Supporting Information

Enantiomeric Pairs of Meroterpenoids with Diverse Heterocyclic Systems from *Rhododendron nyingchiense*

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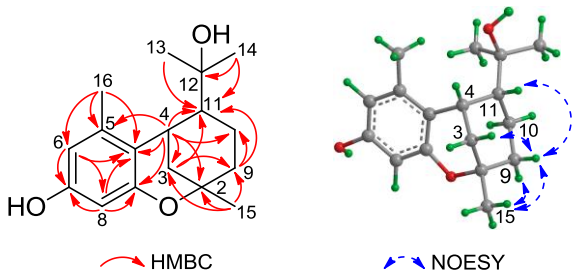

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Figure S1. Key 2D NMR correlations of **7**.

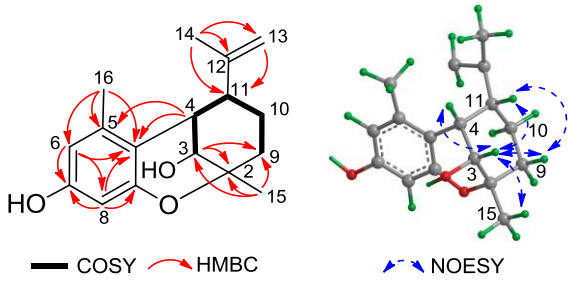

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Figure S2. Key 2D NMR correlations of **8**.

Physical and Spectroscopic Data of Known Compounds

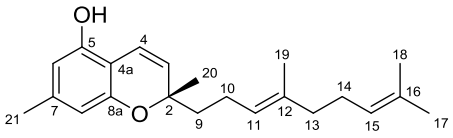
Confluentin (**9**): yellow gum; $[\alpha]^{25}_{D}$ +77.0 (*c* 0.15, MeOH); ^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 5.49 (1H, d, *J* = 10.0 Hz, H-3), 6.62 (1H, d, *J* = 10.0 Hz, H-4), 6.12 (1H, s, H-6), 6.24 (1H, s, H-8), 1.74 (2H, m, H_2-9), 2.12 (2H, m, H_2-10), 5.09 (2H, m, H-11, 15), 1.96 (2H, m, H_2-13), 2.04 (2H, m, H_2-14), 1.59 (3H, s, H_3-17), 1.58 (3H, s, H_3-18), 1.68 (3H, s, H_3-19), 1.38 (3H, s, H_3-20), 2.20 (3H, s, H_3-21); ^{13}C NMR (150 MHz, $CDCl_3$) δ_C: 78.4 (C, C-2), 127.3 (CH, C-3), 116.9 (CH, C-4), 106.9 (C, C-4a), 151.3 (C, C-5), 108.5 (CH, C-6), 139.6 (C, C-7), 109.9 (CH, C-8), 154.2 (C, C-8a), 41.2 (CH_2, C-9), 22.8 (CH_2, C-10), 124.2 (CH, C-11), 135.4 (C, C-12), 39.8 (CH_2, C-13), 26.8 (CH_2, C-14), 124.5 (CH, C-15), 131.4 (C, C-16), 25.8 (CH_3, C-17), 17.8 (CH_3, C-18), 16.1 (CH_3, C-19), 26.4 (CH_3, C-20), 21.6 (CH_3, C-21); positive ESIMS *m/z* 327.2 $[M + H]^+$; negative ESIMS *m/z* 325.0 $[M - H]^-$.

(*E*)-4-(3,7-dimethylocta-2,6-dienyl)-5-methylbenzene-1,3-diol (**10**): light yellow oil;

^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 6.22 (1H, s, H-2), 6.26 (1H, s, H-6), 3.28 (2H, d, J = 6.8 Hz, H_2-7), 5.13 (1H, t, J = 6.8 Hz, H-8), 2.03 (2H, m, H_2-10), 2.08 (2H, m, H_2-11), 5.04 (1H, t, J = 7.2 Hz, H-12), 1.66 (3H, s, H_3-14), 1.58 (3H, s, H_3-15), 1.78 (3H, s, H_3-16), 2.23 (3H, s, H_3-17); ^{13}C NMR (150 MHz, $CDCl_3$) δ_C: 154.4 (C, C-1), 101.2 (CH, C-2), 155.6 (C, C-3), 118.1 (C, C-4), 138.6 (C, C-5), 109.8 (CH, C-6), 25.3 (CH_2, C-7), 122.3 (CH, C-8), 137.7 (C, C-9), 39.8 (CH_2, C-10), 26.6 (CH_2, C-11), 124.1 (CH, C-12), 132.0 (C, C-13), 25.8 (CH_3, C-14), 17.8 (CH_3, C-15), 16.3 (CH_3, C-16), 20.2 (CH_3, C-17); positive ESIMS *m/z* 261.2 $[M + H]^+$; negative ESIMS *m/z* 259.0 $[M - H]^-$.

Grifolin (**11**): light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 6.23 (2H, s, H-4, 6), 3.38 (2H, d, J = 6.4 Hz, H_2-7), 5.26 (1H, t, J = 6.4 Hz, H-8), 1.92–2.14 (8H, m, H_2-10, 11, 14, 15), 5.07 (2H, m, H-12, 16), 1.67 (3H, s, H_3-18), 1.58 (6H, s, H_3-19, 20), 1.81 (3H, s, H_3-21), 2.21 (3H, s, H_3-22); ^{13}C NMR (150 MHz, $CDCl_3$) δ_C: 155.0 (C, C-1, 3), 110.6 (C, C-2), 109.2 (CH, C-4, 6), 137.7 (C, C-5), 22.3 (CH_2, C-7), 121.8 (CH, C-8), 139.1 (C, C-9), 39.8 (CH_2, C-10), 26.8 (CH_2, C-11), 123.8 (CH, C-12), 135.8 (C, C-13), 39.8 (CH_2, C-14), 26.5 (CH_2, C-15), 124.6 (CH, C-16), 131.4 (C, C-17), 25.8 (CH_3, C-18), 17.8 (CH_3, C-19), 16.4 (CH_3, C-20), 16.2 (CH_3, C-21), 21.2 (CH_3, C-22); positive ESIMS *m/z* 329.2 $[M + H]^+$; negative ESIMS *m/z* 327.0 $[M - H]^-$.

Grifolinone A (**12**): light yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ_H: 6.24 (2H, s, H-4, 6), 3.38 (2H, d, J = 7.2 Hz, H_2-7), 5.25 (1H, t, J = 7.2 Hz, H-8), 2.07 (2H, t, J = 7.2 Hz, H_2-10), 2.16 (2H, m, H_2-11), 5.19 (1H, t, J = 6.0 Hz, H-12), 3.04 (2H, s, H_2-14), 6.11 (1H, s, H-16), 2.15 (3H, d, J = 1.2 Hz, H_3-18), 1.87 (3H, d, J = 1.2 Hz, H_3-19), 1.60 (3H, s, H_3-20), 1.79 (3H, s, H_3-21), 2.19 (3H, s, H_3-22); ^{13}C NMR (150 MHz, $CDCl_3$) δ_C: 155.1 (C, C-1, 3), 110.8 (C, C-2), 109.1 (CH, C-4, 6), 137.7 (C, C-5), 22.3 (CH_2, C-7), 122.6 (CH, C-8), 137.5 (C, C-9), 39.4 (CH_2, C-10), 26.5 (CH_2, C-11), 129.0 (CH, C-12), 130.0 (C, C-13), 55.3 (CH_2, C-14), 200.4 (C, C-15), 123.2 (CH, C-16), 156.5 (C, C-17), 27.9 (CH_3, C-18), 21.0 (CH_3, C-19), 16.6 (CH_3, C-20), 16.3 (CH_3, C-21), 21.2 (CH_3, C-22); positive ESIMS *m/z* 343.2 $[M + H]^+$; negative ESIMS *m/z* 341.0 $[M - H]^-$.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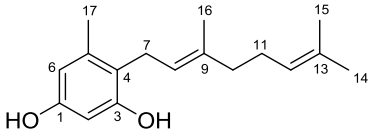
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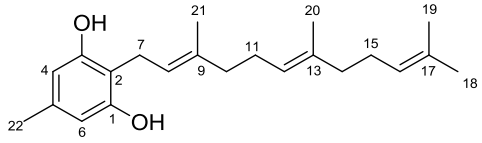
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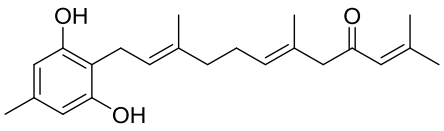
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X-ray Crystallographic Data

X-ray crystallographic data for **1a**

Empirical formula	$C_{17}H_{24}O_5$
Formula weight	308.36
Temperature	296 K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P2121 21
Unit cell dimensions	a = 9.3465 (3)Å, α = 90°
	b = 9.3699 (3) Å, β = 90◦
	c = 18.6281(6) Å, γ = 90°
Volume	1631.37(9)$Å^3$
Z	4
Calculated density	1.255 Mg/m^3
Absorption coefficient	0.751 mm^{-1}
F(000)	664
Crystal size	0.20 x 0.15 x 0.10 mm^3
Theta range for data collection	4.748 to 69.906°
Index ranges	-8<=h<=10, -11<=k<=11,
	-21<=l<=22
Reflections collected	10793
Independent reflections	2906 [R(int) = 0.0316]
Completeness to theta = 67.679°	96.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7533 and 0.4893
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2906 / 0 / 208
Goodness-of-fit on F^2	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0318, wR2 = 0.0871
R indices (all data)	R1 = 0.0328, wR2 = 0.0881
Absolute structure parameter	0.15 (7)
Extinction coefficient	0.0035 (6)
Largest diff. peak and hole	0.131 and -0.180 $e.Å^{-3}$

X-ray crystallographic data for **3a**

Empirical formula	$C_{17}H_{22}O_2$
Formula weight	258.34
Temperature	301.94 K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	C 1 2 1
Unit cell dimensions	a = 29.6580 (19) Å, α = 90°
	b = 6.8498 (5) Å, β = 104.450(2)°
	c = 7.4333(5) Å, γ = 90°
Volume	1462.31(17) $Å^3$
Z	4
Calculated density	1.173 Mg/m^3
Absorption coefficient	0.588 mm^{-1}
F(000)	560
Crystal size	0.15 x 0.05 x 0.02 mm^3
Theta range for data collection	6.151 to 67.487°
Index ranges	-35<=h<=31, -7<=k<=7, -8<=l<=8
Reflections collected	10832
Independent reflections	2508 [R(int) = 0.0457]
Completeness to theta = 67.487°	96.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7533 and 0.5341
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2508 / 1 / 176
Goodness-of-fit on F^2	1.103
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.1056
R indices (all data)	R1 = 0.0397, wR2 = 0.1074
Absolute structure parameter	0.02 (10)
Extinction coefficient	n/a
Largest diff. peak and hole	0.167 and -0.155 e.$Å^{-3}$

X-ray crystallographic data for **4a**

Empirical formula	$C_{17}H_{22}O_2$
Formula weight	258.34
Temperature	293 K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P21 21 21
Unit cell dimensions	a = 6.0879(4) Å, α = 90°
	b = 8.0119(6) Å, β = 90°
	c = 29.617(2) Å, γ = 90°
Volume	1444.57(17) $Å^3$
Z	4
Calculated density	1.188 Mg/m^3
Absorption coefficient	0.596 mm^{-1}
F(000)	560
Crystal size	0.05 x 0.01 x 0.005 mm^3
Theta range for data collection	2.984 to 70.120°
Index ranges	-7<=h<=7, -8<=k<=9, -36<=l<=35
Reflections collected	11826
Independent reflections	2683 [R(int) = 0.0500]
Completeness to theta = 67.487°	97.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7533 and 0.5844
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2683 / 0 / 178
Goodness-of-fit on F^2	1.105
Final R indices [I>2sigma(I)]	R1 = 0.0376, wR2 = 0.1115
R indices (all data)	R1 = 0.0506, wR2 = 0.1208
Absolute structure parameter	0.16 (10)
Extinction coefficient	0.0035 (9)
Largest diff. peak and hole	0.226 and -0.196 e.$Å^{-3}$

X-ray crystallographic data for **5a**

Empirical formula	$C_{17.50}H_{24}O_{3.50}$
Formula weight	290.37
Temperature	296 K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P21 21 21
Unit cell dimensions	a = 10.27200(10) Å, α = 90°
	b = 16.5830(2) Å, β = 90°
	c = 18.9486(2) Å, γ = 90°
Volume	3227.72(6) $Å^3$
Z	8
Calculated density	1.195 Mg/m^3
Absorption coefficient	0.658 mm^{-1}
F(000)	1256
Crystal size	0.22 x 0.2 x 0.15 mm^3
Theta range for data collection	3.542 to 69.746°
Index ranges	-12<=h<=11, -17<=k<=20, -22<=l<=22
Reflections collected	20904
Independent reflections	5872 [R(int) = 0.0399]
Completeness to theta = 67.487°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7532 and 0.5807
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5872 / 0 / 392
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0343, wR2 = 0.0937
R indices (all data)	R1 = 0.0360, wR2 = 0.0959
Absolute structure parameter	0.11 (6)
Extinction coefficient	0.0051 (4)
Largest diff. peak and hole	0.287 and -0.198 $e.Å^{-3}$

X-ray crystallographic data for **6a**

Empirical formula	$C_{18}H_{26}O_3$
Formula weight	290.39
Temperature	296.15 K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P21 21 21
Unit cell dimensions	a = 10.1815(2) Å, α = 90°
	b = 10.1849(2) Å, β = 90°
	c = 15.7912(3) Å, γ = 90°
Volume	1637.51(6) $Å^3$
Z	4
Calculated density	1.178 Mg/m^3
Absorption coefficient	0.622 mm^{-1}
F(000)	632
Crystal size	0.25 x 0.2 x 0.18 mm^3
Theta range for data collection	5.167 to 69.707°
Index ranges	-12<=h<=12, -12<=k<=11, -17<=l<=19
Reflections collected	12421
Independent reflections	2970 [R(int) = 0.0301]
Completeness to theta = 67.487°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7532 and 0.6169
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2970 / 0 / 196
Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R1 = 0.0413, wR2 = 0.1078
R indices (all data)	R1 = 0.0420, wR2 = 0.1087
Absolute structure parameter	-0.03 (8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.192 and -0.241 e.$Å^{-3}$

The structures of **1a**, **3a**, **4a**, **5a**, and **6a** were solved by direct methods using SHELXS-97 program and refined with full-matrix least-squares calculations on F^2 using SHELXL-97. Their crystallographic data have been deposited at the Cambridge Crystallographic Data Center. The deposition numbers of Crystallographic data for **1a**, **3a**, **4a**, **5a**, and **6a** have been deposited at the Cambridge Crystallographic Data Center (deposition no. CCDC 1569502 for **1a**, CCDC 1585591 for **3a**, CCDC 1821249 for **4a**, CCDC 1821254 for **5a**, and CCDC 1821262 for **6a**). Copy of the data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

NMR Calculation Details for 2

In order to determine the relative configurations at C-11 and C-4, 4a, four model compounds **2a'** (2*S*, 3*S*, 4*R*, 4a*R*, 11*S*), **2b'** (2*S*, 3*S*, 4*S*, 4a*S*, 11*S*), **2c'** (2*S*, 3*S*, 4*R*, 4a*R*, 11*R*), and **2d'** (2*S*, 3*S*, 4*S*, 4a*S*, 11*R*) were designed. Conformational analysis was carried out. Conformation search using molecular mechanics calculations was performed in Discovery Studio 3.5 Client with MMFF force field with 20 kcal mol^{-1} upper energy limit.[1] The optimized conformation geometries and thermodynamic parameters of all selected conformations were provided. The predominant conformers were optimized at B3LYP/6-31G (d,p) level. For all optimized structures, vibrational spectra were calculated to ensure that no imaginary frequencies for energy minimum were obtained. NMR calculations were performed at the levels of mPW1PW91/6-31G(d,p) with the gauge-independent atomic orbital (GIAO) method.[2] The solvent effect was considered by using chloroform in the calculations to resemble the experimental condition. The polarized continuum model (PCM) of Tomasi et al. was used.[3] The calculated ^{13}C NMR chemical shifts were analyzed by subtracting the isotopic shifts for TMS calculated with the same methods.[1] Different conformers for the supposed structures were considered. The ^{13}C NMR chemical shifts in each compound were considered as the average values of the same atoms in the different conformers. The average values were obtained by the Boltzmann distributions, using the relative Gibbs free energies as weighting factors.[4] The differences $\Delta\delta$ were determined by subtracting the experimental chemical shifts δexptl from the calculated chemical shifts δcalcd. Largest absolute deviation (LAD) and mean absolute deviation (MAD) were adopted for evaluation of the results.

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ECD Calculation Details for 2a and 2b

Model compounds **2a'** (2*S*, 3*S*, 4*R*, 4a*R*, 11*S*) and *ent*-**2a'** (2*R*, 3*R*, 4*S*, 4a*S*, 11*R*) were designed for the theoretical ECD calculations, which were performed using Gaussian 09[1] and figured using GaussView 5.0.[2] Conformation search using molecular mechanics calculations was performed in Discovery Studio 3.5 Client with MMFF force field with 20 kcal mol^{-1} upper energy limit.[3] The optimized conformation geometries and thermodynamic parameters of all selected conformations were provided. The predominant conformers were optimized at B3LYP/6-31G (d,p) level. The theoretical calculation of ECD was performed using time dependent Density Functional Theory (TDDFT) at B3LYP/6-31G (d,p) level in MeOH with PCM model.[4] The ECD spectra of compounds **2a'** and *ent*-**2a'** were obtained by weighing the Boltzmann distribution rate of each geometric conformation.[5]

The ECD spectra were simulated by overlapping Gaussian functions for each transition according to:

$$\Delta\varepsilon(E) = \frac{1}{2.297\times10^{-39}} \times \frac{1}{\sqrt{2\pi\sigma}} \sum_{i}^{A} \Delta E_i R_i e^{-[(E-E_i)/(2\sigma)]^2} \qquad (1)$$

The σ represented the width of the band at $1/e$ height, and ΔE_i and R_i were the excitation energies and rotational strengths for transition i, respectively. R_{vel} had been used in this work.

The absolute configurations of compounds **2a** and **2b** were determined by comparing the experimental ECD spectra with quantum chemical TDDFT calculated theoretical ECD spectra of the models **2a'** and *ent*-**2a'**.

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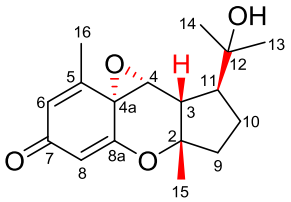
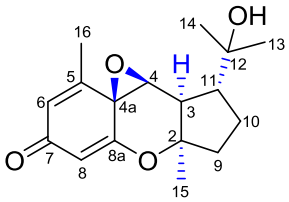
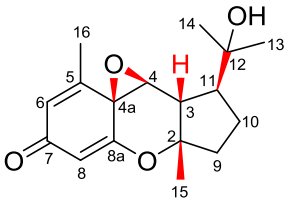


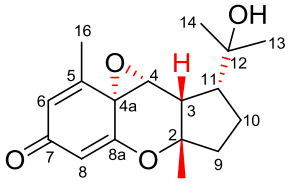
2a'



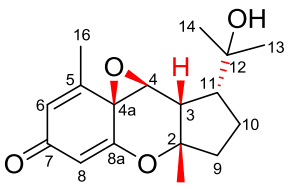
***ent*-2a'**



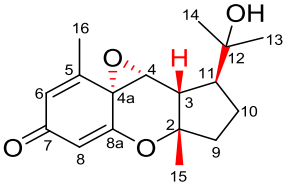
2b'



2c'



2d'



2a'

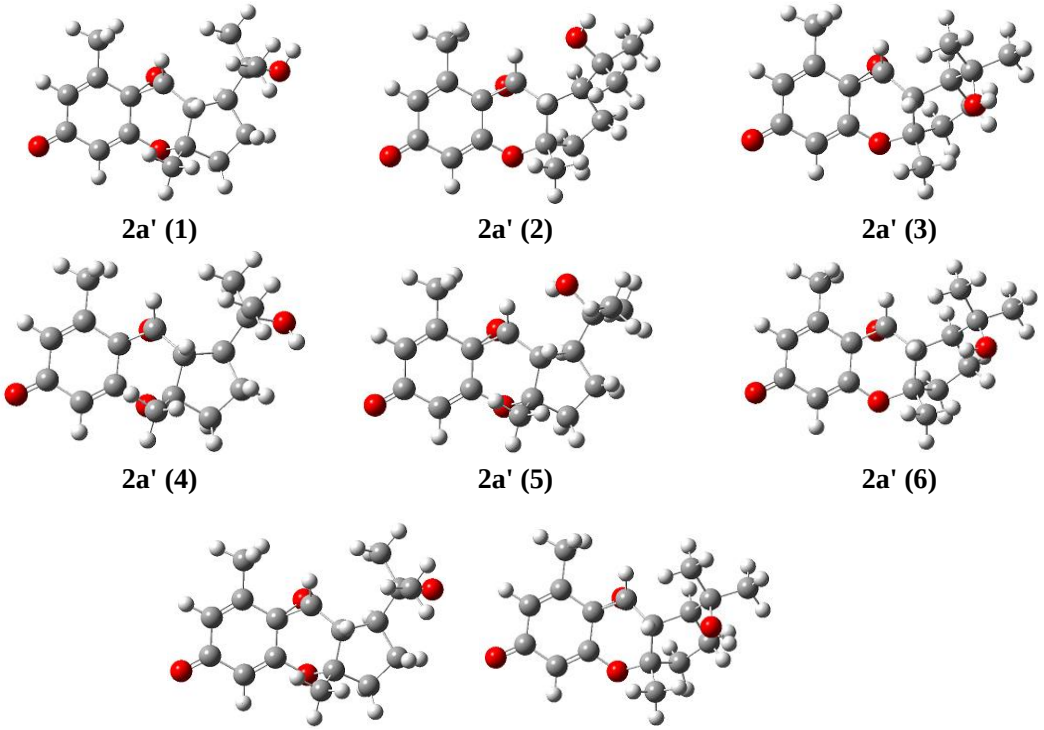


Figure S3. Optimized geometries of predominant conformers for **2a'** at the B3LYP/6-31G(d,p) level in the gas phase**.**

Table S1. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized **2a'** at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
2a' (1)	-961.562809	-961.610321	0.3
2a' (2)	-961.567374	-961.614680	29.5
2a' (3)	-961.567778	-961.614506	24.6
2a' (4)	-961.614506	-961.610301	0.3
2a' (5)	-961.568115	-961.614800	33.6
2a' (6)	-961.566173	-961.612908	4.5
2a' (7)	-961.563347	-961.611463	1.0
2a' (8)	-961.566676	-961.613200	6.2

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S2. Optimized Z-matrixes of **2a'** in the gas phase (Å) at B3LYP/6-31G(d,p) level

2a' (1)				**2a' (2)**			
C	-3.77395	1.161533	0.159956	C	-3.8292	1.14283	0.230353
C	-4.15966	-0.23188	-0.16782	C	-4.18424	-0.28584	0.40617
C	-3.06779	-1.17928	-0.42887	C	-3.11793	-1.26555	0.180143

C	-1.78113	-0.78463	-0.38725	C	-1.87249	-0.87636	-0.16406
C	-1.39888	0.625876	-0.10177	C	-1.51275	0.56053	-0.30719
C	-2.49891	1.588359	0.206836	C	-2.59698	1.566008	-0.10486
O	-0.77156	-1.64805	-0.659	O	-0.92633	-1.79644	-0.44978
C	0.351223	-1.7024	0.278489	C	0.47168	-1.62566	-0.07478
C	0.982812	-0.29269	0.525676	C	0.914913	-0.17066	0.287809
C	0.010385	0.855896	0.332403	C	-0.07945	0.896664	-0.10102
C	1.444382	-2.52686	-0.43989	C	1.331079	-1.99496	-1.29535
C	3.33716	0.810081	-0.06899	C	3.350386	0.801368	0.384615
C	2.247665	-0.24996	-0.37556	C	2.280802	0.056953	-0.44684
C	2.737137	-1.70945	-0.31973	C	2.679764	-1.32309	-1.01565
C	-0.14626	-2.35001	1.570992	C	0.687035	-2.5786	1.104592
C	-2.12974	3.015621	0.50298	C	-2.26033	3.016734	-0.31261
O	-5.3412	-0.57143	-0.19262	O	-5.32305	-0.61714	0.735284
O	4.418376	0.426514	-0.93942	O	2.67971	2.005535	0.808447
C	2.886095	2.229046	-0.45351	C	3.829577	0.030163	1.624504
H	1.905665	-0.05571	-1.39996	H	2.069427	0.7085	-1.30369
H	1.297705	-0.26766	1.576063	H	1.043066	-0.08809	1.371988
O	-0.37428	1.145554	-1.00442	O	-0.60691	0.827518	-1.42317
H	0.195906	1.739911	0.942136	H	0.184737	1.897991	0.234028
C	3.831624	0.786561	1.38666	C	4.548775	1.175129	-0.50111
H	-4.6012	1.837935	0.355322	H	-4.64303	1.845942	0.38345
H	-3.32676	-2.21137	-0.6359	H	-3.35769	-2.3162	0.296589
H	1.14967	-2.61934	-1.48917	H	0.861692	-1.55074	-2.17874
H	1.530382	-3.53798	-0.03158	H	1.39705	-3.07601	-1.44905
H	3.230148	-1.91089	0.639506	H	3.249139	-1.9067	-0.28341
H	3.459875	-1.93059	-1.10601	H	3.300243	-1.23953	-1.91229
H	-0.63172	-3.30446	1.348951	H	0.40281	-3.59564	0.82124
H	0.691959	-2.53677	2.249799	H	1.733435	-2.58522	1.425244
H	-0.86899	-1.71146	2.089893	H	0.072618	-2.27407	1.957739
H	-1.43684	3.397593	-0.25365	H	-1.74067	3.157701	-1.26538
H	-3.01829	3.649763	0.517936	H	-3.16585	3.626681	-0.30834
H	-1.63526	3.109279	1.478079	H	-1.59802	3.393445	0.476672
H	5.110904	1.095961	-0.85454	H	3.309733	2.531524	1.319572
H	3.734004	2.921384	-0.3804	H	4.524076	0.651883	2.201676
H	2.103853	2.614228	0.205988	H	4.364779	-0.88542	1.356898
H	2.514135	2.250805	-1.48101	H	2.997851	-0.2331	2.283231
H	4.194564	-0.205	1.66817	H	4.217941	1.769379	-1.35768
H	4.663542	1.490489	1.505764	H	5.273789	1.769812	0.067337
H	3.052944	1.088308	2.094642	H	5.071672	0.288105	-0.8716
2a' (3)				**2a' (4)**			
C	-3.89527	1.070051	0.219752	C	-3.77782	1.164597	0.167793
C	-4.20035	-0.36217	0.457414	C	-4.1675	-0.23469	-0.12746

C	-3.10138	-1.31068	0.276896	C	-3.07908	-1.18531	-0.39367
C	-1.86734	-0.89818	-0.08811	C	-1.79285	-0.7883	-0.38154
C	-1.56231	0.543054	-0.30578	C	-1.40656	0.625434	-0.12049
C	-2.67919	1.52001	-0.1355	C	-2.50252	1.593268	0.185305
O	-0.89381	-1.80504	-0.29592	O	-0.78635	-1.65337	-0.66304
C	0.527106	-1.53837	-0.09708	C	0.349926	-1.70001	0.255846
C	0.907552	-0.06934	0.264252	C	0.976639	-0.28807	0.506035
C	-0.1402	0.938198	-0.13988	C	0.006105	0.859413	0.300266
C	1.265075	-1.8037	-1.41823	C	1.437983	-2.51095	-0.48377
C	3.393468	0.738397	0.439996	C	3.350612	0.819642	-0.04447
C	2.264263	0.213452	-0.47846	C	2.253573	-0.23359	-0.38106
C	2.611362	-1.09975	-1.22855	C	2.732611	-1.69915	-0.34769
C	0.949929	-2.49947	1.016803	C	-0.12119	-2.36151	1.551537
C	-2.39459	2.972055	-0.40686	C	-2.1296	3.025966	0.448516
O	-5.32876	-0.71464	0.800847	O	-5.34841	-0.57695	-0.12433
O	3.561805	-0.26459	1.457295	O	4.485387	0.560738	-0.89247
C	4.704295	0.904204	-0.34565	C	2.922379	2.237972	-0.4376
H	2.080511	0.993861	-1.22702	H	1.925828	-0.02188	-1.40646
H	1.046031	0.011322	1.346853	H	1.279427	-0.25949	1.559769
O	-0.6856	0.80207	-1.44922	O	-0.38719	1.128602	-1.03779
H	0.067844	1.968096	0.154149	H	0.1986	1.751838	0.895042
C	3.014416	2.075498	1.098778	C	3.804186	0.792032	1.424257
H	-4.73266	1.750694	0.344575	H	-4.60227	1.844067	0.364276
H	-3.30115	-2.36137	0.452675	H	-3.3408	-2.22027	-0.58225
H	0.693877	-1.3342	-2.22475	H	1.142866	-2.5744	-1.53492
H	1.353877	-2.87222	-1.63567	H	1.523436	-3.53209	-0.10149
H	3.280338	-1.70974	-0.61431	H	3.224308	-1.92571	0.608216
H	3.118095	-0.90976	-2.17877	H	3.443008	-1.92484	-1.14751
H	0.754352	-3.53256	0.71624	H	-0.59912	-3.32	1.330614
H	2.010959	-2.38292	1.250458	H	0.727868	-2.54229	2.218542
H	0.37881	-2.29191	1.927068	H	-0.84375	-1.73349	2.083139
H	-1.88147	3.091321	-1.36618	H	-1.44765	3.393364	-0.32501
H	-3.3221	3.547525	-0.42835	H	-3.01809	3.660136	0.464279
H	-1.74924	3.409523	0.365389	H	-1.62112	3.13845	1.414374
H	4.285062	0.014169	2.034685	H	4.886566	-0.27021	-0.60593
H	5.495054	1.286488	0.310961	H	3.779958	2.910062	-0.34547
H	4.588062	1.61642	-1.16914	H	2.122381	2.616266	0.203109
H	5.039536	-0.05032	-0.75689	H	2.577195	2.262525	-1.47446
H	2.120353	1.975658	1.719959	H	4.137735	-0.20591	1.730844
H	3.828305	2.423834	1.745508	H	4.645234	1.47918	1.551415
H	2.835415	2.854079	0.349812	H	3.009588	1.102041	2.110148
2a' (5)				**2a' (6)**			
C	-3.73196	1.158839	0.122084	C	-3.90906	1.05589	0.222939

C	-4.10767	-0.21413	-0.29043	C	-4.20408	-0.37714	0.467797
C	-3.00897	-1.16095	-0.52759	C	-3.09818	-1.31903	0.292505
C	-1.72417	-0.77964	-0.40138	C	-1.86747	-0.90031	-0.0757
C	-1.34917	0.618116	-0.04696	C	-1.57319	0.541799	-0.30337
C	-2.45841	1.572542	0.254147	C	-2.69649	1.512239	-0.13585
O	-0.70872	-1.6493	-0.64144	O	-0.88717	-1.80491	-0.26847
C	0.361298	-1.72897	0.357288	C	0.533304	-1.52042	-0.1139
C	1.007006	-0.33387	0.598582	C	0.901049	-0.05285	0.260676
C	0.04506	0.830237	0.439494	C	-0.15368	0.94861	-0.1446
C	1.467849	-2.59032	-0.30336	C	1.245695	-1.75065	-1.45548
C	3.247868	0.850919	-0.12831	C	3.412974	0.721049	0.457309
C	2.224544	-0.28885	-0.36072	C	2.259925	0.246338	-0.47165
C	2.748008	-1.73491	-0.2924	C	2.590379	-1.0397	-1.27451
C	-0.21712	-2.34896	1.628724	C	1.003749	-2.4943	0.970236
C	-2.09578	2.979559	0.64001	C	-2.42147	2.964858	-0.41406
O	-5.28765	-0.54243	-0.39842	O	-5.3294	-0.73627	0.813355
O	2.552563	2.112789	-0.12987	O	3.724411	-0.29417	1.429518
C	3.939225	0.79776	1.23751	C	4.704218	0.909379	-0.34732
H	1.809875	-0.13634	-1.36802	H	2.074501	1.057981	-1.1865
H	1.368377	-0.31808	1.633838	H	1.006237	0.027078	1.350049
O	-0.29681	1.171695	-0.90126	O	-0.70106	0.80174	-1.45046
H	0.238986	1.690591	1.07461	H	0.051227	1.980522	0.144657
C	4.297547	0.860607	-1.25225	C	3.059127	2.031695	1.176952
H	-4.56435	1.831572	0.308099	H	-4.75077	1.731533	0.345416
H	-3.26402	-2.18319	-0.78308	H	-3.29035	-2.36981	0.476026
H	1.153369	-2.80053	-1.32918	H	0.654707	-1.27059	-2.24072
H	1.594673	-3.55106	0.203567	H	1.339291	-2.81395	-1.69522
H	3.303462	-1.89158	0.640258	H	3.279443	-1.66358	-0.69712
H	3.420905	-1.98778	-1.11633	H	3.072615	-0.81505	-2.22952
H	-0.70556	-3.29936	1.395457	H	0.807854	-3.52427	0.660422
H	0.579126	-2.53737	2.355771	H	2.073763	-2.37786	1.161719
H	-0.9569	-1.69171	2.097148	H	0.461913	-2.30951	1.903499
H	-1.37125	3.397535	-0.06619	H	-1.91125	3.083772	-1.37495
H	-2.9816	3.617525	0.653944	H	-3.35269	3.534163	-0.43609
H	-1.63795	3.016791	1.636201	H	-1.77765	3.409937	0.355143
H	2.029072	2.163264	-0.94305	H	3.069539	-0.24615	2.138176
H	4.583861	1.67399	1.347096	H	5.49789	1.281729	0.306058
H	4.557532	-0.09762	1.341328	H	4.556597	1.625665	-1.16146
H	3.213146	0.819322	2.05473	H	5.038935	-0.03825	-0.77466
H	3.814189	0.923587	-2.23424	H	2.168577	1.925523	1.807972
H	4.94997	1.730798	-1.13853	H	3.888626	2.336988	1.821316
H	4.919055	-0.0403	-1.24219	H	2.865883	2.838225	0.462348
2a' (7)				**2a' (8)**			

C	-3.77752	1.161749	0.160416	C	-3.88766	1.076496	0.219133
C	-4.16373	-0.23383	-0.157	C	-4.19669	-0.35486	0.455429
C	-3.07227	-1.1823	-0.41717	C	-3.1008	-1.30744	0.269314
C	-1.78595	-0.7863	-0.38347	C	-1.86787	-0.89709	-0.09885
C	-1.40323	0.625141	-0.10506	C	-1.55755	0.543273	-0.31235
C	-2.50252	1.589586	0.199966	C	-2.67112	1.523314	-0.13911
O	-0.7763	-1.64905	-0.65783	O	-0.89703	-1.80547	-0.32192
C	0.35086	-1.70246	0.274277	C	0.519223	-1.5478	-0.09299
C	0.978266	-0.29112	0.527901	C	0.909076	-0.07867	0.260777
C	0.005453	0.856235	0.329233	C	-0.13401	0.93328	-0.14463
C	1.442632	-2.51859	-0.45604	C	1.27817	-1.83472	-1.39784
C	3.349435	0.814814	-0.05701	C	3.388588	0.753323	0.443019
C	2.249594	-0.24031	-0.36674	C	2.267697	0.194926	-0.47796
C	2.734293	-1.70185	-0.32802	C	2.623003	-1.13112	-1.19945
C	-0.13692	-2.36003	1.565321	C	0.909667	-2.49895	1.041685
C	-2.13281	3.018629	0.486711	C	-2.38213	2.974876	-0.40787
O	-5.34496	-0.57448	-0.17533	O	-5.32452	-0.7056	0.801374
O	4.470012	0.539428	-0.92019	O	3.610635	-0.13571	1.553163
C	2.871655	2.251355	-0.32758	C	4.69616	0.939098	-0.34147
H	1.896209	-0.03382	-1.38834	H	2.082994	0.950422	-1.25213
H	1.289719	-0.26489	1.579334	H	1.050688	0.00438	1.343083
O	-0.37717	1.139643	-1.01004	O	-0.67869	0.799248	-1.45461
H	0.191019	1.743044	0.933991	H	0.077673	1.961824	0.150283
C	3.925542	0.711238	1.358499	C	2.978747	2.085564	1.081467
H	-4.60435	1.838973	0.354794	H	-4.72243	1.759624	0.347532
H	-3.3316	-2.21555	-0.6181	H	-3.30442	-2.35809	0.440929
H	1.144587	-2.59983	-1.50542	H	0.722632	-1.37041	-2.21811
H	1.53054	-3.53408	-0.05931	H	1.364672	-2.9058	-1.60317
H	3.225829	-1.91161	0.629565	H	3.27872	-1.75015	-0.57436
H	3.461479	-1.92066	-1.11198	H	3.150411	-0.9621	-2.14207
H	-0.6178	-3.31612	1.34045	H	0.729141	-3.5365	0.747582
H	0.70523	-2.54517	2.239687	H	1.961857	-2.37649	1.311057
H	-0.86098	-1.72806	2.090332	H	0.312307	-2.28312	1.932633
H	-1.44131	3.396337	-0.27328	H	-1.86657	3.094091	-1.36587
H	-3.02141	3.652722	0.499718	H	-3.30797	3.55295	-0.43056
H	-1.63645	3.11821	1.460233	H	-1.7374	3.409186	0.366621
H	4.172365	0.664742	-1.83235	H	4.1499	-0.87447	1.242104
H	3.734473	2.923194	-0.30855	H	5.472316	1.339554	0.317169
H	2.156897	2.60223	0.42204	H	4.562965	1.63263	-1.17791
H	2.389831	2.332369	-1.30852	H	5.056121	-0.00991	-0.75357

H	4.346688	-0.27928	1.545152	H	2.10375	1.964772	1.725565
H	4.731834	1.440797	1.47293	H	3.794324	2.46361	1.70367
H	3.167883	0.920435	2.119277	H	2.75011	2.833247	0.31561

Table S3. The computed ^{13}C NMR data for **2a'**.

No.	**2a'**	δexptl	chloroform	
			δcalcd	$\Delta\delta$
1	**6**	132	130.8	-1.2
2	**7**	187.7	180.0	-7.7
3	**8**	115.3	112.2	-3.1
4	**8a**	167.1	165.9	-1.2
5	**4a**	54.7	57.5	2.8
6	**5**	149	148.0	-1.0
7	**2**	90.9	90.6	-0.3
8	**3**	43.7	45.8	2.1
9	**4**	63.7	67.7	4.0
10	**9**	40.5	42.2	1.7
11	**12**	72.3	72.7	0.4
12	**11**	53.8	55.2	1.4
13	**10**	25.5	27.0	1.5
14	**15**	27.3	28.6	1.3
15	**16**	16	18.0	2.0
16	**14**	26	25.1	-0.9
17	**13**	30.4	30.7	0.3
	LAD[a]			7.7
	MAD[b]			1.94

[a] LAD = largest absolute deviation. [b] MAD = mean absolute deviation, computed as $(1/n)\sum_{i}^{n} |\delta_{calcd} - \delta_{exptl}|$

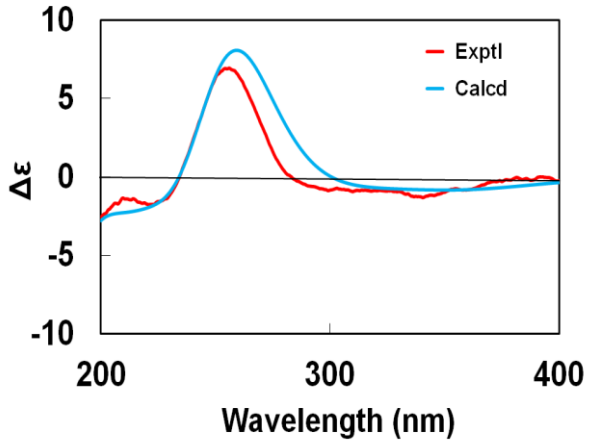
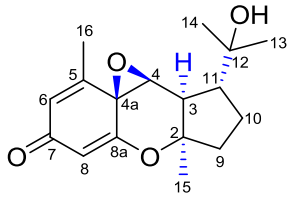
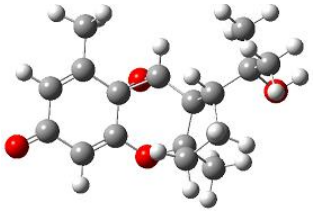


Figure S4. Experimental ECD of **2a** and calculated ECD of **2a'** (blue, calculated at the B3LYP-PCM/6-31G(d,p)//B3LYP/6-31G(d,p) level in CH_3OH; red, experimental in CH_3OH)**.**

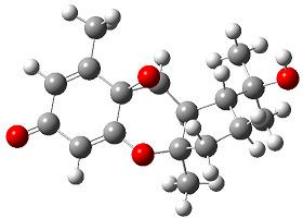


***ent*-2a'**

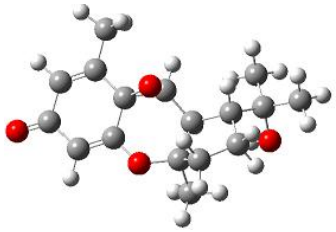
***ent*-2a'(1)**



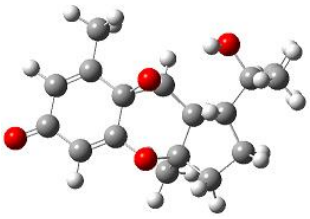
***ent*-2a'(2)**



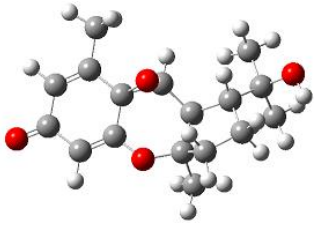
***ent*-2a'(3)**



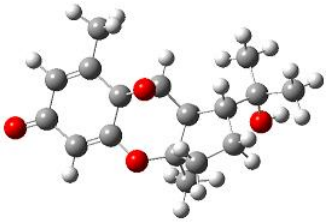
***ent*-2a'(4)**



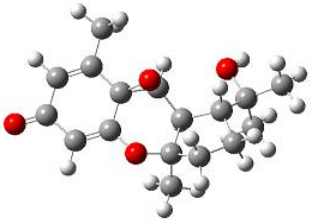
***ent*-2a'(5)**



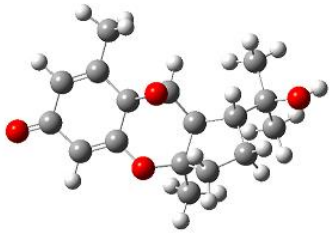
***ent*-2a'(6)**



***ent*-2a'(7)**



***ent*-2a'(8)**



***ent*-2a'(9)**

Figure S5. Optimized geometries of predominant conformers for ***ent*-2a'** at the B3LYP/6-31G(d,p) level in the gas phase**.**

Table S4. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized ***ent*-2a'**at B3LYP/6-31G(d,p) level in the gas phase

Conformations	E+ZPE	G	%
***ent*-2a' (1)**	-961.566677	-961.613203	6.1
***ent*-2a' (2)**	-961.564988	-961.612470	2.8
***ent*-2a' (3)**	-961.563625	-961.610522	0.3
***ent*-2a' (4)**	-961.566173	-961.612907	4.4
***ent*-2a' (5)**	-961.568116	-961.614801	33.0
***ent*-2a' (6)**	-961.563280	-961.610065	0.2
***ent*-2a' (7)**	-961.567776	-961.614503	24.0
***ent*-2a' (8)**	-961.567371	-961.614676	28.9
***ent*-2a' (9)**	-961.563467	-961.610232	0.3

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S5. Optimized Z-matrixes of ***ent*-2a'**in the gas phase (Å) at B3LYP/6-31G(d,p) level

***ent*-2a' (1)**				***ent*-2a' (2)**			
C	-3.88759	1.076567	-0.21922	C	-3.84087	1.128969	-0.23282
C	-4.19676	-0.35477	-0.45505	C	-4.1826	-0.29852	-0.44377
C	-3.10083	-1.30736	-0.26956	C	-3.11192	-1.27514	-0.22661
C	-1.86787	-0.89706	0.09855	C	-1.87244	-0.88524	0.138507
C	-1.55743	0.543245	0.312134	C	-1.52521	0.551862	0.311016
C	-2.67098	1.523357	0.13885	C	-2.61526	1.554035	0.122685
O	-0.89707	-1.80555	0.32138	O	-0.924	-1.80721	0.408734
C	0.519304	-1.54795	0.092707	C	0.487507	-1.6103	0.105273
C	0.909181	-0.07885	-0.26105	C	0.910708	-0.15726	-0.27928
C	-0.13389	0.933179	0.144153	C	-0.09364	0.899149	0.11655
C	-2.38208	2.974901	0.407713	C	-2.29148	3.001677	0.369591
O	-5.32491	-0.70553	-0.8001	O	-5.315	-0.63054	-0.79285
H	1.051057	0.004161	-1.34333	H	1.01995	-0.09289	-1.36914
O	-0.67852	0.799354	1.454205	O	-0.6248	0.80667	1.434387
C	1.27802	-1.8349	1.397734	C	1.303184	-1.91758	1.372173
C	2.622872	-1.13124	1.199588	C	2.656092	-1.24506	1.11046
C	2.267644	0.194757	0.477976	C	2.276562	0.1012	0.447221
C	3.38856	0.753439	-0.44275	C	3.359065	0.797165	-0.42039
C	4.695941	0.9395	0.342007	C	3.874713	-0.05876	-1.58546
C	2.978468	2.08554	-1.08129	C	4.527535	1.249258	0.461308
O	3.611108	-0.13542	-1.55293	O	2.791383	2.019212	-0.94427
C	0.909964	-2.49917	-1.0418	C	0.78146	-2.59388	-1.03152

H	-4.72234	1.759724	-0.34761	H	-4.65912	1.828856	-0.37659
H	-3.30448	-2.358	-0.44119	H	-3.34333	-2.32466	-0.36746
H	0.077802	1.961661	-0.15094	H	0.167047	1.909761	-0.19663
H	-1.86817	3.094279	1.366597	H	-1.78794	3.124003	1.333512
H	-1.7358	3.408872	-0.36567	H	-1.61984	3.402962	-0.39955
H	-3.30781	3.553205	0.428572	H	-3.20105	3.605421	0.365476
H	1.364609	-2.90601	1.602879	H	1.37259	-2.99088	1.572221
H	0.722363	-1.37077	2.21802	H	0.798317	-1.44183	2.218367
H	3.150117	-0.96211	2.142274	H	3.235773	-1.1034	2.026681
H	3.278661	-1.75041	0.574704	H	3.263841	-1.86386	0.440941
H	2.082623	0.950078	1.252245	H	2.063987	0.807894	1.258245
H	5.056058	-0.00948	0.754024	H	3.061197	-0.3988	-2.23742
H	5.472097	1.34021	-0.31647	H	4.566079	0.534187	-2.1916
H	4.562402	1.632878	1.178518	H	4.411151	-0.94509	-1.23636
H	2.103738	1.964364	-1.72571	H	4.17214	1.935088	1.235833
H	3.794128	2.463832	-1.70323	H	5.270988	1.776082	-0.1431
H	2.749281	2.833143	-0.31552	H	5.012592	0.397365	0.946499
H	4.149185	-0.87486	-1.24141	H	2.366269	1.813954	-1.78681
H	0.31302	-2.28333	-1.93302	H	0.202543	-2.33131	-1.92261
H	1.962289	-2.37684	-1.31075	H	1.842206	-2.59049	-1.30003
H	0.729221	-3.53666	-0.74766	H	0.503608	-3.60678	-0.72819
***ent*-2a' (3)**				***ent*-2a' (4)**			
C	-3.87996	1.095331	-0.23384	C	-3.90906	1.0558	-0.22296
C	-4.20402	-0.33612	-0.44907	C	-4.20396	-0.37721	-0.46802
C	-3.11738	-1.2972	-0.25182	C	-3.0981	-1.31905	-0.29265
C	-1.87939	-0.89361	0.106247	C	-1.86742	-0.90035	0.07576
C	-1.55313	0.546348	0.293813	C	-1.57327	0.541786	0.3034
C	-2.65755	1.535234	0.112833	C	-2.69655	1.512178	0.135969
O	-0.91688	-1.80712	0.342676	O	-0.88714	-1.80487	0.268625
C	0.501362	-1.57382	0.099292	C	0.533358	-1.52034	0.11409
C	0.904074	-0.11378	-0.28703	C	0.900988	-0.05285	-0.2606
C	-0.1267	0.917486	0.108532	C	-0.15372	0.948629	0.144729
C	-2.35343	2.987186	0.361831	C	-2.42163	2.964795	0.414344
O	-5.33613	-0.68027	-0.78706	O	-5.32924	-0.73635	-0.81379
H	1.020348	-0.04284	-1.37472	H	1.006126	0.027035	-1.34997
O	-0.66103	0.811608	1.423755	O	-0.70101	0.80177	1.45055
C	1.273746	-1.84579	1.400165	C	1.245748	-1.75051	1.455675
C	2.626399	-1.16524	1.170939	C	2.590408	-1.03951	1.274622
C	2.268472	0.156195	0.446432	C	2.259922	0.246459	0.471648
C	3.412826	0.765341	-0.41153	C	3.412915	0.721077	-0.45745
C	3.038514	2.170472	-0.91142	C	4.704228	0.909458	0.347013
C	3.846543	-0.11173	-1.58997	C	3.059015	2.031594	-1.1773
O	4.586584	0.858374	0.413381	O	3.724272	-0.29431	-1.42955

C	0.863874	-2.56239	-1.01278	C	1.003849	-2.4943	-0.96998
H	-4.70874	1.784717	-0.36767	H	-4.7508	1.731424	-0.3454
H	-3.33241	-2.34838	-0.40546	H	-3.29018	-2.36985	-0.47624
H	0.094843	1.938081	-0.20629	H	0.051215	1.980531	-0.14458
H	-1.83576	3.114035	1.317706	H	-1.9114	3.083661	1.375228
H	-1.70523	3.405055	-0.41882	H	-1.77787	3.409985	-0.35485
H	-3.27337	3.574756	0.377756	H	-3.3529	3.534016	0.436444
H	1.347866	-2.91469	1.620893	H	1.339452	-2.81381	1.695401
H	0.732364	-1.3628	2.219324	H	0.65478	-1.27053	2.240977
H	3.173606	-0.98392	2.098418	H	3.072668	-0.81477	2.229594
H	3.271682	-1.79142	0.547695	H	3.27945	-1.66344	0.697257
H	2.058374	0.89871	1.230147	H	2.074503	1.058178	1.186414
H	2.759474	2.822605	-0.07463	H	5.038974	-0.03814	0.774405
H	3.894599	2.621218	-1.42111	H	5.497841	1.281746	-0.30647
H	2.199191	2.149217	-1.61458	H	4.556704	1.625827	1.161102
H	4.195913	-1.08882	-1.24875	H	2.168389	1.925292	-1.80818
H	4.678456	0.371668	-2.10908	H	3.888469	2.336716	-1.8218
H	3.036002	-0.25805	-2.30903	H	2.86588	2.838288	-0.46285
H	4.380585	1.445013	1.154728	H	3.069261	-0.24646	-2.13809
H	0.316269	-2.32349	-1.92979	H	0.462025	-2.30957	-1.90326
H	1.933908	-2.53762	-1.23696	H	2.07386	-2.3778	-1.16147
H	0.596068	-3.5774	-0.70756	H	0.807993	-3.52425	-0.6601
***ent*-2a' (5)**				***ent*-2a' (6)**			
C	-3.73199	1.158583	-0.12207	C	-3.88285	1.090127	-0.233
C	-4.10751	-0.2142	0.291217	C	-4.20197	-0.34022	-0.4611
C	-3.00875	-1.16099	0.527977	C	-3.11347	-1.30022	-0.26618
C	-1.72398	-0.77972	0.40124	C	-1.87828	-0.89566	0.099415
C	-1.34914	0.618003	0.046423	C	-1.55602	0.543583	0.297485
C	-2.4585	1.572278	-0.25473	C	-2.66286	1.530657	0.12165
O	-0.70846	-1.64933	0.641102	O	-0.91384	-1.80943	0.332252
C	0.361398	-1.72889	-0.35783	C	0.504306	-1.56751	0.102937
C	1.007138	-0.33381	-0.59881	C	0.90259	-0.10794	-0.28544
C	0.045098	0.83029	-0.43996	C	-0.13014	0.919438	0.116106
C	-2.09611	2.979237	-0.64099	C	-2.36311	2.981039	0.38423
O	-5.28746	-0.54235	0.400174	O	-5.33131	-0.68557	-0.80689
H	1.368843	-0.31801	-1.63396	H	1.014428	-0.03595	-1.37356
O	-0.29682	1.171937	0.9007	O	-0.66594	0.802593	1.429708
C	1.467934	-2.59049	0.302501	C	1.265875	-1.82719	1.413057
C	2.748	-1.73486	0.292486	C	2.618483	-1.14331	1.189464
C	2.224375	-0.28886	0.360842	C	2.265099	0.171823	0.446747
C	3.247743	0.85096	0.128833	C	3.410793	0.772506	-0.41655
C	3.939597	0.79796	-1.23675	C	3.034751	2.167172	-0.92784
C	4.297063	0.860554	1.253105	C	3.847562	-0.11821	-1.59043

O	2.552414	2.112825	0.130244	O	4.537885	1.004388	0.445517
C	-0.21729	-2.34854	-1.62932	C	0.882988	-2.56096	-0.99967
H	-4.56448	1.831206	-0.30813	H	-4.71313	1.778218	-0.36386
H	-3.26367	-2.18319	0.78383	H	-3.32561	-2.35077	-0.42788
H	0.238987	1.690508	-1.07526	H	0.091302	1.942293	-0.1906
H	-1.37333	3.398285	0.066384	H	-1.84804	3.100721	1.342391
H	-1.63619	3.016104	-1.63622	H	-1.7136	3.407169	-0.39078
H	-2.98236	3.616544	-0.65722	H	-3.28452	3.566229	0.402716
H	1.595099	-3.55083	-0.20509	H	1.342068	-2.89368	1.644206
H	1.153205	-2.80154	1.328075	H	0.718719	-1.3367	2.223358
H	3.420458	-1.98784	1.116731	H	3.147079	-0.94909	2.126716
H	3.303982	-1.89125	-0.6399	H	3.265173	-1.786	0.580335
H	1.809439	-0.13645	1.36805	H	2.070669	0.923651	1.220475
H	3.213806	0.819647	-2.05422	H	2.766513	2.820053	-0.09205
H	4.584273	1.674206	-1.34599	H	3.889146	2.61365	-1.44373
H	4.557944	-0.0974	-1.3405	H	2.196173	2.127011	-1.62964
H	3.813431	0.923348	2.234978	H	4.198363	-1.09813	-1.24925
H	4.949446	1.730816	1.139699	H	4.67614	0.363673	-2.11649
H	4.918627	-0.04031	1.243076	H	3.040904	-0.28503	-2.31079
H	2.028533	2.163217	0.943173	H	4.877271	0.144493	0.728048
H	-0.95714	-1.69116	-2.09742	H	0.341298	-2.33082	-1.92228
H	0.578825	-2.53677	-2.35656	H	1.95442	-2.53188	-1.21679
H	-0.70569	-3.29899	-1.3962	H	0.618442	-3.5757	-0.69057
***ent*-2a' (7)**				***ent*-2a' (8)**			
C	-3.8952	1.070202	-0.21971	C	-3.82923	1.143048	-0.22991
C	-4.20044	-0.36201	-0.45713	C	-4.18452	-0.2856	-0.40528
C	-3.1014	-1.31051	-0.2773	C	-3.11821	-1.2654	-0.17971
C	-1.86736	-0.89814	0.087914	C	-1.87257	-0.87631	0.163901
C	-1.5623	0.543007	0.305783	C	-1.51261	0.560537	0.306855
C	-2.67907	1.520052	0.13552	C	-2.59679	1.566139	0.104569
O	-0.89389	-1.80508	0.295396	O	-0.92642	-1.79646	0.44928
C	0.527049	-1.53844	0.096834	C	0.471527	-1.62583	0.074176
C	0.907587	-0.06942	-0.2643	C	0.91502	-0.17078	-0.28809
C	-0.14016	0.938138	0.139899	C	-0.07933	0.896586	0.100618
C	-2.39416	2.972155	0.406372	C	-2.25969	3.016904	0.311356
O	-5.32912	-0.71446	-0.79981	O	-5.32356	-0.61682	-0.73376
H	1.046219	0.011343	-1.34687	H	1.043477	-0.08818	-1.37223
O	-0.68551	0.801898	1.449206	O	-0.60676	0.827491	1.422811
C	1.264912	-1.80397	1.418028	C	1.330977	-1.99563	1.294578
C	2.611246	-1.10002	1.228509	C	2.679679	-1.32372	1.015118
C	2.264199	0.213302	0.478517	C	2.280774	0.056558	0.4469
C	3.393499	0.738412	-0.43978	C	3.350479	0.801413	-0.38399
C	4.704148	0.904614	0.346075	C	3.830005	0.030807	-1.62412

C	3.014248	2.075378	-1.09872	C	4.54865	1.174861	0.502151
O	3.562285	-0.26462	-1.45692	O	2.679808	2.005698	-0.8075
C	0.949946	-2.49955	-1.01704	C	0.686654	-2.57848	-1.10547
H	-4.7325	1.750977	-0.34452	H	-4.64303	1.846255	-0.38283
H	-3.30111	-2.36119	-0.45331	H	-3.35812	-2.31605	-0.29597
H	0.067894	1.96805	-0.15411	H	0.184841	1.897912	-0.23444
H	-1.87872	3.09147	1.364431	H	-1.73761	3.158029	1.262776
H	-1.7509	3.409803	-0.36753	H	-1.59949	3.393535	-0.47974
H	-3.32175	3.547401	0.430249	H	-3.16524	3.626824	0.309347
H	1.353702	-2.87252	1.635295	H	1.39689	-3.07674	1.447863
H	0.693701	-1.33458	2.224593	H	0.861618	-1.55172	2.178137
H	3.117911	-0.91013	2.178784	H	3.300186	-1.24057	1.911778
H	3.280233	-1.70998	0.614266	H	3.249023	-1.90704	0.282618
H	2.080407	0.993593	1.227185	H	2.069195	0.707696	1.304013
H	5.039599	-0.04982	0.757353	H	2.99843	-0.23216	-2.28316
H	5.494908	1.287074	-0.31043	H	4.524593	0.65284	-2.20085
H	4.587618	1.616804	1.169548	H	4.365169	-0.88489	-1.35684
H	2.12037	1.975347	-1.72014	H	4.217594	1.768634	1.358962
H	3.82824	2.423953	-1.74521	H	5.273733	1.769894	-0.06585
H	2.834839	2.853901	-0.3498	H	5.071568	0.287699	0.872282
H	4.284536	0.015015	-2.03515	H	3.310209	2.532409	-1.31742
H	0.379106	-2.2918	-1.92744	H	0.072347	-2.27354	-1.95855
H	2.011058	-2.38329	-1.25044	H	1.733072	-2.58525	-1.42606
H	0.754005	-3.53259	-0.71654	H	0.402168	-3.59553	-0.82242
***ent*-2a' (9)**							
C	-3.87709	1.094966	-0.23494				
C	-4.19866	-0.33515	-0.46195				
C	-3.11288	-1.29684	-0.2634				
C	-1.87708	-0.89455	0.103935				
C	-1.55243	0.544467	0.300145				
C	-2.65689	1.533473	0.121426				
O	-0.91527	-1.80831	0.341708				
C	0.503786	-1.57304	0.103934				
C	0.90555	-0.11237	-0.28088				
C	-0.1254	0.917151	0.120153				
C	-2.35516	2.983626	0.383358				
O	-5.32832	-0.67786	-0.81007				
H	1.017159	-0.03964	-1.36918				
O	-0.66306	0.8033	1.432808				
C	1.274944	-1.84393	1.405754				
C	2.628456	-1.16473	1.175149				
C	2.267884	0.156946	0.452498				
C	3.400757	0.768043	-0.40984				

C	3.010302	2.164409	-0.92257				
C	3.845154	-0.11846	-1.58397				
O	4.487441	0.900363	0.522174				
C	0.869189	-2.56135	-1.00768				
H	-4.70584	1.784547	-0.368				
H	-3.32674	-2.3473	-0.42351				
H	0.097004	1.939626	-0.18747				
H	-1.84127	3.102966	1.342207				
H	-1.70379	3.408212	-0.39101				
H	-3.27565	3.570353	0.400117				
H	1.347664	-2.91269	1.627934				
H	0.734238	-1.359	2.224118				
H	3.177865	-0.97586	2.099017				
H	3.270198	-1.7952	0.551909				
H	2.074274	0.899088	1.236219				
H	2.733815	2.814429	-0.08731				
H	3.856247	2.626859	-1.44481				
H	2.177379	2.127326	-1.63266				
H	4.211595	-1.08612	-1.23384				
H	4.664141	0.368959	-2.12603				
H	3.040691	-0.28879	-2.30612				
H	5.237964	1.282406	0.046869				
H	0.324224	-2.32212	-1.92622				
H	1.939919	-2.53787	-1.22858				
H	0.599853	-3.57626	-0.70339				

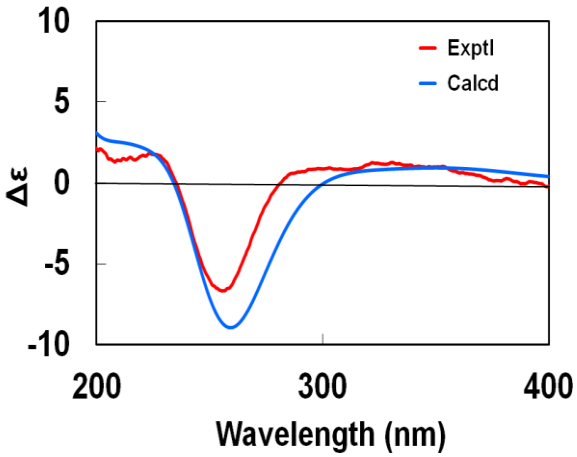
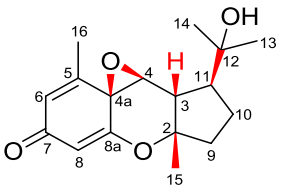
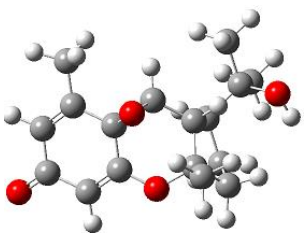


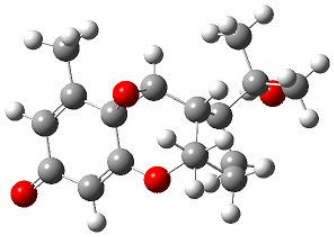
Figure S6. Experimental ECD of **2b** and calculated ECD of ***ent*-2a'** (blue, calculated at the B3LYP-PCM/6-31G(d,p)//B3LYP/6-31G(d,p) level in CH_3OH; red, experimental in CH_3OH).



