Electronic Supplementary Material (ESI) for RSC Advances.

Isolation of lingzhifuran A and lingzhilactones D-F from *Ganoderma lucidum* as specific Smad3 phosphorylation inhibitors and total synthesis of lingzhifuran A

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[d] *Laboratory of Molecular Engineering and Laboratory of Natural Product Synthesis, Guangzhou Institutes of Biomedicine and Health, Chinese Academy of Sciences, Guangzhou, 510530, People's Republic of China*

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Contents of Supplementary Information

Ⅰ. The NMR, HREIMS, and UV spectra of natural lingzhifuran A (1).

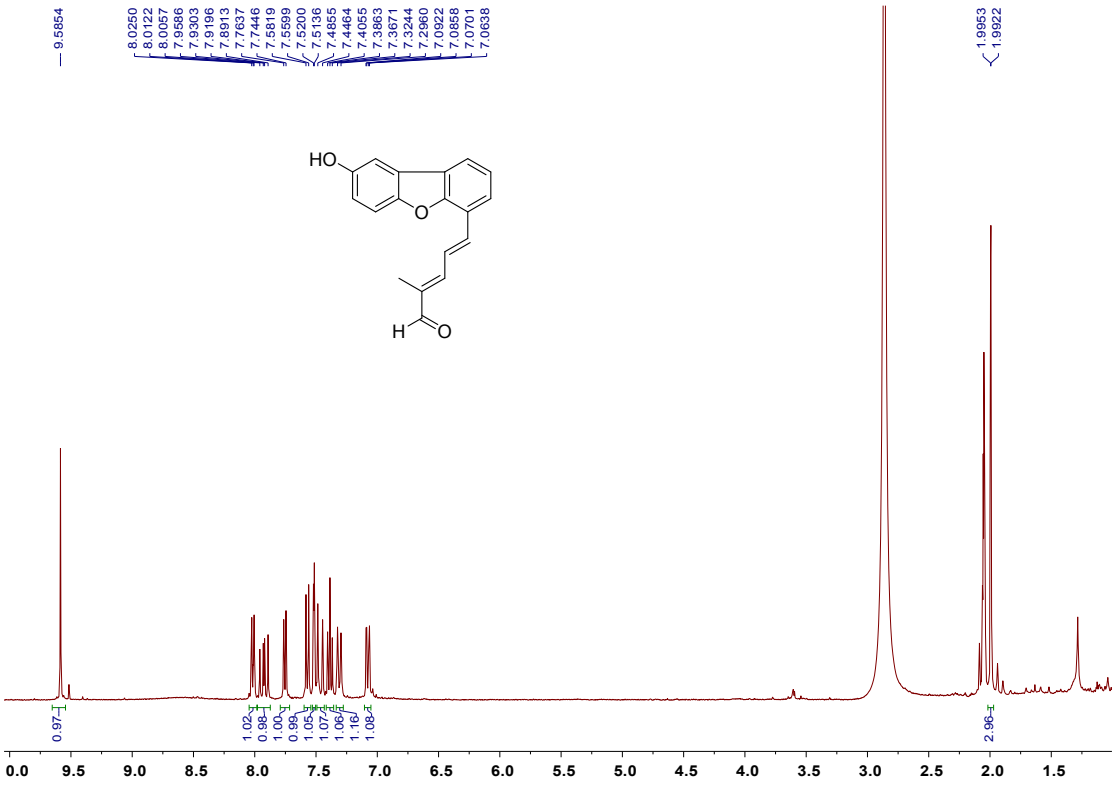


Figure S1. The ^{1}H NMR spectrum (acetone-d_6, 400 MHz) of **1**.

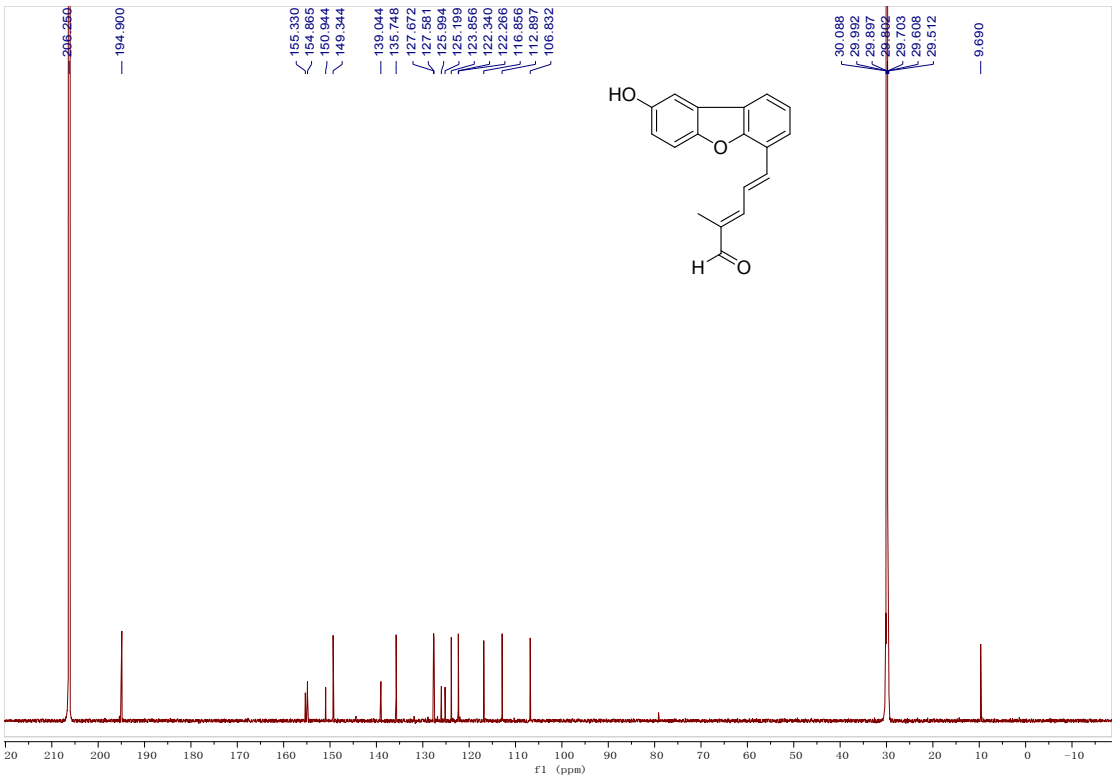


Figure S2. The ^{13}C NMR spectrum (acetone-d_6, 200 MHz) of **1**.

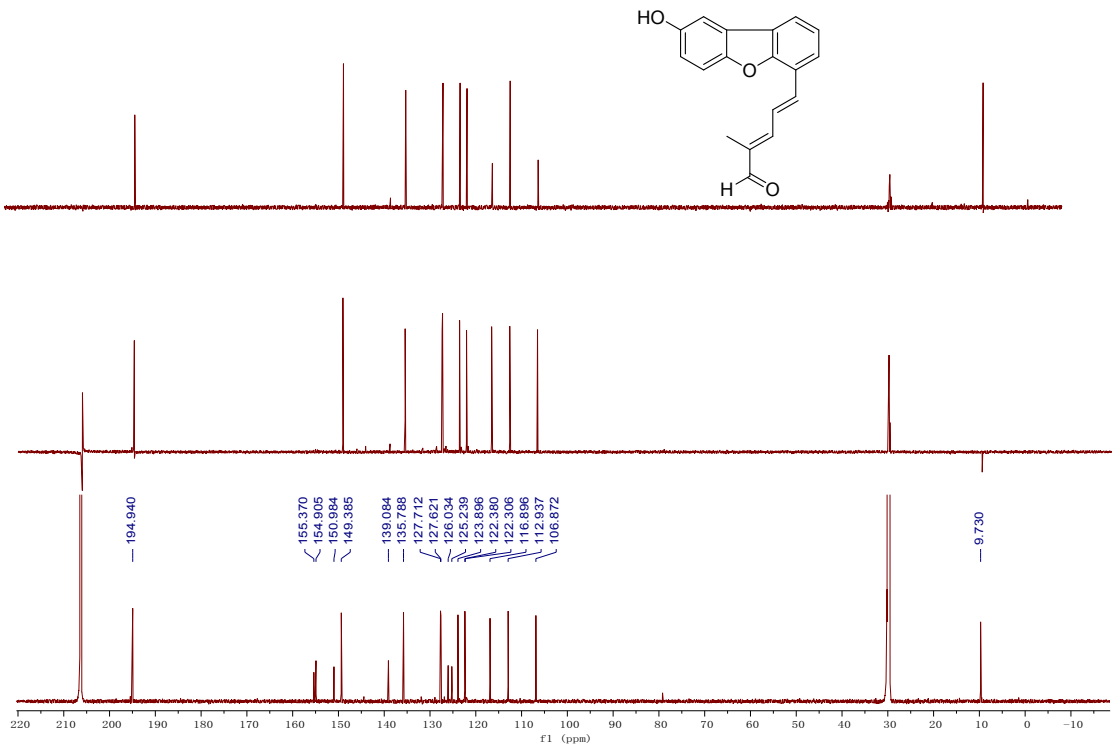


Figure S3. The DEPT spectra (acetone-d_6, 200 MHz) of **1**.

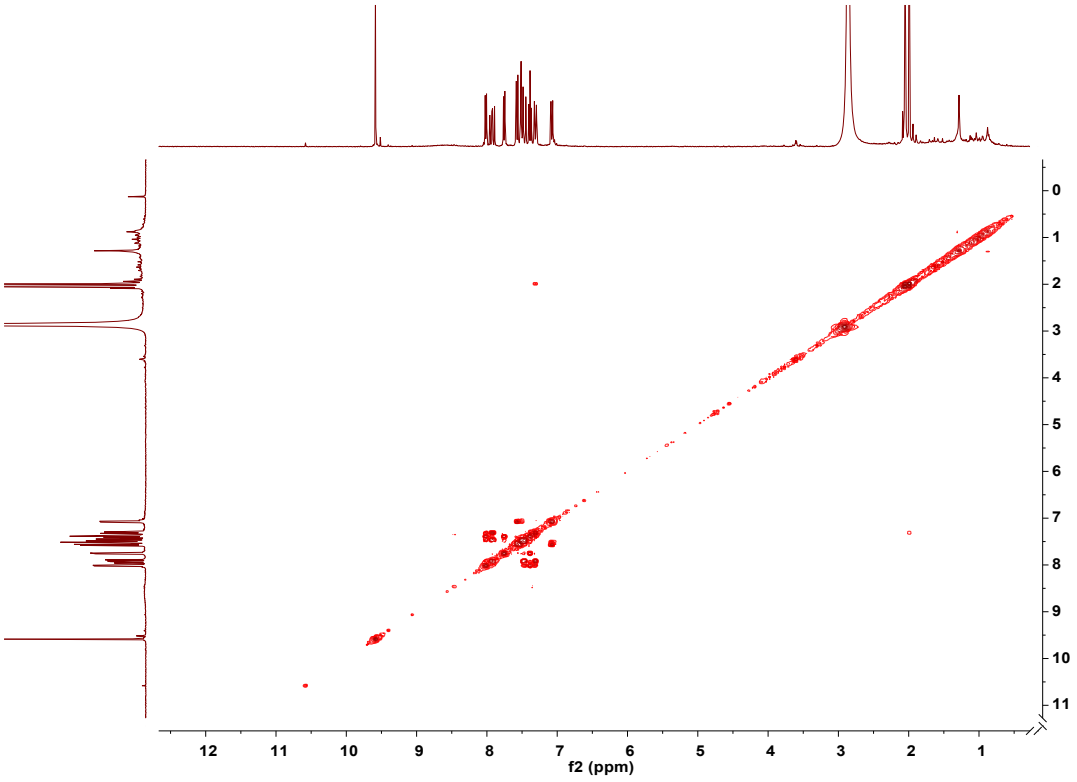


Figure S4. The ^{1}H-^{1}H COSY spectrum (acetone-d_6, 800 MHz) of **1**.

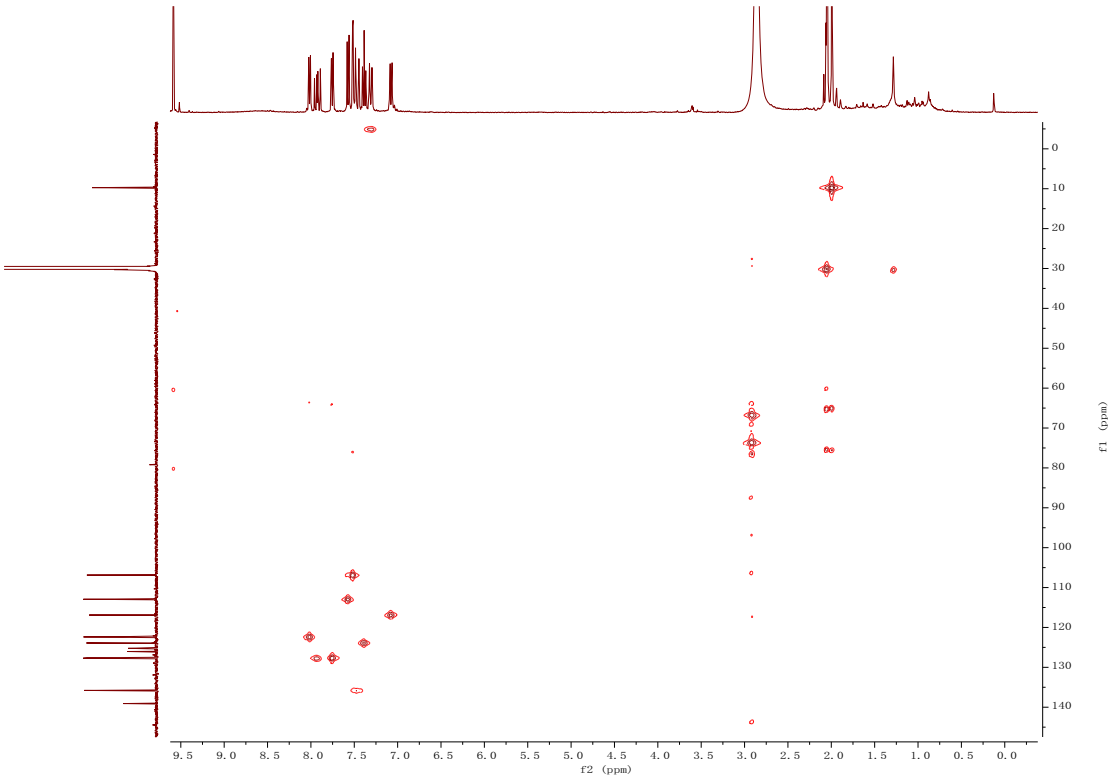


Figure S5. The HMQC spectrum (acetone-d_6, 800 MHz) of **1**.

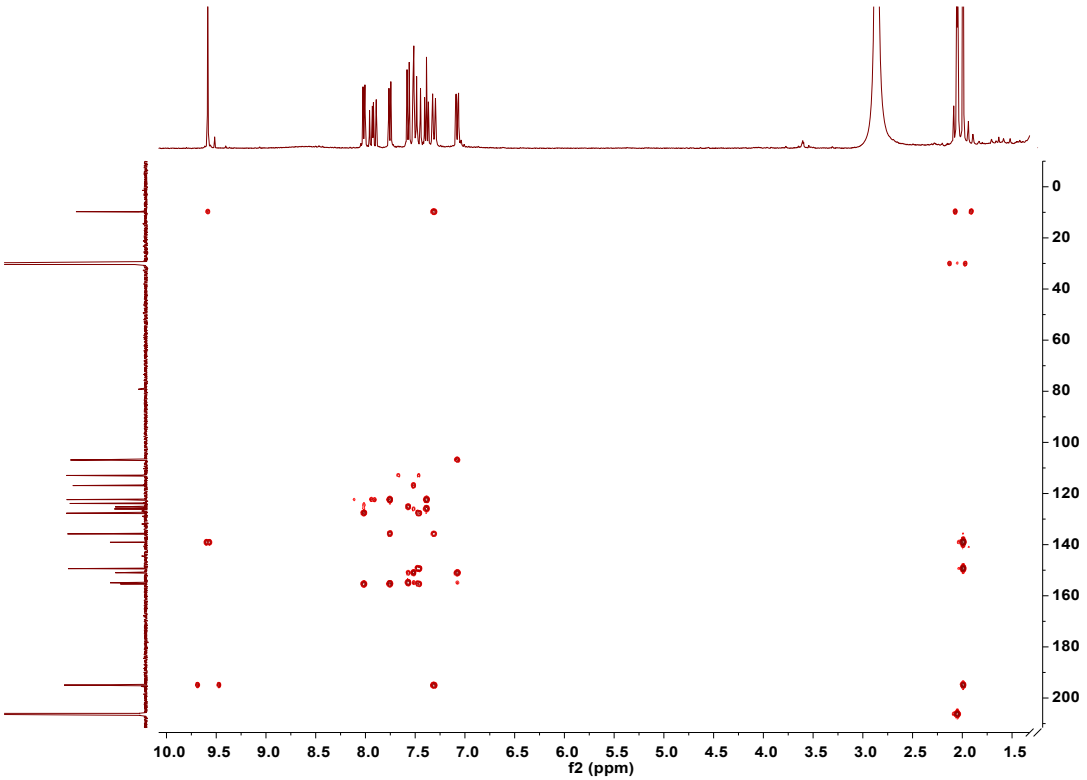


Figure S6. The HMBC spectrum (acetone-d_6, 800 MHz) of **1**.

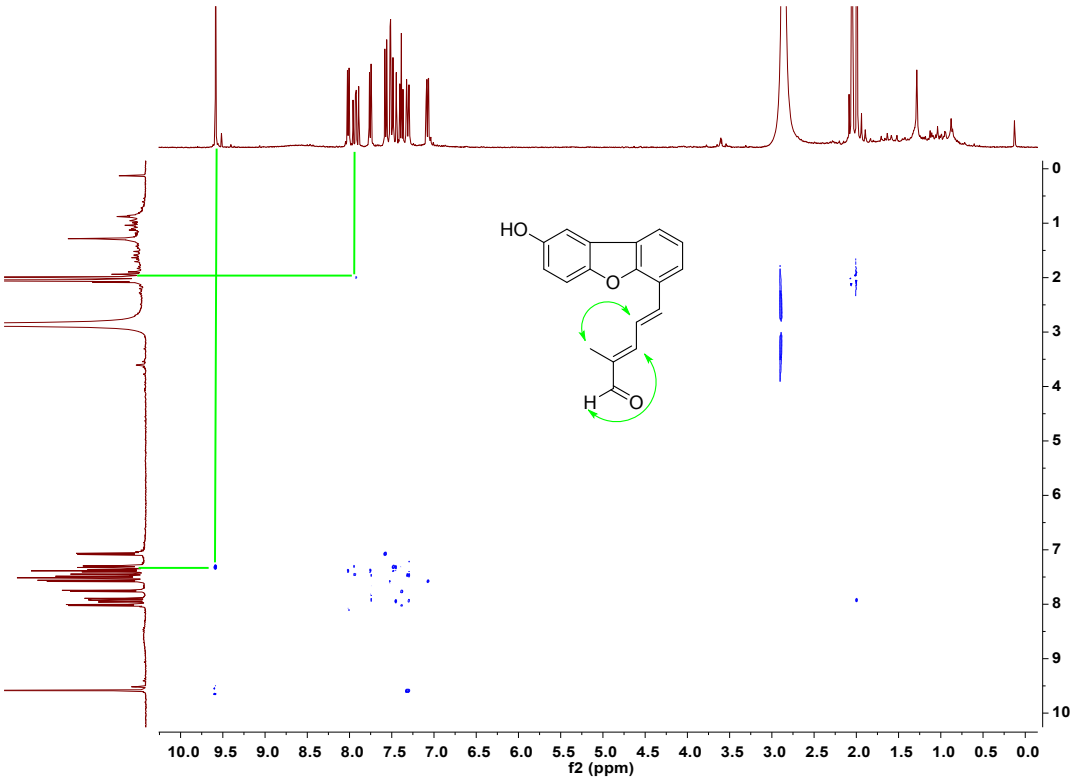


Figure S7. The ROESY spectrum (acetone-d_6, 800 MHz) of **1**.

