Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Euphopias D−F from *Euphorbia* L.: Quantum Chemical Calculation-Based Structure Elucidation and Their Bioactivity Inhibiting NLRP3 Inflammasome Activation

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Table S1. NMR data of **1**−**3** (J in Hz, δ in ppm)

Pos.	**1**[a]		**2**[a]		**2**[b]		**2**[c]		**3**[a]	
	δ_H[d]	δ_C[e]	δ_H[d]	δ_C[e]	δ_H[f]	δ_C[g]	δ_H[f]	δ_C[g]	δ_H[d]	δ_C[e]
1	1.07 dd (13.9, 10.8)	37.7 CH_2	1.08 dd (14.8, 8.5)	37.2 CH_2	1.04 dd (14.7, 8.3)	38.2 CH_2	1.07 dd (14.5, 8.6)	37.3 CH_2	1.90 m	36.3 CH_2
	2.84 dd (13.9, 7.8)		2.81 dd (14.9, 8.7)		2.64 dd (14.7, 8.6)		2.75 dd (14.5, 8.6)		1.94 m	
2	2.12 m	40.5 CH	2.13 m	39.7 CH	2.00 m	41.1 CH	1.92 overlap	39.9 CH	2.09 m	36.3 CH
3	5.46 dd (7.1, 2.4)	80.1 CH	4.62 dd (5.6, 1.3)	80.7 CH	4.47 dd (5.7, 1.4)	82.2 CH	4.70 d (5.7)	80.9 CH	5.50 dd (5.6, 3.9)	78.6 CH
4	2.29 dd (10.6, 7.2)	46.5 CH	2.01 overlap	45.9 CH	2.04 m	47.2 CH	2.06 m	46.3 CH	2.29 dd (11.6, 5.7)	46.4 CH
5	2.73 t (11.5)	35.7 CH	2.42 t (10.8)	36.1 CH	2.39 t (10.9)	37.4 CH	2.43 t (10.8)	36.1 CH	2.90 dd (11.4, 8.5)	31.7 CH
6		148.0 C		48.4 C		49.3 C		48.4 C		140.5 C
7	2.45 d (6.4)	52.8 CH	9.18 s	203.2 CH	9.08 s	205.2 CH	9.24 s	203.3 CH	5.04 t (7.7)	121.7 CH
8	2.54 d (18.7, 6.5)	43.0 CH_2							1.92 m	25.3 CH_2
	1.96 d (18.8)								1.55 m	
9		219.3 C							4.18 t (3.9)	77.9 CH
10		40.9 C		131.2 C		132.4 C		131.1 C		41.0 C
11	2.06 s	56.6 CH	5.49 s	120.9 CH	5.44 s	121.8 CH	5.28 s	121.0 CH	1.23 overlap	47.0 CH
12	1.74 t (11.7)	40.9 CH	2.01 overlap	36.7 CH	1.98 m	38.0 CH	1.92 overlap	36.9 CH	3.80 d (3.5)	80.4 CH
13	1.98 m	31.5 CH	1.85 m	34.9 CH	1.80 ddd (11.7, 6.9, 2.6)	36.1 CH	1.82 m	35.0 CH	2.21 m	44.5 CH
14	5.97 d (2.6)	71.0 CH	5.99 d (2.5)	71.1 CH	5.88 d (2.4)	72.4 CH	6.18 d (2.3)	71.1 CH	5.06 d (5.9)	79.2 CH
15		90.1 C		91.0 C		92.3 C		90.9 C		89.7 C
16	1.30 d (7.1)	19.8 CH_3	1.20 d (7.2)	20.5 CH_3	1.11 d (7.2)	20.5 CH_3	0.96 d (7.2)	20.1 CH_3	0.94 d (6.5)	13.4 CH_3
17	4.70 s	108.2 CH_2	1.08 s	13.0 CH_3	0.96 s	13.3 CH_3	0.90 s	12.9 CH_3	1.70 s	20.4 CH_3
	4.86 s									
18	1.03 s	21.9 CH_3	1.73 s	23.7 CH_3	1.63 s	23.8 CH_3	1.39 s	23.4 CH_3	0.84 s	27.2 CH_3
19	1.01 s	27.8 CH_3	1.41 d (18.1)	36.9 CH_2	1.31 d (17.7)	37.8 CH_2	1.08 d (17.1)	36.7 CH_2	1.01 s	20.6 CH_3
			2.36 d (18.1)		2.31 d (17.7)		2.07 d (17.1)			
20	0.96 d (6.7)	15.8 CH_3	1.05 d (6.7)	15.4 CH_3	0.95 d (6.7)	15.8 CH_3	0.79 d (6.7)	15.3 CH_3	0.99 d (7.2)	13.3 CH_3
OBz-3										
1'		165.7 C		165.1 C		166.7 C		165.1 C		165.4 C
2'		130.6 C		130.5 C		131.7 C		131.1 C		129.8 C
3', 7'	7.95 m	129.2 CH	8.07 m	129.4 CH	7.98 m	130.5 CH	8.12 m	129.7 CH	7.99 m	129.5 CH
4', 6'	7.44 t (7.6)	128.5 CH	7.46 m	128.5 CH	7.42 t (7.8)	129.8 CH	7.27 t (7.7)	128.9 CH	7.37 t (7.7)	128.5 CH
5'	7.56 t (7..4)	133.0 CH	7.57 m	133.1 CH	7.53 m	134.5 CH	7.35 t (7.4)	133.3 CH	7.49 m	133.2 CH
OAc-14										
1''		169.7 C		169.7 C		171.8 C		169.9 C		171.3 C
2''	2.13 s	20.9 CH_3	2.14 s	20.9 CH_3	2.04 s	20.8 CH_3	1.89 s	20.4 CH_3	2.11 s	20.9 CH_3
OAc-9										
1'''										170.4 C
2'''									1.90 s	21.0 CH_3
OAc-15										
1'''		169.3 C		169.4 C		171.4 C		169.6 C		
2'''	2.04 s	22.2 CH_3	2.07 s	22.4 CH_3	1.96 s	22.4 CH_3	1.87 s	22.0 CH_3		

[a]Recorded in $CDCl_3$. [b]Recorded in CD_3OD. [c]Recorded in C_5D_5N. [d]400 MHz. [e]100 MHz. [f]600 MHz. [g]150 MHz.

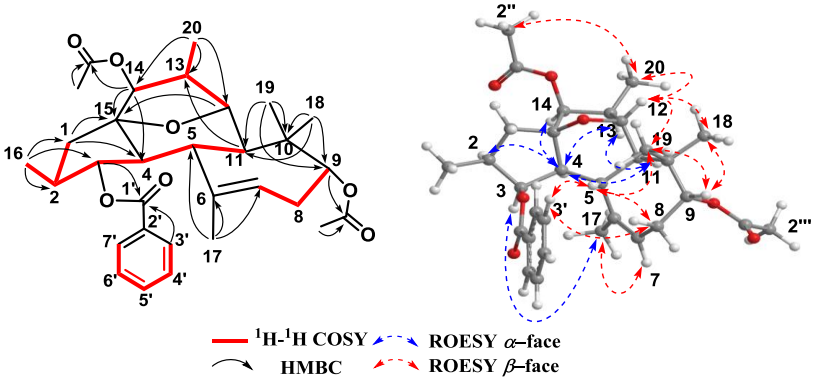

Figure S1. Key 2D NMR correlations of **3**.

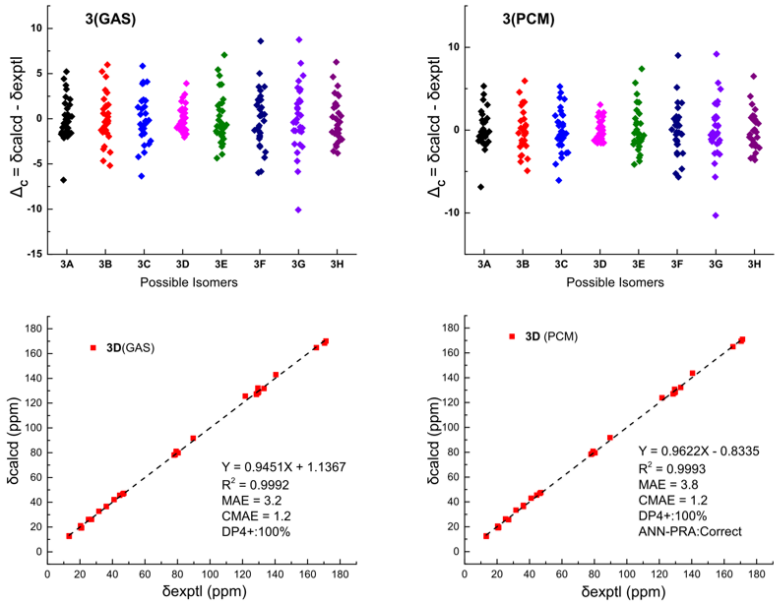

Figure S2. NMR computation of compound **3**.

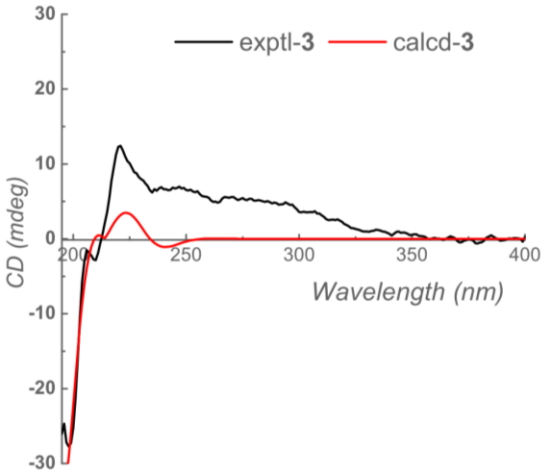

Figure S3. ECD calculation of **3**.

Table S2. NMR computed results for compounds **2** and **3.**

Comp.	Possible Isomers	Basis set	Nuclie	Equation	R^2	MAE	CMAE	DP4+	ANN-PRA
2	(C-5/19,C-6/12)-**2A**	a	**C**	Y = 0.9305X + 3.4472	0.9974	4.2	2.4	0.00%	**Incorrect**
			H	Y = 1.015X – 0.0239	0.9783	0.27	0.26		
		b	**C**	Y = 0.9515X + 1.3834	0.9976	4.0	2.3	0.00%	
			H	Y = 1.0449X + 0.5193	0.9796	0.65	0.22		
	(C-5/12,C-6/19)-**2B**	a	**C**	Y = 0.9429X + 1.2182	0.9994	3.7	1.1	100%	**Correct**
			H	Y = 1.0237X – 0.0995	0.9907	0.18	0.17		
		b	**C**	Y = 0.9648X – 0.881	0.9994	3.9	1.1	100%	
			H	Y = 1.0553X + 0.3864	0.9936	0.55	0.14		
3	**(**5S9S11R)-**3A**	a	**C**	Y = 0.9476X + 1.0201	0.9980	3.5	1.7	0.00%	**Incorrect**
			H	Y = 1.0228X – 0.116	0.9871	0.20	0.19		
		c	**C**	Y = 0.9649X – 0.9534	0.9981	4.0	1.7	0.00%	
			H	Y = 1.0619X + 0.3311	0.9887	0.50	0.20		
	(5S9S11S)-**3B**	a	**C**	Y = 0.9361X + 2.5303	0.9974	3.7	2.0	0.00%	**Incorrect**
			H	Y = 1.0276X – 0.0477	0.9738	0.30	0.30		
		c	**C**	Y = 0.951X + 0.7786	0.9977	3.8	1.9	0.00%	
			H	Y = 1.0669X + 0.3886	0.9796	0.60	0.20		
	(5S9R11S)-**3C**	a	**C**	Y = 0.927X + 3.6835	0.9974	3.9	2.1	0.00%	**Incorrect**
			H	Y = 1.0205X – 0.0098	0.9720	0.30	0.30		
		c	**C**	Y = 0.9428X + 1.8547	0.9976	3.9	2.0	0.00%	
			H	Y = 1.0598X + 0.4289	0.9745	0.60	0.30		
	(5S9R11R)-**3D**	a	**C**	Y = 0.9451X + 1.1367	0.9992	3.2	1.2	100%	**Correct**
			H	Y = 1.0153X – 0.0818	0.9898	0.20	0.20		
		c	**C**	Y = 0.9622X – 0.8335	0.9993	3.8	1.2	100%	
			H	Y = 1.0558X + 0.3555	0.9918	0.50	0.10		
	(5R9S11R)-**3E**	a	**C**	Y = 0.9232X + 3.9661	0.9973	4.2	2.2	0.00%	**Incorrect**
			H	Y = 1.0182X – 0.0468	0.9765	0.30	0.30		
		c	**C**	Y = 0.9395X + 2.0665	0.9974	4.2	2.1	0.00%	
			H	Y = 1.0549X + 0.3859	0.9803	0.60	0.20		
	(5R9S11S)-**3F**	a	**C**	Y = 0.9355X + 2.4288	0.9965	4.1	2.5	0.00%	**Incorrect**
			H	Y = 1.0253X – 0.0994	0.9672	0.30	0.30		
		c	**C**	Y = 0.9521X + 0.5352	0.9968	4.0	2.2	0.00%	
			H	Y = 1.0641X + 0.3399	0.9737	0.50	0.20		
	(5R9R11S)-**3G**	a	**C**	Y = 0.9355X + 2.4374	0.9951	4.4	2.7	0.00%	**Incorrect**
			H	Y = 1.0189X – 0.0742	0.9739	0.30	0.20		
		c	**C**	Y = 0.9523X + 0.5187	0.9955	4.3	2.5	0.00%	
			H	Y = 1.0569X + 0.3699	0.9774	0.50	0.20		
	(5R9R11R)-**3H**	a	**C**	Y = 0.9287X + 3.3127	0.9978	3.8	2.0	0.00%	**Incorrect**
			H	Y = 1.0157X – 0.061	0.9869	0.20	0.20		
		c	**C**	Y = 0.9456X + 1.3659	0.9981	3.8	1.8	0.00%	
			H	Y = 1.0531X + 0.382	0.9897	0.50	0.20		

a mPW1PW91/6-31G*// B3LYP/6-31G* (in gas phase). b mPW1PW91/6-31G**//B3LYP/6-31G* levels (in methanol)
c mPW1PW91/6-31G**//B3LYP/6-31G* levels (in chloroform)

Experimental procedures

General experimental procedures

A Hitachi U-4100 UV-visible spectrophotometer was employed to obtain ultraviolet (UV) spectra. Optical rotations were measured on a Rudolp Autopol VI polarimeter. Circular dichroism (CD) spectra was recorded on an Applied Photophysics V100 Chirascan instrument. Infrared (IR) spectra was obtained with a Nicolet iS10 FT-IR spectrometer. BRUKER Ascend^{TM} 400 and 600 MHz NMR instruments were used to check 1D and 2D NMR spectra. HRESIMS data were obtained from Thermo Fisher LTQ Orbitrap XL hybrid ion trap mass spectrometer. Column chromatography (CC) were performed on Macroporous resin (D-101, Tianjin Haoju Science and Technology Ltd.), Silica gel (100–200; 200–300 mesh, Qingdao Marine Chemical, Ltd.), and MCI gel CHP 20P (75–150 μm, Mitsubishi Chemical Industries, Tokyo, Japan). Preparative HPLC was performed on Agilent 1260 Infinity II Preparative liquid chromatography system equipped with an automatic fraction collector. And the columns used were Megres RP C-18 column (10 μm, 30 mm × 250 mm, 20 ml/min) and CAPCELL PAK-C18 column (5 μm, 20 mm × 250 mm, 10 ml/min). TLC was performed on pre-coated TLC plates (200–300 μm thickness, silica gel 60 F254, Qingdao Marine Chemical Inc.), with spots visualized under UV light (254 and 365 nm) and heated after spraying with 10% aqueous H_2SO_4.

Plant Materials

The samples of *Euphorbia helioscopia* L. were purchased from Bozhou Materia Medica Market in Anhui Province, P. R. China, in September 2019, and authenticate by Pro. Xiwen Li (Kunming Institute of Botany). A voucher specimen (XWL20190926) was maintained in Key Laboratory of Medicinal Chemistry for Natural Resoures, Ministry of Education, Yunnan University.

Extraction and Isolation

The air-dried powder of the whole plant of *E. helioscopia* (20 kg) were extracted with 90% aqueous methanol (100 L) under reflux condition three times at 60°C heating by water bath. The methanol extracts were evaporated in vacuum to afford the crude extract (3 kg). The crude extracts was suspended in H_2O and partitioned with ethyl acetate (3 × 10 L, EtOAc) to afford an EtOAc-soluble extract. The EtOAc extracts (260 g) was fractioned by using D-101 macroporous resin column eluted MeOH/H_2O (30%−100%, v/v) to give five parts (Fr.1−Fr.5), Fr.4 (40 g) was subjected to a column chromatography (CC) over silica gel (100–200 mesh) with PE/EtOAc gradient elution system (1:0, 9:1, 4:1, 3:1, 1:1, and 0:1, v/v) to give six subfractions Fr.4.1−4.6.

Fr.4.2 (PE/EtOAc 9:1, 8 g) was chromatographed on a MCI with a MeOH/H_2O gradient elution system (60:40, 70:30, 80:20, 90:10, and 100:0, v/v) to afford five fractions Fr.4.2.1−4.2.5. Fr.4.2.4 (2.5 g) was further separated by a silica gel CC (200–300 mesh) eluted with PE/Acetone (gradient system, 20:1, 10:1, 5:1, and 2:1 v/v) to obtain four fractions Fr.4.2.4.1−Fr.4.2.4.4. Then Fr.4.2.4.1 (1.2 g) was subjected on a preparative HPLC equipped with Megres RP C-18 column (10 *μ*m, 30 mm × 250 mm, 20 ml/min) eluted with MeCN/H_2O (90:10, v/v) to obtain 7 fractions Fr.4.2.4.1.1−Fr.4.2.4.1.7. Compound **1** (10.4 mg, 5.2 × 10^{-5} % yield) was obtained from Fr.4.2.4.1.5 by recrystallization. Fr.4.2.4.1.4 was further purified by preparative HPLC equipped with CAPCELL PAK-C18 column (5 *μ*m, 20 mm × 250 mm, 10 ml/min) eluted with MeCN/H_2O (90:10, v/v) to give compound **2** (12.4 mg, t_R = 15.4 min, 9.2 × 10^{-5} % yield). Fr.4.2.4.1.7 and Fr.4.2.4.1.6 were separated by preparative HPLC equipped with CAPCELL PAK-C18 column (5 *μ*m, 20 mm × 250 mm, 10 ml/min) eluted with MeCN/H_2O (90:10, v/v) to yield compound **3** (10.5 mg, t_R = 23.5 min, 5.25 × 10^{-5} % yield).

Physical Constants And Spectroscopic Data of Compounds 1−3.

*Euphopia D (**1**)*: Colorless crystals (MeOH); mp: 227−231°C; $[\alpha]_D^{24}$ −12.36 (*c* 0.10, MeOH); ECD (MeOH) λ_{max} ($\Delta\varepsilon$): 198 (-16.28), 229 (-9.21), and 301 (3.42) nm; UV (MeOH) λ_{max} (log ε): 195 (3.71) and 230 (3.11); IR (KBr) ν_{max}: 3451, 2989, 2959, 2936, 1749, 1737, 1713, 1370, 1278, 1233, 1210, 1117, 1025, 714 cm^{-1}; HRMS (ESI) *m/z*: $[M + Na]^+$ Calcd for $C_{31}H_{38}O_7Na$ 545.2510; Found 545.2510.

Euphopia E (***2***): White powder; $[\alpha]_D^{24}$ −13.36 (*c* 0.10, MeOH); ECD (MeOH) λ_{max} ($\Delta\varepsilon$): 232 (-2.38) and 229 (-0.47) nm; UV (MeOH) λ_{max} (log ε): 195 (3.76) and 230 (3.21); IR (KBr) ν_{max}: 3428, 2966, 2936, 2879, 1749, 1728, 1452, 1374, 1277, 1228, 1113, 1025, 714 cm^{-1}; HRMS (ESI) *m/z*: $[M + Na]^+$ Calcd for $C_{29}H_{36}O_7Na$ 519.2353; Found 519.2357.

Euphopia F (***3***): White powder; $[\alpha]_D^{24}$ +6.36 (*c* 0.11, MeOH); ECD (MeOH) λ_{max} ($\Delta\varepsilon$): 198 (-2.31) and 221 (1.04) nm; UV (MeOH) λ_{max} (log ε): 195 (3.42) and 229 (2.81); IR (KBr) ν_{max}: 3429, 2966, 2932, 2877, 1728, 1453, 1373, 1271, 1247, 1109, 1027, 712 cm^{-1}; HRMS (ESI) *m/z*: $[M + Na]^+$ Calcd for $C_{31}H_{40}O_7Na$ 547.2666; Found 547.2667.

Crystal data for euphopia D (**1**): $C_{31}H_{38}O_7 \cdot CH_4O$, M = 554.65, a = 8.1554(2) Å, b = 18.3869(4) Å, c = 19.8665(4) Å, α = 90°, β = 90°, γ = 90°, V = 2979.03(11) $Å^3$, T = 100.(2) K, space group $P212121$, Z = 4, μ(Cu Kα) = 0.717 mm^{-1}, 33939 reflections measured, 5864 independent reflections (R_{int} = 0.0272). The final R_1 values were 0.0327 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0900 ($I > 2\sigma(I)$). The final R_1 values were 0.0329 (all data). The final $wR(F^2)$ values were 0.0902 (all data). The goodness of fit on F^2 was 1.099. Flack parameter = 0.03(3). Crystallographic data for **1** has been deposited at the Cambridge Crystallographic Data Center (https://ccdc.cam.ac.uk) with the deposition number of 2039968.

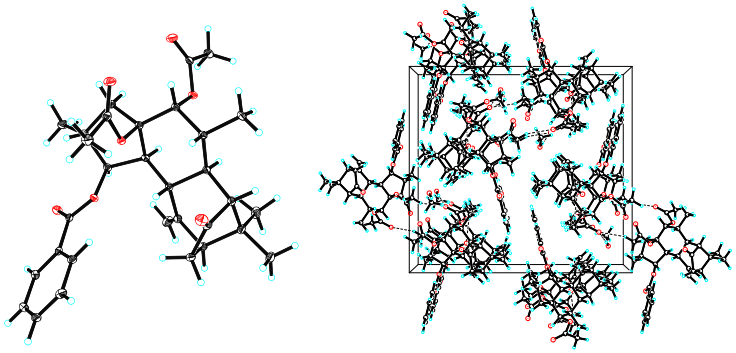

Figure S4. ORTEP drawing of euphopia D (**1**) at the 30% probability levels.

Quantum Chemistry Calculations.

All theoretical calculations were performed using Gaussian 09[1]. Conformation search was initially performed using the program Spartan'14. The conformers were optimized at B3LYP/6-31G* level of theory in gas phase. Room-temperature equilibrium populations were calculated according to Boltzmann distribution law.

NMR calculation of **2** and **3** were calculated with the GIAO method[2] at mPW1PW91/6-31G*// B3LYP/6-31G* (in gas phase) and mPW1PW91/6-31G**//B3LYP/6-31G* levels (in solevent with PCM model). The shielding constants (including ^{13}C and ^{1}H) obtained were directly performed statistical analyses with experimental chemical shifts by using DP4+[3] probability and ANN-PRA[4] analyses.

The theoretical calculation of ECD of compounds **1−3** was performed using time-dependent Density Functional Theory (TDDFT)[5] at wB97XD/6-311+G**//B3LYP/6-31G* level in MeOH with PCM model. The ECD spectra were obtained by weighing the Boltzmann distribution rate of each geometric conformation. The sigma/gamma value for processing calculated ECD was 0.3 eV.[6]

NLRP3 Inflammasome Activation.

J774A.1 macrophages were incubated with gradient concentrations of compounds for 30 min followed by 100 ng/mL lipopolysaccharide (LPS) for 4 h. Next, cells were treated with the NLRP3 stimulus Nigericin (10 μM) for 1 h. The supernatant was collected for LDH release assay and IL-1β/Casp-1 western blot detection. LDH release level was determined according to the manufacturer's manual (Promega, USA). IL-1β levels were detected by mouse IL-1 beta/IL-1F2 DuoSet ELISA kit (R&D Incorporation, USA) according to the manufacturer's manual. Western blot assays were used to detect GSDMD full length (FL) and N-terminal (NT) from cell lysate as well as IL-1β (p17) and Casp-1 (p20) from supernatant.

Pyroptosis Assay.

After inflammasome stimulation, cells were stained by PI (0.5 μg/mL; Thermofisher, USA) for 15 min at room temperature. Fluorescent images were immediately observed by an Axio Observer 3 inverted fluorescent microscope (Zeiss, Germany). Pyroptotic cells were counted by FACSCelestat™ Flow Cytometer (BD, USA).

Cytotoxicity Assay.

Cell viability was performed by MTT methods see previous report.[7]

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Computational details of compounds 1−3

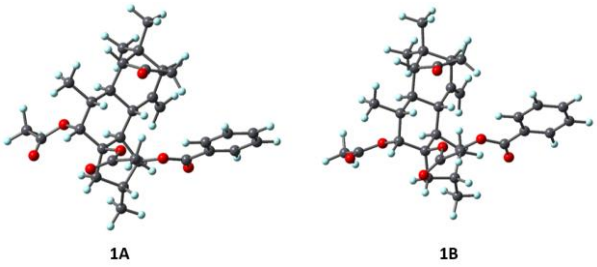


Figure S5. Key conformers of **1**.

