Electronic Supplementary Information

Secondary metabolites from the endolichenic fungus *Ophiosphaerella korrae*

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Table S1 NMR Boltzmann averaged isotropic magnetic shielding values (σ), unscaled (δ_u) and scaled (δ_s) chemical shifts calculated at the PCM/mPW1PW91/6-31+G**//PCM/B3LYP/6-31G* (solvent: DMSO) level of theory for (2*S*,6*R*,7*S*)-**1** and (2*S*,6*S*,7*R*)-**1**. S37

Table S2 NMR Boltzmann averaged isotropic magnetic shielding values (σ), unscaled (δ_u) and scaled (δ_s) chemical shifts calculated at the PCM/mPW1PW91/6-31+G**//PCM/B3LYP/6-31G* (solvent: DMSO) level of theory for (2*S*,5*R*,6*S*)-**1a** and (2*S*,5*S*,6*R*)-**1a**. S38

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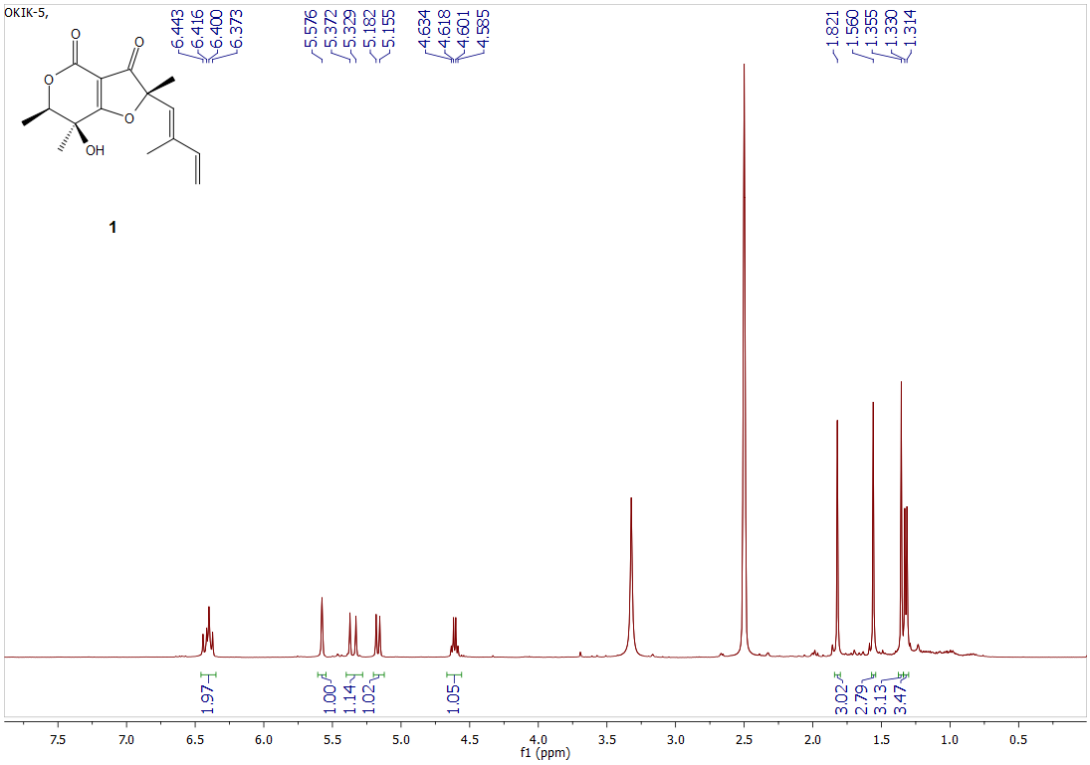
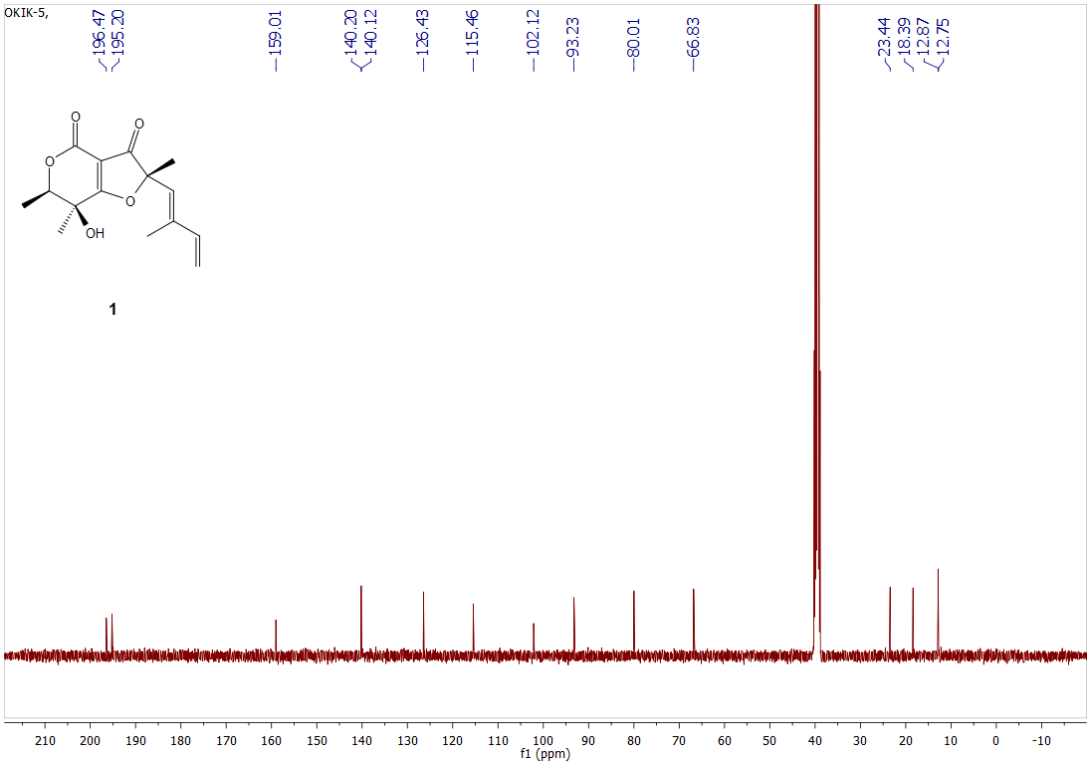


Fig. S1 ^{1}H NMR spectrum (400 MHz) of **1** in DMSO-d_6.



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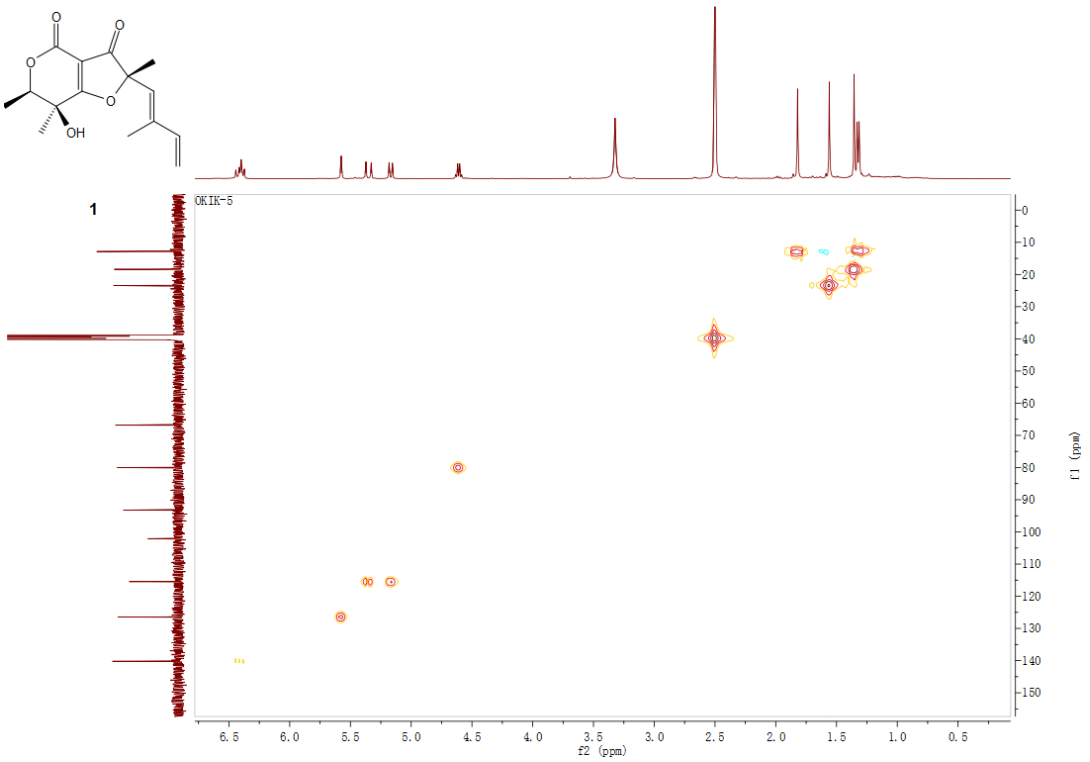
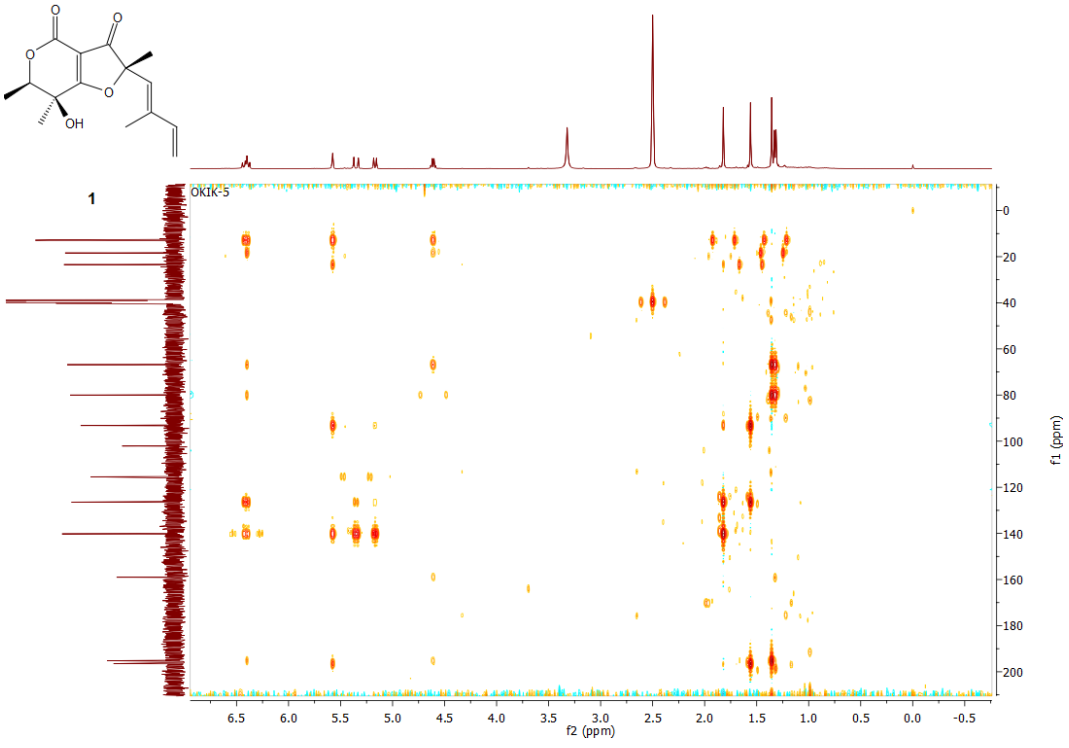


Fig. S3 HSQC spectrum (600 MHz) of **1** in DMSO-d_6.



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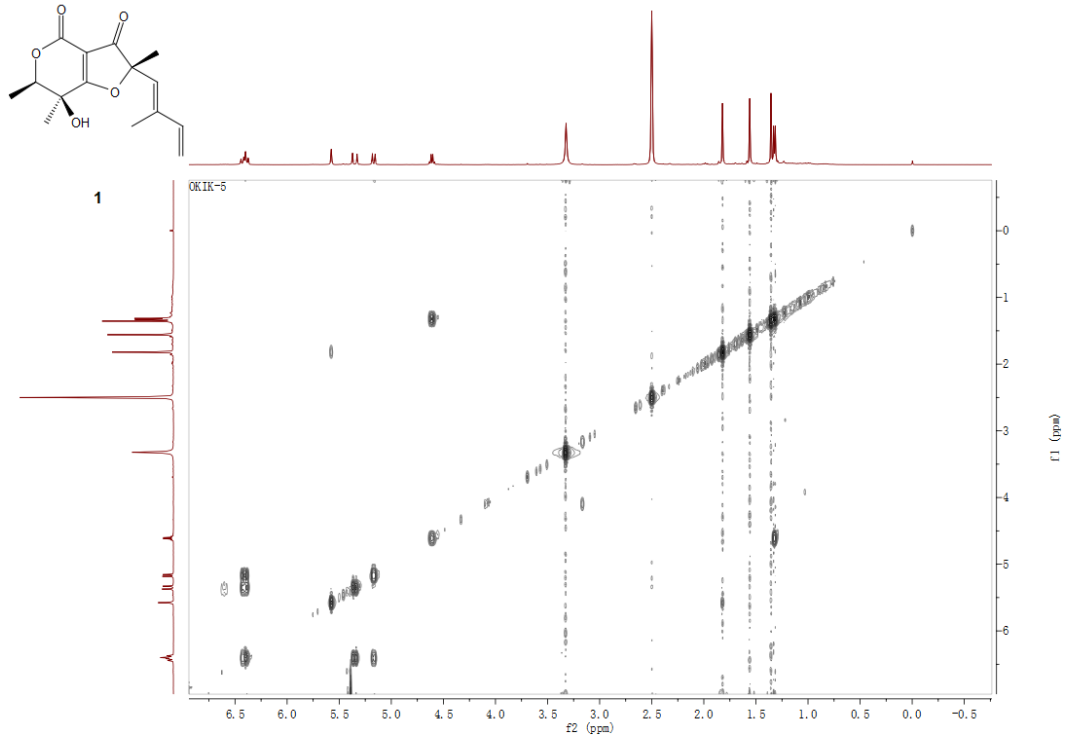

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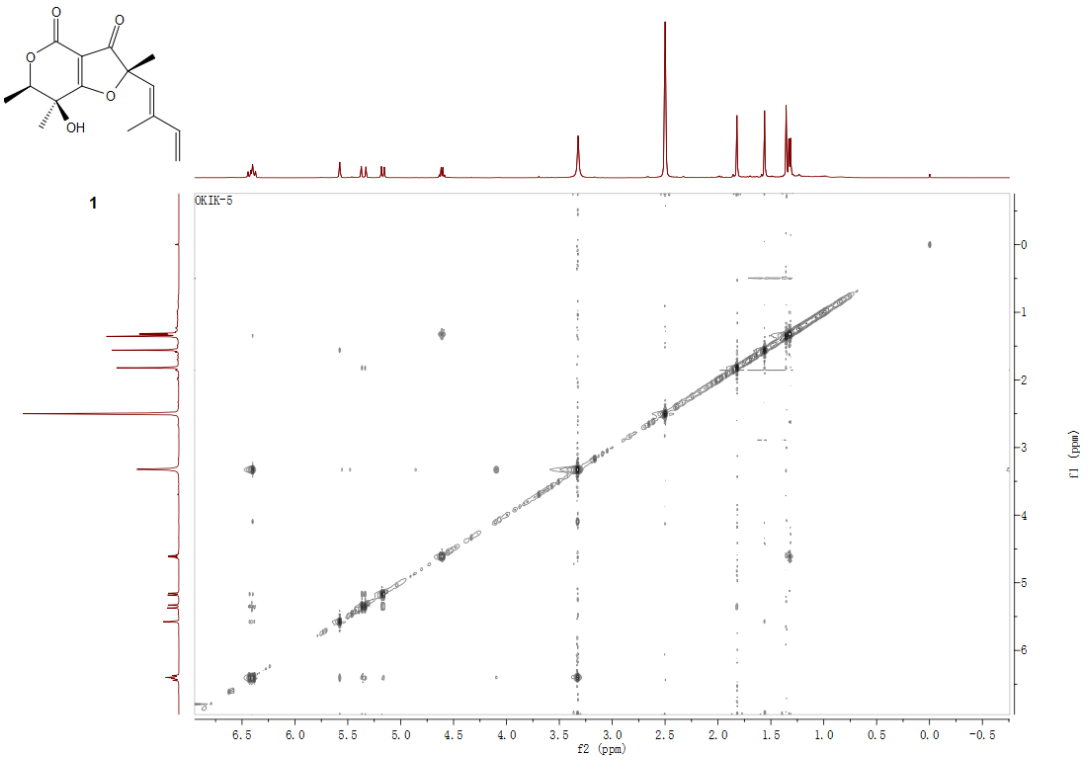

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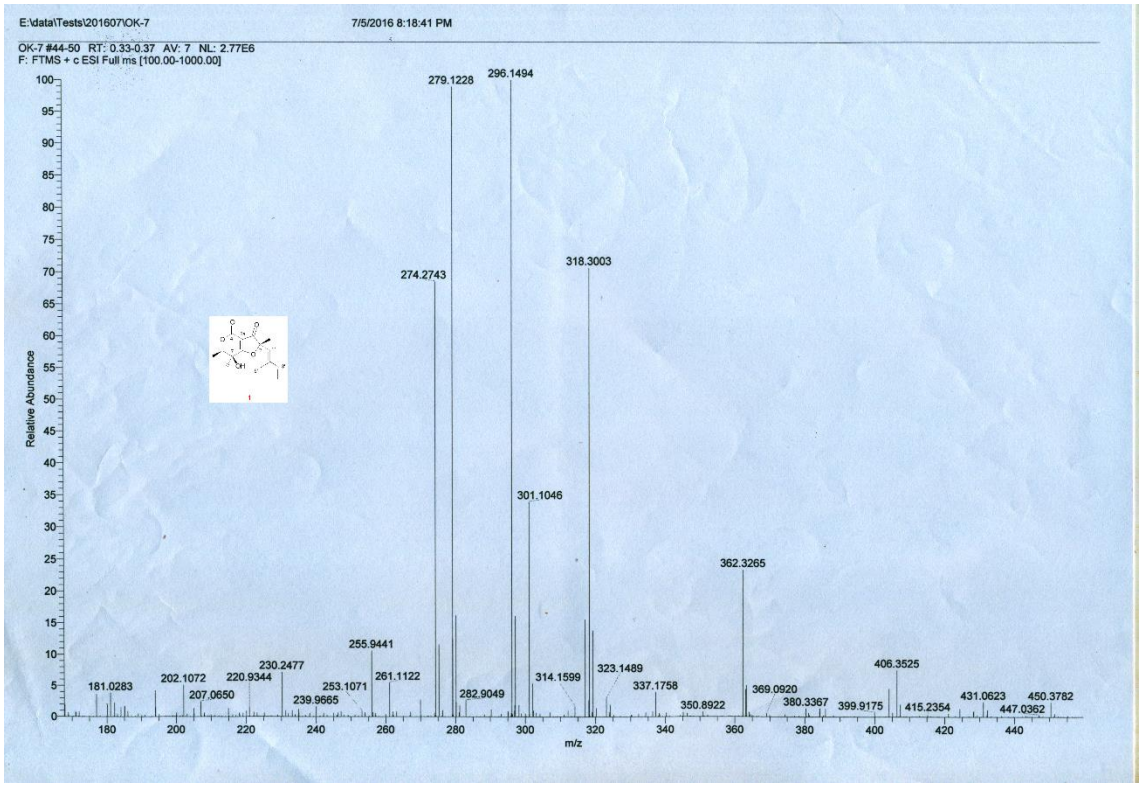


Fig. S7 HRESIMS spectrum of **1**.

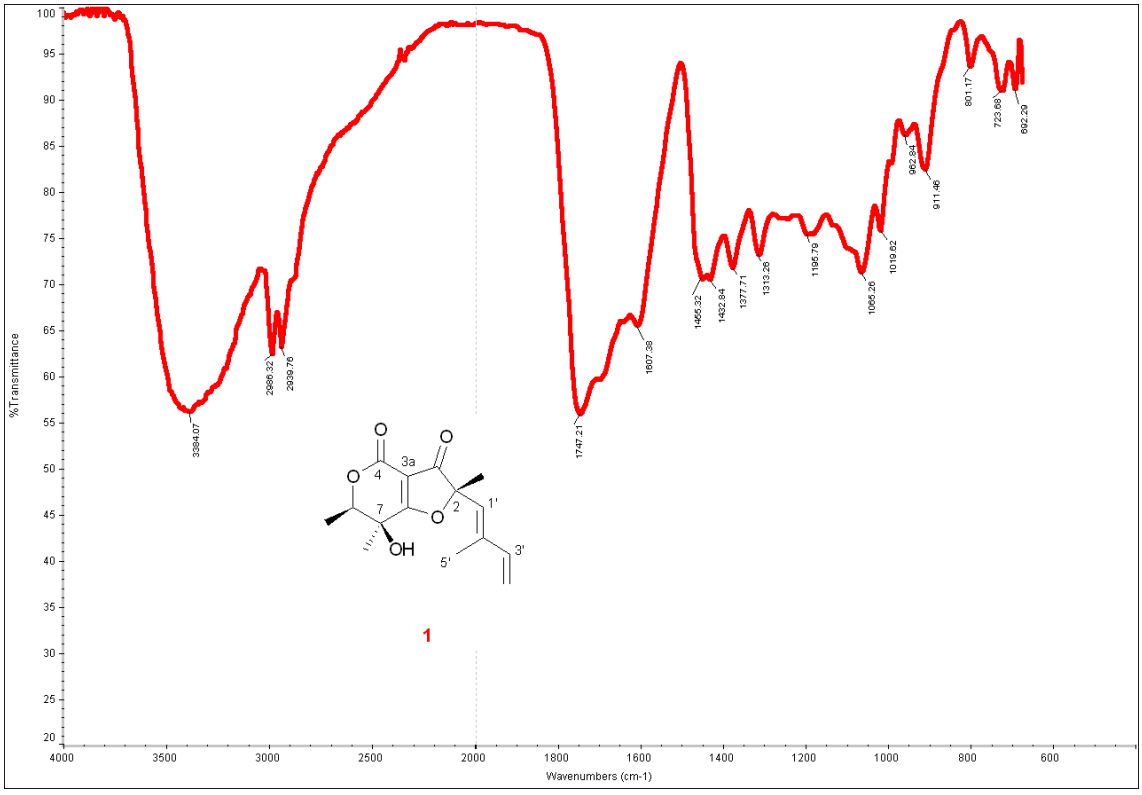


Fig. S8 IR (KBr disc) spectrum of **1**.

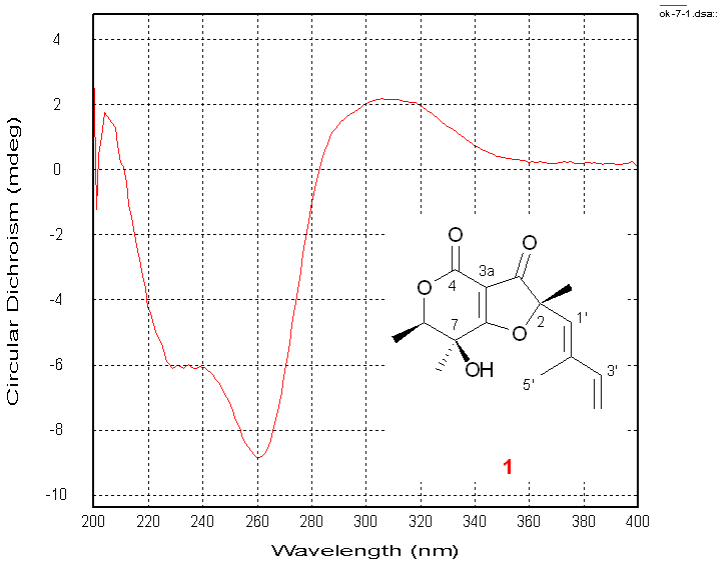


Fig. S9 CD spectrum of **1**.