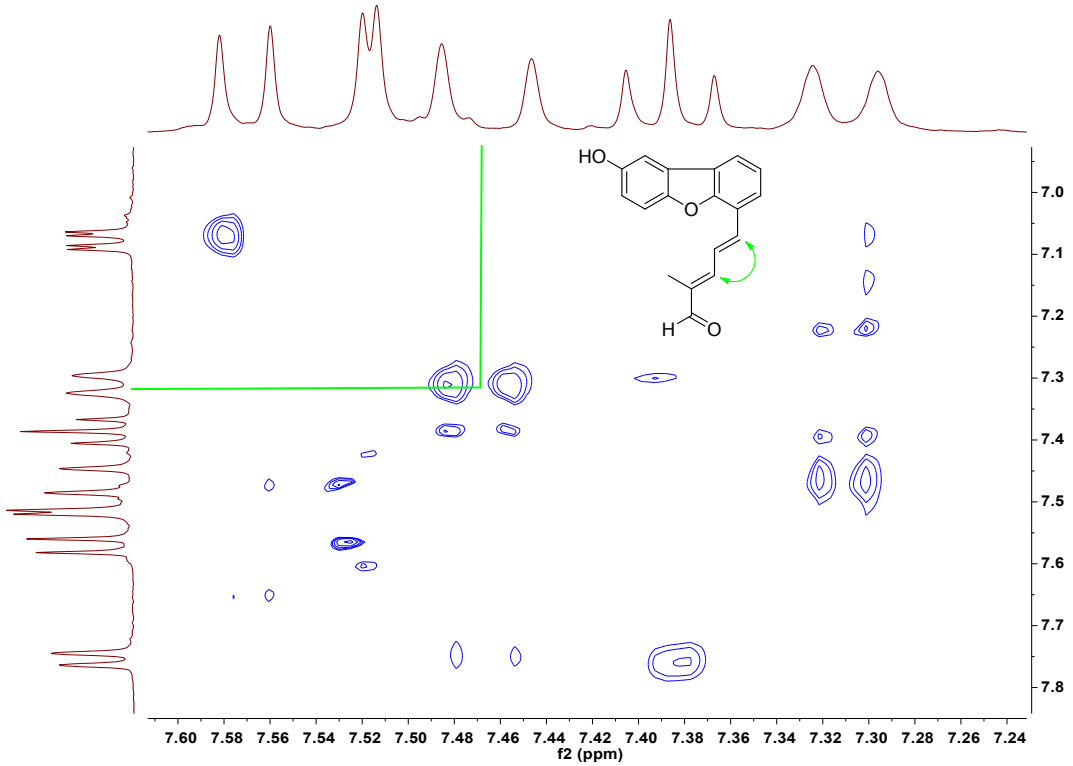
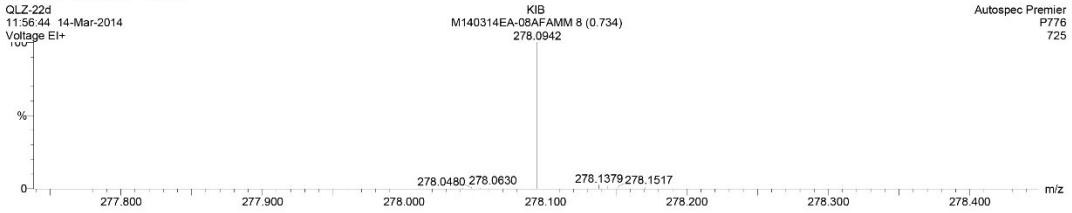


Figure S8. The enlarged ROESY spectrum (acetone-d_6, 800 MHz) of **1**.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
13 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: 3-5



Minimum:		200.0	10.0	-10.0		
Maximum:				120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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Figure S9. The HREI (positive) spectrum of **1**.

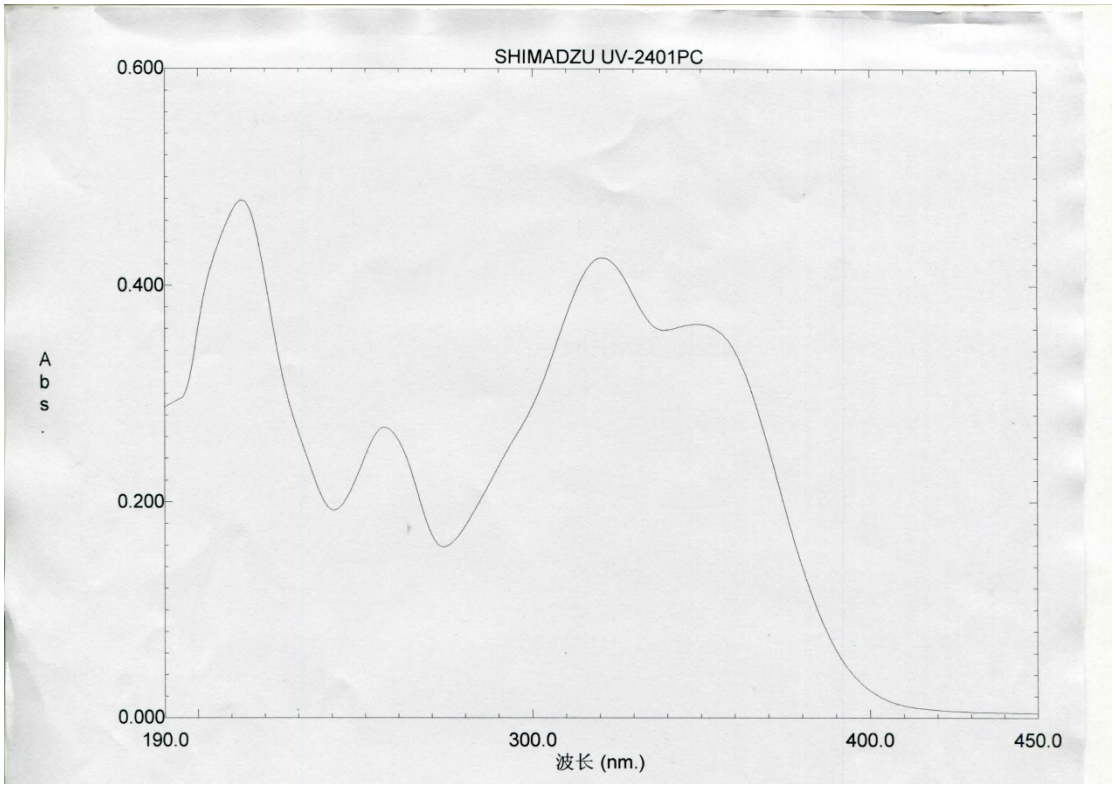


Figure S10. The UV spectrum (MeOH) of **1**.

Ⅱ. The NMR, HRESIMS and CD spectra of lingzhilactone D (2).

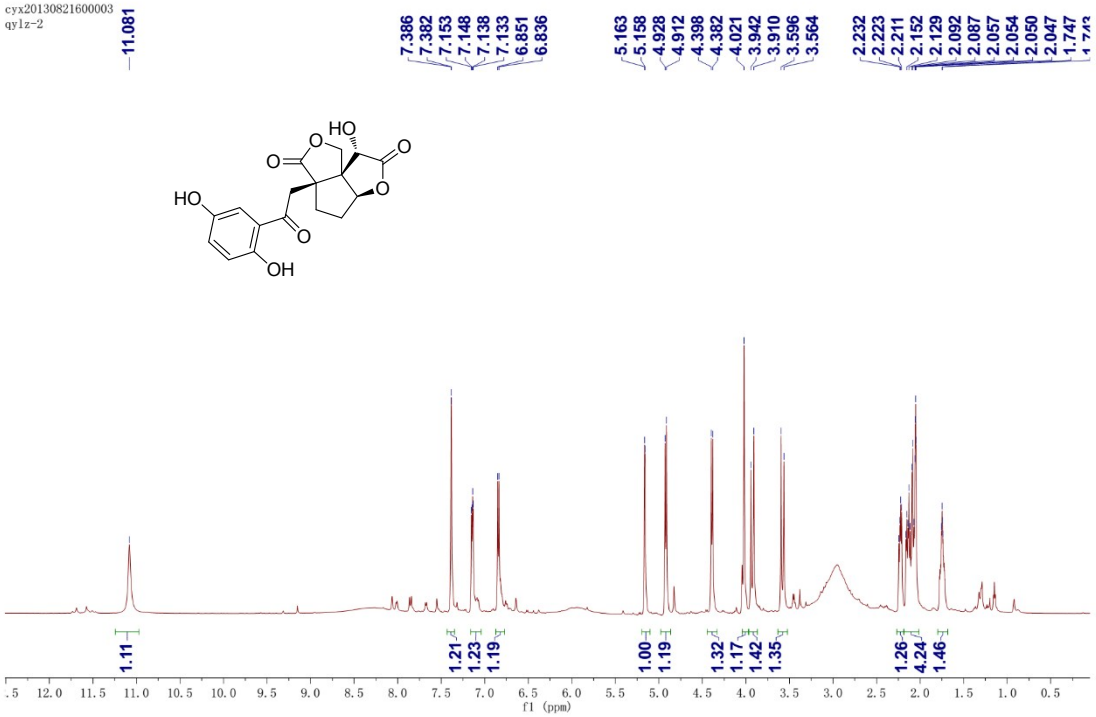


Figure S11. The ^{1}H NMR spectrum (acetone-d_6, 600 MHz) of **2**.

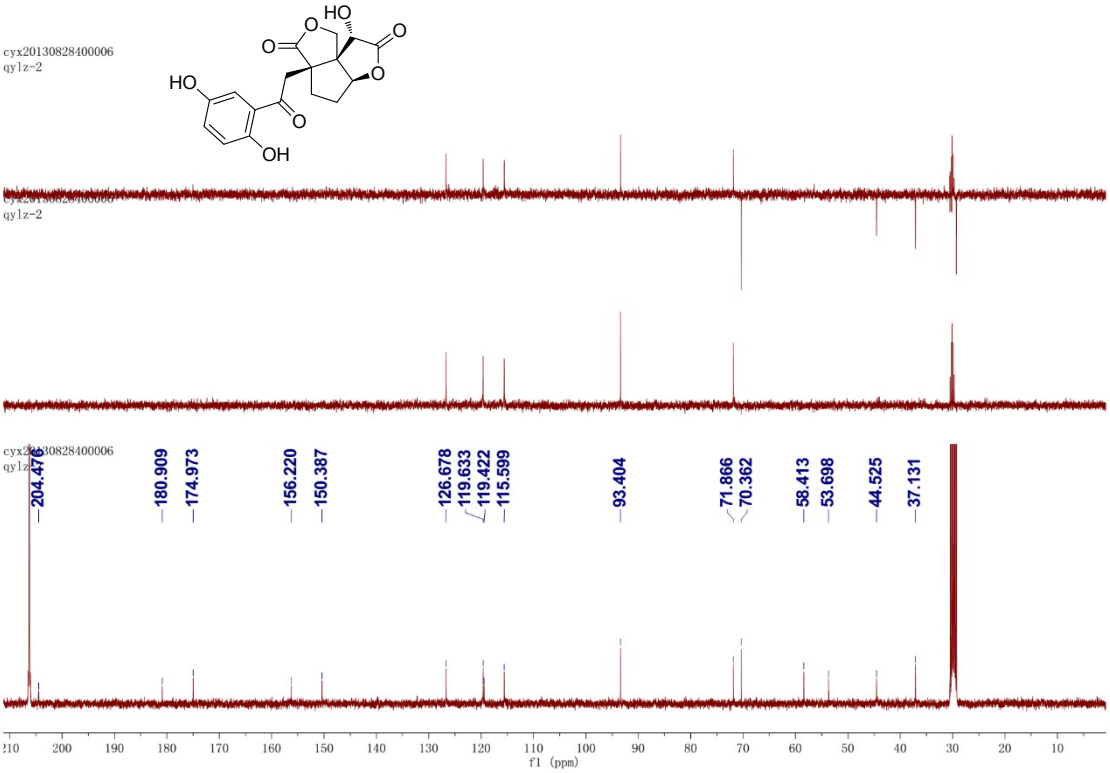


Figure S12. The DEPT spectra (acetone-d_6, 150 MHz) of **2**.

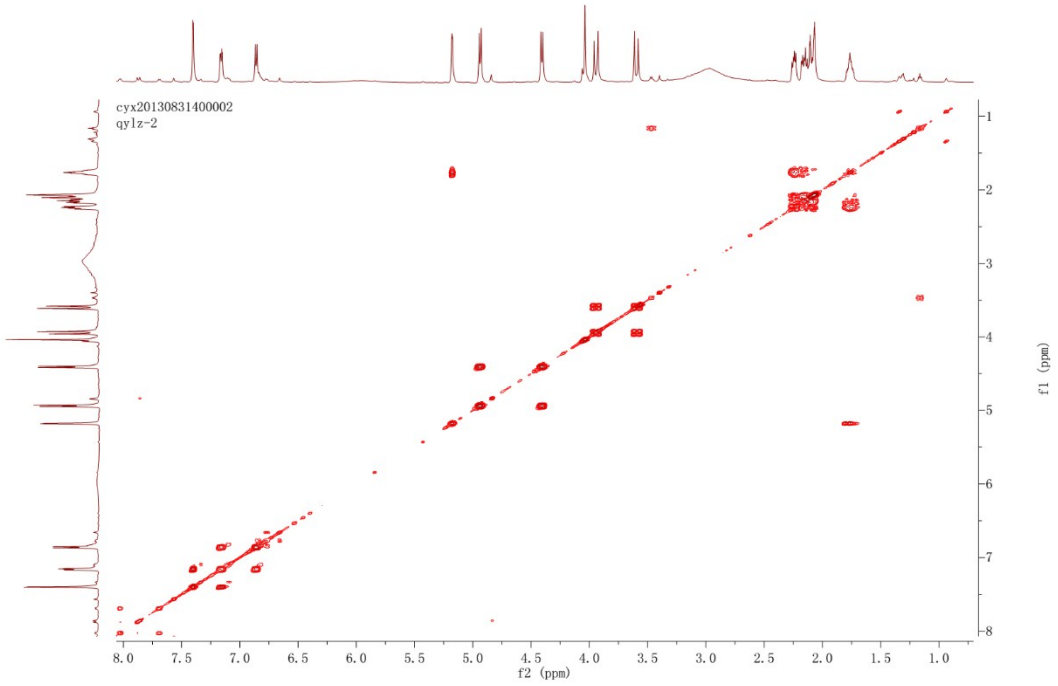


Figure S13. The ^{1}H-^{1}H COSY spectrum (acetone-d_6, 600 MHz) of **2**.

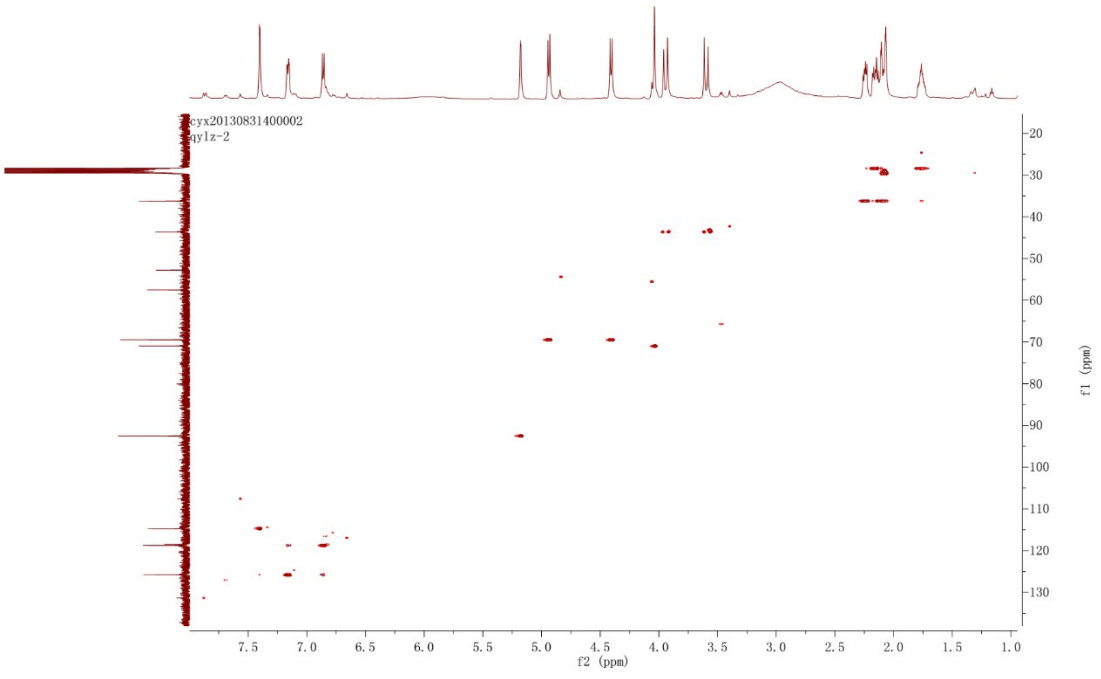


Figure S14. The HSQC spectrum (acetone-d_6, 600 MHz) of **2**.

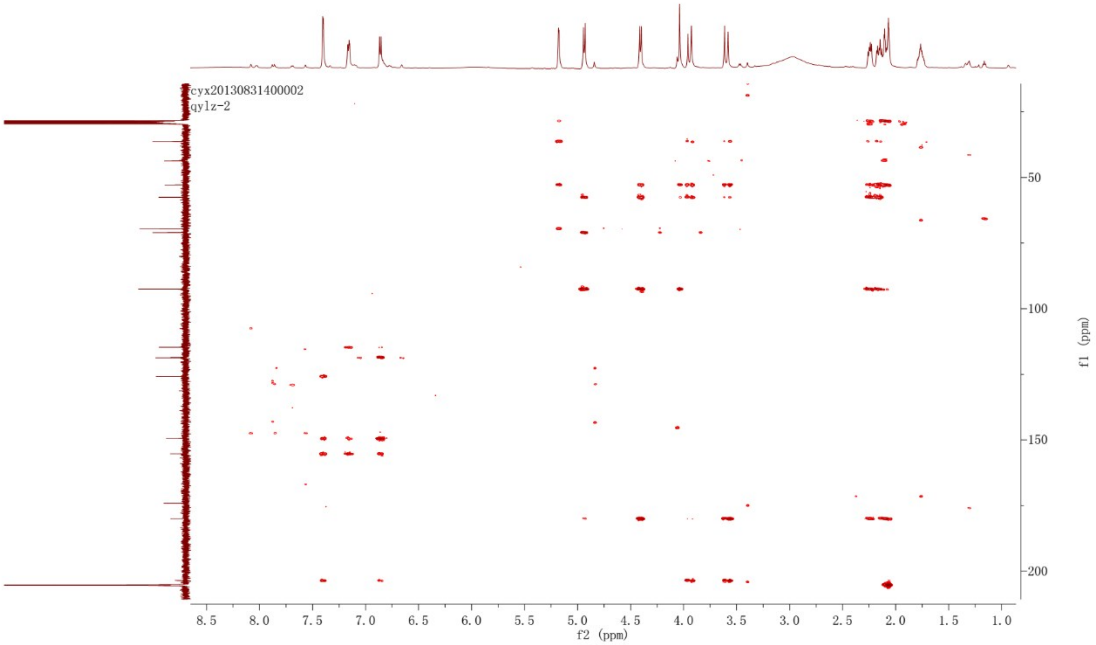


Figure S15. The HMBC spectrum (acetone-d_6, 600 MHz) of **2**.

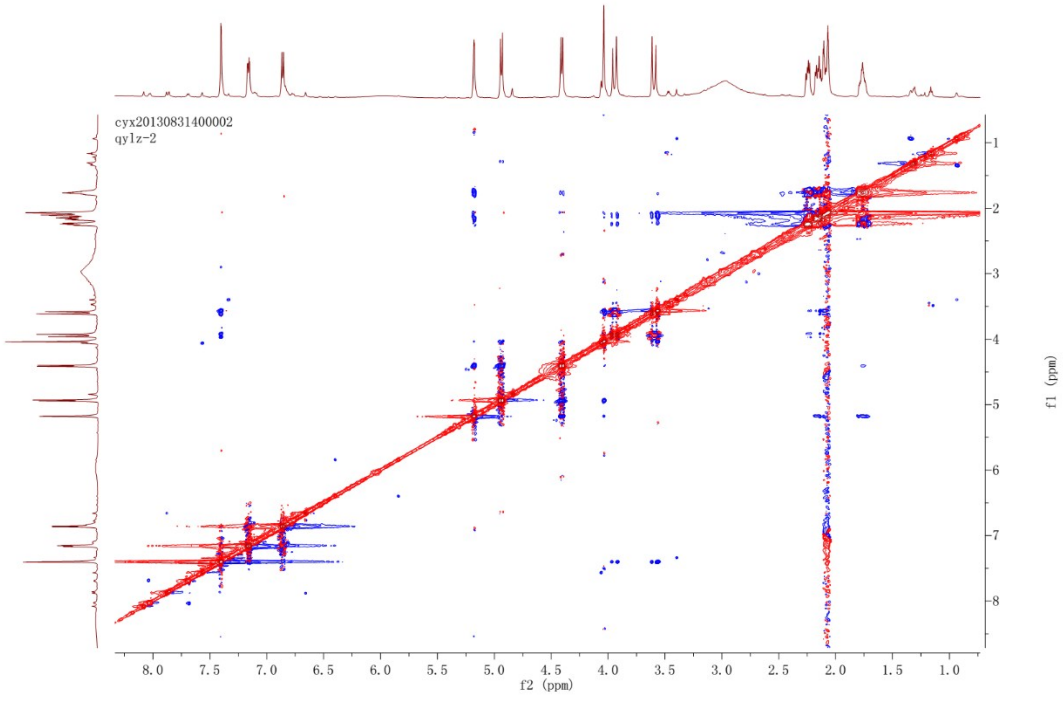


Figure S16. The ROESY spectrum (acetone-d_6, 600 MHz) of **2**.

