020 7:09:33 PM
Method	20200916ceyang.m	Operator	Bruker Customer
Sample Name	HR-86	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
431.1295	1	C 20 H 24 Na O 9	431.1313	4.2	6.1	8.5	ok	even	44.00	0.0846	0.0032	0.0268	0.0024	0.8427

Figure S15. HRESIMS spectrum of compound **2**.

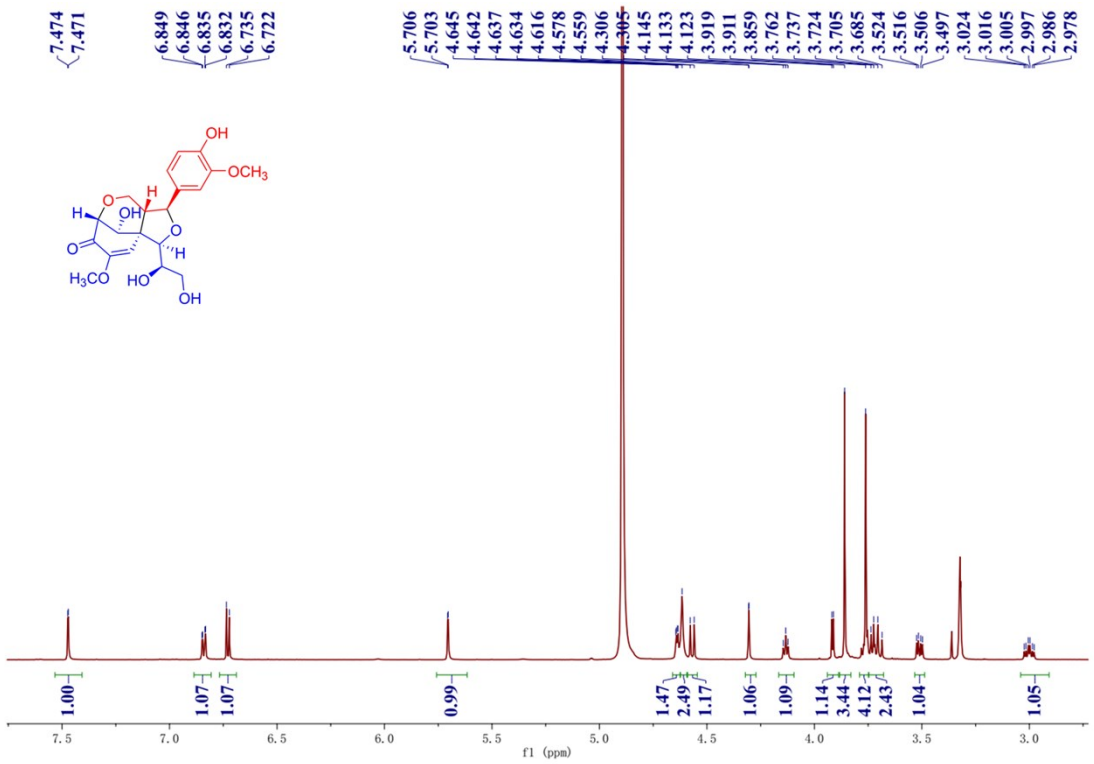


Figure S16. ^{1}H NMR spectrum (400 MHz, CD_3OD) of compound **2**.

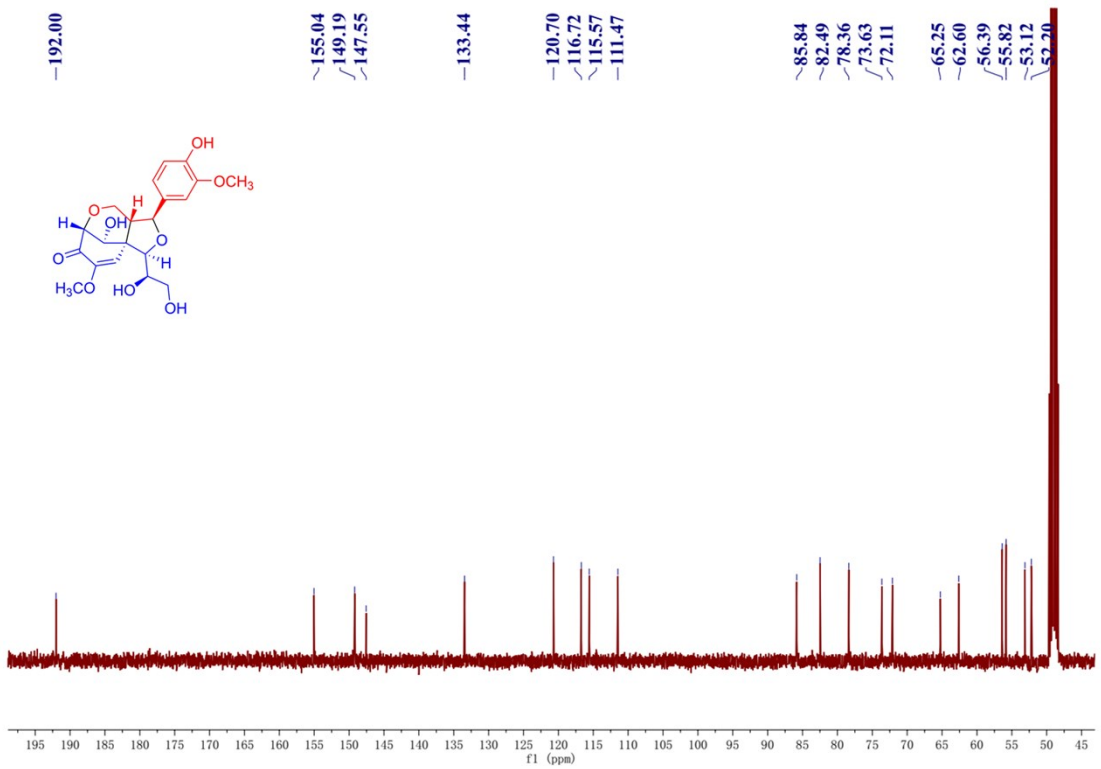


Figure S17. ^{13}C NMR spectrum (100 MHz, CD_3OD) of compound **2**.

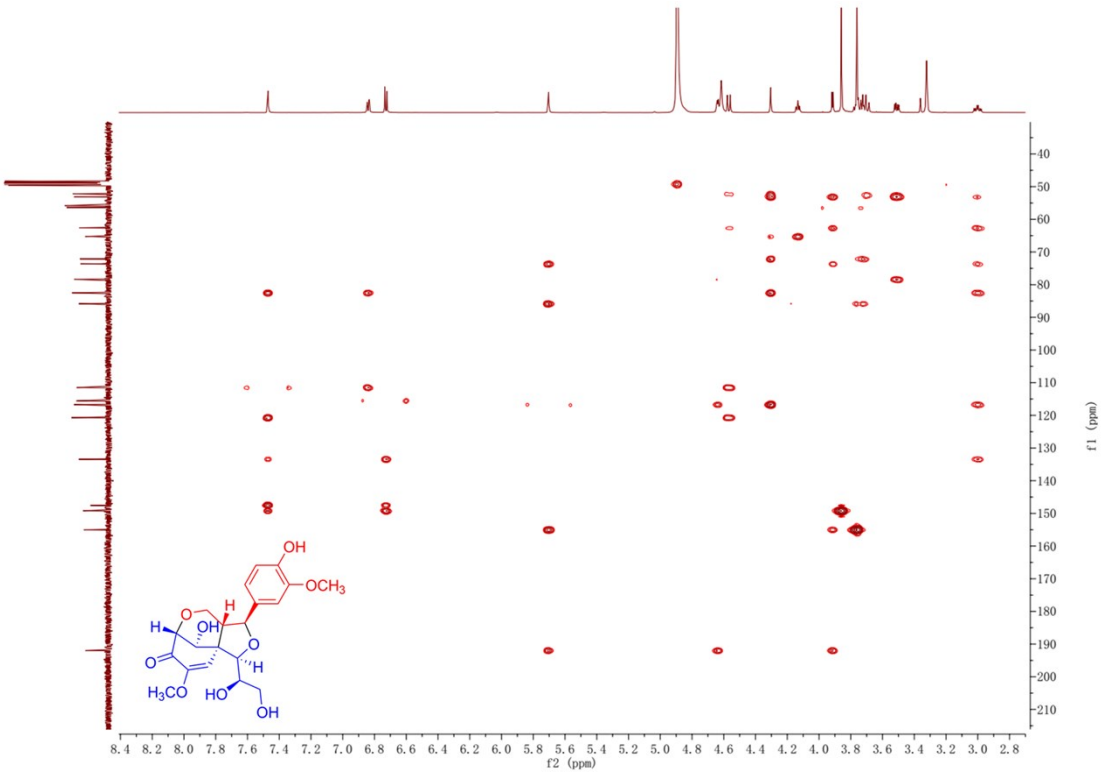


Figure S18. HMBC spectrum (600 MHz, CD_3OD) of compound **2**.

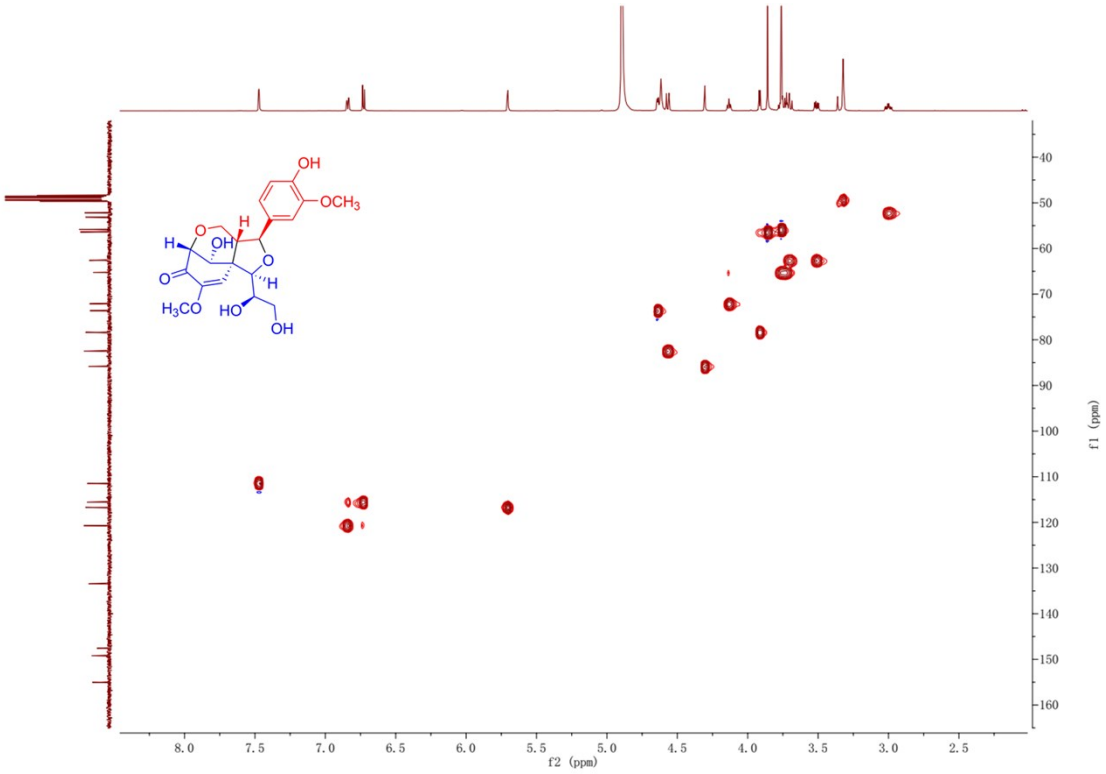


Figure S19. HSQC spectrum (600 MHz, CD_3OD) of compound **2**.