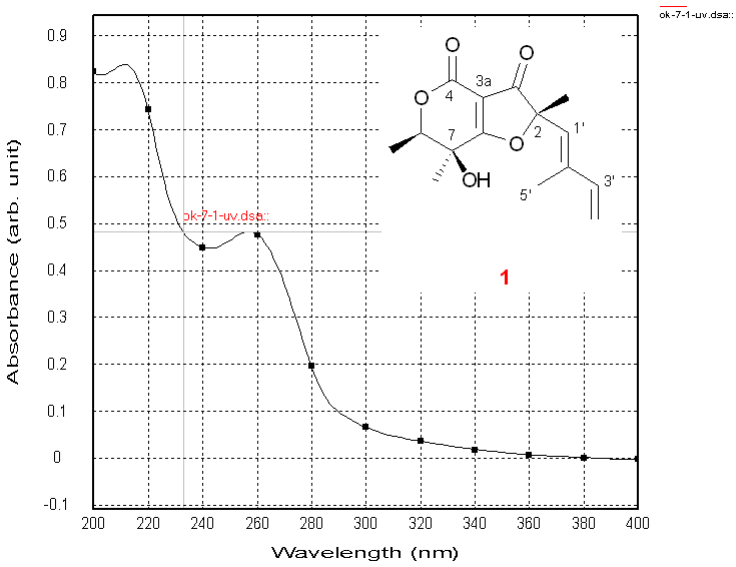


Fig. S10 UV spectrum of **1**.

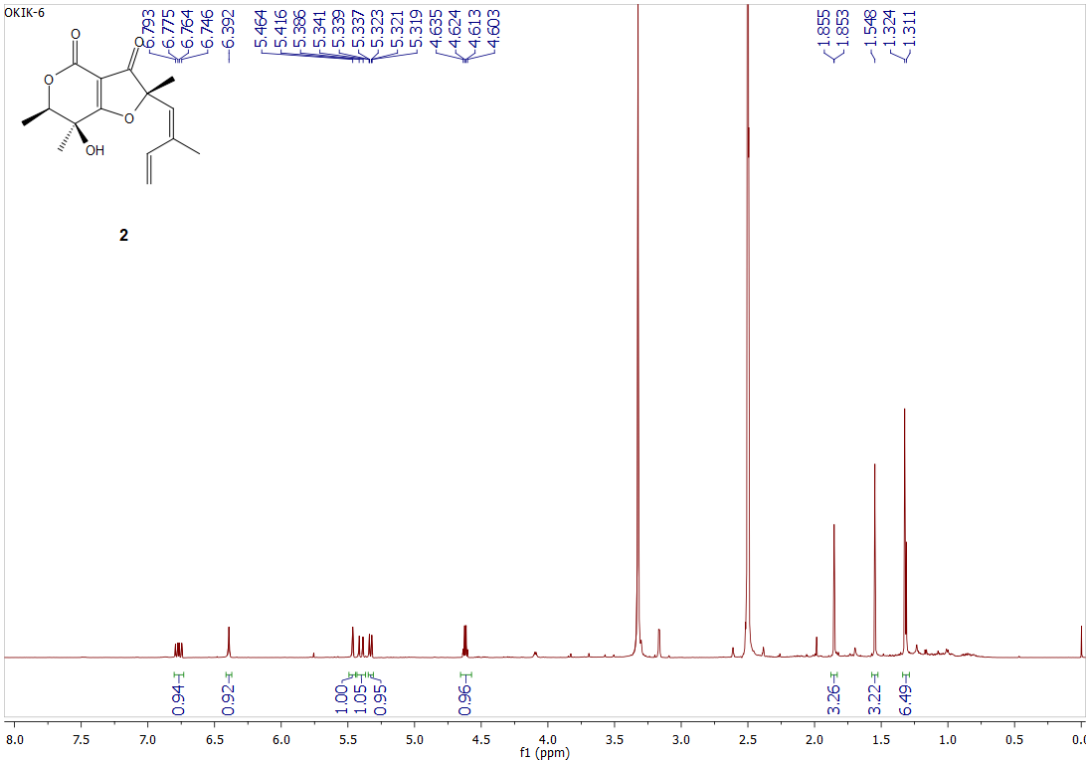


Fig. S11 ^{1}H NMR spectrum (600 MHz) of **2** in DMSO-d_6.

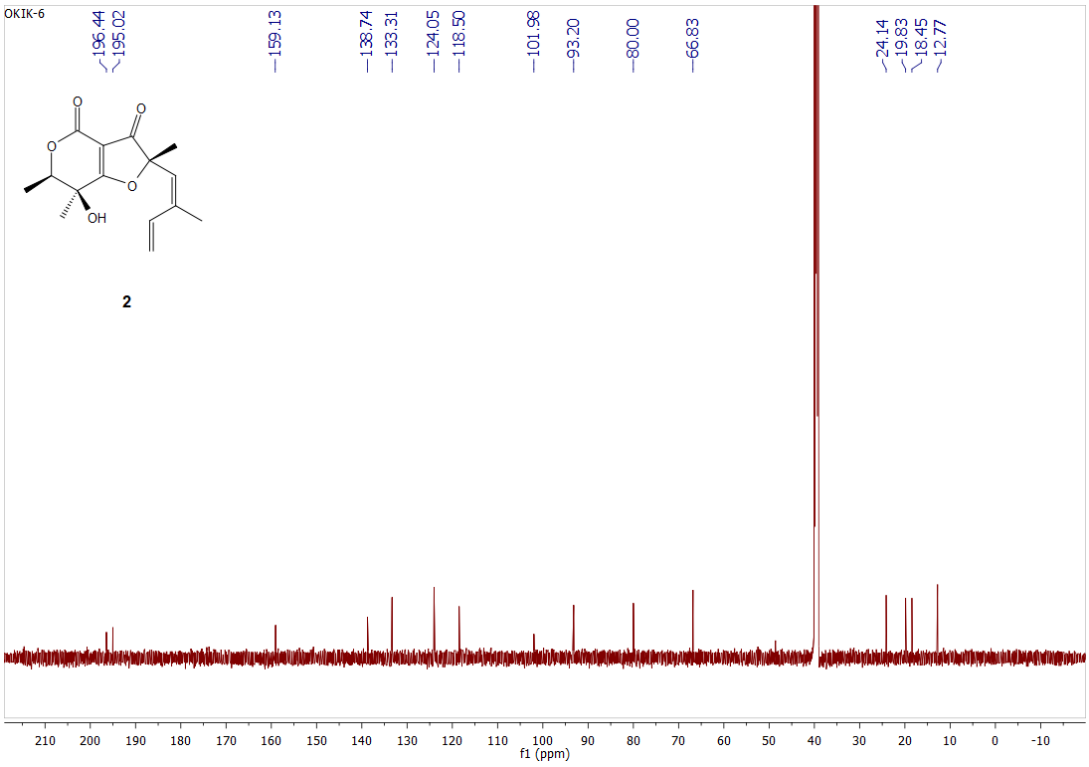


Fig. S12 ^{13}C NMR spectrum (150 MHz) of **2** in DMSO-d_6.

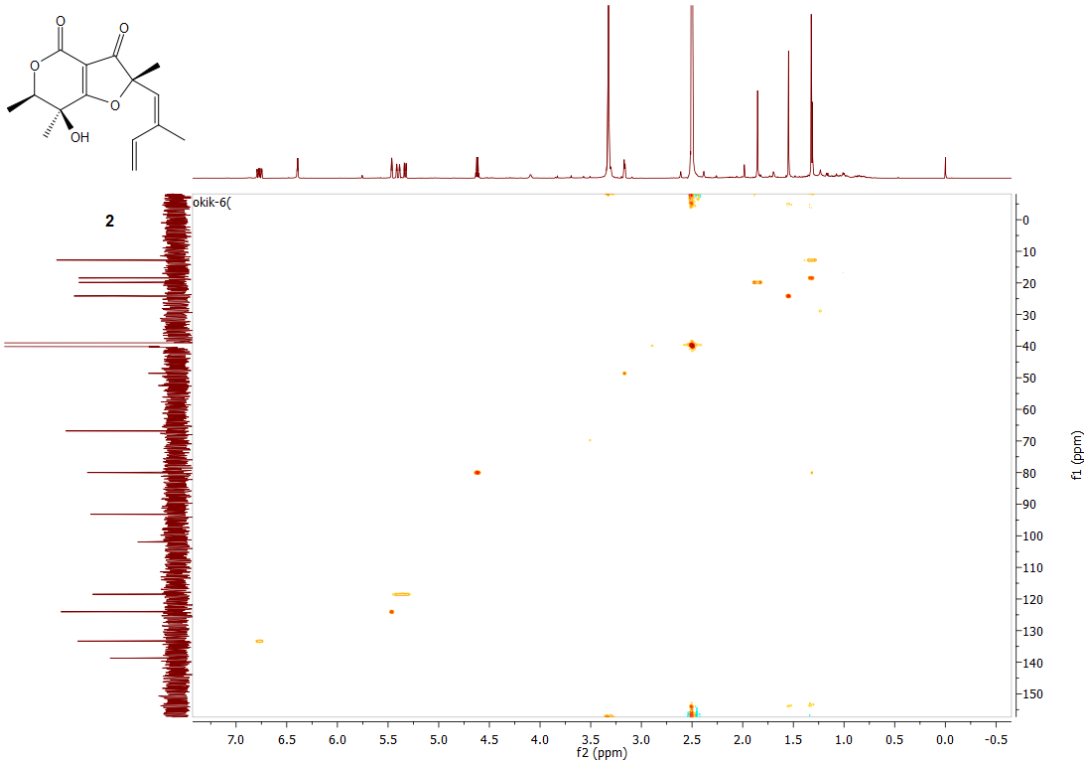
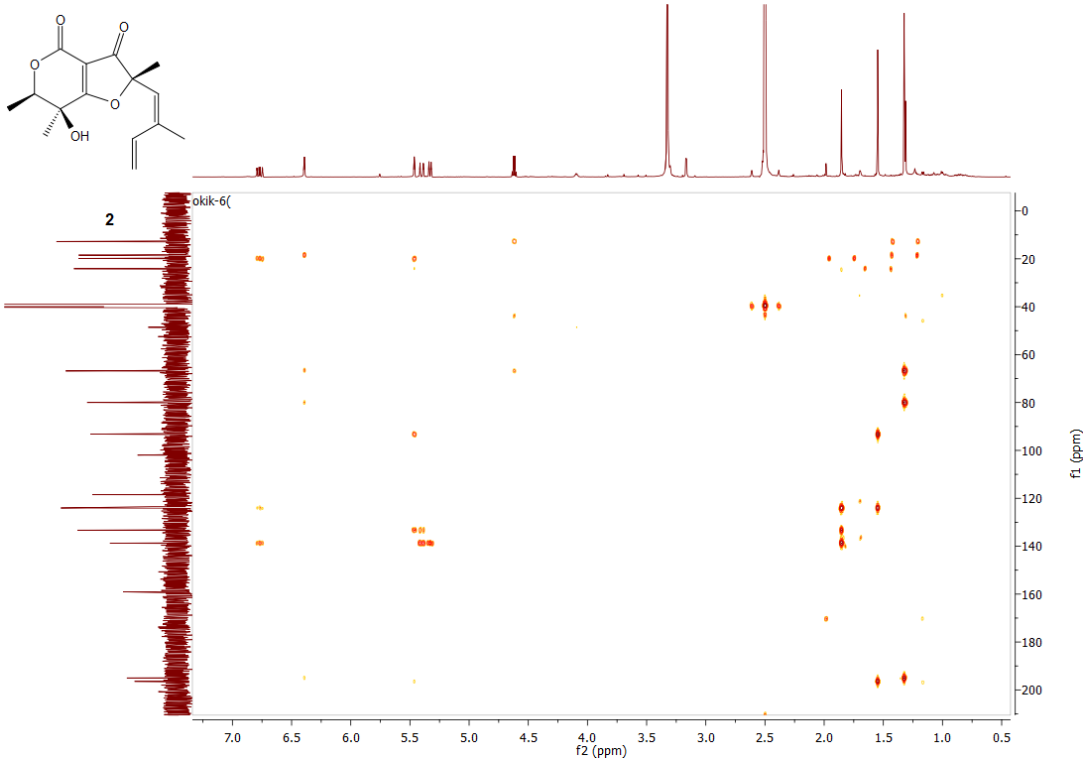


Fig. S13 HSQC spectrum (600 MHz) of **2** in DMSO-d_6.



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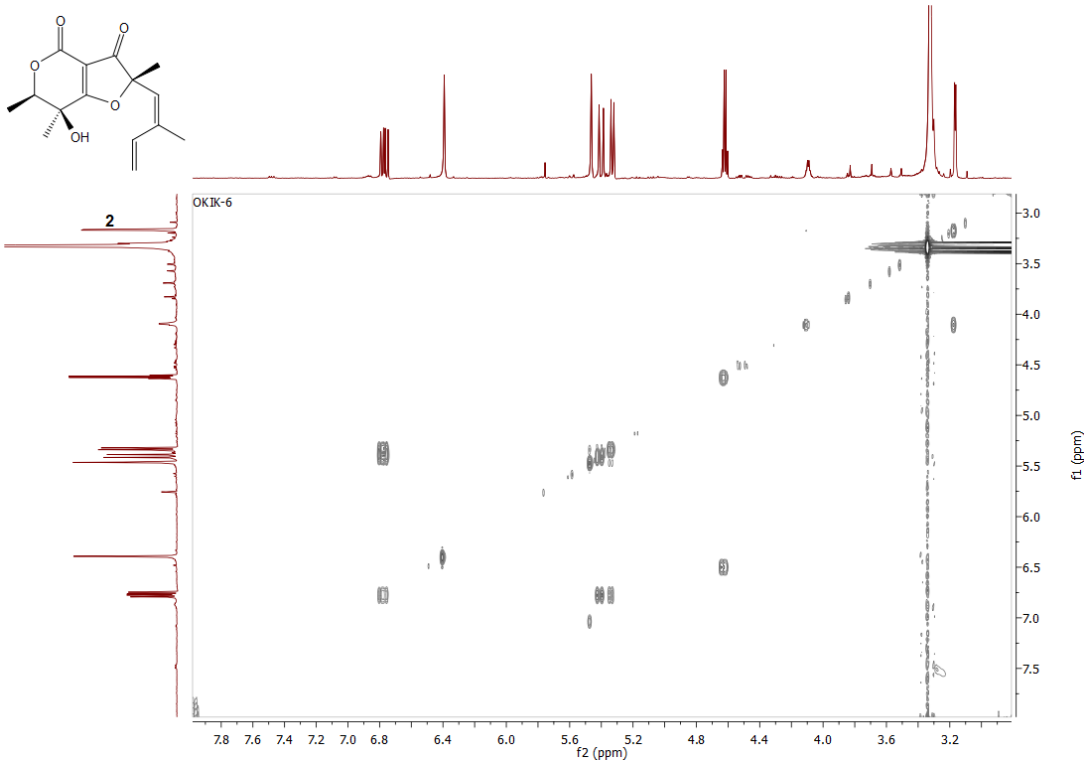


Fig. S15 ^{1}H-^{1}H COSY spectrum (600 MHz) of **2** in DMSO-d_6.

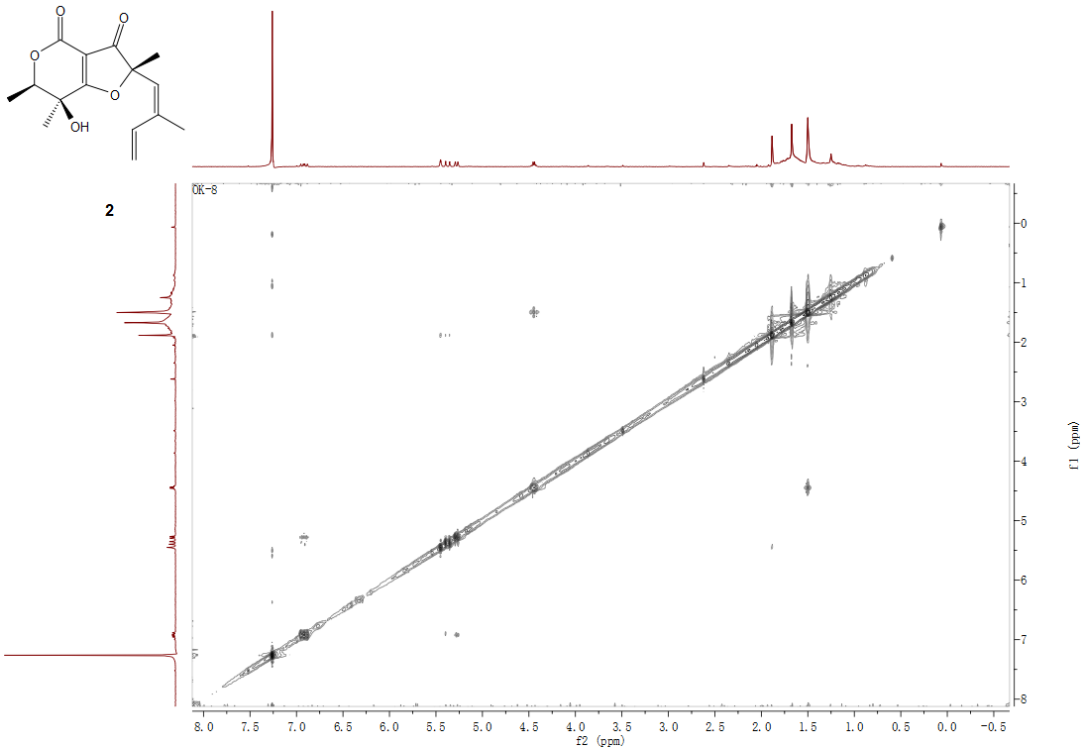


Fig. S16 NOESY spectrum (600 MHz) of **2** in $CDCl_3$.

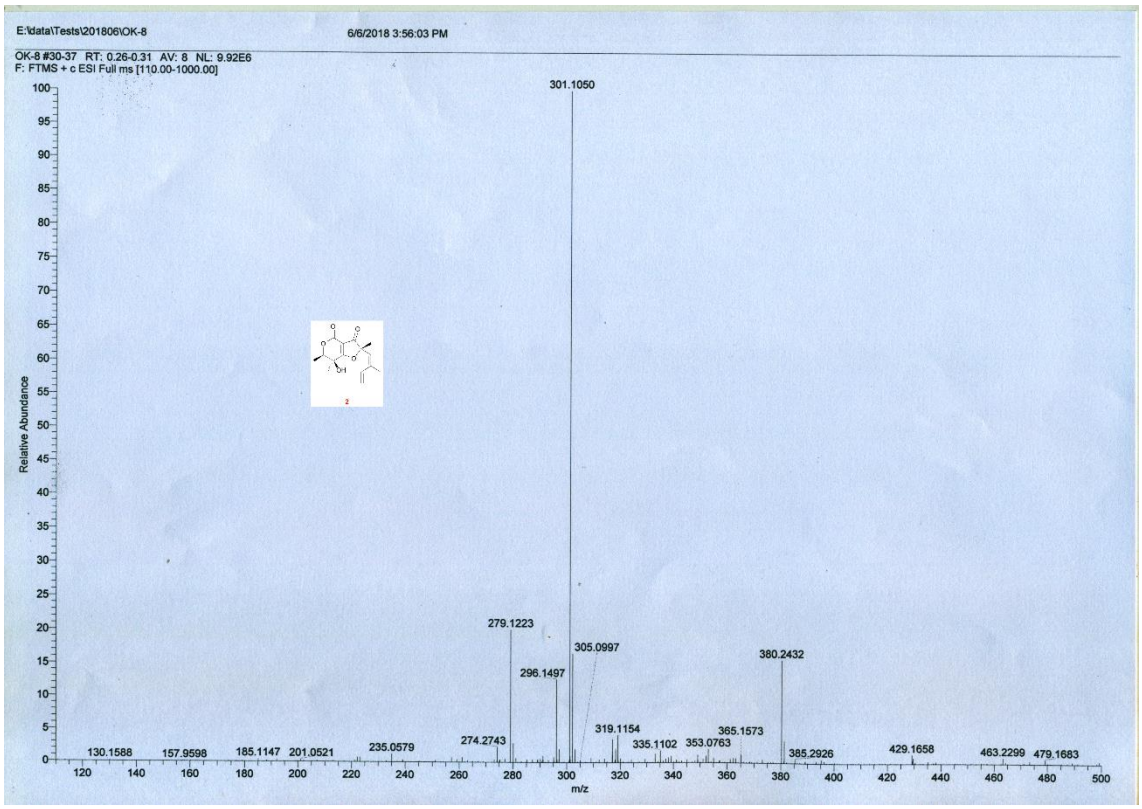


Fig. S17 HRESIMS spectrum of **2**.

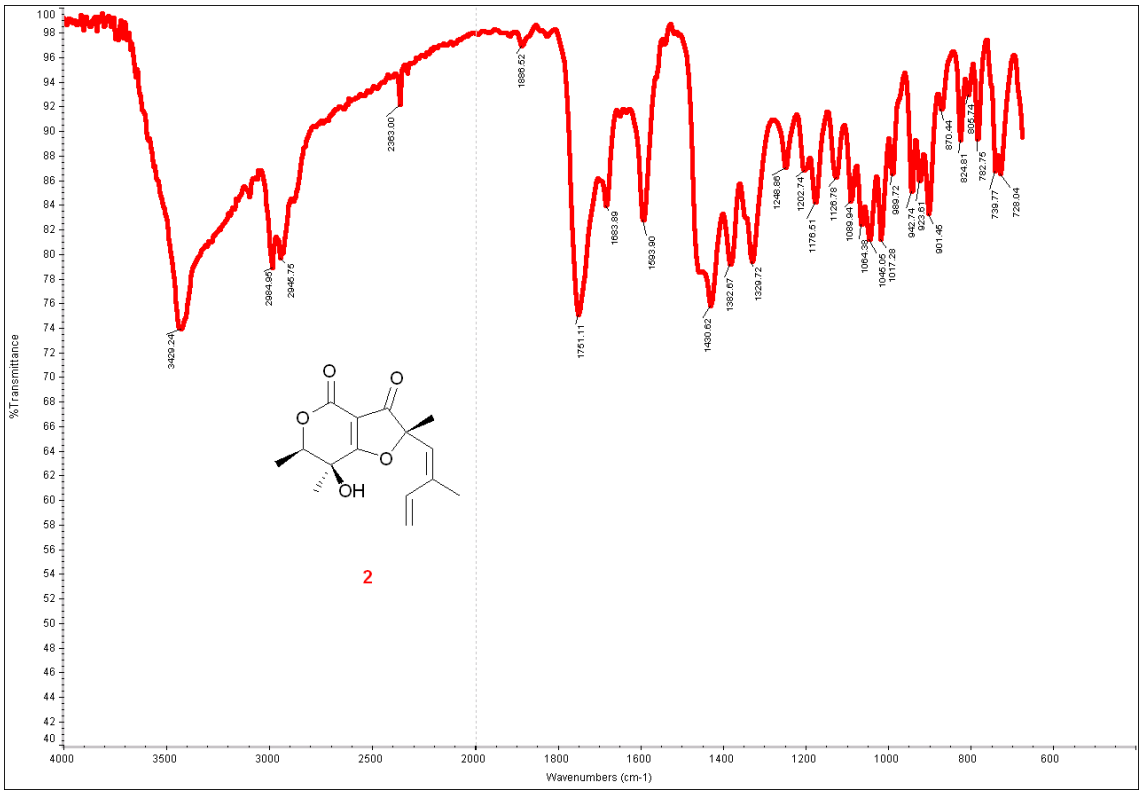


Fig. S18 IR (KBr disc) spectrum of **2**.