2b'



2b' (1)



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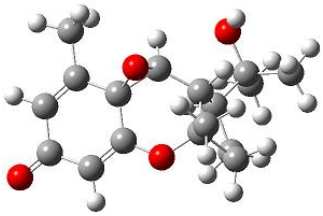
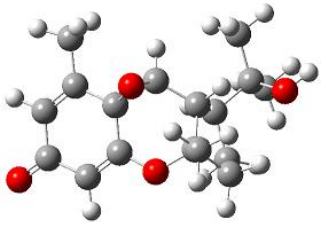
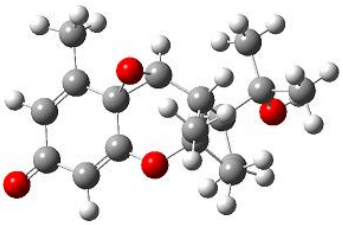


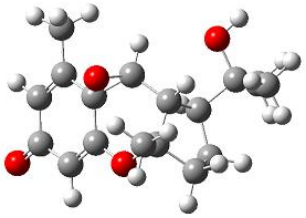
2b' (3)



2b' (4)



2b' (5)



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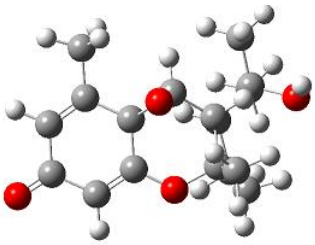
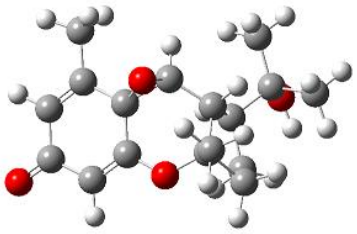
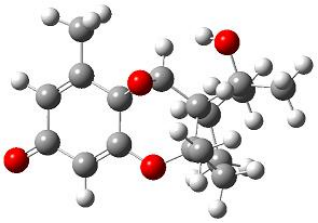


2b' (7)



2b' (8)



2b' (9)

Figure S7. Optimized geometries of predominant conformers for **2b'** at the B3LYP/6-31G (d,p) level in the gas phase.

Table S6. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized **2b'** at B3LYP/6-31G (d,p) level in the gas phase

Conformations	E+ZPE	G	%
2b' (1)	-961.568401	-961.614975	5.3
2b' (2)	-961.566746	-961.613367	1.0
2b' (3)	-961.567892	-961.614716	4.0
2b' (4)	-961.569074	-961.615803	12.6
2b' (5)	-961.566376	-961.612824	0.5
2b' (6)	-961.570158	-961.617112	50.5
2b' (7)	-961.567133	-961.614198	2.3
2b' (8)	-961.565849	-961.612396	0.3
2b' (9)	-961.569194	-961.616387	23.5

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S7. Optimized Z-matrixes of **2b'** in the gas phase (Å) at B3LYP/6-31G (d,p) level.

2b' (1)				**2b' (2)**			
C	-3.55906	1.07602	-0.47795	C	-3.56488	1.073904	-0.45125
C	-3.67255	-0.23198	-1.16693	C	-3.67888	-0.22777	-1.15263
C	-2.60776	-1.20191	-0.91915	C	-2.612	-1.19885	-0.91816
C	-1.57209	-0.92611	-0.09406	C	-1.57448	-0.92967	-0.09336
C	-1.46649	0.390233	0.601843	C	-1.46951	0.379033	0.61578
C	-2.54391	1.393849	0.343732	C	-2.54787	1.385014	0.370478
O	-0.60204	-1.85237	0.056718	O	-0.60329	-1.85562	0.047196
C	0.670187	-1.61427	0.742696	C	0.676318	-1.62843	0.722519
C	1.063561	-0.11809	0.720421	C	1.064067	-0.12675	0.732037
C	-0.09957	0.792142	1.031597	C	-0.10347	0.77765	1.047246
C	0.590292	-2.26112	2.12262	C	0.60711	-2.30114	2.090673
C	-2.46414	2.711824	1.064546	C	-2.46701	2.696192	1.103595
O	-4.61885	-0.46622	-1.91898	O	-4.62732	-0.45525	-1.90371
H	1.828177	0.006042	1.495698	H	1.800759	-0.00354	1.53498
O	-1.03559	0.323312	1.997672	O	-1.03556	0.297283	2.010746
C	1.720576	-2.24991	-0.17462	C	1.716267	-2.24578	-0.223
C	1.877373	-1.24549	-1.32288	C	1.872447	-1.21163	-1.34466
C	1.721961	0.165328	-0.67231	C	1.733598	0.174865	-0.65159
C	3.057963	0.960613	-0.56134	C	3.066708	0.978677	-0.5827
C	2.877381	2.273729	0.20954	C	4.196756	0.242784	0.145005
C	3.635181	1.273848	-1.95134	C	2.845605	2.365245	0.043741
O	4.013691	0.210029	0.208565	O	3.561221	1.145907	-1.92131
H	-4.36568	1.776885	-0.67293	H	-4.37283	1.775624	-0.63745
H	-2.6557	-2.15196	-1.43895	H	-2.65975	-2.14334	-1.4479
H	0.120823	1.857153	1.096096	H	0.11736	1.842228	1.122047
H	-0.17688	-1.78421	2.732837	H	-0.15184	-1.83207	2.717533
H	0.351587	-3.32358	2.017838	H	0.361914	-3.36003	1.968098
H	1.553587	-2.17392	2.635331	H	1.575739	-2.23023	2.596295
H	-2.29835	2.557452	2.135208	H	-2.30012	2.532111	2.172675
H	-1.63604	3.32781	0.69176	H	-1.63966	3.316065	0.735497
H	-3.38688	3.279155	0.928568	H	-3.38997	3.264629	0.974155
H	2.655842	-2.34263	0.388731	H	2.655563	-2.37545	0.327009
H	1.41423	-3.24803	-0.49933	H	1.39283	-3.23034	-0.5717

H	1.08358	-1.402	-2.05839	H	1.06467	-1.34187	-2.07071
H	2.823508	-1.3739	-1.85746	H	2.812526	-1.29497	-1.89357
H	1.042583	0.772035	-1.28398	H	1.049279	0.801828	-1.24137
H	2.566978	2.093438	1.241734	H	4.407479	-0.71986	-0.32679
H	3.827501	2.813242	0.244108	H	5.108523	0.84376	0.091847
H	2.134604	2.914119	-0.27643	H	3.963007	0.075066	1.199927
H	3.836678	0.365243	-2.52804	H	2.061825	2.916009	-0.49111
H	4.576732	1.820031	-1.84508	H	3.768756	2.947962	-0.01765
H	2.944535	1.88853	-2.53743	H	2.55415	2.303872	1.097455
H	4.327486	-0.5212	-0.34025	H	2.894636	1.633962	-2.42503
2b' (3)				**2b' (4)**			
C	-3.53385	1.127216	-0.40135	C	-3.56033	1.081272	-0.47462
C	-3.69617	-0.16097	-1.11621	C	-3.67958	-0.229	-1.159
C	-2.63938	-1.15456	-0.93275	C	-2.61664	-1.20021	-0.91237
C	-1.57386	-0.92045	-0.13418	C	-1.57668	-0.92484	-0.09164
C	-1.43288	0.36583	0.611047	C	-1.46665	0.393096	0.600691
C	-2.48944	1.402452	0.398642	C	-2.54166	1.399199	0.342457
O	-0.60237	-1.85826	-0.06954	O	-0.60899	-1.85129	0.058643
C	0.660532	-1.6921	0.646998	C	0.669906	-1.6169	0.737336
C	1.08096	-0.20506	0.71187	C	1.063815	-0.12043	0.719734
C	-0.05933	0.722613	1.052425	C	-0.09834	0.792075	1.027917
C	0.542759	-2.41079	1.98892	C	0.592958	-2.26574	2.116409
C	-2.35736	2.703091	1.142872	C	-2.45603	2.719621	1.05831
O	-4.67221	-0.36122	-1.83931	O	-4.63007	-0.46209	-1.90648
H	1.822056	-0.13131	1.518812	H	1.823173	0.002312	1.499779
O	-1.00266	0.241817	2.005921	O	-1.03421	0.328382	1.996511
C	1.71391	-2.30071	-0.28959	C	1.71462	-2.25097	-0.18643
C	1.934603	-1.2356	-1.37484	C	1.875719	-1.2448	-1.33106
C	1.743021	0.137464	-0.66049	C	1.727224	0.162205	-0.67268
C	3.017083	1.023367	-0.53125	C	3.060239	0.948416	-0.56437
C	3.400056	1.594092	-1.90014	C	2.88584	2.274451	0.196787
C	4.213838	0.29842	0.10033	C	3.645637	1.245591	-1.95521
O	2.683913	2.178728	0.269851	O	3.949575	0.08881	0.169161
H	-4.3281	1.85119	-0.55902	H	-4.36586	1.783531	-0.66937
H	-2.71484	-2.083	-1.48711	H	-2.66792	-2.15146	-1.42958
H	0.200545	1.776552	1.136511	H	0.123223	1.857362	1.089076
H	-0.22357	-1.94802	2.61135	H	-0.16882	-1.78699	2.732285
H	0.281963	-3.46013	1.823591	H	0.348823	-3.32679	2.010186
H	1.49812	-2.37526	2.522966	H	1.559902	-2.18529	2.623273
H	-2.17711	2.523567	2.207406	H	-2.28482	2.568699	2.128629
H	-1.51805	3.30015	0.765114	H	-1.62911	3.333225	0.678851
H	-3.2655	3.299258	1.035434	H	-3.37867	3.287888	0.925357
H	2.632435	-2.47014	0.284618	H	2.655697	-2.34526	0.364823

H	1.382294	-3.266	-0.68183	H	1.40044	-3.24599	-0.51387
H	1.181969	-1.35051	-2.1596	H	1.081953	-1.39129	-2.06946
H	2.911018	-1.3314	-1.85757	H	2.830106	-1.36983	-1.84463
H	1.034695	0.744137	-1.23612	H	1.054786	0.781166	-1.27912
H	2.584435	2.210254	-2.28927	H	2.54818	2.108578	1.222787
H	4.289029	2.22443	-1.81101	H	3.842183	2.80792	0.248187
H	3.607723	0.798719	-2.62169	H	2.172172	2.935364	-0.30656
H	3.973328	-0.1054	1.091196	H	3.846196	0.328585	-2.51273
H	5.04379	1.00128	0.218088	H	4.591022	1.792398	-1.8582
H	4.56218	-0.53233	-0.5192	H	2.965905	1.867643	-2.54664
H	2.821194	1.949451	1.198115	H	4.800843	0.539521	0.250648
2b' (5)				**2b' (6)**			
C	-3.57274	1.07613	-0.45722	C	3.514925	-1.12214	-0.39625
C	-3.70065	-0.2397	-1.12905	C	3.648661	0.137929	-1.16485
C	-2.63192	-1.20783	-0.89155	C	2.594781	1.134713	-0.98468
C	-1.58287	-0.92502	-0.08633	C	1.55359	0.926084	-0.14707
C	-1.46816	0.394492	0.600509	C	1.432464	-0.3388	0.637306
C	-2.54417	1.400514	0.344621	C	2.494503	-1.37214	0.442433
O	-0.60939	-1.84871	0.054163	O	0.590593	1.870995	-0.07108
C	0.669998	-1.61894	0.727486	C	-0.67634	1.703056	0.642594
C	1.064933	-0.11859	0.722497	C	-1.0824	0.214683	0.72894
C	-0.10015	0.794298	1.022839	C	0.063607	-0.69393	1.098465
C	0.596836	-2.27642	2.102965	C	-0.57193	2.445159	1.972536
C	-2.44788	2.727707	1.046304	C	2.392878	-2.64223	1.24208
O	-4.66208	-0.4811	-1.85906	O	4.600817	0.313368	-1.926
H	1.796483	0.008631	1.529899	H	-1.83601	0.130302	1.519297
O	-1.0314	0.332673	1.996672	O	1.011142	-0.17414	2.028424
C	1.70753	-2.25088	-0.21104	C	-1.7299	2.288299	-0.30846
C	1.872024	-1.22672	-1.34071	C	-1.9312	1.206951	-1.38136
C	1.739592	0.166956	-0.65982	C	-1.71845	-0.15317	-0.65036
C	3.072387	0.959414	-0.58277	C	-2.97817	-1.04808	-0.52919
C	4.203881	0.205901	0.135172	C	-3.36622	-1.61278	-1.90393
C	2.861429	2.339718	0.06115	C	-4.18036	-0.34151	0.116935
O	3.427673	1.141375	-1.96357	O	-2.5528	-2.13208	0.32088
H	-4.37987	1.777348	-0.64877	H	4.310371	-1.84647	-0.54658
H	-2.68725	-2.16125	-1.40426	H	2.654232	2.046388	-1.56814
H	0.124292	1.859165	1.079216	H	-0.19325	-1.74319	1.225804
H	-0.16005	-1.79636	2.72409	H	0.196227	2.000499	2.605552
H	0.346264	-3.33534	1.991964	H	-0.32133	3.494546	1.791578
H	1.565436	-2.20482	2.608694	H	-1.5294	2.40733	2.502442
H	-2.26183	2.587576	2.115666	H	2.239348	-2.41998	2.30265
H	-1.62661	3.33694	0.648121	H	1.547108	-3.25871	0.913214
H	-3.37218	3.294947	0.920998	H	3.302082	-3.23673	1.133691

H	2.644584	-2.38304	0.342692	H	-2.65416	2.454239	0.257331
H	1.377985	-3.23635	-0.55157	H	-1.40667	3.251792	-0.71201
H	1.064065	-1.35397	-2.06652	H	-1.17863	1.323694	-2.16573
H	2.809639	-1.32415	-1.89087	H	-2.90797	1.282277	-1.86704
H	1.078895	0.797055	-1.26635	H	-0.99301	-0.75216	-1.21279
H	4.414162	-0.74882	-0.35266	H	-2.53458	-2.18467	-2.32511
H	5.123213	0.802999	0.108421	H	-4.23039	-2.28179	-1.81453
H	3.977534	0.018227	1.189439	H	-3.63683	-0.82191	-2.61011
H	2.083978	2.89492	-0.47213	H	-3.93734	0.038208	1.112777
H	3.786569	2.925818	0.011502	H	-5.01172	-1.04757	0.227389
H	2.584031	2.268124	1.118012	H	-4.54339	0.490067	-0.49391
H	4.271697	1.612328	-1.99158	H	-3.29535	-2.74392	0.415514
2b' (7)				**2b' (8)**			
C	-3.56378	1.08803	-0.47116	C	-3.56899	1.078096	-0.45728
C	-3.69106	-0.22385	-1.15091	C	-3.69773	-0.23597	-1.13178
C	-2.62692	-1.19637	-0.91153	C	-2.6299	-1.2061	-0.89512
C	-1.58116	-0.92117	-0.09922	C	-1.58167	-0.9256	-0.08868
C	-1.46684	0.395448	0.59509	C	-1.46593	0.392071	0.601266
C	-2.53911	1.405427	0.338407	C	-2.54068	1.399755	0.346162
O	-0.60941	-1.84726	0.037757	O	-0.60743	-1.85068	0.04841
C	0.660512	-1.6235	0.730207	C	0.667206	-1.62335	0.729734
C	1.059927	-0.12719	0.720663	C	1.065854	-0.1252	0.724888
C	-0.09934	0.790356	1.026069	C	-0.09776	0.789535	1.025849
C	0.566423	-2.27831	2.105979	C	0.588846	-2.28257	2.104096
C	-2.44504	2.727857	1.049433	C	-2.44307	2.725619	1.050026
O	-4.64795	-0.458	-1.88913	O	-4.65787	-0.47584	-1.86371
H	1.798176	-0.01107	1.525503	H	1.79912	0.000709	1.530827
O	-1.03742	0.328187	1.99287	O	-1.0307	0.326468	1.997507
C	1.713641	-2.25527	-0.18567	C	1.707821	-2.25664	-0.2035
C	1.892913	-1.24511	-1.32411	C	1.872013	-1.23353	-1.33429
C	1.735072	0.159487	-0.66423	C	1.742497	0.165336	-0.65742
C	3.077011	0.947035	-0.56222	C	3.073438	0.97357	-0.58432
C	2.918211	2.260857	0.219958	C	4.217624	0.222608	0.116387
C	3.627355	1.263081	-1.95858	C	2.852736	2.337469	0.079082
O	4.082851	0.131063	0.064149	O	3.473472	1.301672	-1.92383
H	-4.36835	1.792065	-0.66302	H	-4.37498	1.780738	-0.64822
H	-2.68197	-2.14698	-1.42946	H	-2.68631	-2.15855	-1.40959
H	0.127766	1.854409	1.08775	H	0.128776	1.853534	1.084762
H	-0.19903	-1.79882	2.716636	H	-0.17057	-1.8026	2.721977
H	0.318671	-3.3375	1.991686	H	0.338542	-3.34137	1.99131
H	1.528004	-2.20735	2.625104	H	1.555154	-2.21089	2.61408
H	-2.27138	2.580256	2.119861	H	-2.25781	2.583627	2.119267
H	-1.61703	3.336668	0.664723	H	-1.6208	3.334253	0.653132

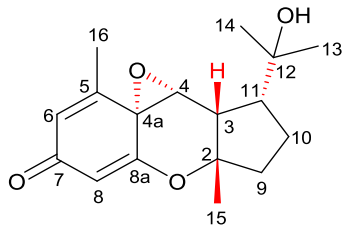
H	-3.36564	3.299563	0.917608	H	-3.36654	3.294231	0.925086
H	2.649732	-2.35544	0.374551	H	2.644985	-2.38342	0.350679
H	1.403635	-3.24969	-0.51836	H	1.382033	-3.24283	-0.54511
H	1.114492	-1.39131	-2.07839	H	1.068813	-1.36419	-2.06455
H	2.858915	-1.3666	-1.81602	H	2.812569	-1.36747	-1.87924
H	1.056418	0.774991	-1.26811	H	1.07766	0.791147	-1.26342
H	2.595727	2.089609	1.253548	H	4.444048	-0.72569	-0.38289
H	3.876381	2.786901	0.255967	H	5.122024	0.83652	0.087888
H	2.185219	2.92188	-0.25405	H	3.992721	0.002833	1.16483
H	3.835652	0.351338	-2.52206	H	2.058643	2.888233	-0.43415
H	4.563839	1.819853	-1.86796	H	3.769245	2.929306	0.009628
H	2.915479	1.866928	-2.52954	H	2.591172	2.238361	1.136632
H	3.943773	0.157458	1.01986	H	3.697878	0.479989	-2.38052
2b' (9)							
C	3.485037	-1.12816	-0.37164				
C	3.593224	0.085597	-1.21584				
C	2.545464	1.092878	-1.05997				
C	1.528022	0.932402	-0.18332				
C	1.424683	-0.29341	0.664711				
C	2.48832	-1.33115	0.507185				
O	0.571628	1.884607	-0.124				
C	-0.68826	1.741884	0.609778				
C	-1.08978	0.255968	0.741508				
C	0.060009	-0.62921	1.154315				
C	-0.57144	2.527152	1.913677				
C	2.417135	-2.54861	1.388341				
O	4.521487	0.215426	-2.01438				
H	-1.85296	0.195727	1.524723				
O	1.014721	-0.06411	2.048501				
C	-1.75342	2.298032	-0.34477				
C	-1.97138	1.188865	-1.38559				
C	-1.70888	-0.15382	-0.63364				
C	-2.92978	-1.10934	-0.51014				
C	-3.33829	-1.63874	-1.89259				
C	-4.13647	-0.48028	0.193326				
O	-2.55458	-2.22396	0.32675				
H	4.280648	-1.8568	-0.49877				
H	2.590965	1.97305	-1.6911				
H	-0.19184	-1.67072	1.343842				
H	0.206644	2.109893	2.552699				
H	-0.33032	3.571432	1.69426				
H	-1.5226	2.501618	2.455386				
H	2.301174	-2.26	2.437553				

H	1.561235	-3.18559	1.132241				
H	3.322359	-3.14983	1.284809				
H	-2.66961	2.479835	0.229109				
H	-1.43614	3.250312	-0.77842				
H	-1.25473	1.301541	-2.20344				
H	-2.96916	1.235087	-1.83028				
H	-0.95061	-0.7197	-1.19209				
H	-2.49147	-2.1321	-2.38608				
H	-4.14731	-2.36764	-1.78983				
H	-3.68083	-0.83797	-2.55419				
H	-3.89384	-0.18154	1.216274				
H	-4.94582	-1.21284	0.250081				
H	-4.50305	0.395517	-0.34859				
H	-1.97408	-2.79528	-0.19515				

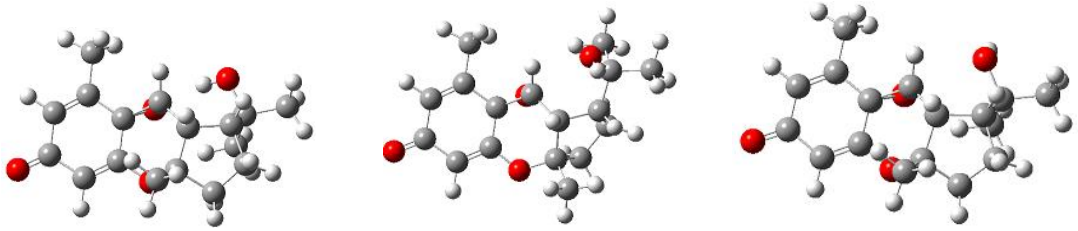
Table S8. The computed ^{13}C NMR data for **2b'**.

No.	**2b'**	δexptl	chloroform	
			δcalcd	$\Delta\delta$
1	**6**	132	130.7	-1.3
2	**7**	187.6	179.3	-8.3
3	**8**	115.3	107.7	-7.6
4	**8a**	167.1	166.2	-0.9
5	**4a**	54.7	55.4	0.7
6	**5**	149	147.3	-1.7
7	**2**	90.9	91.8	0.9
8	**3**	43.7	45.2	1.5
9	**4**	63.7	66.6	2.9
10	**10**	25.5	27.0	1.5
11	**16**	16	17.8	1.8
12	**9**	40.5	43.1	2.6
13	**15**	27.3	28.7	1.4
14	**11**	53.8	52.5	-1.3
15	**12**	72.4	73.7	1.3
16	**14**	30.4	30.2	-0.2
17	**13**	26	24.2	-1.8
	LAD[a]			8.3
	MAD[b]			2.21

[a] LAD = largest absolute deviation. [b] MAD = mean absolute deviation, computed as (1/*n*) $\sum_{i}^{n} |\delta_{\text{calcd}} - \delta_{\text{exptl}}|$



2c'



2c'(1) **2c'(2)** **2c'(3)**

Figure S8. Optimized geometries of predominant conformers for **2c'** at the B3LYP/6-31G(d,p) level in the gas phase**.**

Table S9. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized **2c'** at B3LYP/6-31G(d,p) level in the gas phase.

Conformations	E+ZPE	G	%
2c'(1)	-961.559096	-961.604606	3.8
2c'(2)	-961.560887	-961.607634	95.2
2c'(3)	-961.557052	-961.603291	1.0

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S10. Optimized Z-matrixes of **2c'** in the gas phase (Å) at B3LYP/6-31G(d,p) level.

2c'(1)				**2c'(2)**			
C	-3.72939	-0.95351	-0.10056	C	-3.62307	-1.35129	-0.11018
C	-3.94354	0.36678	0.539146	C	-4.16406	0.025577	-0.20787
C	-2.74967	1.186739	0.791296	C	-3.19835	1.120261	-0.12544
C	-1.52307	0.743045	0.461733	C	-1.87771	0.887693	0.044913
C	-1.3083	-0.60337	-0.14331	C	-1.3402	-0.49668	0.155539
C	-2.51672	-1.43112	-0.43473	C	-2.3169	-1.62407	0.053069
O	-0.4094	1.473467	0.725882	O	-1.03416	1.940101	0.093951
C	0.52622	1.663797	-0.3827	C	0.409026	1.847472	-0.0541
C	0.977695	0.312412	-1.02777	C	0.927022	0.500245	-0.62807
C	0.007152	-0.83095	-0.81663	C	0.096477	-0.67655	-0.17874
C	-0.14527	2.585235	-1.40458	C	0.740424	3.018919	-0.98369
C	-2.3181	-2.78944	-1.04803	C	-1.79115	-3.02704	0.186484
O	-5.07448	0.756121	0.821852	O	-5.36971	0.218267	-0.36604
H	0.944213	0.480454	-2.11221	H	0.891164	0.506019	-1.72344
O	-0.21239	-1.3251	0.503325	O	-0.31844	-0.68182	1.188367
C	1.803296	2.278911	0.215645	C	1.103779	1.99603	1.325726
C	2.968958	1.566976	-0.49016	C	2.34176	1.064554	1.299398
C	2.504298	0.103382	-0.71011	C	2.405885	0.474464	-0.13331
C	2.950854	-0.90638	0.39959	C	3.198348	-0.85782	-0.30688
C	2.595896	-0.49407	1.836169	C	2.969302	-1.89266	0.803536
C	4.467822	-1.12604	0.282295	C	4.702096	-0.55348	-0.40715
O	2.38967	-2.19589	0.10278	O	2.772681	-1.51401	-1.52013
H	-4.63063	-1.53272	-0.28	H	-4.35995	-2.1469	-0.1721
H	-2.88843	2.166177	1.234711	H	-3.56792	2.133674	-0.23159
H	0.057889	-1.61986	-1.56501	H	0.412181	-1.63836	-0.57451
H	-0.50273	3.493721	-0.91177	H	0.35067	3.946035	-0.55486
H	0.567717	2.870952	-2.18454	H	1.821034	3.131311	-1.11025
H	-0.99883	2.098378	-1.88766	H	0.283934	2.876193	-1.96755
H	-1.98115	-2.71551	-2.08936	H	-1.17082	-3.31038	-0.67274
H	-1.55798	-3.35431	-0.49866	H	-1.16955	-3.1237	1.082181
H	-3.2504	-3.35726	-1.03761	H	-2.61543	-3.73987	0.252222
H	1.808375	2.070786	1.287815	H	0.40443	1.689131	2.104308
H	1.831523	3.365589	0.092829	H	1.368021	3.041681	1.510333
H	3.156411	2.037248	-1.46342	H	3.265992	1.590155	1.557653
H	3.901445	1.642224	0.074864	H	2.208846	0.267031	2.032929
H	2.965044	-0.29693	-1.61948	H	2.925751	1.207952	-0.76568
H	1.524827	-0.31398	1.953788	H	1.913444	-2.05577	1.02402
H	2.88733	-1.29987	2.517358	H	3.404977	-2.84326	0.484422
H	3.136481	0.407188	2.140351	H	3.461048	-1.587	1.730296

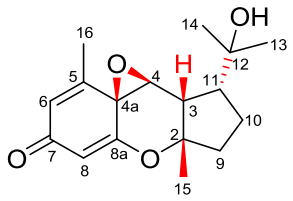
H	4.71547	-1.52576	-0.70571	H	4.913877	0.088526	-1.27114
H	4.786057	-1.85772	1.029641	H	5.269306	-1.48118	-0.5245
H	5.035908	-0.20489	0.438073	H	5.066493	-0.03589	0.485989
H	1.53541	-2.25706	0.551512	H	3.023413	-0.94948	-2.26459
2c'(3)							
C	-3.72564	-1.05114	-0.14152				
C	-4.02958	0.316674	0.340527				
C	-2.88329	1.193225	0.619293				
C	-1.62156	0.760195	0.438506				
C	-1.319	-0.6166	-0.03882				
C	-2.47524	-1.51423	-0.32666				
O	-0.55279	1.536991	0.750246				
C	0.478926	1.697483	-0.26775				
C	0.935448	0.34924	-0.93049				
C	0.035083	-0.83643	-0.63707				
C	-0.0635	2.676251	-1.31368				
C	-2.18601	-2.91909	-0.77773				
O	-5.19125	0.694853	0.483441				
H	0.812822	0.487648	-2.01218				
O	-0.22005	-1.23232	0.699612				
C	1.723444	2.240489	0.448853				
C	2.911101	1.656569	-0.32675				
C	2.492861	0.213421	-0.71189				
C	3.031432	-0.88922	0.242548				
C	2.674321	-0.70152	1.724477				
C	4.560787	-1.00371	0.087953				
O	2.452013	-2.10664	-0.26402				
H	-4.59172	-1.67902	-0.33083				
H	-3.08408	2.200285	0.966802				
H	0.15389	-1.67046	-1.32379				
H	-0.39917	3.596433	-0.82742				
H	0.712438	2.930362	-2.0432				
H	-0.91099	2.245195	-1.85649				
H	-1.78513	-2.93854	-1.7987				
H	-1.4388	-3.38418	-0.12691				
H	-3.09414	-3.52498	-0.76279				
H	1.707996	1.869734	1.476776				
H	1.732808	3.333717	0.49147				
H	3.084462	2.240537	-1.23849				
H	3.840832	1.696434	0.246427				
H	2.928906	-0.04745	-1.68191				

H	1.597658	-0.61889	1.874364				
H	3.037172	-1.56374	2.298826				
H	3.166376	0.181992	2.141968				
H	4.824807	-1.1962	-0.95596				
H	4.929819	-1.84244	0.68846				
H	5.087022	-0.10466	0.422562				
H	2.546068	-2.78457	0.417821				

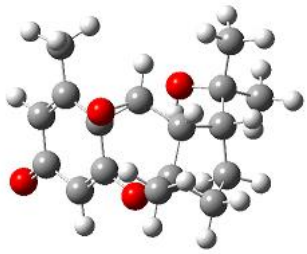
Table S11. The computed ^{13}C NMR data for **2c'**.

No.	**3c'**	δexptl	chloroform	
			δcalcd	$\Delta\delta$
1	6	132	131.1	-0.9
2	7	187.7	179.4	-8.3
3	8	115.3	108.5	-6.8
4	8a	167.1	164.6	-2.5
5	4a	54.7	56.6	1.9
6	5	149	147.1	-1.9
7	2	90.9	88.3	-2.6
8	3	43.7	47.2	3.5
9	4	63.7	63.9	0.2
10	15	27.3	30.9	3.6
11	16	16	18.0	2.0
12	9	40.5	41.7	1.2
13	10	25.5	26.3	0.8
14	11	53.8	54.7	0.9
15	12	72.3	73.3	1.0
16	13	26	25.4	-0.6
17	14	30.4	33.5	3.1
		LAD[a]		8.3
		MAD[b]		2.47

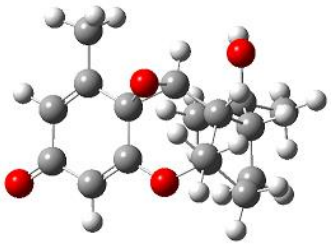
[a] LAD = largest absolute deviation. [b] MAD = mean absolute deviation, computed as $(1/n)\sum_{i}^{n} |\delta_{calcd} - \delta_{exptl}|$



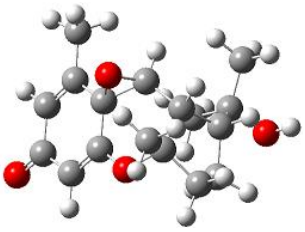
2d'



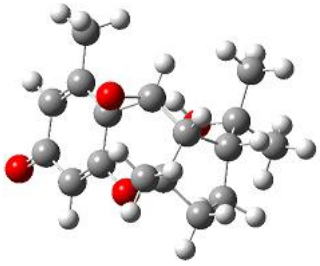
2d'(1)



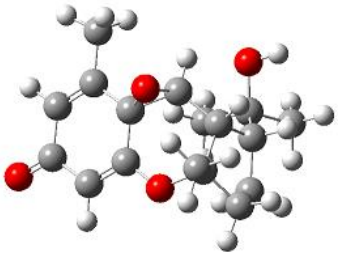
2d'(2)



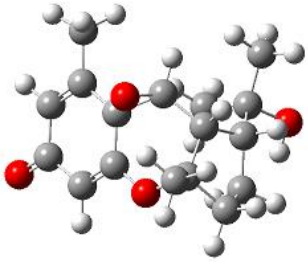
2d'(3)



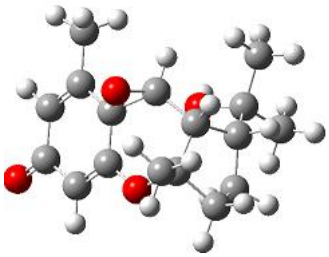
2d'(4)



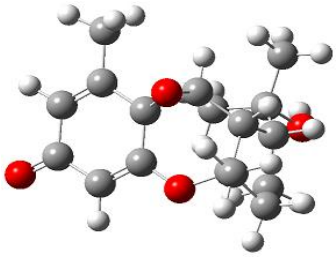
2d'(5)



2d'(6)



2d'(7)



2d'(8)

Figure S9. Optimized geometries of predominant conformers for **2d'** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S12. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized **2d'** at B3LYP/6-31G(d,p) level in the gas phase.

Conformations	E+ZPE	G	%
2d'(1)	-961.563412	-961.609927	26.9
2d'(2)	-961.563915	-961.610396	44.2
2d'(3)	-961.558655	-961.605808	0.4
2d'(4)	-961.559190	-961.605992	0.4
2d'(5)	-961.563231	-961.609537	17.8
2d'(6)	-961.558948	-961.605751	0.3
2d'(7)	-961.562587	-961.608965	9.7
2d'(8)	-961.558866	-961.605676	0.3

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

Table S13. Optimized Z-matrixes of **2d'** in the gas phase (Å) at B3LYP/6-31G(d,p) level.

2d'(1)				**2d'(2)**			
C	3.202293	-1.06328	-0.1448	C	3.243653	-1.05855	-0.14684
C	3.266821	-0.08205	-1.25355	C	3.305346	-0.08384	-1.26269
C	2.224854	0.944453	-1.28738	C	2.248377	0.923915	-1.3164
C	1.261608	1.004011	-0.3396	C	1.266448	0.973976	-0.38707
C	1.199716	0.015824	0.768764	C	1.221868	0.00749	0.746218
C	2.248667	-1.04721	0.802816	C	2.285421	-1.04295	0.796039
O	0.322147	1.96668	-0.42479	O	0.280134	1.881882	-0.54015
C	-0.93585	1.995546	0.328528	C	-0.91024	1.979428	0.307667
C	-1.33952	0.602842	0.911462	C	-1.30962	0.606897	0.925293
C	-0.13383	-0.18908	1.375602	C	-0.11007	-0.19559	1.377151
C	-0.81635	3.111383	1.361381	C	-0.6781	3.105513	1.312026
C	2.196176	-2.04823	1.922827	C	2.25821	-2.01295	1.945444
O	4.150444	-0.15207	-2.10839	O	4.20299	-0.14704	-2.10338
H	-1.91416	0.806612	1.82301	H	-1.85142	0.831826	1.851297
O	0.850709	0.582304	2.071534	O	0.89042	0.576647	2.047066
C	-1.98666	2.255492	-0.76172	C	-2.03968	2.270264	-0.69312
C	-2.20957	0.875185	-1.38165	C	-2.36554	0.901211	-1.29531
C	-2.32272	-0.04737	-0.14599	C	-2.35494	-0.04233	-0.07089
C	-2.21757	-1.57527	-0.41552	C	-2.27617	-1.55635	-0.38961
C	-3.06057	-1.973	-1.63967	C	-1.05966	-1.98628	-1.22406
C	-2.6985	-2.38287	0.798565	C	-3.56624	-1.99667	-1.10407

O	-0.85745	-1.98426	-0.63064	O	-2.23223	-2.19299	0.905347
H	3.985045	-1.81634	-0.14193	H	4.040646	-1.79638	-0.1271
H	2.239507	1.65746	-2.10388	H	2.249885	1.616662	-2.15021
H	-0.32857	-1.16013	1.818666	H	-0.33144	-1.15946	1.825039
H	-0.04665	2.871526	2.096202	H	0.141897	2.859001	1.986994
H	-0.55411	4.050391	0.865341	H	-0.43855	4.031521	0.781048
H	-1.77035	3.250439	1.88044	H	-1.58271	3.273473	1.905543
H	2.061628	-1.54709	2.886439	H	2.171013	-1.48022	2.897336
H	1.356937	-2.74147	1.787588	H	1.402148	-2.6956	1.876322
H	3.11499	-2.63715	1.956441	H	3.167756	-2.61677	1.959706
H	-2.91284	2.615949	-0.29677	H	-2.90547	2.66538	-0.14753
H	-1.63935	3.01627	-1.4652	H	-1.72996	3.019375	-1.4264
H	-1.34237	0.61088	-2.0005	H	-1.58373	0.627628	-2.01105
H	-3.0954	0.8316	-2.02034	H	-3.32175	0.886774	-1.82569
H	-3.3351	0.10713	0.250535	H	-3.32389	0.072843	0.429217
H	-2.67333	-1.5172	-2.55646	H	-0.1148	-1.72268	-0.74856
H	-3.03186	-3.05877	-1.7663	H	-1.07348	-3.07455	-1.35752
H	-4.10554	-1.66533	-1.52874	H	-1.07559	-1.54107	-2.22253
H	-2.18072	-2.10106	1.718303	H	-4.44364	-1.7448	-0.50142
H	-2.51953	-3.44714	0.624003	H	-3.56023	-3.08222	-1.25877
H	-3.77031	-2.23219	0.957517	H	-3.66978	-1.52861	-2.08729
H	-0.53876	-1.57396	-1.4465	H	-2.2518	-3.14924	0.761715
2d'(3)				**2d'(4)**			
C	3.243791	-1.09423	-0.15267	C	3.215258	-1.00989	-0.15463
C	3.306492	-0.11884	-1.26896	C	3.215987	-0.09821	-1.32688
C	2.267674	0.90865	-1.30664	C	2.147369	0.895287	-1.39127
C	1.299016	0.971466	-0.3649	C	1.201441	0.98115	-0.42894
C	1.243118	-0.0074	0.75524	C	1.212472	0.072559	0.751471
C	2.296098	-1.06839	0.799998	C	2.299115	-0.95267	0.827008
O	0.344985	1.916598	-0.47499	O	0.216007	1.889642	-0.56159
C	-0.87675	1.99078	0.331629	C	-0.9775	1.975635	0.284953
C	-1.29253	0.608296	0.930481	C	-1.3374	0.612113	0.953281
C	-0.09253	-0.19716	1.37871	C	-0.09769	-0.1141	1.431886
C	-0.68303	3.104948	1.356363	C	-0.78002	3.14288	1.24886
C	2.272972	-2.03538	1.95256	C	2.347818	-1.84194	2.041
O	4.193749	-0.19502	-2.11864	O	4.084496	-0.19775	-2.19309
H	-1.83651	0.828624	1.857003	H	-1.89005	0.859272	1.867948
O	0.908897	0.561294	2.057478	O	0.90208	0.716156	2.022826
C	-1.96919	2.282794	-0.70864	C	-2.11306	2.193939	-0.723
C	-2.26433	0.91422	-1.32312	C	-2.38146	0.796931	-1.27882
C	-2.32926	-0.01734	-0.09245	C	-2.34966	-0.11734	-0.03137
C	-2.34604	-1.53918	-0.42788	C	-2.16127	-1.62737	-0.36606
C	-2.70662	-2.38895	0.802791	C	-3.14781	-2.04383	-1.46869

C	-1.07884	-2.06706	-1.10668	C	-2.40497	-2.53097	0.856607
O	-3.37351	-1.73859	-1.41859	O	-0.8682	-1.87246	-0.93822
H	4.033013	-1.84044	-0.14096	H	4.027382	-1.73065	-0.12507
H	2.277769	1.611452	-2.13178	H	2.11189	1.548374	-2.25544
H	-0.29825	-1.16019	1.840375	H	-0.25423	-1.04206	1.977798
H	0.112683	2.852184	2.05798	H	0.050943	2.952923	1.92846
H	-0.42429	4.036499	0.844762	H	-0.57535	4.056325	0.682885
H	-1.60956	3.266695	1.91689	H	-1.68888	3.301672	1.838457
H	2.19191	-1.50054	2.903905	H	2.292888	-1.24634	2.957533
H	1.419494	-2.72252	1.890837	H	1.511754	-2.55288	2.066167
H	3.182485	-2.63911	1.963729	H	3.272381	-2.42217	2.052412
H	-2.857	2.675006	-0.1964	H	-2.99444	2.575266	-0.19201
H	-1.63123	3.03565	-1.42531	H	-1.8265	2.931138	-1.47756
H	-1.44487	0.627682	-1.98977	H	-1.58072	0.50734	-1.96683
H	-3.18492	0.882796	-1.90827	H	-3.3304	0.731801	-1.81669
H	-3.31184	0.162706	0.369952	H	-3.33352	-0.04425	0.450606
H	-3.64733	-2.04287	1.248636	H	-2.90674	-1.54863	-2.41094
H	-2.83896	-3.43124	0.499609	H	-3.07824	-3.12263	-1.63211
H	-1.94325	-2.3588	1.585281	H	-4.1787	-1.79872	-1.1948
H	-0.82994	-1.47987	-1.9933	H	-1.75206	-2.3002	1.7032
H	-1.25637	-3.09626	-1.43002	H	-2.23523	-3.57519	0.578107
H	-0.21763	-2.06271	-0.43725	H	-3.43677	-2.4365	1.209664
H	-4.21862	-1.48239	-1.02305	H	-0.2122	-1.93364	-0.23376
2d'(5)				**2d'(6)**			
C	3.248639	-1.07634	-0.15262	C	3.240087	-1.06251	-0.14058
C	3.333443	-0.07199	-1.23981	C	3.273074	-0.12577	-1.29045
C	2.279085	0.939642	-1.28631	C	2.223817	0.890556	-1.34395
C	1.282991	0.969263	-0.37213	C	1.269475	0.974921	-0.3892
C	1.221149	-0.02047	0.740052	C	1.239201	0.029824	0.761107
C	2.275388	-1.08157	0.77486	C	2.30705	-1.01499	0.825872
O	0.295291	1.877248	-0.52615	O	0.303613	1.906402	-0.51558
C	-0.88915	1.979212	0.325925	C	-0.90745	1.98857	0.307248
C	-1.30491	0.60244	0.924947	C	-1.30225	0.613842	0.933358
C	-0.11489	-0.22422	1.360411	C	-0.0893	-0.16029	1.400941
C	-0.64003	3.08704	1.346818	C	-0.71231	3.126225	1.305553
C	2.220812	-2.08657	1.892658	C	2.314412	-1.94155	2.01145
O	4.245836	-0.11369	-2.06557	O	4.144546	-0.22321	-2.15426
H	-1.83769	0.825805	1.857306	H	-1.85342	0.845108	1.852927
O	0.888656	0.523948	2.052515	O	0.907754	0.630707	2.048481
C	-2.01789	2.299686	-0.66674	C	-2.01602	2.251771	-0.72256
C	-2.36547	0.944124	-1.28667	C	-2.3005	0.871063	-1.31535
C	-2.361	-0.0204	-0.07688	C	-2.32845	-0.0526	-0.07433
C	-2.29997	-1.53708	-0.41165	C	-2.30171	-1.57863	-0.39763

C	-1.08658	-1.97127	-1.2396	C	-2.66806	-2.41898	0.83167
C	-3.58818	-1.95604	-1.14134	C	-1.00624	-2.08813	-1.04611
O	-2.20703	-2.28922	0.817874	O	-3.3951	-1.82463	-1.30475
H	4.040107	-1.8202	-0.14151	H	4.038495	-1.79855	-0.11591
H	2.293907	1.650444	-2.10465	H	2.214656	1.56705	-2.19088
H	-0.34554	-1.19783	1.782579	H	-0.27855	-1.11204	1.892305
H	0.17828	2.819766	2.015999	H	0.096456	2.898559	2.000424
H	-0.38952	4.017457	0.82885	H	-0.47331	4.050008	0.770684
H	-1.54072	3.258667	1.945395	H	-1.63256	3.288011	1.876216
H	2.116176	-1.58339	2.858855	H	2.244927	-1.3747	2.944948
H	1.364739	-2.76358	1.78243	H	1.466732	-2.63818	1.989766
H	3.128303	-2.69347	1.90705	H	3.229976	-2.53594	2.026613
H	-2.87591	2.700515	-0.11295	H	-2.90373	2.635343	-0.20483
H	-1.6995	3.054166	-1.39081	H	-1.69876	2.999576	-1.45381
H	-1.59002	0.668161	-2.00813	H	-1.48912	0.599673	-2.00068
H	-3.32354	0.949716	-1.81377	H	-3.24128	0.832425	-1.87025
H	-3.33201	0.110459	0.423071	H	-3.31585	0.091982	0.380014
H	-0.14229	-1.71946	-0.75712	H	-3.64137	-2.10722	1.221456
H	-1.11575	-3.05651	-1.36942	H	-2.7409	-3.47206	0.546806
H	-1.09828	-1.50978	-2.22976	H	-1.93074	-2.33233	1.633661
H	-4.47659	-1.69209	-0.55409	H	-0.72777	-1.49357	-1.92286
H	-3.58889	-3.03904	-1.29241	H	-1.16108	-3.11949	-1.37559
H	-3.68046	-1.4729	-2.11828	H	-0.15534	-2.07764	-0.36272
H	-3.02745	-2.14607	1.310395	H	-3.14292	-1.48011	-2.17175
2d'(7)				**2d'(8)**			
C	3.215009	-1.10905	-0.16654	C	3.238224	-1.08377	-0.14598
C	3.323558	-0.07781	-1.22684	C	3.286178	-0.1293	-1.2812
C	2.294708	0.959299	-1.24525	C	2.247903	0.898019	-1.32384
C	1.296788	0.979831	-0.33294	C	1.289138	0.976665	-0.37258
C	1.20497	-0.04135	0.742648	C	1.242537	0.012466	0.76062
C	2.235923	-1.12247	0.753776	C	2.30058	-1.04256	0.816169
O	0.351886	1.93626	-0.42642	O	0.33858	1.923867	-0.48142
C	-0.88354	1.991822	0.356975	C	-0.89156	1.992488	0.316064
C	-1.3185	0.602401	0.925631	C	-1.29801	0.611192	0.924457
C	-0.12774	-0.23123	1.35186	C	-0.0925	-0.17808	1.386141
C	-0.70633	3.083881	1.408138	C	-0.71425	3.117039	1.332004
C	2.14728	-2.16586	1.832737	C	2.292953	-1.98674	1.98778
O	4.236808	-0.12023	-2.05245	O	4.161951	-0.22299	-2.14128
H	-1.86428	0.809556	1.854182	H	-1.84862	0.834813	1.846318
O	0.876138	0.495181	2.067548	O	0.904632	0.595488	2.054291
C	-1.9522	2.305947	-0.70037	C	-1.97899	2.265126	-0.73451
C	-2.24213	0.94632	-1.33653	C	-2.25715	0.888515	-1.33921
C	-2.35203	0.004724	-0.11715	C	-2.32482	-0.02752	-0.09709

C	-2.29684	-1.50922	-0.436	C	-2.32805	-1.54891	-0.40785
C	-3.19336	-1.84673	-1.64036	C	-2.67617	-2.38372	0.837341
C	-2.75102	-2.3545	0.769924	C	-1.05725	-2.07691	-1.08976
O	-0.93108	-1.80413	-0.76794	O	-3.42786	-1.66447	-1.33375
H	3.990165	-1.87013	-0.17544	H	4.03004	-1.82717	-0.12848
H	2.333602	1.700617	-2.03509	H	2.250246	1.588772	-2.15916
H	-0.34355	-1.20967	1.769099	H	-0.29062	-1.1359	1.861555
H	0.072848	2.807779	2.119865	H	0.078892	2.878016	2.041354
H	-0.42871	4.024103	0.922845	H	-0.46036	4.04635	0.813924
H	-1.64327	3.240678	1.952753	H	-1.64621	3.275411	1.884346
H	2.018272	-1.69917	2.814394	H	2.222245	-1.43323	2.929177
H	1.290208	-2.83103	1.668851	H	1.439605	-2.67585	1.950747
H	3.049741	-2.78032	1.850665	H	3.203453	-2.589	1.9998
H	-2.85038	2.694843	-0.20383	H	-2.87453	2.652254	-0.23228
H	-1.59527	3.064819	-1.40121	H	-1.6427	3.015677	-1.45443
H	-1.40448	0.643889	-1.97348	H	-1.42942	0.605978	-1.99802
H	-3.14909	0.950589	-1.947	H	-3.17685	0.838891	-1.92322
H	-3.34612	0.169621	0.318849	H	-3.31427	0.143652	0.344691
H	-2.82488	-1.36554	-2.54862	H	-3.61592	-2.03363	1.273871
H	-3.20174	-2.93044	-1.80901	H	-2.80562	-3.43596	0.557629
H	-4.22934	-1.53444	-1.474	H	-1.90228	-2.35218	1.6093
H	-2.18323	-2.12787	1.674888	H	-0.83492	-1.51555	-1.99986
H	-2.62233	-3.421	0.55324	H	-1.20399	-3.1261	-1.37374
H	-3.81097	-2.18729	0.98733	H	-0.17928	-2.04138	-0.44161
H	-0.89454	-2.70229	-1.1234	H	-3.48989	-2.59311	-1.596

Table S14. The computed ^{13}C NMR data for **2d'**.