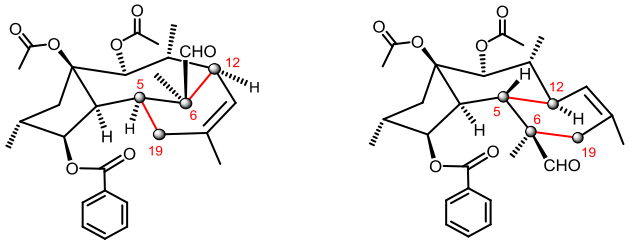
Table S3. Important thermodynamic parameters and Boltzmann distributions of the optimized **1** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
1A	-1728.832521	0	50.21%	0
1B	-1728.832513	0.005082774	49.79%	0

Table S4. Optimized Z-matrixes of **1** in the gas phase (Å) at B3LYP/6-31G* level

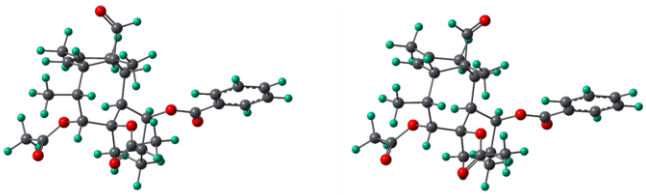
1A				**1B**			
C	-2.693	1.8629	0.1981	C	-2.5599	2.0888	-0.205
C	-2.1167	0.4534	0.4868	C	-2.1325	0.6735	0.2619
C	-1.0615	0.2098	-0.6178	C	-1.0074	0.2503	-0.7097
C	-0.5831	1.656	-0.9503	C	-0.368	1.619	-1.0959
C	-1.9352	2.3688	-1.0435	C	-1.6346	2.4299	-1.3885
C	-4.1979	1.8468	-0.0403	C	-4.0262	2.1553	-0.6145
H	-1.5941	-0.2032	-1.4874	H	-1.495	-0.1855	-1.5944
C	0.1506	-0.6997	-0.3043	C	0.0817	-0.7312	-0.2174
C	1.1488	-0.6937	-1.53	C	1.1781	-0.9097	-1.3434
C	1.5647	0.7539	-1.9373	C	1.7632	0.4594	-1.8111
C	0.31	1.6374	-2.2083	C	0.6275	1.4269	-2.2585
C	-0.0778	-2.1543	0.144	C	-0.3203	-2.1198	0.311
C	1.2101	-2.9857	0.31	C	0.8644	-3.0449	0.6542
C	1.9138	-3.1177	-1.0652	C	1.6668	-3.3472	-0.6374
C	2.3582	-1.6405	-1.263	C	2.2646	-1.9355	-0.8983
C	2.4769	0.7676	-3.1724	C	2.7886	0.2951	-2.9406
C	-1.2643	-2.7523	0.3384	C	-1.5697	-2.5956	0.4368
C	2.8973	-1.3473	0.1363	C	2.7074	-1.5803	0.5204
C	2.2445	-2.238	1.1786	C	1.8866	-2.3241	1.5588
O	3.7167	-0.4757	0.3936	O	3.5803	-0.7662	0.7898
H	0.6087	-1.0961	-2.3965	H	0.6792	-1.3287	-2.2266
H	0.6634	-0.219	0.5386	H	0.5618	-0.2302	0.6329
C	1.0105	-3.6754	-2.182	C	0.8134	-3.9099	-1.7903
C	3.1419	-4.0621	-1.0049	C	2.7901	-4.3884	-0.3968
O	-1.4747	0.444	1.7718	O	-1.6098	0.735	1.5984
C	-2.2534	0.1443	2.8373	C	-2.5062	0.6194	2.6058
C	0.0143	0.1277	6.4761	C	-0.582	0.7602	6.4348
C	0.6645	0.3891	5.2704	C	0.1963	0.824	5.2795
C	-0.057	0.4003	4.0746	C	-0.4118	0.7807	4.0229
C	-1.4369	0.1485	4.0815	C	-1.8065	0.6728	3.9182
C	-2.082	-0.1141	5.2975	C	-2.5808	0.6081	5.0843
C	-1.3572	-0.1238	6.4909	C	-1.969	0.6523	6.3386
O	-3.4486	-0.0993	2.8072	O	-3.7129	0.4892	2.4813
O	0.163	2.1423	0.2079	O	0.3101	2.1379	0.0876
O	0.4975	4.2517	-0.6347	O	0.8527	4.1553	-0.8646
C	0.6261	3.4181	0.2468	C	0.86	3.3796	0.0777
C	1.3314	3.6586	1.5461	C	1.4833	3.6664	1.409
O	-0.3966	1.067	-3.3358	O	-0.0743	0.8568	-3.389
O	-0.8878	3.1506	-4.1745	O	0.8429	2.3856	-4.8448
C	-0.9181	1.9325	-4.2462	C	0.1137	1.4363	-4.6054
C	-1.5645	1.1668	-5.3595	C	-0.7094	0.7242	-5.6348
H	-2.4867	2.5332	1.0428	H	-2.3945	2.8156	0.6009

H	-2.898	-0.3113	0.4429	H	-2.9687	-0.03	0.2113
H	-1.8605	3.4595	-1.0245	H	-1.4684	3.5091	-1.4389
H	-2.4712	2.0871	-1.9568	H	-2.089	2.1217	-2.338
H	-4.5608	2.8505	-0.2845	H	-4.2802	3.1561	-0.979
H	-4.7282	1.5052	0.8542	H	-4.6767	1.9317	0.2369
H	-4.4653	1.1793	-0.8665	H	-4.2527	1.4371	-1.4098
H	2.1329	1.2032	-1.1135	H	2.2917	0.9205	-0.9674
H	0.6621	2.6449	-2.4534	H	1.0743	2.3896	-2.5254
H	0.9906	-3.9668	0.7476	H	0.5168	-3.9651	1.1387
H	3.1492	-1.5752	-2.0126	H	3.1194	-2.0011	-1.5741
H	2.6313	1.7915	-3.5301	H	3.0752	1.2695	-3.3505
H	3.4664	0.3635	-2.9395	H	3.7083	-0.1722	-2.5763
H	2.0534	0.1813	-3.9944	H	2.3959	-0.3185	-3.7577
H	-1.3266	-3.7956	0.6386	H	-1.7544	-3.6025	0.8037
H	-2.2161	-2.2617	0.1931	H	-2.4558	-2.0385	0.1686
H	1.7901	-1.6483	1.9786	H	1.4233	-1.6348	2.2691
H	2.9929	-2.9174	1.5953	H	2.5291	-3.0312	2.0905
H	1.5242	-3.6328	-3.1493	H	1.4098	-3.9906	-2.7064
H	0.7578	-4.7237	-1.9839	H	0.4454	-4.9124	-1.5419
H	0.0624	-3.1455	-2.2996	H	-0.0659	-3.3088	-2.0331
H	2.8381	-5.072	-0.7069	H	2.3675	-5.3409	-0.0572
H	3.6216	-4.1329	-1.9882	H	3.3433	-4.5791	-1.324
H	3.9149	-3.7339	-0.3042	H	3.528	-4.0752	0.3473
H	0.5775	0.12	7.4063	H	-0.1068	0.7945	7.4124
H	1.7343	0.5844	5.2611	H	1.2779	0.9072	5.3568
H	0.4707	0.6056	3.1465	H	0.2148	0.8306	3.1359
H	-3.1522	-0.3119	5.3194	H	-3.6641	0.5234	5.0197
H	-1.8633	-0.3272	7.4315	H	-2.575	0.6025	7.24
H	0.6313	3.5322	2.3758	H	0.7144	3.662	2.1857
H	2.1728	2.9679	1.644	H	2.2533	2.9214	1.6256
H	1.7163	4.6821	1.566	H	1.952	4.6542	1.385
H	-0.8288	0.5147	-5.8371	H	-0.3856	-0.3168	-5.7121
H	-2.4014	0.5825	-4.969	H	-1.7675	0.7797	-5.3664
H	-1.9445	1.8673	-6.1086	H	-0.5717	1.2066	-6.6067



2A (C-5/19,C-6/12) **2B** (C-5/12,C-6/19)

Figure S6. Possible isomers **2A** and **2B** for compound **2**.



2A-1 **2A-2**

Figure S7. Key conformers of isomer **2A**.

Table S5. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **2A** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
2A-1	-1653.351334	0	57.41%	0
2A-2	-1653.351052	0.176918168	42.59%	0

Table S6. Optimized Z-matrixes of isomer **2A** in the gas phase (Å) at B3LYP/6-31G* level.

2A-1				**2A-2**			
C	-0.4437	-2.4981	1.0751	C	-0.7008	-2.5913	0.6581
C	-0.8878	-1.0492	1.3708	C	-1.0109	-1.1727	1.1817
C	0.2592	-0.1578	0.8188	C	0.2268	-0.3203	0.7894
C	0.8047	-0.9692	-0.3833	C	0.7225	-0.9811	-0.5229
C	0.8694	-2.3703	0.284	C	0.6438	-2.4682	-0.0803
C	-0.1379	1.3554	0.7323	C	-0.025	1.218	0.9487
C	2.2273	0.8665	-1.6127	C	2.3221	0.8904	-1.4383
C	2.2076	-0.4901	-0.8568	C	2.1705	-0.5618	-0.9067
C	-0.2443	-3.3191	2.3439	C	-0.6245	-3.6238	1.7764
C	1.7261	2.1304	-0.8397	C	1.9244	2.0588	-0.4762
C	3.6404	1.1259	-2.1794	C	3.7625	1.1041	-1.9533
H	1.0424	-0.2376	1.5884	H	0.9811	-0.5968	1.5425
O	-0.1997	-1.0015	-1.4243	O	-0.2576	-0.7626	-1.5659
C	0.1977	2.1828	-0.5463	C	0.4023	2.2033	-0.1833
C	-0.6902	1.896	-1.7694	C	-0.5022	2.1816	-1.4278
C	-0.0421	-1.7884	-2.5218	C	-0.1395	-1.3834	-2.771
O	0.9544	-2.4346	-2.8023	O	0.7959	-2.0797	-3.1299
C	-1.2821	-1.7455	-3.362	C	-1.3431	-1.0929	-3.615
O	3.0942	-0.4233	0.289	O	3.0376	-0.756	0.239
C	4.2758	-1.0925	0.237	C	4.1464	-1.5275	0.0921
C	5.0227	-0.8919	1.52	C	4.8998	-1.5738	1.3862
O	4.6867	-1.754	-0.7033	O	4.4943	-2.1006	-0.9283
C	0.5549	2.0575	1.9496	C	0.7089	1.6471	2.2643
C	2.003	2.4066	1.6724	C	2.1843	1.8952	2.0512
C	2.5192	2.417	0.4277	C	2.7171	2.0584	0.8247
C	2.8321	2.7438	2.8788	C	3.0234	1.9636	3.2948
O	-2.1092	-0.772	0.6607	O	-2.1812	-0.6633	0.5144
C	-3.2508	-1.1765	1.2724	C	-3.3727	-1.021	1.0552
C	-6.7291	-0.3327	-1.0881	C	-6.6758	0.5472	-1.1822
C	-5.4726	0.027	-1.5743	C	-5.3801	0.7265	-1.6655
C	-4.3275	-0.2394	-0.82	C	-4.2909	0.2225	-0.951

C	-4.4362	-0.8666	0.4285	C	-4.4954	-0.4631	0.2546
C	-5.7029	-1.2251	0.9095	C	-5.801	-0.6418	0.7312
C	-6.8454	-0.9584	0.1523	C	-6.8874	-0.1367	0.0142
O	-3.3215	-1.7307	2.3576	O	-3.5276	-1.6959	2.0597
C	-0.1825	3.6597	-0.2686	C	0.1202	3.6442	0.3166
O	-1.2819	4.0135	0.1538	O	0.7721	4.6389	0.0113
H	-1.1884	-3.0058	0.4488	H	-1.4712	-2.9114	-0.0551
H	-1.0232	-0.8463	2.4408	H	-1.1506	-1.132	2.2693
H	0.9557	-3.1925	-0.4321	H	0.679	-3.1767	-0.9126
H	1.7279	-2.4455	0.9623	H	1.4705	-2.7243	0.5934
H	-1.2155	1.4471	0.9193	H	-1.0918	1.3812	1.1492
H	1.6031	0.7471	-2.5046	H	1.7037	0.971	-2.3386
H	2.5875	-1.2413	-1.5572	H	2.4967	-1.2229	-1.7163
H	0.1196	-4.3229	2.1009	H	-0.3538	-4.6066	1.3767
H	-1.1869	-3.4261	2.8895	H	-1.5905	-3.7202	2.2818
H	0.4818	-2.8483	3.0154	H	0.1224	-3.3457	2.5279
H	1.9392	2.9796	-1.5075	H	2.2315	2.9765	-0.9994
H	3.9609	0.2894	-2.81	H	4.0163	0.3516	-2.708
H	4.3898	1.2594	-1.3943	H	4.5073	1.0412	-1.1549
H	3.6464	2.0246	-2.8057	H	3.8614	2.0861	-2.4286
H	-0.632	2.7164	-2.4973	H	-0.3731	3.0934	-2.0261
H	-0.4315	1.0052	-2.3263	H	-0.3148	1.3682	-2.1156
H	-1.7425	1.8098	-1.4767	H	-1.5594	2.1411	-1.1418
H	-1.1855	-2.4583	-4.1859	H	-2.2444	-1.4445	-3.1066
H	-2.1478	-2.0332	-2.7599	H	-1.4084	-0.0217	-3.8189
H	-1.4175	-0.7443	-3.7771	H	-1.2539	-1.6239	-4.567
H	4.4274	-1.265	2.3574	H	5.7835	-2.2075	1.2692
H	5.9619	-1.4512	1.4845	H	5.2255	-0.5672	1.6608
H	5.2515	0.1686	1.6529	H	4.2666	-2.0003	2.1683
H	0.0199	2.9765	2.2183	H	0.2575	2.5603	2.6716
H	0.4848	1.4171	2.8385	H	0.5612	0.8845	3.04
H	3.5687	2.6741	0.292	H	3.785	2.2491	0.7312
H	3.8617	3.004	2.6119	H	4.0761	2.1667	3.0718
H	2.3984	3.5973	3.4098	H	2.6613	2.76	3.9528
H	2.8708	1.8896	3.5626	H	2.9751	1.0135	3.8367
H	-7.6198	-0.1224	-1.6755	H	-7.5232	0.9396	-1.7398
H	-5.385	0.519	-2.54	H	-5.2193	1.2582	-2.6004
H	-3.3588	0.05	-1.2163	H	-3.2905	0.3677	-1.3482
H	-5.8048	-1.7127	1.8773	H	-5.9774	-1.1757	1.6634
H	-7.8253	-1.2373	0.5321	H	-7.8983	-0.2782	0.3892
H	0.5772	4.4207	-0.5183	H	-0.8009	3.7636	0.9159

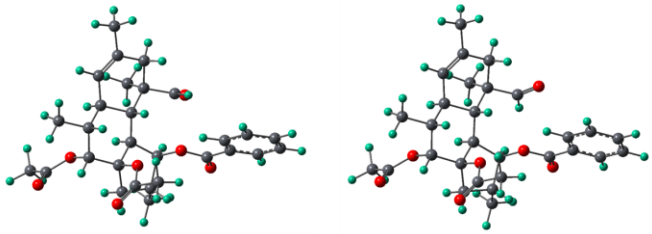


Figure S8. Key conformers of isomer **2B**.

Table S7. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **2B** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
2B-1	-1653.372565	0	93.82%	0
2B-2	-1653.369999	1.610341867	6.18%	0

Table S8. Optimized Z-matrixes of isomer **2B** in the gas phase (Å) at B3LYP/6-31G* level.

2B-1	**2B-2**

C	-2.939	0.1973	0.2731	C	-2.629	1.2713	-0.1111
C	-1.5893	0.6509	0.8904	C	-1.2201	1.3754	0.5265
C	-0.6359	-0.5403	0.6448	C	-0.7615	-0.0866	0.7001
C	-1.1312	-1.0848	-0.7289	C	-1.391	-0.7801	-0.5461
C	-2.6448	-1.1155	-0.4788	C	-2.8165	-0.2122	-0.4848
C	0.9036	-0.3207	0.6421	C	0.7514	-0.4236	0.8281
C	1.0804	-2.2758	-1.0549	C	0.231	-2.71	-0.2792
C	-0.4653	-2.4432	-1.0312	C	-1.2658	-2.3125	-0.4212
C	-4.0163	-0.0131	1.3323	C	-3.728	1.7406	0.8363
C	1.5899	-1.6996	0.305	C	0.873	-1.9934	0.9529
C	1.7329	-3.6184	-1.4223	C	0.3484	-4.2413	-0.2172
H	-0.8688	-1.2887	1.4165	H	-1.2685	-0.4655	1.6
O	-0.7887	-0.0955	-1.7431	O	-0.6813	-0.2911	-1.7194
C	1.5248	0.2853	1.9467	C	1.5469	0.2741	1.9837
C	1.2587	-0.5811	3.1925	C	0.9728	-0.0457	3.378
C	-1.2199	-0.2507	-3.0223	C	-1.1017	-0.6191	-2.9676
O	-1.8698	-1.1917	-3.4481	O	-2.046	-1.3449	-3.2345
C	-0.7898	0.9219	-3.8488	C	-0.2374	0.0567	-3.9872
O	-0.828	-3.3869	0.0067	O	-1.9882	-2.7488	0.7574
C	-1.2756	-4.6119	-0.3813	C	-2.8484	-3.7943	0.619
C	-1.6281	-5.4255	0.8262	C	-3.5136	-4.0762	1.9314
O	-1.3729	-5.0094	-1.5316	O	-3.0543	-4.4249	-0.4058
C	3.054	0.4833	1.7491	C	3.0391	-0.1598	1.9112
C	3.7607	-0.637	1.0383	C	3.2658	-1.627	1.6721
C	3.0961	-1.6099	0.3954	C	2.2878	-2.4386	1.2413
C	5.2625	-0.6056	1.098	C	4.6579	-2.1267	1.938
H	1.1407	0.3773	-0.1751	H	1.242	-0.1238	-0.1101
H	1.2987	-2.4266	1.0762	H	0.2942	-2.3102	1.8324
O	-1.0897	1.8129	0.2018	O	-0.3381	2.0602	-0.3768
C	-1.7333	2.9817	0.4541	C	-0.4379	3.414	-0.3956
C	0.0399	6.2483	-1.6818	C	1.9917	5.1303	-3.4776
C	-0.9884	6.4702	-0.7667	C	0.9821	5.8765	-2.8703
C	-1.5558	5.3955	-0.0795	C	0.2024	5.3058	-1.8624
C	-1.0951	4.0916	-0.304	C	0.4273	3.9823	-1.4616
C	-0.0612	3.8757	-1.227	C	1.4478	3.2401	-2.071
C	0.5034	4.9535	-1.9128	C	2.227	3.8151	-3.0772
O	-2.6947	3.1274	1.1897	O	-1.1695	4.0799	0.3197
C	1.0117	1.6985	2.2005	C	1.557	1.7957	1.848
O	0.4275	2.0553	3.2188	O	2.2974	2.4227	1.0952
H	-3.3019	0.9394	-0.4488	H	-2.6812	1.8746	-1.0263
H	-1.6656	0.8668	1.9622	H	-1.2358	1.8842	1.497
H	-3.242	-1.1645	-1.3933	H	-3.3637	-0.2938	-1.4277
H	-2.9246	-1.9787	0.1368	H	-3.4119	-0.7245	0.2801
H	1.3426	-1.5671	-1.8521	H	0.7644	-2.3876	-1.1837
H	-0.7921	-2.8046	-2.0109	H	-1.6695	-2.7895	-1.3194
H	-4.9424	-0.3761	0.8745	H	-4.714	1.6135	0.3775
H	-4.2418	0.9248	1.8493	H	-3.6035	2.8008	1.0786
H	-3.7001	-0.7439	2.0846	H	-3.7147	1.1768	1.7753
H	1.236	-4.0687	-2.2885	H	-0.2513	-4.71	-1.005
H	1.6878	-4.331	-0.5925	H	0.0136	-4.6345	0.7481
H	2.7822	-3.4881	-1.7036	H	1.3798	-4.5683	-0.3804
H	1.686	-0.1194	4.0912	H	1.5201	0.4965	4.159
H	1.6978	-1.5793	3.1102	H	1.0325	-1.1098	3.6239
H	0.186	-0.6957	3.3803	H	-0.0749	0.2624	3.4608
H	-1.3252	1.8173	-3.5245	H	-0.5094	-0.2977	-4.9854
H	0.2902	1.0651	-3.7586	H	-0.3903	1.1377	-3.9417
H	-1.0235	0.7298	-4.8998	H	0.8122	-0.1912	-3.8086
H	-2.0116	-6.3992	0.5082	H	-4.2208	-4.9015	1.8098
H	-0.7371	-5.5833	1.4389	H	-2.7634	-4.3645	2.672
H	-2.4062	-4.917	1.4012	H	-4.0646	-3.193	2.2646
H	3.2493	1.398	1.1716	H	3.5591	0.3695	1.1014
H	3.5239	0.6434	2.7292	H	3.5431	0.1399	2.8403
H	3.6764	-2.4171	-0.0449	H	2.5134	-3.4973	1.1397
H	5.7157	-1.4374	0.5484	H	4.7617	-3.1952	1.722
H	5.639	0.3256	0.6623	H	5.3788	-1.5892	1.3135
H	5.6027	-0.6673	2.1367	H	4.9228	-1.9714	2.9888

H	0.4799	7.0872	-2.2161	H	2.6026	5.5775	-4.258
H	-1.3496	7.48	-0.5867	H	0.8044	6.9039	-3.1779
H	-2.3573	5.579	0.6342	H	-0.5814	5.8957	-1.3914
H	0.3122	2.8747	-1.4253	H	1.6591	2.2213	-1.7551
H	1.3043	4.7848	-2.6287	H	3.0246	3.2397	-3.5404
H	1.2052	2.4277	1.3941	H	0.8124	2.3408	2.4542

Table S9. Experimental chemical shifts of **2**, calculated shielding tensors and chemical shifts of isomers **2A** and **2B** in gas phase with TMS as reference at mPW1PW91/6-31G* level.

Nuclie	δ(exptl)	**2A**					**2B**				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
C-1	38.2	155.0	38.0	37.2	0.2	1.0	157.5	35.5	36.4	2.7	1.8
C-2	41.1	153.4	39.6	38.8	1.5	2.3	152.2	40.8	41.9	0.3	0.8
C-3	82.2	112.1	80.9	83.2	1.3	1.0	113.9	79.1	82.6	3.1	0.4
C-4	47.2	139.6	53.4	53.7	6.2	6.5	146.2	46.8	48.3	0.4	1.1
C-5	37.4	159.2	33.8	32.7	3.6	4.7	156.7	36.3	37.2	1.1	0.2
C-6	49.3	141.9	51.1	51.2	1.8	1.9	144.6	48.4	50.0	0.9	0.7
C-9	205.2	-1.7	194.7	205.5	10.5	0.3	-3.3	196.3	206.8	8.9	1.6
C-10	132.4	65.3	127.7	133.6	4.7	1.2	66.3	126.7	133.1	5.7	0.7
C-11	121.8	69.8	123.2	128.7	1.4	6.9	74.1	118.9	124.8	2.9	3.0
C-12	38.0	149.0	44.0	43.5	6.0	5.5	155.6	37.4	38.4	0.6	0.4
C-13	36.1	158.9	34.1	33.0	2.0	3.1	157.1	35.9	36.8	0.2	0.7
C-14	72.4	122.7	70.3	71.9	2.1	0.5	123.4	69.6	72.5	2.8	0.1
C-15	92.3	100.0	93.0	96.2	0.7	3.9	102.1	90.9	95.1	1.4	2.8
C-16	20.5	173.6	19.4	17.2	1.1	3.3	173.2	19.8	19.7	0.7	0.8
C-17	13.3	173.9	19.1	16.9	5.8	3.6	179.0	14.0	13.5	0.7	0.2
C-18	23.8	168.4	24.6	22.7	0.8	1.1	168.9	24.1	24.3	0.3	0.5
C-19	37.8	154.9	38.1	37.2	0.3	0.6	157.9	35.1	35.9	2.7	1.9
C-20	15.8	173.8	19.2	16.9	3.4	1.1	177.1	15.9	15.6	0.1	0.2
C-1'	166.7	34.1	158.9	167.0	7.8	0.3	35.3	157.7	166.0	9.0	0.7
C-2'	131.7	68.4	124.6	130.2	7.1	1.5	67.6	125.4	131.7	6.3	0.0
C-3',7'	130.5	69.3	123.7	129.2	6.8	1.3	66.1	126.9	133.3	3.6	2.8
C-3',7'	130.5	66.3	126.7	132.4	3.8	1.9	69.8	123.2	129.4	7.3	1.1
C-4',6'	129.8	71.1	121.9	127.3	7.9	2.5	70.3	122.7	128.9	7.1	0.9
C-4',6'	129.8	70.5	122.5	128.0	7.3	1.8	71.3	121.7	127.8	8.1	2.0
C-5'	134.5	66.3	126.7	132.5	7.8	2.0	66.5	126.5	132.9	8.0	1.6
C-1''	171.8	31.6	161.4	169.8	10.4	2.0	31.8	161.2	169.7	10.6	2.1
C-2''	20.8	172.4	20.6	18.4	0.2	2.4	172.6	20.4	20.4	0.4	0.4
C-1'''	171.4	31.5	161.5	169.8	9.9	1.6	31.3	161.7	170.2	9.7	1.2
C-2'''	22.4	171.0	22.0	19.9	0.4	2.5	171.4	21.6	21.6	0.8	0.8
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|; **2A**: Y = 0.9305X + 3.4472, R^2 = 0.9974, MAE = 4.2 ppm, CMAE = 2.4 ppm; **2B**: Y = 0.9429X + 1.2182, R^2 = 0.9994, MAE = 3.7 ppm, CMAE = 1.1 ppm;										

Nuclie	δ(exptl)	**2A**					**2B**				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
H-1a	1.04	30.94	1.06	1.02	0.02	0.02	30.93	1.07	1.14	0.03	0.10
H-1b	2.64	29.24	2.76	2.69	0.12	0.05	29.25	2.75	2.78	0.11	0.14
H-2	2.00	29.93	2.07	2.01	0.07	0.01	29.95	2.05	2.10	0.05	0.10
H-3	4.47	27.14	4.86	4.77	0.39	0.30	27.49	4.51	4.50	0.04	0.03
H-4	2.04	29.97	2.03	1.97	0.01	0.07	30.05	1.95	2.00	0.09	0.04
H-5	2.39	29.44	2.56	2.50	0.17	0.11	29.51	2.49	2.53	0.10	0.14
H-7	9.08	22.65	9.35	9.18	0.27	0.10	22.59	9.41	9.29	0.33	0.21
H-11	5.44	26.07	5.93	5.82	0.49	0.38	26.44	5.56	5.53	0.12	0.09
H-12	1.98	29.69	2.31	2.25	0.33	0.27	29.82	2.18	2.22	0.20	0.24
H-13	1.80	29.91	2.09	2.03	0.29	0.23	30.20	1.80	1.86	0.00	0.06
H-14	5.88	25.72	6.28	6.16	0.40	0.28	25.96	6.04	5.99	0.16	0.11
H-16	1.11	31.14	0.86	0.82	0.25	0.29	31.15	0.85	0.92	0.26	0.19
H-16	1.11	30.03	1.97	1.91	0.86	0.80	29.98	2.02	2.07	0.91	0.96
H-16	1.11	31.35	0.65	0.61	0.46	0.50	31.39	0.61	0.70	0.50	0.41
H-17	0.96	31.51	0.49	0.46	0.47	0.50	31.19	0.81	0.89	0.15	0.07
H-17	0.96	29.48	2.52	2.46	1.56	1.50	31.14	0.86	0.94	0.10	0.02
H-17	0.96	31.22	0.78	0.75	0.18	0.21	30.97	1.03	1.10	0.07	0.14
H-18	1.63	30.47	1.53	1.48	0.10	0.15	30.47	1.53	1.59	0.10	0.04
H-18	1.63	30.52	1.48	1.44	0.15	0.19	30.45	1.55	1.61	0.08	0.02

H-18	1.63	30.56	1.44	1.39	0.19	0.24	30.54	1.46	1.52	0.17	0.11
H-19a	1.31	30.49	1.51	1.46	0.20	0.15	30.91	1.09	1.16	0.22	0.15
H-19b	2.31	29.84	2.16	2.11	0.15	0.20	29.91	2.09	2.14	0.22	0.17
H-20	0.95	30.86	1.14	1.10	0.19	0.15	30.96	1.04	1.11	0.09	0.16
H-20	0.95	30.76	1.24	1.20	0.29	0.25	31.41	0.59	0.67	0.36	0.28
H-20	0.95	31.19	0.81	0.78	0.14	0.17	30.82	1.18	1.25	0.23	0.30
H-3',7'	7.98	23.86	8.14	7.99	0.16	0.01	23.77	8.23	8.14	0.25	0.16
H-3',7'	7.98	23.77	8.23	8.08	0.25	0.10	23.96	8.04	7.95	0.06	0.03
H-4',6'	7.42	24.73	7.27	7.14	0.15	0.28	24.59	7.41	7.34	0.01	0.08
H-4',6'	7.42	24.60	7.40	7.27	0.02	0.15	24.73	7.27	7.20	0.15	0.22
H-5'	7.53	24.56	7.44	7.31	0.09	0.22	24.57	7.43	7.35	0.10	0.18
H-2''	2.04	30.27	1.73	1.68	0.31	0.36	30.43	1.57	1.63	0.47	0.41
H-2''	2.04	30.30	1.70	1.65	0.34	0.39	30.14	1.86	1.92	0.18	0.12
H-2''	2.04	30.16	1.84	1.79	0.20	0.25	30.12	1.88	1.94	0.16	0.10
H-2'''	1.96	30.30	1.70	1.65	0.26	0.31	30.05	1.95	2.00	0.01	0.04
H-2'''	1.96	30.00	2.00	1.94	0.04	0.02	30.01	1.99	2.04	0.03	0.08
H-2'''	1.96	30.21	1.79	1.74	0.17	0.22	30.51	1.49	1.55	0.47	0.41
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|; **2A**: Y = 1.015X – 0.0239, R^2 = 0.9783, MAE = 0.27 ppm, CMAE = 0.26 ppm; **2B**: Y = 1.0237X – 0.0995, R^2 = 0.9907, MAE = 0.18 ppm, CMAE = 0.17 ppm;										

Table S10. Experimental chemical shifts of **2**, calculated shielding tensors and chemical shifts of isomers **2A** and **2B** in methanol with TMS as reference at mPW1PW91/6-31G** level.