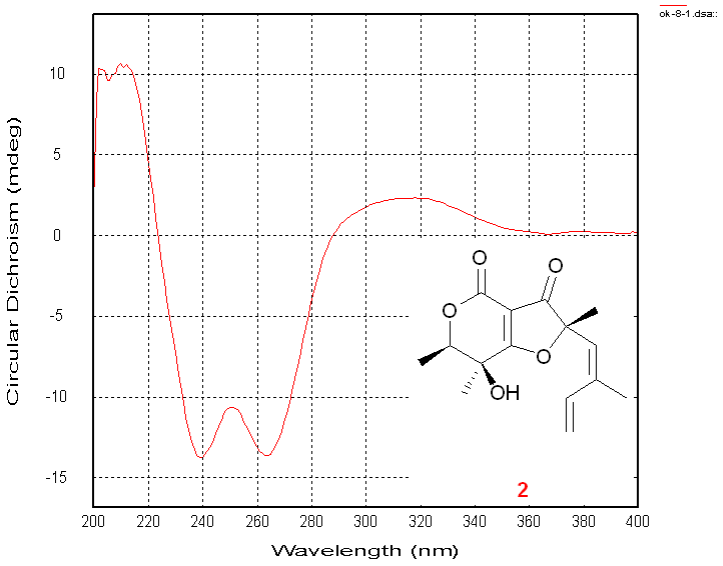


Fig. S19 CD spectrum of **2**.

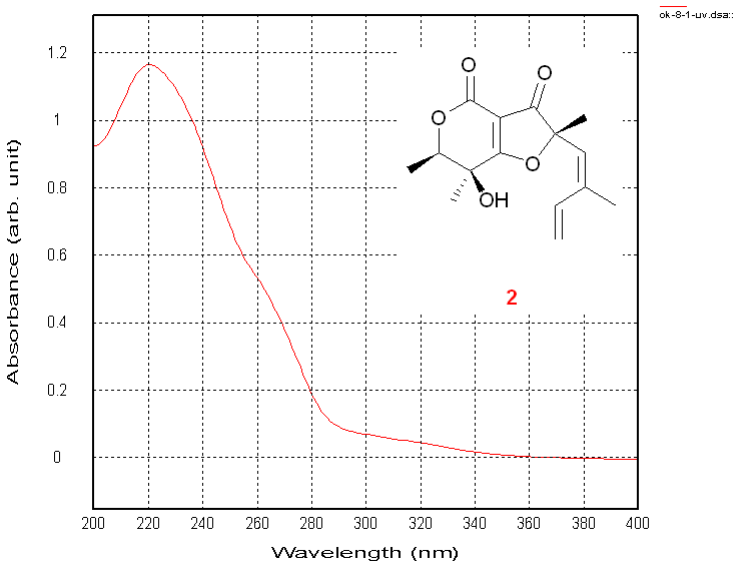


Fig. S20 UV spectrum of **2.**

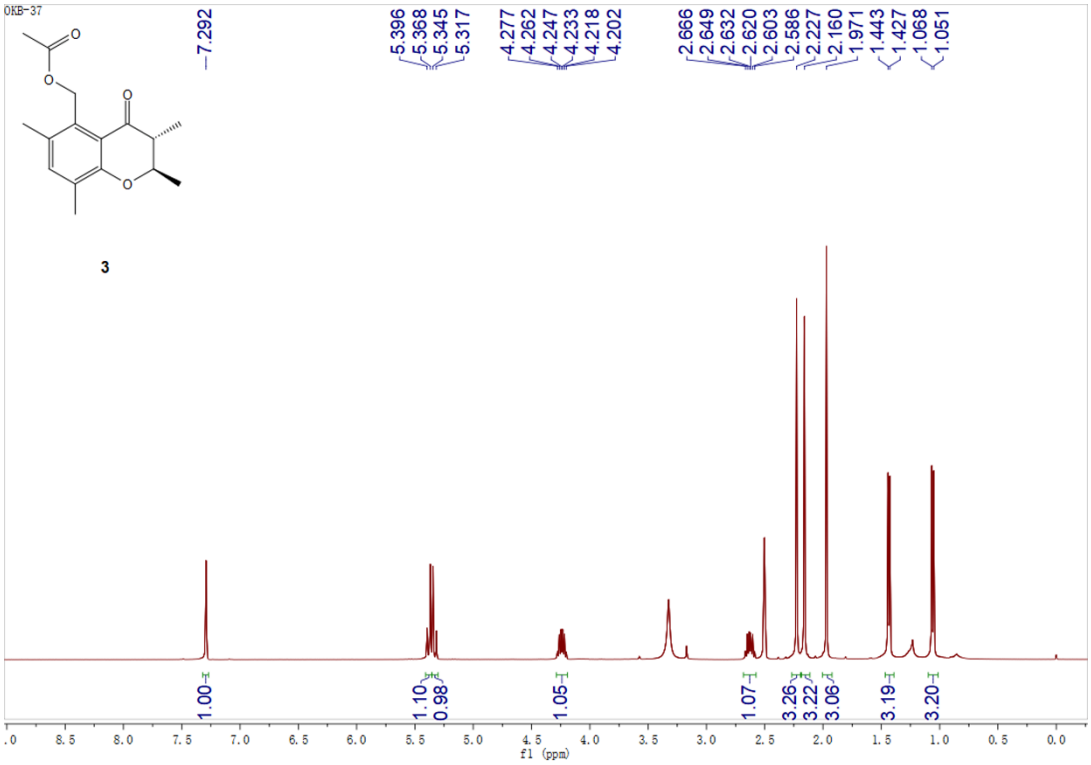


Fig. S21 ^{1}H NMR spectrum (400 MHz) of **3** in DMSO-d_6.

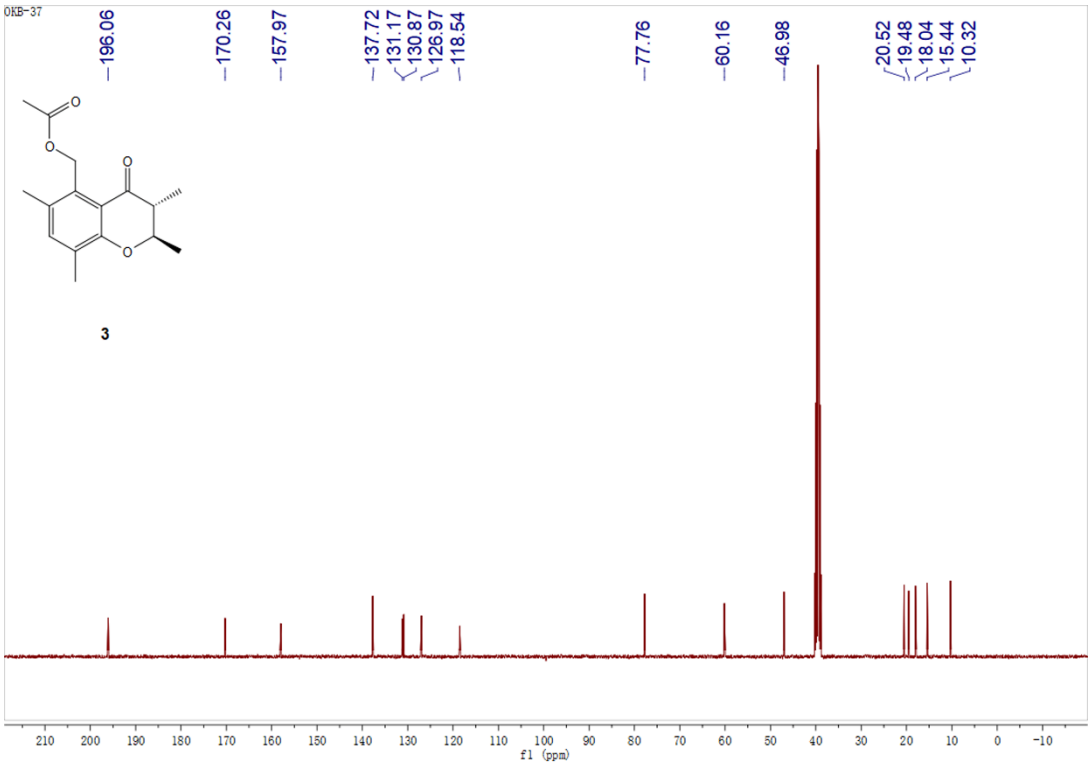


Fig. S22 ^{13}C NMR spectrum (100 MHz) of **3** in DMSO-d_6.

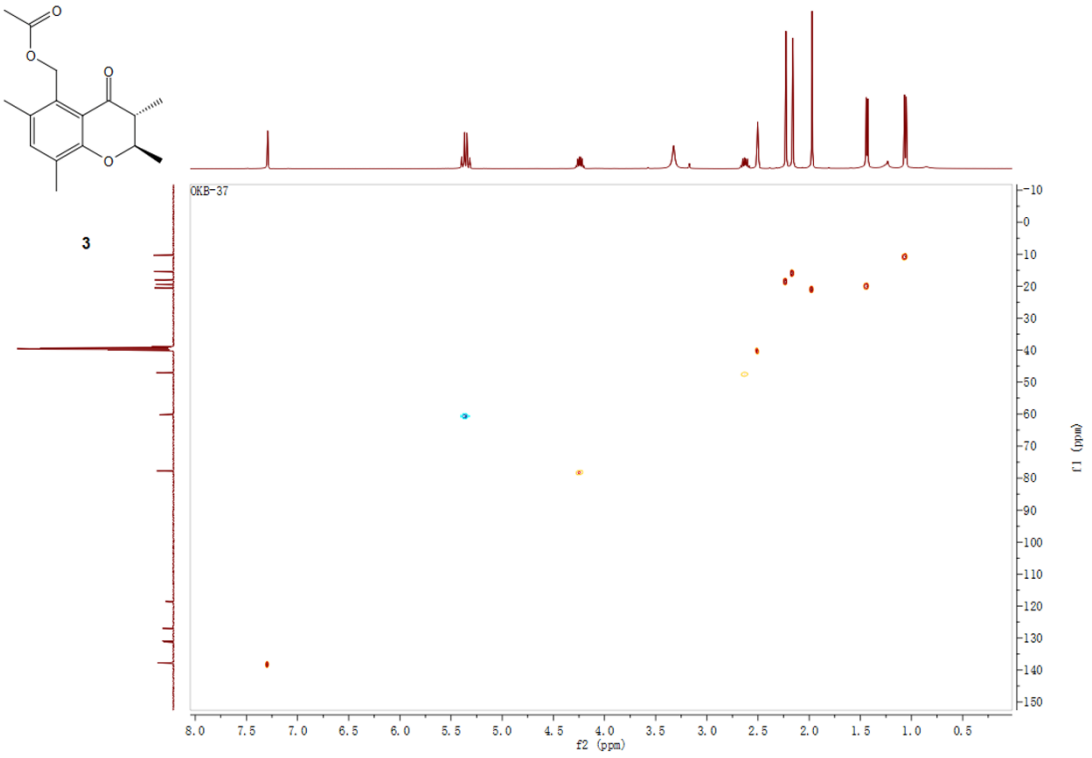


Fig. S23 HSQC spectrum (400 MHz) of **3** in DMSO-d_6.

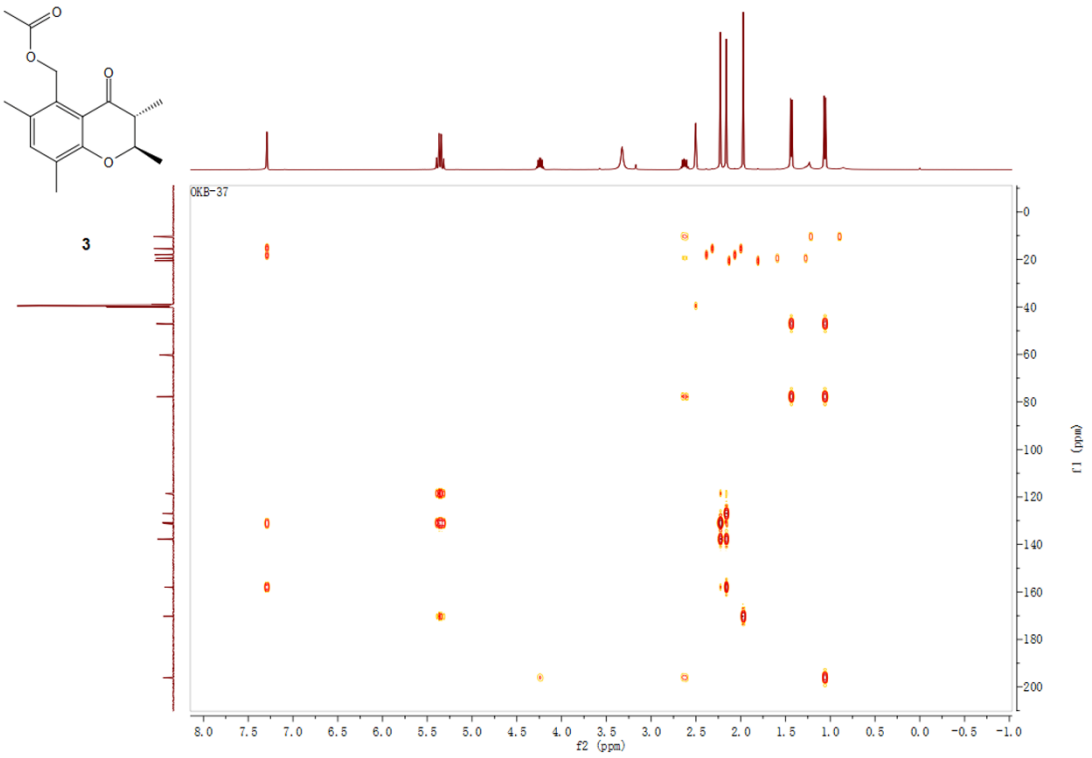


Fig. S24 HMBC spectrum (400 MHz) of **3** in DMSO-d_6.

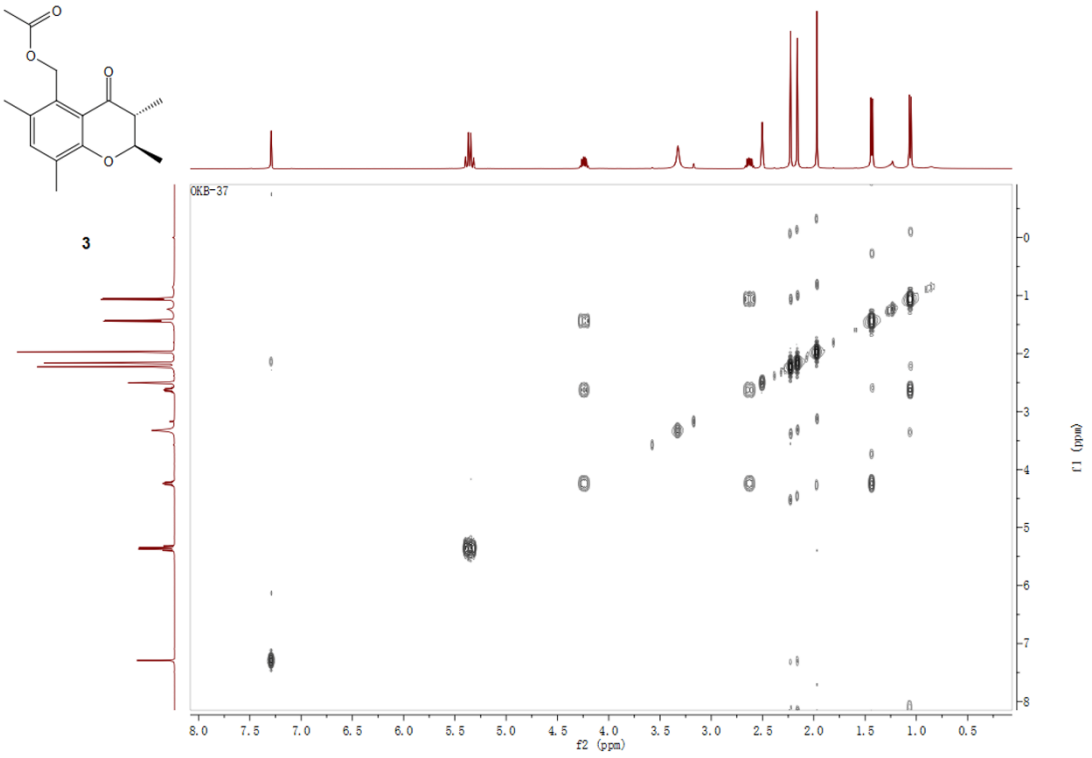


Fig. S25 ^{1}H-^{1}H COSY spectrum (400 MHz) of **3** in DMSO-d_6.

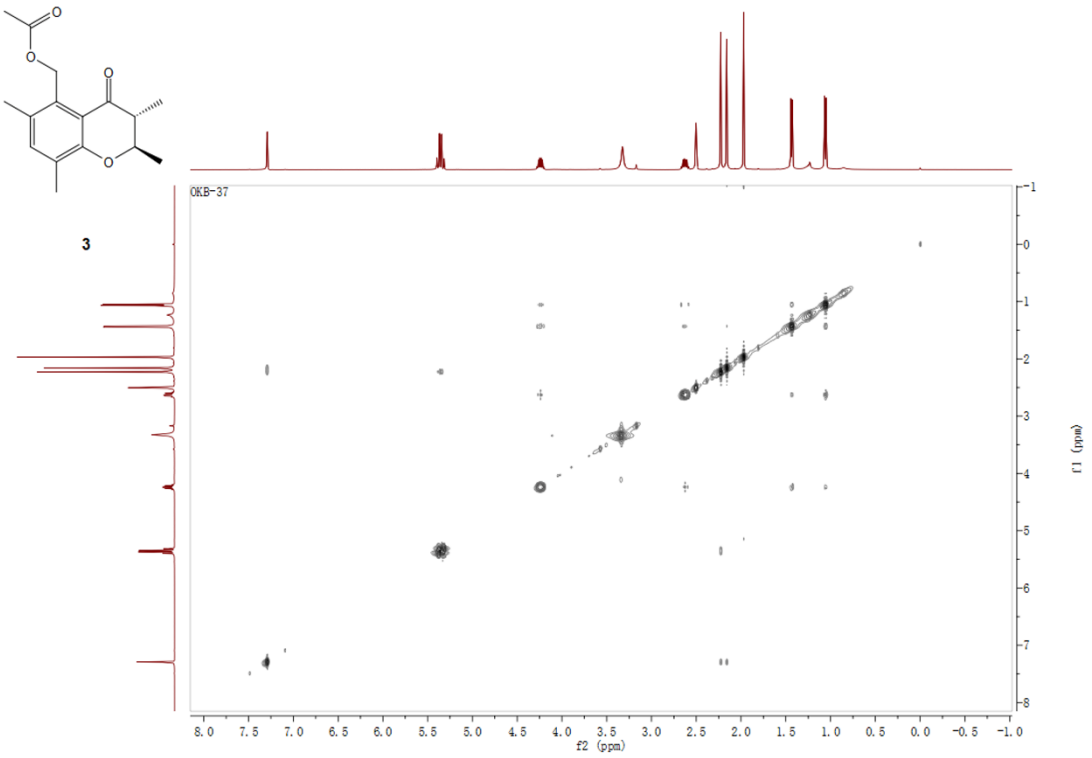


Fig. S26 NOESY spectrum (400 MHz) of **3** in DMSO-d_6.

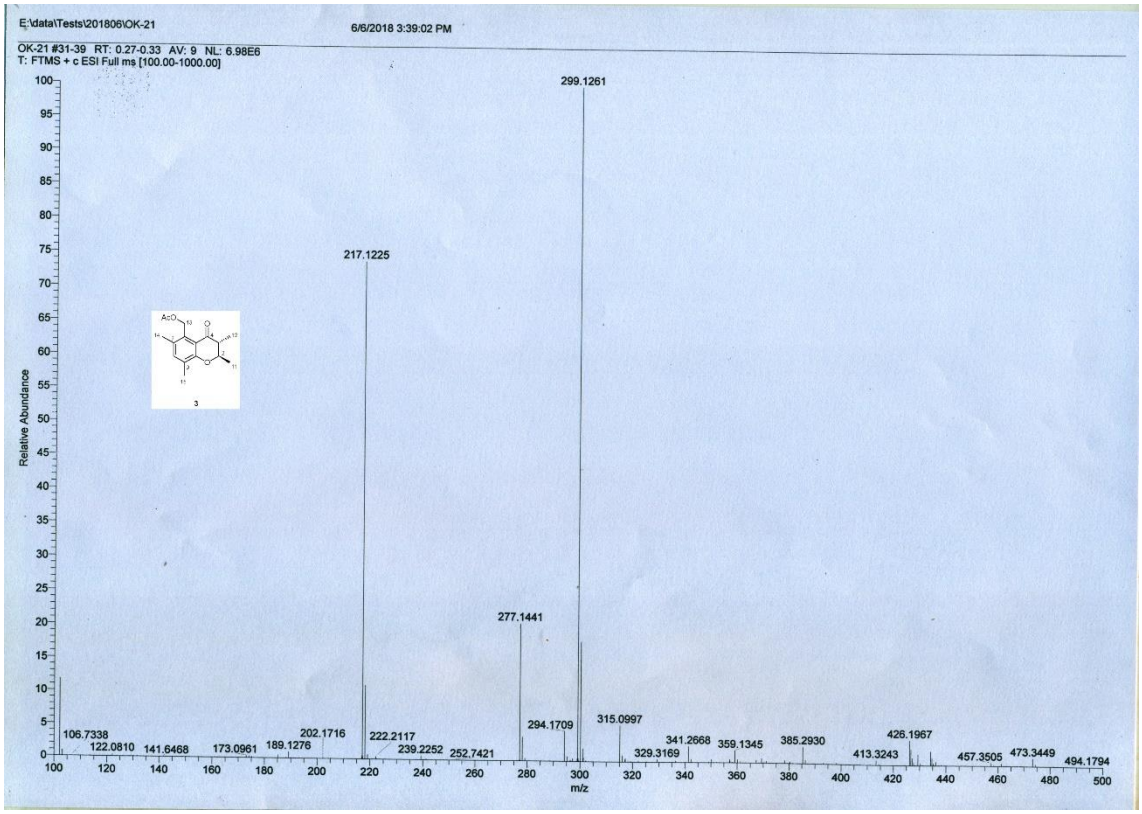


Fig. S27 HRESIMS spectrum of **3**.

