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Electronic Supplementary Information

Modified diterpenoids from the tuber of *Icacina oliviformis* as protein tyrosine phosphatase 1B inhibitors

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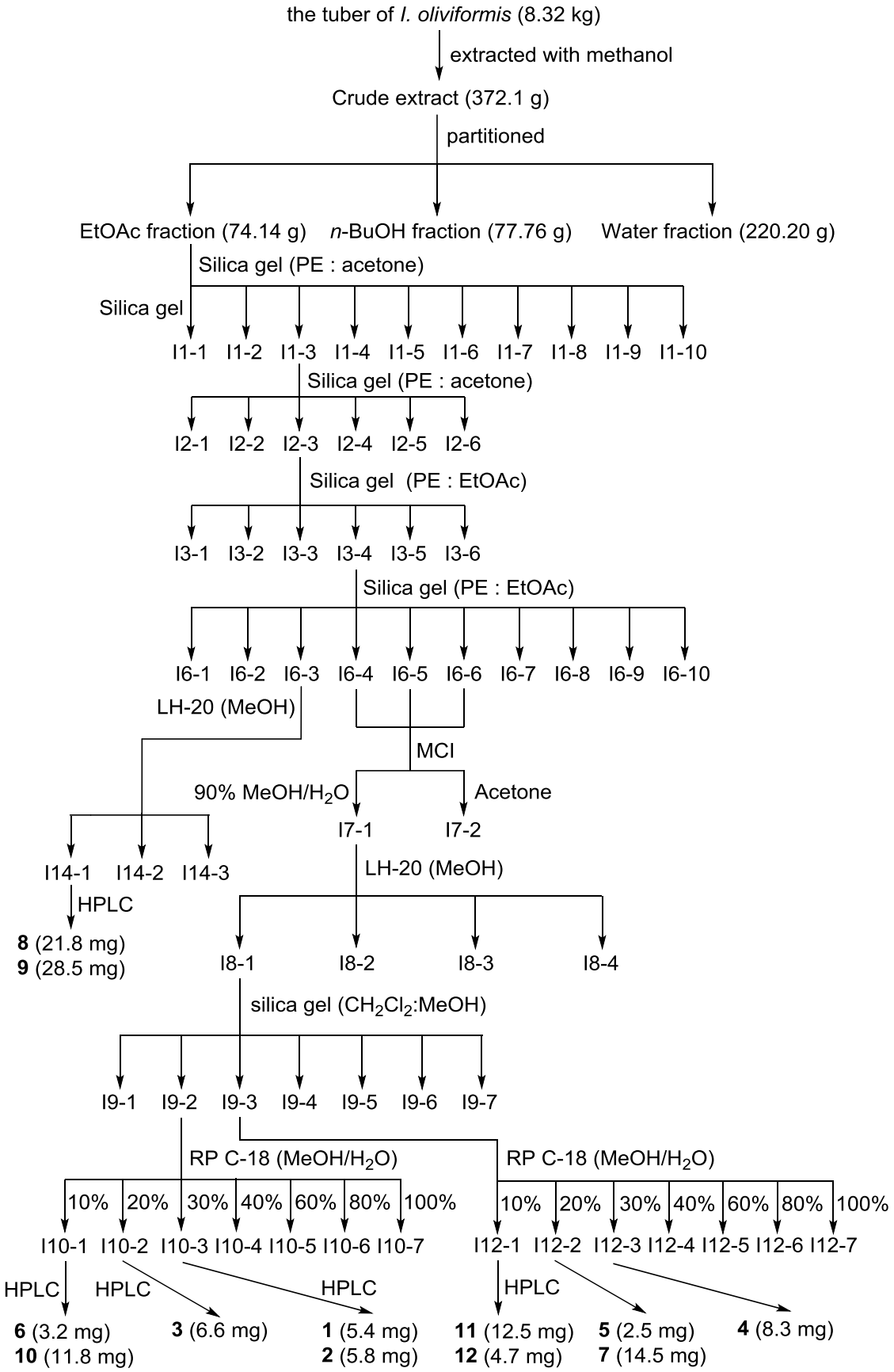

Fig. S1 Flow charts of the extraction and isolation processes.

Table S1 ^{1}H NMR [δ, mult, (J in Hz)] spectroscopic data for compounds **1**–**3** and **1a** (^{1}H: 400 MHz, ^{13}C: 100 MHz).

	1 ($CDCl_3$)		**1a** ($CDCl_3$)		**2** ($CDCl_3$)		**3** ($CDCl_3$)	
No.	δ_H (J in Hz)	δ_C	δ_H, (J in Hz)	δ_C	δ_H, (J in Hz)	δ_C	δ_H, (J in Hz)	δ_C
1a	1.63, m	28.5	1.64, m	28.4	1.66, m	27.7	1.79, m	26.0
1b	1.68, m		1.69, m		2.33, m		1.96, m	
2a	2.25, ddd (15.7, 11.6, 4.0)	27.9	2.23, ddd (15.5, 11.3, 4.3)	27.9	2.38, ddd (14.8, 12.2, 8.9)	28.5	2.19, ddd (16.1, 11.0, 5.2)	30.0
2b	2.37, ddd (15.7, 11.3, 6.8)		2.38, ddd (15.5, 11.5, 6.1)		2.48, ddd (14.8, 11.9, 4.8)		2.46, ddd (16.1, 11.5, 5.9)	
3		173.3		173.2		173.26		174.1
4	2.57, qd (7.1, 7.0)	40.4	2.59, qd (7.0, 7.1)	40.4	3.02, qd (7.0, 6.7)	34.5		119.1
5	1.95, overlap	41.8	1.97, overlap	41.8	2.23, brs	38.4		149.3
6	5.92, dd (10.1, 3.4)	131.5	5.94, dd (10.1, 3.5)	131.8	6.09, dd (10.2, 1.6)	127.0	6.15, d (9.7)	117.7
7	5.65, dd (10.1, 0.8)	122.4	5.65, dd (10.1, 1.4)	122.1	5.76, dd (10.2, 2.9)	125.9	6.82, d (9.7)	130.2
8		58.2		58.0		58.4		103.8
9β	2.39, dd (11.3, 6.8)	45.4	2.42, dd (11.2, 6.5)	45.5	2.01, dd (11.6, 6.5)	46.3	2.43, dd (11.5, 6.6)	41.8
10		37.0		37.0		37.6		38.5
11α	1.62, m	27.3	1.67, m	27.2	1.63, m	27.5	1.71, ddd (13.6, 11.6, 3.4)	18.2
11β	1.91, m		1.95, m		1.87, m		1.59, ddt (13.6, 6.7, 3.5)	
12α	1.54, m	32.8	1.65, m	32.9	1.55, m	32.3	1.99, overlap	32.4
12β	1.77, m		1.76, m		1.70, m		1.33, td (13.0, 3.1)	
13		52.5		52.7		53.7		42.0
14		179.1		179.0		179.4		162.6
15α	4.31, dd (6.9, 3.8)	85.9	4.52, dd (8.2, 2.8)	82.6	4.30, dd (7.6, 3.5)	85.9		77.6
15β							4.15, dd (9.0, 7.6)	
16α	3.85, overlap	61.8	4.41, dd (12.0, 8.2)	63.5	3.82, overlap	61.7	3.96, dd (9.0, 8.5)	72.3
16β	3.88, overlap		4.65, dd (12.0, 2.8)		3.88, overlap		4.29, dd (8.5, 7.6)	
17	1.09, s	21.1	1.15, s	20.6	0.98, s	20.7	1.19, s	17.6
18	1.36, d (7.0)	16.9	1.37, d (7.0)	16.9	1.38, d (7.0)	14.0	1.98, s	12.3
19		174.4		174.3		173.30		166.6
20α	3.91, d (12.2)	71.3	3.93, d (12.1)	71.3	3.91, dd (12.5, 1.3)	71.1	4.34, d (11.1)	75.6
20β	4.50, d (12.2)		4.49, d (12.1)		4.81, dd (12.5, 1.0)		4.19, dd (11.1, 1.7)	
3-OCH_3	3.67, s	52.1	3.68, s	52.1	3.69, s	52.2	3.62, s	51.8
1′				165.7				
2′				128.3				
3′			7.91, d (8.6)	131.4				
4′			7.61, d (8.6)	132.1				

5′		128.9
6′	7.61, d (8.6)	132.1
7′	7.91, d (8.6)	131.4

Table S2 ^{1}H NMR [δ, mult, (J in Hz)] spectroscopic data for compounds **4**−**7** (^{1}H: 400 MHz, ^{13}C: 100 MHz).

	4 ($CDCl_3$)		**5** (CD_3OD)		**6** (CD_3OD)		**7** ($CDCl_3$)	
No.	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C
1α	2.00, m	37.4	1.74, overlap	30.2	1.76, overlap	30.3	1.70, overlap	29.6
1β	2.25, m		1.69, overlap		1.70, overlap		1.65, overlap	
2α	2.11, m	29.3	2.33, ddd (12.7, 11.6, 3.9)	23.4	2.33, ddd (12.9, 12.2, 3.9)	23.4	2.31, ddd (13.7, 10.3, 5.8)	22.7
2β	2.18, m		1.81, ddd (12.7, 10.1, 4.1)		1.84, ddd (12.9, 11.8, 4.8)		1.81, ddd (13.7, 10.6, 6.2)	
3		173.2		100.9		100.9		99.1
4		120.4		52.9		52.9		51.1
5		149.7	2.40, dd (7.0, 1.6)	46.5	2.38, dd (7.0, 1.8)	46.0	2.19, dd (7.0, 1.9)	45.2
6	6.65, d (10.2)	122.5	4.93, dd (7.0, 4.6)	73.5	5.02, dd (6.9, 5.0)	73.4	4.88, dd (7.0, 4.8)	70.7
7	7.06, d (10.2)	130.4	5.94, brd (4.6)	118.4	6.18, dd (4.8, 0.8)	117.5	5.96, brd (4.8)	117.0
8		129.3		147.0		147.5		142.4
9β		134.8	1.93, dd (12.7, 3.1)	38.0	1.92, dd (11.7, 3.2)	40.0	1.88, dd (10.5, 3.2)	38.7
10		40.5		31.5		31.6		30.6
11α	6.89, d (7.9)	122.3	1.27, m	26.6	1.29, m	26.6	1.15, m	26.2
11β			1.65, m		1.65, m		1.63, m	
12α	7.08, d (7.9)	131.0	1.42, overlap	33.7	1.45, m	35.5	1.45, m	34.5
12β			1.42, overlap		1.31, m		1.29, m	
13		135.9		50.6		53.6		53.5
14		140.7	3.99, s	87.5		107.1		110.0
15α	2.76, dq (14.6, 7.6)	21.9		79.9		79.8		78.6
15β	2.79, dq (14.6, 7.6)		3.79, d (4.6)		3.80, dd (5.4, 0.9)		3.70, dd (12.1, 4.7)	
16α	1.15, t (7.6)	14.9	3.70, d (10.1)	76.6	3.93, dd (10.1, 0.9)	76.0	3.83, dd (10.5, 1.3)	76.6
16β			4.39, dd (10.1, 4.9)		4.43, dd (10.1, 5.4)		4.51, dd (10.5, 5.6)	
17	2.32, s	19.7	0.94, s	15.7	0.99, s	14.0	0.96, s	12.7
18	2.03, s	12.4	1.36, s	19.0	1.37, s	19.0	1.40, s	19.2
19		165.7		180.6		180.7		177.0
20α	4.72, d (10.9)	72.8	3.57, dd (9.2, 1.9)	73.8	3.56, dd (9.2, 1.9)	73.9	3.56, dd (9.3, 2.0)	72.7
20β	4.41, d (10.9)		3.99, dd (9.2, 3.4)		3.96, dd (9.2, 3.3)		4.07, dd (9.3, 2.8)	
OCH_3-3	3.54, s	51.8	3.30, s	50.1	3.30, s	50.1	3.38, s	50.1
OCH_3-14							3.29, s	50.1

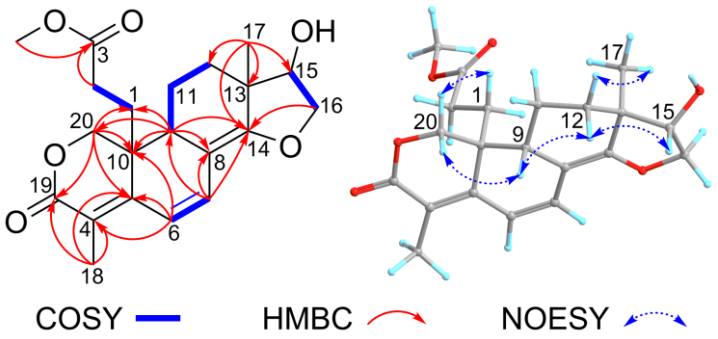

Fig. S2 ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **3**.

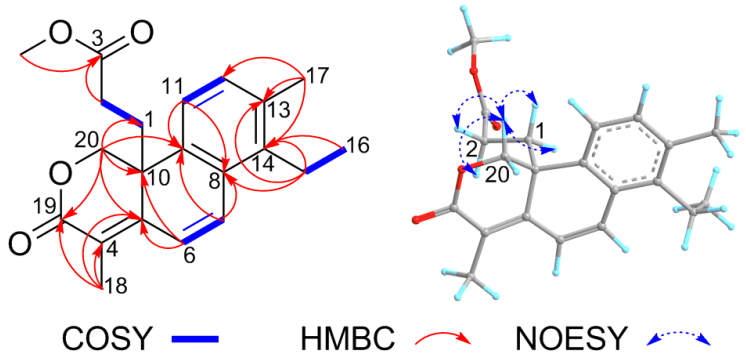

Fig. S3 ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **4**.

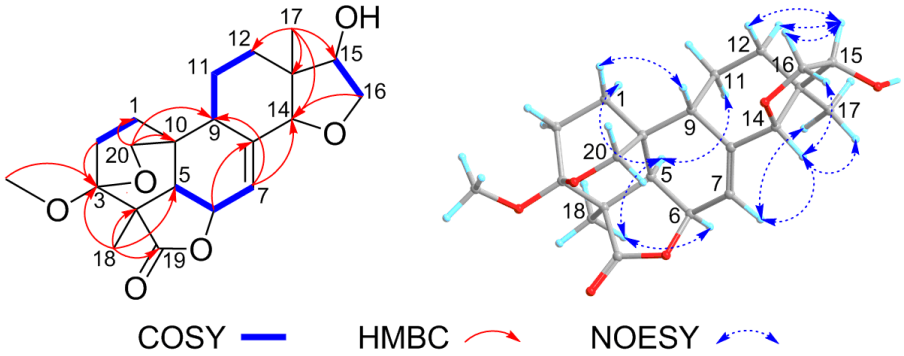

Fig. S4 ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **5**.

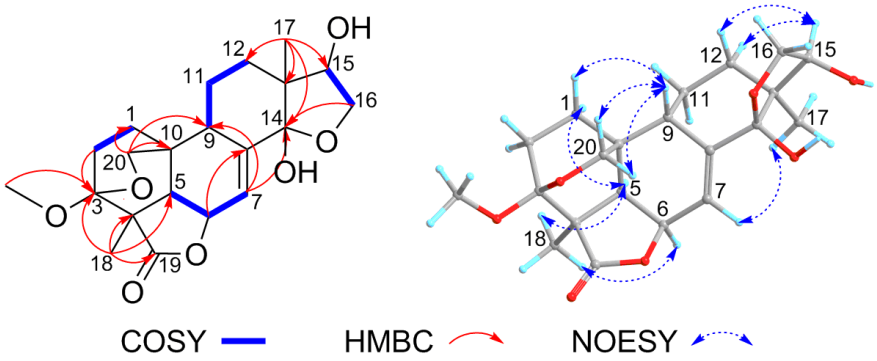

Fig. S5 ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **6**.

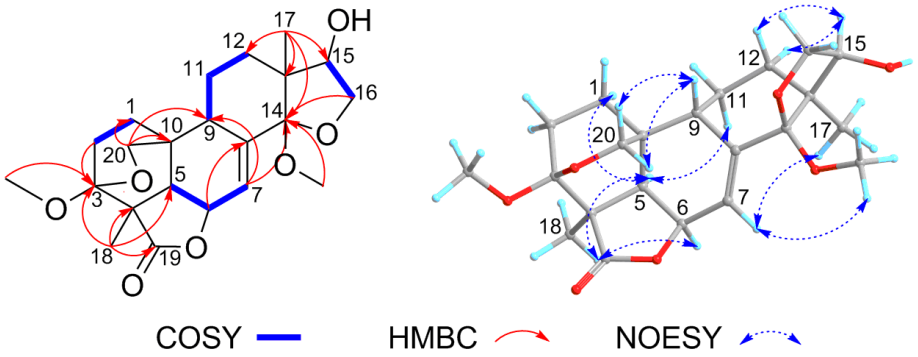

Fig. S6 ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **7**.

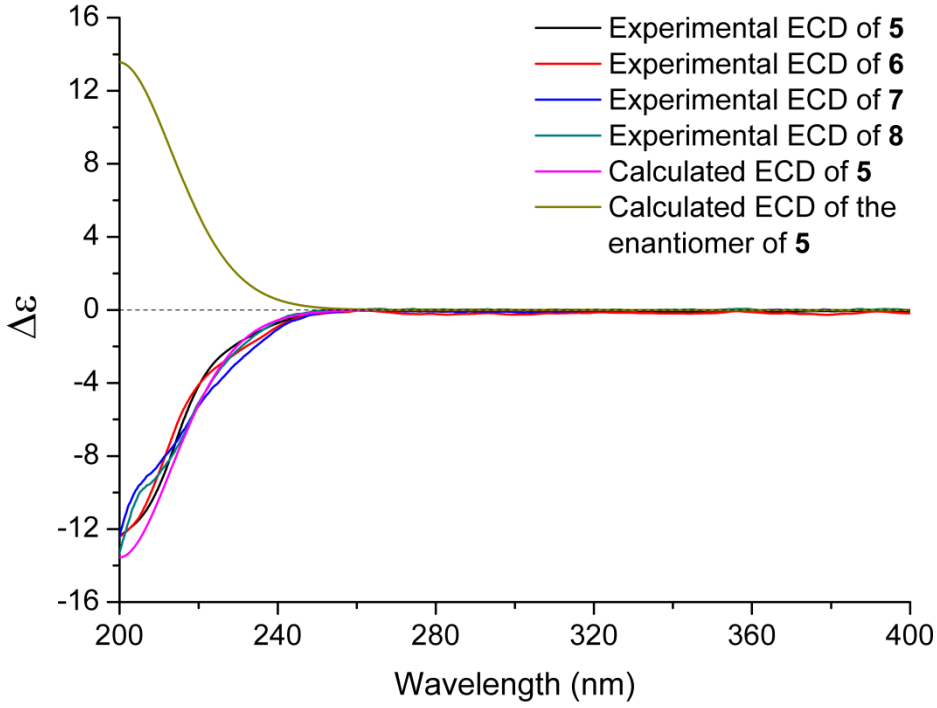

Fig. S7 Experimental ECD spectra of **5**–**8** and the calculated ECD spectra for **5** and its enantiomer.

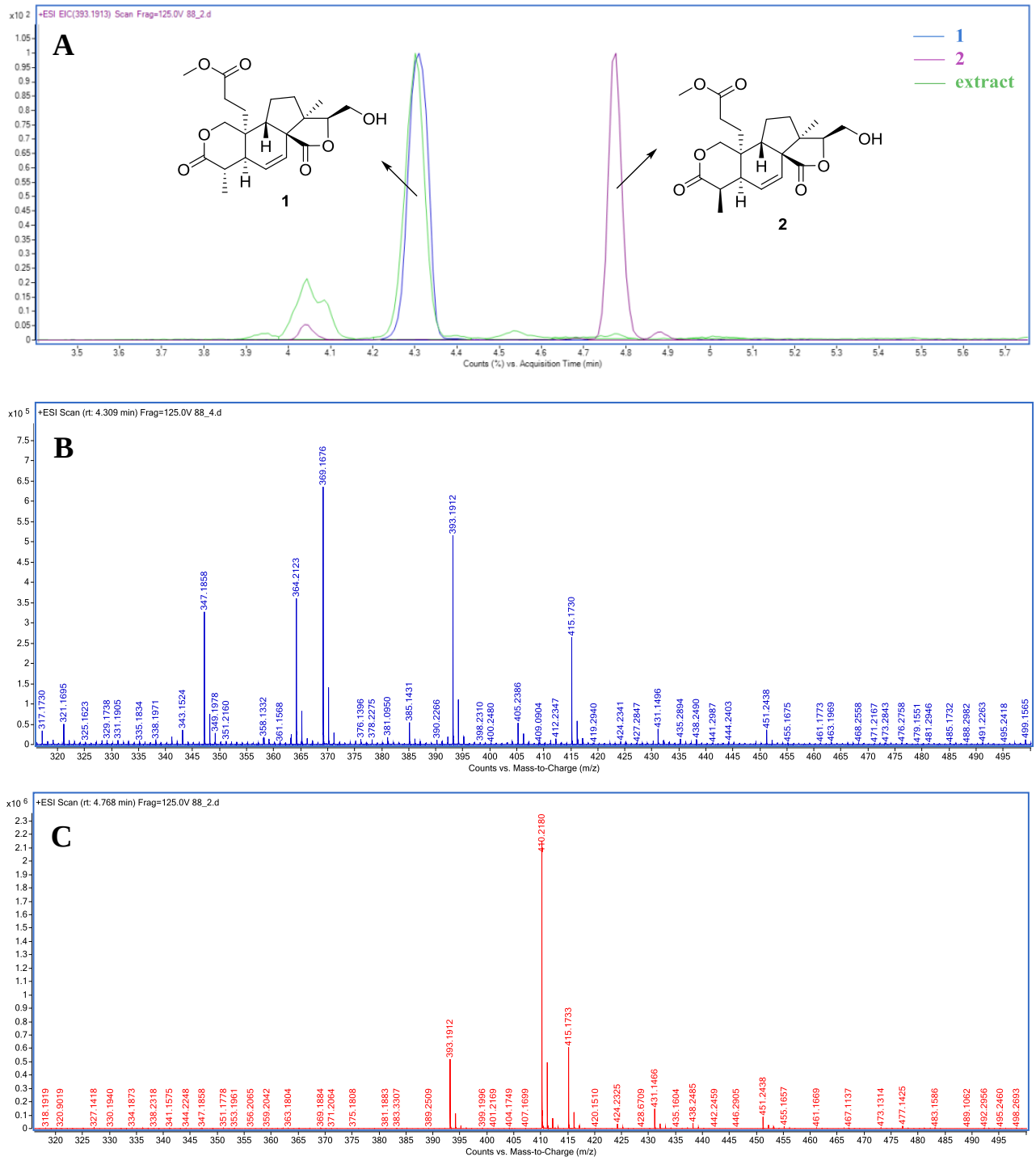

Fig. S8 A: HRESIMS chromatogram of compounds **1**, **2**, and extract with the scan of *m*/*z* 393.1913.

B: HRESIMS spectrum of extract at 4.309 min. **C**: HRESIMS spectrum of extract at 4.769 min.

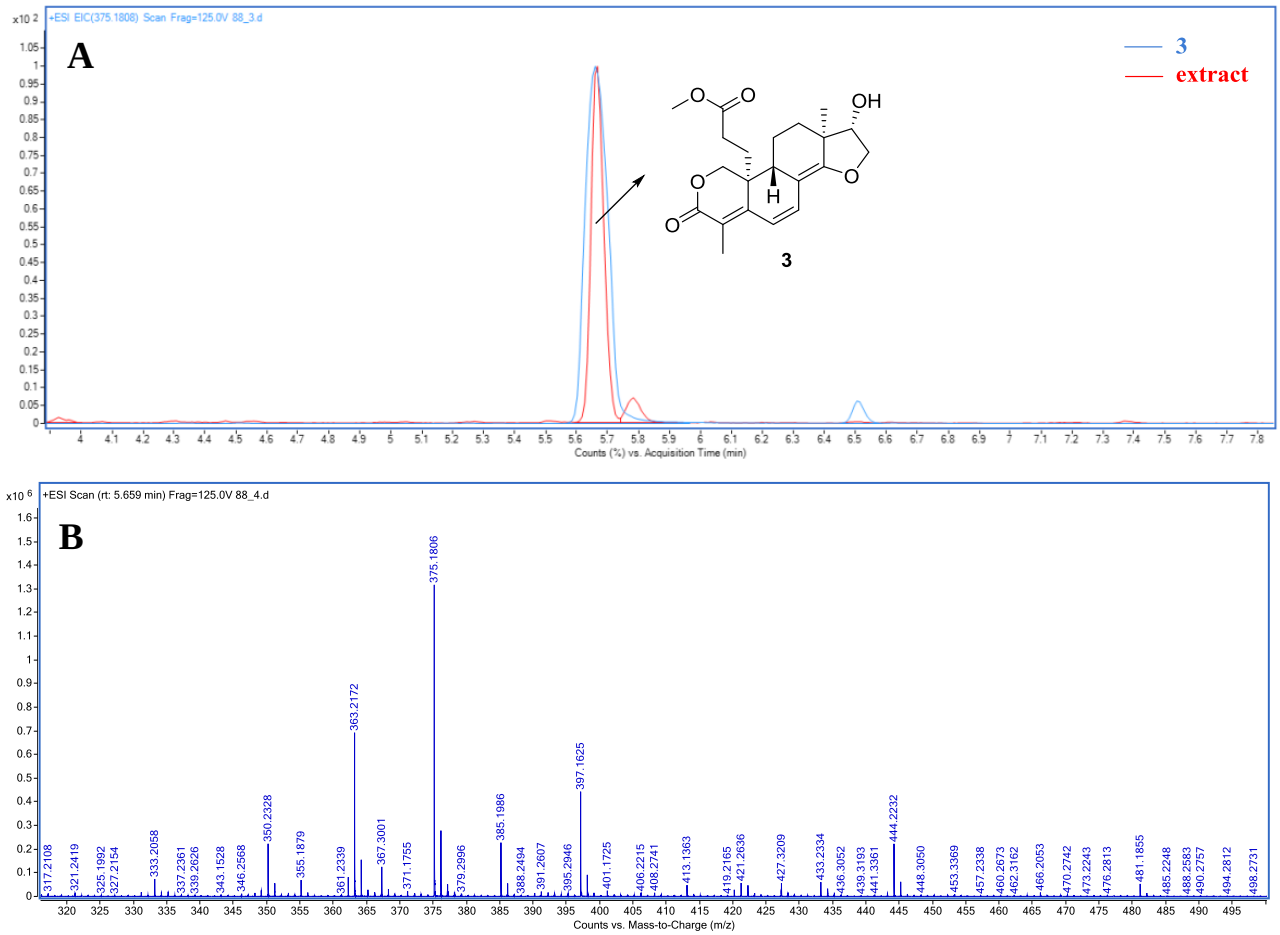

Fig. S9 A: HRESIMS chromatogram of compound **3** and extract with the scan of *m/z* 375.1808.

B: HRESIMS spectrum of extract at 5.659 min.

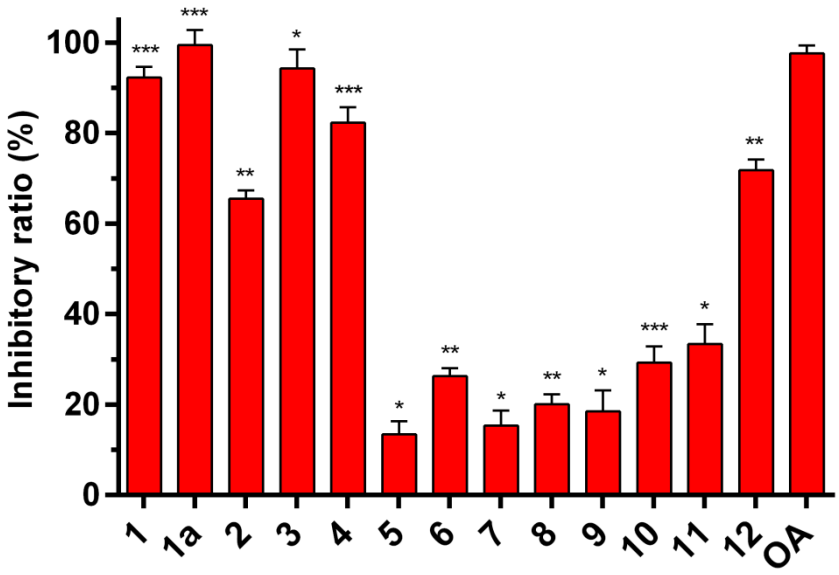

Fig. S10 PTP1B inhibitory ratio (%) of compounds **1**−**12** and **1a** with a concentration of 80 μM.

Oleanolic acid (OA) was used as control drugs. Mean ± SD of three replicates are shown; * means 0.01 < p < 0.05, ** means p < 0.01, and *** means p < 0.001 compared with the control group (OA).

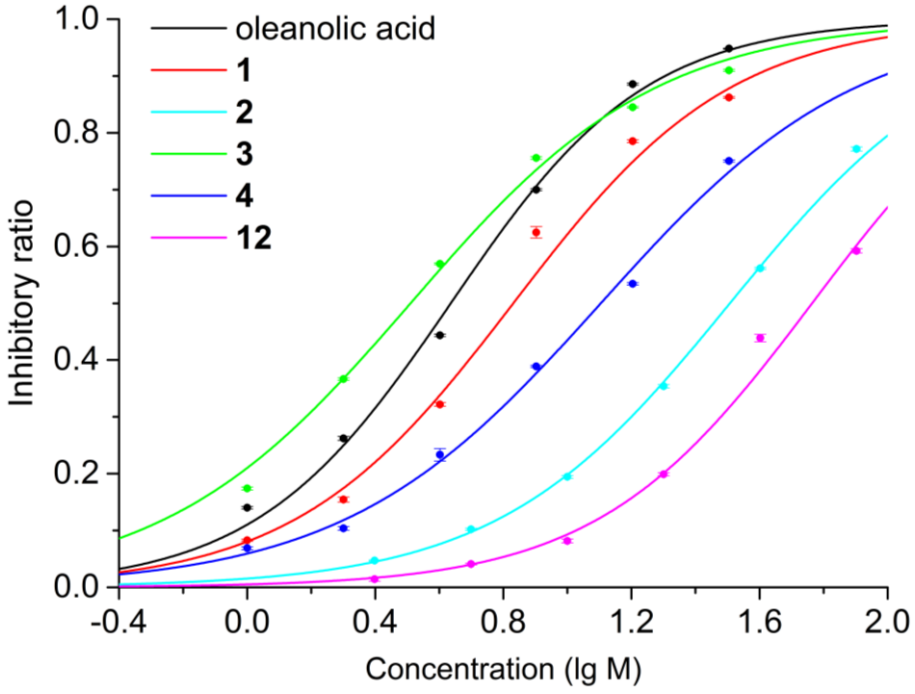

Fig. S11 Concentration-inhibition ratio curves of **1**−**4**, **12**, and oleanolic acid.

The final concentrations of **1**, **3**, **4**, and oleanolic acid were 1, 2, 4, 8, 16, and 32 μM.

The final concentrations of **2** and **12** were 2.5, 5, 10, 20, 40, and 80 μM.

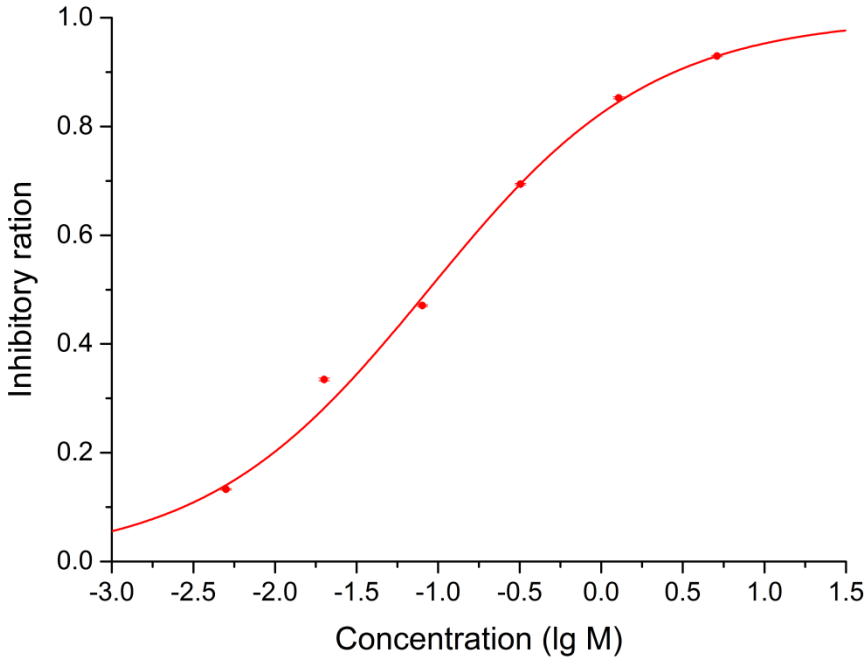

Fig. S12 Concentration-inhibition ratio curve of **1a**.

The final concentrations of **1a** were 0.005, 0.02, 0.08, 0.32, 1.28, and 5.12 μM.

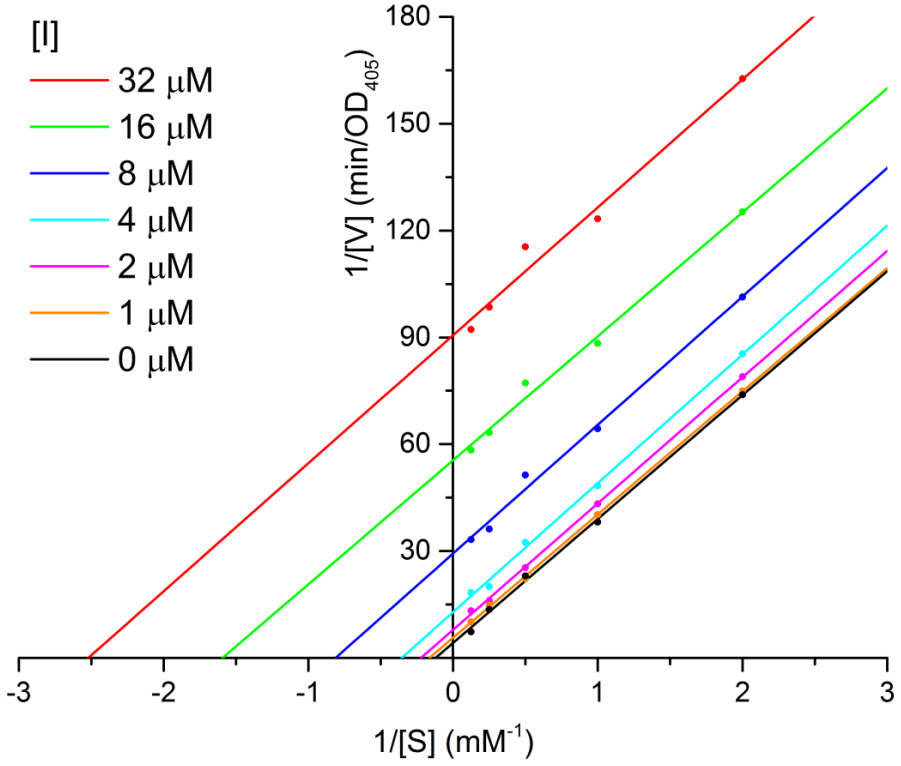

Fig. S13 Lineweaver-Burk plot for the inhibition of PTP1B by **1**.

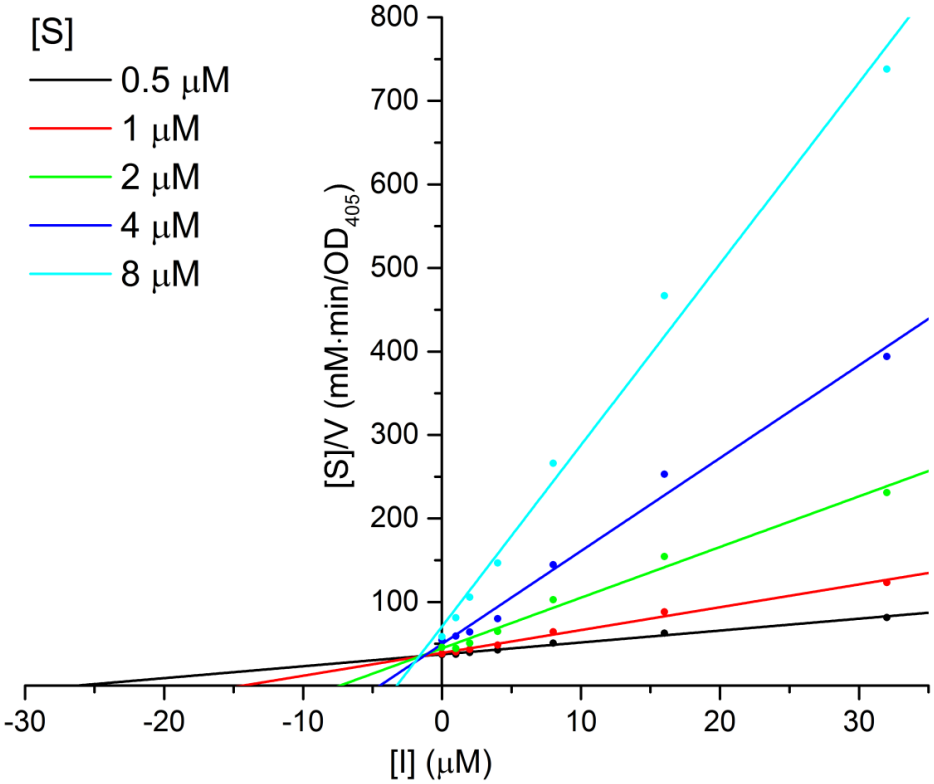

Fig. S14 The plot of [S]/V against [I] for the inhibition of PTP1B by **1**.

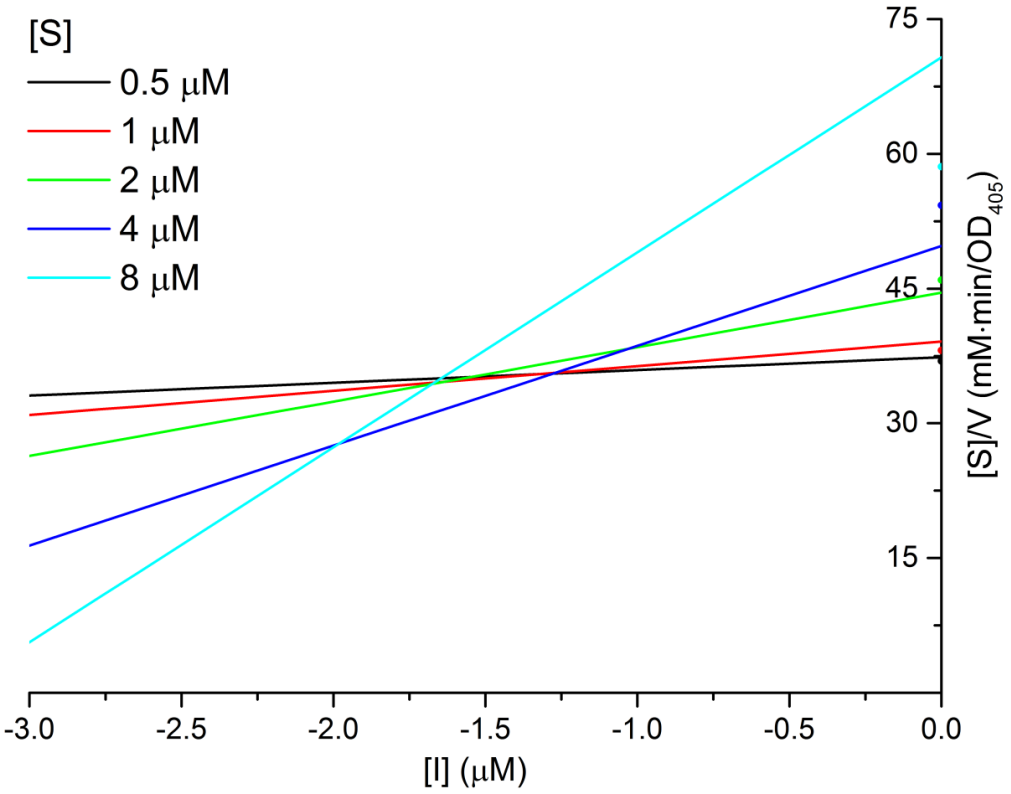

Fig. S15 The plot of [S]/V against [I] for the inhibition of PTP1B by **1** (amplified).

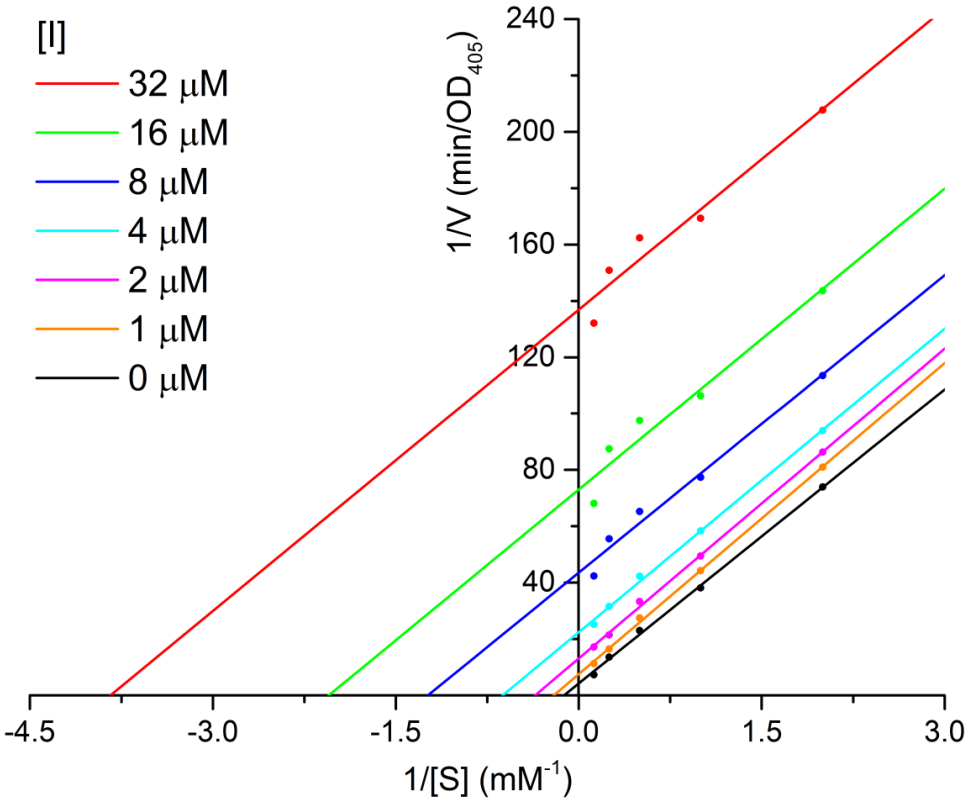

Fig. S16 Lineweaver-Burk plot for the inhibition of PTP1B by **3**.

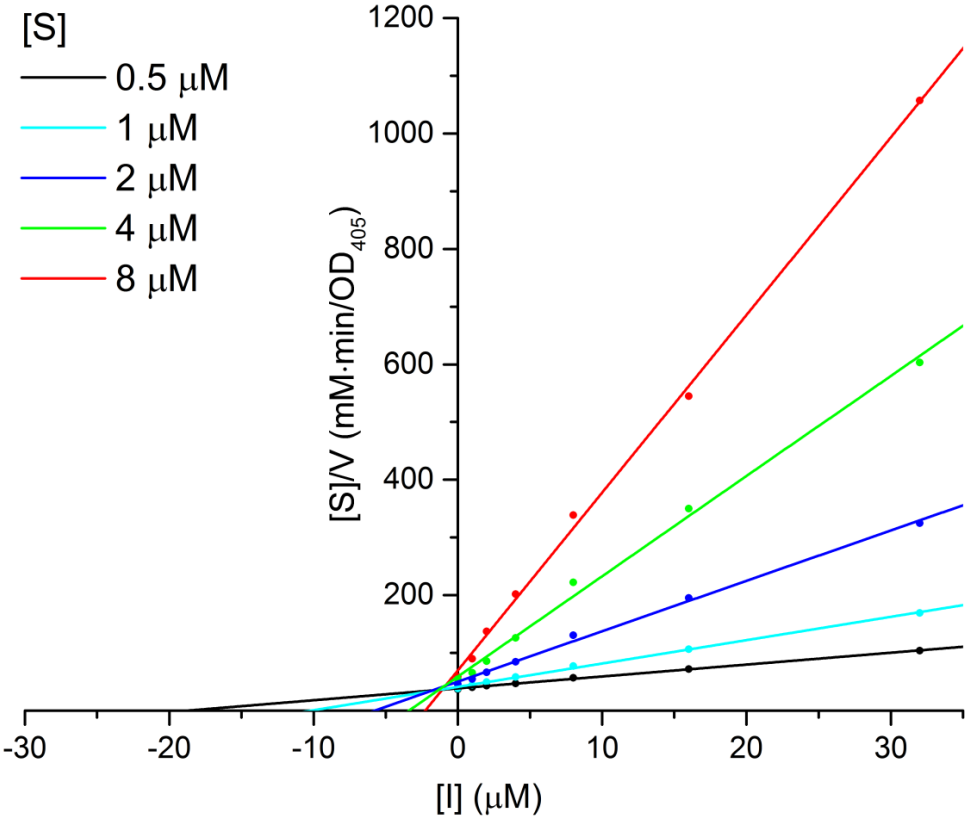

Fig. S17 The plot of [S]/V against [I] for the inhibition of PTP1B by **3**.

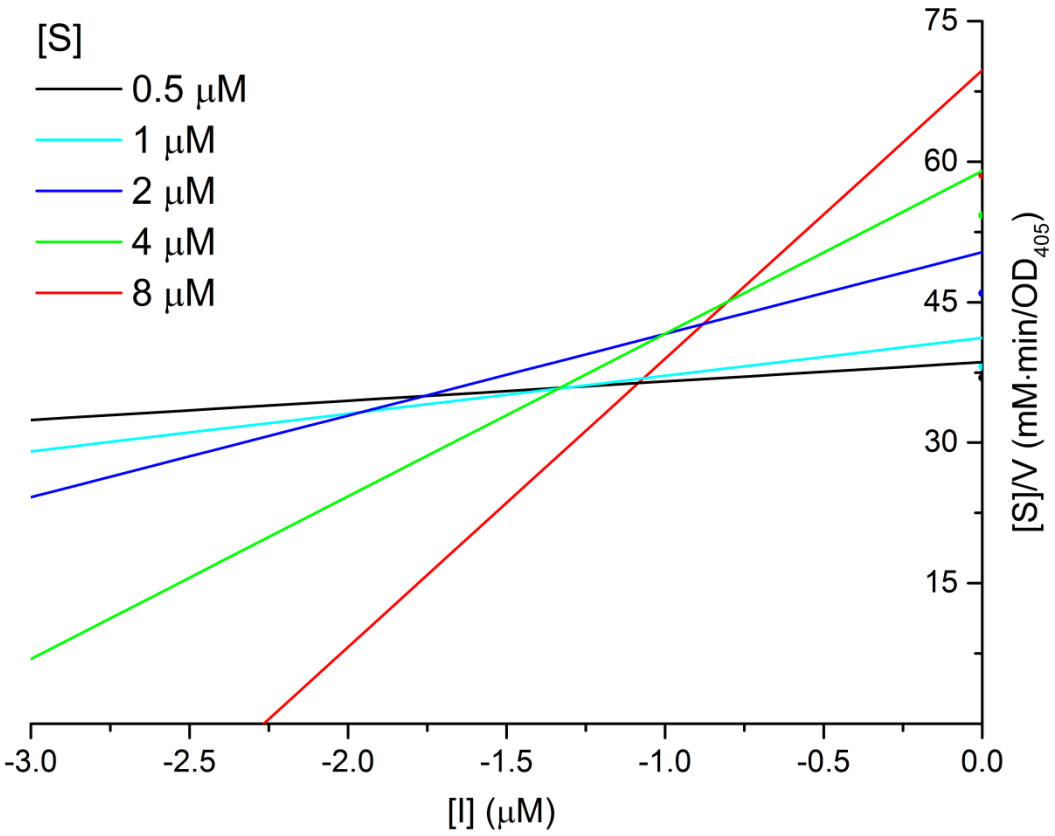

Fig. S18 The plot of [S]/V against [I] for the inhibition of PTP1B by **3** (amplified).

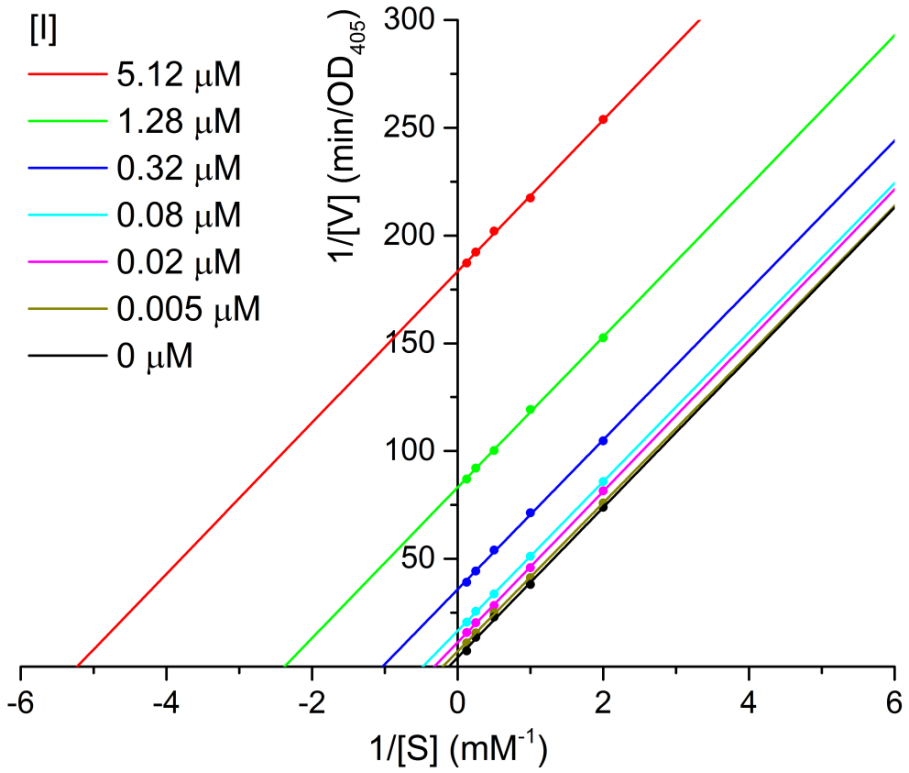

Fig. S19 Lineweaver-Burk plot for the inhibition of PTP1B by **1a**.

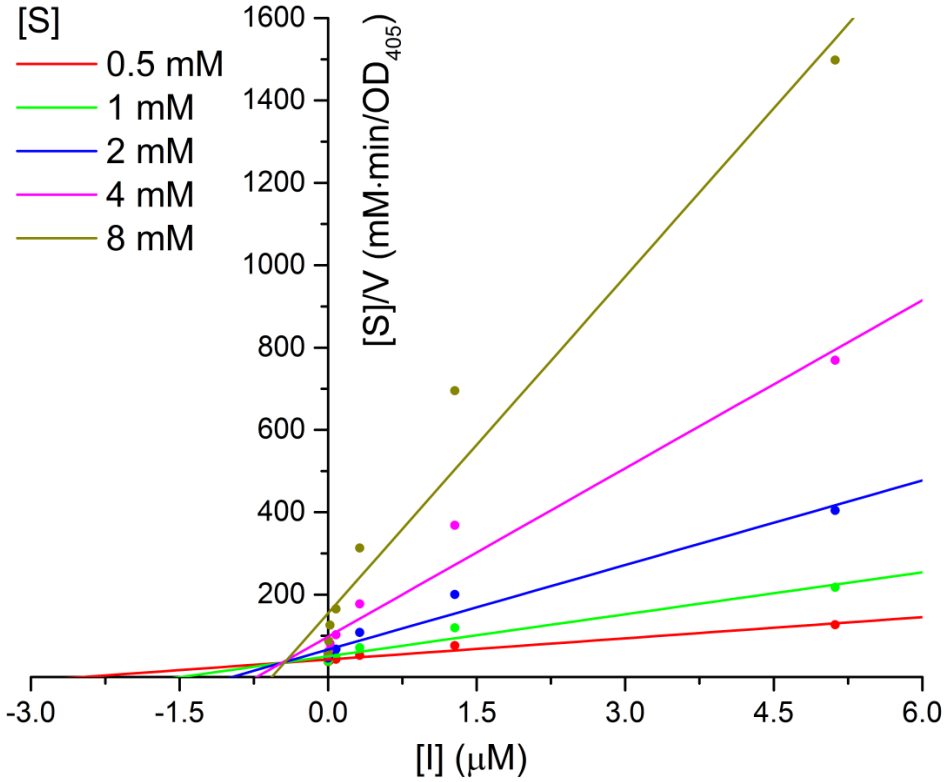

Fig. S20 The plot of [S]/V against [I] for the inhibition of PTP1B by **1a**.

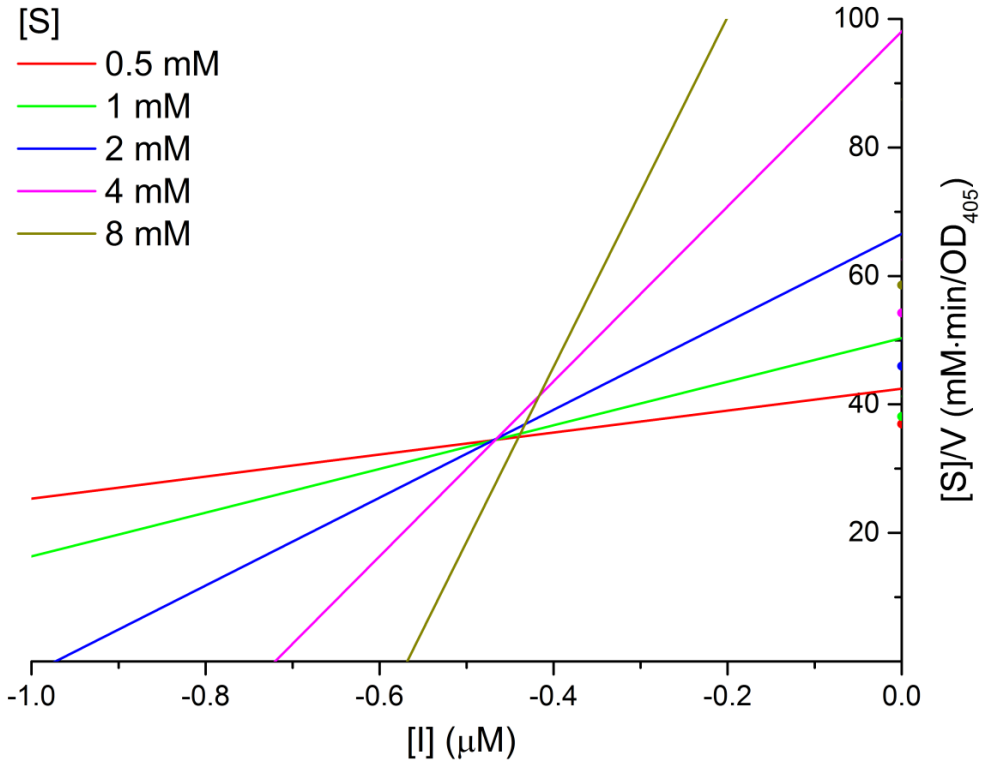

Fig. S21 The plot of [S]/V against [I] for the inhibition of PTP1B by **1a** (amplified).

Table S3 Effect of different concentrations of **1** on V_{max}, K_m, and the K_{ik} to K_{iv} ratio.

V_{max} and K_m values were calculated according to Lineweaver-Burk from the data shown in Fig. S13. K_{ik}/K_{iv} ratio was calculated based on published methods.[S1]

Inhibitor (**1**)	Substrate (*p*NPP)				
[I] (μM)	V_{max}	K_m	K_{iv}	K_{ik}	K_{ik}/K_{iv} or K_{ik}/K_{iv}[a]
0	0.2374	8.258			
1	0.1766	6.111	2.907	2.846	1.021
2	0.1270	4.505	1.151	1.201	1.043
4	0.07775	2.813	0.4871	0.5165	1.060
8	0.03411	1.231	0.1678	0.1752	1.044
16	0.01802	0.6274	0.08217	0.08222	1.001
32	0.01104	0.3966	0.04878	0.05045	1.034

[a] The ratio of the larger one of K_{ik} and K_{iv} to the smaller one.

Table S4 Effect of different concentrations of **3** on V_{max}, K_m, and the K_{ik} to K_{iv} ratio.

V_{max} and K_m values were calculated according to Lineweaver-Burk from the data shown in Fig. S16. K_{ik}/K_{iv} ratio was calculated based on published methods.[S1]

Inhibitor (**3**)	Substrate (*p*NPP)				
[I] (μM)	V_{max}	K_m	K_{iv}	K_{ik}	K_{ik}/K_{iv} or K_{ik}/K_{iv}[a]
0	0.2374	8.258			
1	0.1330	4.899	1.275	1.459	1.144
2	0.07644	2.803	0.4750	0.5137	1.081
4	0.04466	1.604	0.2317	0.2410	1.040
8	0.02298	0.8088	0.1072	0.1086	1.013
16	0.01370	0.4880	0.06124	0.06281	1.026
32	0.007307	0.2604	0.03176	0.03256	1.025

[a] The ratio of the larger one of K_{ik} and K_{iv} to the smaller one.

Table S5 Effect of different concentrations of **1a** on V_{max}, K_m, and the K_{ik} to K_{iv} ratio.

V_{max} and K_m values were calculated according to Lineweaver-Burk from the data shown in Fig. S19. K_{ik}/K_{iv} ratio was calculated based on published methods.[S1]

Inhibitor (**1a**)	Substrate (*p*NPP)				
[I] (μM)	V_{max}	K_m	K_{iv}	K_{ik}	K_{ik}/K_{iv} or K_{ik}/K_{iv} [a]
0	0.2374	8.258			
0.005	0.1418	4.886	1.484	1.449	1.024
0.02	0.08913	3.123	0.6013	0.6082	1.011
0.08	0.06037	2.090	0.3411	0.3388	1.007
0.32	0.02793	0.9691	0.1334	0.1330	1.003
1.28	0.01203	0.4206	0.05339	0.05366	1.005
5.12	0.005453	0.1914	0.02351	0.02373	1.009

[a] The ratio of the larger one of K_{ik} and K_{iv} to the smaller one.

Table S6 The calculated energies (kcal/mol) of **1**−**12**, **1a**, and oleanolic acid to PTP1B by Autodock 4.2.6.[S2]

Inhibitors	Binding Energy	Intermolecular	Internal Energy	Torsional Energy	Unbound Extended Energy
1	−8.63	−10.42	−1.57	1.79	−1.57
1a	−10.89	−11.94	−1.69	1.05	−1.69
2	−6.41	−8.20	−0.93	1.79	−0.93
3	−7.52	−9.02	−0.80	1.49	−0.80
4	−9.91	−11.4	−0.32	1.49	−0.32
5	−8.48	−9.08	−0.19	0.60	−0.19
6	−7.98	−8.87	−1.51	0.89	−1.51
7	−7.80	−8.69	−0.29	0.89	−0.29
8	−8.51	−9.11	−0.59	0.60	−0.59
9	−7.86	−8.76	−1.53	0.89	−1.53
10	−7.54	−8.43	−0.72	0.89	−0.72
11	−8.17	−8.47	−0.01	0.30	−0.01
12	−10.13	−10.73	−0.53	0.60	−0.53
oleanolic acid	−9.19	−10.08	0.13	0.89	0.13

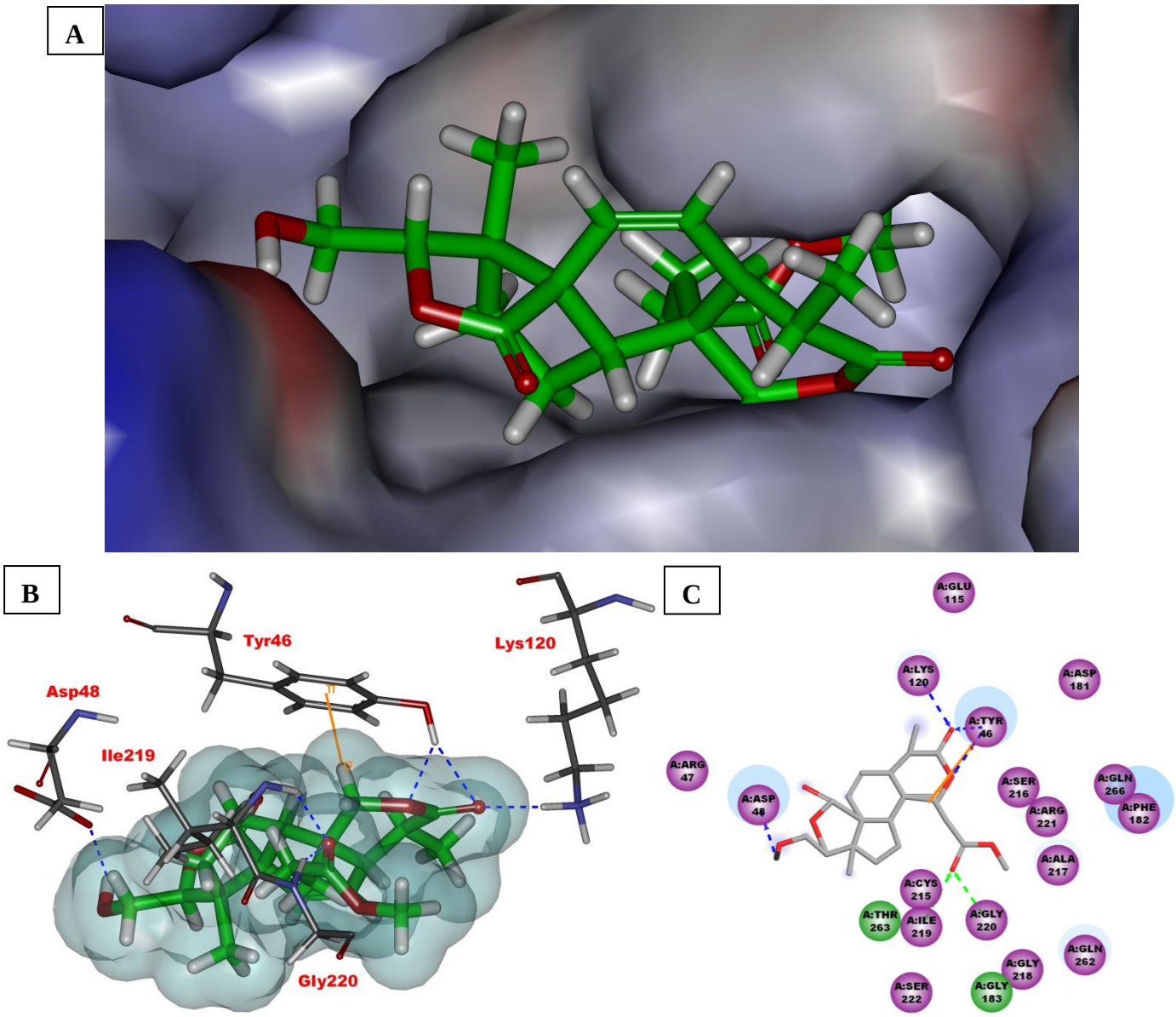

Fig. S22 Molecular docking models for PTP1B inhibition of **1**.

A: 3D docking surfaces of the PTP1B protein active site and **1**. **B** and **C**: Ligand interaction models of **1**.

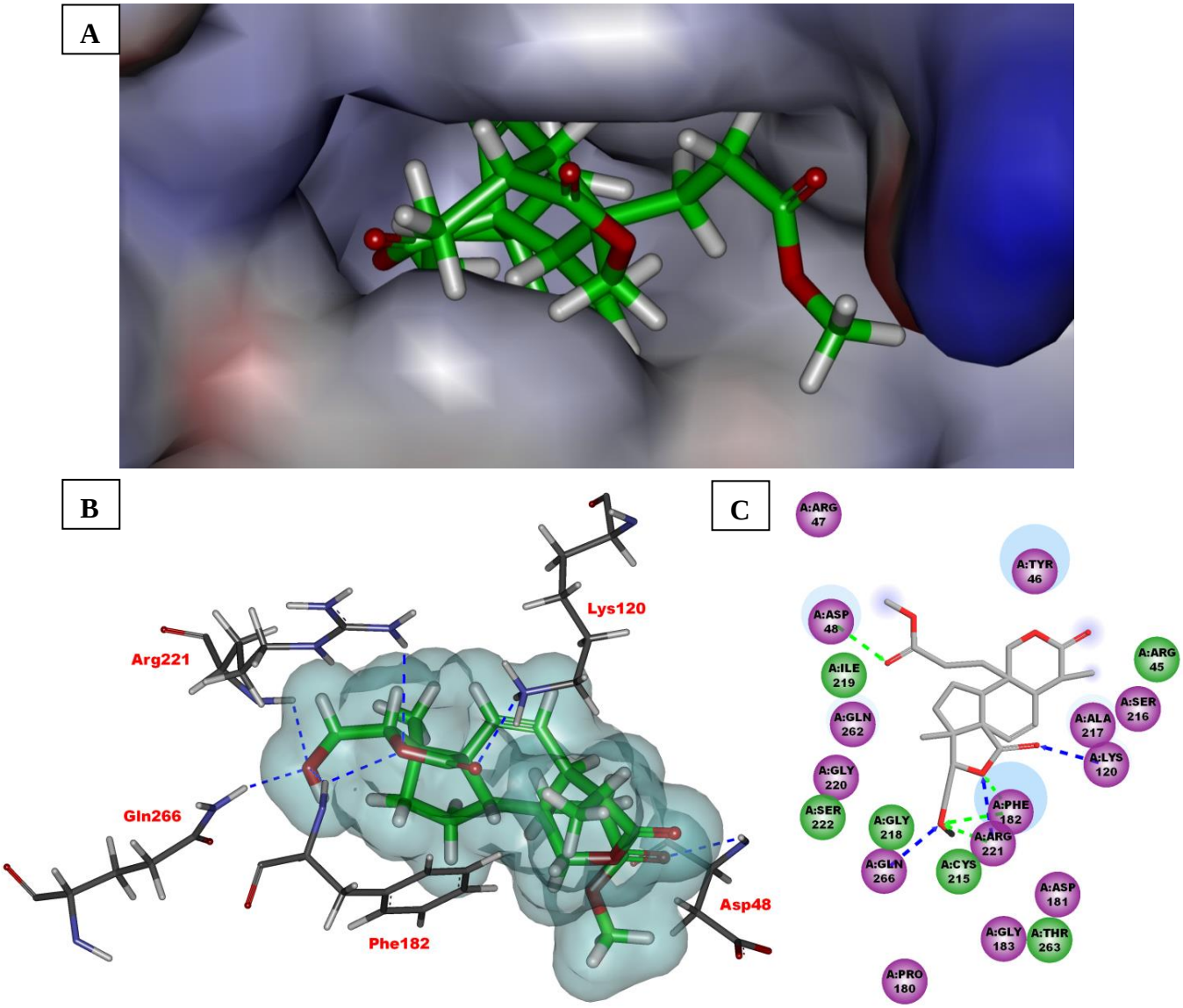

Fig. S23 Molecular docking models for PTP1B inhibition of **2**.

A: 3D docking surfaces of the PTP1B protein active site and **2**. **B** and **C**: Ligand interaction models of **2**.