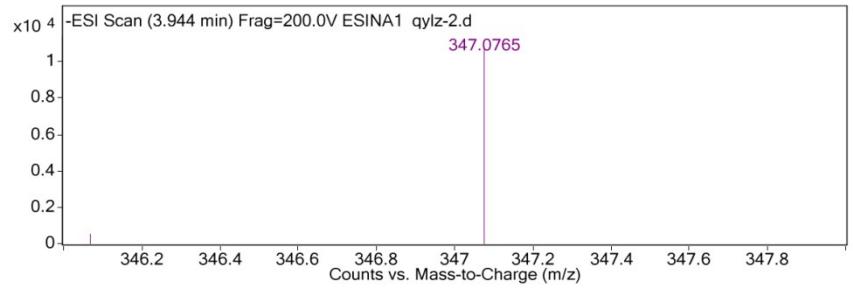
Qualitative Analysis Report

Data Filename	ESINA1 qylz-2.d	**Sample Name**	qylz-2
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESIN.m	**Acquired Time**	9/25/2013 12:18:11 PM
IRM Calibration Status	Success	**DA Method**	demo.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	9

Formula Calculator Results

Formula	Calculated Mass	Measured Mass	Diff. (mDa)	Diff. (ppm)	DBE
C17 H15 O8	347.0767	347.0760	0.7	2.1	10.5

--- End Of Report ---

Figure S17. HRESIMS (negative) spectrum of **2**.

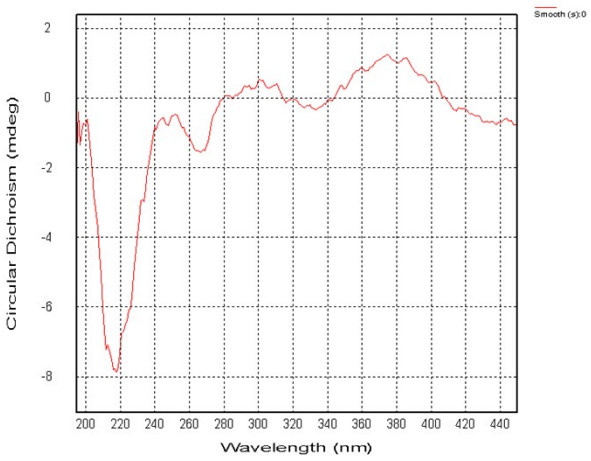


Figure S18. The experiment CD spectrum (+)-(**2**).

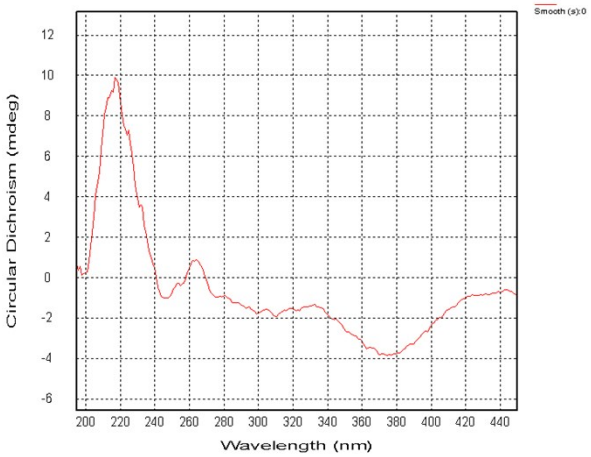


Figure S19. The experiment CD spectrum (–)-(**2**).

Ⅲ. The NMR, HRESIMS and CD spectra of lingzhilactone E (3).

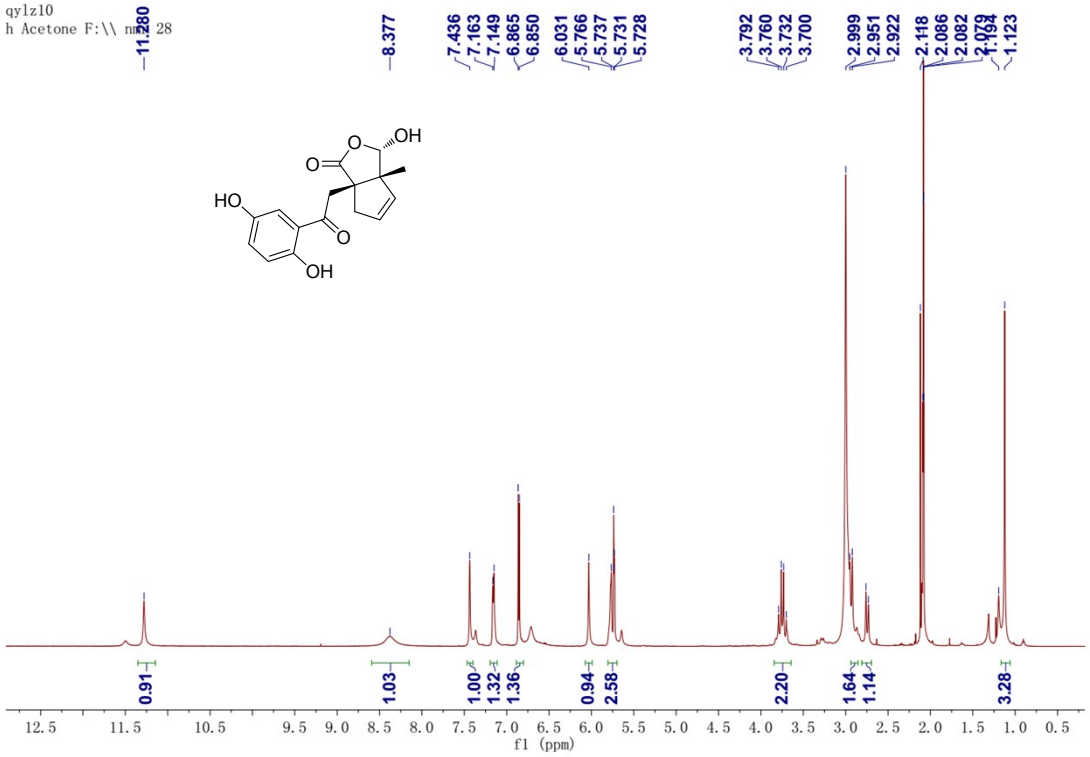


Figure S20. The ^{1}H NMR spectrum (acetone-d_6, 600 MHz) of **3**.

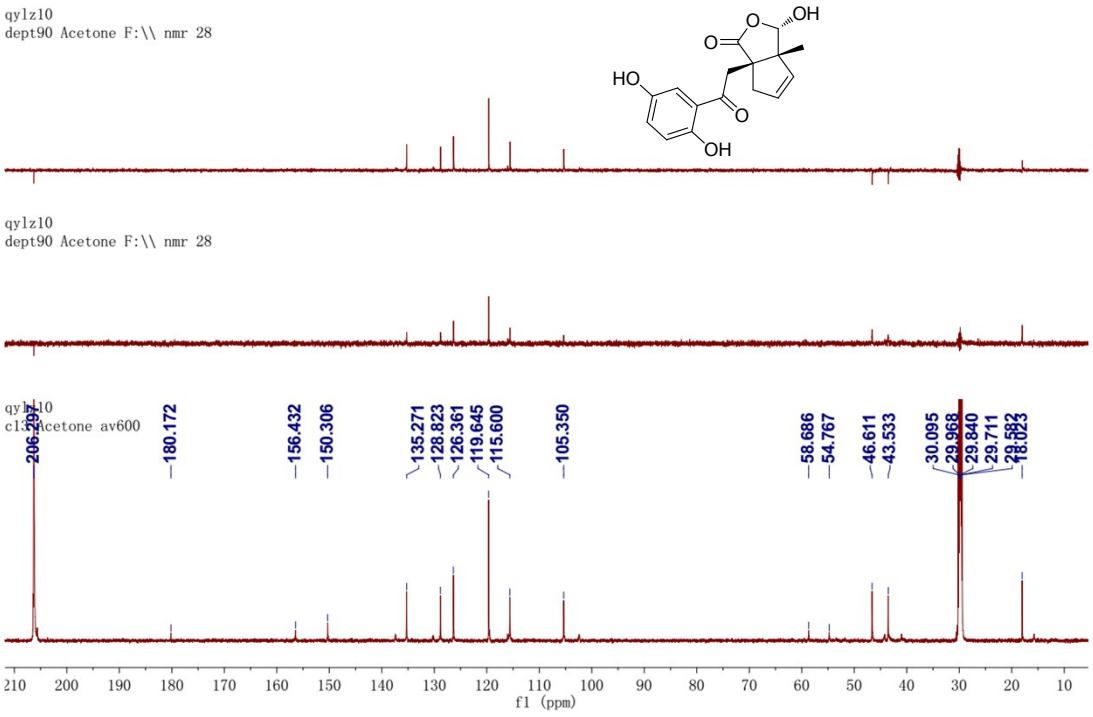


Figure S21. The DEPT spectra (acetone-d_6, 150 MHz) of **3**.

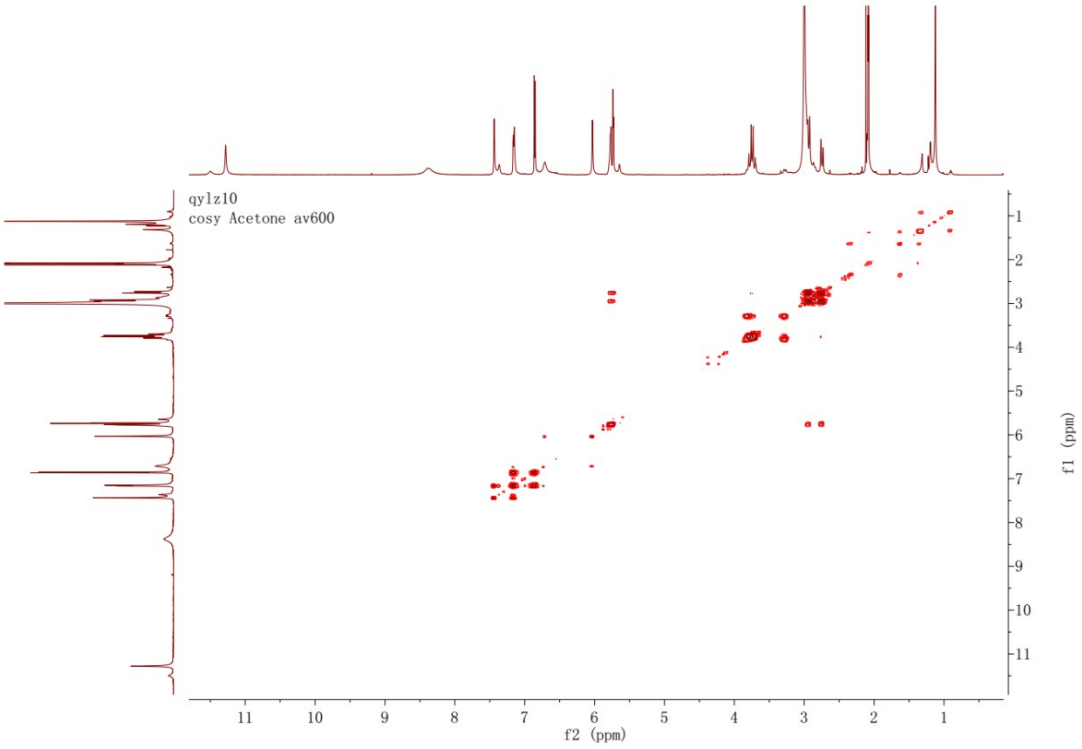


Figure S22. The ^{1}H-^{1}H COSY spectrum (acetone-d_6, 600 MHz) of **3**.

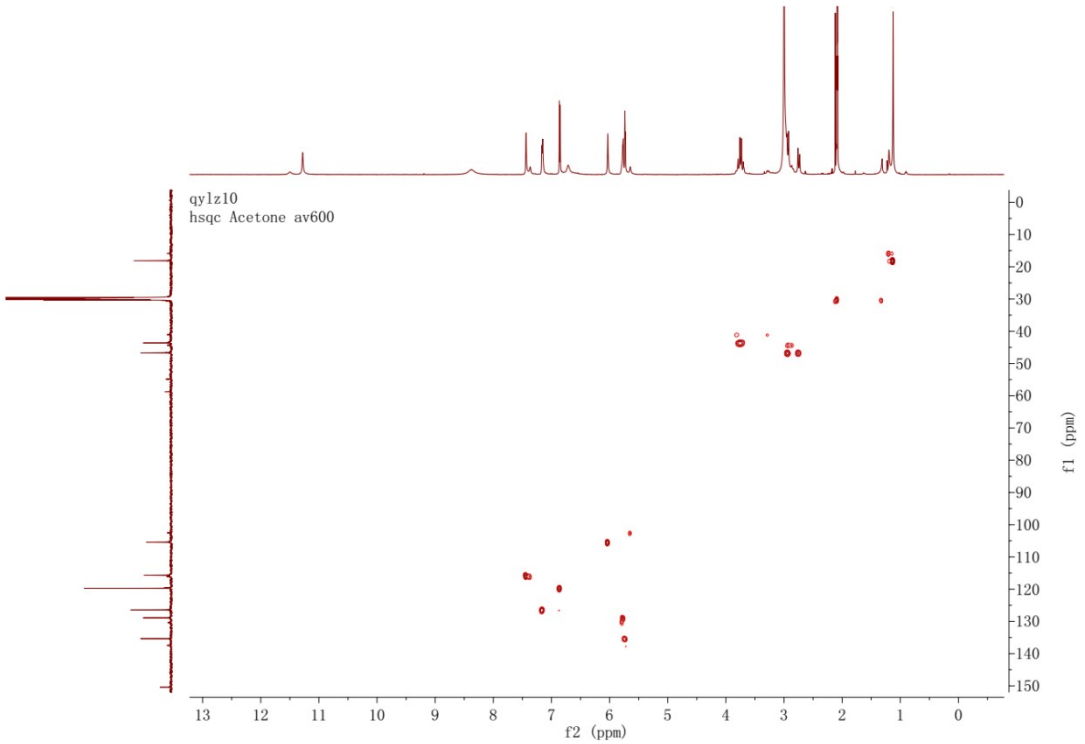


Figure S23. The HSQC spectrum (acetone-d_6, 600 MHz) of **3**.

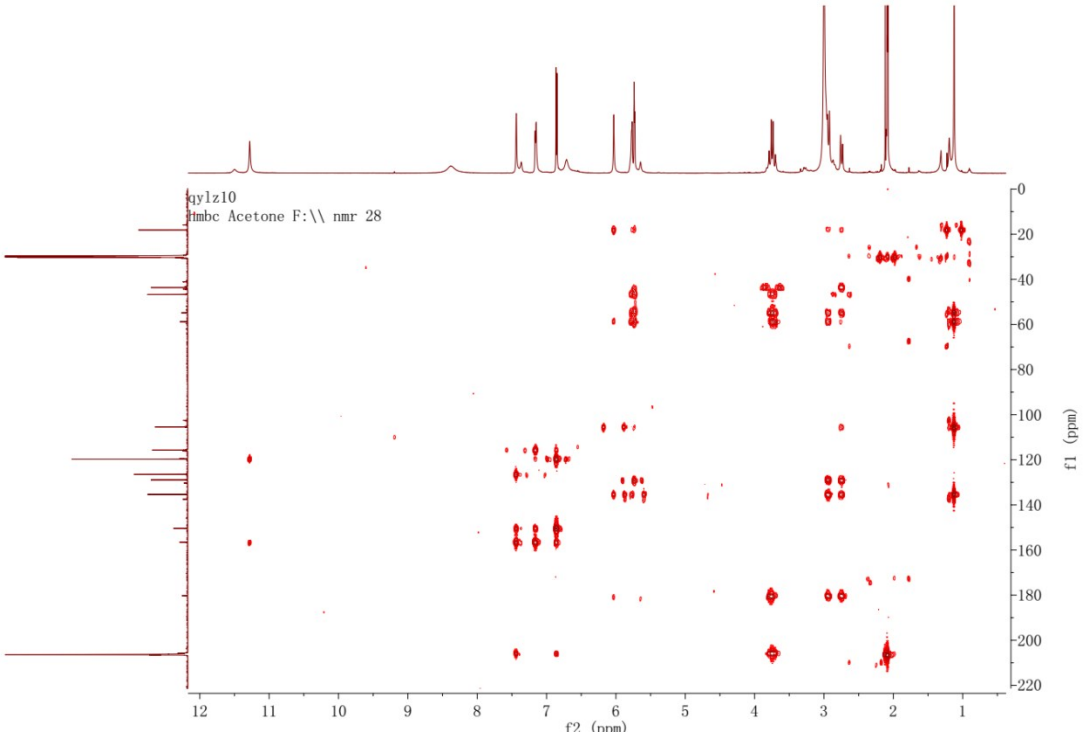


Figure S24. The HMBC spectrum (acetone-d_6, 600 MHz) of **3**.

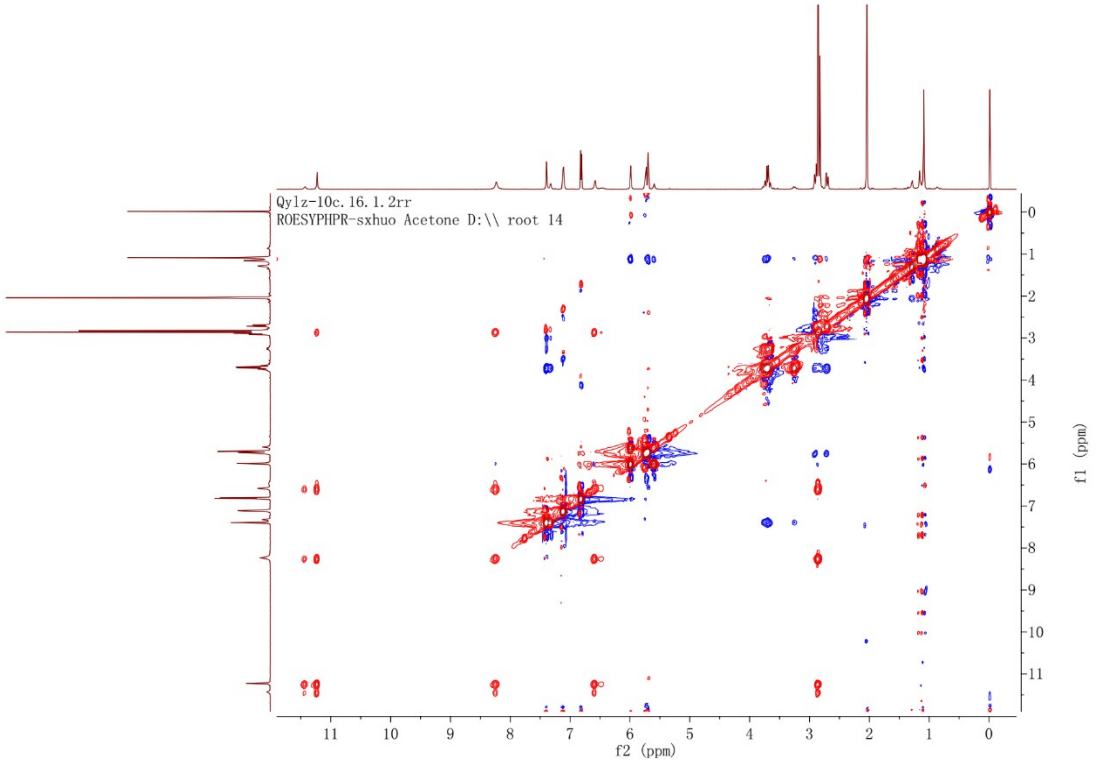


Figure S25. The ROESY spectrum (acetone-d_6, 600 MHz) of **3**.