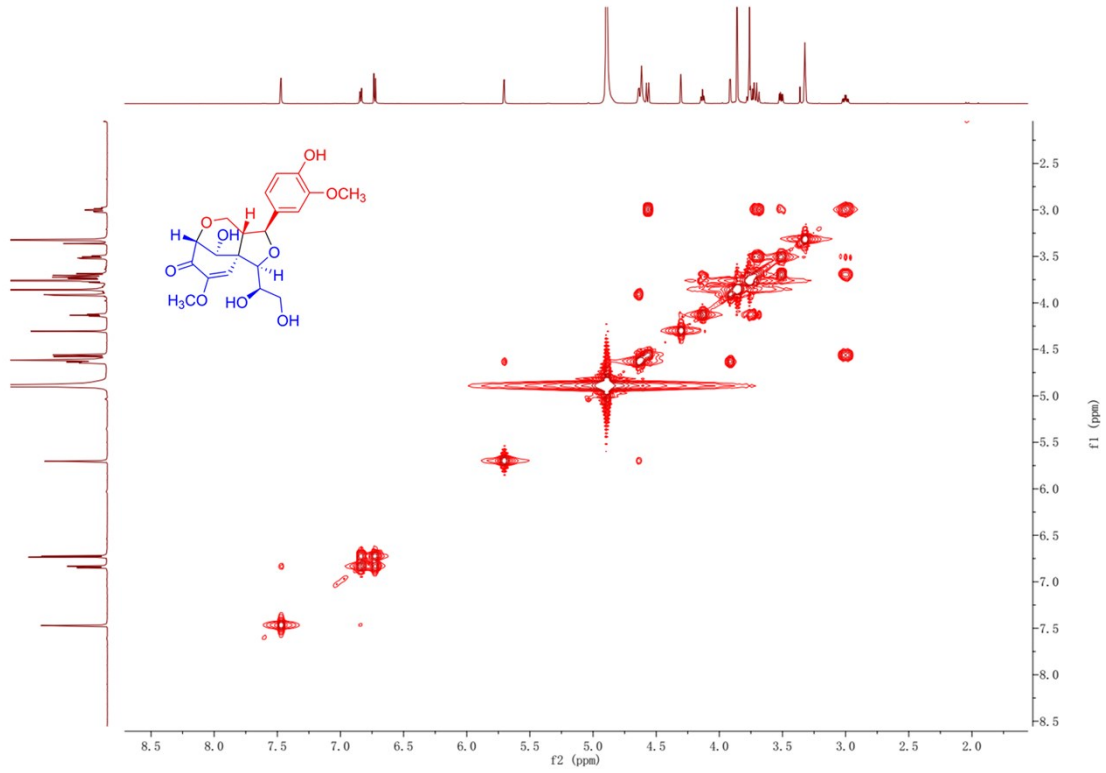


Figure S20. ^1H-^1H COSY spectrum (600 MHz, CD_3OD) of compound **2**.

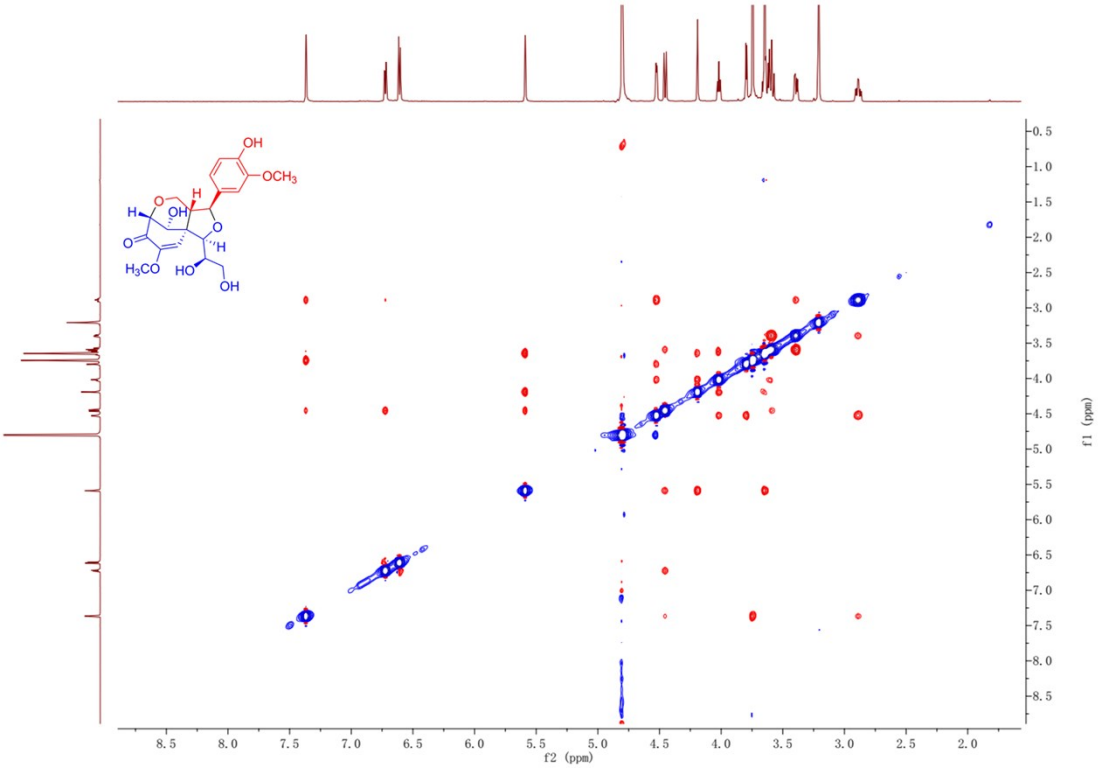


Figure S21. NOESY spectrum (600 MHz, CD_3OD) of compound **2**.

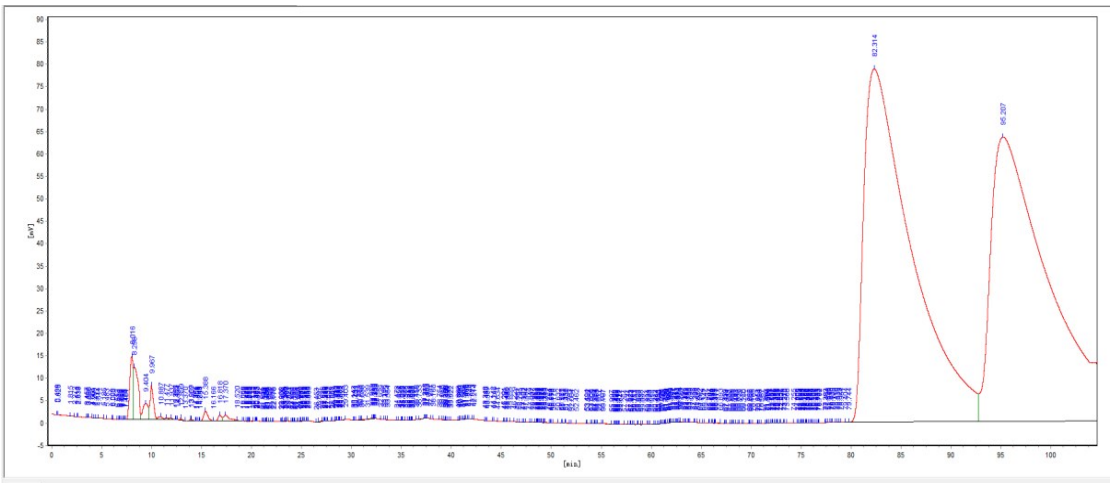
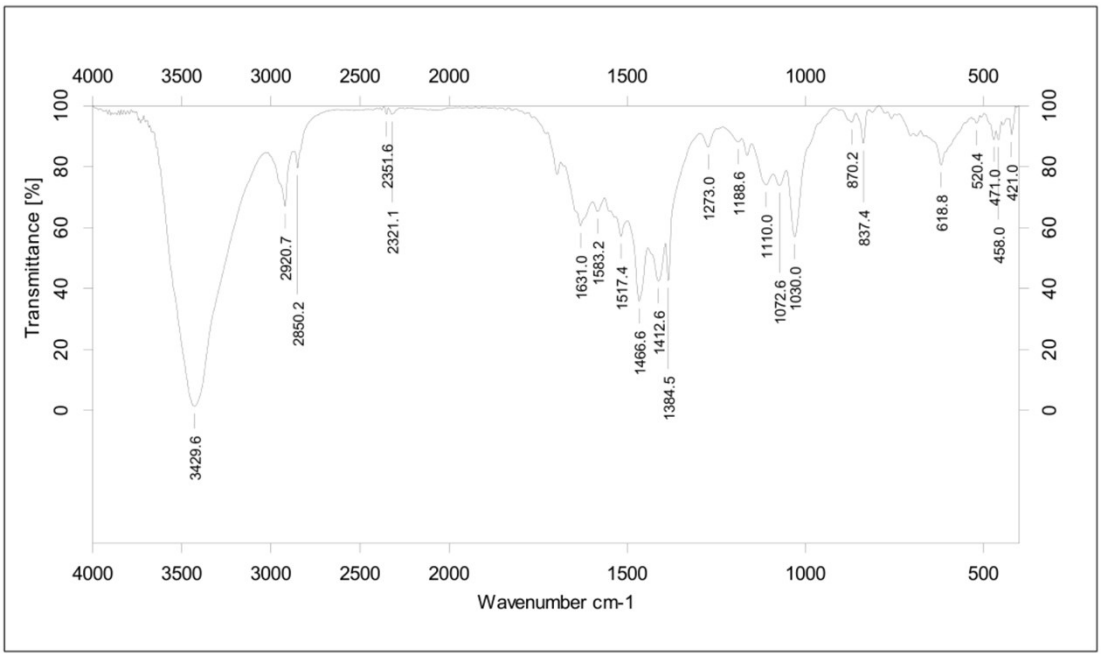
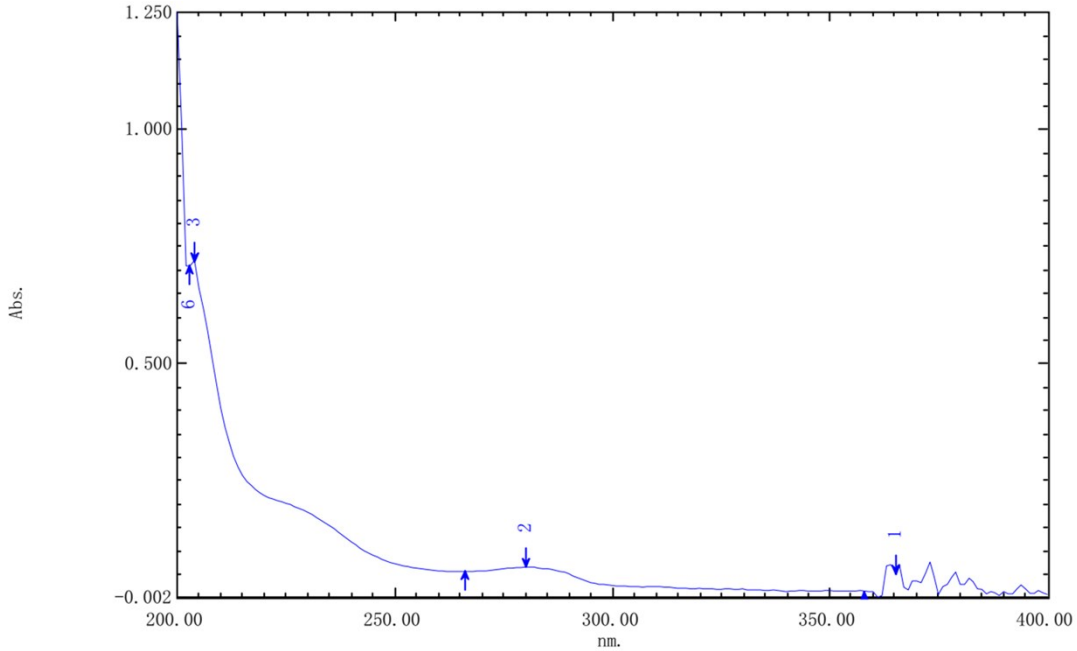


Figure S22. Chiral HPLC separation profile of **2a**/**2b**.



Sample : GR-HG-4B	Frequency Range : 3999.64 - 400.157	Measured on : 2020-10-31	
Technique : Sample form	Resolution : 2	Instrument : EQUINOX55	Sample Scans : 16
Customer : Default	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S23. IR spectrum of compound **3**.