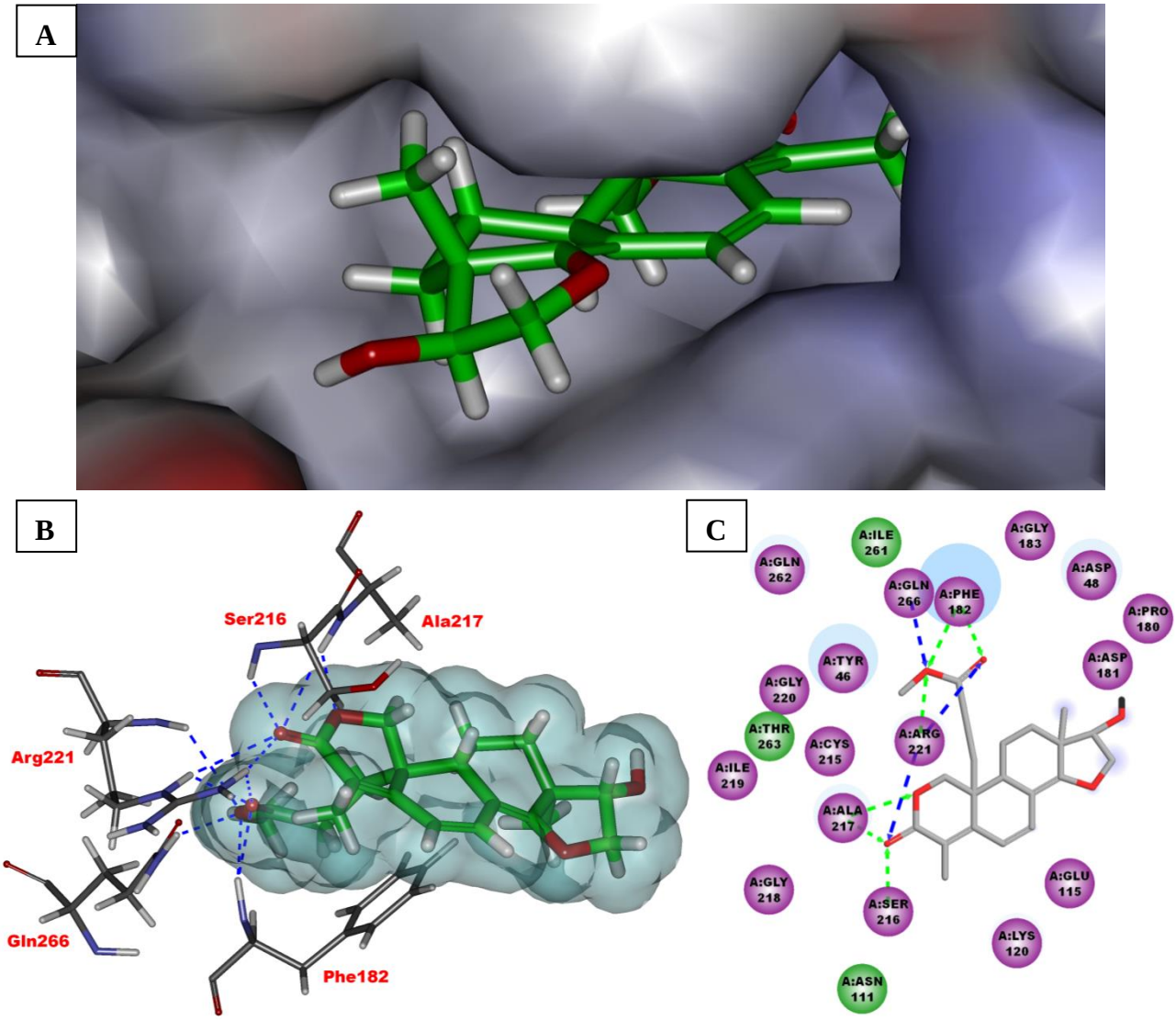

Fig. S24 Molecular docking models for PTP1B inhibition of **3**.

A: 3D docking surfaces of the PTP1B protein active site and **3**. **B** and **C**: Ligand interaction models of **3**.

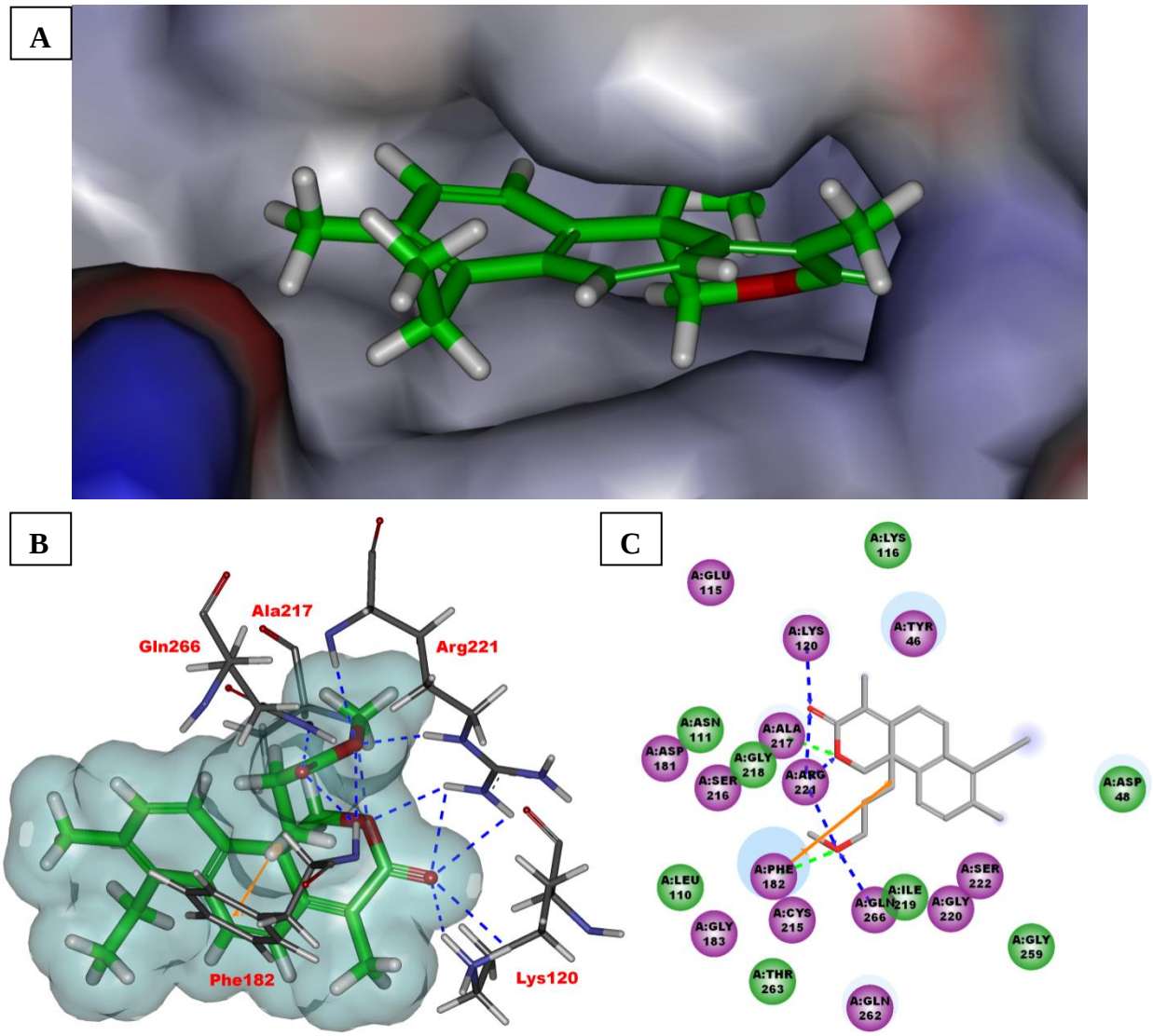

Fig. S25 Molecular docking models for PTP1B inhibition of **4**.

A: 3D docking surfaces of the PTP1B protein active site and **4**. **B** and **C**: Ligand interaction models of **4**.

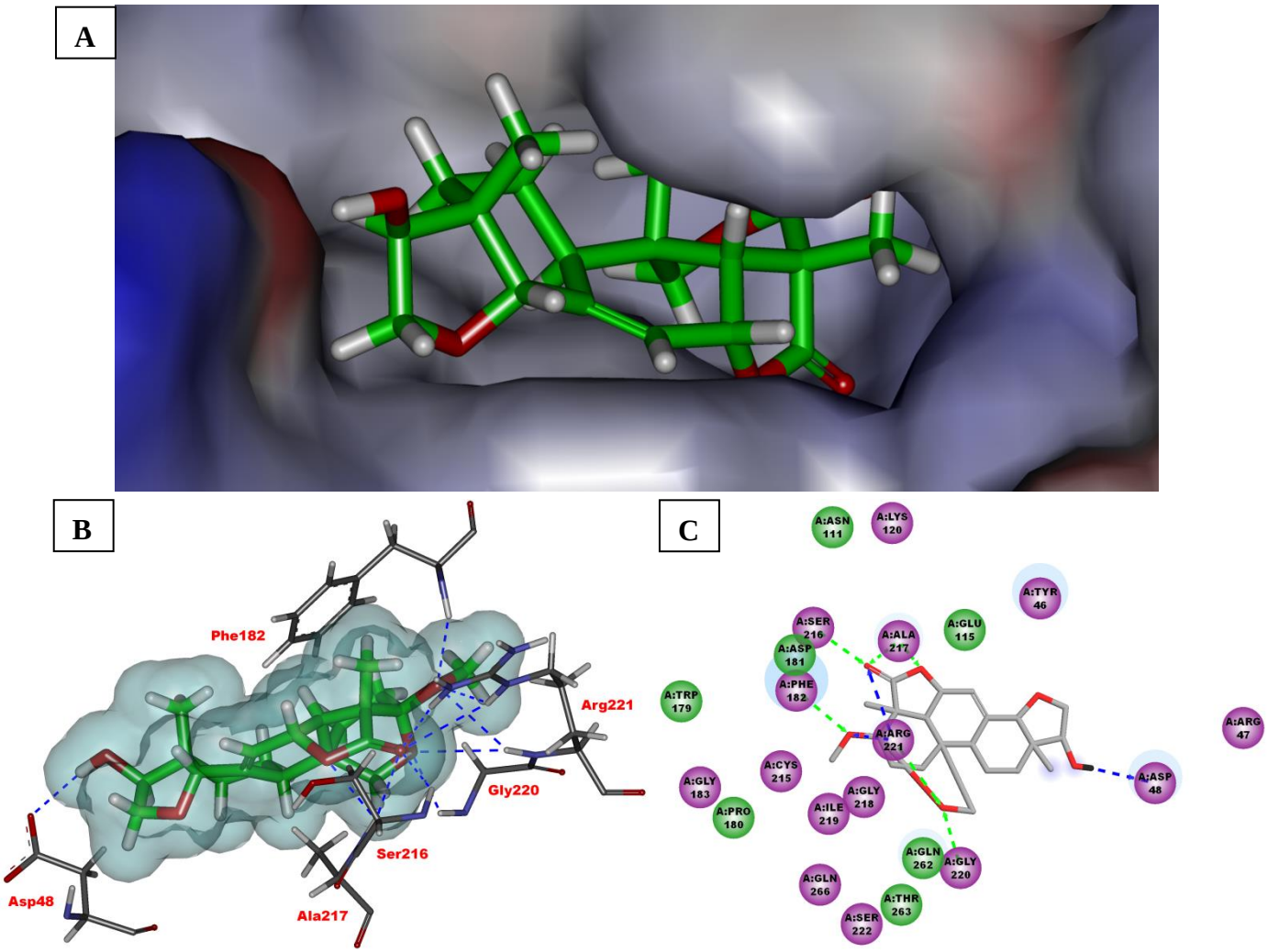

Fig. S26 Molecular docking models for PTP1B inhibition of **5**.

A: 3D docking surfaces of the PTP1B protein active site and **5**. **B** and **C**: Ligand interaction models of **5**.

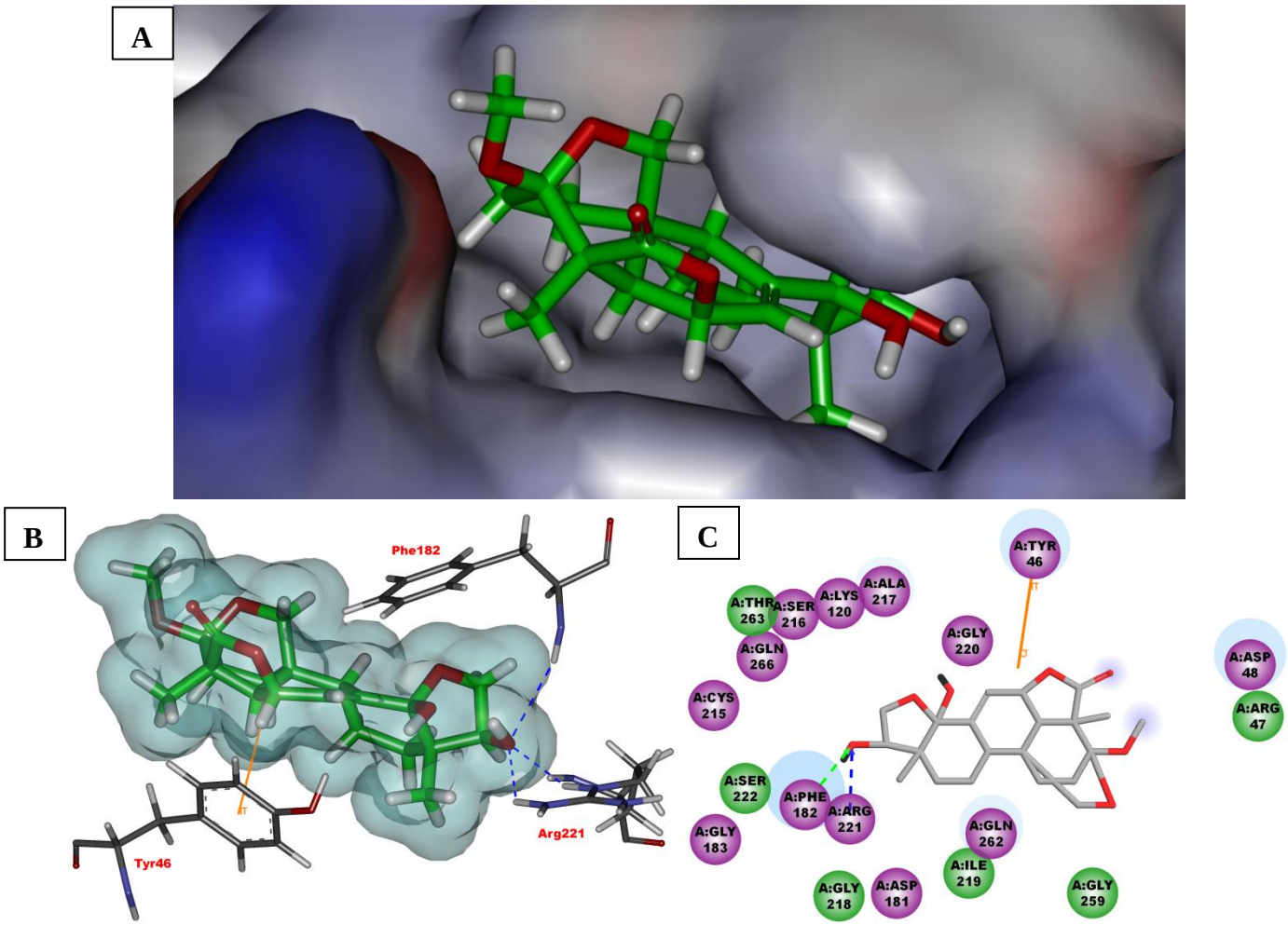

Fig. S27 Molecular docking models for PTP1B inhibition of **6**.

A: 3D docking surfaces of the PTP1B protein active site and **6**. **B** and **C**: Ligand interaction models of **6**.

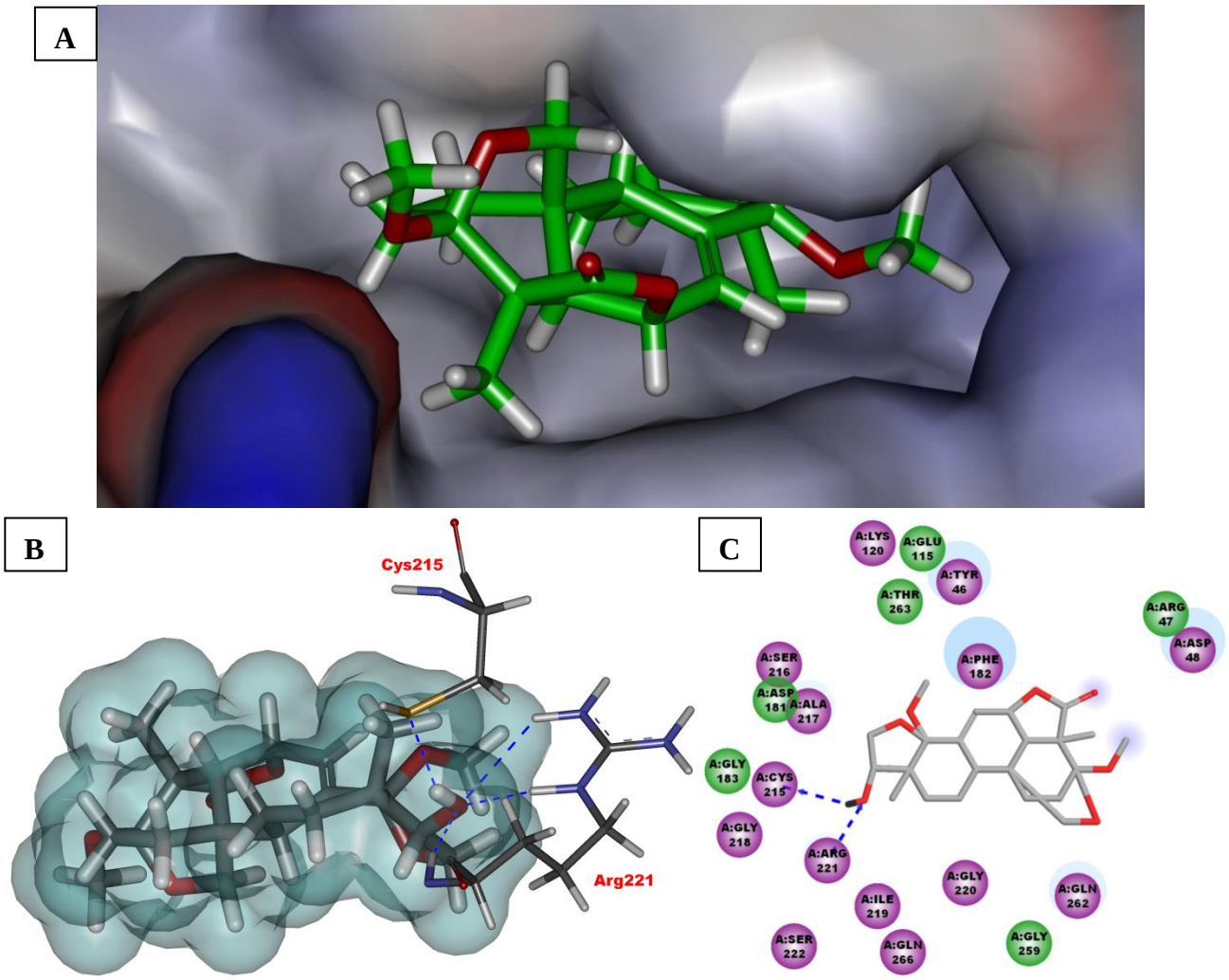

Fig. S28 Molecular docking models for PTP1B inhibition of **7**.

A: 3D docking surfaces of the PTP1B protein active site and **7**. **B** and **C**: Ligand interaction models of **7**.

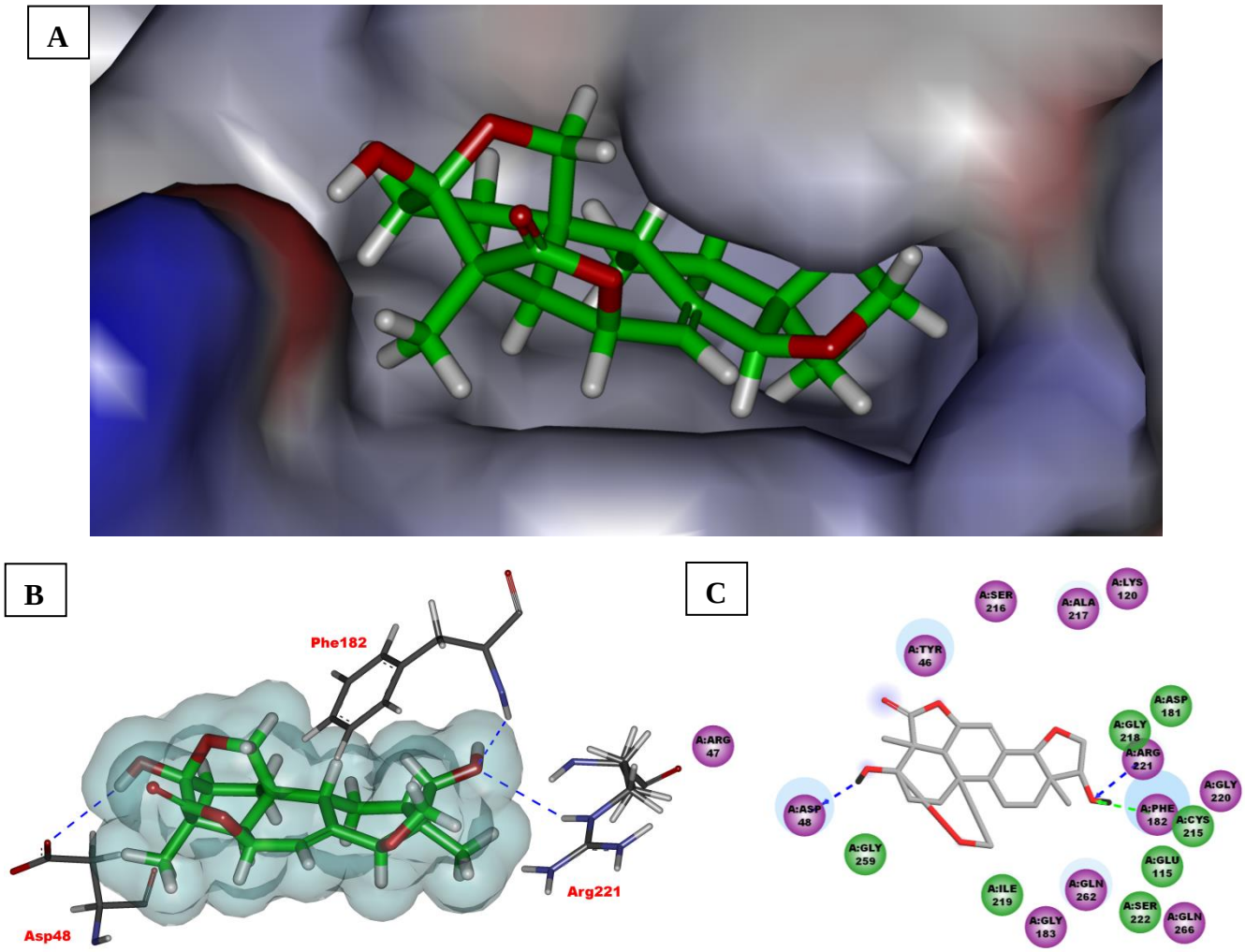

Fig. S29 Molecular docking models for PTP1B inhibition of **8**.

A: 3D docking surfaces of the PTP1B protein active site and **8**. **B** and **C**: Ligand interaction models of **8**.

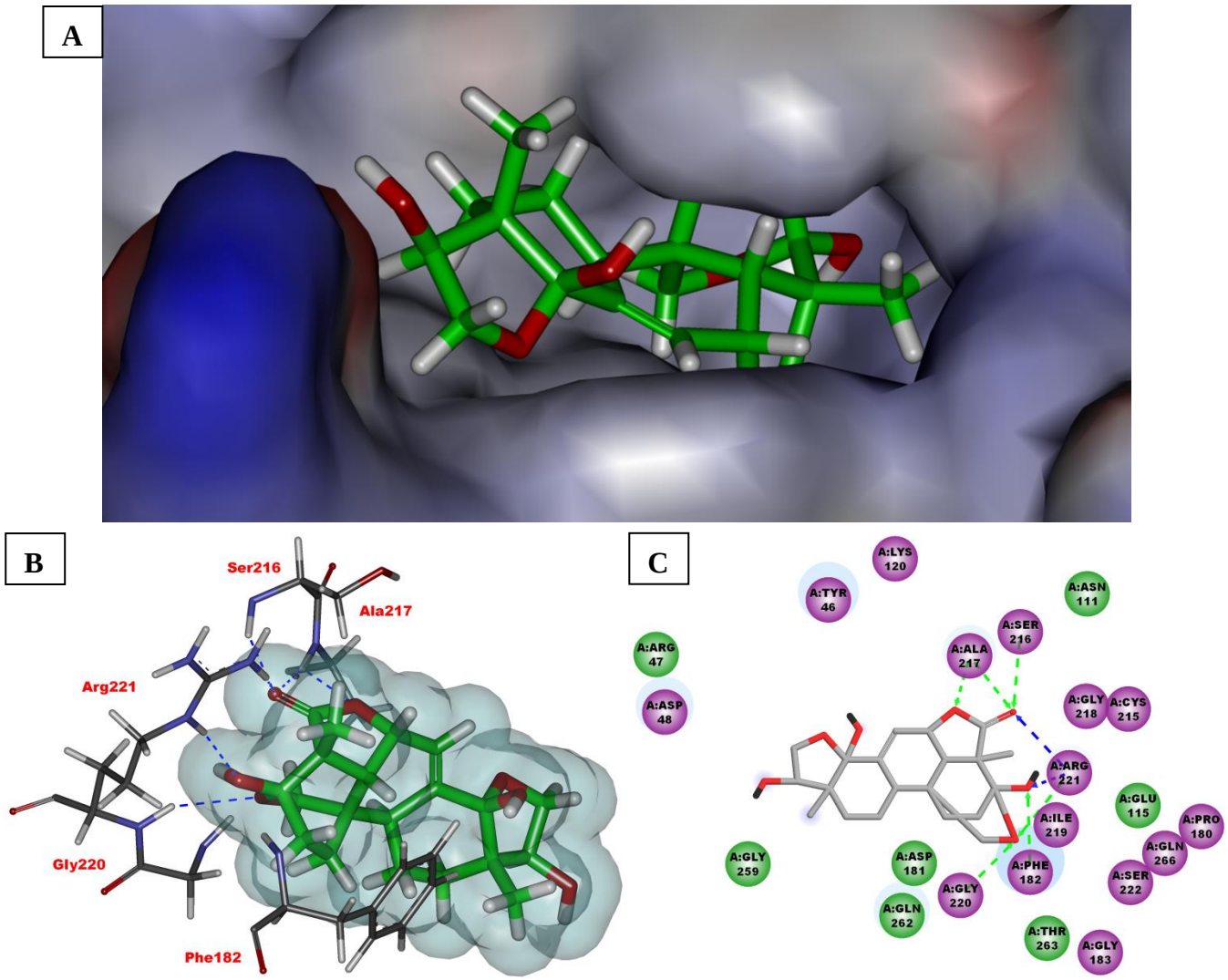

Fig. S30 Molecular docking models for PTP1B inhibition of **9**.

A: 3D docking surfaces of the PTP1B protein active site and **9**. **B** and **C**: Ligand interaction models of **9**.

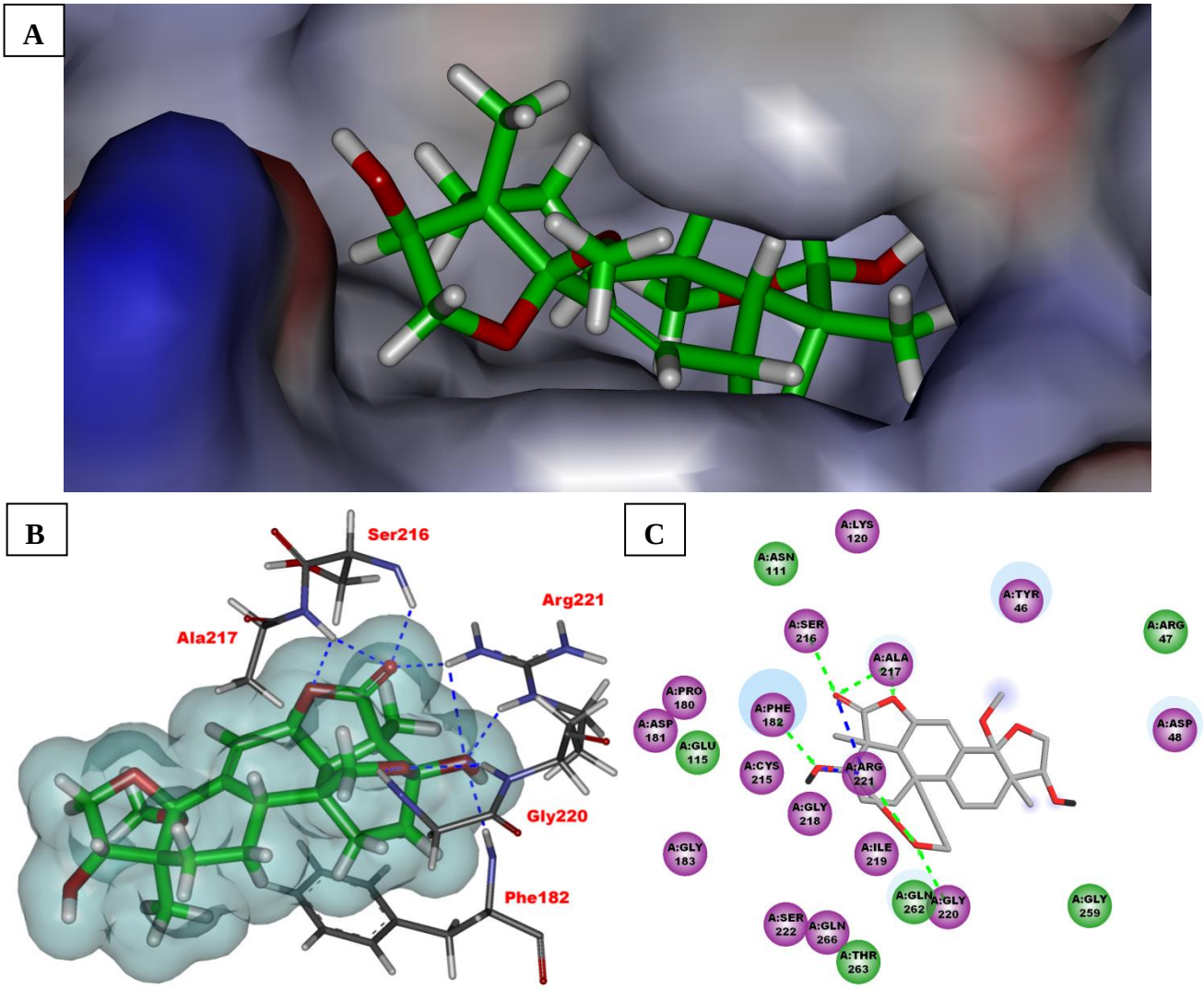

Fig. S31 Molecular docking models for PTP1B inhibition of **10**.

A: 3D docking surfaces of the PTP1B protein active site and **10**. **B** and **C**: Ligand interaction models of **10**.

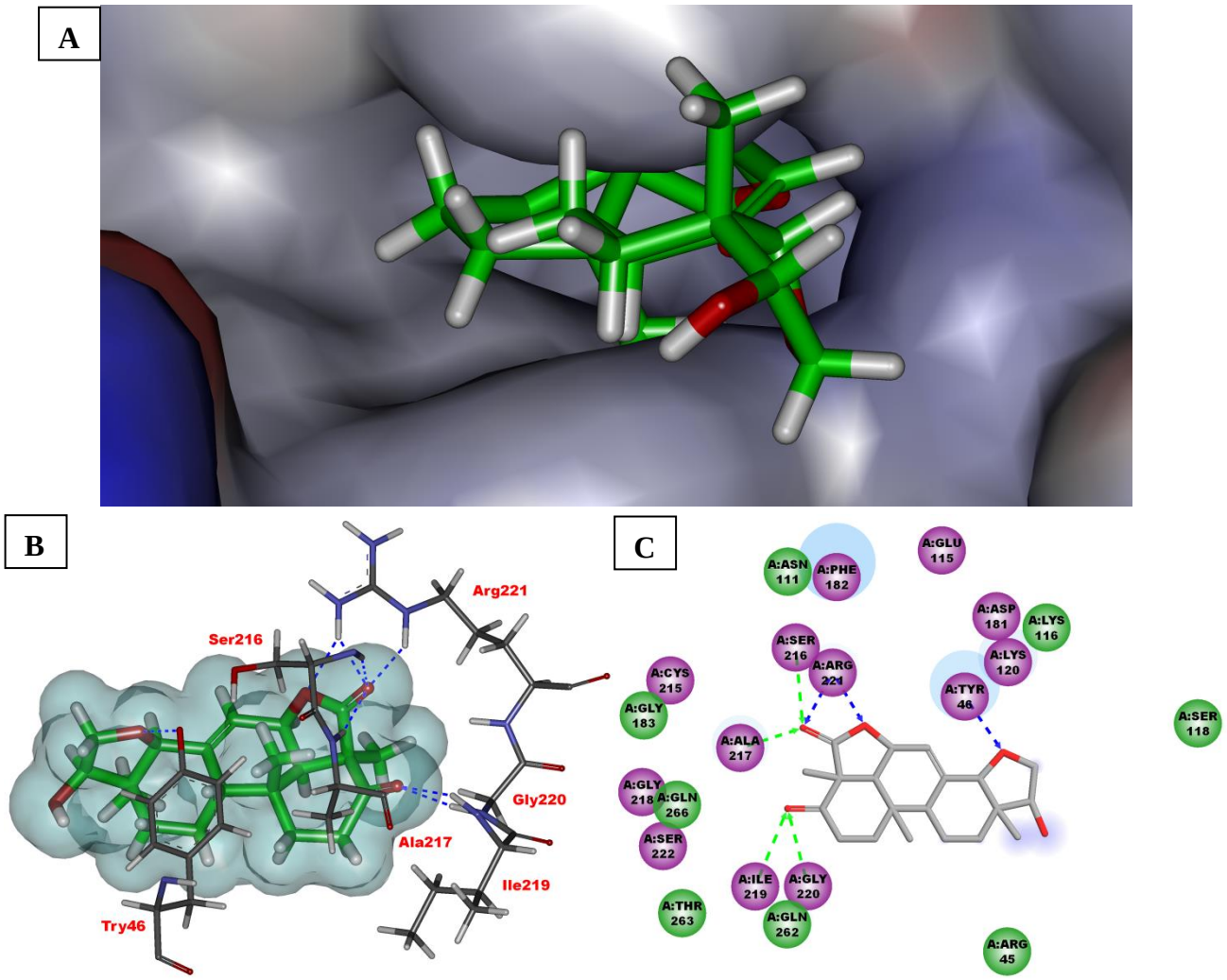

Fig. S32 Molecular docking models for PTP1B inhibition of **11**.

A: 3D docking surfaces of the PTP1B protein active site and **11**. **B** and **C**: Ligand interaction models of **11**.

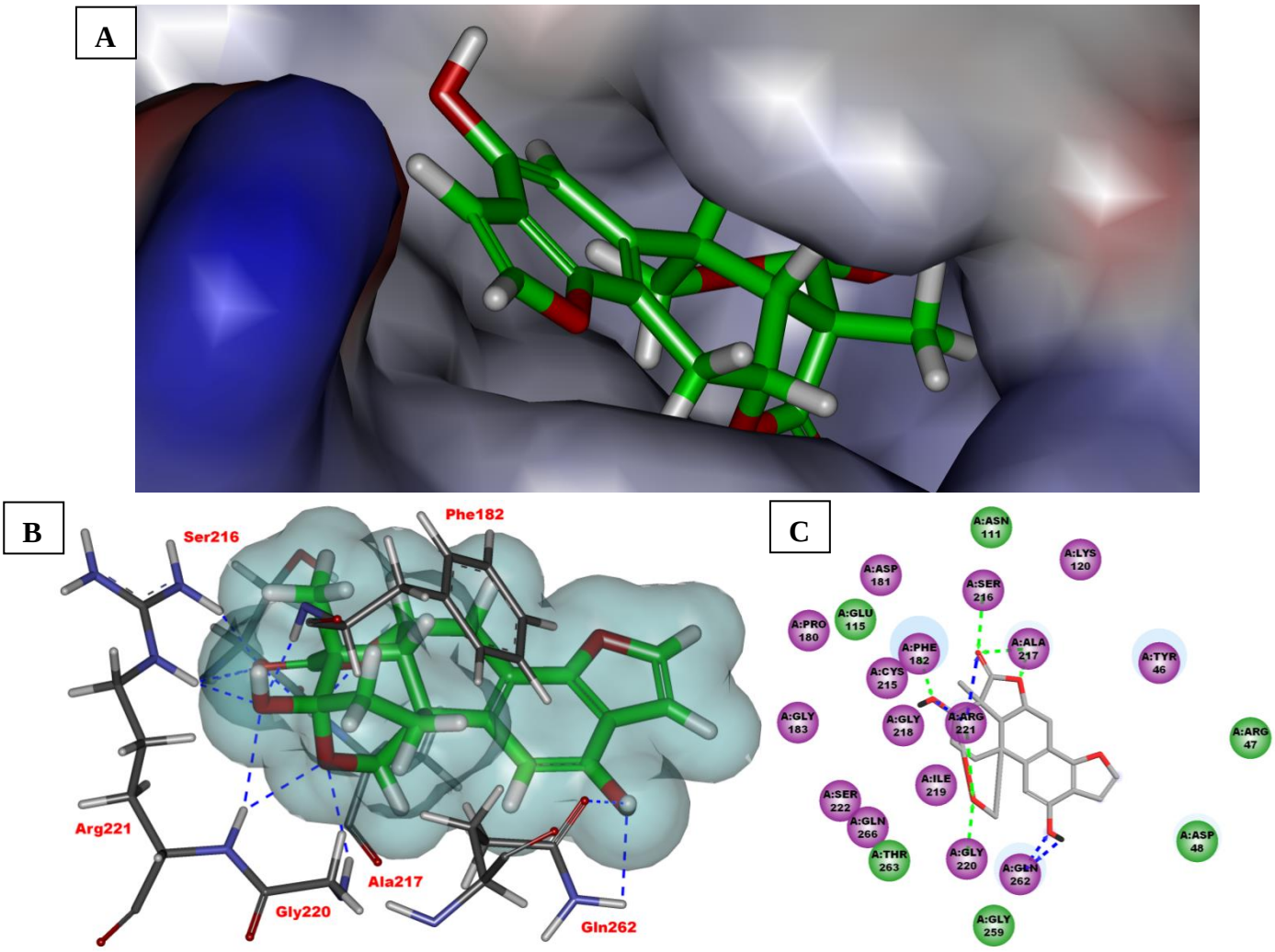

Fig. S33 Molecular docking models for PTP1B inhibition of **12**.

A: 3D docking surfaces of the PTP1B protein active site and **12**. **B** and **C**: Ligand interaction models of **12**.

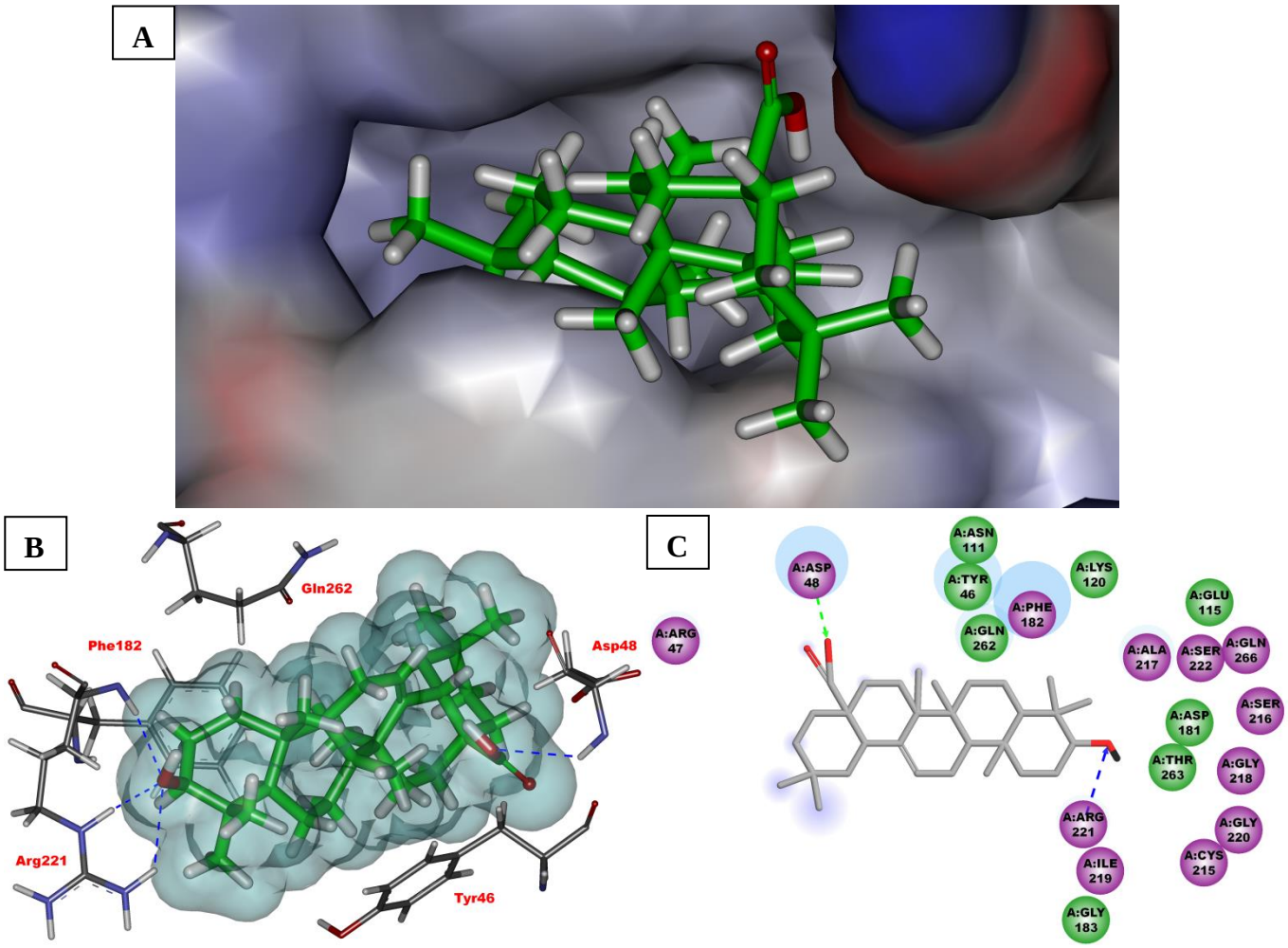

Fig. S34 Molecular docking models for PTP1B inhibition of oleanolic acid.

A: 3D docking surfaces of the PTP1B protein active site and oleanolic acid. **B** and **C**: Ligand interaction models of oleanolic acid.

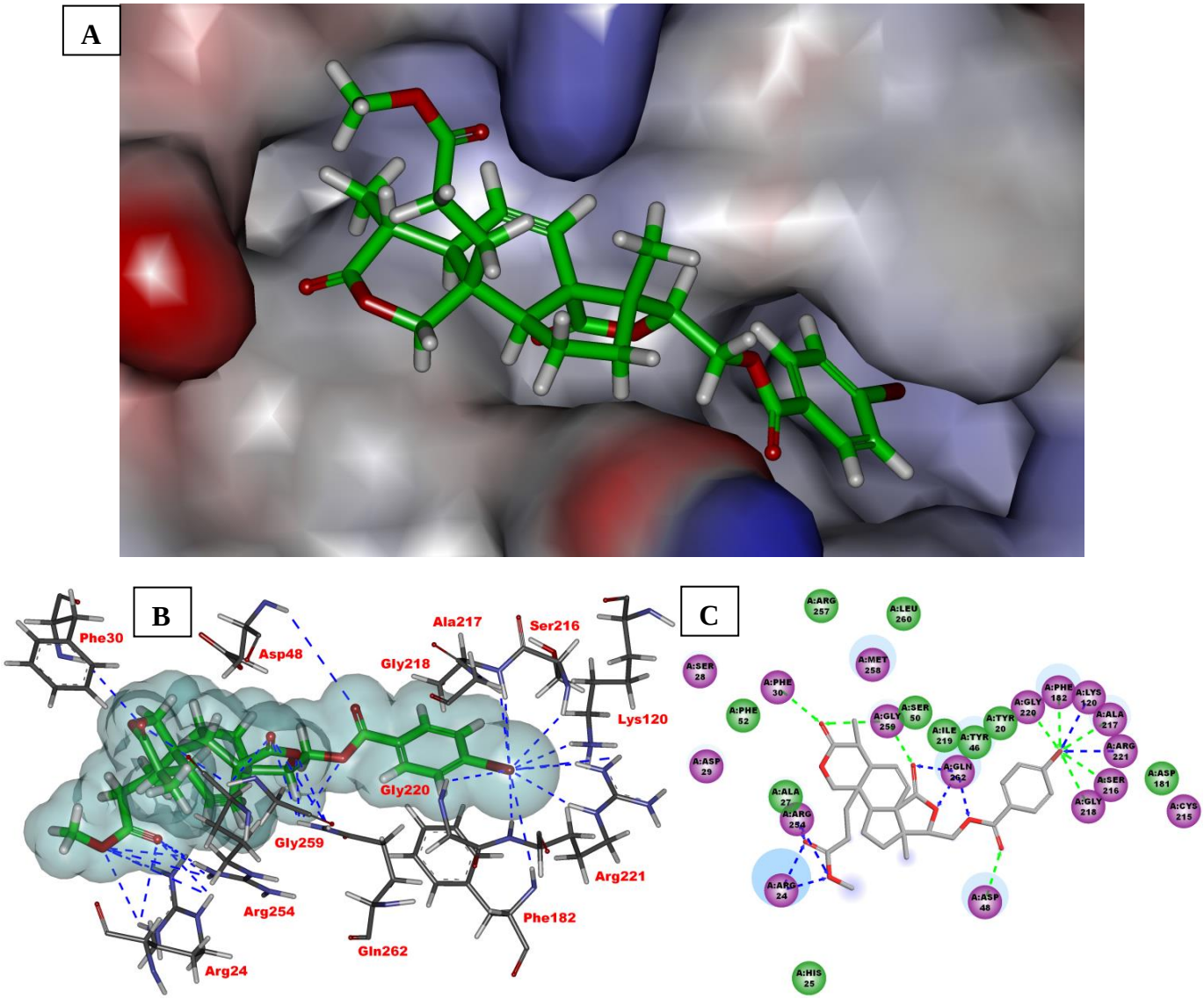

Fig. S35 Molecular docking models for PTP1B inhibition of **1a.**

A: 3D docking surfaces of the PTP1B protein active site and **1a**. **B** and **C**: Ligand interaction models of **1a**.

Table S7 Important thermodynamic parameters and Boltzmann distributions of the different optimized isomers of compound **1** at B3LYP/6-31+G(d) level in gas phase.

Conformations	Energy (a.u.)	Relative energy (a.u.)	Nuclear repulsion energy (Hartrees)	Boltzmann factor (%)
1A	−1343.70504058	0.00310509	2962.3450224001	0.42
1B	−1343.70694792	0.00119775	2924.6328793056	6.53
1C	−1343.70814567	0	2904.5235547101	9.54
1D	−1343.70459203	0.00355364	3019.7095929764	38.32
1E	−1343.70510386	0.00304181	2915.1714423055	3.61
1F	−1343.70706989	0.00107578	2927.5010214520	41.59

Table S8 Important thermodynamic parameters and Boltzmann distributions of the different optimized isomers of compound **2** at B3LYP/6-31+G(d) level in gas phase.

Conformations	Energy (a.u.)	Relative energy (a.u.)	Nuclear repulsion energy (Hartrees)	Boltzmann factor (%)
2A	−1343.70528970	0.00140642	2915.8210517709	4.28
2B	-1343.70286231	0.00383381	2895.1077100429	1.96
2C	-1343.70669612	0	2899.6568145182	26.18
2D	-1343.70669612	0	2899.6568007855	26.18
2E	-1343.70014788	0.00654824	2945.4804778632	1.01
2F	-1343.70669612	0	2899.6568049749	26.18
2G	-1343.70088613	0.00580999	2966.8819092253	5.98
2H	-1343.70164669	0.00504943	2931.6113237176	8.24

Table S9 Important thermodynamic parameters and Boltzmann distributions of the different optimized isomers of compound **3** at B3LYP/6-31+G(d) level in gas phase.

Conformations	Energy (a.u.)	Relative energy (a.u.)	Nuclear repulsion energy (Hartrees)	Boltzmann factor (%)
3A	-1267.25736159	0	2667.7048075713	49.87
3B	-1267.25569699	0.00166460	2697.5717406589	0.02
3C	-1267.25432256	0.00303903	2715.4179401750	0.02
3D	-1267.25367450	0.00368709	2711.7339290538	0.01
3E	-1267.25336634	0.00399525	2721.7823617983	0.02
3F	-1267.25709272	0.00026887	2664.5182114449	0.2
3G	-1267.25736159	0	2667.7048389274	49.87

Table S10 Important thermodynamic parameters and Boltzmann distributions of the different optimized isomers of compound **4** at B3LYP/6-31+G(d) level in gas phase.

Conformations	Energy (a.u.)	Relative energy (a.u.)	Nuclear repulsion energy (Hartrees)	Boltzmann factor (%)
4A	-1115.63978501	0.00003512	2237.2214986488	14.29
4B	-1115.63687272	0.00294741	2295.9160304179	2.54
4C	-1115.63978515	0.00003498	2237.2232150598	14.29
4D	-1115.63854459	0.00127554	2238.2205188774	5.89
4E	-1115.63689965	0.00292048	2291.2010454473	2.75
4F	-1115.63685131	0.00296882	2303.8204851092	9.8
4G	-1115.63707566	0.00274447	2301.6169425981	9.18
4H	-1115.63982013	0	2233.1938773129	15.83
4I	-1115.63893831	0.00088182	2225.2080968314	1.52
4J	-1115.63819442	0.00162571	2224.3157442050	10.3
4K	-1115.63638591	0.00343422	2321.8691267000	13.62

Table S11 Important thermodynamic parameters and Boltzmann distributions of the different optimized isomers of compound **5** at B3LYP/6-31+G(d) level in gas phase.

Conformations	Energy (a.u.)	Relative energy (a.u.)	Nuclear repulsion energy (Hartrees)	Boltzmann factor (%)
5A	-1268.43705711	0	2846.7047877104	4.03
5B	-1268.43534770	0.00170941	2846.7923327887	91.94
5C	-1268.43705711	0	2846.7037766298	4.03

Table S12 Experimental and calculated chemical shifts of **1** for DP4 probability statistical analysis.

Functional	Solvent	Basis Set				Type of Data			
mPW1PW91	Chloroform	6-311g (d,p)				Scaled Shifts			
DP4		4*R**,5*S**-**1**		4*R**,5*R**-**1**		4*S**,5*R**-**1**		4*S**,5*S**-**1**	
Bayes's theorem probability		0.25%		0%		0%		99.75%	
Nuclei	$\delta_{experimental}$	$\delta_{calculated}$	$\delta_{corrected}$	$\delta_{calculated}$	$\delta_{corrected}$	$\delta_{calculated}$	$\delta_{corrected}$	$\delta_{calculated}$	$\delta_{corrected}$
C-1	28.5	28.26	26.74	25.65	23.42	28.63	25.90	29.85	27.75
C-2	27.9	29.49	27.93	33.01	30.54	35.16	32.27	29.42	27.34
C-3	173.3	181.09	174.44	181.62	174.13	181.63	175.29	181.20	174.10
C-4	40.4	37.97	36.13	41.43	38.67	40.81	37.80	43.61	41.06
C-5	41.8	43.07	41.05	49.52	46.49	48.19	44.99	45.39	42.79
C-6	131.5	135.51	130.39	141.81	135.66	138.86	133.52	136.08	130.47
C-7	122.4	132.37	127.35	131.89	126.09	130.79	125.64	130.39	124.98
C-8	58.2	63.29	60.59	66.66	63.05	66.21	62.60	66.02	62.73
C-9	45.4	49.87	47.63	55.46	52.23	55.58	52.21	49.77	47.02
C-10	37.0	41.56	39.60	40.01	37.30	42.11	39.06	40.80	38.34
C-11	27.3	29.73	28.17	28.60	26.27	29.30	26.56	29.40	27.32
C-12	32.8	34.63	32.90	35.15	32.60	36.42	33.51	34.97	32.71
C-13	52.5	59.86	57.27	55.47	52.24	56.39	53.00	57.14	54.14
C-14	179.1	185.25	178.45	185.98	178.35	184.14	177.73	185.57	178.33
C-15	85.9	88.54	84.99	87.85	83.53	84.95	80.89	88.91	84.87
C-16	61.8	63.56	60.86	63.95	60.43	61.38	57.88	64.22	60.99
C-17	21.1	21.11	19.83	17.11	15.18	18.10	15.62	20.26	18.48
C-18	16.9	15.78	14.68	18.09	16.12	16.70	14.25	16.06	14.43
C-19	174.4	177.62	171.08	178.18	170.81	177.07	170.83	179.71	172.66
C-20	71.3	73.08	70.06	78.16	74.17	75.90	72.05	73.75	70.21
OCH_3-3	52.1	53.85	51.47	53.99	50.81	53.28	49.96	53.80	50.91

Table S13 Experimental and calculated chemical shifts of **2** for DP4 probability statistical analysis.

Functional	Solvent	Basis Set				Type of Data			
mPW1PW91	Chloroform	6-311g (d,p)				Scaled Shifts			
DP4		4*R**,5*S**-**2**		4*R**,5*R**-**2**		4*S**,5*R**-**2**		4*S**,5*S**-**2**	
Bayes's theorem probability		98.03%		0%		0%		1.97%	
Nuclei	$\delta_{experimental}$	$\delta_{calculated}$	$\delta_{corrected}$	$\delta_{calculated}$	$\delta_{corrected}$	$\delta_{calculated}$	$\delta_{corrected}$	$\delta_{calculated}$	$\delta_{corrected}$
C-1	27.7	28.26	25.97	25.65	22.49	28.63	25.10	29.85	26.95
C-2	28.5	29.49	27.17	33.01	29.61	35.16	31.50	29.42	27.34
C-3	173.26	181.09	174.29	181.62	173.33	181.63	175.22	181.20	174.10
C-4	34.5	37.97	35.40	41.43	37.75	40.81	37.05	43.61	41.06
C-5	38.4	43.07	40.34	49.52	45.58	48.19	44.29	45.39	42.79
C-6	127.0	135.51	130.05	141.81	134.83	138.86	133.25	136.08	130.47
C-7	125.9	132.37	127.00	131.89	125.24	130.79	125.34	130.39	124.98
C-8	58.4	63.29	59.97	66.66	62.16	66.21	61.98	66.02	62.73
C-9	46.3	49.87	46.95	55.46	51.32	55.58	51.54	49.77	47.02
C-10	37.6	41.56	38.89	40.01	36.38	42.11	38.33	40.80	38.34
C-11	27.5	29.73	27.41	28.60	25.34	29.30	25.76	29.40	27.32
C-12	32.3	34.63	32.16	35.15	31.68	36.42	32.74	34.97	32.71
C-13	53.7	59.86	56.64	55.47	51.33	56.39	52.34	57.14	54.14
C-14	179.4	185.25	178.32	185.98	177.55	184.14	177.68	185.57	178.33
C-15	85.9	88.54	84.47	87.85	82.65	84.95	80.36	88.91	84.87
C-16	61.7	63.56	60.24	63.95	59.53	61.38	57.24	64.22	60.99
C-17	20.7	21.11	19.04	17.11	14.24	18.10	14.77	20.26	18.48
C-18	14.0	15.78	13.86	18.09	15.18	16.70	13.39	16.06	14.43
C-19	173.30	177.62	170.92	178.18	170.00	177.07	170.74	179.71	172.66
C-20	71.1	73.08	69.47	78.16	73.28	75.90	71.48	73.75	70.21
OCH_3-3	52.2	53.85	50.81	53.99	49.90	53.28	49.28	53.80	50.91

Table S14 Cartesian coordinate of **1** [E(RB3LYP) = −1343.70706989 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.157637	2.863946	1.70819
2	6	0	0.89101	3.598736	0.590989
3	8	0	0.871213	4.80407	0.689566
4	6	0	0.486348	2.860661	−0.6855
5	1	0	−0.60845	2.802681	−0.60785
6	6	0	0.823432	3.701019	−1.92617
7	1	0	0.388439	3.247972	−2.82335
8	1	0	0.424885	4.712446	−1.82197
9	1	0	1.908555	3.779441	−2.07049
10	6	0	1.036746	1.408373	−0.79541
11	1	0	2.092109	1.503779	−1.0832
12	6	0	0.319609	0.617974	−1.86695
13	1	0	0.71208	0.646247	−2.88182
14	6	0	−0.76679	−0.11806	−1.60356
15	1	0	−1.25822	−0.66645	−2.4062
16	6	0	−1.4242	−0.14278	−0.24225
17	6	0	−0.52267	0.387231	0.932202
18	1	0	−0.92624	1.361878	1.223792
19	6	0	0.974545	0.637102	0.550584
20	6	0	1.780802	−0.69513	0.484985
21	1	0	1.962847	−1.04832	1.506181
22	1	0	1.170086	−1.46546	0.010635
23	6	0	3.130901	−0.66476	−0.24348
24	1	0	3.005775	−0.4992	−1.32077
25	1	0	3.788571	0.139846	0.107429
26	6	0	3.88694	−1.97268	−0.08796
27	8	0	5.106177	−1.89436	−0.66438
28	6	0	5.91806	−3.08383	−0.59881
29	1	0	6.84667	−2.82645	−1.10853
30	1	0	6.110256	−3.35539	0.442432
31	1	0	5.41664	−3.91409	−1.10308
32	8	0	3.472343	−2.97133	0.465594
33	6	0	1.641062	1.511413	1.621925
34	1	0	1.482134	1.09908	2.622358
35	1	0	2.723999	1.563735	1.451652
36	6	0	−0.7869	−0.60422	2.101086
37	1	0	−0.83691	−0.09142	3.067477
38	1	0	0.005112	−1.35416	2.180121
39	6	0	−2.11618	−1.29814	1.755011
40	1	0	−2.95277	−0.64264	2.028656
41	1	0	−2.25379	−2.24192	2.294891
42	6	0	−2.06781	−1.49896	0.216017
43	6	0	−3.44839	−1.45184	−0.47177
44	1	0	−3.37115	−1.81271	−1.50595
45	8	0	−3.79469	−0.03991	−0.54453
46	6	0	−2.69596	0.739491	−0.38311
47	8	0	−2.76471	1.943914	−0.37161
48	6	0	−4.61295	−2.17415	0.193541
49	1	0	−4.37654	−3.23823	0.290507
50	1	0	−4.79064	−1.76672	1.197781
51	8	0	−5.79303	−2.10758	−0.59641
52	1	0	−6.04248	−1.17322	−0.68819
53	6	0	−1.32249	−2.78565	−0.16238
54	1	0	−1.92772	−3.66281	0.097773
55	1	0	−1.11052	−2.83553	−1.23598
56	1	0	−0.37284	−2.88331	0.37047

Table S15 Cartesian coordinate of **2** [E(RB3LYP) = −1343.70669612 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	2.201702	1.981745	1.586481
2	6	0	2.442042	2.926635	0.643238
3	8	0	3.127599	3.88178	0.934469
4	6	0	1.957944	2.664809	−0.78632
5	1	0	2.798341	2.122596	−1.24119
6	6	0	1.825143	3.975983	−1.57658
7	1	0	2.795753	4.472857	−1.64259
8	1	0	1.136481	4.682345	−1.10343
9	1	0	1.468656	3.769861	−2.59317
10	6	0	0.727596	1.721771	−0.87614
11	1	0	0.688152	1.372313	−1.92097
12	6	0	0.909147	0.481637	0.053534
13	6	0	2.145775	−0.35006	−0.39444
14	1	0	2.008729	−0.67052	−1.43212
15	1	0	3.034433	0.287321	−0.39722
16	6	0	2.48709	−1.57856	0.463041
17	1	0	2.852952	−1.2983	1.455679
18	1	0	1.6127	−2.22055	0.634731
19	6	0	3.536657	−2.4565	−0.19595
20	8	0	4.139377	−3.25489	0.710829
21	6	0	5.127756	−4.16905	0.195308
22	1	0	5.939235	−3.61741	−0.2862
23	1	0	5.49449	−4.71546	1.064385
24	1	0	4.673905	−4.8512	−0.5285
25	8	0	3.799048	−2.47567	−1.38216
26	6	0	1.115704	1.028548	1.476988
27	1	0	0.214188	1.511385	1.856977
28	1	0	1.378467	0.235965	2.180124
29	6	0	−0.36867	−0.41318	0.040755
30	1	0	−0.30359	−1.05915	0.925641
31	6	0	−1.75426	0.339271	0.138235
32	6	0	−1.66173	1.824915	−0.0919
33	1	0	−2.55379	2.414133	0.118416
34	6	0	−0.57235	2.433303	−0.56897
35	1	0	−0.61745	3.504577	−0.74584
36	6	0	−2.40424	0.066242	1.508247
37	8	0	−3.65253	−0.44719	1.36004
38	6	0	−4.05071	−0.48323	−0.03795
39	1	0	−4.66546	0.410127	−0.20761
40	6	0	−2.74569	−0.39083	−0.86239
41	6	0	−2.02038	−1.73312	−1.12961
42	1	0	−2.37258	−2.22356	−2.0442
43	1	0	−2.17407	−2.43602	−0.30019
44	6	0	−0.53896	−1.34302	−1.18215
45	1	0	0.120682	−2.21528	−1.147
46	1	0	−0.31582	−0.81309	−2.11648
47	6	0	−3.01619	0.337671	−2.18845
48	1	0	−3.72636	−0.24045	−2.79288
49	1	0	−3.44218	1.333354	−2.03222
50	1	0	−2.10327	0.461098	−2.77895
51	6	0	−4.9396	−1.70511	−0.23086
52	1	0	−5.23137	−1.78206	−1.28303
53	1	0	−4.39682	−2.61933	0.044763
54	8	0	−6.15162	−1.59627	0.503409
55	1	0	−5.92924	−1.53302	1.446931
56	8	0	−1.91326	0.241572	2.596968

Table S16 Cartesian coordinate of **3** [E(RB3LYP) = −1267.25736159 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	3.343571	−1.26005	−1.731332
2	6	0	4.013224	−1.45364	−0.557645
3	6	0	3.214114	−1.60368	0.684019
4	6	0	1.887893	−1.27453	0.698104
5	6	0	1.096842	−1.32342	1.914194
6	1	0	1.61105	−1.5143	2.851185
7	6	0	−0.246936	−1.10819	1.930683
8	1	0	−0.780179	−1.08414	2.87767
9	6	0	1.002186	−0.91875	0.715499
10	6	0	−0.284723	−1.28379	−0.579427
11	1	0	−0.201072	−2.38461	−0.544049
12	6	0	1.202164	−0.78587	−0.584795
13	6	0	1.924414	−1.47509	−1.752068
14	1	0	1.734767	−2.55714	−1.730096
15	1	0	1.604517	−1.08152	−2.719735
16	6	0	1.368647	0.754724	−0.772739
17	1	0	2.414198	0.941757	−1.043667
18	1	0	0.774314	1.066398	−1.637433
19	6	0	1.014784	1.671628	0.413873
20	1	0	0.019548	1.434229	0.803945
21	1	0	1.726822	1.56052	1.234575
22	6	0	0.963537	3.119614	−0.028528
23	8	0	1.718961	3.920465	0.753051
24	6	0	1.713164	5.322201	0.418132
25	1	0	2.088317	5.470837	−0.59773
26	1	0	0.70006	5.726407	0.49251
27	1	0	2.372495	5.794607	1.146619
28	8	0	0.307885	3.532444	−0.967444
29	6	0	−1.097768	−0.95048	−1.849257
30	1	0	−0.726544	−1.54867	−2.689737
31	1	0	−0.961726	0.09742	−2.135947
32	6	0	−2.601019	−1.23233	−1.664838
33	1	0	−3.142499	−1.0194	−2.594623
34	1	0	−2.748347	−2.29953	−1.447205
35	6	0	−3.179778	−0.39785	−0.510317
36	6	0	−2.308724	−0.56759	0.708488
37	8	0	−3.037433	−0.39123	1.859203
38	6	0	−4.445389	−0.41727	1.539974
39	1	0	−4.859432	0.593885	1.648088
40	1	0	−4.941097	−1.07869	2.254981
41	6	0	−4.526307	−0.9111	0.080397
42	1	0	−4.529115	−2.0059	0.061762
43	8	0	−5.715214	−0.54102	−0.590708
44	1	0	−5.777679	0.427204	−0.629857
45	6	0	−3.301787	1.097353	−0.901345
46	1	0	−3.694258	1.708785	−0.079995
47	1	0	−2.330568	1.520978	−1.168836
48	1	0	−3.963415	1.210666	−1.769431
49	6	0	3.977575	−2.06208	1.905796
50	1	0	3.498035	−2.92687	2.37963
51	1	0	4.995854	−2.33831	1.626613
52	1	0	4.047649	−1.26836	2.661748
53	8	0	5.229462	−1.46629	−0.585292

Table S17 Cartesian coordinate of **4** [E(RB3LYP) = −1115.63982013 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	−2.31129	−2.10183	1.750578
2	6	0	−0.94488	−1.66214	1.819406
3	1	0	−0.28679	−2.54043	1.808905
4	1	0	−0.87096	−1.17817	2.794253
5	6	0	−0.57788	−0.71323	0.664253
6	6	0	0.901711	−0.31337	0.767752
7	6	0	1.424957	0.111815	1.989007
8	1	0	0.803697	0.13676	2.879288
9	6	0	2.752946	0.524326	2.093053
10	1	0	3.134574	0.841581	3.060848
11	6	0	3.602214	0.545595	0.982006
12	6	0	3.093887	0.143111	−0.27134
13	6	0	1.744274	−0.29103	−0.37216
14	6	0	1.183347	−0.73012	−1.64726
15	1	0	1.79273	−0.64614	−2.54016
16	6	0	−0.04797	−1.28198	−1.7644
17	1	0	−0.38034	−1.63954	−2.7343
18	6	0	−0.90815	−1.47828	−0.61742
19	6	0	−1.992	−2.30667	−0.6598
20	6	0	−2.81837	−2.5198	0.556694
21	8	0	−3.9195	−3.03577	0.545843
22	6	0	−2.43805	−3.0484	−1.89879
23	1	0	−3.39122	−3.54455	−1.70746
24	1	0	−2.57377	−2.37302	−2.75245
25	1	0	−1.7076	−3.81211	−2.19626
26	6	0	4.005914	0.14758	−1.4872
27	1	0	3.461042	0.484999	−2.37599
28	1	0	4.801722	0.884368	−1.3419
29	6	0	4.64744	−1.225	−1.77474
30	1	0	5.240667	−1.57036	−0.92012
31	1	0	3.886326	−1.98757	−1.97494
32	1	0	5.310417	−1.16782	−2.64646
33	6	0	5.032591	1.011262	1.160432
34	1	0	5.758016	0.270257	0.804327
35	1	0	5.231016	1.94433	0.616898
36	1	0	5.245113	1.198274	2.21769
37	6	0	−1.46265	0.576359	0.777552
38	1	0	−2.51353	0.273344	0.836935
39	1	0	−1.22675	1.068792	1.726995
40	6	0	−1.29475	1.588401	−0.35879
41	1	0	−0.23683	1.850701	−0.49757
42	1	0	−1.6376	1.189315	−1.31856
43	6	0	−2.03296	2.883951	−0.08341
44	8	0	−2.4021	3.273262	1.006129
45	8	0	−2.21517	3.590558	−1.22293
46	6	0	−2.86804	4.866434	−1.07693
47	1	0	−2.92474	5.27806	−2.08502
48	1	0	−3.86817	4.7355	−0.65554
49	1	0	−2.28401	5.52069	−0.42397