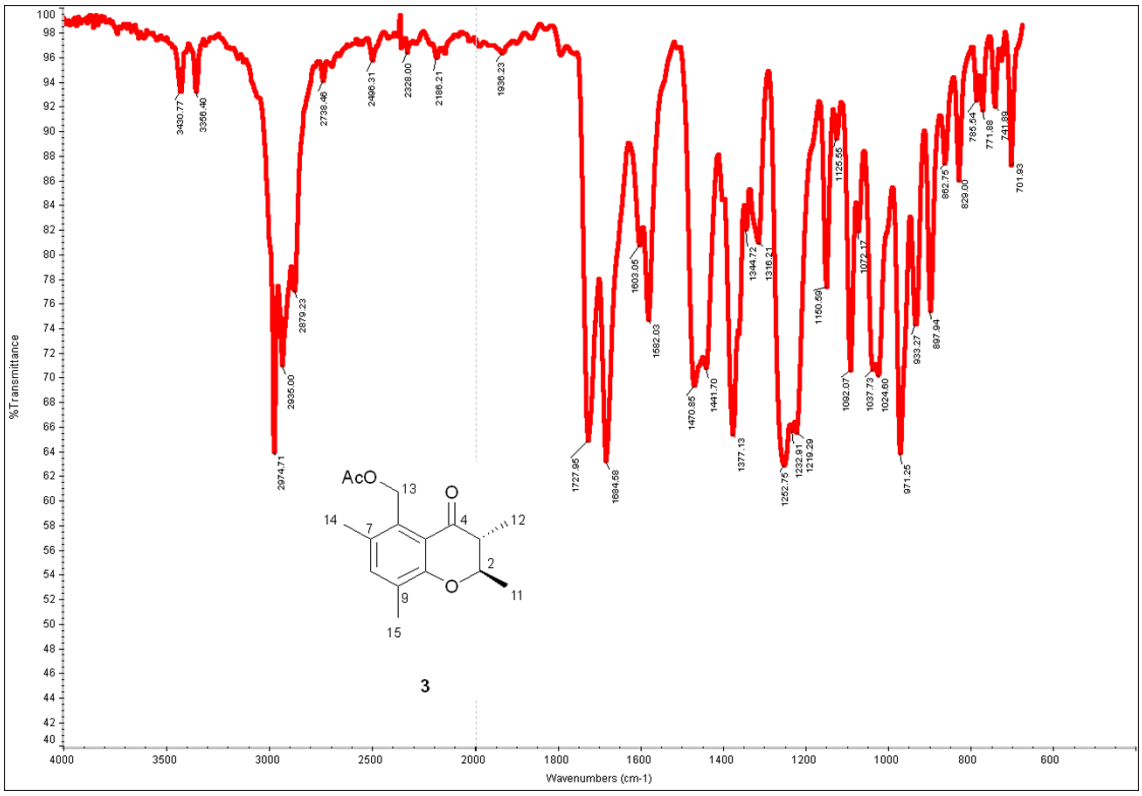


Fig. S28 IR (KBr disc) spectrum of **3**.

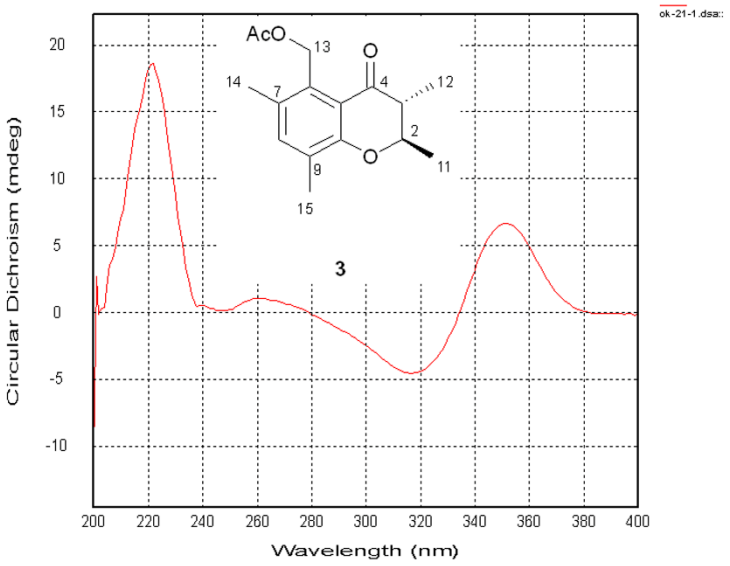


Fig. S29 CD spectrum of 3.

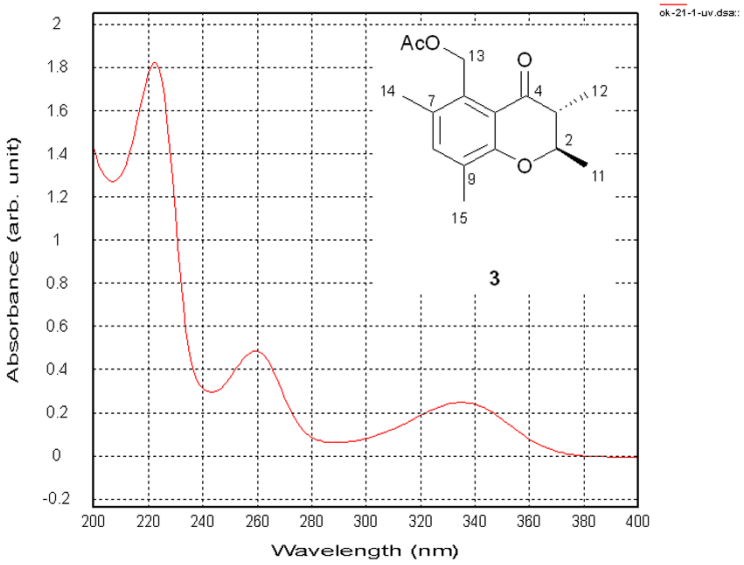


Fig. S30 UV spectrum of **3**.

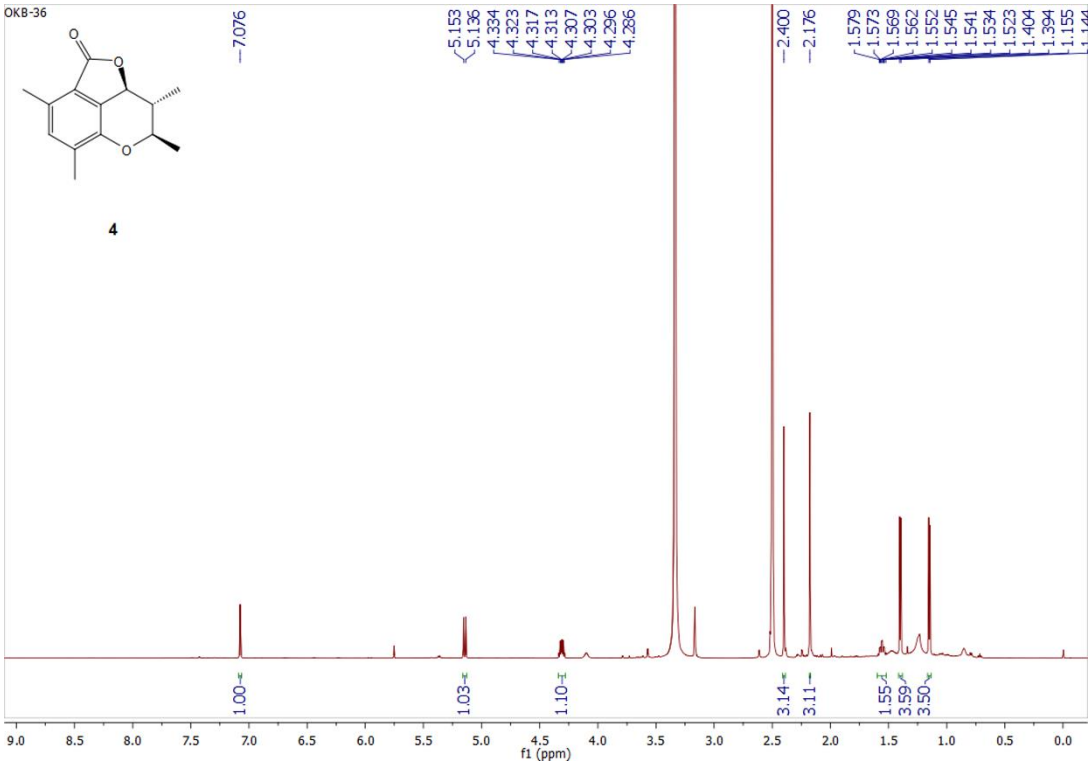


Fig. S31 ^{1}H NMR spectrum (600 MHz) of **4** in DMSO-d_6.

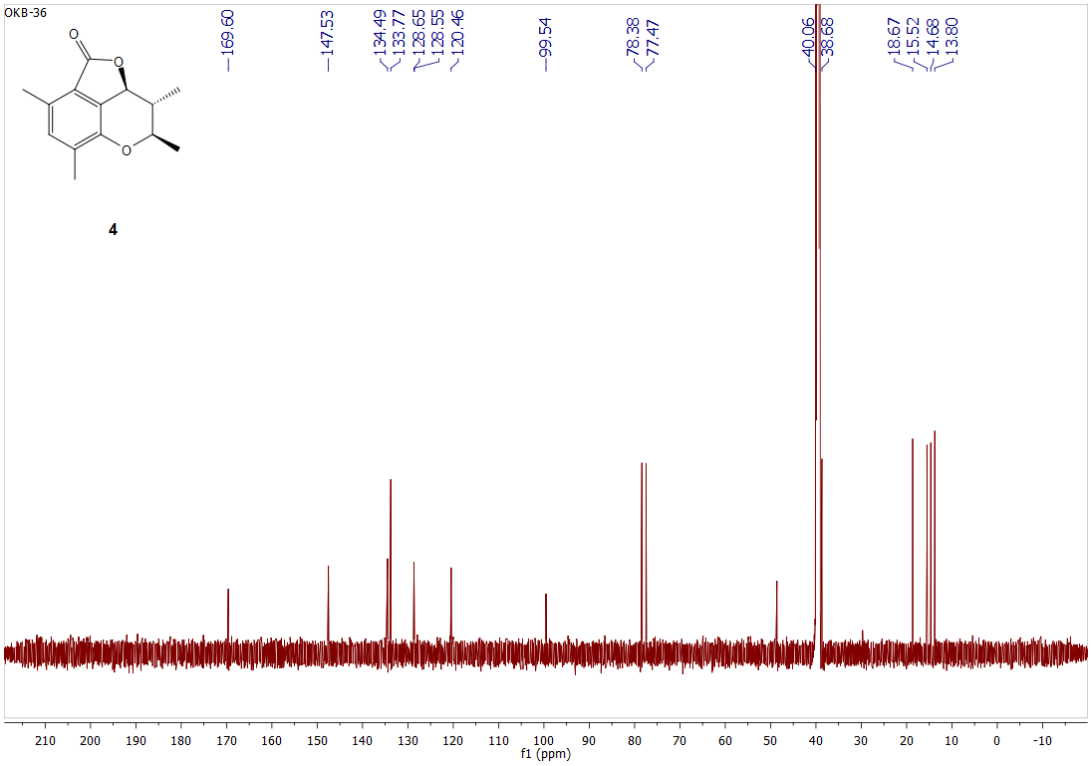


Fig. S32 ^{13}C NMR spectrum (150 MHz) of **4** in DMSO-d_6.

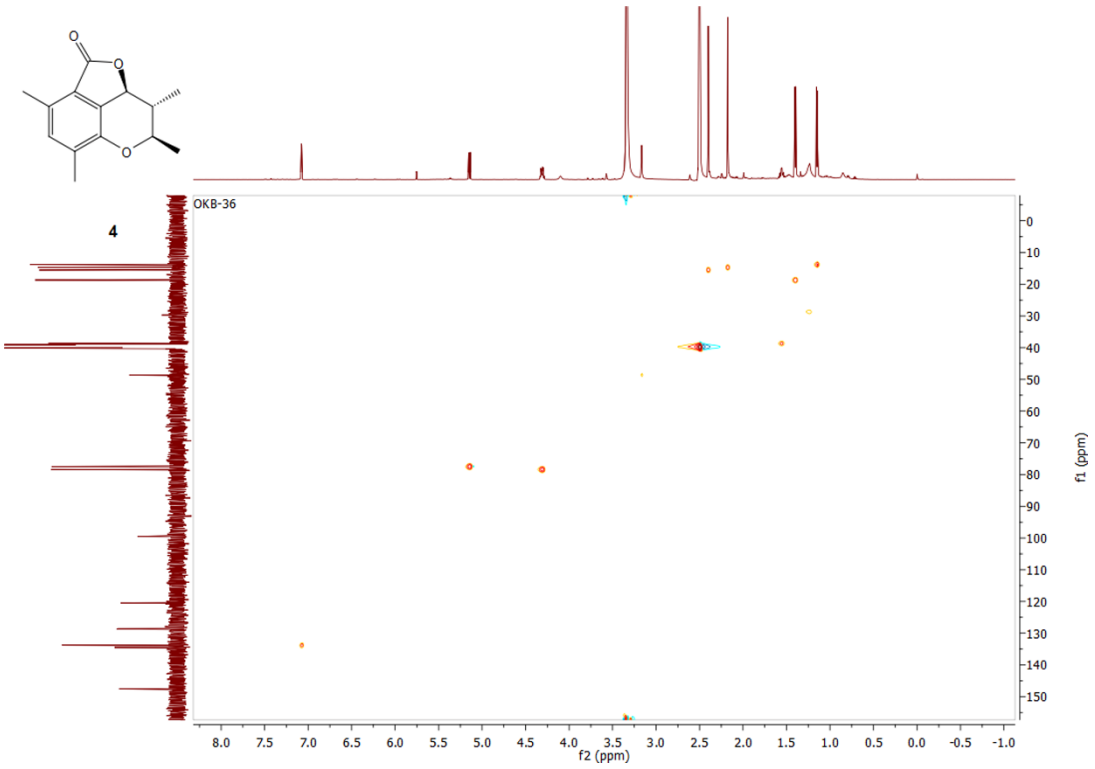
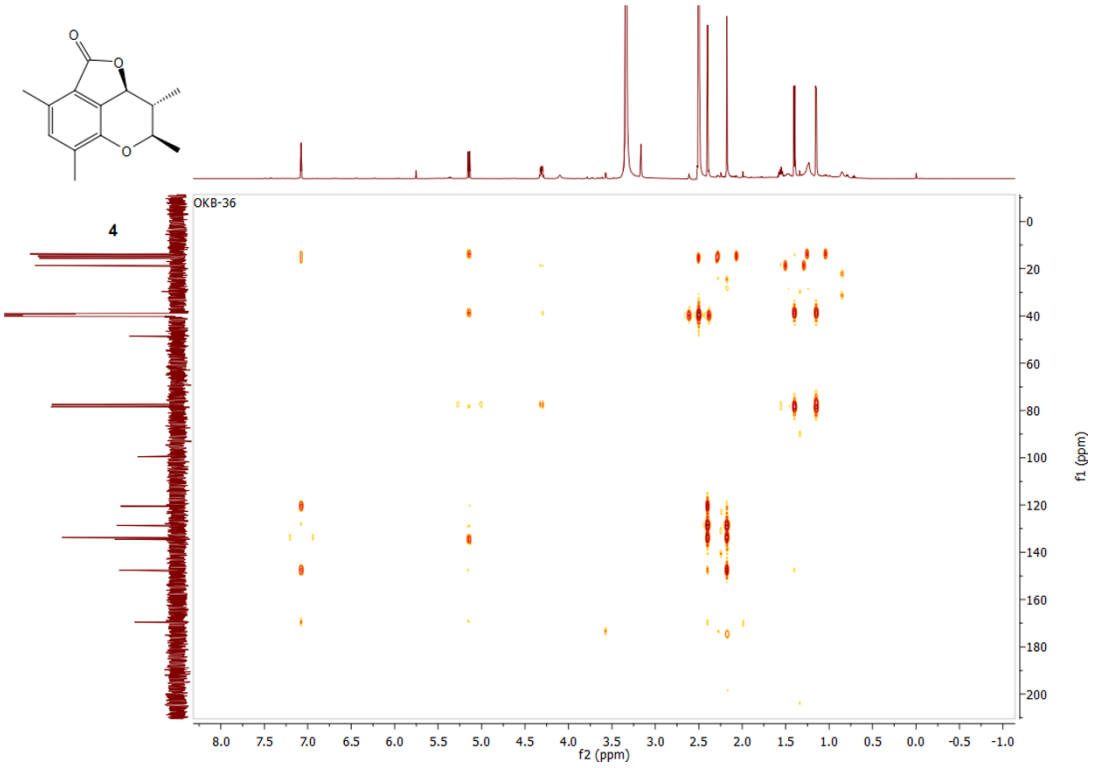


Fig. S33 HSQC spectrum (600 MHz) of **4** in DMSO-d_6.



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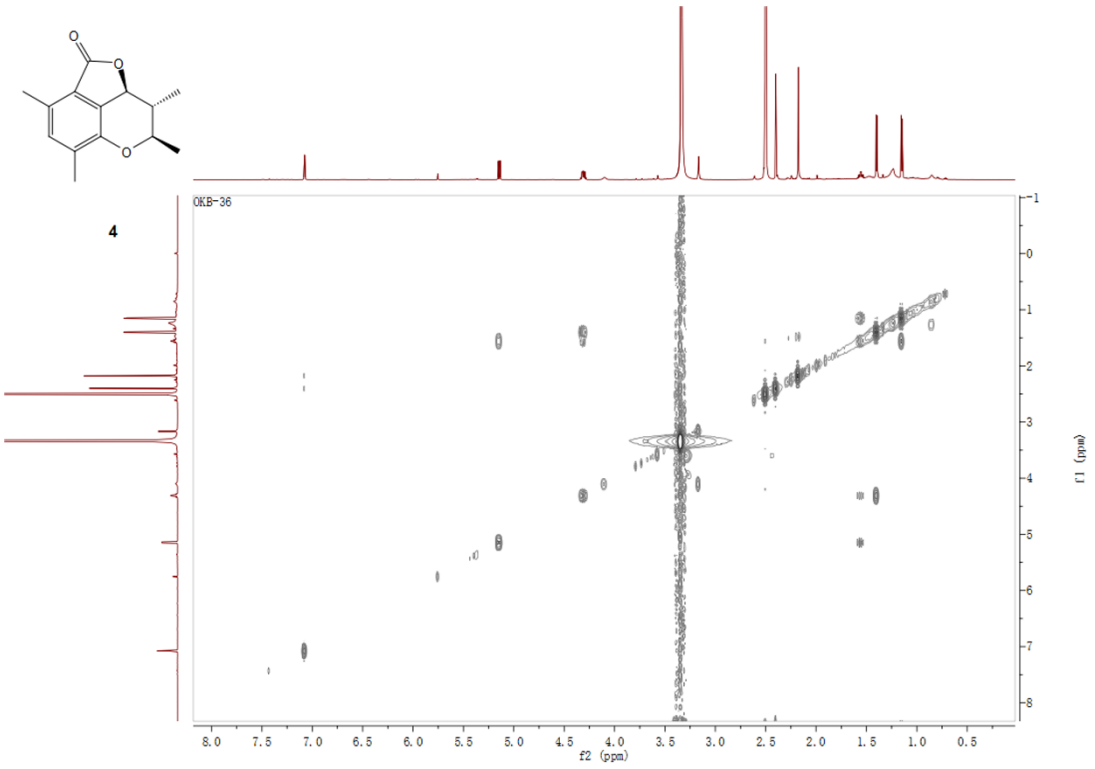
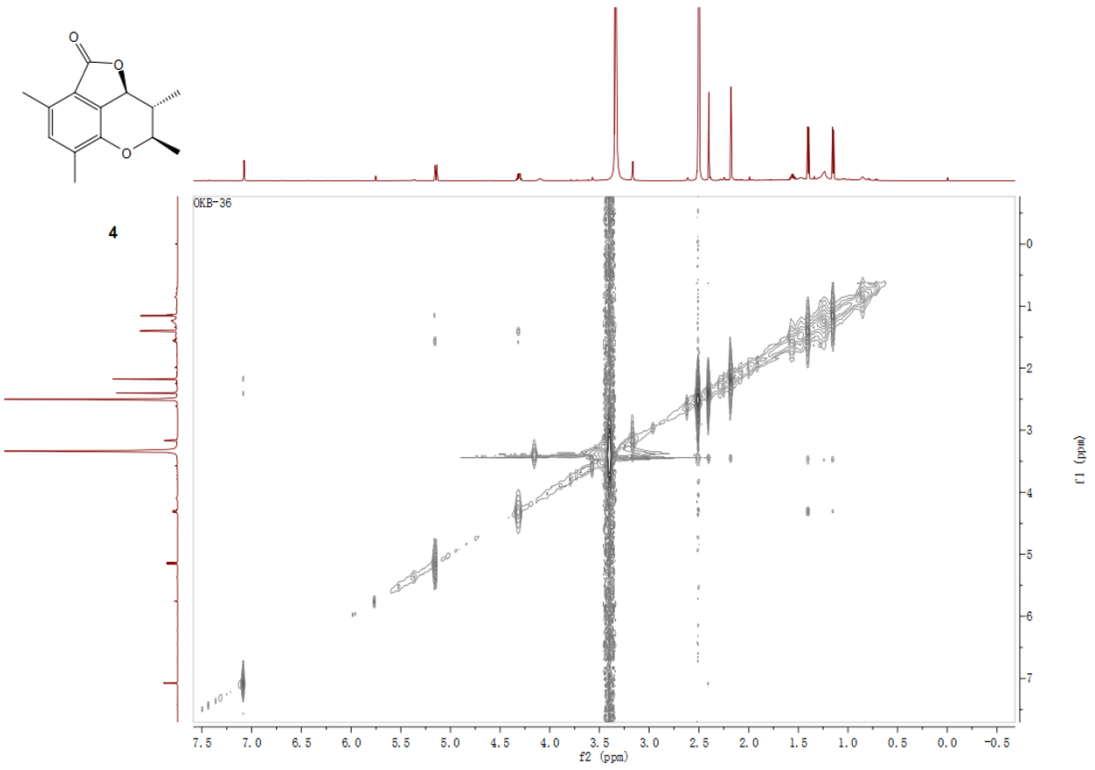


Fig. S35 ^{1}H-^{1}H COSY spectrum (600 MHz) of **4** in DMSO-d_6.