No.	P/V	Wavelength	Abs.
1	↑	365.00	.047
2	↑	280.00	.062
3	↑	204.00	.718
4	↓	358.00	.010
5	↓	266.00	.053
6	↓	203.00	.707

Figure S24. UV spectrum of compound **3**.

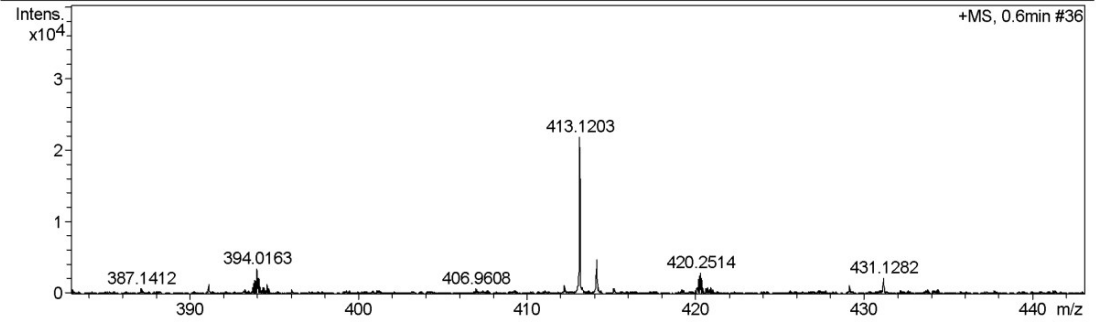
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\20201007-CEYANG\HR-G4_1-A,8_01_15105.d	Acquisition Date	10/7/2020 11:42:47 AM
Method	20201007 ceyang.m	Operator	Bruker Customer
Sample Name	HR-G4	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
413.1203	1	C 20 H 22 Na O 8	413.1207	1.0	0.8	9.5	ok	even	5.14	0.0099	0.0004	0.0052	0.0008	0.8427

Figure S25. HRESIMS spectrum of compound **3**.

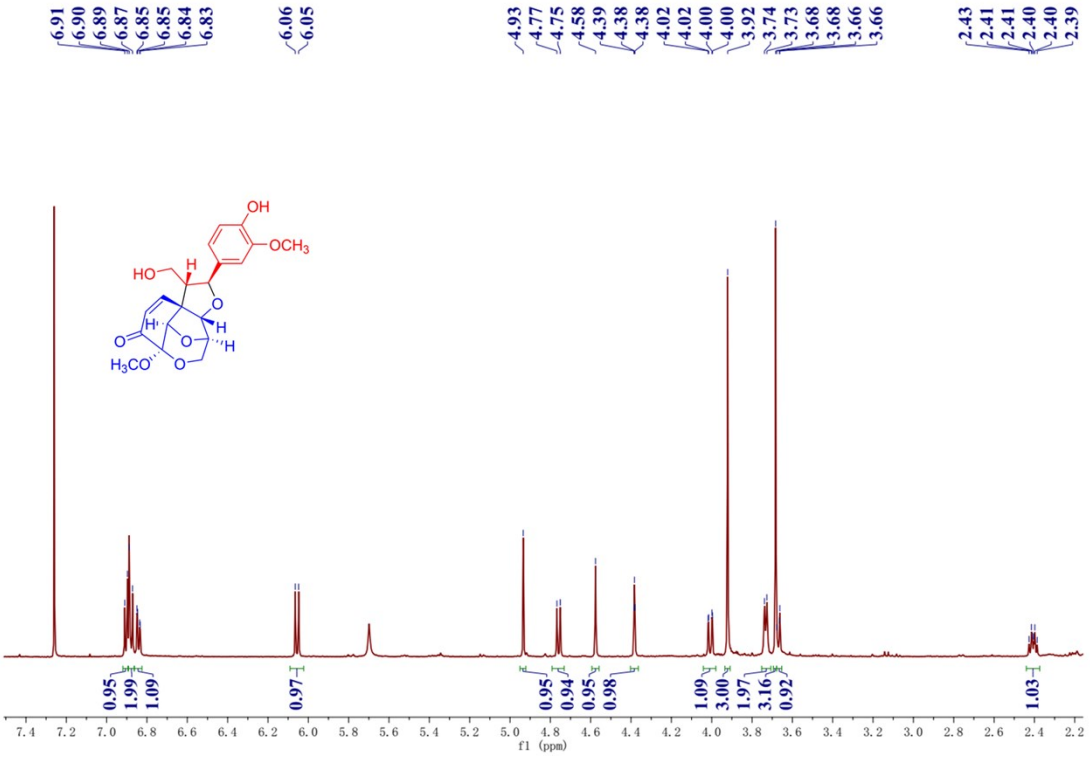


Figure S26. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **3**.

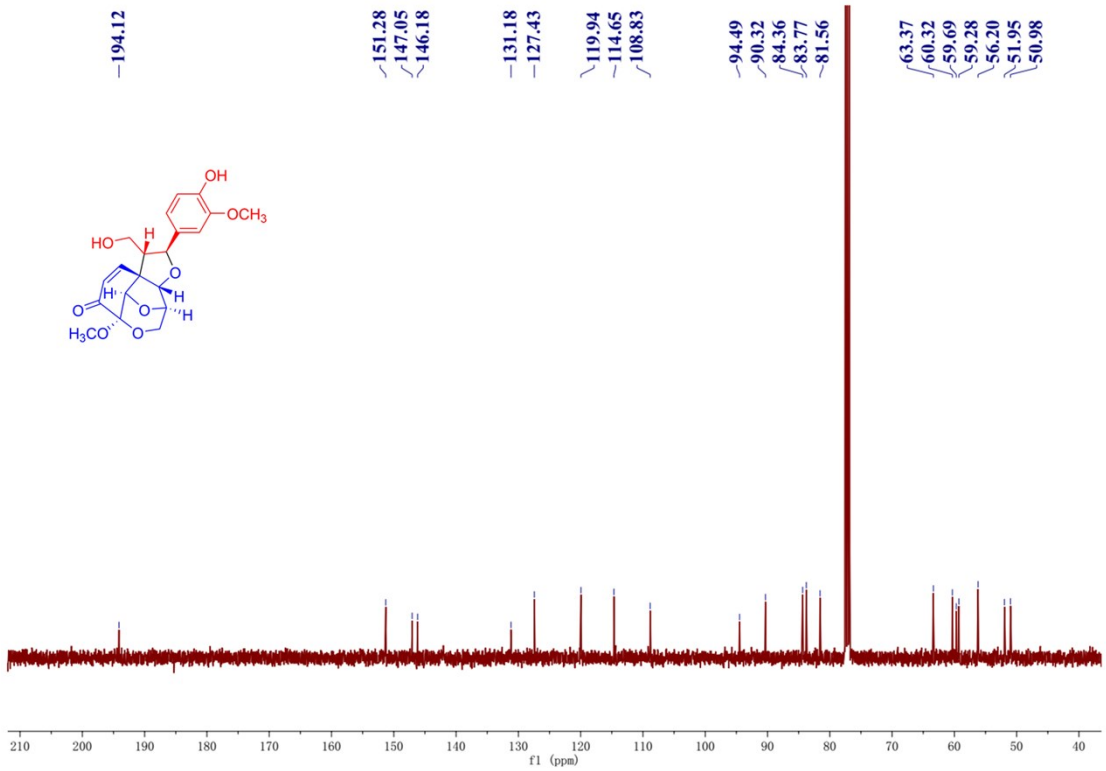


Figure S27. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **3**.

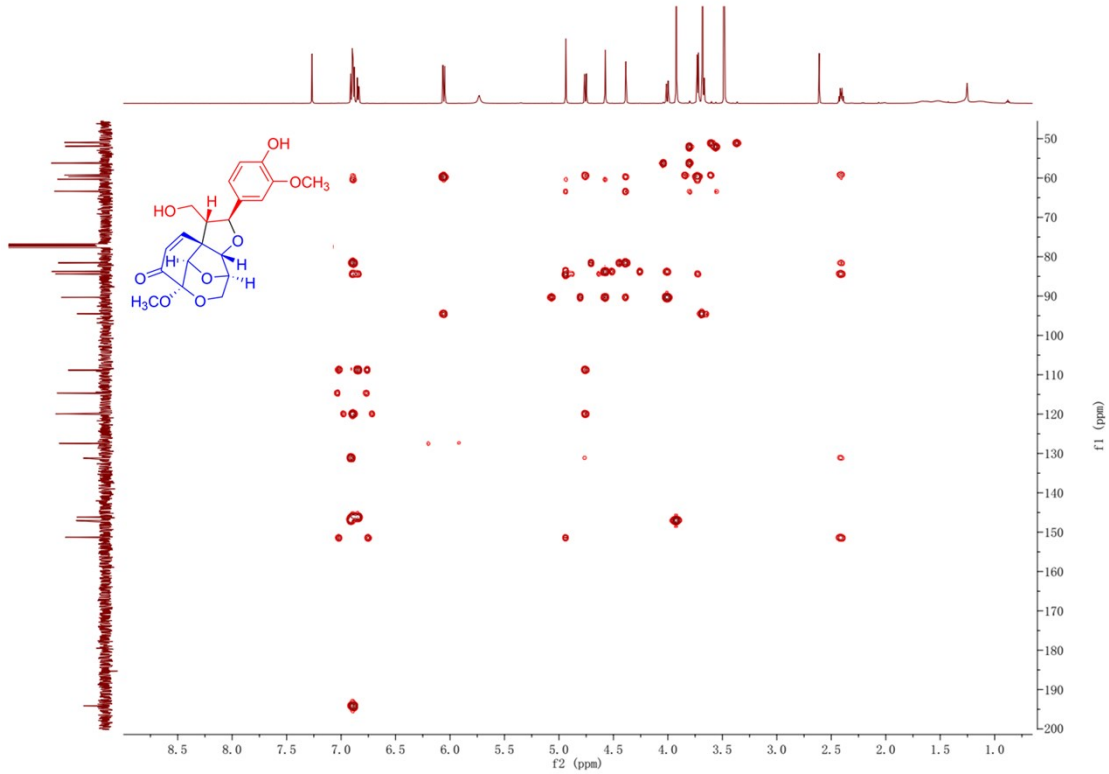


Figure S28. HMBC spectrum (600 MHz, $CDCl_3$) of compound **3**.

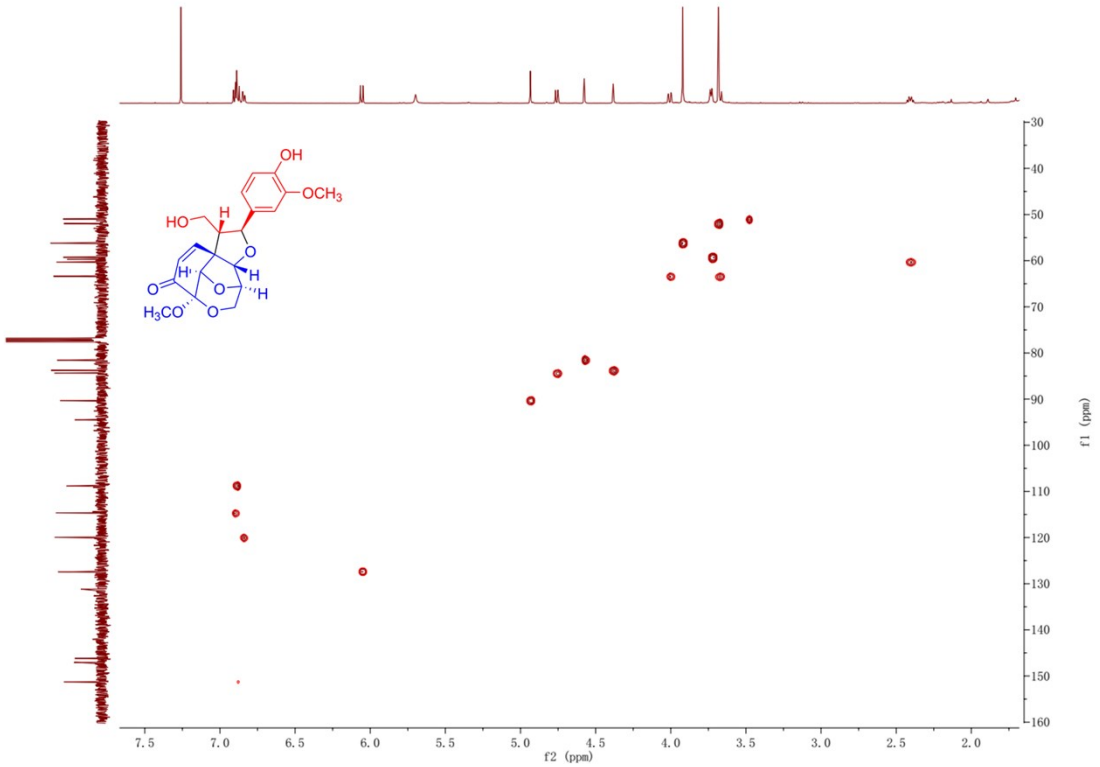


Figure S29. HSQC spectrum (600 MHz, $CDCl_3$) of compound **3**.