Table S18 Cartesian coordinate of **5** [E(RB3LYP) = −1268.43534770 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	−2.76978	−2.08897	0.645715
2	6	0	−3.23193	−0.80867	−0.07752
3	6	0	−2.74605	0.466154	0.706014
4	6	0	−1.21535	0.310819	0.9507
5	6	0	−0.64344	−0.85285	0.102042
6	6	0	−1.22022	−2.1524	0.702873
7	6	0	−0.63956	1.693163	0.603482
8	6	0	0.732931	1.691604	0.006879
9	6	0	1.439672	0.574133	−0.21227
10	6	0	0.903161	−0.82156	0.028022
11	6	0	2.90459	0.637841	−0.54737
12	6	0	3.800655	−0.04708	0.524282
13	6	0	3.196301	−1.4231	0.923388
14	6	0	1.686679	−1.4087	1.228936
15	8	0	3.180922	−0.07492	−1.76247
16	6	0	4.530644	−0.56748	−1.72815
17	6	0	5.088374	−0.29826	−0.31302
18	8	0	6.030294	0.773894	−0.28771
19	6	0	4.034507	0.828241	1.75908
20	1	0	1.193505	−1.42752	−0.8438
21	6	0	−1.1929	−0.76394	−1.34223
22	6	0	−3.55293	0.712422	1.992634
23	6	0	−2.83076	1.740366	−0.16128
24	8	0	−1.60428	2.318854	−0.28971
25	8	0	−3.81322	2.243186	−0.64807
26	8	0	−2.63242	−0.77863	−1.37134
27	1	0	3.204267	1.694041	−0.66361
28	1	0	−1.01072	0.09688	2.006593
29	8	0	−4.62145	−0.90171	−0.20307
30	6	0	−5.27338	−0.44106	−1.39888
31	1	0	−3.21803	−2.13264	1.643153
32	1	0	−3.18569	−2.9248	0.07602
33	1	0	−0.84684	−3.01746	0.1396
34	1	0	−0.8783	−2.27573	1.736388
35	1	0	−0.62387	2.326337	1.502247
36	1	0	1.18255	2.667476	−0.17148
37	1	0	3.748795	−1.80551	1.791751
38	1	0	3.363368	−2.14506	0.112793
39	1	0	1.478988	−0.82665	2.137021
40	1	0	1.365769	−2.4371	1.430064
41	1	0	4.507724	−1.63475	−1.97781
42	1	0	5.137228	−0.05217	−2.48412
43	1	0	5.650364	−1.15286	0.075291
44	1	0	5.656118	1.549622	−0.73632
45	1	0	4.417782	1.817861	1.492401
46	1	0	3.104297	0.97	2.320578
47	1	0	4.768395	0.363399	2.427341
48	1	0	−0.8417	−1.63029	−1.9186
49	1	0	−0.85313	0.14274	−1.85329
50	1	0	−4.60047	0.907353	1.751049
51	1	0	−3.50568	−0.15701	2.656599
52	1	0	−3.15743	1.576048	2.541559
53	1	0	−4.93399	−1.00974	−2.26977
54	1	0	−6.33362	−0.63831	−1.22252
55	1	0	−5.11555	0.626345	−1.56017

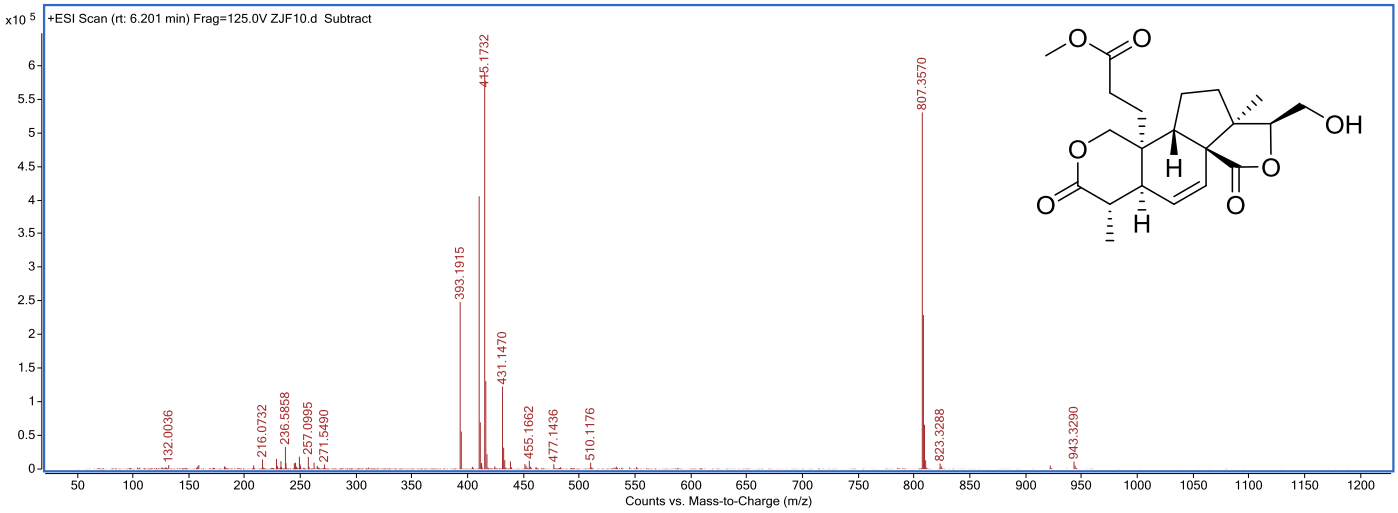

Fig. S36 HR-ESI-MS spectrum of **1**

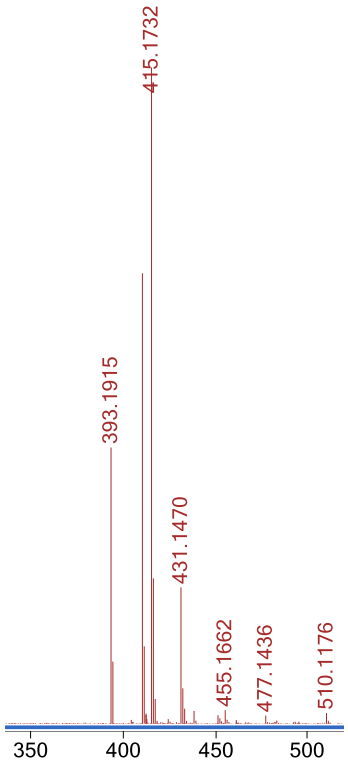

Fig. S37 HR-ESI-MS spectrum of **1** (amplified)

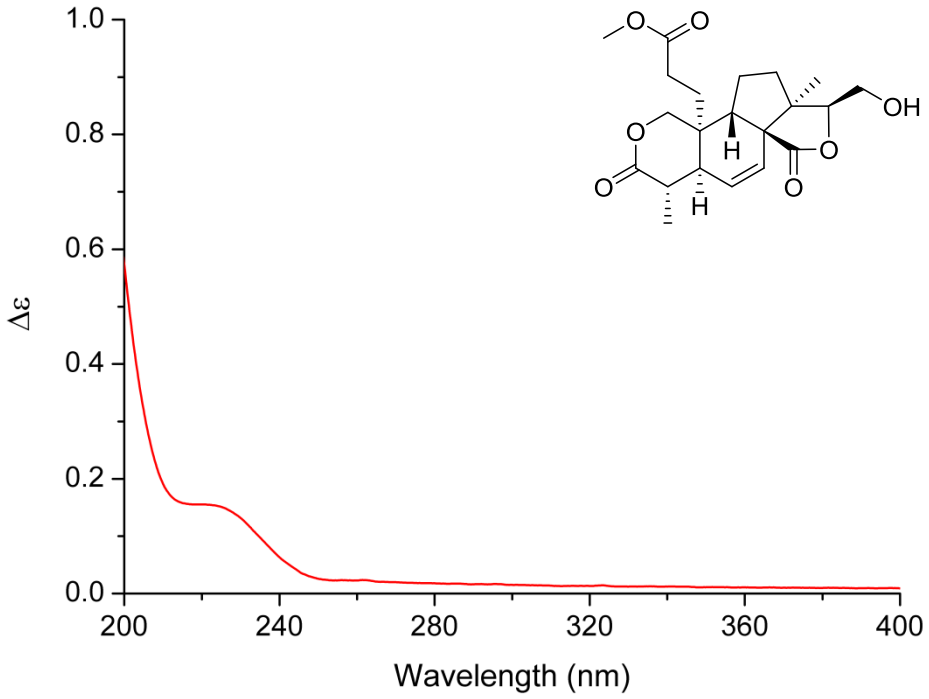

Fig. S38 UV spectrum of **1**

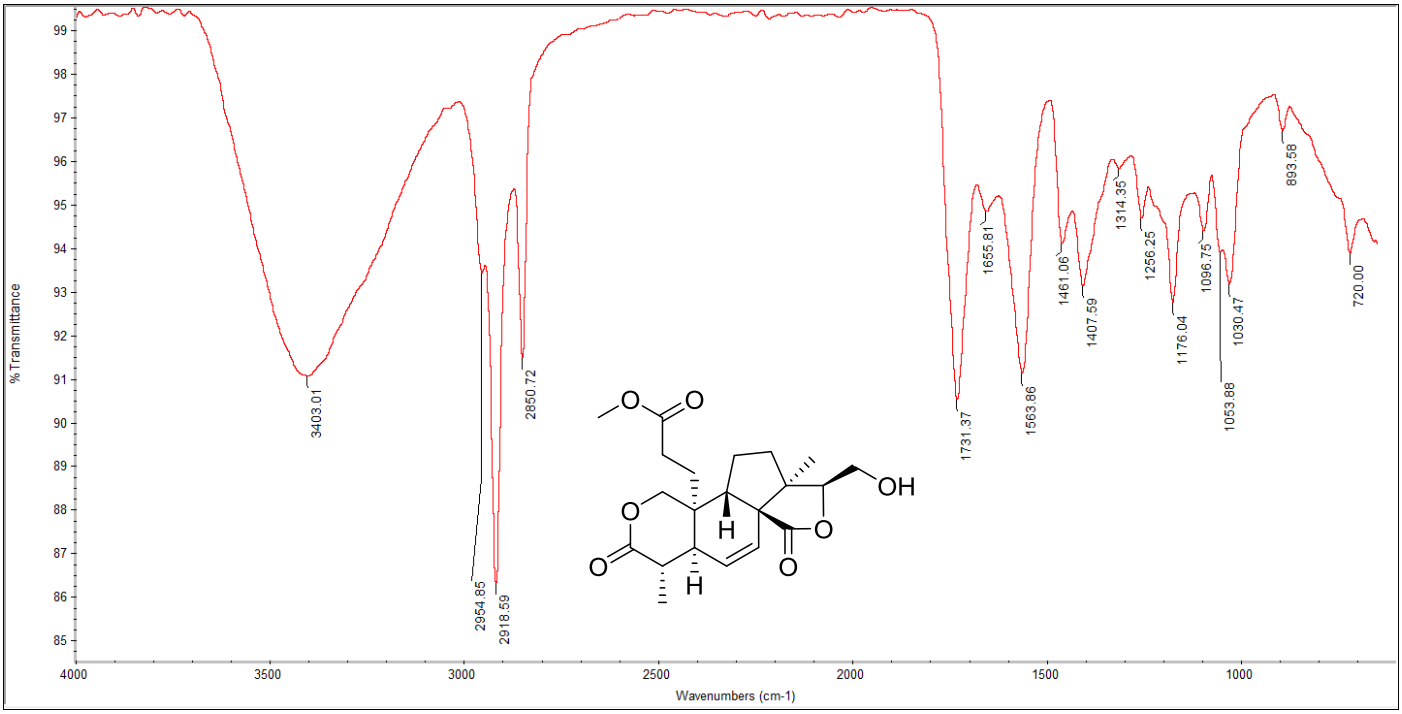

Fig. S39 IR spectrum of **1**

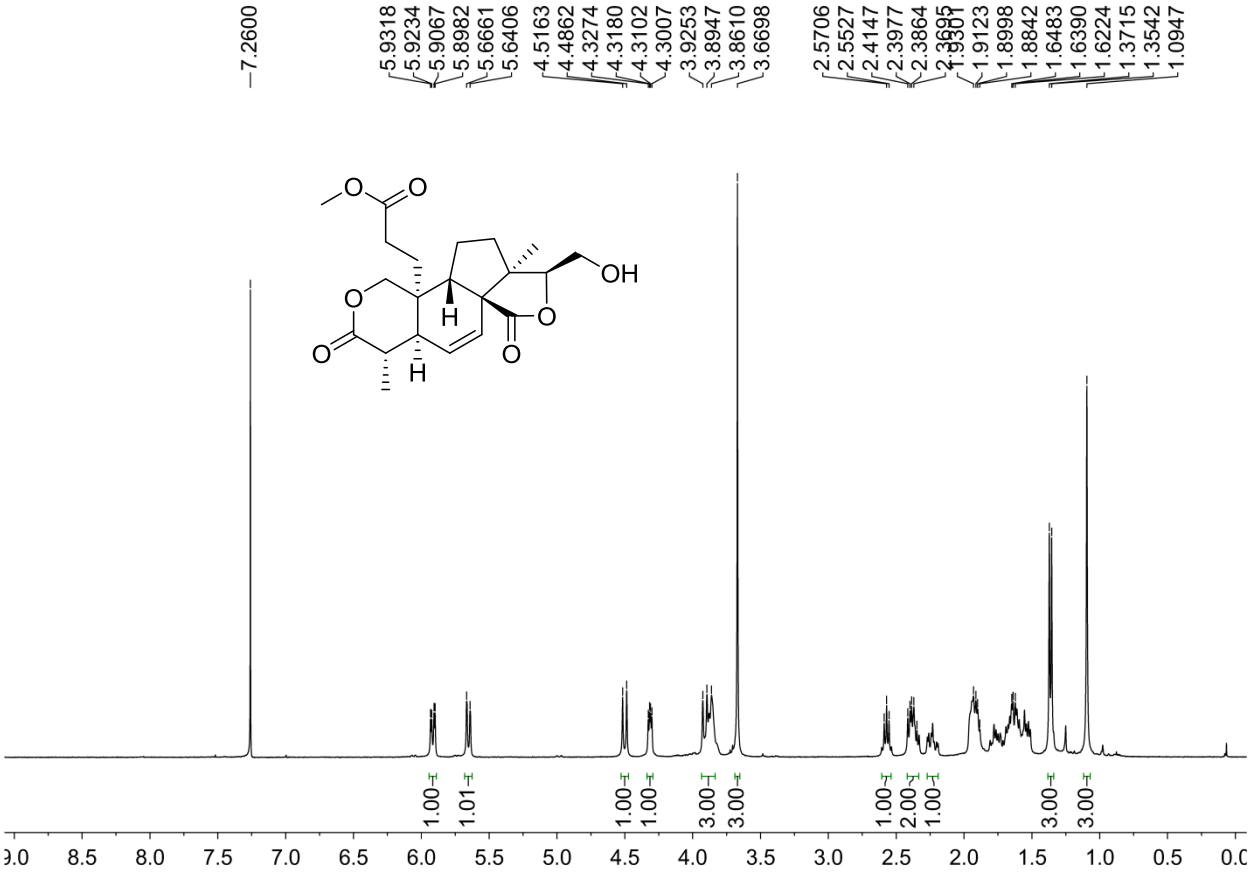

Fig. S40 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **1**

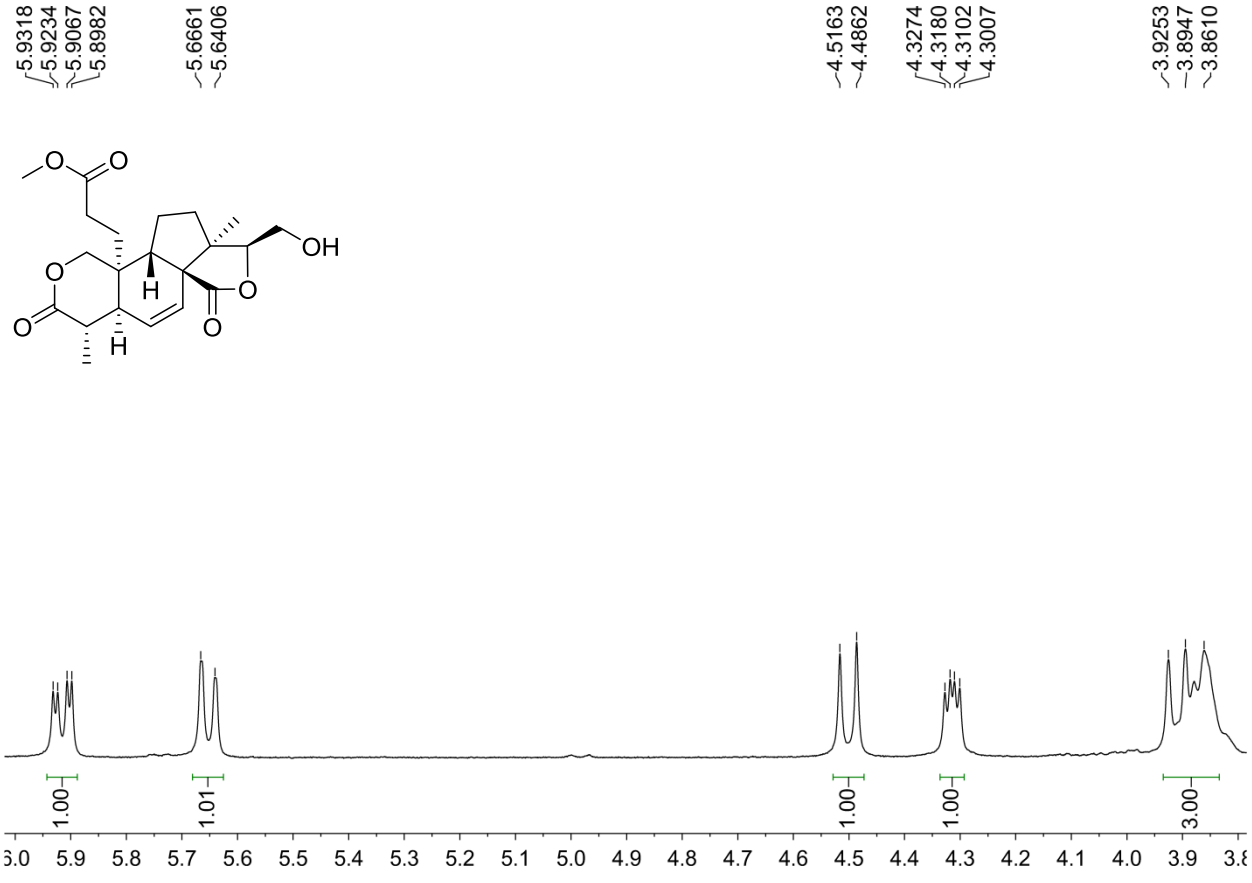

Fig. S41 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **1** (amplified)

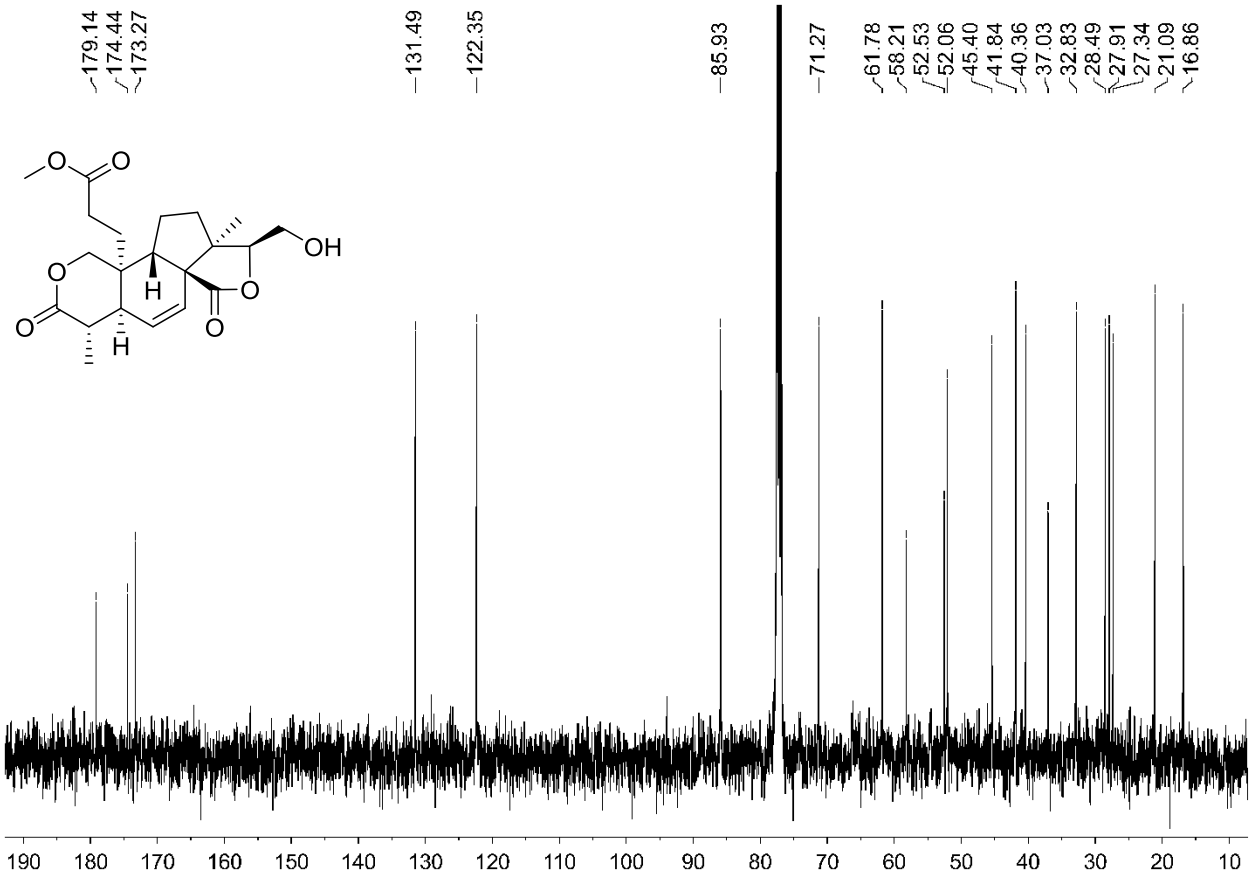

Fig. S42 ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of **1**

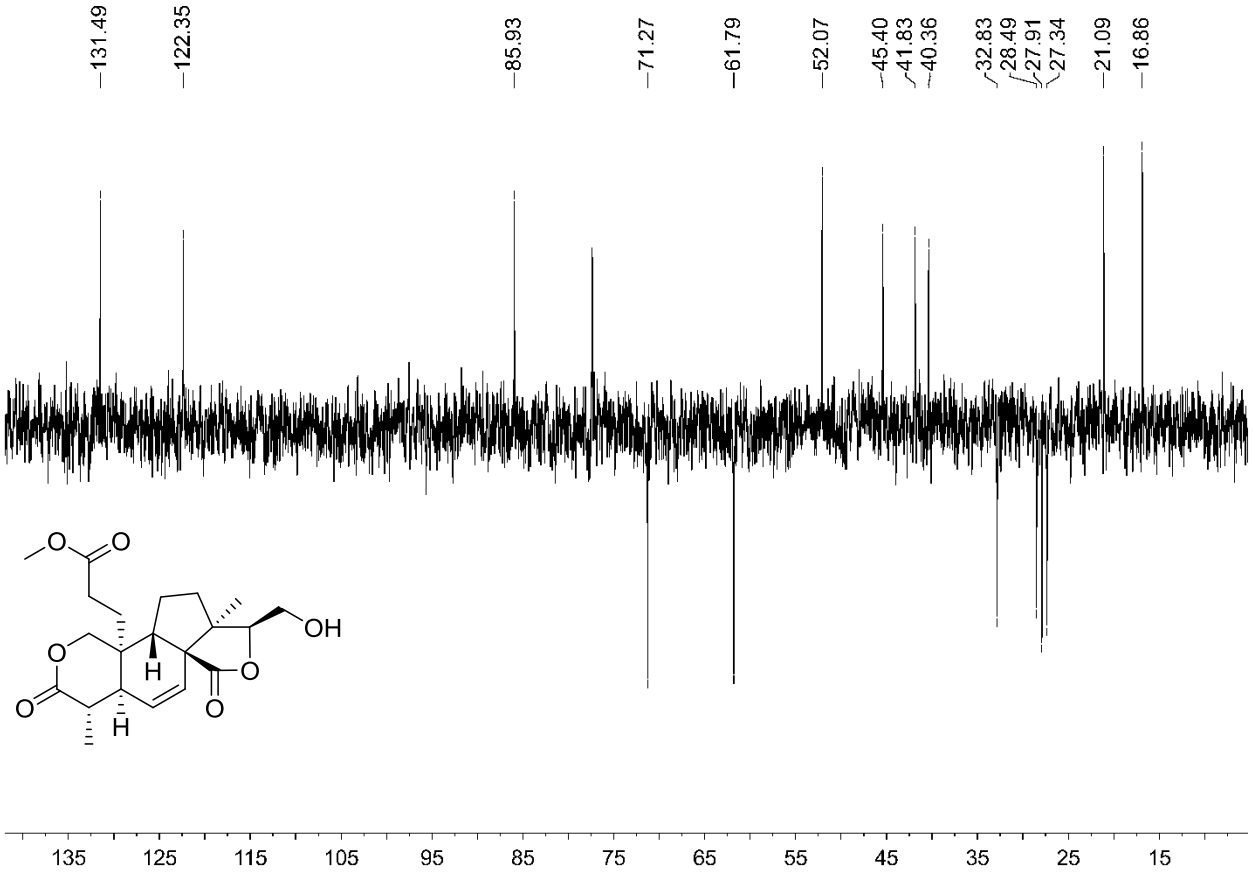

Fig. S43 DEPT135 (100 MHz, chloroform-*d*) spectrum of **1**

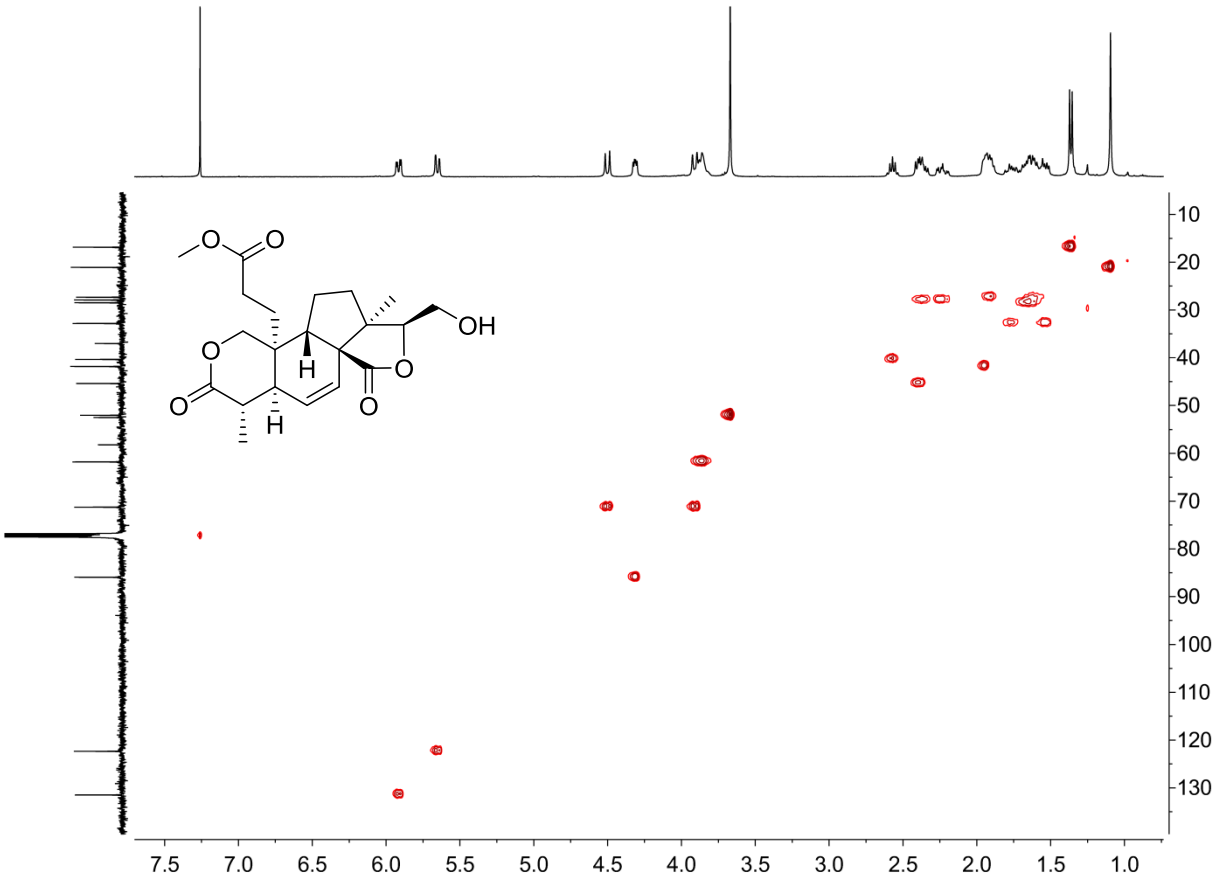

Fig. S44 HSQC spectrum (chloroform-*d*) of **1** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

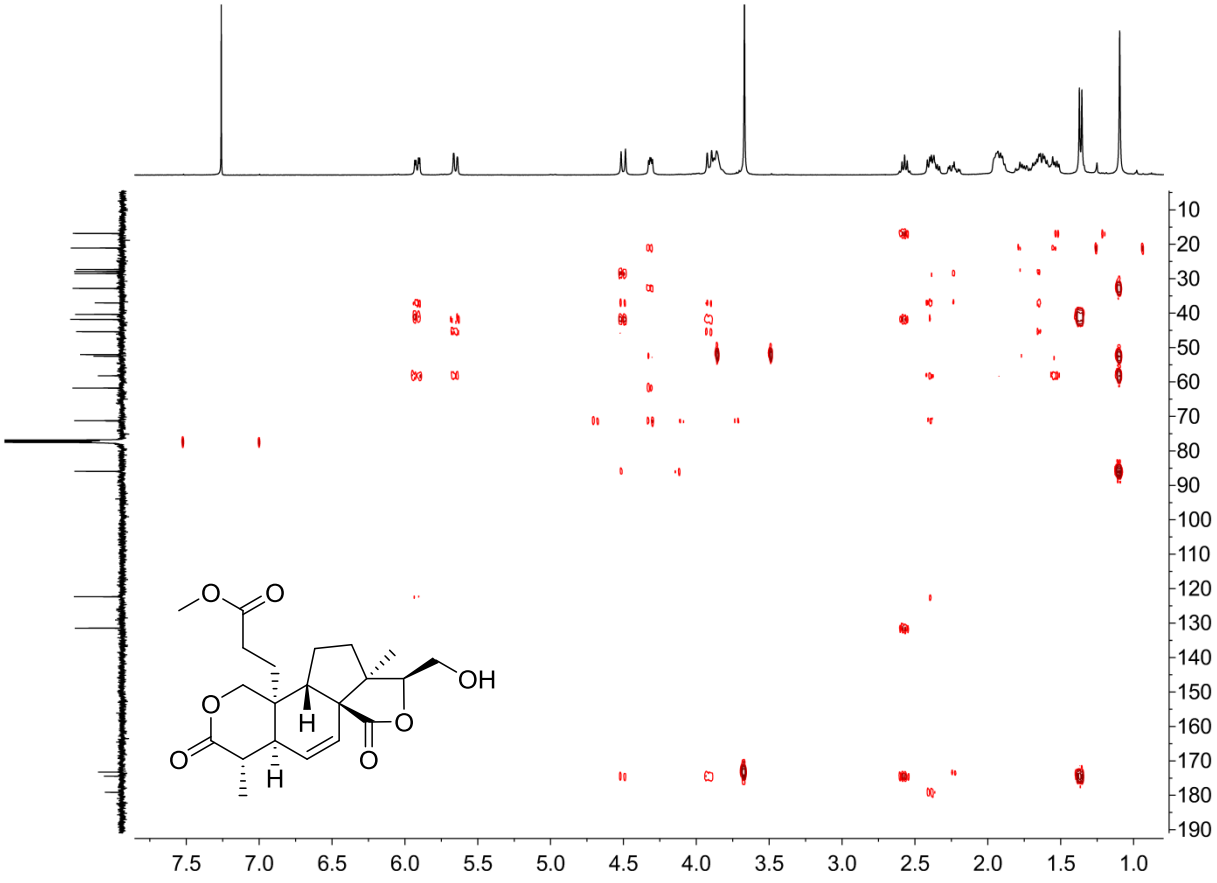

Fig. S45 HMBC spectrum (chloroform-*d*) of **1** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

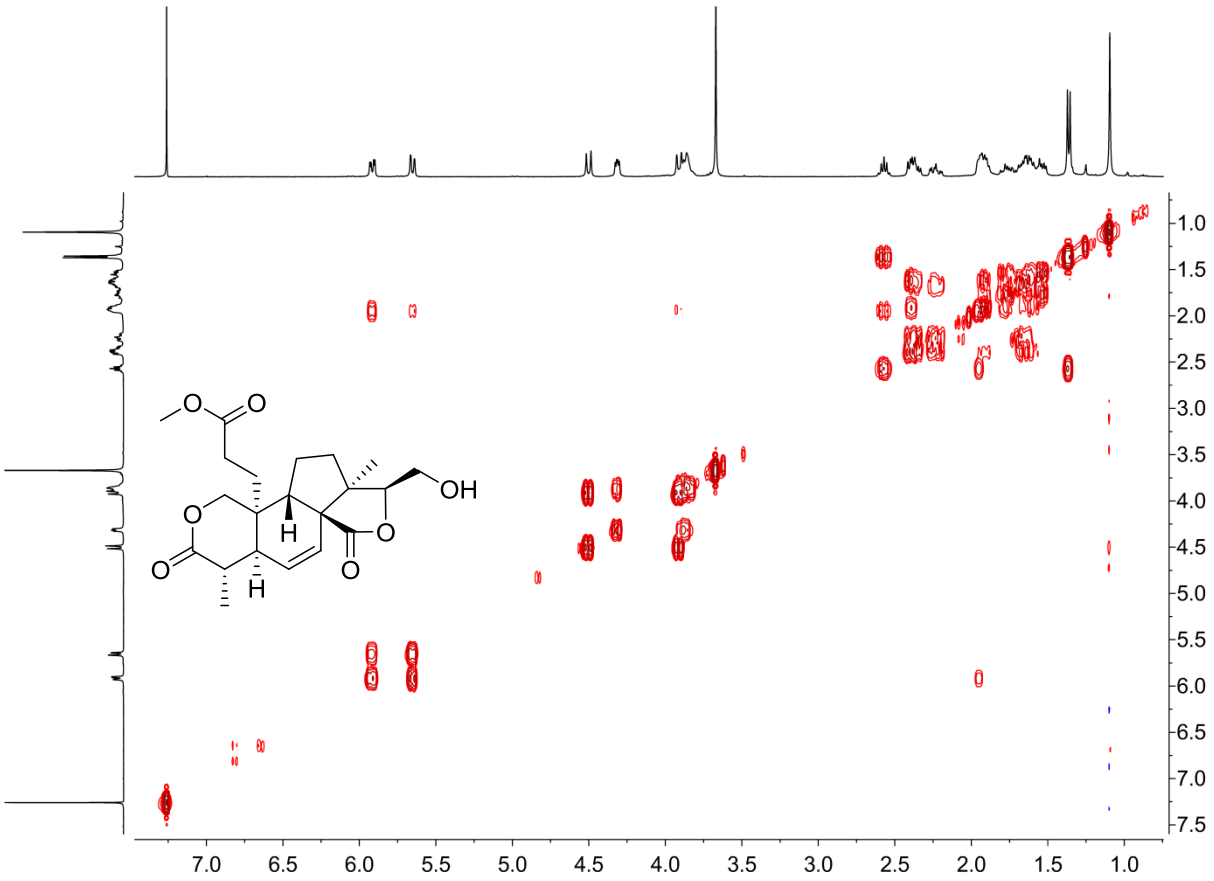

Fig. S46 ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of **1**

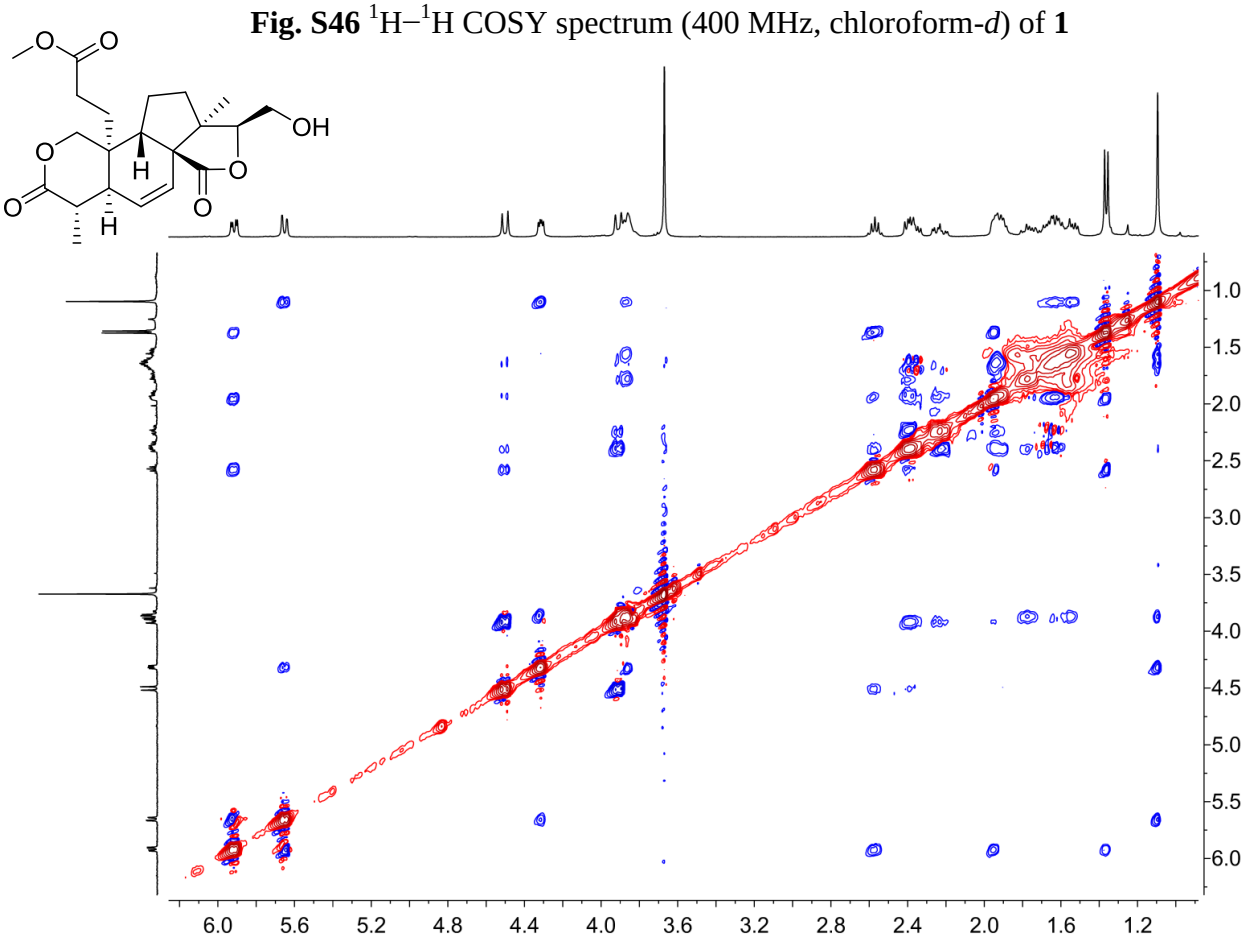

Fig. S47 NOESY spectrum (400 MHz, chloroform-*d*) of **1**

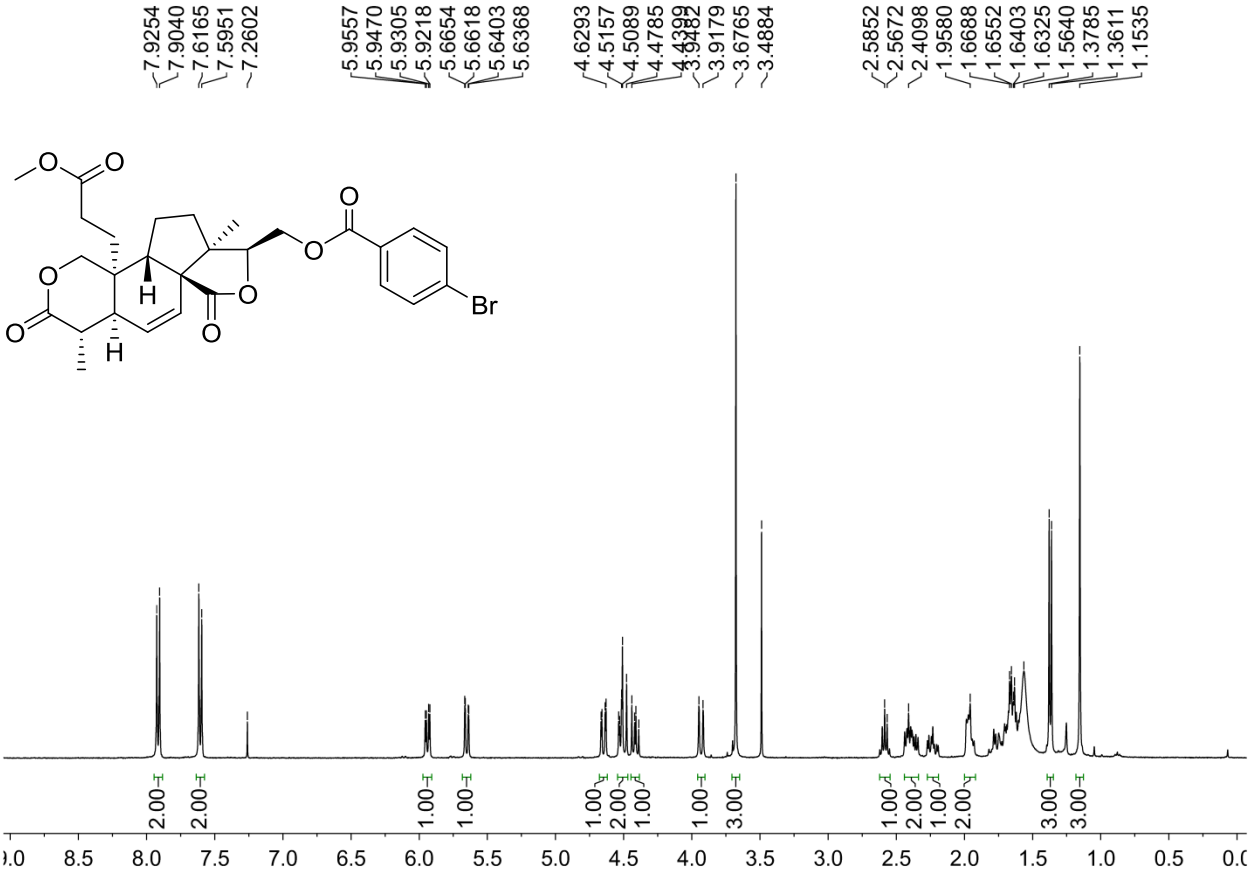

Fig. S48 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **1a**

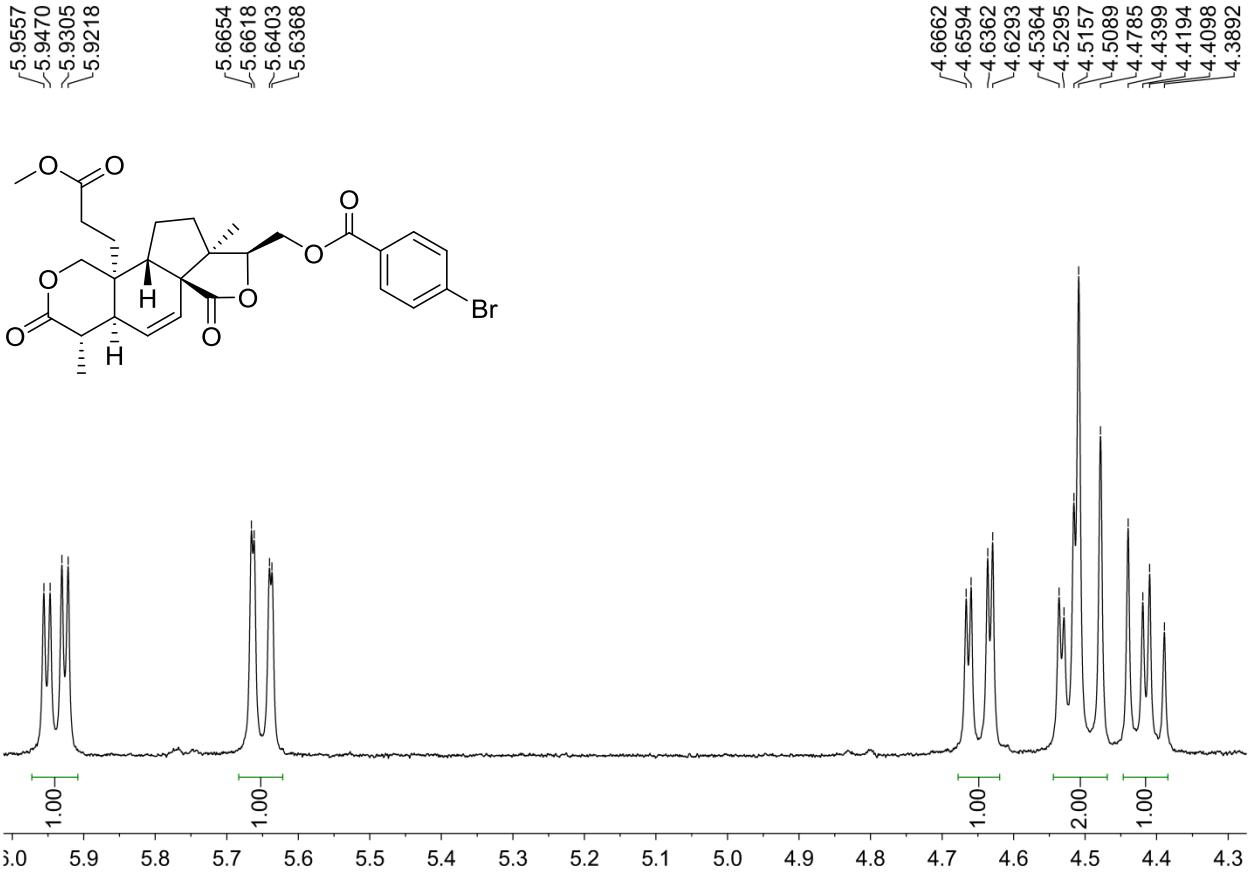

Fig. S49 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **1a** (amplified)

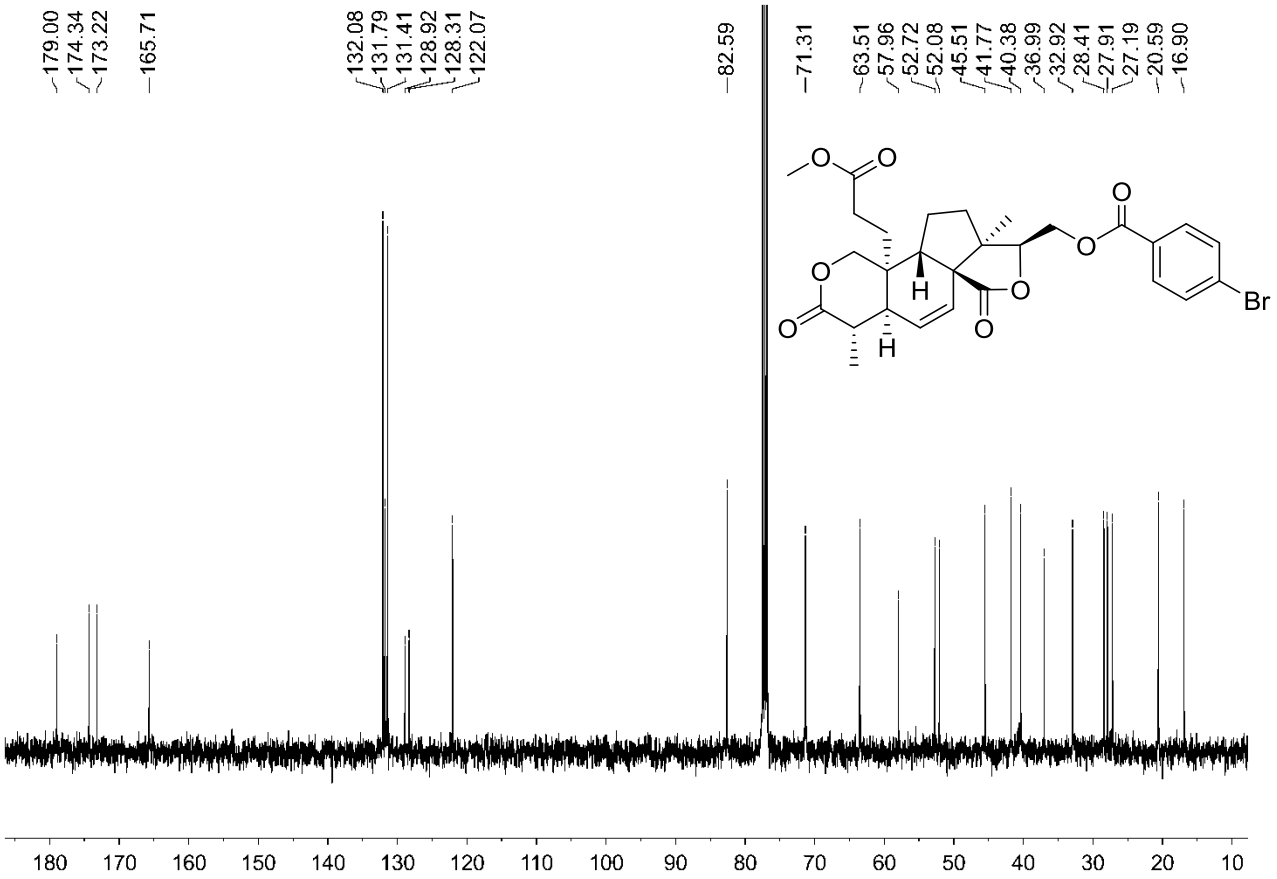

Fig. S50 ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of **1a**

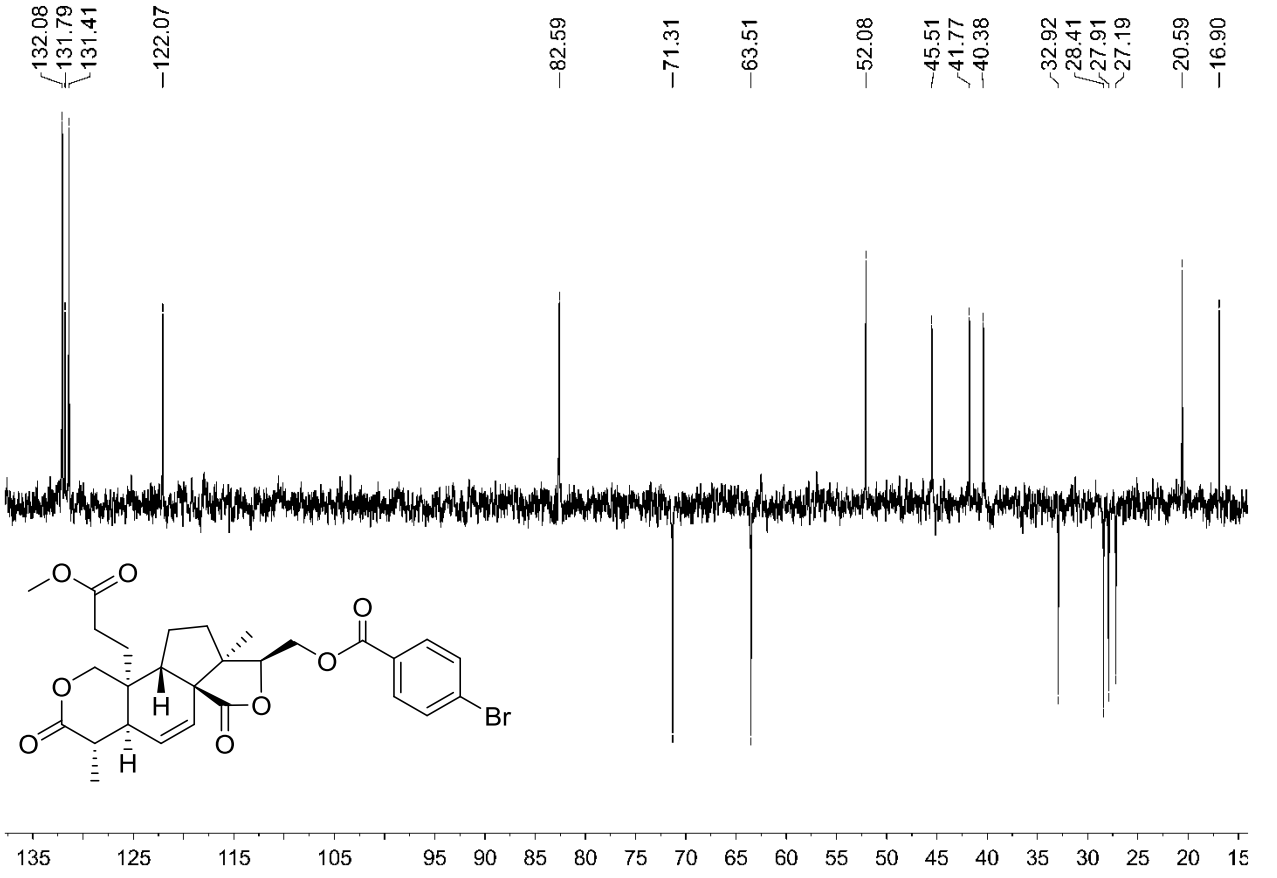

Fig. S51 DEPT135 (100 MHz, chloroform-*d*) spectrum of **1a**

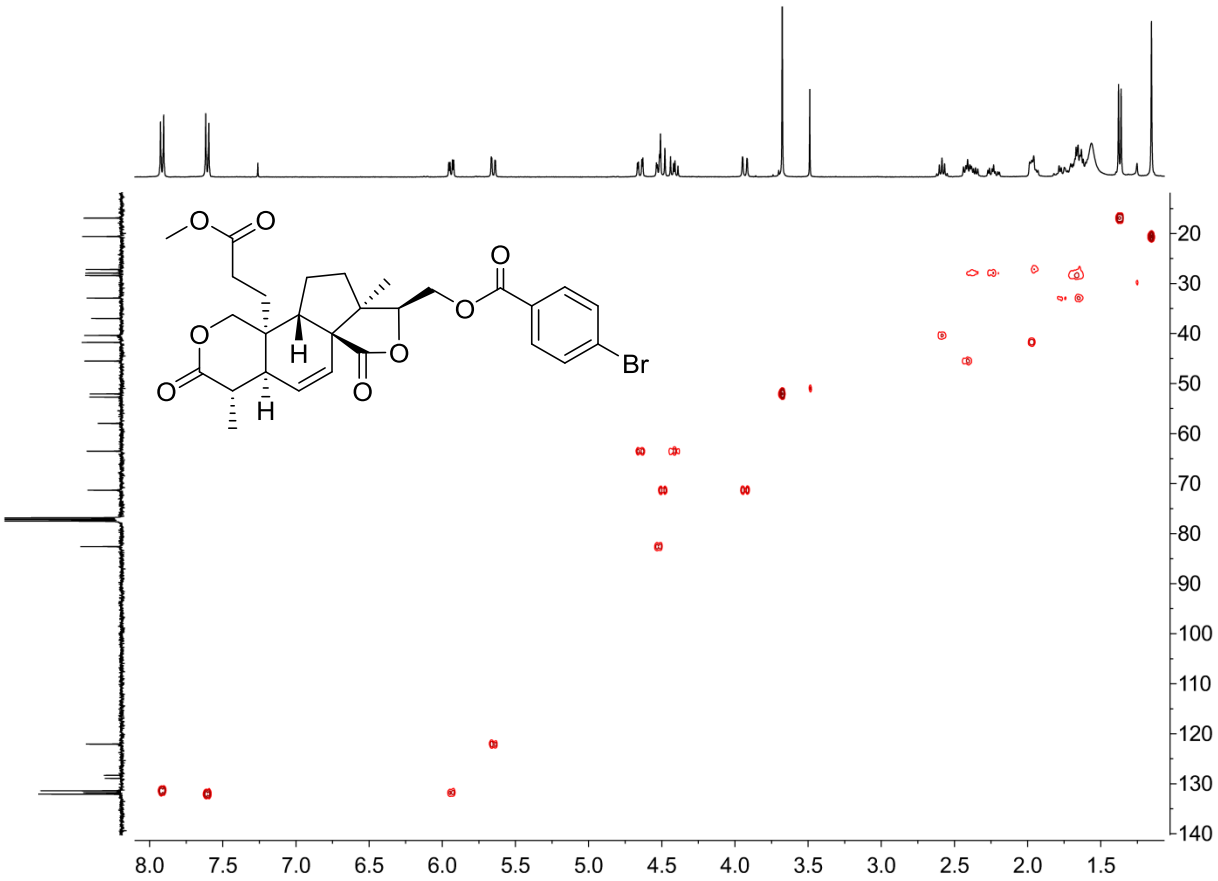

Fig. S52 HSQC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **1a**

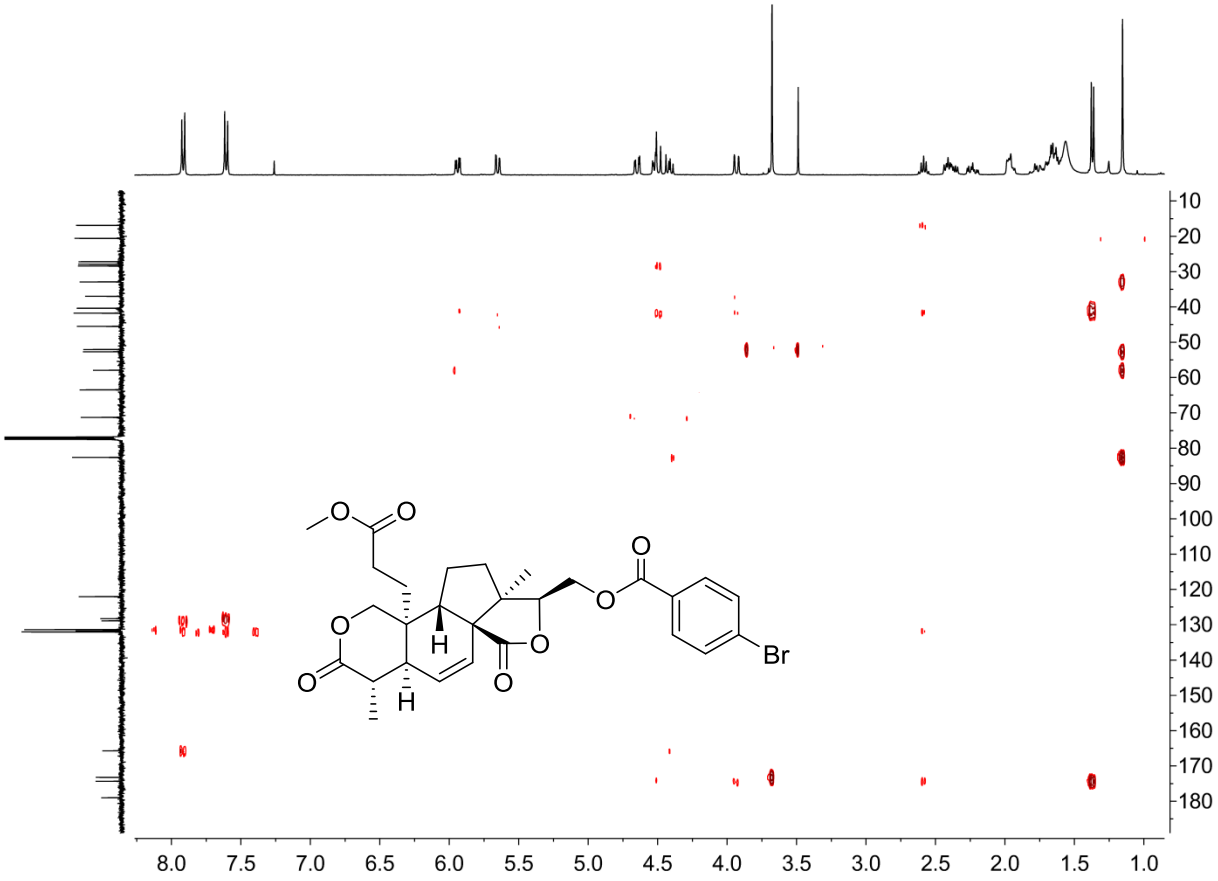

Fig. S53 HMBC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **1a**

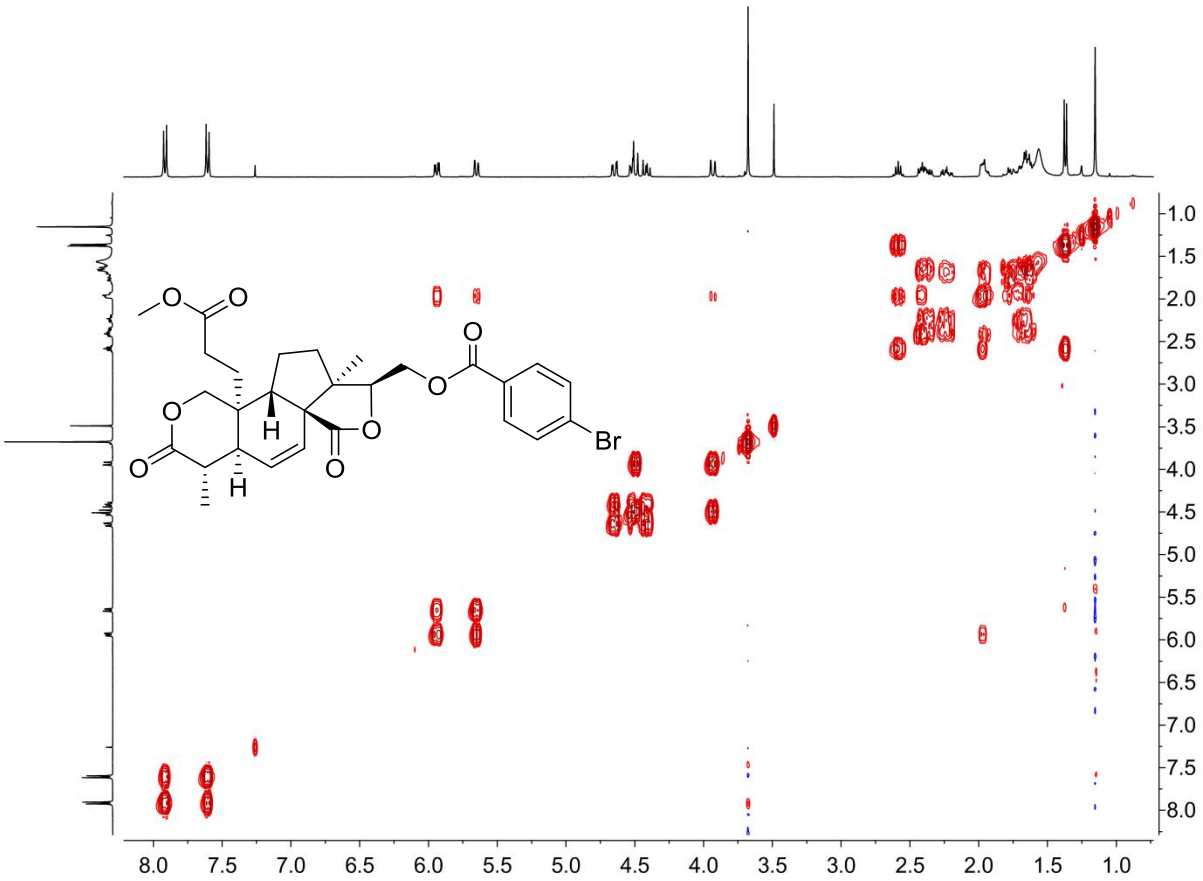

Fig. S54 ^{1}H–^{1}H COSY spectrum (^{1}H: 400 MHz, chloroform-*d*) of **1a**

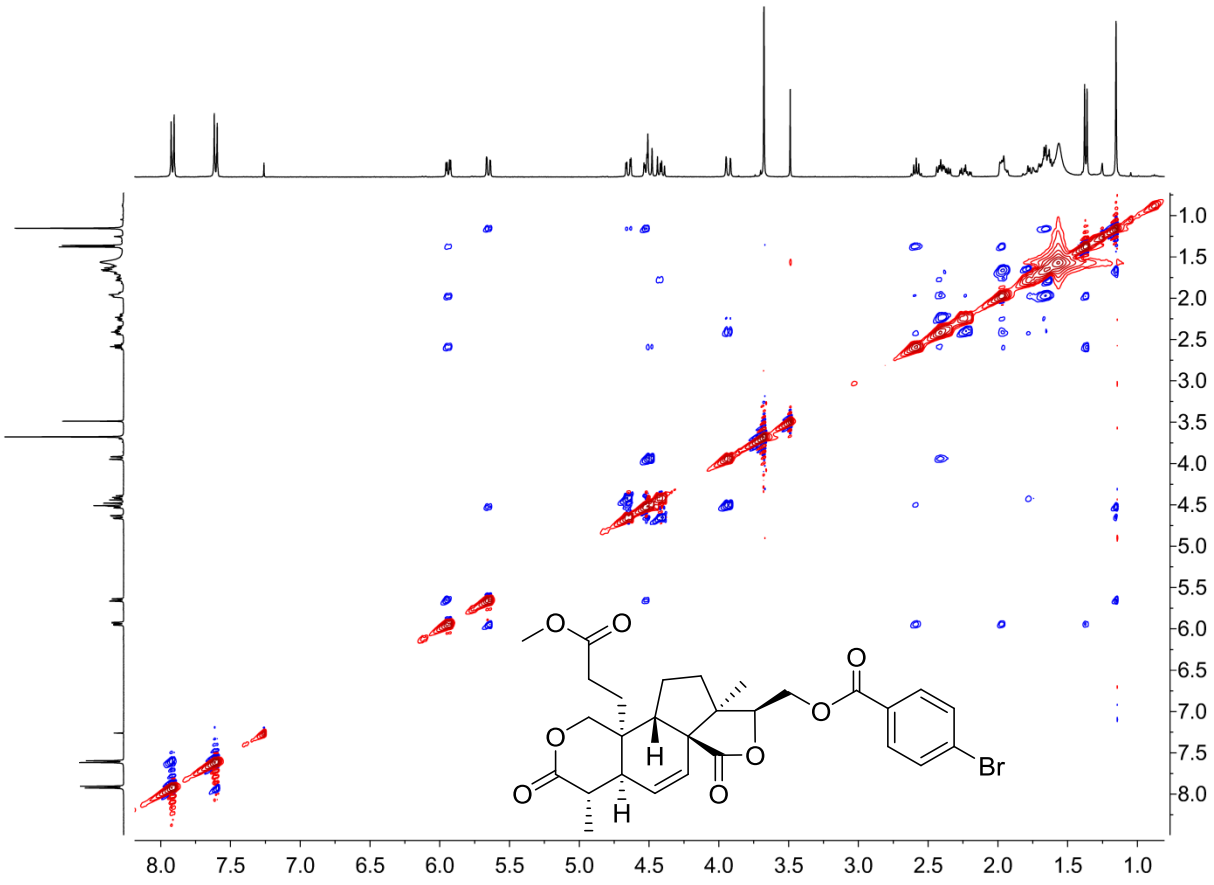

Fig. S55 NOESY spectrum (^{1}H: 400 MHz, chloroform-*d*) of **1a**

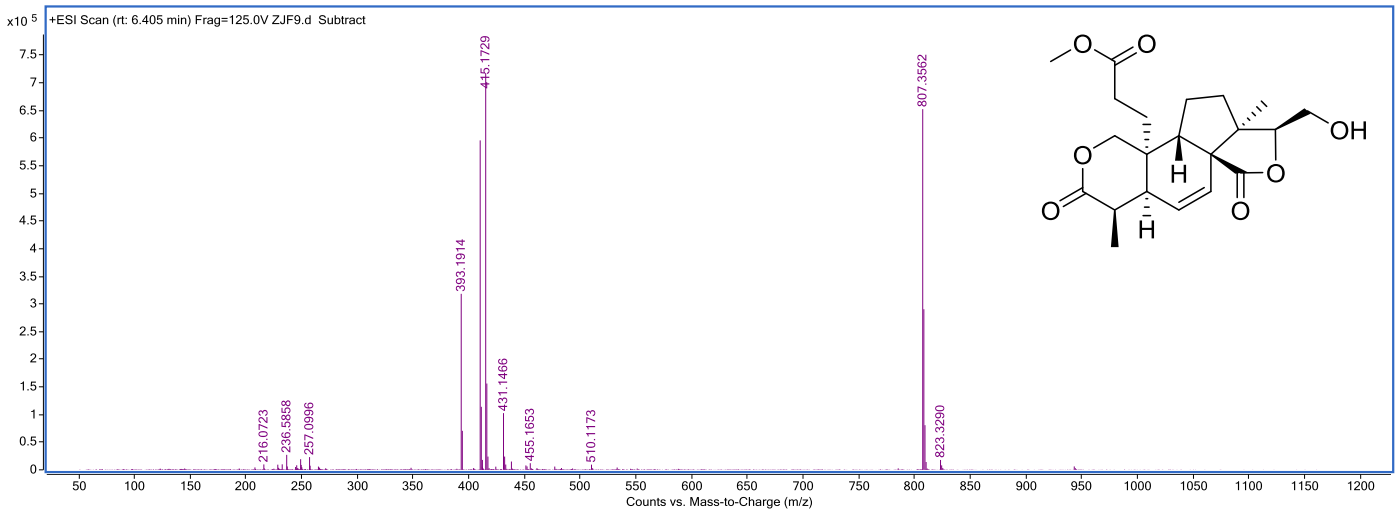

Fig. S56 HR-ESI-MS spectrum of **2**

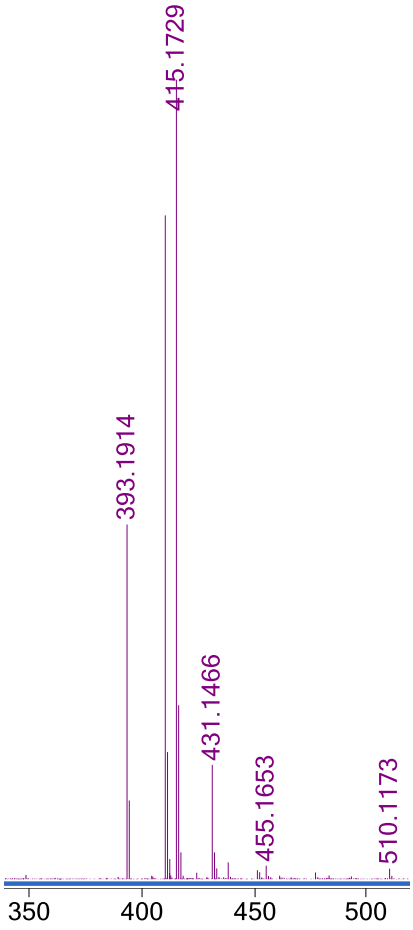

Fig. S57 HR-ESI-MS spectrum of **2** (amplified)