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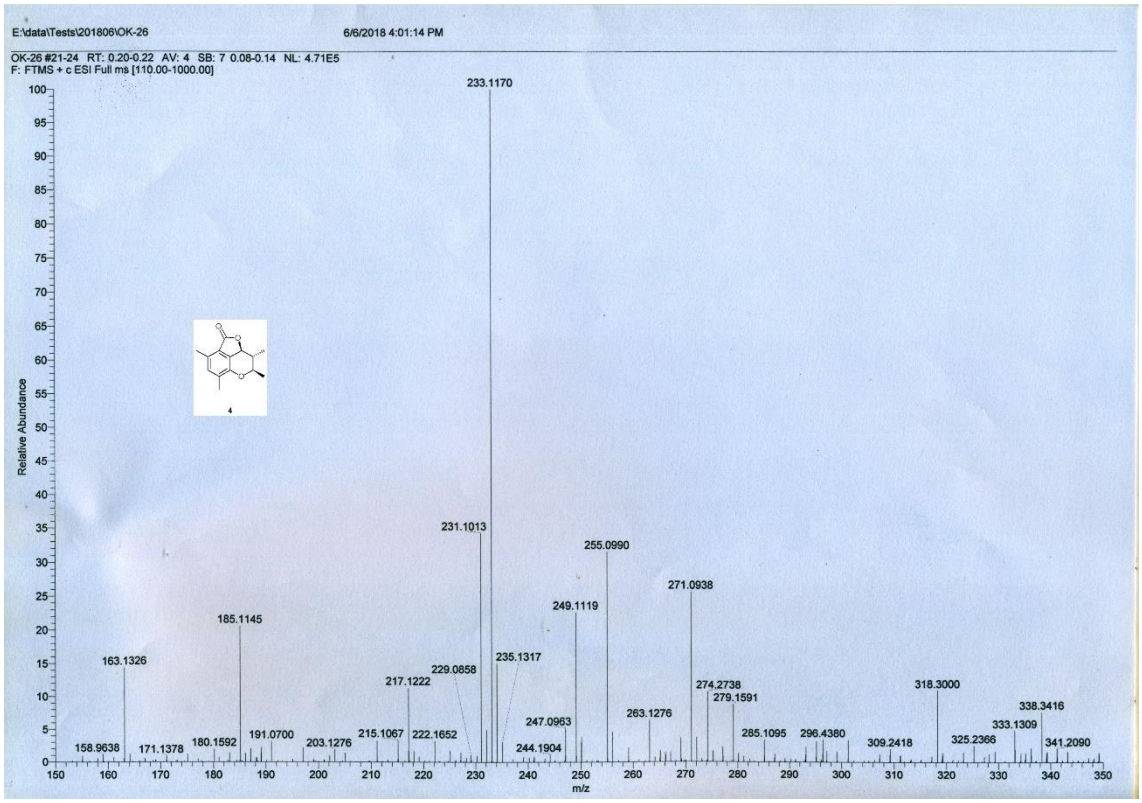

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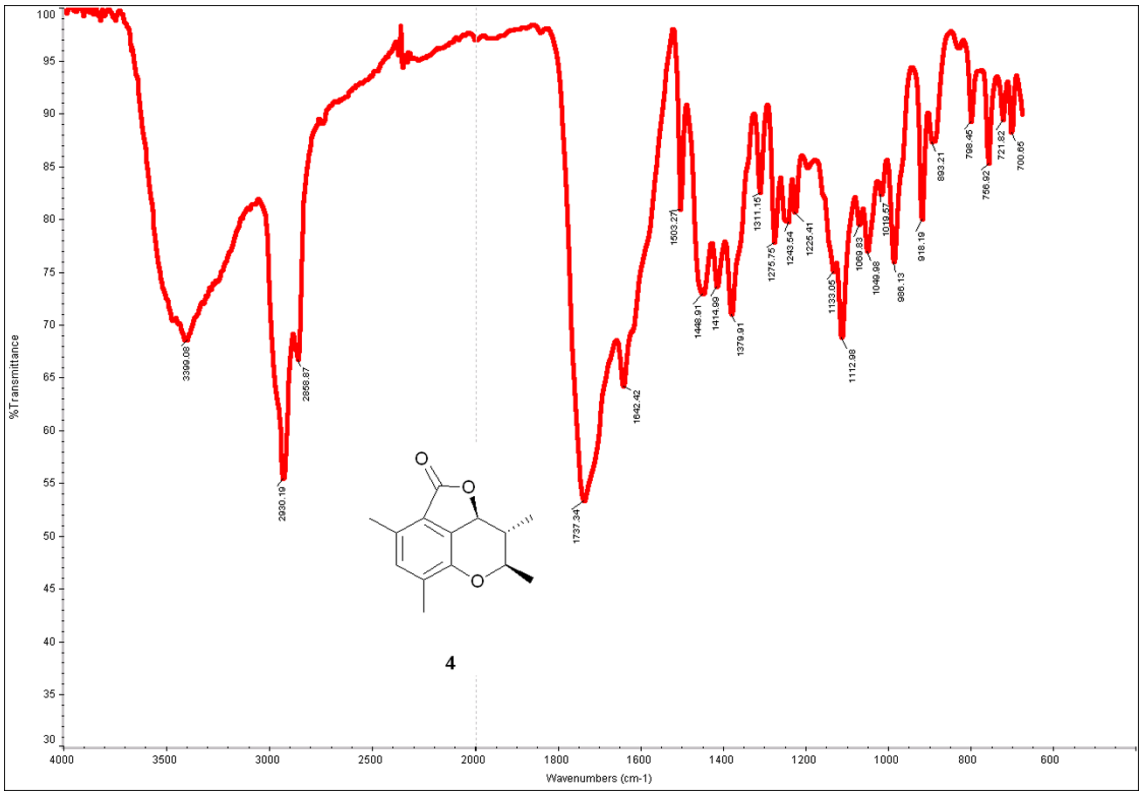


Fig. S38 IR (KBr disc) spectrum of **4**.

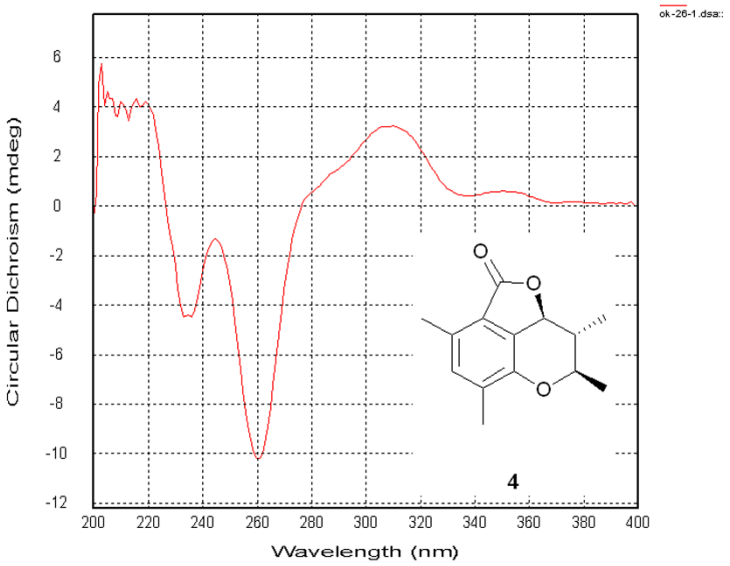


Fig. S39 CD spectrum of **4**.

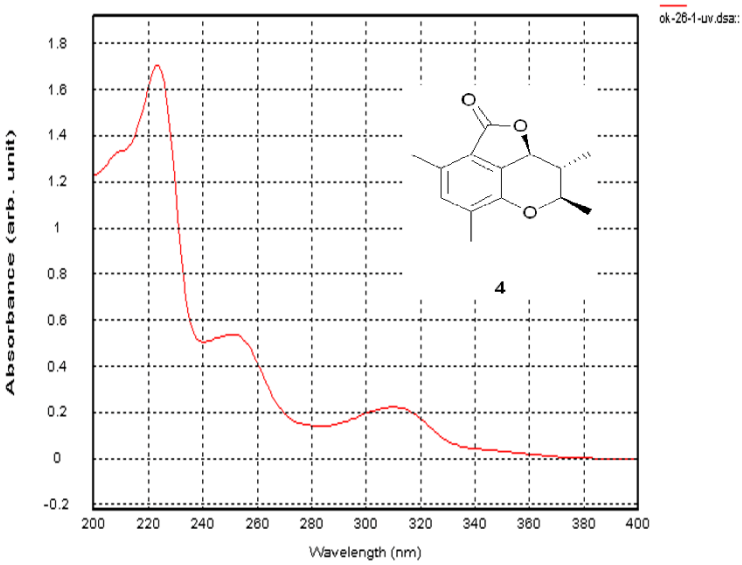


Fig. S40 UV spectrum of **4**.

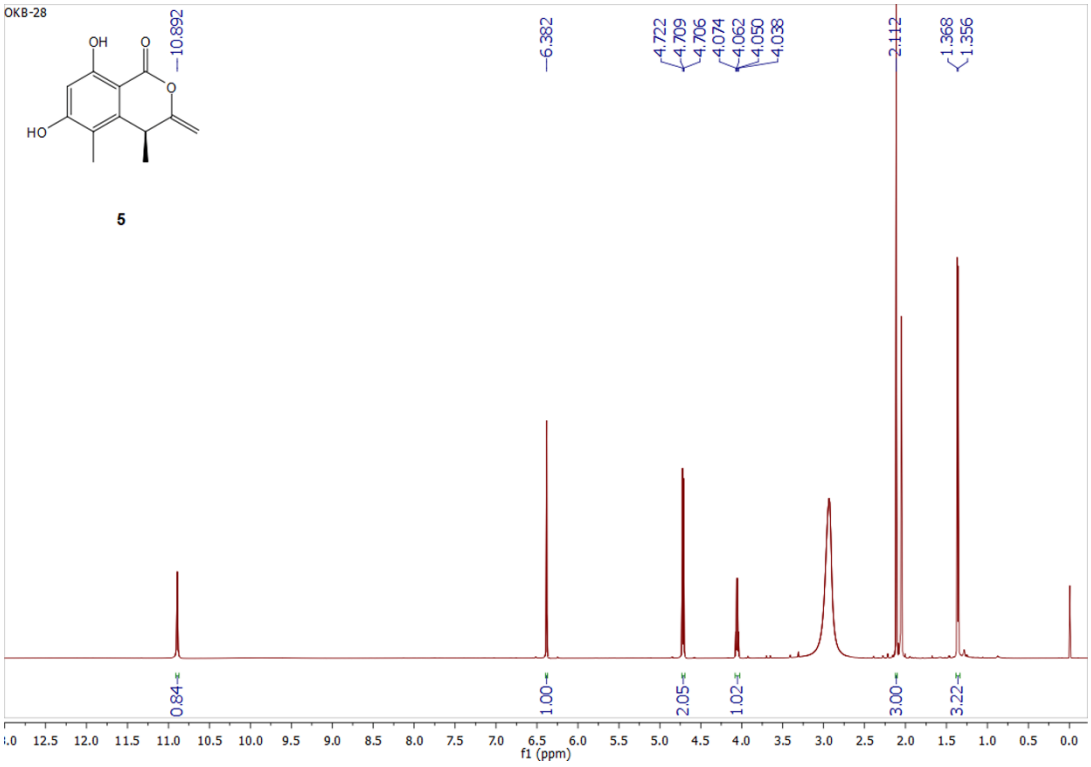


Fig. S41 ^{1}H NMR spectrum (600 MHz) of **5** in Acetone-d_6.

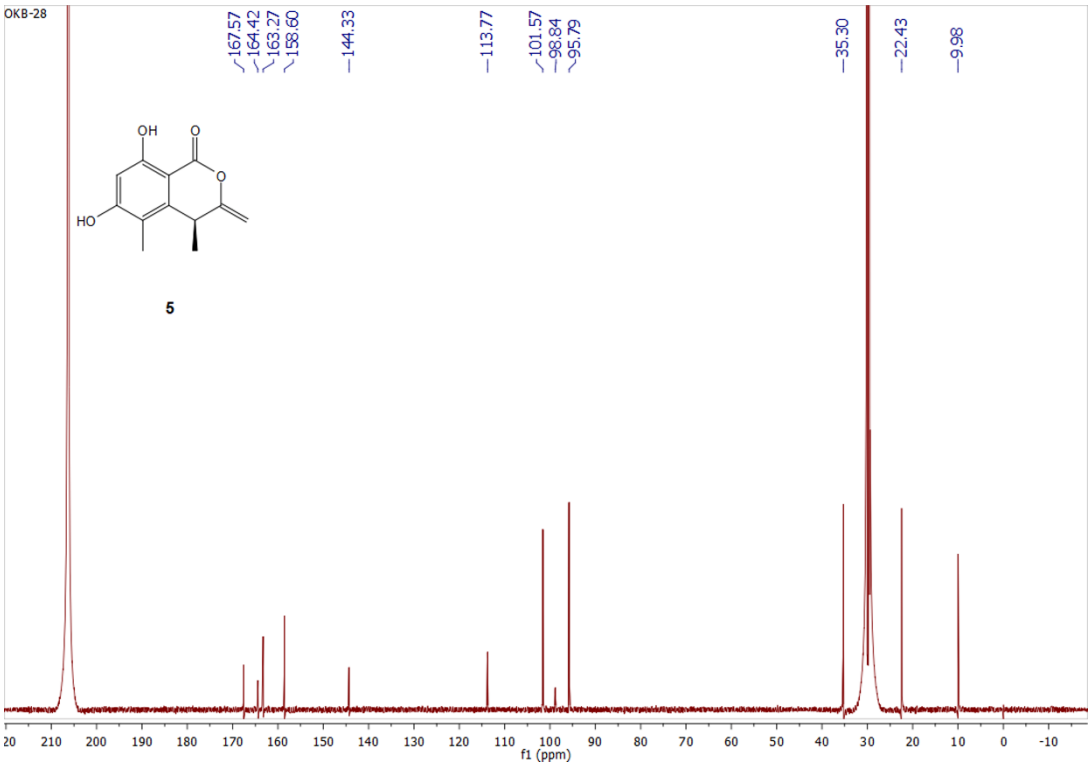


Fig. S42 ^{13}C NMR spectrum (150 MHz) of **5** in Acetone-d_6.

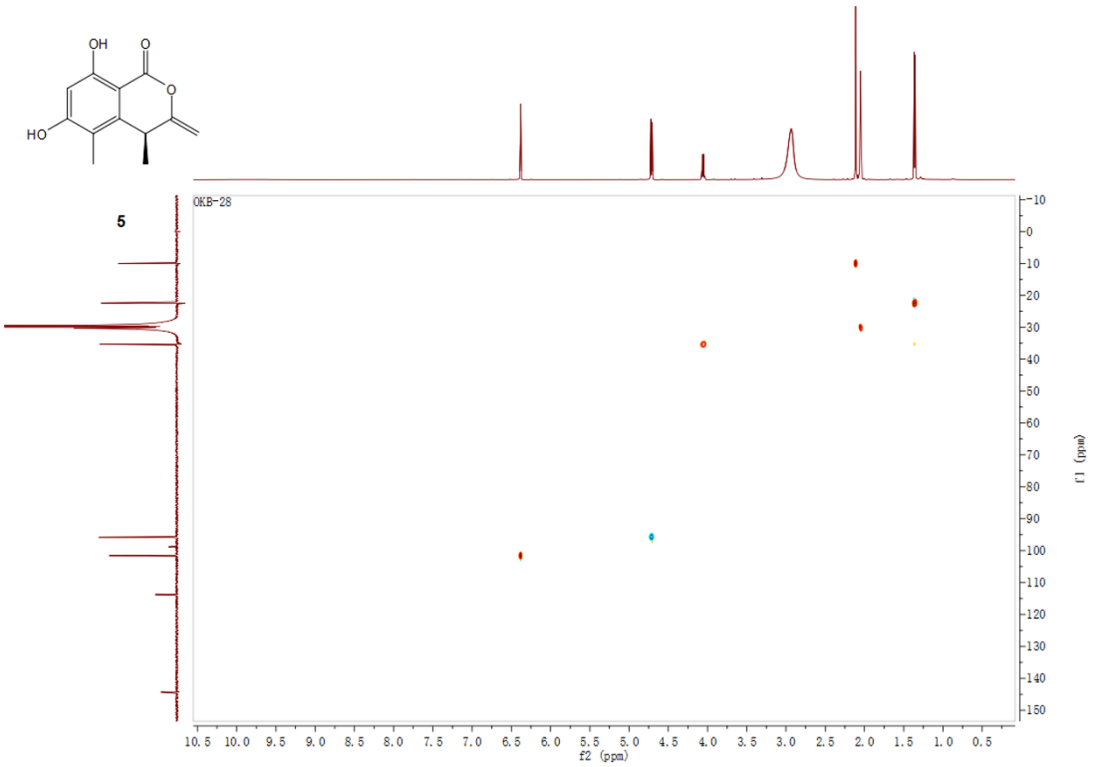


Fig. S43 HSQC spectrum (600 MHz) of **5** in Acetone-d_6.

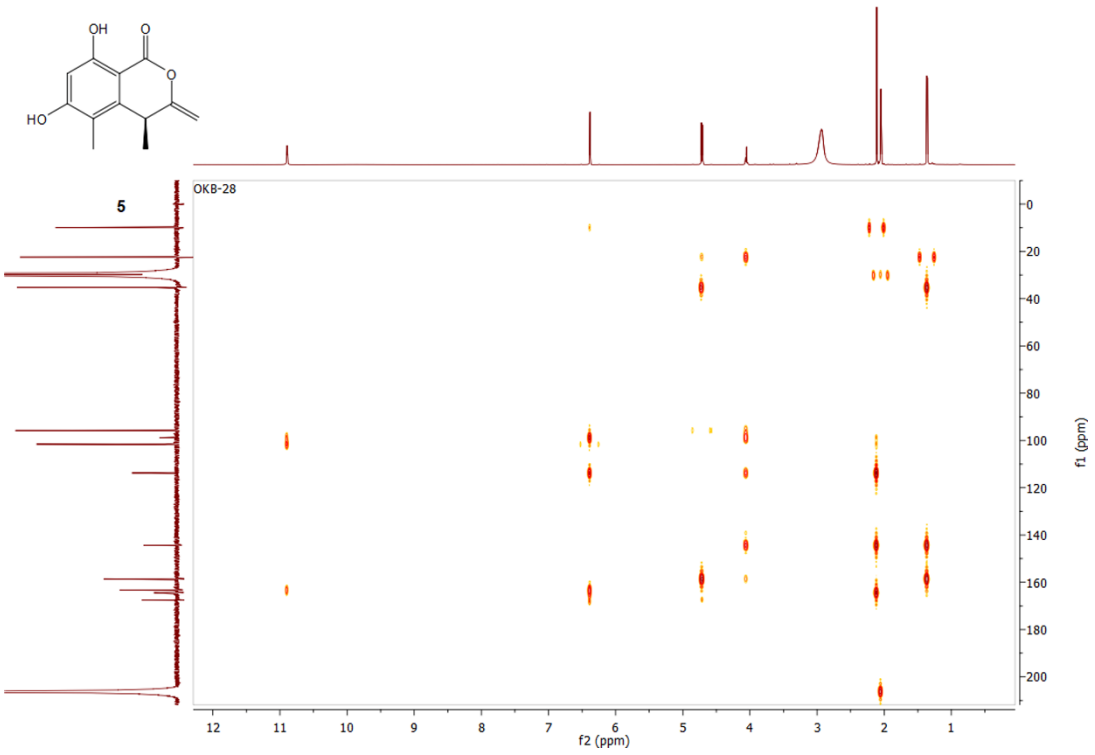


Fig. S44 HMBC spectrum (600 MHz) of **5** in Acetone-d_6.

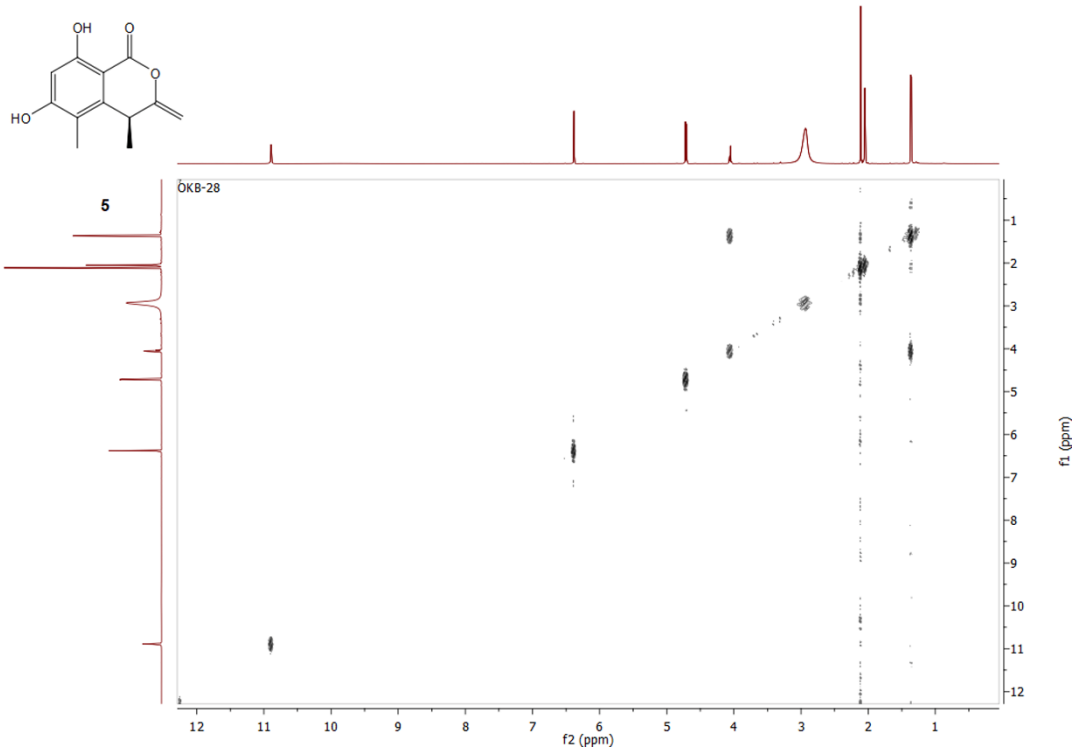


Fig. S45 ^{1}H-^{1}H COSY spectrum (600 MHz) of **5** in Acetone-d_6.

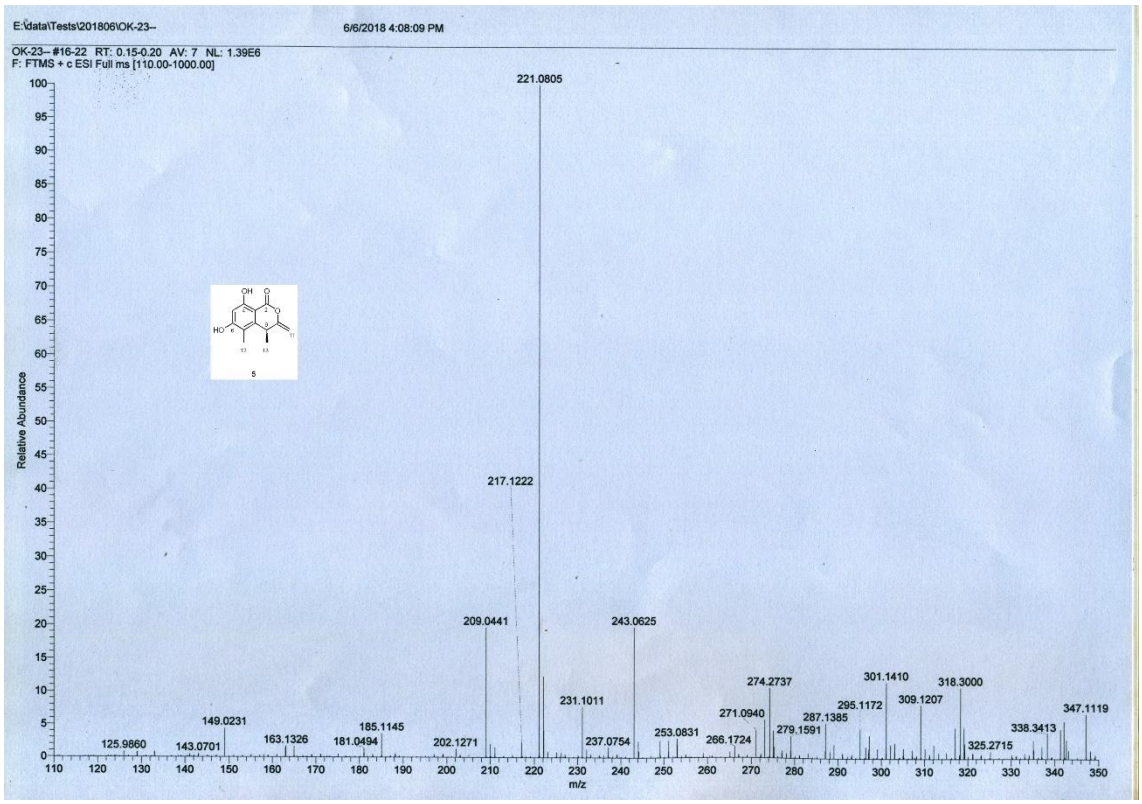


Fig. S46 HRESIMS spectrum of **5**.