Qualitative Analysis Report

Data Filename	Qylz-10c.d	**Sample Name**	Qylz-10c
Sample Type	Sample	**Position**	P1-C4
Instrument Name	Instrument 1	**User Name**	
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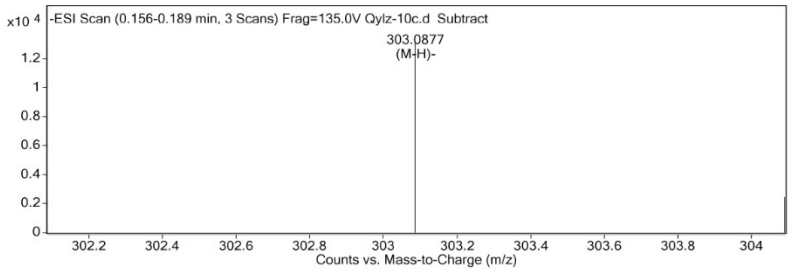
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

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68.9958		1350.24		
112.9856	1	10002.41		
201.0556	1	2158.59		
259.0977	1	1117.12		
303.0877	1	13112.16	C16 H16 O6	(M-H)-
304.0911	1	2398.74	C16 H16 O6	(M-H)-
417.0798	1	2817.1		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C16 H16 O6	304.0947	303.0874	303.0877	-0.3	-0.8	9.0000

--- End Of Report ---

Figure S26. The HRESIMS (negative) spectrum of **3**.

Ⅳ. The NMR, HRESIMS and CD spectra of lingzhilactone F (4).

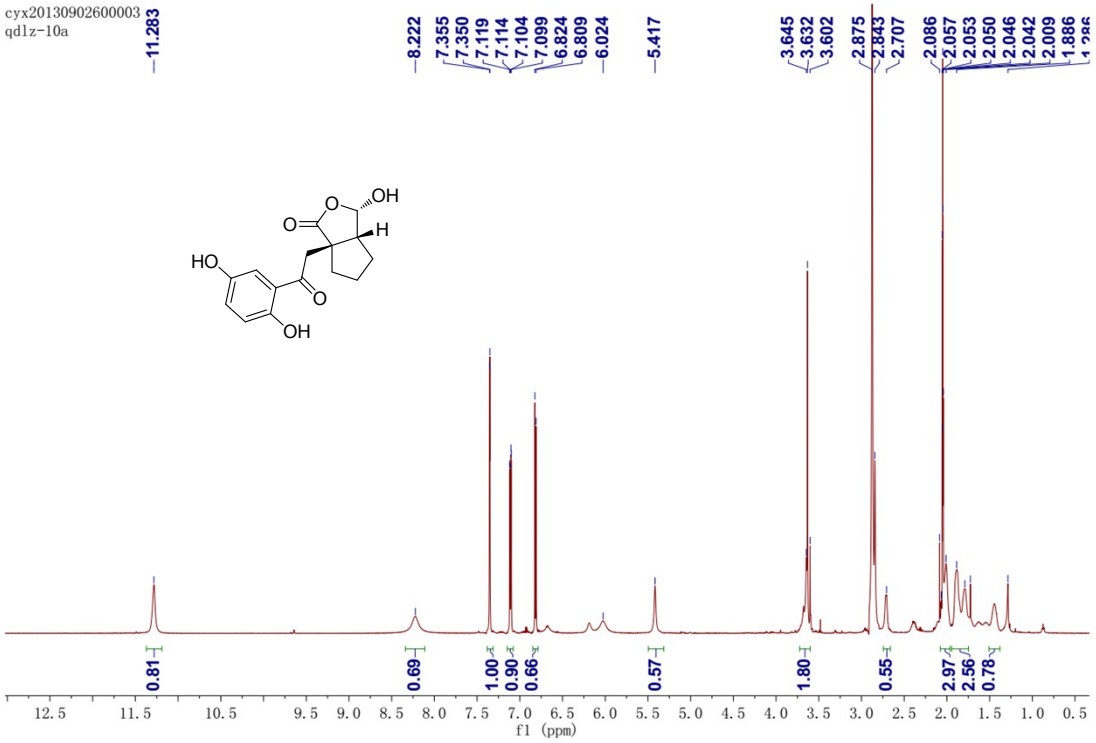


Figure S27. The ^{1}H NMR spectrum (acetone-d_6, 600 MHz) of **4**.

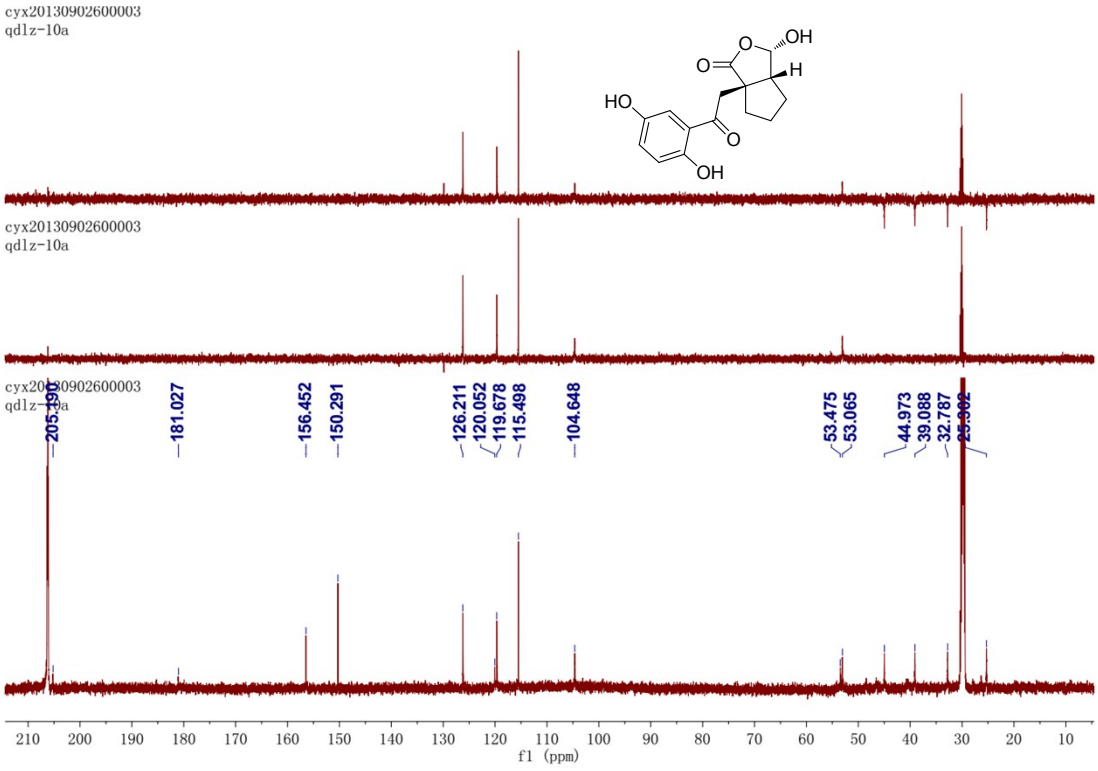


Figure S28. The DEPT spectra (acetone-d_6, 150 MHz) of **4**.

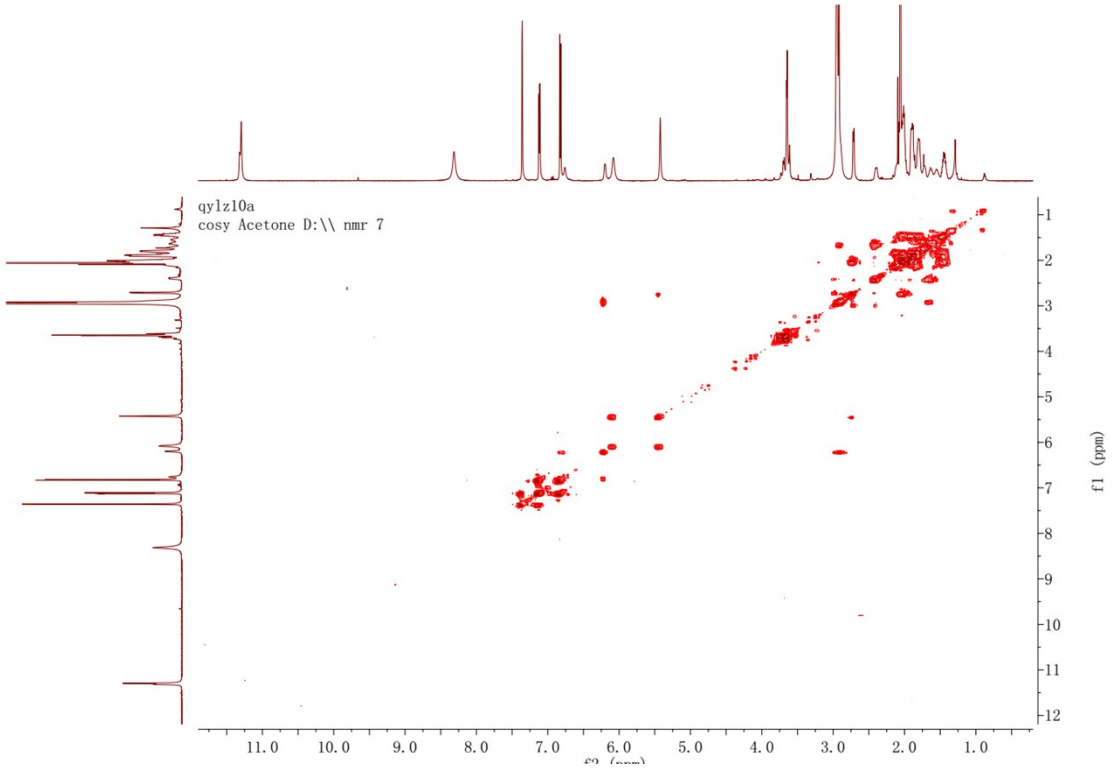


Figure S29. The ^{1}H-^{1}H COSY spectrum (acetone-d_6, 600 MHz) of **4**.

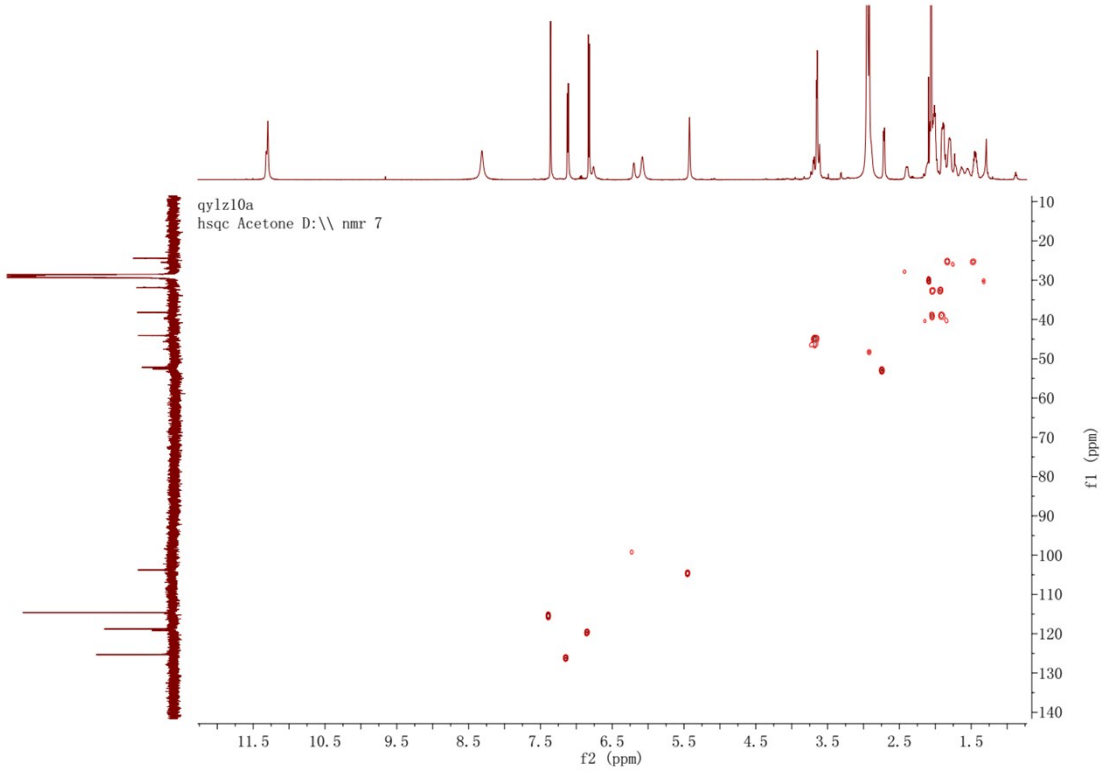


Figure S30. The HSQC spectrum (acetone-d_6, 600 MHz) of **4**.

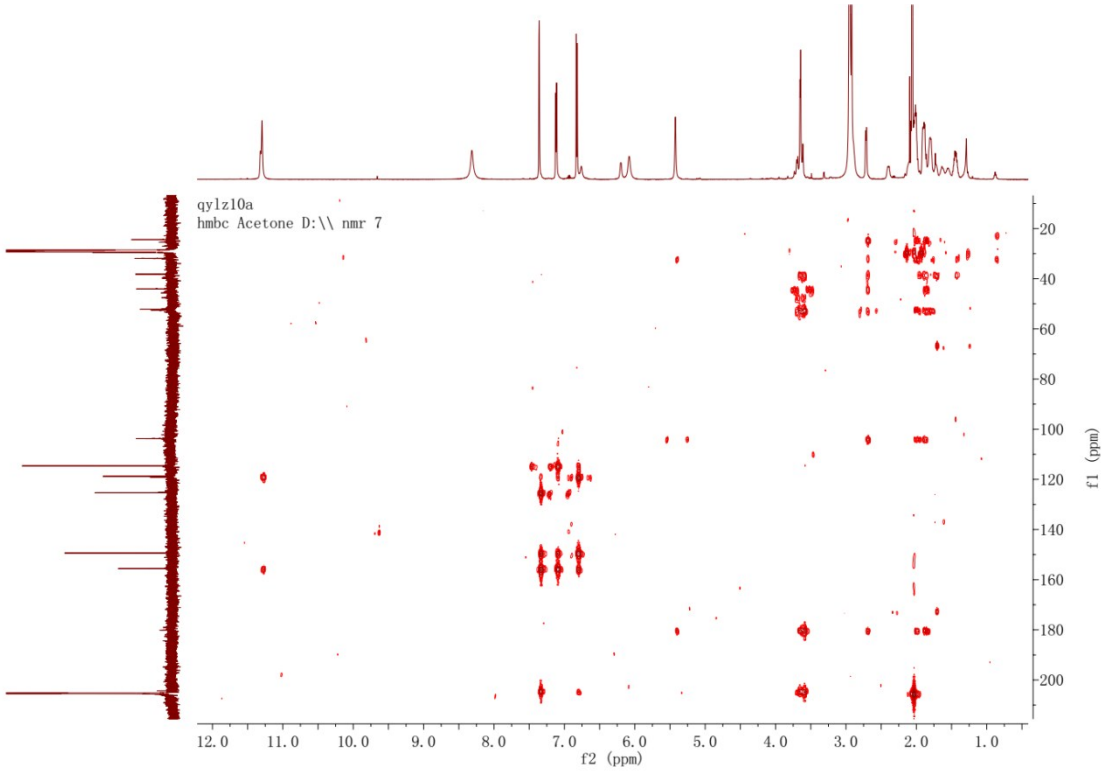


Figure S31. The HMBC spectrum (acetone-d_6, 600 MHz) of **4**.

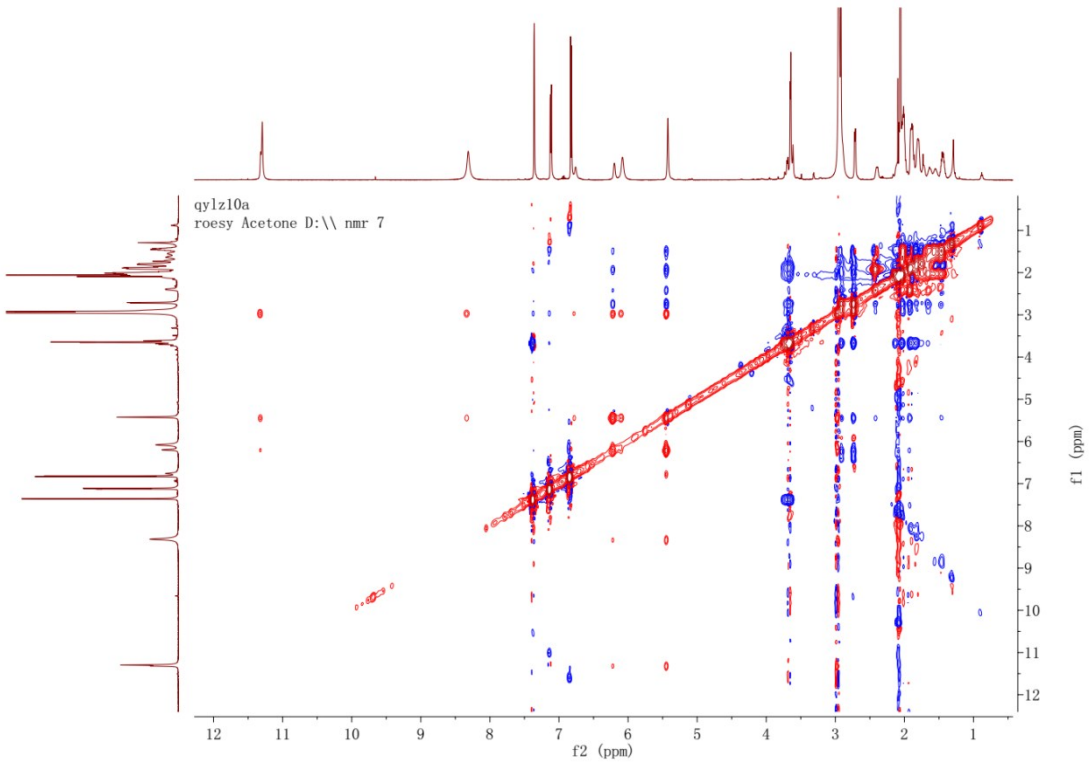


Figure S32. The ROESY spectrum (acetone-d_6, 600 MHz) of **4**.

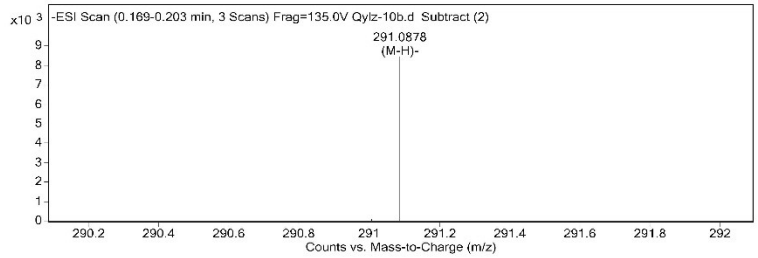
Qualitative Analysis Report

Data Filename	Qylz-10b.d	**Sample Name**	Qylz-10b
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU-ESI-i.m	**Acquired Time**	6/28/2016 3:48:06 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

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95.0502	1	1025.16		
112.9856		1370.31		
139.0401	1	6231		
151.0403		682.73		
291.0878	1	8447.57	C15 H16 O6	(M-H)-
292.0921	1	2117.58	C15 H16 O6	(M-H)-
405.0788	1	1053.73		
564.1878	1	1040.49		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H16 O6	292.0947	291.0874	291.0878	-0.6	-2.2	8.0000

--- End Of Report ---

Figure S33. The HRESIMS (negative) spectrum of **4**.

Ⅴ. The NMR spectra of synthetic intermediates 5-10.

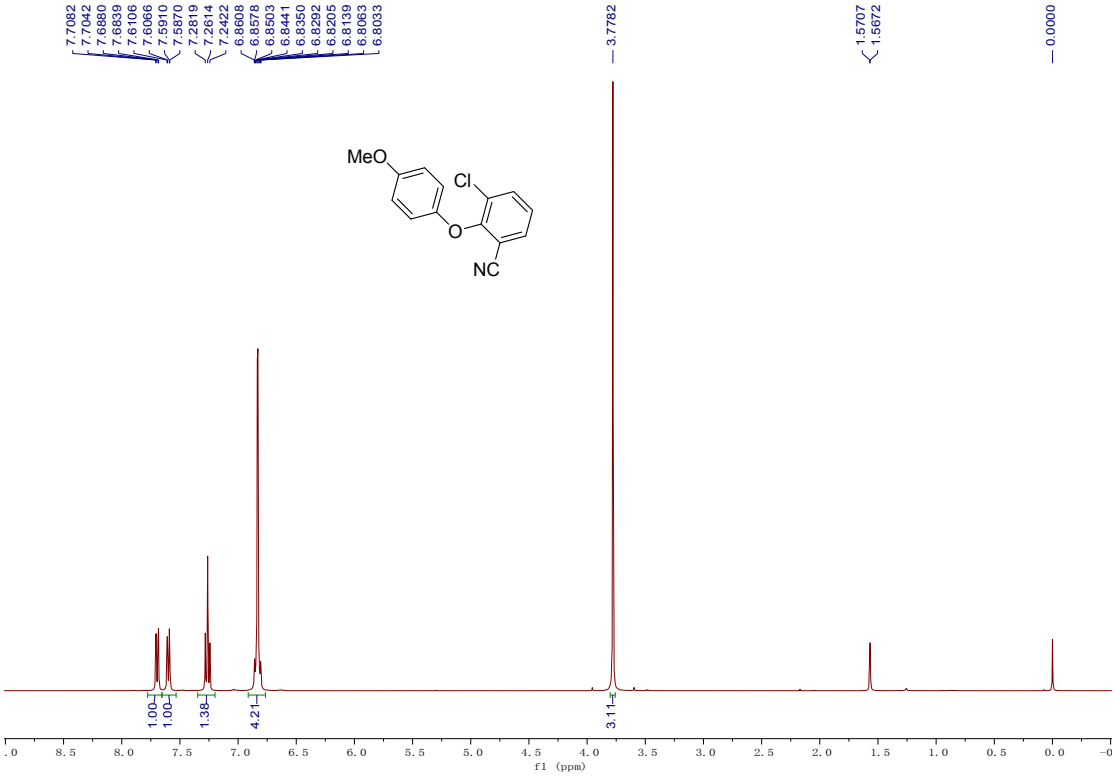


Figure S34. The ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of synthetic intermediate **6**.