No.	2d'	δexptl	chloroform	
			δcalcd	Δδ
1	6	132	130.5	-1.5
2	7	187.6	179.5	-8.1
3	8	115.3	106.6	-8.7
4	8a	167.1	166.8	-0.3
5	4a	54.7	56.4	1.7
6	5	149	148.3	-0.7
7	2	90.9	91.1	0.2
8	3	43.7	45.1	1.4
9	4	63.7	64.8	1.1
10	10	25.5	28.6	3.1
11	16	16	17.4	1.4
12	9	40.5	42.3	1.8
13	15	27.3	29.8	2.5
14	11	53.8	53.5	-0.3
15	12	72.4	73.5	1.1
16	13	26	27.0	1.0
17	14	30.4	31.5	1.1
	LAD[a]			8.7
	MAD[b]			2.12

[a] LAD = largest absolute deviation. [b] MAD = mean absolute deviation, computed as (1/*n*) $\sum_{i}^{n} |\delta_{calcd} - \delta_{exptl}|$

Original Spectroscopic Data

Figure S10. Positive ESIMS spectrum of **1**

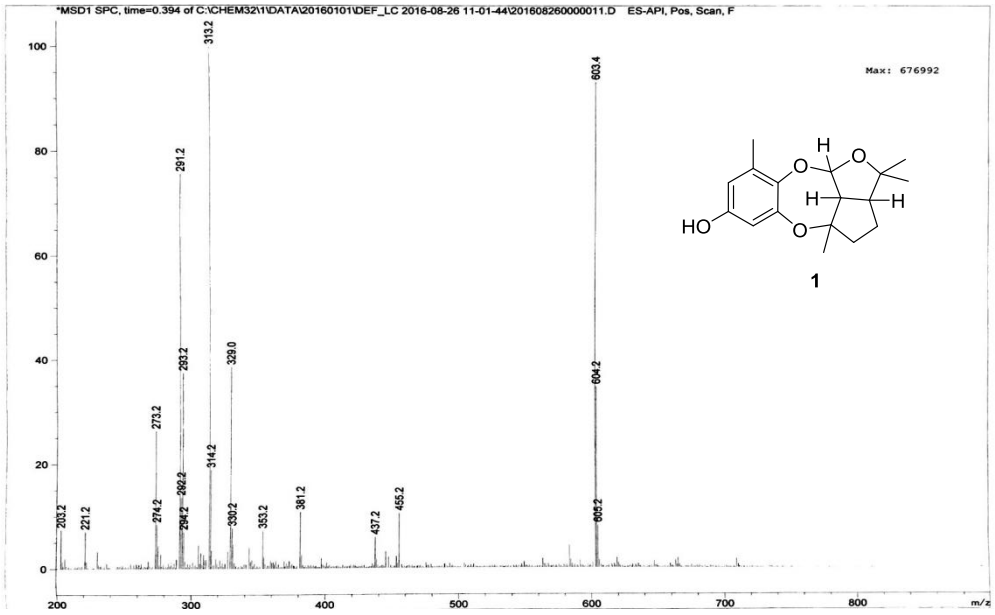


Figure S11. Negative ESIMS spectrum of **1**

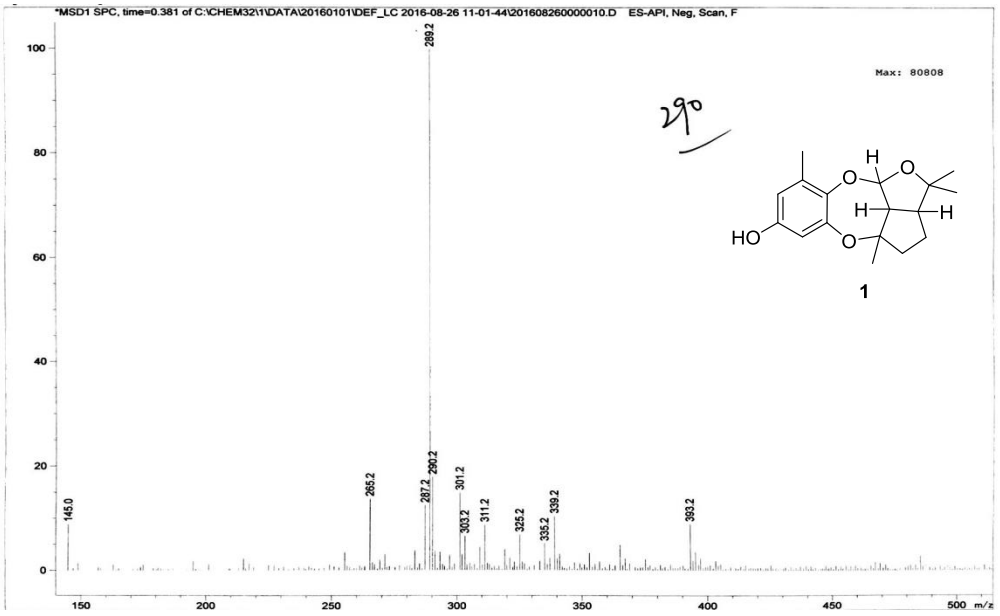


Figure S12. Positive HR-ESIMS spectrum of **1**

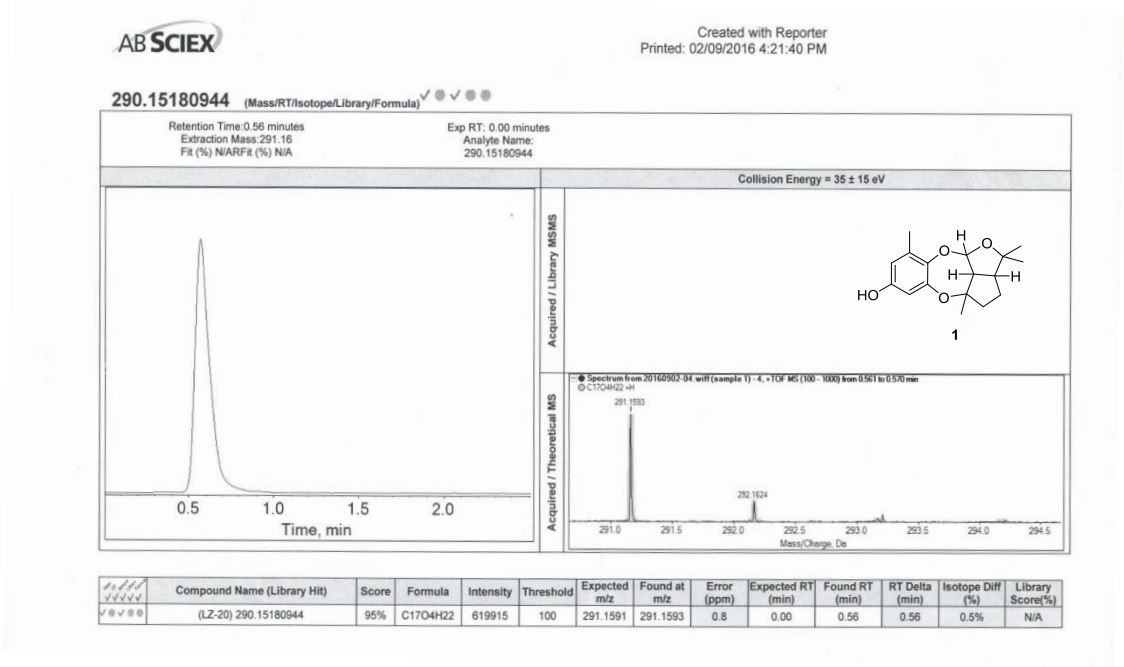


Figure S13. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **1**

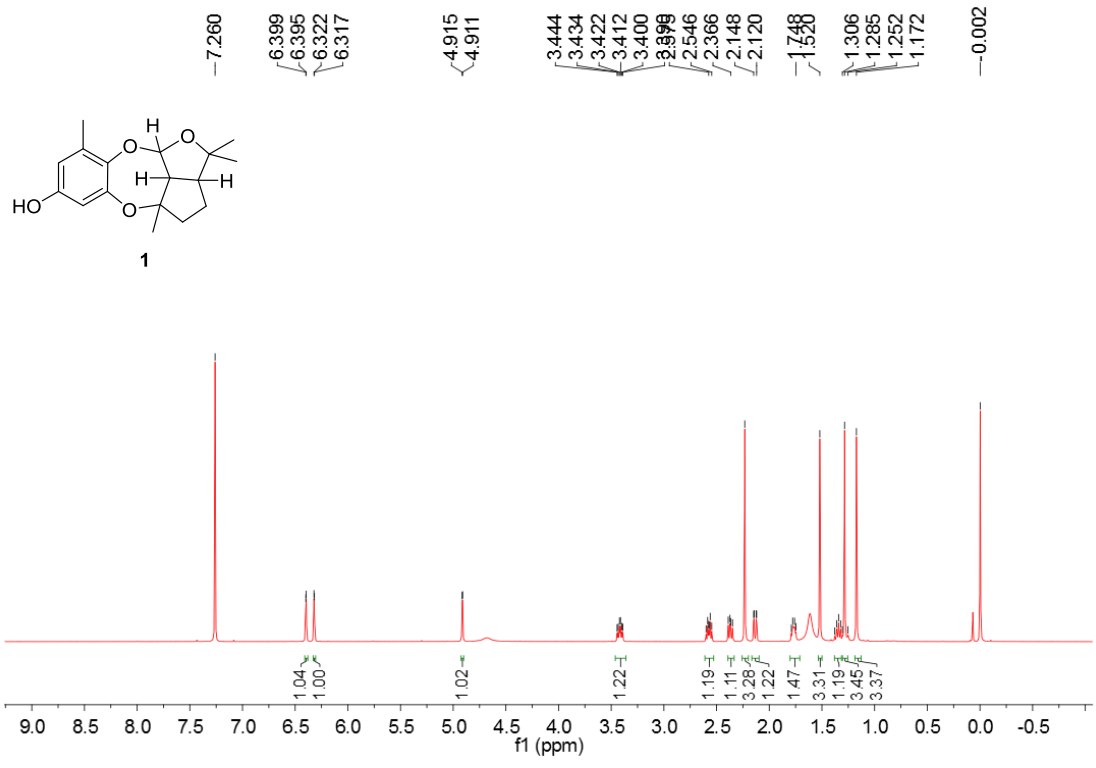


Figure S14. ^{13}C NMR and DEPT (150 MHz, $CDCl_3$) spectra of **1**

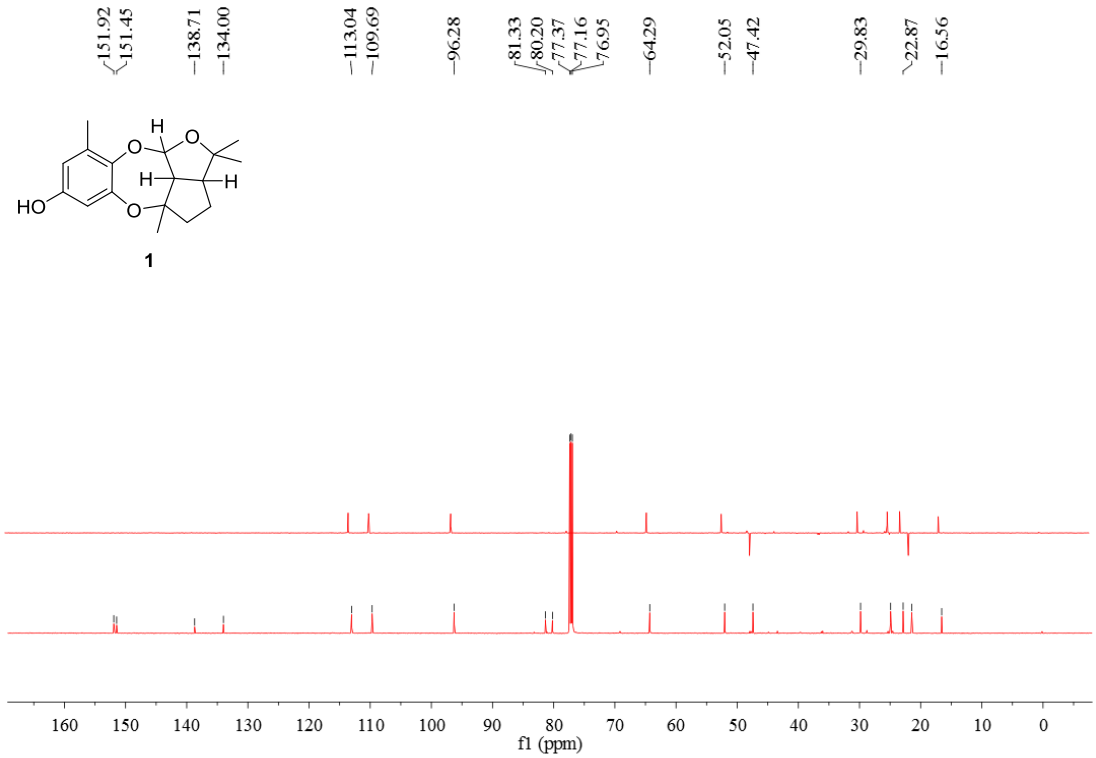


Figure S15. HSQC (600 MHz, $CDCl_3$) spectrum of **1**

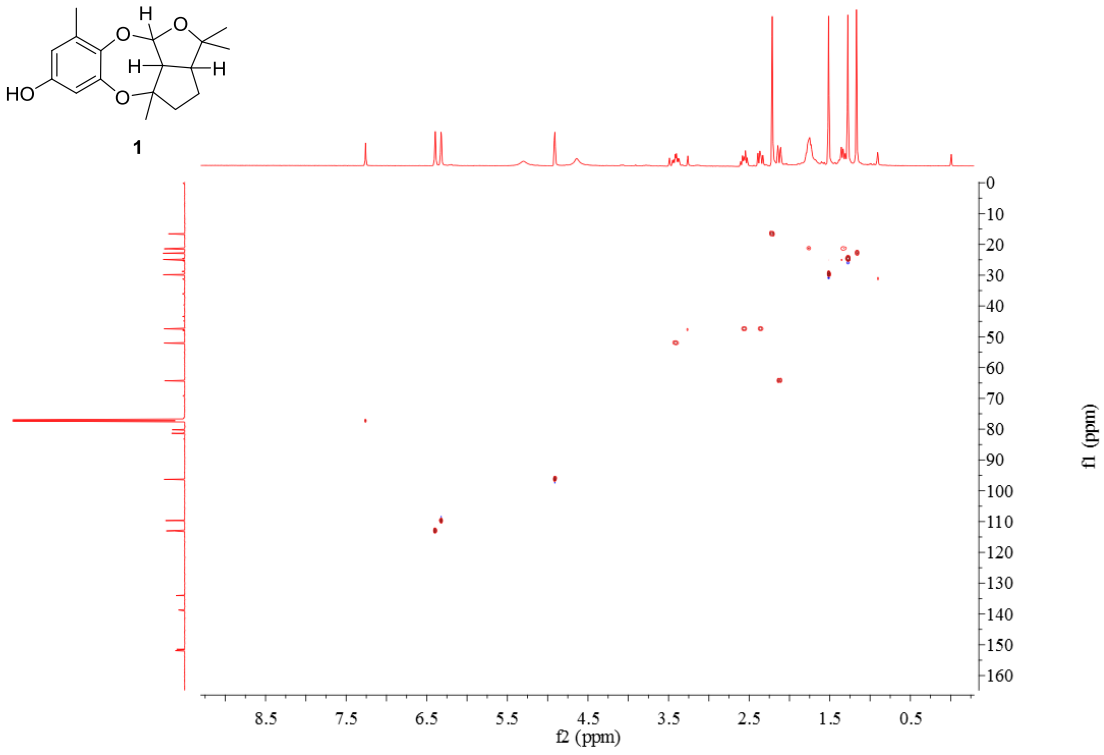


Figure S16. HSQC (600 MHz, $CDCl_3$) spectrum of **1**

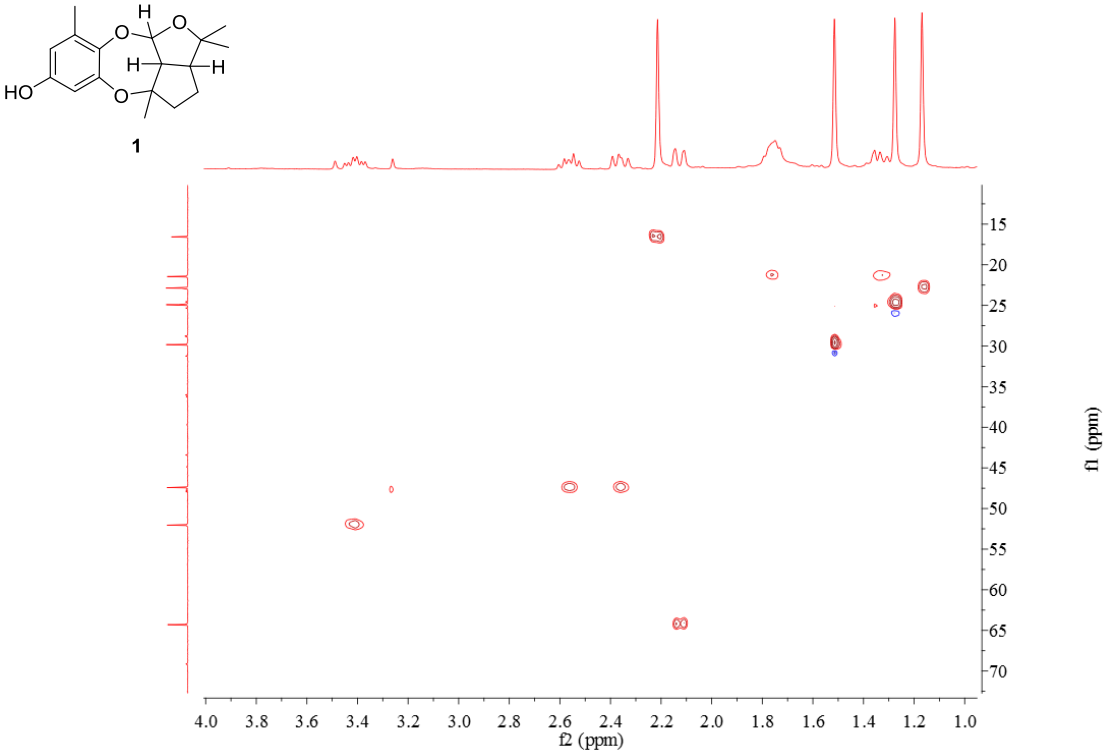


Figure S17. HMBC (600 MHz, $CDCl_3$) spectrum of **1**

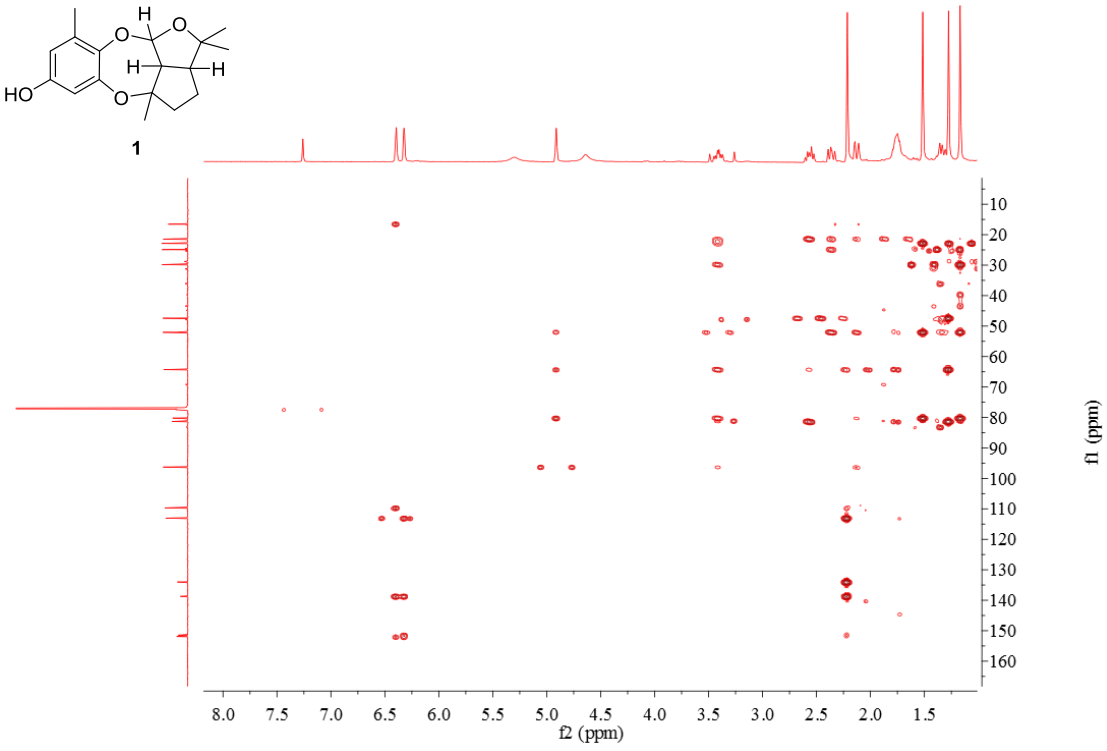


Figure S18. HMBC (600 MHz, $CDCl_3$) spectrum of **1**

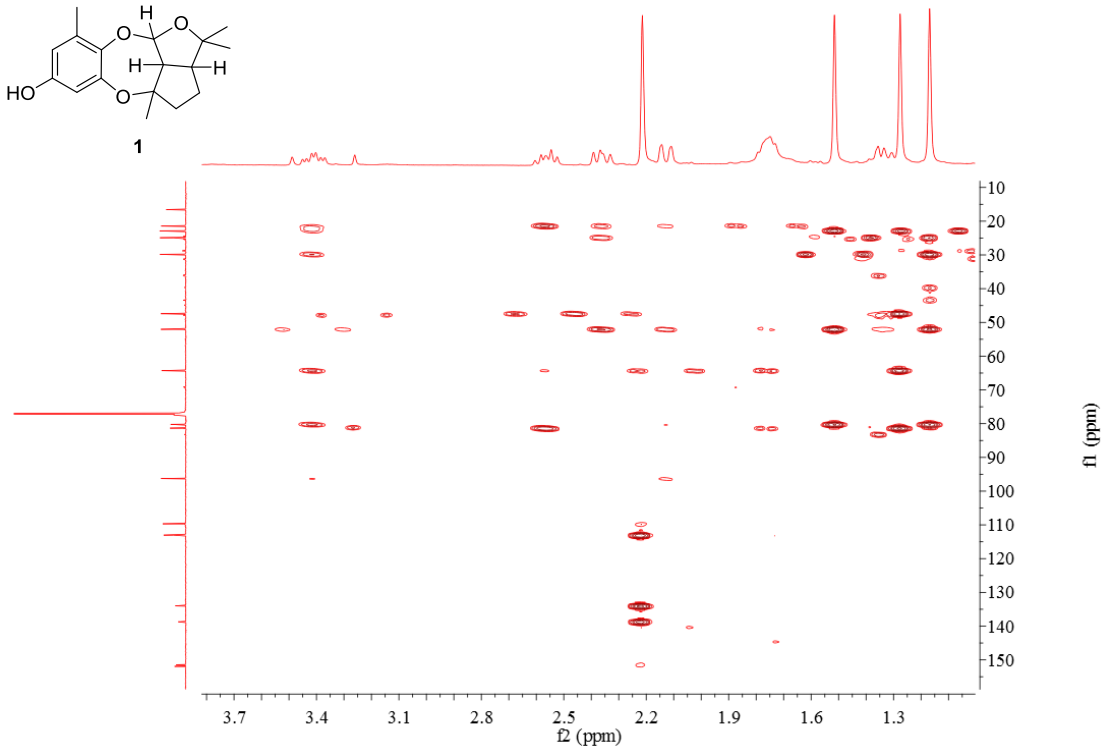


Figure S19. ^{1}H-^{1}H COSY (600 MHz, $CDCl_3$) spectrum of **1**

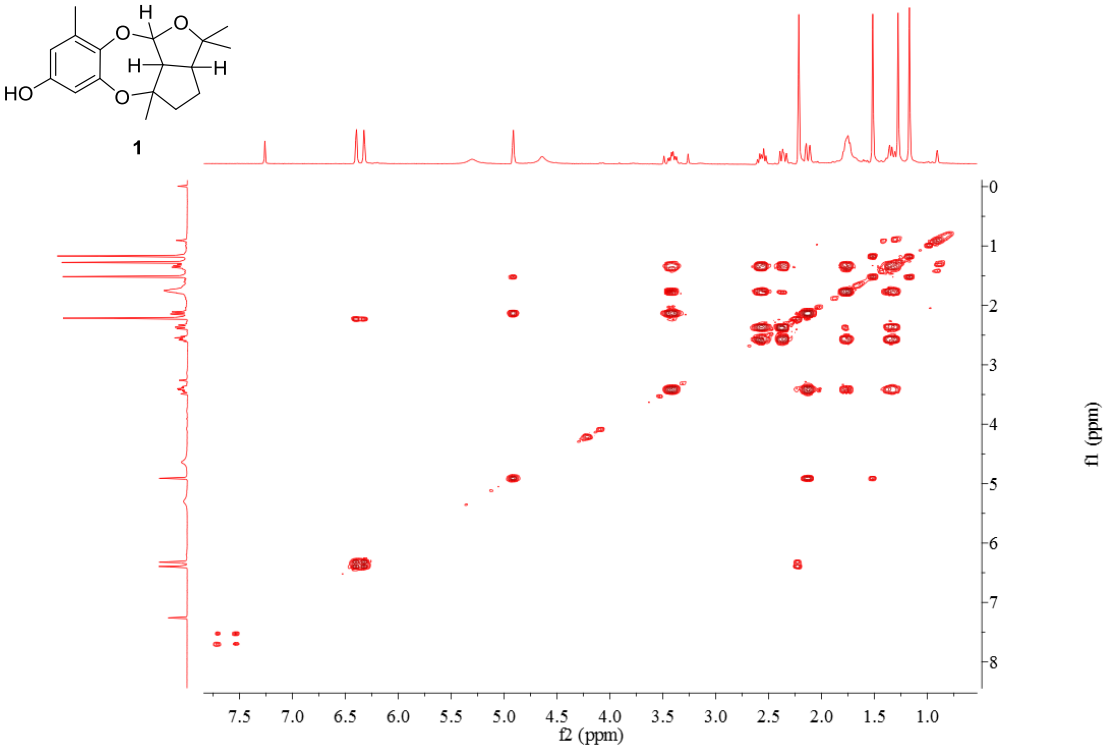


Figure S20. NOESY (600 MHz, $CDCl_3$) spectrum of **1**

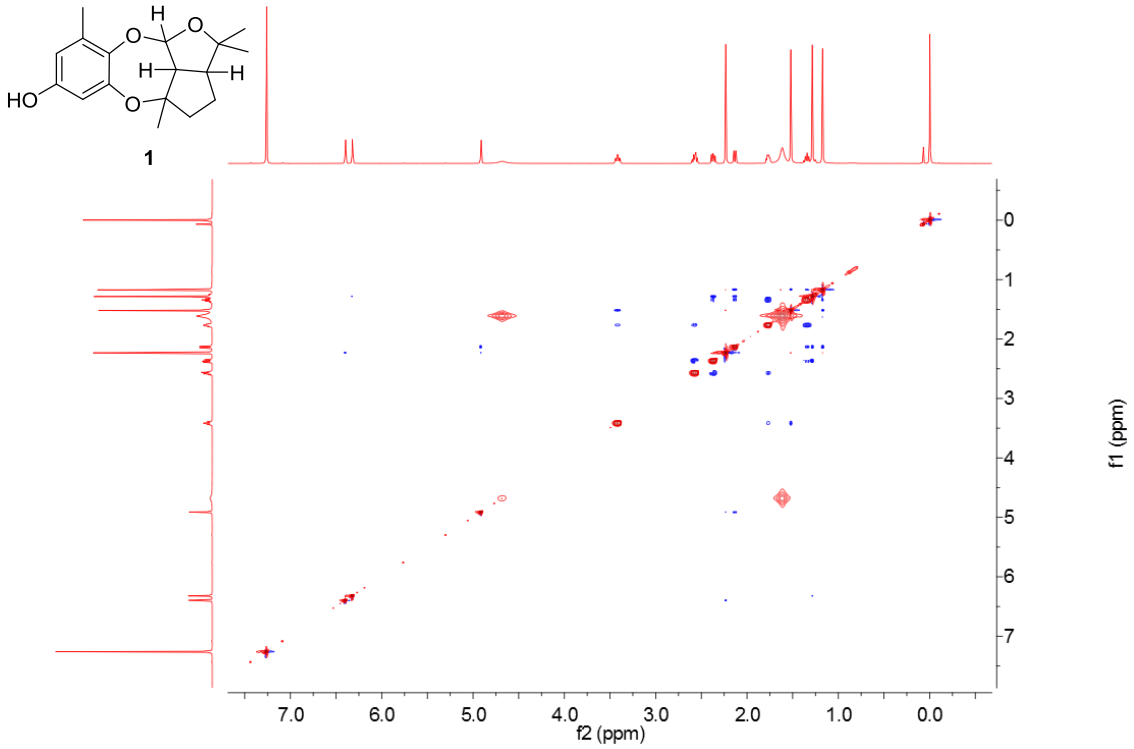


Figure S21. IR spectrum of **1**

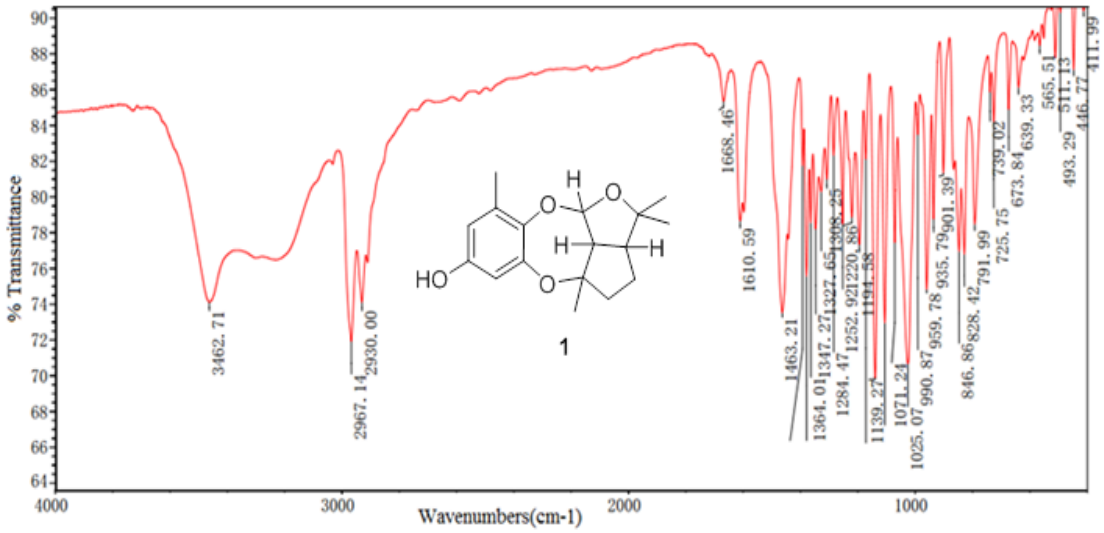


Figure S22. Positive ESIMS spectrum of **1a**

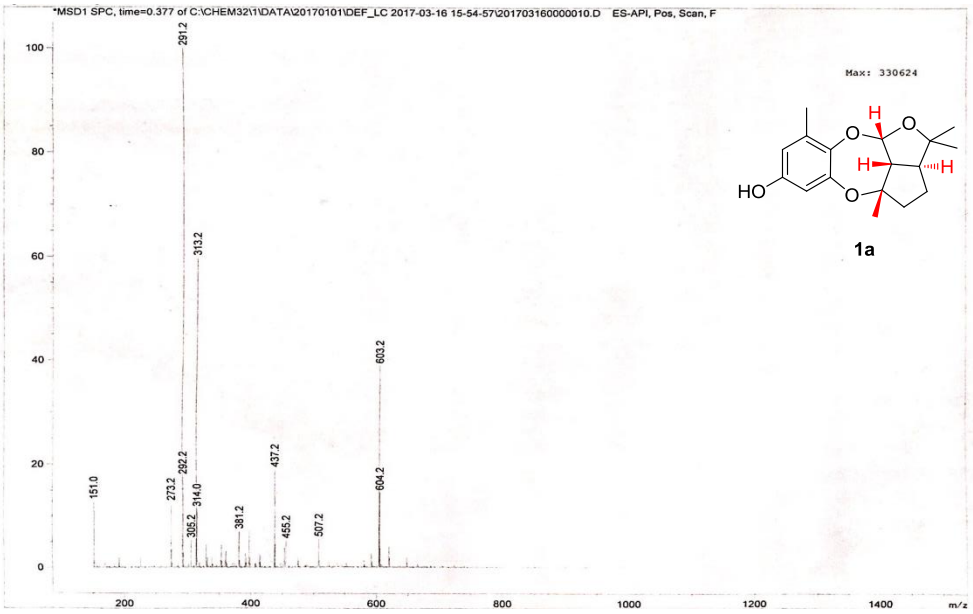


Figure S23. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **1a**

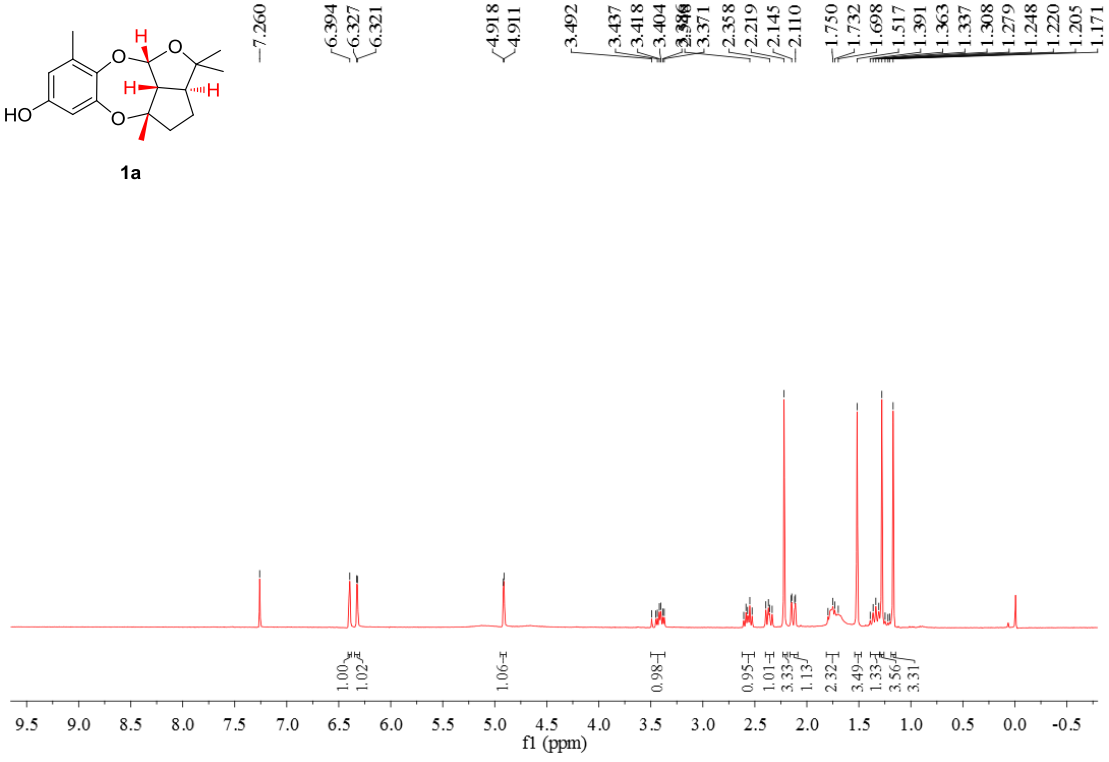


Figure S24. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **1a**

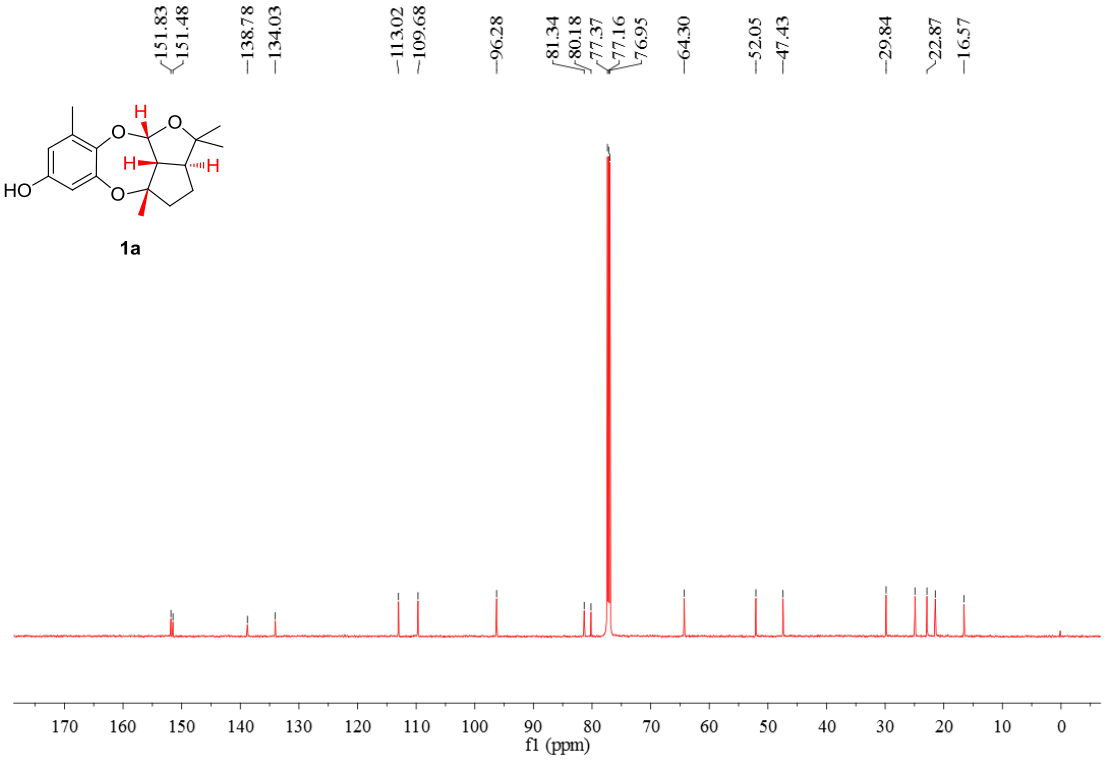


Figure S25. Positive ESIMS spectrum of **1b**

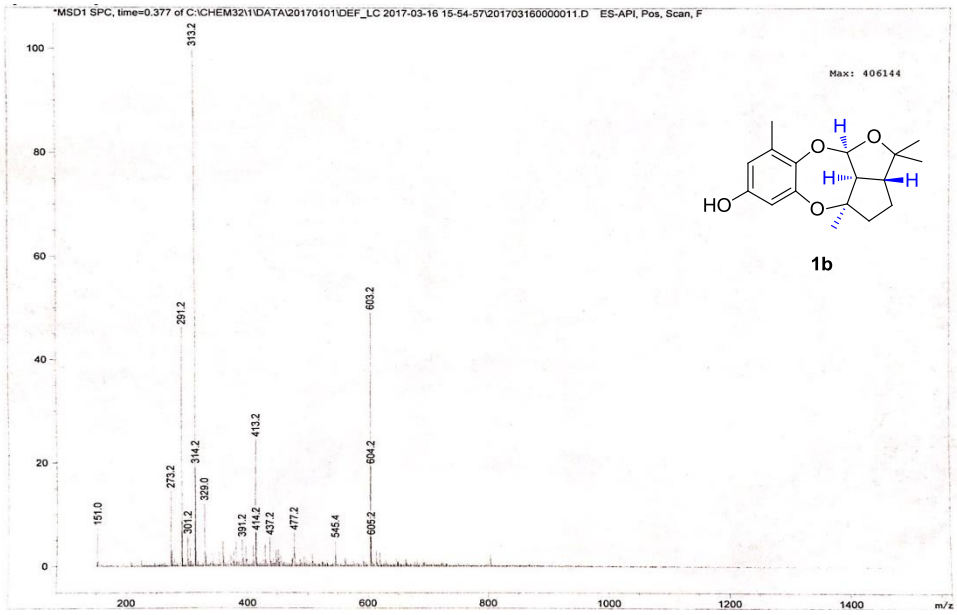


Figure S26. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **1b**

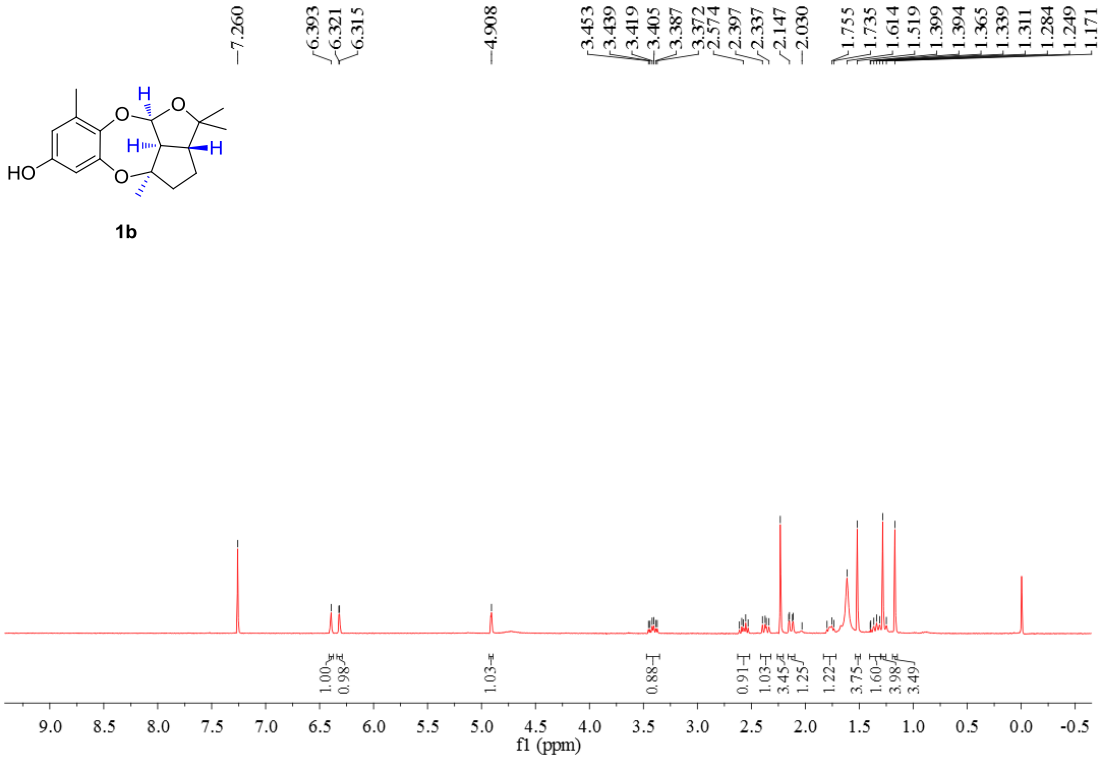


Figure S27. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **1b**

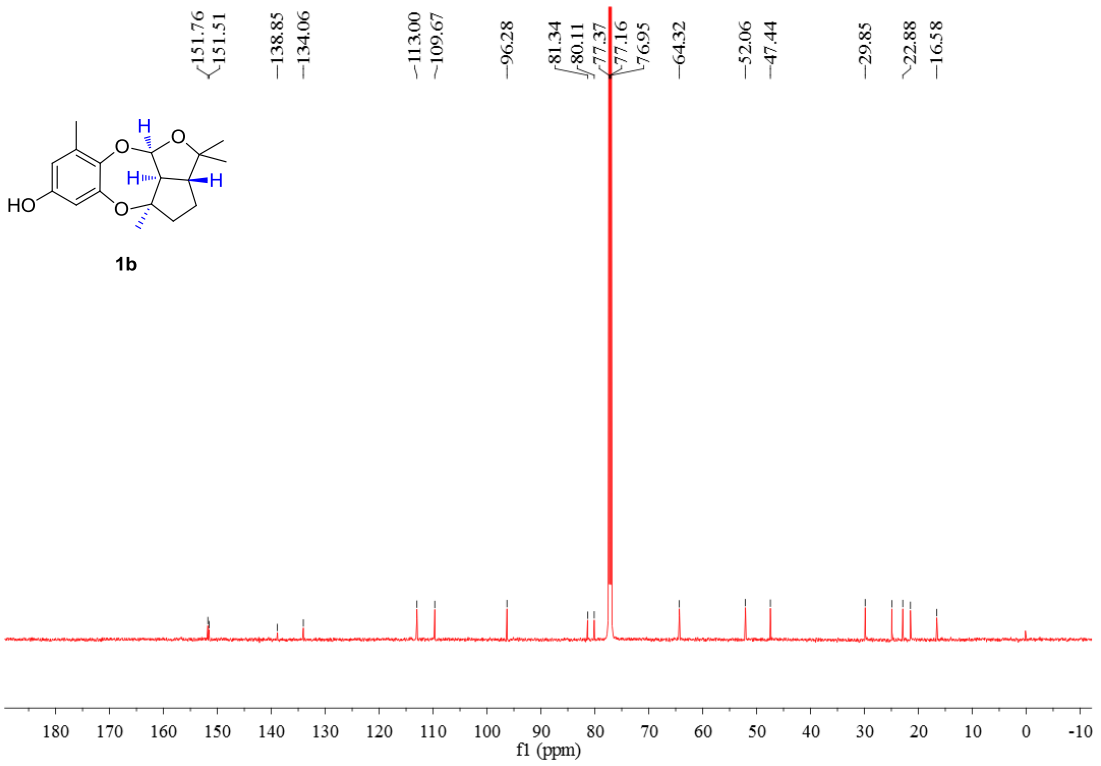


Figure S28. Positive ESIMS spectrum of **2**

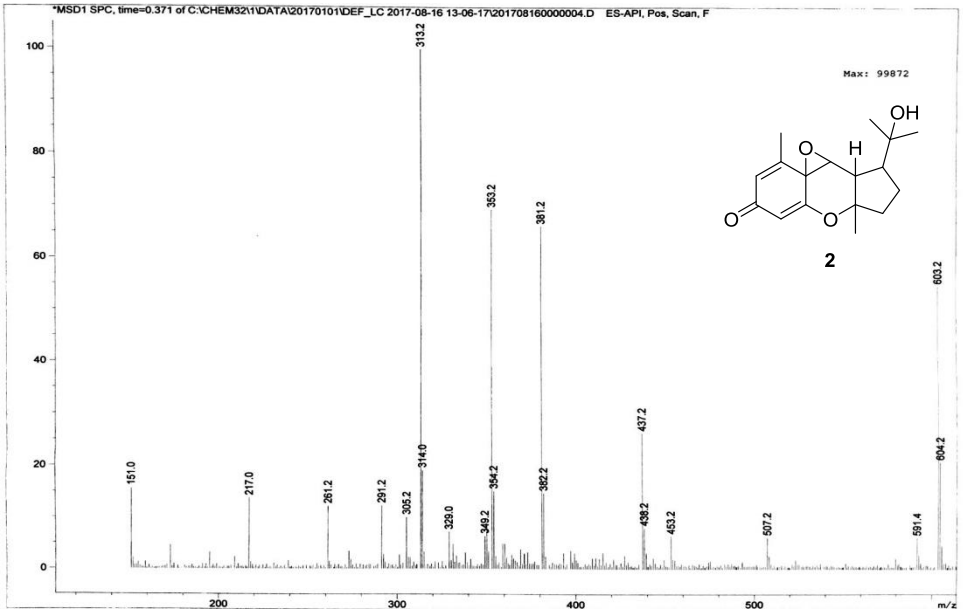


Figure S29. Negative ESIMS spectrum of **2**

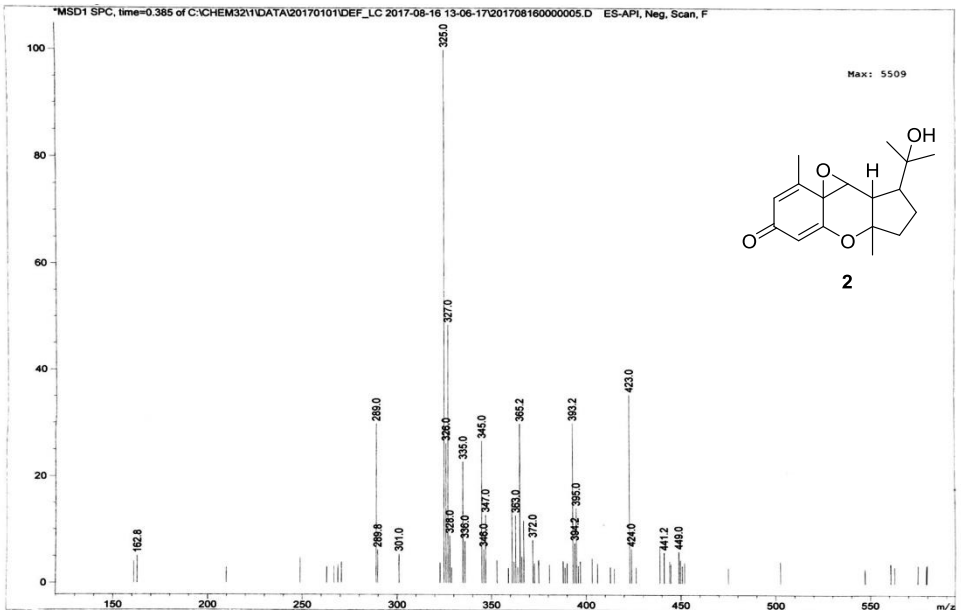
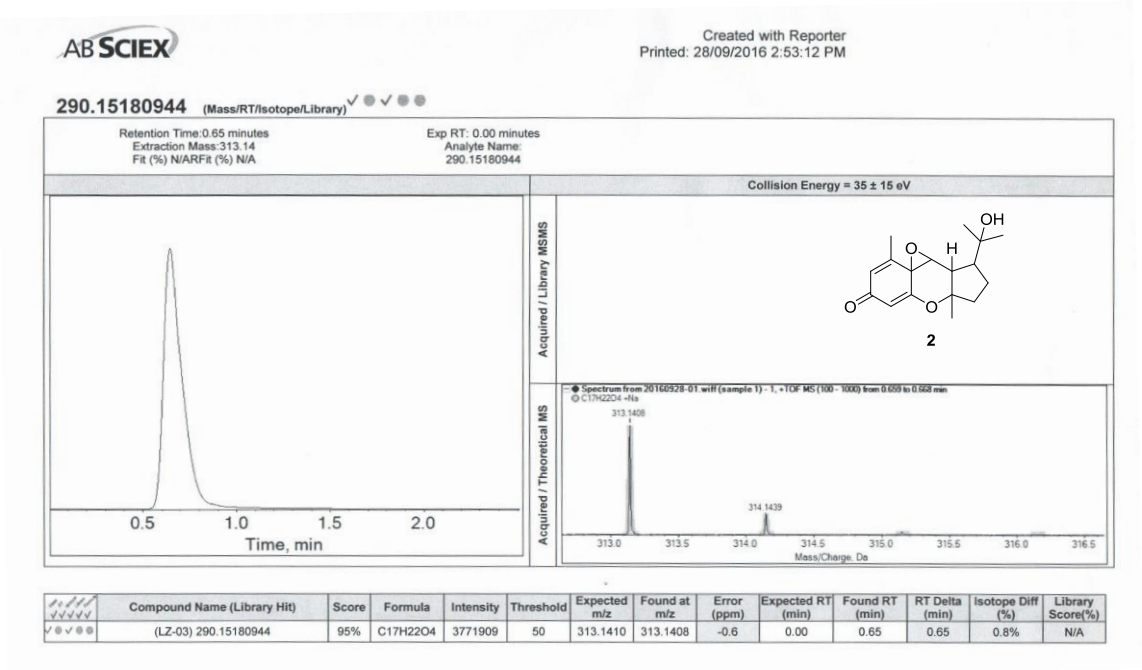


Figure S30. Positive HR-ESIMS spectrum of **2**



Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
(LZ-03) 290.15180944	95%	C17H22O4	3771909	50	313.1410	313.1408	-0.6	0.00	0.65	0.65	0.8%	N/A