Nuclie	δ(exptl)	**2A**					**2B**				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
C-1	38.2	156.3	36.7	37.1	1.5	1.1	158.8	34.2	36.4	4.0	1.8
C-2	41.1	154.4	38.6	39.1	2.5	2.0	153.1	39.9	42.3	1.2	1.2
C-3	82.2	112.4	80.6	83.3	1.6	1.1	114.0	79.0	82.8	3.2	0.6
C-4	47.2	140.4	52.6	53.8	5.4	6.6	146.9	46.1	48.7	1.1	1.5
C-5	37.4	159.9	33.1	33.4	4.3	4.0	157.5	35.5	37.7	1.9	0.3
C-6	49.3	141.4	51.6	52.8	2.3	3.5	144.0	49.0	51.7	0.3	2.4
C-9	205.2	-5.6	198.6	207.3	6.6	2.1	-7.5	200.5	208.7	4.7	3.5
C-10	132.4	64.5	128.5	133.6	3.9	1.2	65.6	127.4	133.0	5.0	0.6
C-11	121.8	70.9	122.1	126.8	0.3	5.0	75.8	117.2	122.4	4.6	0.6
C-12	38.0	150.0	43.0	43.7	5.0	5.7	156.4	36.6	38.8	1.4	0.8
C-13	36.1	160.0	33.0	33.3	3.1	2.8	157.9	35.1	37.3	1.0	1.2
C-14	72.4	122.7	70.3	72.5	2.1	0.1	123.5	69.5	72.9	2.9	0.5
C-15	92.3	100.3	92.7	96.0	0.4	3.7	102.3	90.7	94.9	1.6	2.6
C-16	20.5	175.6	17.4	16.8	3.1	3.7	175.3	17.7	19.2	2.8	1.3
C-17	13.3	175.6	17.4	16.9	4.1	3.6	181.1	11.9	13.2	1.4	0.1
C-18	23.8	170.6	22.4	22.1	1.4	1.7	171.0	22.0	23.7	1.8	0.1
C-19	37.8	156.3	36.7	37.1	1.1	0.7	159.4	33.6	35.8	4.2	2.0
C-20	15.8	175.7	17.3	16.7	1.5	0.9	179.0	14.0	15.4	1.8	0.4
C-1'	166.7	32.9	160.1	166.8	6.6	0.1	33.6	159.4	166.1	7.3	0.6
C-2'	131.7	68.8	124.2	129.0	7.5	2.7	68.5	124.5	130.0	7.2	1.7
C-3',7'	130.5	69.3	123.7	128.6	6.8	1.9	67.9	125.1	130.6	5.4	0.1
C-3',7'	130.5	67.8	125.2	130.2	5.3	0.3	69.3	123.7	129.1	6.8	1.4
C-4',6'	129.8	70.5	122.5	127.3	7.3	2.5	70.4	122.6	127.9	7.2	1.9
C-4',6'	129.8	70.6	122.4	127.2	7.4	2.6	70.3	122.7	128.0	7.1	1.8
C-5'	134.5	65.4	127.6	132.6	6.9	1.9	65.3	127.7	133.3	6.8	1.2
C-1''	171.8	28.8	164.2	171.1	7.6	0.7	28.9	164.1	171.0	7.7	0.8
C-2''	20.8	173.8	19.2	18.7	1.6	2.1	173.9	19.1	20.7	1.7	0.1
C-1'''	171.4	29.1	163.9	170.8	7.5	0.6	28.9	164.1	171.0	7.3	0.4
C-2'''	22.4	172.2	20.8	20.4	1.6	2.0	172.6	20.4	22.1	2.0	0.3
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|; **2A**: Y = 0.9515X + 1.3834, R^2 = 0.9976, MAE = 4.0 ppm, CMAE = 2.3 ppm; **2B**: Y = 0.9648X – 0.881, R^2 = 0.9994, MAE = 3.9 ppm, CMAE = 1.1 ppm;										

Nuclie	δ(exptl)	**2A**					**2B**				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
H-1a	1.04	30.35	1.65	1.08	0.61	0.04	30.3	1.69	1.24	0.60	0.20
H-1b	2.64	28.82	3.18	2.55	0.54	0.09	28.8	3.19	2.66	0.50	0.00
H-2	2.00	29.44	2.56	1.95	0.56	0.05	29.5	2.50	2.00	0.50	0.00
H-3	4.47	26.59	5.41	4.69	0.94	0.22	27.1	4.92	4.30	0.50	0.20
H-4	2.04	29.43	2.57	1.96	0.53	0.08	29.5	2.54	2.04	0.50	0.00

H-5	2.39	29.01	2.99	2.36	0.60	0.03	29.0	2.99	2.47	0.60	0.10
H-7	9.08	22.05	9.95	9.02	0.87	0.06	22.0	9.99	9.10	0.90	0.00
H-11	5.44	25.38	6.62	5.84	1.18	0.40	25.8	6.24	5.55	0.80	0.10
H-12	1.98	29.22	2.78	2.17	0.80	0.19	29.3	2.66	2.16	0.70	0.20
H-13	1.80	29.28	2.72	2.10	0.92	0.30	29.6	2.36	1.87	0.60	0.10
H-14	5.88	25.30	6.70	5.92	0.82	0.04	25.5	6.45	5.75	0.60	0.10
H-16	1.11	30.66	1.34	0.79	0.23	0.32	30.7	1.35	0.91	0.20	0.20
H-16	1.11	29.84	2.16	1.57	1.05	0.46	29.8	2.17	1.69	1.10	0.60
H-16	1.11	30.72	1.28	0.73	0.17	0.38	30.8	1.24	0.81	0.10	0.30
H-17	0.96	30.90	1.10	0.55	0.14	0.41	30.8	1.19	0.76	0.20	0.20
H-17	0.96	28.69	3.31	2.67	2.35	1.71	30.5	1.45	1.01	0.50	0.10
H-17	0.96	30.74	1.26	0.71	0.30	0.25	30.5	1.52	1.07	0.60	0.10
H-18	1.63	29.94	2.06	1.47	0.43	0.16	30.0	2.04	1.57	0.40	0.10
H-18	1.63	30.05	1.95	1.37	0.32	0.26	29.9	2.11	1.64	0.50	0.00
H-18	1.63	29.95	2.05	1.47	0.42	0.16	30.0	2.00	1.52	0.40	0.10
H-19a	1.31	29.91	2.09	1.50	0.78	0.19	30.4	1.62	1.17	0.30	0.10
H-19b	2.31	29.45	2.55	1.94	0.24	0.37	29.3	2.74	2.23	0.40	0.10
H-20	0.95	30.65	1.35	0.79	0.40	0.16	30.7	1.26	0.83	0.30	0.10
H-20	0.95	30.24	1.76	1.19	0.81	0.24	30.9	1.12	0.69	0.20	0.30
H-20	0.95	30.63	1.37	0.81	0.42	0.14	30.2	1.80	1.34	0.80	0.40
H-3',7'	7.98	23.04	8.96	8.07	0.98	0.09	23.2	8.81	7.99	0.80	0.00
H-3',7'	7.98	23.14	8.86	7.98	0.88	0.00	23.1	8.91	8.07	0.90	0.10
H-4',6'	7.42	23.84	8.16	7.31	0.74	0.11	23.8	8.23	7.43	0.80	0.00
H-4',6'	7.42	23.78	8.22	7.37	0.80	0.05	23.8	8.19	7.40	0.80	0.00
H-5'	7.53	23.68	8.32	7.47	0.79	0.06	23.7	8.33	7.53	0.80	0.00
H-2''	2.04	29.58	2.42	1.82	0.38	0.22	29.9	2.10	1.62	0.10	0.40
H-2''	2.04	29.67	2.33	1.73	0.29	0.31	29.3	2.65	2.15	0.60	0.10
H-2''	2.04	29.39	2.61	2.00	0.57	0.04	29.3	2.67	2.16	0.60	0.10
H-2'''	1.96	29.69	2.31	1.71	0.35	0.25	29.4	2.59	2.09	0.60	0.10
H-2'''	1.96	29.28	2.72	2.11	0.76	0.15	29.2	2.81	2.30	0.80	0.30
H-2'''	1.96	29.50	2.50	1.89	0.54	0.07	30.0	2.03	1.56	0.10	0.40
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|;										
	2A: Y = 1.0449X + 0.5193, R^2 = 0.9796, MAE = 0.65 ppm, CMAE = 0.22 ppm;										
	2B: Y = 1.0553X + 0.3864, R^2 = 0.9936, MAE = 0.55 ppm, CMAE = 0.14 ppm;										

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	Gas Phase		6-31G(d)		Shielding Tensors	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.00%	100.00%	-	-	-	-
sDP4+ (C data)	0.00%	100.00%	-	-	-	-
sDP4+ (all data)	0.00%	100.00%	-	-	-	-
uDP4+ (H data)	0.00%	100.00%	-	-	-	-
uDP4+ (C data)	0.00%	100.00%	-	-	-	-
uDP4+ (all data)	0.00%	100.00%	-	-	-	-
DP4+ (H data)	0.00%	100.00%	-	-	-	-
DP4+ (C data)	0.00%	100.00%	-	-	-	-
DP4+ (all data)	0.00%	100.00%	-	-	-	-

Figure S9. Detailed DP4+ probability of **2** calculated at mPW1PW91/6-31G* level in gas phase.

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCM		6-31G(d,p)		Shielding Tensors	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.00%	100.00%	-	-	-	-
sDP4+ (C data)	0.00%	100.00%	-	-	-	-
sDP4+ (all data)	0.00%	100.00%	-	-	-	-
uDP4+ (H data)	0.00%	100.00%	-	-	-	-
uDP4+ (C data)	0.00%	100.00%	-	-	-	-
uDP4+ (all data)	0.00%	100.00%	-	-	-	-
DP4+ (H data)	0.00%	100.00%	-	-	-	-
DP4+ (C data)	0.00%	100.00%	-	-	-	-
DP4+ (all data)	0.00%	100.00%	-	-	-	-

Figure S10. Detailed DP4+ probability of compound **2** calculated at mPW1PW91/6-31G** level in methanol with PCM model.

Experimental		mPW1PW91/6-31G* gas phase		mPW1PW91/6-31G** PCM		
δ ^{13}C	δ ^{1}H	σ ^{13}C	σ ^{1}H	sp2	σ ^{13}C	σ ^{1}H
38.2	1.04	155.0	30.94		156.27	30.3482
	2.64		29.24			28.8186
41.1	2.00	153.4	29.93		154.393	29.4386
82.2	4.47	112.094	27.139		112.368	26.5851
47.2	2.04	139.559	29.973		140.424	29.4348
37.4	2.39	159.158	29.438		159.882	29.0138
49.3		141.911			141.413	
205.2	9.08	-1.699	22.654	x	-5.5867	22.051
132.4		65.266		x	64.4539	
121.8	5.44	69.777	26.071	x	70.9373	25.3771
38.0	1.98	149.035	29.692		150.03	29.2153
36.1	1.80	158.860	29.911		159.97	29.2839
72.4	5.88	122.689	25.720		122.678	25.2972
92.3		100.032			100.319	
20.5	1.11	173.593	31.141		175.641	30.659
13.3	0.96	173.861	31.511		175.583	30.9023
23.8	1.63	168.419	30.475		170.591	29.9428
37.8	1.31	154.930	30.492		156.329	29.9117
	2.31		29.838			29.4507
15.8	0.95	173.790	30.857		175.745	30.6538
166.7		34.124		x	32.9263	
131.7		68.442		x	68.8476	
130.5	7.98	69.340	23.864	x	69.2682	23.0445
130.5	7.98	66.313	23.771	x	67.7775	23.1445
129.8	7.42	71.064	24.729	x	70.4937	23.8402
129.8	7.42	70.483	24.599	x	70.5929	23.7764
134.5	7.53	66.268	24.559	x	65.4342	23.6791
171.8		31.591		x	28.7965	
20.8	2.04	172.419	30.268		173.781	29.5796
171.4		31.523		x	29.1079	
22.4	1.96	171.045	30.302		172.198	29.6941

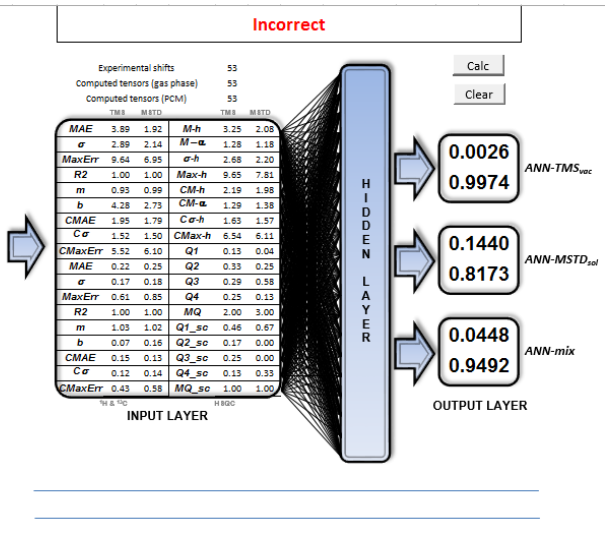


Figure S11. The result of ANN-PRA statistical analysis between compound **2** and isomer **2A**.

Experimental		mPW1PW91/6-31G* gas phase		mPW1PW91/6-31G** PCM		
δ ^{13}C	δ ^{1}H	σ ^{13}C	σ ^{1}H	sp2	σ ^{13}C	σ ^{1}H
38.2	1.04	157.5	30.93		158.809	30.3101
	2.64		29.25			28.8111
41.1	2.00	152.2	29.95		153.083	29.5021
82.2	4.47	113.854	27.494		113.97	27.0779
47.2	2.04	146.236	30.054		146.902	29.4567
37.4	2.39	156.731	29.510		157.538	29.007
49.3		144.611			144.014	
205.2	9.08	-3.253	22.594	x	-7.4729	22.0112
132.4		66.264		x	65.5873	
121.8	5.44	74.104	26.435	x	75.7929	25.7618
38.0	1.98	155.587	29.822		156.443	29.3391
36.1	1.80	157.053	30.199		157.925	29.638
72.4	5.88	123.413	25.964		123.547	25.5497
92.3		102.127			102.309	
20.5	1.11	173.238	31.153		175.337	30.6537
13.3	0.96	179.031	31.187		181.117	30.812
23.8	1.63	168.886	30.467		171.042	29.9587
37.8	1.31	157.889	30.911		159.358	30.3795
	2.31		29.906			29.2588
15.8	0.95	177.102	30.965		179.008	30.7364
166.7		35.269		x	33.6377	
131.7		67.646		x	68.4896	
130.5	7.98	66.122	23.769	x	67.9165	23.1868
130.5	7.98	69.807	23.960	x	69.2898	23.094
129.8	7.42	70.266	24.587	x	70.4418	23.7723
129.8	7.42	71.275	24.731	x	70.3452	23.8065
134.5	7.53	66.512	24.572	x	65.3117	23.6667
171.8		31.756		x	28.8662	
20.8	2.04	172.556	30.434		173.894	29.9004
171.4		31.331		x	28.8871	
22.4	1.96	171.434	30.053		172.597	29.4083

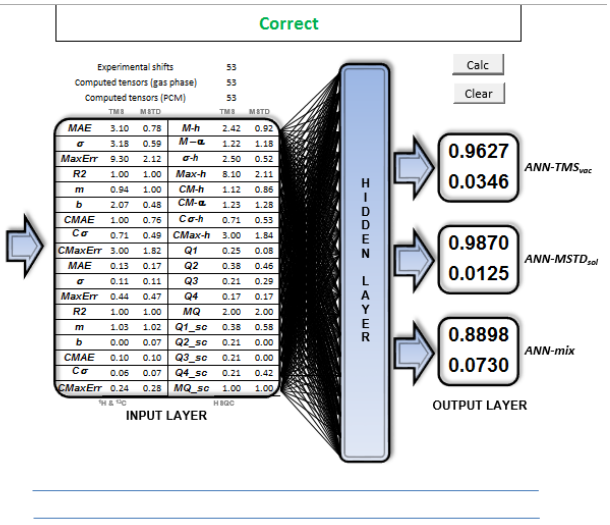


Figure S12. The result of ANN-PRA statistical analysis between compound **2** and isomer **2B**.

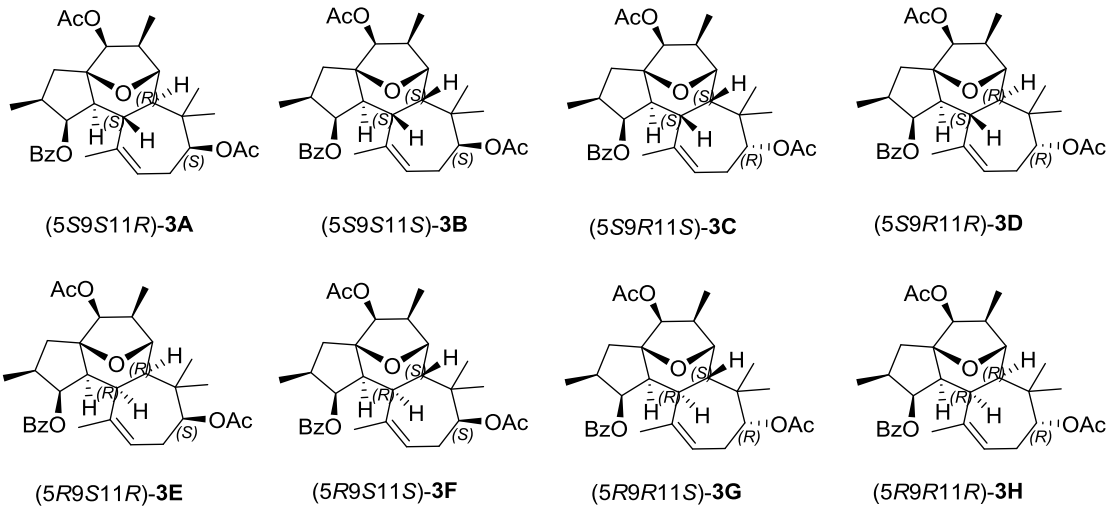


Figure S13. Possible isomers **3A−3H** of compound **3**.

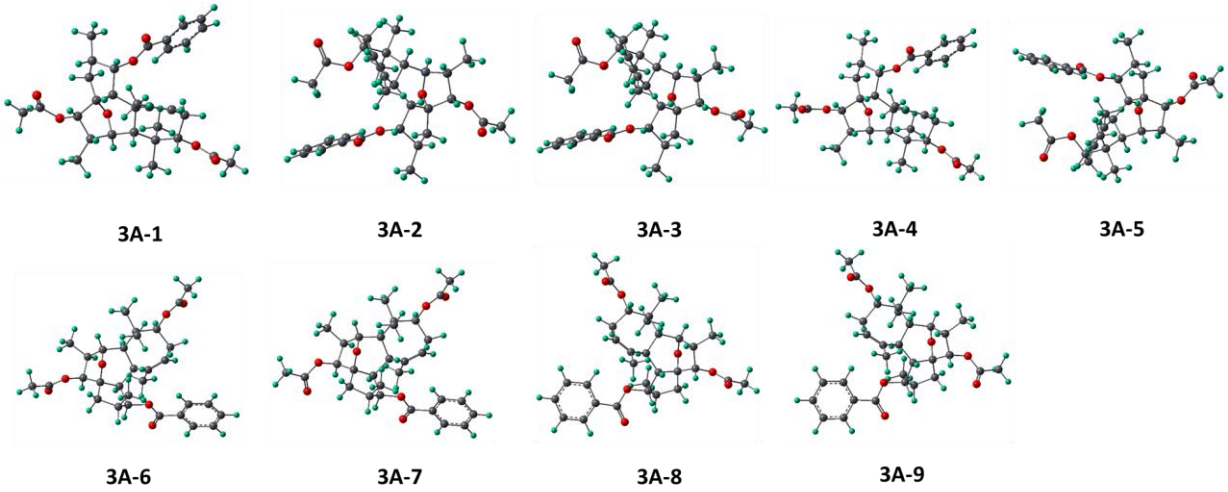


Figure S14. Key conformers of isomer **3A**.

Table S11. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **3A** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
3A-1	-1731.987491	0	45.88%	0
3A-2	-1731.984505	1.873290682	1.94%	0
3A-3	-1731.984542	1.8500668	2.02%	0
3A-4	-1731.987436	0.034117333	43.31%	0
3A-5	-1731.984102	2.126594778	1.26%	0
3A-6	-1731.984245	2.036918339	1.47%	0
3A-7	-1731.984042	2.164150827	1.19%	0
3A-8	-1731.983881	2.264990543	1.00%	0
3A-9	-1731.984505	1.873303232	1.94%	0

Table S12. Optimized Z-matrixes of isomer **3A** in the gas phase (Å) at B3LYP/6-31G* level.