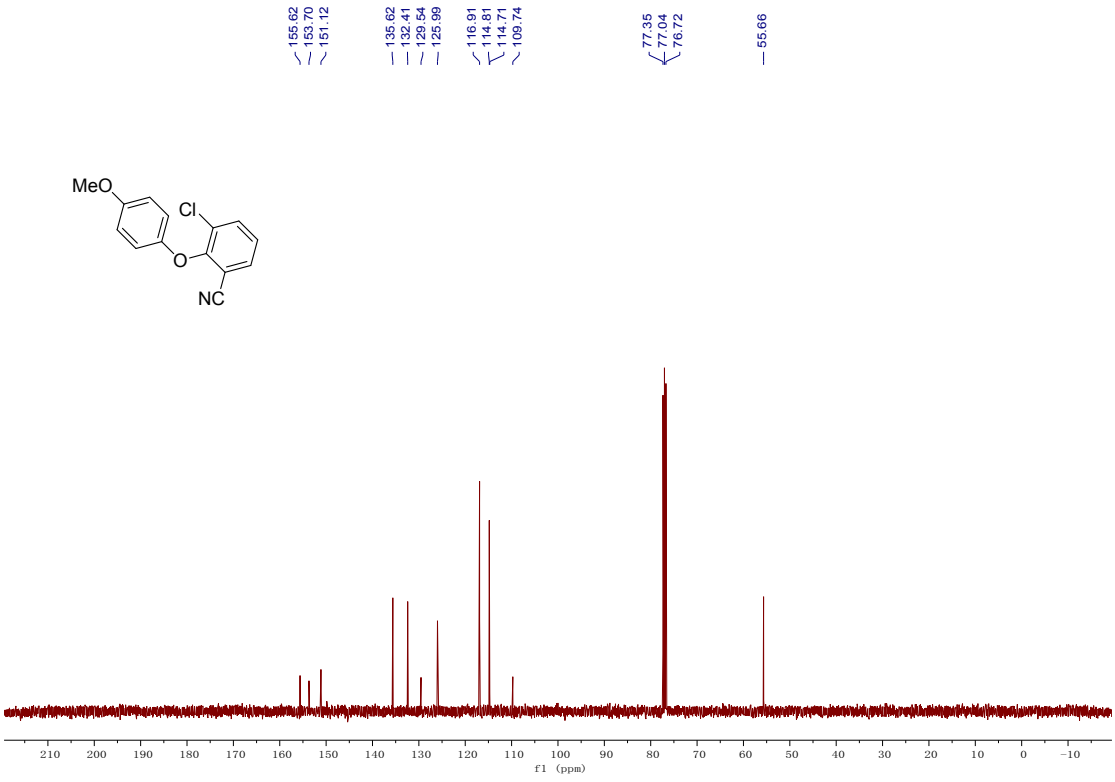


Figure S35. The ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of synthetic intermediate **6**.

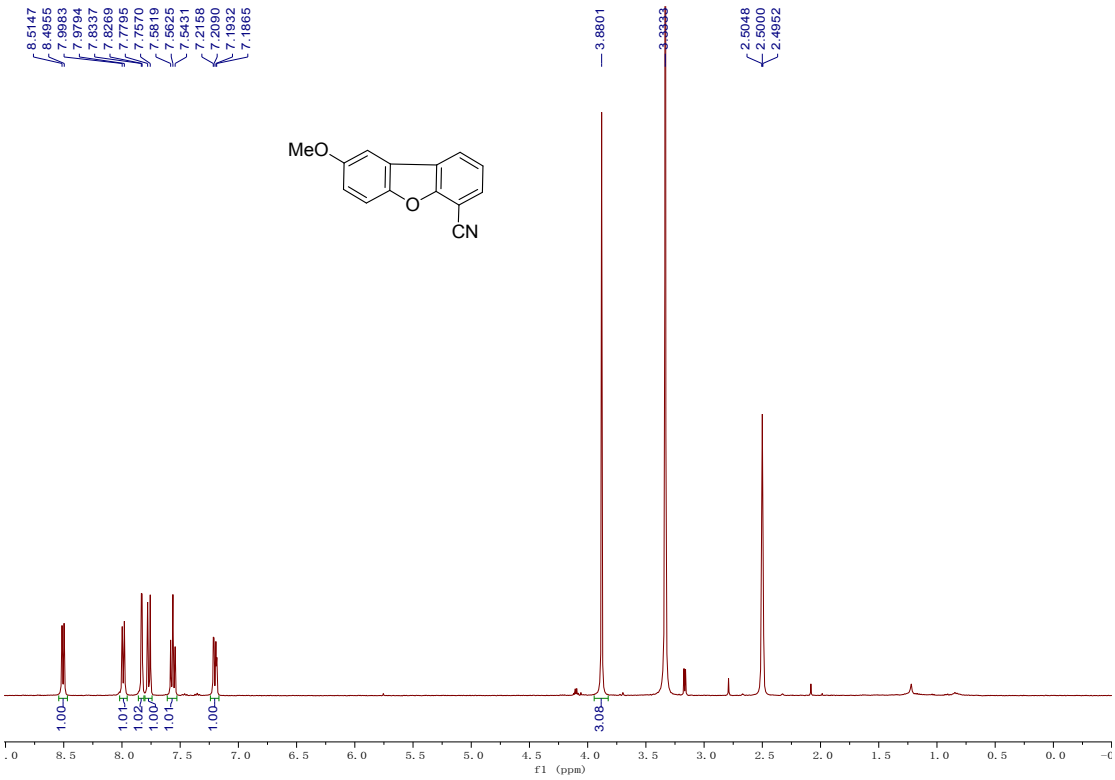


Figure S36. The ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of intermediate **7**.

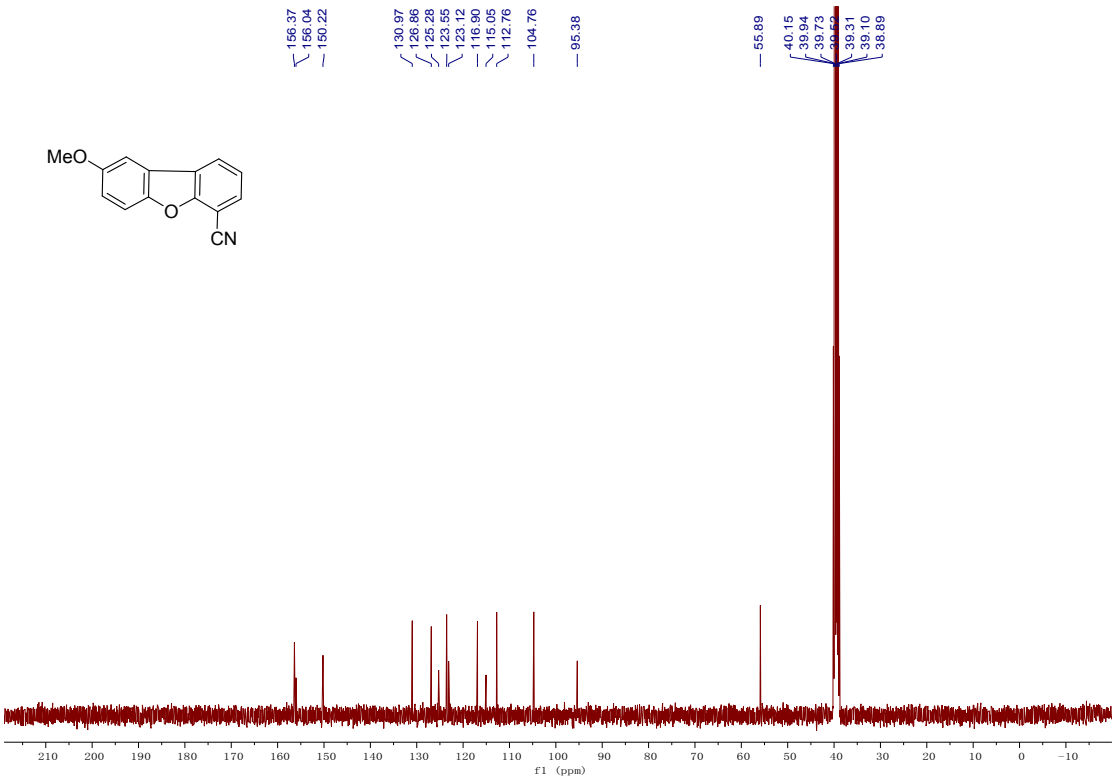


Figure S37. The ^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of intermediate **7**.

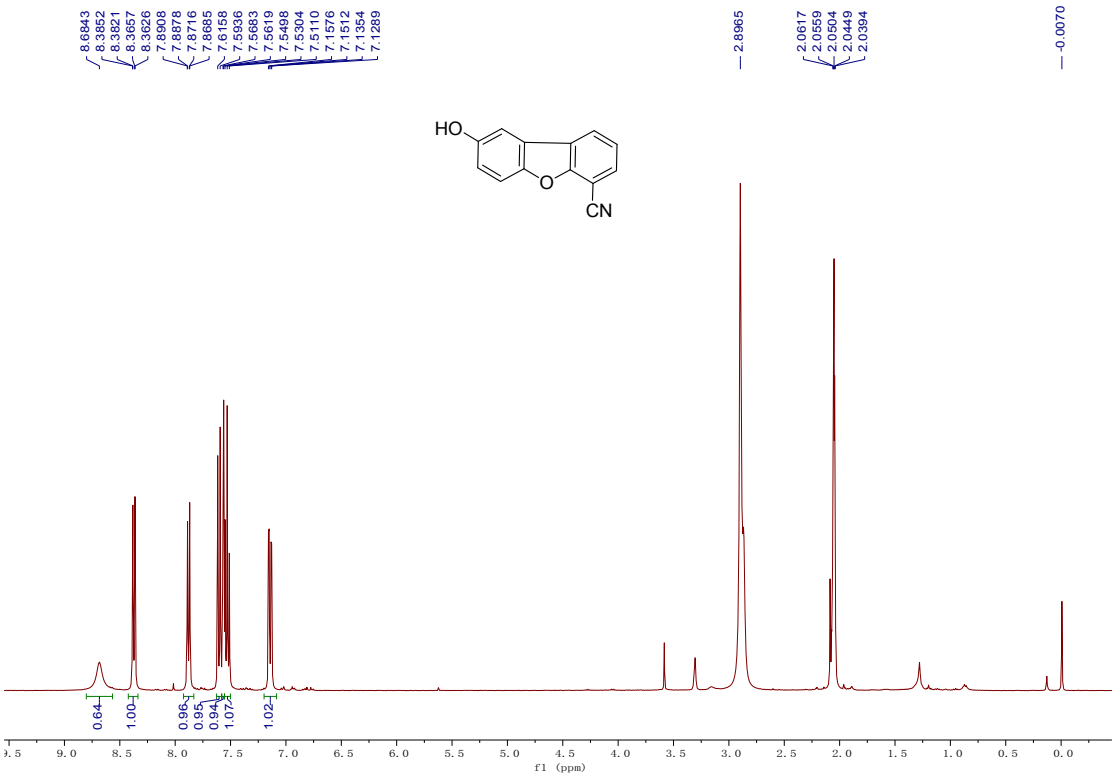


Figure S38. The ^{1}H NMR spectrum (acetone-d_6, 400 MHz) of intermediate **8**.

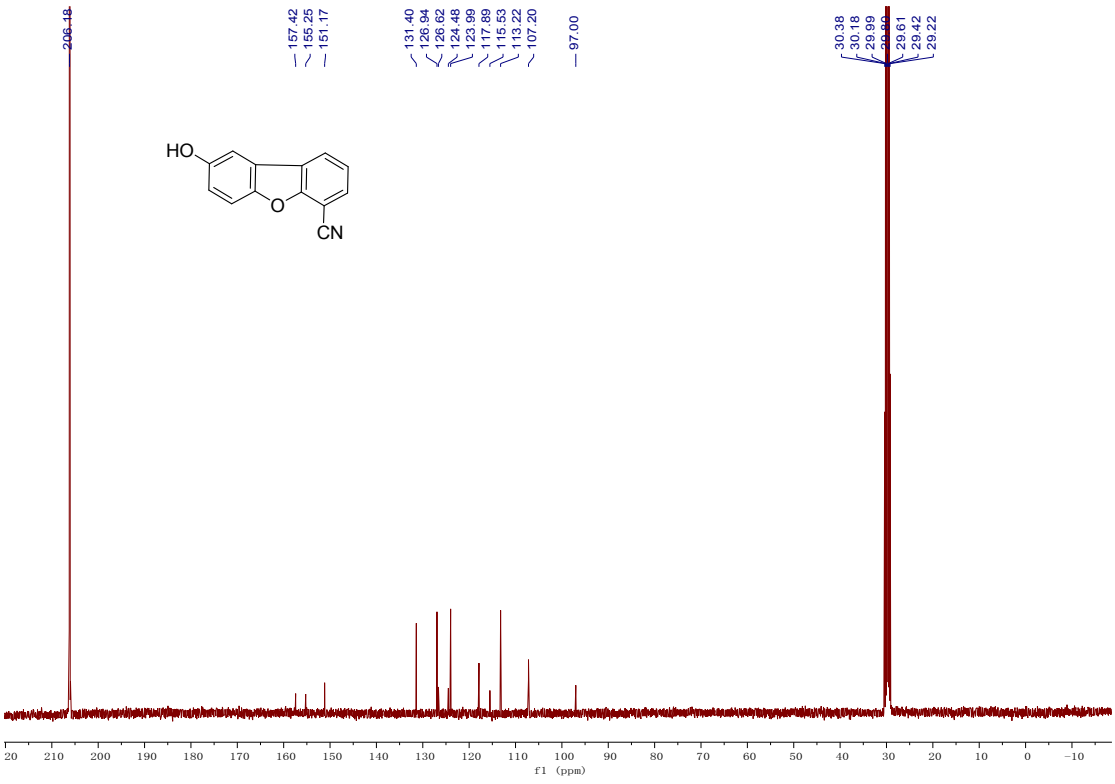


Figure S39. The ^{13}C NMR spectrum (acetone-d_6, 100 MHz) of intermediate **8**.

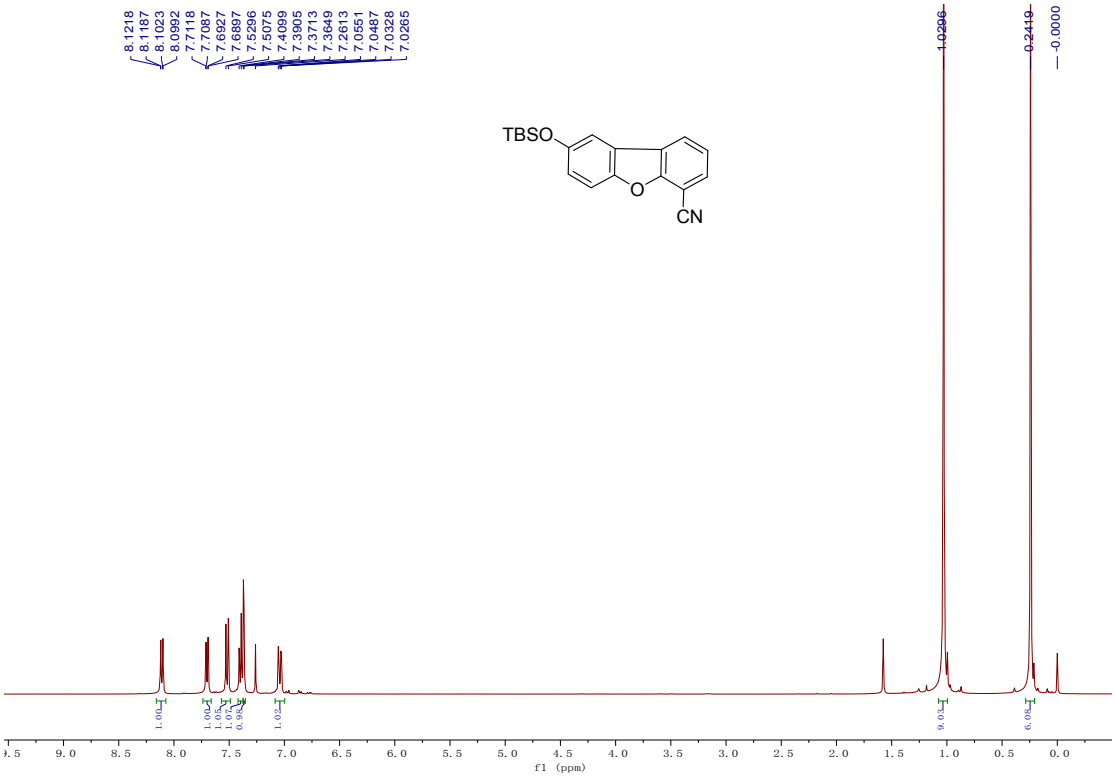


Figure S40. The ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of synthetic intermediate **9**.

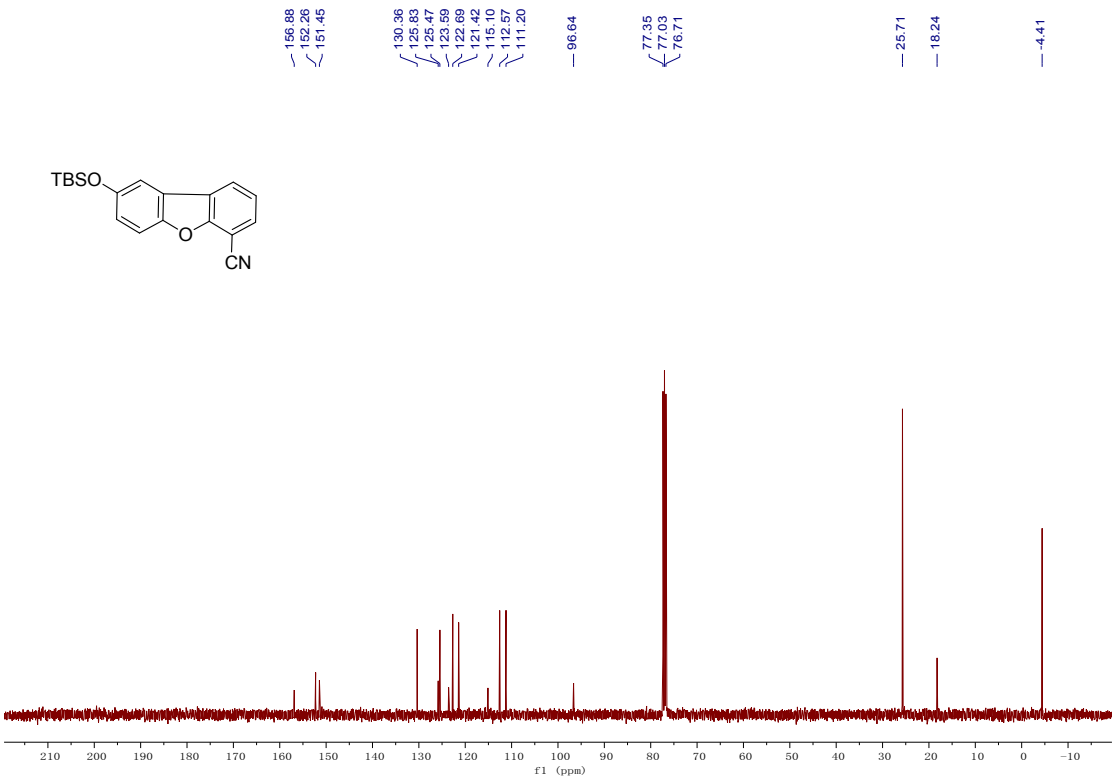


Figure S41. The ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of synthetic intermediate **9**.