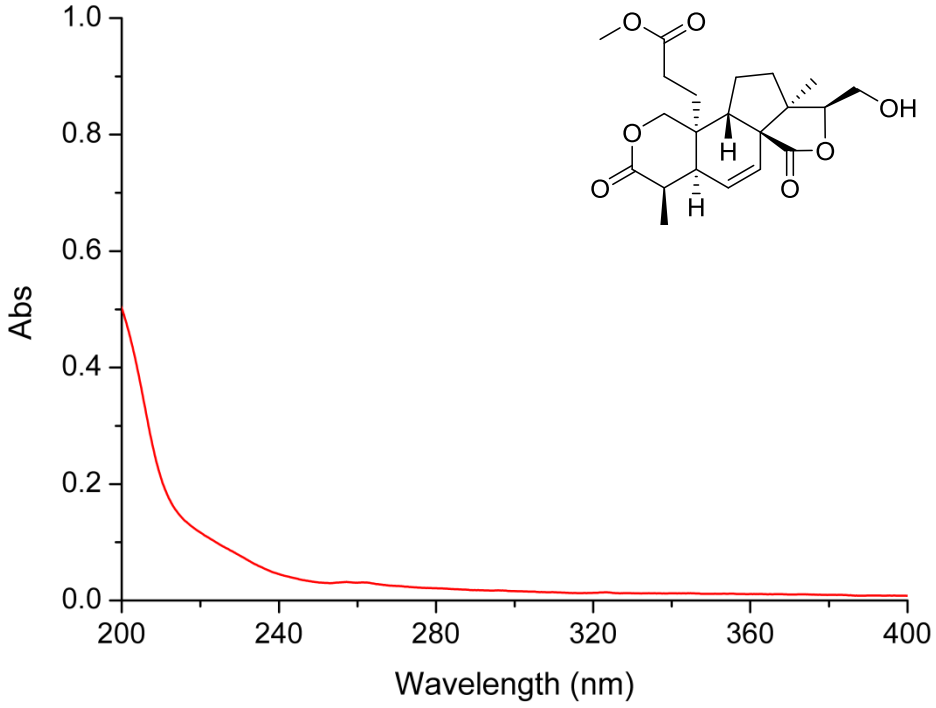

Fig. S58 UV spectrum of **2**

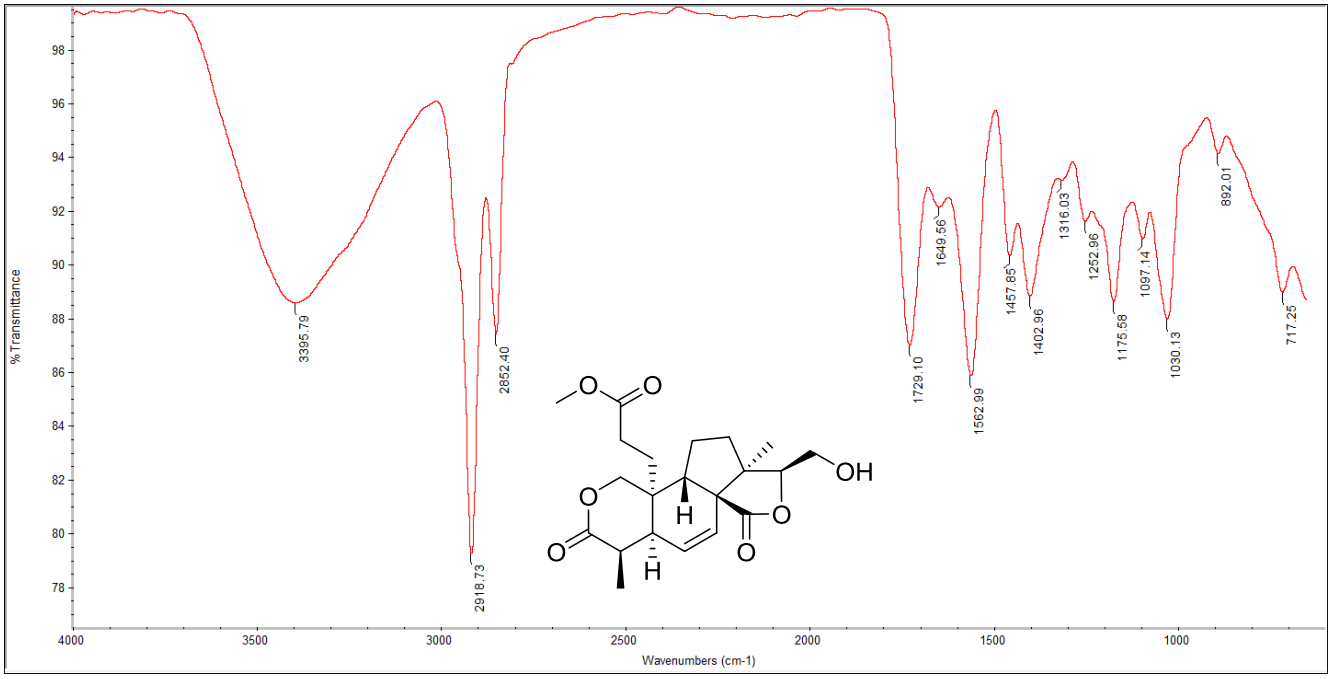

Fig. S59 IR spectrum of **2**

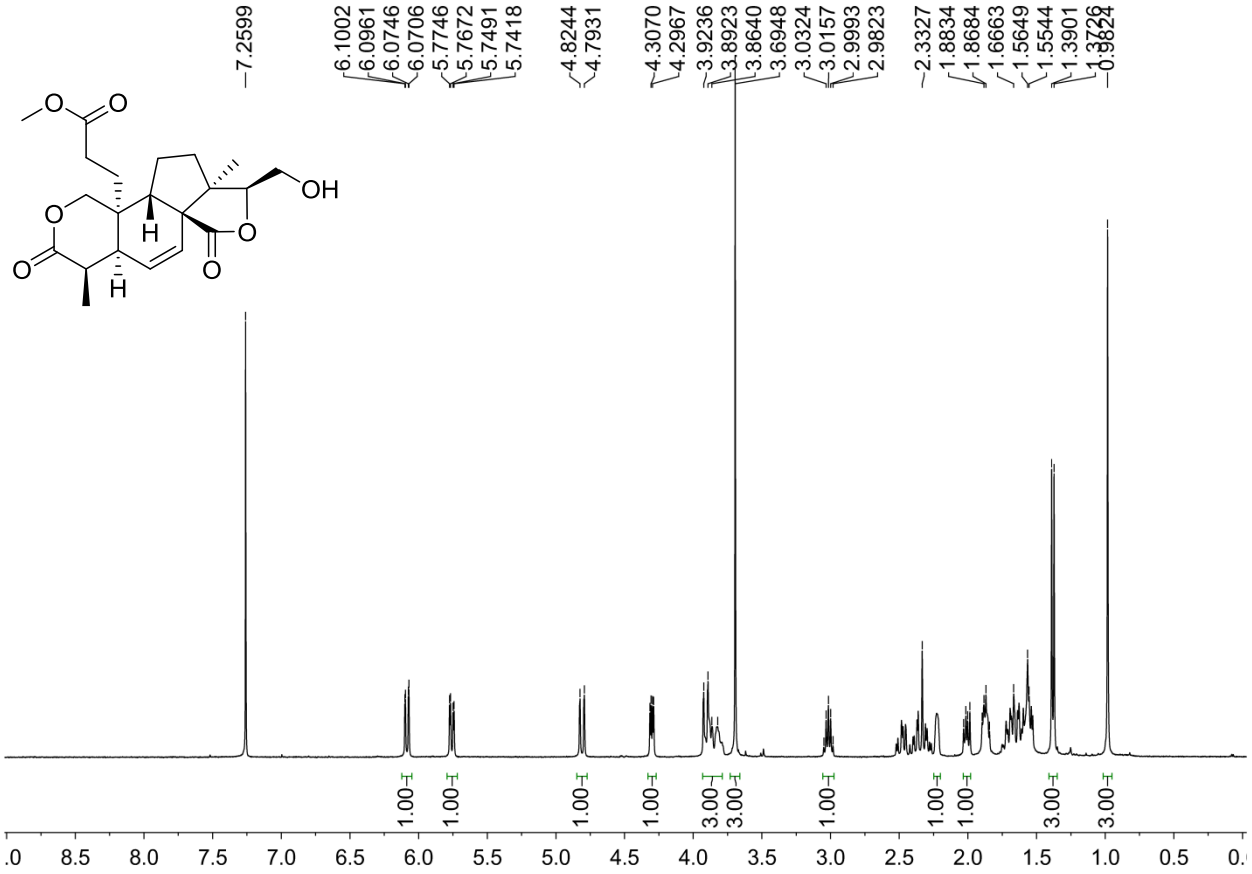

Fig. S60 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **2**

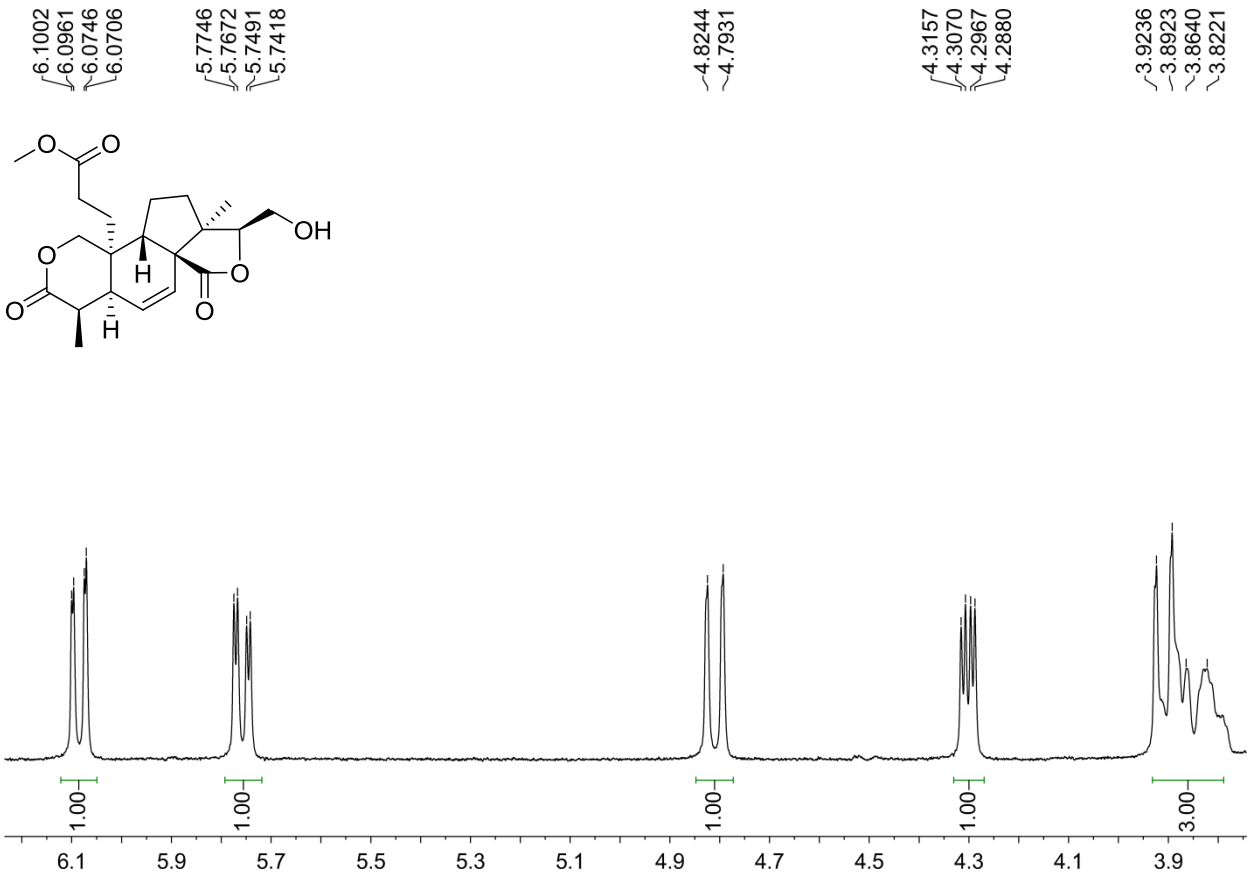

Fig. S61 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **2** (amplified)

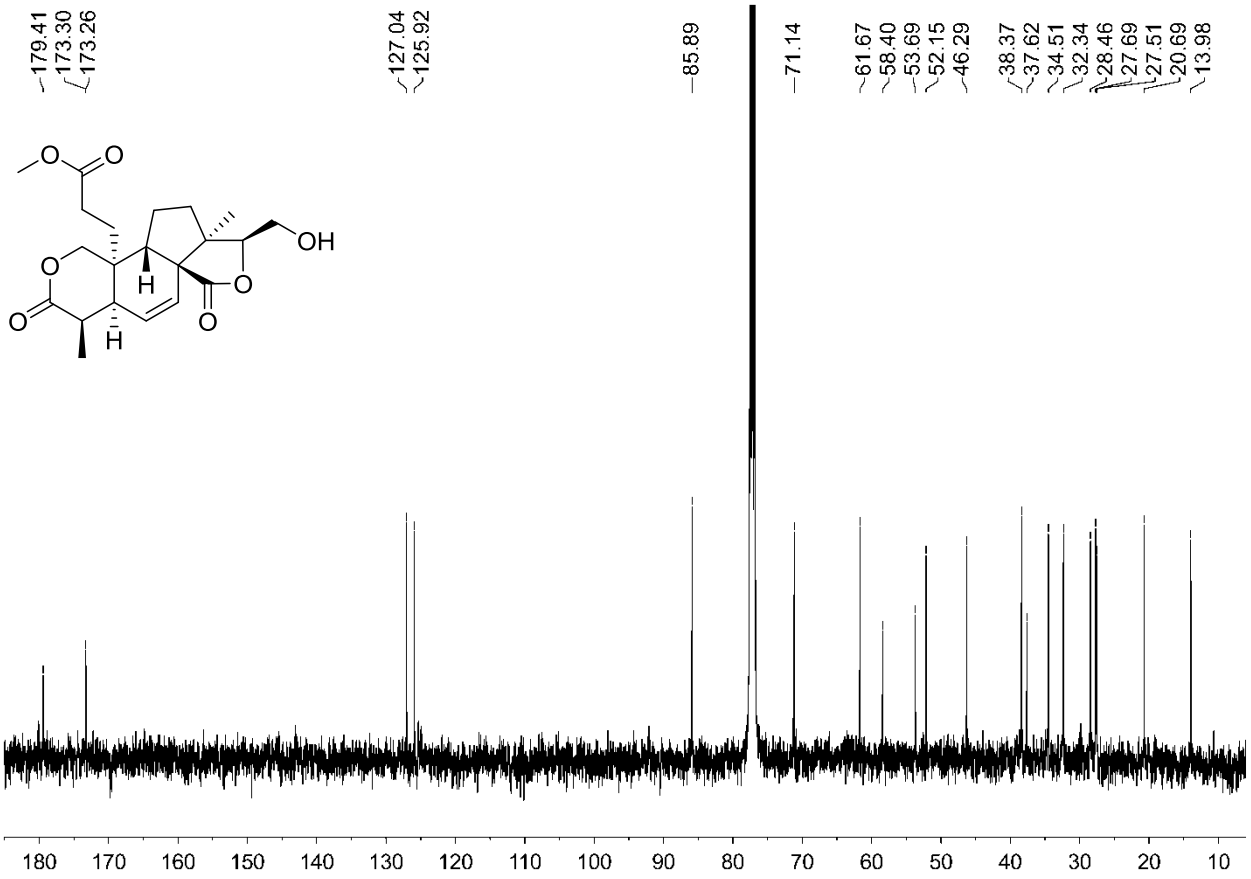

Fig. S62 ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of **2**

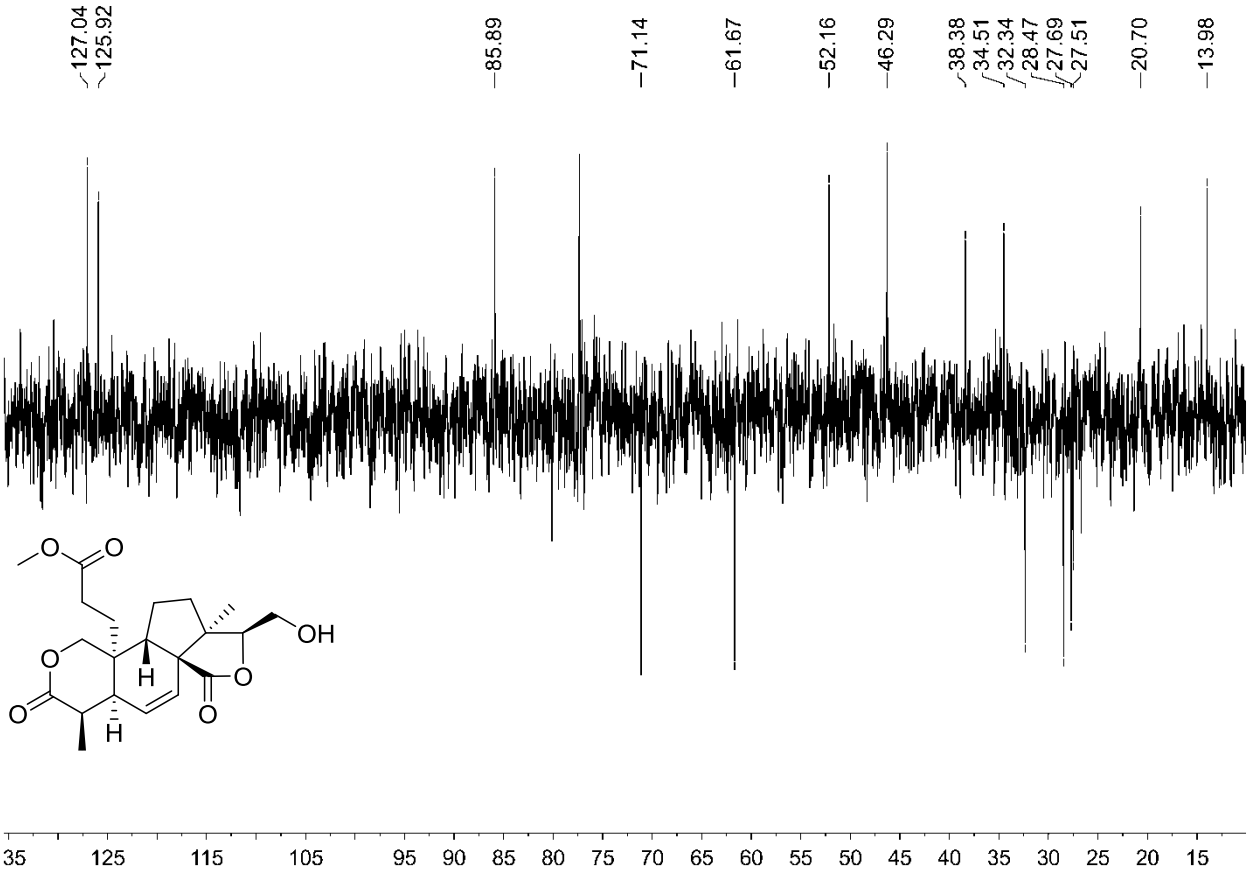

Fig. S63 DEPT135 (100 MHz, chloroform-*d*) spectrum of **2**

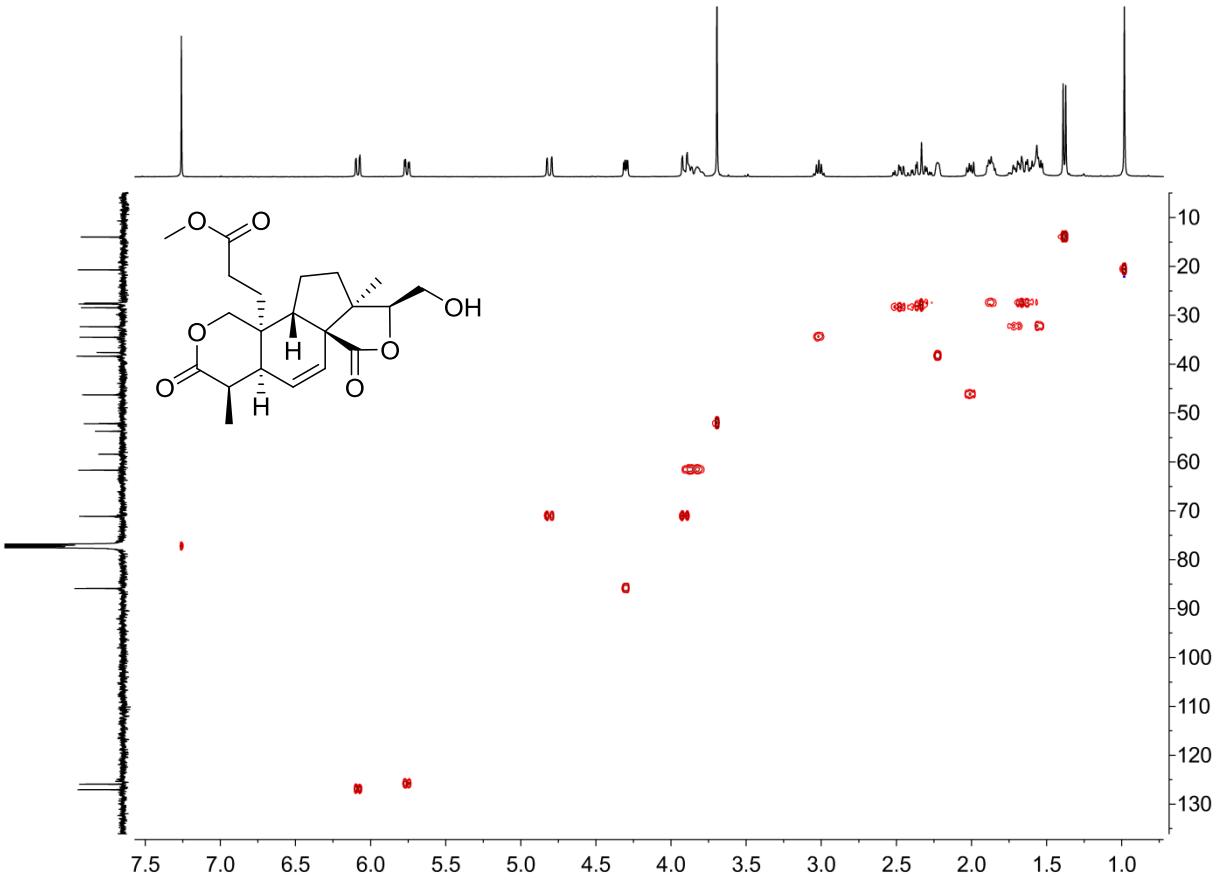

Fig. S64 HSQC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **2**

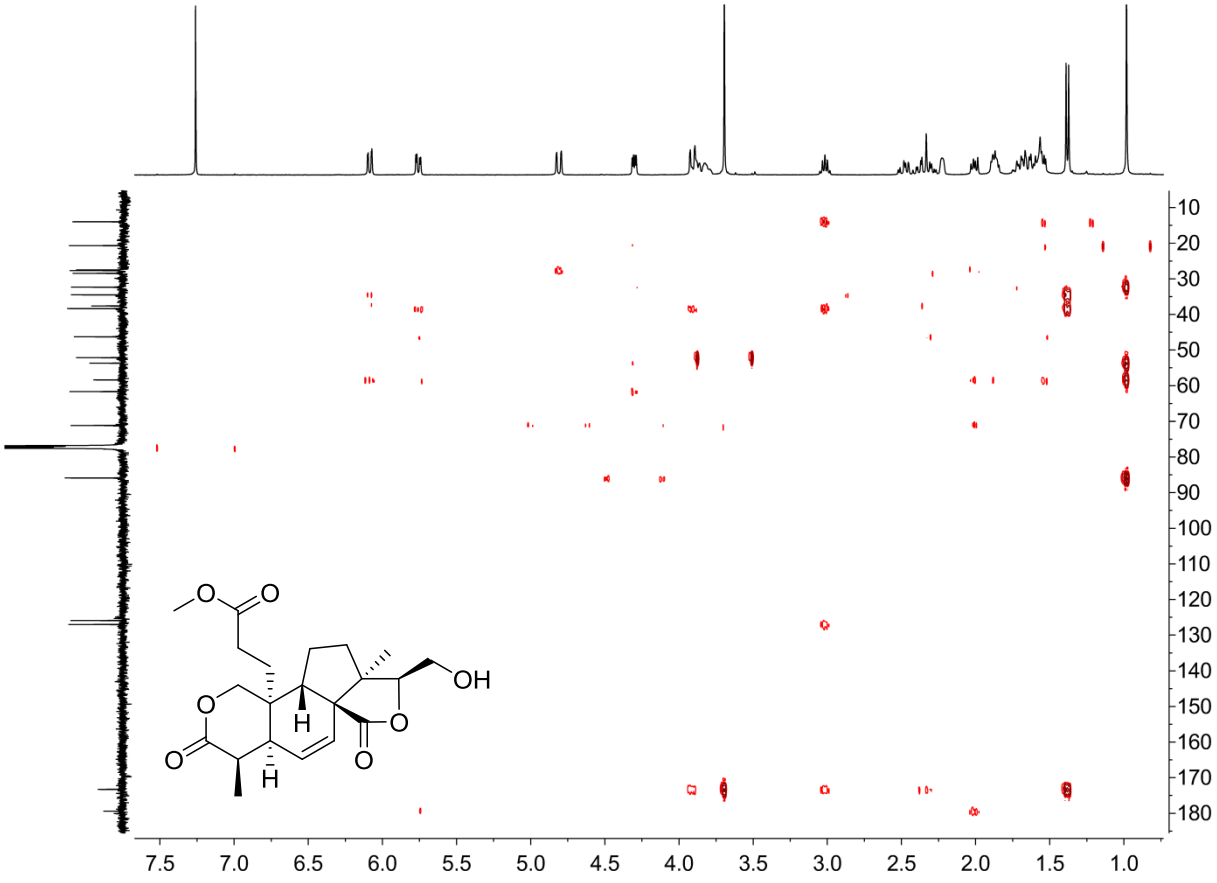

Fig. S65 HMBC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **2**

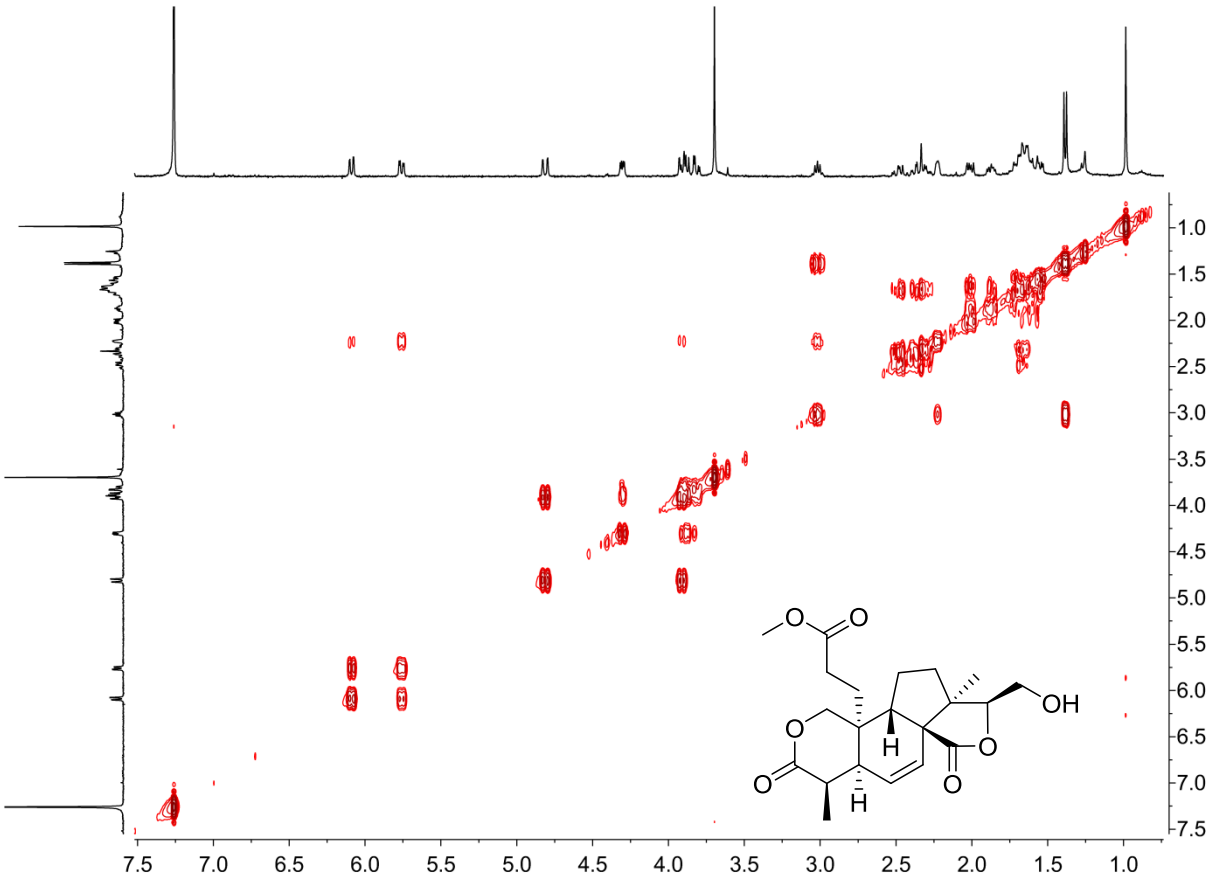

Fig. S66 ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of **2**

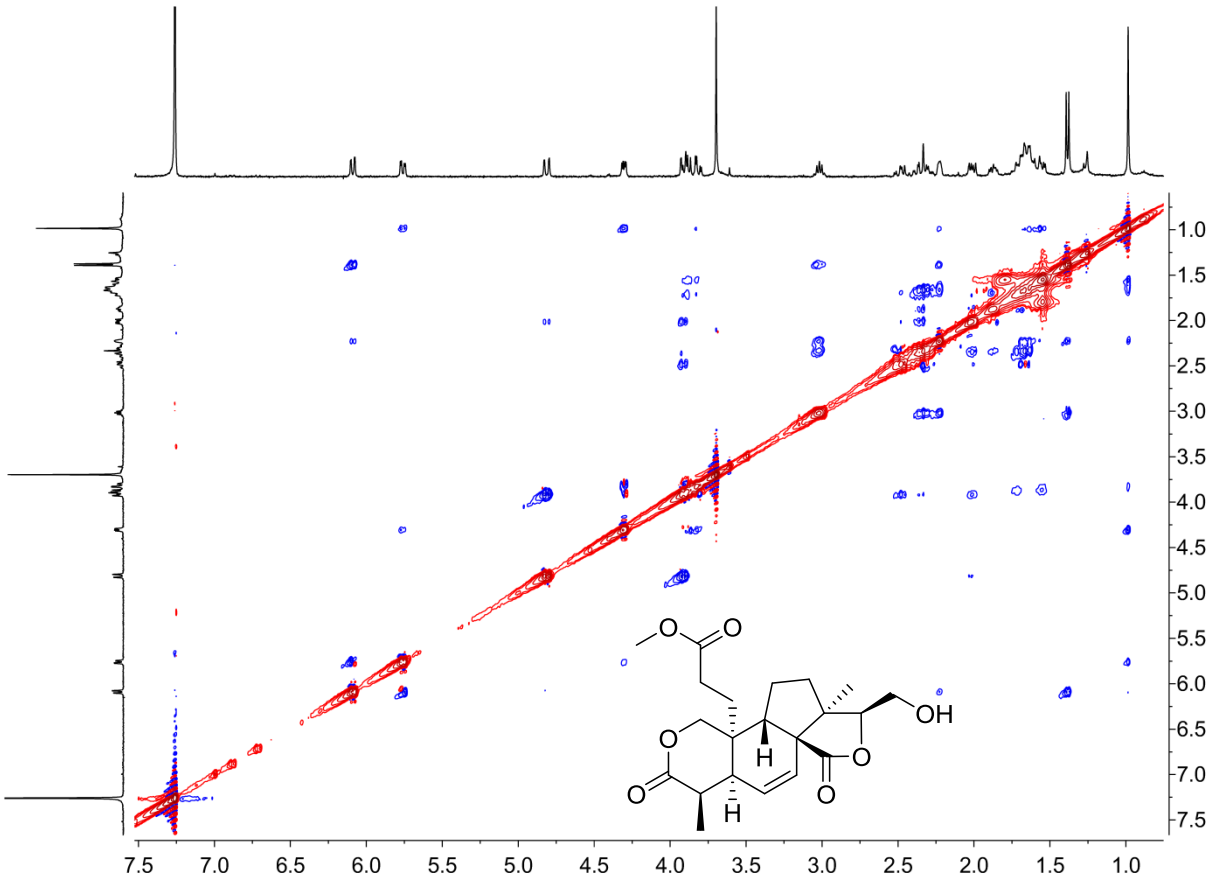

Fig. S67 NOESY spectrum (400 MHz, chloroform-*d*) of **2**

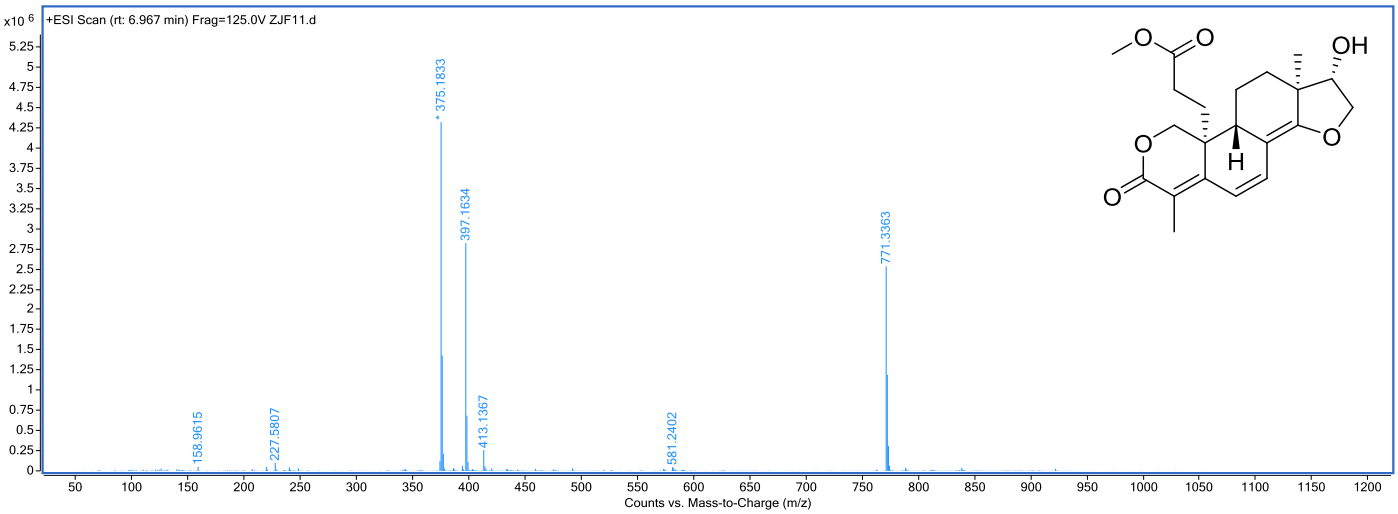

Fig. S68 HR-ESI-MS spectrum of **3**

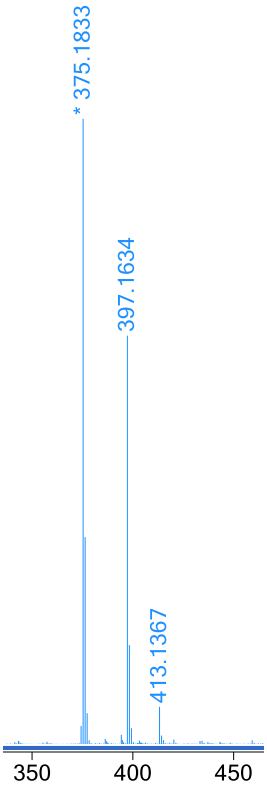

Fig. S69 HR-ESI-MS spectrum of **3** (amplified)

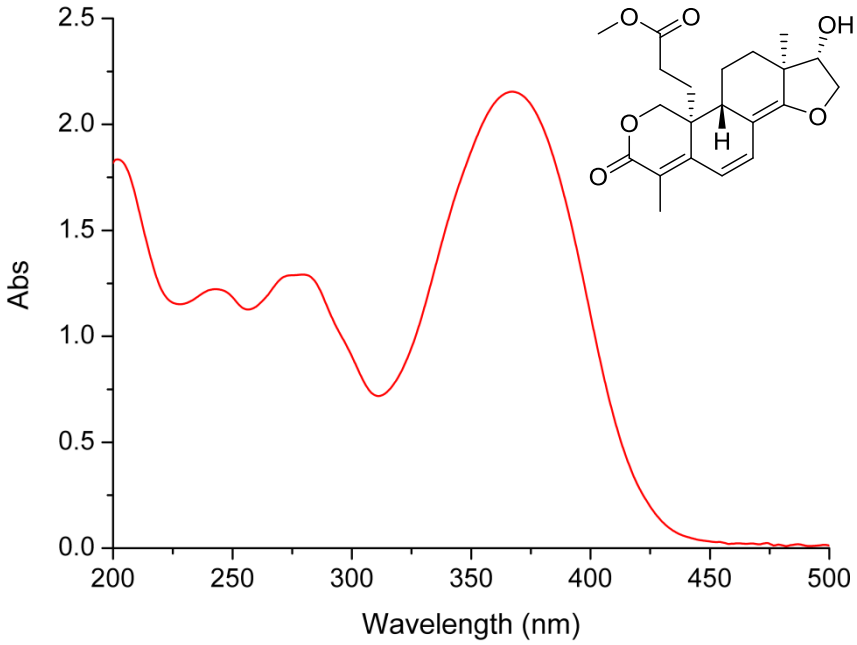

Fig. S70 UV spectrum of **3**

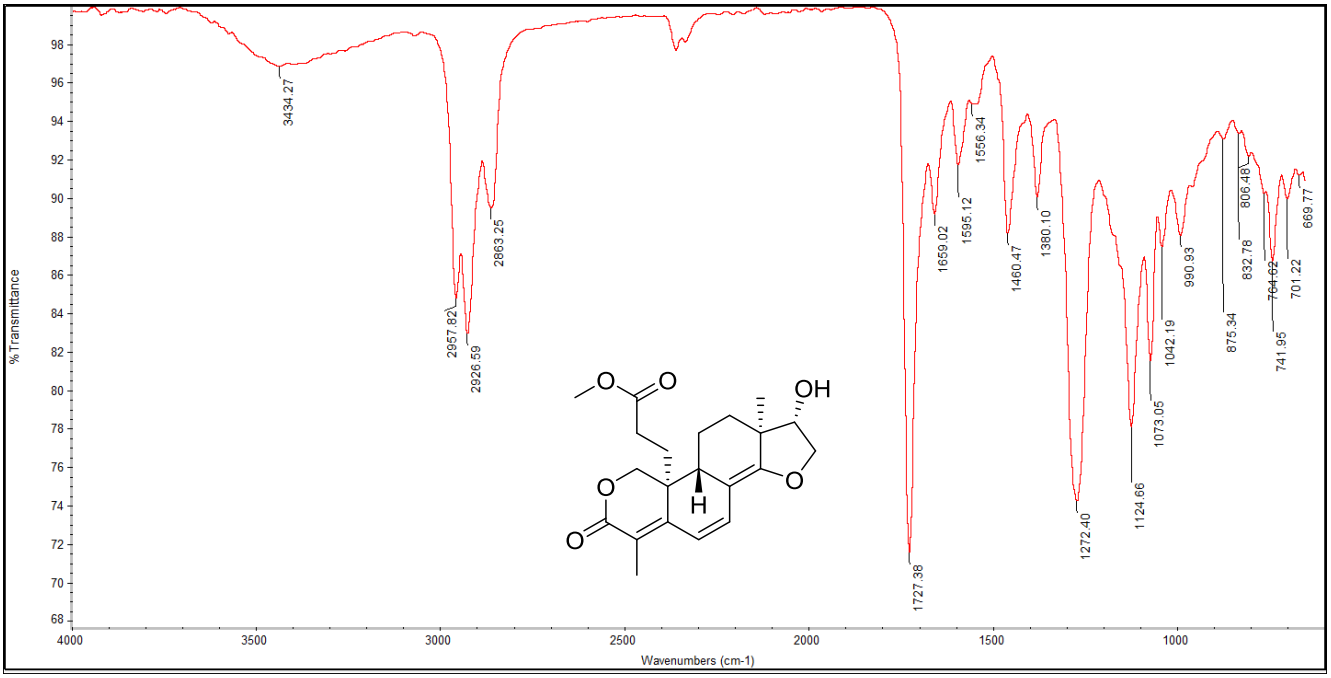

Fig. S71 IR spectrum of **3**

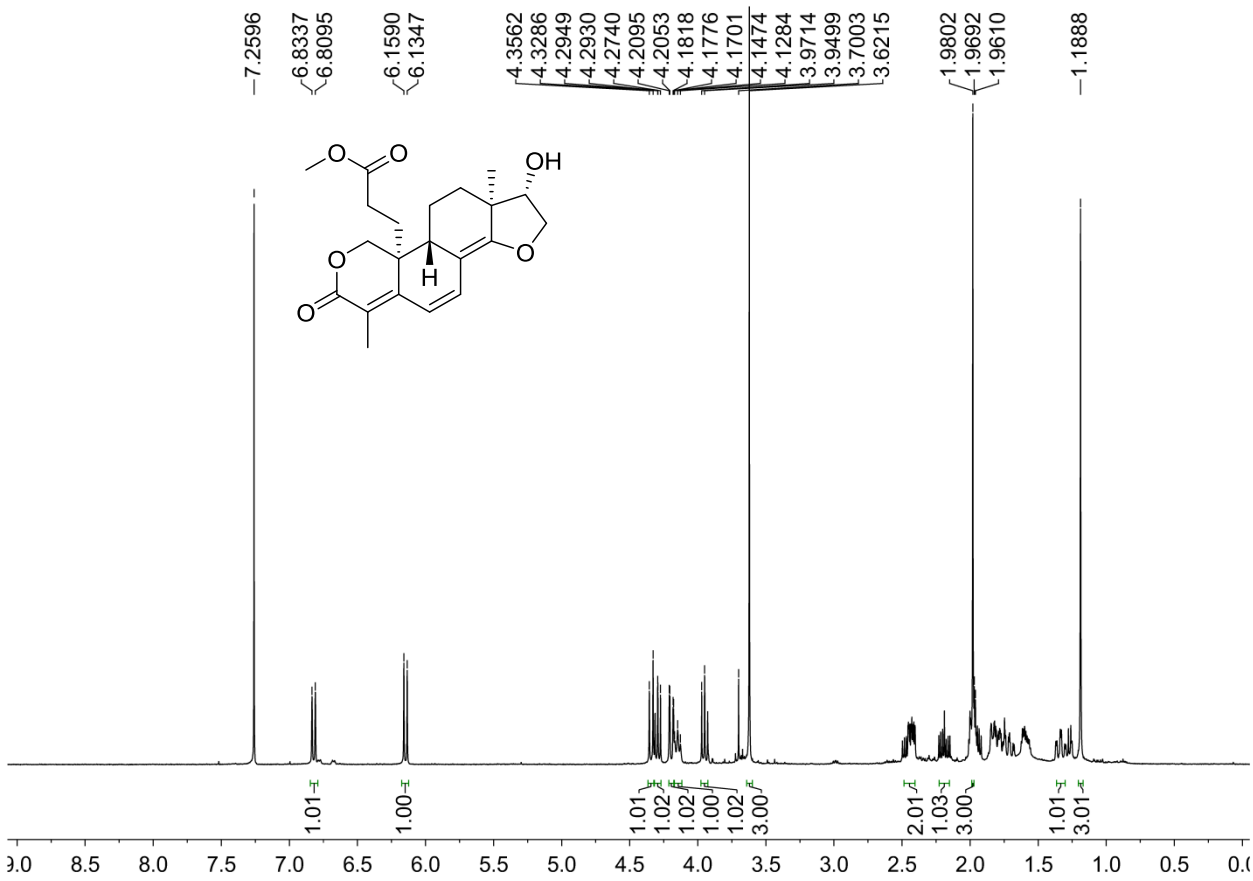

Fig. S72 [1]H NMR (400 MHz, chloroform-*d*) spectru

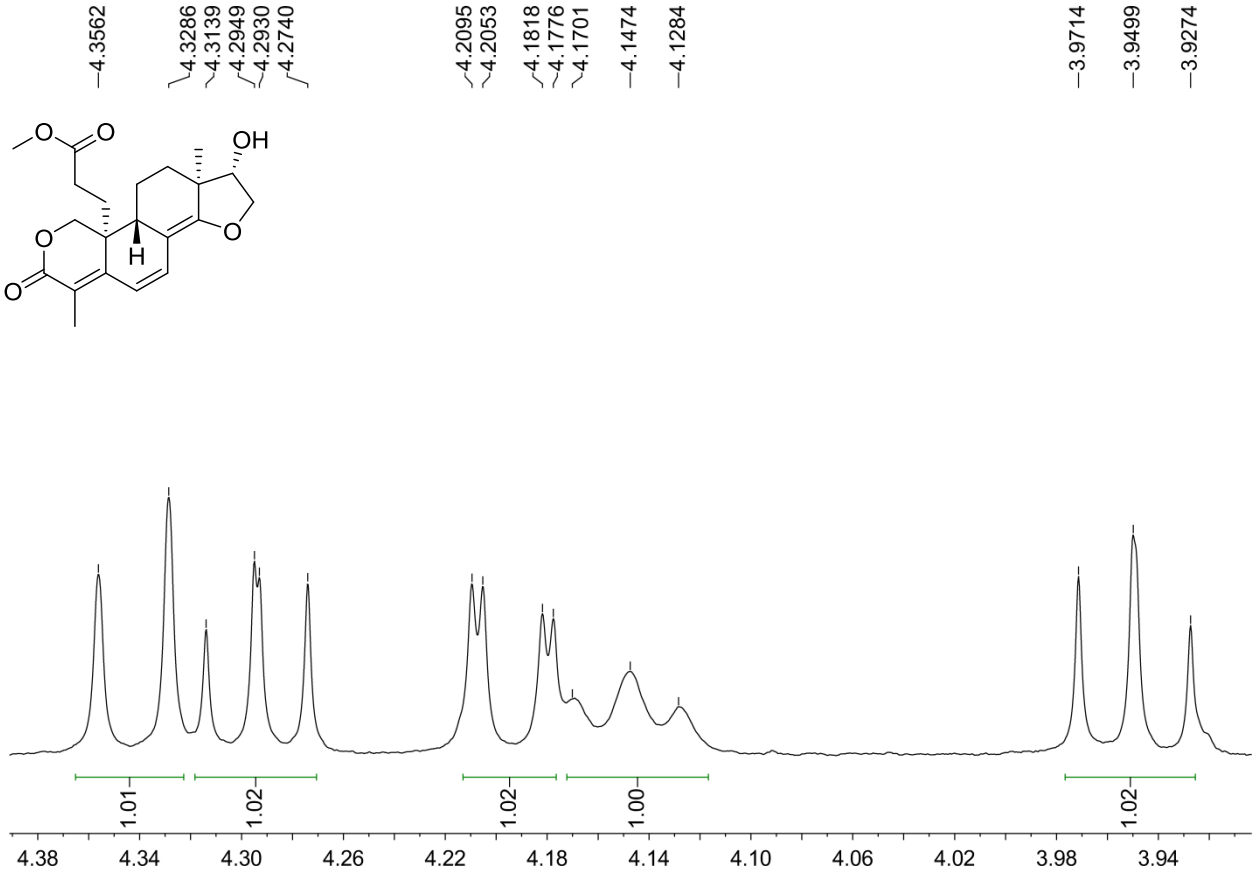

Fig. S73 [1]H NMR (400 MHz, chloroform-*d*) spectrum of **3** (amplified)

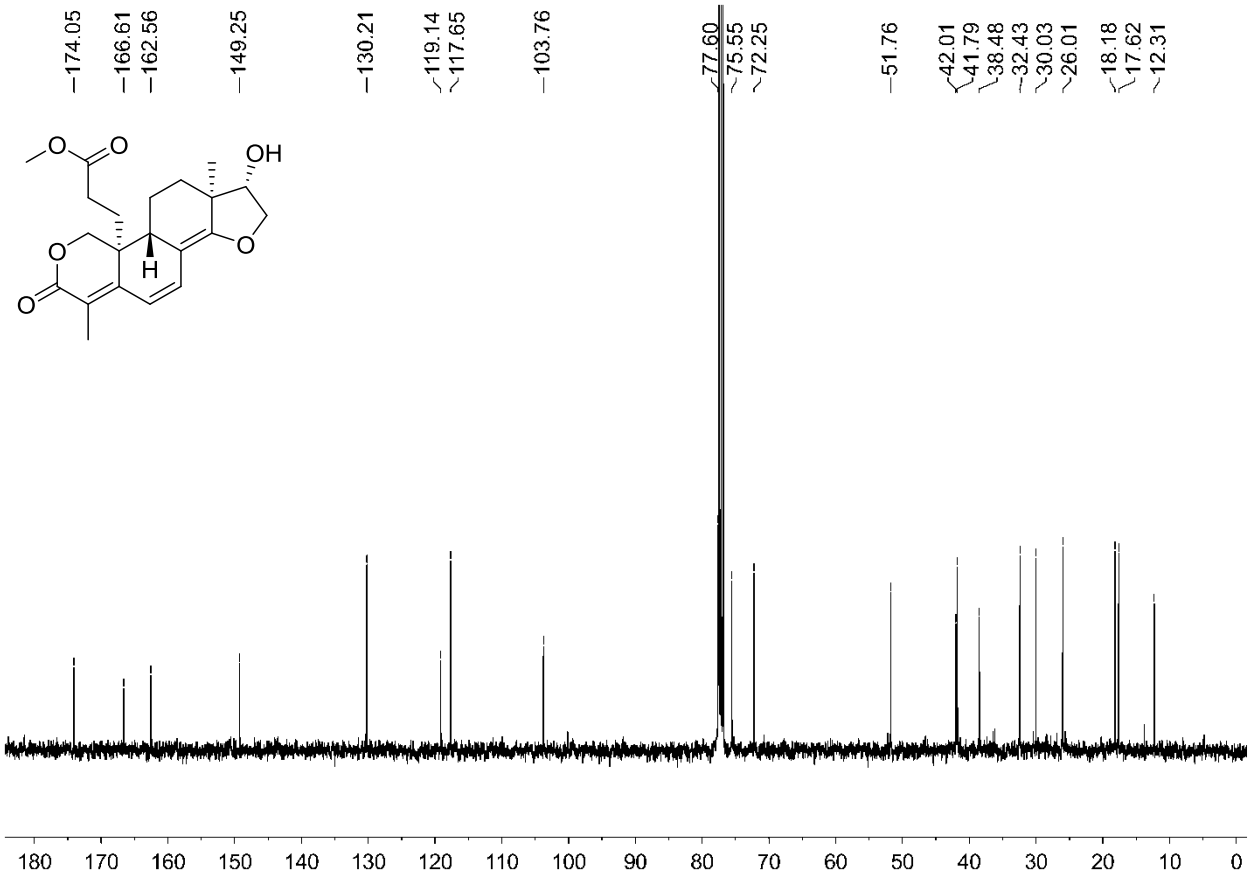

Fig. S74 ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of **3**

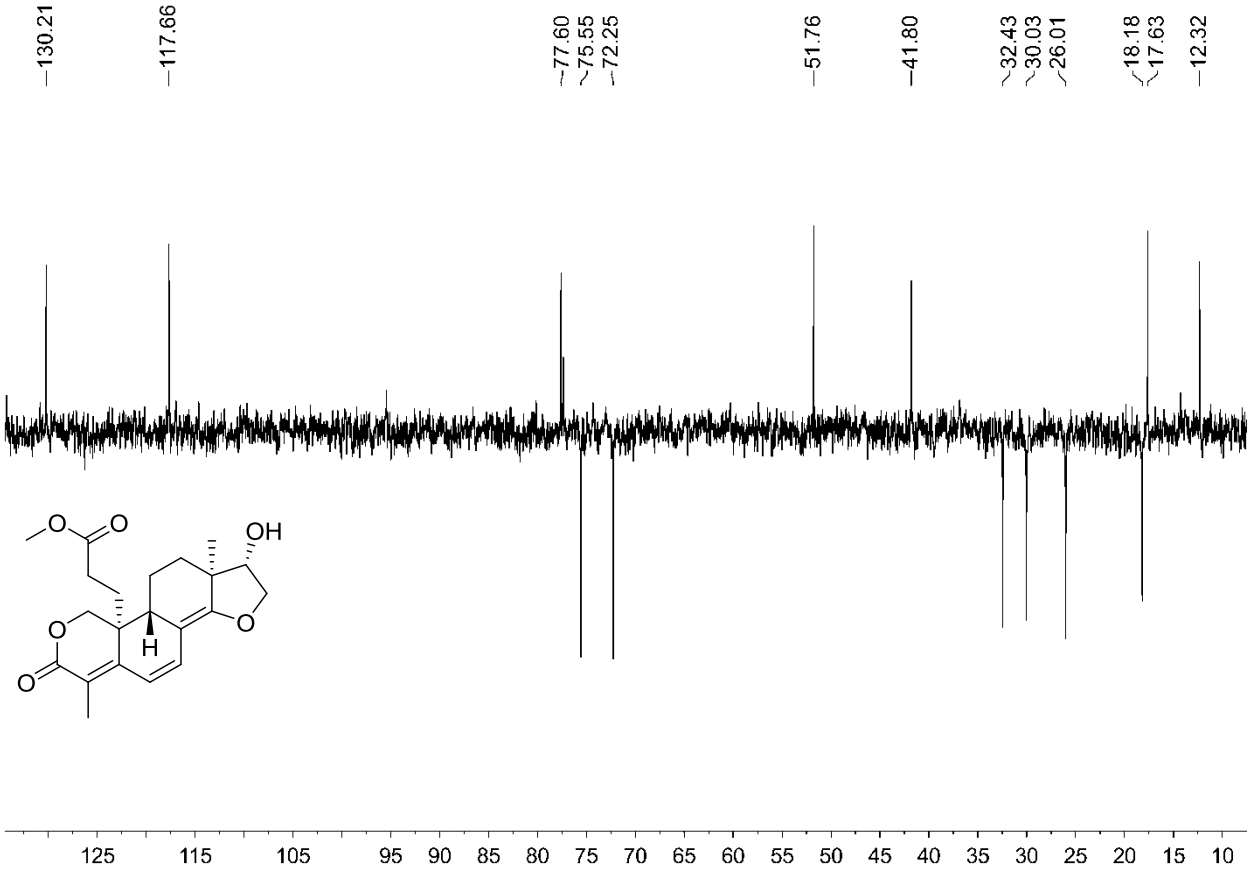

Fig. S75 DEPT135 (100 MHz, chloroform-*d*) spectrum of **3**

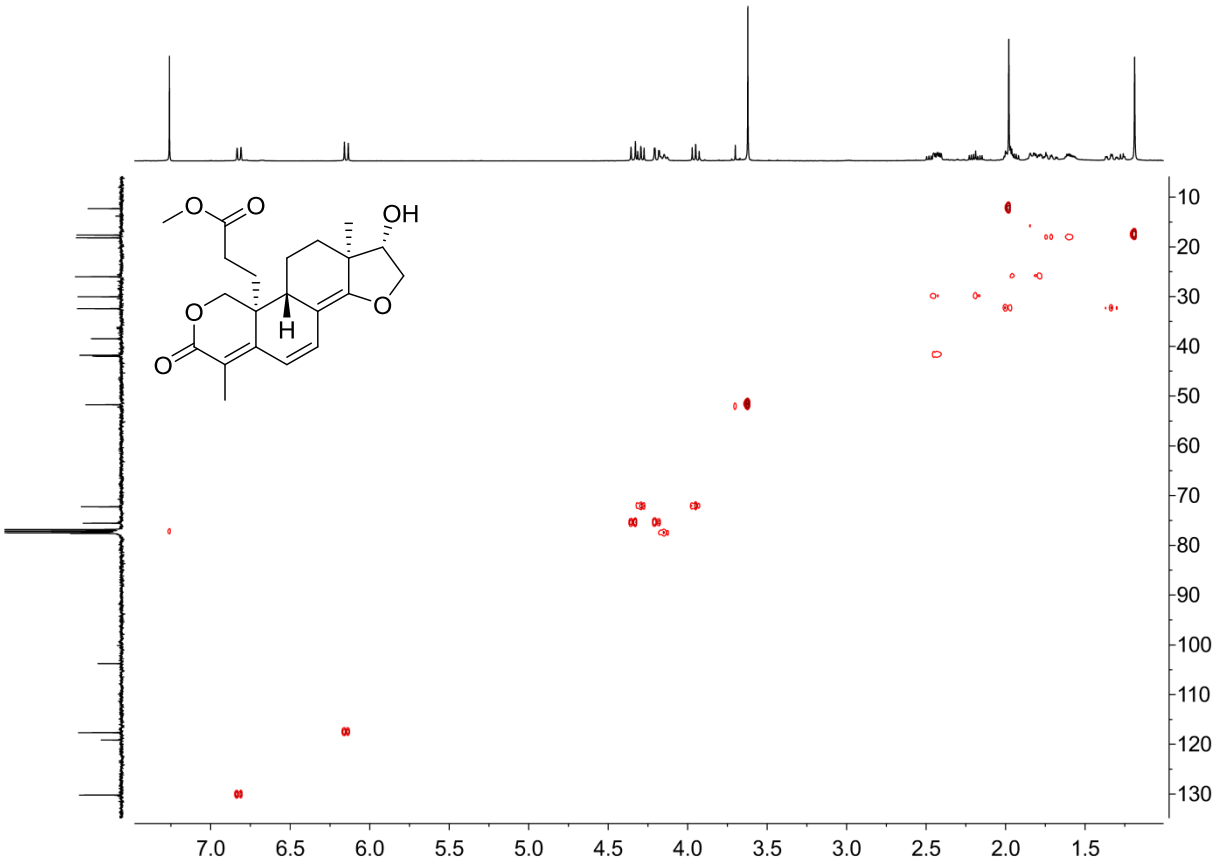

Fig. S76 HSQC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **3**

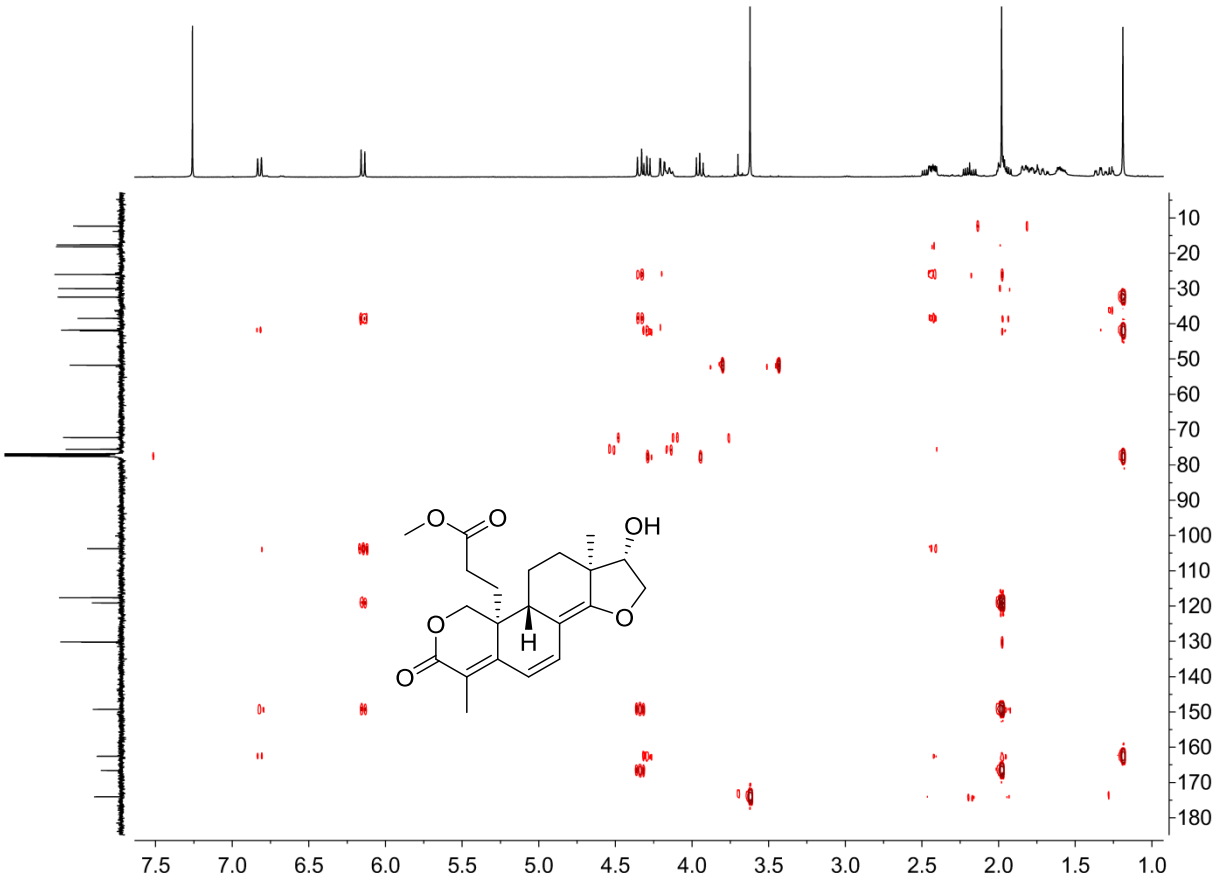

Fig. S77 HMBC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **3**

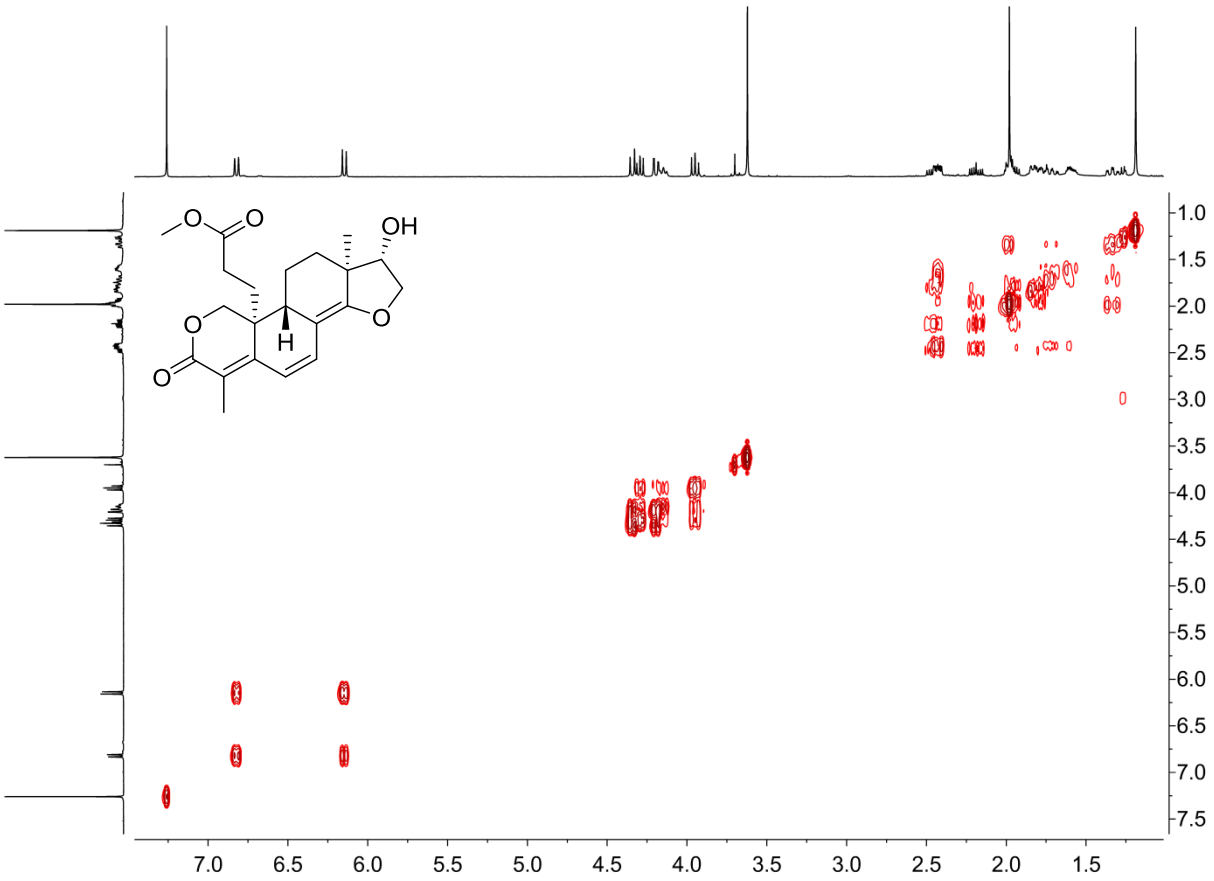

Fig. S78 ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of **3**

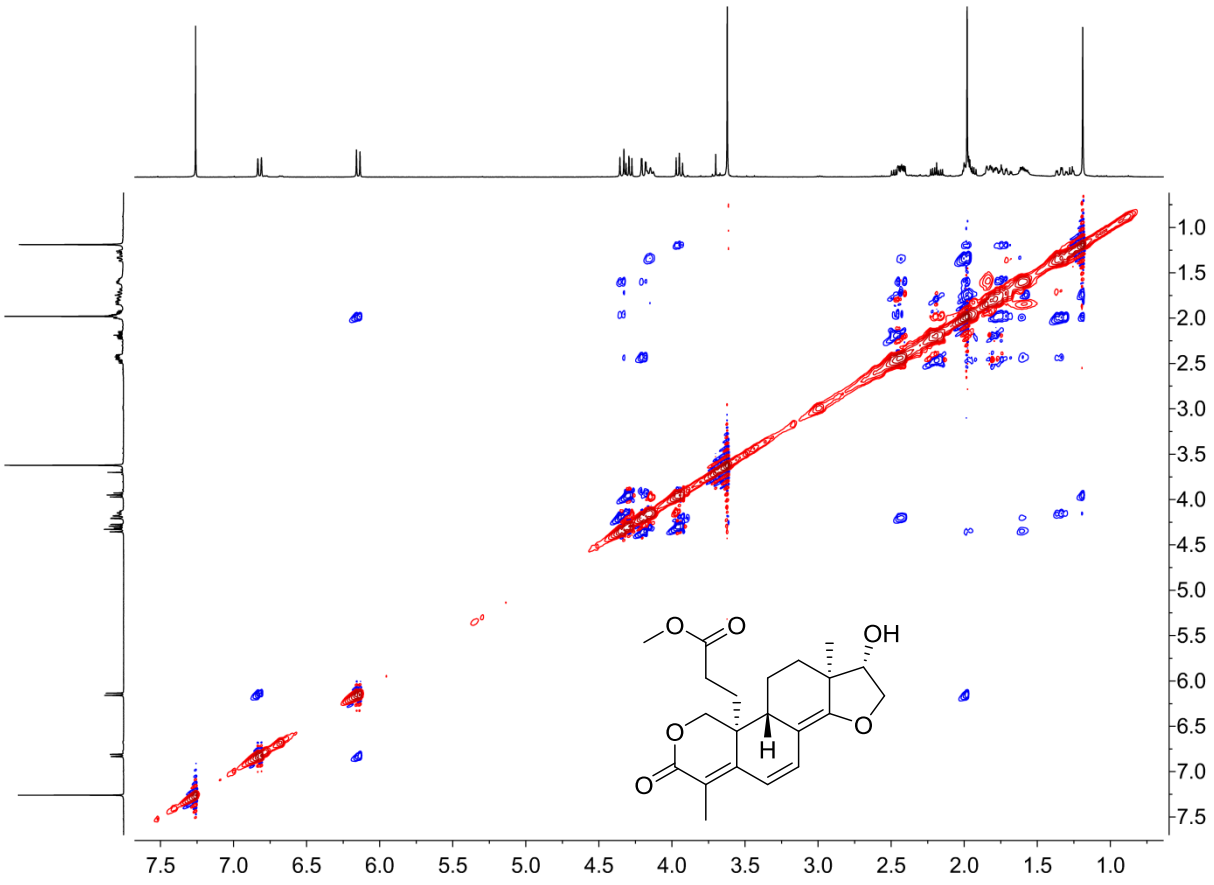

Fig. S79 NOESY spectrum (400 MHz, chloroform-*d*) of **3**

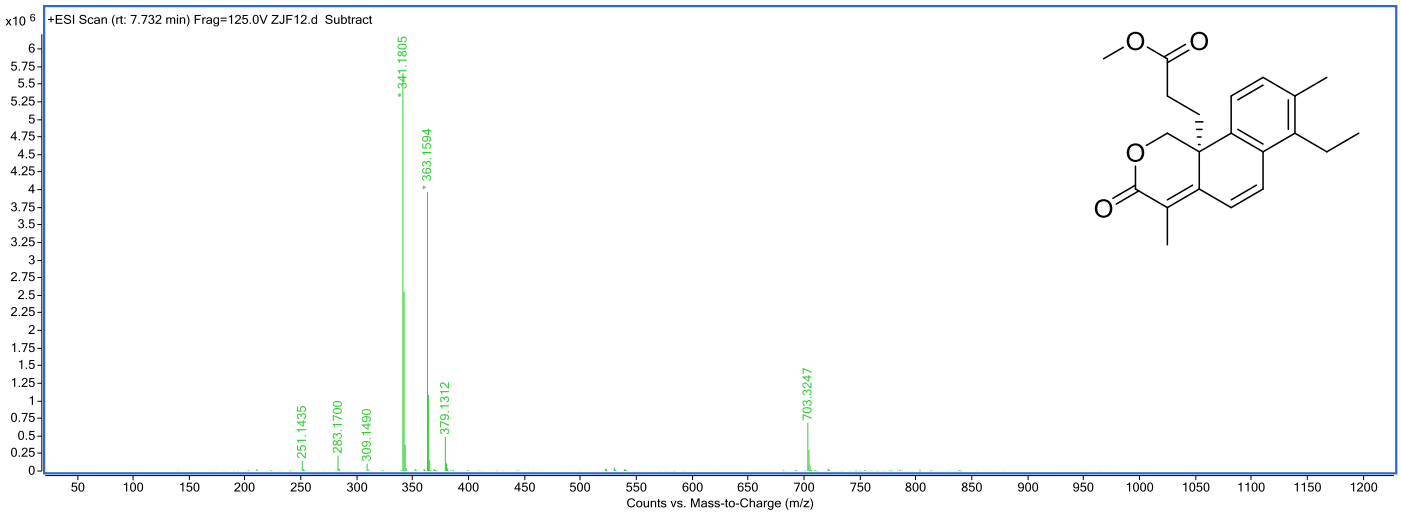

Fig. S80 HR-ESI-MS spectrum of **4**

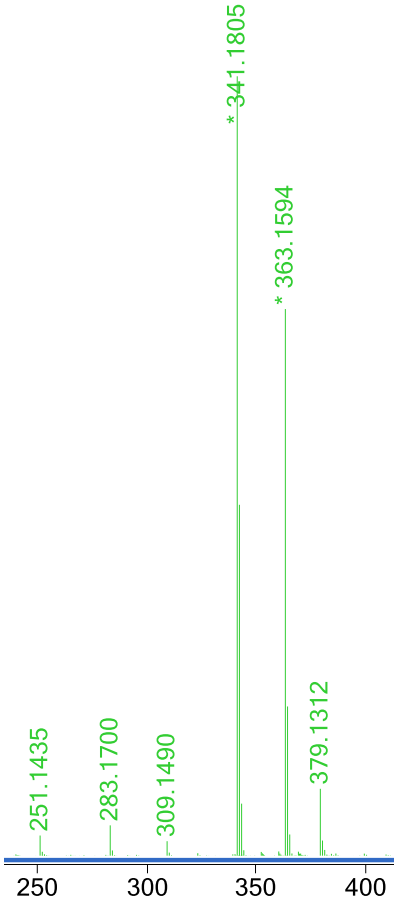

Fig. S81 HR-ESI-MS spectrum of **4** (amplified)