3A-1				**3A-2**				**3A-3**			
C	-1.8149	-2.987	-1.0147	C	-2.7833	-1.4622	-0.9518	C	-2.6019	-1.7044	-1.1784
C	-0.5601	-2.5902	-0.2221	C	-1.4097	-1.7553	-0.3306	C	-1.3462	-1.8563	-0.3081

C	0.0308	-1.411	-1.0419	C	-0.4325	-0.908	-1.1959	C	-0.258	-1.0844	-1.1078
C	-1.1876	-0.816	-1.8086	C	-1.3164	0.2891	-1.6721	C	-1.0747	0.0208	-1.8473
C	-2.4075	-1.6331	-1.395	C	-2.7293	0.0491	-1.1433	C	-2.5557	-0.2284	-1.5599
C	0.809	-0.3341	-0.2245	C	0.9165	-0.4938	-0.4964	C	0.9563	-0.5506	-0.2575
C	0.1141	0.4584	-3.317	C	0.2185	1.1084	-3.2733	C	0.6759	0.733	-3.2657
C	-0.8881	-0.7037	-3.3131	C	-1.1873	0.5104	-3.19	C	-0.7127	0.1001	-3.3405
C	-2.7979	-3.8612	-0.2514	C	-3.9774	-1.8989	-0.1174	C	-3.9085	-2.0878	-0.5008
C	2.1572	-0.818	0.3029	C	1.9823	-1.6189	-0.4659	C	2.0249	-1.6273	0.0603
C	2.7207	-0.2339	1.3742	C	3.3016	-1.4235	-0.2532	C	3.2899	-1.3631	0.4525
C	2.1643	0.9782	2.0501	C	4.0434	-0.1748	0.1375	C	3.9361	-0.0544	0.8159
C	2.1869	2.2003	1.1156	C	3.2485	0.8916	0.9109	C	3.0083	1.0569	1.3368
C	0.9522	1.058	-0.9496	C	1.5212	0.8486	-1.0772	C	1.6174	0.7461	-0.878
C	-0.1921	1.21	-1.9978	C	0.4559	1.6697	-1.8503	C	0.669	1.4434	-1.8882
C	2.893	-1.9231	-0.4065	C	1.541	-3.0543	-0.649	C	1.6449	-3.0888	-0.0294
C	0.0384	1.3723	-4.5356	C	0.4114	2.1674	-4.3538	C	1.0313	1.6879	-4.3998
O	-2.0617	-0.3312	-4.0601	O	-2.1467	1.473	-3.6685	O	-1.6382	0.9728	-4.0186
H	0.6953	-1.8668	-1.7873	H	-0.206	-1.5105	-2.0854	H	0.1138	-1.7743	-1.8766
O	-1.3504	0.5591	-1.4376	O	-0.7824	1.5046	-1.1413	O	-0.663	1.3013	-1.366
C	-2.6779	-1.3272	-4.7505	C	-3.2034	0.9789	-4.3671	C	-1.9753	0.6308	-5.2903
C	-3.8613	-0.7817	-5.4884	C	-4.0896	2.1002	-4.8141	C	-2.9447	1.628	-5.8462
O	-2.3332	-2.5001	-4.7643	O	-3.4161	-0.2038	-4.592	O	-1.5537	-0.3394	-5.9026
C	1.0192	2.3051	0.0572	C	2.2687	1.7251	0.0165	C	2.1666	1.7575	0.2165
C	-0.3331	2.5449	0.7737	C	1.277	2.4827	0.9324	C	1.0291	2.5707	0.8806
C	1.3185	3.5942	-0.7709	C	3.1284	2.7985	-0.7132	C	3.1101	2.779	-0.4836
O	2.1487	3.3853	1.9583	O	2.5393	0.2812	2.0163	O	2.144	0.5389	2.3771
H	1.9075	1.0741	-1.4943	H	2.2896	0.5852	-1.8182	H	2.4977	0.4363	-1.4596
C	3.3399	3.8353	2.4381	C	3.2768	-0.0454	3.111	C	2.7031	0.3547	3.6028
C	3.1214	5.0615	3.2701	C	2.4088	-0.707	4.1353	C	1.6947	-0.2273	4.5436
O	4.4316	3.3255	2.2332	O	4.4702	0.1769	3.2601	O	3.8529	0.6336	3.9123
H	0.1781	-0.1441	0.6489	H	0.661	-0.3014	0.5492	H	0.536	-0.2606	0.7093
O	-0.9408	-2.1485	1.0901	O	-1.3905	-1.2911	1.0291	O	-1.5657	-1.2231	0.9625
C	-0.3026	-2.717	2.1418	C	-1.3907	-2.2235	2.0098	C	-1.7009	-2.0237	2.0453
C	-1.3286	-0.7844	5.8293	C	-1.3559	-0.4058	5.893	C	-2.3216	0.2667	5.6163
C	-0.4223	-1.8437	5.8088	C	-1.3123	-1.7927	5.7559	C	-2.2376	-1.1242	5.6685
C	-0.1024	-2.4655	4.6002	C	-1.3247	-2.3695	4.4843	C	-2.0361	-1.856	4.4965
C	-0.6895	-2.0306	3.4044	C	-1.3783	-1.5598	3.3417	C	-1.9152	-1.1983	3.2648
C	-1.5999	-0.9643	3.433	C	-1.421	-0.1656	3.4874	C	-2.0001	0.2008	3.2203
C	-1.9167	-0.3444	4.6439	C	-1.411	0.4073	4.7613	C	-2.2038	0.929	4.3947
O	0.4902	-3.6433	2.0912	O	-1.4015	-3.4337	1.8551	O	-1.6597	-3.2431	2.0501
H	-1.508	-3.513	-1.9287	H	-2.8427	-1.9493	-1.9345	H	-2.4831	-2.3141	-2.0844
H	0.1378	-3.433	-0.1864	H	-1.1842	-2.8228	-0.4058	H	-1.0885	-2.9138	-0.2041
H	-3.1667	-1.7295	-2.1738	H	-3.5238	0.394	-1.808	H	-3.2116	-0.027	-2.4122
H	-2.9051	-1.1652	-0.5354	H	-2.8752	0.5754	-0.1908	H	-2.9004	0.4095	-0.736
H	1.133	0.0517	-3.2855	H	0.9341	0.3034	-3.4844	H	1.4288	-0.0655	-3.2735
H	-0.4274	-1.6065	-3.7301	H	-1.2429	-0.4208	-3.7649	H	-0.6954	-0.8946	-3.7997
H	-3.1946	-3.3571	0.6359	H	-4.0189	-1.382	0.8466	H	-4.1236	-1.4573	0.3679
H	-3.6482	-4.125	-0.889	H	-4.9111	-1.6818	-0.647	H	-4.7451	-1.9811	-1.1995
H	-2.3163	-4.7896	0.0718	H	-3.9406	-2.9762	0.0737	H	-3.8782	-3.13	-0.1673
H	3.6825	-0.5845	1.7455	H	3.9619	-2.2919	-0.29	H	3.9644	-2.2062	0.6136
H	1.1673	0.79	2.4611	H	4.8645	-0.5068	0.7864	H	4.6505	-0.2872	1.6166
H	2.7854	1.1753	2.9335	H	4.5263	0.2517	-0.7481	H	4.5446	0.2949	-0.0249
H	3.1309	2.2061	0.5511	H	3.9695	1.5993	1.3438	H	3.6377	1.831	1.798
H	-0.4614	2.2465	-2.1988	H	0.6837	2.7361	-1.8896	H	0.8742	2.509	-2.0028
H	2.3669	-2.8757	-0.3086	H	0.8805	-3.3531	0.1684	H	0.8703	-3.3226	0.7049
H	3.0066	-1.6829	-1.4687	H	1.0393	-3.2032	-1.6083	H	1.3024	-3.3565	-1.0319
H	3.9014	-2.0708	-0.0038	H	2.3825	-3.7568	-0.6344	H	2.4869	-3.7552	0.1916
H	0.819	2.1389	-4.4841	H	1.4549	2.4995	-4.3774	H	2.0501	2.0686	-4.2694
H	-0.9254	1.8877	-4.6029	H	-0.2114	3.051	-4.1786	H	0.3592	2.5516	-4.4351
H	0.1876	0.8005	-5.4573	H	0.1642	1.7625	-5.3405	H	0.9877	1.1761	-5.3663
H	-4.3273	-1.583	-6.0689	H	-3.5223	2.7949	-5.4387	H	-3.2223	1.3357	-6.8629
H	-4.5938	-0.393	-4.7767	H	-4.9149	1.6957	-5.4069	H	-3.8481	1.6489	-5.2315
H	-3.5392	0.0032	-6.1774	H	-4.5029	2.6147	-3.943	H	-2.4795	2.6162	-5.8815
H	-1.1399	2.7415	0.0605	H	0.7091	3.2415	0.3845	H	0.5406	3.2484	0.173
H	-0.2889	3.4197	1.4322	H	1.8116	3.008	1.7328	H	1.4208	3.1945	1.693
H	-0.6377	1.6948	1.3887	H	0.5562	1.8082	1.4042	H	0.2555	1.9236	1.3048
H	0.5071	3.8597	-1.4531	H	2.5189	3.5194	-1.2653	H	2.5818	3.4148	-1.1996

H	1.4603	4.4689	-0.1265	H	3.7217	3.3811	0.0016	H	3.5709	3.4547	0.2466
H	2.2309	3.4717	-1.3653	H	3.8237	2.3425	-1.4255	H	3.9183	2.2764	-1.0248
H	2.6657	5.8461	2.6609	H	3.0357	-1.1117	4.9349	H	1.2449	-1.1196	4.1011
H	2.486	4.82	4.1258	H	1.7204	0.0259	4.5606	H	2.1926	-0.5219	5.4717
H	4.0842	5.4241	3.6412	H	1.862	-1.5363	3.6796	H	0.9323	0.5201	4.7718
H	-1.5769	-0.3007	6.771	H	-1.3492	0.0424	6.8838	H	-2.4811	0.8357	6.5293
H	0.037	-2.1859	6.7329	H	-1.2719	-2.4262	6.6387	H	-2.3318	-1.6401	6.621
H	0.6094	-3.2889	4.5936	H	-1.2937	-3.4532	4.3876	H	-1.9744	-2.9415	4.5471
H	-2.0676	-0.6024	2.5203	H	-1.463	0.4878	2.6187	H	-1.9098	0.7383	2.2789
H	-2.6226	0.4825	4.6614	H	-1.4462	1.4888	4.8694	H	-2.2702	2.0137	4.3551
3A-4				**3A-5**				**3A-6**			
C	-3.1071	-1.7975	-0.7902	C	-2.718	-1.5856	-0.1507	C	-3.0997	-0.7898	-0.0216
C	-1.7477	-2.0435	-0.1192	C	-1.2948	-2.1327	0.048	C	-1.8686	-1.7064	0.0756
C	-0.7576	-1.2422	-1.0061	C	-0.3739	-1.2883	-0.8784	C	-0.7927	-1.0886	-0.8614
C	-1.6228	-0.1095	-1.6295	C	-1.3456	-0.6933	-1.9314	C	-1.6087	-0.1913	-1.8265
C	-3.0511	-0.3088	-1.1276	C	-2.7346	-1.2546	-1.642	C	-3.0859	-0.3741	-1.4915
C	0.5122	-0.7004	-0.279	C	0.5092	-0.215	-0.1544	C	0.382	-0.3387	-0.1481
C	-0.0336	0.5182	-3.2628	C	0.314	0.1405	-3.3936	C	0.1338	0.2398	-3.3635
C	-1.4543	-0.0453	-3.156	C	-0.8481	-0.8534	-3.3738	C	-1.2497	-0.4092	-3.3007
C	-4.312	-2.1569	0.0656	C	-3.082	-0.3912	0.7292	C	-3.0919	0.4034	0.9328
C	1.5225	-1.7857	0.083	C	1.7326	-0.7946	0.5621	C	1.4276	-1.2689	0.4743
C	2.3976	-1.5966	1.0854	C	2.327	-0.1186	1.5608	C	2.2291	-0.836	1.4629
C	2.543	-0.309	1.8318	C	1.9235	1.2531	1.9984	C	2.2424	0.5695	1.9727
C	3.0398	0.8193	0.9111	C	2.1789	2.3005	0.903	C	2.7321	1.5583	0.9027
C	1.2139	0.5102	-1.003	C	0.9419	1.0044	-1.0574	C	1.0934	0.7595	-1.0307
C	0.1723	1.2391	-1.9054	C	-0.0386	1.131	-2.2577	C	0.129	1.2191	-2.1624
C	1.5817	-3.0594	-0.7171	C	2.3054	-2.1159	0.1227	C	1.5939	-2.6711	-0.0488
C	0.2206	1.4447	-4.4464	C	0.5422	0.8434	-4.7274	C	0.4741	0.9433	-4.6723
O	-2.4177	0.8723	-3.7093	O	-1.8597	-0.4343	-4.3116	O	-2.201	0.2914	-4.1256
H	-0.4658	-1.9163	-1.8217	H	0.2775	-2.0027	-1.396	H	-0.3841	-1.9206	-1.4473
O	-1.0954	1.1575	-1.2201	O	-1.3372	0.7342	-1.7745	O	-1.2026	1.1676	-1.615
C	-2.9314	0.5523	-4.9264	C	-2.5434	-1.4196	-4.9504	C	-2.5157	-0.289	-5.3137
C	-3.9169	1.5958	-5.3541	C	-3.5581	-0.8208	-5.8747	C	-3.52	0.5505	-6.0414
O	-2.6376	-0.4335	-5.5866	O	-2.3687	-2.6197	-4.7983	O	-2.0502	-1.3358	-5.7398
C	1.9564	1.5188	-0.001	C	1.1126	2.3819	-0.2583	C	1.6802	1.9919	-0.1919
C	0.9526	2.3122	0.8721	C	-0.238	2.9082	0.2838	C	0.5569	2.844	0.4465
C	2.738	2.5715	-0.8484	C	1.6496	3.4691	-1.2423	C	2.4558	2.9359	-1.1645
O	3.6446	1.8324	1.7619	O	2.2443	3.5985	1.5558	O	3.1887	2.7521	1.5967
H	2.0059	0.1173	-1.6571	H	1.94	0.7959	-1.4706	H	1.9715	0.3049	-1.5129
C	4.9491	1.6479	2.1025	C	3.4471	3.9621	2.0781	C	4.4668	2.7386	2.0637
C	5.4142	2.7822	2.963	C	3.3455	5.3275	2.6856	C	4.7809	4.0463	2.723
O	5.6484	0.703	1.7682	O	4.4645	3.2851	2.0664	O	5.2505	1.8053	1.972
H	0.1364	-0.2945	0.6647	H	-0.1447	0.1892	0.6252	H	-0.0999	0.1883	0.6819
O	-1.7688	-1.5132	1.2148	O	-0.8849	-2.1172	1.4155	O	-1.4143	-1.8787	1.4177
C	-1.4199	-2.354	2.2186	C	-1.3209	-3.1503	2.1782	C	-2.0809	-2.8005	2.1562
C	-1.1102	-0.2845	5.9611	C	0.0399	-2.837	6.2317	C	-0.523	-3.0959	6.1394
C	-0.8464	-1.6511	5.8793	C	-0.6458	-3.9705	5.797	C	-1.5116	-3.973	5.6953
C	-0.9561	-2.3112	4.6539	C	-1.0831	-4.0572	4.4737	C	-2.0093	-3.8635	4.3952
C	-1.3321	-1.6064	3.5025	C	-0.8345	-3.0092	3.5769	C	-1.5182	-2.8752	3.5312
C	-1.5956	-0.2319	3.5926	C	-0.1493	-1.8713	4.0229	C	-0.5281	-1.9944	3.9867
C	-1.4839	0.425	4.8202	C	0.2878	-1.7881	5.3469	C	-0.0317	-2.1074	5.2874
O	-1.1904	-3.5478	2.1136	O	-2.0099	-4.0824	1.7949	O	-3.0105	-3.4907	1.7689
H	-3.1518	-2.3732	-1.7246	H	-3.4511	-2.3733	0.0623	H	-4.0089	-1.3646	0.1929
H	-1.5108	-3.1121	-0.1349	H	-1.2571	-3.1635	-0.3349	H	-2.1256	-2.6863	-0.3537
H	-3.816	-0.0432	-1.8635	H	-2.8916	-2.1878	-2.1949	H	-3.511	-1.1889	-2.091
H	-3.2351	0.3085	-0.2391	H	-3.539	-0.5578	-1.8991	H	-3.678	0.5299	-1.6673
H	0.6742	-0.3157	-3.3524	H	1.2411	-0.3946	-3.1509	H	0.895	-0.5357	-3.2097
H	-1.5445	-1.0385	-3.61	H	-0.4949	-1.8666	-3.5961	H	-1.2219	-1.4767	-3.5473
H	-4.3589	-1.5599	0.9822	H	-2.4036	0.4537	0.5961	H	-2.2138	1.0396	0.8053
H	-5.2397	-1.9828	-0.4896	H	-4.0929	-0.0415	0.4933	H	-3.9773	1.0267	0.7672
H	-4.2807	-3.2137	0.3495	H	-3.0703	-0.6675	1.7883	H	-3.1168	0.0705	1.9753
H	3.1161	-2.3748	1.3383	H	3.1991	-0.5378	2.0604	H	2.9729	-1.5038	1.8952
H	1.6205	-0.0395	2.3561	H	0.8874	1.2727	2.3519	H	1.2688	0.8568	2.3833
H	3.2695	-0.4772	2.6374	H	2.5135	1.4982	2.8911	H	2.9152	0.5968	2.8397
H	3.8149	0.4226	0.2392	H	3.152	2.0991	0.4315	H	3.5874	1.1182	0.3692
H	0.3944	2.2948	-2.0595	H	-0.129	2.1453	-2.6445	H	0.3047	2.2405	-2.4979

H	0.684	-3.6637	-0.5655	H	1.602	-2.932	0.3115	H	0.7014	-3.2725	0.1465
H	1.6873	-2.8336	-1.7832	H	2.5475	-2.0887	-0.9447	H	1.788	-2.6539	-1.1262
H	2.4387	-3.682	-0.4368	H	3.2314	-2.3612	0.6545	H	2.4382	-3.1887	0.42
H	1.2646	1.7762	-4.4512	H	1.4218	1.4934	-4.6681	H	1.4871	1.3578	-4.6278
H	-0.4088	2.3399	-4.4094	H	-0.3103	1.4681	-5.0137	H	-0.2114	1.7705	-4.8834
H	0.0305	0.9273	-5.392	H	0.7155	0.1129	-5.5243	H	0.4379	0.2415	-5.5113
H	-4.3365	1.3213	-6.3262	H	-4.0904	-1.6213	-6.3963	H	-3.783	0.0644	-6.9852
H	-4.7317	1.6557	-4.6282	H	-4.2817	-0.2362	-5.301	H	-4.4259	0.6509	-5.4382
H	-3.4147	2.5616	-5.4506	H	-3.0586	-0.1939	-6.6176	H	-3.0923	1.5319	-6.2609
H	0.2632	2.9033	0.2609	H	-0.9693	3.0472	-0.5187	H	-0.1385	3.2269	-0.3073
H	1.4663	3.0247	1.5273	H	-0.1222	3.8854	0.7663	H	0.9636	3.7212	0.9623
H	0.3506	1.6632	1.5123	H	-0.6821	2.2374	1.0226	H	-0.0276	2.2837	1.1797
H	2.0806	3.2226	-1.4298	H	0.9211	3.7456	-2.0088	H	1.8013	3.4408	-1.8794
H	3.3343	3.2406	-0.2181	H	1.8975	4.4021	-0.7242	H	2.976	3.7369	-0.6276
H	3.4241	2.0778	-1.5457	H	2.5579	3.1226	-1.7479	H	3.2089	2.3773	-1.7315
H	5.3201	3.7243	2.417	H	4.3205	5.6195	3.0861	H	4.6706	4.8605	2.0023
H	4.8291	2.8114	3.8855	H	3.0528	6.0521	1.9215	H	5.8153	4.0341	3.0781
H	6.4666	2.6335	3.2213	H	2.6209	5.3159	3.5036	H	4.1192	4.1975	3.5795
H	-1.0241	0.2287	6.916	H	0.3806	-2.7704	7.2621	H	-0.1355	-3.1822	7.1517
H	-0.5539	-2.2038	6.7688	H	-0.8407	-4.7874	6.4875	H	-1.8958	-4.7426	6.3604
H	-0.7441	-3.3775	4.5991	H	-1.618	-4.946	4.144	H	-2.7813	-4.5527	4.058
H	-1.8849	0.3419	2.7152	H	0.049	-1.041	3.3509	H	-0.1355	-1.2143	3.3406
H	-1.6882	1.4909	4.8854	H	0.8213	-0.904	5.6872	H	0.7384	-1.4231	5.6352
3A-7				**3A-8**				**3A-9**			
C	-3.1001	-1.1019	0.0581	C	-3.2734	-0.5805	0.3009	C	-2.416	-2.1247	-1.0498
C	-1.7832	-1.8716	0.2535	C	-2.0934	-1.5669	0.3198	C	-1.2271	-1.9187	-0.1022
C	-0.7741	-1.2766	-0.7735	C	-1.0774	-1.0538	-0.7426	C	-0.2191	-1.167	-1.0065
C	-1.6746	-0.5629	-1.8168	C	-1.9164	-0.1069	-1.6384	C	-1.1205	-0.212	-1.8195
C	-3.1235	-0.8691	-1.4512	C	-3.3667	-0.203	-1.1762	C	-2.5492	-0.7721	-1.7546
C	0.3306	-0.3525	-0.1588	C	0.2148	-0.3866	-0.166	C	0.9639	-0.469	-0.2504
C	0.0322	-0.0679	-3.3762	C	-0.294	0.2345	-3.3234	C	0.0861	1.471	-3.067
C	-1.2746	-0.8551	-3.2685	C	-1.699	-0.3401	-3.1374	C	-0.4778	0.0554	-3.2083
C	-3.2243	0.1891	0.8654	C	-3.1168	0.6319	1.2177	C	-3.7035	-2.5587	-0.3653
C	1.4952	-1.1087	0.4817	C	1.2717	-1.3824	0.3137	C	2.2025	-1.4027	-0.1426
C	2.2225	-0.5359	1.4566	C	2.1631	-1.0262	1.2548	C	3.4821	-0.9976	-0.003
C	2.0427	0.8818	1.9014	C	2.276	0.3599	1.8072	C	4.0181	0.3738	0.2865
C	2.3989	1.8775	0.7814	C	2.7179	1.3649	0.7271	C	3.0867	1.2883	1.098
C	0.8991	0.7637	-1.1112	C	0.8947	0.6914	-1.09	C	1.3123	0.9652	-0.8312
C	-0.1019	1.0092	-2.2724	C	-0.1391	1.2092	-2.1283	C	0.112	1.6634	-1.5482
C	1.8872	-2.4654	-0.0401	C	1.3722	-2.7398	-0.33	C	1.9765	-2.9019	-0.1043
C	0.3131	0.5375	-4.7471	C	-0.0334	0.9229	-4.6583	C	-0.7796	2.5438	-3.738
O	-2.2432	-0.3082	-4.1861	O	-2.6799	0.4134	-3.8773	O	-1.3747	-0.032	-4.3226
H	-0.3056	-2.1331	-1.2722	H	-0.803	-1.926	-1.3474	H	0.1682	-1.9085	-1.7157
O	-1.4234	0.8486	-1.7212	O	-1.4173	1.2269	-1.4647	O	-1.1043	1.0504	-1.1267
C	-3.1215	-1.185	-4.739	C	-3.1295	-0.1456	-5.0318	C	-1.5304	-1.2781	-4.8493
C	-4.0563	-0.4608	-5.6579	C	-4.1443	0.7513	-5.6711	C	-2.4488	-1.2256	-6.0308
O	-3.1577	-2.3874	-4.5222	O	-2.7637	-1.2161	-5.4942	O	-1.0151	-2.2979	-4.4141
C	1.3118	2.1086	-0.3439	C	1.6051	1.8744	-0.2744	C	1.9596	1.951	0.2413
C	0.0834	2.8471	0.2393	C	0.5804	2.7648	0.4691	C	0.8968	2.534	1.2097
C	1.9686	3.0855	-1.3687	C	2.3452	2.8032	-1.2872	C	2.6078	3.1484	-0.5126
O	2.6768	3.1564	1.4158	O	3.2741	2.5191	1.4157	O	2.4979	0.5643	2.206
H	1.8356	0.402	-1.5613	H	1.7091	0.2118	-1.6532	H	2.0813	0.8195	-1.6032
C	3.9422	3.3499	1.8774	C	4.5856	2.4476	1.7716	C	3.2879	0.3184	3.2825
C	4.0603	4.7172	2.4774	C	4.9991	3.72	2.4451	C	2.5236	-0.4728	4.2995
O	4.8546	2.5387	1.8225	O	5.3264	1.4942	1.5821	O	4.4435	0.693	3.42
H	-0.1886	0.1721	0.6493	H	-0.1407	0.1494	0.7196	H	0.6319	-0.3178	0.7799
O	-1.3502	-1.7848	1.6126	O	-1.5501	-1.6747	1.637	O	-1.6362	-1.0957	1.0019
C	-0.9241	-2.9252	2.2055	C	-1.3108	-2.9195	2.1132	C	-1.336	-1.5277	2.249
C	0.5049	-2.2035	6.1837	C	0.5291	-2.808	5.985	C	-2.4965	1.3328	5.2236
C	0.5385	-3.4856	5.6369	C	0.2668	-4.0244	5.3563	C	-1.9455	0.1063	5.5928
C	0.0666	-3.7044	4.3411	C	-0.3355	-4.0437	4.0967	C	-1.5769	-0.8166	4.6121
C	-0.4427	-2.64	3.5848	C	-0.6795	-2.844	3.459	C	-1.7593	-0.5167	3.2552
C	-0.4741	-1.3539	4.1422	C	-0.4134	-1.6249	4.0983	C	-2.3142	0.7185	2.8915
C	-0.0002	-1.1386	5.4384	C	0.1902	-1.6095	5.3578	C	-2.6806	1.6394	3.8756
O	-0.9118	-4.0376	1.7031	O	-1.5549	-3.9692	1.54	O	-0.7876	-2.5786	2.5392
H	-3.9434	-1.7403	0.3501	H	-4.1891	-1.0983	0.6124	H	-2.1439	-2.8838	-1.7955

H	-1.978	-2.914	-0.0354	H	-2.4816	-2.5333	-0.0314	H	-0.8449	-2.8896	0.2243
H	-3.4513	-1.7967	-1.9341	H	-3.8825	-1.0078	-1.7149	H	-3.0304	-0.9016	-2.726
H	-3.8136	-0.0668	-1.7315	H	-3.9247	0.7271	-1.3261	H	-3.1969	-0.0992	-1.1778
H	0.8687	-0.7402	-3.1456	H	0.4347	-0.5816	-3.2365	H	1.0913	1.5442	-3.4978
H	-1.1029	-1.92	-3.4619	H	-1.7504	-1.4066	-3.3838	H	0.3737	-0.6133	-3.3919
H	-2.4041	0.8842	0.6769	H	-2.2048	1.1972	1.0157	H	-4.059	-1.8128	0.3532
H	-4.1589	0.7039	0.6184	H	-3.9647	1.3142	1.0948	H	-4.4966	-2.7111	-1.1048
H	-3.242	-0.0243	1.9393	H	-3.0941	0.3242	2.2683	H	-3.5547	-3.5015	0.1709
H	3.0593	-1.0716	1.9021	H	2.9223	-1.7333	1.5856	H	4.2644	-1.7581	0.0262
H	1.039	1.0564	2.3024	H	1.354	0.6731	2.3076	H	4.9268	0.2223	0.8842
H	2.7051	1.0412	2.7621	H	3.0206	0.3315	2.6132	H	4.3556	0.8468	-0.6411
H	3.3131	1.534	0.2753	H	3.5111	0.9087	0.1167	H	3.6935	2.0984	1.5268
H	-0.0397	2.0106	-2.6973	H	0.0652	2.2209	-2.4777	H	0.0474	2.7279	-1.3217
H	1.1098	-3.2076	0.153	H	0.491	-3.3488	-0.117	H	1.2887	-3.1595	0.7048
H	2.0694	-2.416	-1.1187	H	1.4772	-2.6356	-1.4149	H	1.5908	-3.2804	-1.0539
H	2.8078	-2.835	0.4251	H	2.2441	-3.3002	0.0252	H	2.8995	-3.459	0.095
H	1.2894	1.034	-4.7497	H	1.0005	1.2817	-4.7045	H	-0.3797	3.5426	-3.5324
H	-0.4369	1.2844	-5.0279	H	-0.689	1.7868	-4.809	H	-1.8142	2.5157	-3.3792
H	0.3281	-0.2404	-5.5173	H	-0.1819	0.2269	-5.4898	H	-0.7897	2.4138	-4.8252
H	-4.745	-1.178	-6.1134	H	-4.5152	0.2837	-6.5877	H	-2.0483	-0.54	-6.7819
H	-4.6378	0.2713	-5.0921	H	-4.9873	0.9008	-4.9918	H	-2.5233	-2.2217	-6.4762
H	-3.4888	0.0292	-6.4532	H	-3.6827	1.7078	-5.9288	H	-3.4443	-0.908	-5.7112
H	-0.6583	3.0716	-0.5336	H	-0.1625	3.1852	-0.2159	H	0.2063	3.2235	0.7156
H	0.3674	3.8094	0.6804	H	1.0687	3.6184	0.9529	H	1.3769	3.1044	2.014
H	-0.4162	2.2732	1.0227	H	0.0425	2.2212	1.2489	H	0.2966	1.7472	1.6748
H	1.2595	3.4569	-2.1131	H	1.6594	3.3515	-1.9383	H	1.873	3.7531	-1.0518
H	2.3759	3.977	-0.8788	H	2.9428	3.5676	-0.778	H	3.1142	3.8255	0.1854
H	2.7928	2.5971	-1.9002	H	3.0246	2.2242	-1.9226	H	3.35	2.8103	-1.2429
H	5.0839	4.8707	2.8312	H	4.8594	4.5625	1.7631	H	3.1921	-0.7521	5.1187
H	3.8368	5.4742	1.7215	H	4.4156	3.8623	3.3581	H	1.7069	0.1326	4.7
H	3.3796	4.8087	3.3275	H	6.058	3.661	2.7126	H	2.1362	-1.388	3.844
H	0.8738	-2.0339	7.1924	H	0.9995	-2.7941	6.9653	H	-2.7829	2.0515	5.9877
H	0.933	-4.3155	6.2179	H	0.5321	-4.9586	5.8452	H	-1.8027	-0.1321	6.6439
H	0.0994	-4.7084	3.9222	H	-0.5336	-4.9984	3.613	H	-1.1463	-1.7709	4.9095
H	-0.8601	-0.5094	3.5771	H	-0.6658	-0.6792	3.6253	H	-2.4581	0.9813	1.8453
H	-0.0243	-0.1393	5.866	H	0.3971	-0.6619	5.849	H	-3.1079	2.5972	3.5887

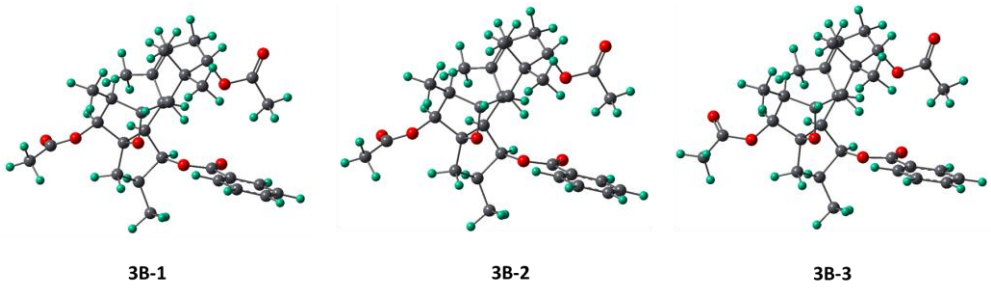


Figure S15. Key conformers of isomer **3B**.