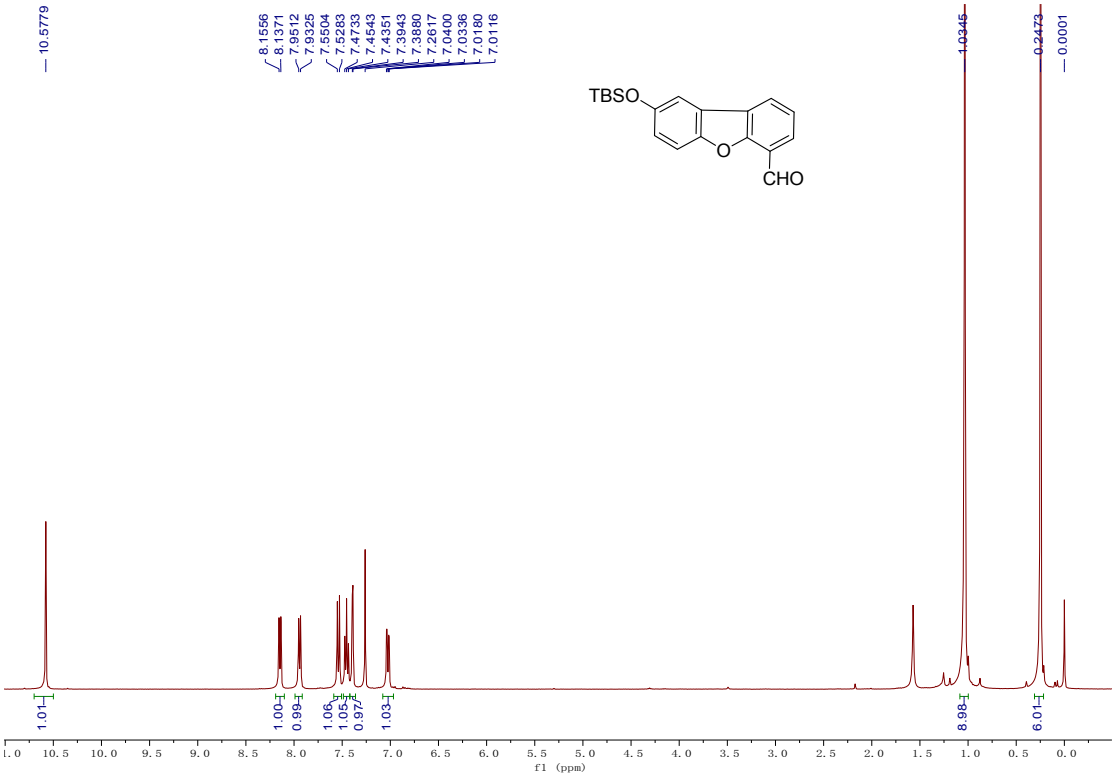


Figure S42. The ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of synthetic intermediate **5**.

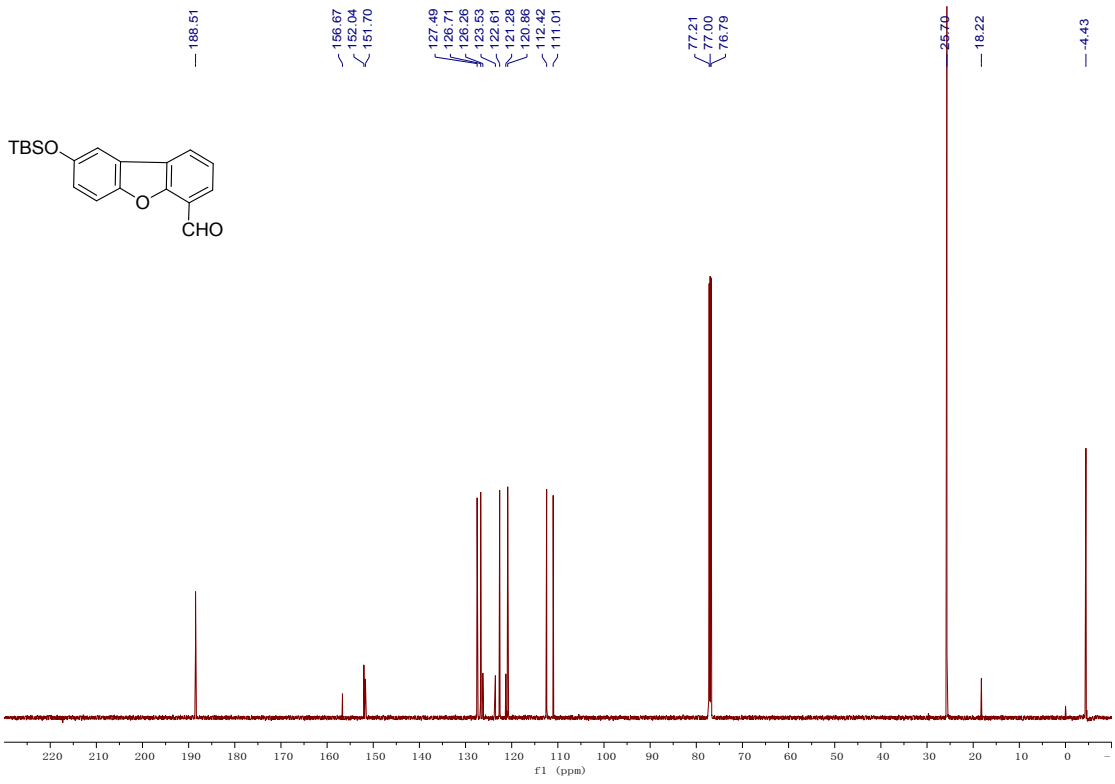


Figure S43. The ^{13}C NMR spectrum ($CDCl_3$, 150 MHz) of synthetic intermediate **5**.

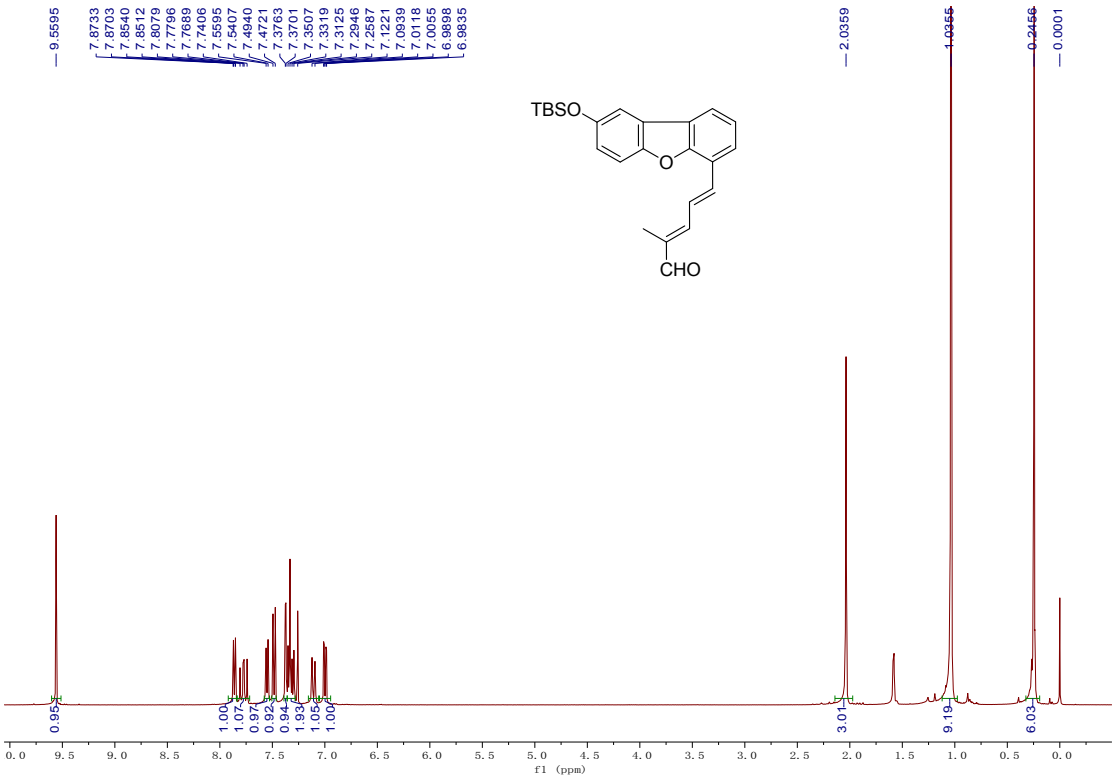


Figure S44. The ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of synthetic intermediate **10**.

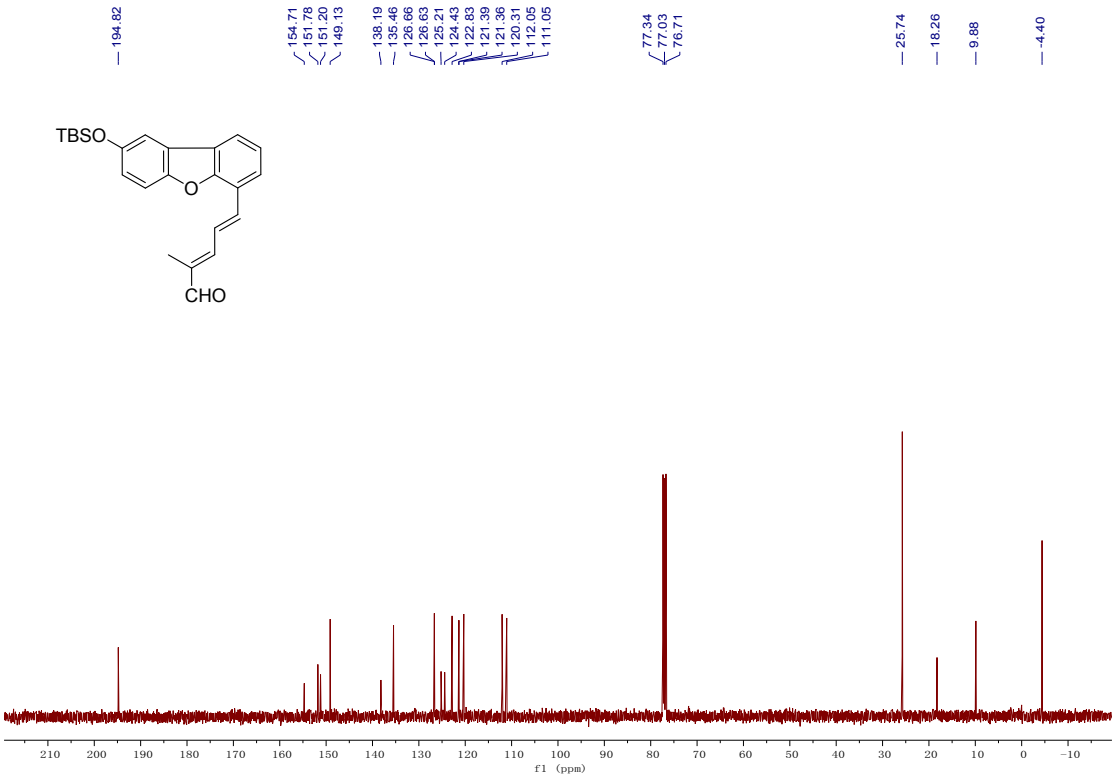


Figure S45. The ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of synthetic intermediate **10**.

Ⅵ. The NMR, HREIMS, and UV spectra of synthetic lingzhifuran A(1).

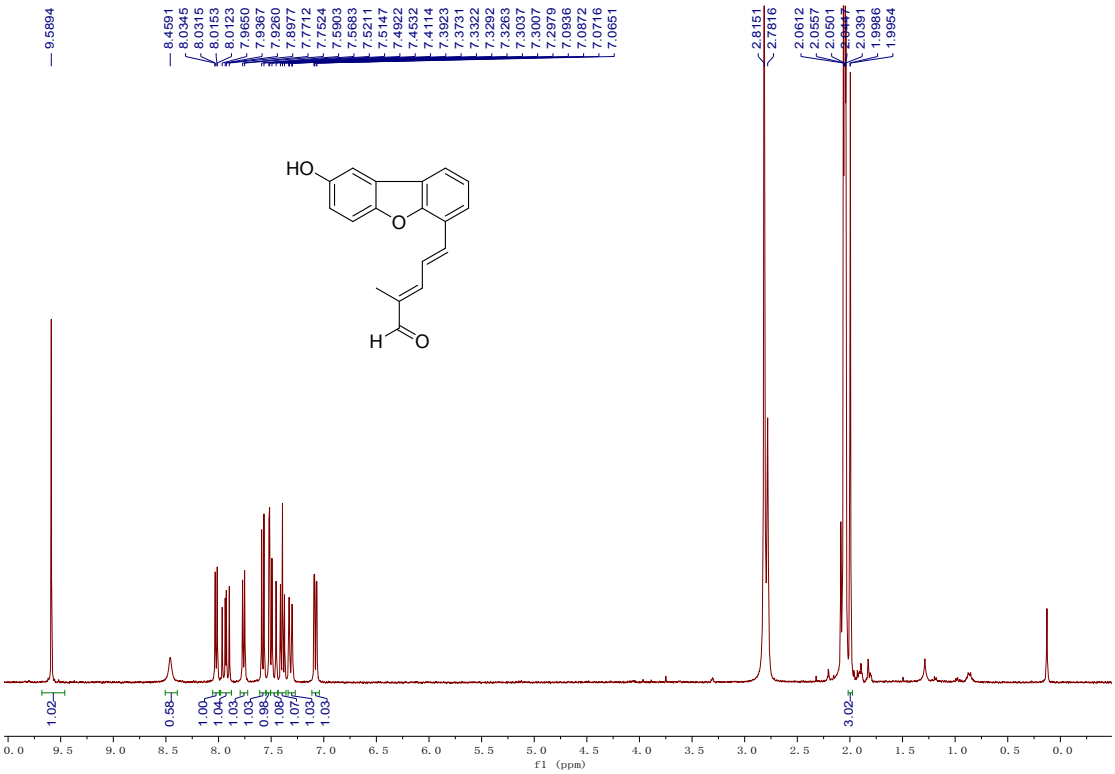


Figure S46. The ^{1}H NMR spectrum (acetone-d_6, 400 MHz) of synthetic **1**.

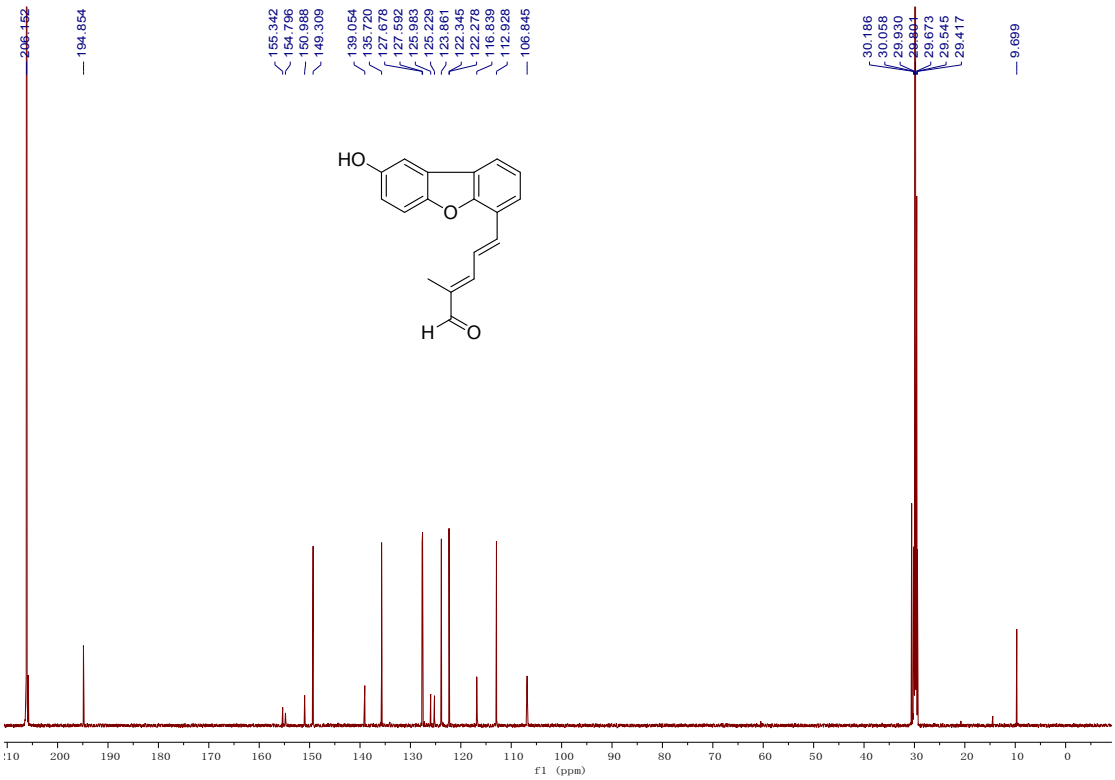


Figure S47. The ^{13}C NMR spectrum (acetone-d_6, 150 MHz) of synthetic **1**.

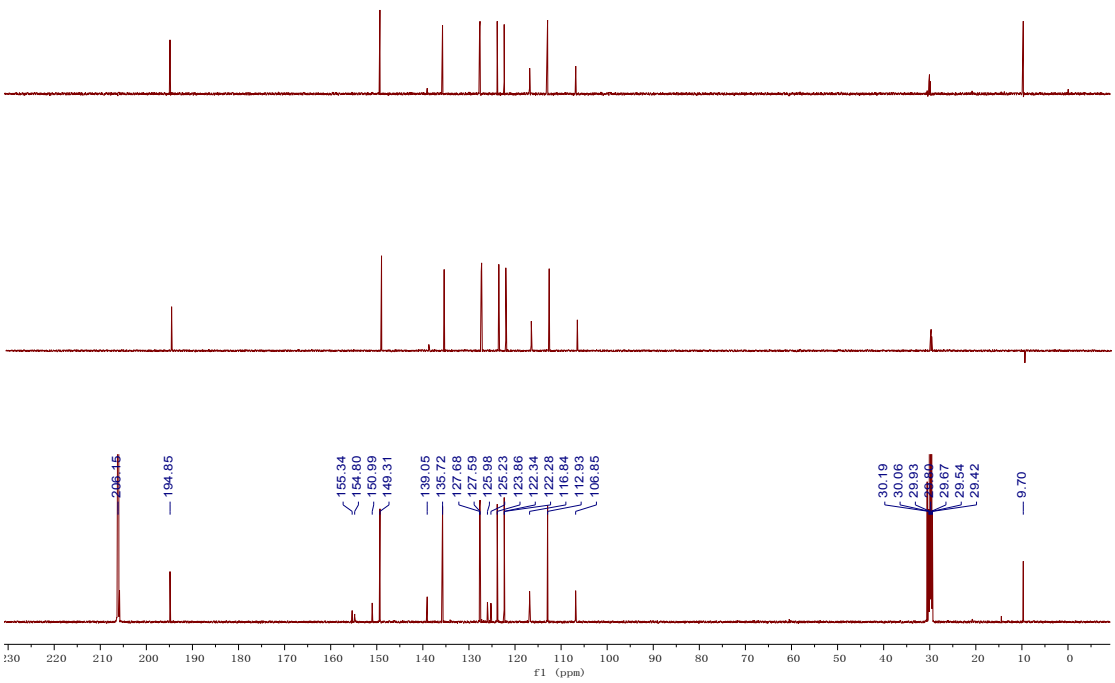


Figure S48. The DEPT spectra (acetone-d_6, 150 MHz) of synthetic **1**.

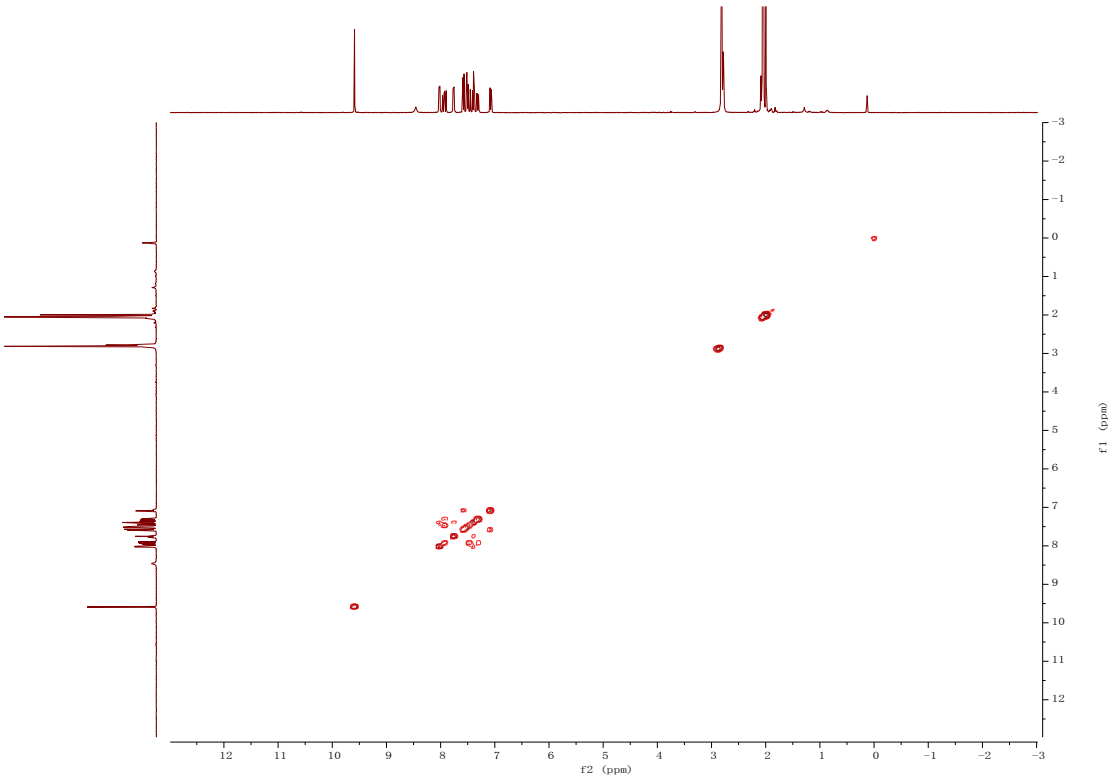


Figure S49. The ^{1}H-^{1}H COSY spectrum (acetone-d_6, 600 MHz) of synthetic **1**.