Figure S31. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2**

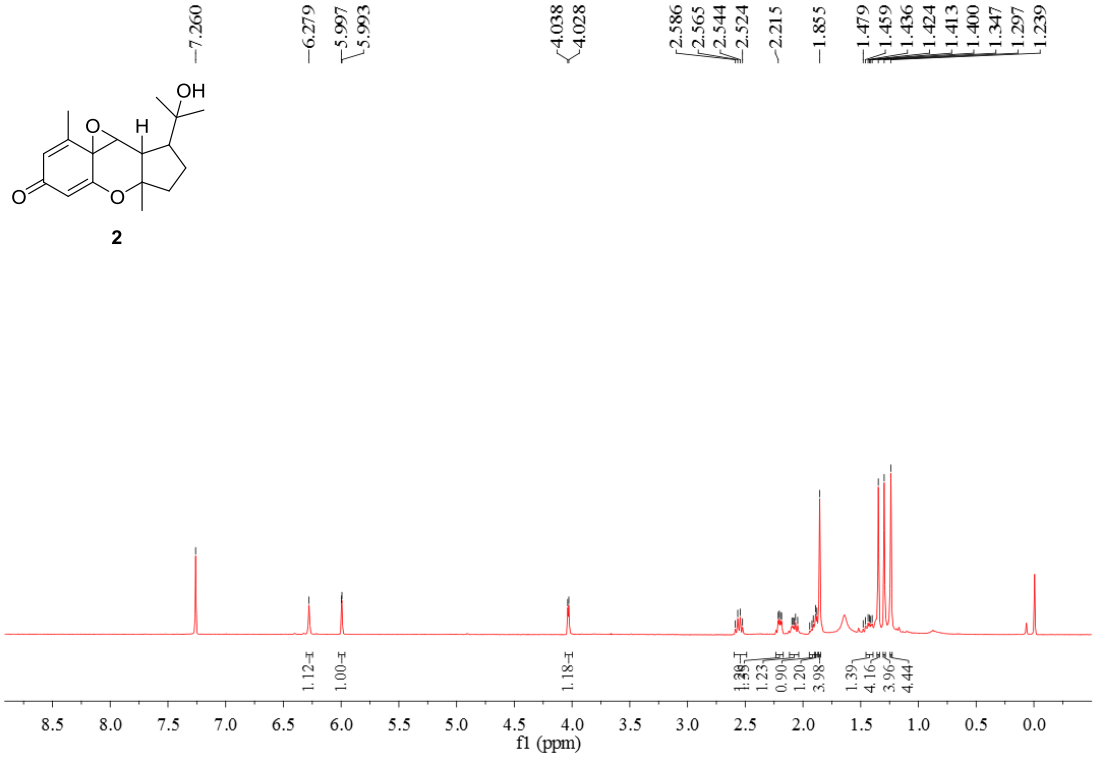


Figure S32. ^{13}C NMR and DEPT (150 MHz, $CDCl_3$) spectra of **2**

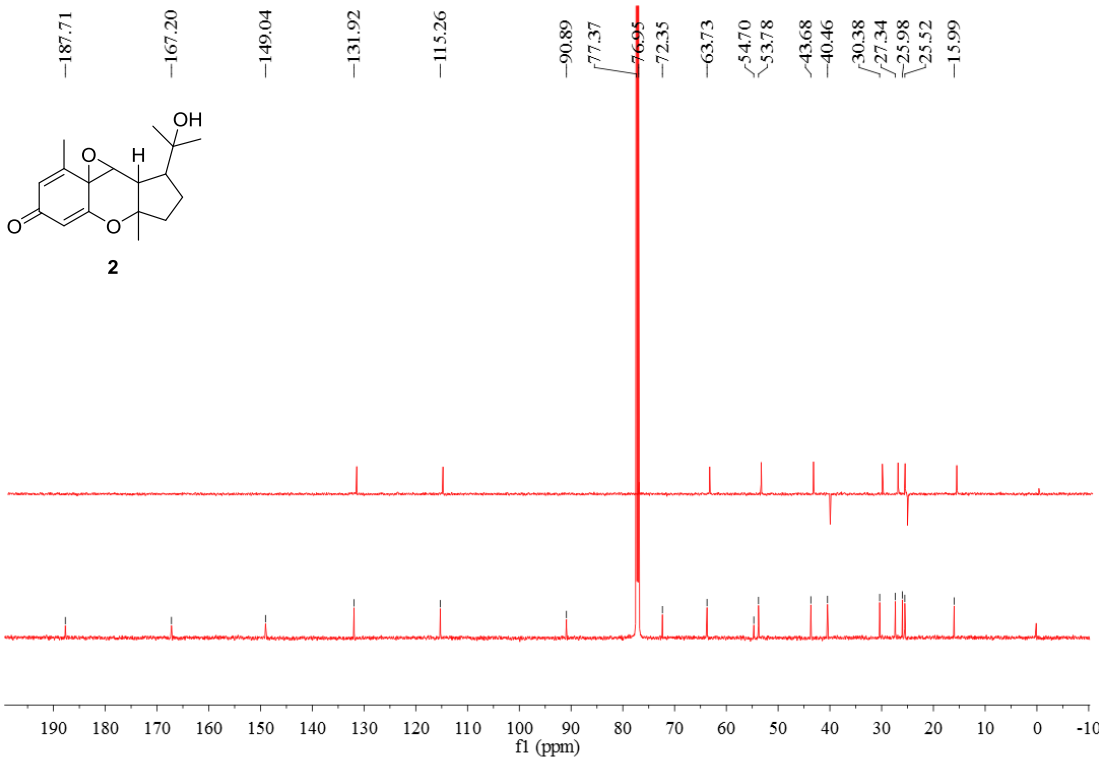


Figure S33. HSQC (600 MHz, $CDCl_3$) spectrum of **2**

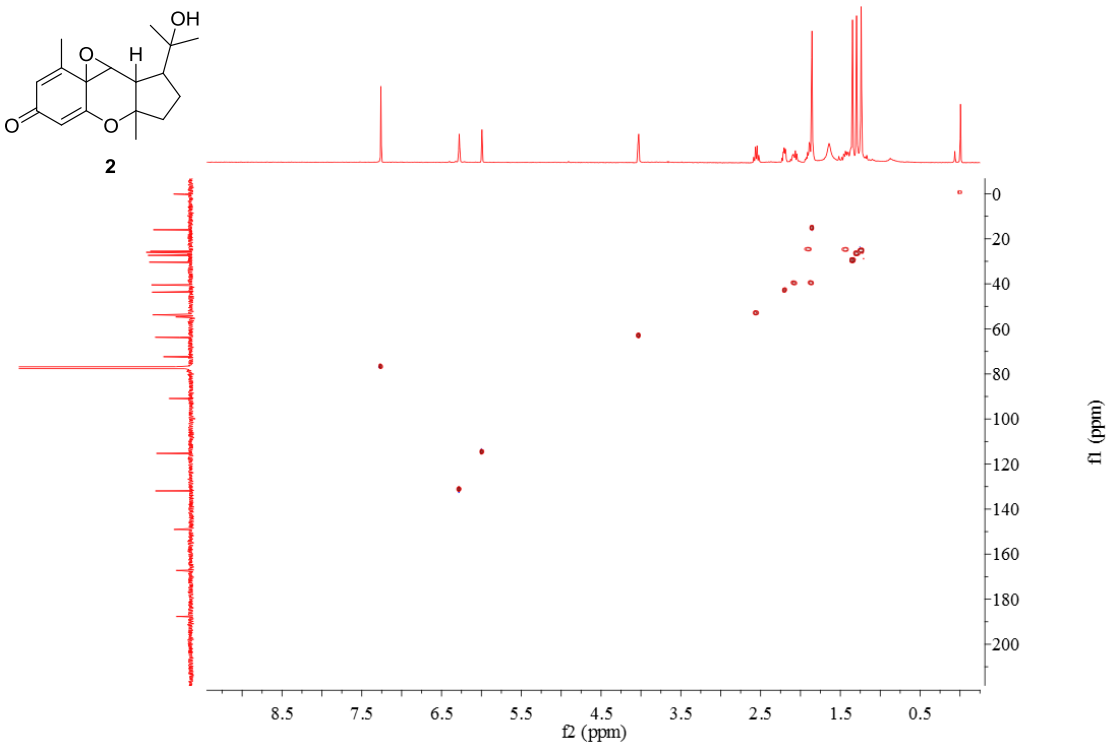


Figure S34. HSQC (600 MHz, $CDCl_3$) spectrum of **2**

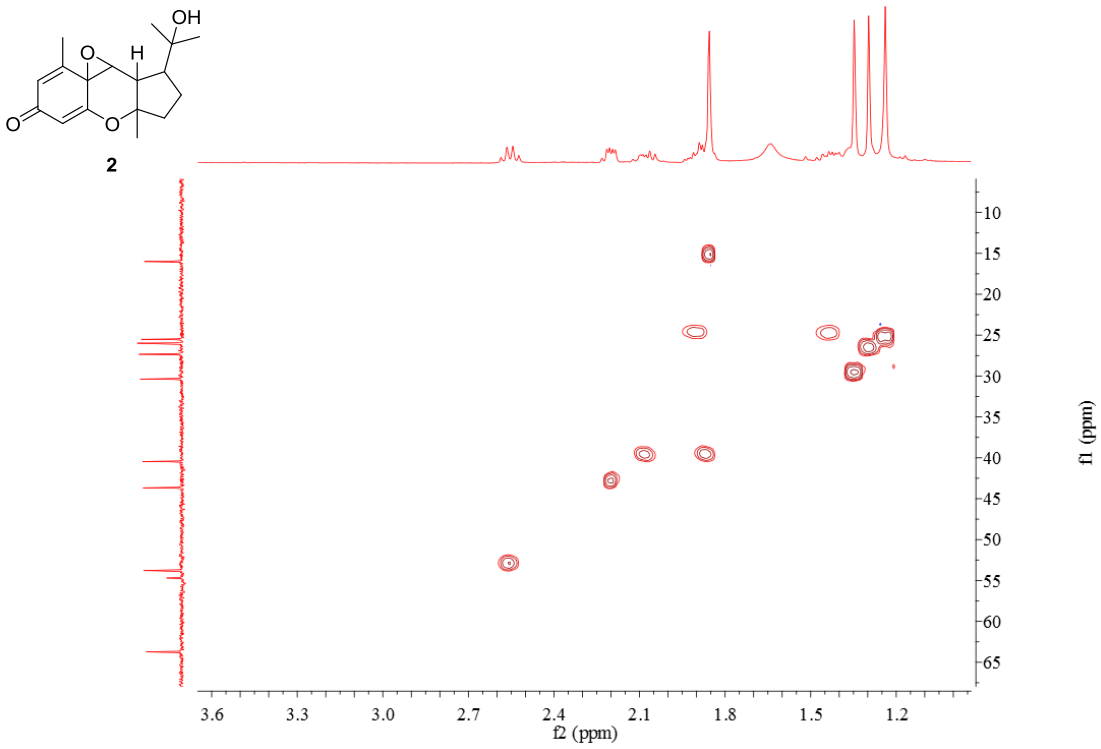


Figure S35. HMBC (600 MHz, $CDCl_3$) spectrum of **2**

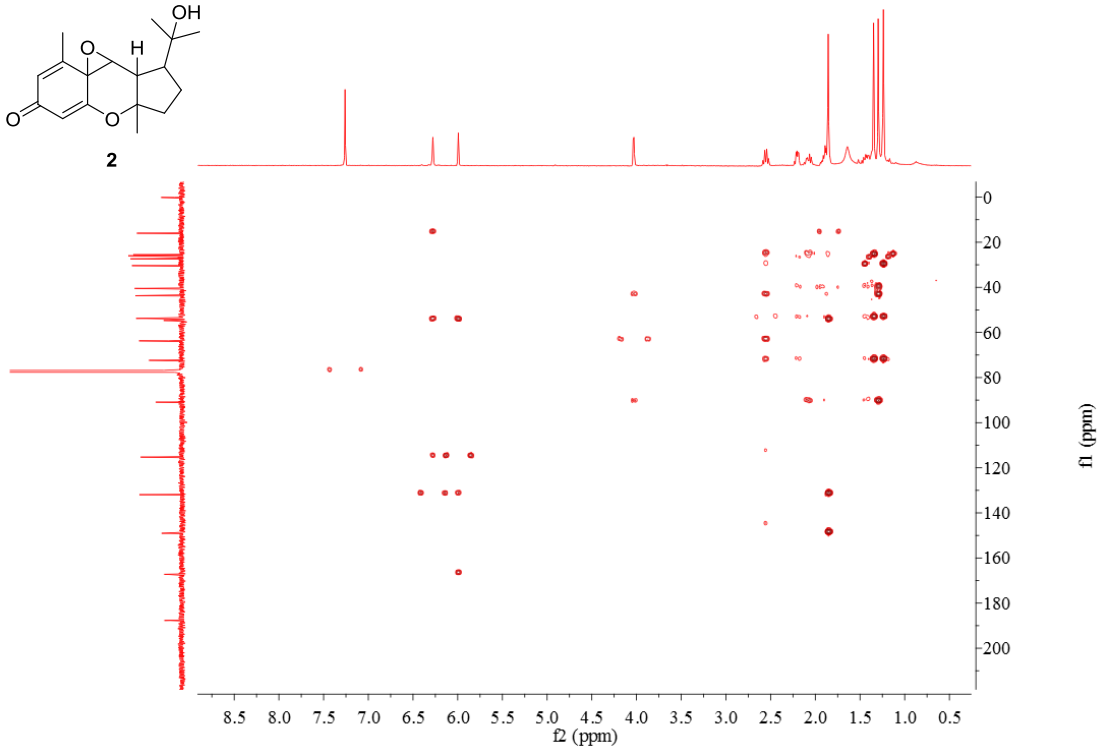


Figure S36. HMBC (600 MHz, $CDCl_3$) spectrum of **2**

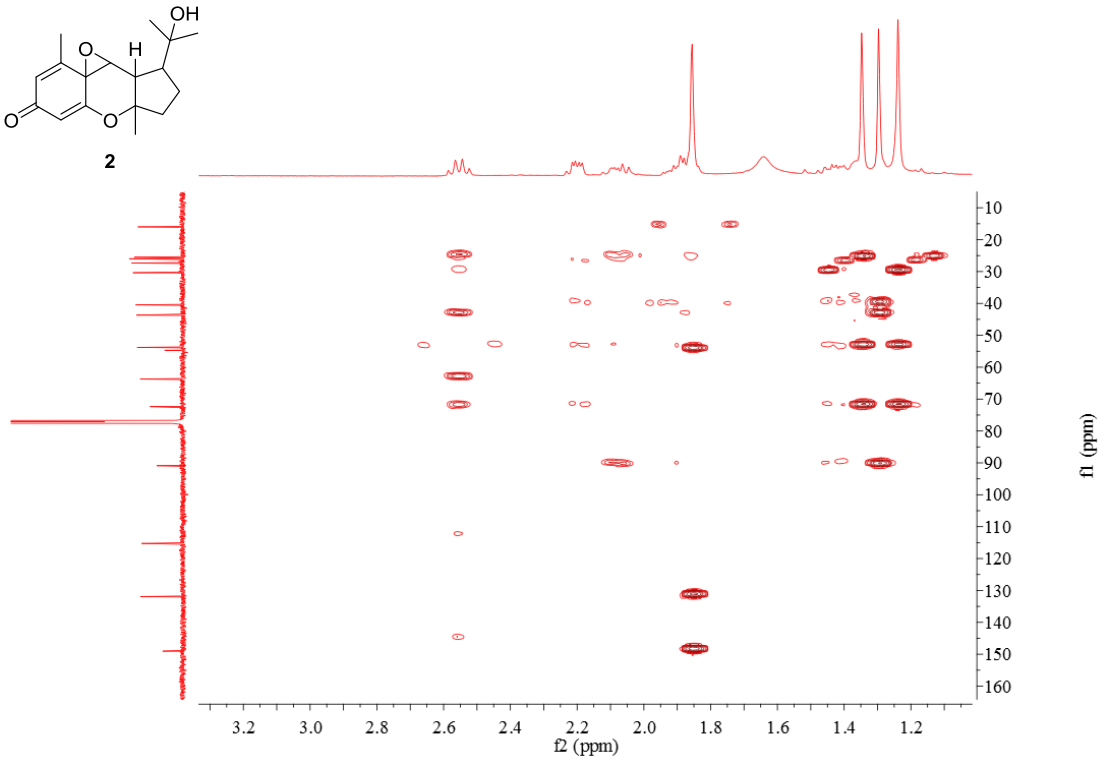


Figure S37. ^{1}H-^{1}H COSY (600 MHz, $CDCl_3$) spectrum of **2**

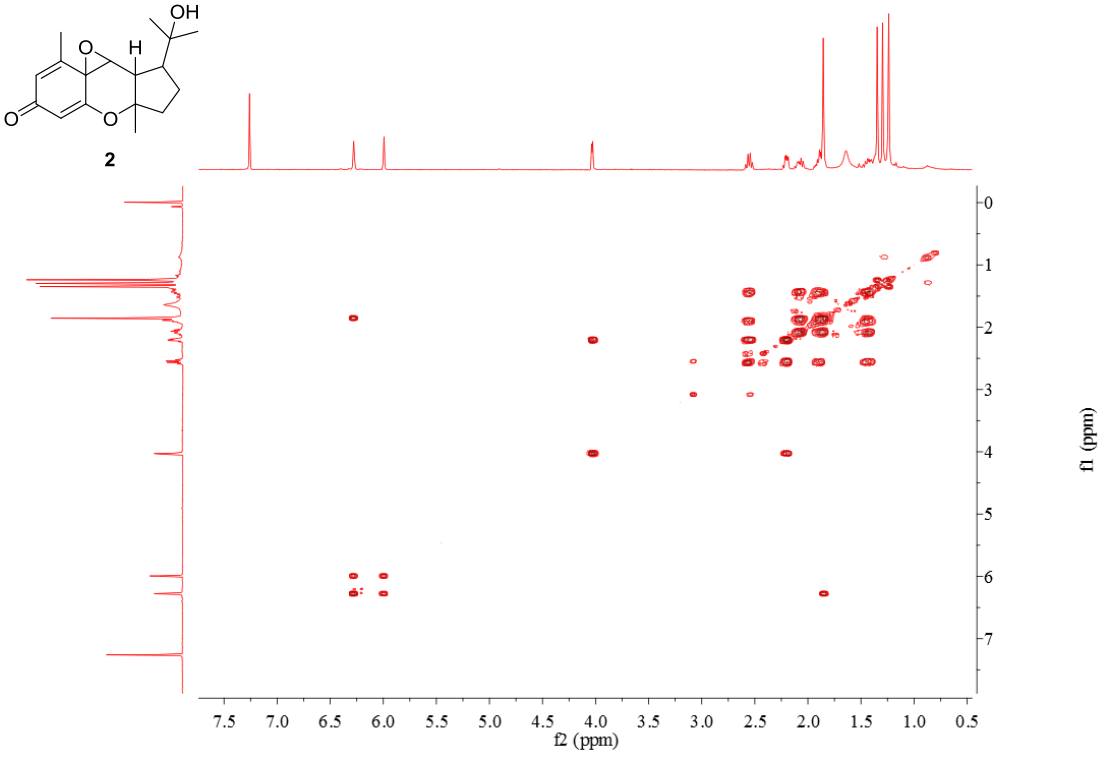


Figure S38. ROESY (600 MHz, $CDCl_3$) spectrum of **2**

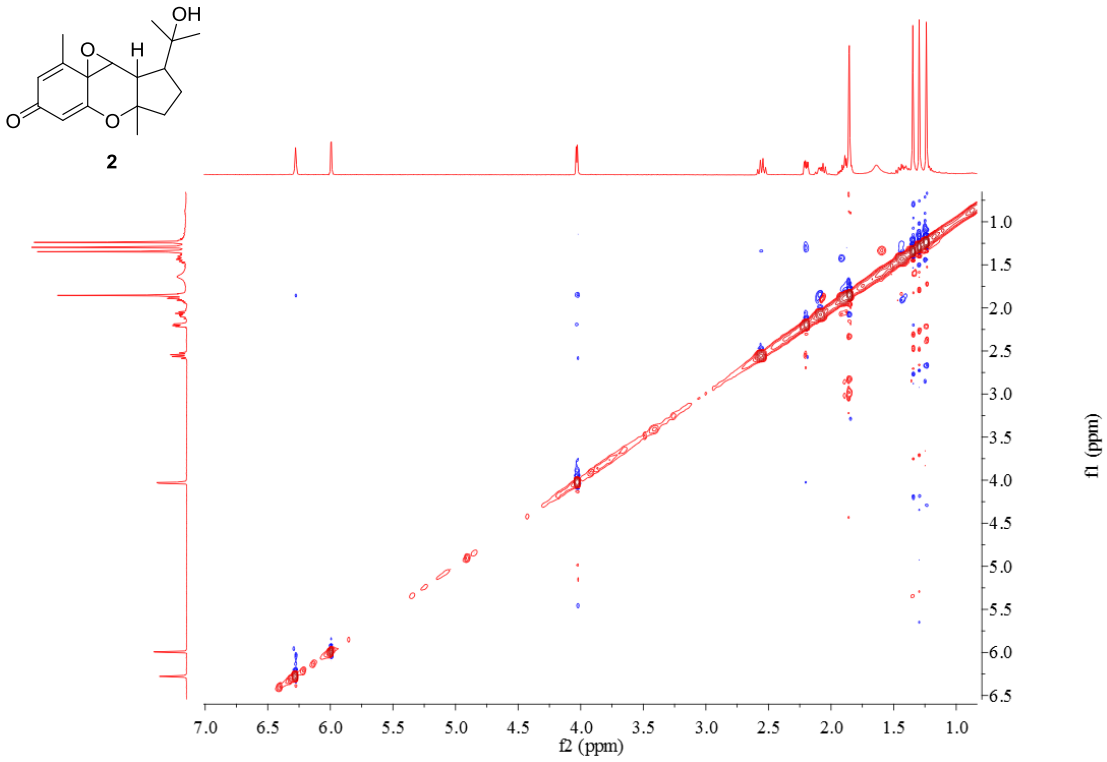


Figure S39. IR spectrum of **2**

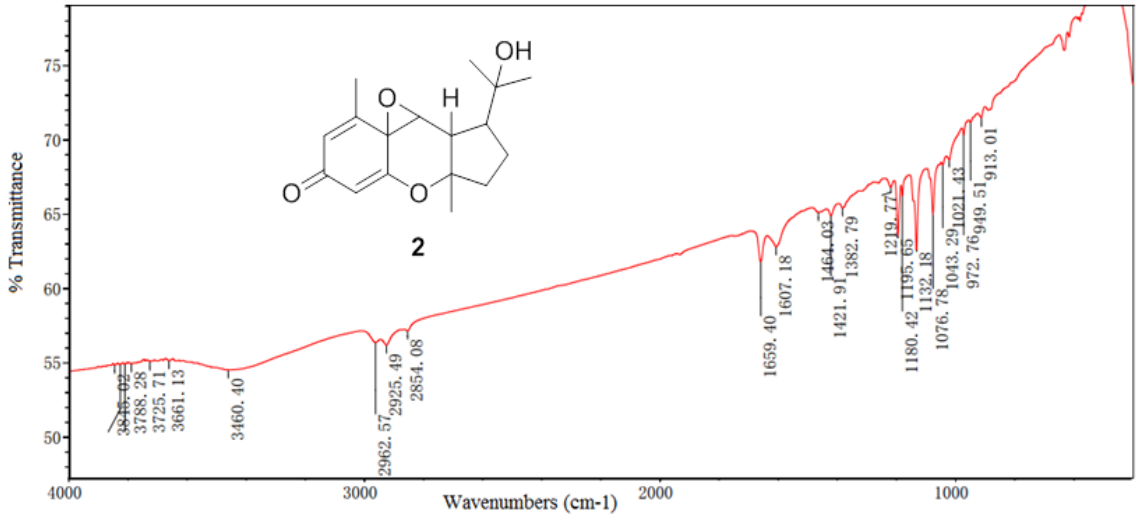


Figure S40. Positive ESIMS spectrum of **2a**

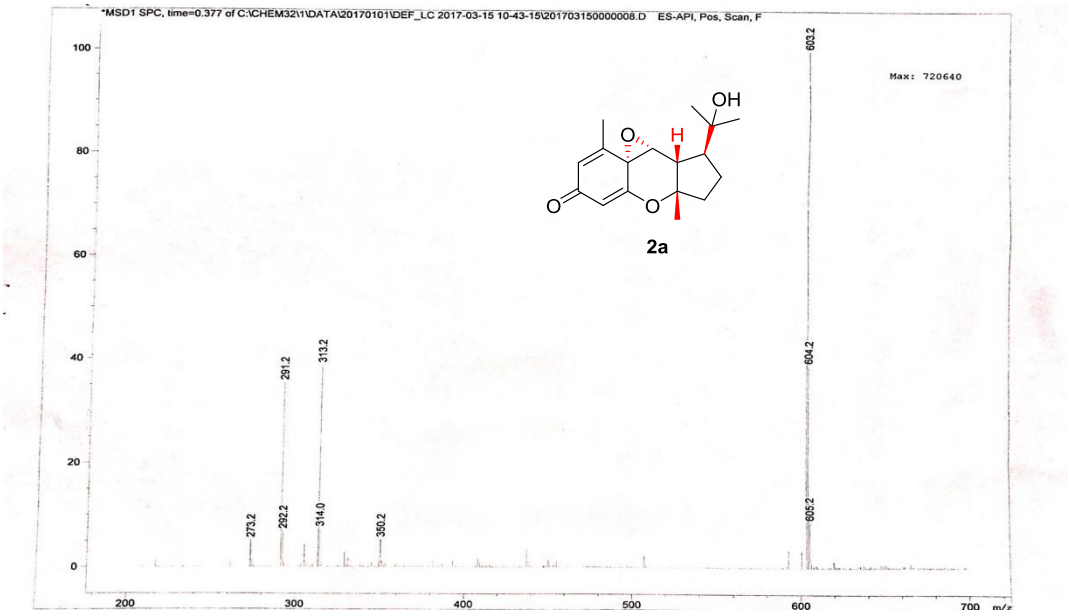


Figure S41. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2a**

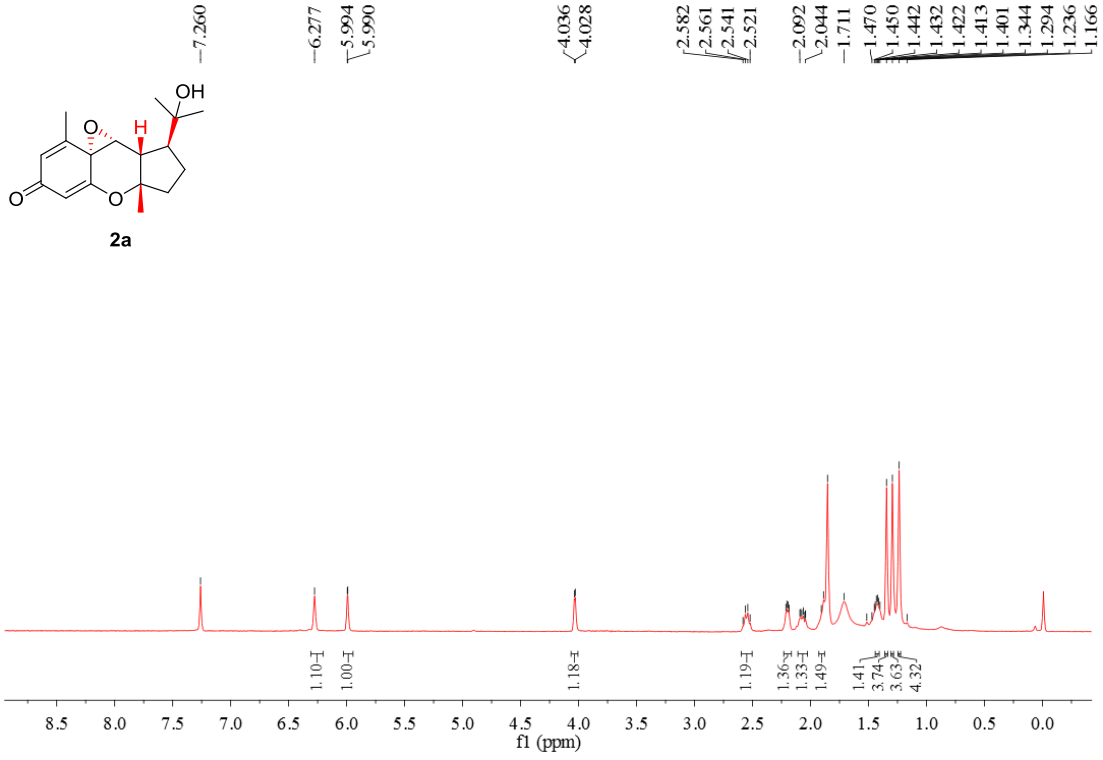


Figure S42. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **2a**

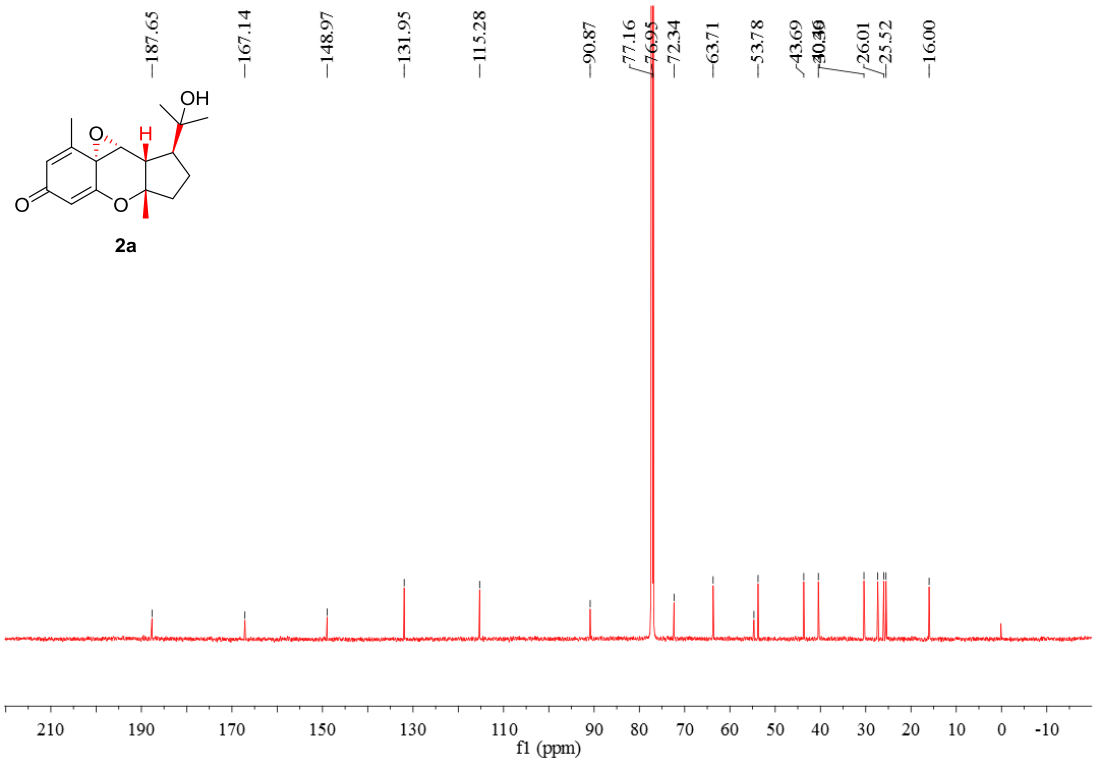


Figure S43. Positive ESIMS spectrum of **2b**

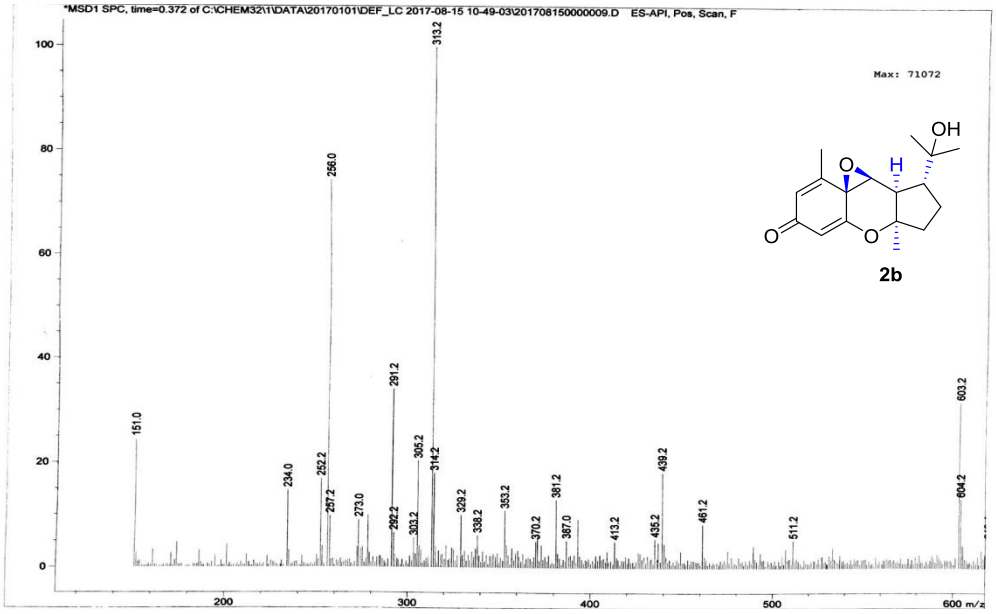


Figure S44. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2b**

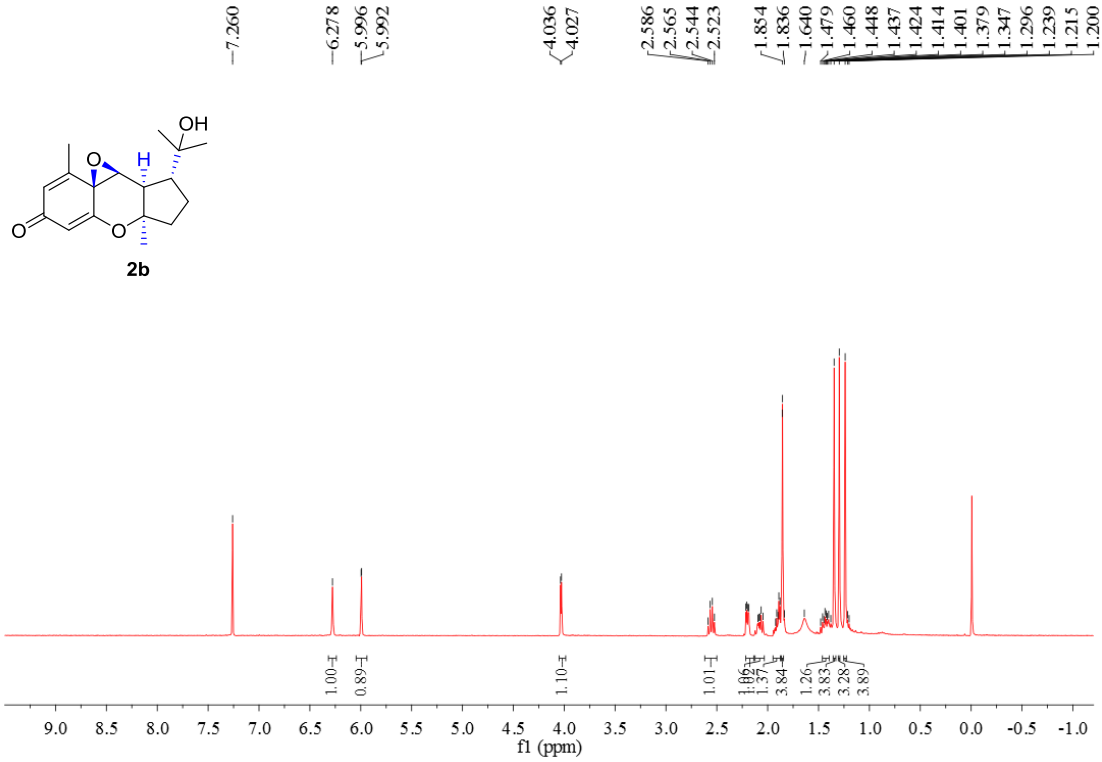


Figure S45. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **2b**

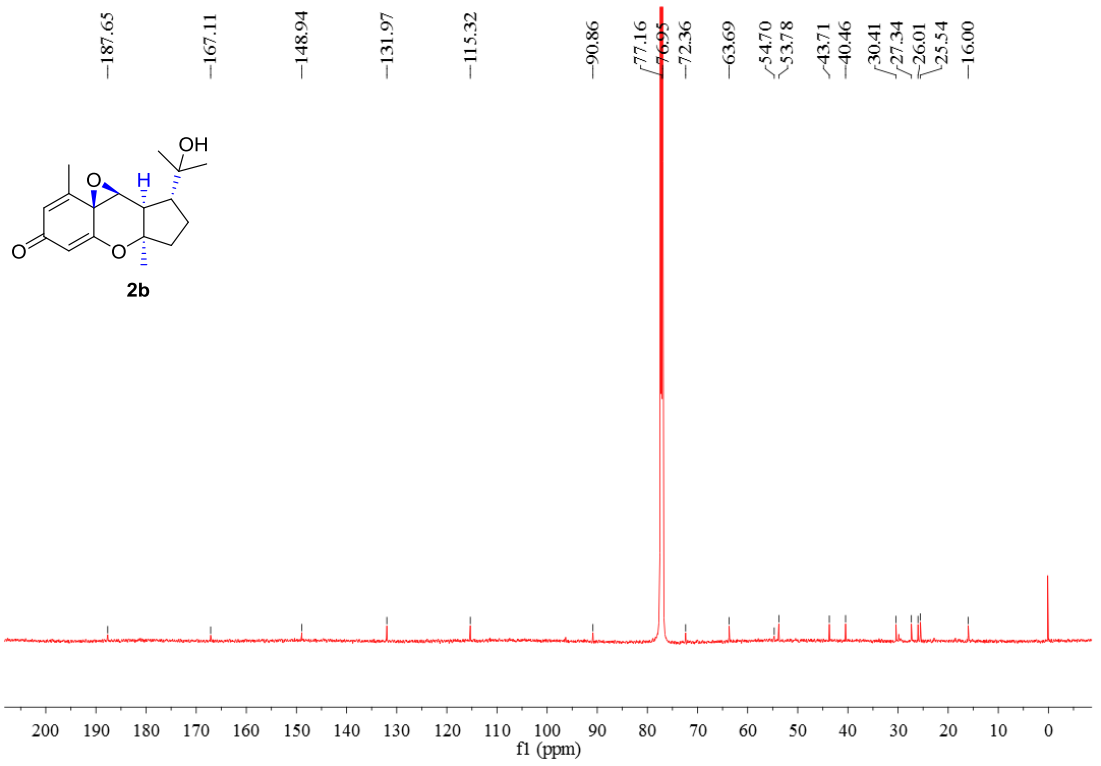


Figure S46. Positive ESIMS spectrum of **3**

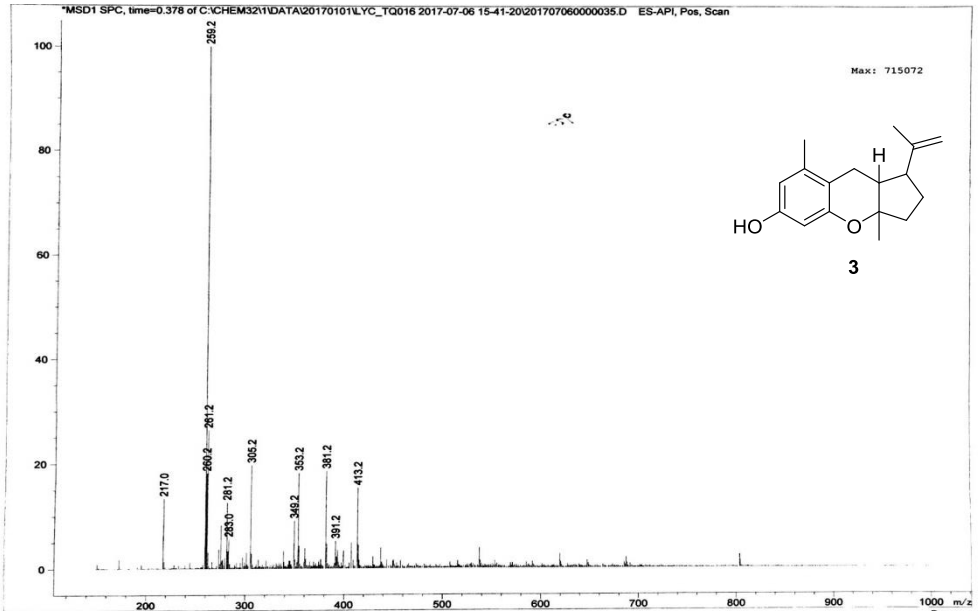
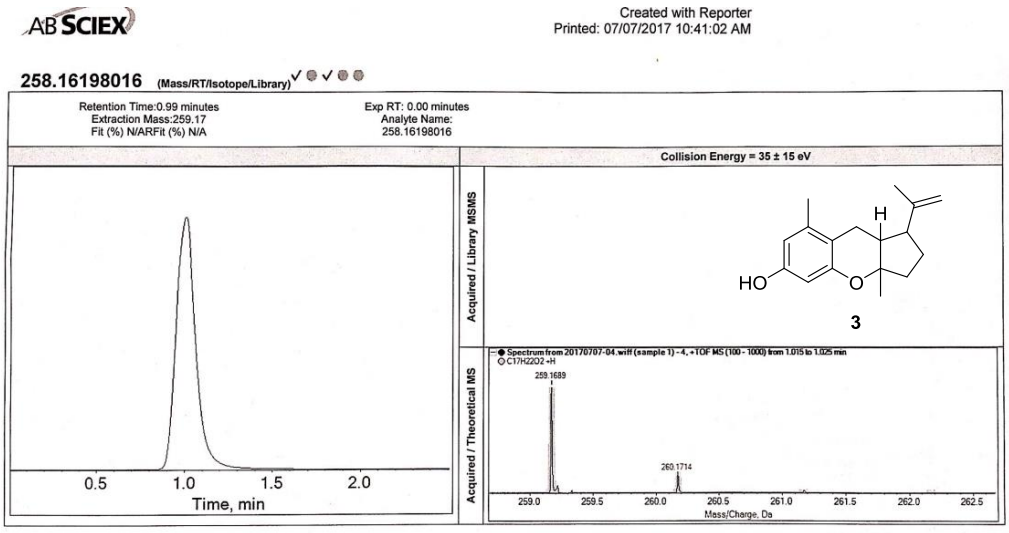


Figure S47. Positive HR-ESIMS spectrum of **3**



	Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
✓●✓●●	258.16198016(LZ-22)	93%	C17H22O2	5560216	50	259.1693	259.1689	-1.3	0.00	0.99	0.99	0.2%	N/A