Table S13. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **3B** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
3B-1	-1731.977572	3.13751E-05	33.83%	0
3B-2	-1731.977572	0	33.83%	0
3B-3	-1731.977529	0.026907324	32.33%	0

Table S14. Optimized Z-matrixes of isomer **3B** in the gas phase (Å) at B3LYP/6-31G* level.

3B-1				**3B-2**				**3B-3**			
C	-2.2229	-1.4161	2.2411	C	-2.7473	-1.1692	1.7606	C	-2.3283	-1.4112	2.2026
C	-0.8373	-1.5409	1.5865	C	-1.2604	-1.397	1.4487	C	-0.8987	-1.521	1.6436
C	-1.1651	-1.3267	0.0874	C	-1.2328	-1.2633	-0.0924	C	-1.1352	-1.371	0.1206
C	-2.1545	-0.1378	0.139	C	-2.1327	-0.0257	-0.3288	C	-2.1514	-0.2062	0.067

C	-2.9774	-0.3522	1.4164	C	-3.215	-0.0939	0.7587	C	-3.0514	-0.394	1.2952
C	0.1056	-1.1388	-0.8158	C	0.2157	-1.2026	-0.6941	C	0.1808	-1.184	-0.7139
C	-1.8863	0.853	-2.025	C	-1.3539	0.7671	-2.45	C	-1.799	0.6986	-2.1199
C	-2.9265	0.1165	-1.1575	C	-2.6002	0.1621	-1.7742	C	-2.8604	-0.0352	-1.2768
C	-2.2156	-1.103	3.7302	C	-3.0593	-0.8005	3.2035	C	-2.4252	-1.0494	3.6774
C	0.1279	-1.9748	-2.1061	C	0.4758	-2.1555	-1.872	C	0.3023	-2.0727	-1.9626
C	1.2195	-2.1107	-2.8851	C	1.7072	-2.4227	-2.3492	C	1.4448	-2.215	-2.6637
C	2.5753	-1.474	-2.8117	C	3.0469	-1.8411	-2.0063	C	2.7771	-1.539	-2.5332
C	2.8038	-0.2304	-1.939	C	3.1468	-0.5011	-1.2599	C	2.9153	-0.2454	-1.7157
C	0.4717	0.3844	-0.9606	C	0.6967	0.2837	-0.8761	C	0.5125	0.3411	-0.9076
C	-0.797	1.276	-1.02	C	-0.4751	1.2222	-1.2684	C	-0.7738	1.1927	-1.0774
C	-1.0657	-2.8258	-2.482	C	-0.6582	-2.9644	-2.4632	C	-0.8484	-2.9618	-2.3812
C	-2.455	2.0491	-2.7899	C	-1.6675	1.9179	-3.4072	C	-2.3503	1.8533	-2.9568
O	-4.0529	0.9869	-0.9095	O	-3.6878	1.1119	-1.8295	O	-4.0334	0.7851	-1.084
H	-1.7317	-2.2153	-0.208	H	-1.7768	-2.1387	-0.4604	H	-1.6616	-2.2843	-0.1739
O	-1.4167	1.0921	0.2707	O	-1.3595	1.1727	-0.1281	O	-1.457	1.0474	0.1856
C	-5.2842	0.4117	-0.9086	C	-4.9326	0.6098	-2.0404	C	-5.1274	0.4664	-1.8251
C	-6.3321	1.4501	-0.6505	C	-5.9335	1.7236	-2.0684	C	-6.2508	1.4034	-1.5038
O	-5.5151	-0.7763	-1.0813	O	-5.209	-0.5731	-2.177	O	-5.1965	-0.4425	-2.6395
C	1.6393	0.8104	-1.927	C	2.0603	0.5648	-1.6123	C	1.7222	0.7572	-1.8254
C	1.1763	1.1363	-3.3608	C	1.9281	0.7324	-3.1386	C	1.3352	0.9967	-3.2981
C	2.2526	2.1349	-1.3691	C	2.6105	1.9287	-1.084	C	2.2625	2.1265	-1.3015
O	3.1246	-0.6085	-0.5796	O	3.167	-0.7198	0.1716	O	3.1648	-0.5437	-0.3217
H	0.8888	0.6063	0.0334	H	0.9131	0.5762	0.1641	H	0.866	0.6183	0.0975
C	4.3977	-1.0278	-0.3468	C	4.3565	-1.1081	0.7083	C	4.434	-0.9065	0.0075
C	4.5711	-1.3662	1.1011	C	4.2241	-1.2897	2.1876	C	4.5299	-1.1628	1.4793
O	5.2869	-1.1003	-1.1832	O	5.3982	-1.265	0.0869	O	5.3738	-0.9923	-0.7702
H	0.916	-1.6002	-0.2322	H	0.852	-1.6357	0.0923	H	0.9677	-1.5946	-0.0638
O	0.0428	-0.5217	2.0757	O	-0.4638	-0.3816	2.0695	O	-0.0772	-0.46	2.1452
C	1.0262	-0.8971	2.9248	C	0.343	-0.7512	3.0893	C	0.8524	-0.7747	3.0757
C	3.3532	2.4617	4.2238	C	2.3574	2.6416	4.7633	C	3.0281	2.688	4.3639
C	2.2814	2.6709	3.3567	C	1.492	2.8368	3.6871	C	2.0129	2.8346	3.4192
C	1.5074	1.5908	2.9266	C	0.8092	1.7523	3.1321	C	1.2883	1.72	2.9911
C	1.8076	0.292	3.361	C	1.0395	0.441	3.644	C	1.5816	0.4492	3.5057
C	2.8827	0.0916	4.2379	C	1.8584	0.2776	4.7398	C	2.5994	0.3118	4.4598
C	3.6535	1.1741	4.6663	C	2.5407	1.3639	5.2904	C	3.3208	1.4287	4.8859
O	1.2644	-2.0349	3.2963	O	0.4968	-1.8833	3.5154	O	1.0844	-1.8889	3.5163
H	-2.7457	-2.3727	2.0998	H	-3.2864	-2.0976	1.5245	H	-2.8182	-2.3848	2.0604
H	-0.4198	-2.5434	1.7367	H	-0.9471	-2.4042	1.7458	H	-0.4661	-2.5052	1.8583
H	-3.9749	-0.7468	1.1997	H	-4.1837	-0.4098	0.3605	H	-4.027	-0.8118	1.0202
H	-3.0978	0.5833	1.9745	H	-3.3512	0.8791	1.2448	H	-3.2244	0.5574	1.811
H	-1.4708	0.1703	-2.7701	H	-0.8366	0.0017	-3.0335	H	-1.3253	0.0013	-2.8151
H	-3.2557	-0.8067	-1.6399	H	-2.8866	-0.7786	-2.251	H	-3.1382	-1.005	-1.6966
H	-1.6552	-1.8638	4.2827	H	-2.6935	-1.5736	3.887	H	-1.8852	-1.7778	4.2906
H	-1.7671	-0.1265	3.94	H	-2.6036	0.1531	3.4898	H	-2.0131	-0.0559	3.8821
H	-3.2382	-1.0879	4.122	H	-4.141	-0.7069	3.3484	H	-3.4712	-1.0466	4.0017
H	1.1535	-2.794	-3.7349	H	1.7951	-3.1811	-3.1312	H	1.4486	-2.9338	-3.4863
H	3.2869	-2.2626	-2.5402	H	3.6103	-2.6167	-1.4738	H	3.4875	-2.2926	-2.1736
H	2.8236	-1.1869	-3.843	H	3.5605	-1.7029	-2.968	H	3.0876	-1.2983	-3.5596
H	3.6862	0.2769	-2.3563	H	4.119	-0.0706	-1.5412	H	3.8059	0.2685	-2.1066
H	-0.5394	2.3346	-1.1032	H	-0.1434	2.2584	-1.3696	H	-0.5389	2.2535	-1.1928
H	-0.9289	-3.341	-3.44	H	-0.3427	-3.5567	-3.3303	H	-0.6392	-3.5112	-3.3065
H	-1.2372	-3.6056	-1.7336	H	-1.0525	-3.6745	-1.7296	H	-1.0558	-3.7153	-1.615
H	-1.9644	-2.2195	-2.5941	H	-1.4616	-2.3182	-2.8178	H	-1.7481	-2.3785	-2.5769
H	-2.8116	2.8341	-2.1144	H	-0.7581	2.2711	-3.9021	H	-2.7963	2.6345	-2.332
H	-3.2874	1.7384	-3.4299	H	-2.1075	2.7748	-2.8861	H	-3.1083	1.4957	-3.6608
H	-1.6922	2.4962	-3.4342	H	-2.3633	1.5925	-4.1874	H	-1.5546	2.3216	-3.544
H	-6.2877	2.2217	-1.4234	H	-6.9297	1.3114	-2.2522	H	-5.9643	2.4263	-1.7606
H	-7.3206	0.9833	-0.6824	H	-5.941	2.2382	-1.1042	H	-7.1313	1.1288	-2.0917
H	-6.1832	1.8876	0.3398	H	-5.6907	2.4201	-2.8748	H	-6.5039	1.3286	-0.4432
H	0.5943	0.3327	-3.8159	H	1.4181	-0.1024	-3.6208	H	0.8034	0.1542	-3.7441
H	0.5611	2.0406	-3.3862	H	1.3772	1.6415	-3.3936	H	0.697	1.8789	-3.4052
H	2.0369	1.3268	-4.0131	H	2.9155	0.8251	-3.605	H	2.2269	1.1812	-3.909
H	3.0928	2.4705	-1.9887	H	3.5868	2.1569	-1.5287	H	3.13	2.4561	-1.8858
H	1.5248	2.9518	-1.3539	H	1.9496	2.7646	-1.3328	H	1.513	2.9205	-1.3735
H	2.6301	2.0075	-0.3484	H	2.7408	1.9199	0.0043	H	2.5791	2.0628	-0.2544

H	5.5059	-1.9179	1.2344	H	3.2999	-1.824	2.4189	H	5.4737	-1.6704	1.6975
H	4.6105	-0.4466	1.6886	H	5.059	-1.8934	2.5526	H	4.5006	-0.2134	2.0177
H	3.7507	-2.0054	1.4375	H	4.2399	-0.315	2.6781	H	3.7134	-1.815	1.8001
H	3.9531	3.3048	4.5586	H	2.8869	3.4881	5.1942	H	3.5894	3.5578	4.6969
H	2.0446	3.6761	3.0162	H	1.3455	3.8345	3.28	H	1.7819	3.8178	3.0164
H	0.6722	1.7778	2.2545	H	0.1367	1.9278	2.2945	H	0.4967	1.8584	2.2574
H	3.1244	-0.9097	4.5894	H	2.0064	-0.7157	5.1591	H	2.8349	-0.667	4.8736
H	4.4865	1.0124	5.346	H	3.2132	1.2133	6.1314	H	4.1094	1.3159	5.6259

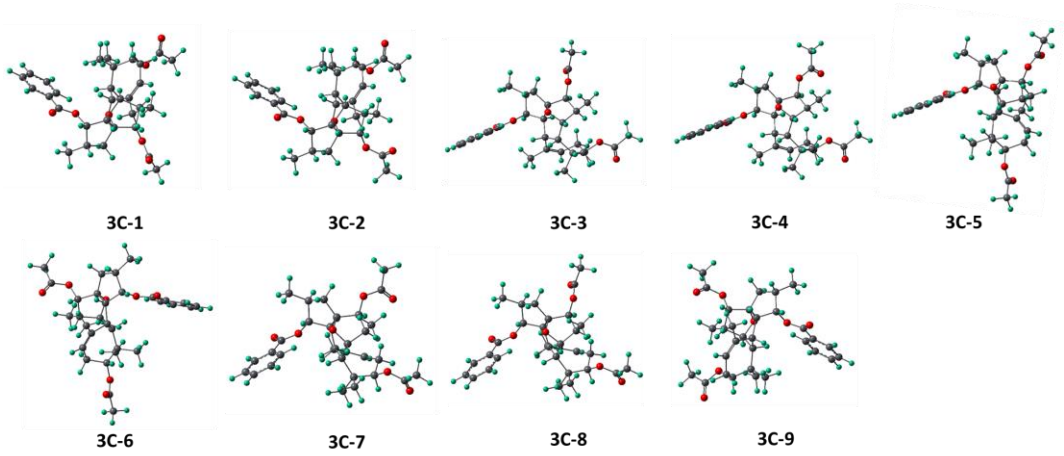


Figure S16. Key conformers of isomer **3C**.

Table S15. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **3C** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
3C-1	-1731.97338	0	26.98%	0
3C-2	-1731.973347	0.020745246	26.05%	0
3C-3	-1731.9723	0.677765882	8.59%	0
3C-4	-1731.972226	0.724201097	7.94%	0
3C-5	-1731.970019	2.108968222	0.77%	0
3C-6	-1731.970043	2.093701076	0.79%	0
3C-7	-1731.970696	1.683791082	1.57%	0
3C-8	-1731.970502	1.805928246	1.28%	0
3C-9	-1731.973347	0.020751521	26.05%	0

Table S16. Optimized Z-matrixes of isomer **3C** in the gas phase (Å) at B3LYP/6-31G* level.

3C-1				**3C-2**				**3C-3**			
C	-1.9964	-3.0905	0.7479	C	-1.7111	-3.3464	0.698	C	-2.0085	-2.4478	-0.8282
C	-0.5082	-2.6871	0.824	C	-0.2706	-2.8019	0.8194	C	-0.6992	-2.3367	-0.0313
C	-0.317	-1.8661	-0.4713	C	-0.1306	-1.9454	-0.4585	C	-0.1619	-0.9373	-0.4495
C	-1.6081	-1.0329	-0.5394	C	-1.4921	-1.2345	-0.5368	C	-1.4498	-0.1143	-0.7592
C	-2.7074	-1.9878	-0.07	C	-2.5063	-2.2991	-0.1146	C	-2.6315	-1.072	-0.6017
C	1.0032	-1.0293	-0.579	C	1.1075	-0.9898	-0.5287	C	0.8176	-0.2622	0.561
C	-1.1002	1.0511	-1.6378	C	-1.1714	0.8898	-1.621	C	-0.4146	1.7796	-1.7553
C	-1.7659	-0.3206	-1.8897	C	-1.7069	-0.5343	-1.8839	C	-1.3476	0.6143	-2.1082
C	-2.6632	-3.3464	2.0927	C	-2.379	-3.6939	2.0215	C	-2.9426	-3.5749	-0.4177
C	1.594	-1.0594	-1.9971	C	1.7339	-0.964	-1.9303	C	2.1847	-0.9413	0.5173
C	2.1818	-0.0778	-2.7071	C	2.2238	0.0721	-2.6366	C	3.1814	-0.581	-0.3096
C	2.5623	1.352	-2.4706	C	2.4326	1.5379	-2.4069	C	3.092	0.5068	-1.3201
C	2.2797	2.1346	-1.1817	C	2.0777	2.2847	-1.1139	C	3.0227	1.9354	-0.7559
C	0.8156	0.3637	0.0964	C	0.7767	0.3772	0.1433	C	0.7679	1.325	0.56
C	-0.5863	0.9759	-0.1913	C	-0.6724	0.8544	-0.1648	C	-0.4684	1.86	-0.22
C	1.6462	-2.4425	-2.6384	C	1.9579	-2.3373	-2.5547	C	2.4215	-2.0507	1.5135

C	-2.0786	2.2228	-1.7905	C	-2.2449	1.9753	-1.7722	C	-0.782	3.1022	-2.4255
O	-3.1492	-0.1523	-2.2535	O	-3.107	-0.5434	-2.2215	O	-2.6266	1.132	-2.5266
H	-0.3749	-2.6048	-1.2783	H	-0.1048	-2.6723	-1.278	H	0.3664	-1.099	-1.4002
O	-1.5226	0.0517	0.406	O	-1.5249	-0.1579	0.4164	O	-1.5522	0.9782	0.1619
C	-3.6581	-1.0572	-3.1317	C	-3.4034	-0.5209	-3.5489	C	-3.2422	0.478	-3.5475
C	-5.0868	-0.7262	-3.435	C	-4.8889	-0.5413	-3.739	C	-4.539	1.1509	-3.8765
O	-3.0548	-2.0127	-3.5984	O	-2.5901	-0.4816	-4.4604	O	-2.8167	-0.5191	-4.1125
C	2.0489	1.3314	0.117	C	1.9112	1.4587	0.1808	C	2.1056	2.1698	0.4977
C	3.3444	0.5587	0.4824	C	3.2711	0.8136	0.5597	C	2.9444	1.9019	1.7887
C	1.8485	2.3583	1.2752	C	1.6	2.457	1.3396	C	1.7647	3.6866	0.5985
O	1.1897	3.0648	-1.3993	O	0.9102	3.1154	-1.3339	O	2.5848	2.8044	-1.8333
H	0.7372	0.0946	1.1585	H	0.7085	0.0985	1.2042	H	0.4379	1.5191	1.5981
C	1.5246	4.2338	-2.0203	C	1.1419	4.3097	-1.954	C	3.5331	3.2161	-2.7186
C	0.333	5.1331	-2.1284	C	-0.1274	5.0932	-2.0781	C	2.9117	4.1085	-3.7487
O	2.633	4.5162	-2.4536	O	2.2244	4.6941	-2.3738	O	4.7148	2.9071	-2.693
H	1.7498	-1.5753	0.0155	H	1.8863	-1.4652	0.085	H	0.428	-0.4945	1.563
O	-0.2726	-1.9224	2.0107	O	-0.1392	-2.034	2.0199	O	-0.9816	-2.351	1.3797
C	0.8371	-2.2085	2.731	C	0.9779	-2.2174	2.7619	C	-0.8106	-3.5224	2.0377
C	1.2006	0.3659	6.1403	C	1.0207	0.3508	6.1948	C	-1.6881	-3.1249	6.2152
C	0.1132	0.523	5.2816	C	-0.054	0.4168	5.3086	C	-1.8493	-2.0214	5.3778
C	-0.0257	-0.3091	4.1685	C	-0.0889	-0.4152	4.1874	C	-1.57	-2.1305	4.0135
C	0.9275	-1.3049	3.9103	C	0.9563	-1.3194	3.9487	C	-1.1263	-3.3497	3.4814
C	2.0179	-1.4552	4.7777	C	2.0332	-1.3783	4.8434	C	-0.9679	-4.4539	4.3297
C	2.1526	-0.6217	5.8897	C	2.0637	-0.5453	5.9635	C	-1.2482	-4.3405	5.6928
O	1.6697	-3.06	2.465	O	1.8937	-2.9828	2.5081	O	-0.443	-4.5767	1.5456
H	-2.0589	-4.0175	0.1604	H	-1.6706	-4.2618	0.091	H	-1.7682	-2.5646	-1.8937
H	0.1139	-3.5896	0.8016	H	0.4369	-3.6393	0.8013	H	0.0144	-3.1207	-0.3086
H	-3.2105	-2.4755	-0.9101	H	-2.9397	-2.8027	-0.9868	H	-3.4557	-0.8914	-1.2946
H	-3.4686	-1.4668	0.5215	H	-3.3266	-1.866	0.4686	H	-3.0563	-0.9902	0.4074
H	-0.2857	1.2143	-2.3449	H	-0.365	1.1276	-2.3156	H	0.5867	1.5199	-2.0853
H	-1.2316	-0.8415	-2.692	H	-1.1357	-1.0447	-2.6677	H	-0.9013	-0.0064	-2.8932
H	-2.7092	-2.4384	2.703	H	-2.5255	-2.8079	2.6481	H	-3.2922	-3.4678	0.6139
H	-3.6892	-3.7012	1.9491	H	-3.3627	-4.1424	1.847	H	-3.8279	-3.5874	-1.0626
H	-2.1178	-4.1107	2.6556	H	-1.7746	-4.4142	2.5822	H	-2.4443	-4.5445	-0.5143
H	2.5403	-0.3686	-3.7006	H	2.6329	-0.183	-3.6205	H	4.1352	-1.1053	-0.2651
H	3.6545	1.3693	-2.602	H	3.5132	1.6851	-2.5517	H	3.9714	0.4336	-1.9739
H	2.1631	1.9161	-3.3239	H	1.9598	2.0483	-3.2564	H	2.2599	0.3023	-2.0007
H	3.1764	2.7447	-0.9933	H	2.9154	2.9713	-0.9174	H	4.039	2.2416	-0.4699
H	-0.7046	1.926	0.3351	H	-0.8878	1.7853	0.3651	H	-0.74	2.86	0.1326
H	0.6941	-2.6821	-3.122	H	1.0553	-2.6818	-3.0687	H	1.8581	-2.9438	1.2371
H	2.4285	-2.5207	-3.4022	H	2.7716	-2.3349	-3.2892	H	3.4779	-2.3364	1.5675
H	1.8748	-3.2075	-1.8883	H	2.2398	-3.0686	-1.7893	H	2.1235	-1.7372	2.5192
H	-1.5948	3.1683	-1.5363	H	-1.858	2.9499	-1.4659	H	-0.0384	3.8723	-2.2008
H	-2.9452	2.1182	-1.1282	H	-3.1228	1.77	-1.1498	H	-1.7533	3.4765	-2.0851
H	-2.4367	2.2995	-2.8224	H	-2.5687	2.0651	-2.8136	H	-0.8188	2.9867	-3.5138
H	-5.154	0.2834	-3.8485	H	-5.3314	0.3521	-3.2915	H	-4.3561	2.191	-4.1579
H	-5.4724	-1.4307	-4.1775	H	-5.1174	-0.5468	-4.8086	H	-5.0081	0.6401	-4.7222
H	-5.6869	-0.8109	-2.5257	H	-5.3077	-1.4453	-3.2898	H	-5.2121	1.0968	-3.0172
H	3.2158	-0.004	1.4143	H	3.186	0.2356	1.4874	H	2.3483	2.0847	2.6907
H	4.1839	1.2481	0.6326	H	4.0373	1.5807	0.7245	H	3.8093	2.5752	1.8374
H	3.6544	-0.1478	-0.2912	H	3.6591	0.1455	-0.2126	H	3.3394	0.8901	1.865
H	0.976	3.0004	1.1262	H	0.6702	3.0111	1.184	H	1.1781	4.0462	-0.2499
H	1.7249	1.8505	2.2387	H	1.5173	1.9359	2.3004	H	1.1909	3.9024	1.5075
H	2.7185	3.0196	1.3677	H	2.4002	3.1999	1.4424	H	2.678	4.2927	0.6351
H	-0.1773	5.1963	-1.1638	H	-0.6479	5.1174	-1.1172	H	2.469	4.982	-3.2636
H	0.6641	6.1398	-2.3995	H	0.1106	6.1237	-2.3575	H	3.6826	4.4504	-4.445
H	-0.3423	4.7596	-2.9012	H	-0.7597	4.6515	-2.8513	H	2.1545	3.5547	-4.3094
H	1.3064	1.0146	7.0066	H	1.0455	0.9994	7.0673	H	-1.9068	-3.0376	7.2768
H	-0.6278	1.2943	5.4771	H	-0.8659	1.1172	5.4888	H	-2.1941	-1.0746	5.7866
H	-0.8782	-0.1654	3.5073	H	-0.9333	-0.3427	3.5046	H	-1.7049	-1.2574	3.379
H	2.7673	-2.2217	4.5892	H	2.8532	-2.0726	4.6701	H	-0.6255	-5.4073	3.9313
H	3.0003	-0.7433	6.5595	H	2.9016	-0.5956	6.6546	H	-1.1237	-5.2008	6.3459
3C-4				**3C-5**				**3C-6**			
C	-2.1495	-2.3797	-0.8553	C	-2.2111	-3.1212	0.0277	C	-2.2235	-3.1822	-0.12
C	-0.8199	-2.3527	-0.0866	C	-0.7727	-2.64	0.3156	C	-0.8039	-2.7066	0.2595
C	-0.231	-0.9658	-0.4727	C	-0.5112	-1.6629	-0.8521	C	-0.4814	-1.708	-0.8733