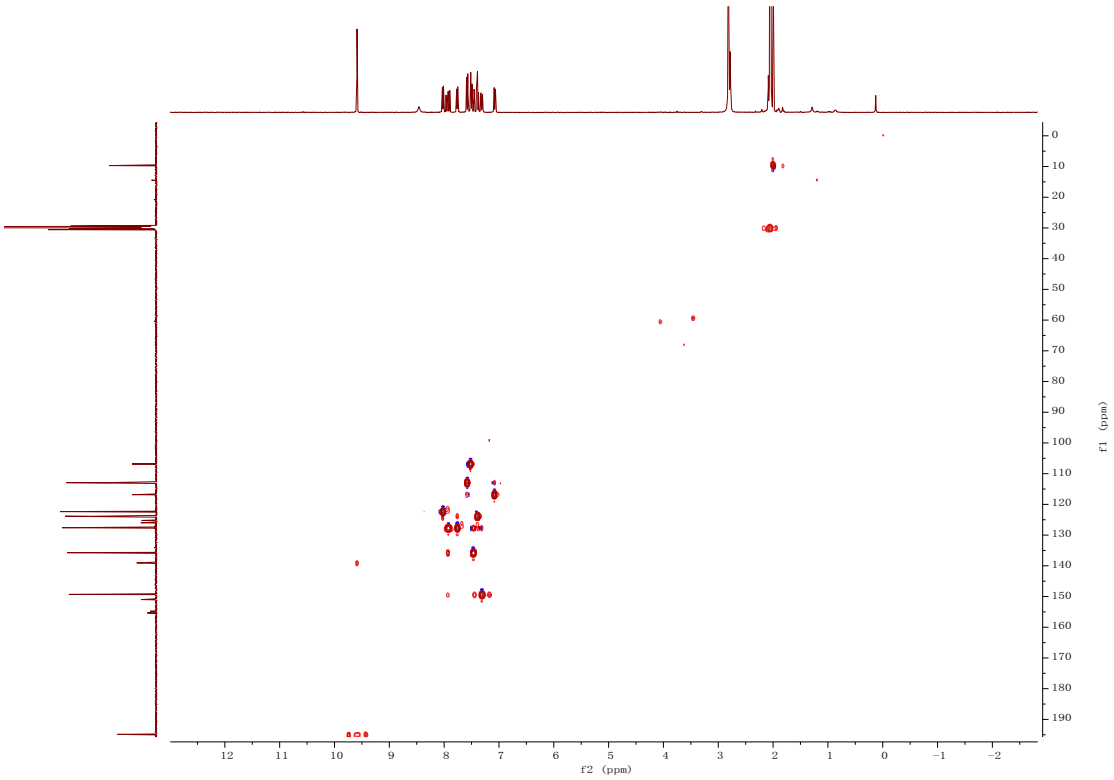


Figure S50. The HSQC spectrum (acetone-d_6, 600 MHz) of synthetic **1**.

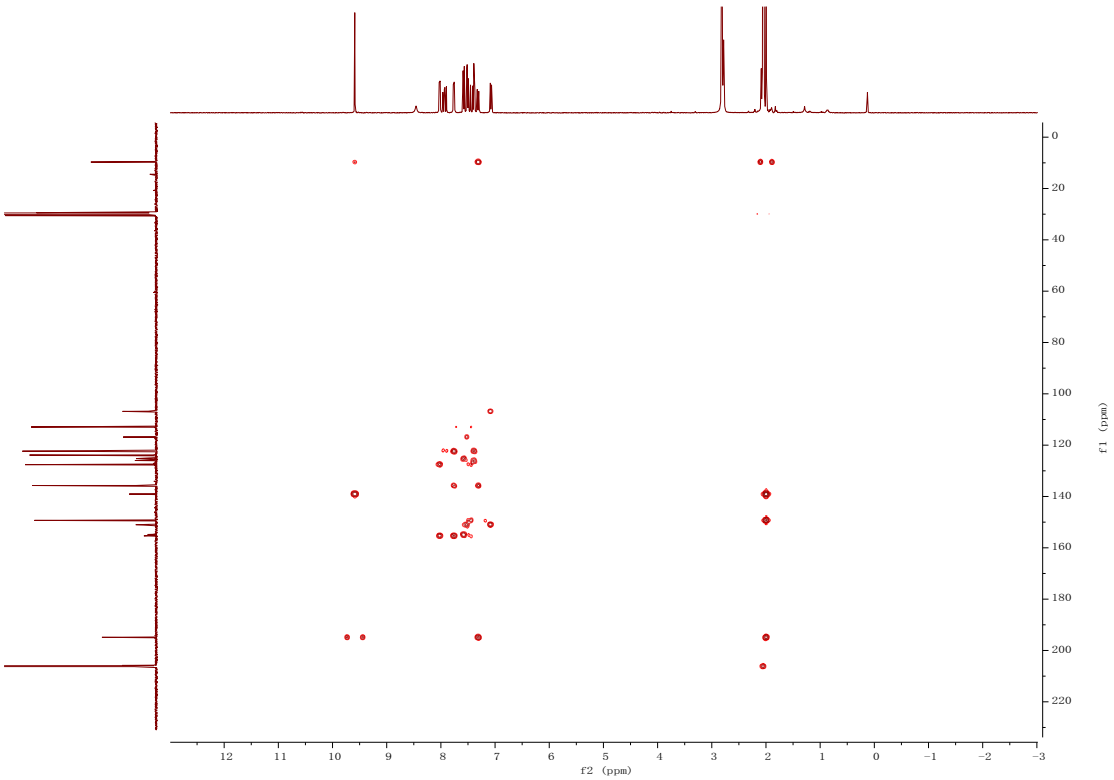


Figure S51. The HMBC spectrum (acetone-d_6, 600 MHz) of synthetic **1**.

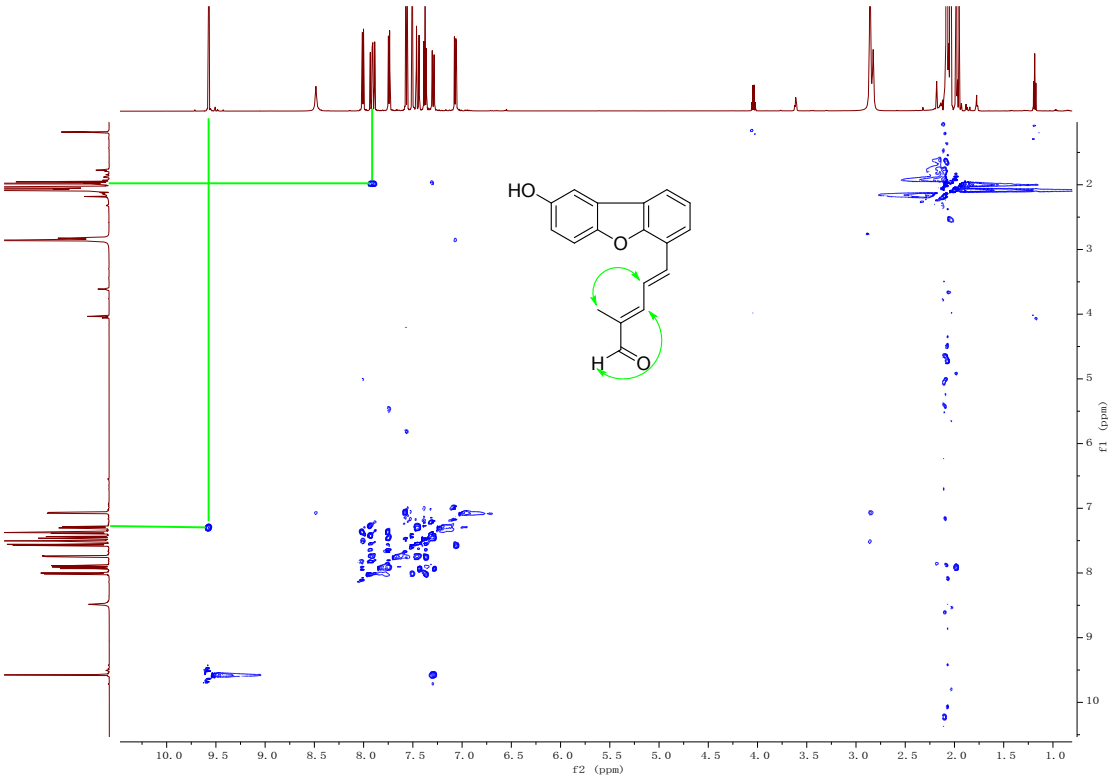


Figure S52. The ROESY spectrum (acetone-d_6, 600 MHz) of synthetic **1**.

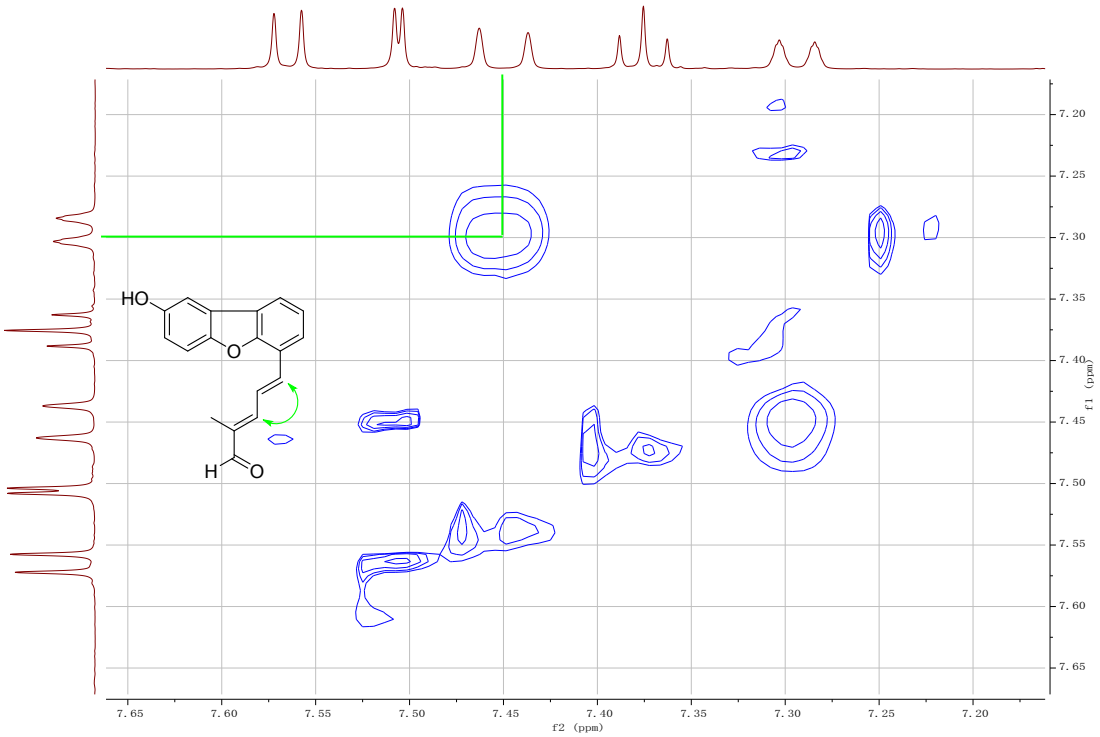


Figure S53. The enlarged ROESY spectrum (acetone-d_6, 600 MHz) of synthetic **1**.

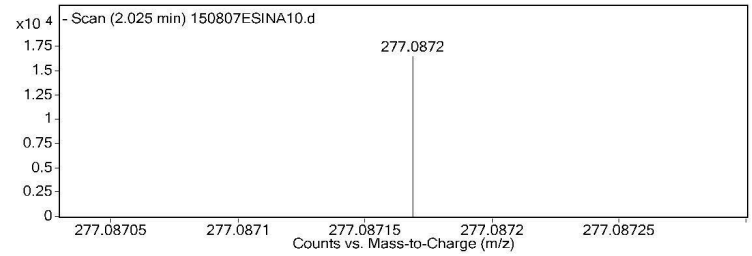
Qualitative Analysis Report

Data Filename	150807ESINA10.d	**Sample Name**	qlz-22
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESIN.m	**Acquired Time**	8/7/2015 3:53:52 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
112.9856		22250.12		
154.9733		1103.86		
277.0872	1	16477.71	C18 H13 O3	M-
278.0904	1	1478.03	C18 H13 O3	M-
313.0634	1	3722.93		
555.1803	1	892.39		
1033.9881	1	42752.42		
1034.9894	1	4595.79		
1933.9295	1	6599.81		
1934.9323	1	1130.7		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	6

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C18 H13 O3	277.0865	277.0870	277.0872	-0.1	-0.5	12.5000

--- End Of Report ---

Figure S54. The HRESIMS (negative) spectrum of synthetic **1**.

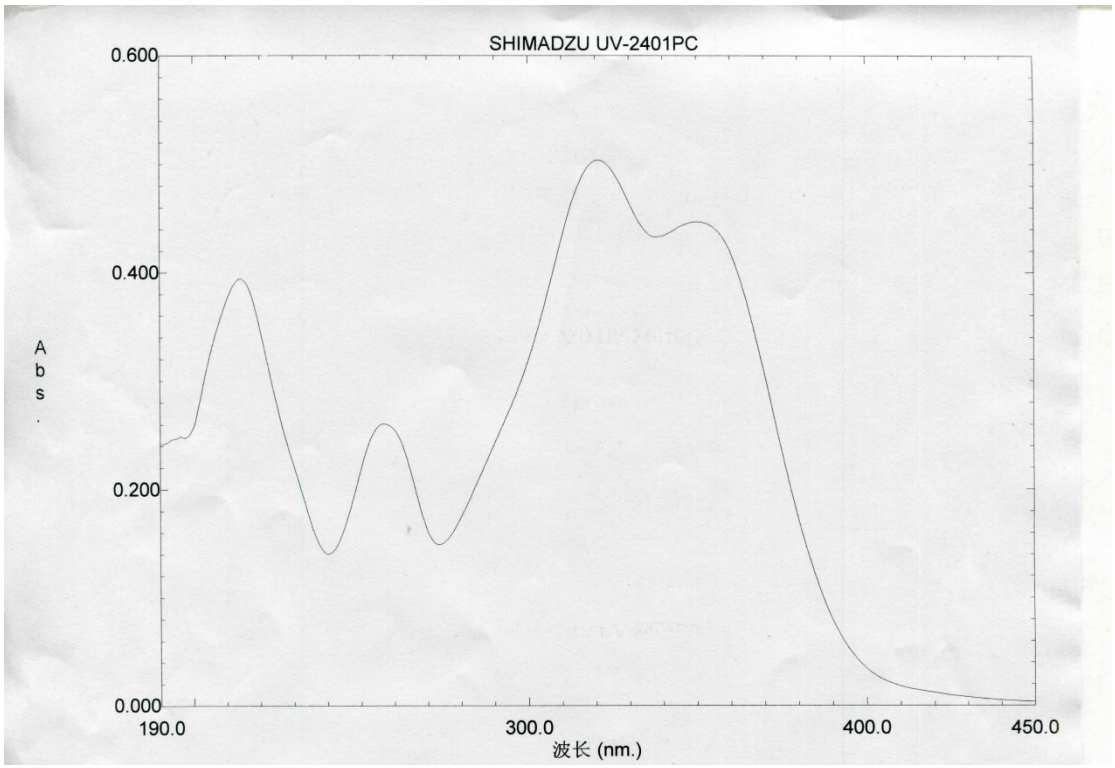


Figure S55. The UV spectrum (MeOH) of synthetic **1**.

Ⅶ Comparison of natural 1 and synthetic 1.

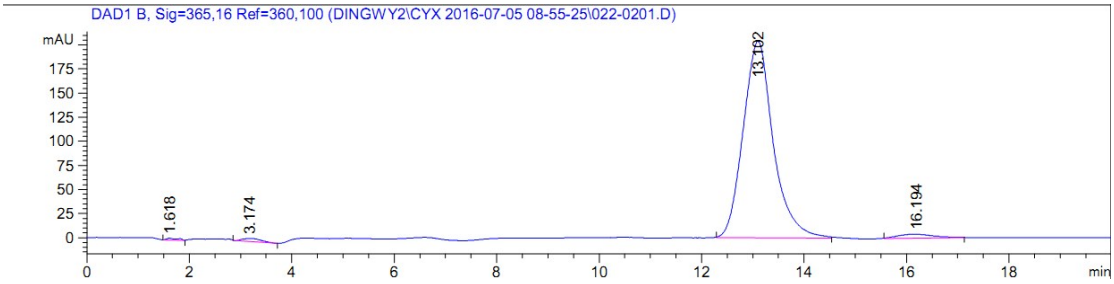
Table S1. ^{1}H and ^{13}C NMR data of **1** in acetone-d_6 (δ in ppm, J in Hz).

	1 (natural)			**1** (synthetic)	
No.	δ_H[a]	δ_C[b]	No.	δ_H[c]	δ_C[d]
1		154.9 s	1		154.8 s
2	7.52 (d, 2.6)	106.9 d	2	7.52 (d, 2.6)	106.8 d
3		125.2 s	3		125.2 s
4		150.9 s	4		151.0 s
5	7.57 (d, 8.8)	112.9 d	5	7.58 (d, 8.8)	112.9 d
6	7.08 (dd,8.8, 2.6)	116.9 d	6	7.08 (dd, 8.8, 2.6)	116.8 d
1′		126.0 s	1′		126.0 s
2′		155.3 s	2′		155.3 s
3′		122.3 s	3′		122.3 s
4′	7.47 (d, 15.6)	135.7 d	4′	7.47 (d, 15.6)	135.7 d
5′	7.92 (dd, 15.6, 11.4)	127.7 d	5′	7.93 (dd, 15.6, 11.3)	127.7 d
6′	7.31 (d, 11.4)	149.3 d	6′	7.32 (d, 11.3)	149.3 d
7′		139.0 s	7′		139.1 s
8′	9.59 (s)	194.9 s	8′	9.59 (s)	194.9 d
9′	1.99 (d, 1.2)	9.7 q	9′	2.00 (d, 1.2)	9.7 q
10′	7.76 (d, 7.6)	127.6 d	10′	7.76 (d,7.6)	127.6 d
11′	7.39 (dd, 7.7, 7.7)	123.9 d	11′	7.39 (dd, 7.6, 7.6)	123.9 d
12′	8.01 (d, 7.7)	122.3 d	12′	8.02 (dd,7.6, 1.2)	122.3 d
1-OH			1-OH	8.46 (br)	

[a] Recorded at 800 MHz; [b] Recorded at 200 MHz; [c] Recorded at 400 MHz; [d] Recorded at 150 MHz.