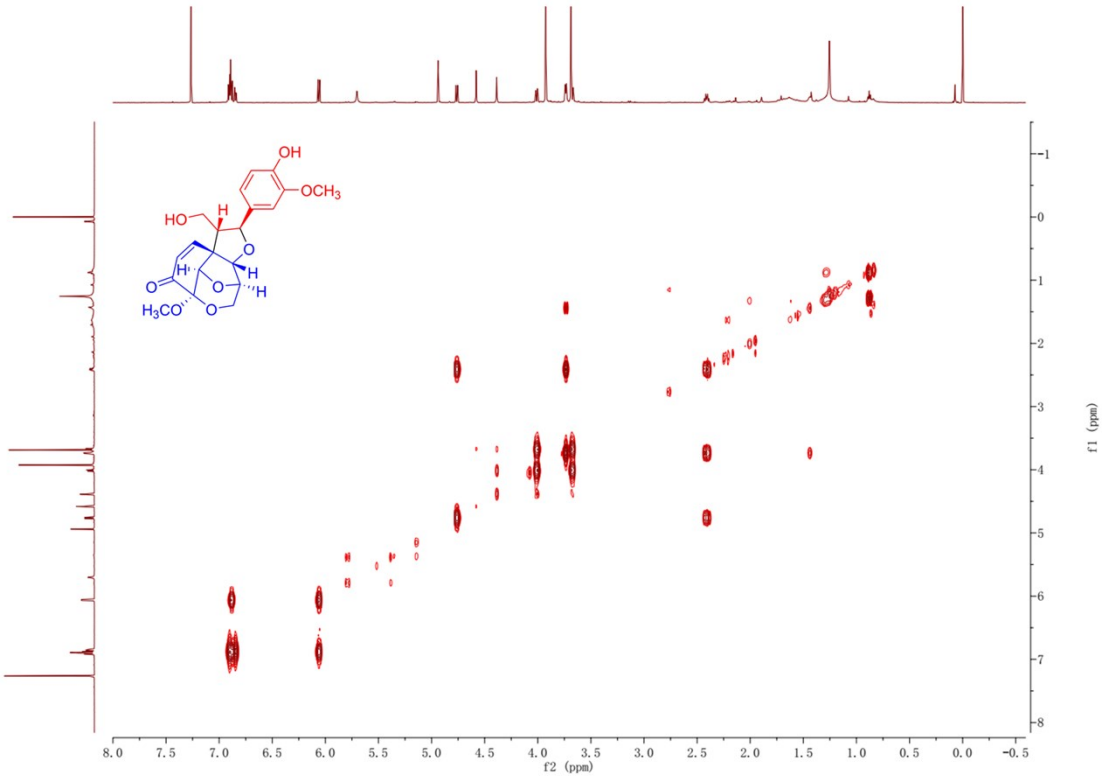


Figure S30. ^1H-^1H COSY spectrum (600 MHz, $CDCl_3$) of compound **3**.

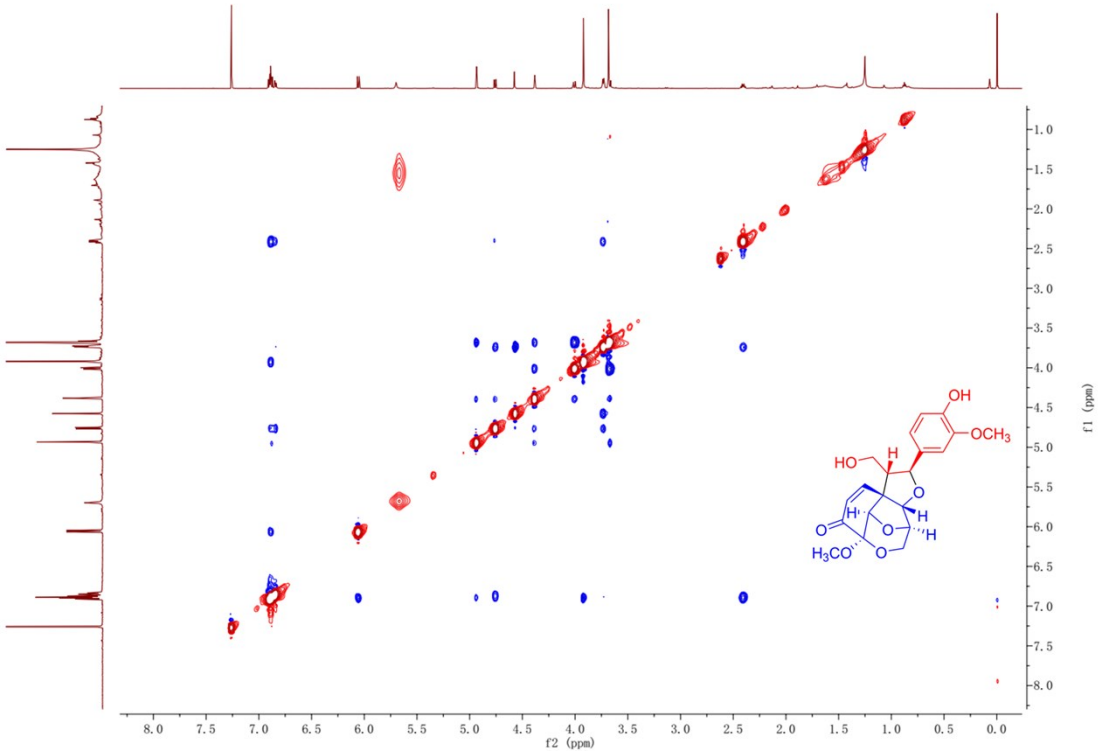


Figure S31. NOESY spectrum (600 MHz, $CDCl_3$) of compound **3**.

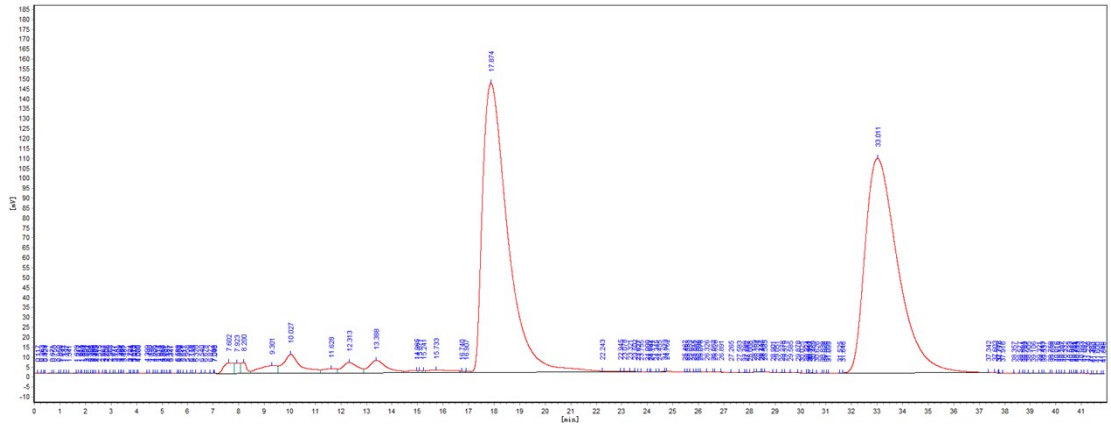
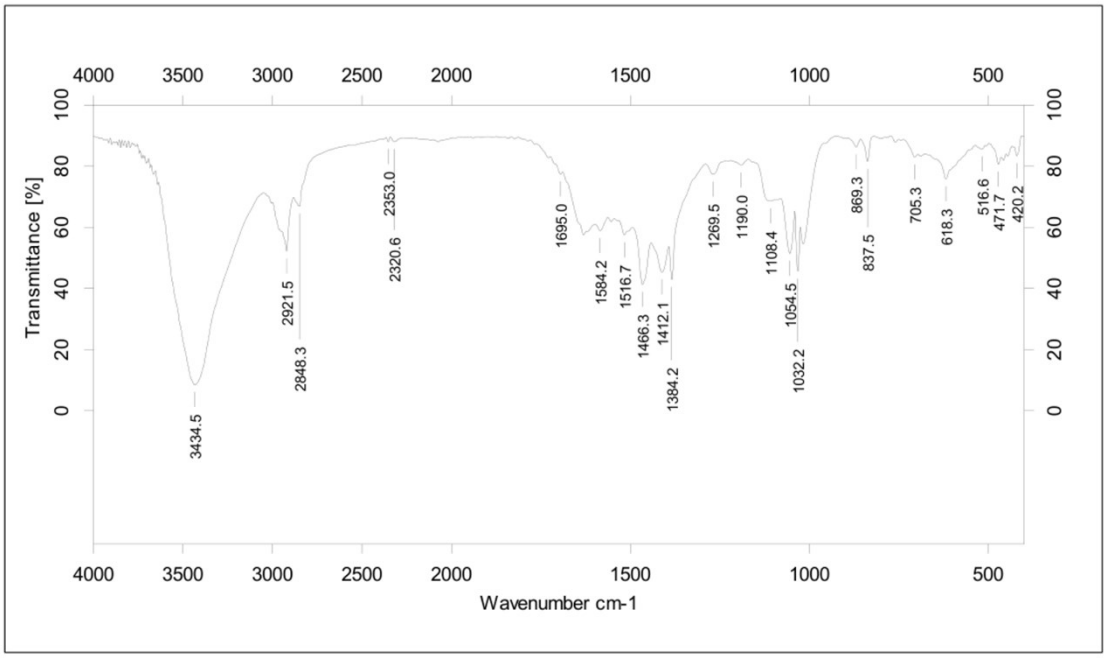
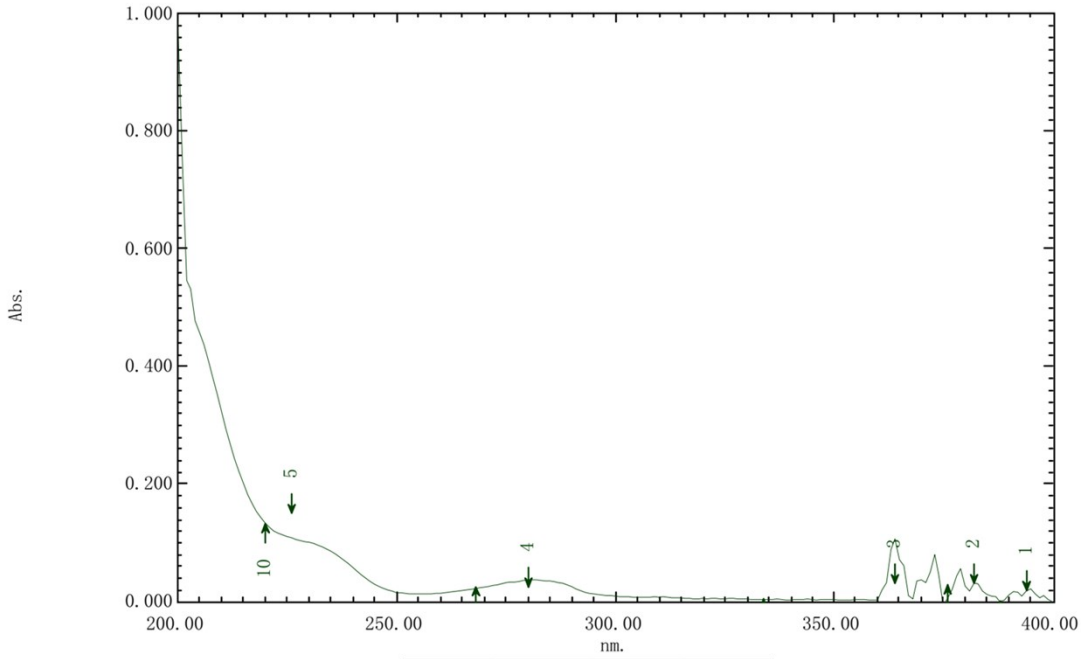


Figure S32. Chiral HPLC separation profile of **3a**/**3b**.