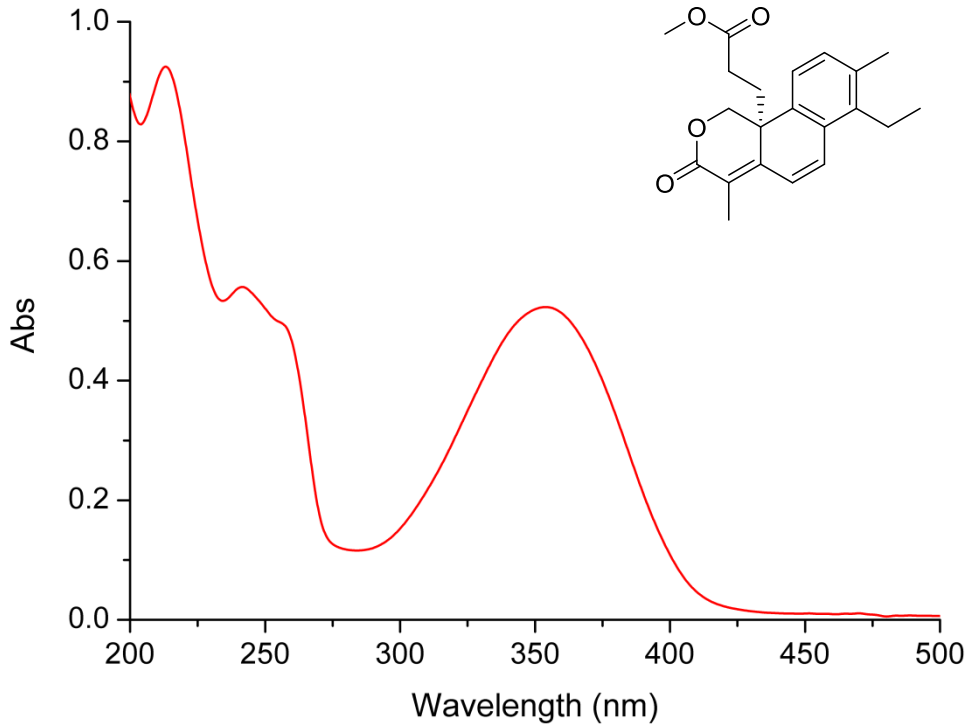

Fig. S82 UV spectrum of **4**

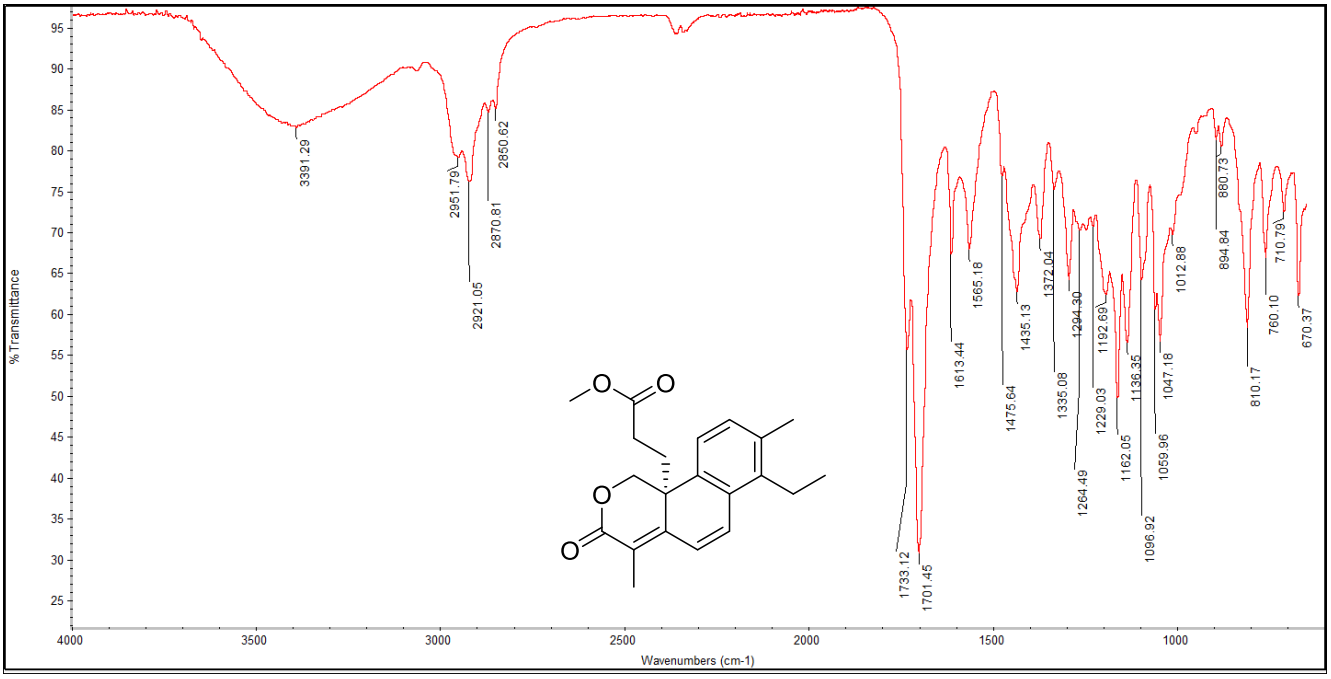

Fig. S83 IR spectrum of **4**

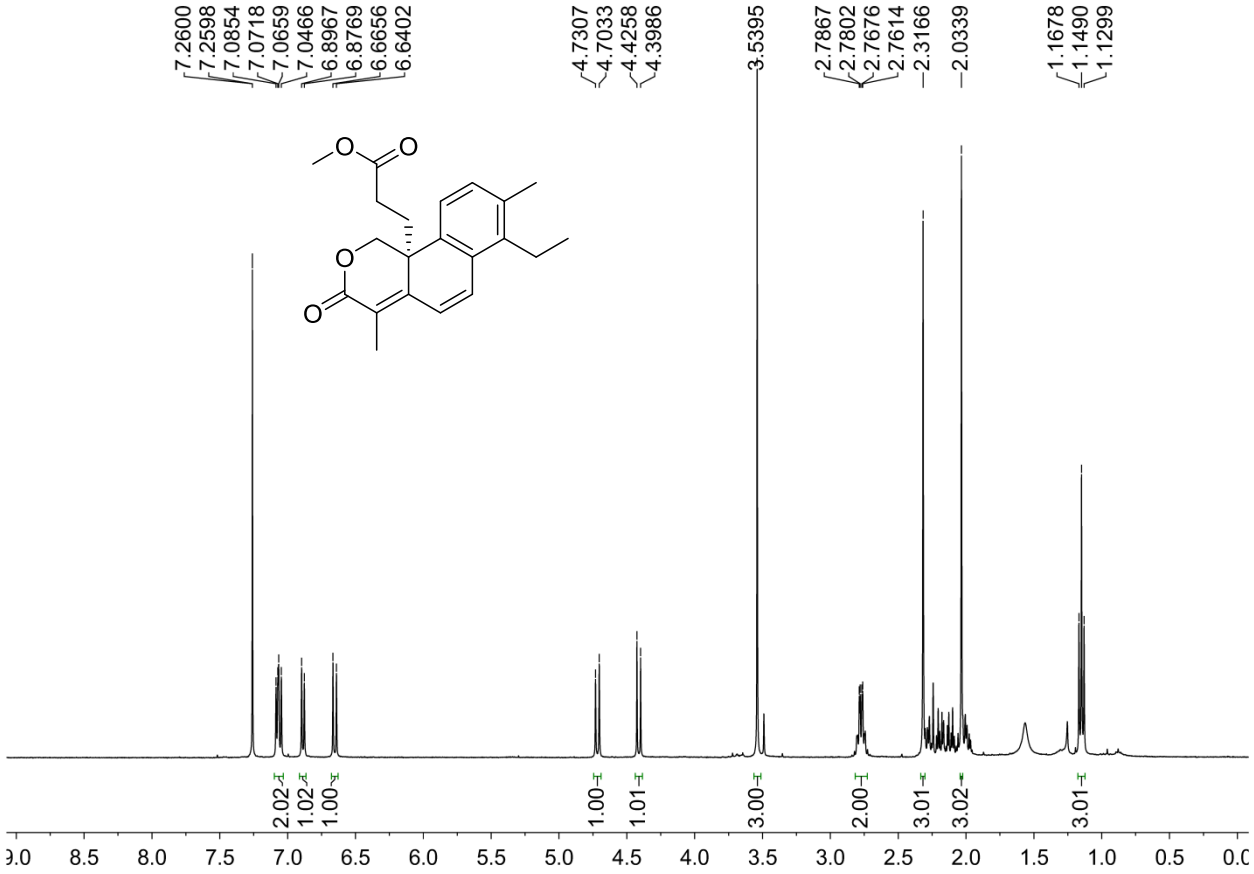

Fig. S84 [1]H NMR (400 MHz, chloroform-*d*) spectrum of **4**

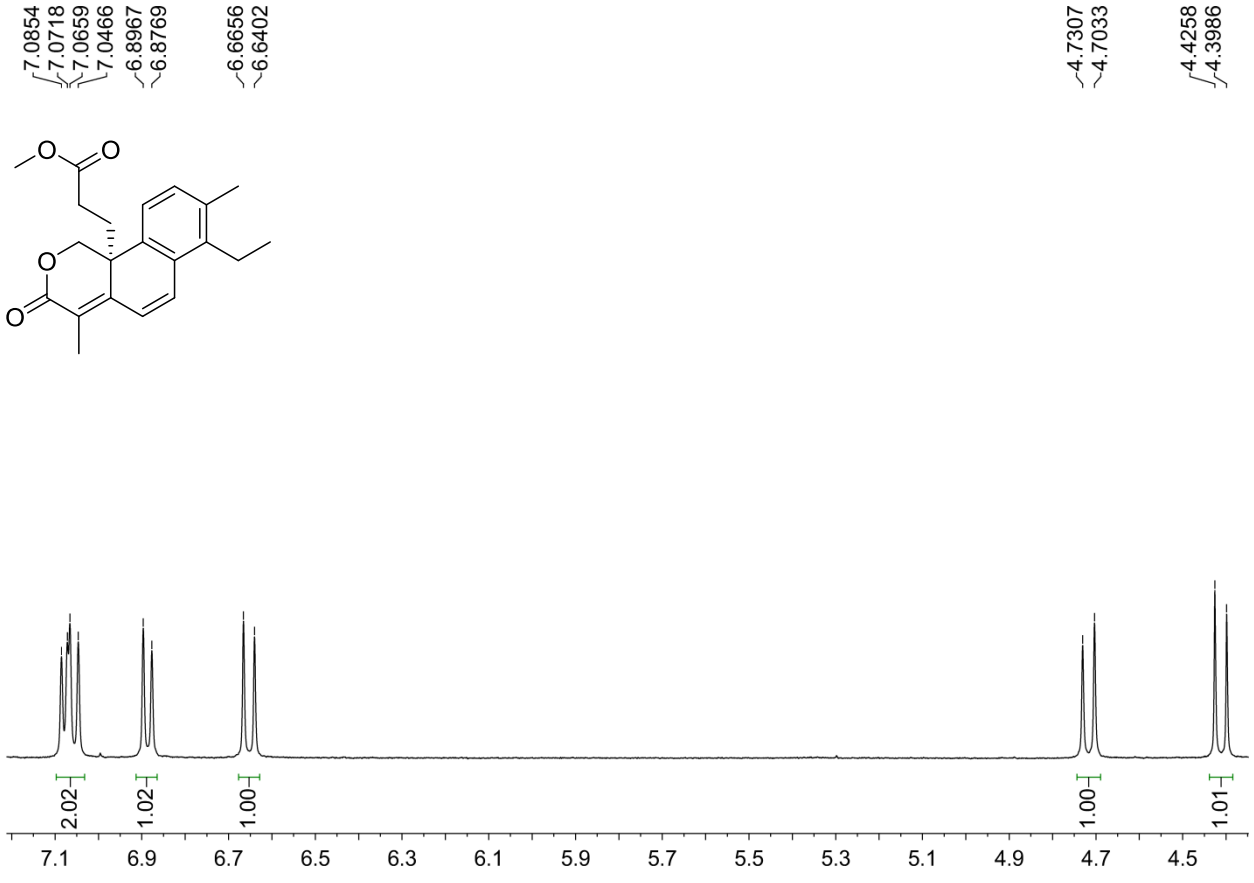

Fig. S85 [1]H NMR (400 MHz, chloroform-*d*) spectrum of **4** (amplified)

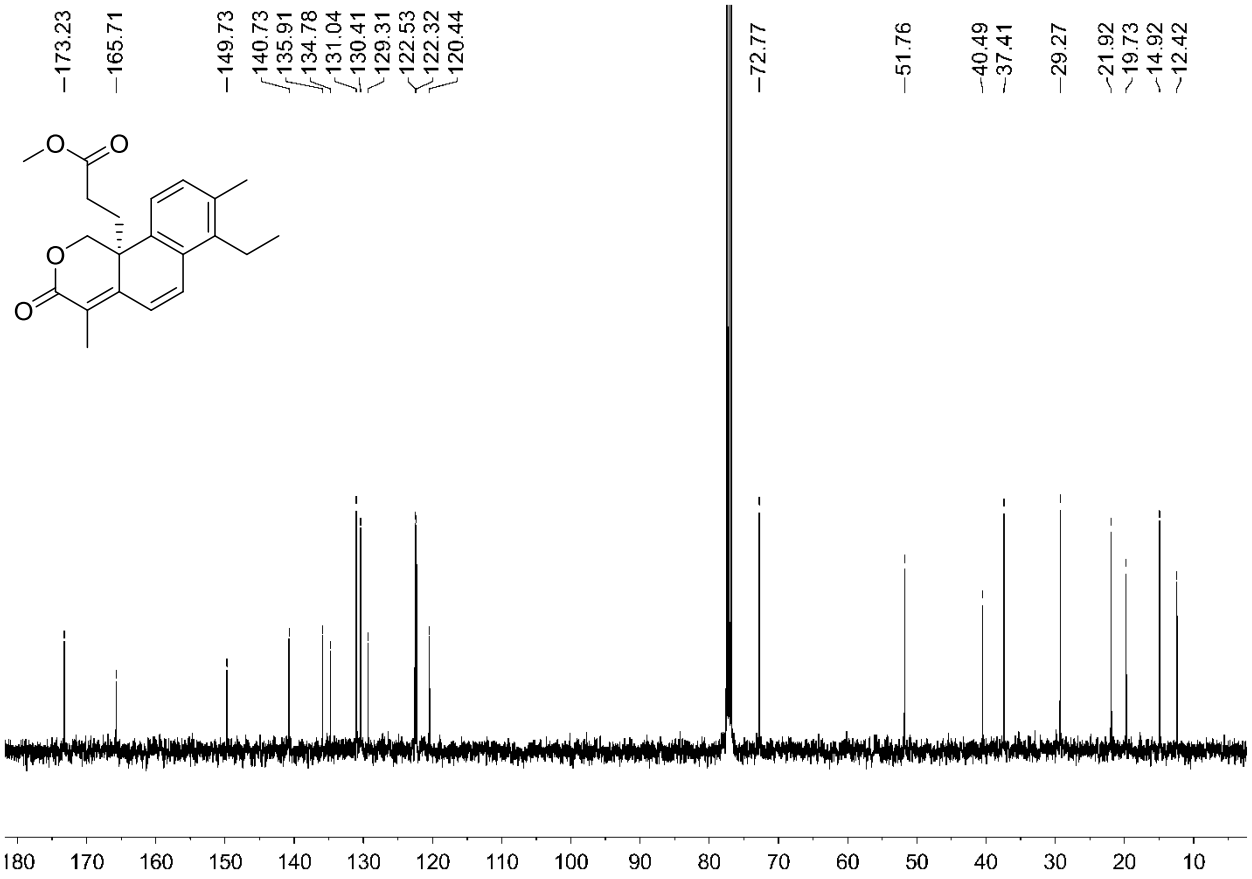

Fig. S86 ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of **4**

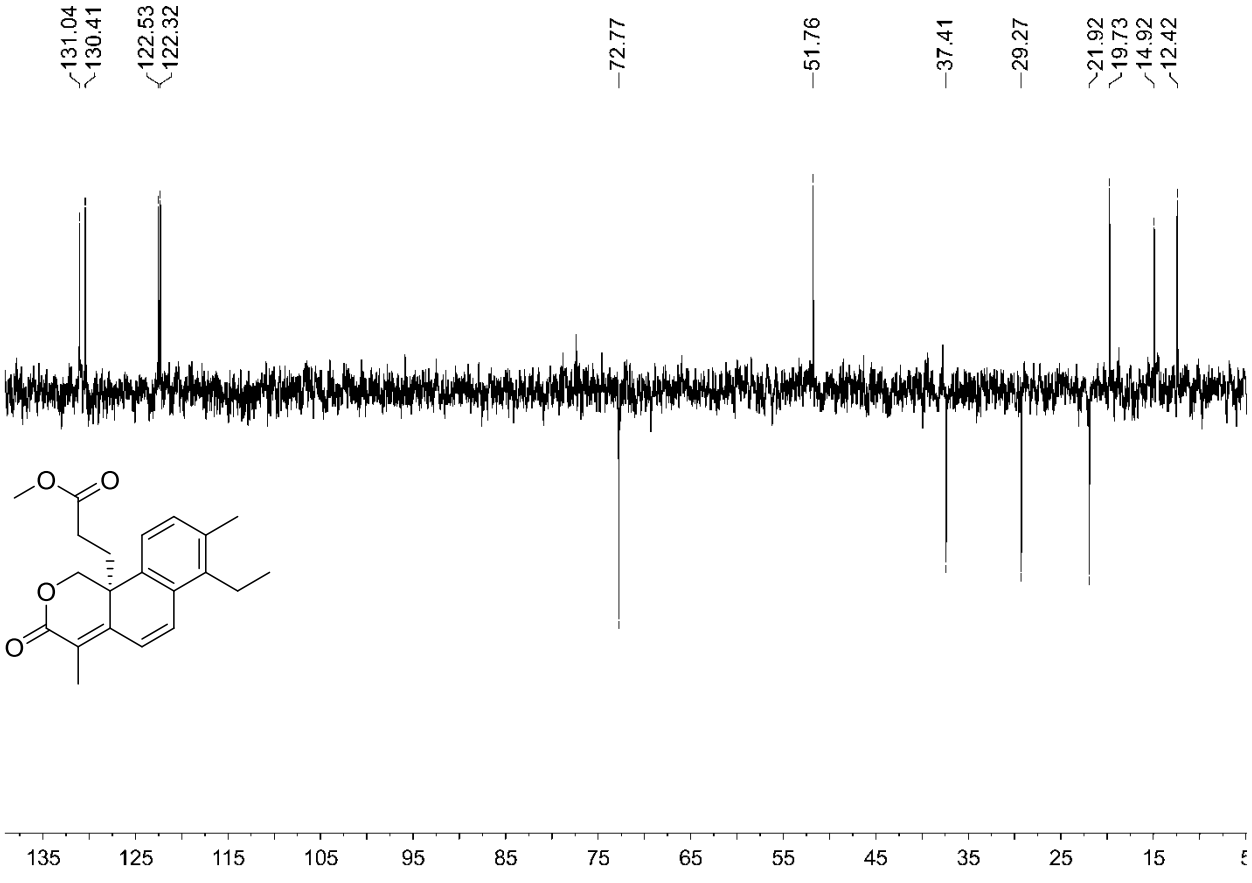

Fig. S87 DEPT135 (100 MHz, chloroform-*d*) spectrum of **4**

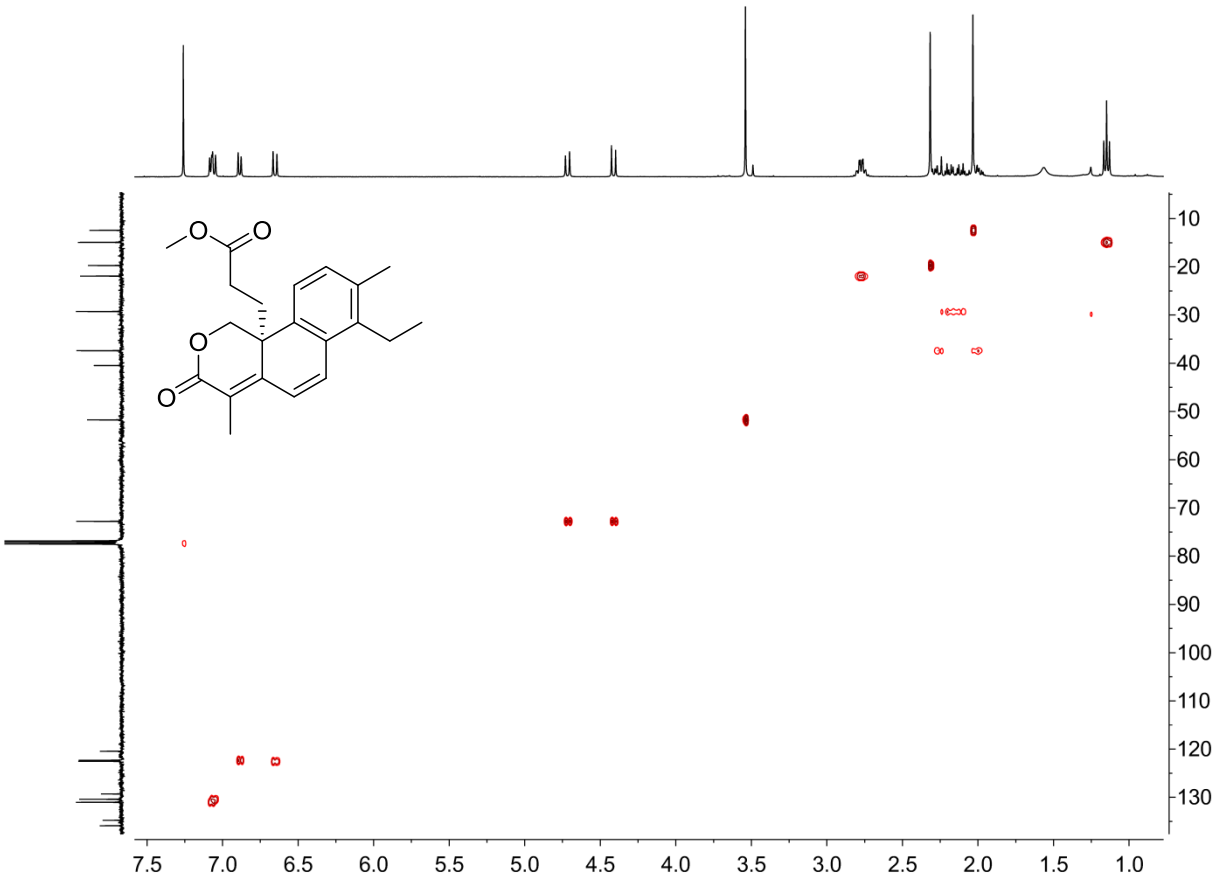

Fig. S88 HSQC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **4**

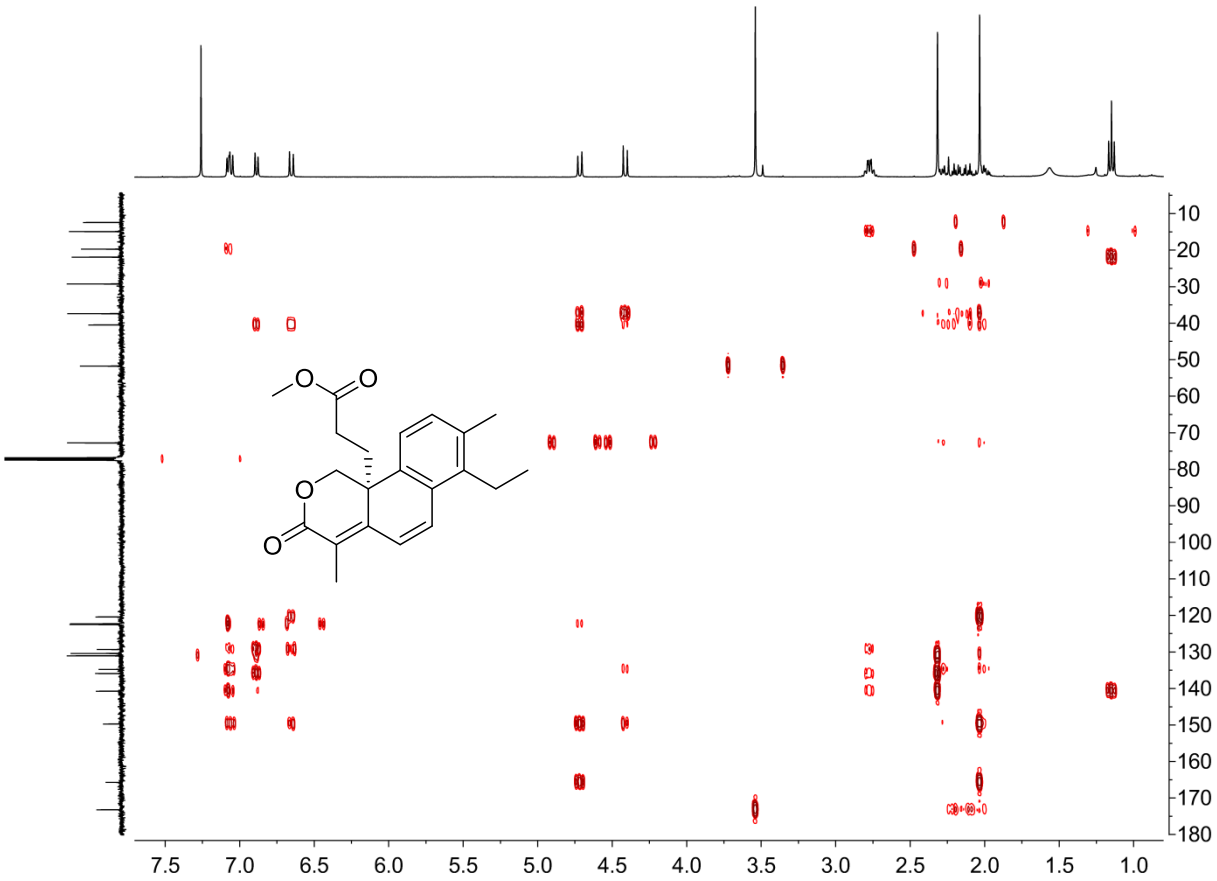

Fig. S89 HMBC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **4**

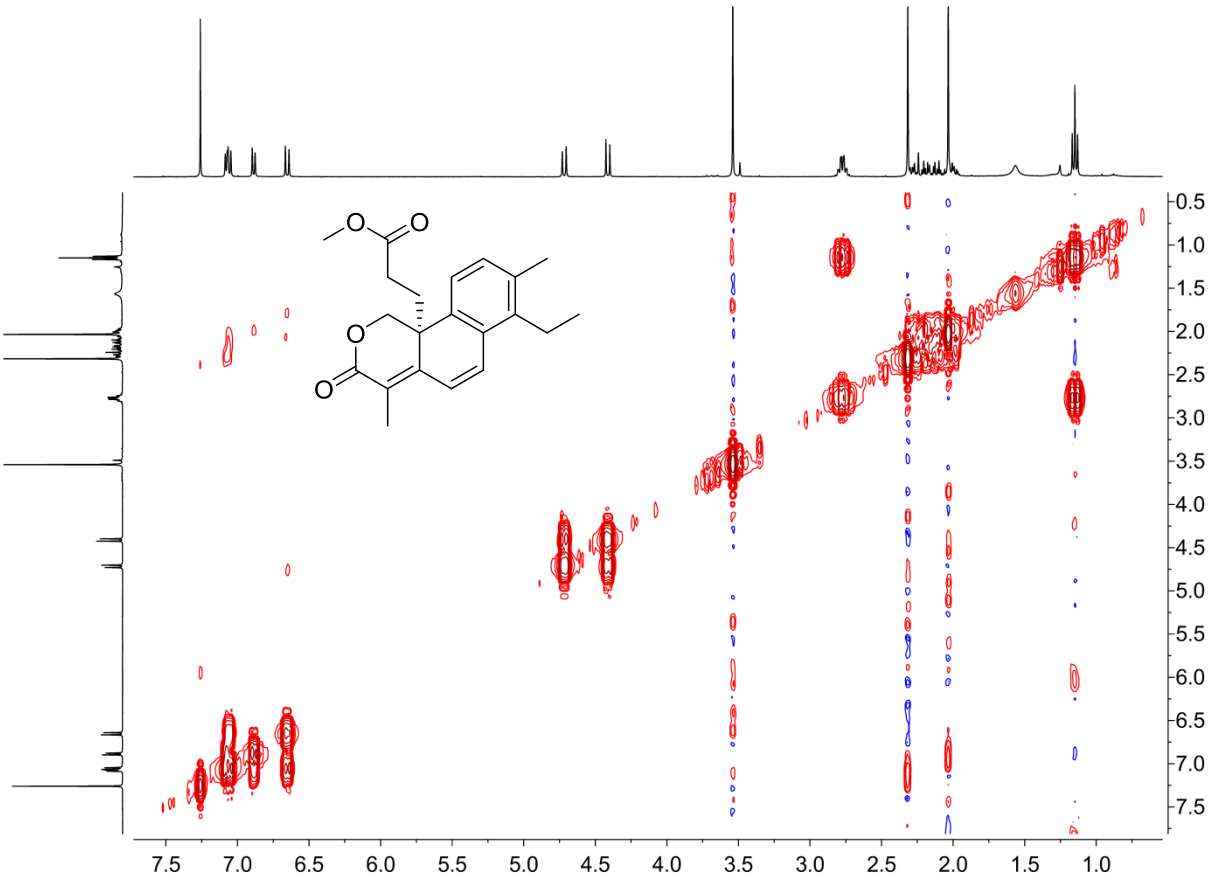

Fig. S90 $^{1}H-^{1}H$ COSY spectrum (400 MHz, chloroform-*d*) of **4**

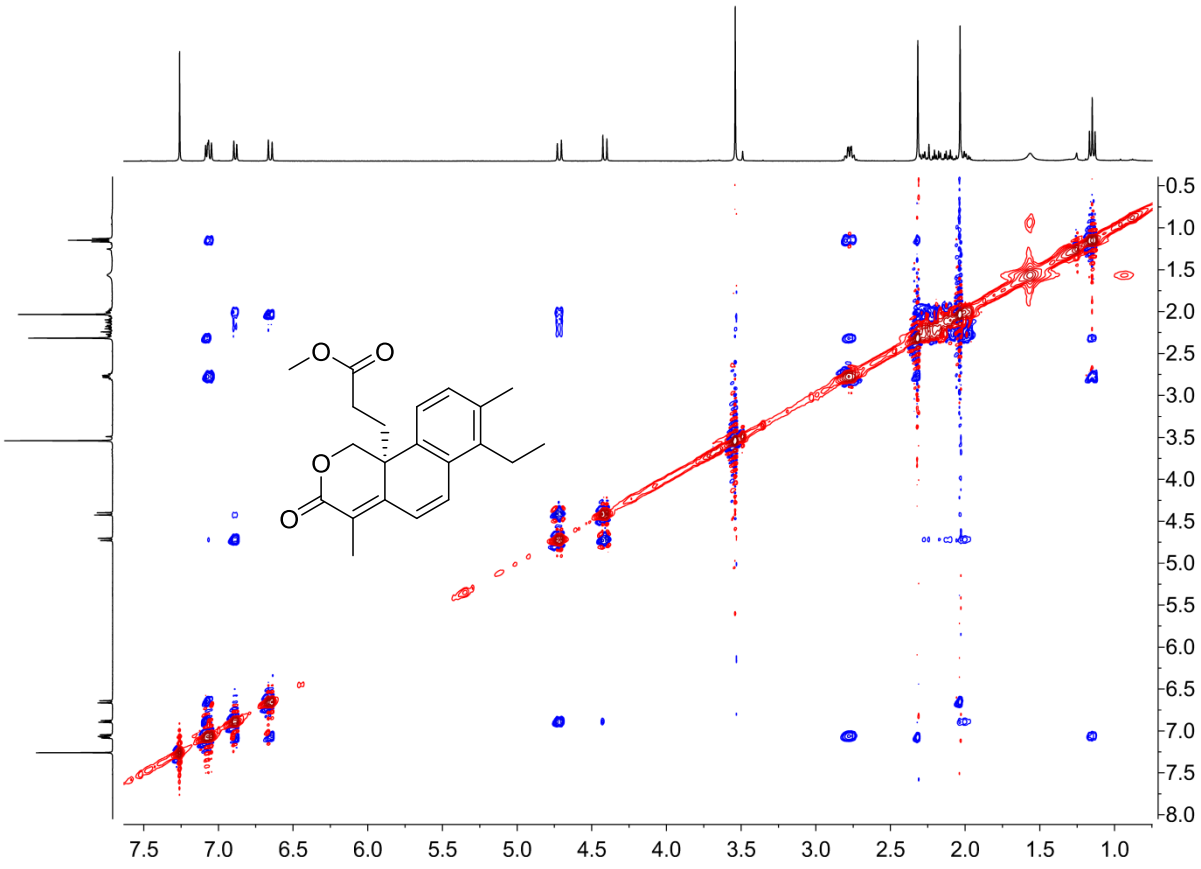

Fig. S91 NOESY spectrum (400 MHz, chloroform-*d*) of **4**

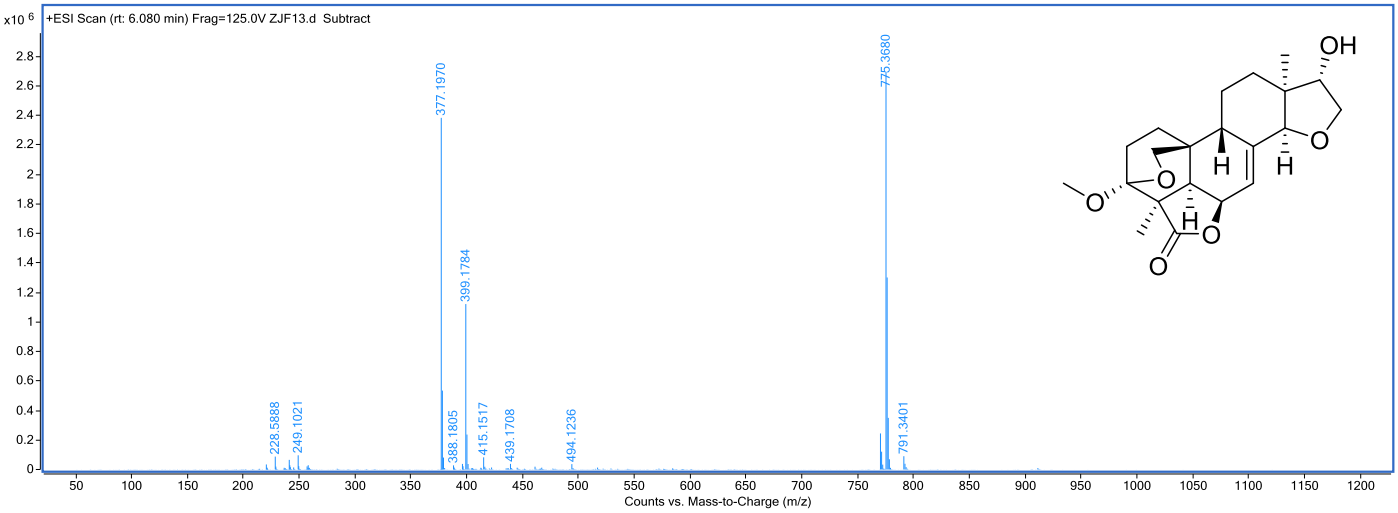

Fig. S92 HR-ESI-MS spectrum of **5**

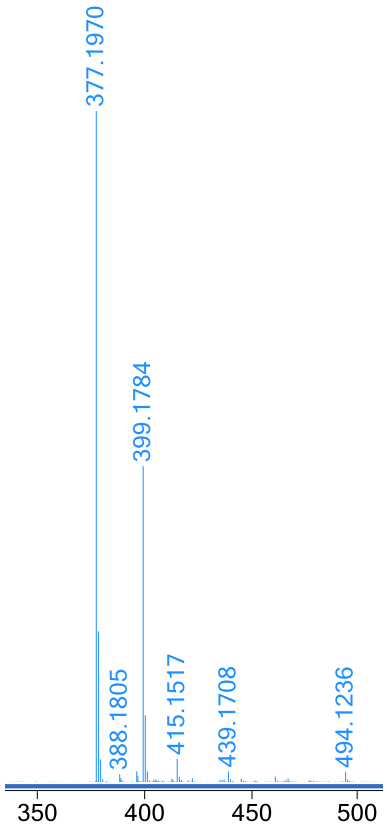

Fig. S93 HR-ESI-MS spectrum of **5** (amplified)

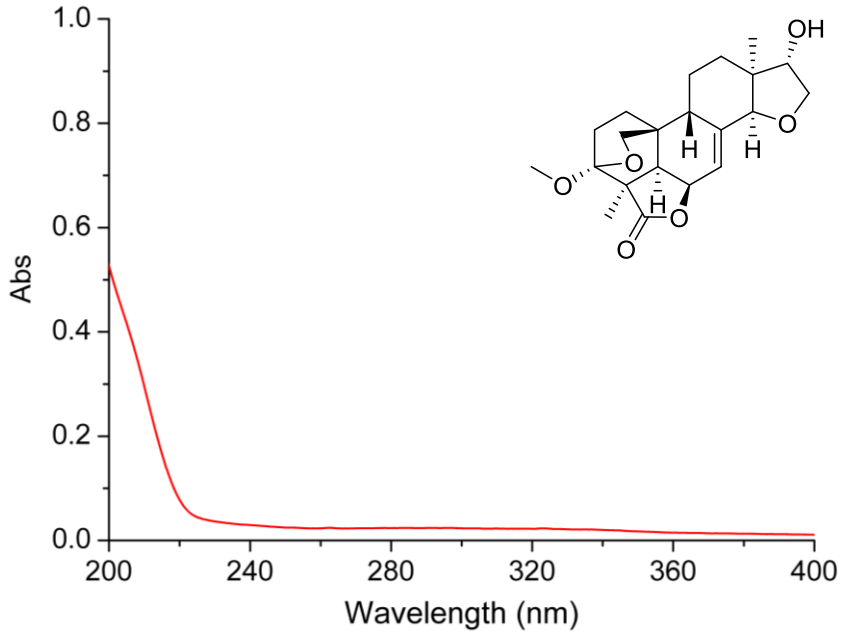

Fig. S94 UV spectrum of **5**

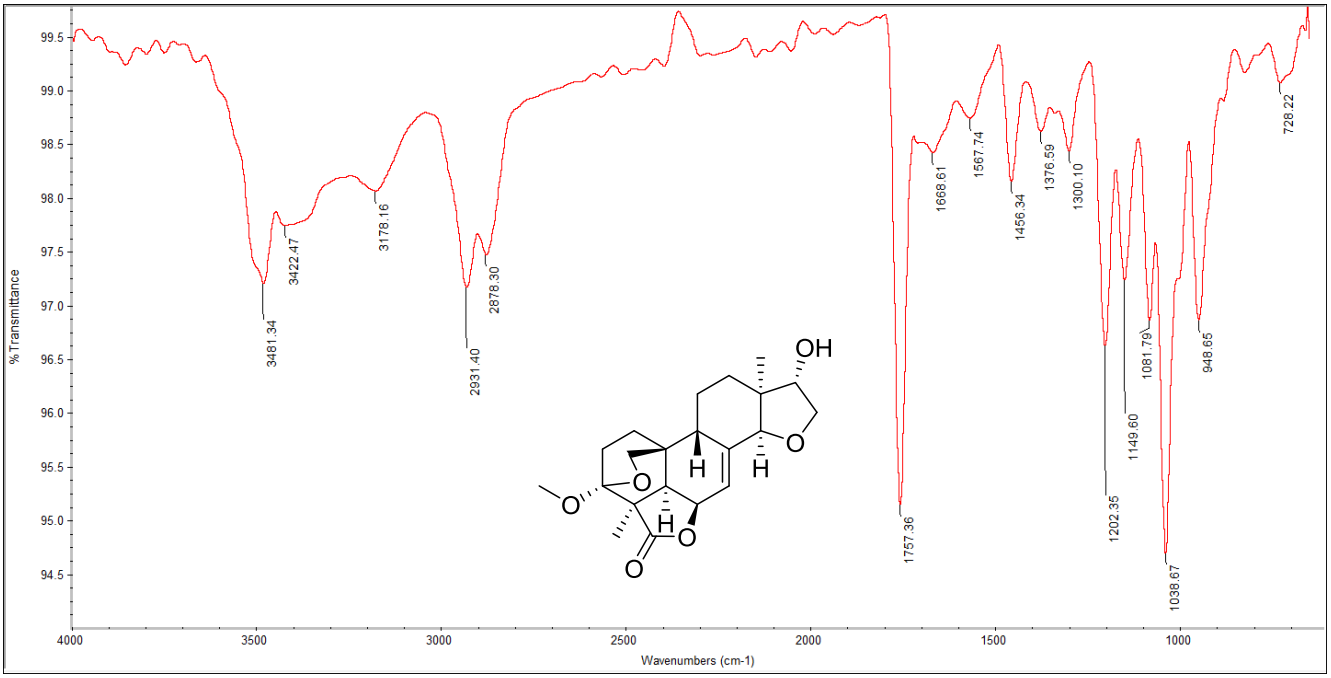

Fig. S95 IR spectrum of **5**

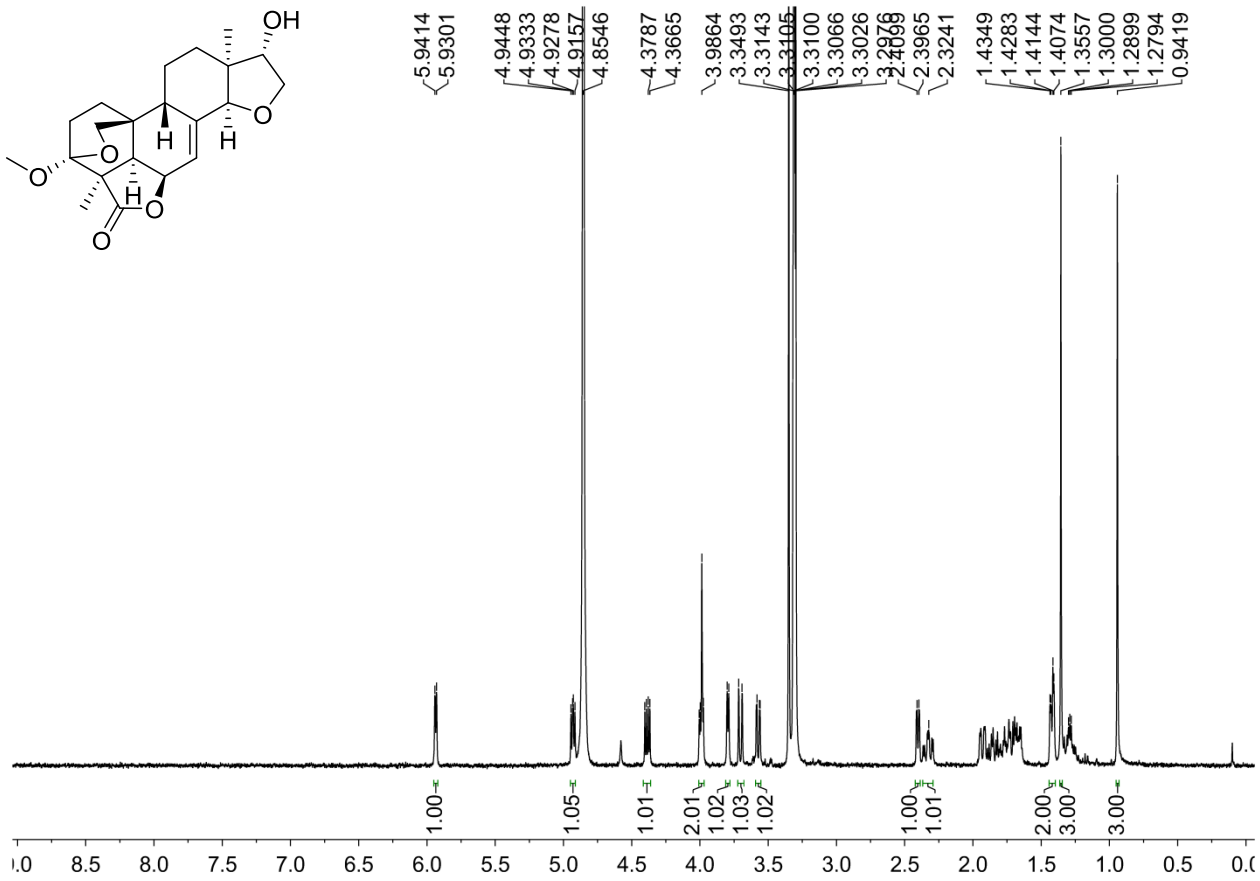

Fig. S96 ^{1}H NMR (400 MHz, methanol-d_4) spectrum of **5**

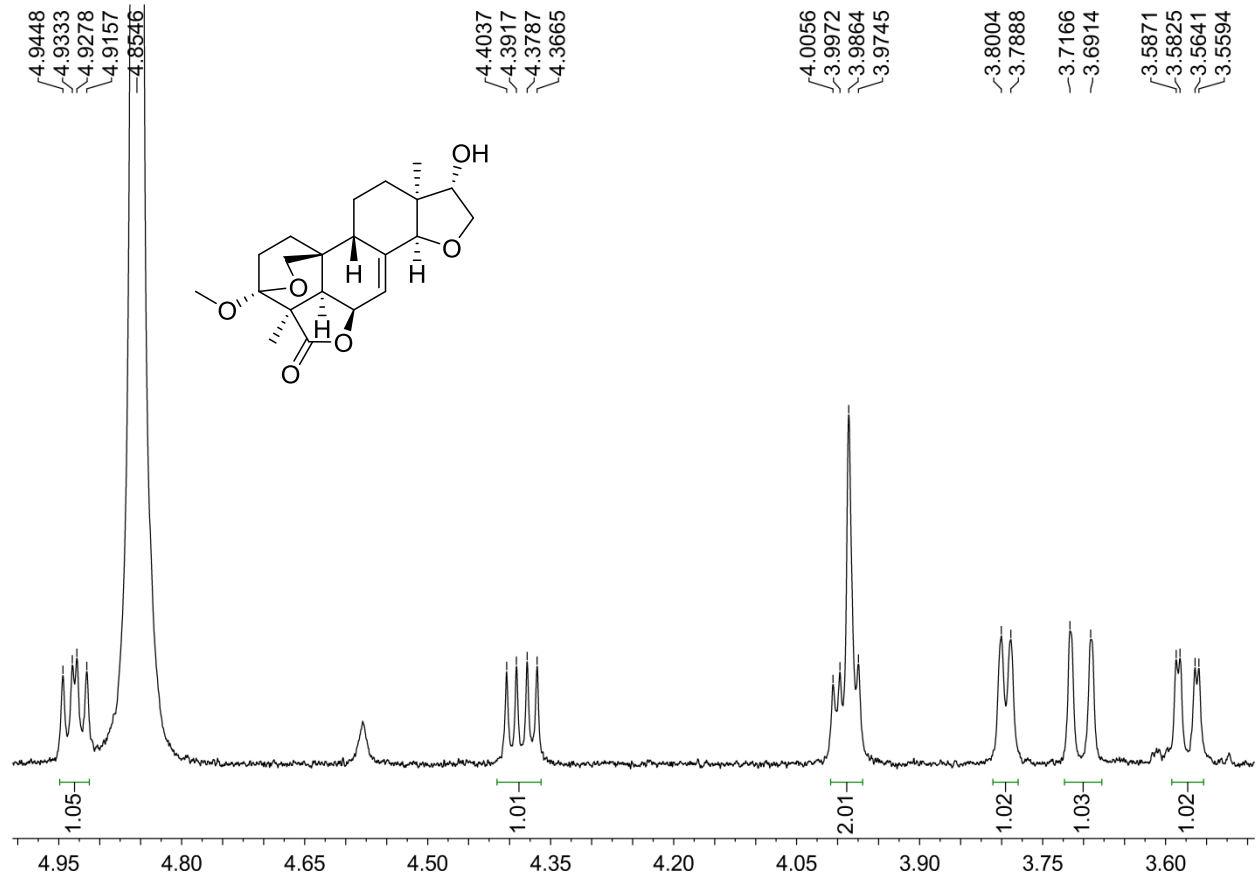

Fig. S97 ^{1}H NMR (400 MHz, methanol-d_4) spectrum of **5** (amplified)

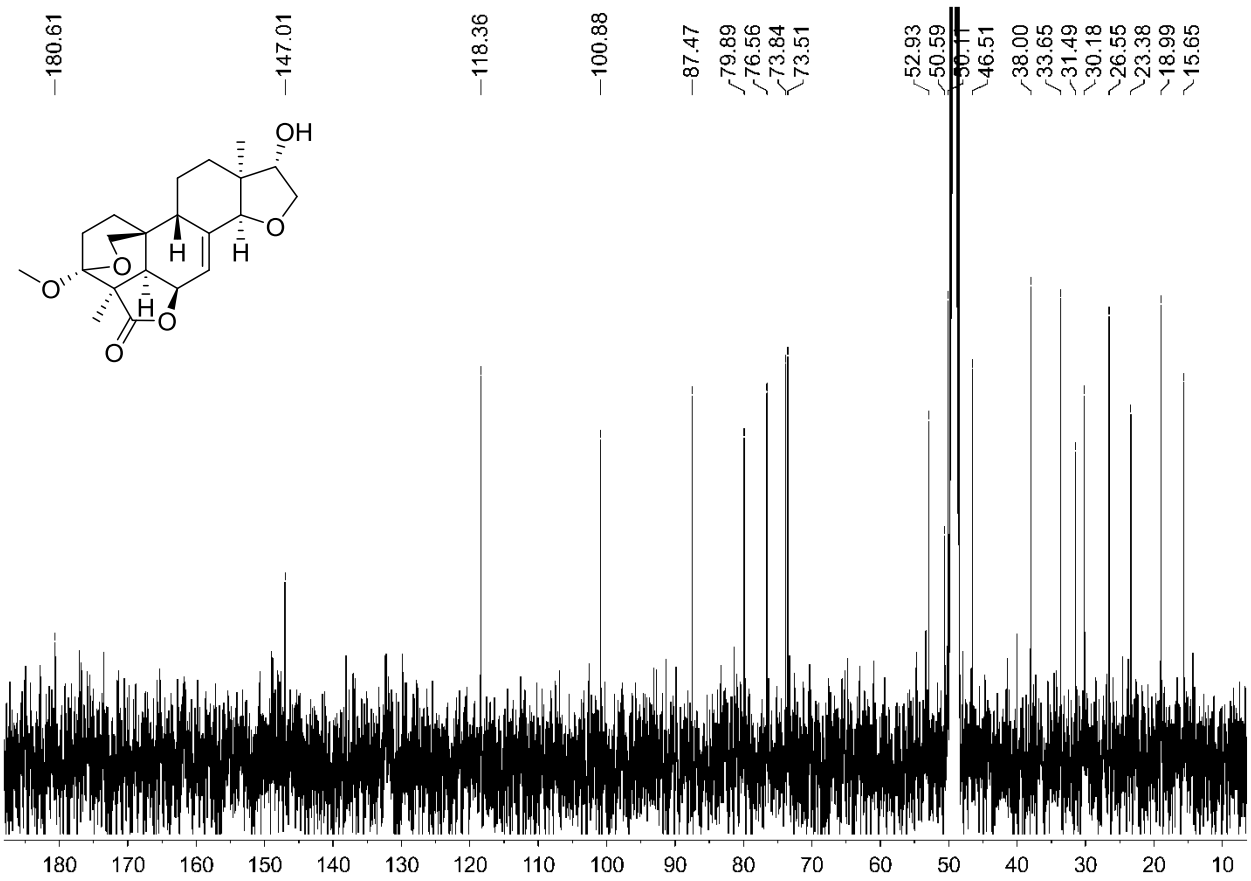

Fig. S98 ^{13}C NMR (100 MHz, methanol-d_4) spectrum of **5**

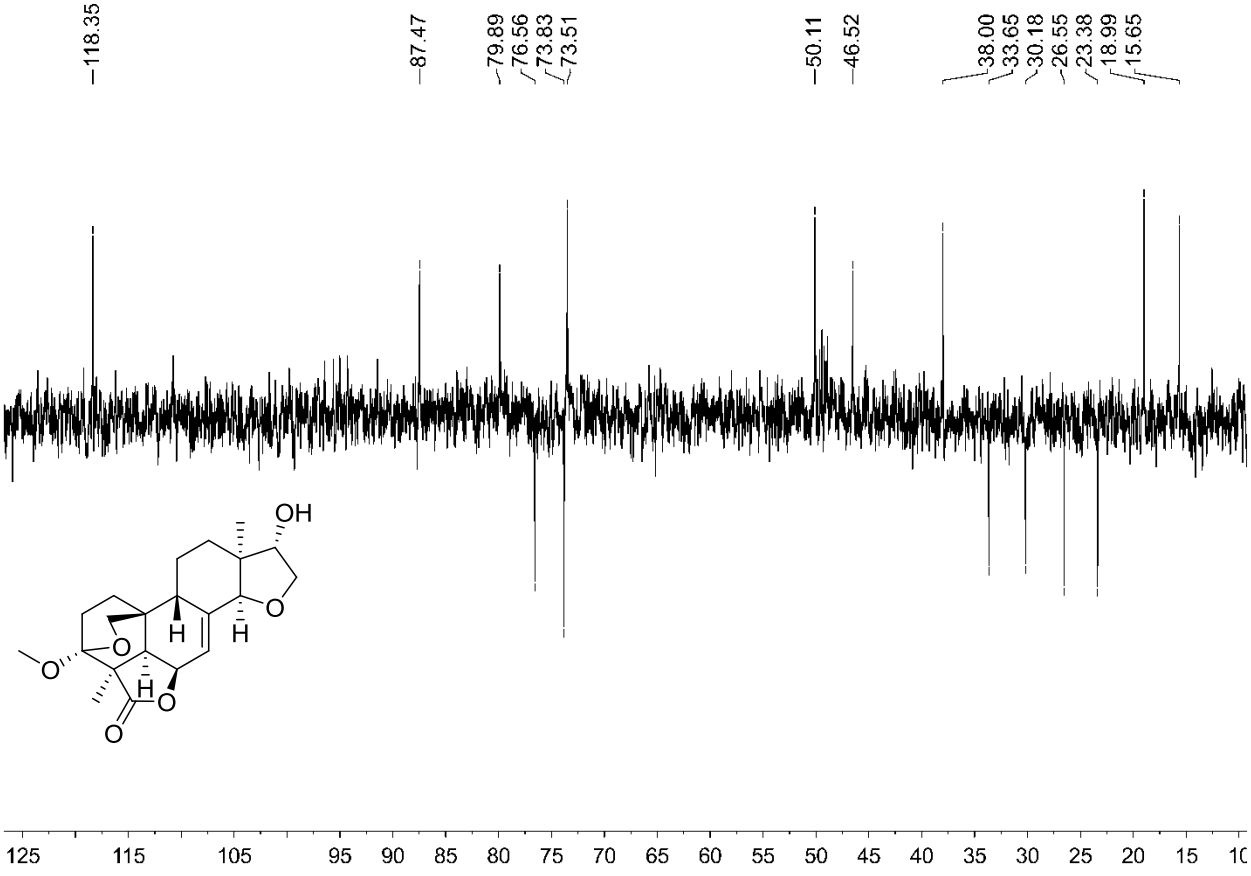

Fig. S99 DEPT135 (100 MHz, methanol-d_4) spectrum of **5**

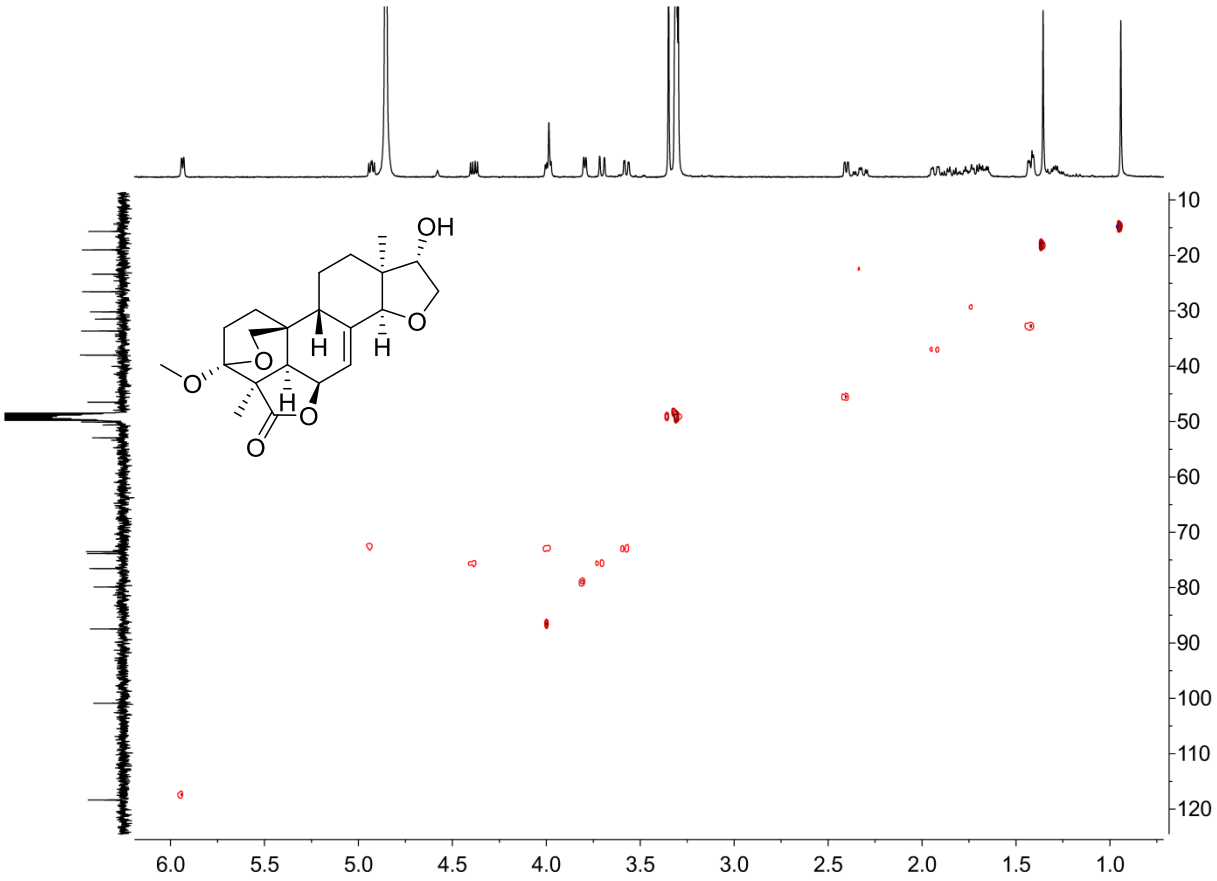

Fig. S100 HSQC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, methanol-d_4) of **5**

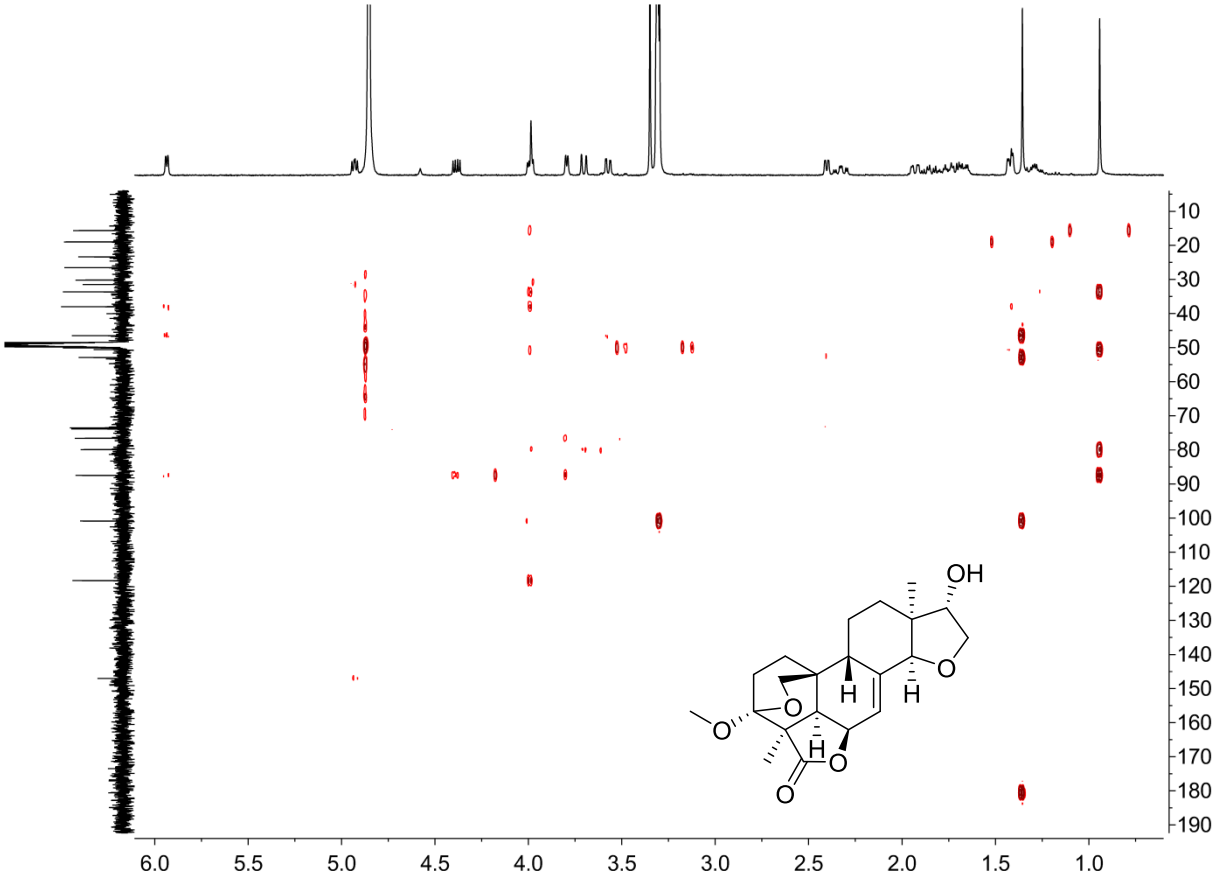

Fig. S101 HMBC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, methanol-d_4) of **5**