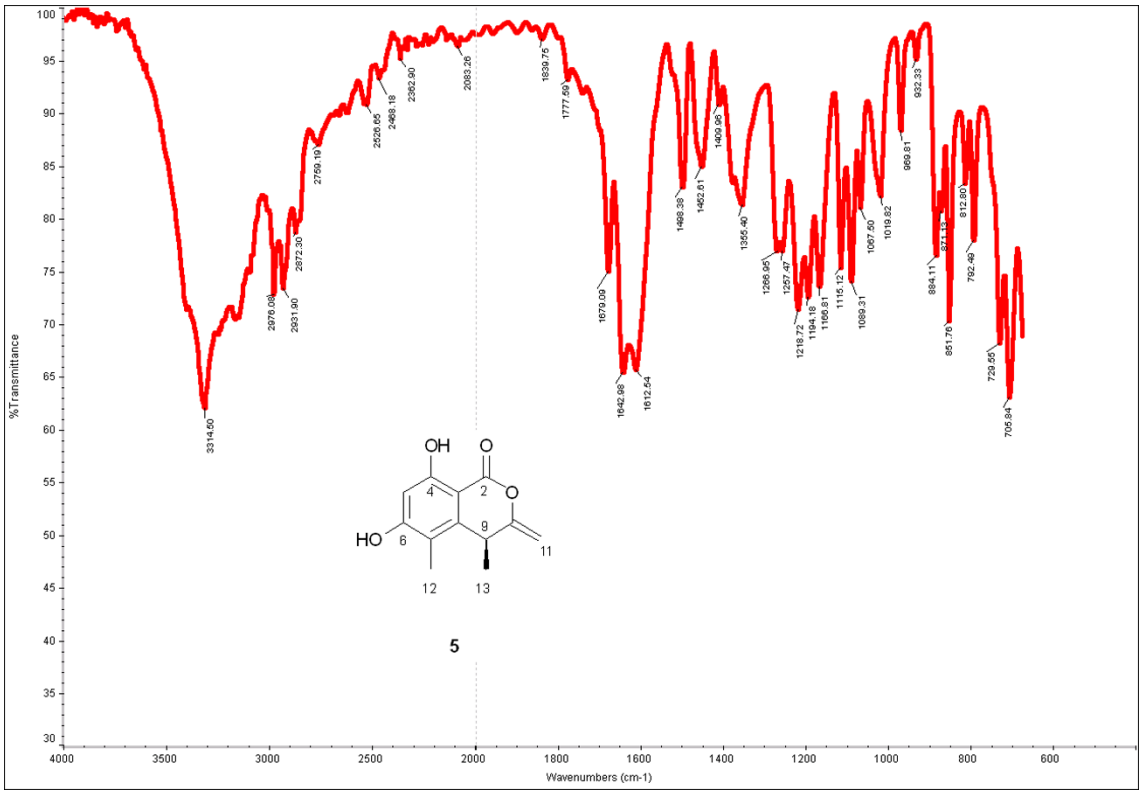


Fig. S47 IR (KBr disc) spectrum of **5**.

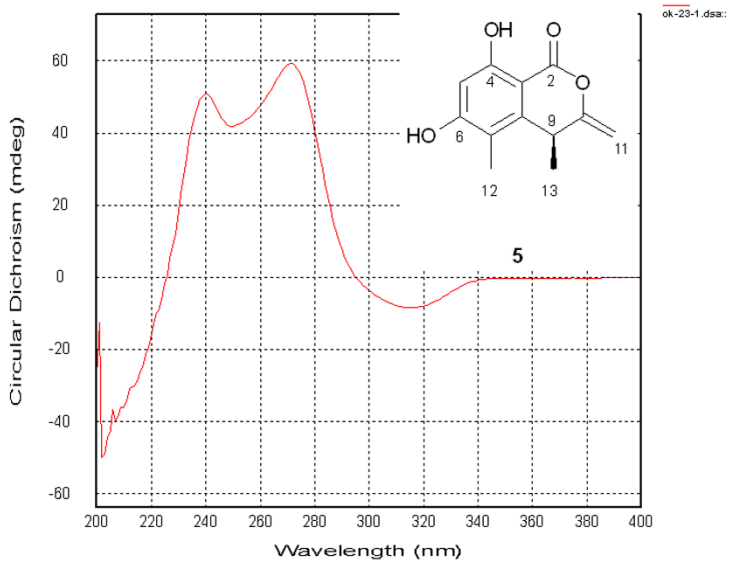


Fig. S48 CD spectrum of **5**.

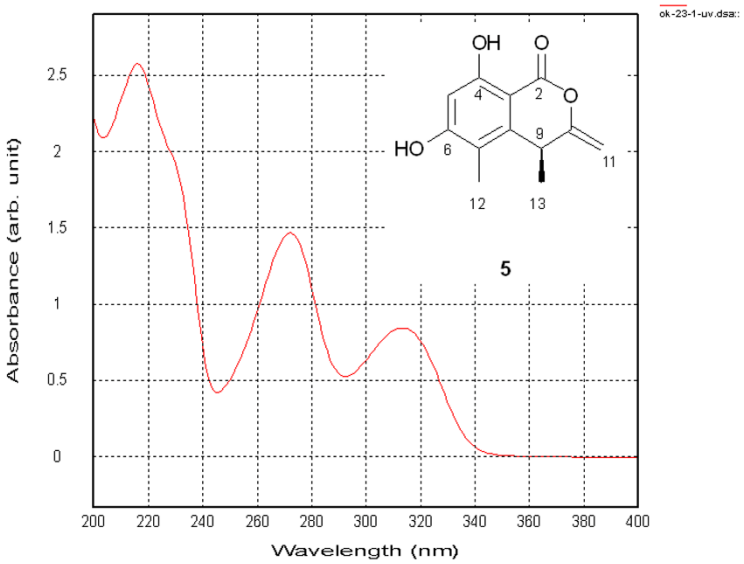


Fig. S49 UV spectrum of **5**.

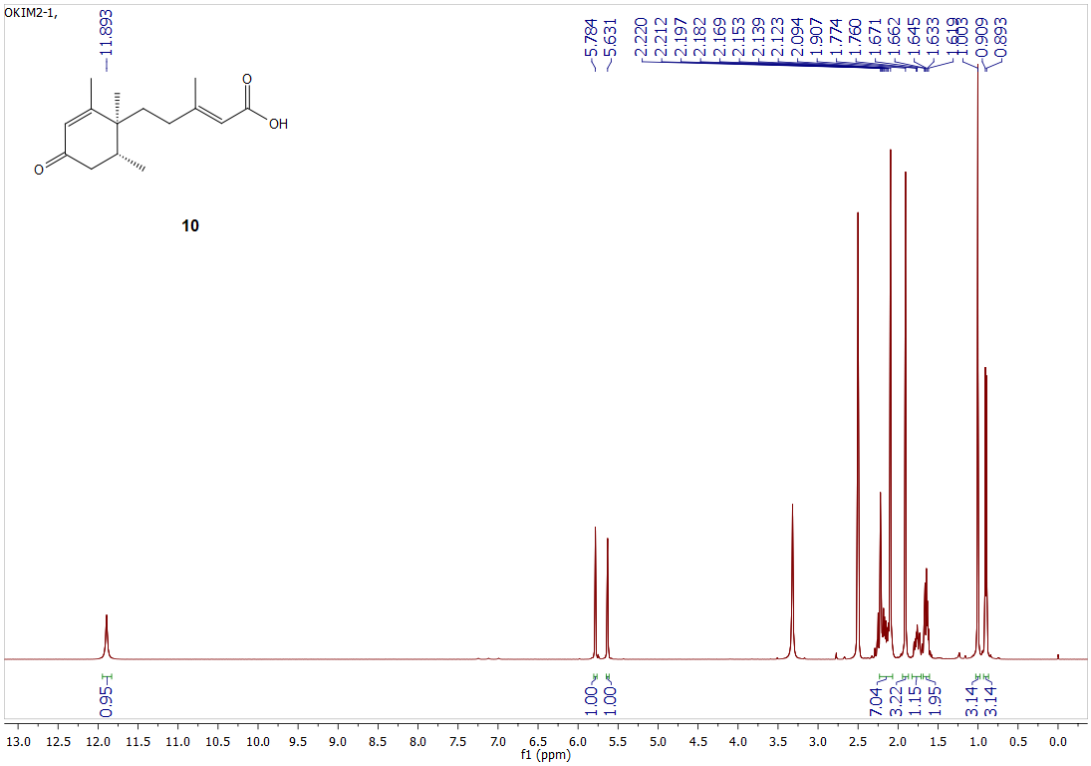


Fig. S50 ^{1}H NMR spectrum (400 MHz) of **10** in DMSO-d_6.

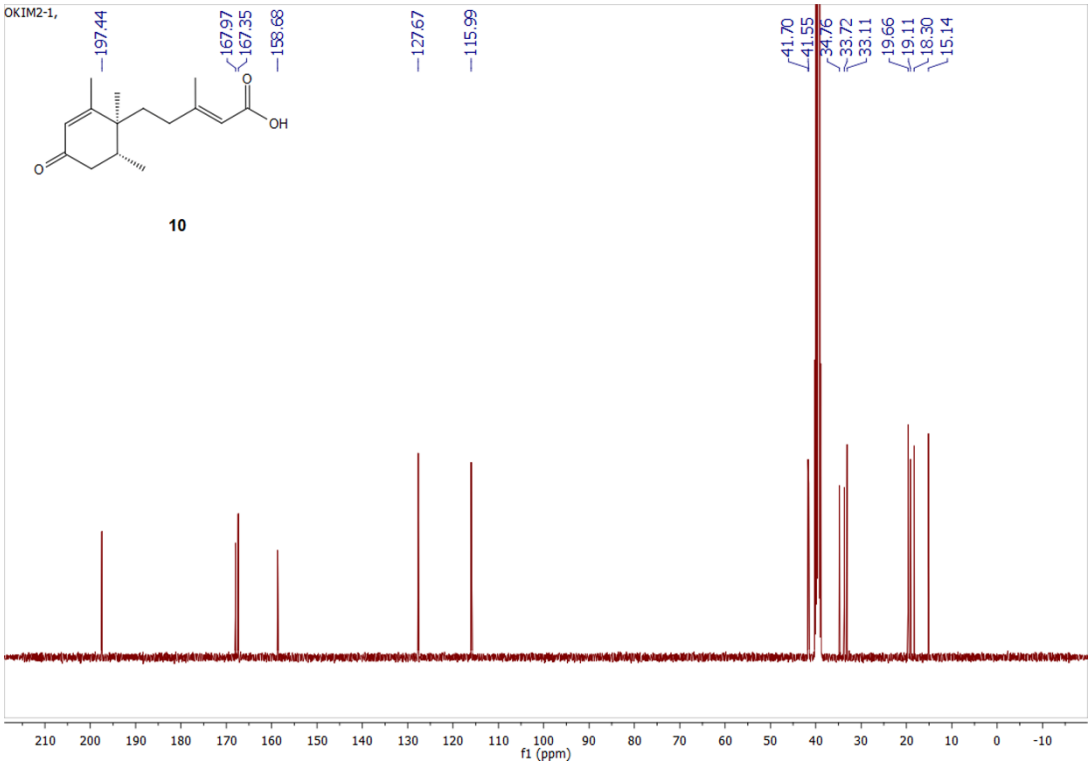


Fig. S51 ^{13}C NMR spectrum (100 MHz) of **10** in DMSO-d_6.

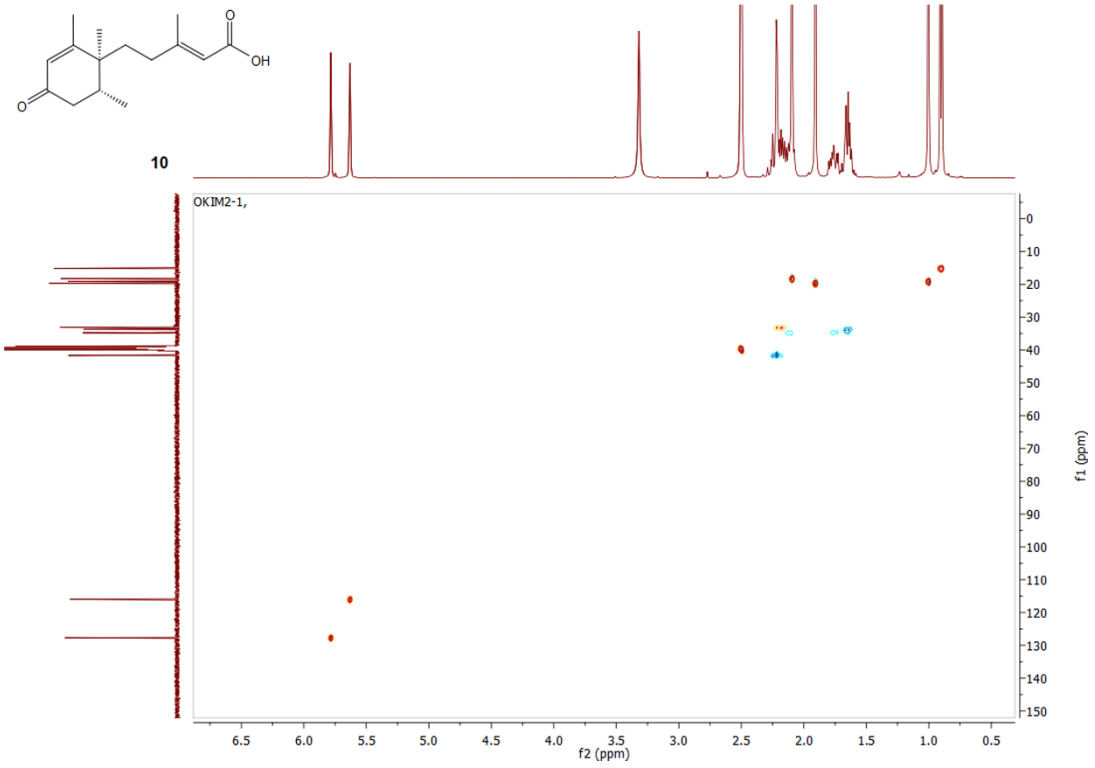


Fig. S52 HSQC spectrum (400 MHz) of **10** in DMSO-d_6.

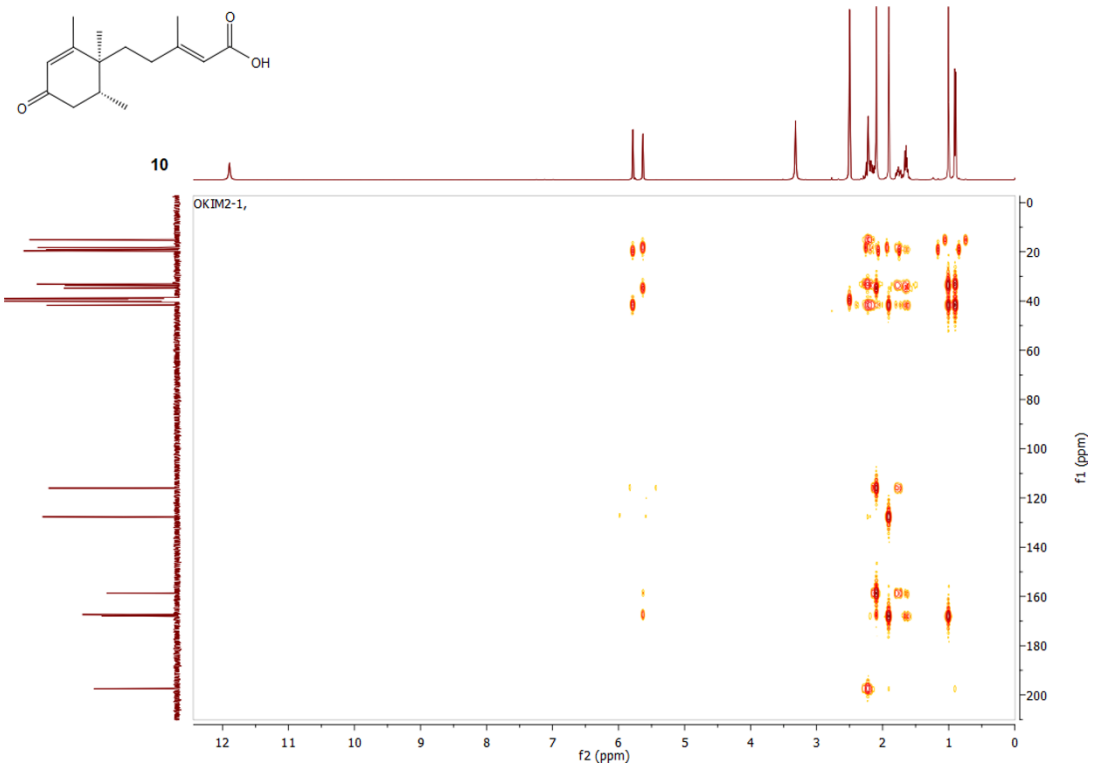


Fig. S53 HMBC spectrum (400 MHz) of **10** in DMSO-d_6.

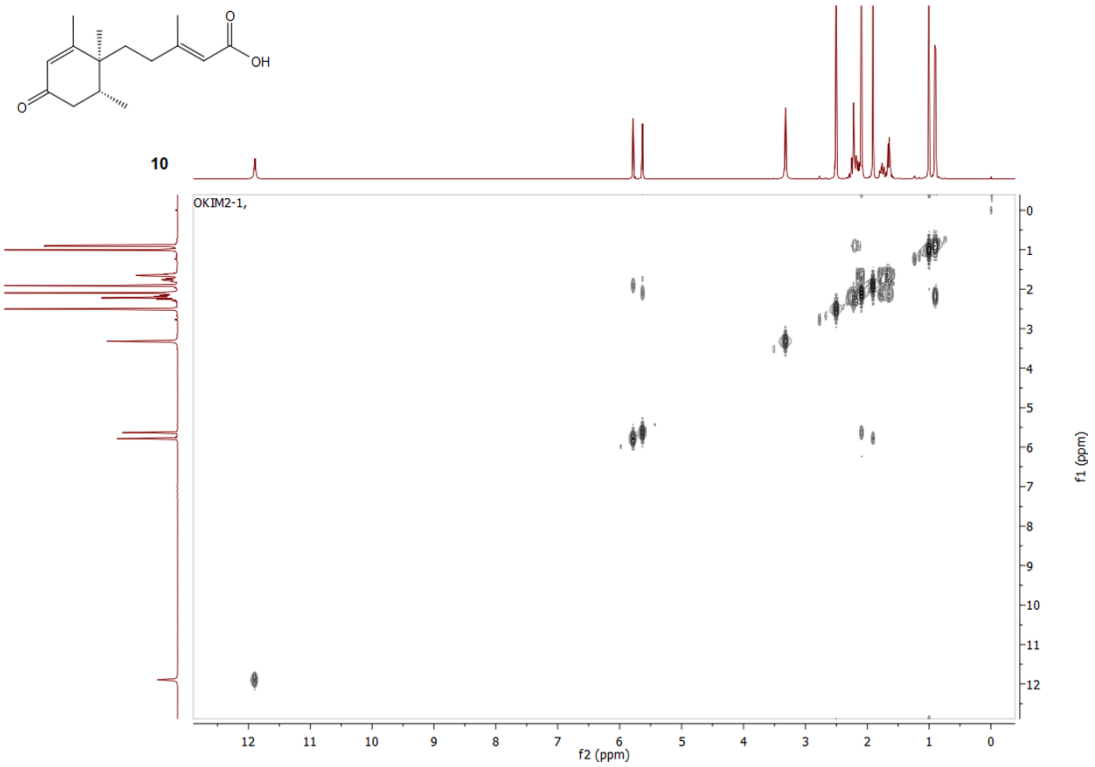


Fig. S54 ^{1}H-^{1}H COSY spectrum (400 MHz) of **10** in DMSO-d_6.

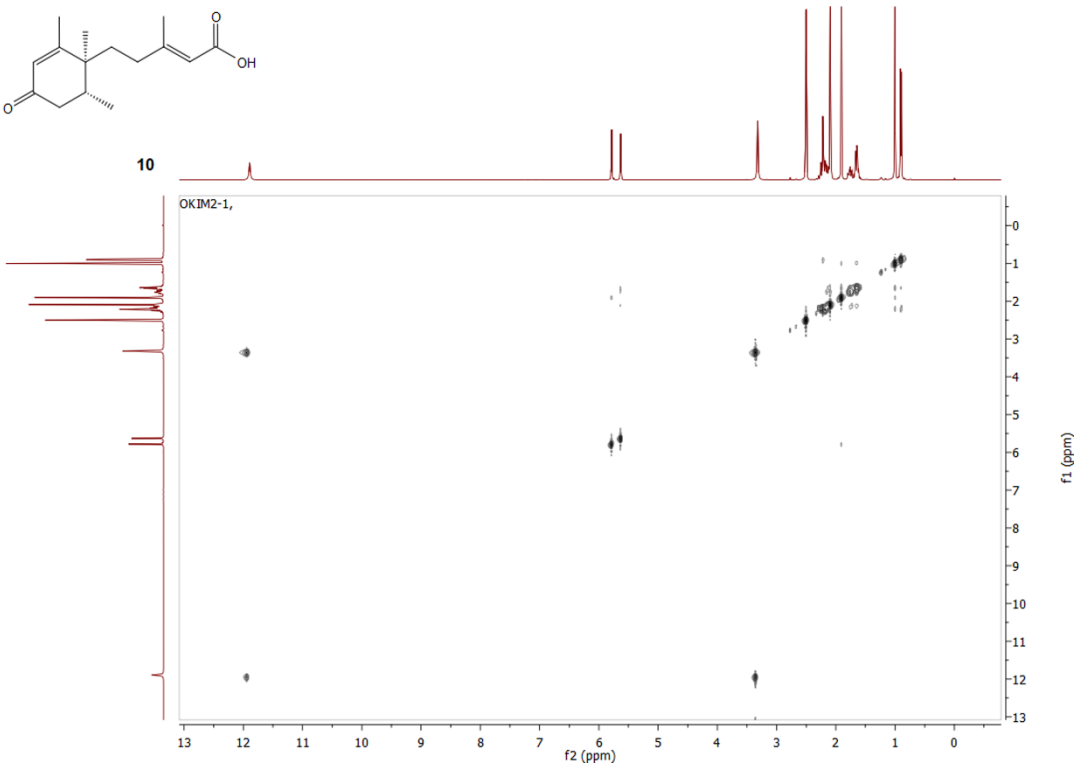


Fig. S55 NOESY spectrum (400 MHz) of **10** in DMSO-d_6.

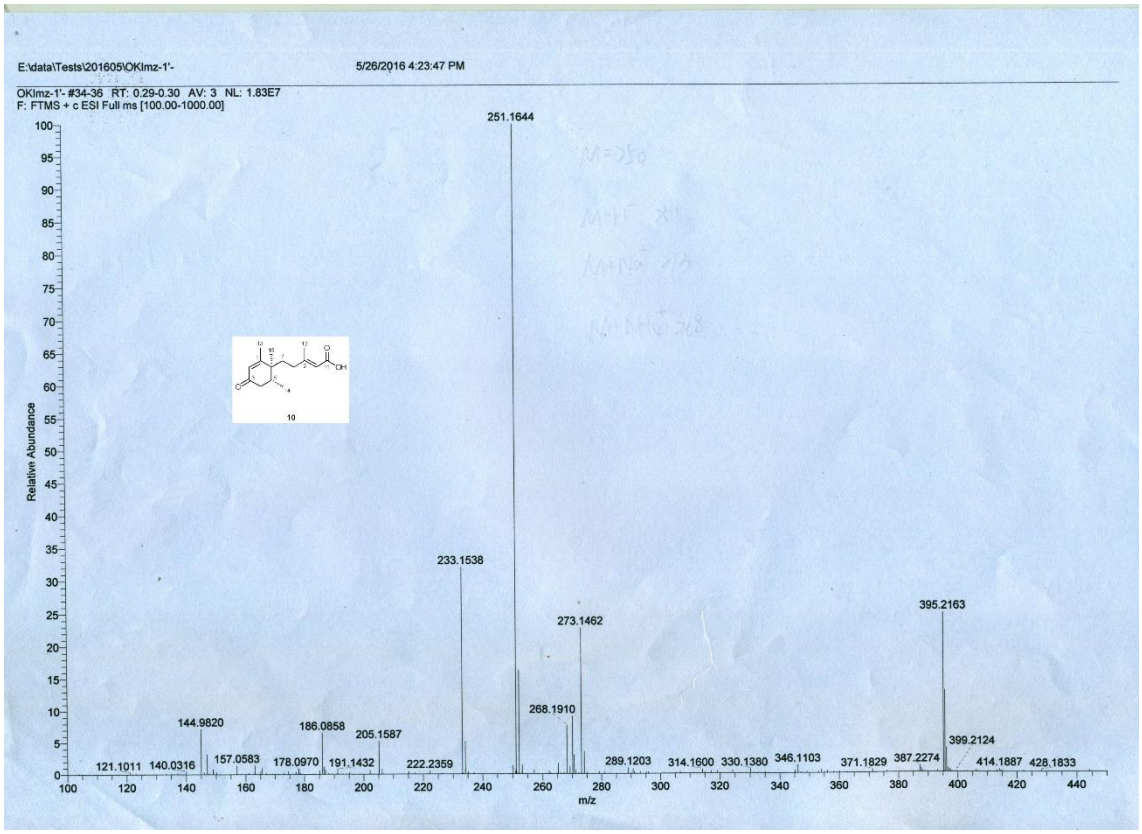


Fig. S56 HRESIMS spectrum of **10**.