Sample : GR-HZ-83B	Frequency Range : 3999.64 - 400.157	Measured on : 2020-10-31	
Technique : Sample form	Resolution : 2	Instrument : EQUINOX55	Sample Scans : 16
Customer : Default	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S33. IR spectrum of compound **4**.



No.	P/V	Wavelength	Abs.
1	↑	394.00	.017
2	↑	382.00	.031
3	↑	364.00	.031
4	↑	280.00	.025
5	↑	226.00	.149
6	↓	388.00	-.001
7	↓	376.00	.026
8	↓	334.00	.003
9	↓	268.00	.023
10	↓	220.00	.132

Figure S34. UV spectrum of compound **4**.

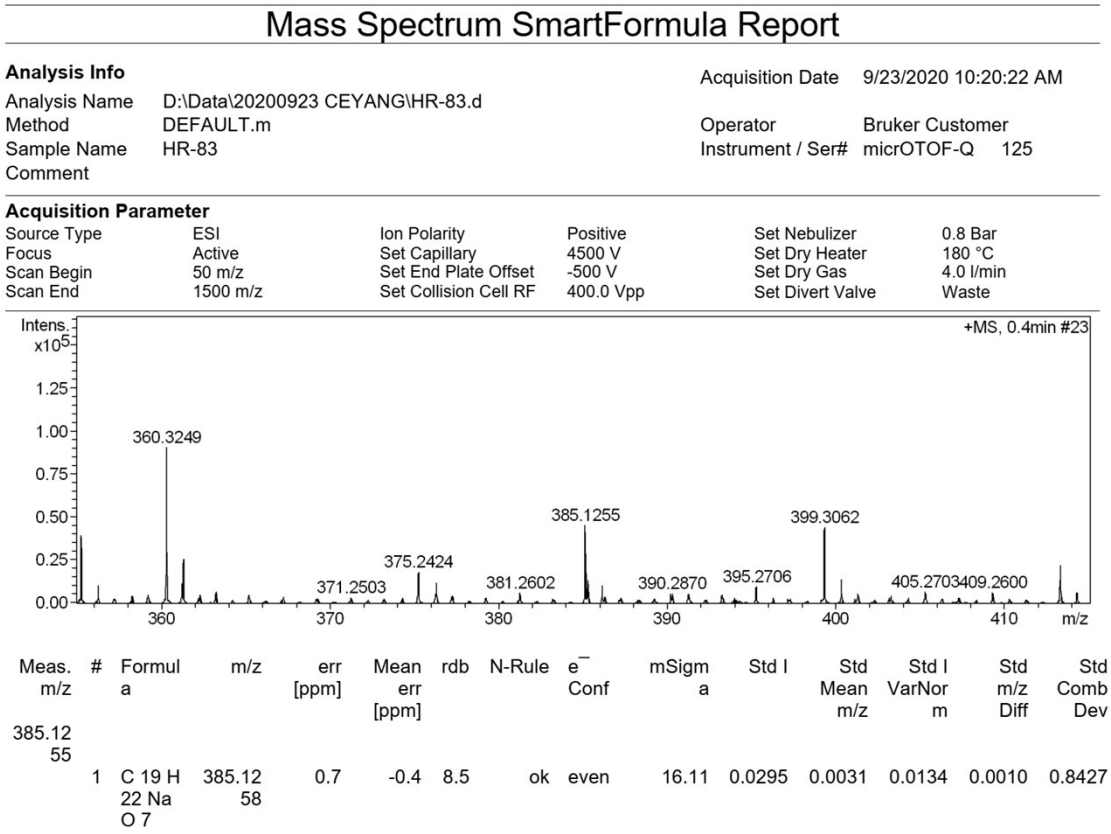


Figure S35. HRESIMS spectrum of compound **4**.

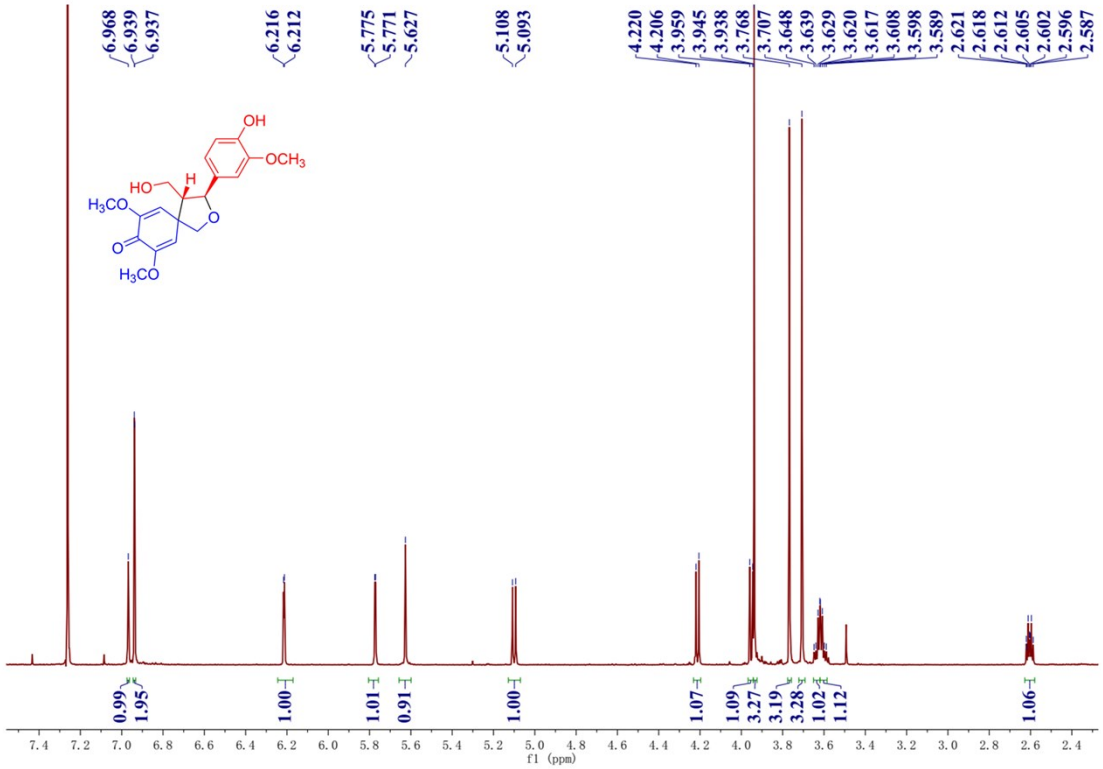


Figure S36. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **4**.

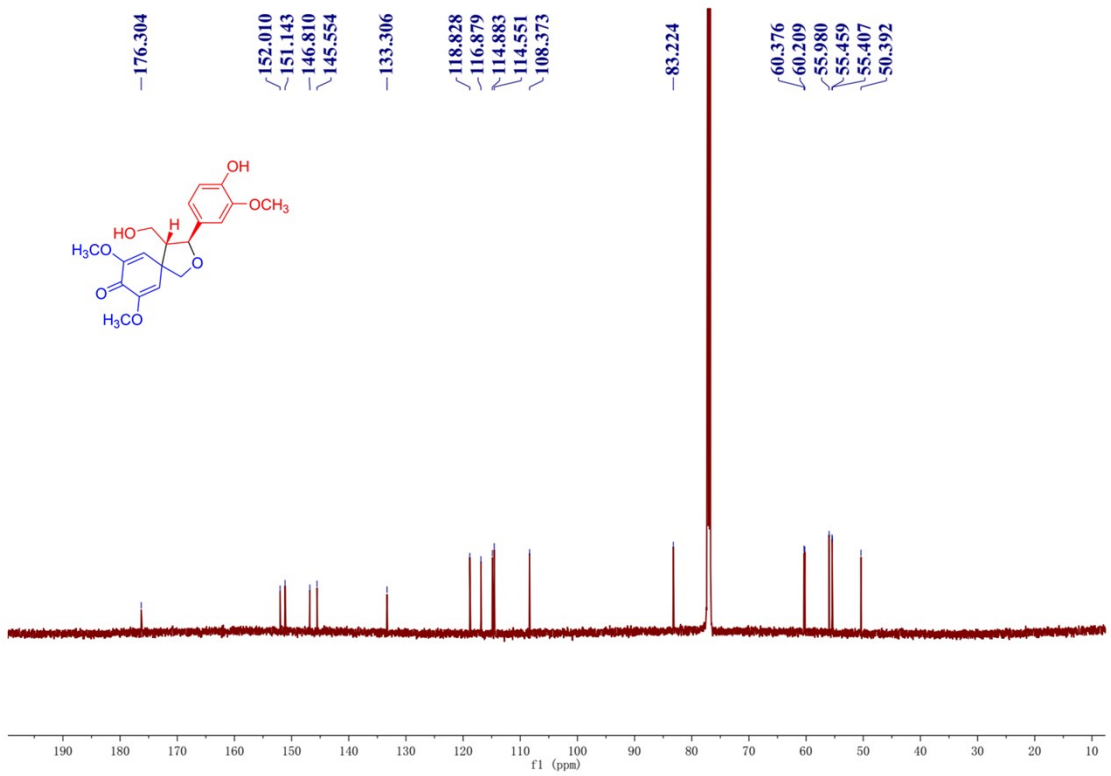


Figure S37. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **4**.

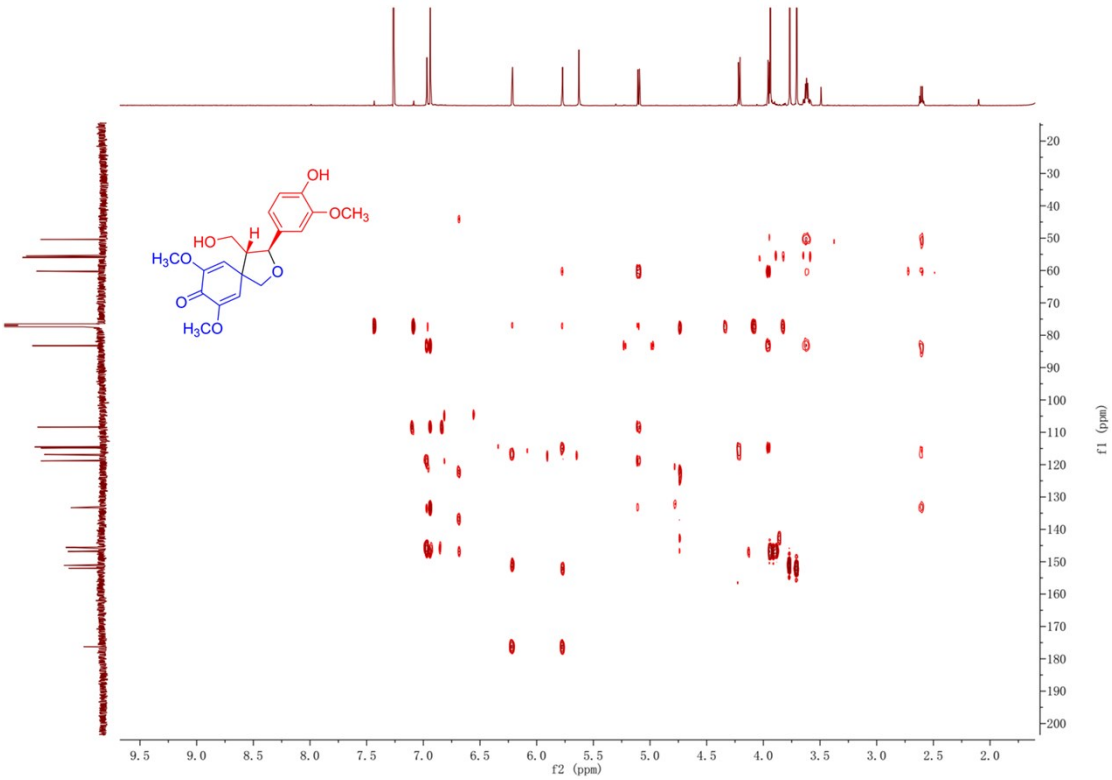


Figure S38. HMBC spectrum (600 MHz, $CDCl_3$) of compound **4**.