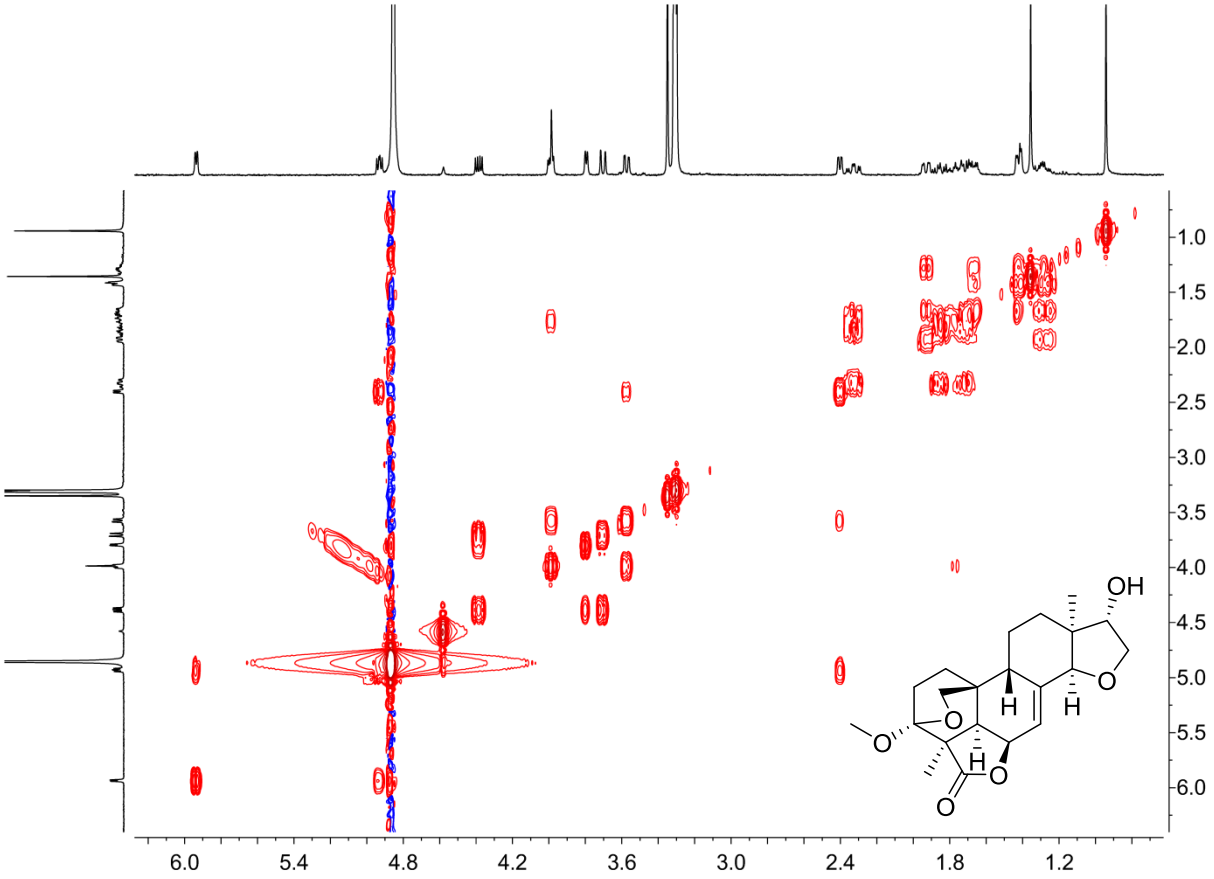

Fig. S102 ^{1}H–^{1}H COSY spectrum (400 MHz, methanol-d_4) of **5**

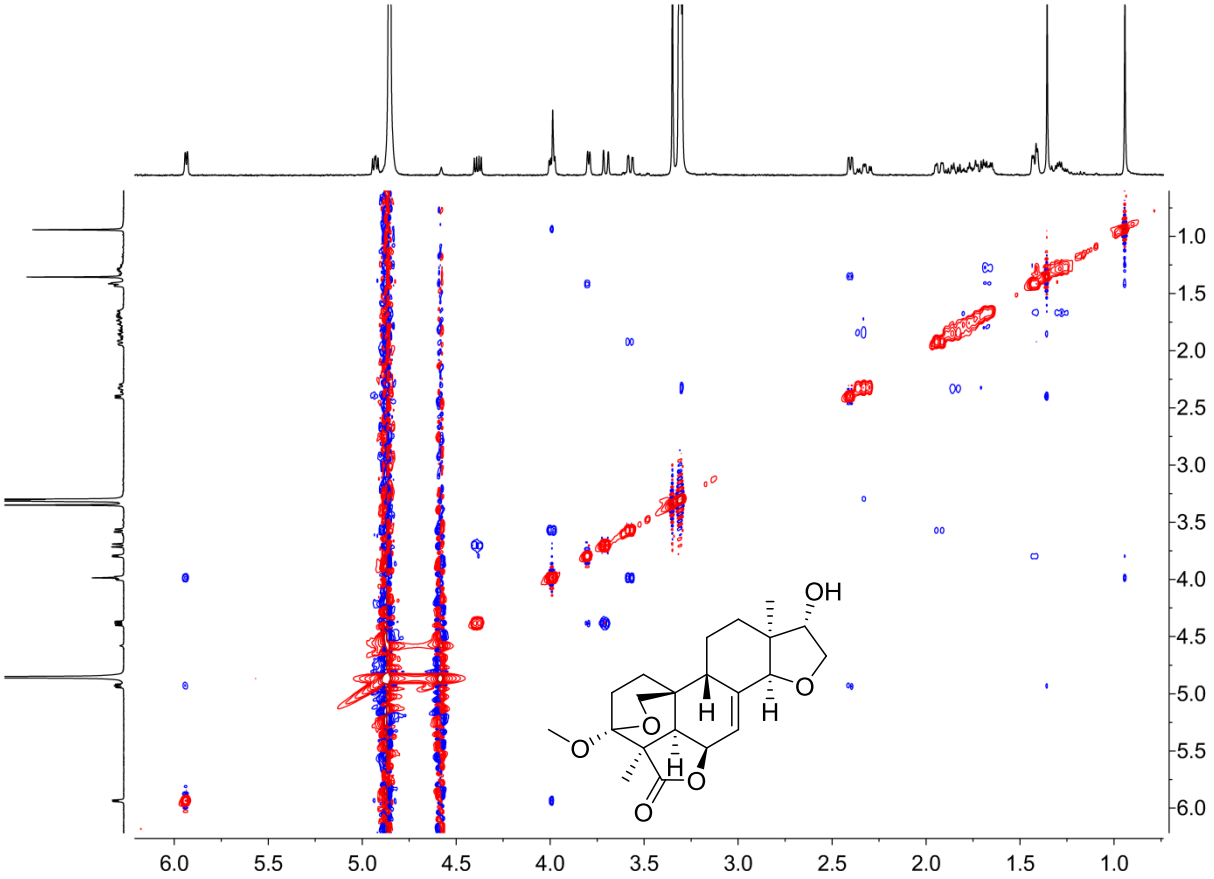

Fig. S103 NOESY spectrum (400 MHz, methanol-d_4) of **5**

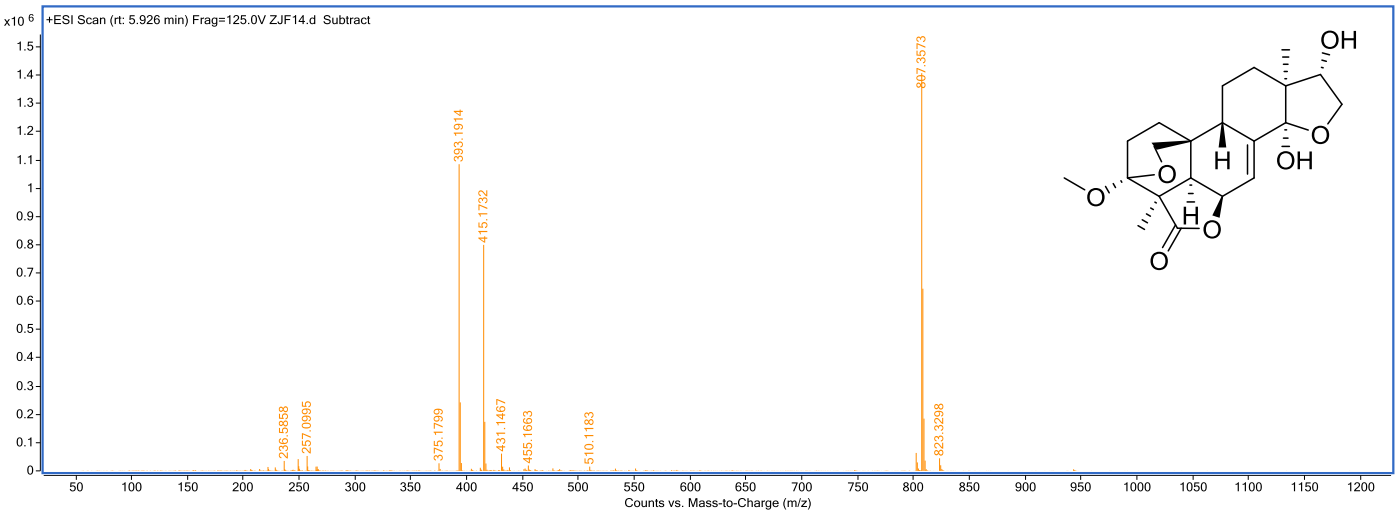

Fig. S104 HR-ESI-MS spectrum of **6**

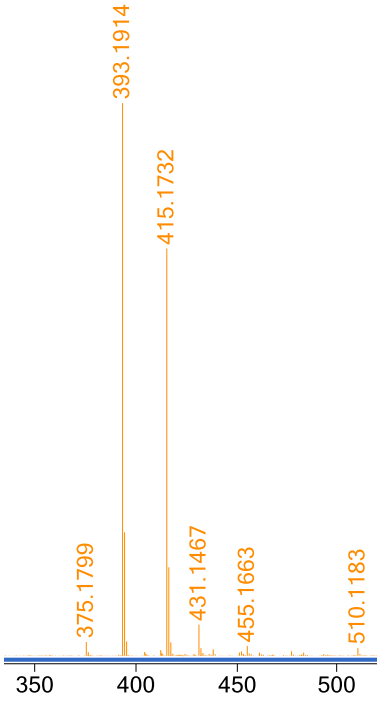

Fig. S105 HR-ESI-MS spectrum of **6** (amplified)

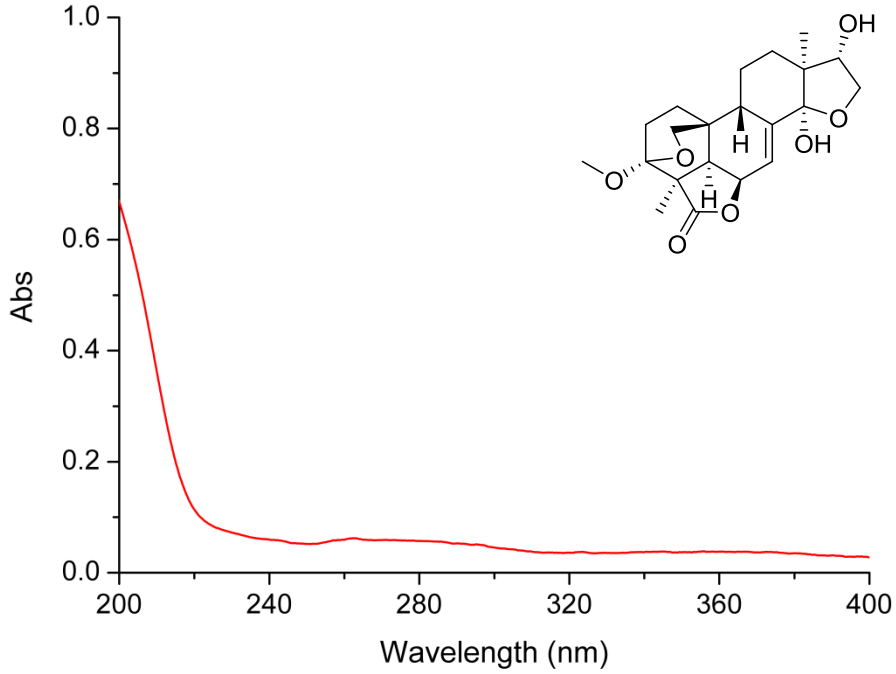

Fig. S106 UV spectrum of **6**

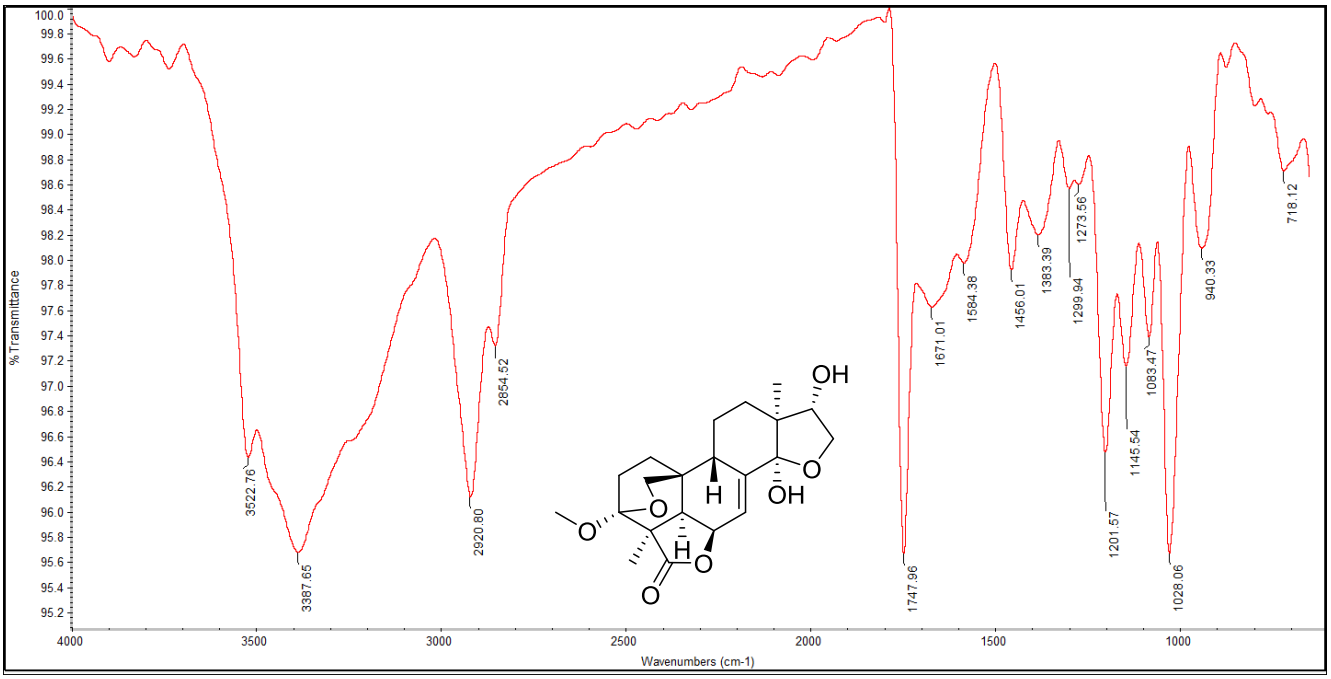

Fig. S107 IR spectrum of **6**

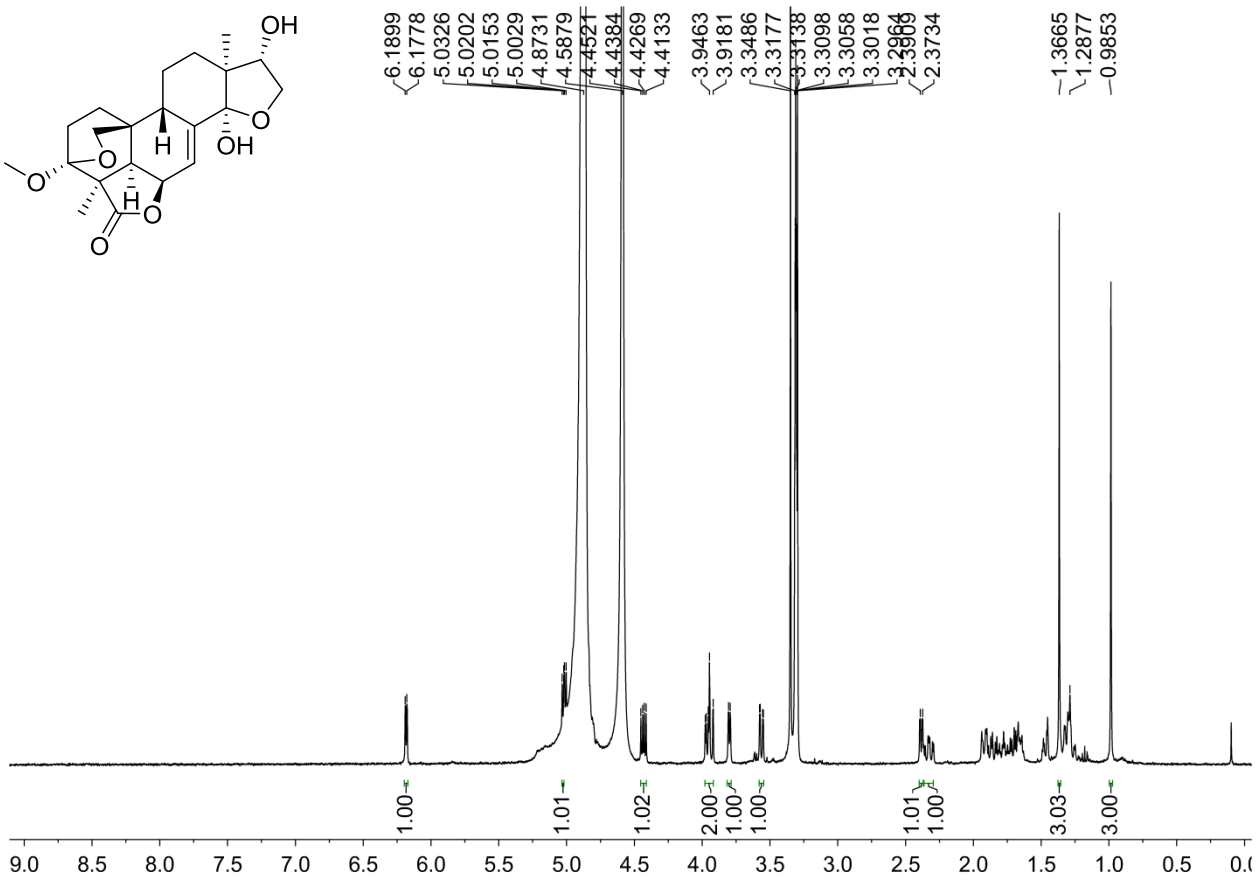

Fig. S108 ^{1}H NMR (400 MHz, methanol-d_4) spectrum of **6**

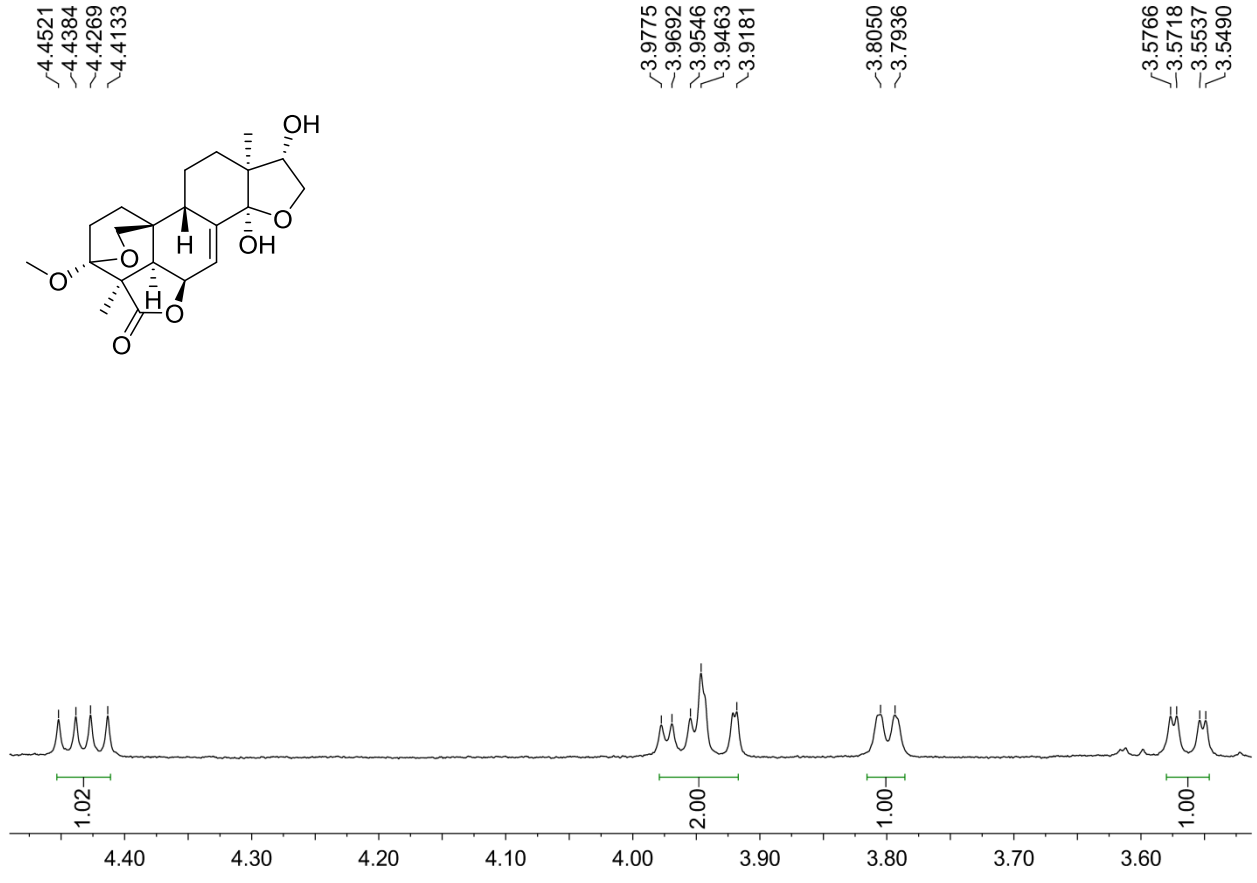

Fig. S109 ^{1}H NMR (400 MHz, methanol-d_4) spectrum of **6** (amplified)

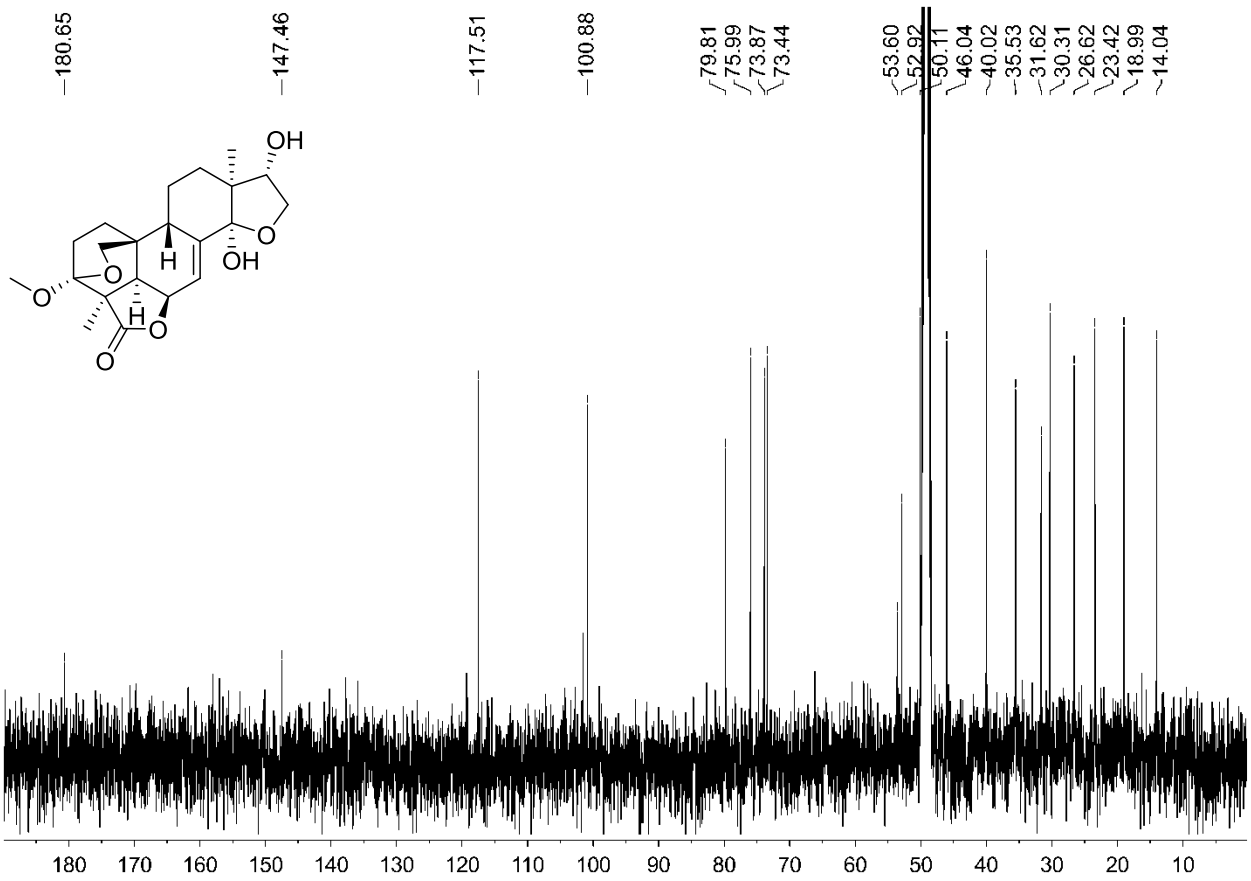

Fig. S110 ^{13}C NMR (100 MHz, methanol-d_4) spectrum of **6**

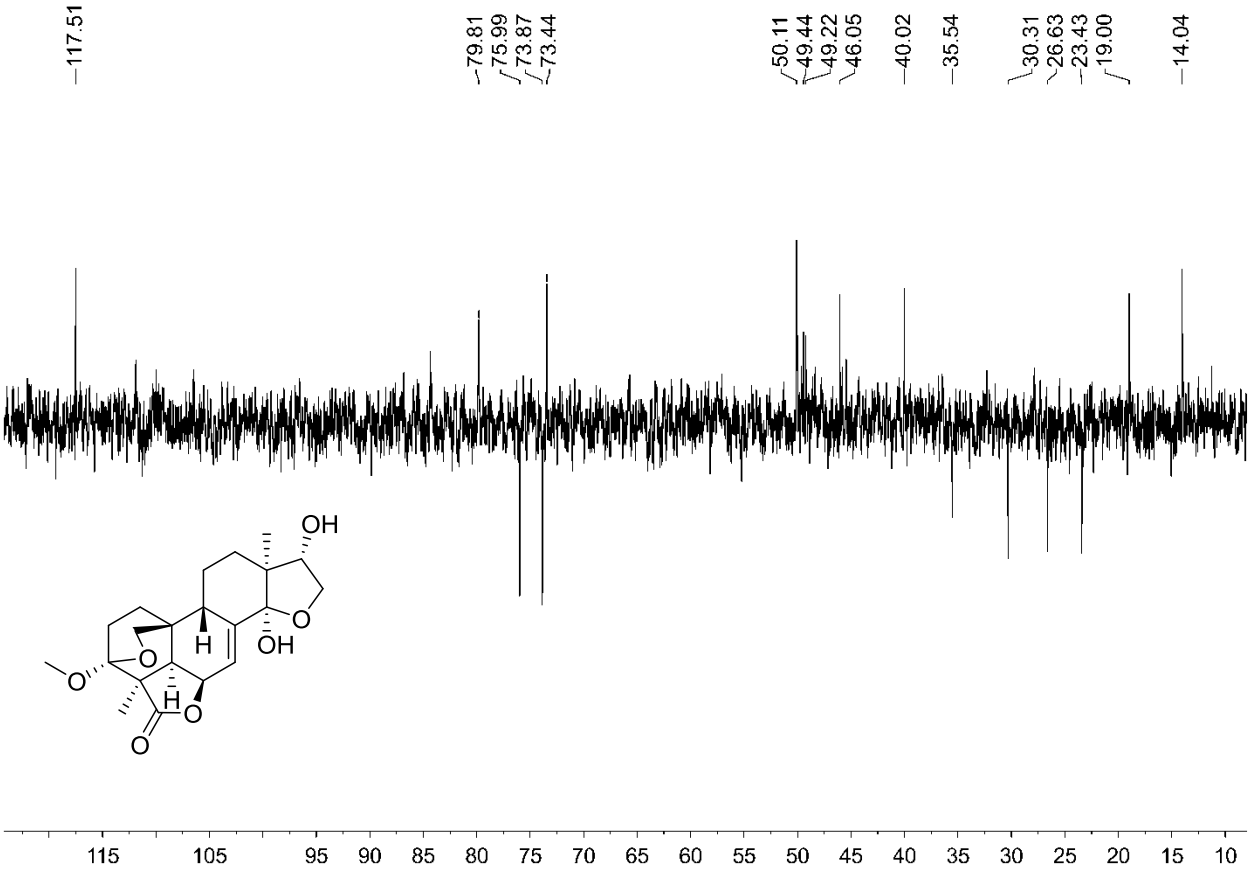

Fig. S111 DEPT135 (100 MHz, methanol-d_4) spectrum of **6**

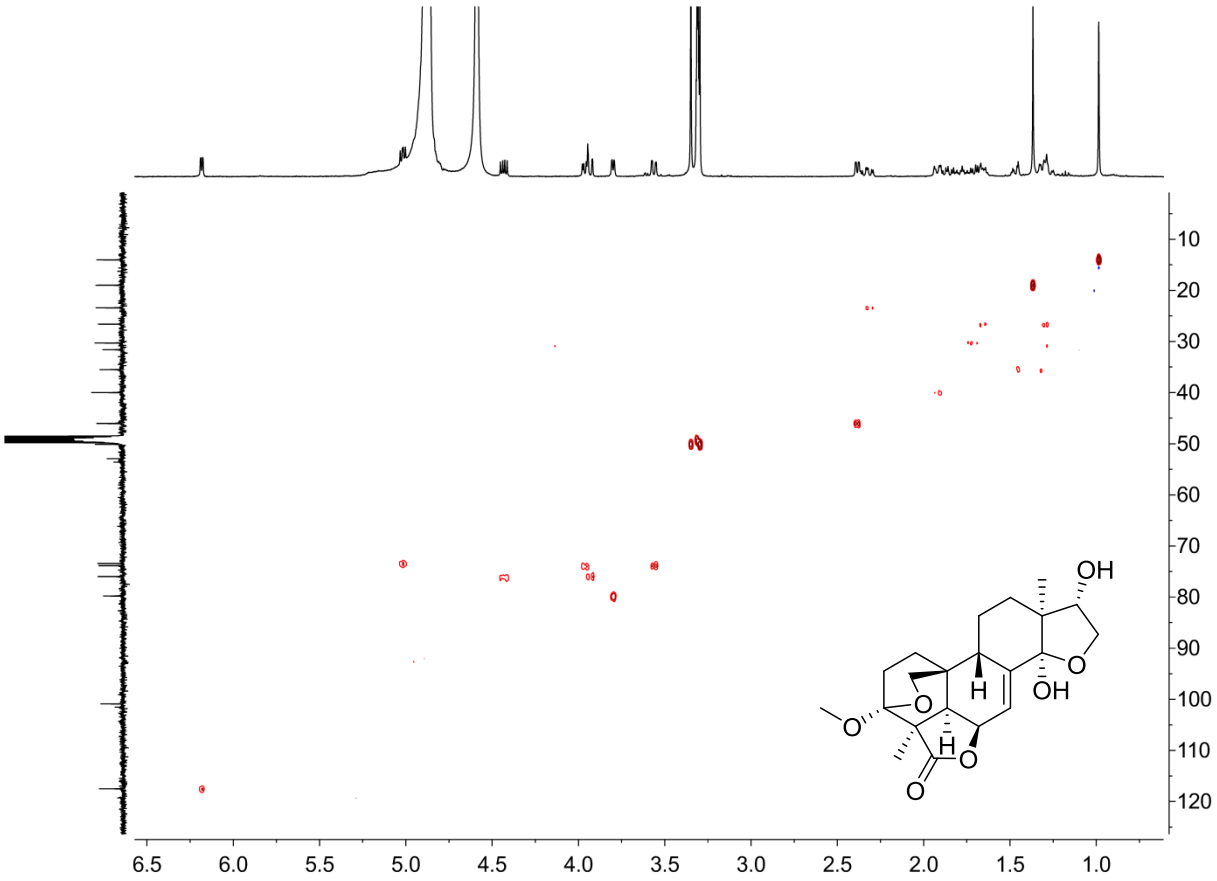

Fig. S112 HSQC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, methanol-d_4) of **6**

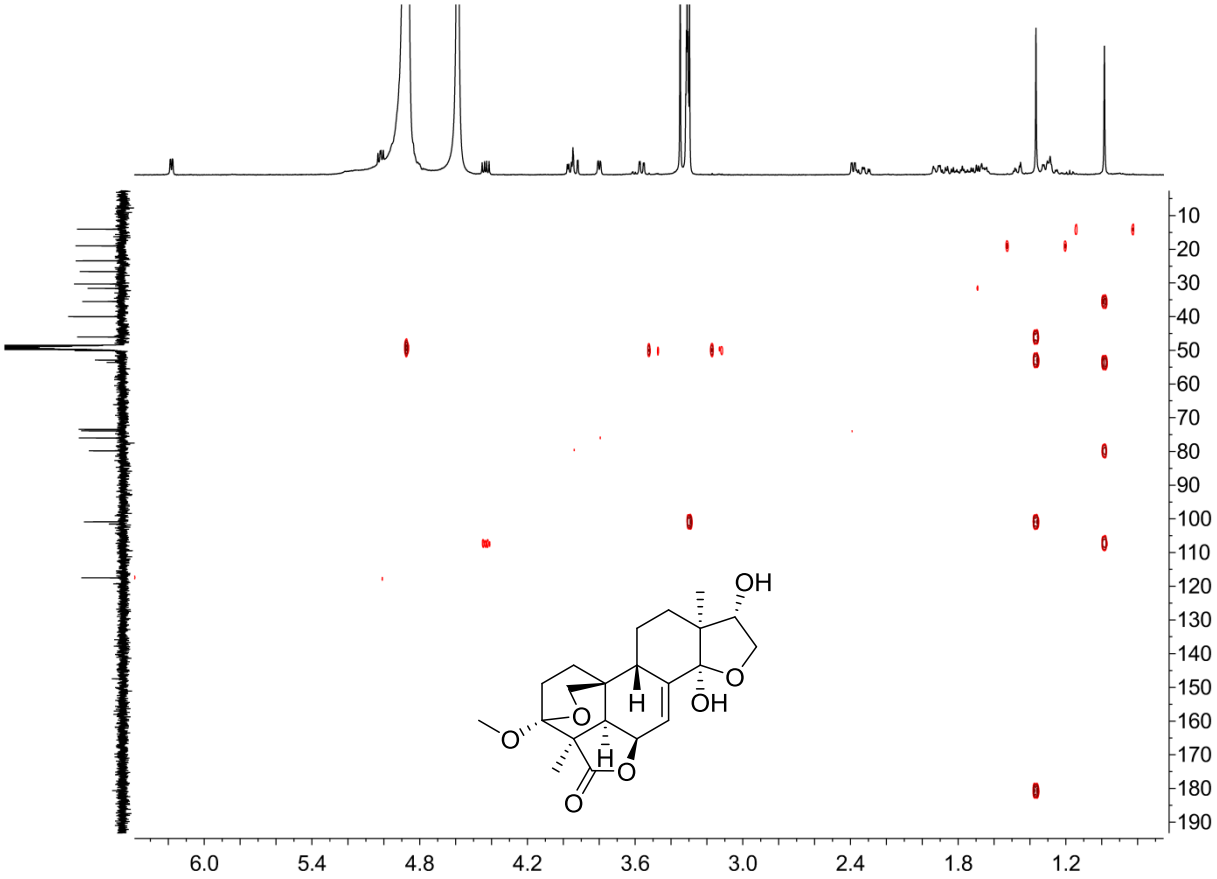

Fig. S113 HMBC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, methanol-d_4) of **6**

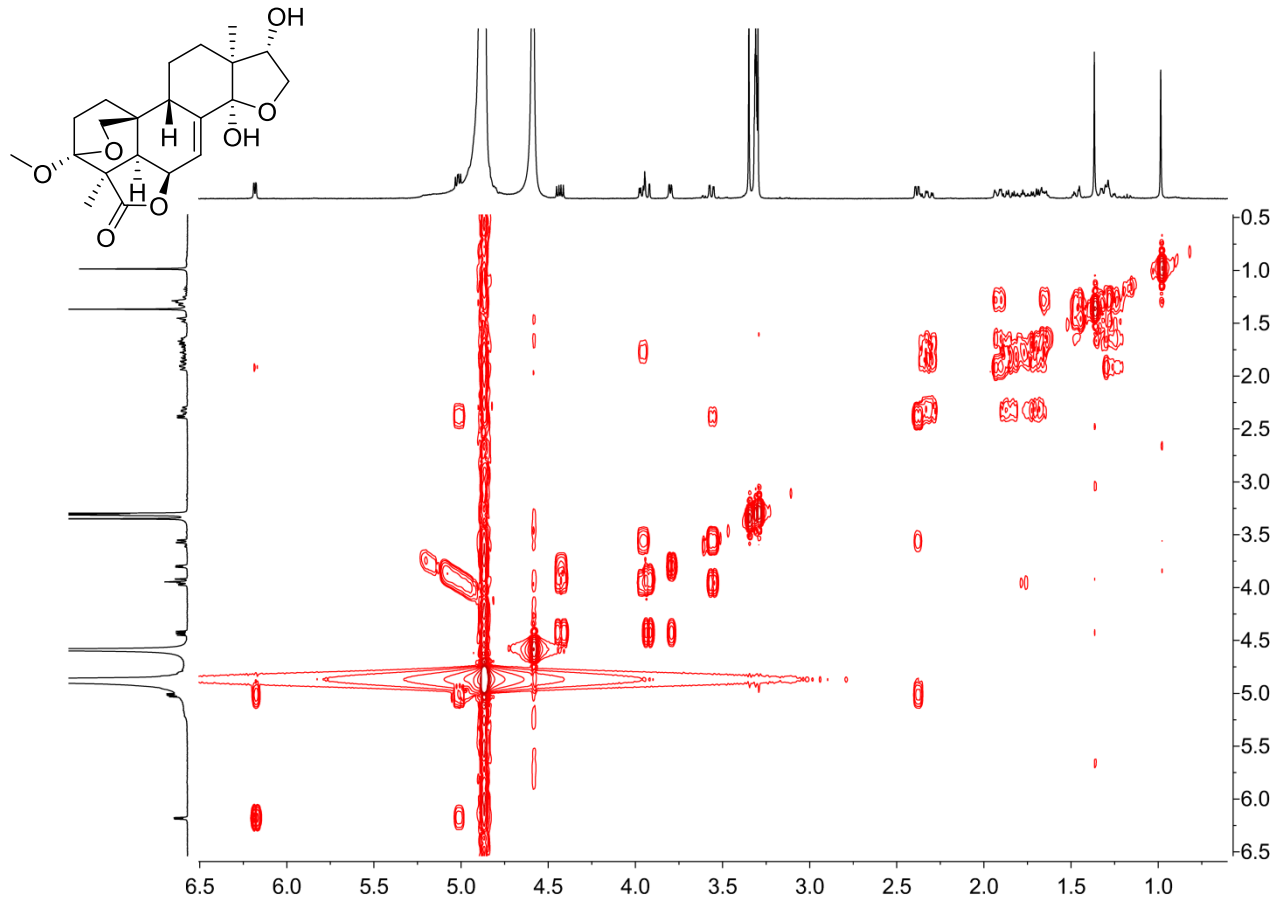

Fig. S114 ^{1}H–^{1}H COSY spectrum (400 MHz, methanol-d_4) of **6**

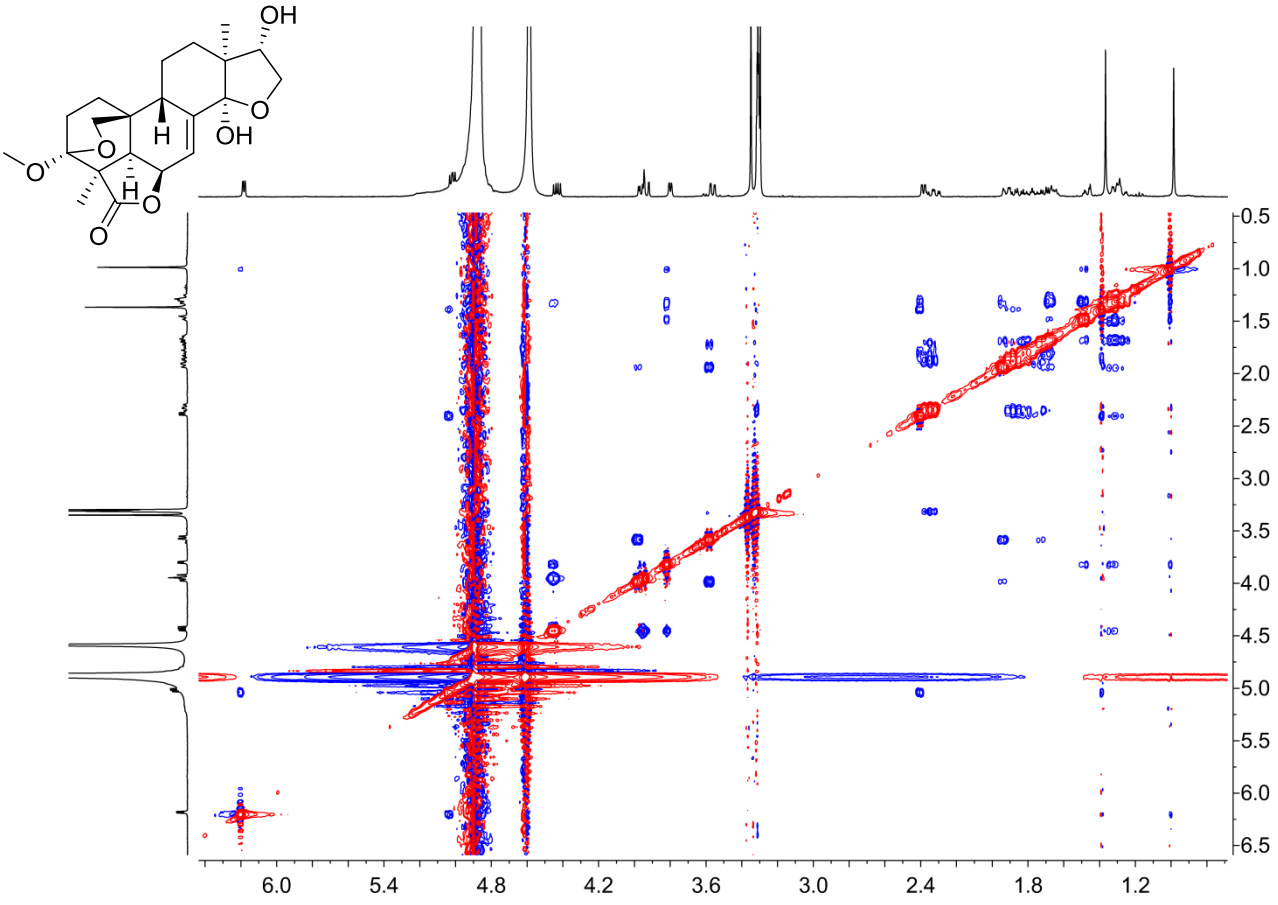

Fig. S115 NOESY spectrum (400 MHz, methanol-d_4) of **6**

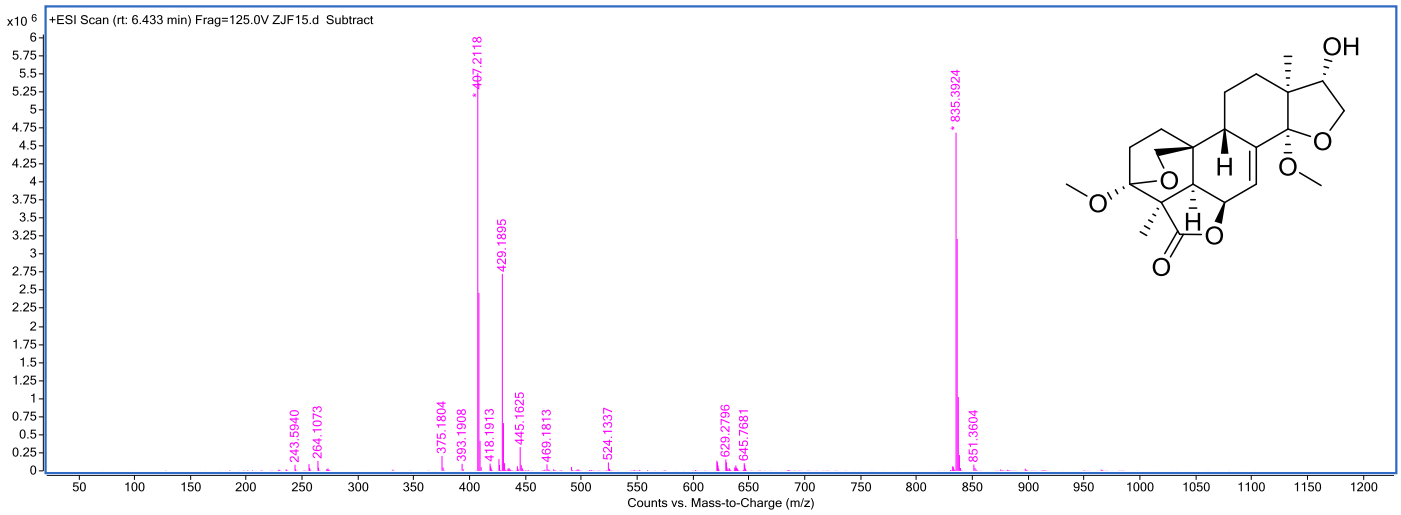

Fig. S116 HR-ESI-MS spectrum of **7**

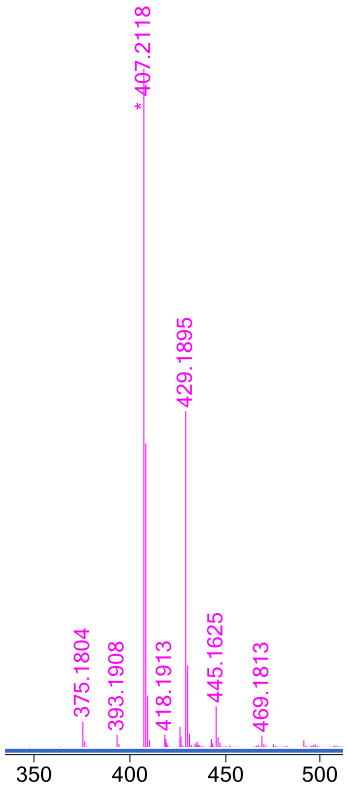

Fig. S117 HR-ESI-MS spectrum of **7** (amplified)

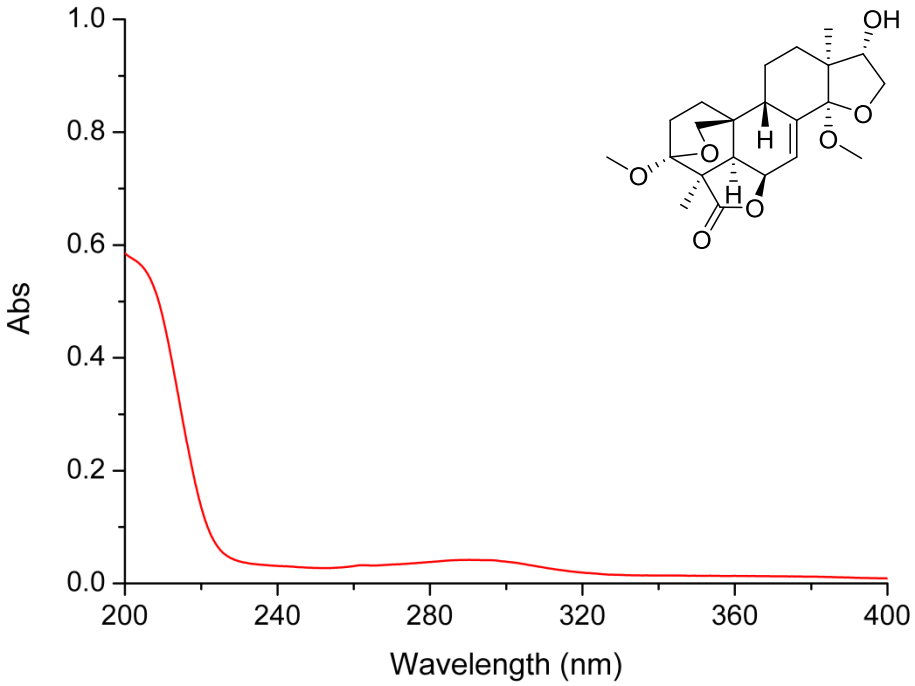

Fig. S118 UV spectrum of **7**

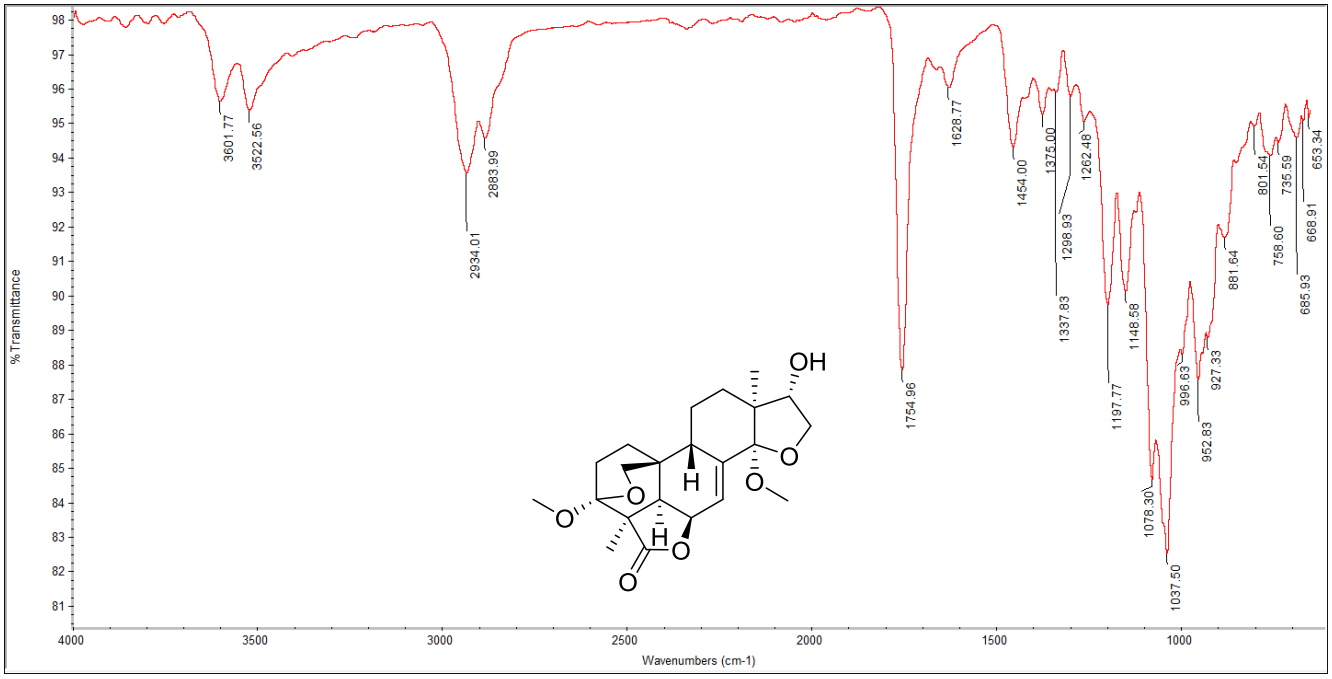

Fig. S119 IR spectrum of **7**

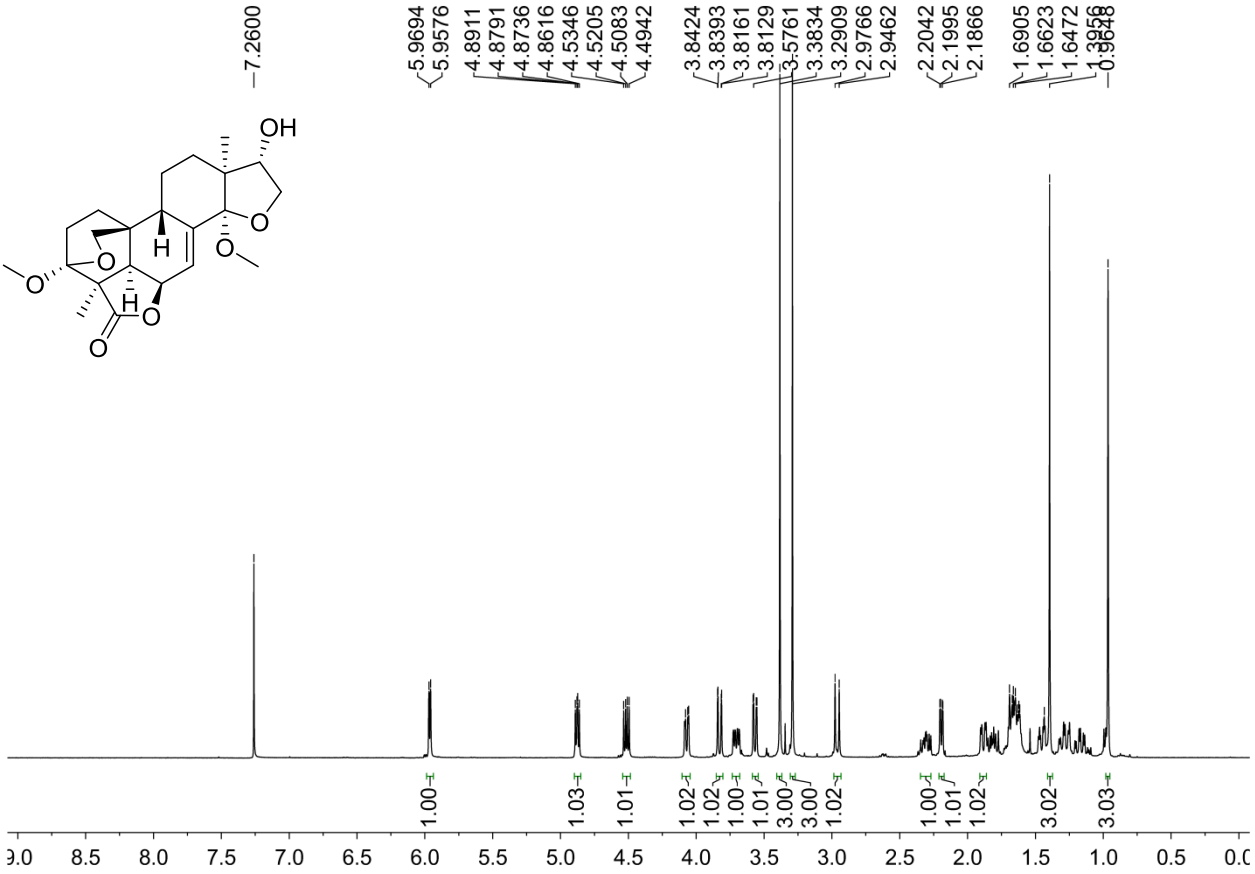

Fig. S120 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **7**

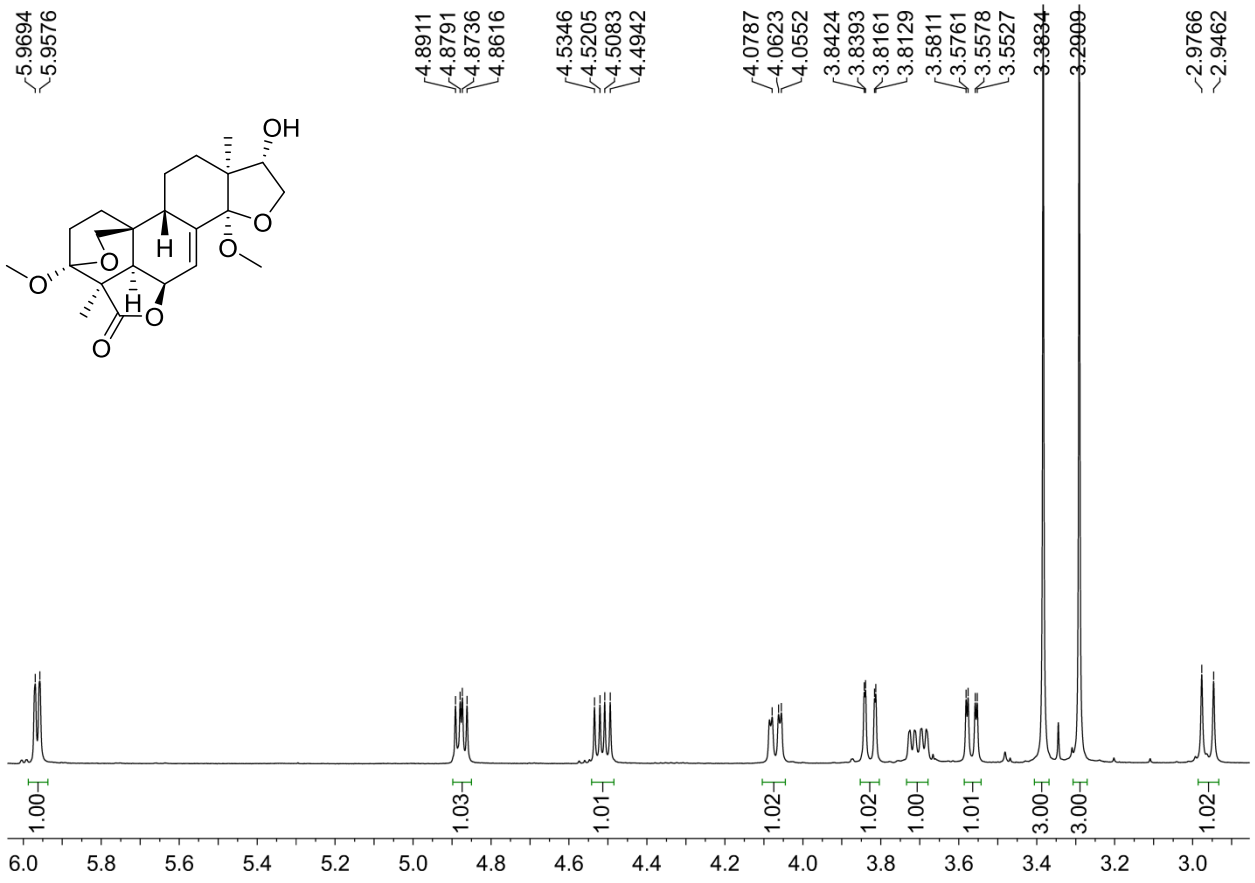

Fig. S121 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **7** (amplified)

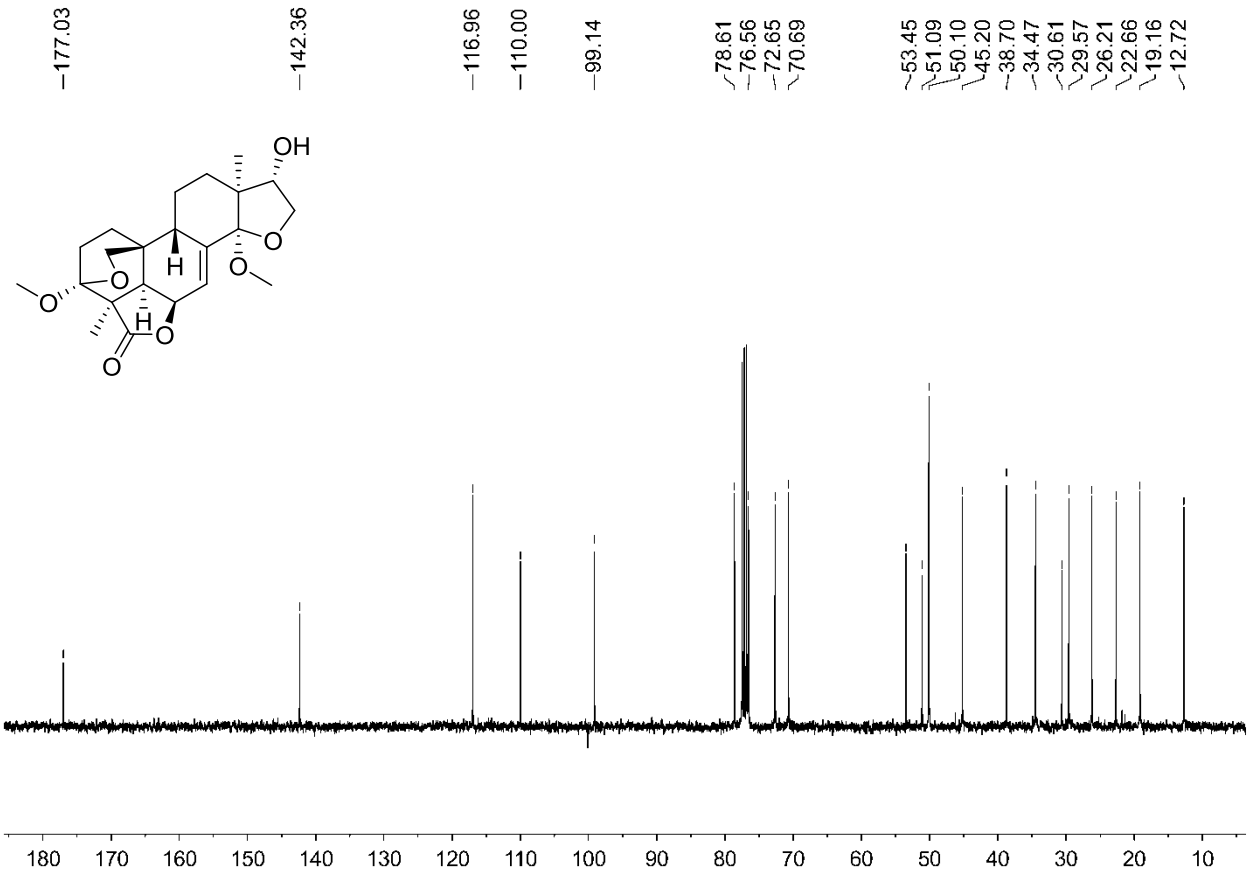

Fig. S122 ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of **7**.