Figure S48. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3**

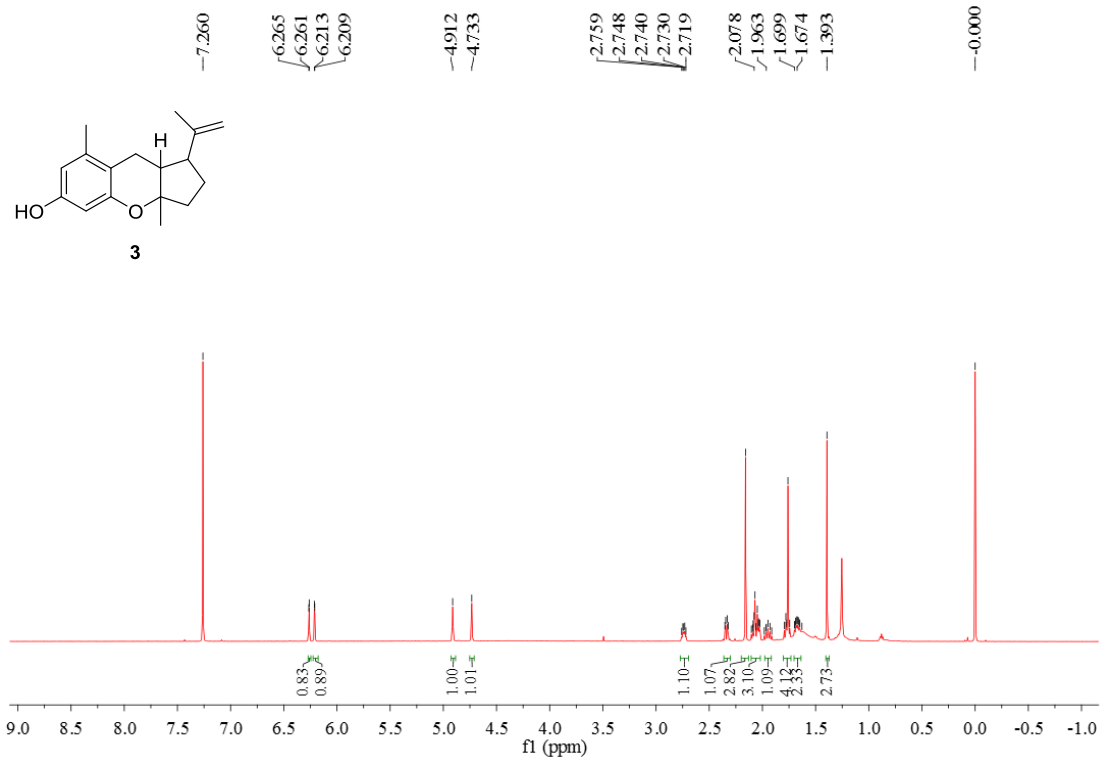


Figure S49. ^{13}C NMR and DEPT (150 MHz, $CDCl_3$) spectra of **3**

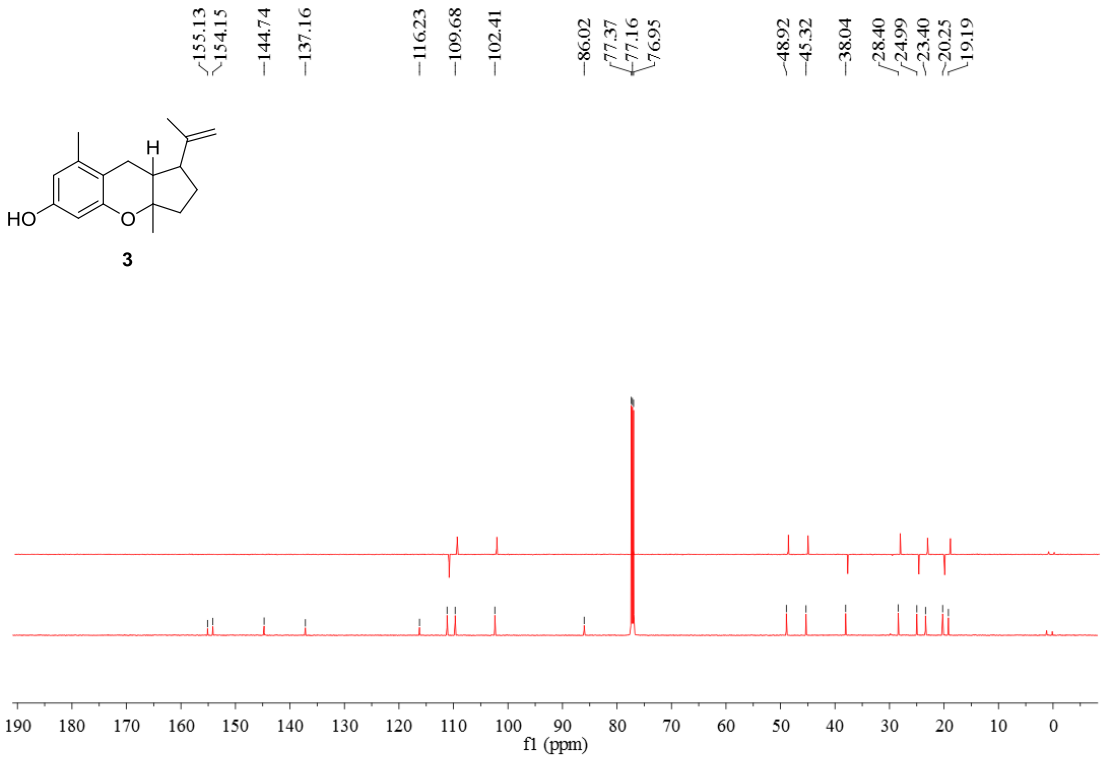


Figure S50. HSQC (600 MHz, $CDCl_3$) spectrum of **3**

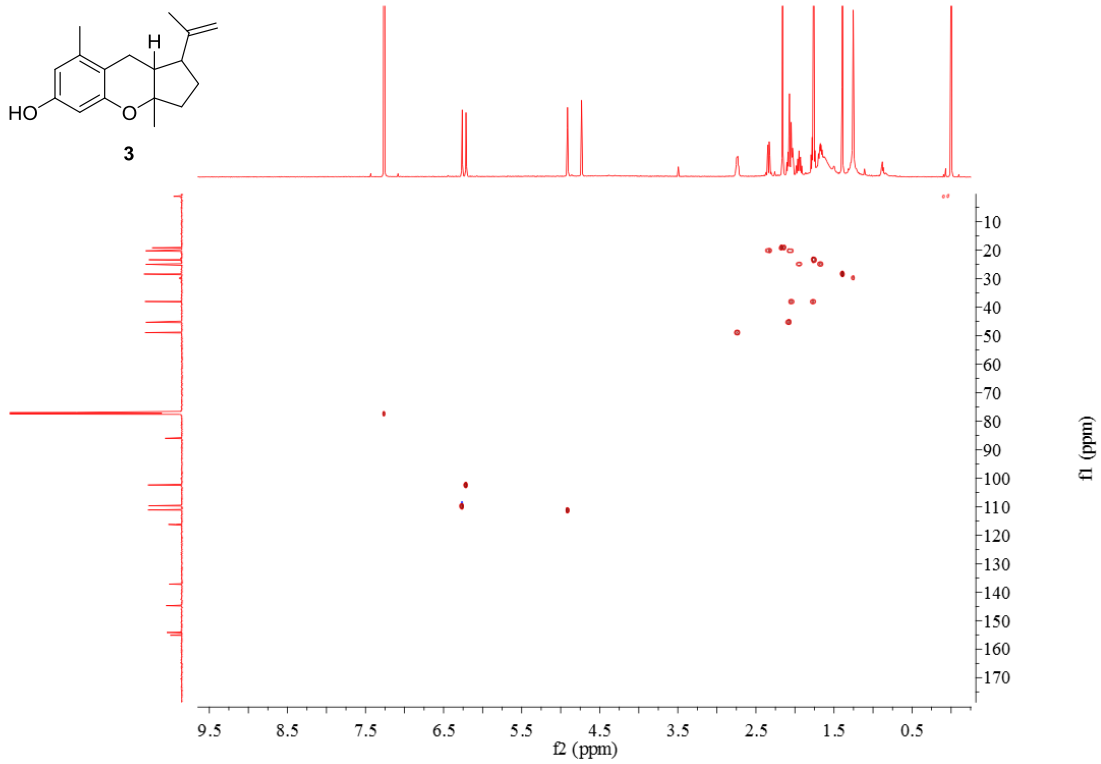


Figure S51. HSQC (600 MHz, $CDCl_3$) spectrum of **3**

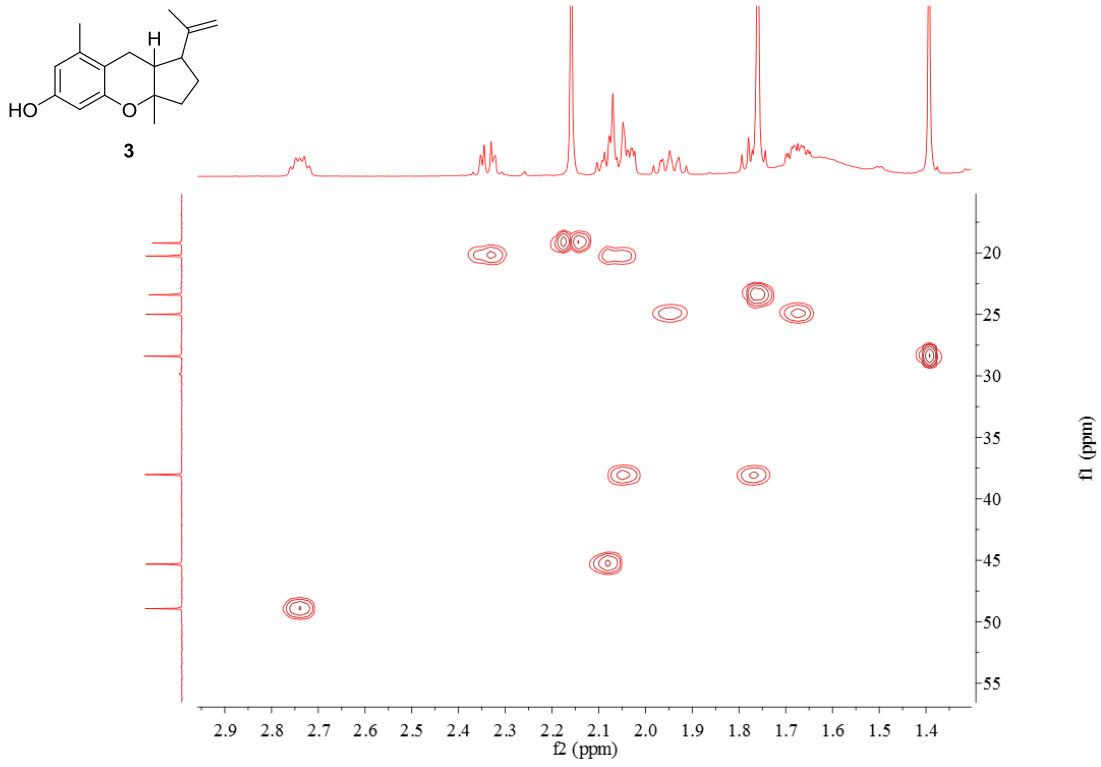


Figure S52. HMBC (600 MHz, $CDCl_3$) spectrum of **3**

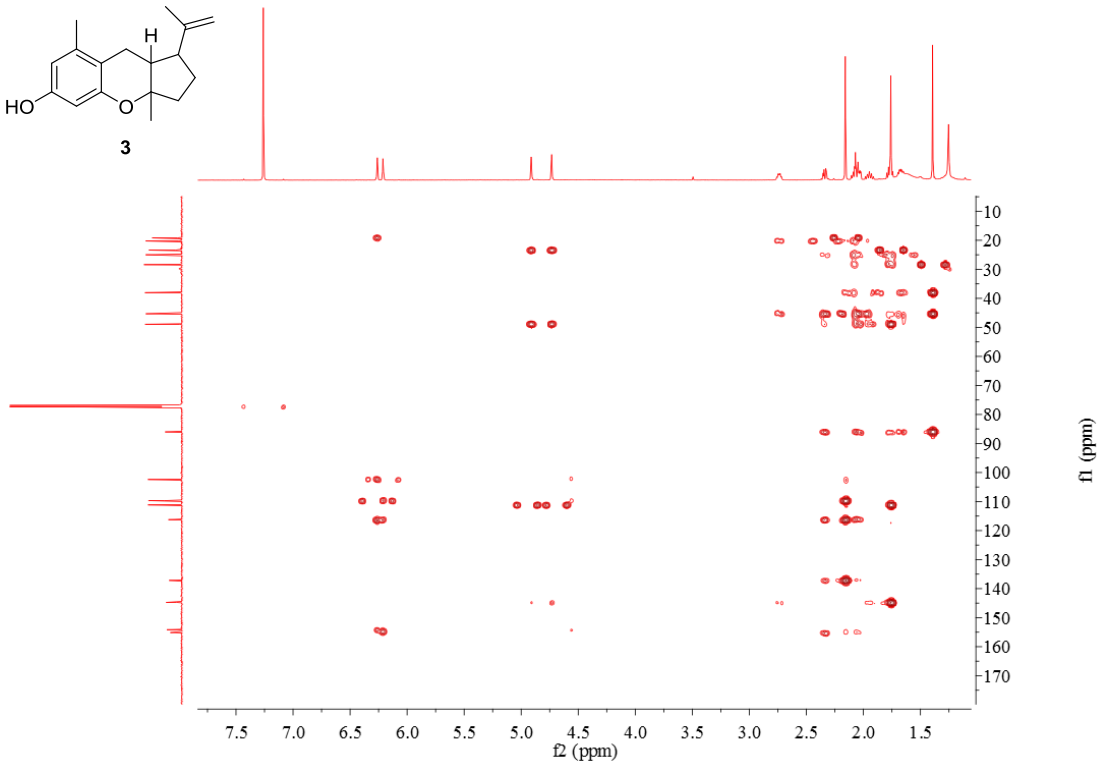


Figure S53. HMBC (600 MHz, $CDCl_3$) spectrum of **3**

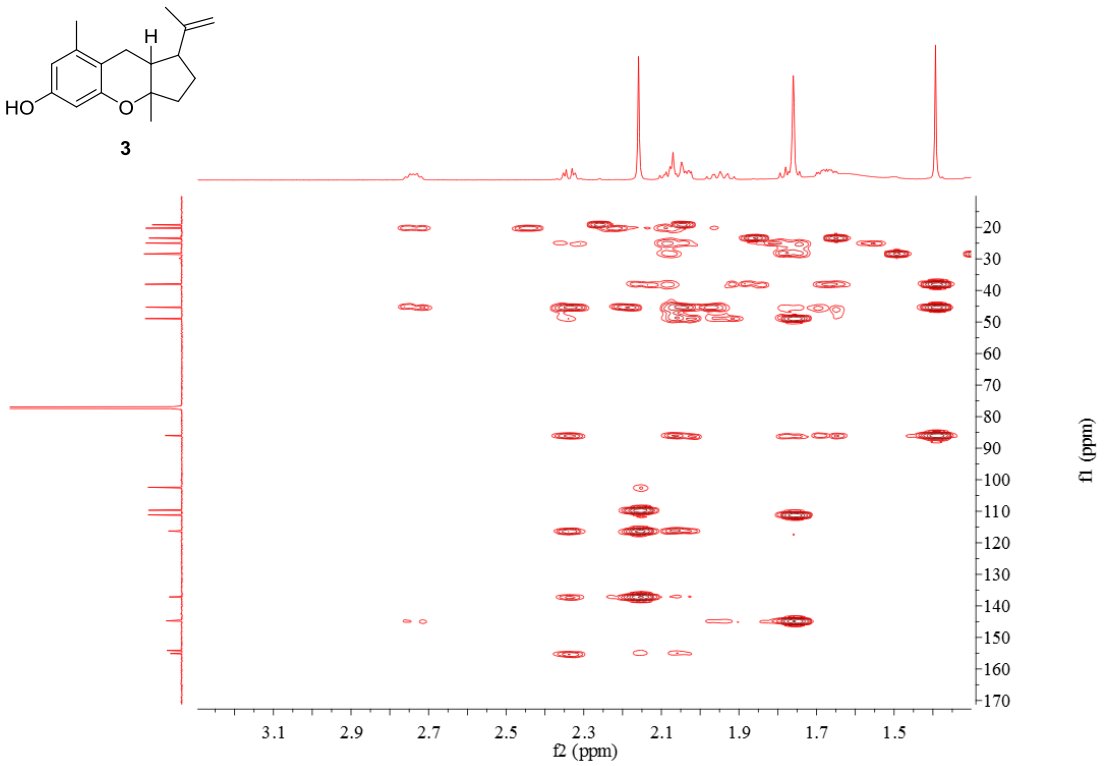


Figure S54. NOESY (600 MHz, $CDCl_3$) spectrum of **3**

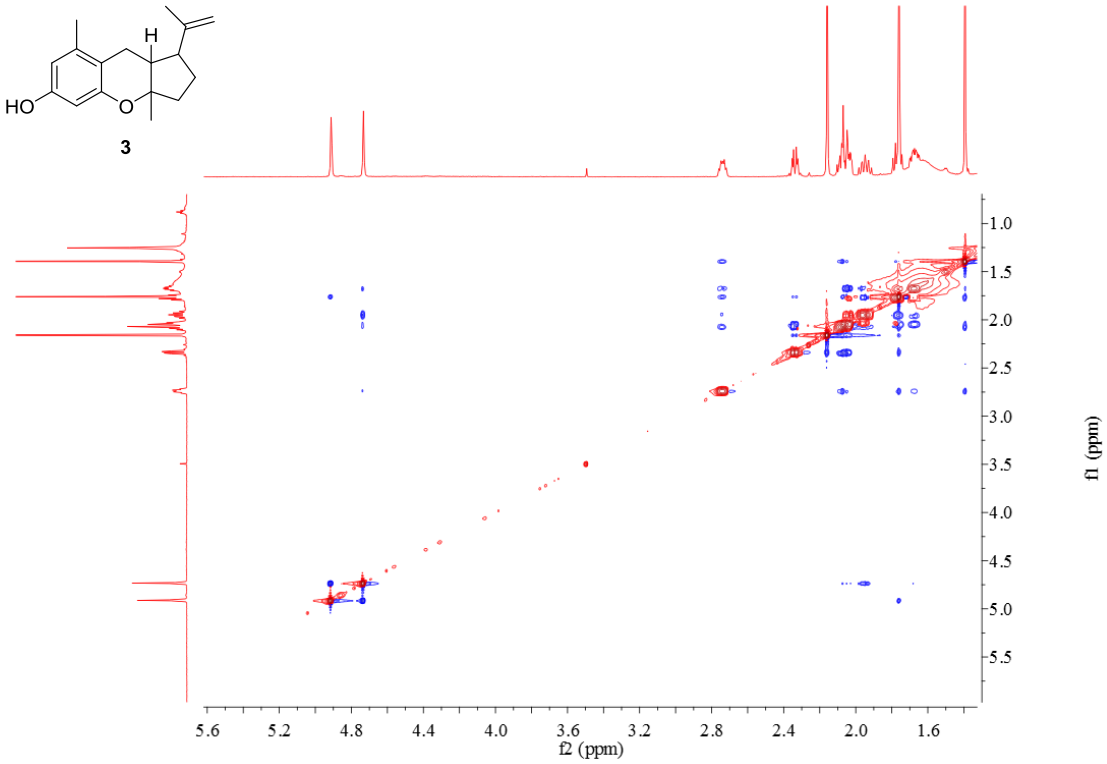


Figure S55. IR spectrum of **3**

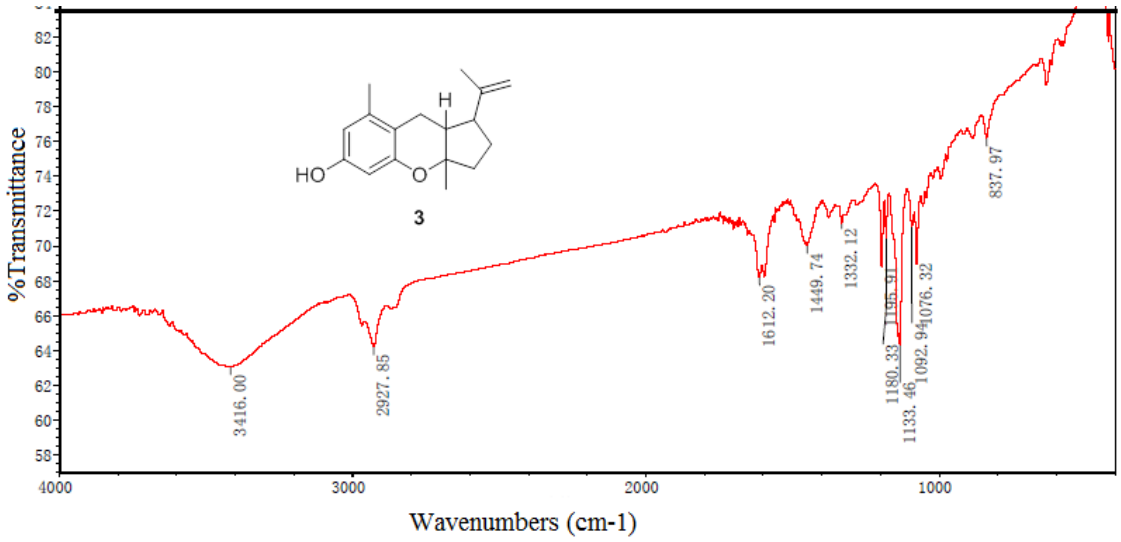


Figure S56. Positive ESIMS spectrum of **3a**

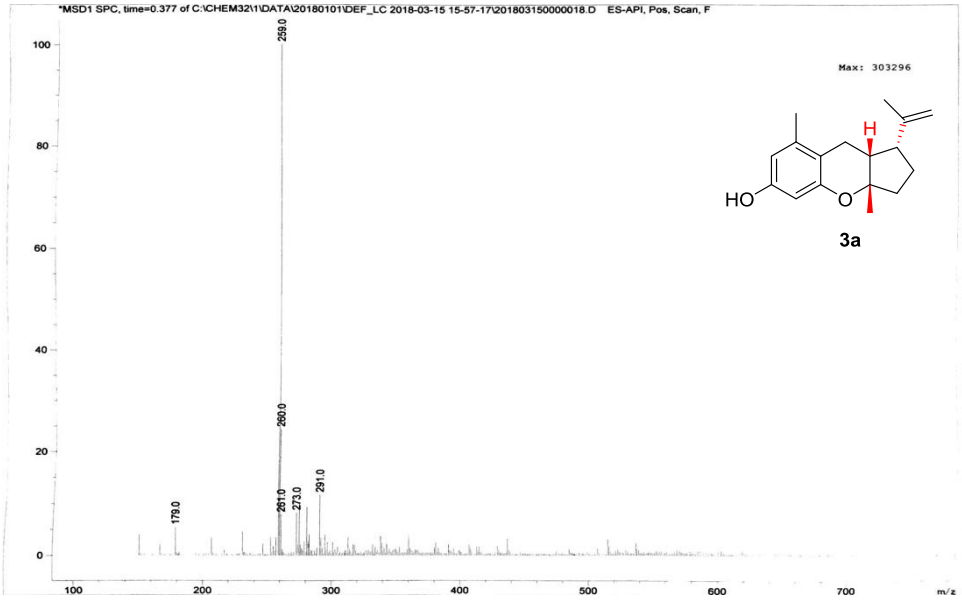


Figure S57. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3a**

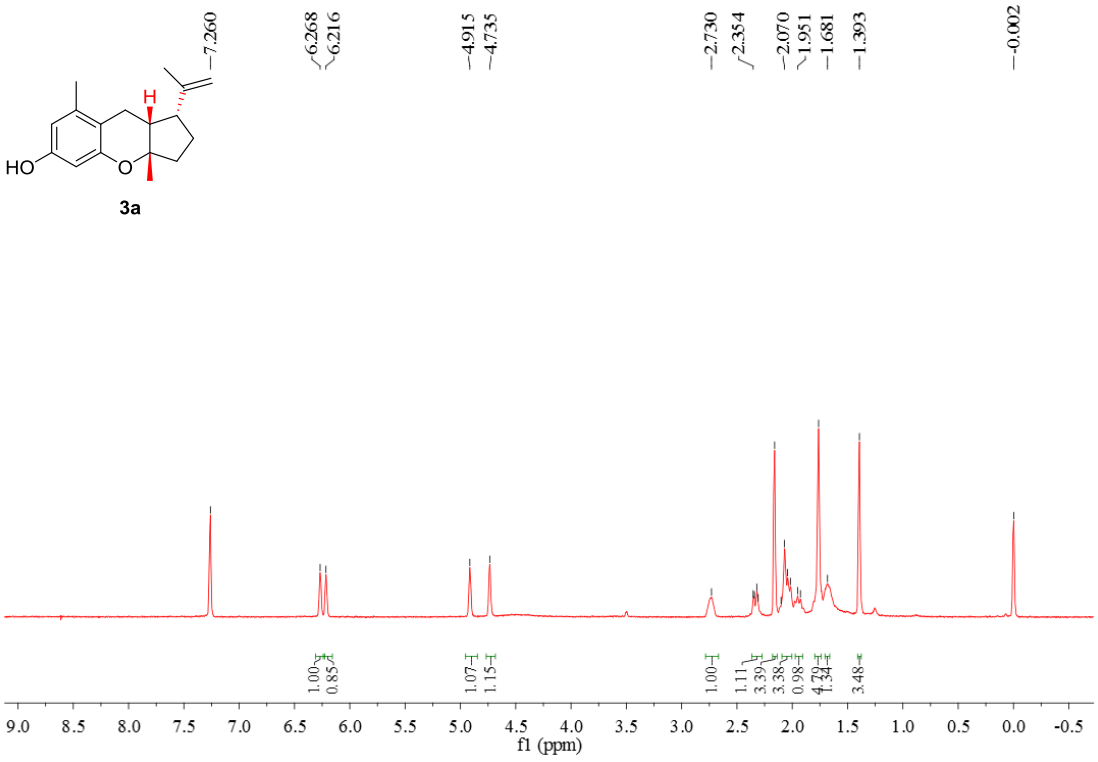


Figure S58. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **3a**

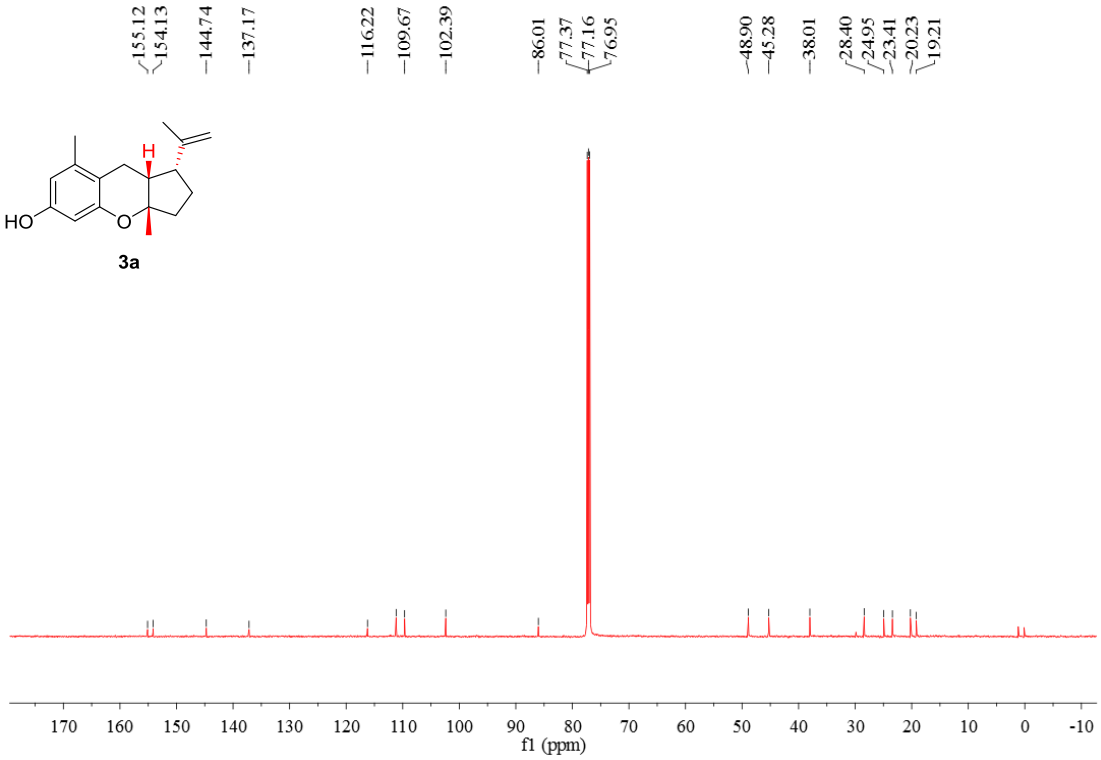


Figure S59. Positive ESIMS spectrum of **3b**

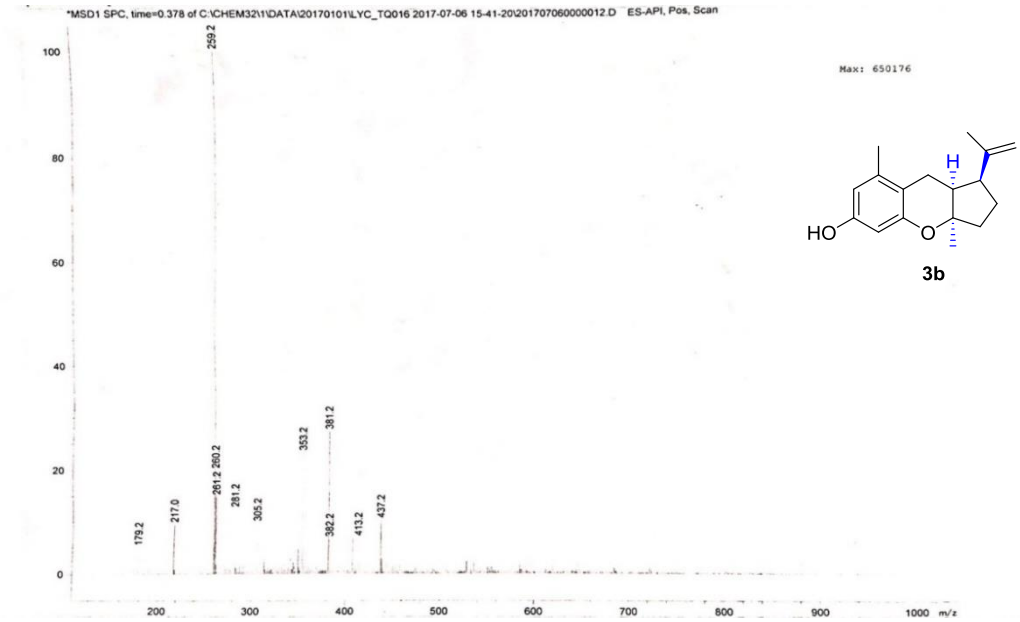


Figure S60. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3b**

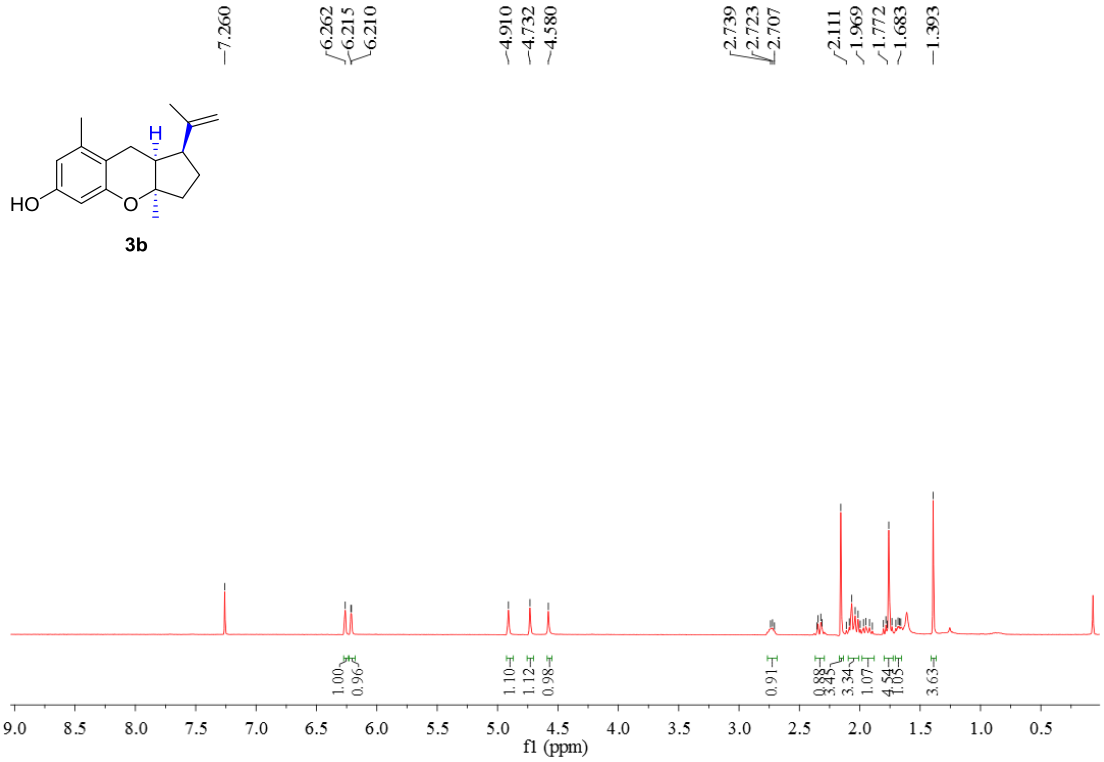


Figure S61. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **3b**

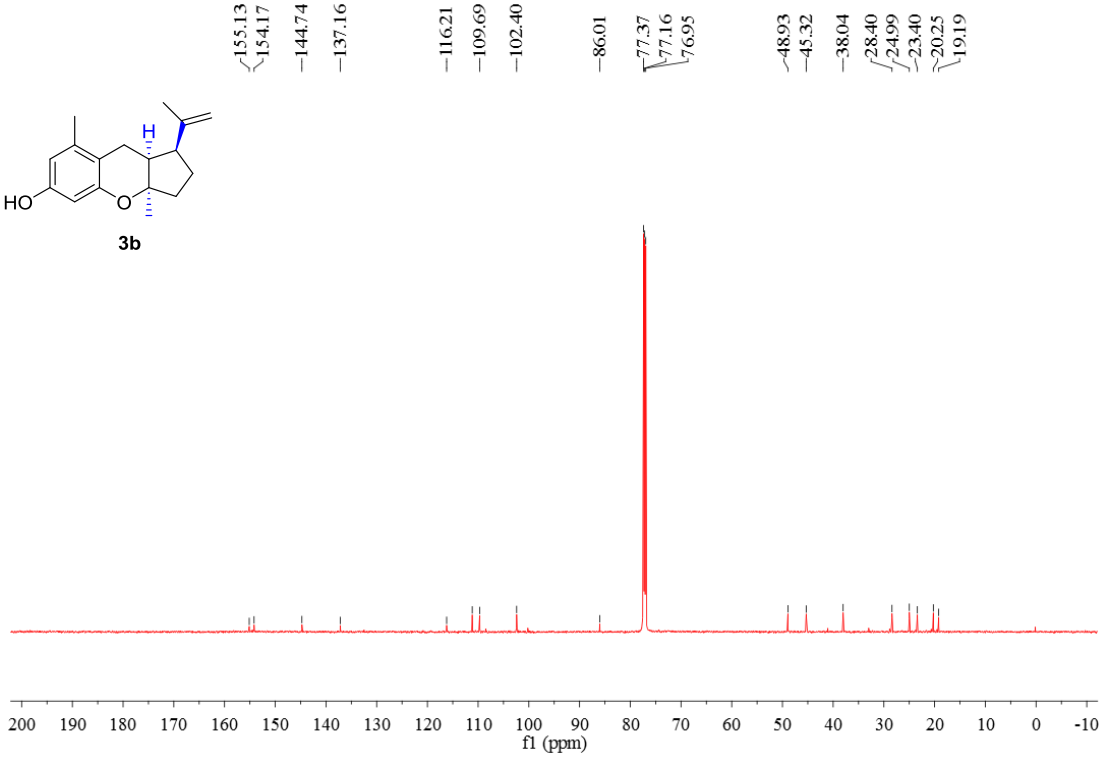


Figure S62. Positive ESIMS spectrum of **4**

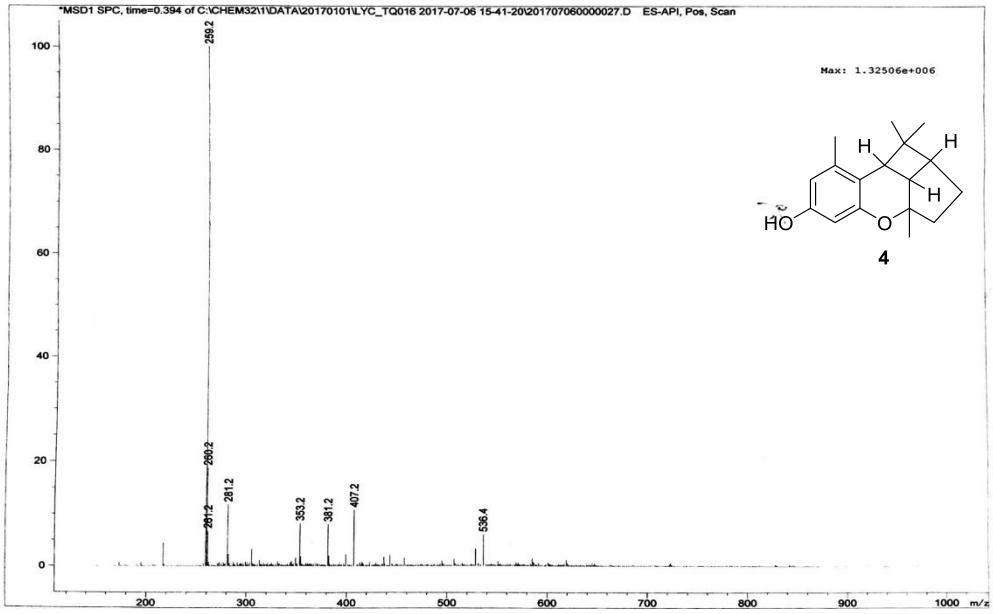
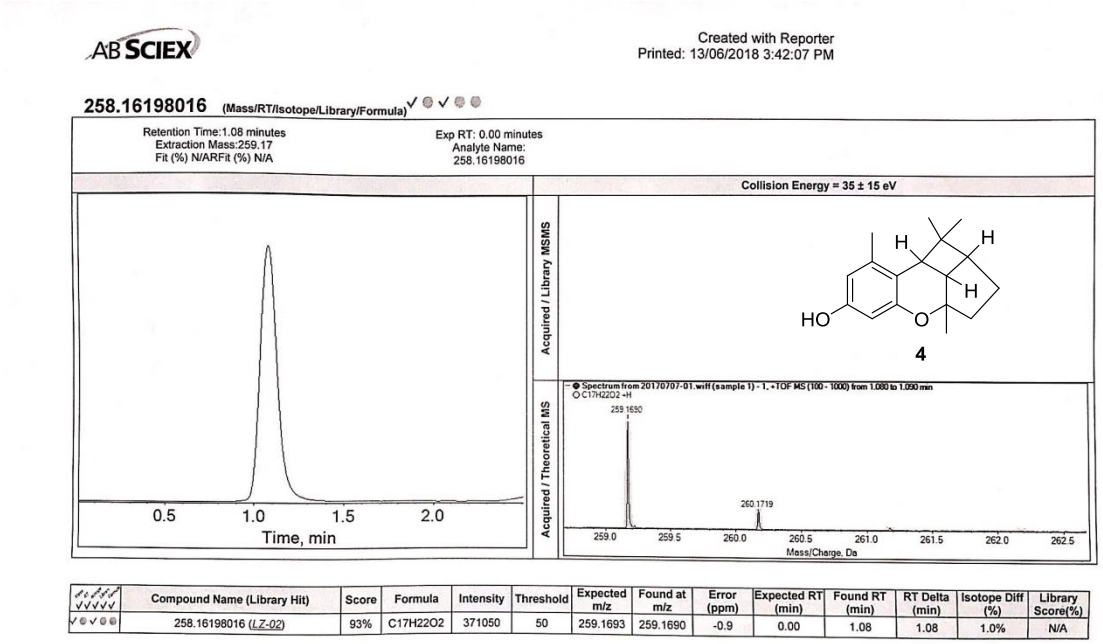


Figure S63. Positive HR-ESIMS spectrum of **4**



Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
258.16198016 (LZ-02)	93%	C17H22O2	371050	50	259.1693	259.1690	-0.9	0.00	1.08	1.08	1.0%	N/A