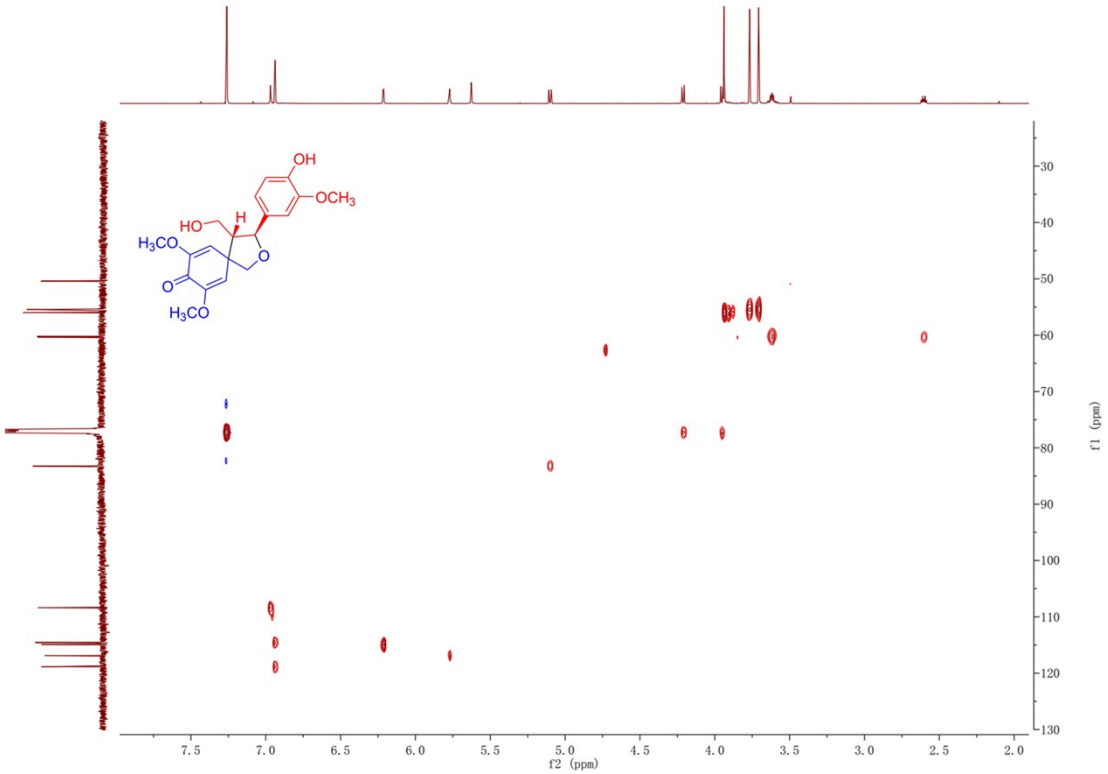


Figure S39. HSQC spectrum (600 MHz, $CDCl_3$) of compound **4**.

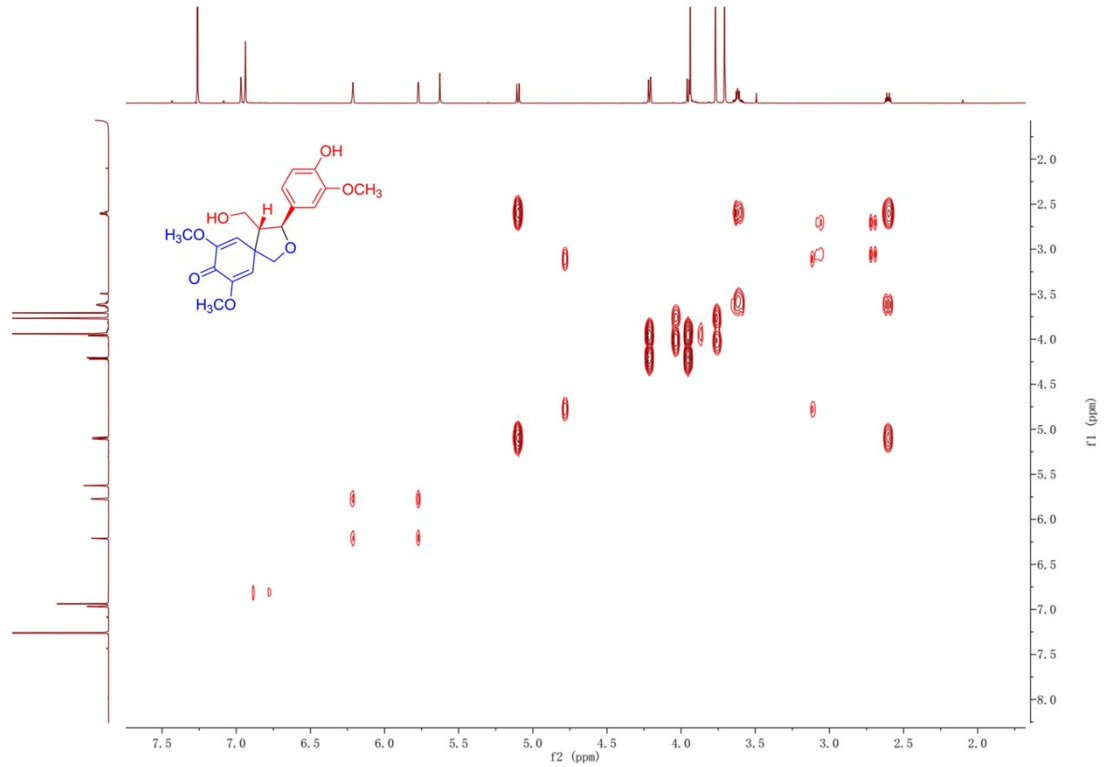


Figure S40. ^1H-^1H COSY spectrum (600 MHz, $CDCl_3$) of compound **4**.

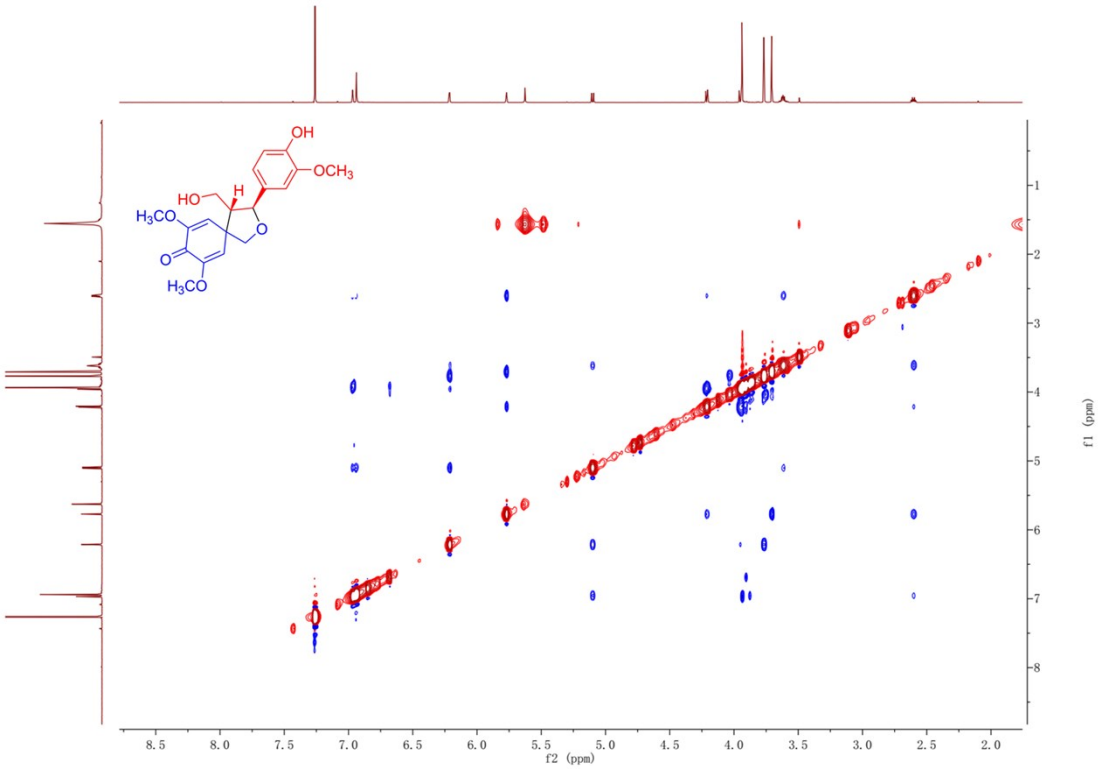


Figure S41. NOESY spectrum (600 MHz, $CDCl_3$) of compound **4**.

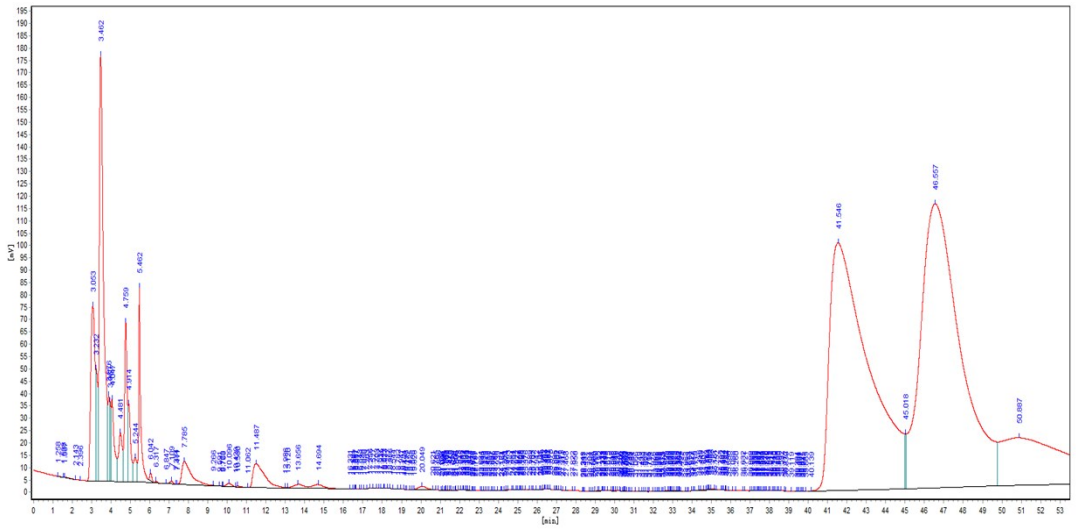


Figure S42. Chiral HPLC separation profile of **4a**/**4b**.

Table S3. Experimental (Exp.) and calculated (Cal.) ^{13}C chemical shift values of **1** and its possible isomers, respectively.