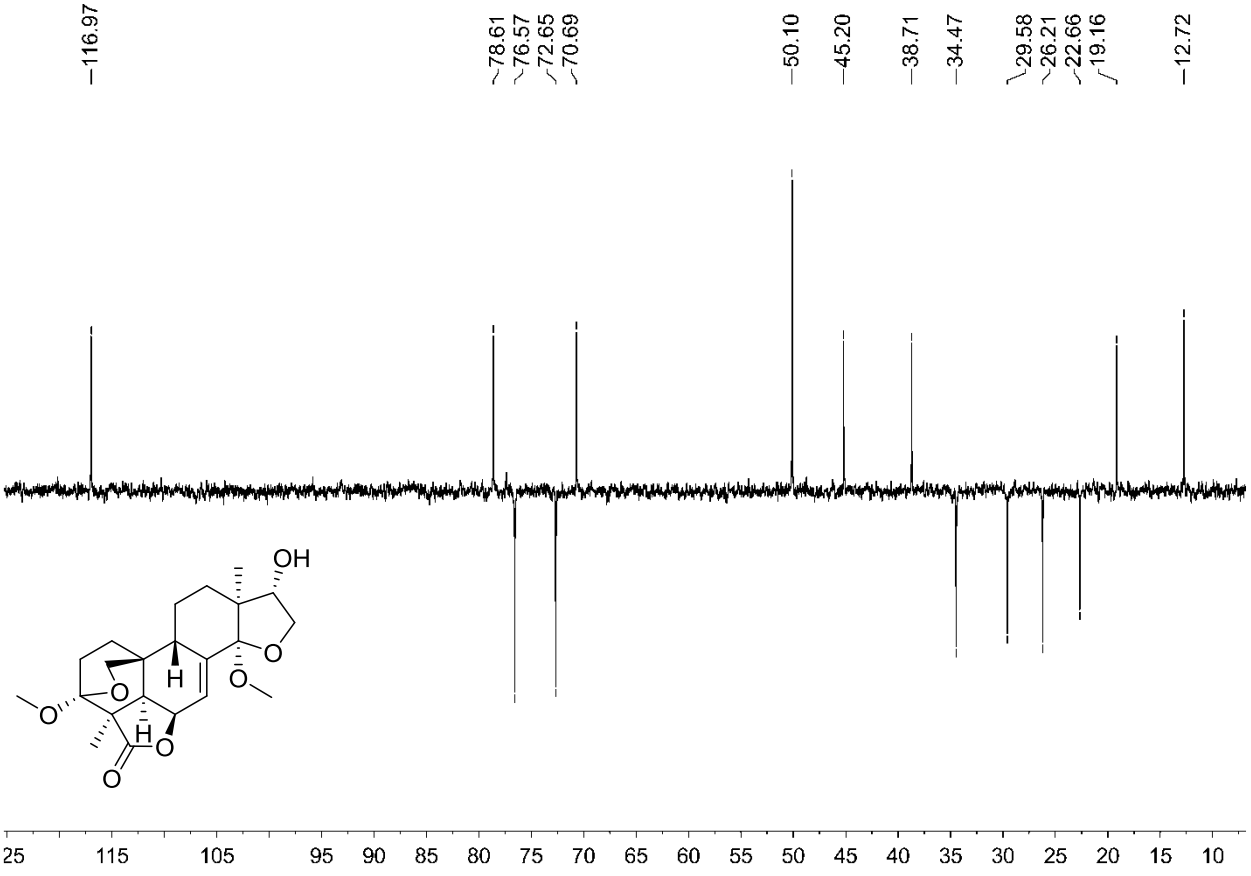

Fig. S123 DEPT135 (100 MHz, chloroform-*d*) spectrum of **7**

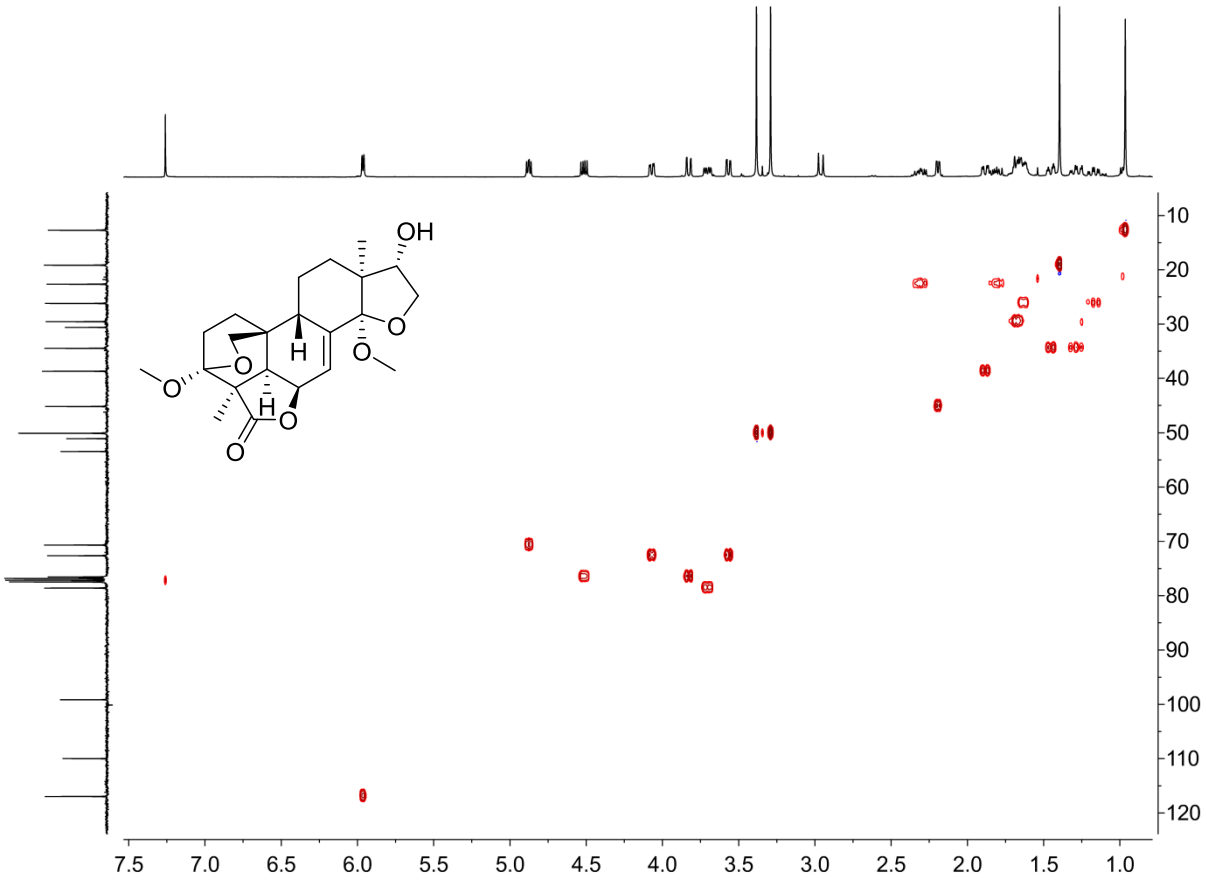

Fig. S124 HSQC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **7**

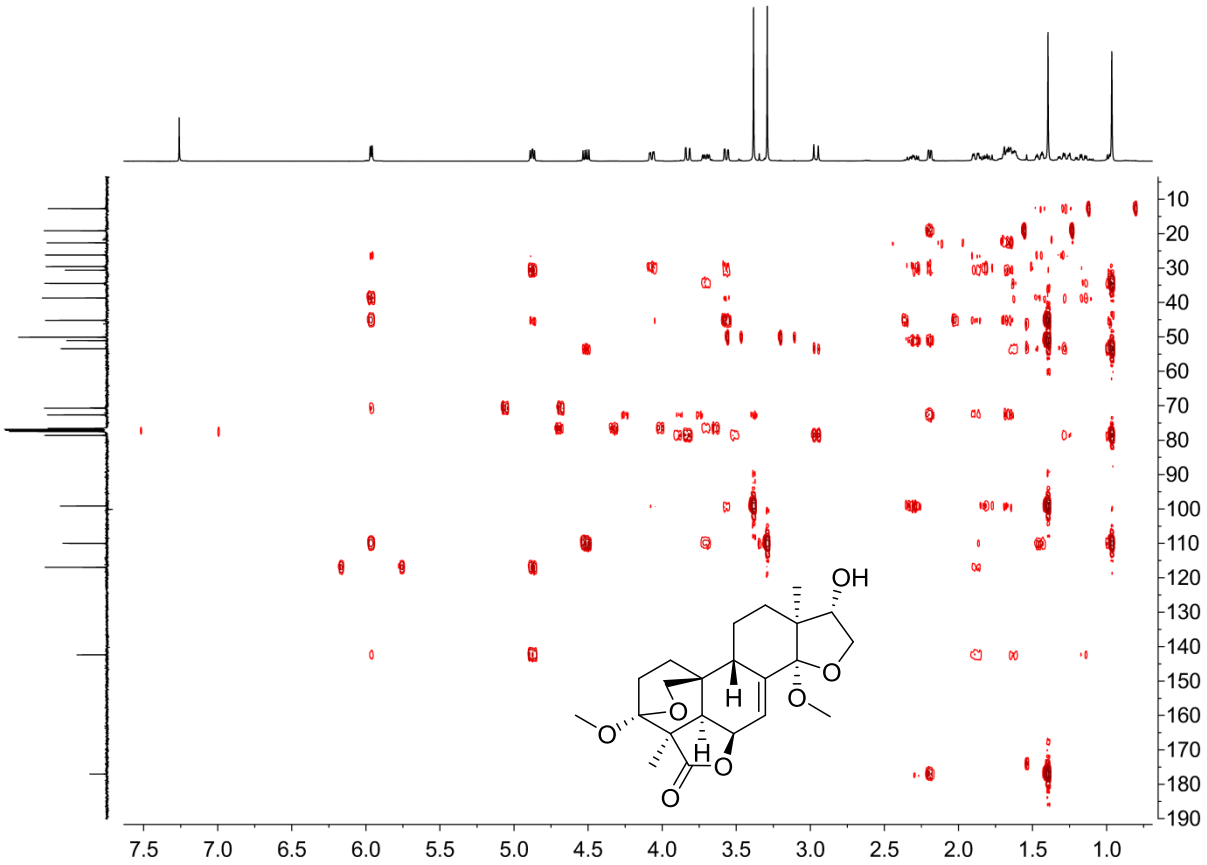

Fig. S125 HMBC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **7**

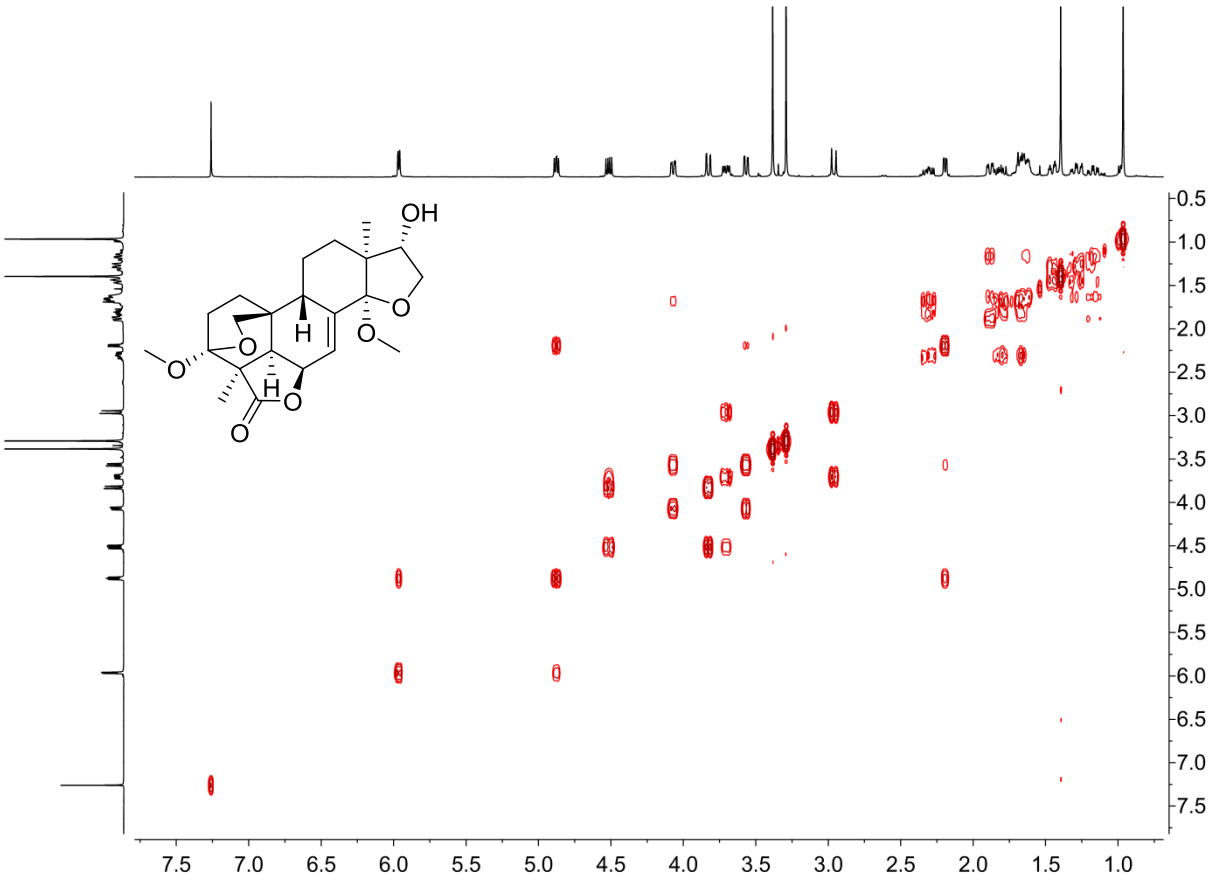

Fig. S126 ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of **7**

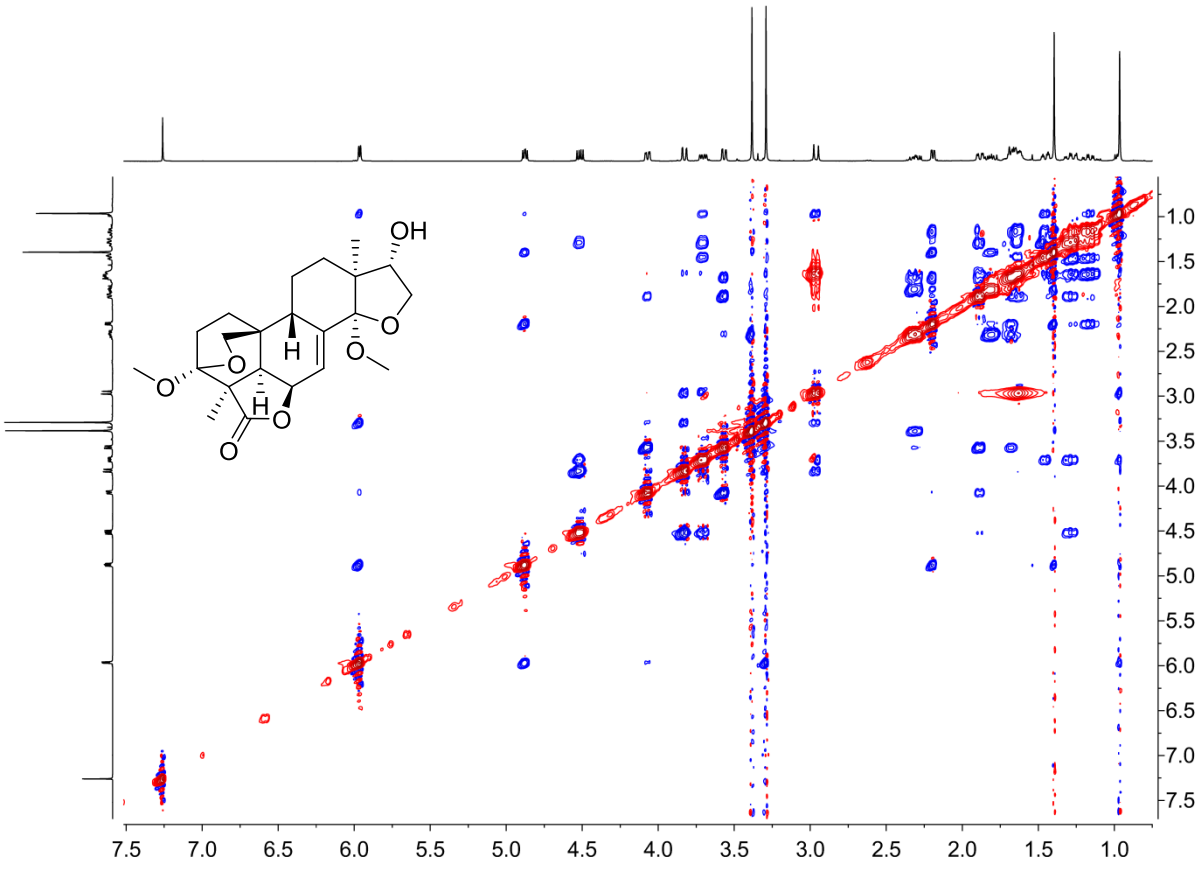

Fig. S127 NOESY spectrum (400 MHz, chloroform-*d*) of **7**

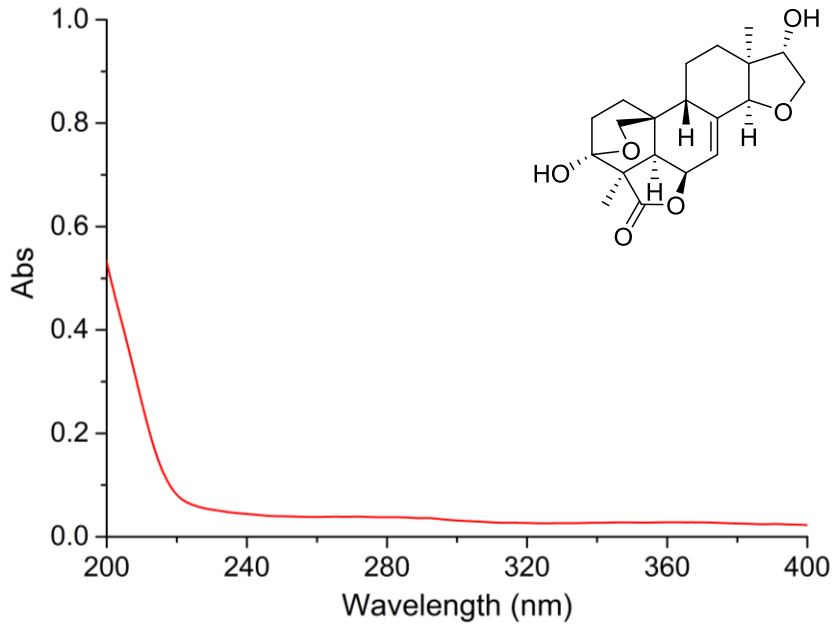

Fig. S128 UV spectrum of **8**

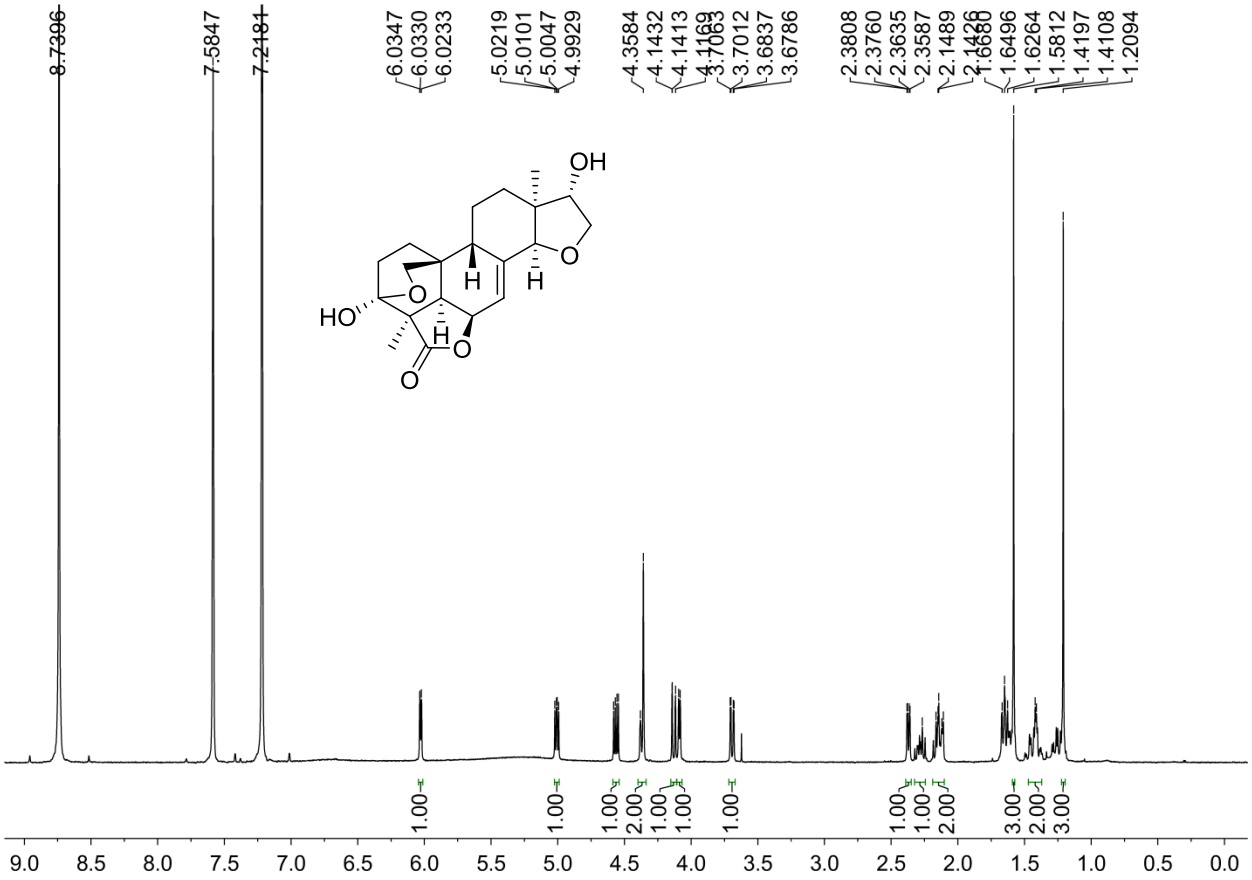

Fig. S129 ^{1}H NMR (400 MHz, pyridin-d_5) spectrum of **8**

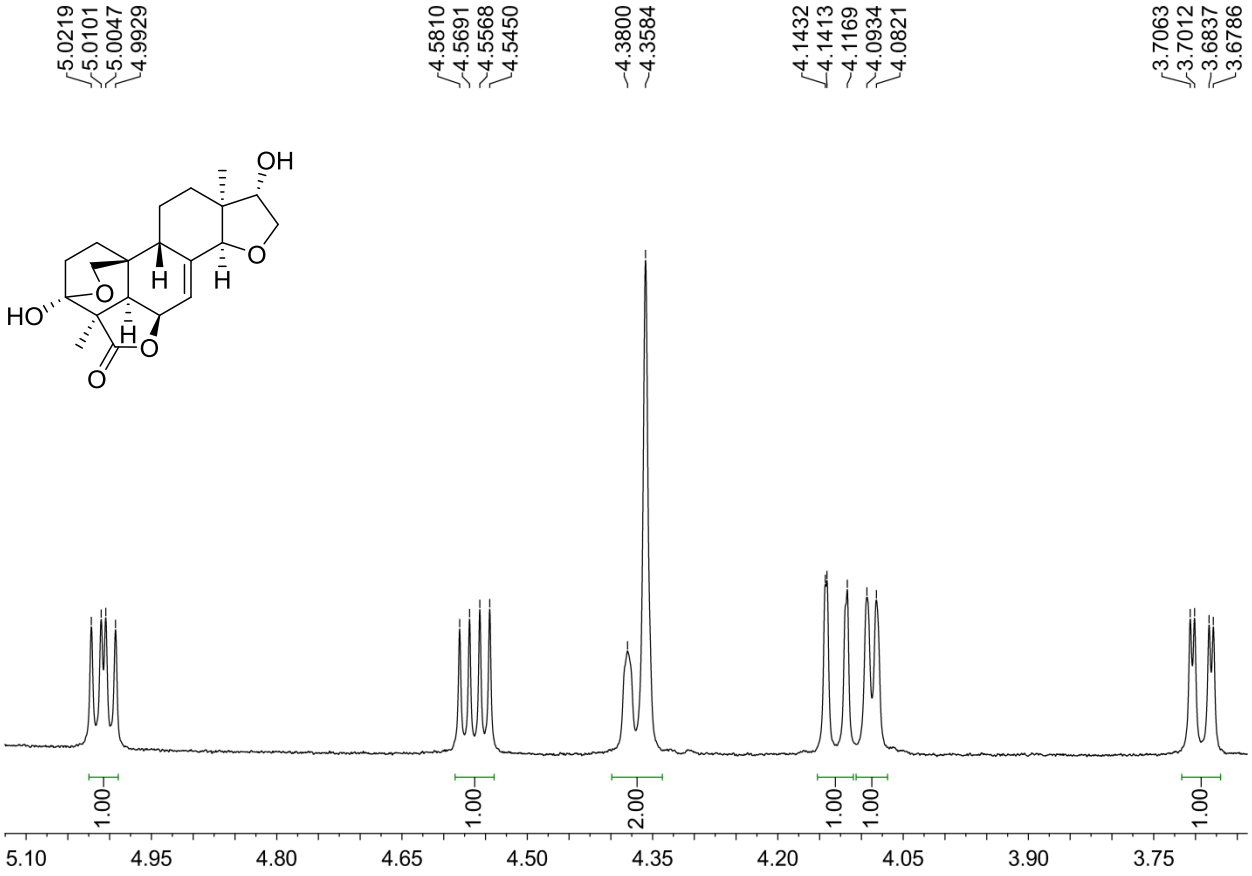

Fig. S130 ^{1}H NMR (400 MHz, pyridin-d_5) spectrum of **8** (amplified)

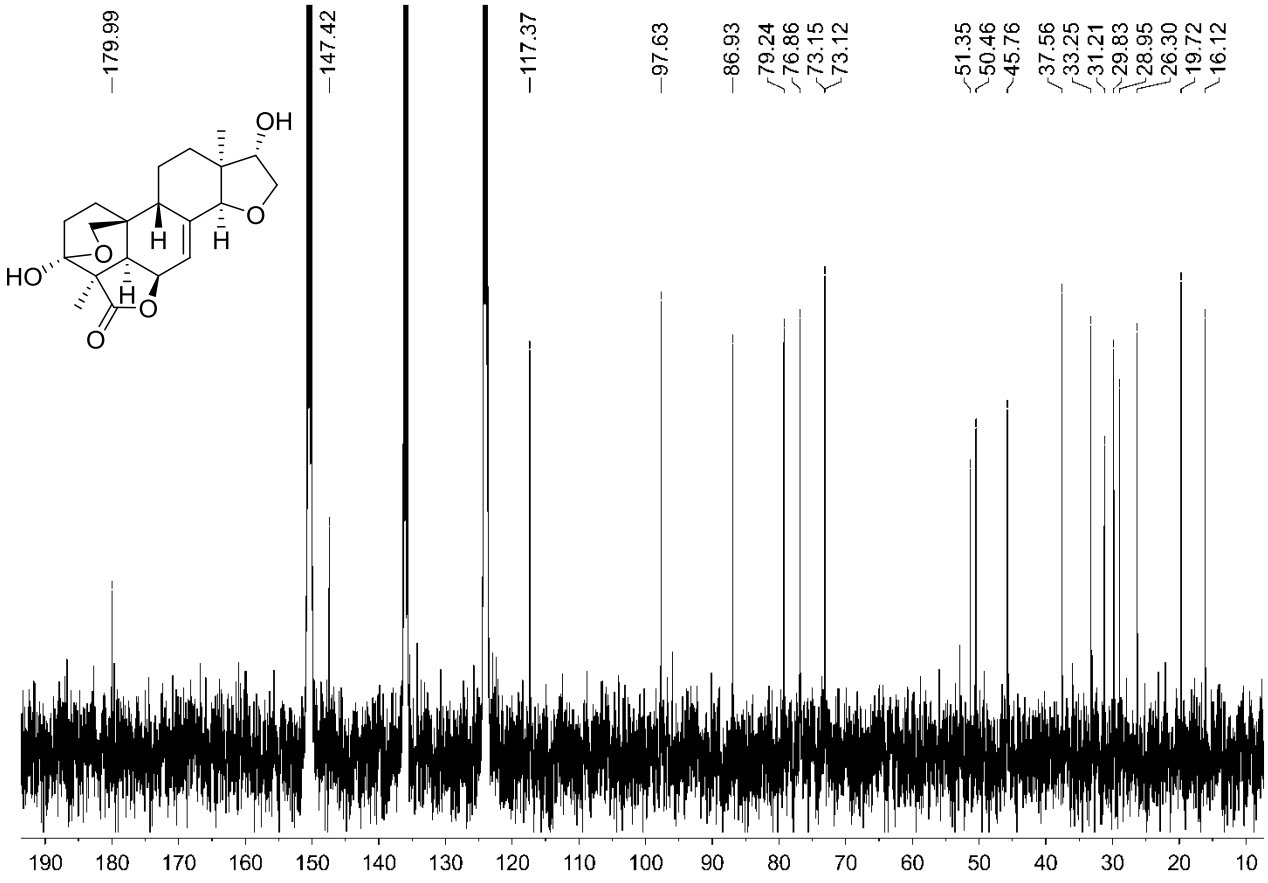

Fig. S131 ^{13}C NMR (100 MHz, pyridin-d_5) spectrum of **8**

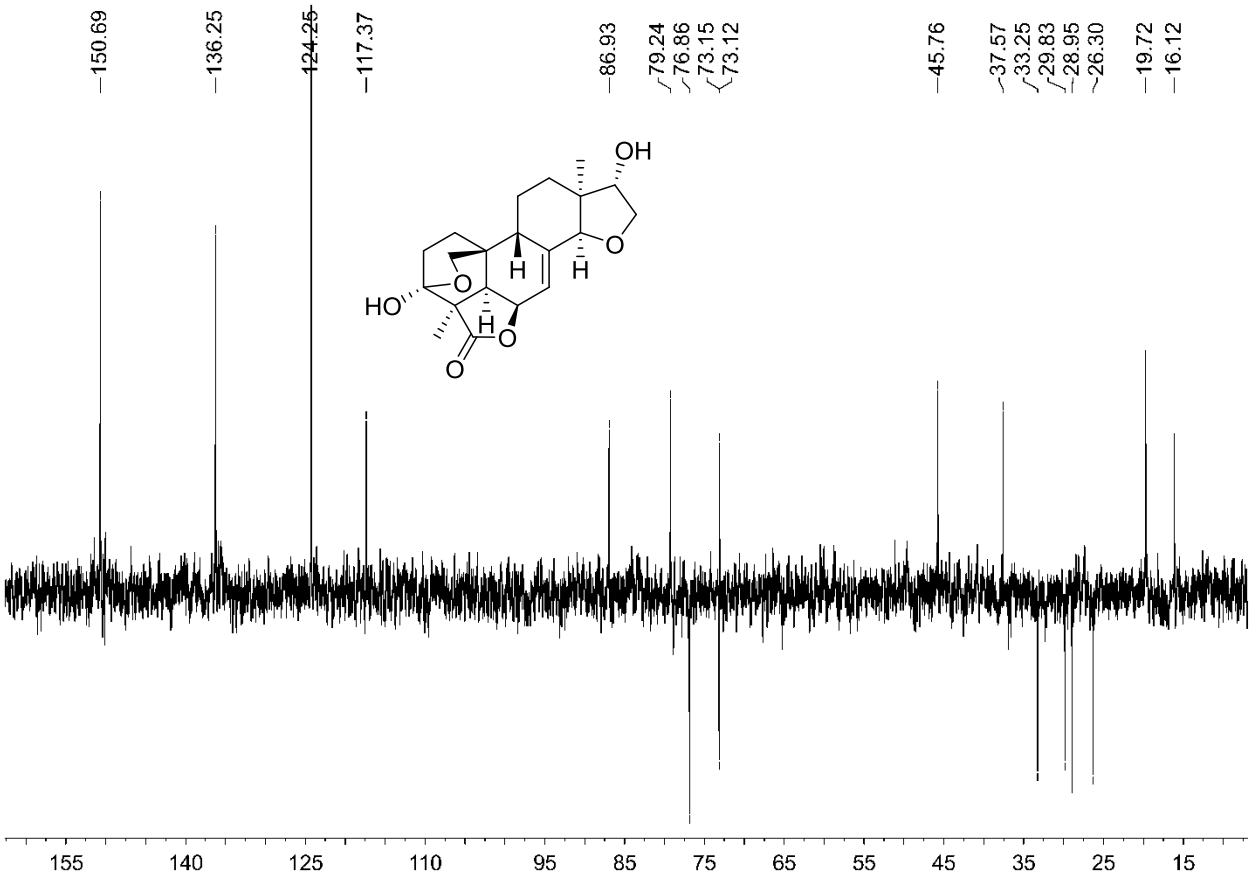

Fig. S132 DEPT135 (100 MHz, pyridin-d_5) spectrum of **8**

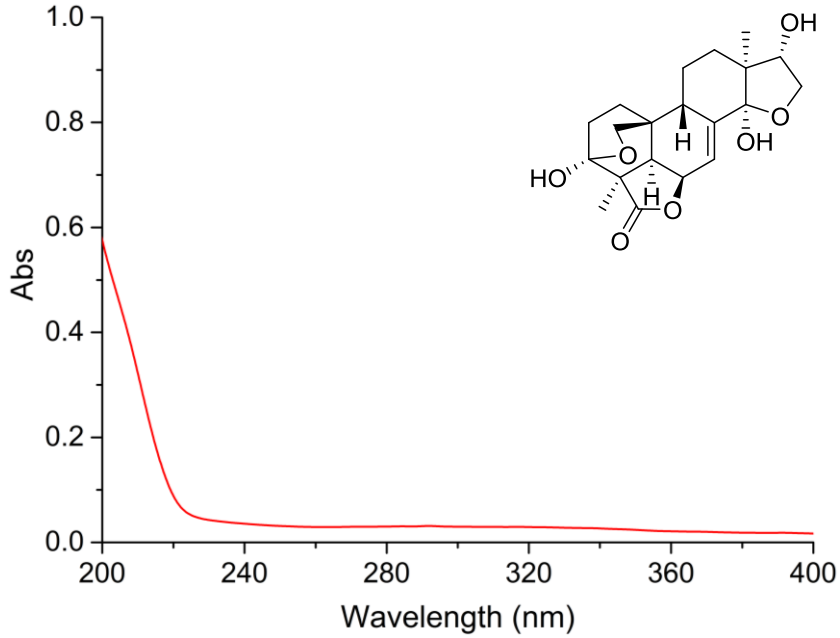

Fig. S133 UV spectrum of **9**

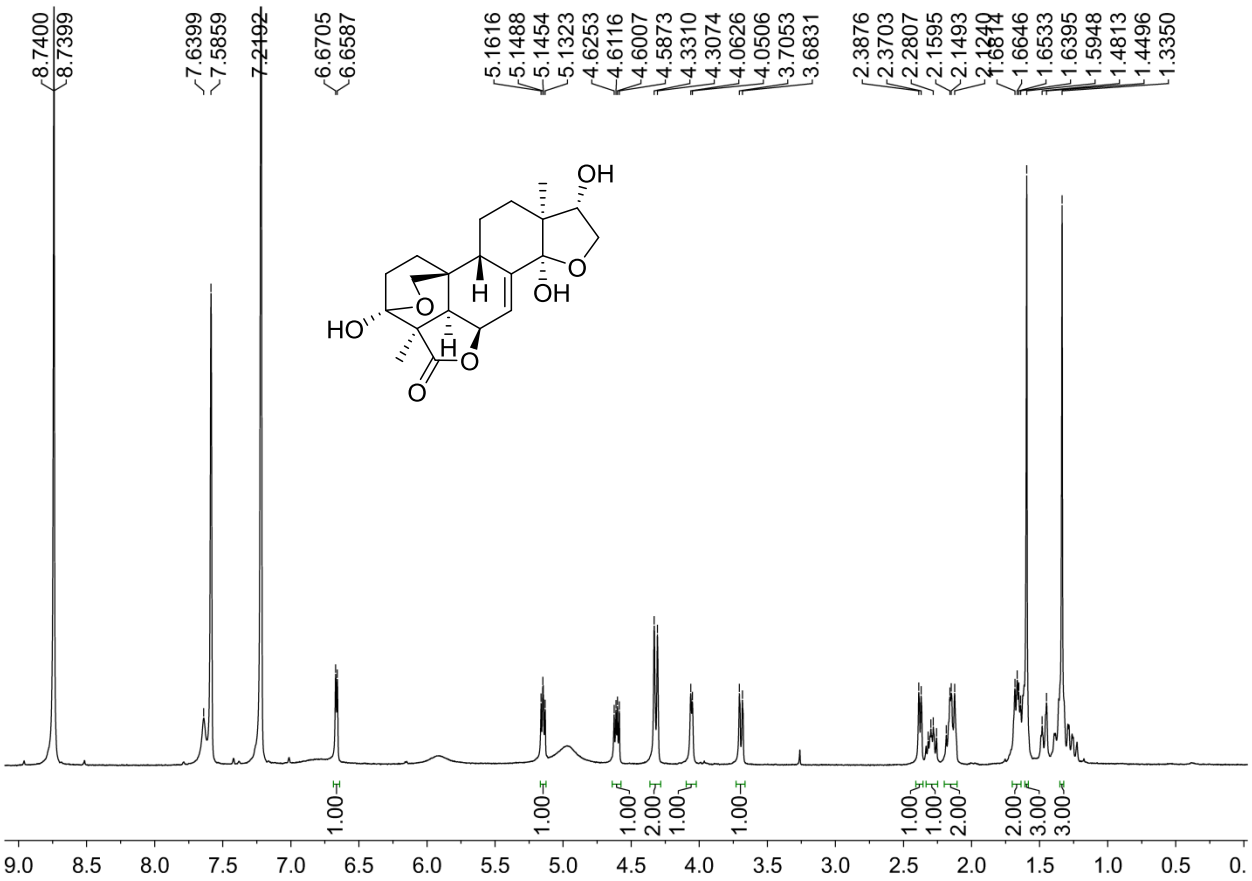

Fig. S134 ^{1}H NMR (400 MHz, pyridin-d_5) spectrum of **9**

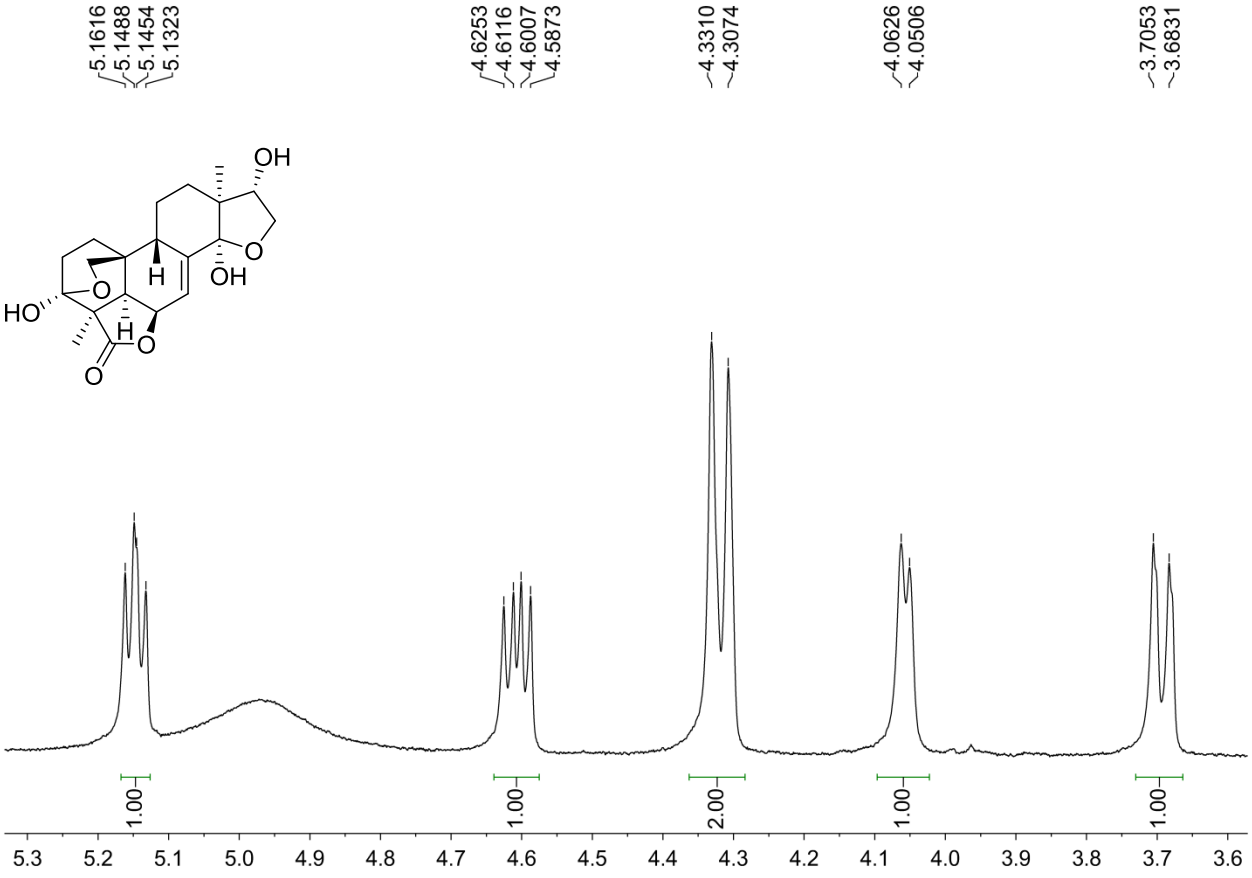

Fig. S135 ^{1}H NMR (400 MHz, pyridin-d_5) spectrum of **9** (amplified)

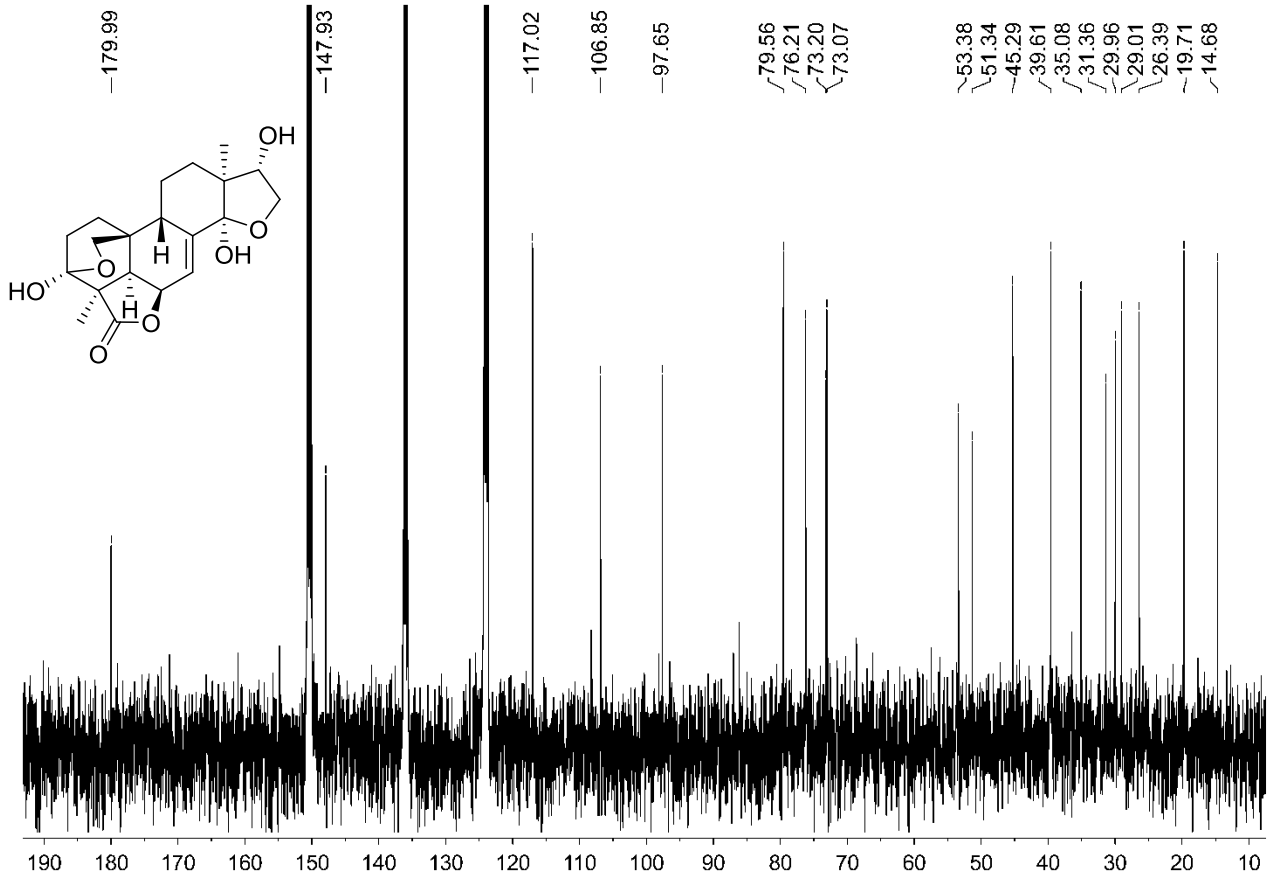

Fig. S136 ^{13}C NMR (100 MHz, pyridin-d_5) spectrum of **9**

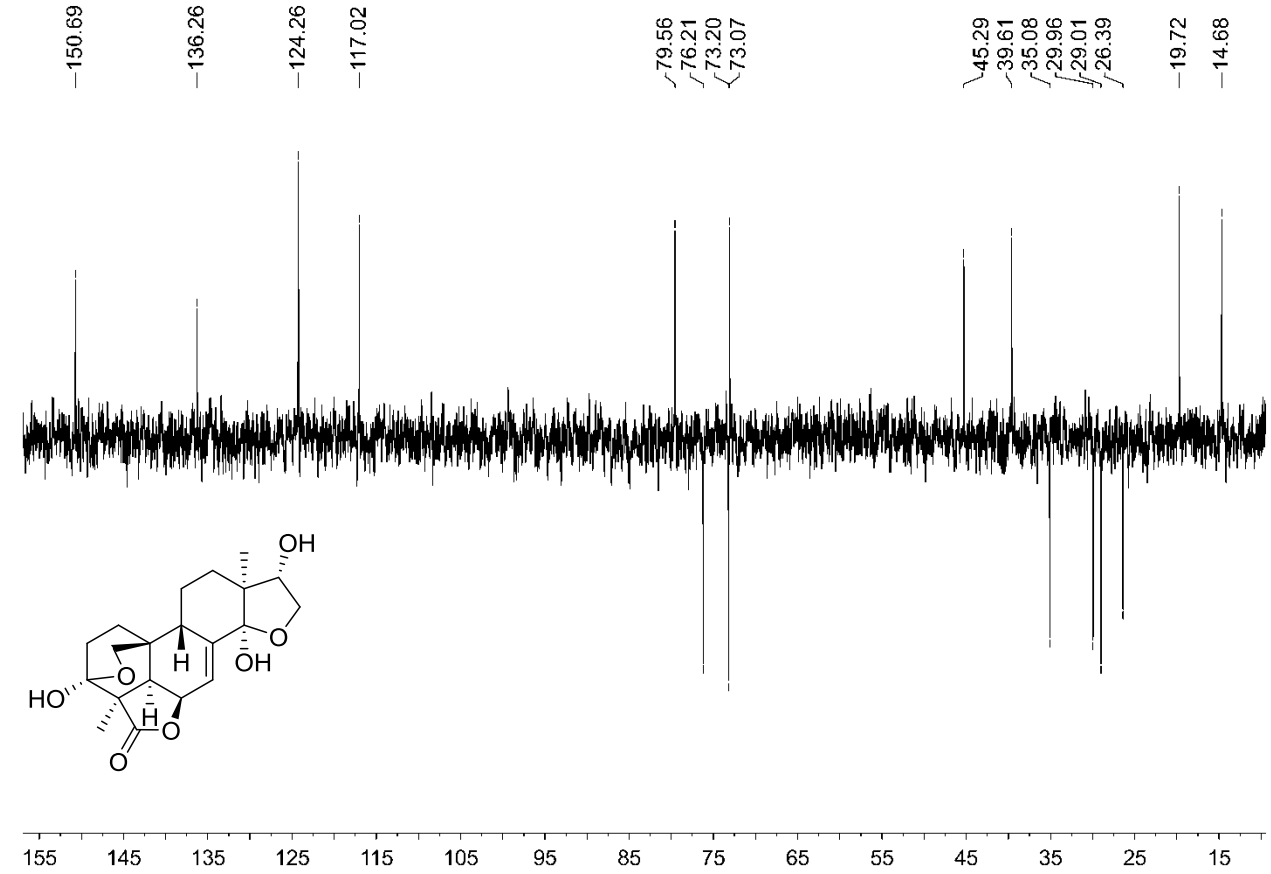

Fig. S137 DEPT135 (100 MHz, pyridin-d_5) spectrum of **9**

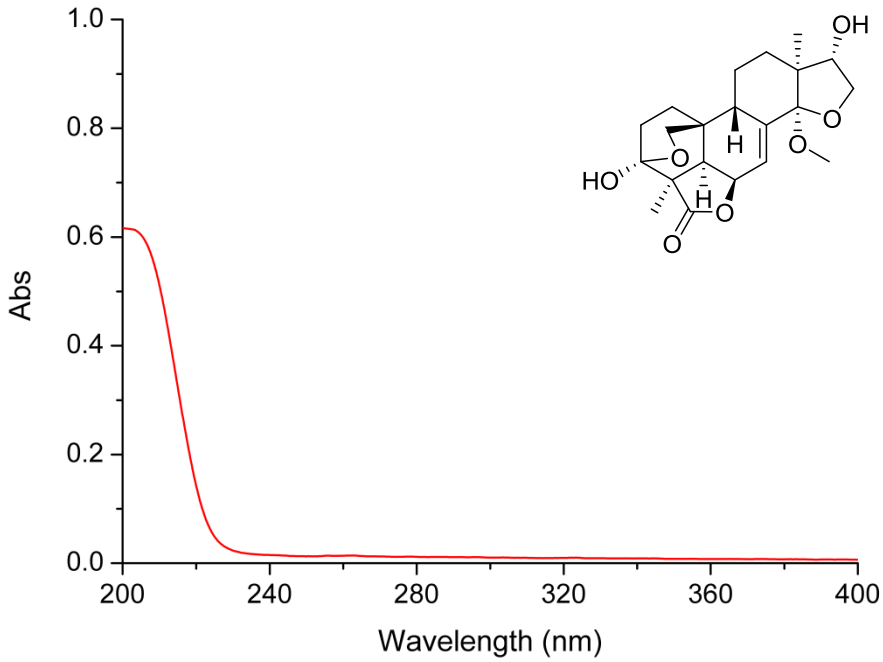

Fig. S138 UV spectrum of **10**

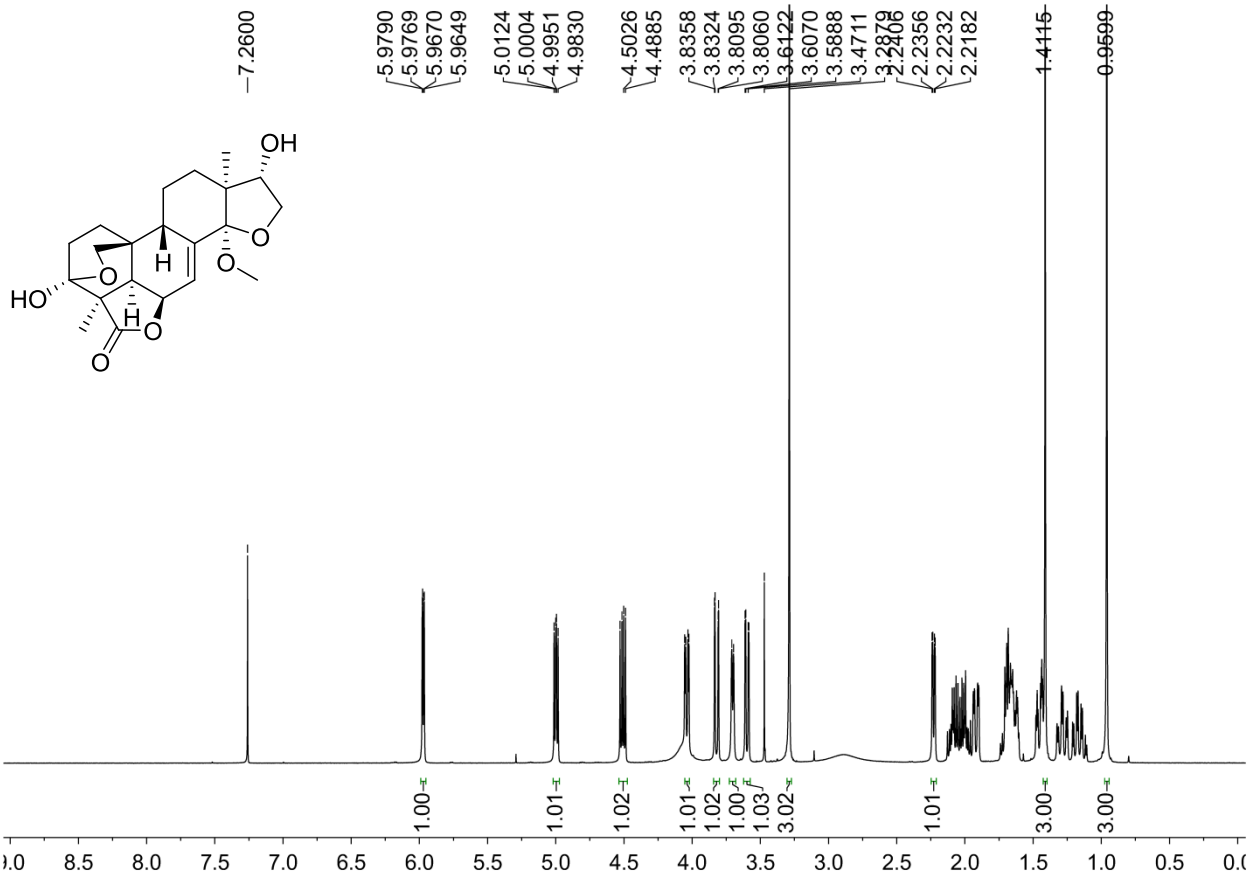

Fig. S139 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **10**

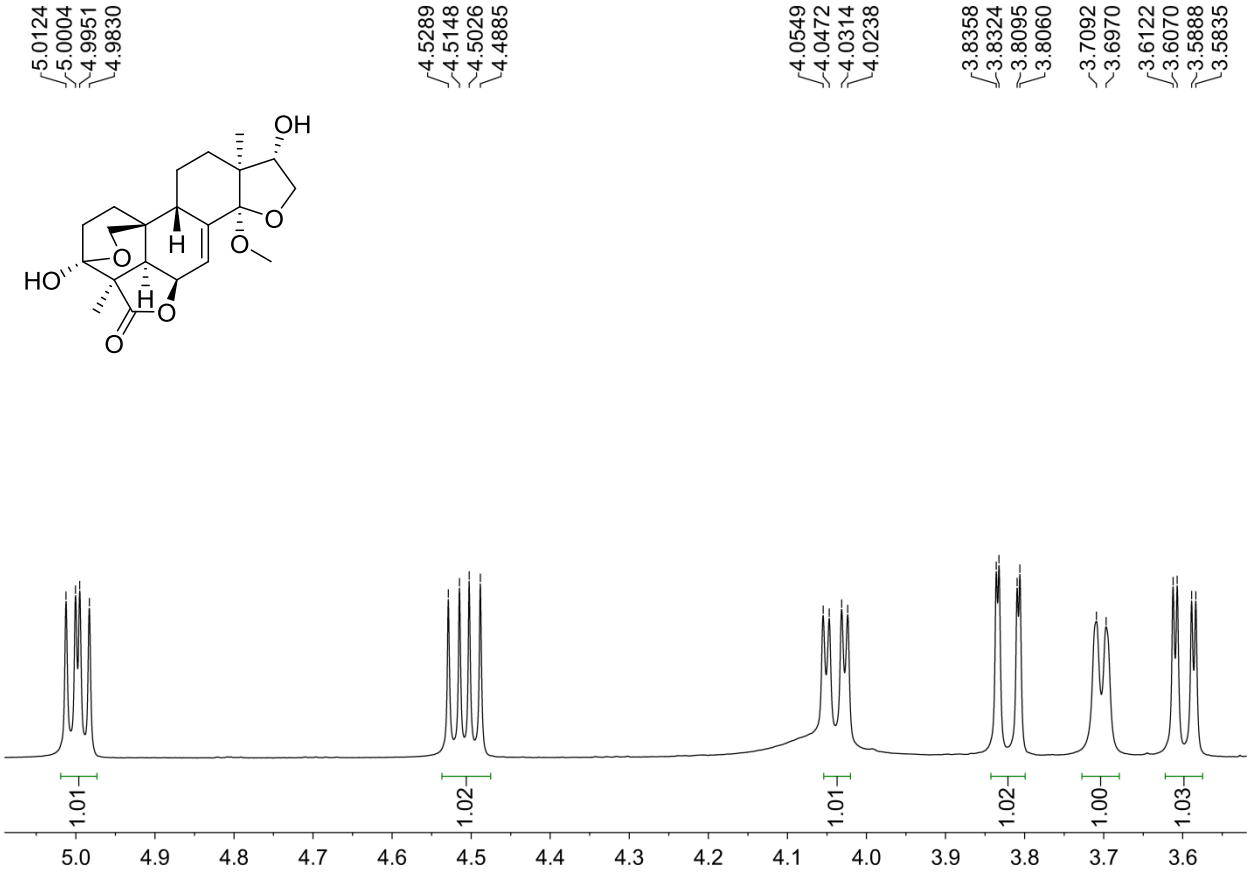

Fig. S140 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **10** (amplified)