Figure S64. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4**

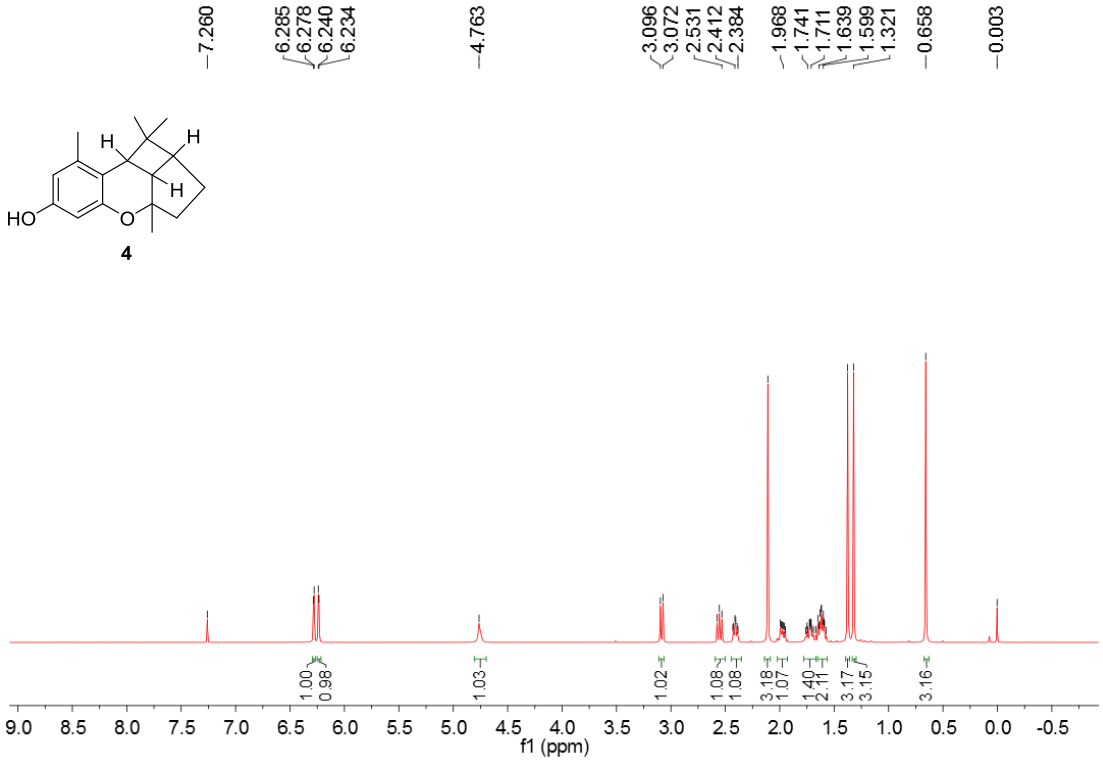


Figure S65. ^{13}C NMR and DEPT (150 MHz, $CDCl_3$) spectra of **4**

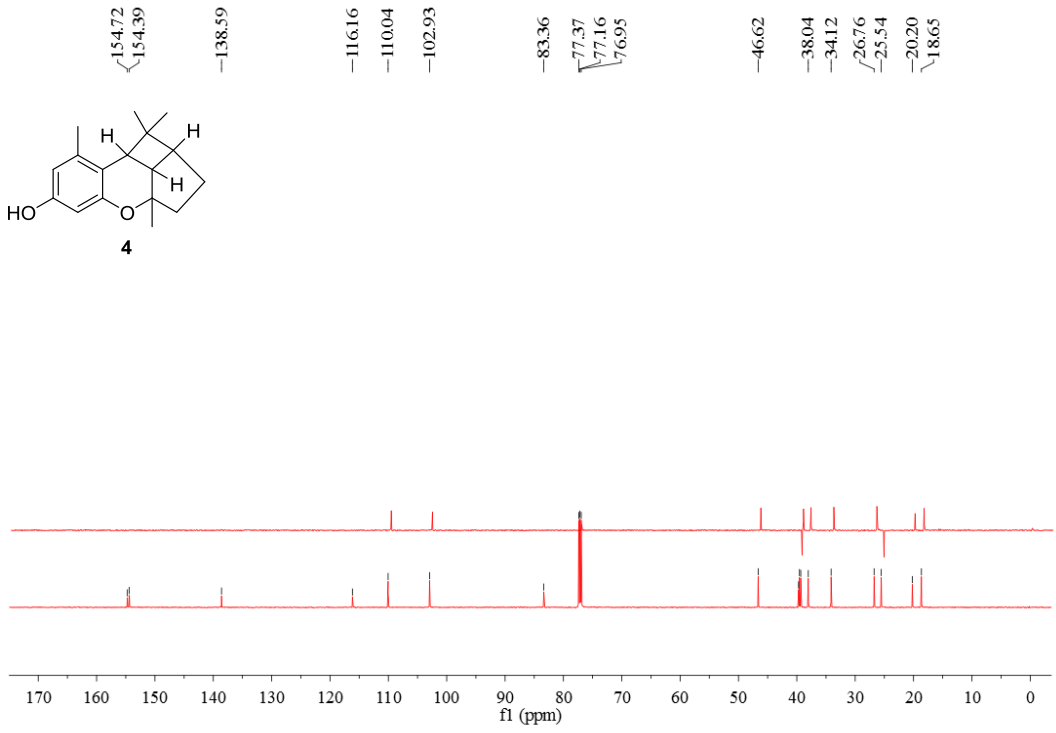


Figure S66. HSQC (600 MHz, $CDCl_3$) spectrum of **4**

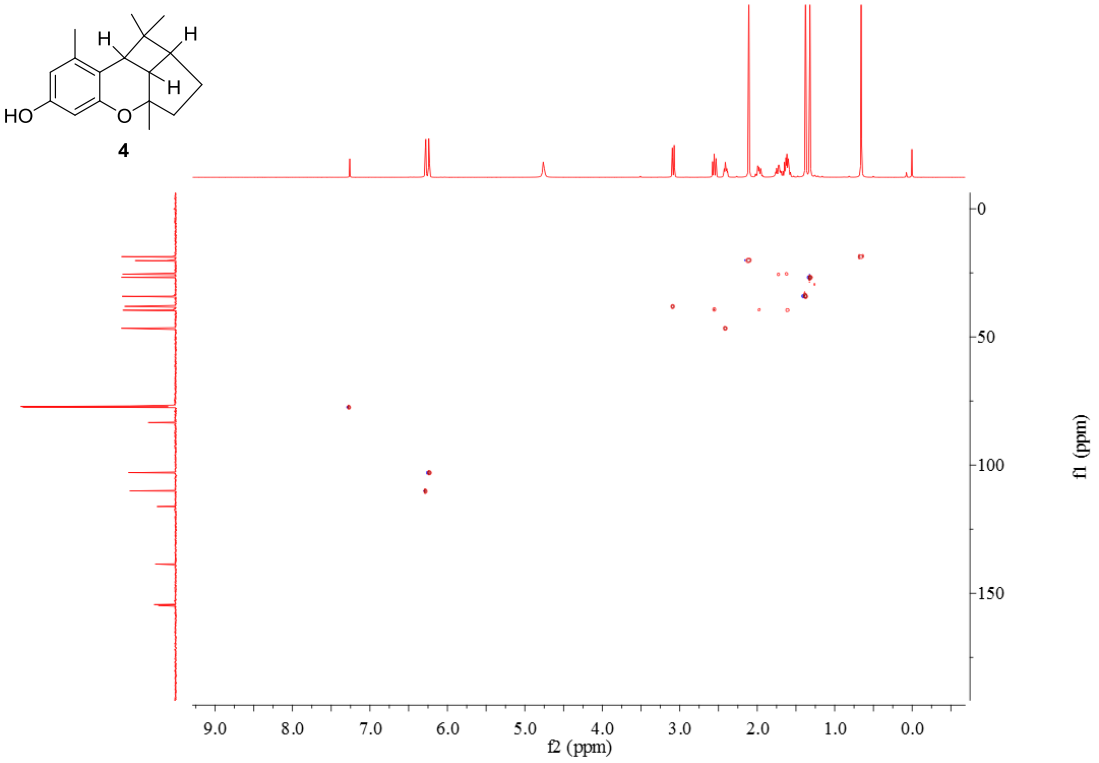


Figure S67. HSQC (600 MHz, $CDCl_3$) spectrum of **4**

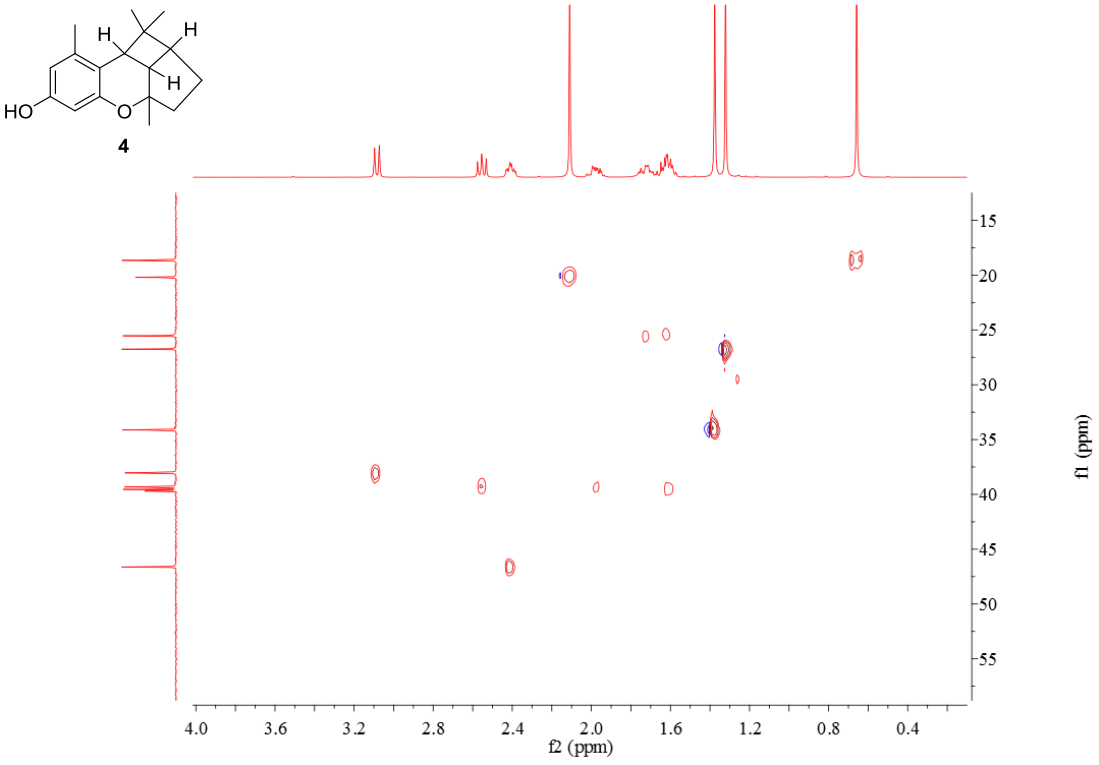


Figure S68. HMBC (600 MHz, $CDCl_3$) spectrum of **4**

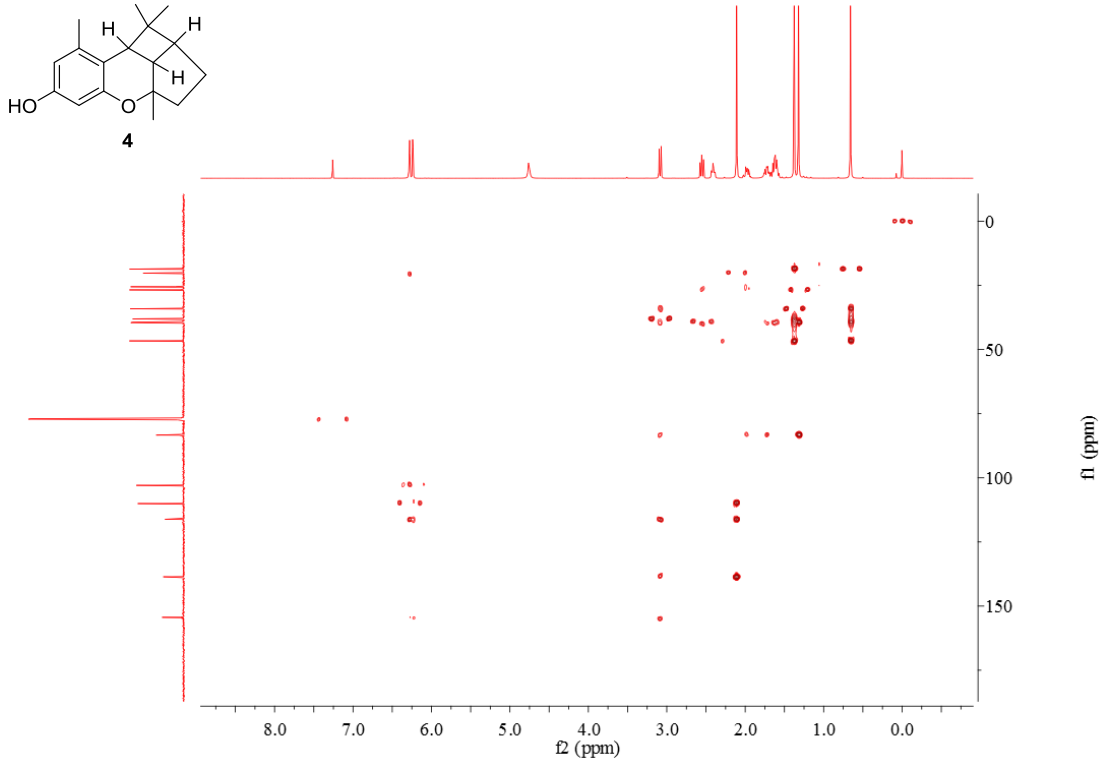


Figure S69. HMBC (600 MHz, $CDCl_3$) spectrum of **4**

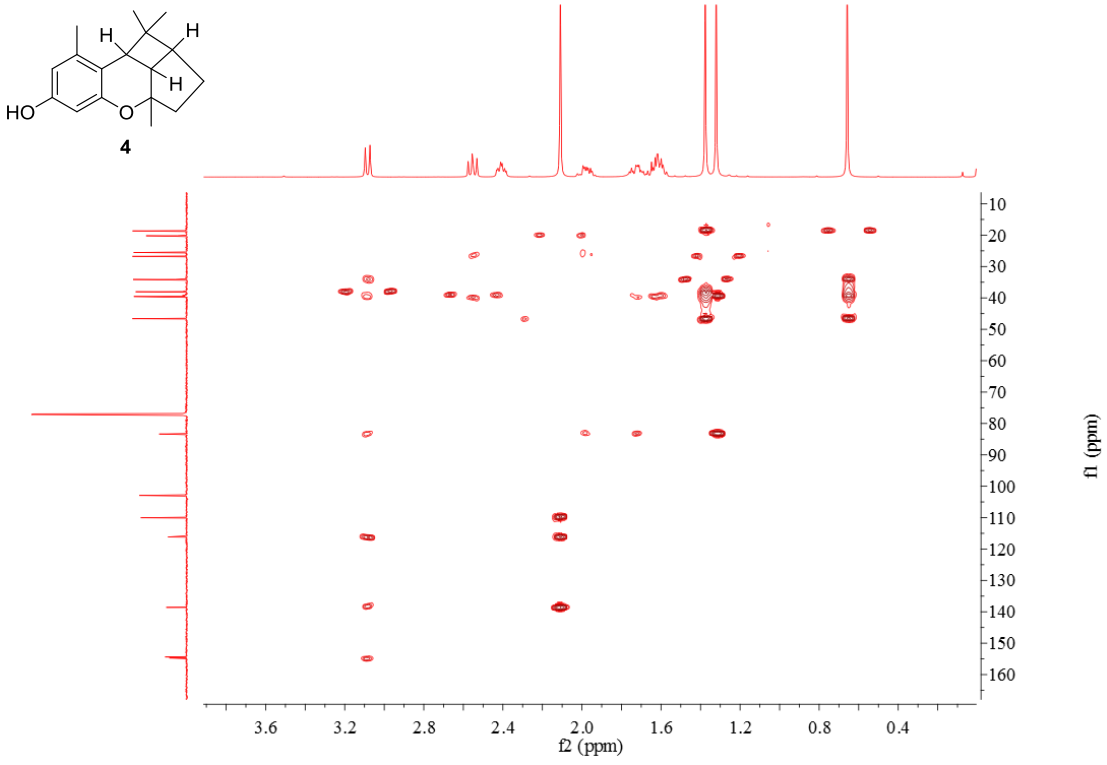


Figure S70. NOESY (600 MHz, $CDCl_3$) spectrum of **4**

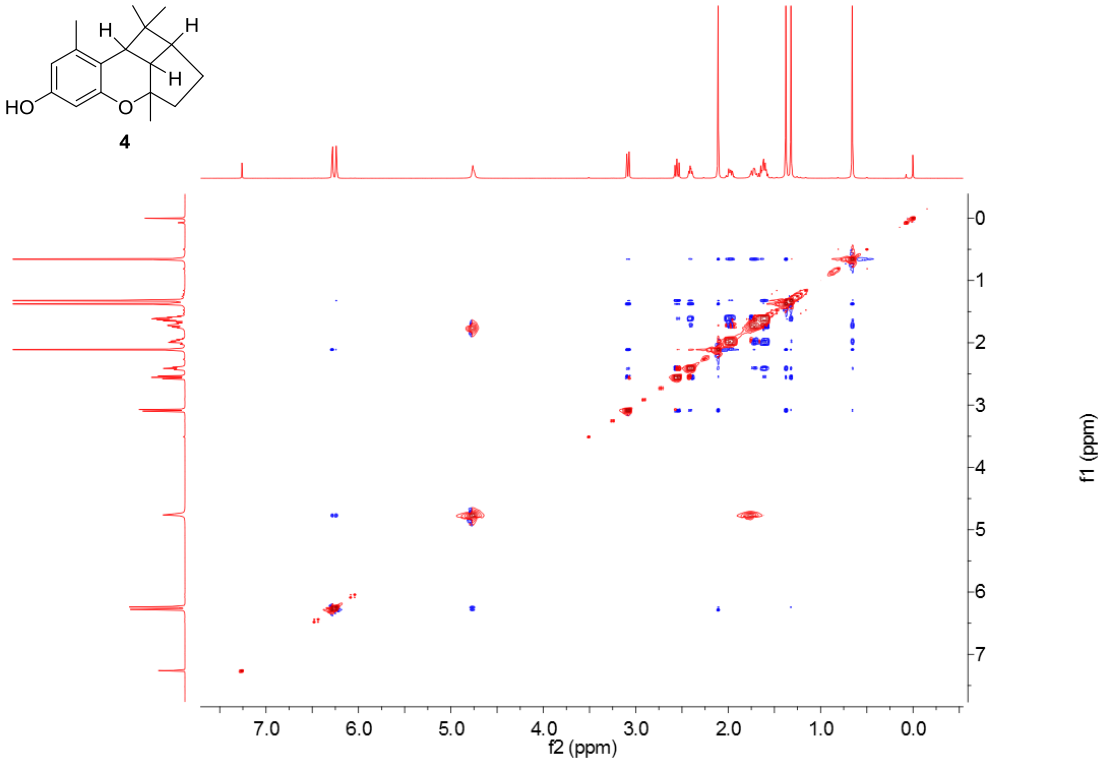


Figure S71. IR spectrum of **4**

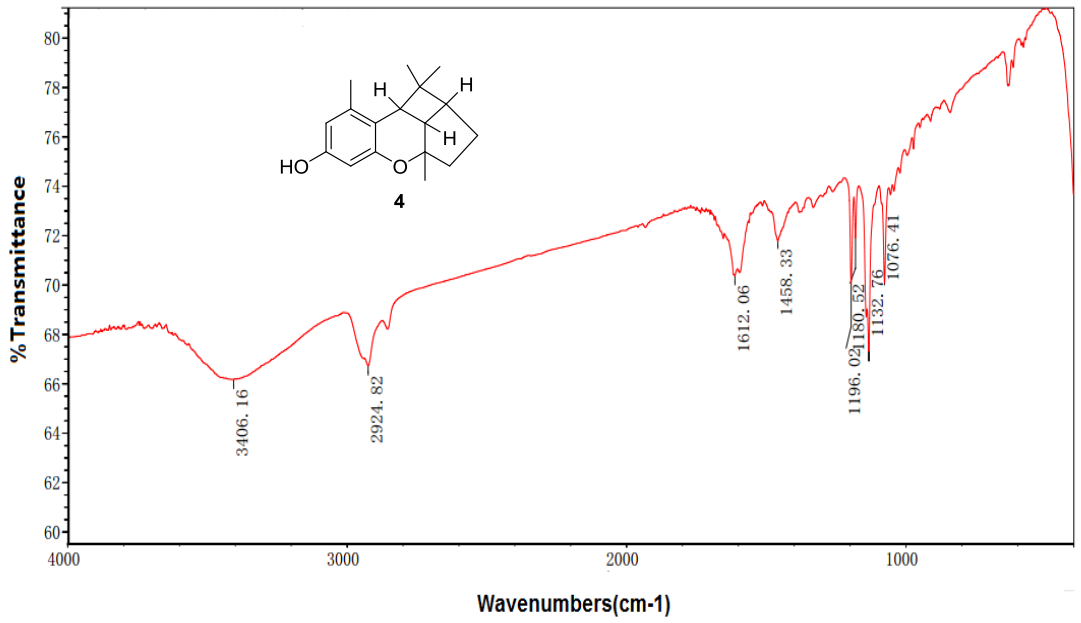


Figure S72. Positive ESIMS spectrum of **4a**

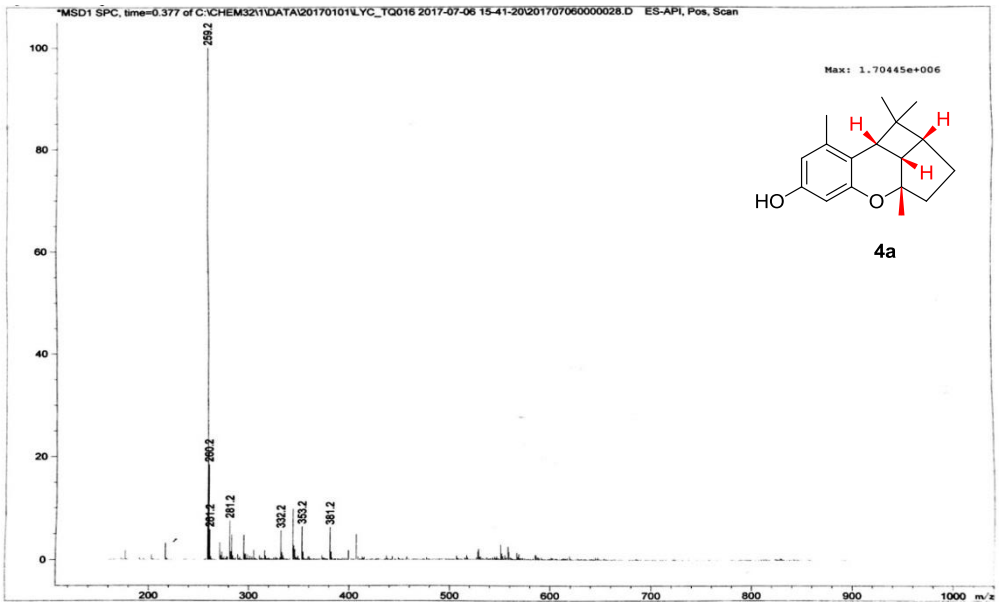


Figure S73. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4a**

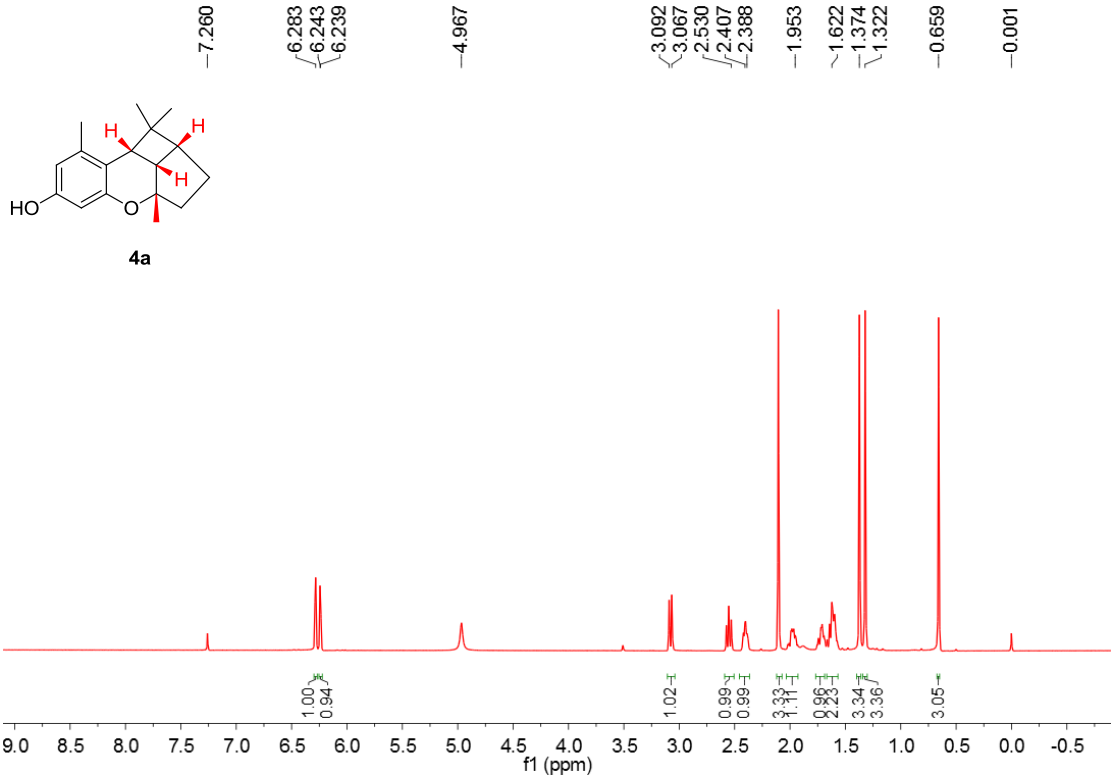


Figure S74. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **4a**

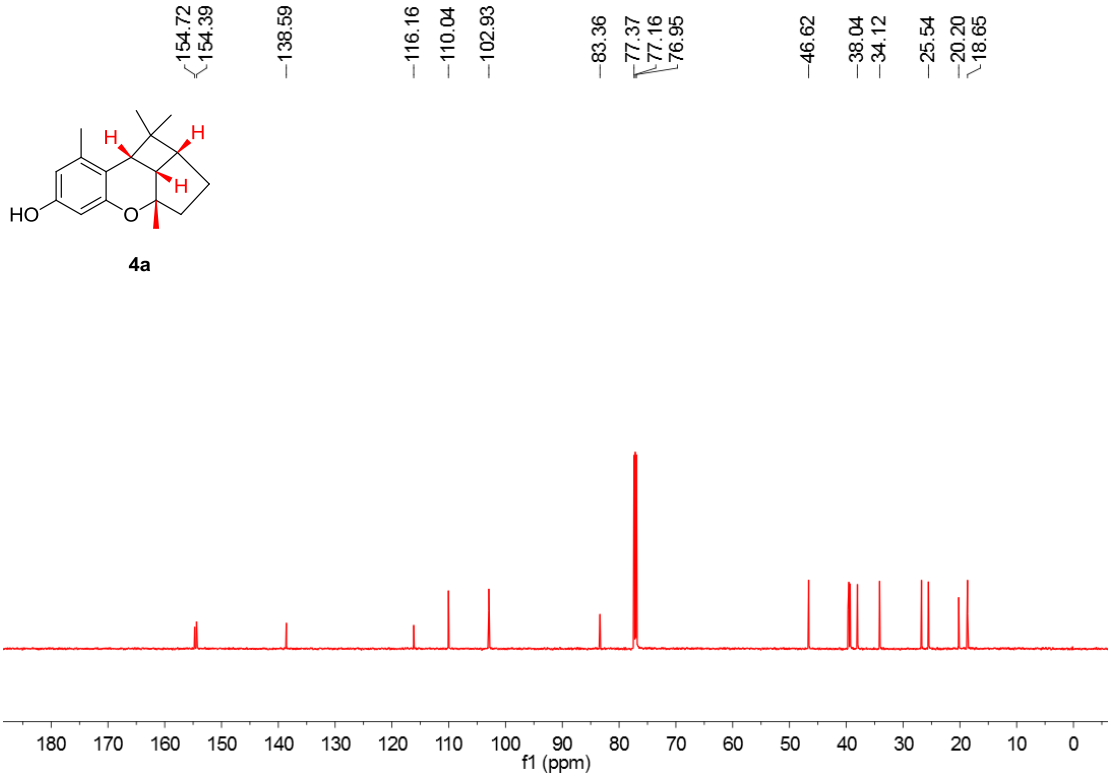


Figure S75. Positive ESIMS spectrum of **4b**

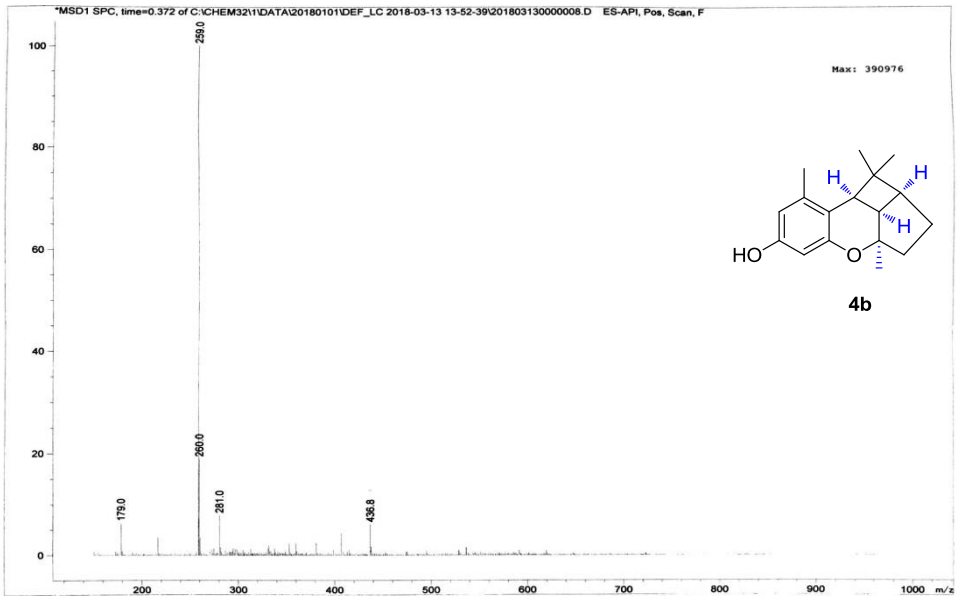


Figure S76. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4b**

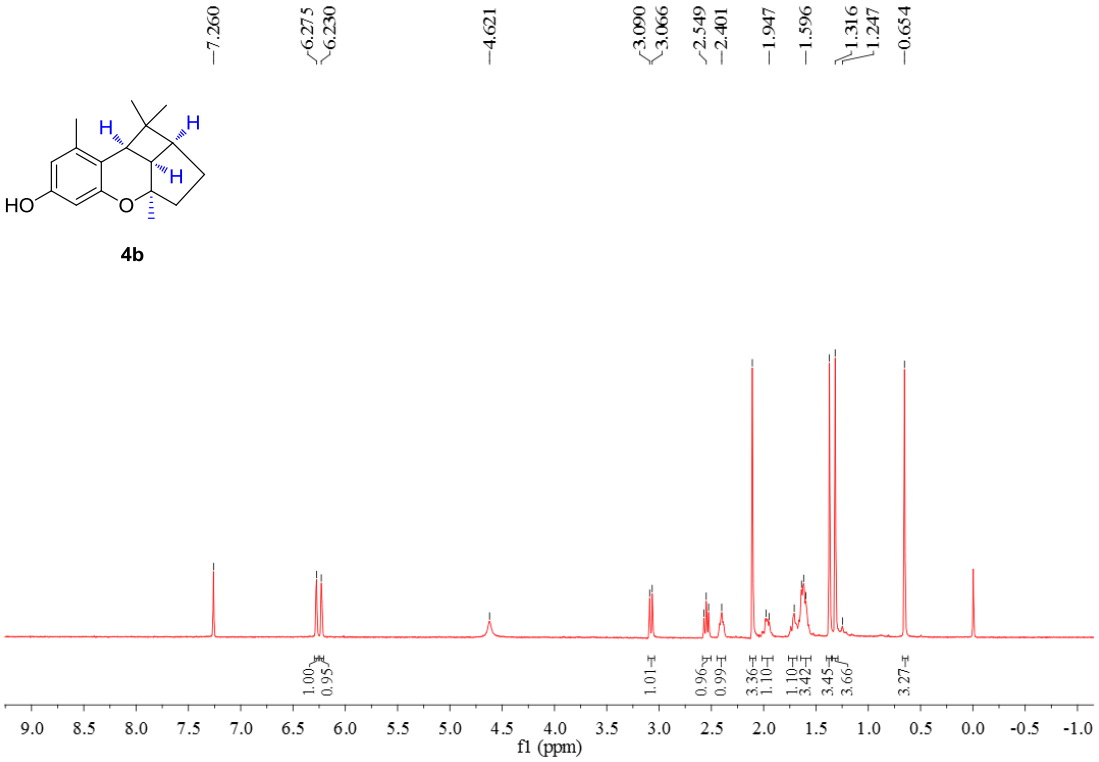


Figure S77. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **4b**

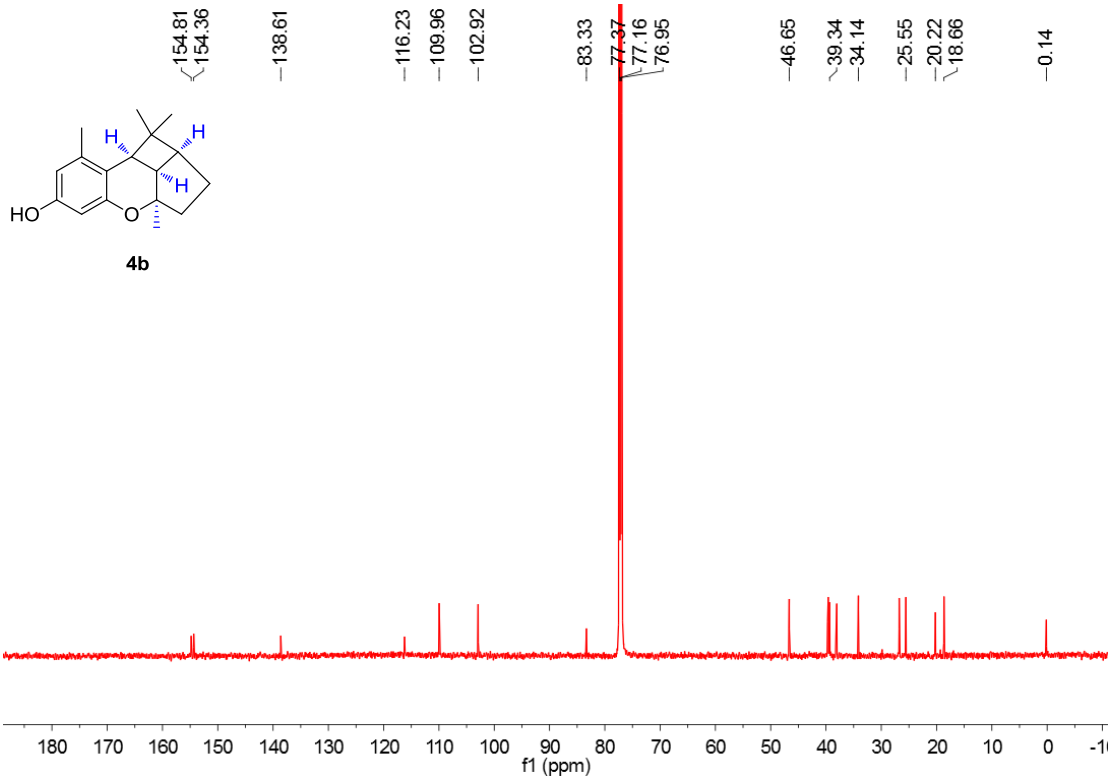


Figure S78. Positive ESIMS spectrum of **5**

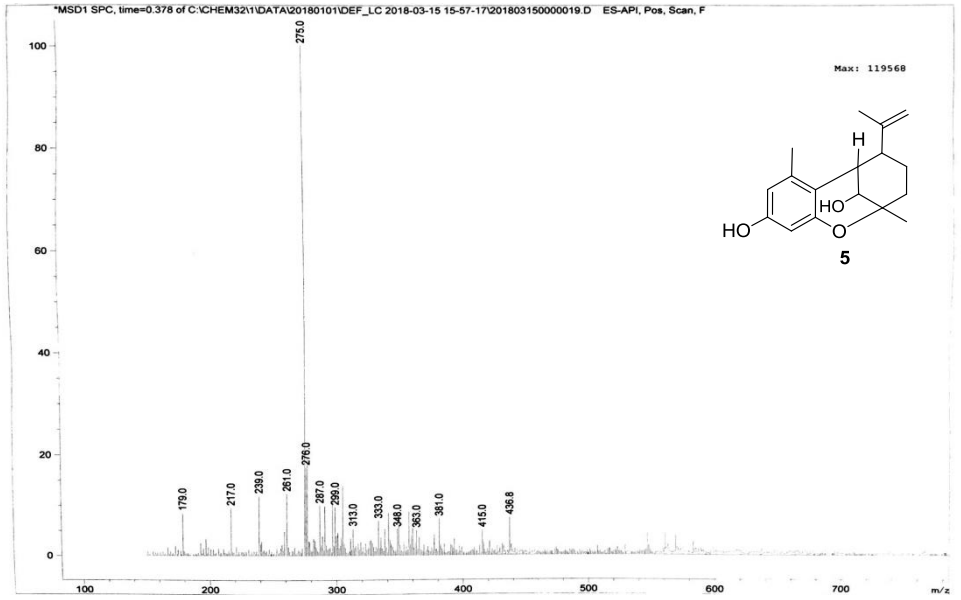


Figure S79. Positive HR-ESIMS spectrum of **5**

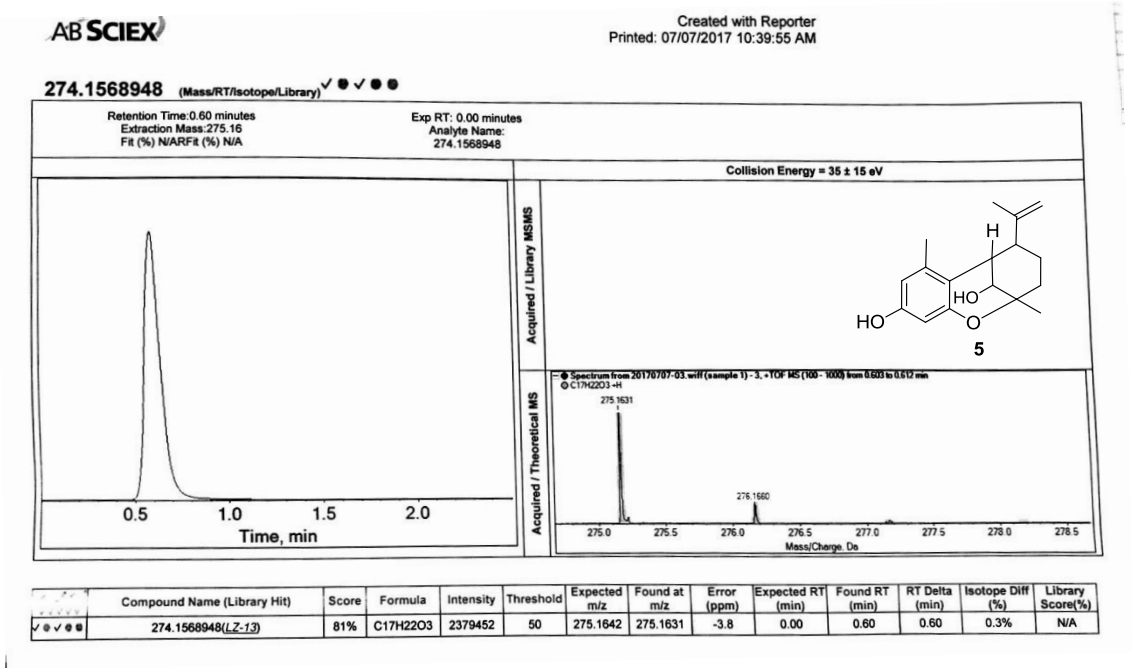


Figure S80. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **5**

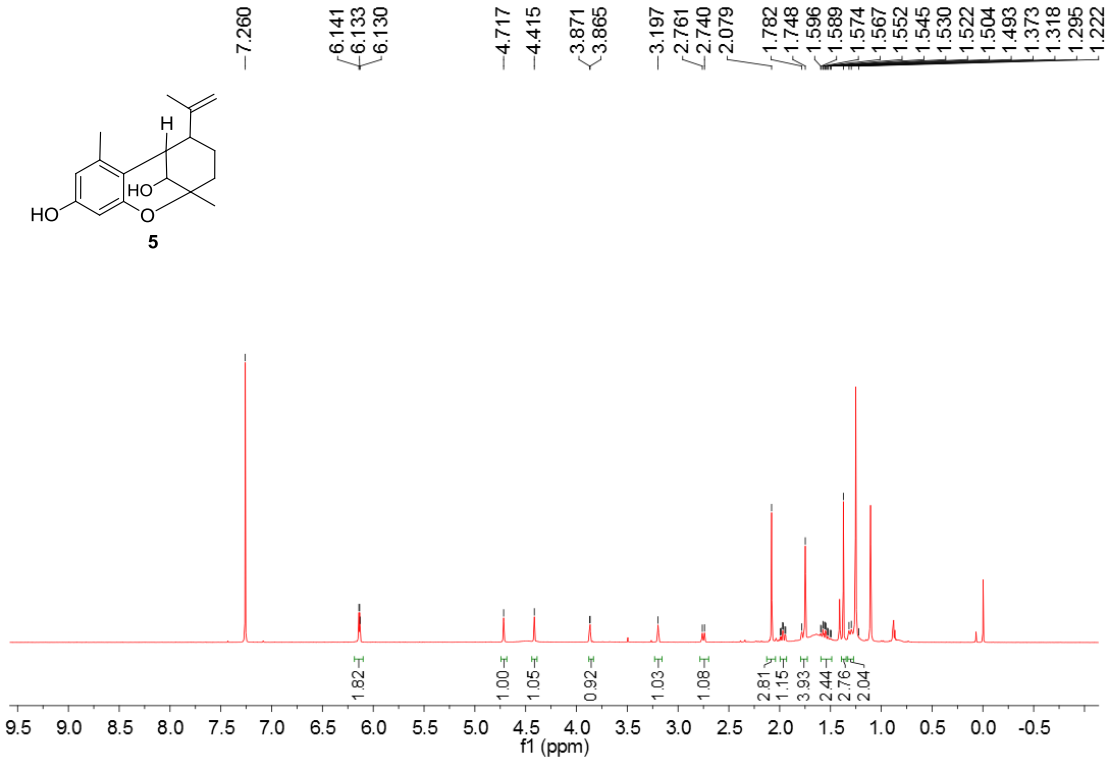


Figure S81. ^{13}C NMR and DEPT (150 MHz, $CDCl_3$) spectra of **5**

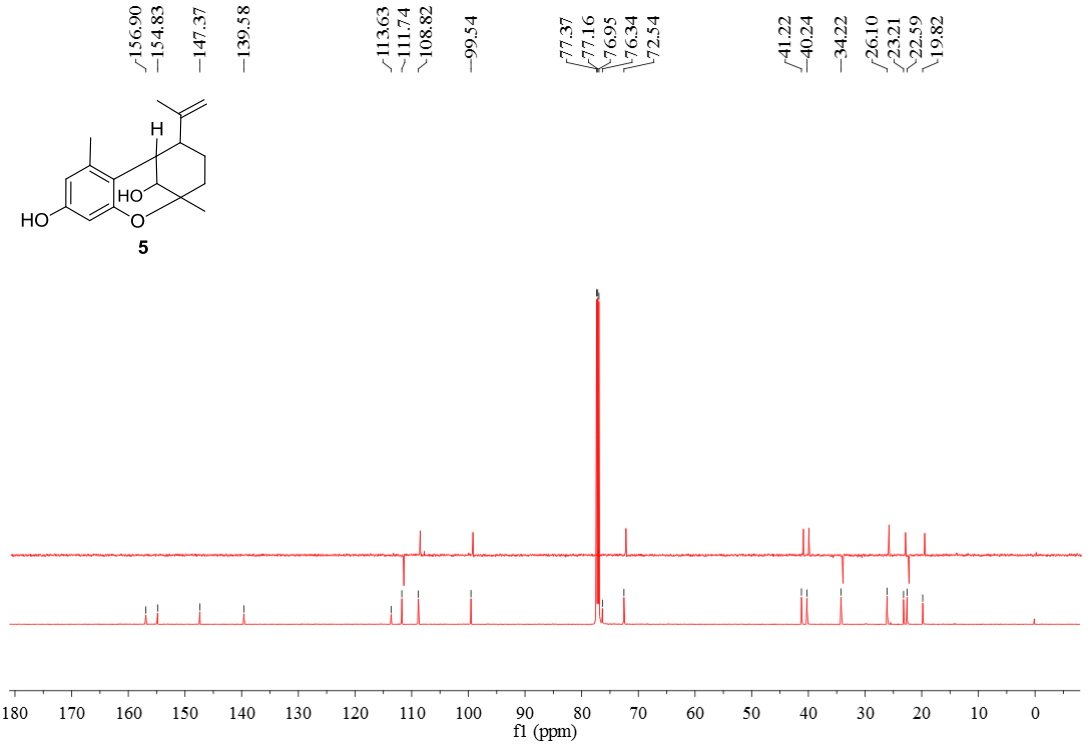


Figure S82. HSQC (600 MHz, $CDCl_3$) spectrum of **5**

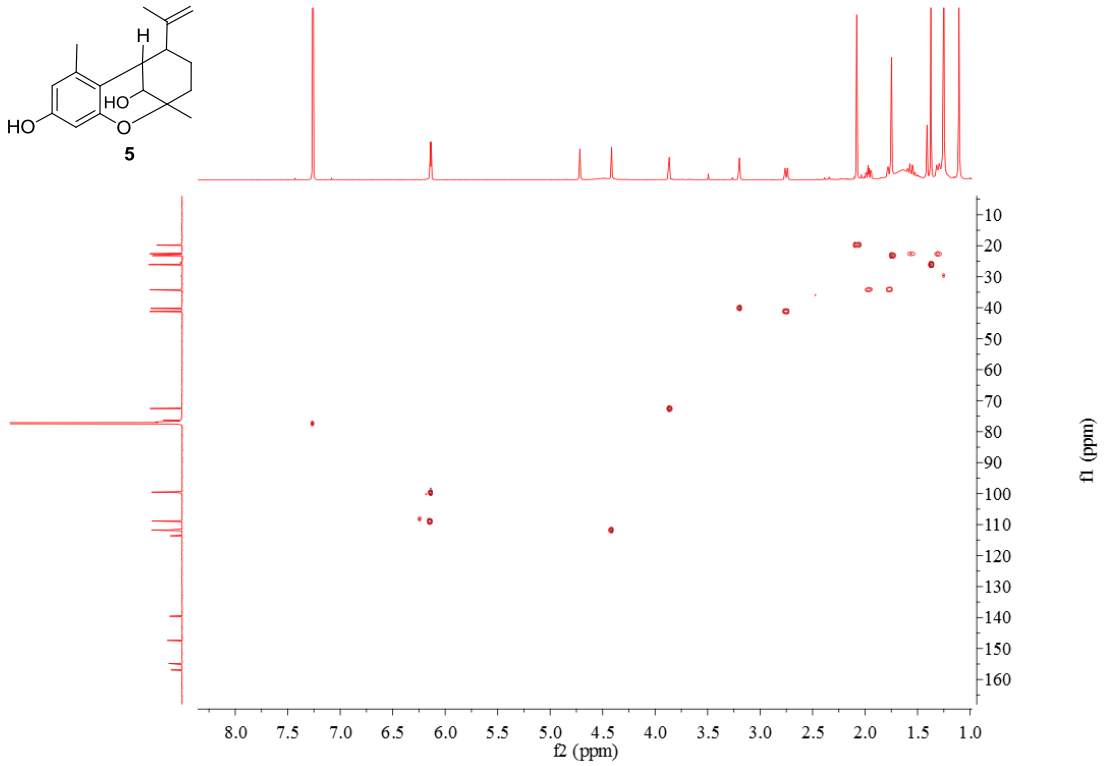


Figure S83. HSQC (600 MHz, $CDCl_3$) spectrum of **5**

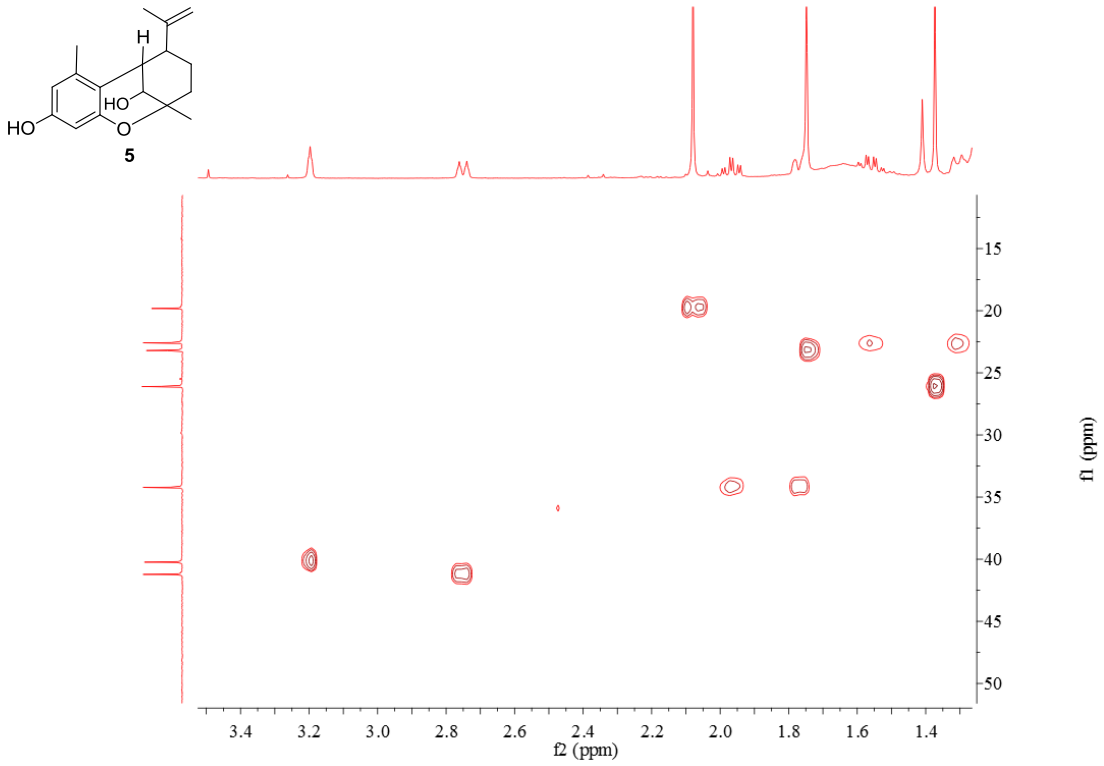


Figure S84. HMBC (600 MHz, $CDCl_3$) spectrum of **5**

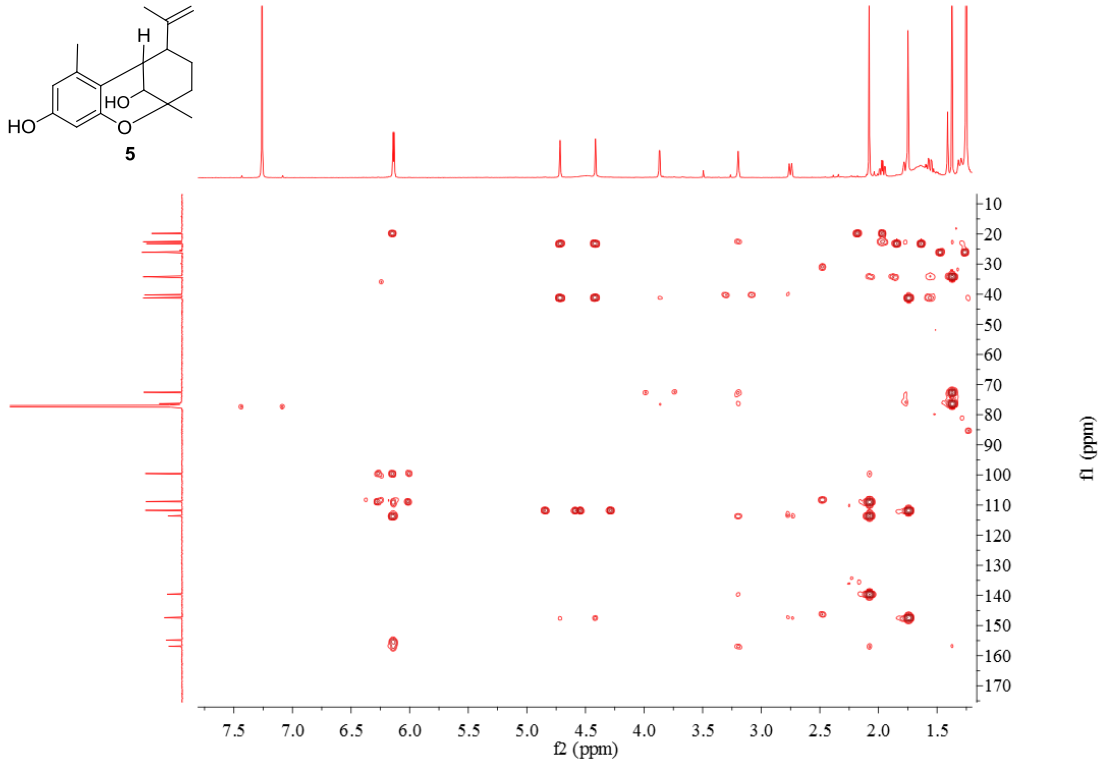


Figure S85. HMBC (600 MHz, $CDCl_3$) spectrum of **5**

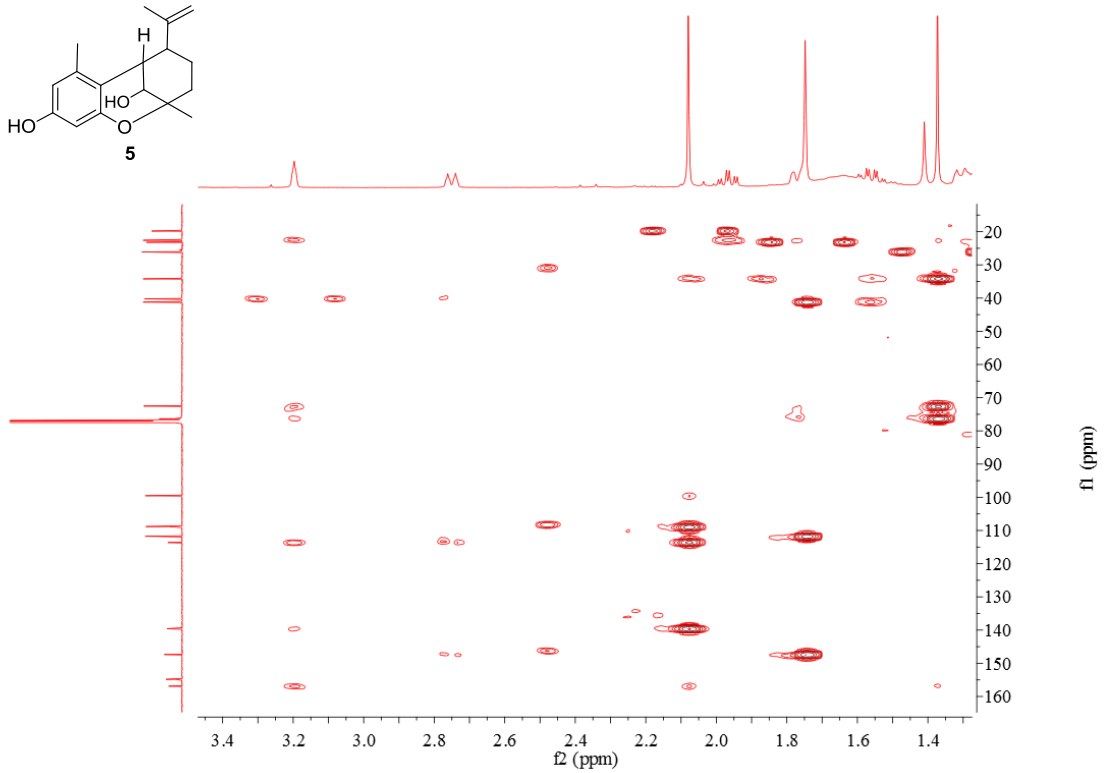


Figure S86. NOESY (600 MHz, $CDCl_3$) spectrum of **5**

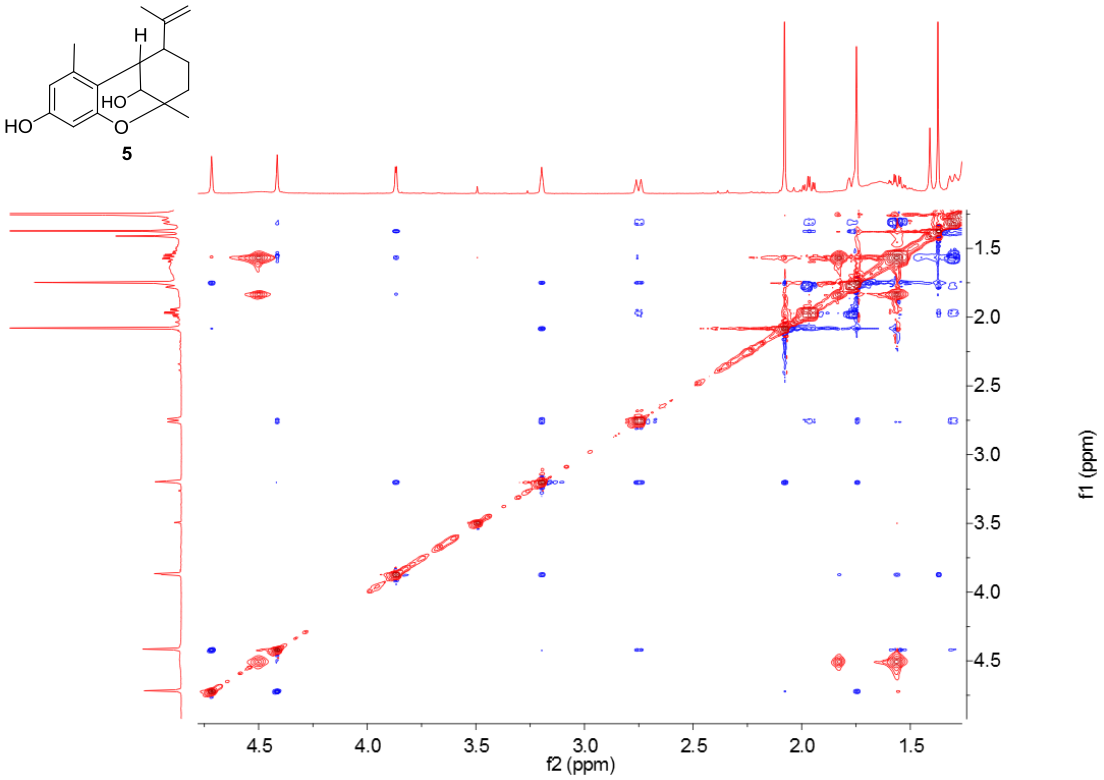


Figure S87. IR spectrum of **5**

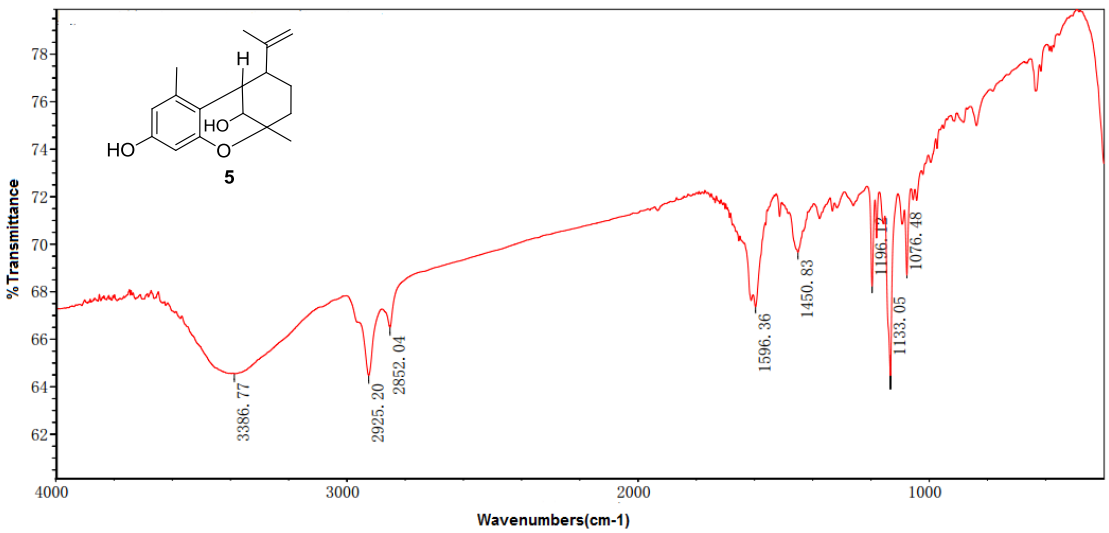


Figure S88. Positive ESIMS spectrum of **5a**

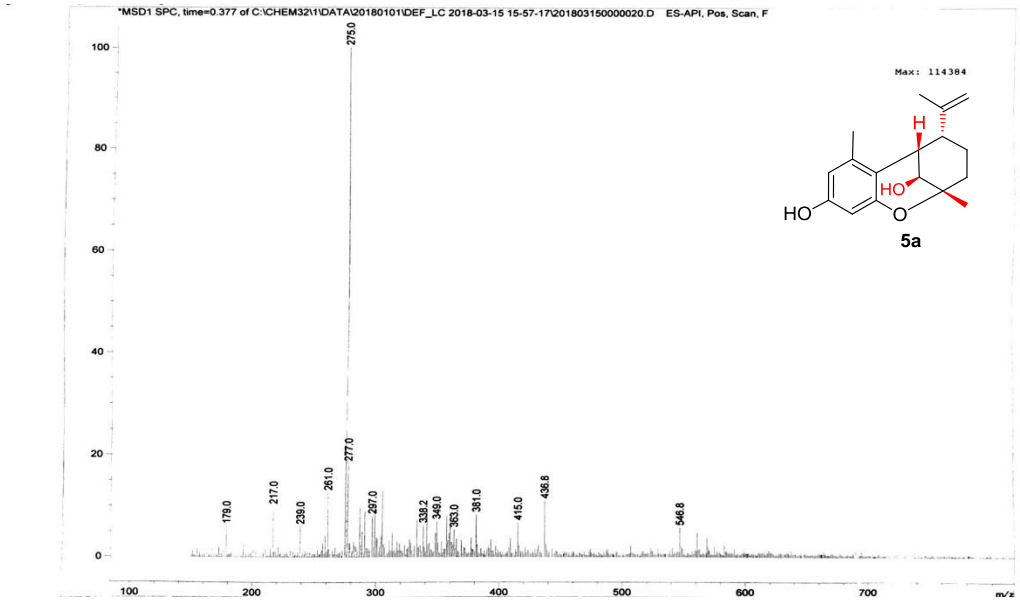


Figure S89. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5a**

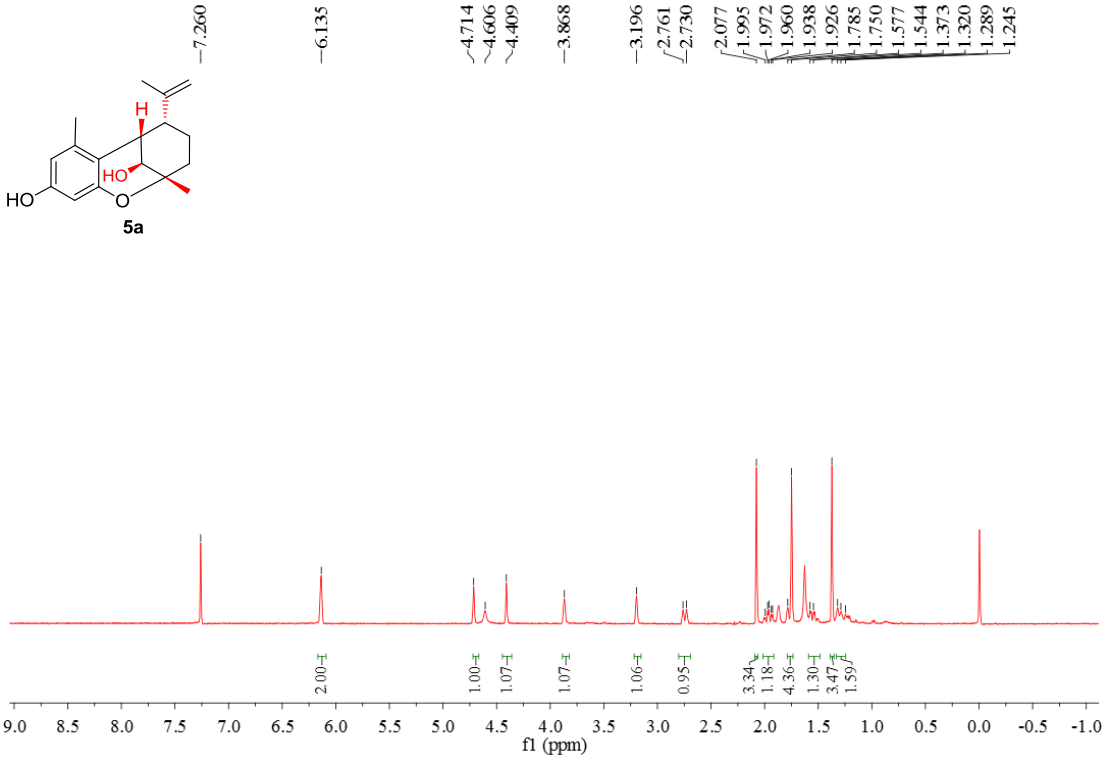


Figure S90. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **5a**

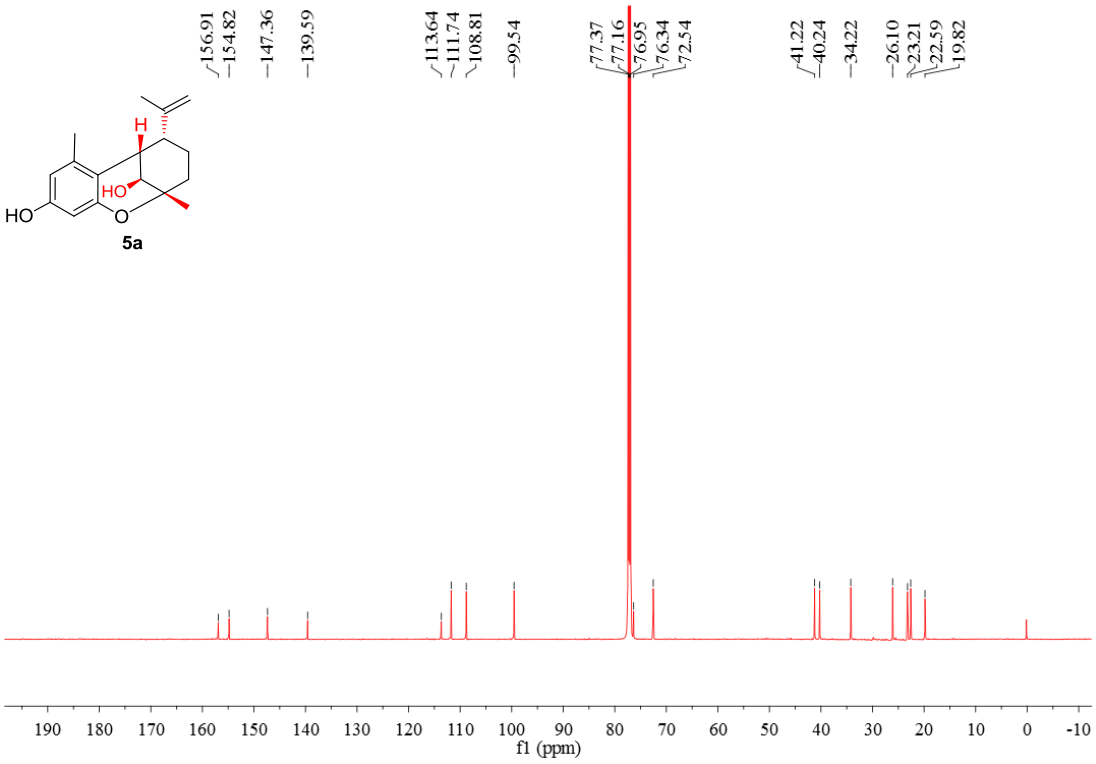


Figure S91. Positive ESIMS spectrum of **5b**

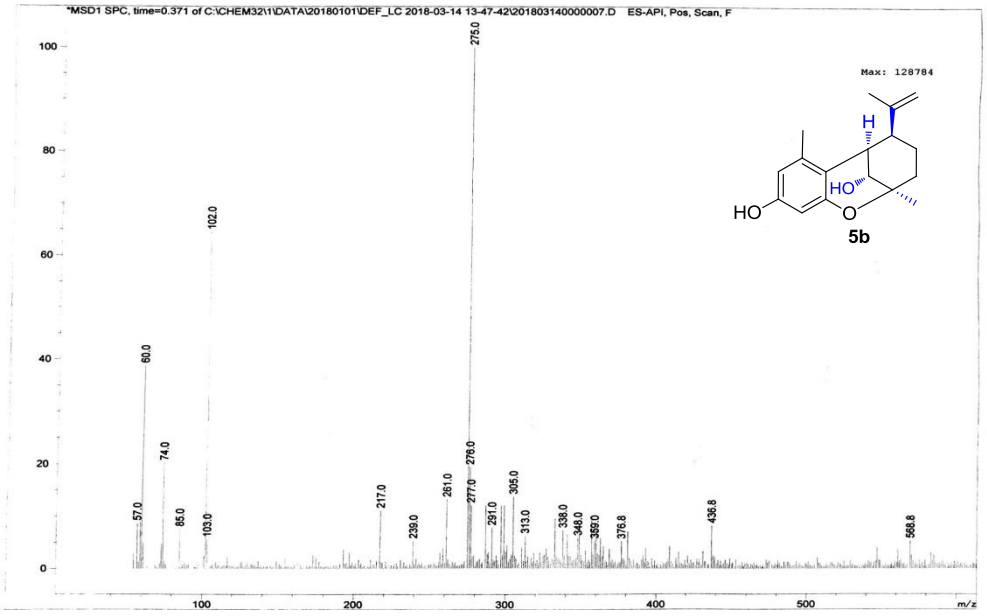


Figure S92. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5b**

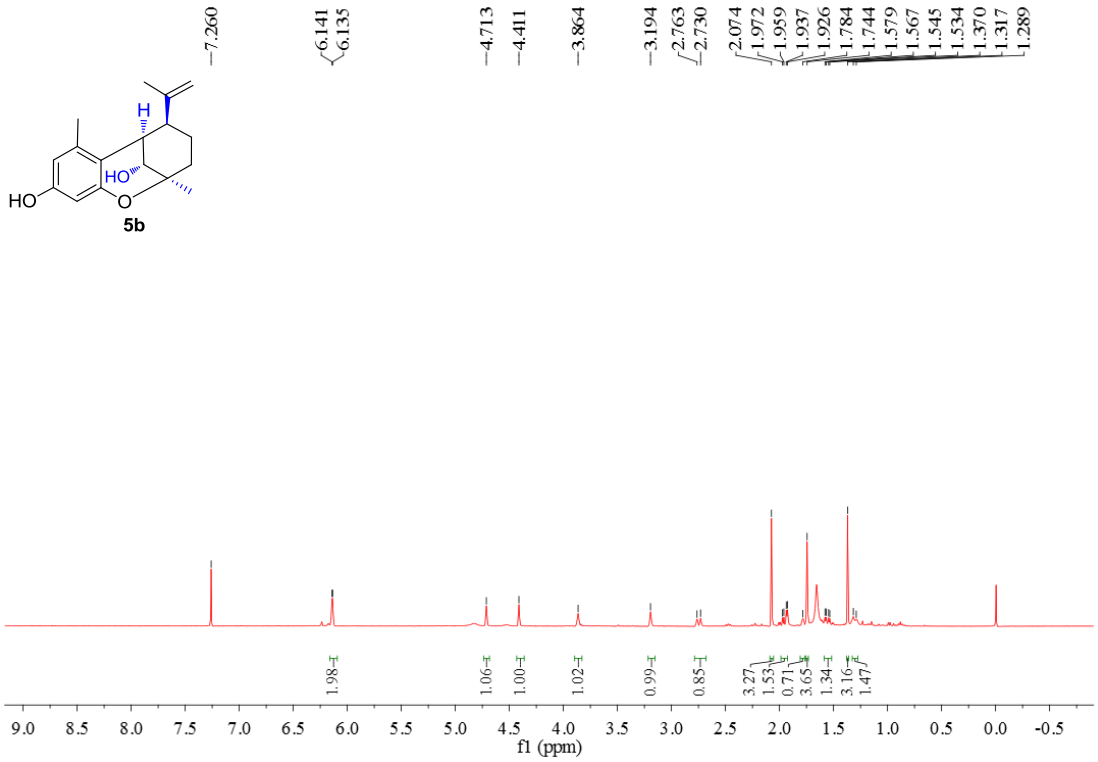


Figure S93. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **5b**

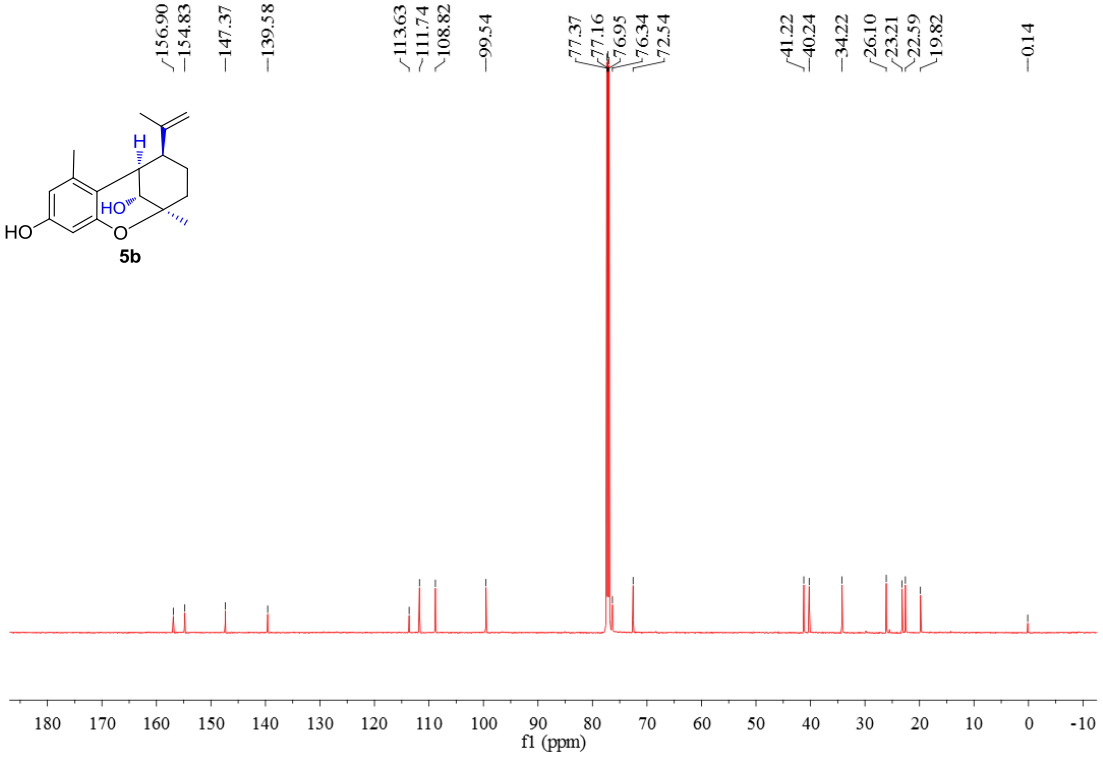


Figure S94. Positive ESIMS spectrum of **6**

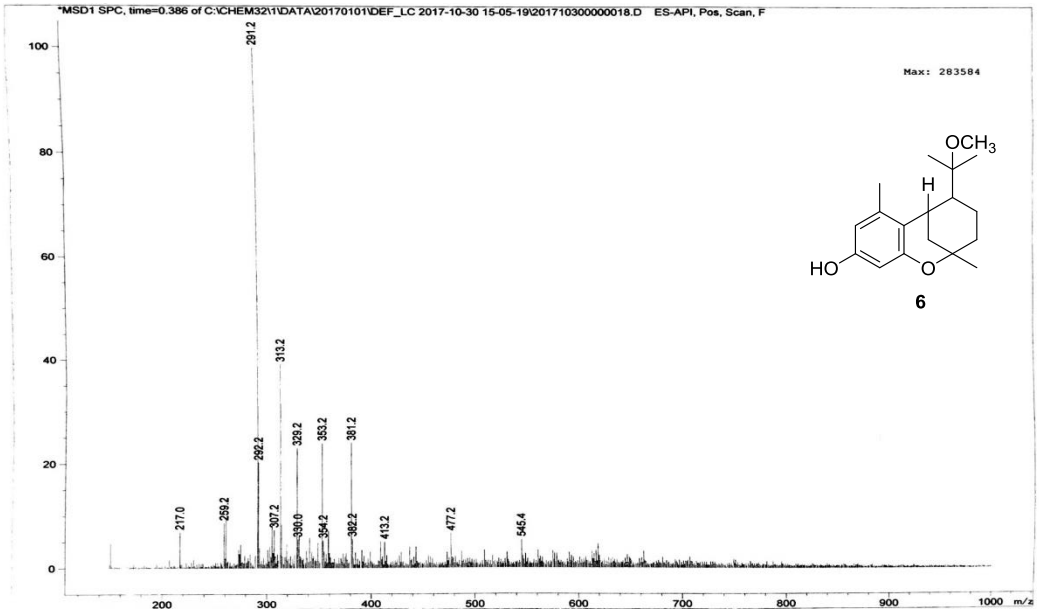
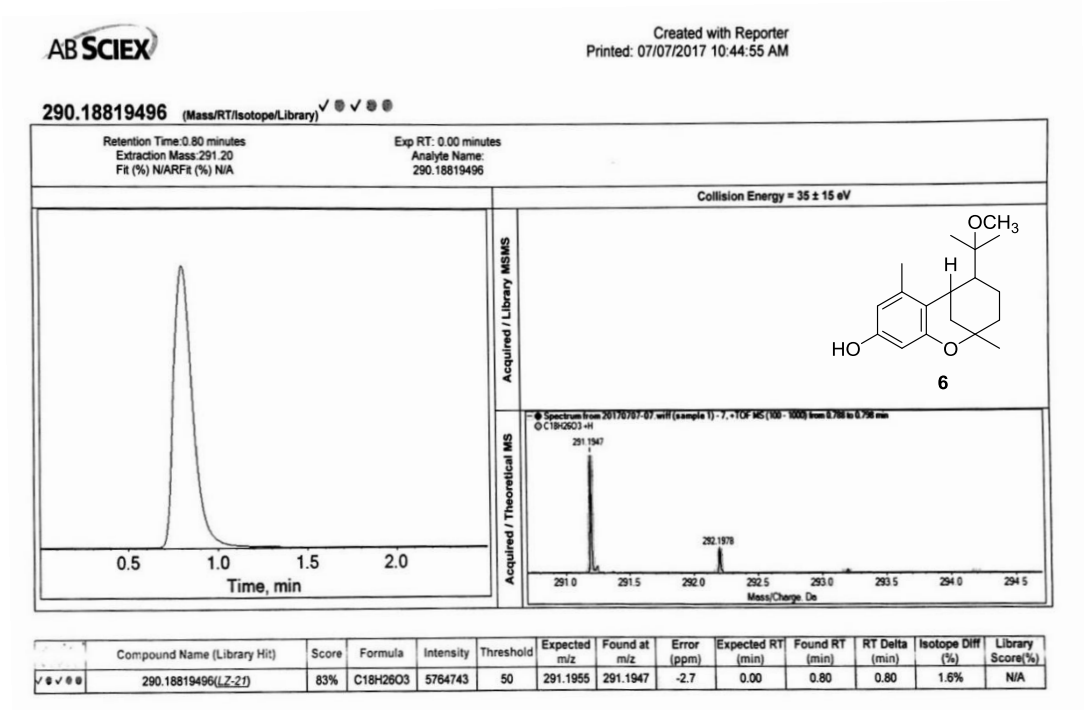


Figure S95. Positive HR-ESIMS spectrum of **6**



	Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
✓●✓●●	290.18819496(LZ-21)	83%	C18H26O3	5764743	50	291.1955	291.1947	-2.7	0.00	0.80	0.80	1.6%	N/A