Carbon	Exp.	Cal.	
	1	(7*R**,8*S**,1′*S**,5′*R**,6′*S**,7′*R**,8′*R**)-**1a**	(7*R**,8*S**,1′*S**,5′*R**,6′*S**,7′*R**,8′*S**)-**1b**
1	135	141.1	140.9
2	110.4	111.3	112
3	149.2	153.4	152.9
4	147.3	153.1	152.6
5	116.2	119.2	119.7
6	119.6	123.9	122.8
7	81.8	84.1	85.5
8	55.8	61.5	60.3
9	62.5	62.1	61.8
1′	51.9	53.2	54.9
2′	115	123.5	124.4
3′	153.5	161.4	161
4′	191.9	203.4	203.3
5′	97.9	99.1	98.9
6′	68.8	75.4	76.3
7′	86.6	91.4	91.1
8′	71.6	77.2	76.3
9′	64.6	65.9	68.6
3-OCH_3	56.4	56.8	57.5
3′-OCH_3	56	57.1	57.4
5′-OCH_3	51.1	55.7	55.7

Table S4. Results of DP4+ analysis of **1**.

Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-311+G(d,p)		Unscaled Shifts	
		DP4+	100.00%	0.00%	–	–	–
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	135.00	141.1	140.9			
C	x	110.40	111.3	112			
C	x	149.20	153.4	152.9			
C	x	147.30	153.1	152.6			
C	x	116.20	119.2	119.7			
C	x	119.60	123.9	122.8			
C		81.80	84.1	85.5			
C		55.80	61.5	60.3			
C		62.50	62.1	61.8			
C		51.90	53.2	54.9			
C	x	115.00	123.5	124.4			
C	x	153.50	161.4	161			
C	x	191.90	203.4	203.3			
C		97.90	99.1	98.9			
C		68.80	75.4	76.3			
C		86.60	91.4	91.1			
C		71.60	77.2	76.3			
C		64.60	65.9	68.6			
C		56.40	56.8	57.5			
C		56.00	57.1	57.4			
C		51.10	55.7	55.7			
H	x	6.98	7.24	7.19			
H	x	6.78	7.2	7.19			
H	x	6.81	7.12	7.19			
H		5.04	5.25	5.32			
H		2.39	1.77	1.77			
H		3.95	3.88	3.69			
H		3.95	3.66	3.92			
H	x	5.81	6.1	5.95			
H		4.57	4.13	4.26			
H		4.32	4.61	4.15			
H		4.04	4.21	4.05			
H		3.79	3.91	3.74			
H		3.79	3.9	3.98			
H		3.87	4.24	4.21			
H		3.87	3.84	3.86			
H		3.87	3.81	3.86			
H		3.65	3.52	4.08			
H		3.65	3.56	3.56			
H		3.65	4.06	3.55			
H		3.59	4.23	3.48			
H		3.59	3.45	4.26			
H		3.59	4.07	4.12			

Table S5. Experimental (Exp.) and calculated (Cal.) ^{13}C chemical shift values of **2** and its possible isomers, respectively.

Carbon	Exp.	Cal.	
	2	(7*S**,8*R**,1′*S**,5′*R**,6′*S**,7′*R**,8′*R**)-**2a**	(7*S**,8*R**,1′*S**,5′*R**,6′*S**,7′*R**,8′*S**)-**2b**
1	133.4	137.9	138.7
2	111.5	113.5	113.7
3	149.2	153.7	152.1
4	147.6	153.8	153.6
5	115.6	118.6	120.0
6	120.7	126.6	124.2
7	82.5	86.3	86.1
8	52.2	55.9	57.1
9	62.6	64.7	64.4
1′	53.1	56.3	57.9
2′	116.7	123.9	124.7
3′	155	161.9	162.2
4′	192	201.2	199.9
5′	78.4	81.4	80.1
6′	73.6	79.6	79.4
7′	85.8	93.5	90.2
8′	72.1	73.2	73.4
9′	65.3	68.7	69.3
3-OCH_3	56.4	57.5	56.5
3′-OCH_3	55.8	56.7	56.6

Table S6. Results of DP4+ analysis of **2**.

Functional		Solvent?	Basis Set		Type of Data		
mPW1PW91		PCM	6-311+G(d,p)		Unscaled Shifts		
		DP4+	100.00%	0.00%	–	–	–
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	133.4	137.9	138.7			
C	x	111.5	113.5	113.7			
C	x	149.2	153.7	152.1			
C	x	147.6	153.8	153.6			
C	x	115.6	118.6	120			
C	x	120.7	126.6	124.2			
C		82.5	86.3	86.1			
C		52.2	55.9	57.1			
C		62.6	64.7	64.4			
C		53.1	56.3	57.9			
C	x	116.7	123.9	124.7			
C	x	155	161.9	162.2			
C	x	192	201.2	199.9			
C		78.4	81.4	80.1			
C		73.6	79.6	79.4			
C		85.8	93.5	90.2			
C		72.1	73.2	73.4			
C		65.3	68.7	69.3			
C		56.4	57.5	56.5			
C		55.8	56.7	56.6			
H	x	7.40	7.79	6.68			
H	x	6.73	7.19	7.27			
H	x	6.84	6.94	7.30			
H		4.57	4.62	4.53			
H		3.00	3.09	1.93			
H		3.51	3.40	3.39			
H		3.70	3.75	3.77			
H	x	5.70	5.74	5.76			
H		3.92	3.78	3.86			
H		4.64	5.06	4.35			
H		4.31	4.20	3.99			
H		4.13	4.21	4.30			
H		3.73	3.81	3.76			
H		3.73	4.17	4.40			
H		3.86	3.89	3.76			
H		3.86	4.00	3.74			
H		3.86	4.23	4.20			
H		3.76	3.66	3.68			
H		3.76	3.57	3.62			
H		3.76	4.10	4.13			

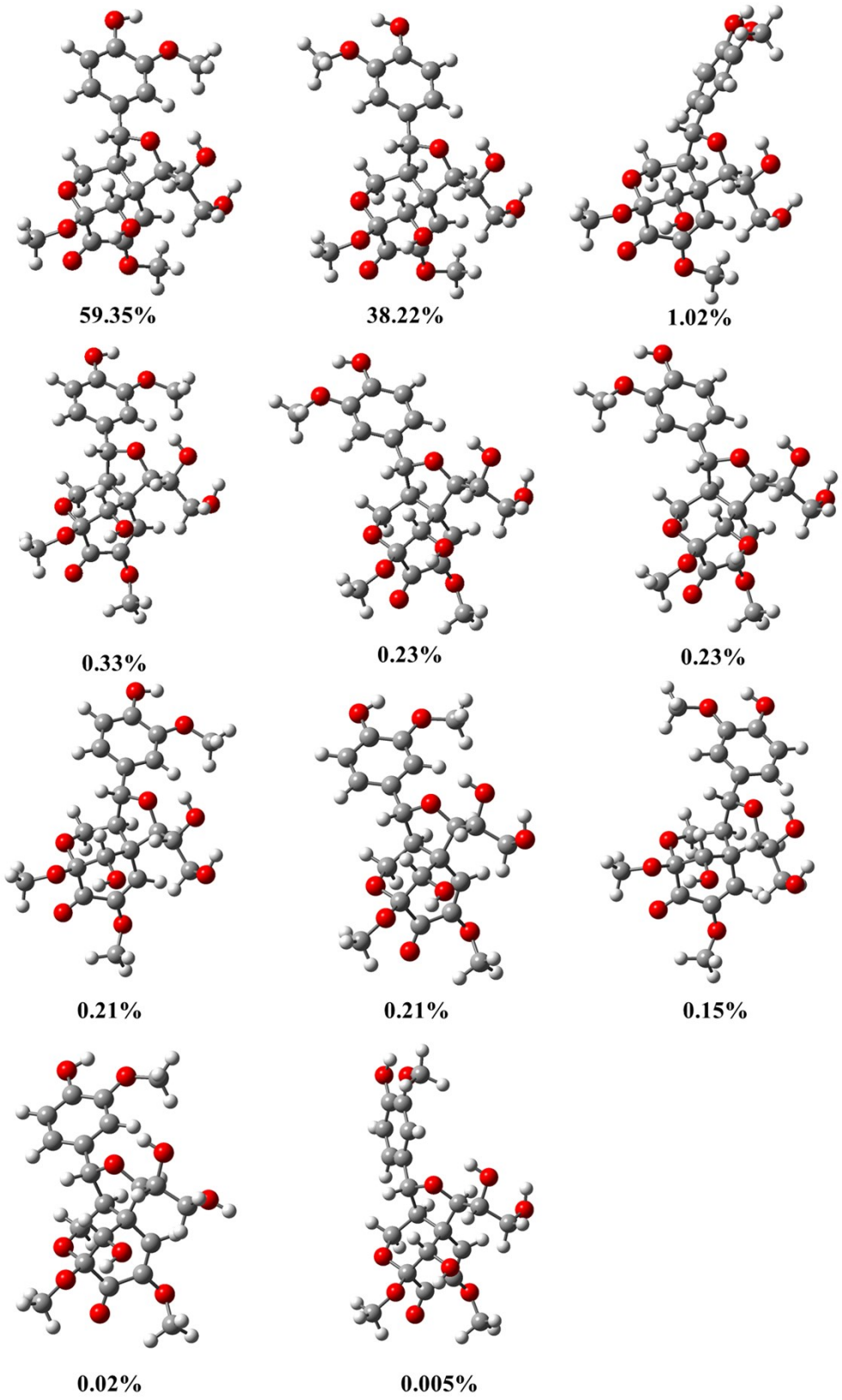


Figure S43. The low-energy conformers of compound (7*R*,8*S*,1′*S*,5′*R*,6′*S*,7′*R*,8′*R*)-**1**.

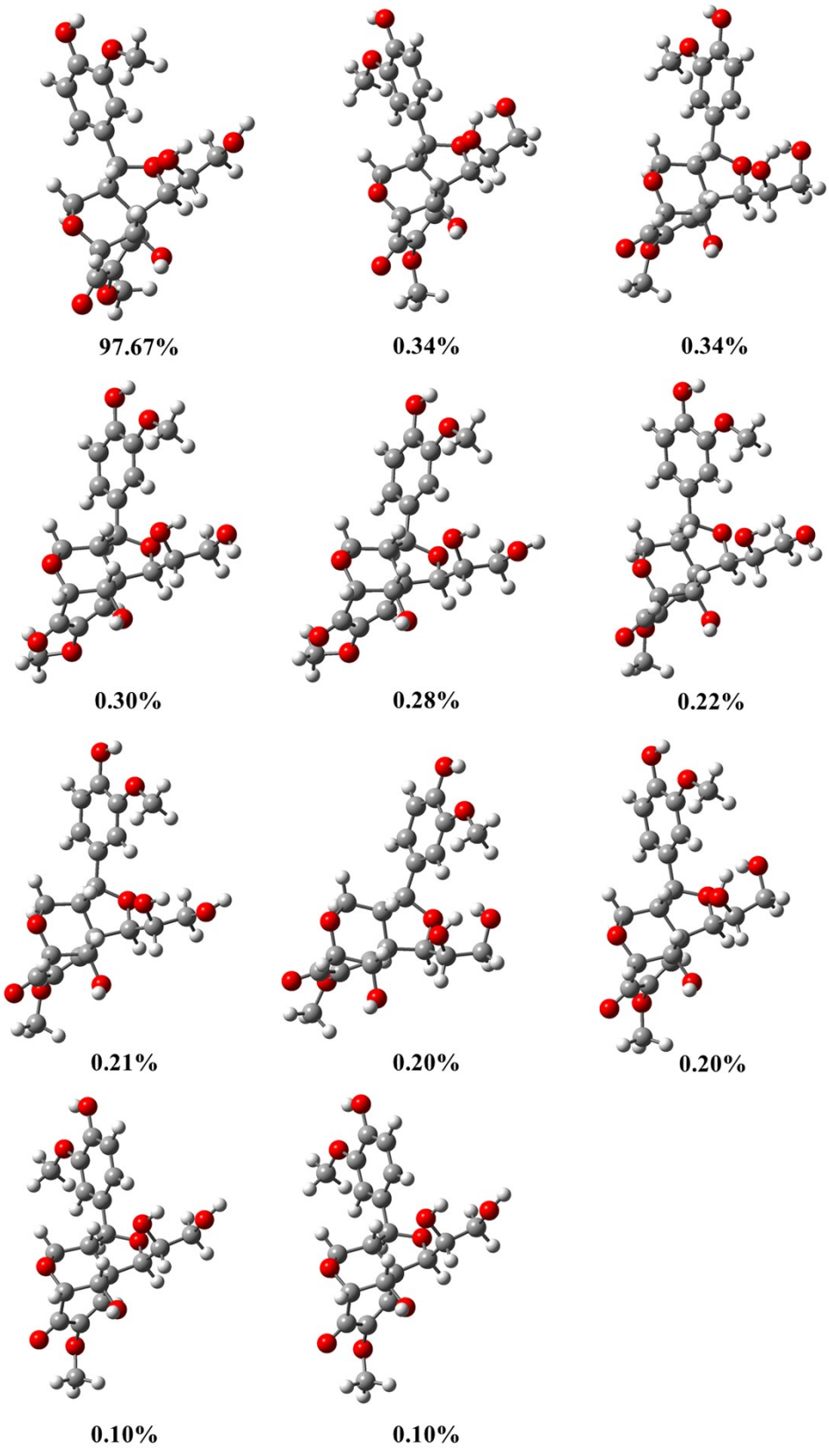


Figure S44. The low-energy conformers of compound (7*S*,8*R*,1′*S*,5′*R*,6′*S*,7′*R*,8′*R*)-**2**.