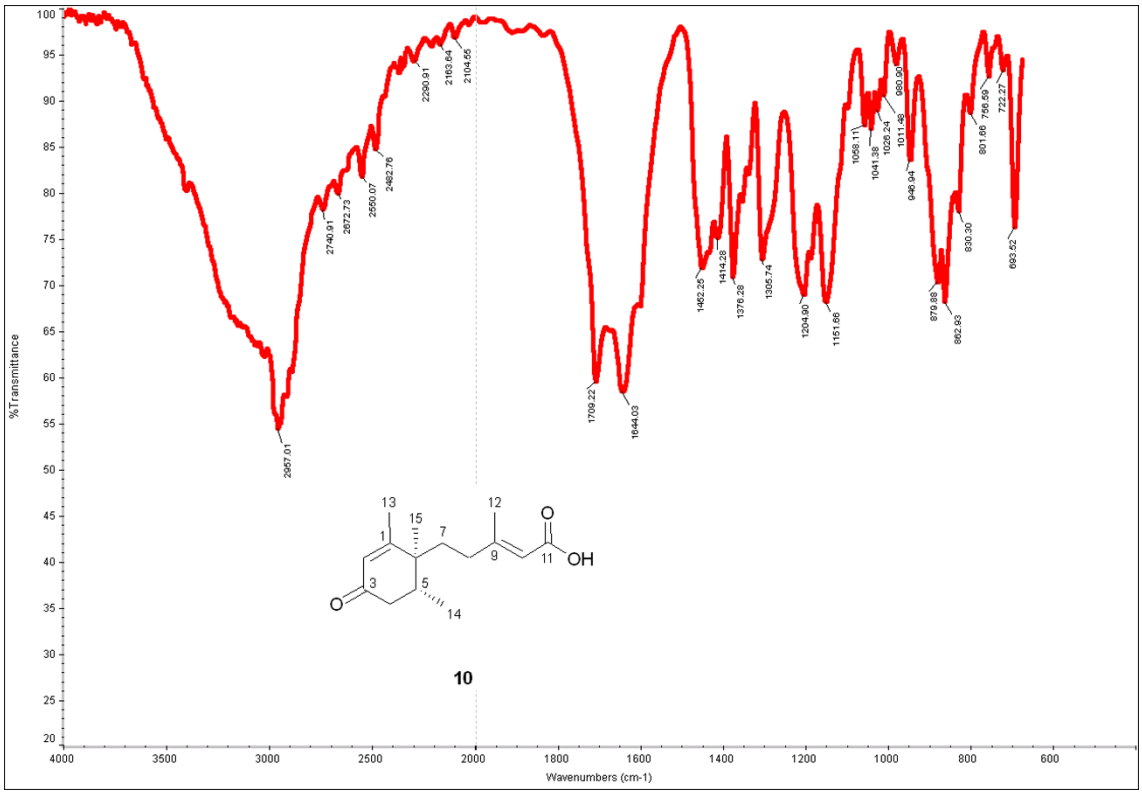


Fig. S57 IR (KBr disc) spectrum of **10**.

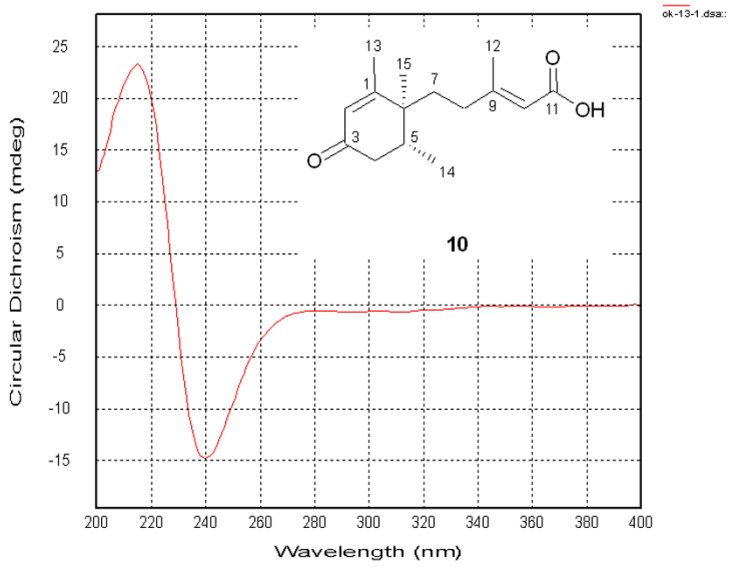


Fig. S58 CD spectrum of **10**.

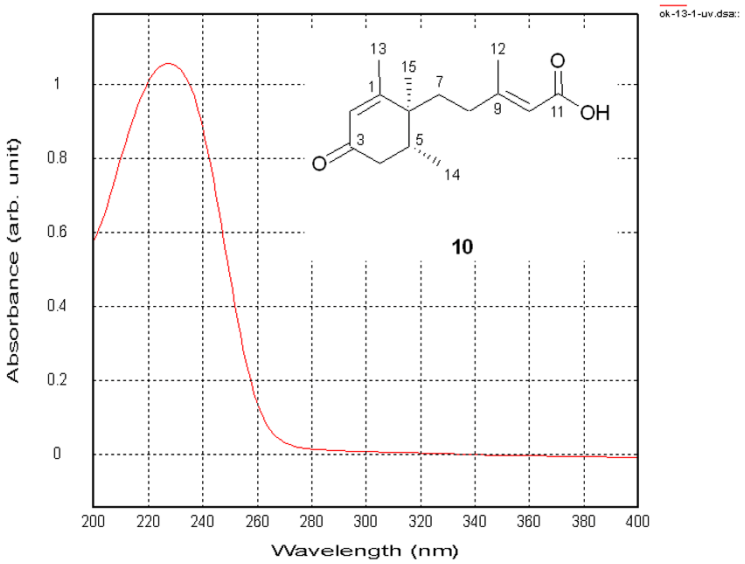


Fig. S59 UV spectrum of **10**.

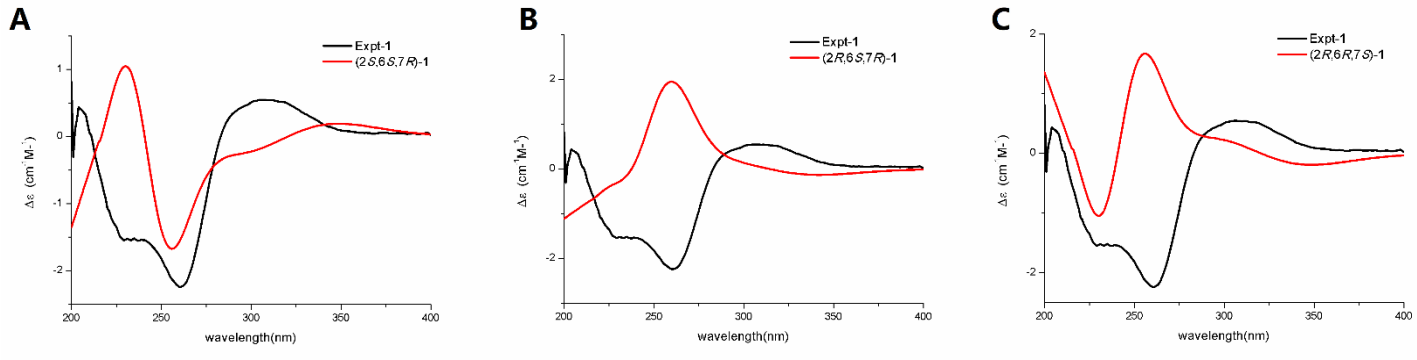
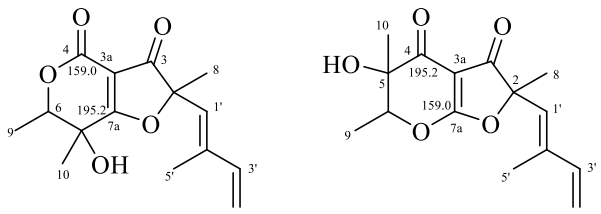


Fig. S60 Experimental ECD (balck) and calculated ECD (red) curves of compound **1**.



1
in DMSO-d_6

1a
in DMSO-d_6

Fig. S61 Compounds **1** and **1a** for the GIAO NMR shift calculation.

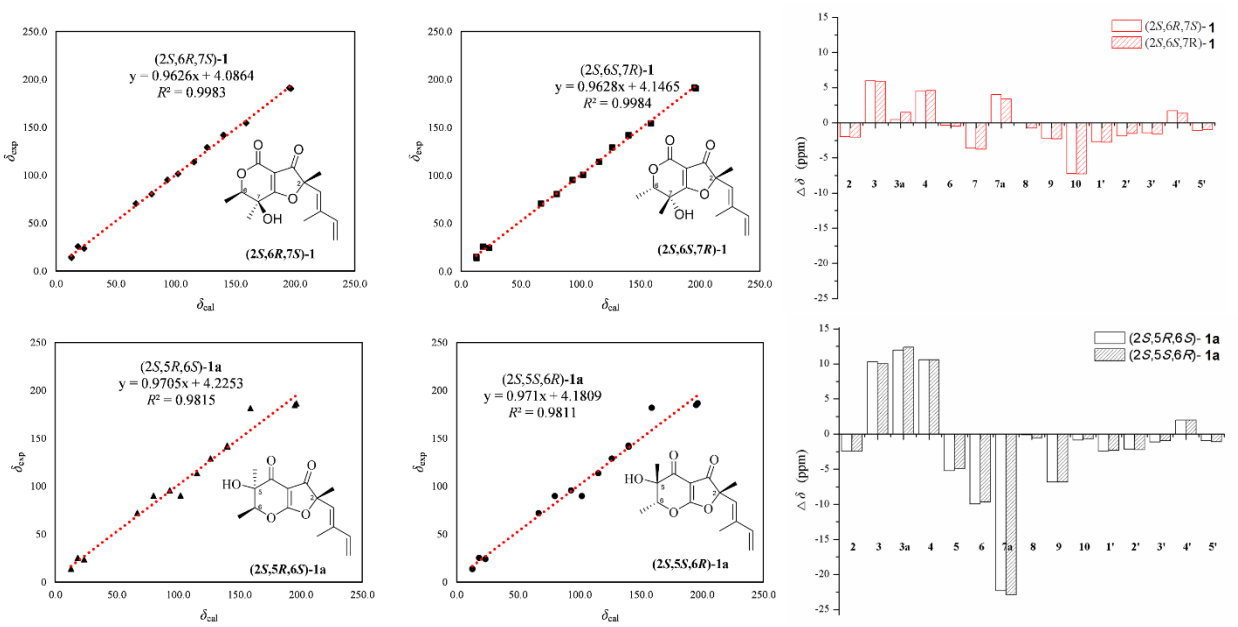


Fig. S62 Linear correlation between the experimental and calculated ^{13}C NMR chemical shifts for compounds **1** and **1a** and their compared ^{13}C NMR data ($\Delta\delta = \delta_{exp} - \delta_{cal\ (scaled)}$).

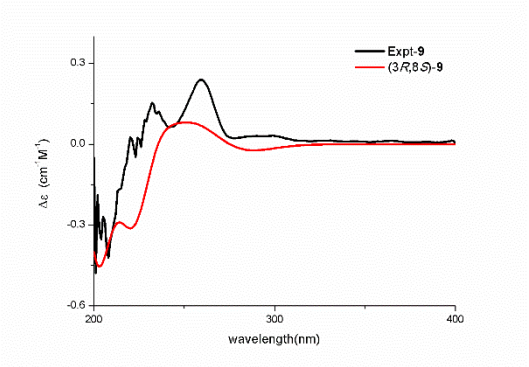


Fig. S63 Experimental ECD (balck) and calculated ECD (red) curves of compound **9**.

A	B	C	D	E	F	G	H
Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-31+G(d,p)		Unscaled Shifts	
		DP4+	1.98%	98.02%	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		93.2	99.9	100.0			
C	x	196.5	199.9	200.1			
C	x	102.1	106.7	105.6			
C	x	159.0	162.1	162.1			
C		80.0	84.3	84.5			
C		66.8	73.9	74.1			
C	x	195.2	200.7	201.4			
C		23.4	24.6	25.4			
C		12.8	15.7	15.8			
C		18.4	26.9	26.9			
C	x	126.4	135.6	135.6			
C	x	140.1	149.0	148.7			
C	x	140.2	148.7	148.9			
C	x	115.5	119.4	119.8			
C		12.9	14.7	14.6			
H		4.61	4.32	4.36			
H		1.56	1.46	1.56			
H		1.32	1.26	1.30			
H		1.36	1.57	1.51			
H	x	5.58	5.86	5.81			
H	x	6.41	6.77	6.77			
H	x	5.17	5.33	5.37			
H	x	5.35	5.46	5.42			
H		1.82	2.10	2.08			

Fig. S64 The outcome of DP4$^+$ analysis ("main" sheet) of isomers (2*S*,6*R*,7*S*)-**1** and (2*S*,6*S*,7*R*)-**1.**

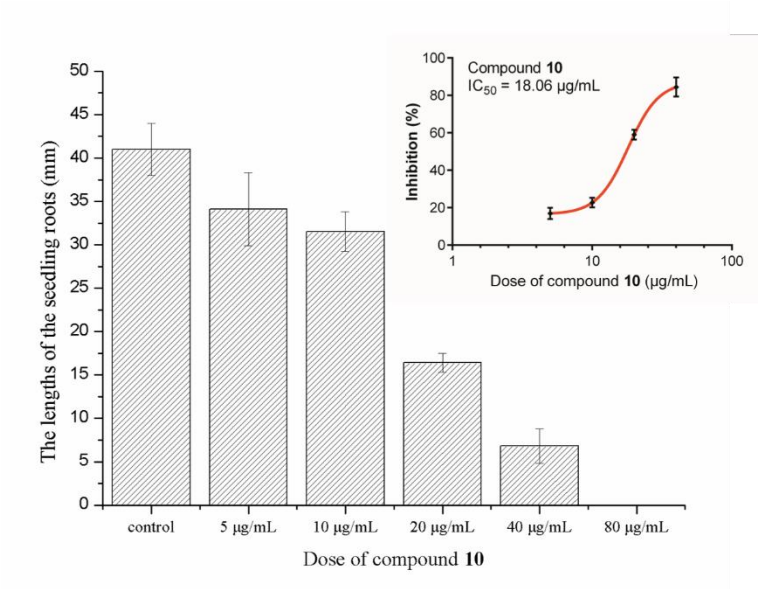


Fig. S65 The lengths of the seedling roots with different concentrations of compound 10 (5, 10, 20, 40 and 80 μg/mL).

Table S1 NMR Boltzmann averaged isotropic magnetic shielding values (σ), unscaled (δ_u) and scaled (δ_s) chemical shifts calculated at the PCM/mPW1PW91/6-31+G**//PCM/B3LYP/6-31G* (solvent: DMSO) level of theory for (2*S*,6*R*,7*S*)-**1** and (2*S*,6*S*,7*R*)-**1**.

				σ		$\delta_{unscaled}$ (δ_u)		δ_{scaled} (δ_s)	
Atom	δ_{exp}	TMS	Slope	(2*S*,6*R*,7*S*)-**1**	(2*S*,6*S*,7*R*)-**1**	(2*S*,6*R*,7*S*)-**1**	(2*S*,6*S*,7*R*)-**1**	(2*S*,6*R*,7*S*)-**1**	(2*S*,6*S*,7*R*)-**1**
C-2	93.2	186.4939	1.0496	86.5698	86.4758	99.9	100.0	95.2	95.3
C-3	196.5	186.4939	1.0496	-13.4433	-13.5678	199.9	200.1	190.5	190.6
C-3a	102.1	186.4939	1.0496	79.7905	80.8482	106.7	105.6	101.7	100.7
C-4	159.0	186.4939	1.0496	24.3731	24.3793	162.1	162.1	154.5	154.5
C-6	80.0	186.4939	1.0496	102.1537	102.0166	84.3	84.5	80.4	80.5
C-7	66.8	186.4939	1.0496	112.5693	112.3707	73.9	74.1	70.4	70.6
C-7a	195.2	186.4939	1.0496	-14.2131	-14.8627	200.7	201.4	191.2	191.8
C-8	23.4	186.4939	1.0496	161.8683	161.0807	24.6	25.4	23.5	24.2
C-9	12.8	186.4939	1.0496	170.7929	170.7022	15.7	15.8	15.0	15.0
C-10	18.4	186.4939	1.0496	159.5739	159.5718	26.9	26.9	25.6	25.6
C-1'	126.4	186.4939	1.0496	50.9395	50.8863	135.6	135.6	129.1	129.2
C-2'	140.1	186.4939	1.0496	37.4466	37.8124	149.0	148.7	142.0	141.7
C-3'	140.2	186.4939	1.0496	37.8256	37.6225	148.7	148.9	141.6	141.8
C-4'	115.5	186.4939	1.0496	67.1028	66.7341	119.4	119.8	113.7	114.1
C-5'	12.9	186.4939	1.0496	171.7836	171.9252	14.7	14.6	14.0	13.9
H-6	4.61	31.69683	1.058	27.3765	27.3381	4.32	4.36	4.08	4.12
H_3-8	1.56	31.69683	1.058	30.2377	30.1333	1.46	1.56	1.38	1.48
H_3-9	1.32	31.69683	1.058	30.4400	30.3946	1.26	1.30	1.19	1.23
H_3-10	1.36	31.69683	1.058	30.1240	30.1846	1.57	1.51	1.49	1.43
H-1'	5.58	31.69683	1.058	25.8377	25.8852	5.86	5.81	5.54	5.49
H-3'	6.41	31.69683	1.058	24.9267	24.9220	6.77	6.77	6.40	6.40
H-4'a	5.17	31.69683	1.058	26.3687	26.3250	5.33	5.37	5.04	5.08
H-4'b	5.35	31.69683	1.058	26.2330	26.2810	5.46	5.42	5.16	5.12
H-5'	1.82	31.69683	1.058	29.5937	29.6179	2.10	2.08	1.99	1.96

Table S2 NMR Boltzmann averaged isotropic magnetic shielding values (σ), unscaled (δ_u) and scaled (δ_s) chemical shifts calculated at the PCM/mPW1PW91/6-31+G**//PCM/B3LYP/6-31G* (solvent: DMSO) level of theory for (2*S*,5*R*,6*S*)-**1a** and (2*S*,5*S*,6*R*)-**1a**.

				σ		$\delta_{unscaled}$ (δ_u)		δ_{scaled} (δ_s)	
Atom	δ_{exp}	TMS	Slope	(2*S*,5*R*,6*S*)-**1a**	(2*S*,5*S*,6*R*)-**1a**	(2*S*,5*R*,6*S*)-**1a**	(2*S*,5*S*,6*R*)-**1a**	(2*S*,5*R*,6*S*)-**1a**	(2*S*,5*S*,6*R*)-**1a**
C-2	93.2	186.4939	1.0496	86.05436	86.2609	100.4	100.4	95.7	95.6
C-3	196.5	186.4939	1.0496	-8.9506	-9.413	195.4	195.7	186.2	186.4
C-3a	102.1	186.4939	1.0496	91.85392	92.30765	94.6	94.2	90.1	89.8
C-4	195.2	186.4939	1.0496	-7.31666	-7.3199	193.8	193.8	184.6	184.6
C-5	66.8	186.4939	1.0496	110.8191	111.1848	75.7	75.3	72.1	71.8
C-6	80.0	186.4939	1.0496	92.05365	92.30765	94.4	94.2	90.0	89.7
C-7a	159.0	186.4939	1.0496	-3.83011	-4.6716	190.3	190.9	181.3	181.9
C-8	23.4	186.4939	1.0496	161.7541	161.186	24.7	25.2	23.6	24.0
C-9	18.4	186.4939	1.0496	160.0093	159.9813	26.5	26.5	25.2	25.2
C-10	12.8	186.4939	1.0496	172.1976	172.3801	14.3	14.1	13.6	13.5
C-1'	126.4	186.4939	1.0496	51.2433	51.0413	135.2	135.1	128.8	128.8
C-2'	140.1	186.4939	1.0496	37.14134	36.9771	149.3	149.4	142.3	142.3
C-3'	140.2	186.4939	1.0496	38.11391	38.4509	148.4	148.1	141.4	141.1
C-4'	115.5	186.4939	1.0496	67.40093	67.3397	119.1	119.1	113.4	113.5
C-5'	12.9	186.4939	1.0496	171.9472	171.9303	14.5	14.6	13.8	13.9
H-6	4.61	31.69683	1.058	26.80258	26.82989	4.89	4.87	4.62	4.60
H_3-8	1.56	31.69683	1.058	30.14883	30.16767	1.54	1.53	1.46	1.45
H_3-9	1.32	31.69683	1.058	30.36583	30.38525	1.33	1.31	1.26	1.24
H_3-10	1.36	31.69683	1.058	30.49309	30.45296	1.20	1.24	1.13	1.18
H-1'	5.58	31.69683	1.058	25.81519	25.74167	5.88	5.96	5.56	5.63
H-3'	6.41	31.69683	1.058	24.91815	25.02007	6.78	6.68	6.40	6.31
H-4'a	5.17	31.69683	1.058	26.26495	26.14303	5.43	5.55	5.13	5.25
H-4'b	5.35	31.69683	1.058	26.42626	26.37193	5.27	5.32	4.98	5.03
H-5'	1.82	31.69683	1.058	29.60473	29.65284	2.09	2.04	1.97	1.93

Table S3 Boltzmann distributions of all conformers.