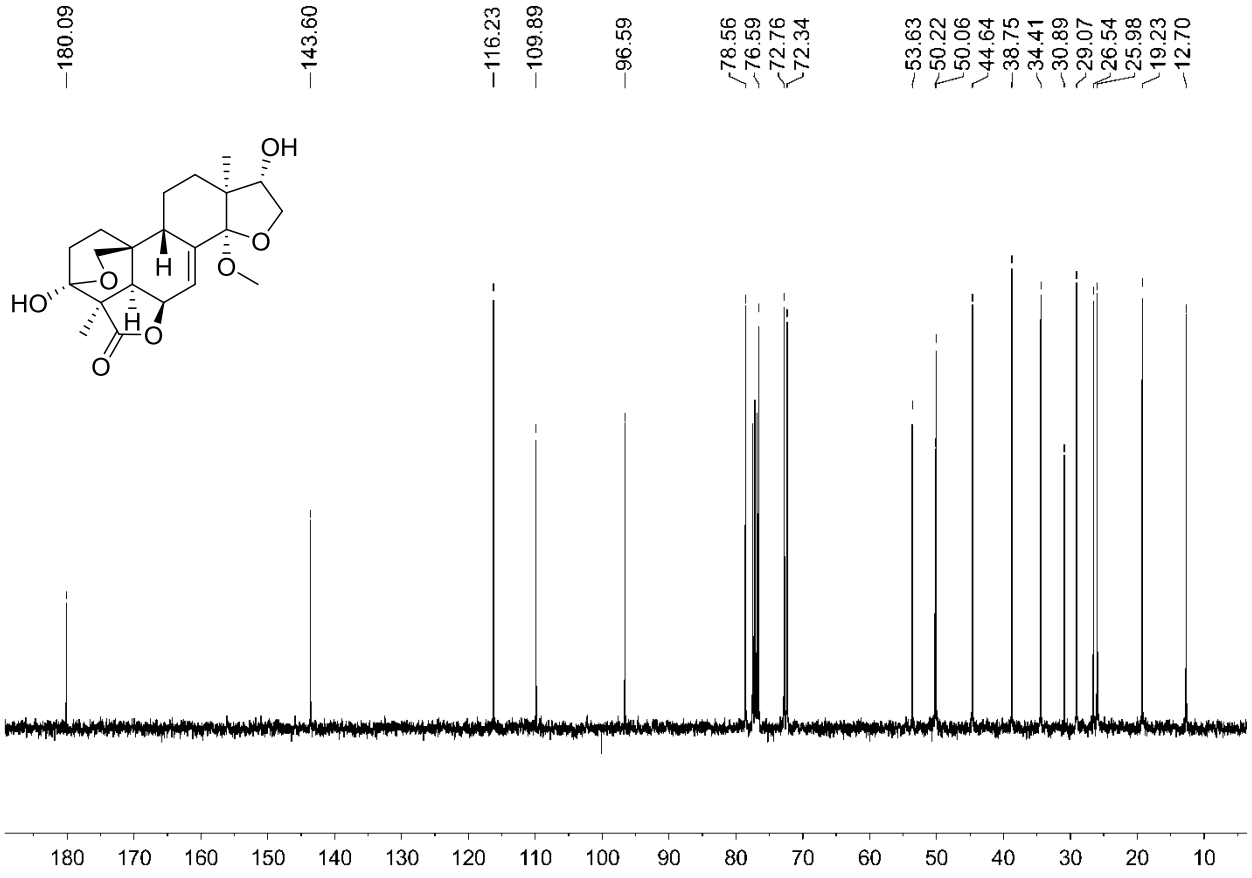

Fig. S141 ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of **10**

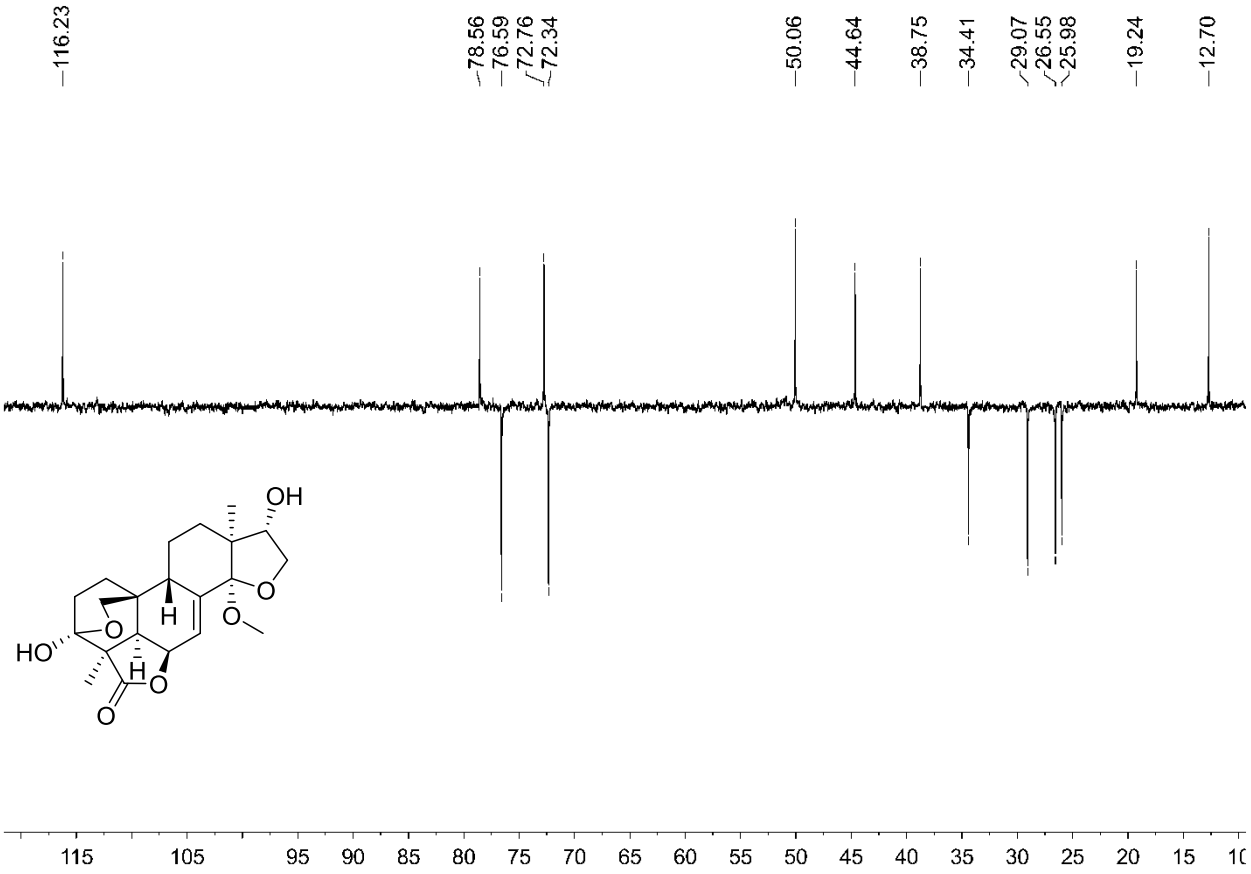

Fig. S142 DEPT135 (100 MHz, chloroform-*d*) spectrum of **10**

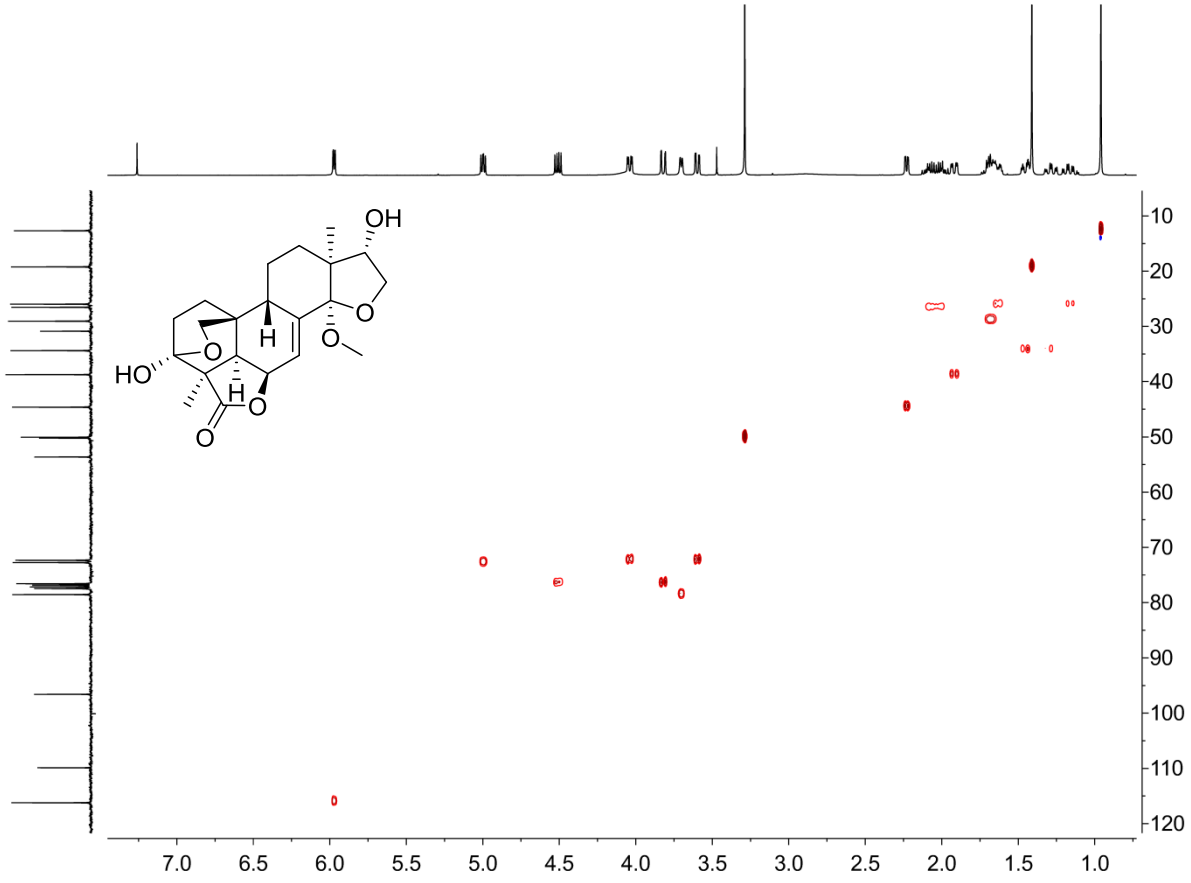

Fig. S143 HSQC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **10**

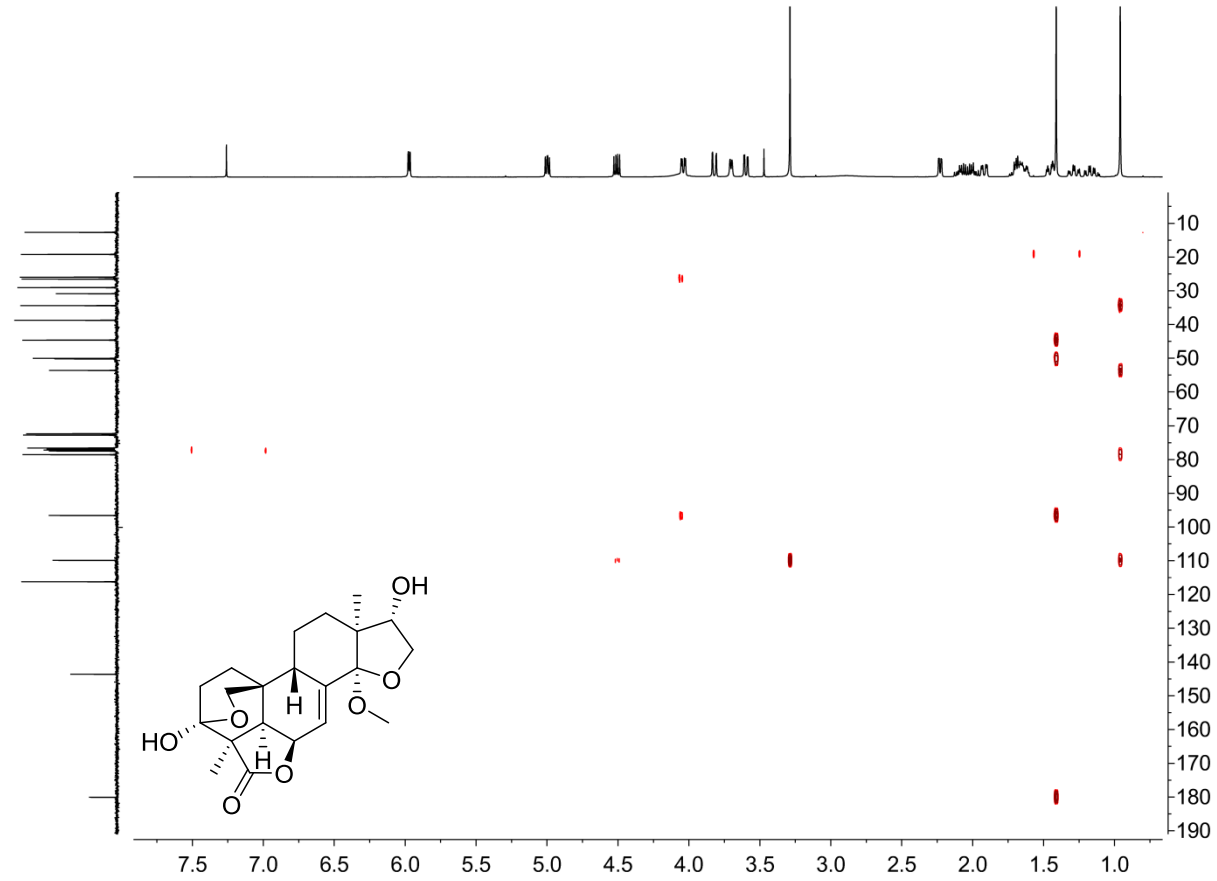

Fig. S144 HMBC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **10**

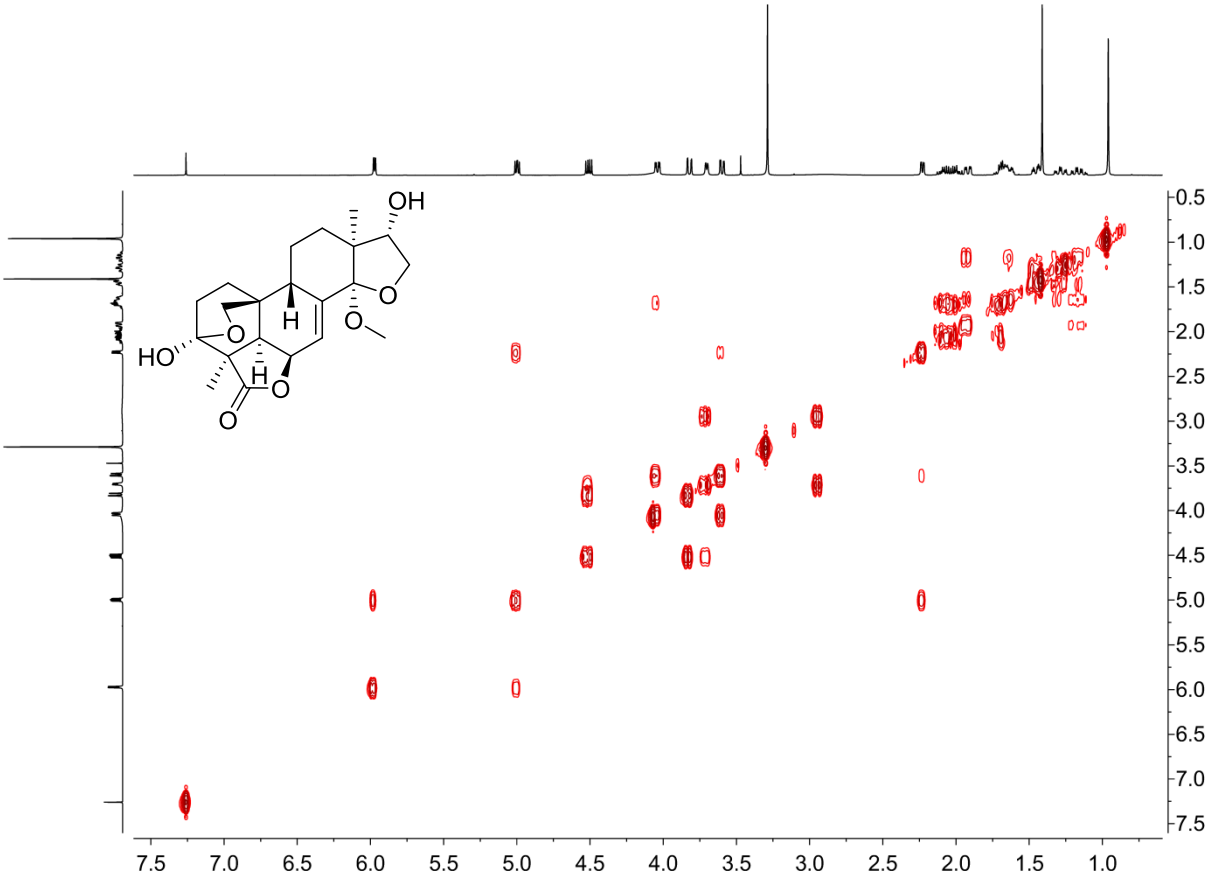

Fig. S145 ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of **10**

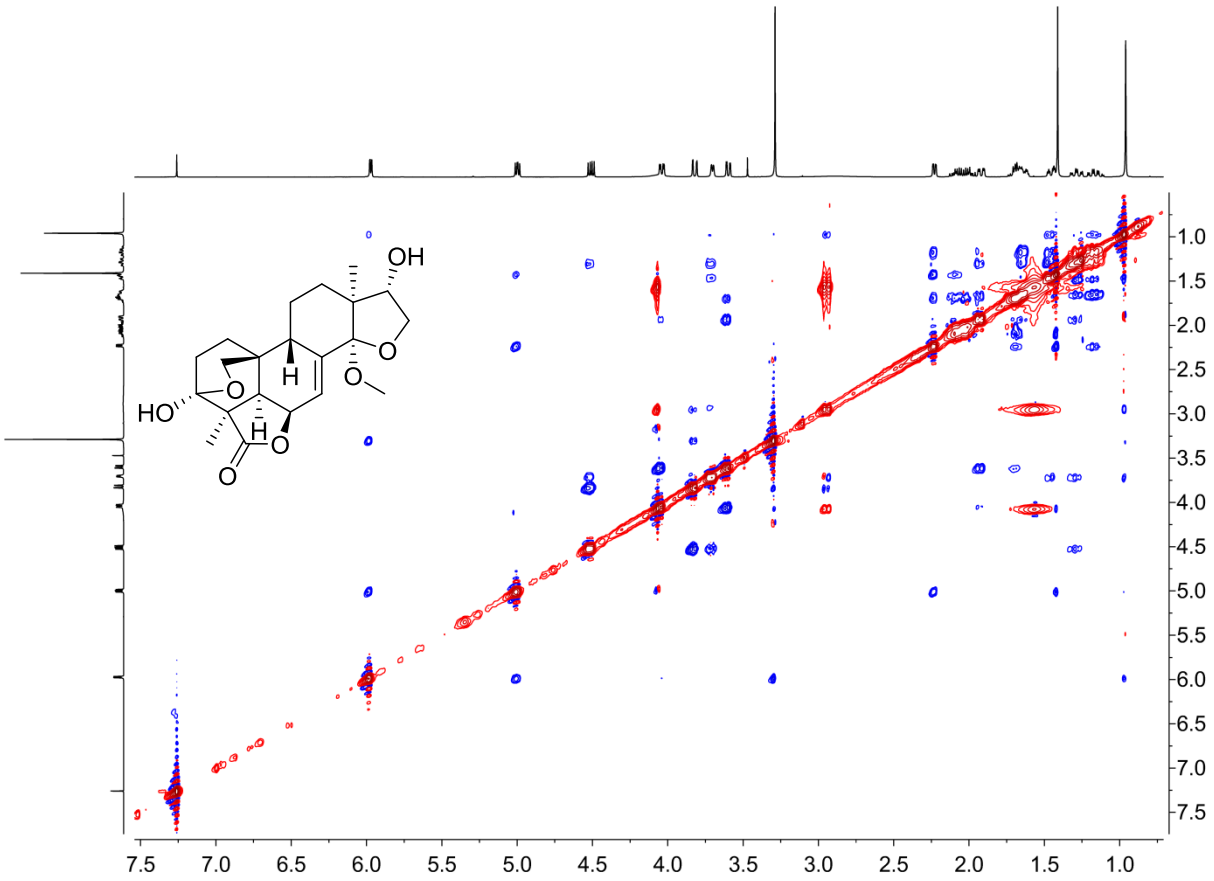

Fig. S146 NOESY spectrum (400 MHz, chloroform-*d*) of **10**

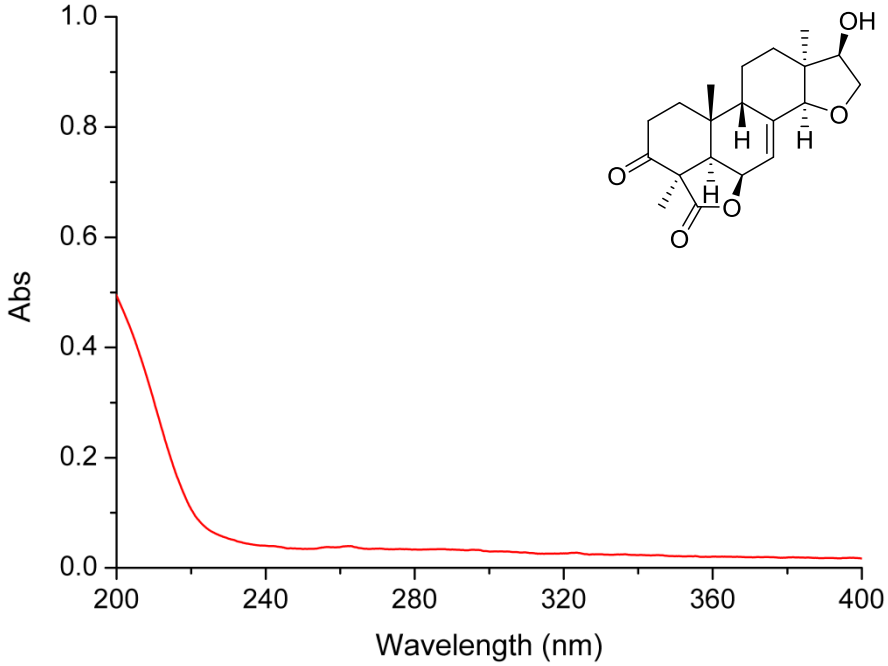

Fig. S147 UV spectrum of **11**

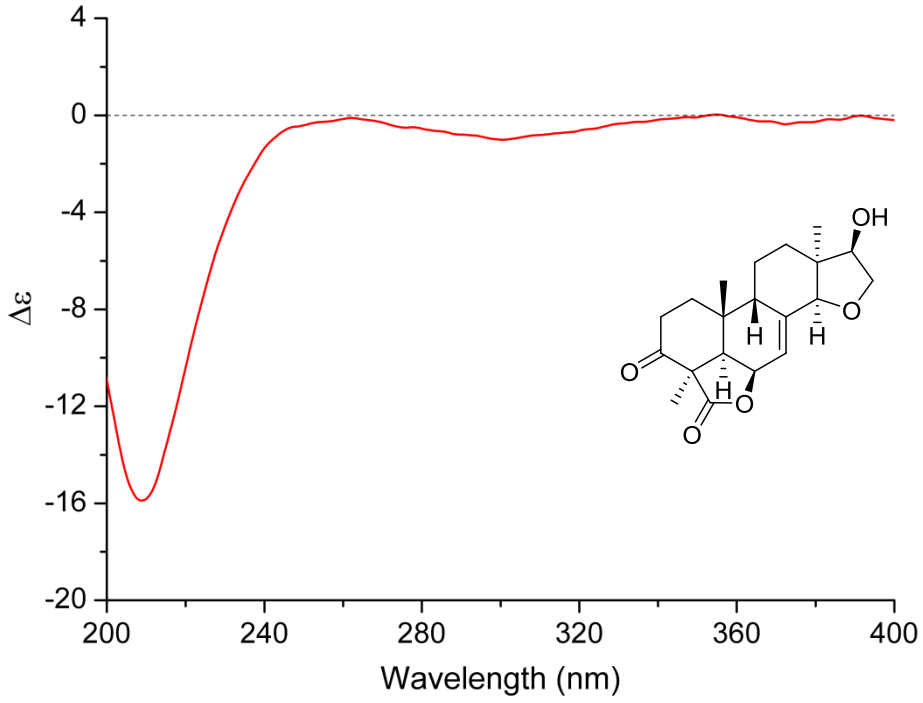

Fig. S148 Experimental ECD spectrum of **11**

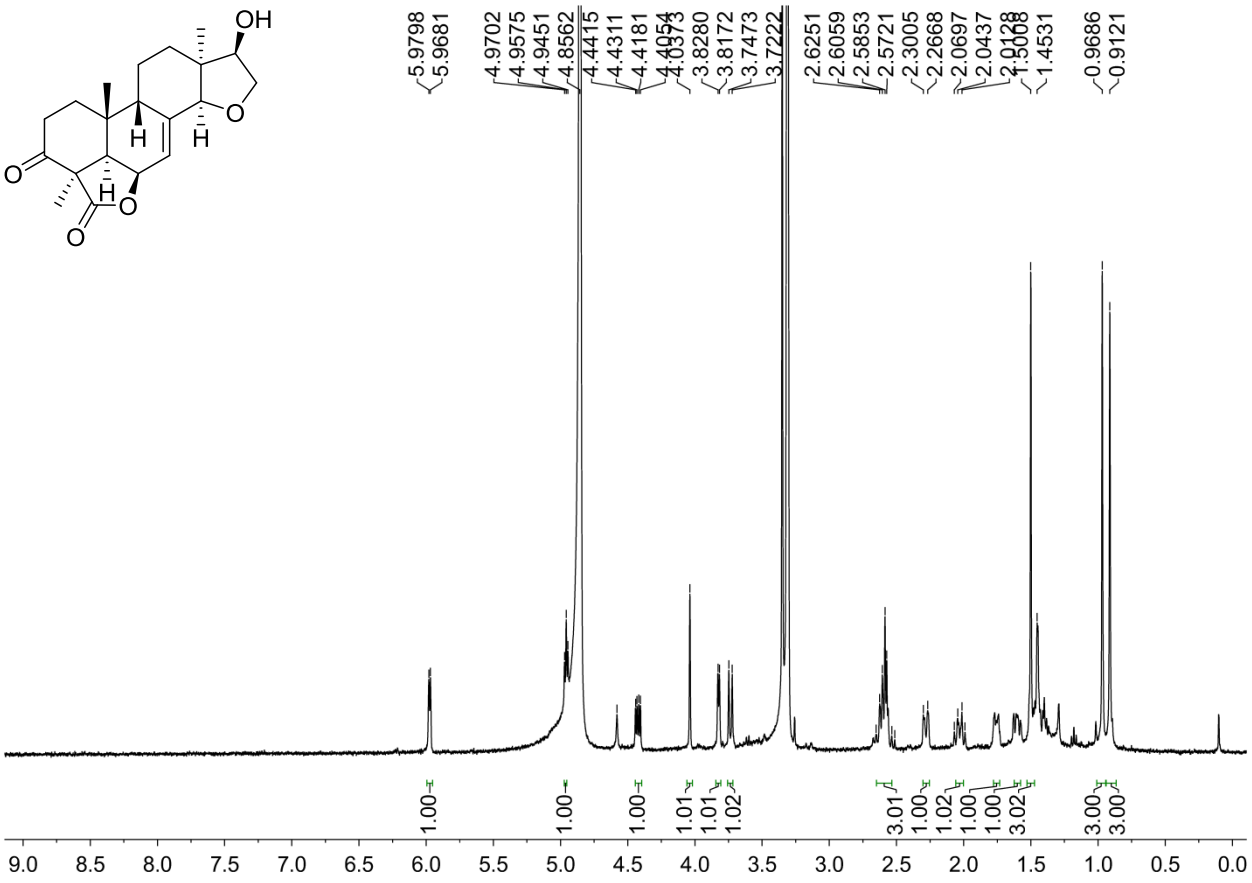

Fig. S149 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **11**

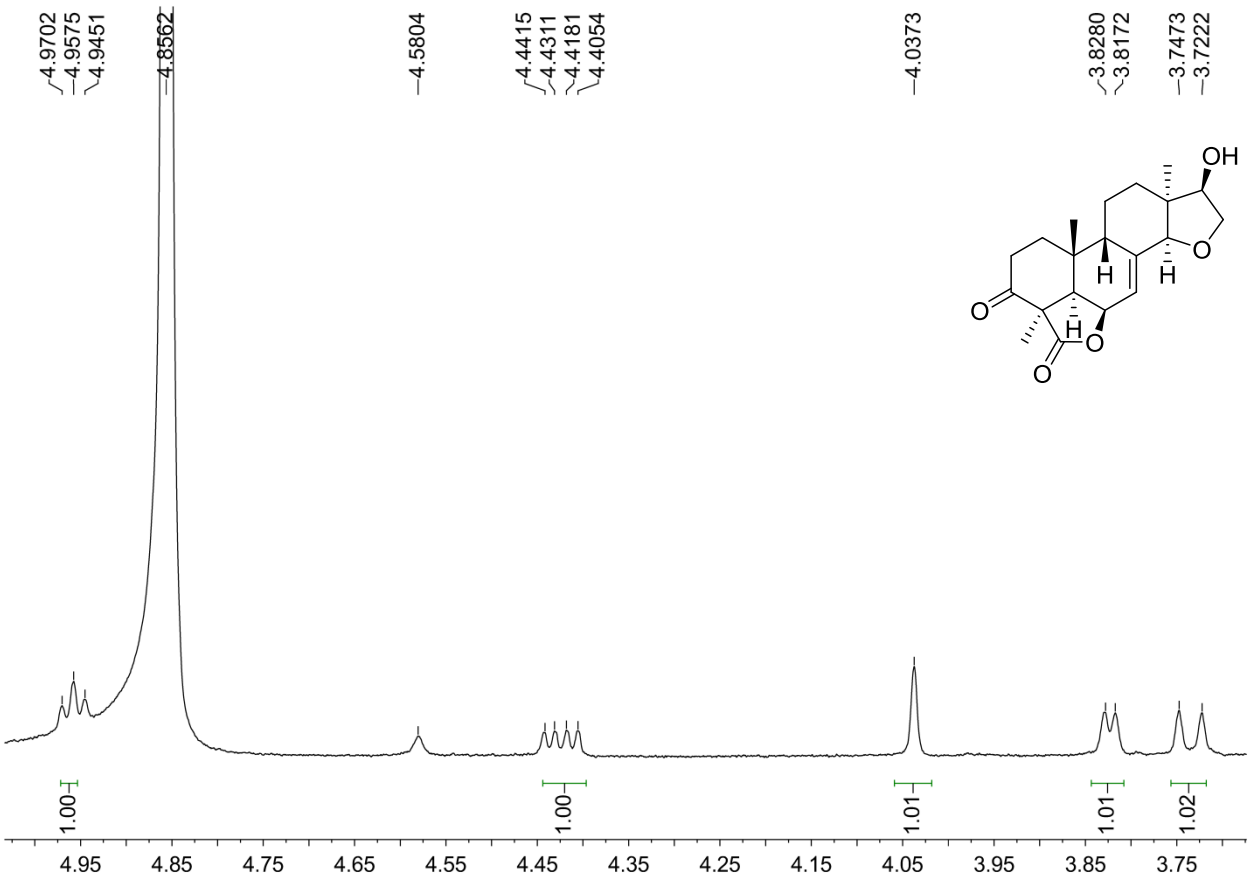

Fig. S150 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **11** (amplified)

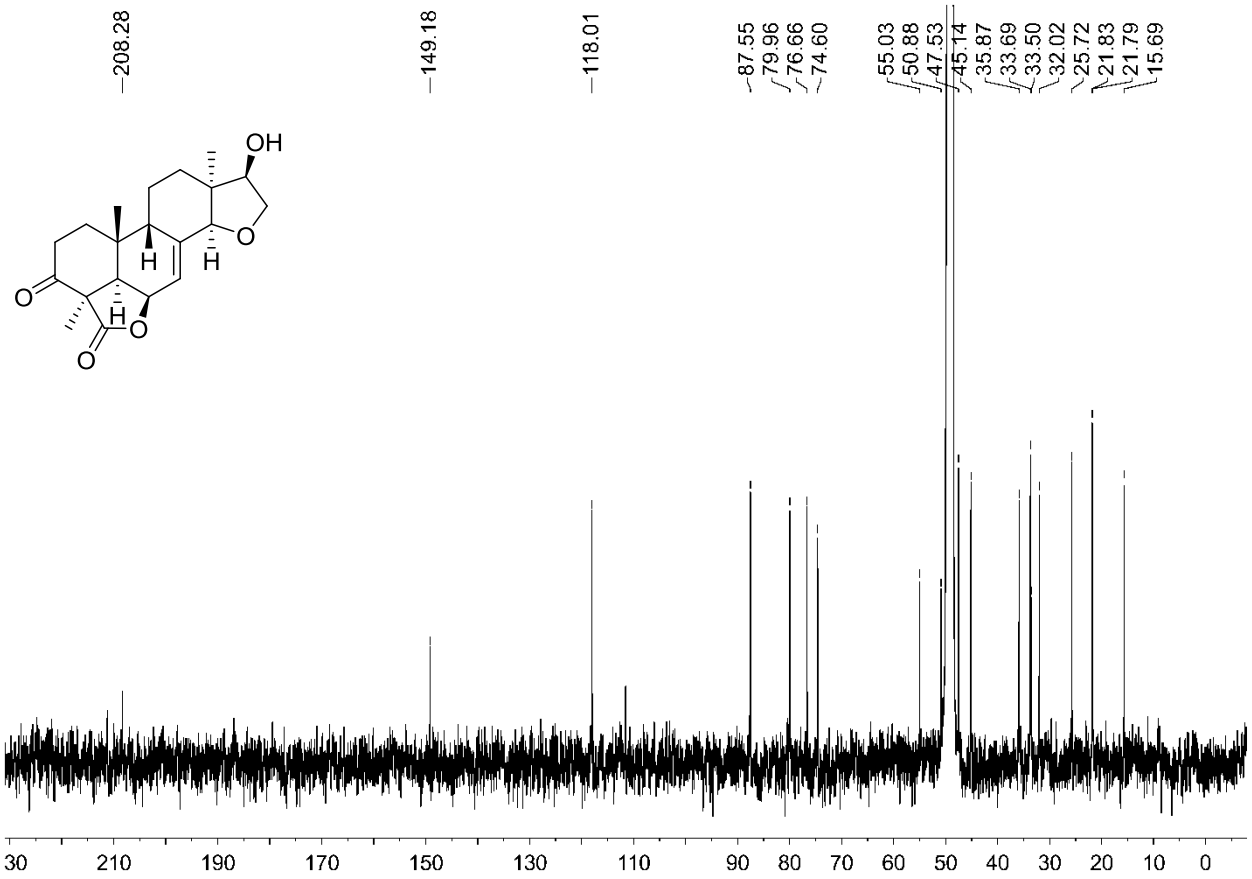

Fig. S151 ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of **11**

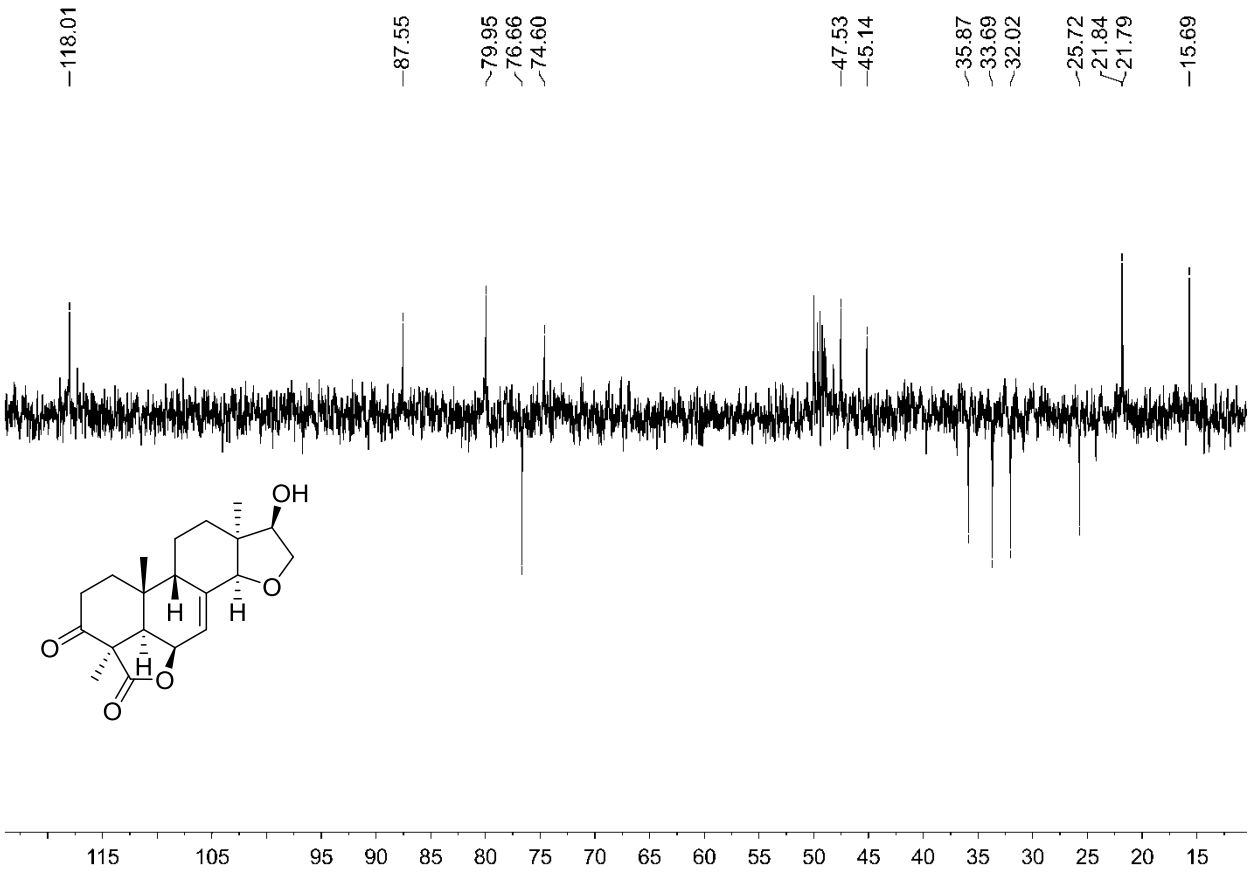

Fig. S152 DEPT135 (100 MHz, chloroform-*d*) spectrum of **11**

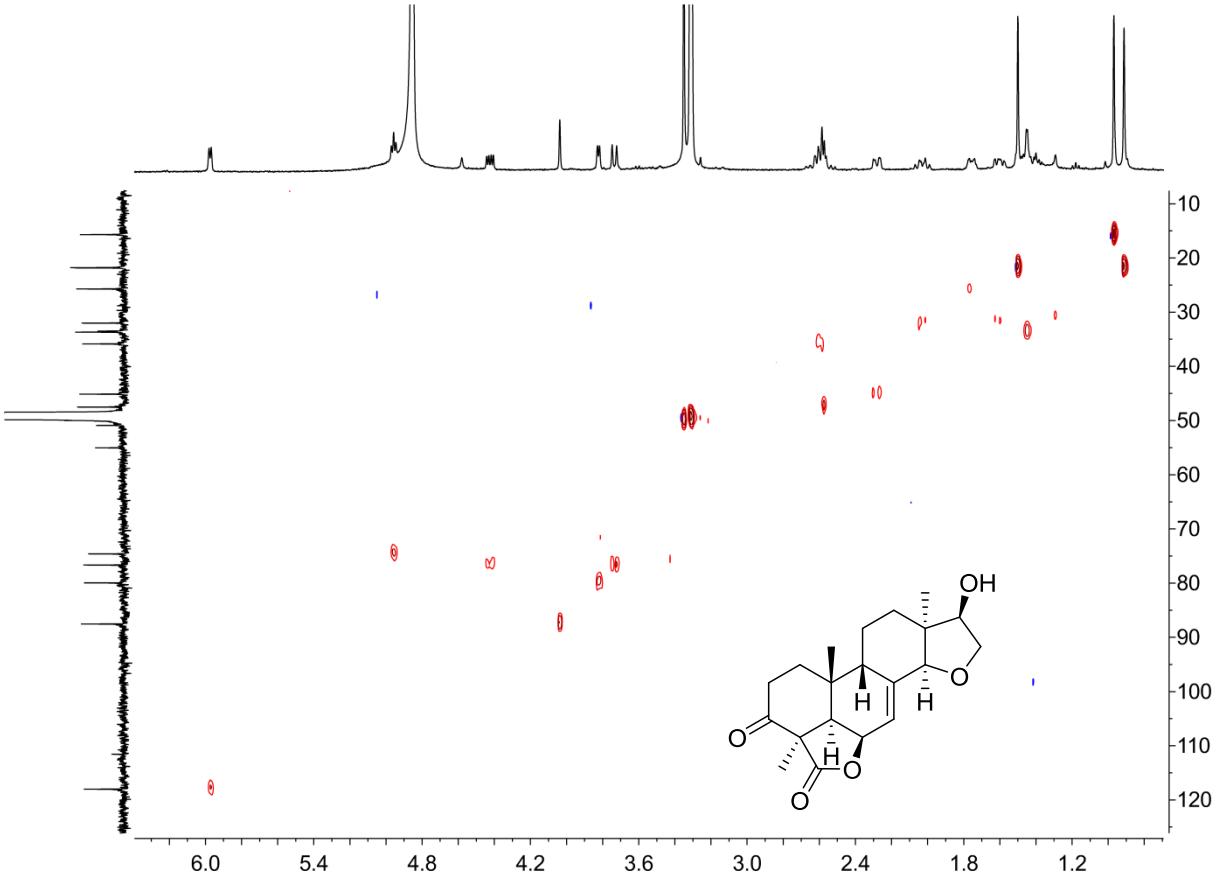

Fig. S153 HSQC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **11**

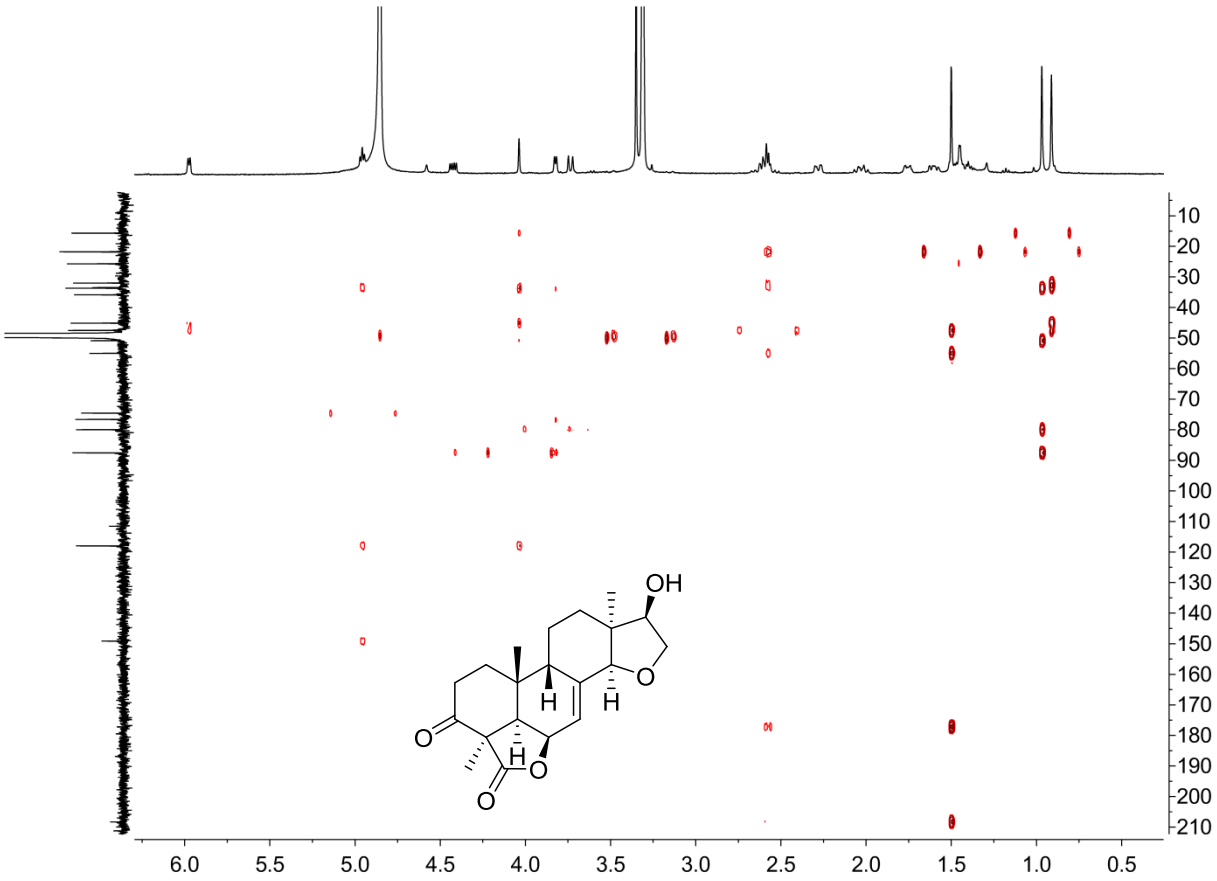

Fig. S154 HMBC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **11**

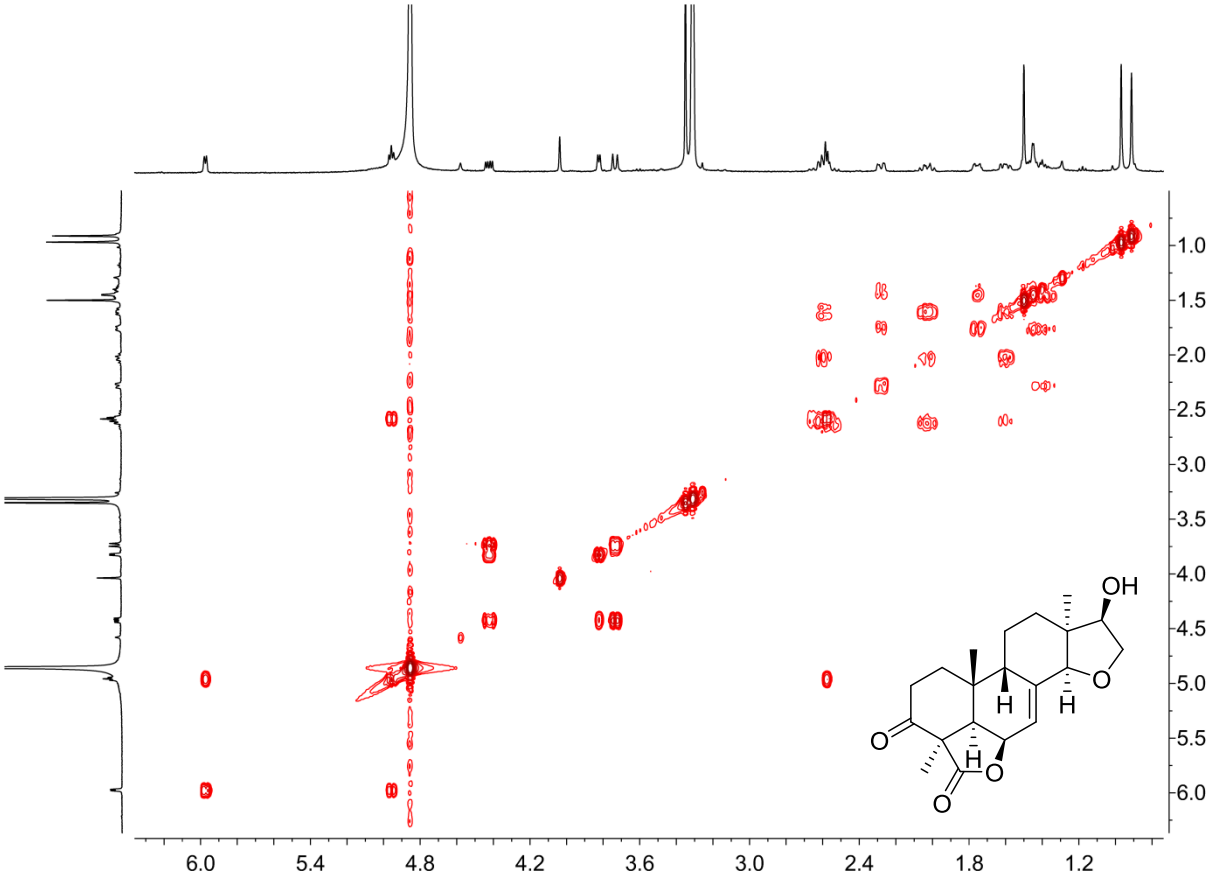

Fig. S155 ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of **11**

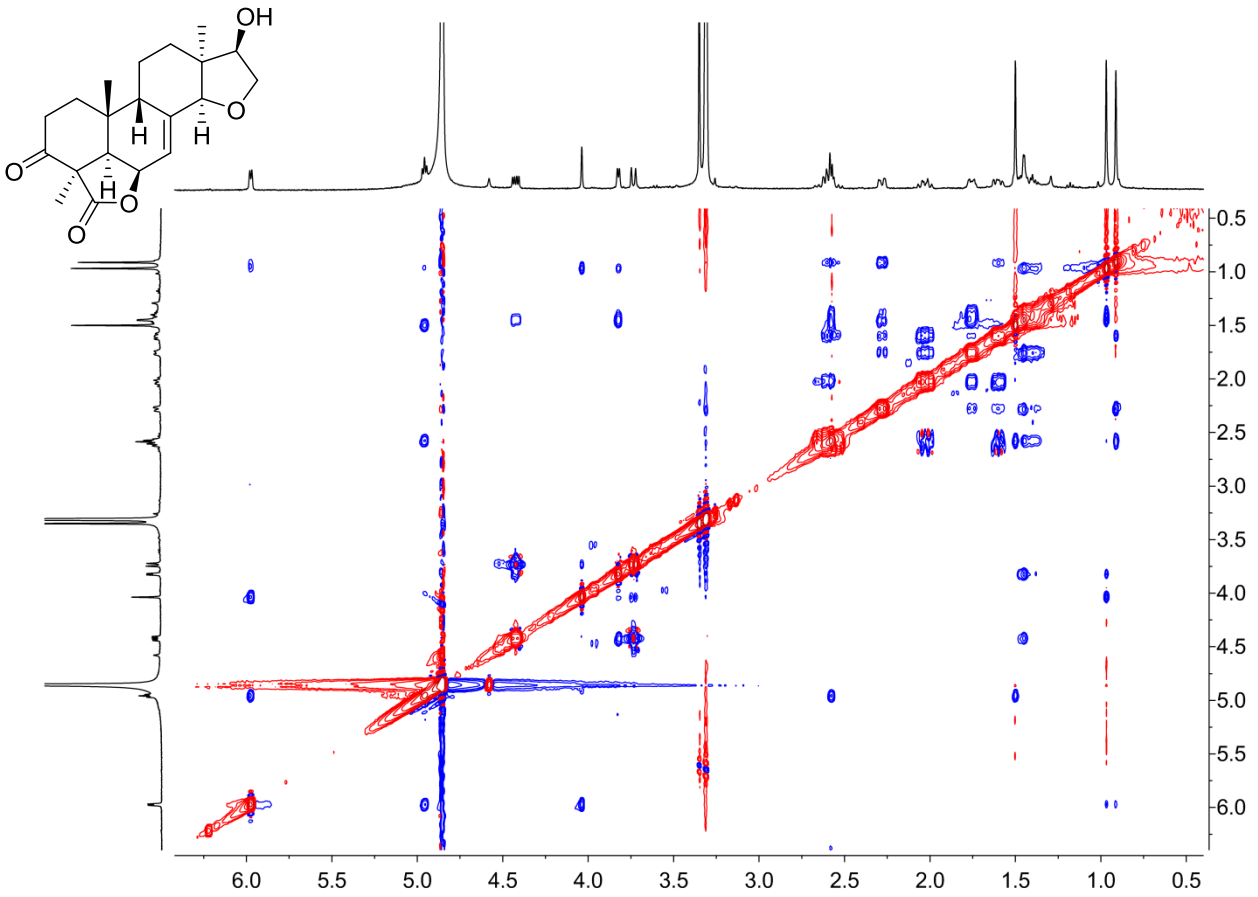

Fig. S156 NOESY spectrum (400 MHz, chloroform-*d*) of **11**

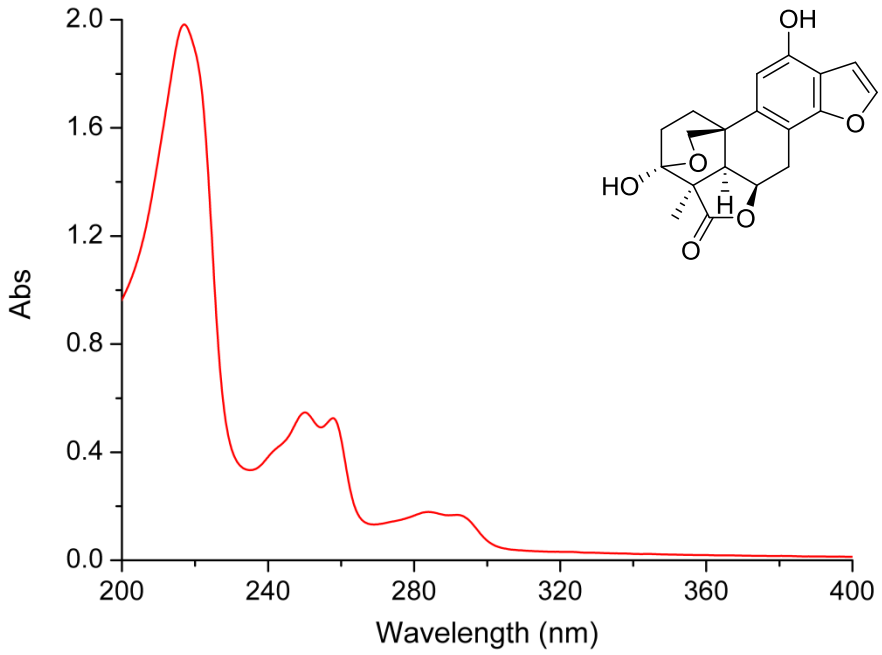

Fig. S157 UV spectrum of **12**

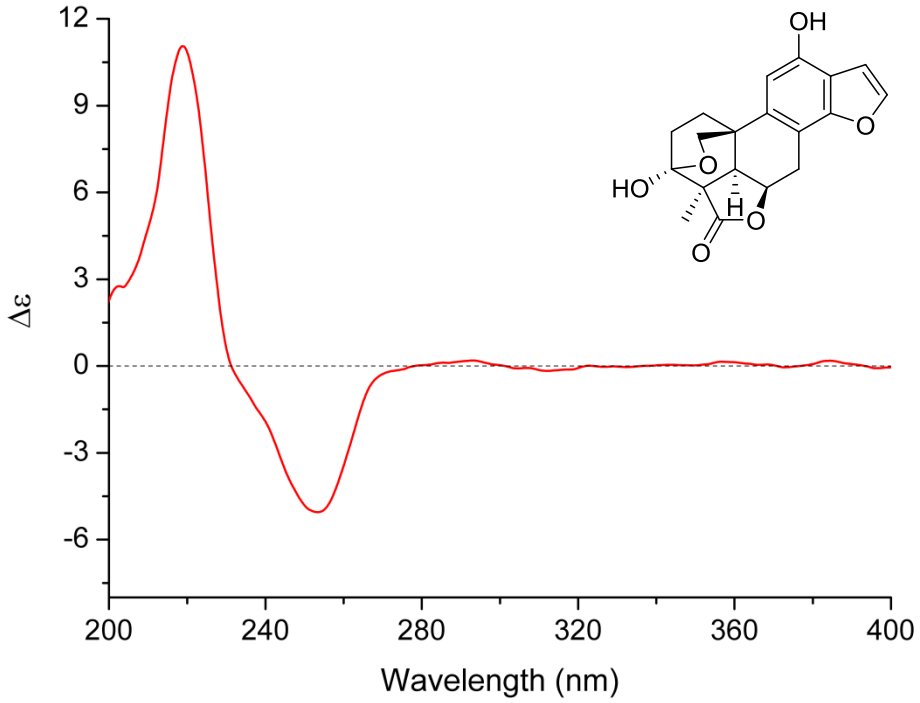

Fig. S158 Experimental ECD spectrum of **12**

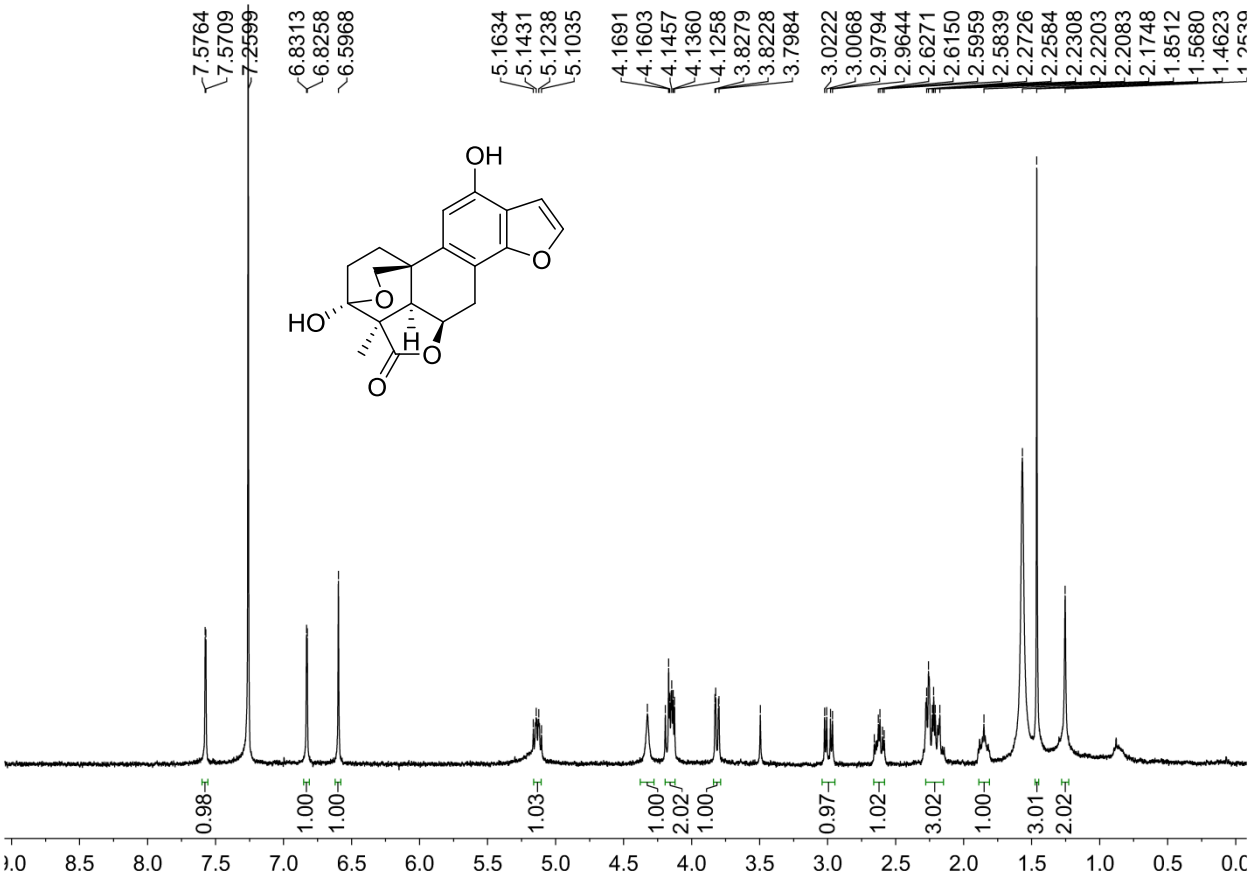

Fig. S159 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **12**

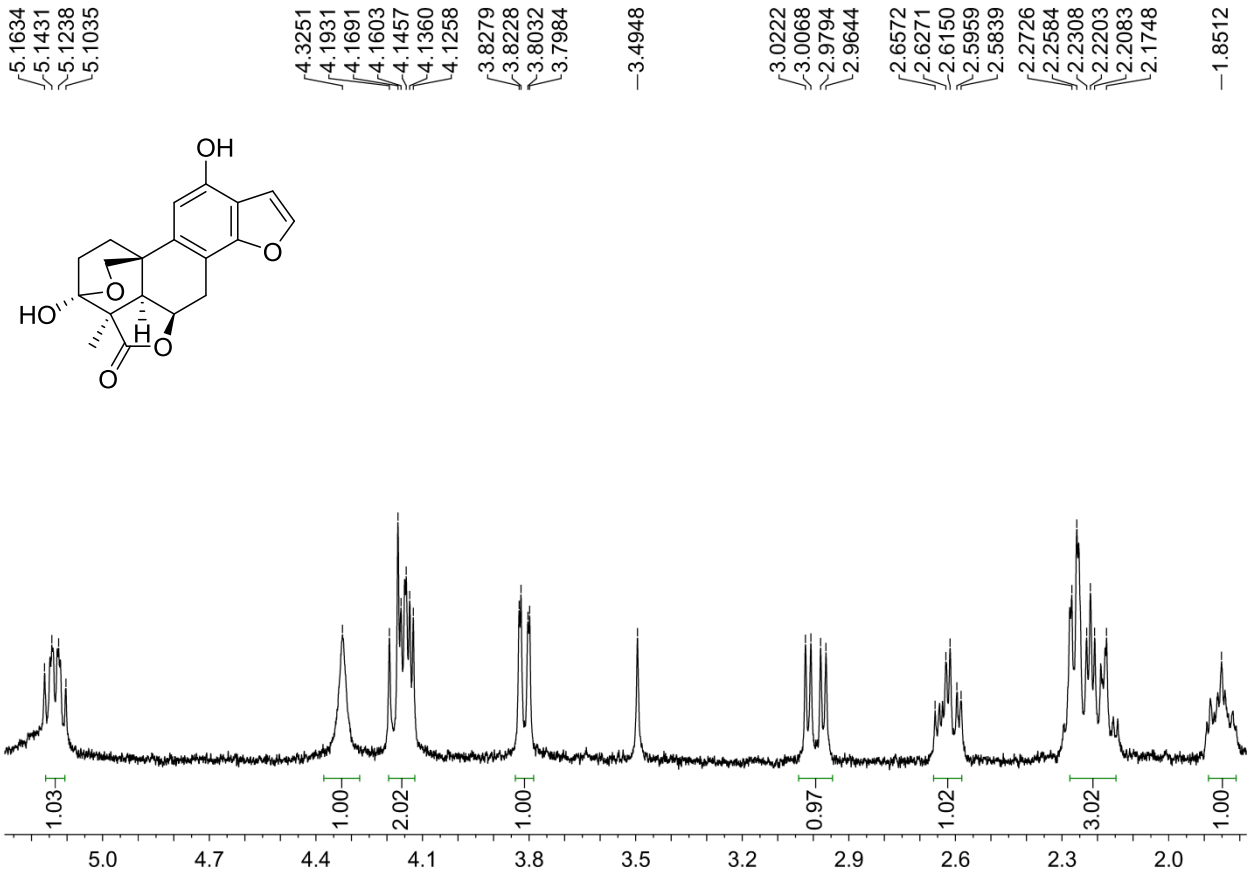

Fig. S160 ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of **12** (amplified)

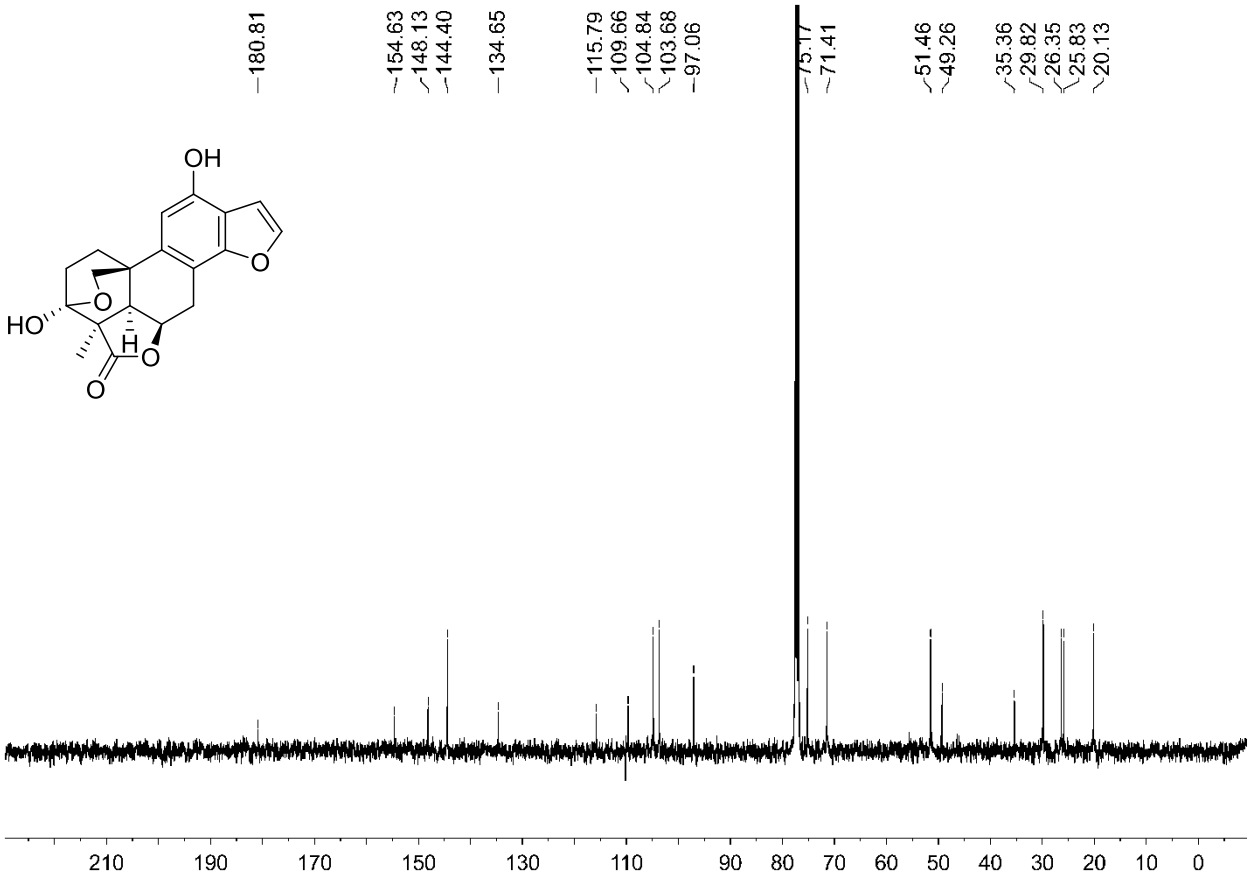

Fig. S161 ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of **12**

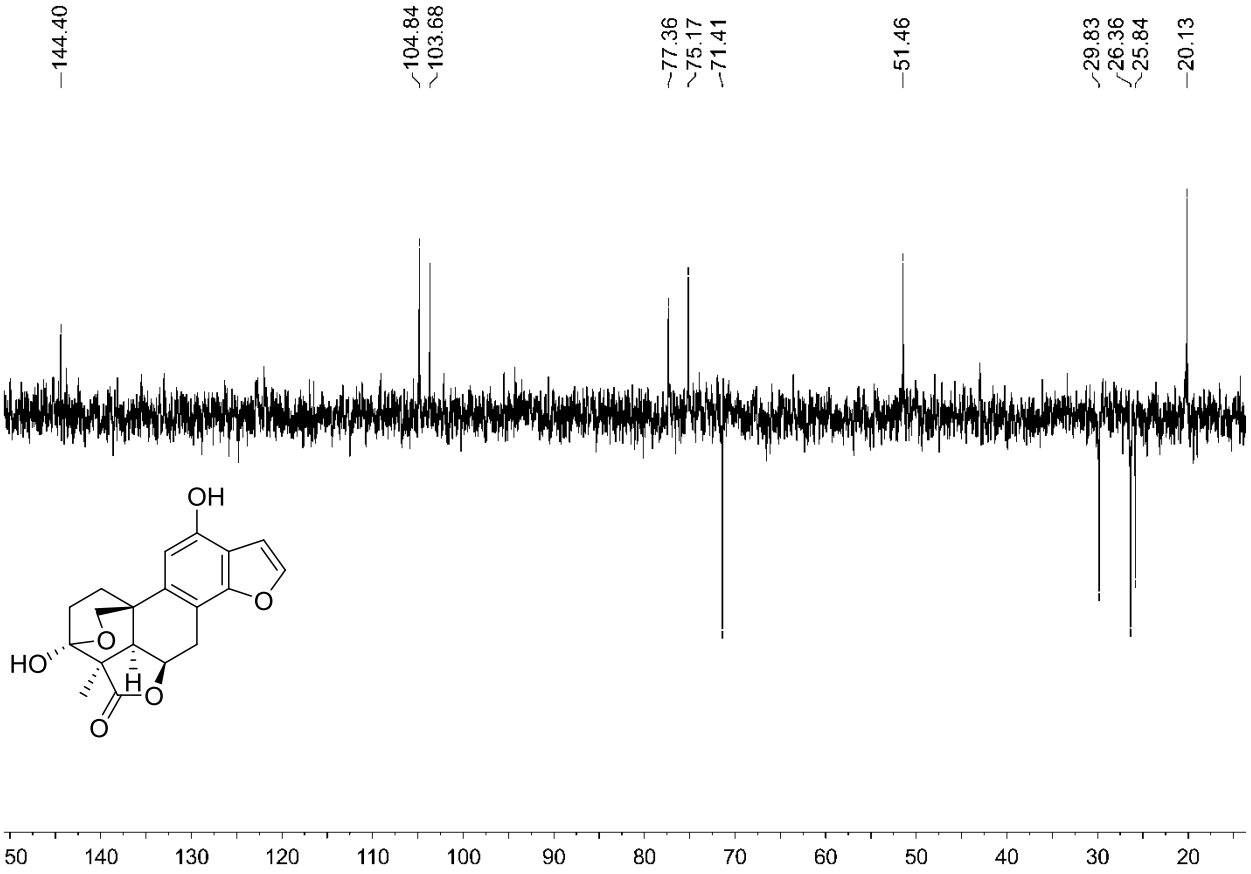

Fig. S162 DEPT135 (100 MHz, chloroform-*d*) spectrum of **12**

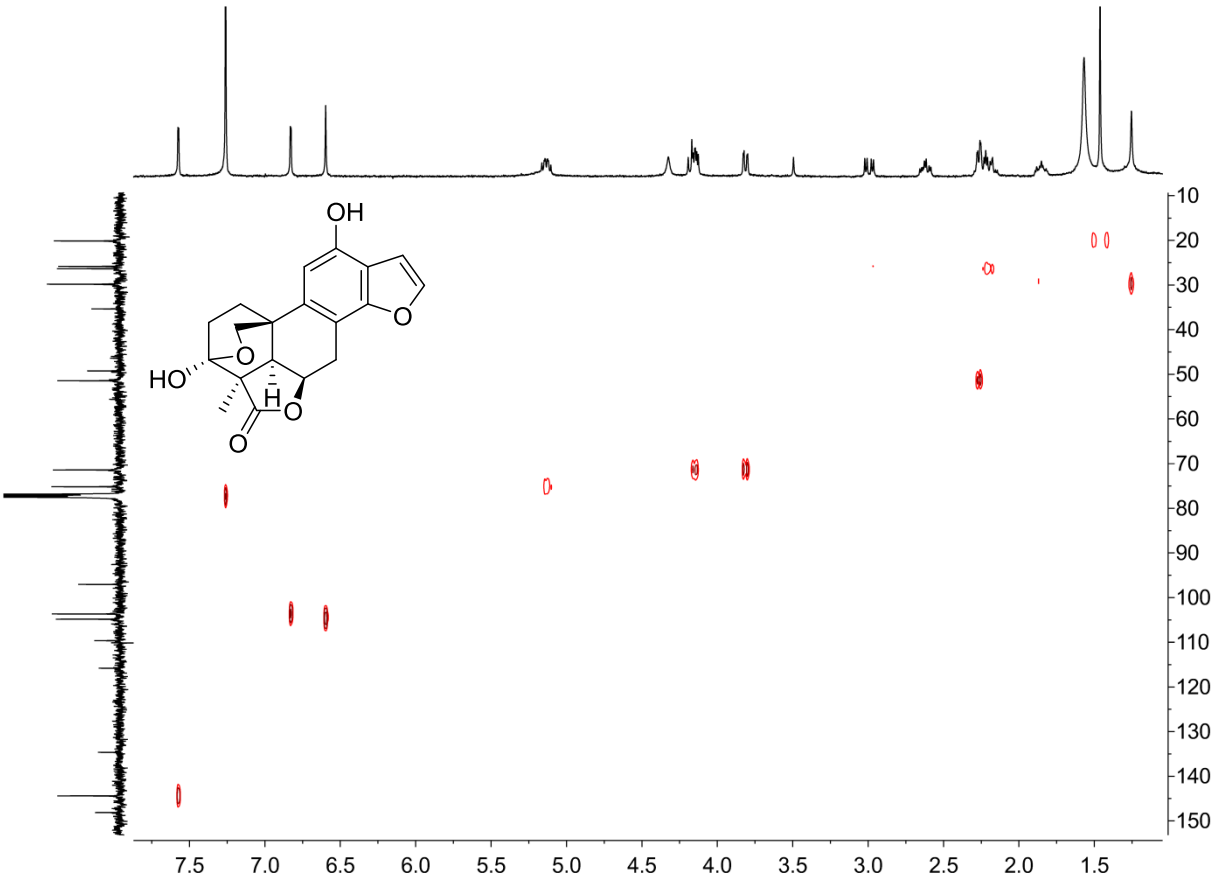

Fig. S163 HSQC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **12**

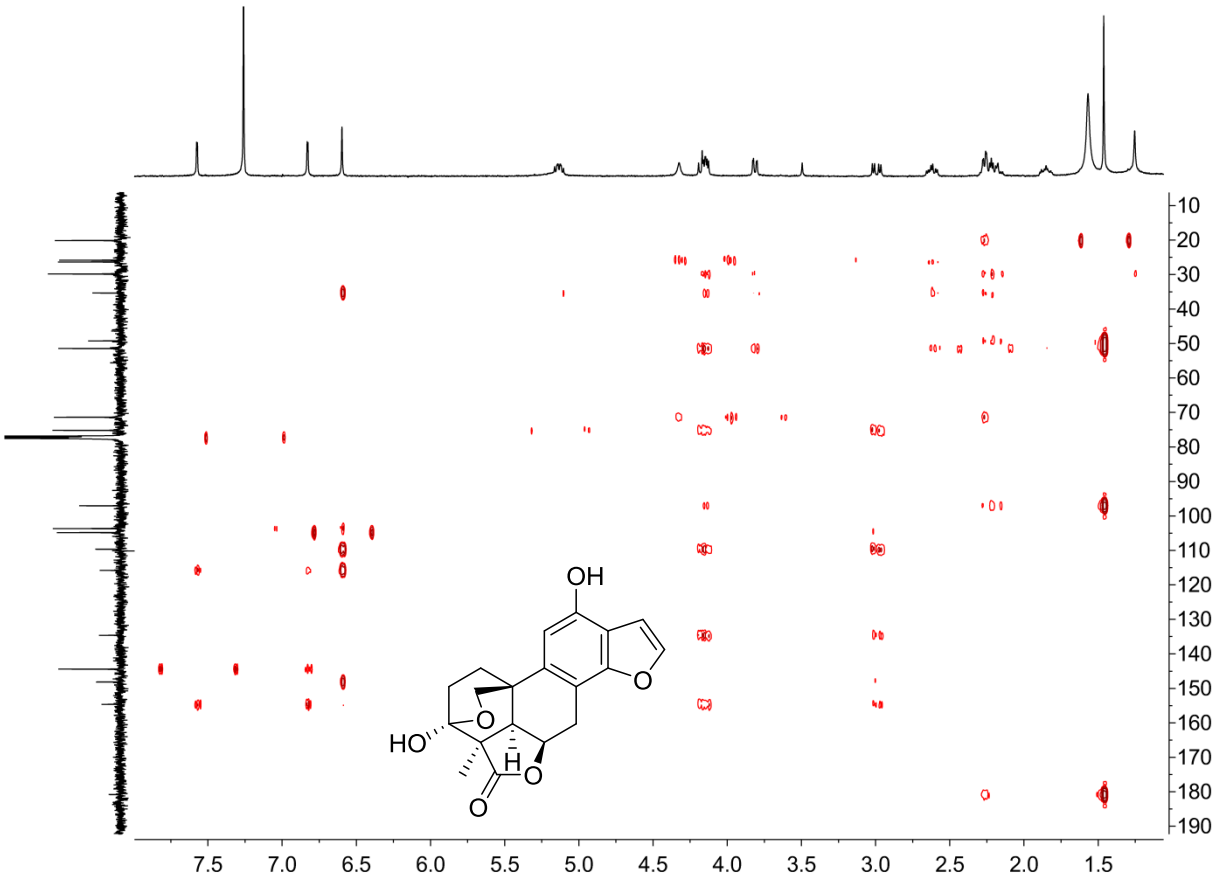

Fig. S164 HMBC spectrum (^{1}H: 400 MHz, ^{13}C: 100 MHz, chloroform-*d*) of **12**

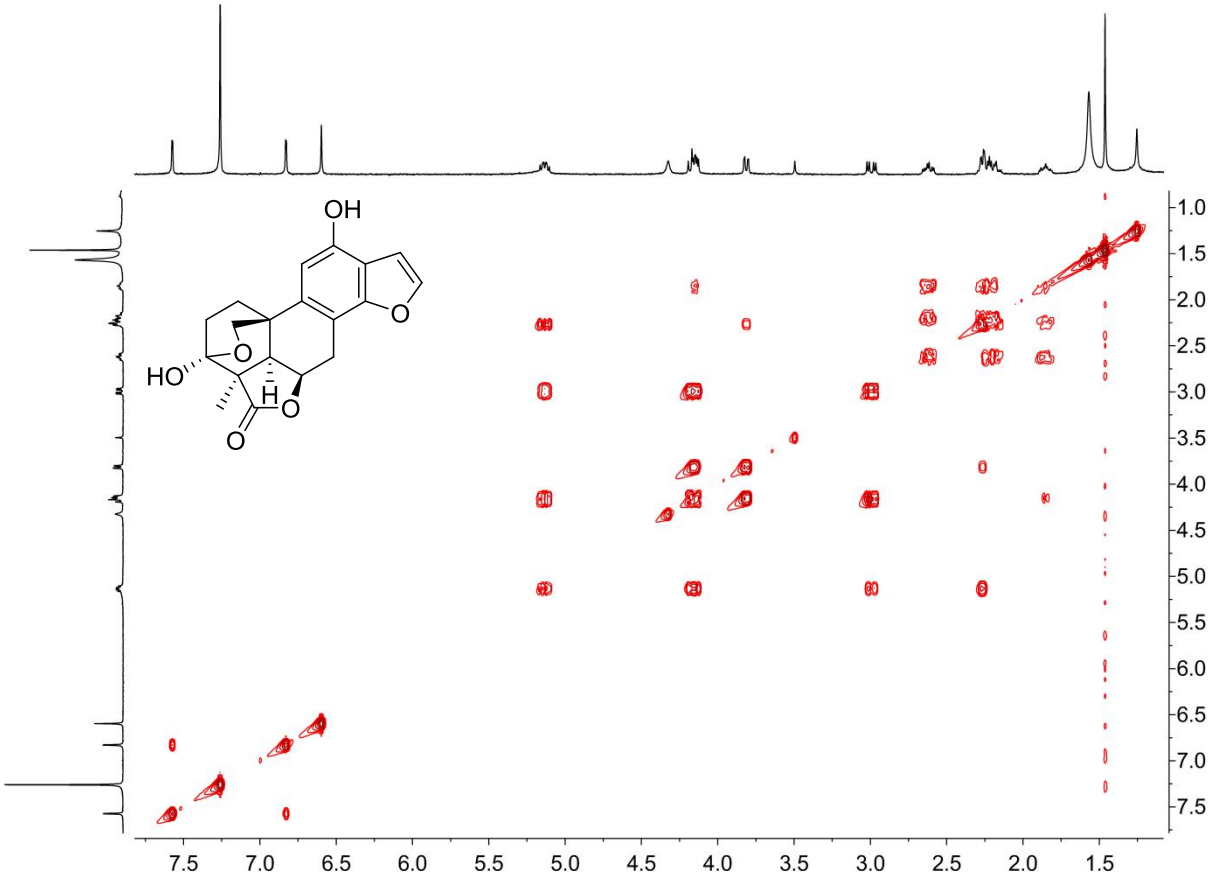

Fig. S165 ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of **12**

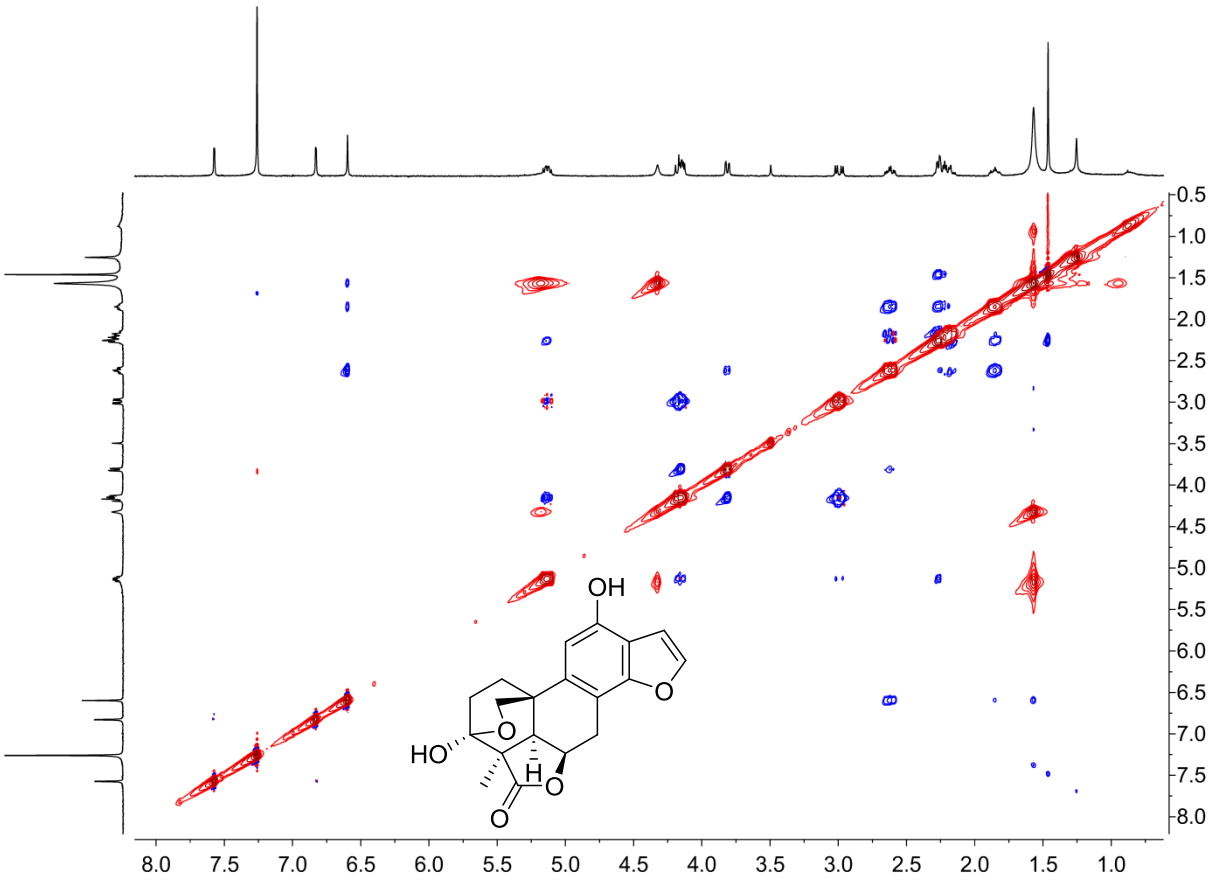

Fig. S166 NOESY spectrum (400 MHz, chloroform-*d*) of **12**

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