C	-1.4884	-0.0734	-0.6962	C	-1.8468	-0.9002	-0.9669	C	-1.8079	-0.9377	-1.0335
C	-2.7107	-0.9868	-0.573	C	-2.9186	-1.9641	-0.7146	C	-2.8959	-2.0004	-0.8553
C	0.8158	-0.383	0.528	C	0.768	-0.757	-0.7357	C	0.7946	-0.8115	-0.6808
C	-0.4118	1.8243	-1.6371	C	-1.3218	1.3058	-1.7933	C	-1.238	1.2631	-1.8306
C	-1.4104	0.7227	-2.0074	C	-1.9587	-0.0334	-2.2296	C	-1.8716	-0.0668	-2.2945
C	-3.1218	-3.4803	-0.4615	C	-2.987	-3.5973	1.2482	C	-3.0579	-3.7024	1.0424
C	2.148	-1.1175	0.3966	C	1.4369	-0.6084	-2.1255	C	1.5359	-0.6559	-2.032
C	3.1274	-0.7592	-0.4516	C	1.9939	0.493	-2.6656	C	2.1172	0.4494	-2.5374
C	3.0482	0.3815	-1.4033	C	2.2971	1.8026	-2.0167	C	2.3819	1.7568	-1.8671
C	3.0625	1.7822	-0.7685	C	2.7435	1.6238	-0.5696	C	2.7645	1.5677	-0.4032
C	0.8359	1.2022	0.6062	C	0.4084	0.5448	0.0774	C	0.4007	0.4853	0.1227
C	-0.4052	1.8261	-0.0968	C	-0.9944	1.1077	-0.3085	C	-0.9779	1.0587	-0.3302
C	2.3723	-2.2835	1.3292	C	1.5888	-1.8824	-2.9427	C	1.735	-1.9259	-2.8446
C	-0.7339	3.2	-2.2163	C	-2.2249	2.5264	-1.9924	C	-2.1119	2.4999	-2.0563
O	-2.7042	1.282	-2.3134	O	-3.3355	0.178	-2.6009	O	-3.2481	0.1075	-2.685
H	0.2528	-1.1111	-1.4492	H	-0.4492	-2.3091	-1.7337	H	-0.3802	-2.3367	-1.7639
O	-1.5113	0.9696	0.2841	O	-1.9255	0.0748	0.0872	O	-1.9303	0.0283	0.0214
C	-3.0453	1.3427	-3.628	C	-3.8135	-0.5843	-3.62	C	-3.4859	0.2302	-4.0182
C	-4.4168	1.9268	-3.7721	C	-5.24	-0.2245	-3.9004	C	-4.9545	0.398	-4.2596
O	-2.344	0.9853	-4.5631	O	-3.1877	-1.4483	-4.217	O	-2.6381	0.2147	-4.8984
C	2.2068	1.9907	0.5322	C	1.5594	1.5775	0.4357	C	1.5372	1.5082	0.5482
C	3.0824	1.6207	1.7725	C	2.1821	1.1354	1.7985	C	2.0983	1.0424	1.9296
C	1.9389	3.5133	0.7237	C	1.0016	3.0017	0.685	C	0.9717	2.9296	0.7956
O	2.6186	2.7207	-1.7831	O	3.6219	2.724	-0.213	O	3.6225	2.6673	0.0014
H	0.5542	1.3579	1.6648	H	0.1826	0.1354	1.0703	H	0.1227	0.0684	1.0996
C	3.5444	3.1315	-2.6923	C	4.9306	2.6035	-0.5669	C	4.9464	2.5526	-0.2933
C	2.9176	4.0915	-3.6561	C	5.6975	3.7985	-0.09	C	5.6866	3.7479	0.2235
O	4.7121	2.7742	-2.7317	O	5.4202	1.6719	-1.1879	O	5.4671	1.6254	-0.8951
H	0.4566	-0.6481	1.5331	H	1.5085	-1.3114	-0.1418	H	1.4999	-1.3752	-0.0537
O	-1.0717	-2.4012	1.329	O	-0.7229	-2.0105	1.5992	O	-0.8281	-2.0975	1.5535
C	-0.9319	-3.5988	1.9459	C	0.3054	-2.3361	2.4165	C	0.1605	-2.4258	2.4175
C	-1.6843	-3.2992	6.1557	C	0.0461	-0.2674	6.1628	C	-0.2954	-0.3978	6.1671
C	-1.8178	-2.1632	5.3579	C	-0.9344	-0.0493	5.1954	C	-1.2211	-0.1651	5.1504
C	-1.5784	-2.24	3.9838	C	-0.8702	-0.7171	3.9705	C	-1.0926	-0.8197	3.9233
C	-1.2027	-3.4594	3.4022	C	0.1801	-1.609	3.7091	C	-0.0327	-1.7129	3.7096
C	-1.0716	-4.5965	4.211	C	1.1618	-1.8217	4.6863	C	0.8939	-1.94	4.736
C	-1.3119	-4.5152	5.584	C	1.0935	-1.1523	5.9096	C	0.7614	-1.2838	5.9613
O	-0.6217	-4.6507	1.4111	O	1.222	-3.0973	2.1539	O	1.0932	-3.1796	2.1924
H	-1.9369	-2.4707	-1.9293	H	-2.1442	-3.9625	-0.6766	H	-2.117	-3.9975	-0.8494
H	-0.1491	-3.1577	-0.4067	H	-0.087	-3.4938	0.2616	H	-0.1151	-3.559	0.2296
H	-3.5184	-0.7468	-1.2707	H	-3.3159	-2.3685	-1.6506	H	-3.2589	-2.3632	-1.8243
H	-3.1362	-0.9238	0.4367	H	-3.7582	-1.5617	-0.137	H	-3.7538	-1.6087	-0.2974
H	0.5624	1.5346	-2.0187	H	-0.4235	1.5	-2.3738	H	-0.3131	1.4447	-2.3715
H	-1.0505	0.0949	-2.8303	H	-1.3975	-0.4571	-3.0697	H	-1.3011	-0.533	-3.1055
H	-3.4435	-3.3945	0.5812	H	-3.1625	-2.785	1.9613	H	-3.2714	-2.9164	1.7742
H	-4.0208	-3.4336	-1.0854	H	-3.9638	-3.9925	0.9497	H	-4.0172	-4.0884	0.6816
H	-2.6673	-4.466	-0.6021	H	-2.4438	-4.3953	1.7646	H	-2.5383	-4.5173	1.5568
H	4.0582	-1.3248	-0.4708	H	2.4053	0.4212	-3.6746	H	2.58	0.3841	-3.5244
H	3.8986	0.3043	-2.094	H	3.1153	2.2604	-2.5883	H	3.2217	2.2243	-2.398
H	2.1831	0.2462	-2.0597	H	1.4685	2.5076	-2.1209	H	1.5539	2.4573	-2.0018
H	4.1014	2.0327	-0.5113	H	3.319	0.6928	-0.4646	H	3.338	0.6375	-0.2808
H	-0.6209	2.8164	0.3165	H	-1.2555	1.9801	0.2931	H	-1.2632	1.9301	0.2617
H	1.7496	-3.1329	1.0422	H	0.6776	-2.0949	-3.5102	H	0.8588	-2.1349	-3.4659
H	3.4133	-2.625	1.318	H	2.4122	-1.8156	-3.6635	H	2.5998	-1.8564	-3.5147
H	2.1387	-2.0026	2.3613	H	1.8196	-2.732	-2.2911	H	1.9257	-2.779	-2.1845
H	0.0386	3.9264	-1.949	H	-1.7057	3.439	-1.6798	H	-1.6049	3.397	-1.6843
H	-1.6885	3.5867	-1.8442	H	-3.1462	2.4521	-1.4046	H	-3.0718	2.4219	-1.5347
H	-0.7779	3.1604	-3.3093	H	-2.4938	2.6444	-3.0474	H	-2.3054	2.6545	-3.1223
H	-5.1417	1.3068	-3.2386	H	-5.3115	0.8354	-4.1578	H	-5.3064	1.3136	-3.7778
H	-4.426	2.9491	-3.386	H	-5.602	-0.8122	-4.7488	H	-5.1386	0.4755	-5.335
H	-4.6917	1.9499	-4.8305	H	-5.857	-0.4516	-3.0276	H	-5.4949	-0.4713	-3.8765
H	2.5302	1.7806	2.7062	H	1.437	1.1574	2.6019	H	1.319	1.055	2.7001
H	3.9771	2.2538	1.8198	H	3.0007	1.7959	2.106	H	2.905	1.6948	2.2824
H	3.4356	0.5907	1.7815	H	2.5812	0.1166	1.7381	H	2.4961	0.0231	1.8709
H	1.3365	3.942	-0.0799	H	0.5609	3.4296	-0.2204	H	0.5785	3.3755	-0.123
H	1.4114	3.7055	1.6654	H	0.2392	2.997	1.4723	H	0.1707	2.9131	1.5435

H	2.8793	4.0768	0.753	H	1.7788	3.6948	1.0264	H	1.7327	3.6134	1.1883
H	2.5315	4.9597	-3.1161	H	5.3137	4.7011	-0.5718	H	5.3207	4.6518	-0.2698
H	3.6722	4.4332	-4.3702	H	5.6196	3.8791	0.9972	H	5.5605	3.8221	1.3066
H	2.1158	3.5926	-4.2062	H	6.7523	3.6817	-0.3547	H	6.7524	3.6367	0.0047
H	-1.8718	-3.2369	7.225	H	-0.0063	0.2533	7.1159	H	-0.3977	0.1128	7.1217
H	-2.1097	-1.216	5.8052	H	-1.7501	0.642	5.3934	H	-2.0438	0.5273	5.3113
H	-1.6904	-1.3416	3.3809	H	-1.642	-0.5278	3.227	H	-1.8219	-0.6187	3.1409
H	-0.7817	-5.5503	3.7741	H	1.9844	-2.509	4.4971	H	1.7235	-2.628	4.5841
H	-1.2088	-5.4007	6.2064	H	1.8578	-1.3218	6.6642	H	1.4831	-1.4643	6.7542
3C-7				**3C-8**				**3C-9**			
C	-2.9197	-1.5484	0.9297	C	-2.8034	-1.8361	0.0215	C	-3.0075	-1.1692	1.0801
C	-1.5026	-2.0761	0.6292	C	-1.3096	-2.193	0.1398	C	-1.6884	-1.8861	0.7403
C	-0.7877	-0.9877	-0.2397	C	-0.508	-1.0002	-0.487	C	-0.8968	-0.9416	-0.2274
C	-1.8531	0.1018	-0.4699	C	-1.5863	-0.0688	-1.081	C	-1.8985	0.1849	-0.5737
C	-3.1909	-0.5876	-0.2279	C	-2.8416	-0.9261	-1.2048	C	-3.2739	-0.3357	-0.1713
C	0.5962	-0.4796	0.2644	C	0.5549	-0.3171	0.4266	C	0.5308	-0.4954	0.2345
C	-0.9009	2.0737	-1.4903	C	-0.5543	1.9825	-1.8308	C	-0.6122	1.667	-1.9357
C	-1.6923	0.8035	-1.8332	C	-1.1174	0.6538	-2.358	C	-1.7843	0.68	-2.0192
C	-3.0745	-0.8919	2.303	C	-3.402	-1.1916	1.2732	C	-2.9549	-0.3347	2.3614
C	1.7019	-1.3023	-0.402	C	1.9194	-0.9764	0.196	C	1.5821	-1.4294	-0.3767
C	2.4263	-0.9055	-1.4613	C	2.9107	-0.4709	-0.5564	C	2.4889	-1.1393	-1.3251
C	2.2377	0.3749	-2.1918	C	2.8342	0.7849	-1.3451	C	2.7075	0.1299	-2.0685
C	2.6681	1.6341	-1.4287	C	2.7805	2.0828	-0.5276	C	2.8963	1.449	-1.3019
C	0.7482	1.0955	0.3607	C	0.4571	1.2615	0.5171	C	0.7645	1.0622	0.2409
C	-0.5318	1.8877	-0.02	C	-0.6994	1.8773	-0.3152	C	-0.3783	1.8632	-0.4321
C	1.9889	-2.6502	0.2186	C	2.1494	-2.2906	0.9073	C	1.6035	-2.8323	0.2022
C	-1.692	3.377	-1.6643	C	-1.2792	3.2266	-2.3568	C	-0.8533	3.0068	-2.6318
O	-2.977	1.0927	-2.4126	O	-2.2072	0.9057	-3.2659	O	-3.0127	1.3374	-2.3916
H	-0.6366	-1.4826	-1.2116	H	0.0179	-1.4498	-1.3434	H	-0.7778	-1.5366	-1.1461
O	-1.6456	1.1373	0.4978	O	-1.825	0.9964	-0.1506	O	-1.5802	1.3551	0.1849
C	-2.9972	1.2335	-3.7663	C	-2.3438	0.0385	-4.3044	C	-3.3799	1.2395	-3.6971
C	-4.3947	1.5042	-4.2313	C	-3.505	0.4431	-5.159	C	-4.6782	1.9532	-3.9163
O	-2.0228	1.164	-4.5014	O	-1.6371	-0.9369	-4.5121	O	-2.7489	0.6663	-4.573
C	2.1475	1.7693	0.0477	C	1.779	2.1169	0.6814	C	2.2351	1.6068	0.1028
C	3.2249	1.175	1.0081	C	2.5333	1.6511	1.9659	C	3.1467	0.9351	1.1742
C	2.092	3.2777	0.4327	C	1.401	3.5976	0.9859	C	2.2556	3.1194	0.4864
O	2.222	2.7781	-2.2024	O	2.4547	3.1578	-1.448	O	2.4281	2.5174	-2.1688
H	0.698	1.2191	1.4601	H	0.0123	1.3651	1.526	H	0.5494	1.2897	1.3033
C	3.009	3.1681	-3.242	C	3.4809	3.692	-2.1647	C	3.286	2.9339	-3.1419
C	2.3901	4.3447	-3.932	C	2.9658	4.7879	-3.0463	C	2.6598	4.0344	-3.9416
O	4.0622	2.6453	-3.5744	O	4.6489	3.3381	-2.1107	O	4.3997	2.4767	-3.3524
H	0.6785	-0.7629	1.3226	H	0.3161	-0.5988	1.4615	H	0.6091	-0.7227	1.3069
O	-0.7903	-2.4252	1.8188	O	-0.9378	-2.5012	1.4861	O	-0.9616	-2.26	1.9131
C	-1.0674	-3.6444	2.3453	C	-1.2312	-3.7543	1.9155	C	-1.3714	-3.395	2.5333
C	1.2141	-4.4007	5.8952	C	-0.0419	-4.3582	5.9896	C	0.9459	-4.2188	6.0448
C	1.2745	-3.1395	5.3031	C	0.0266	-3.0769	5.4433	C	1.1374	-3.0133	5.3703
C	0.5377	-2.8726	4.1468	C	-0.3572	-2.8592	4.1179	C	0.3917	-2.7256	4.2247
C	-0.2631	-3.8719	3.576	C	-0.8097	-3.928	3.3316	C	-0.5497	-3.6483	3.7475
C	-0.3211	-5.1354	4.1797	C	-0.8801	-5.2115	3.8898	C	-0.7389	-4.8556	4.4337
C	0.4168	-5.3981	5.3355	C	-0.4957	-5.425	5.215	C	0.0083	-5.1393	5.5786
O	-1.851	-4.461	1.8885	O	-1.7552	-4.6356	1.2536	O	-2.2752	-4.127	2.1635
H	-3.6398	-2.3751	0.8881	H	-3.3878	-2.742	-0.1819	H	-3.8121	-1.9038	1.2073
H	-1.5877	-2.9663	-0.0113	H	-1.1037	-3.0654	-0.4978	H	-1.9212	-2.7902	0.1584
H	-3.4877	-1.1676	-1.1107	H	-2.7968	-1.5544	-2.1013	H	-3.68	-0.9846	-0.9574
H	-3.9927	0.119	0.0109	H	-3.7597	-0.3305	-1.24	H	-3.993	0.4667	0.0242
H	-0.0269	2.1593	-2.1282	H	0.4812	2.0922	-2.1326	H	0.258	1.2137	-2.3979
H	-1.131	0.157	-2.5173	H	-0.3209	0.1021	-2.8706	H	-1.5744	-0.1518	-2.7011
H	-2.2851	-0.1651	2.5129	H	-2.7797	-0.3851	1.6702	H	-2.0734	0.311	2.406
H	-4.0398	-0.3809	2.3817	H	-4.3968	-0.7855	1.0624	H	-3.8461	0.2952	2.4505
H	-3.0421	-1.6466	3.0958	H	-3.517	-1.9347	2.0695	H	-2.9268	-0.9849	3.2422
H	3.204	-1.5579	-1.857	H	3.8503	-1.016	-0.6428	H	3.1635	-1.9359	-1.6452
H	2.8062	0.3173	-3.1295	H	3.7117	0.8242	-2.0044	H	3.6227	-0.0127	-2.6625
H	1.2016	0.4487	-2.5323	H	2.0003	0.7114	-2.0482	H	1.9377	0.2109	-2.8424
H	3.7661	1.6617	-1.3914	H	3.7832	2.2797	-0.123	H	3.9758	1.5958	-1.1504
H	-0.5308	2.8441	0.5136	H	-0.9925	2.8356	0.1259	H	-0.3201	2.92	-0.1589
H	1.1348	-3.3211	0.0917	H	1.4949	-3.0668	0.5015	H	0.6773	-3.3636	-0.0334

H	2.8571	-3.1393	-0.2363	H	3.1798	-2.6466	0.7984	H	2.4283	-3.4364	-0.1916
H	2.2027	-2.5424	1.2867	H	1.9595	-2.1842	1.9798	H	1.73	-2.7937	1.2885
H	-1.0956	4.2332	-1.3298	H	-0.8298	4.1346	-1.9398	H	0.004	3.6731	-2.4962
H	-2.621	3.3696	-1.0841	H	-2.3403	3.225	-2.0846	H	-1.7297	3.5249	-2.2281
H	-1.9401	3.5526	-2.7153	H	-1.1997	3.2933	-3.4471	H	-0.9957	2.8677	-3.7079
H	-4.7478	2.449	-3.8107	H	-3.3505	1.4561	-5.5392	H	-4.5573	3.0167	-3.6961
H	-4.4053	1.5801	-5.3223	H	-3.5833	-0.2387	-6.0106	H	-4.9798	1.844	-4.962
H	-5.0501	0.6814	-3.9346	H	-4.429	0.3862	-4.5783	H	-5.454	1.5143	-3.2838
H	2.9054	1.249	2.0543	H	2.9573	0.6499	1.8913	H	2.7089	1.0263	2.1752
H	4.1694	1.7265	0.9229	H	1.8696	1.6606	2.8385	H	4.1304	1.4194	1.2091
H	3.4603	0.1288	0.8133	H	3.369	2.3247	2.1927	H	3.3342	-0.1237	0.9965
H	1.3729	3.8396	-0.1713	H	0.8656	4.0744	0.1592	H	1.6729	3.7405	-0.2
H	1.8091	3.4065	1.484	H	0.762	3.6671	1.874	H	1.8531	3.2767	1.4938
H	3.0702	3.7543	0.2958	H	2.297	4.1999	1.1785	H	3.2797	3.5117	0.4776
H	3.0236	4.6482	-4.7703	H	3.795	5.2129	-3.619	H	3.395	4.4338	-4.646
H	1.4059	4.0704	-4.3203	H	2.229	4.3847	-3.7458	H	1.8081	3.6438	-4.5036
H	2.3089	5.1822	-3.2346	H	2.5233	5.5781	-2.4345	H	2.3456	4.8441	-3.2779
H	1.7877	-4.606	6.796	H	0.2563	-4.5253	7.0219	H	1.5268	-4.4403	6.937
H	1.8942	-2.3621	5.7435	H	0.377	-2.2457	6.0505	H	1.8668	-2.2954	5.7379
H	0.595	-1.8808	3.7054	H	-0.3022	-1.8514	3.7142	H	0.5533	-1.7774	3.7182
H	-0.9417	-5.9204	3.7511	H	-1.2346	-6.0504	3.2936	H	-1.4696	-5.5801	4.0787
H	0.368	-6.3805	5.7989	H	-0.5518	-6.4233	5.6422	H	-0.1426	-6.0779	6.1063

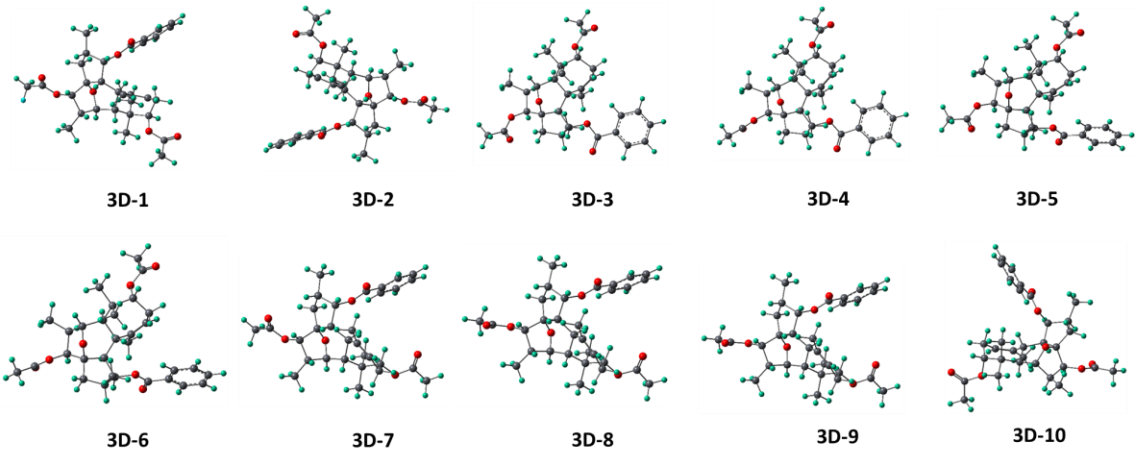


Figure S17. Key conformers of isomer **3D**.

Table S17. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **3D** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	ΔG(kcal/mol)	%	Number of imaginary frequencies
3D-1	-1731.987387	0	44.36%	0
3D-2	-1731.987309	0.048606375	40.86%	0
3D-3	-1731.984	2.125396248	1.22%	0
3D-4	-1731.984134	2.040934357	1.41%	0
3D-5	-1731.983833	2.230164132	1.03%	0
3D-6	-1731.983745	2.285133386	0.94%	0
3D-7	-1731.984934	1.539214413	3.30%	0
3D-8	-1731.984848	1.592953762	3.01%	0
3D-9	-1731.984848	1.593035337	3.01%	0
3D-10	-1731.98367	2.332309054	0.86%	0

Table S18. Optimized Z-matrixes of isomer **3D** in the gas phase (Å) at B3LYP/6-31G* level.

3D-1				**3D-2**				**3D-3**			
C	-3.4031	-1.0165	0.286	C	-2.9458	-1.8667	0.8943	C	-2.914	0.4566	1.2257

C	-1.9841	-1.4681	0.6639	C	-1.4476	-1.7745	1.2191	C	-2.0257	-0.791	1.0899
C	-1.1086	-0.9351	-0.5033	C	-0.8143	-1.3174	-0.1225	C	-1.2495	-0.6265	-0.2485
C	-1.9123	0.2701	-1.0773	C	-1.9559	-0.548	-0.8482	C	-2.0975	0.3962	-1.0503
C	-3.1727	0.4015	-0.2283	C	-3.1856	-0.614	0.0544	C	-3.3369	0.7148	-0.2193
C	0.3616	-0.5591	-0.1396	C	0.4975	-0.4798	-0.0017	C	0.2601	-0.2279	-0.1079
C	-0.6672	0.4173	-3.0823	C	-0.894	-0.5052	-2.9591	C	-0.969	0.1333	-3.1105
C	-2.0951	0.1322	-2.5983	C	-2.1539	-1.0576	-2.285	C	-2.3598	-0.0374	-2.4983
C	-4.4103	-1.0685	1.4244	C	-3.8561	-1.9368	2.1108	C	-2.24	1.6643	1.8742
C	1.2517	-1.7623	0.1576	C	1.7108	-1.2936	0.4383	C	1.1764	-1.3829	0.3058
C	2.3567	-1.631	0.9118	C	2.7612	-0.6979	1.0291	C	2.3718	-1.1482	0.8753
C	2.9006	-0.3226	1.4029	C	2.9215	0.7852	1.1843	C	2.976	0.2112	1.0657
C	3.2963	0.6346	0.2597	C	2.971	1.5327	-0.1642	C	3.2411	0.9553	-0.2574
C	1.0514	0.4289	-1.1568	C	0.8235	0.407	-1.2634	C	0.8615	0.53	-1.3545
C	-0.0437	1.2309	-1.9213	C	-0.4912	0.6853	-2.051	C	-0.2901	1.1677	-2.1804
C	0.9209	-3.1075	-0.4318	C	1.7608	-2.7746	0.1726	C	0.7533	-2.8048	0.0464
C	-0.5718	1.1467	-4.4181	C	-1.0564	-0.0843	-4.4153	C	-0.9537	0.5677	-4.572
O	-2.9897	1.1346	-3.1169	O	-3.3426	-0.4677	-2.8465	O	-3.2853	0.8624	-3.1403
H	-1.1135	-1.7243	-1.2661	H	-0.6228	-2.2337	-0.6956	H	-1.3212	-1.5914	-0.7647
O	-1.1145	1.4575	-0.9833	O	-1.5413	0.8049	-1.0688	O	-1.2993	1.5757	-1.2364
C	-4.2497	0.721	-3.4166	C	-4.068	-1.249	-3.6896	C	-4.5613	0.4196	-3.2889
C	-5.0478	1.8653	-3.9608	C	-5.2678	-0.4965	-4.1766	C	-5.3922	1.4706	-3.958
O	-4.6818	-0.4116	-3.258	O	-3.791	-2.3943	-4.0147	O	-4.9819	-0.6705	-2.9298
C	2.1281	1.3938	-0.4712	C	1.6015	1.7583	-0.905	C	1.9949	1.5907	-0.9764
C	1.4798	2.3877	0.5234	C	0.736	2.7323	-0.0685	C	1.4497	2.7503	-0.1099
C	2.8083	2.2581	-1.5785	C	1.9511	2.5053	-2.23	C	2.5446	2.2396	-2.2852
O	4.0689	-0.0844	-0.7382	O	3.8745	0.8488	-1.0725	O	3.907	0.0672	-1.194
H	1.6094	-0.1601	-1.8987	H	1.4957	-0.1557	-1.9269	H	1.3599	-0.2038	-2.0046
C	5.3781	-0.3123	-0.4514	C	5.2047	1.059	-0.8865	C	5.2393	-0.1303	-1.009
C	6.0142	-1.0853	-1.5654	C	5.9885	0.2617	-1.8832	C	5.7603	-1.08	-2.0433
O	5.9635	0.0529	0.5576	O	5.7024	1.7866	-0.0398	O	5.9231	0.3821	-0.1348
H	0.2759	-0.0032	0.7982	H	0.296	0.2268	0.808	H	0.2716	0.4795	0.7271
O	-1.5993	-0.8537	1.9032	O	-1.2387	-0.7849	2.2379	O	-1.1705	-0.9817	2.2171
C	-1.1093	-1.6683	2.8692	C	-0.5225	-1.1613	3.3252	C	-1.7323	-1.5806	3.2962
C	0.4185	0.5781	6.1865	C	0.3338	2.1801	5.8718	C	1.0548	-1.9969	6.5274
C	0.5012	-0.8137	6.1706	C	0.8113	0.9075	6.1823	C	-0.2173	-2.5622	6.6077
C	-0.0059	-1.5308	5.0853	C	0.5194	-0.1712	5.3454	C	-1.1138	-2.4174	5.547
C	-0.5998	-0.8581	4.009	C	-0.2537	0.0182	4.192	C	-0.7408	-1.7066	4.3981
C	-0.6795	0.5419	4.0322	C	-0.7307	1.301	3.8863	C	0.5377	-1.1373	4.3272
C	-0.1706	1.2557	5.1196	C	-0.4359	2.3777	4.7259	C	1.4325	-1.2848	5.3895
O	-1.0606	-2.887	2.8308	O	-0.127	-2.2885	3.5745	O	-2.8839	-1.9774	3.3762
H	-3.7685	-1.6419	-0.5397	H	-3.1203	-2.7533	0.2696	H	-3.7958	0.2194	1.8334
H	-1.9468	-2.561	0.7175	H	-1.0709	-2.7584	1.5166	H	-2.6725	-1.6724	0.966
H	-4.0411	0.7797	-0.7717	H	-4.1298	-0.6827	-0.4944	H	-4.1491	0.021	-0.4643
H	-3.0009	1.0989	0.6022	H	-3.2475	0.2825	0.6845	H	-3.6973	1.7383	-0.365
H	-0.1325	-0.5341	-3.1989	H	-0.1109	-1.2738	-2.9344	H	-0.4385	-0.8261	-3.056
H	-2.4094	-0.8715	-2.9062	H	-2.1995	-2.1519	-2.3181	H	-2.6941	-1.0776	-2.581
H	-4.4925	-2.0864	1.819	H	-3.6072	-2.8062	2.7278	H	-1.9629	1.4478	2.9108
H	-4.1331	-0.4052	2.2502	H	-3.7766	-1.0419	2.7366	H	-1.3381	1.9785	1.3453
H	-5.4004	-0.761	1.0719	H	-4.9019	-2.0306	1.7998	H	-2.9264	2.5177	1.8902
H	2.9729	-2.503	1.1252	H	3.6133	-1.2958	1.3485	H	3.0037	-1.9848	1.1692
H	2.2152	0.1459	2.1159	H	2.1614	1.1948	1.8568	H	2.3789	0.8097	1.7608
H	3.8022	-0.559	1.9827	H	3.8774	0.9418	1.7007	H	3.9363	0.0552	1.574
H	3.944	1.4067	0.7005	H	3.3846	2.5312	0.0401	H	3.9271	1.7837	-0.027
H	0.3003	2.2029	-2.2745	H	-0.4651	1.6132	-2.6222	H	0.0132	2.0504	-2.7426
H	1.7129	-3.8427	-0.2503	H	2.7396	-3.2036	0.4148	H	1.5385	-3.5232	0.3072
H	0.0029	-3.5145	-0.0017	H	1.0203	-3.31	0.7714	H	-0.1292	-3.0678	0.6364
H	0.8048	-3.0279	-1.5176	H	1.5797	-2.9762	-0.8882	H	0.5317	-2.9468	-1.0163
H	-1.0127	2.148	-4.3715	H	-1.7851	0.725	-4.5297	H	-1.398	1.5589	-4.7106
H	-1.0835	0.582	-5.2042	H	-1.3798	-0.9301	-5.0301	H	-1.5052	-0.1457	-5.1928
H	0.4766	1.2619	-4.7135	H	-0.1015	0.2735	-4.8153	H	0.0757	0.6133	-4.9435
H	-4.5644	2.2614	-4.8574	H	-5.8947	-0.2096	-3.3286	H	-4.9774	1.6997	-4.9428
H	-6.0472	1.5135	-4.2322	H	-4.9488	0.3863	-4.7362	H	-6.4122	1.0979	-4.0882
H	-5.1449	2.6434	-3.1996	H	-5.8535	-1.1386	-4.8407	H	-5.425	2.3681	-3.3353
H	0.9688	1.8921	1.3515	H	0.4291	2.314	0.8924	H	1.0741	2.4186	0.8601
H	0.7521	3.0394	0.0294	H	-0.1715	3.0303	-0.6033	H	0.6388	3.2858	-0.6138
H	2.2392	3.0446	0.9646	H	1.2894	3.6543	0.1471	H	2.2373	3.4868	0.0904