Figure S96. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **6**

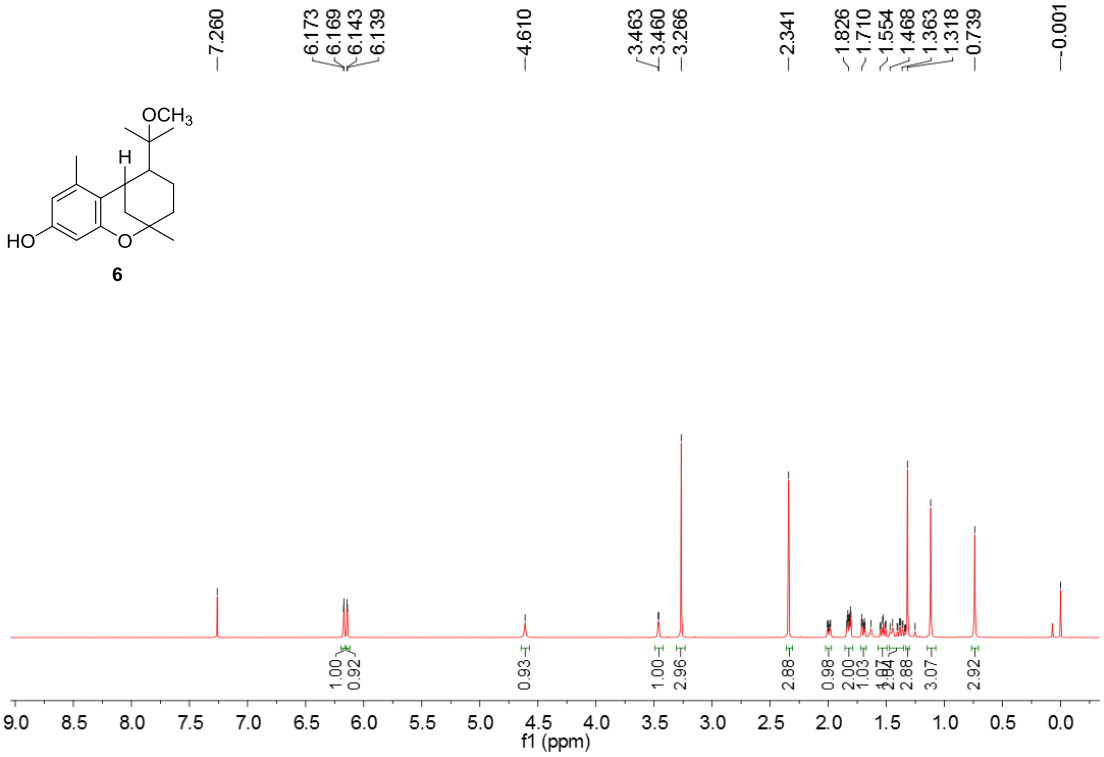


Figure S97. ^{13}C NMR and DEPT (150 MHz, $CDCl_3$) spectra of **6**

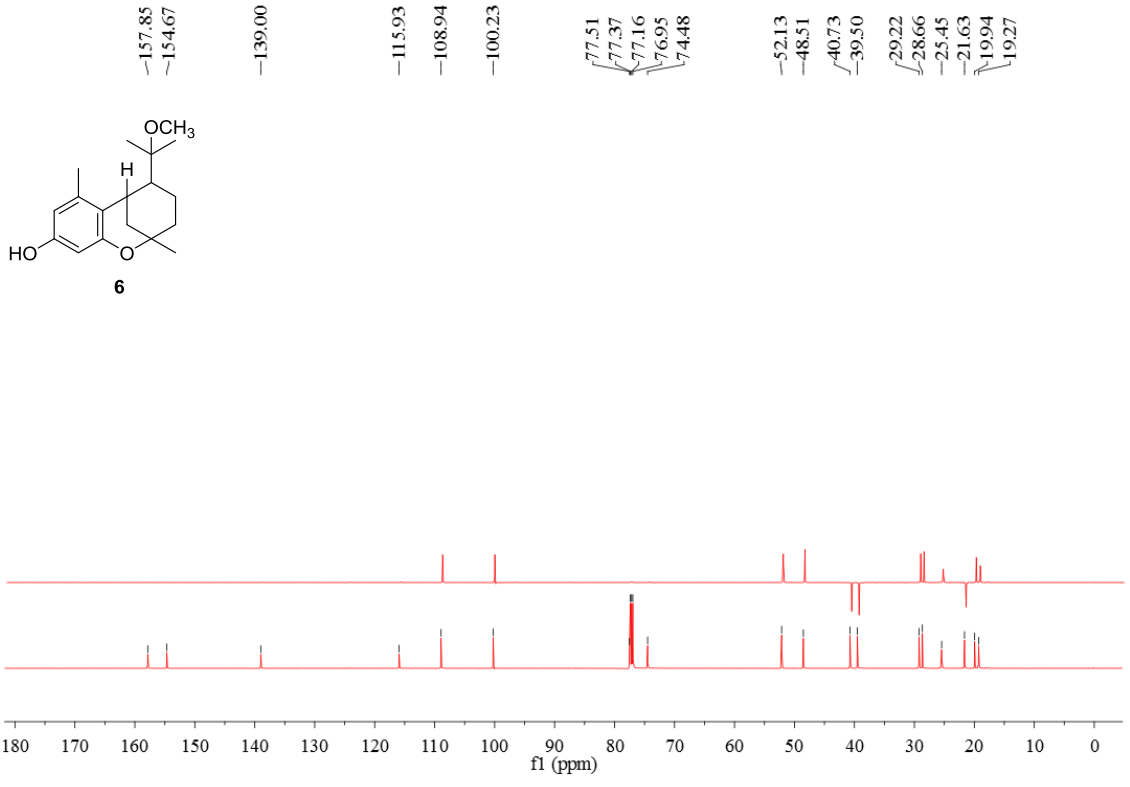


Figure S98. HSQC (600 MHz, $CDCl_3$) spectrum of **6**

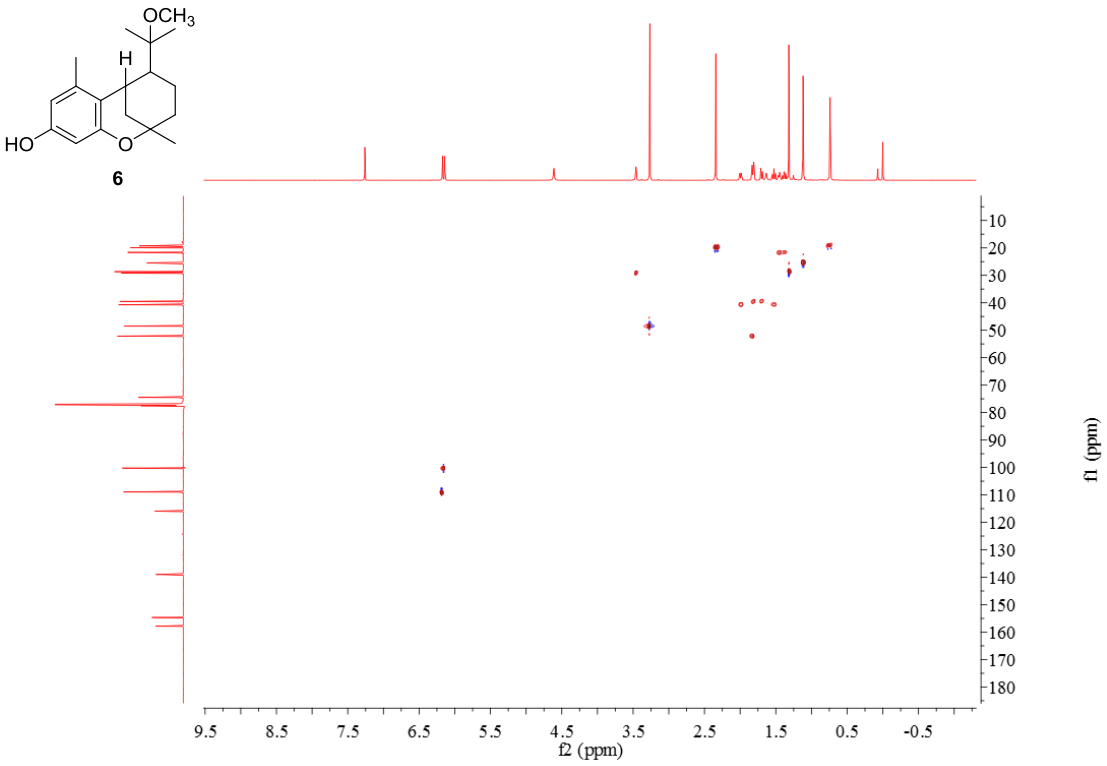


Figure S99. HSQC (600 MHz, $CDCl_3$) spectrum of **6**

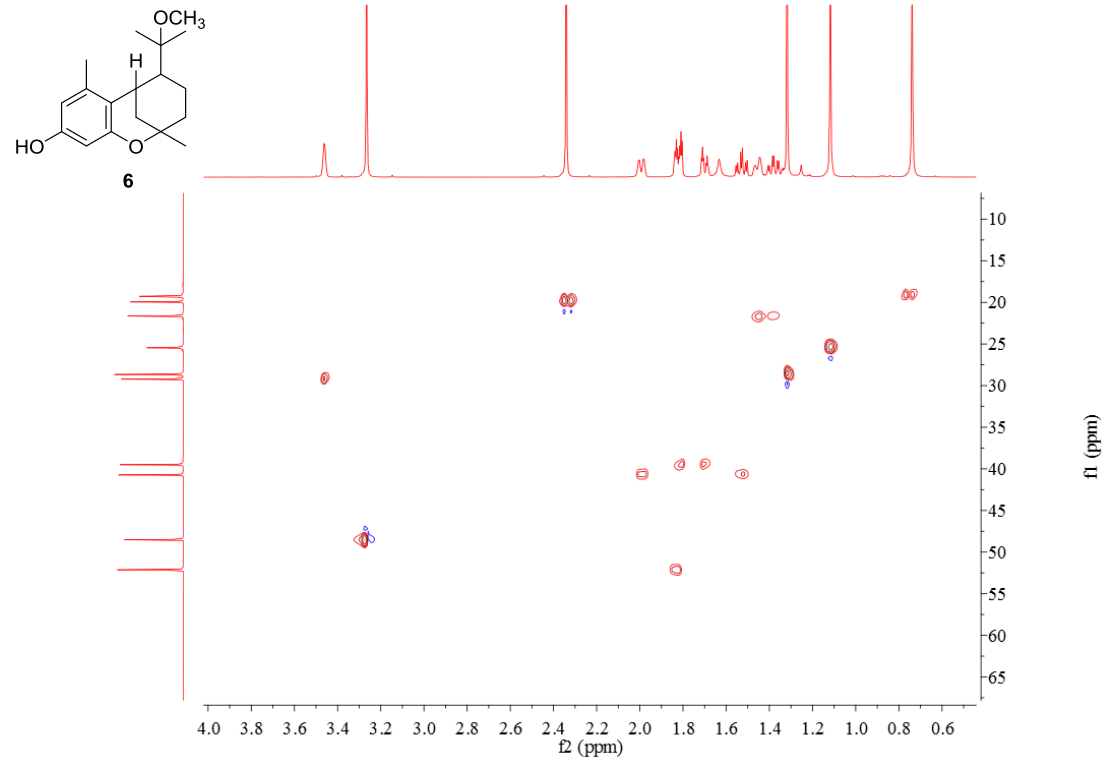


Figure S100. HMBC (600 MHz, $CDCl_3$) spectrum of **6**

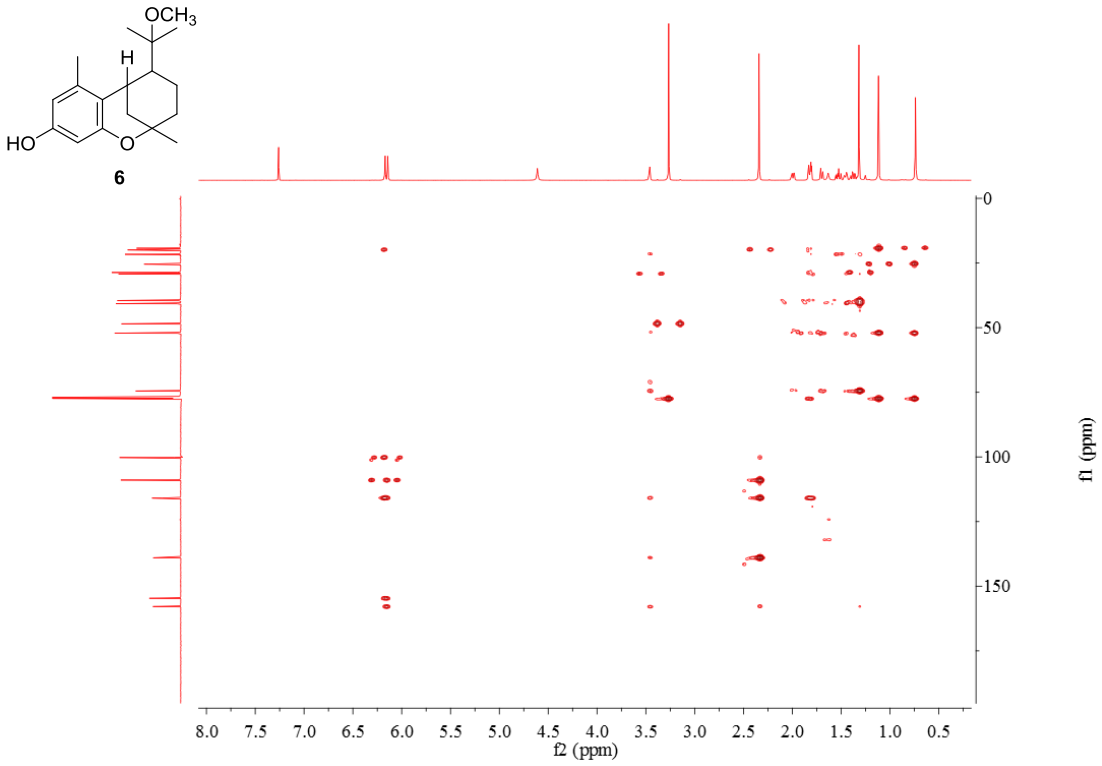


Figure S101. HMBC (600 MHz, $CDCl_3$) spectrum of **6**

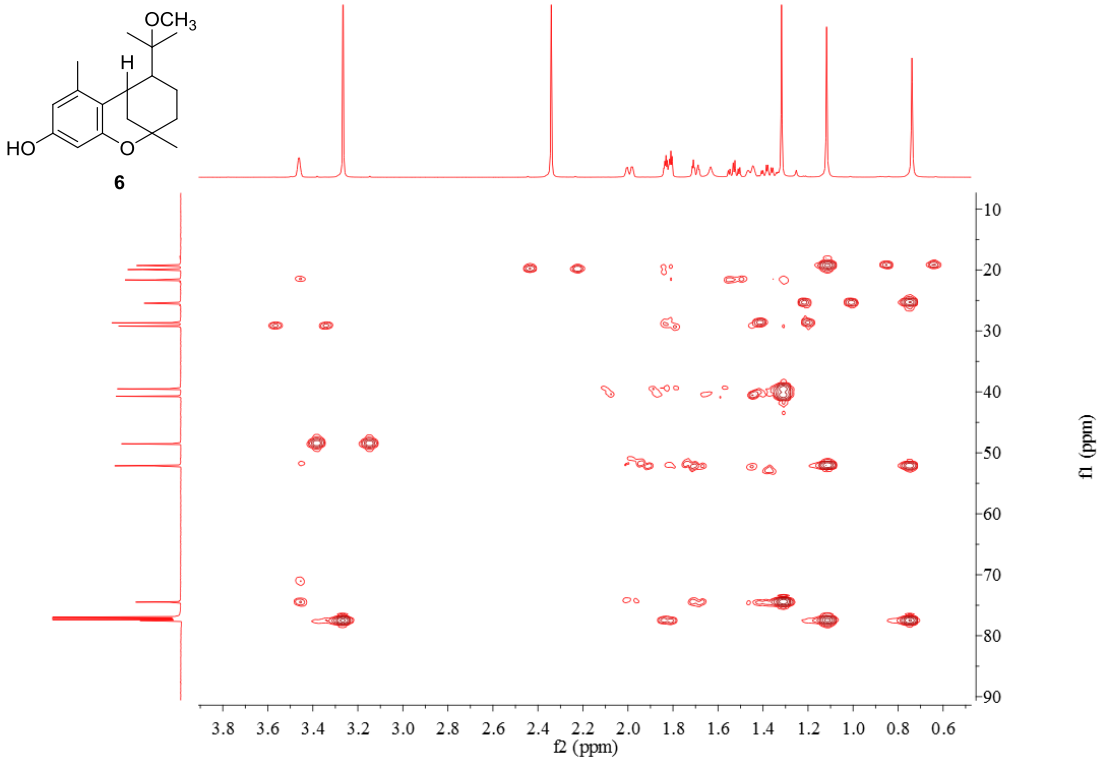


Figure S102. NOESY (600 MHz, $CDCl_3$) spectrum of **6**

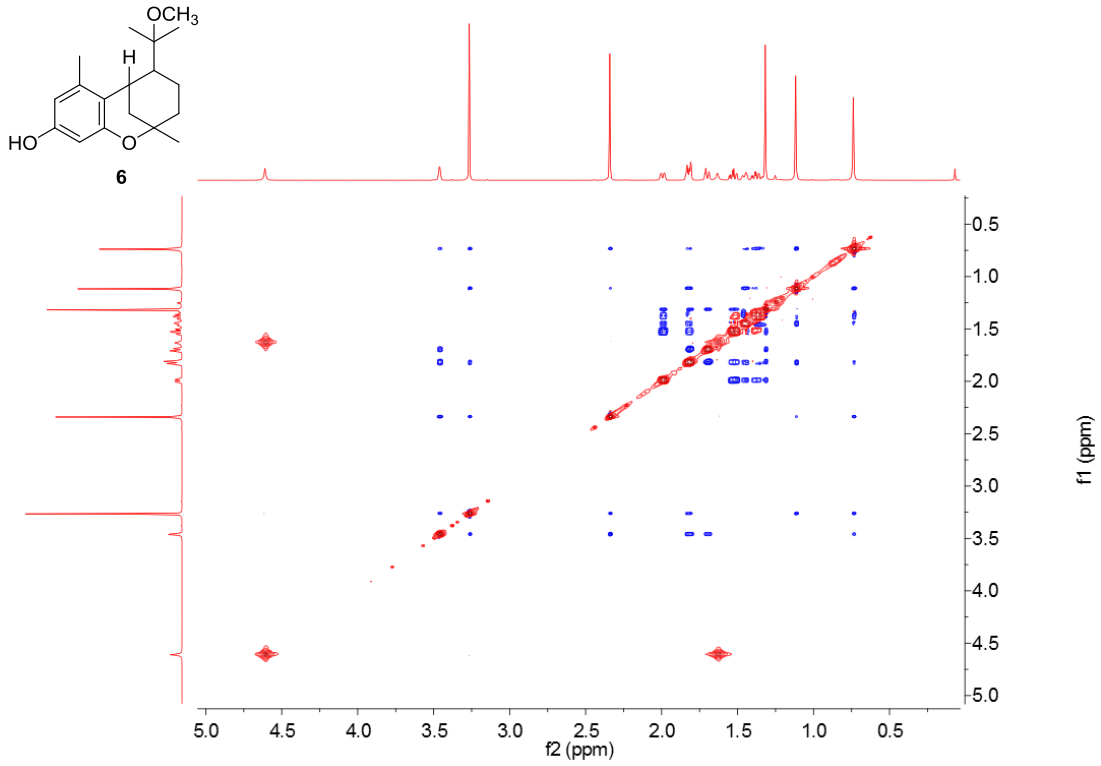


Figure S103. IR spectrum of **6**

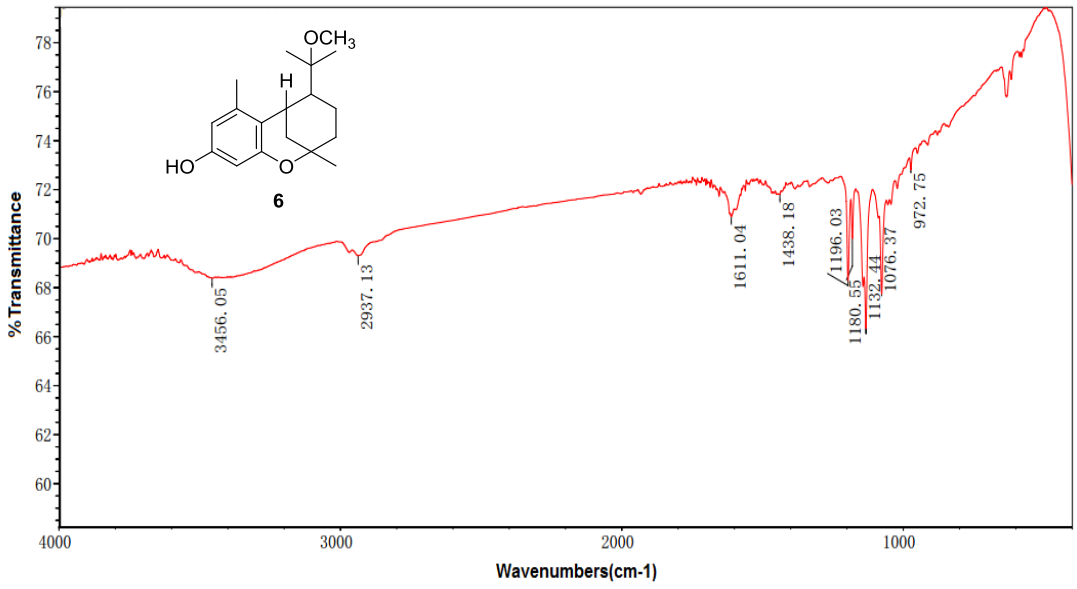


Figure S104. Positive ESIMS spectrum of **6a**

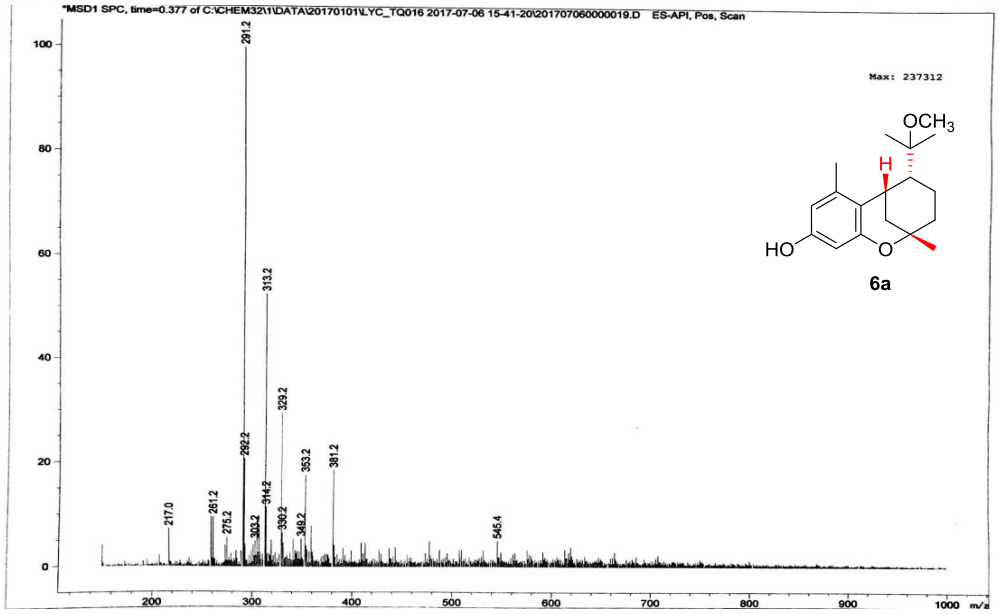


Figure S105. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **6a**

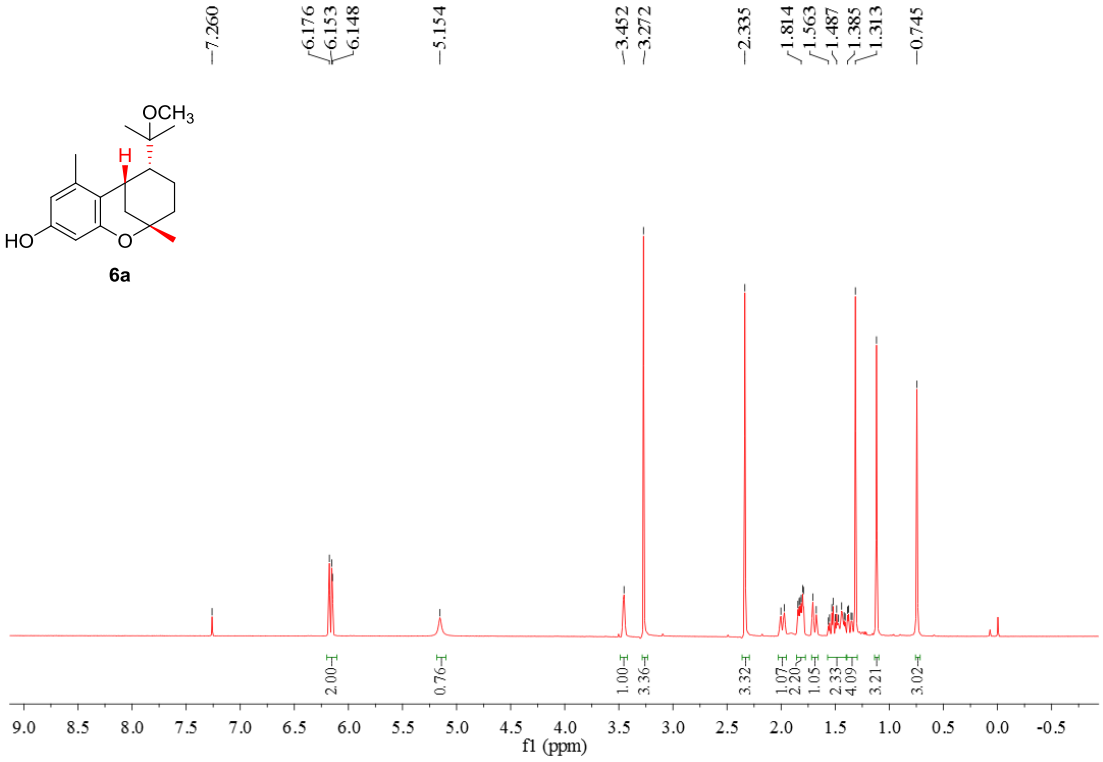


Figure S106. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **6a**

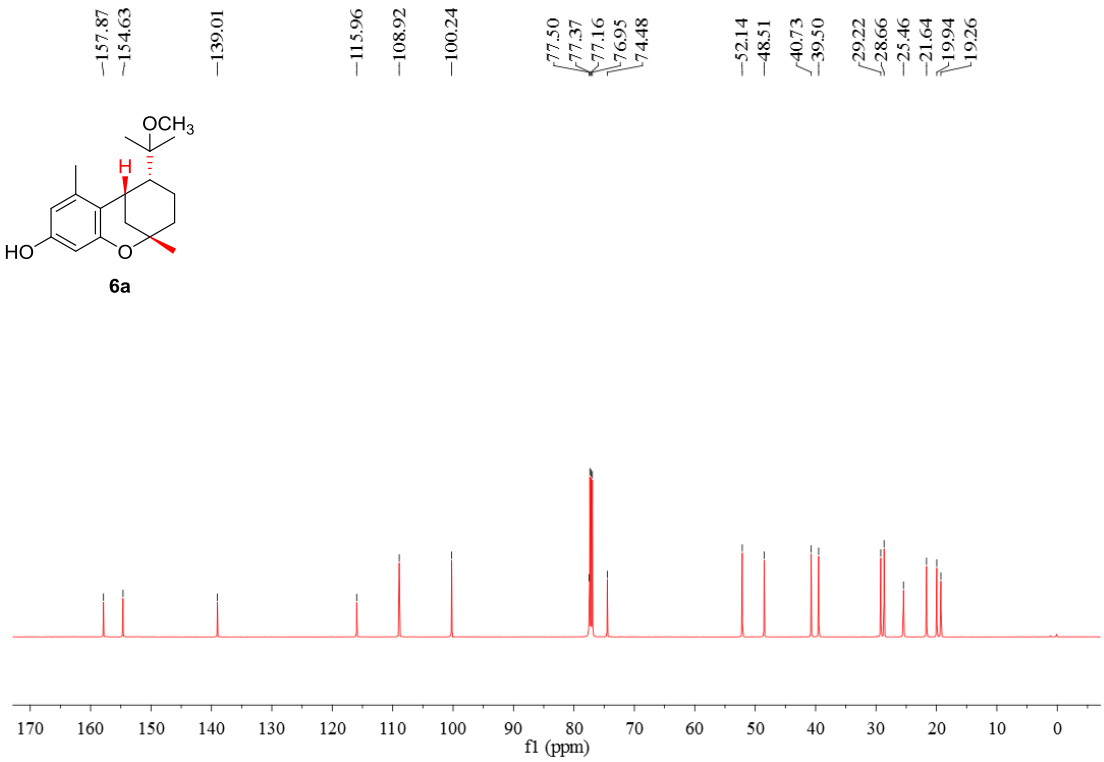


Figure S107. Positive ESIMS spectrum of **6b**

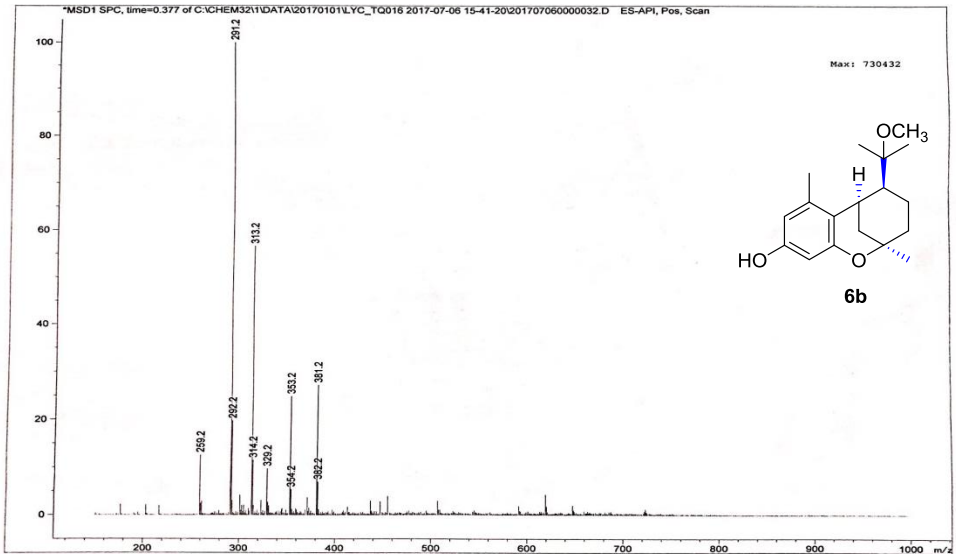


Figure S108. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **6b**

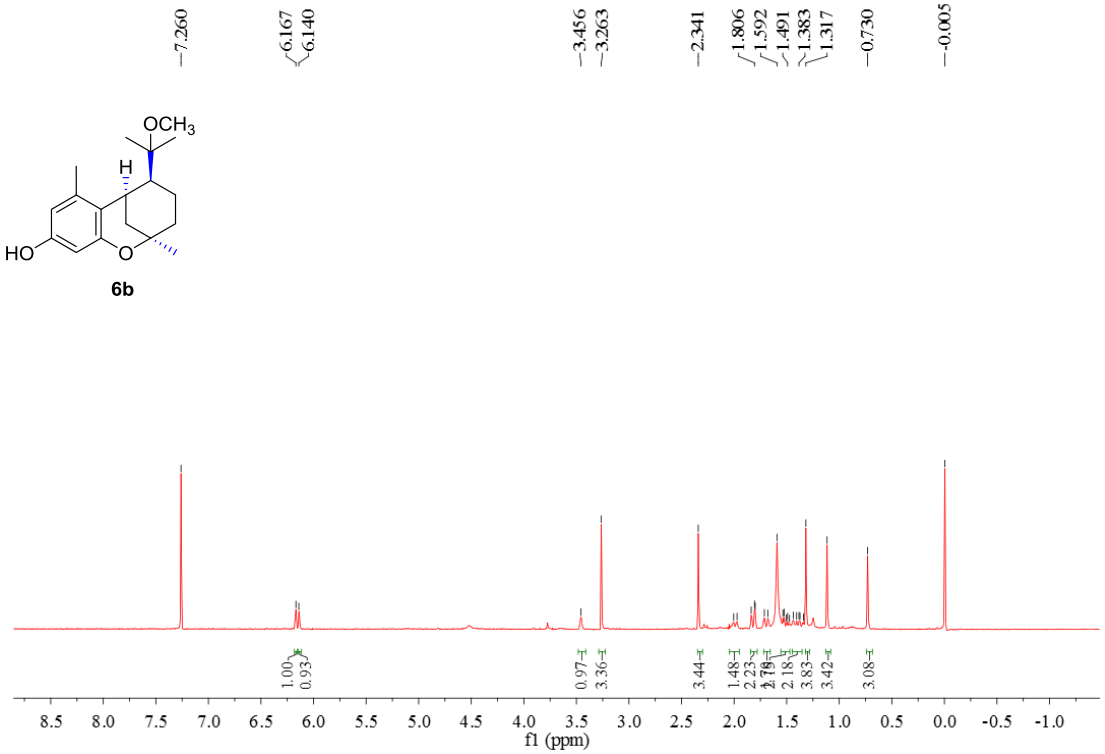


Figure S109. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **6b**

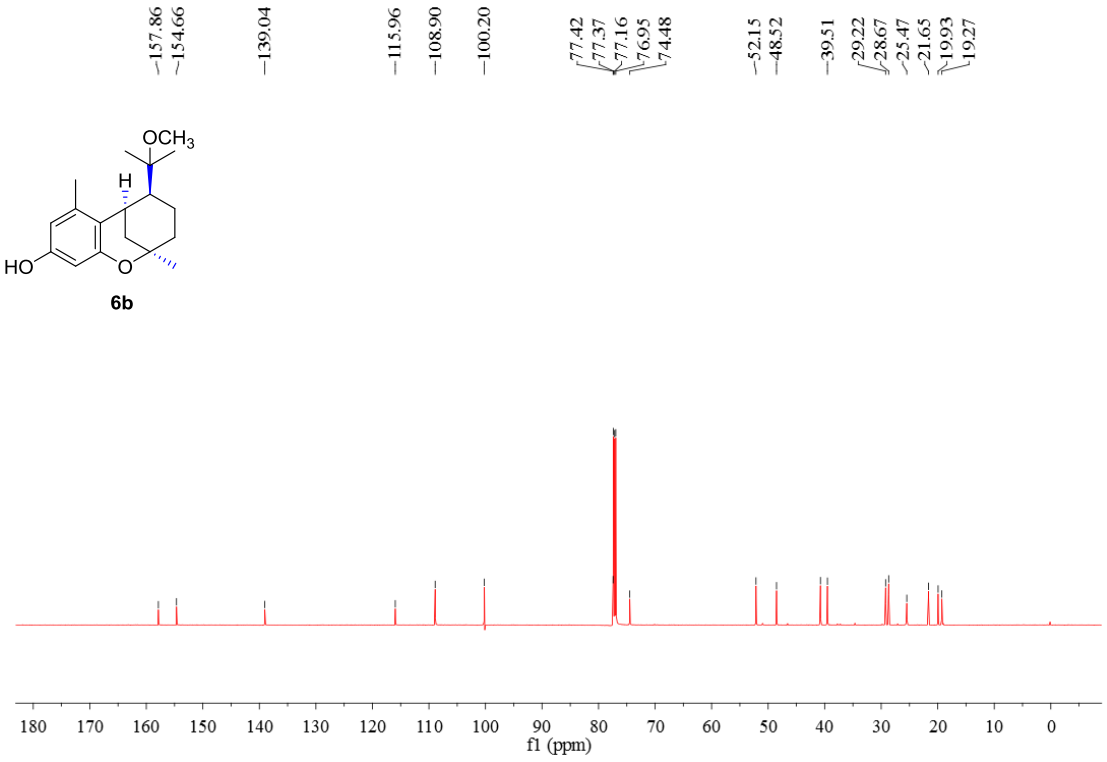


Figure S110. Positive ESIMS spectrum of **7**

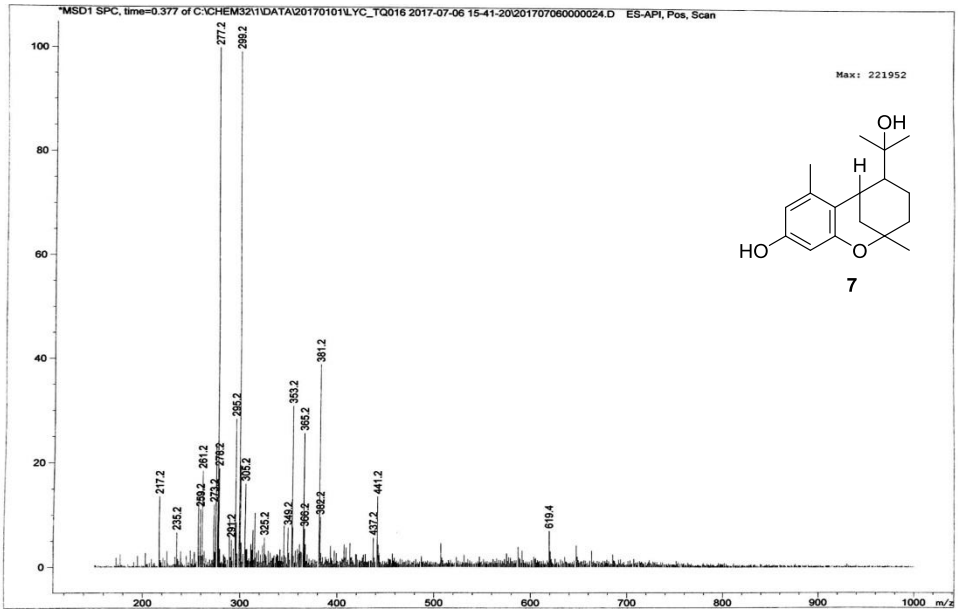


Figure S111. Positive HR-ESIMS spectrum of **7**

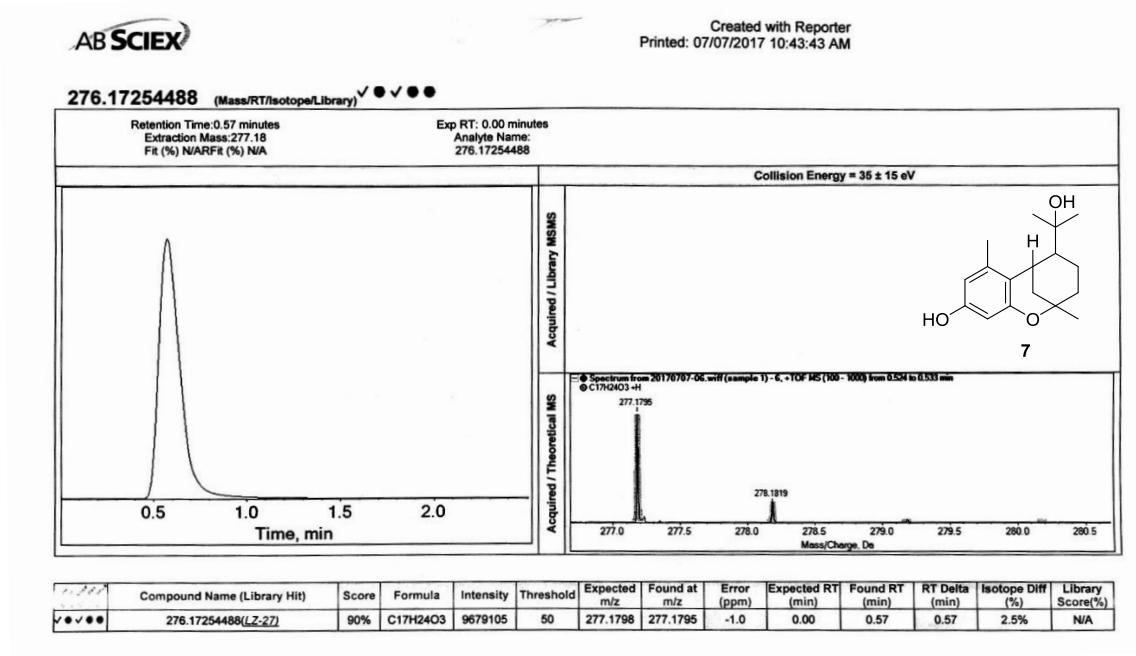


Figure S112. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **7**

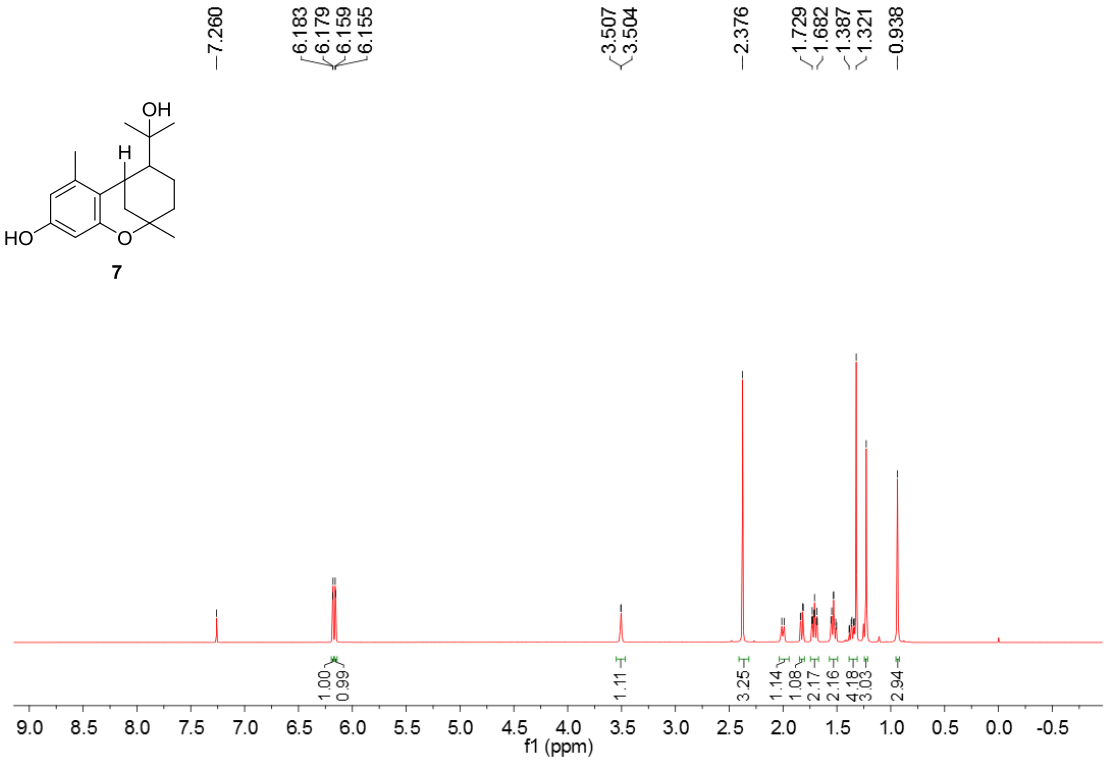


Figure S113. ^{13}C NMR and DEPT (150 MHz, $CDCl_3$) spectra of **7**

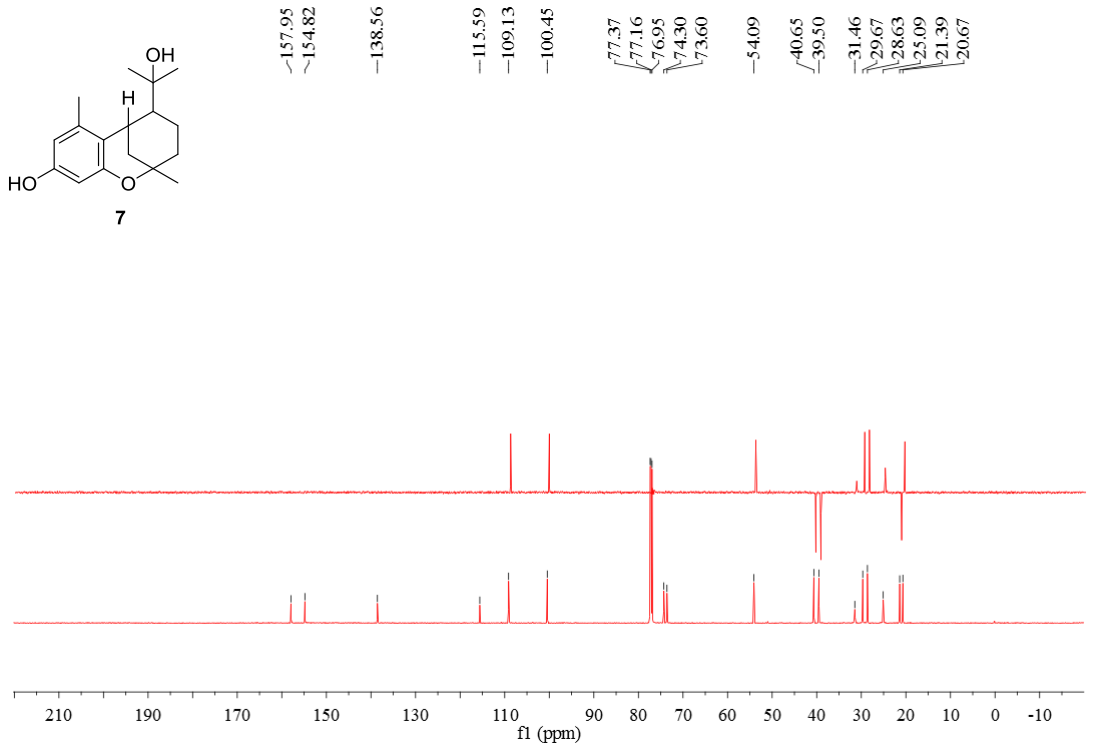


Figure S114. HSQC (600 MHz, $CDCl_3$) spectrum of **7**

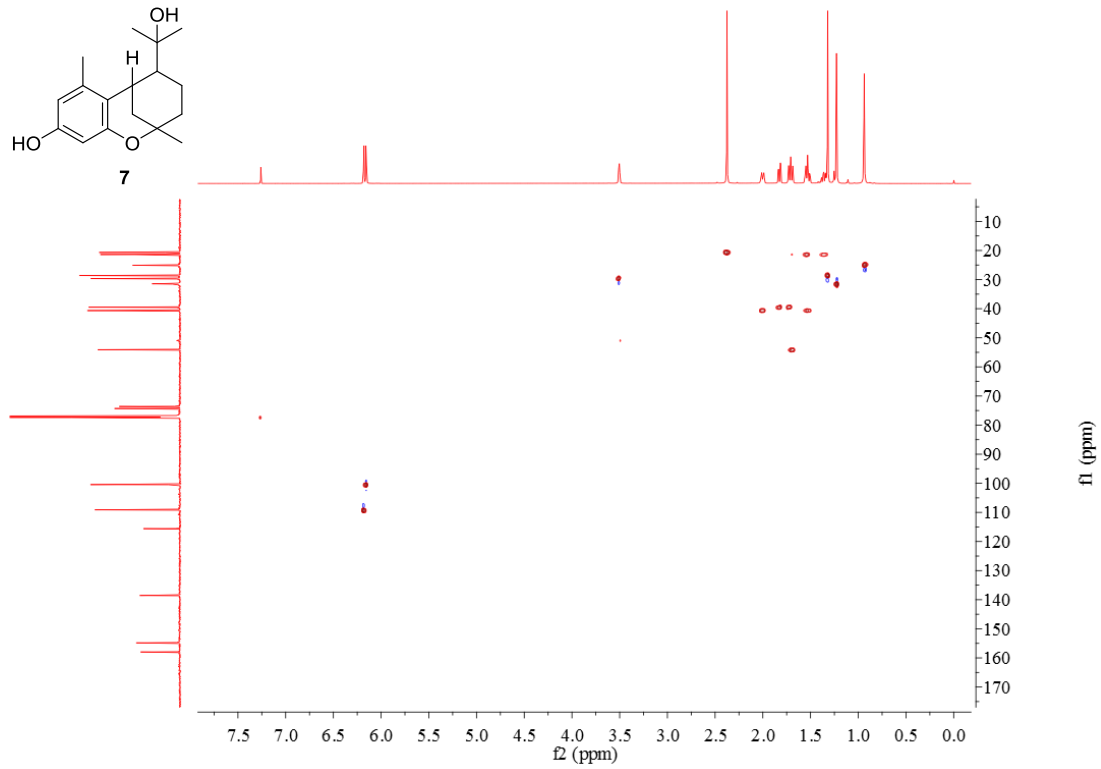


Figure S115. HSQC (600 MHz, $CDCl_3$) spectrum of **7**

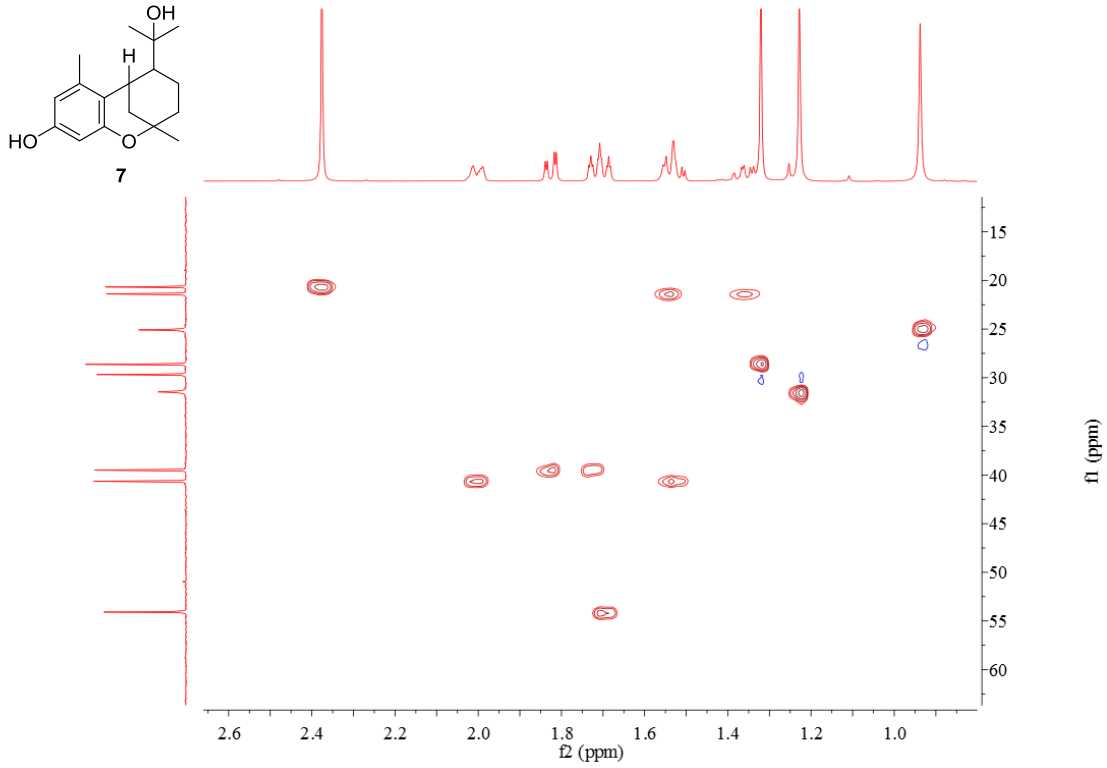


Figure S116. HMBC (600 MHz, $CDCl_3$) spectrum of **7**

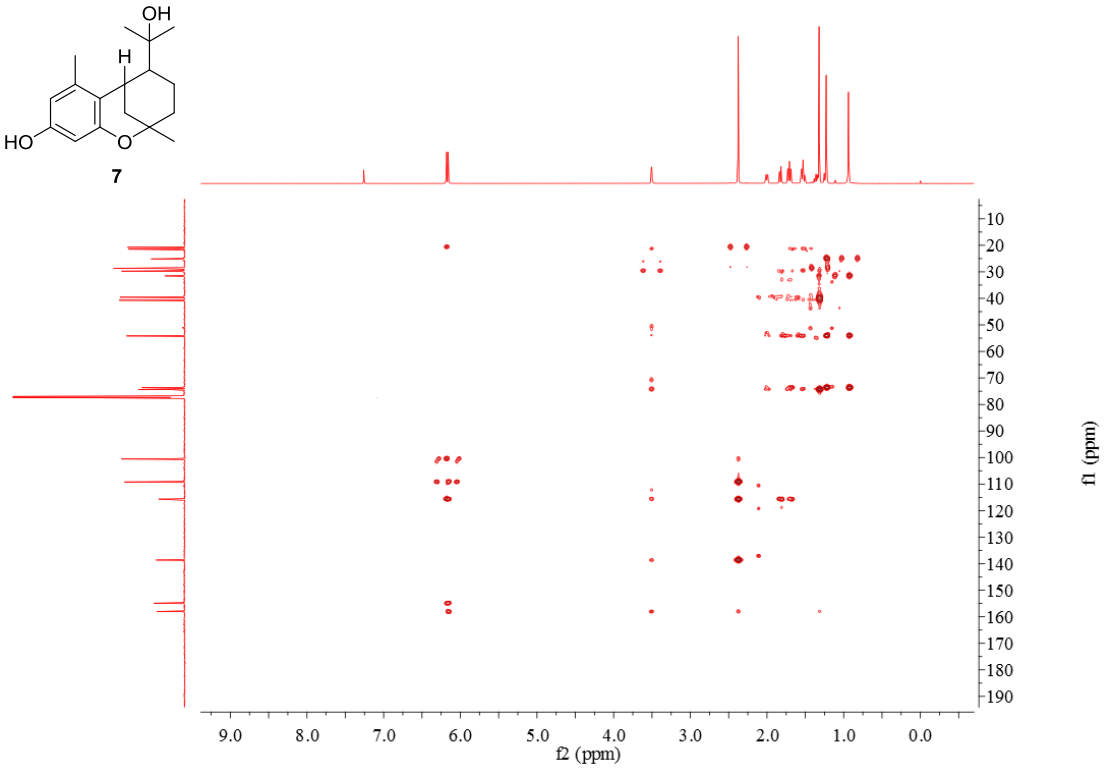


Figure S117. HMBC (600 MHz, $CDCl_3$) spectrum of **7**

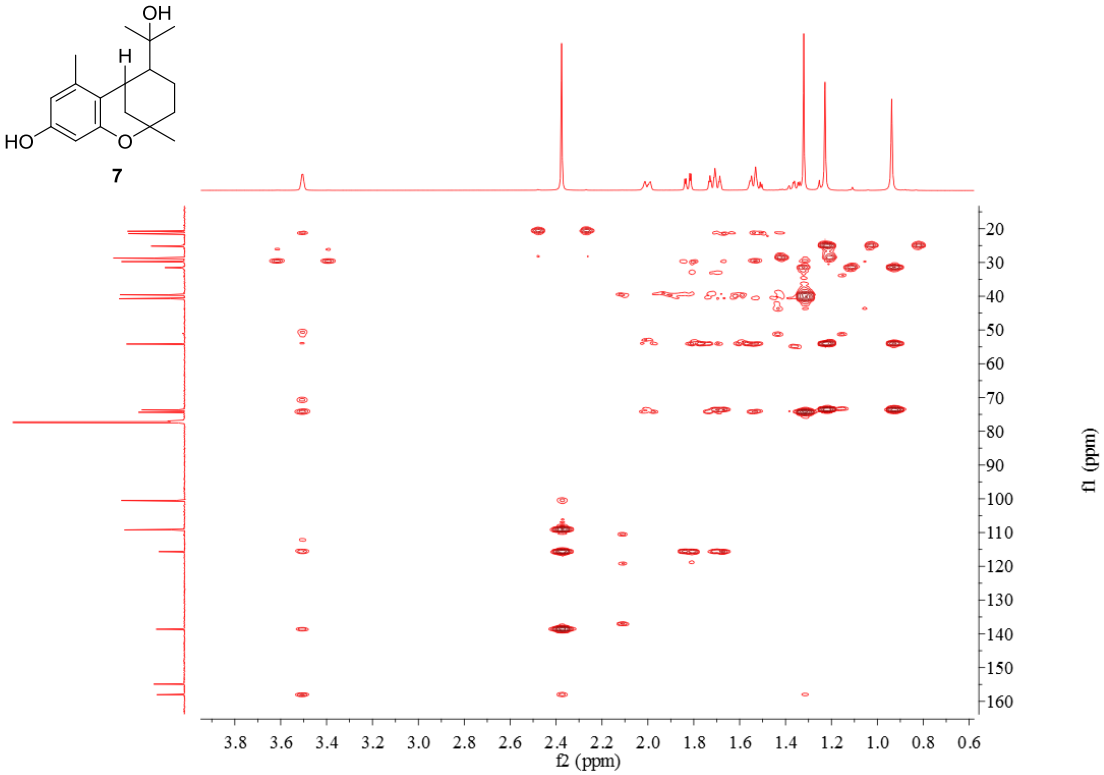


Figure S118. NOESY (600 MHz, $CDCl_3$) spectrum of **7**

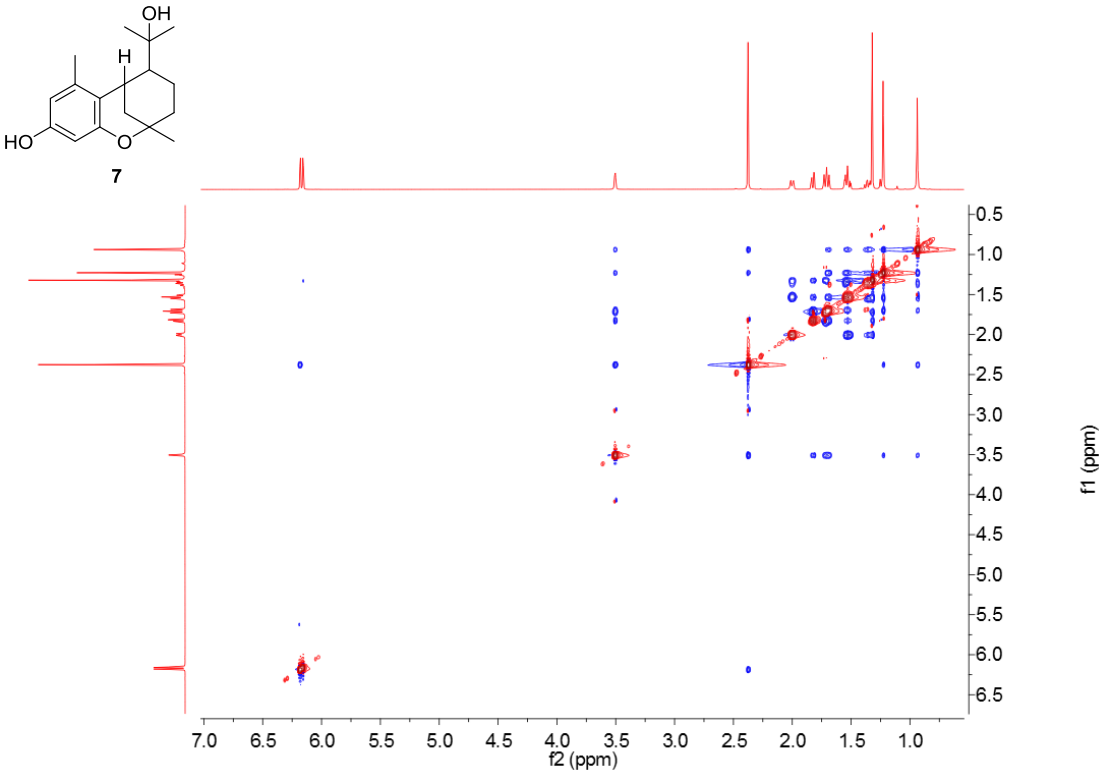