HPLC analysis were recorded on a Agilent 1200 spectrometer using Eclipse XDB-C18 column (5 μm, 4.6 × 150 mm). HPLC (65% aq. MeOH; flow rate: 1.0 mL/min; 25 ℃; Detection: 365 nm)

(a) natural **1**



(b) synthetic **1**

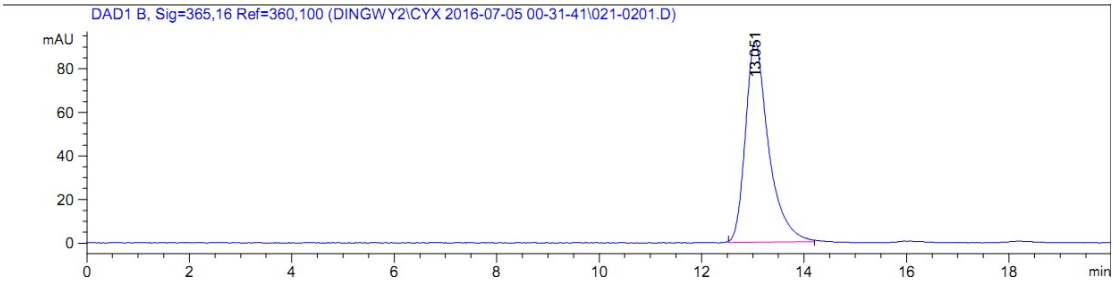
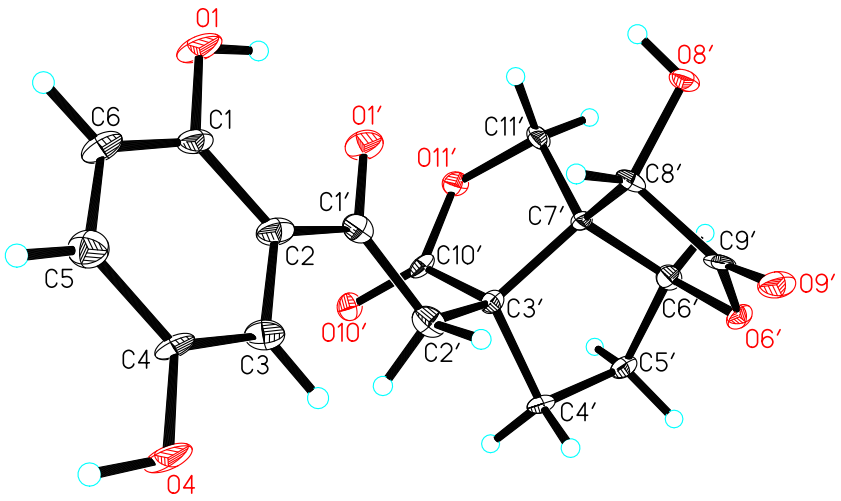


Figure S56. HPLC chromatograms of natural and synthetic of **1**.

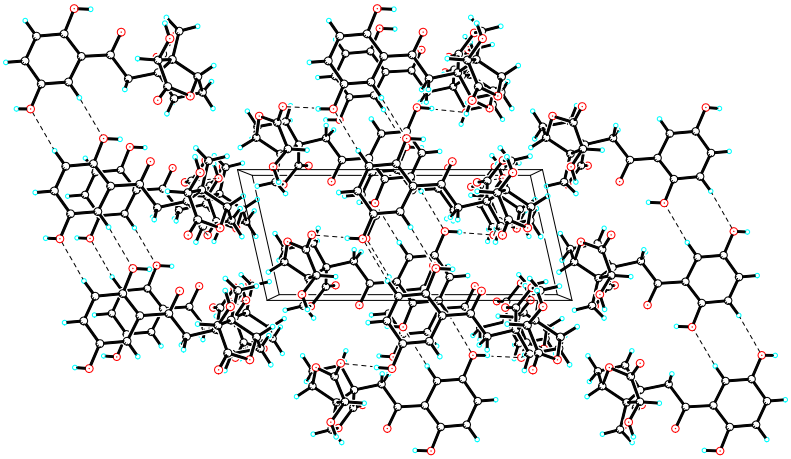
Ⅷ. X-ray data of (-)-2.

Crystal data for cu_qylz2b_0m: $C_{17}H_{16}O_8$, M = 348.30, monoclinic, a = 6.7105(3) Å, b = 7.8030(4) Å, c = 15.2397(9) Å, α = 90.00°, β = 102.694(2)°, γ = 90.00°, V = 778.48(7) Å^3, T = 100(2) K, space group $P21$, Z = 2, μ(CuKα) = 1.020 mm^{-1}, 5682 reflections measured, 2079 independent reflections (R_{int} = 0.0482). The final R_1 values were 0.1075 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.2890 ($I > 2\sigma(I)$). The final R_1 values were 0.1080 (all data). The final $wR(F^2)$ values were 0.2892 (all data). The goodness of fit on F^2 was 1.212. Flack parameter = -0.2(8). The deposition number CCDC 1491784 for (-)-**2** can be obtained free of charge from The Cambridge Crystallographic Data Centre via www. ccdc.cam.ac.uk/data_request/cif.



View of a molecule of qylz2b with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the hydrogen-bonded motif of qylz2b.

Hydrogen-bonds are shown as dashed lines.

Table 1. Crystal data and structure refinement for qylz2b.

Identification code	qylz2b
Empirical formula	C17 H16 O8
Formula weight	348.30
Temperature	100(2) K
Wavelength	1.54178 A
Crystal system, space group	Monoclinic, P 21
Unit cell dimensions	a = 6.7105(3) A alpha = 90 deg. b = 7.8030(4) A beta = 102.694(2) deg. c = 15.2397(9) A gamma = 90 deg.
Volume	778.48(7) A^3
Z, Calculated density	2, 1.486 Mg/m^3
Absorption coefficient	1.020 mm^-1
F(000)	364

Crystal size	0.32 x 0.16 x 0.12 mm
Theta range for data collection	2.97 to 68.81 deg.
Limiting indices	-7<=h<=7, -7<=k<=9, -18<=l<=18
Reflections collected / unique	5682 / 2079 [R(int) = 0.0482]
Completeness to theta = 68.81	97.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8874 and 0.7361
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2079 / 7 / 228
Goodness-of-fit on F^2	1.212
Final R indices [I>2sigma(I)]	R1 = 0.1075, wR2 = 0.2890
R indices (all data)	R1 = 0.1080, wR2 = 0.2892
Absolute structure parameter	-0.2(8)
Largest diff. peak and hole	0.588 and -0.622 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for qylz2b.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(9')	5006(10)	8089(10)	1892(5)	27(2)
O(4)	5291(10)	4260(15)	6418(4)	40(3)
O(1')	-672(11)	3946(11)	2877(5)	29(2)
O(11')	-860(10)	2304(10)	1127(4)	21(2)
O(6')	4460(10)	5879(10)	954(4)	19(2)
O(8')	345(10)	7526(9)	1098(4)	21(2)
O(10')	795(10)	410(9)	2117(5)	22(2)
O(1)	-2422(10)	4344(14)	4222(5)	37(2)
C(5)	1610(17)	4419(17)	6226(7)	31(3)
C(4)	3368(14)	4257(16)	5879(7)	25(2)
C(3)	3196(15)	4101(16)	4978(7)	25(2)
C(2)	1225(15)	4122(15)	4362(7)	25(2)
C(1')	1075(15)	3889(13)	3407(7)	23(2)
C(2')	2878(16)	3530(14)	3020(6)	24(2)
C(3')	2365(14)	3176(13)	2009(6)	16(2)
C(7')	1531(13)	4659(14)	1344(6)	17(2)
C(8')	1810(16)	6459(13)	1697(7)	20(2)
C(9')	3861(14)	6929(13)	1553(6)	20(2)
C(10')	734(15)	1816(13)	1797(6)	18(2)
C(11')	-719(14)	4143(14)	936(6)	20(2)
C(6')	2835(14)	4589(14)	636(6)	19(2)
C(5')	3855(14)	2828(14)	693(6)	20(2)
C(4')	4312(13)	2483(13)	1714(6)	16(2)
C(1)	-490(14)	4317(15)	4745(7)	25(2)
C(6)	-288(15)	4440(17)	5663(7)	28(3)

Table 3. Bond lengths [A] and angles [deg] for qylz2b.

O(9')-C(9')	1.226(13)
O(4)-C(4)	1.369(11)
O(4)-H(4)	0.8400
O(1')-C(1')	1.270(12)
O(11')-C(10')	1.361(12)
O(11')-C(11')	1.471(13)
O(6')-C(9')	1.351(12)
O(6')-C(6')	1.485(11)
O(8')-C(8')	1.449(11)
O(8')-H(8')	0.8400
O(10')-C(10')	1.197(13)
O(1)-C(1)	1.365(12)
O(1)-H(1)	0.8400
C(5)-C(6)	1.370(15)
C(5)-C(4)	1.401(13)
C(5)-H(5)	0.9500
C(4)-C(3)	1.358(15)
C(3)-C(2)	1.444(13)
C(3)-H(3)	0.9500
C(2)-C(1)	1.408(13)
C(2)-C(1')	1.448(15)
C(1')-C(2')	1.485(14)
C(2')-C(3')	1.528(12)
C(2')-H(2'1)	0.9900
C(2')-H(2'2)	0.9900
C(3')-C(10')	1.508(13)
C(3')-C(7')	1.559(14)
C(3')-C(4')	1.568(12)
C(7')-C(8')	1.500(15)
C(7')-C(6')	1.532(12)
C(7')-C(11')	1.555(12)
C(8')-C(9')	1.486(14)
C(8')-H(8'1)	1.0000
C(11')-H(11A)	0.9900
C(11')-H(11B)	0.9900
C(6')-C(5')	1.529(15)
C(6')-H(6')	1.0000
C(5')-C(4')	1.543(13)
C(5')-H(5'1)	0.9900
C(5')-H(5'2)	0.9900

C(4')-H(4'1)	0.9900
C(4')-H(4'2)	0.9900
C(1)-C(6)	1.379(15)
C(6)-H(6)	0.9500

C(4)-O(4)-H(4)	109.5
C(10')-O(11')-C(11')	110.3(7)
C(9')-O(6')-C(6')	109.0(7)
C(8')-O(8')-H(8')	109.5
C(1)-O(1)-H(1)	109.5
C(6)-C(5)-C(4)	120.6(10)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(3)-C(4)-O(4)	117.8(8)
C(3)-C(4)-C(5)	119.9(10)
O(4)-C(4)-C(5)	122.3(9)
C(4)-C(3)-C(2)	121.2(9)
C(4)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4
C(1)-C(2)-C(3)	116.6(9)
C(1)-C(2)-C(1')	123.2(9)
C(3)-C(2)-C(1')	120.2(9)
O(1')-C(1')-C(2)	119.1(9)
O(1')-C(1')-C(2')	118.2(9)
C(2)-C(1')-C(2')	122.7(8)
C(1')-C(2')-C(3')	114.4(8)
C(1')-C(2')-H(2'1)	108.7
C(3')-C(2')-H(2'1)	108.7
C(1')-C(2')-H(2'2)	108.7
C(3')-C(2')-H(2'2)	108.7
H(2'1)-C(2')-H(2'2)	107.6
C(10')-C(3')-C(2')	109.6(8)
C(10')-C(3')-C(7')	104.1(8)
C(2')-C(3')-C(7')	119.3(9)
C(10')-C(3')-C(4')	107.9(8)
C(2')-C(3')-C(4')	109.5(8)
C(7')-C(3')-C(4')	105.9(7)
C(8')-C(7')-C(6')	103.9(8)
C(8')-C(7')-C(11')	114.8(8)
C(6')-C(7')-C(11')	111.3(8)
C(8')-C(7')-C(3')	117.6(8)
C(6')-C(7')-C(3')	104.6(7)
C(11')-C(7')-C(3')	104.3(7)
O(8')-C(8')-C(9')	106.7(8)

O(8')-C(8')-C(7')	107.4(8)
C(9')-C(8')-C(7')	103.0(8)
O(8')-C(8')-H(8'1)	113.0
C(9')-C(8')-H(8'1)	113.0
C(7')-C(8')-H(8'1)	113.0
O(9')-C(9')-O(6')	118.7(9)
O(9')-C(9')-C(8')	129.4(9)
O(6')-C(9')-C(8')	111.9(9)
O(10')-C(10')-O(11')	120.8(9)
O(10')-C(10')-C(3')	126.8(9)
O(11')-C(10')-C(3')	112.2(8)
O(11')-C(11')-C(7')	105.8(8)
O(11')-C(11')-H(11A)	110.6
C(7')-C(11')-H(11A)	110.6
O(11')-C(11')-H(11B)	110.6
C(7')-C(11')-H(11B)	110.6
H(11A)-C(11')-H(11B)	108.7
O(6')-C(6')-C(5')	107.6(7)
O(6')-C(6')-C(7')	103.8(7)
C(5')-C(6')-C(7')	108.1(8)
O(6')-C(6')-H(6')	112.3
C(5')-C(6')-H(6')	112.3
C(7')-C(6')-H(6')	112.3
C(6')-C(5')-C(4')	101.6(8)
C(6')-C(5')-H(5'1)	111.5
C(4')-C(5')-H(5'1)	111.5
C(6')-C(5')-H(5'2)	111.5
C(4')-C(5')-H(5'2)	111.5
H(5'1)-C(5')-H(5'2)	109.3
C(5')-C(4')-C(3')	103.6(7)
C(5')-C(4')-H(4'1)	111.0
C(3')-C(4')-H(4'1)	111.0
C(5')-C(4')-H(4'2)	111.0
C(3')-C(4')-H(4'2)	111.0
H(4'1)-C(4')-H(4'2)	109.0
O(1)-C(1)-C(6)	117.4(9)
O(1)-C(1)-C(2)	121.2(10)
C(6)-C(1)-C(2)	121.4(9)
C(5)-C(6)-C(1)	120.3(9)
C(5)-C(6)-H(6)	119.8
C(1)-C(6)-H(6)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for qylz2b.
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(9')	16(3)	19(4)	44(4)	-5(3)	2(3)	0(3)
O(4)	7(3)	93(8)	18(3)	-4(4)	-2(2)	5(4)
O(1')	20(4)	40(5)	25(3)	-7(3)	-1(3)	0(4)
O(11')	16(3)	17(4)	27(3)	0(3)	2(3)	-3(3)
O(6')	12(3)	18(4)	27(3)	-2(3)	4(3)	-5(3)
O(8')	16(3)	19(4)	24(3)	4(3)	-2(3)	4(3)
O(10')	23(3)	13(4)	30(4)	0(3)	7(3)	-5(3)
O(1)	10(3)	68(7)	30(4)	-8(5)	0(3)	6(4)
C(5)	31(6)	31(7)	30(5)	-3(5)	7(4)	3(5)
C(4)	7(4)	34(7)	34(5)	-3(5)	5(4)	-2(5)
C(3)	17(5)	31(6)	24(5)	-5(5)	-4(4)	-1(5)
C(2)	15(5)	23(6)	37(5)	-4(5)	3(4)	-1(5)
C(1')	15(4)	16(6)	33(5)	4(4)	-5(4)	-8(4)
C(2')	25(5)	22(6)	21(5)	-3(4)	-5(4)	-3(4)
C(3')	14(4)	16(5)	20(4)	-1(4)	6(3)	-1(4)
C(7')	9(4)	15(5)	26(5)	6(4)	4(3)	0(4)
C(8')	21(5)	14(5)	22(5)	4(4)	0(4)	7(4)
C(9')	14(5)	21(6)	24(5)	4(4)	1(4)	11(4)
C(10')	15(5)	20(6)	23(5)	-6(4)	11(4)	-2(4)
C(11')	21(5)	12(5)	26(5)	6(4)	3(4)	1(4)
C(6')	18(2)	18(3)	20(2)	0(2)	1(2)	-2(2)
C(5')	13(4)	22(6)	26(5)	-4(4)	6(4)	-2(4)
C(4')	9(4)	16(5)	22(4)	-6(4)	2(3)	1(4)
C(1)	12(4)	18(6)	46(6)	3(5)	6(4)	0(4)
C(6)	13(4)	37(7)	37(6)	-7(5)	7(4)	-4(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for qylz2b.

	x	y	z	U(eq)
H(4)	5246	3867	6926	60
H(8')	-839	7293	1159	31
H(1)	-2365	4403	3678	55
H(5)	1734	4514	6857	37
H(3)	4394	3975	4748	31
H(2'1)	3611	2525	3332	29
H(2'2)	3817	4523	3139	29
H(8'1)	1709	6555	2340	24
H(11A)	-1669	4809	1217	24
H(11B)	-1063	4354	279	24
H(6')	2023	4848	18	23
H(5'1)	5125	2863	463	24
H(5'2)	2922	1954	355	24
H(4'1)	5552	3103	2026	19
H(4'2)	4501	1242	1843	19
H(6)	-1471	4540	5907	34

Table 6. Torsion angles [deg] for qylz2b.

C(6)-C(5)-C(4)-C(3)	-1(2)
C(6)-C(5)-C(4)-O(4)	178.9(12)
O(4)-C(4)-C(3)-C(2)	-178.7(12)
C(5)-C(4)-C(3)-C(2)	0.9(19)
C(4)-C(3)-C(2)-C(1)	0.2(18)
C(4)-C(3)-C(2)-C(1')	-177.7(11)
C(1)-C(2)-C(1')-O(1')	3.6(17)
C(3)-C(2)-C(1')-O(1')	-178.7(11)
C(1)-C(2)-C(1')-C(2')	-174.4(11)
C(3)-C(2)-C(1')-C(2')	3.3(16)
O(1')-C(1')-C(2')-C(3')	-3.0(14)
C(2)-C(1')-C(2')-C(3')	175.0(10)
C(1')-C(2')-C(3')-C(10')	-51.3(12)
C(1')-C(2')-C(3')-C(7')	68.4(12)
C(1')-C(2')-C(3')-C(4')	-169.5(9)
C(10')-C(3')-C(7')-C(8')	139.2(8)
C(2')-C(3')-C(7')-C(8')	16.7(12)
C(4')-C(3')-C(7')-C(8')	-107.2(9)
C(10')-C(3')-C(7')-C(6')	-106.3(8)
C(2')-C(3')-C(7')-C(6')	131.2(9)
C(4')-C(3')-C(7')-C(6')	7.3(10)
C(10')-C(3')-C(7')-C(11')	10.7(9)
C(2')-C(3')-C(7')-C(11')	-111.8(9)
C(4')-C(3')-C(7')-C(11')	124.3(8)
C(6')-C(7')-C(8')-O(8')	85.0(9)
C(11')-C(7')-C(8')-O(8')	-36.8(10)
C(3')-C(7')-C(8')-O(8')	-160.1(7)
C(6')-C(7')-C(8')-C(9')	-27.4(9)
C(11')-C(7')-C(8')-C(9')	-149.2(8)
C(3')-C(7')-C(8')-C(9')	87.5(9)
C(6')-O(6')-C(9')-O(9')	-179.9(8)
C(6')-O(6')-C(9')-C(8')	0.1(10)
O(8')-C(8')-C(9')-O(9')	84.9(13)
C(7')-C(8')-C(9')-O(9')	-162.2(10)
O(8')-C(8')-C(9')-O(6')	-95.0(9)
C(7')-C(8')-C(9')-O(6')	17.9(10)
C(11')-O(11')-C(10')-O(10')	172.4(8)
C(11')-O(11')-C(10')-C(3')	-11.7(10)
C(2')-C(3')-C(10')-O(10')	-55.7(12)
C(7')-C(3')-C(10')-O(10')	175.6(9)
C(4')-C(3')-C(10')-O(10')	63.5(12)

C(2')-C(3')-C(10')-O(11')	128.7(8)
C(7')-C(3')-C(10')-O(11')	0.0(10)
C(4')-C(3')-C(10')-O(11')	-112.1(8)
C(10')-O(11')-C(11')-C(7')	18.3(9)
C(8')-C(7')-C(11')-O(11')	-147.4(8)
C(6')-C(7')-C(11')-O(11')	94.9(9)
C(3')-C(7')-C(11')-O(11')	-17.3(9)
C(9')-O(6')-C(6')-C(5')	-132.1(8)
C(9')-O(6')-C(6')-C(7')	-17.7(10)
C(8')-C(7')-C(6')-O(6')	27.9(9)
C(11')-C(7')-C(6')-O(6')	152.0(8)
C(3')-C(7')-C(6')-O(6')	-96.0(8)
C(8')-C(7')-C(6')-C(5')	142.0(8)
C(11')-C(7')-C(6')-C(5')	-93.9(9)
C(3')-C(7')-C(6')-C(5')	18.1(10)
O(6')-C(6')-C(5')-C(4')	75.1(8)
C(7')-C(6')-C(5')-C(4')	-36.4(9)
C(6')-C(5')-C(4')-C(3')	39.7(9)
C(10')-C(3')-C(4')-C(5')	81.3(9)
C(2')-C(3')-C(4')-C(5')	-159.4(8)
C(7')-C(3')-C(4')-C(5')	-29.6(10)
C(3)-C(2)-C(1)-O(1)	-179.6(11)
C(1')-C(2)-C(1)-O(1)	-1.8(17)
C(3)-C(2)-C(1)-C(6)	-1.5(17)
C(1')-C(2)-C(1)-C(6)	176.3(11)
C(4)-C(5)-C(6)-C(1)	-1(2)
O(1)-C(1)-C(6)-C(5)	179.9(12)
C(2)-C(1)-C(6)-C(5)	1.7(19)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for qylz2b [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4)...O(9')#1	0.84	1.94	2.780(11)	175.8
O(1)-H(1)...O(1')	0.84	1.88	2.596(10)	143.0

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