H	2.1503	3.0425	-1.9638	H	1.0768	2.9706	-2.6943	H	1.8497	2.965	-2.7185
H	3.6942	2.7726	-1.1869	H	2.6642	3.3181	-2.0467	H	3.4726	2.7912	-2.0913
H	3.1291	1.6437	-2.4268	H	2.4004	1.8291	-2.9654	H	2.7611	1.4837	-3.048
H	7.0658	-1.2674	-1.3262	H	7.057	0.4337	-1.7256	H	6.8324	-1.2316	-1.8892
H	5.5116	-2.0488	-1.6815	H	5.7836	-0.8034	-1.7486	H	5.2548	-2.0444	-1.9484
H	5.9622	-0.5093	-2.4928	H	5.7301	0.5787	-2.8967	H	5.6075	-0.6614	-3.0412
H	0.8146	1.1356	7.0319	H	0.5627	3.0197	6.5239	H	1.7524	-2.11	7.3537
H	0.9619	-1.3416	7.002	H	1.4128	0.7542	7.0751	H	-0.5124	-3.1155	7.4959
H	0.0673	-2.6168	5.0798	H	0.9005	-1.16	5.5938	H	-2.1049	-2.8616	5.6195
H	-1.1316	1.0909	3.2095	H	-1.3297	1.4787	2.9962	H	0.8495	-0.5741	3.4521
H	-0.2334	2.3411	5.1333	H	-0.8067	3.371	4.4848	H	2.424	-0.8427	5.3287
3D-4				**3D-5**				**3D-6**			
C	-2.9321	-0.0536	1.3831	C	-3.1625	0.5395	0.9318	C	-2.9802	-0.512	1.5227
C	-1.8191	-1.107	1.254	C	-2.2428	-0.6911	1.0005	C	-1.7018	-1.3581	1.3986
C	-1.1333	-0.849	-0.1177	C	-1.347	-0.6381	-0.273	C	-1.1027	-1.043	-0.0035
C	-2.1869	-0.0385	-0.9154	C	-2.1118	0.3129	-1.2324	C	-2.2885	-0.4254	-0.7885
C	-3.4405	0.0666	-0.0523	C	-3.439	0.6599	-0.5654	C	-3.5267	-0.5247	0.0967
C	0.2746	-0.1658	-0.0572	C	0.141	-0.2181	-0.0217	C	0.1807	-0.1476	0.0011
C	-1.122	-0.1706	-3.0207	C	-0.7577	-0.053	-3.1355	C	-1.2564	-0.3854	-2.9147
C	-2.4218	-0.5831	-2.329	C	-2.2046	-0.2174	-2.6688	C	-2.4528	-1.01	-2.1958
C	-2.487	1.2854	1.969	C	-2.585	1.817	1.5385	C	-2.77	0.8999	2.0679
C	1.4083	-1.1064	0.3606	C	1.0284	-1.341	0.5151	C	1.4654	-0.8962	0.356
C	2.5561	-0.6239	0.8685	C	2.1299	-1.0585	1.2327	C	2.5174	-0.2413	0.8778
C	2.8967	0.8325	0.9766	C	2.6642	0.3271	1.4524	C	2.5964	1.2502	1.0262
C	2.969	1.5467	-0.3869	C	3.0758	1.0345	0.1428	C	2.5249	1.9988	-0.3224
C	0.6731	0.6321	-1.3597	C	0.861	0.4962	-1.2257	C	0.4072	0.7173	-1.2954
C	-0.6096	1.008	-2.1545	C	-0.2023	1.0551	-2.208	C	-0.9351	0.8683	-2.062
C	1.2566	-2.5931	0.1733	C	0.713	-2.773	0.1733	C	1.5852	-2.3658	0.0506
C	-1.2493	0.2142	-4.4902	C	-0.5875	0.2865	-4.6122	C	-1.4761	-0.0362	-4.3821
O	-3.5628	0.0813	-2.9061	O	-3.0665	0.6183	-3.4677	O	-3.7013	-0.5526	-2.752
H	-1.0353	-1.8294	-0.5992	H	-1.3784	-1.6428	-0.7102	H	-0.8719	-2.0123	-0.4608
O	-1.6392	1.2604	-1.1795	O	-1.3153	1.4962	-1.4066	O	-1.9726	0.9464	-1.0662
C	-4.3372	-0.6605	-3.7413	C	-4.3182	0.1481	-3.709	C	-4.3543	-1.4196	-3.5702
C	-5.4817	0.1649	-4.2434	C	-5.0813	1.1312	-4.542	C	-5.6303	-0.8019	-4.0533
O	-4.1365	-1.8258	-4.0508	O	-4.7684	-0.9147	-3.3068	O	-3.9661	-2.5365	-3.8794
C	1.6002	1.9023	-1.0753	C	1.917	1.6028	-0.7612	C	1.1078	2.1238	-0.9992
C	0.8776	2.9801	-0.233	C	1.2469	2.7884	-0.0275	C	0.2222	3.0538	-0.1363
C	1.9708	2.5785	-2.4324	C	2.6105	2.2035	-2.023	C	1.3412	2.8688	-2.35
O	3.7559	0.7538	-1.3149	O	3.8842	0.1355	-0.6625	O	3.4318	1.3789	-1.2727
H	1.2742	-0.0256	-2.0042	H	1.4519	-0.2484	-1.7789	H	1.102	0.1845	-1.9608
C	5.1074	0.8169	-1.1812	C	5.1883	-0.0021	-0.3039	C	4.7507	1.6846	-1.1493
C	5.7601	-0.0679	-2.1981	C	5.8656	-0.9769	-1.2173	C	5.5418	0.9469	-2.1852
O	5.7136	1.4891	-0.3596	O	5.7402	0.5756	0.6213	O	5.2339	2.4452	-0.3232
H	0.1795	0.5694	0.7482	H	0.0689	0.5248	0.7782	H	0.0017	0.559	0.8171
O	-0.9079	-1.0816	2.3525	O	-1.5095	-0.6996	2.2272	O	-0.8115	-1.0857	2.4826
C	-1.3067	-1.736	3.4713	C	-1.4665	-1.8609	2.922	C	-0.2971	-2.1449	3.1509
C	1.6079	-1.4728	6.6045	C	1.009	-1.5307	6.408	C	2.4875	-0.913	6.1704
C	0.4706	-2.2653	6.7554	C	0.3711	-2.7314	6.099	C	2.2098	-2.2641	5.9668
C	-0.4697	-2.3402	5.7259	C	-0.4341	-2.8216	4.9619	C	1.2984	-2.6487	4.9814
C	-0.2756	-1.6226	4.5377	C	-0.6063	-1.709	4.1272	C	0.6583	-1.6818	4.1942
C	0.8676	-0.8248	4.3956	C	0.0374	-0.5048	4.4455	C	0.9419	-0.3252	4.406
C	1.8068	-0.7529	5.427	C	0.8433	-0.4187	5.5831	C	1.8554	0.0556	5.3916
O	-2.3553	-2.3462	3.6077	O	-2.0296	-2.9017	2.6224	O	-0.5513	-3.3206	2.943
H	-3.7319	-0.4352	2.0293	H	-4.0962	0.3282	1.4678	H	-3.6862	-1.0115	2.1978
H	-2.2835	-2.1021	1.1847	H	-2.888	-1.5768	0.9163	H	-2.0158	-2.4113	1.3943
H	-4.1128	-0.7757	-0.2586	H	-4.2043	-0.0783	-0.831	H	-4.0396	-1.4791	-0.0767
H	-3.9931	0.9978	-0.2147	H	-3.8056	1.6554	-0.8358	H	-4.2401	0.288	-0.0752
H	-0.4136	-1.0073	-2.9693	H	-0.2213	-0.9943	-2.9594	H	-0.4151	-1.0892	-2.8756
H	-2.5614	-1.67	-2.3159	H	-2.5118	-1.268	-2.7209	H	-2.4048	-2.1047	-2.1779
H	-2.1452	1.1661	3.0021	H	-2.4357	1.7022	2.6171	H	-2.4148	0.868	3.1032
H	-1.6771	1.746	1.3996	H	-1.627	2.0968	1.0967	H	-2.0465	1.4725	1.4842
H	-3.3246	1.9912	1.9809	H	-3.2757	2.6542	1.3908	H	-3.7144	1.4545	2.0627
H	3.3463	-1.3113	1.1663	H	2.754	-1.8673	1.6093	H	3.4264	-0.7864	1.1267
H	2.2212	1.3409	1.6717	H	1.9667	0.9292	2.0428	H	1.8507	1.6153	1.7391
H	3.8863	0.8853	1.4486	H	3.5562	0.2193	2.083	H	3.5676	1.4648	1.4905
H	3.4944	2.4989	-0.222	H	3.7012	1.8938	0.4261	H	2.8746	3.0251	-0.1374

H	-0.4991	1.9086	-2.7578	H	0.149	1.9074	-2.7895	H	-0.9879	1.7723	-2.6687
H	2.1732	-3.1368	0.4279	H	1.4901	-3.461	0.5241	H	2.5923	-2.7477	0.2515
H	0.4613	-2.992	0.8093	H	-0.2276	-3.0943	0.6254	H	0.8922	-2.9569	0.6532
H	1.0302	-2.8225	-0.8731	H	0.6437	-2.8941	-0.9128	H	1.3785	-2.5482	-1.0091
H	-1.9057	1.079	-4.6322	H	-1.0293	1.2562	-4.8644	H	-2.2727	0.7036	-4.5127
H	-1.6449	-0.6203	-5.0774	H	-1.0557	-0.478	-5.2408	H	-1.7355	-0.9292	-4.9593
H	-0.2676	0.4747	-4.9005	H	0.4758	0.3316	-4.871	H	-0.5612	0.3849	-4.8129
H	-6.0873	0.5098	-3.4015	H	-4.5672	1.2887	-5.4935	H	-6.2705	-0.5594	-3.2015
H	-5.1018	1.0132	-4.8181	H	-6.0795	0.7343	-4.7476	H	-5.4092	0.0952	-4.6371
H	-6.1106	-0.4468	-4.8965	H	-5.185	2.074	-3.9992	H	-6.1584	-1.5144	-4.6934
H	0.6014	2.6293	0.7634	H	0.773	2.4962	0.9116	H	0.031	2.6556	0.8622
H	-0.0346	3.3337	-0.7241	H	0.4862	3.2717	-0.6486	H	-0.7461	3.2451	-0.6093
H	1.5207	3.8574	-0.0934	H	1.9877	3.5585	0.2196	H	0.7042	4.0295	-0.0001
H	1.1368	3.1396	-2.8643	H	1.9554	2.8818	-2.5778	H	0.4165	3.2762	-2.7695
H	2.7844	3.3024	-2.3023	H	3.4912	2.7944	-1.7439	H	2.0148	3.7239	-2.2163
H	2.2986	1.8403	-3.1725	H	2.9419	1.4185	-2.7115	H	1.7882	2.2083	-3.1011
H	6.8465	-0.0094	-2.0858	H	6.9136	-1.0822	-0.9224	H	6.6011	1.198	-2.0794
H	5.4488	-1.1038	-2.0418	H	5.3821	-1.9539	-1.1401	H	5.4234	-0.1303	-2.0436
H	5.4955	0.2663	-3.2044	H	5.8283	-0.6085	-2.2456	H	5.2115	1.243	-3.184
H	2.3398	-1.415	7.4067	H	1.6371	-1.4617	7.2929	H	3.1988	-0.6144	6.9368
H	0.3148	-2.8249	7.6745	H	0.5009	-3.5983	6.7422	H	2.7035	-3.019	6.5738
H	-1.3546	-2.961	5.8535	H	-0.9258	-3.764	4.7278	H	1.0903	-3.706	4.8285
H	1.039	-0.2519	3.4885	H	-0.0749	0.3728	3.8139	H	0.4636	0.4458	3.8073
H	2.6931	-0.1338	5.3111	H	1.3432	0.5162	5.8247	H	2.075	1.1086	5.5504
3D-7				**3D-8**				**3D-9**			
C	-2.8512	-2.0453	0.0068	C	-3.0476	-1.8268	0.0499	C	-2.9817	-2.122	0.1268
C	-1.3866	-2.0615	0.471	C	-1.5905	-1.9484	0.5196	C	-1.5091	-2.1144	0.5583
C	-0.6147	-1.4218	-0.7192	C	-0.7716	-1.3856	-0.6769	C	-0.7847	-1.5227	-0.6851
C	-1.6795	-0.5045	-1.4001	C	-1.7504	-0.3695	-1.3426	C	-1.8367	-0.5431	-1.2871
C	-2.9774	-0.6591	-0.6129	C	-3.0739	-0.44	-0.5833	C	-3.1476	-0.7511	-0.5249
C	0.7337	-0.6956	-0.3602	C	0.6421	-0.7923	-0.3213	C	0.622	-0.8877	-0.3949
C	-0.4312	-0.1459	-3.3736	C	-0.4869	-0.0816	-3.3164	C	-0.6248	-0.0367	-3.2529
C	-1.7503	-0.7746	-2.9138	C	-1.8537	-0.5951	-2.8608	C	-1.941	-0.6801	-2.8153
C	-3.8813	-2.2876	1.0988	C	-4.0959	-1.9857	1.1402	C	-3.9719	-2.3543	1.2581
C	1.9284	-1.6519	-0.1179	C	1.7449	-1.8592	-0.1056	C	1.8016	-1.8834	-0.3789
C	3.2217	-1.2652	-0.0759	C	3.0693	-1.596	-0.0777	C	3.0938	-1.5118	-0.2517
C	3.8128	0.1134	-0.1089	C	3.786	-0.278	-0.1022	C	3.6871	-0.1517	-0.0166
C	2.8862	1.2445	0.3538	C	2.9762	0.9254	0.3967	C	2.7575	0.9248	0.5601
C	1.1174	0.4368	-1.402	C	1.1186	0.3191	-1.3465	C	0.9797	0.358	-1.2928
C	-0.1063	0.8689	-2.2513	C	-0.0687	0.8771	-2.1732	C	-0.261	0.8784	-2.0571
C	1.663	-3.1233	0.1137	C	1.3451	-3.301	0.1186	C	1.525	-3.3619	-0.5274
C	-0.4703	0.5054	-4.752	C	-0.4585	0.6038	-4.6778	C	-0.6689	0.7314	-4.5688
O	-2.8537	-0.0791	-3.5251	O	-2.9154	0.2168	-3.4001	O	-3.0682	0.0812	-3.2932
H	-0.405	-2.2402	-1.4201	H	-0.647	-2.2164	-1.3833	H	-0.684	-2.3478	-1.4
O	-1.2328	0.8532	-1.3596	O	-1.187	0.9415	-1.2714	O	-1.3653	0.7983	-1.1387
C	-3.9358	-0.834	-3.8537	C	-3.6257	-0.3171	-4.4286	C	-3.7553	-0.4433	-4.3421
C	-4.9824	0.0243	-4.4944	C	-4.6909	0.6413	-4.8641	C	-4.8923	0.4597	-4.7092
O	-4.0532	-2.0337	-3.6501	O	-3.431	-1.412	-4.936	O	-3.4924	-1.4914	-4.9134
C	1.8368	1.6825	-0.723	C	1.9571	1.48	-0.6552	C	1.7173	1.5016	-0.4664
C	0.8295	2.6253	-0.0149	C	1.0495	2.4958	0.0855	C	0.72	2.369	0.3449
C	2.5366	2.5208	-1.8303	C	2.7164	2.2734	-1.7564	C	2.4311	2.4524	-1.4663
O	3.6977	2.3966	0.7056	O	3.896	1.9899	0.7575	O	3.5709	2.0216	1.0575
H	1.8486	0.0198	-2.1098	H	1.8011	-0.1502	-2.07	H	1.6987	0.0397	-2.0622
C	4.219	2.4221	1.9622	C	4.4384	1.9385	2.0042	C	4.0747	1.8939	2.3155
C	4.9974	3.6861	2.1627	C	5.3323	3.1213	2.2175	C	4.839	3.1289	2.6819
O	4.0871	1.5518	2.8095	O	4.242	1.0641	2.8347	O	3.9417	0.9241	3.0471
H	0.5573	-0.1961	0.5978	H	0.5228	-0.2962	0.6473	H	0.5553	-0.513	0.6272
O	-1.2306	-1.2511	1.6463	O	-1.3791	-1.135	1.6838	O	-1.3642	-1.2493	1.6967
C	-1.0407	-1.8961	2.8226	C	-1.2289	-1.7761	2.868	C	-0.5854	-1.6936	2.7139
C	-0.4238	0.8583	6.0496	C	-0.4183	0.9737	6.0557	C	0.1672	1.4613	5.5092
C	-0.3999	-0.5176	6.2739	C	-0.4586	-0.3996	6.2934	C	1.0065	0.3492	5.4491
C	-0.6047	-1.4015	5.2126	C	-0.7259	-1.282	5.2449	C	0.7415	-0.678	4.5419
C	-0.835	-0.9122	3.9198	C	-0.9542	-0.7938	3.9513	C	-0.3621	-0.5915	3.6848
C	-0.8596	0.4729	3.7023	C	-0.9141	0.5888	3.7202	C	-1.2028	0.5284	3.7489
C	-0.6532	1.3537	4.7665	C	-0.6457	1.4681	4.7717	C	-0.9368	1.5513	4.6617
O	-1.0324	-3.1055	2.9857	O	-1.3009	-2.9812	3.0462	O	-0.0771	-2.7983	2.8057

H	-2.9843	-2.803	-0.7772	H	-3.2332	-2.5792	-0.7287	H	-3.1263	-2.8999	-0.6353
H	-1.06	-3.0923	0.638	H	-1.3444	-2.9985	0.7021	H	-1.1841	-3.1363	0.7745
H	-3.8823	-0.5699	-1.2174	H	-3.9547	-0.3166	-1.2205	H	-4.0353	-0.7359	-1.1647
H	-3.0477	0.1154	0.1622	H	-3.1212	0.3469	0.1803	H	-3.2831	0.0348	0.2289
H	0.3425	-0.9237	-3.4093	H	0.2111	-0.9269	-3.3697	H	0.133	-0.8227	-3.3665
H	-1.7727	-1.8421	-3.1608	H	-2.0037	-1.6542	-3.0983	H	-2.0141	-1.7306	-3.1178
H	-3.7165	-3.259	1.5758	H	-4.0032	-2.963	1.6246	H	-3.7788	-3.3148	1.7467
H	-3.8497	-1.5156	1.8744	H	-4.0101	-1.2126	1.9106	H	-3.919	-1.5696	2.0198
H	-4.8915	-2.2871	0.6757	H	-5.1022	-1.9149	0.714	H	-4.9962	-2.371	0.8712
H	3.9844	-2.0327	0.0688	H	3.7584	-2.4331	0.0487	H	3.857	-2.2913	-0.2856
H	4.6893	0.0945	0.5524	H	4.6691	-0.3893	0.541	H	4.5217	-0.2934	0.6828
H	4.2252	0.3122	-1.104	H	4.1966	-0.1015	-1.1022	H	4.1624	0.1978	-0.9401
H	2.3481	0.9275	1.2571	H	2.4234	0.6419	1.3024	H	2.2125	0.5074	1.4164
H	-0.0071	1.8765	-2.6593	H	0.115	1.8813	-2.5597	H	-0.1536	1.917	-2.3774
H	2.5869	-3.7028	0.2263	H	2.2117	-3.9657	0.2145	H	2.4387	-3.965	-0.4727
H	1.0993	-3.266	1.0384	H	0.7824	-3.3974	1.0501	H	0.874	-3.7199	0.2724
H	1.1253	-3.5726	-0.7249	H	0.7566	-3.6907	-0.7156	H	1.0699	-3.5783	-1.4982
H	-1.163	1.3529	-4.7862	H	-1.089	1.4987	-4.7002	H	-1.3639	1.5765	-4.5277
H	-0.7759	-0.2194	-5.5134	H	-0.7987	-0.0786	-5.4631	H	-0.9706	0.0754	-5.3913
H	0.5225	0.8806	-5.0226	H	0.5626	0.9143	-4.9246	H	0.3224	1.1318	-4.8075
H	-4.5751	0.4988	-5.3908	H	-4.2323	1.5656	-5.2244	H	-4.5059	1.4336	-5.0199
H	-5.8324	-0.5984	-4.7873	H	-5.2677	0.1961	-5.6798	H	-5.4482	0.022	-5.5433
H	-5.3288	0.7781	-3.7829	H	-5.3681	0.8463	-4.0311	H	-5.5697	0.5672	-3.8583
H	0.2439	2.0911	0.7399	H	0.4279	2.0021	0.839	H	0.1221	1.7567	1.0274
H	0.1307	3.0883	-0.7184	H	0.386	3.0339	-0.5986	H	0.0332	2.9234	-0.3023
H	1.3441	3.4483	0.4944	H	1.6437	3.2584	0.6021	H	1.2427	3.1174	0.9515
H	1.8266	2.9064	-2.5677	H	2.0353	2.7373	-2.4757	H	1.7273	2.9185	-2.1624
H	3.0495	3.3961	-1.417	H	3.3126	3.0897	-1.3339	H	2.9446	3.2731	-0.9537
H	3.278	1.9274	-2.3744	H	3.3933	1.6261	-2.3227	H	3.1746	1.9179	-2.066
H	5.3975	3.7078	3.1804	H	5.7493	3.0832	3.2279	H	5.2198	3.0301	3.7025
H	5.832	3.7227	1.4582	H	6.1552	3.0981	1.4988	H	5.6861	3.2554	2.0032
H	4.3417	4.5502	2.0287	H	4.7563	4.0444	2.1142	H	4.1789	3.9991	2.6408
H	-0.2599	1.5458	6.8759	H	-0.2061	1.6597	6.8721	H	0.3775	2.2607	6.2154
H	-0.2181	-0.9033	7.2739	H	-0.2783	-0.7846	7.294	H	1.8747	0.2838	6.1004
H	-0.5803	-2.4738	5.3972	H	-0.7515	-2.3525	5.4399	H	1.4103	-1.5353	4.493
H	-1.0355	0.8815	2.7103	H	-1.088	0.9964	2.7274	H	-2.0639	0.6176	3.0911
H	-0.6683	2.4269	4.593	H	-0.6114	2.5391	4.5878	H	-1.5882	2.4204	4.708
3D-10											
C	-2.9072	-1.9208	0.2665								
C	-1.4888	-1.7755	0.8337								
C	-0.7169	-1.2397	-0.3944								
C	-1.7079	-0.2699	-1.0688								
C	-3.1012	-0.6206	-0.5251								
C	0.669	-0.6058	-0.0671								
C	-0.6922	1.0286	-2.8456								
C	-1.4731	-0.2681	-2.6043								
C	-3.9993	-2.1384	1.3024								
C	1.7927	-1.6501	-0.0148								
C	2.9401	-1.4176	0.6455								
C	3.3268	-0.1113	1.2625								
C	3.4122	1.032	0.2352								
C	1.0451	0.6492	-0.9462								
C	-0.2327	1.4132	-1.4371								
C	1.639	-2.9712	-0.7261								
C	-1.5378	2.147	-3.4654								
O	-2.6688	-0.3024	-3.3947								
H	-0.6143	-2.0958	-1.0699								
O	-1.3525	1.0514	-0.6223								
C	-3.1342	-1.5462	-3.6961								
C	-4.3569	-1.4434	-4.5542								
O	-2.6415	-2.5967	-3.3107								
C	2.053	1.6687	-0.2252								
C	1.3956	2.3638	0.9941								
C	2.4424	2.7958	-1.235								
O	4.1341	0.5908	-0.9446								
H	1.5779	0.2866	-1.8367								

C	5.4898	0.5452	-0.8511								
C	6.0703	0.0419	-2.1367								
O	6.1502	0.8652	0.1264								
H	0.5809	-0.2303	0.9564								
O	-1.4783	-0.7995	1.8868								
C	-1.3384	-1.2525	3.1541								
C	-1.1621	1.9933	5.9499								
C	-1.0086	0.6754	6.3789								
C	-1.0707	-0.371	5.4565								
C	-1.2864	-0.1031	4.098								
C	-1.4423	1.2249	3.6742								
C	-1.3789	2.2687	4.6001								
O	-1.2577	-2.4197	3.4995								
H	-2.9207	-2.7657	-0.4352								
H	-1.0777	-2.7372	1.1599								
H	-3.8661	-0.7556	-1.2923								
H	-3.4636	0.1796	0.1334								
H	0.1623	0.8588	-3.5107								
H	-0.8233	-1.097	-2.9138								
H	-3.7997	-3.041	1.8887								
H	-4.0853	-1.2943	1.994								
H	-4.9704	-2.2627	0.8116								
H	3.7082	-2.189	0.682								
H	2.6757	0.1315	2.1075								
H	4.3234	-0.2559	1.6997								
H	3.9925	1.8386	0.7074								
H	-0.1267	2.4951	-1.3693								
H	2.5599	-3.5648	-0.7023								
H	0.8575	-3.5788	-0.26								
H	1.3971	-2.8097	-1.7818								
H	-2.4285	2.3634	-2.8657								
H	-1.8605	1.8783	-4.4767								
H	-0.9535	3.0703	-3.5438								
H	-4.1228	-0.8938	-5.4694								
H	-4.6918	-2.4475	-4.8293								
H	-5.1567	-0.9459	-4								
H	1.0932	1.6585	1.7708								
H	0.5065	2.9368	0.7136								
H	2.0921	3.0725	1.4579								
H	1.6308	3.5056	-1.4171								
H	3.2812	3.3916	-0.8551								
H	2.7434	2.3787	-2.2023								
H	7.1601	0.0039	-2.0522								
H	5.7015	-0.9668	-2.3396								
H	5.8072	0.7198	-2.9526								
H	-1.1137	2.8074	6.6693								
H	-0.8404	0.4613	7.4315								
H	-0.9488	-1.3964	5.8004								
H	-1.613	1.462	2.6259								
H	-1.4999	3.2966	4.267								

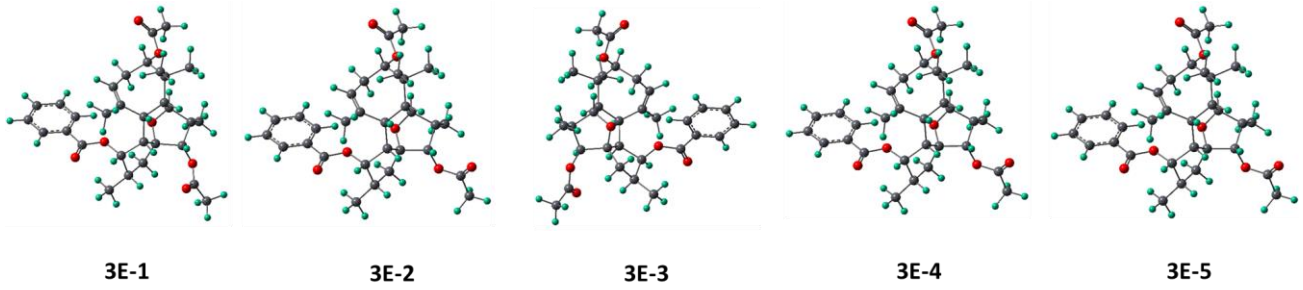


Figure S18. Key conformers of isomer **3E**.