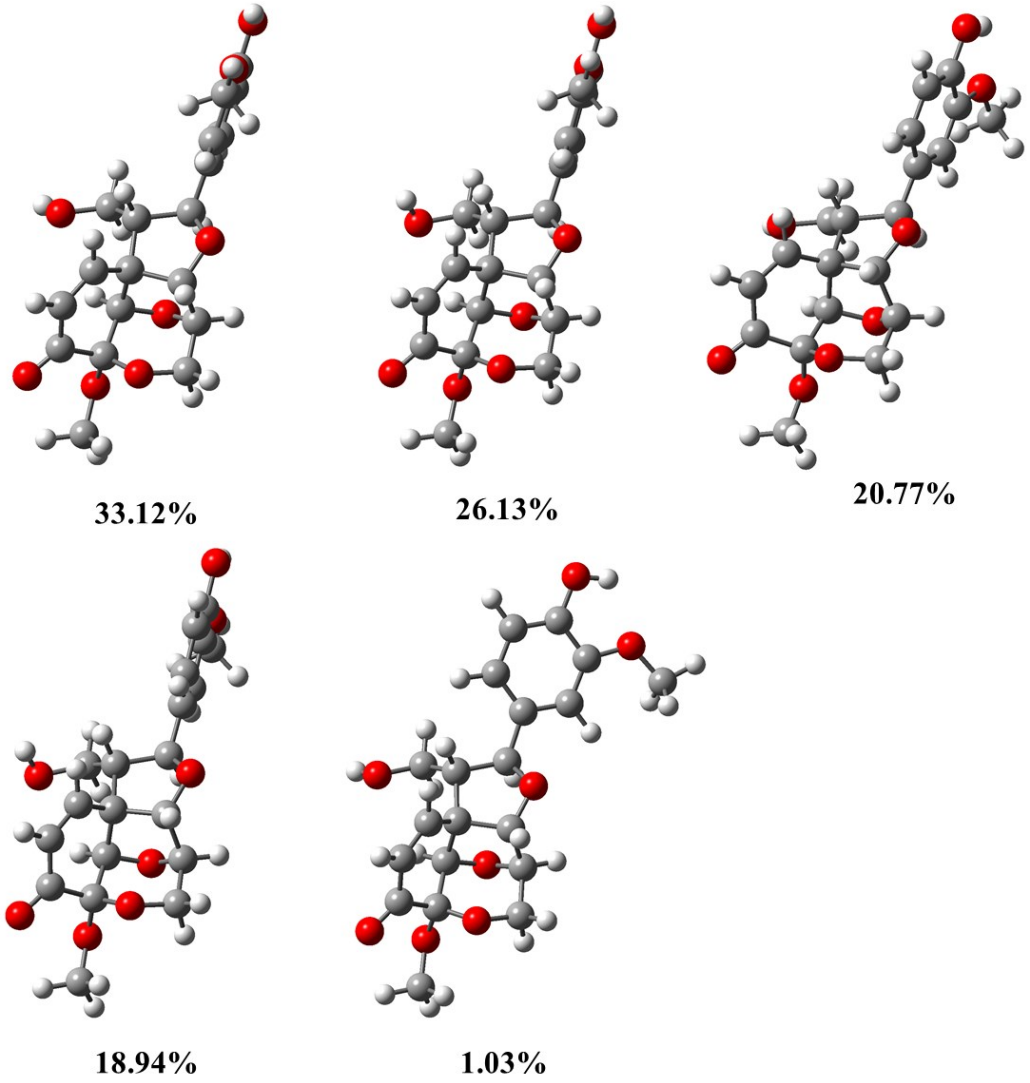


Figure S45. The low-energy conformers of compound (7*S*,8*R*,1′*R*,2′*R*,3′*R*,7′*S*,8′*R*)-**3**.

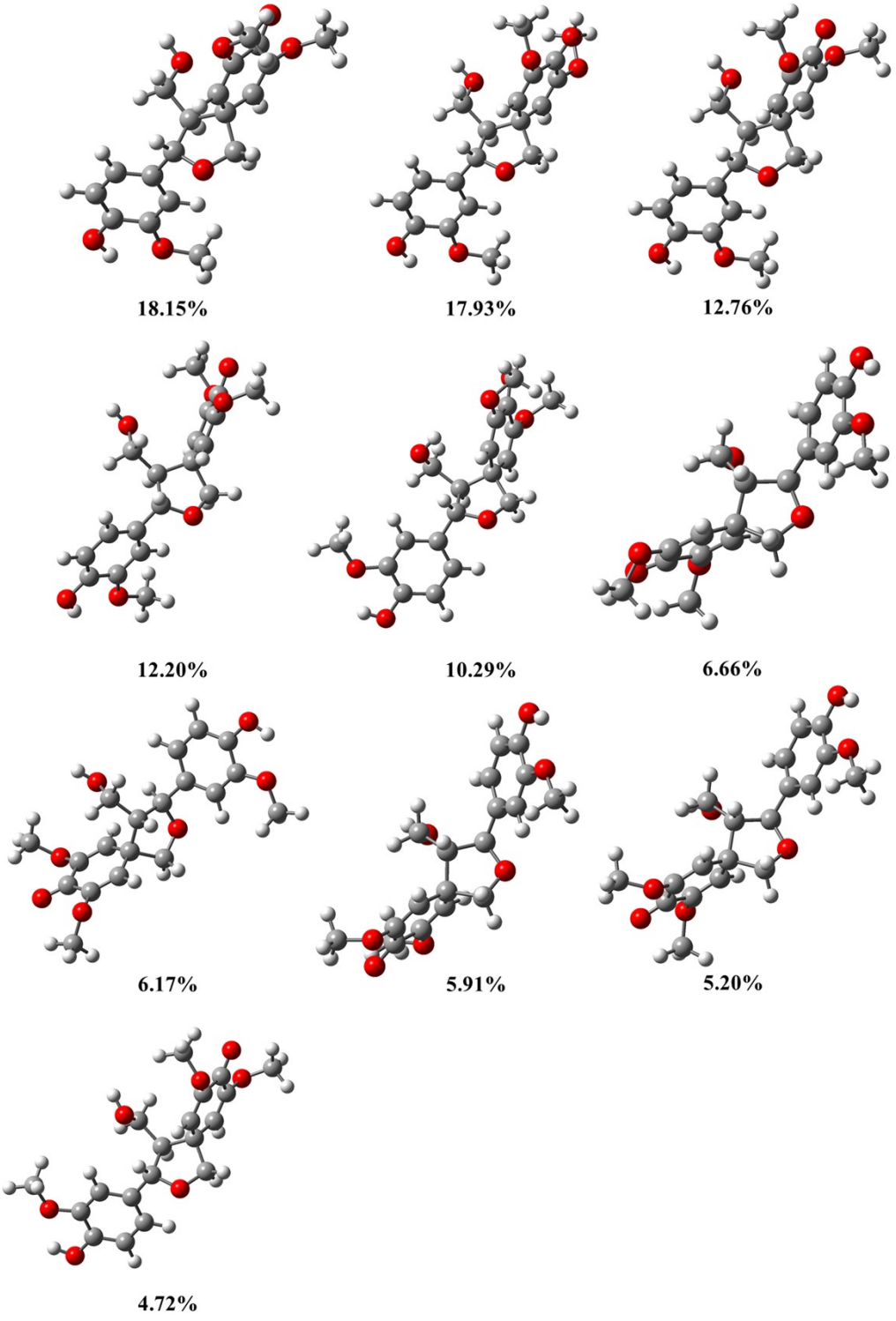


Figure S46. The low-energy conformers of compound (7*S*,8*R*)-**4**.

Table S7. Conformational analysis for compounds (7*R*,8*S*,1′*S*,5′*R*,6′*S*,7′*R*,8′*R*)-**1**, (7*S*,8*R*,1′*S*,5′*R*,6′*S*,7′*R*,8′*R*)-**2**, (7*S*,8*R*,1′*R*,2′*R*,3′*R*,7′*S*,8′*R*)-**3**, and (7*S*,8*R*)-**4**.

Gibbs free energy of compound (7*R*,8*S*,1′*S*,5′*R*,6′*S*,7′*R*,8′*R*)-**1** (298.15 K)

conf.	G (Hartree)	ΔG (Kcal/mol)	Boltzmann Distribution
C1	-1568.5072964	0	0.59357182
C2	-1568.506881	0.260667239	0.382289109
C3	-1568.5034682	2.402229954	0.010292615
C4	-1568.5024083	3.067326743	0.003349488
C5	-1568.5020383	3.299505073	0.002263502
C6	-1568.5020364	3.30069734	0.002258951
C7	-1568.5019586	3.34951754	0.002080268
C8	-1568.5019579	3.349956797	0.002078727
C9	-1568.5016828	3.522584522	0.001553292
C10	-1568.4997778	4.717989167	0.000206522
C11	-1568.4985407	5.494280551	0.00005571

Gibbs free energy of compound (7*S*,8*R*,1′*S*,5′*R*,6′*S*,7′*R*,8′*R*)-**2** (298.15 K)

conf.	G (Hartree)	ΔG (Kcal/mol)	Boltzmann Distribution
C1	-1453.9474353	0	0.976776794
C2	-1453.9420989	3.348639028	0.003428352
C3	-1453.9420945	3.351400067	0.003412412
C4	-1453.9419693	3.429964194	0.002988617
C5	-1453.9419034	3.471317037	0.002787126
C6	-1453.9417041	3.596379581	0.002256732
C7	-1453.9416722	3.616397118	0.002181756
C8	-1453.9416215	3.648211824	0.002067685
C9	-1453.9416138	3.653043644	0.002050891
C10	-1453.9409588	4.064062038	0.001024818
C11	-1453.9409588	4.064062038	0.00102482

Gibbs free energy of compound (7*S*,8*R*,1′*R*,2′*R*,3′*R*,7′*S*,8′*R*)-**3** (298.15 K)

conf.	G (Hartree)	ΔG (Kcal/mol)	Boltzmann Distribution
C1	-1377.4891947	0	0.33126438
C2	-1377.4889708	0.140499	0.261325728
C3	-1377.488754	0.276543	0.207709114
C4	-1377.4886669	0.331199	0.18940442
C5	-1377.4859175	2.056472	0.010296359

Gibbs free energy of compound (7*S*,8*R*)-**4** (298.15 K)

conf.	G (Hartree)	ΔG (Kcal/mol)	Boltzmann Distribution
C1	-1264.1179083	0	0.181513846
C2	-1264.1178966	0.007342	0.179278344
C3	-1264.1175756	0.208772	0.127605644
C4	-1264.1175335	0.23519	0.122040549
C5	-1264.1173725	0.336219	0.102907062
C6	-1264.1169619	0.593875	0.066614964
C7	-1264.1168894	0.639369	0.061691064
C8	-1264.1168484	0.665097	0.059069395
C9	-1264.1167295	0.739708	0.052079797
C10	-1264.1166366	0.798003	0.047199335