Figure S119. IR spectrum of **7**

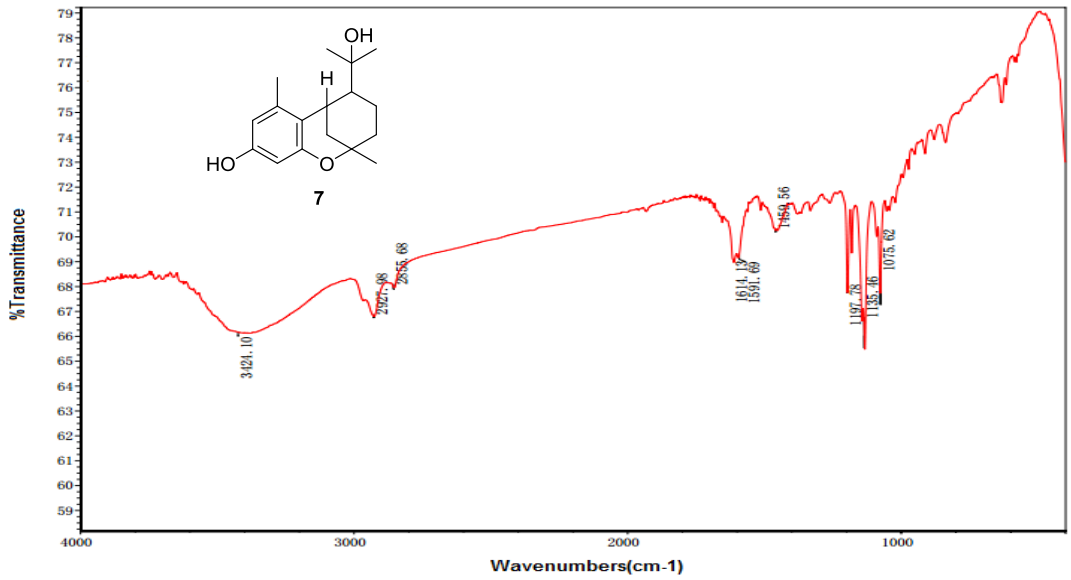


Figure S120. Positive ESIMS spectrum of **7a**

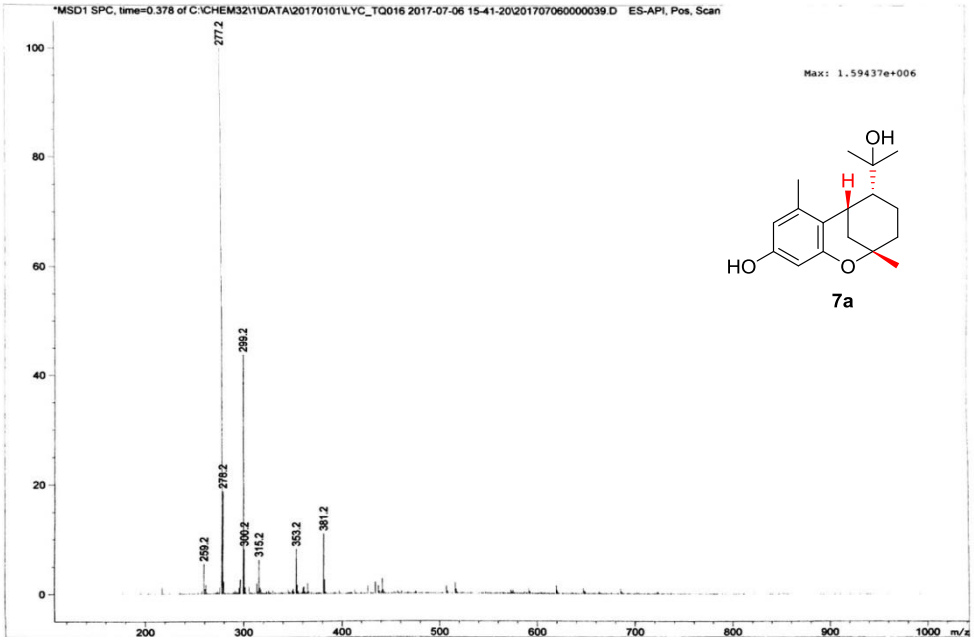


Figure S121. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **7a**

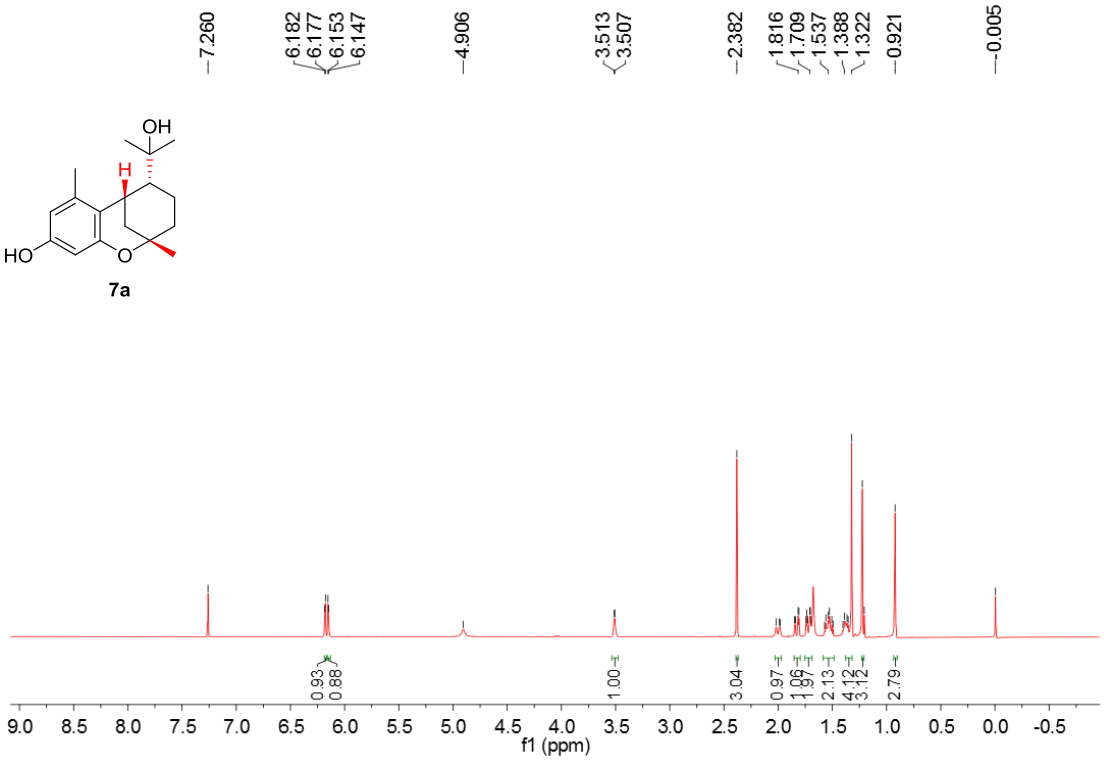


Figure S122. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **7a**

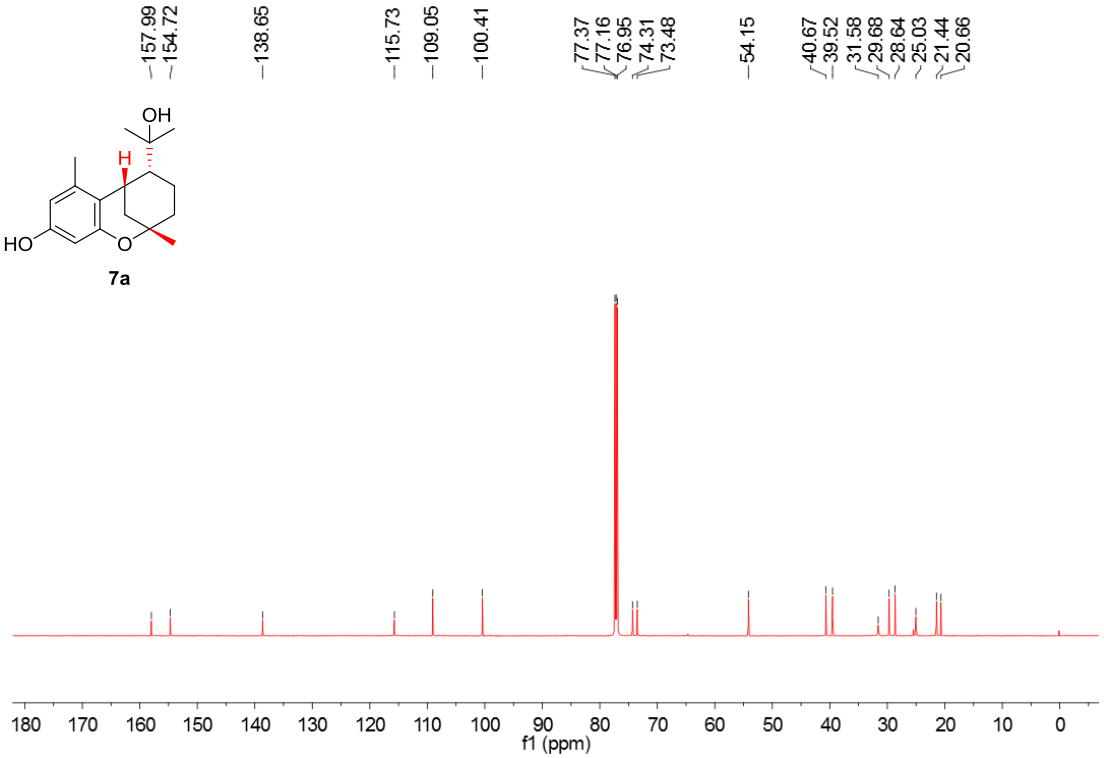


Figure S123. Positive ESIMS spectrum of **7b**

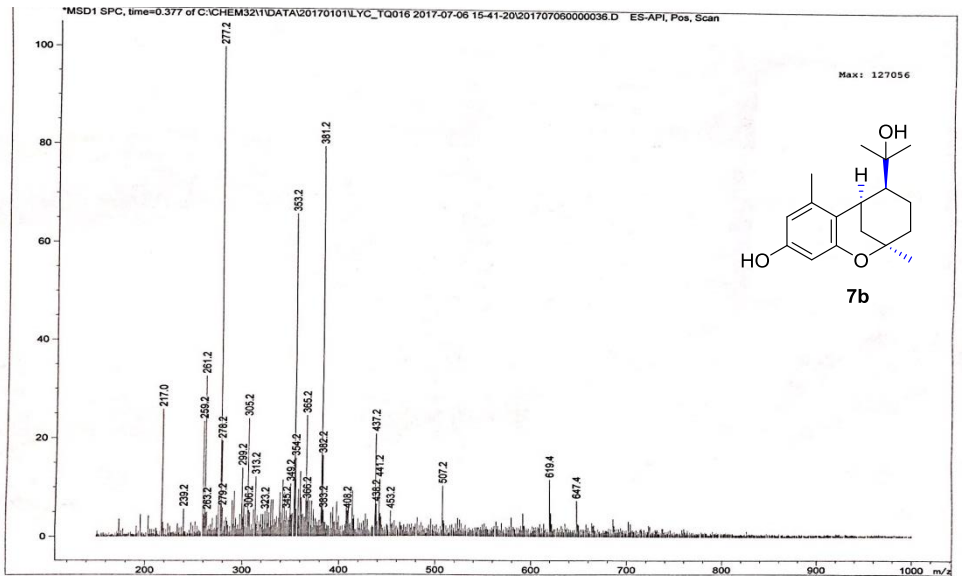


Figure S124. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **7b**

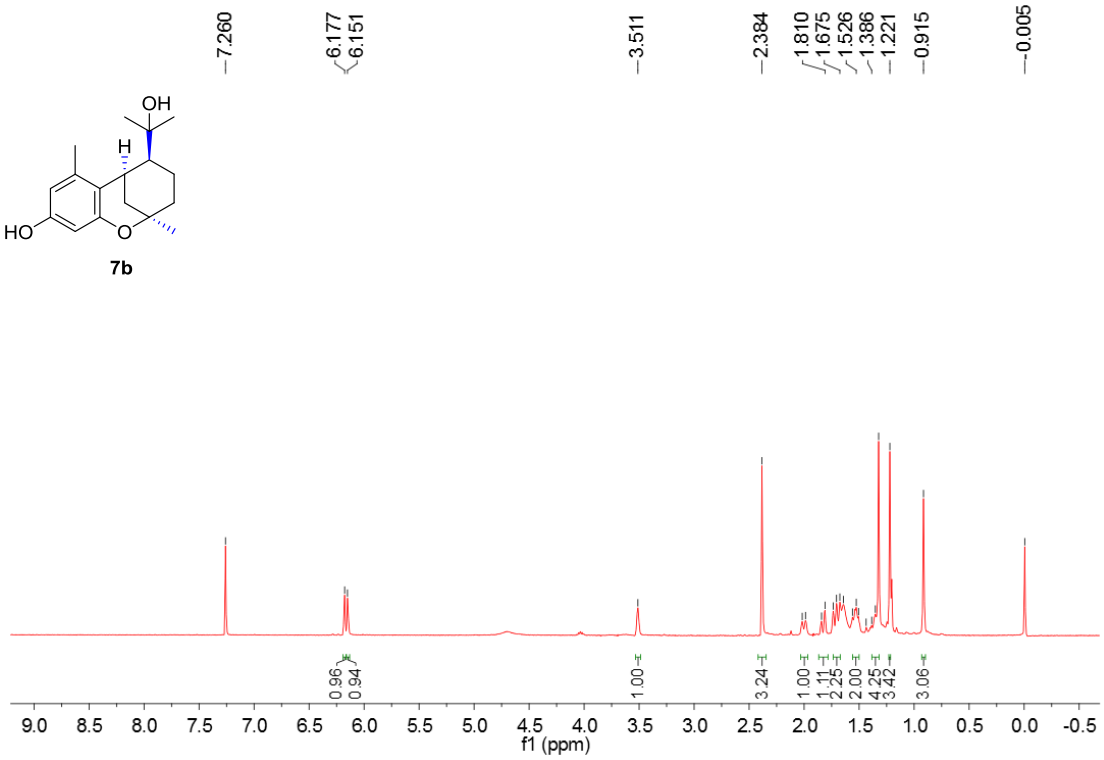


Figure S125. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **7b**

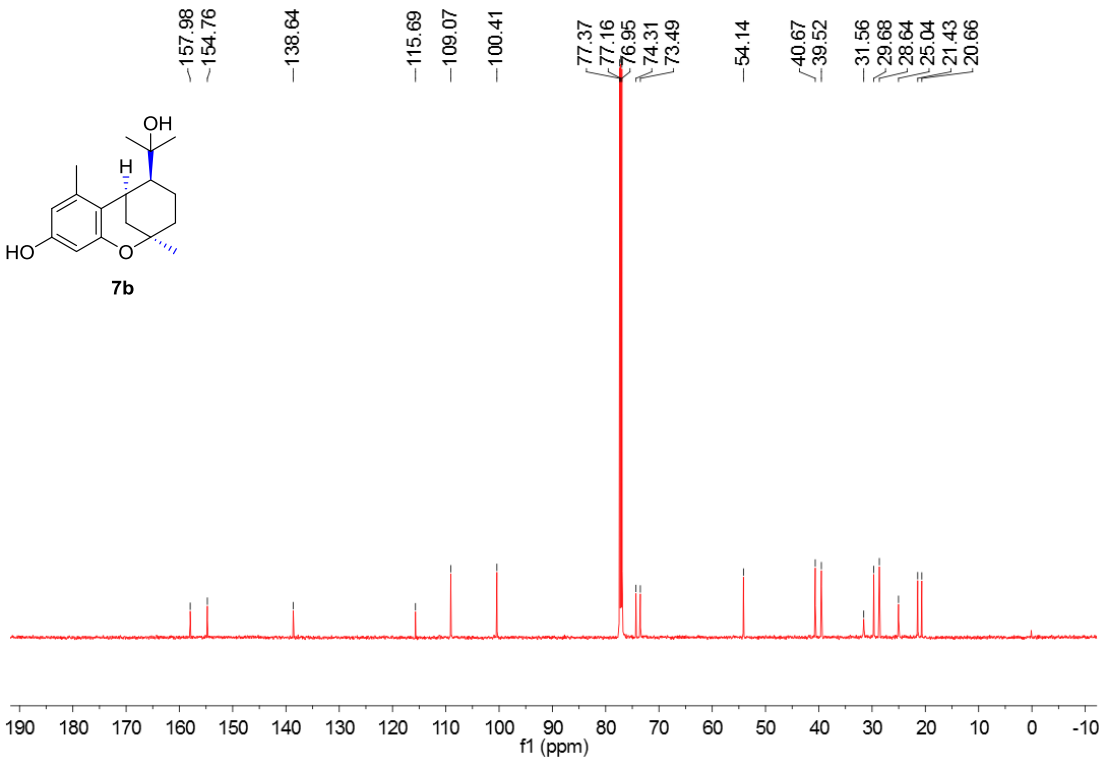


Figure S126. Positive ESIMS spectrum of **8**

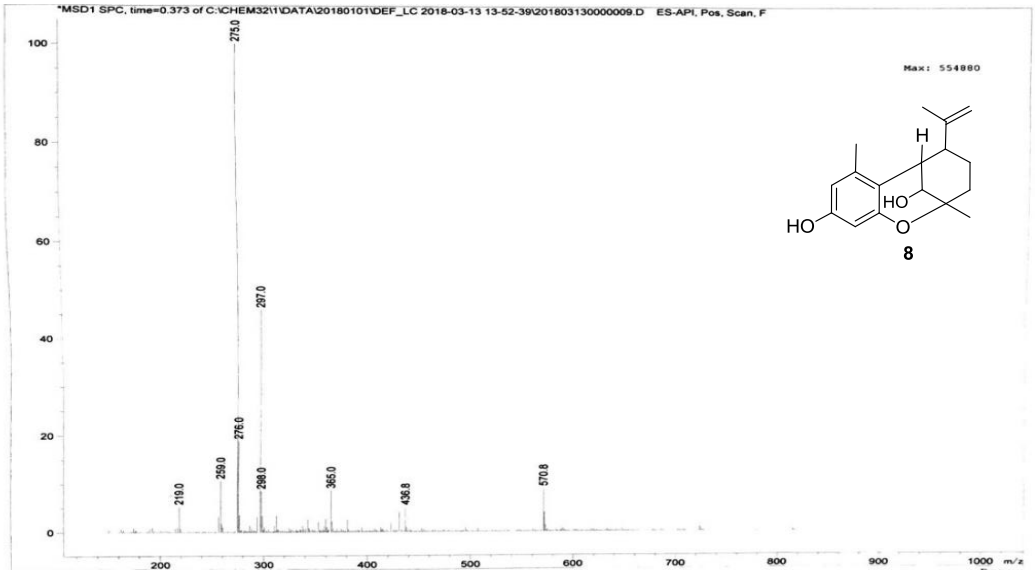
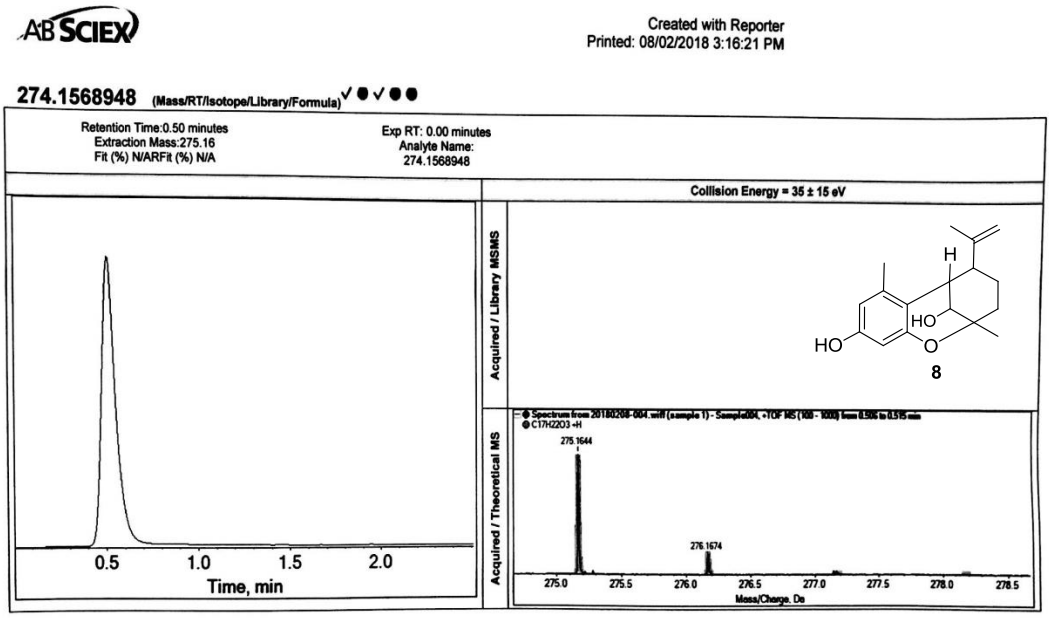


Figure S127. Positive HR-ESIMS spectrum of **8**



Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
274.1568948(LZ-33)	96%	C17H22O3	51845	100	275.1642	275.1644	0.7	0.00	0.50	0.50	0.5%	N/A

Figure S128. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **8**

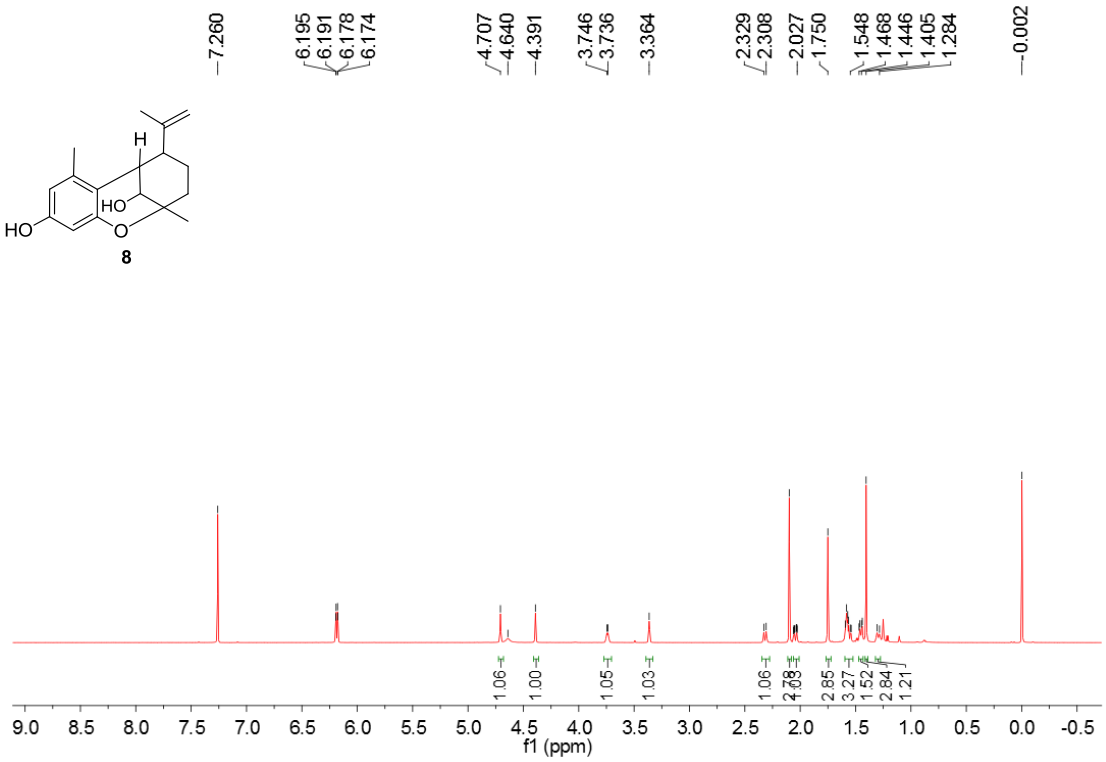


Figure S129. ^{13}C NMR and DEPT (150 MHz, $CDCl_3$) spectra of **8**

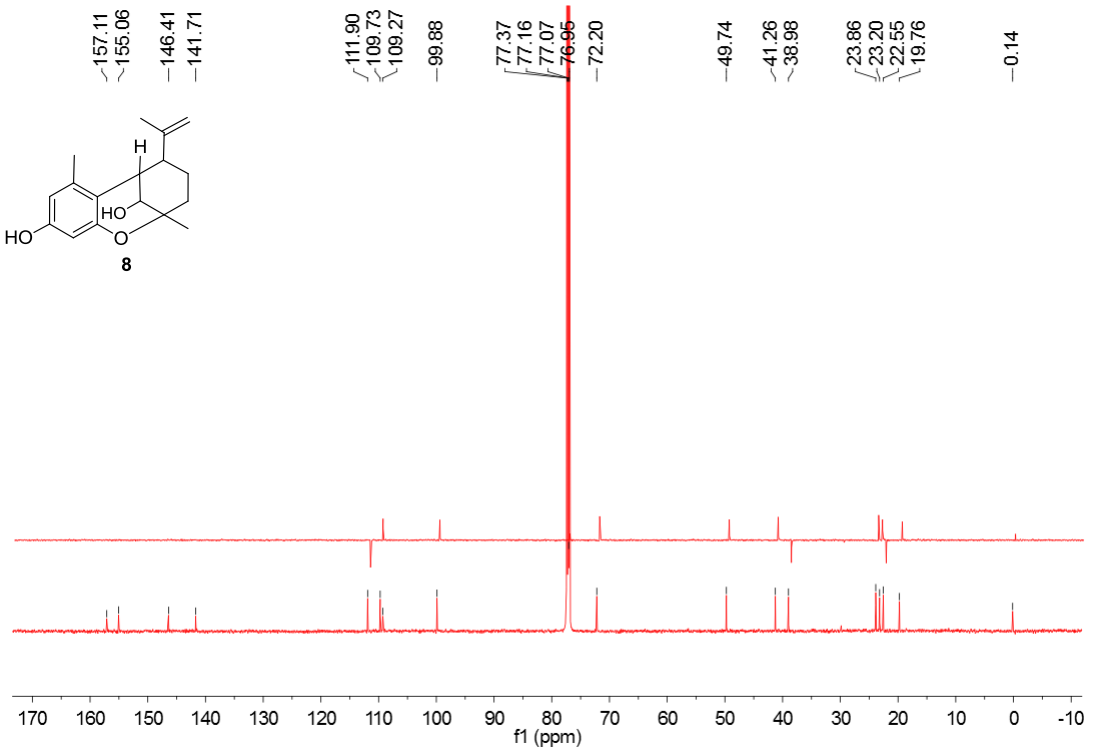


Figure S130. HSQC (600 MHz, $CDCl_3$) spectrum of **8**

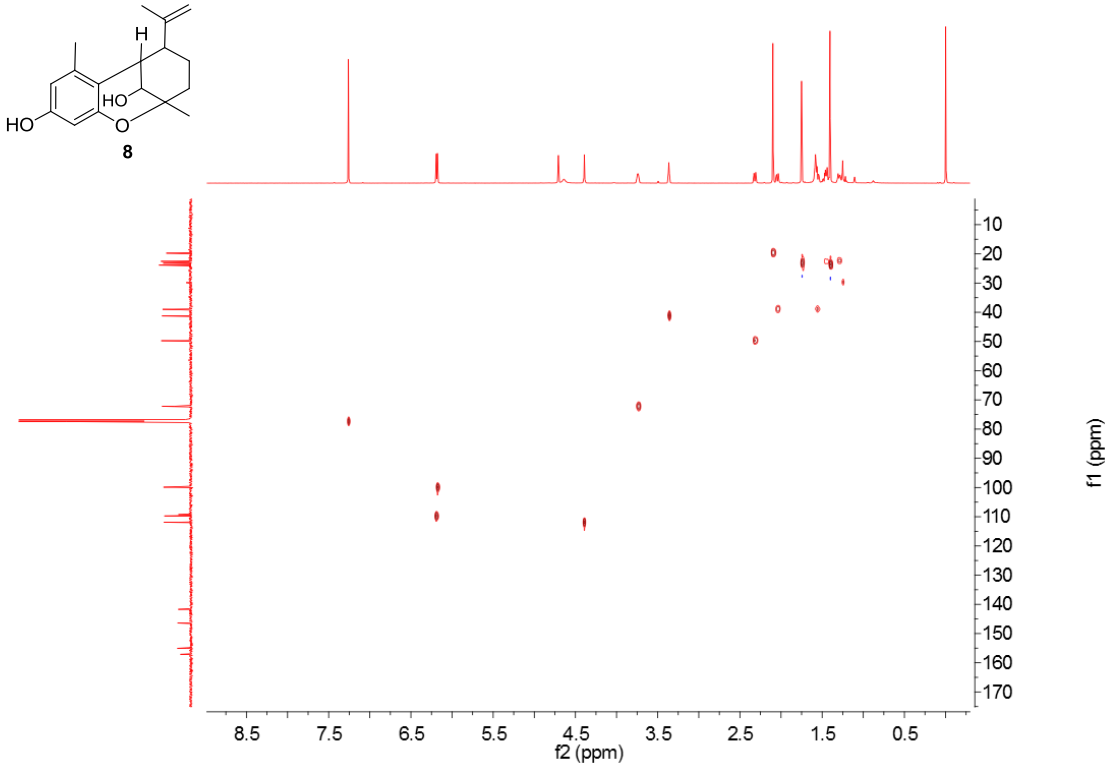


Figure S131. HSQC (600 MHz, $CDCl_3$) spectrum of **8**

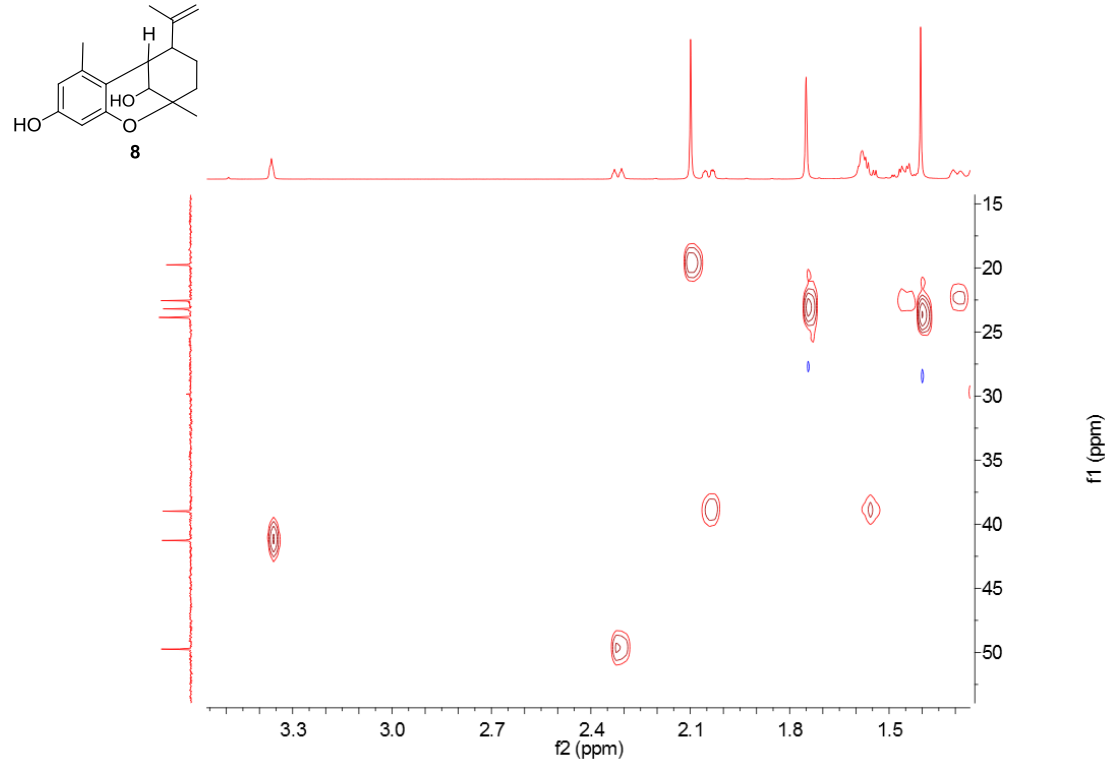


Figure S132. HMBC (600 MHz, $CDCl_3$) spectrum of **8**

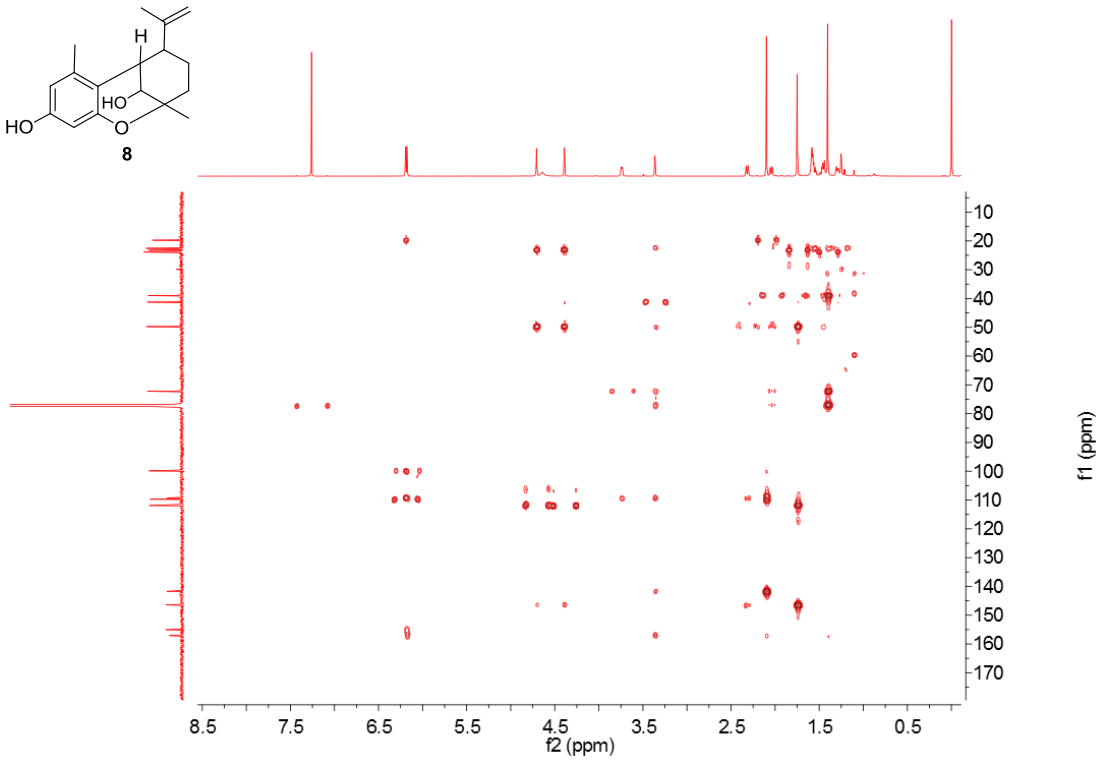


Figure S133. HMBC (600 MHz, $CDCl_3$) spectrum of **8**

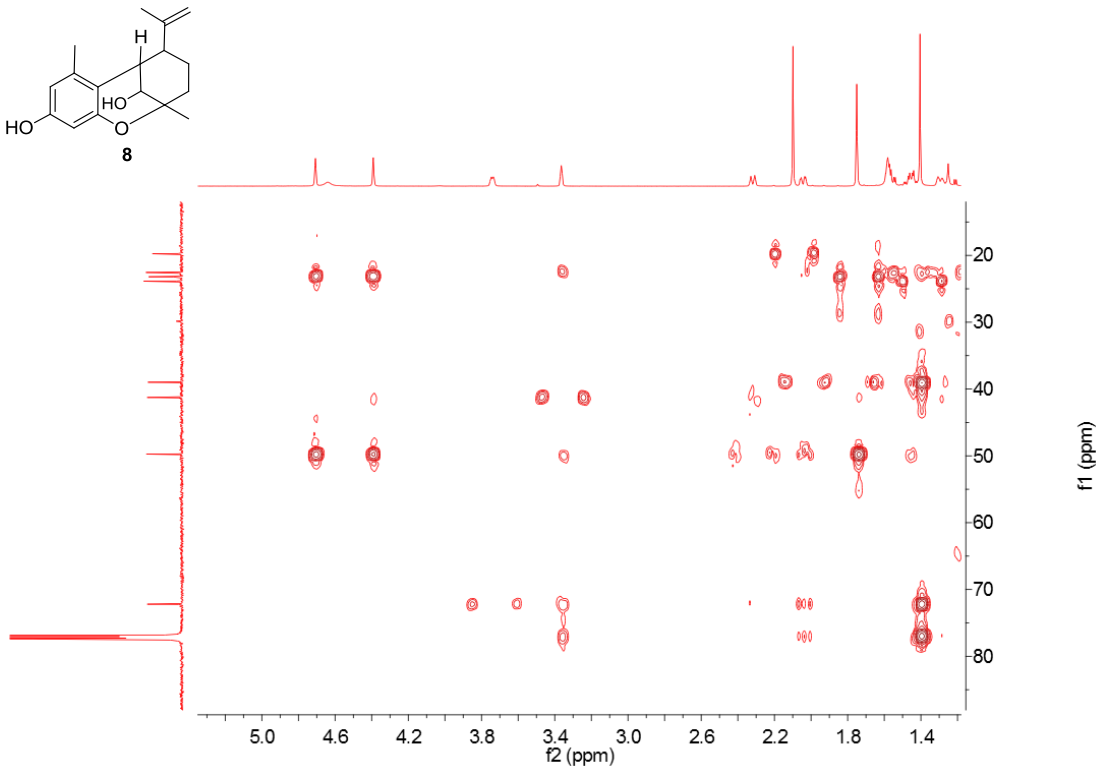


Figure S134. ^{1}H-^{1}H COSY (600 MHz, $CDCl_3$) spectrum of **8**

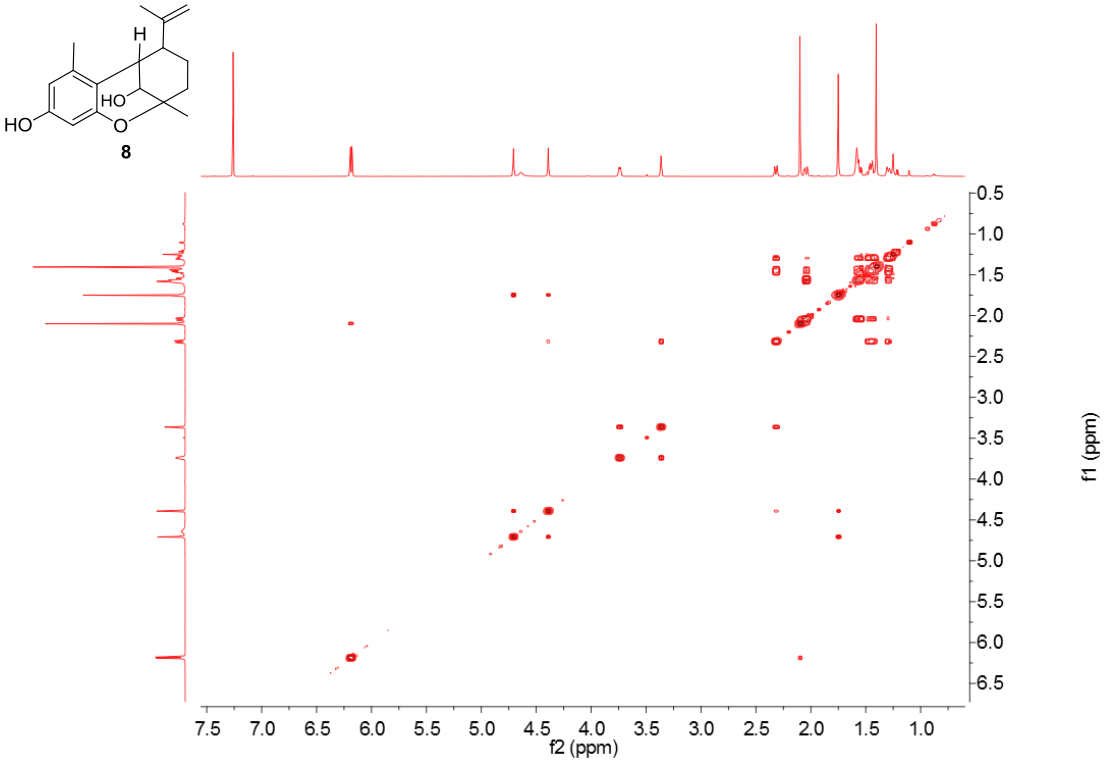


Figure S135. NOESY (600 MHz, $CDCl_3$) spectrum of **8**

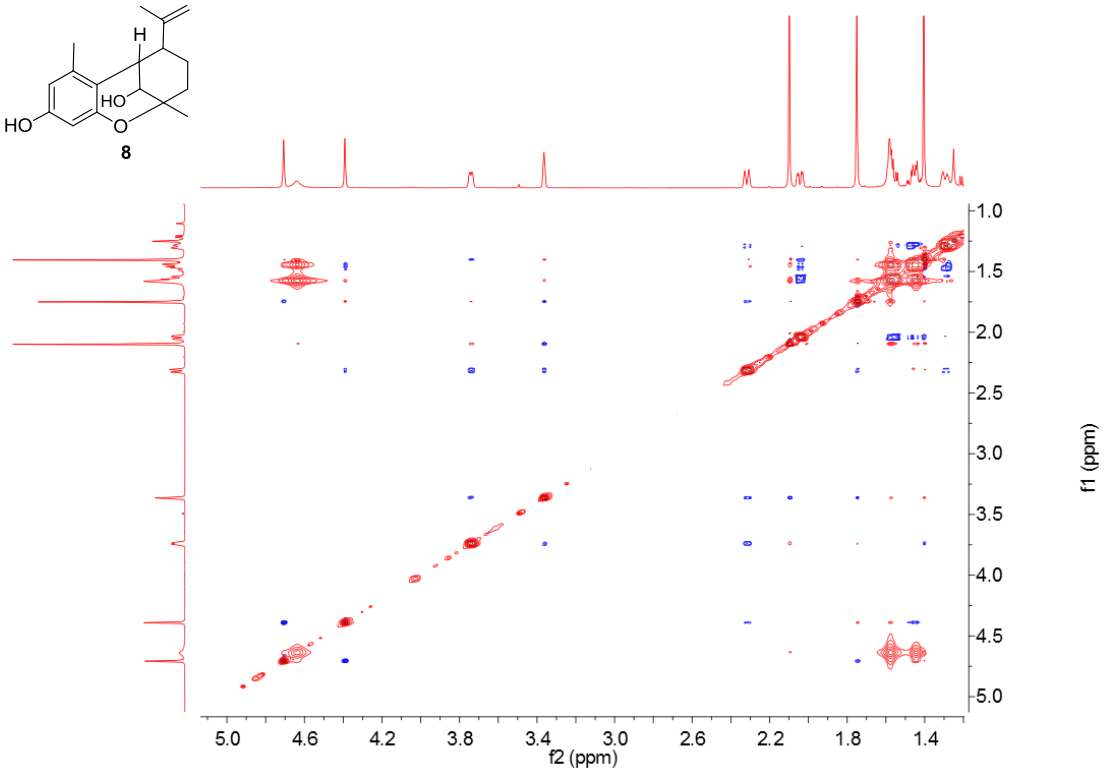


Figure S136. IR spectrum of **8**

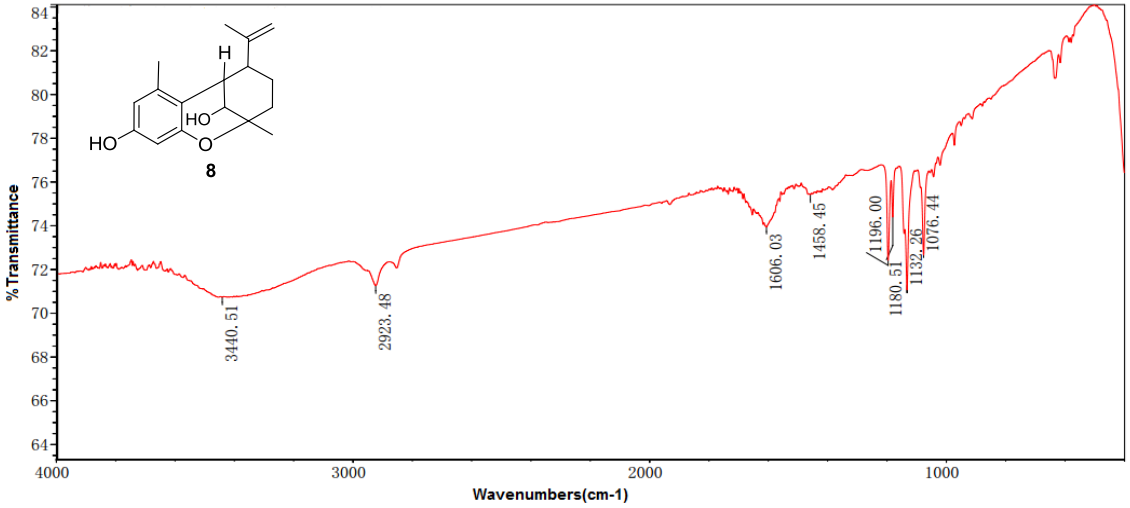


Figure S137. Positive ESIMS spectrum of **8a**

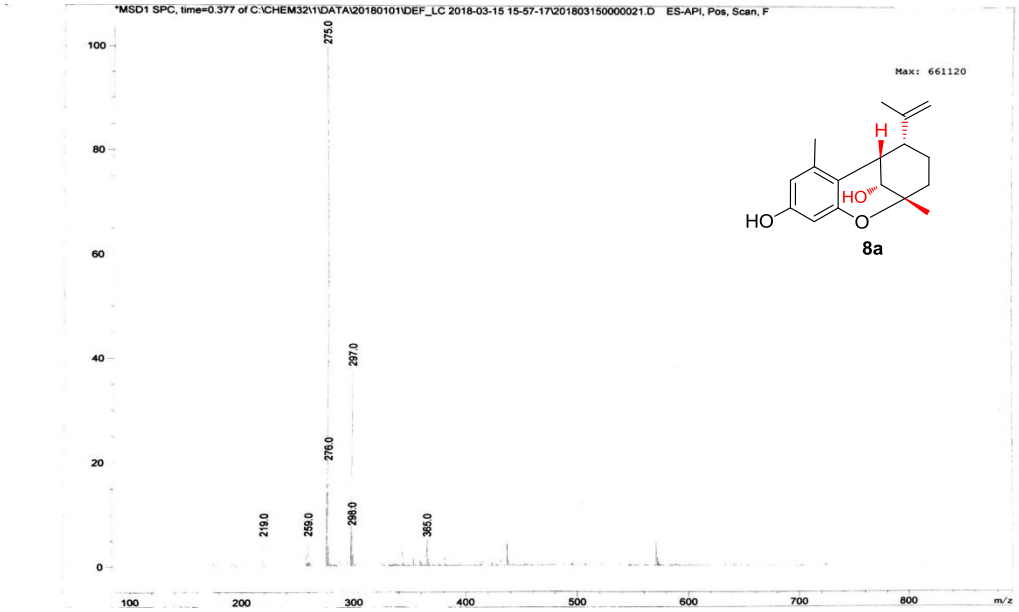


Figure S138. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8a**

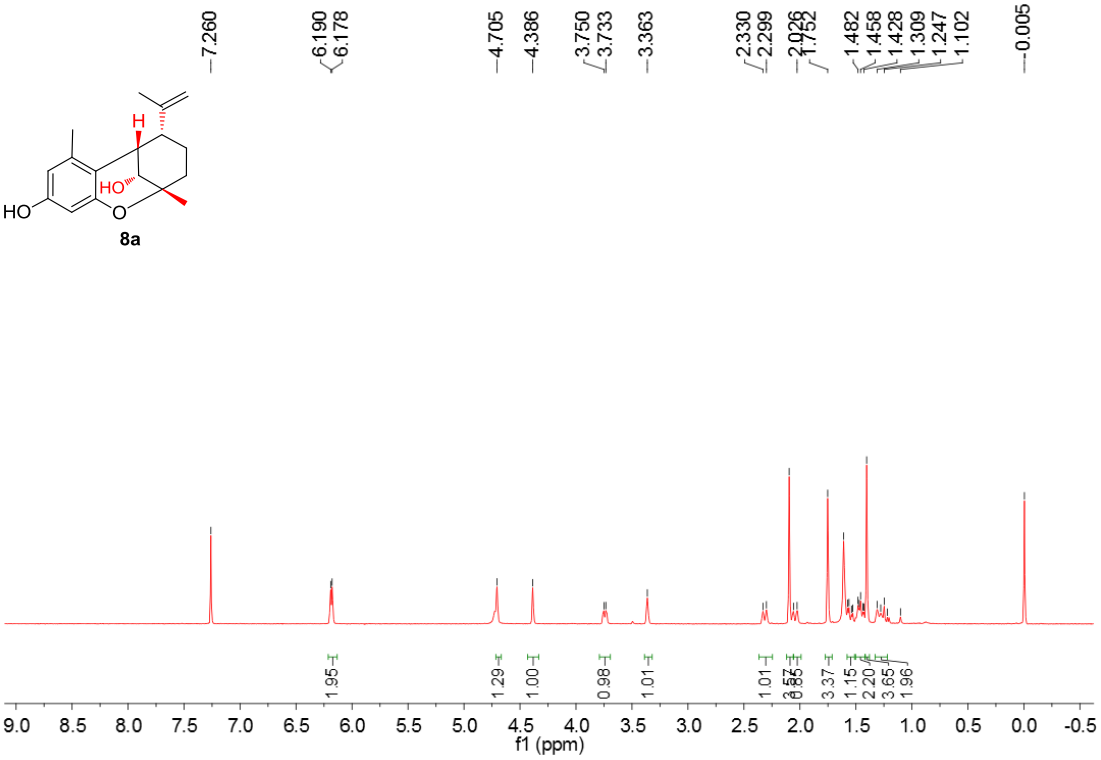


Figure S139. Positive ESIMS spectrum of **8b**

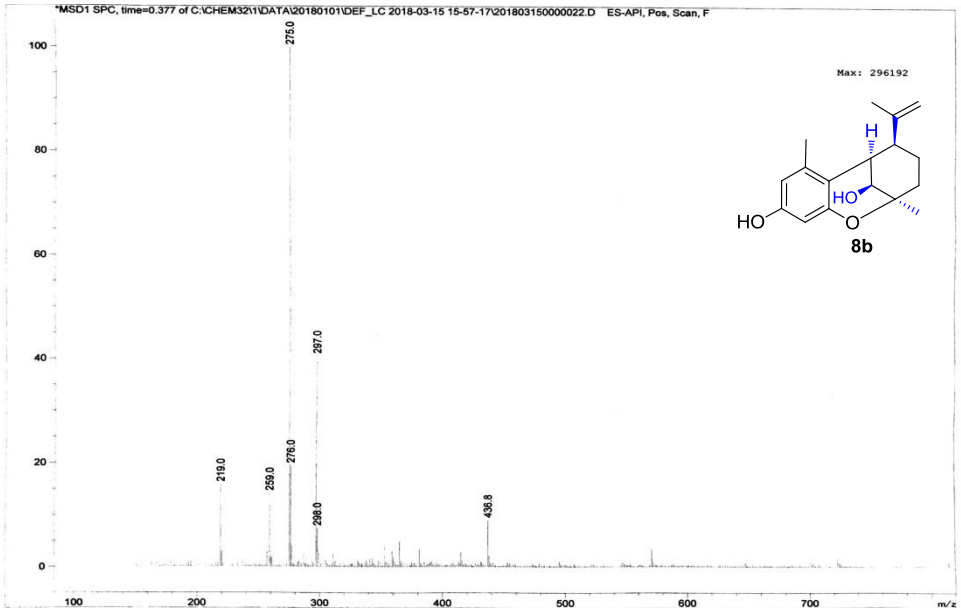


Figure S140. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8b**