		(2*S*,6*R*,7*S*)-**1**	(2*S*,6*S*,7*R*)-**1**	(2*S*,5*R*,6*S*)-**1a**	(2*S*,5*S*,6*R*)-**1a**
E(Hartree)	Conformer **1**	-958.527001	-958.527010	-958.5710123	-958.5710071
	Conformer **2**	-958.522711	-958.522745	-958.5658775	-958.5657506
	Conformer **3**	-958.525744	-958.525690	-958.5695947	-958.5695199
E(kcal/mol)	Conformer **1**	-601478.473	-601478.478	-601506.0901	-601506.0868
	Conformer **2**	-601475.781	-601475.802	-601502.868	-601502.7883
	Conformer **3**	-601477.684	-601477.650	-601505.2006	-601505.1536
Boltzmann populations	Conformer **1**	78.46%	79.50%	81.50%	82.61%
	Conformer **2**	0.83%	0.86%	0.35%	0.31%
	Conformer **3**	20.71%	19.64%	18.14%	17.08%

Cartesian coordinates of conformers in the GIAO NMR shift calculation

Conformer (2*S*,6*R*,7*S*)-**1-1**

O	-3.33863300	0.21749300	-0.66688500
C	-2.83259300	-1.15009100	-0.68345000
C	-1.83037500	-1.38559400	0.48166100
C	-0.84541800	-0.24674800	0.42136500
C	-1.15696700	0.98981700	-0.06572900
C	-2.49099300	1.28934400	-0.57782500
O	0.38142200	-0.39512700	0.89393800
C	1.08886400	0.90682900	0.75443500
C	0.02380800	1.82383200	0.08342900
O	-2.90650300	2.39244900	-0.87070300
O	0.23696200	2.98565400	-0.22284700
C	-2.29335600	-1.48770400	-2.06955200
C	-2.54326800	-1.37918100	1.84570000
O	-1.20258300	-2.63282300	0.22967500
C	2.29539900	0.78183000	-0.13949500
C	3.21948800	-0.20097000	-0.19849800
C	3.21670000	-1.44685100	0.65389200
C	4.31168200	-0.03990900	-1.17113900
C	5.31069300	-0.90821300	-1.38678500
C	1.41339600	1.40527400	2.16554500
H	-3.72217200	-1.75096200	-0.48130600
H	-2.04434500	-2.54960200	-2.12507800
H	-1.39718600	-0.90818100	-2.31313400
H	-3.06287600	-1.26751400	-2.81502300
H	-3.12367300	-0.46348900	1.98776700
H	-3.21922800	-2.23872800	1.88942400
H	-1.81668800	-1.45780200	2.66130900
H	-0.67160300	-2.86730600	1.00935100
H	2.42099600	1.64869700	-0.78615500
H	3.12626900	-2.34267700	0.02704300
H	4.16523300	-1.53502400	1.19679000
H	2.40259900	-1.46158400	1.37683500
H	4.28164500	0.87751200	-1.75845500
H	6.07705800	-0.70252700	-2.12832900
H	5.40366200	-1.84402600	-0.84333800
H	1.84769600	2.40633300	2.08859100
H	2.13690700	0.74342200	2.64824900
H	0.50802900	1.46229900	2.77870600

Conformer (2*S*,6*R*,7*S*)-**1**-**2**

O	3.23022000	0.51396800	0.66074400
C	2.84118700	-0.88073100	0.83595400
C	1.89727700	-1.34279800	-0.31029300
C	0.82165500	-0.29360400	-0.41538200
C	1.01091500	1.01474300	-0.07501100
C	2.29813700	1.48935200	0.42432400
O	-0.36901800	-0.60340300	-0.90177800
C	-1.18713700	0.63920800	-0.94163700
C	-0.22884900	1.71894800	-0.35784100
O	2.61039100	2.65172600	0.58764300
O	-0.54928100	2.88598100	-0.20209600
C	2.28980200	-1.09278500	2.24204700
C	2.64603200	-1.44834500	-1.65061900
O	1.36381800	-2.59729600	0.08440700
C	-2.41087700	0.51740300	-0.07153500
C	-3.21727900	-0.54614700	0.11035100
C	-3.08105300	-1.88115300	-0.58600100
C	-4.35963500	-0.45032000	1.04658200
C	-4.37749200	0.22983600	2.19993100
C	-1.49581200	0.93768200	-2.41149200
H	3.78429600	-1.42122800	0.72796900
H	2.13140100	-2.15772800	2.42501900
H	1.33991400	-0.56994900	2.39187800
H	3.01359000	-0.71483800	2.96983100
H	3.15223300	-0.51183900	-1.90056400
H	3.39152500	-2.24564500	-1.57226300
H	1.95055300	-1.69275400	-2.46056900
H	0.86378800	-2.96061200	-0.66574900
H	-2.65848500	1.45069900	0.42977300
H	-4.04423100	-2.16854900	-1.02613400
H	-2.32679600	-1.88293000	-1.37239400
H	-2.82002800	-2.66687800	0.13490300
H	-5.24292400	-1.02457100	0.76372600
H	-5.26643500	0.25687500	2.82383900
H	-3.50730400	0.77050600	2.56386300
H	-2.01032900	1.90137700	-2.46842600
H	-2.14606700	0.16608400	-2.83139100
H	-0.57494400	0.99644200	-3.00093900

Conformer (2*S*,6*R*,7*S*)-**1-3**

O	-3.16299400	0.99469600	-0.77454900
C	-3.17740900	-0.46128700	-0.85699000
C	-2.42862800	-1.09270100	0.35071500
C	-1.10373100	-0.38136300	0.43763200
C	-0.90710300	0.89946100	0.01169800
C	-1.99956300	1.68414600	-0.55671900
O	-0.05901900	-0.97764800	0.98758700
C	1.09038400	-0.03034100	0.95729000
C	0.46858900	1.25725000	0.32162200
O	-1.97037000	2.87516300	-0.79265800
O	1.06805400	2.30888000	0.17331500
C	-2.67482900	-0.90906900	-2.22564300
C	-3.20803000	-0.89757100	1.66291200
O	-2.25973400	-2.46882700	0.04789200
C	2.13135500	-0.70167700	0.08849700
C	3.37936200	-0.29652700	-0.23201300
C	4.02144400	1.00008900	0.19935000
C	4.18016400	-1.21029700	-1.06310700
C	5.44471300	-1.01195200	-1.46318000
C	1.49474200	0.19858100	2.41464200
H	-4.23645600	-0.70950000	-0.75737200
H	-2.81580100	-1.98582200	-2.34177900
H	-1.61369000	-0.68047000	-2.36634800
H	-3.24752500	-0.39383400	-3.00209800
H	-3.43465100	0.15749500	1.83939200
H	-4.14664900	-1.45655700	1.59779600
H	-2.62967900	-1.27436600	2.51328100
H	-1.91299800	-2.91122800	0.84083700
H	1.79195900	-1.65916300	-0.30029400
H	4.85897100	0.80884000	0.88217300
H	4.43616800	1.52210500	-0.67104800
H	3.31480200	1.67713900	0.67587800
H	3.67894200	-2.13100100	-1.36099500
H	5.95837400	-1.75088300	-2.07121100
H	6.01097600	-0.12213400	-1.20398600
H	2.29853500	0.93588300	2.46274100
H	1.84777000	-0.73715700	2.85598300
H	0.64469400	0.57211000	2.99410500

Conformer (2*S*,6*S*,7*R*)-**1-1**

O	-3.25979900	0.32336900	-0.95524600
C	-3.16657400	-0.90198100	-0.16967600
C	-1.72654900	-1.48620000	-0.22020500
C	-0.80009700	-0.34311900	0.10354500
C	-1.09538000	0.96225200	-0.16500200
C	-2.35592100	1.34000700	-0.79739100
O	0.38746000	-0.57418100	0.63943800
C	1.07620500	0.73454200	0.81248100
C	0.05808400	1.75566500	0.22492700
O	-2.63080200	2.44220900	-1.22720300
O	0.27699400	2.95389300	0.15206500
C	-3.70960100	-0.66058800	1.23496500
C	-1.39305200	-2.04066900	-1.61661500
O	-1.66651800	-2.50203300	0.76885800
C	2.36236400	0.77847500	0.02892100
C	3.31493700	-0.16966000	-0.10176800
C	3.26688700	-1.53998400	0.53001000
C	4.48865800	0.16292100	-0.92438400
C	5.52540900	-0.64770700	-1.18201900
C	1.25640400	0.96616000	2.31537100
H	-3.82397300	-1.59332100	-0.70167500
H	-3.77265400	-1.60542000	1.77900800
H	-3.07718900	0.02695800	1.80559000
H	-4.71237500	-0.23009400	1.16078600
H	-2.04292700	-2.89848700	-1.81517300
H	-0.34922000	-2.36911300	-1.66161200
H	-1.55190700	-1.28760200	-2.39332500
H	-0.82295300	-2.97354400	0.66524800
H	2.52259100	1.74229100	-0.45139200
H	2.38872500	-1.68567700	1.15721600
H	4.16170400	-1.70520600	1.14183600
H	3.26278800	-2.32026000	-0.24120200
H	4.49000100	1.16511000	-1.35225200
H	6.35280100	-0.31466700	-1.80167500
H	5.58989600	-1.65974600	-0.79298700
H	0.29656600	0.90135900	2.83808200
H	1.94877600	0.23289500	2.73646500
H	1.67001700	1.96777500	2.46481200

Conformer (2*S*,6*S*,7*R*)-**1**-**2**

O	-3.13345800	0.62443300	-0.94744800
C	-3.16984800	-0.68259500	-0.30195200
C	-1.78181500	-1.37877800	-0.37873000
C	-0.77723000	-0.36138800	0.09610700
C	-0.95254300	0.98624200	-0.03542600
C	-2.15374000	1.53646300	-0.65706200
O	0.36496600	-0.75061200	0.63812000
C	1.15483800	0.46631100	0.97058000
C	0.24626300	1.63006700	0.47611500
O	-2.32108400	2.69712200	-0.97357800
O	0.56469000	2.80582200	0.54915600
C	-3.74214400	-0.55187000	1.10586600
C	-1.44443000	-1.80479900	-1.81852500
O	-1.84046900	-2.49838200	0.49124100
C	2.46338700	0.48394600	0.22399200
C	3.30388900	-0.53772200	-0.02998700
C	3.12066500	-1.96340300	0.43865500
C	4.53710600	-0.29896700	-0.81274800
C	4.66833400	0.55447100	-1.83628700
C	1.30675500	0.51771900	2.49313600
H	-3.86199100	-1.25284500	-0.92571300
H	-3.90001400	-1.54225000	1.53820600
H	-3.07810200	0.01354800	1.76735400
H	-4.70399700	-0.03367900	1.05357300
H	-2.15701200	-2.57481200	-2.12991400
H	-0.43167100	-2.21839100	-1.86979800
H	-1.50858200	-0.96068400	-2.51058400
H	-1.03202500	-3.02197600	0.36088600
H	2.74419900	1.48327500	-0.10164800
H	2.96803000	-2.63350100	-0.41742900
H	2.27916000	-2.09012000	1.11920200
H	4.03235700	-2.30617100	0.94417700
H	5.39302500	-0.91362700	-0.53080700
H	5.61811700	0.67583300	-2.34948900
H	3.83499700	1.14942600	-2.20185200
H	0.32961300	0.47576800	2.98517300
H	1.92596600	-0.31100800	2.84556100
H	1.79384900	1.45996300	2.76076000

Conformer (2*S*,6*S*,7*R*)-**1-3**

O	-3.10311200	0.99277800	-0.97578700
C	-3.45913500	-0.19887600	-0.21463900
C	-2.31208200	-1.24812200	-0.25772700
C	-1.05313300	-0.50387900	0.10430500
C	-0.86768700	0.82440100	-0.14483900
C	-1.90498200	1.62852800	-0.78447000
O	-0.03601800	-1.13720400	0.66414600
C	1.07499700	-0.16291000	0.85499000
C	0.46709800	1.17452500	0.31574100
O	-1.77120900	2.76393200	-1.19424600
O	1.04001700	2.25087800	0.34339700
C	-3.91232600	0.19533500	1.18722900
C	-2.16481500	-1.85941100	-1.66256900
O	-2.63028000	-2.23742000	0.70820100
C	2.21592000	-0.69972300	0.01887300
C	3.47220800	-0.22665600	-0.13067300
C	4.02167800	1.02561400	0.50883200
C	4.38079100	-1.01277400	-0.98113200
C	5.66850900	-0.73315900	-1.23048100
C	1.33254200	-0.09756800	2.36142400
H	-4.30510900	-0.61004100	-0.77004000
H	-4.30816300	-0.67742200	1.71092200
H	-3.09265500	0.61341100	1.78022400
H	-4.70301300	0.94701500	1.10880500
H	-3.06948100	-2.43203900	-1.88920700
H	-1.30120000	-2.53171100	-1.70297400
H	-2.03511700	-1.08476400	-2.42327400
H	-2.00729400	-2.97586200	0.60089500
H	1.94965200	-1.61246400	-0.50942500
H	3.24839300	1.62005700	0.99201100
H	4.49372700	1.65974600	-0.25086800
H	4.80003900	0.77631900	1.24117600
H	3.94519600	-1.90462800	-1.43129300
H	6.26525700	-1.37923700	-1.86769200
H	6.17250900	0.13470200	-0.81511000
H	0.41807400	0.18332600	2.89318100
H	1.67534300	-1.07027800	2.72387200
H	2.10116900	0.64819800	2.57392400

Conformer (2*S*,5*R*,6*S*)-**1a-1**

C	-3.33711800	-0.99325400	1.76112500
C	2.54066300	0.64802900	-0.16165600
C	1.72794800	1.29710600	2.16066000
O	0.39778200	2.76976500	-0.21177800
O	-2.76669000	1.91394300	-0.91080300
O	0.71975400	-0.57802600	0.98028900
C	1.36752100	0.75205300	0.77730900
C	0.23838000	1.60570100	0.12429600
O	-1.23857300	-1.58026800	0.66044000
C	-0.51824700	-0.49829600	0.53800100
C	-0.90464800	0.72882500	0.01302000
C	-2.21835900	0.87226300	-0.55379100
C	-2.96436400	-0.47079600	-0.75331800
C	-2.70357300	-1.41633400	0.44578300
C	-2.49913000	-1.10820700	-2.07740800
O	-4.35277100	-0.20787900	-0.81103900
C	3.50322300	-0.29675600	-0.22774900
C	3.58963200	-1.51165000	0.66441200
C	4.54589000	-0.12488700	-1.25158100
C	5.57090200	-0.95855700	-1.48126200
H	-3.00771100	0.00410300	2.07042200
H	-3.07777700	-1.70862600	2.54633500
H	-4.42251700	-0.97562100	1.64346200
H	2.60291700	1.49650100	-0.84082300
H	2.49337000	0.67526100	2.63181900
H	2.12279200	2.31009100	2.04081200
H	0.84527800	1.33928100	2.80716900
H	-3.01470000	-2.42802300	0.18041700
H	-2.65920700	-0.40417500	-2.89972600
H	-1.44182500	-1.38981700	-2.06005000
H	-3.09688400	-2.00566500	-2.26686600
H	-4.40922600	0.75259100	-0.99996000
H	2.80972000	-1.53526400	1.42387500
H	3.50975500	-2.43160500	0.07201600
H	4.56375500	-1.54247400	1.16678800
H	4.45195800	0.76958000	-1.86687200
H	6.29630600	-0.74794300	-2.26159500
H	5.72566400	-1.86990900	-0.91114800

Conformer (2*S*,5*R*,6*S*)-**1a-2**

C	-3.39377700	-1.53412200	1.20101400
C	2.59473200	0.36730400	-0.00923900
C	1.83608600	-0.06360600	2.38579300
O	0.63512200	2.42936800	1.00713300
O	-2.59349500	2.22726600	0.13003200
O	0.67601100	-1.10509800	0.51621400
C	1.43378600	0.11913900	0.92175500
C	0.37932900	1.25599900	0.77921800
O	-1.36199700	-1.70001900	-0.14262300
C	-0.55234900	-0.73966500	0.21452900
C	-0.83544900	0.61607300	0.32802800
C	-2.13486600	1.10023800	-0.05215200
C	-2.99600700	0.05818500	-0.80947000
C	-2.80913600	-1.34913800	-0.19003800
C	-2.59792200	0.07016200	-2.29854800
O	-4.35667000	0.42039500	-0.67558100
C	3.49974400	-0.51343000	-0.47782900
C	3.49148900	-2.00343900	-0.22282200
C	4.60944000	-0.05165200	-1.34448000
C	5.25522700	1.11689800	-1.24781600
H	-2.97796800	-0.81742200	1.91665400
H	-3.19010800	-2.54712800	1.55860600
H	-4.47466200	-1.38637400	1.15519300
H	2.69607700	1.41345400	-0.28751400
H	2.54775600	-0.88636400	2.49028200
H	2.31278900	0.85884300	2.72993000
H	0.95985000	-0.25972900	3.01244100
H	-3.20828300	-2.09991600	-0.87387700
H	-2.69809800	1.08450400	-2.69674100
H	-1.57049900	-0.26906200	-2.46224600
H	-3.27614500	-0.58835900	-2.85073400
H	-4.32948800	1.36288900	-0.40650800
H	2.68028800	-2.32749100	0.42794100
H	3.40003500	-2.54649200	-1.17289500
H	4.44488600	-2.31447500	0.22255300
H	4.93752500	-0.76911500	-2.09793900
H	6.06043600	1.37235900	-1.93078500
H	5.01188000	1.85090600	-0.48342600

Conformer (2*S*,5*R*,6*S*)-**1a-3**

C	3.75312300	1.64661300	0.16441200
C	-2.41127100	0.40032700	-0.61075900
C	-1.76584200	2.16318000	1.14837100
O	-0.98797900	-0.71645000	2.01740800
O	2.16805400	-1.70619600	1.62221400
O	-0.31163700	1.53520100	-0.67293200
C	-1.33278800	0.98880800	0.27128300
C	-0.52674200	-0.08291600	1.08059900
O	1.81154800	1.22732300	-1.25432400
C	0.81039500	0.86885600	-0.49731200
C	0.79032600	-0.11355100	0.48383000
C	1.96040400	-0.92108700	0.69818600
C	3.02965200	-0.77801400	-0.41418100
C	3.14850000	0.70077200	-0.86058100
C	2.64431000	-1.68797300	-1.59712200
O	4.27932000	-1.17999900	0.11151900
C	-3.58128600	-0.18330300	-0.27163900
C	-4.07254400	-0.41709500	1.13658500
C	-4.45226800	-0.61468800	-1.37715300
C	-5.65959000	-1.18571000	-1.25501400
H	3.18312500	1.65352300	1.09925900
H	3.78114300	2.66305100	-0.23756800
H	4.77301200	1.32545000	0.38552200
H	-2.18041000	0.49704200	-1.66930100
H	-2.23875300	2.93412700	0.53420700
H	-2.48440200	1.82067800	1.89549900
H	-0.90290000	2.59345600	1.66613000
H	3.70390500	0.74961300	-1.79857200
H	2.52600800	-2.71723400	-1.24488400
H	1.71418500	-1.37567400	-2.08156600
H	3.44991700	-1.66455500	-2.33802400
H	4.04976700	-1.69087200	0.91644500
H	-3.31282900	-0.19975900	1.88518900
H	-4.96648000	0.18639400	1.33877900
H	-4.36416500	-1.46642000	1.26378800
H	-4.06009600	-0.43563500	-2.37812800
H	-6.23469600	-1.46498500	-2.13297300
H	-6.11707200	-1.39254000	-0.29191100

Conformer (2*S*,5*S*,6*R*)-**1a-1**

C	-2.22787200	-2.38467200	-1.09826700
C	2.55454700	0.62415600	-0.31189600
C	1.65146400	1.75610400	1.78142200
O	0.36746200	2.61440700	-0.89921500
O	-2.76544200	1.54930000	-1.43747800
O	0.72907700	-0.37050200	1.02196100
C	1.35000100	0.90291000	0.54742800
C	0.21962500	1.55824400	-0.30246100
O	-1.20746500	-1.45740700	0.91684400
C	-0.51318200	-0.40253100	0.58552900
C	-0.92304900	0.68255300	-0.18005900
C	-2.28703900	0.75492800	-0.62910600
C	-3.22307100	-0.27865300	0.04605400
C	-2.50003300	-1.64042200	0.19888300
C	-3.67045000	0.27252000	1.41422500
O	-4.35169000	-0.47015800	-0.78428200
C	3.54793800	-0.27138000	-0.12613800
C	3.64234500	-1.23477500	1.03240200
C	4.61900600	-0.30856200	-1.13437200
C	5.67586700	-1.13391600	-1.13070200
H	-1.69947000	-3.31858100	-0.88814600
H	-1.62683900	-1.78795800	-1.79204600
H	-3.17947700	-2.61762500	-1.58036000
H	2.61150900	1.28771200	-1.17296500
H	2.41902000	1.28181800	2.39817600
H	2.02054900	2.73031200	1.44807500
H	0.74760500	1.90935200	2.37999200
H	-3.06277100	-2.27076400	0.88923400
H	-4.41133500	-0.40895700	1.84456200
H	-4.13722600	1.25302300	1.27954200
H	-2.83894000	0.37497900	2.11804200
H	-4.34354300	0.30456100	-1.38529000
H	4.59294300	-1.09718800	1.56145500
H	2.82971300	-1.11763900	1.74781000
H	3.62745400	-2.27141700	0.67361100
H	4.51941900	0.40914700	-1.94829700
H	6.42132700	-1.08875500	-1.91919600
H	5.83793800	-1.87616700	-0.35448700

Conformer (2*S*,5*S*,6*R*)-**1a-2**

C	-2.36654700	-2.02196500	-1.55134800
C	2.60717800	0.34850800	-0.18265200
C	1.77934700	1.12966600	2.09883300
O	0.60115900	2.60196300	-0.35248800
O	-2.59287200	1.93151400	-1.08936500
O	0.68761900	-0.72224700	0.94351600
C	1.42105500	0.56371100	0.72404100
C	0.36063100	1.46453900	0.02490100
O	-1.32777600	-1.60401200	0.61841200
C	-0.54435900	-0.56496800	0.50672900
C	-0.85171300	0.68015000	-0.02830100
C	-2.19584200	0.95274600	-0.45842500
C	-3.22488600	-0.11687500	-0.01389800
C	-2.61271700	-1.53502100	-0.13256300
C	-3.66449600	0.18266400	1.43268300
O	-4.34297500	-0.04766700	-0.87739700
C	3.53671600	-0.62509400	-0.13308400
C	3.53611600	-1.79186200	0.82790500
C	4.66709800	-0.62552900	-1.09100800
C	5.29549100	0.45344900	-1.57352800
H	-1.91658500	-3.01828600	-1.53071500
H	-1.70430600	-1.34741900	-2.10378000
H	-3.32094500	-2.07534700	-2.07895000
H	2.70320600	1.12116200	-0.94161200
H	2.49549900	0.48006100	2.60832300
H	2.23624500	2.11359700	1.95868200
H	0.88569300	1.24375800	2.72121100
H	-3.23850300	-2.24458400	0.41114600
H	-4.46433200	-0.51156400	1.70997300
H	-4.05409700	1.20343600	1.49367000
H	-2.84591900	0.07789400	2.15125700
H	-4.26580800	0.83295900	-1.30166200
H	4.48253700	-1.82416000	1.38214500
H	2.71412600	-1.76347100	1.54229000
H	3.46798600	-2.73653700	0.27213600
H	5.02711200	-1.61339200	-1.38189400
H	6.11850100	0.35746800	-2.27603700
H	5.01991700	1.46331100	-1.27931900

Conformer (2*S*,5*S*,6*R*)-**1a-3**

C	2.69360800	2.27616500	-0.99660600
C	-2.44587600	0.61760000	0.33710300
C	-1.73474800	-1.02685500	2.18187400
O	-0.96524700	-2.02755800	-0.65711700
O	2.17798600	-1.62587900	-1.68016300
O	-0.33883200	0.80230400	1.43414900
C	-1.33721800	-0.20270500	0.95714700
C	-0.51795700	-1.05359000	-0.07127600
O	1.77277400	1.40494500	1.09008600
C	0.79548400	0.58941400	0.80092400
C	0.80513700	-0.47049900	-0.09614000
C	2.03131600	-0.82362800	-0.75918500
C	3.28239400	-0.11638500	-0.18006400
C	2.95352400	1.35330400	0.18295300
C	3.77106800	-0.89989300	1.05401900
O	4.29077100	-0.10850100	-1.17173400
C	-3.61433700	0.21651400	-0.20931000
C	-4.07064000	-1.21474600	-0.36008600
C	-4.52127100	1.27409200	-0.68448100
C	-5.73501300	1.09010300	-1.22443300
H	2.45222000	3.28032800	-0.63747600
H	1.86893000	1.91755400	-1.62117400
H	3.59390100	2.32778800	-1.61224800
H	-2.24266900	1.68553800	0.37303900
H	-2.21425500	-0.38369100	2.92456900
H	-2.43826800	-1.80821200	1.88829900
H	-0.85435700	-1.49956300	2.62836800
H	3.74870900	1.75489200	0.81305500
H	4.71311100	-0.46259600	1.40024800
H	3.95325100	-1.94297200	0.77784500
H	3.05159200	-0.87753300	1.87816100
H	4.00844500	-0.79902000	-1.80793600
H	-4.38030700	-1.40346000	-1.39485500
H	-3.28541100	-1.93005700	-0.12217300
H	-4.94591900	-1.41005100	0.27241100
H	-4.15274500	2.29303100	-0.56745100
H	-6.33814900	1.93643400	-1.53985100
H	-6.17053000	0.10575300	-1.36923200