Table S19. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **3E** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	ΔG(kcal/mol)	%	Number of imaginary frequencies
3E-1	-1731.970919	0.000225901	35.80%	0
3E-2	-1731.969664	0.788131092	9.46%	0
3E-3	-1731.97092	0	35.81%	0
3E-4	-1731.969664	0.788118542	9.46%	0
3E-5	-1731.969664	0.788055792	9.46%	0

Table S20. Optimized Z-matrixes of isomer **3E** in the gas phase (Å) at B3LYP/6-31G* level.

3E-1				**3E-2**				**3E-3**			
C	-3.3577	-0.8569	-0.3307	C	-3.4467	-0.8869	-0.304	C	-3.1852	-0.7384	-0.2756
C	-2.1204	-1.4366	0.3742	C	-2.2081	-1.4808	0.3833	C	-2.0334	-1.4676	0.4391
C	-1.078	-1.4263	-0.7706	C	-1.1735	-1.4577	-0.7697	C	-0.9146	-1.4602	-0.6457
C	-1.3545	-0.0713	-1.4671	C	-1.4337	-0.0782	-1.4241	C	-1.1769	-0.1487	-1.4468
C	-2.7927	0.335	-1.1109	C	-2.8879	0.3001	-1.0984	C	-2.4569	0.4646	-0.8734
C	0.445	-1.674	-0.4575	C	0.3439	-1.7366	-0.4604	C	0.5898	-1.7414	-0.2609
C	0.2953	0.8245	-2.9925	C	0.2514	0.8683	-2.8828	C	0.2962	-0.519	-3.2782
C	-0.9395	-0.0878	-2.9651	C	-1.0001	-0.0229	-2.9153	C	-1.1934	-0.3765	-2.9709
C	-4.5052	-0.4597	0.5858	C	-4.5812	-0.4817	0.6253	C	-4.3554	-0.3255	0.6037
C	0.7732	-2.0436	0.9871	C	0.6569	-2.1824	0.9659	C	0.8725	-1.8571	1.2315
C	1.4246	-1.2523	1.858	C	1.3077	-1.4407	1.8799	C	1.3781	-0.8655	1.987
C	1.9043	0.1292	1.5752	C	1.7985	-0.05	1.6687	C	1.688	0.5024	1.4841
C	3.0927	0.2091	0.603	C	2.9964	0.0691	0.7127	C	2.8938	0.6052	0.5356
C	1.415	-0.6805	-1.233	C	1.3274	-0.7175	-1.177	C	1.661	-0.9868	-1.1713
C	0.778	0.7125	-1.5427	C	0.7029	0.6918	-1.4296	C	0.9883	0.1094	-2.0433
C	0.4247	-3.4564	1.4033	C	0.2934	-3.6108	1.308	C	0.6114	-3.211	1.8507
C	-0.0244	2.2766	-3.3623	C	-0.0316	2.3434	-3.1899	C	0.7608	0.1215	-4.5833
O	-1.9309	0.3675	-3.8921	O	-2.0187	0.4932	-3.7811	O	-1.7131	0.7714	-3.672
H	-1.3933	-2.2252	-1.4599	H	-1.5029	-2.2316	-1.4809	H	-1.1984	-2.2883	-1.3153
O	-0.4508	0.8572	-0.8286	O	-0.5408	0.8193	-0.7333	O	-0.0583	0.7207	-1.2731
C	-2.8307	-0.5752	-4.2874	C	-1.8582	0.2188	-5.1048	C	-2.9479	0.6388	-4.2259
C	-3.7876	0.0104	-5.279	C	-2.984	0.816	-5.8913	C	-3.3267	1.9015	-4.9364
O	-2.8677	-1.728	-3.8819	O	-0.9328	-0.4157	-5.5899	O	-3.6583	-0.3532	-4.151
C	2.9174	-0.5801	-0.7466	C	2.8267	-0.6515	-0.6752	C	3.0395	-0.5394	-0.5242
C	3.7625	0.0976	-1.8686	C	3.6855	0.0741	-1.756	C	4.0167	-0.0688	-1.652
C	3.5419	-1.9969	-0.6078	C	3.4404	-2.078	-0.601	C	3.7877	-1.7622	0.0866
O	3.3018	1.616	0.31	O	3.2172	1.4871	0.491	O	2.7778	1.8707	-0.1663
H	1.5238	-1.1668	-2.2167	H	1.4416	-1.1598	-2.1808	H	1.9952	-1.7552	-1.8873
C	4.0375	2.3285	1.2054	C	3.9495	2.1496	1.4266	C	3.1556	2.9886	0.5078
C	4.1408	3.7535	0.7557	C	4.068	3.5938	1.0473	C	2.9393	4.1956	-0.3523
O	4.5438	1.8885	2.2268	O	4.4418	1.6569	2.4307	O	3.6064	3.0214	1.6434
H	0.6544	-2.6241	-0.9802	H	0.5469	-2.6614	-1.0291	H	0.7311	-2.7839	-0.5969
O	-1.7352	-0.5632	1.4438	O	-1.8145	-0.6288	1.466	O	-1.6796	-0.7018	1.6002
C	-1.9929	-0.9802	2.7059	C	-2.0728	-1.067	2.721	C	-2.0845	-1.186	2.8007
C	-0.7081	1.9113	5.5968	C	-0.7756	1.7679	5.6615	C	-0.9714	1.4198	6.015
C	-0.7273	2.2601	4.2467	C	-0.8067	2.1447	4.3192	C	-0.894	1.8851	4.7026
C	-1.1464	1.3325	3.2906	C	-1.2299	1.2358	3.3472	C	-1.2577	1.052	3.6425
C	-1.5436	0.0467	3.6837	C	-1.6191	-0.0595	3.7166	C	-1.6926	-0.2565	3.8929
C	-1.5276	-0.2938	5.0427	C	-1.5915	-0.4283	5.068	C	-1.7755	-0.714	5.2147
C	-1.1091	0.6367	5.9958	C	-1.1688	0.4837	6.0369	C	-1.4139	0.1227	6.2723
O	-2.5121	-2.0374	3.0276	O	-2.5965	-2.1277	3.0234	O	-2.6803	-2.2345	2.992
H	-3.7317	-1.6	-1.0482	H	-3.8355	-1.6276	-1.0168	H	-3.5659	-1.3743	-1.0865
H	-2.3218	-2.4561	0.716	H	-2.4124	-2.505	0.7088	H	-2.31	-2.4977	0.6895
H	-2.7925	1.2409	-0.4913	H	-2.9222	1.2237	-0.5077	H	-2.2128	1.2088	-0.104
H	-3.4306	0.5476	-1.9711	H	-3.5156	0.4562	-1.98	H	-3.082	0.9791	-1.6059
H	1.0452	0.459	-3.7034	H	1.01	0.5199	-3.5928	H	0.5341	-1.5875	-3.3504
H	-0.615	-1.0929	-3.2672	H	-0.7415	-1.0379	-3.2442	H	-1.7318	-1.2877	-3.2543
H	-4.2215	0.3372	1.2805	H	-4.2834	0.3127	1.3171	H	-4.0618	0.3946	1.374
H	-5.3539	-0.0959	-0.0031	H	-5.4336	-0.1111	0.0463	H	-5.1365	0.1461	-0.0022
H	-4.8455	-1.3193	1.1719	H	-4.9217	-1.3389	1.2148	H	-4.7939	-1.1983	1.0975
H	1.6445	-1.6224	2.8586	H	1.5181	-1.8616	2.8623	H	1.5739	-1.0357	3.0443
H	2.1928	0.5905	2.5289	H	2.0793	0.3638	2.6461	H	1.8691	1.1486	2.353
H	1.0765	0.7566	1.2306	H	0.9781	0.5978	1.3447	H	0.7932	0.9383	1.0273

H	3.9934	-0.1776	1.0995	H	3.89	-0.348	1.1972	H	3.8184	0.6237	1.1294
H	1.4246	1.5485	-1.2749	H	1.3508	1.5092	-1.1117	H	1.6712	0.9018	-2.346
H	-0.6283	-3.6827	1.2292	H	-0.7592	-3.8197	1.1104	H	-0.409	-3.5466	1.6489
H	1.0236	-4.1718	0.8297	H	0.8938	-4.3019	0.7067	H	1.3031	-3.9521	1.4364
H	0.6237	-3.636	2.4653	H	0.4782	-3.8439	2.3622	H	0.7455	-3.2014	2.9376
H	-0.3484	2.3496	-4.4057	H	-0.3168	2.4784	-4.2379	H	0.2077	-0.2887	-5.4346
H	0.8662	2.9042	-3.2501	H	0.8651	2.9482	-3.0164	H	1.8254	-0.0789	-4.7459
H	-0.8146	2.6978	-2.7317	H	-0.8354	2.7468	-2.565	H	0.6276	1.2084	-4.5769
H	-4.3675	0.8072	-4.8068	H	-3.9353	0.3972	-5.5535	H	-3.391	2.724	-4.2198
H	-3.2385	0.3935	-6.1429	H	-2.9792	1.9029	-5.7772	H	-2.5917	2.1243	-5.714
H	-4.4747	-0.768	-5.6226	H	-2.8542	0.575	-6.9502	H	-4.304	1.7717	-5.4101
H	3.7335	-0.4926	-2.7921	H	3.6592	-0.4695	-2.7078	H	4.1565	-0.8564	-2.4018
H	4.8133	0.1849	-1.5676	H	4.7346	0.1382	-1.4433	H	5.0035	0.169	-1.2361
H	3.4127	1.1027	-2.1211	H	3.3453	1.0932	-1.961	H	3.6855	0.8263	-2.1829
H	3.1712	-2.5623	0.2471	H	3.0583	-2.6821	0.2217	H	3.343	-2.1711	0.9909
H	3.359	-2.5963	-1.507	H	3.2614	-2.6312	-1.5302	H	3.8542	-2.5802	-0.6405
H	4.6292	-1.9305	-0.4778	H	4.5269	-2.0259	-0.4587	H	4.8147	-1.4903	0.3612
H	3.1438	4.1979	0.7019	H	3.0751	4.0487	1.0076	H	1.8803	4.2832	-0.6078
H	4.7366	4.3194	1.4776	H	4.6627	4.1189	1.8002	H	3.2404	5.0917	0.1978
H	4.6362	3.8	-0.2174	H	4.5716	3.683	0.0814	H	3.5486	4.1202	-1.2565
H	-0.3801	2.6345	6.3396	H	-0.4443	2.4766	6.4167	H	-0.6872	2.0702	6.8388
H	-0.4149	3.2541	3.9368	H	-0.5005	3.1463	4.0278	H	-0.5487	2.8968	4.5035
H	-1.1544	1.6217	2.2416	H	-1.2471	1.5468	2.3046	H	-1.194	1.4333	2.6263
H	-1.8379	-1.2867	5.3622	H	-1.8957	-1.4287	5.369	H	-2.1195	-1.7251	5.424
H	-1.0953	0.3662	7.0487	H	-1.1455	0.1914	7.0838	H	-1.477	-0.238	7.2959
3E-4				**3E-5**							
C	-3.2314	-0.6786	-0.401	C	-3.16	-1.072	-0.018				
C	-2.1206	-1.4326	0.3505	C	-1.8284	-1.4223	0.668				
C	-0.9613	-1.432	-0.6898	C	-0.8966	-1.6322	-0.551				
C	-1.1576	-0.0944	-1.464	C	-1.2885	-0.4705	-1.4778				
C	-2.4663	0.5221	-0.9579	C	-2.7671	-0.1677	-1.1965				
C	0.5178	-1.7597	-0.2461	C	0.6501	-1.7788	-0.3287				
C	0.392	-0.4373	-3.2349	C	0.3177	0.224	-3.1426				
C	-1.1046	-0.2625	-2.9944	C	-0.8692	-0.7263	-2.9469				
C	-4.4315	-0.2601	0.4346	C	-4.2158	-0.4391	0.8762				
C	0.7297	-1.9249	1.2538	C	0.9896	-2.2982	1.0616				
C	1.227	-0.9696	2.0599	C	1.6181	-1.6562	2.0614				
C	1.5954	0.4033	1.613	C	2.2717	-0.3142	2.1566				
C	2.8445	0.5008	0.7221	C	2.7618	0.4529	0.9211				
C	1.645	-1.0042	-1.0839	C	1.5594	-0.7229	-1.0797				
C	1.0365	0.136	-1.9461	C	0.7618	0.4758	-1.6953				
C	0.4067	-3.2882	1.8212	C	0.5946	-3.7482	1.3003				
C	0.9508	0.2272	-4.4894	C	-0.0569	1.5456	-3.8261				
O	-1.5813	0.9386	-3.6355	O	-1.9313	-0.4822	-3.8784				
H	-1.2371	-2.2355	-1.392	H	-1.2412	-2.567	-1.0227				
O	-0.0337	0.7443	-1.204	O	-0.491	0.6414	-1.0295				
C	-2.2897	0.7742	-4.7841	C	-1.7815	-1.0561	-5.1037				
C	-2.7197	2.1078	-5.3129	C	-2.9553	-0.7225	-5.9718				
O	-2.54	-0.2956	-5.3196	O	-0.8306	-1.7392	-5.4551				
C	3.0054	-0.6145	-0.366	C	2.9351	-0.3217	-0.4143				
C	4.0413	-0.1368	-1.437	C	3.7332	0.6053	-1.3903				
C	3.6946	-1.875	0.2372	C	3.8625	-1.5554	-0.2464				
O	2.7943	1.7902	0.0567	O	1.9026	1.5929	0.6924				
H	1.9908	-1.7576	-1.8102	H	1.9102	-1.276	-1.9677				
C	3.1728	2.8755	0.7817	C	2.1557	2.7159	1.4142				
C	3.0289	4.1139	-0.0483	C	1.3024	3.8435	0.9195				
O	3.5731	2.8605	1.9365	O	2.9985	2.8246	2.2935				
H	0.6511	-2.7952	-0.6063	H	0.8803	-2.6704	-0.9412				
O	-1.8004	-0.6836	1.5318	O	-1.4105	-0.34	1.5061				
C	-2.2626	-1.1717	2.7099	C	-1.55	-0.5325	2.8417				
C	-1.2274	1.3769	5.9951	C	-0.6289	3.0114	5.0548				
C	-1.0899	1.8548	4.6923	C	-0.9521	3.1154	3.702				
C	-1.4275	1.0406	3.6092	C	-1.2422	1.9681	2.9607				
C	-1.8963	-0.262	3.8273	C	-1.2173	0.7115	3.5784				
C	-2.0397	-0.7322	5.1394	C	-0.9059	0.6144	4.9407				
C	-1.704	0.0858	6.2199	C	-0.6059	1.7627	5.6748				

O	-2.8877	-2.2091	2.8651	O	-1.9058	-1.5602	3.3973				
H	-3.5873	-1.3006	-1.2338	H	-3.5794	-1.9997	-0.433				
H	-2.4236	-2.4604	0.5787	H	-1.9447	-2.3539	1.2298				
H	-2.2638	1.269	-0.1798	H	-2.9065	0.8918	-0.9513				
H	-3.0527	1.026	-1.7317	H	-3.4265	-0.4006	-2.038				
H	0.6031	-1.5099	-3.3268	H	1.1103	-0.2422	-3.7385				
H	-1.6836	-1.1358	-3.3146	H	-0.5438	-1.7701	-3.0466				
H	-4.1602	0.4466	1.2252	H	-3.8932	0.5302	1.2693				
H	-5.1807	0.2293	-0.1968	H	-5.1419	-0.2751	0.315				
H	-4.9014	-1.1326	0.8992	H	-4.4473	-1.0928	1.7232				
H	1.3709	-1.1755	3.1193	H	1.7282	-2.2054	3.0002				
H	1.7542	1.0185	2.5085	H	3.1708	-0.4901	2.7662				
H	0.7341	0.8772	1.1306	H	1.632	0.3249	2.7748				
H	3.742	0.4747	1.356	H	3.7584	0.843	1.1773				
H	1.7482	0.9241	-2.1877	H	1.2953	1.4227	-1.6337				
H	-0.6131	-3.5892	1.5684	H	-0.4507	-3.9343	1.044				
H	1.0949	-4.0362	1.4137	H	1.2151	-4.4049	0.6807				
H	0.4958	-3.3136	2.9125	H	0.7294	-4.0556	2.3429				
H	0.4613	-0.1627	-5.3874	H	-0.3398	1.3824	-4.8706				
H	2.0233	0.0232	-4.5803	H	0.797	2.2317	-3.8257				
H	0.8231	1.3145	-4.4691	H	-0.8902	2.0458	-3.3211				
H	-3.3469	2.6143	-4.5749	H	-3.8741	-1.0951	-5.5121				
H	-1.8409	2.712	-5.5516	H	-3.0098	0.3588	-6.1205				
H	-3.3041	1.9644	-6.2262	H	-2.8338	-1.2039	-6.9463				
H	4.1947	-0.9062	-2.203	H	3.7743	0.1757	-2.3978				
H	5.0146	0.0643	-0.9728	H	4.7676	0.7334	-1.0479				
H	3.7543	0.7807	-1.9552	H	3.3174	1.6131	-1.4701				
H	3.2014	-2.2976	1.1097	H	3.4454	-2.361	0.3551				
H	3.7698	-2.6729	-0.5111	H	4.1039	-1.9928	-1.2229				
H	4.716	-1.64	0.5621	H	4.8102	-1.2676	0.2245				
H	1.985	4.2406	-0.3463	H	0.2976	3.4856	0.681				
H	3.3307	4.9835	0.5424	H	1.2152	4.6022	1.7019				
H	3.675	4.0479	-0.9272	H	1.7608	4.284	0.031				
H	-0.9632	2.0126	6.8368	H	-0.3966	3.9058	5.6281				
H	-0.7178	2.8617	4.5186	H	-0.9786	4.0919	3.2255				
H	-1.3166	1.4316	2.6007	H	-1.4939	2.0622	1.9066				
H	-2.4103	-1.7387	5.3235	H	-0.8941	-0.3566	5.4317				
H	-1.8137	-0.2847	7.2361	H	-0.3576	1.6833	6.7302				

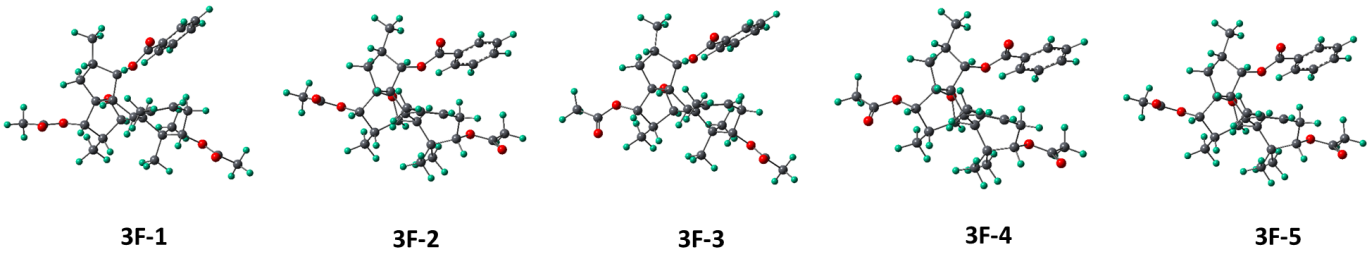


Figure S19. Key conformers of isomer **3F**.

Table S21. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **3F** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
3F-1	-1731.979819	0.960236313	6.90%	0
3F-2	-1731.981021	0.206216278	24.67%	0
3F-3	-1731.980051	0.814950566	8.82%	0
3F-4	-1731.98135	0	34.94%	0
3F-5	-1731.981021	0.206210003	24.67%	0

Table S22. Optimized Z-matrixes of isomer **3F** in the gas phase (Å) at B3LYP/6-31G* level.

3F-1	**3F-2**	**3F-3**

C	-3.5882	0.9405	-0.4486	C	-3.501	0.4664	-0.6127	C	-3.5515	1.2535	-0.4133
C	-2.5943	-0.1423	0.0181	C	-2.4112	-0.5851	-0.3153	C	-2.6528	0.1034	0.087
C	-1.6051	-0.2434	-1.1716	C	-1.4098	-0.3413	-1.4626	C	-1.6935	-0.1271	-1.1079
C	-1.4187	1.2368	-1.5581	C	-1.3422	1.1983	-1.5347	C	-1.3735	1.3174	-1.5385
C	-2.8046	1.8636	-1.4049	C	-2.7802	1.658	-1.2865	C	-2.6915	2.0783	-1.3933
C	-0.2658	-1.0283	-0.9378	C	-0.0149	-1.014	-1.3652	C	-0.431	-1.0284	-0.8708
C	0.7986	1.3636	-2.4726	C	0.8799	1.707	-2.3371	C	0.8183	1.2083	-2.5074
C	-0.6855	1.4394	-2.8874	C	-0.6051	1.729	-2.7732	C	-0.6617	1.4126	-2.8897
C	-4.2854	1.7118	0.6633	C	-4.3437	0.8995	0.5783	C	-4.1784	2.1121	0.6761
C	-0.5802	-2.4019	-0.3273	C	-0.098	-2.5227	-1.143	C	-0.8615	-2.3449	-0.208
C	-0.0196	-2.9387	0.7726	C	0.4976	-3.2144	-0.1553	C	-0.3312	-2.8961	0.8998
C	1.1908	-2.4354	1.4921	C	1.3013	-2.681	0.9827	C	0.9375	-2.4876	1.5782
C	2.2989	-2.1335	0.4735	C	2.5637	-1.8452	0.6857	C	2.0464	-2.3284	0.5282
C	0.8113	-0.0967	-0.2629	C	0.9849	-0.1756	-0.4938	C	0.7441	-0.1834	-0.2489
C	0.7656	1.3193	-0.9299	C	0.8298	1.3362	-0.8451	C	0.8187	1.209	-0.9613
C	-1.5723	-3.2555	-1.0956	C	-0.863	-3.2906	-2.201	C	-1.9438	-3.1261	-0.9299
C	1.646	2.5353	-2.9752	C	1.6167	3.0299	-2.5552	C	1.7658	2.2807	-3.0504
O	-0.9747	2.7352	-3.4475	O	-1.0066	3.0792	-3.0762	O	-0.8932	2.7145	-3.461
H	-2.1433	-0.7307	-1.999	H	-1.8917	-0.6916	-2.3885	H	-2.2879	-0.5853	-1.9134
O	-0.5306	1.8564	-0.6107	O	-0.5163	1.6827	-0.4587	O	-0.4118	1.8768	-0.6297
C	-1.86	2.7687	-4.4785	C	-1.8842	3.236	-4.1025	C	-0.9639	2.7731	-4.8177
C	-2.0384	4.1777	-4.9532	C	-2.1863	4.6895	-4.2992	C	-1.2175	4.1828	-5.2551
O	-2.4394	1.8006	-4.9492	O	-2.3704	2.3315	-4.7658	O	-0.8336	1.825	-5.5782
C	2.2794	-0.6598	-0.0554	C	2.4575	-0.748	-0.4479	C	2.1558	-0.8781	-0.0521
C	3.1208	-0.6422	-1.3487	C	2.9221	-1.377	-1.7858	C	2.9624	-0.9845	-1.3632
C	3.017	0.2539	0.9685	C	3.4952	0.3678	-0.1483	C	3.0024	-0.0067	0.9231
O	3.5909	-2.4201	1.0664	O	2.8858	-1.173	1.9382	O	3.3182	-2.7186	1.1053
H	0.4392	0.0704	0.7548	H	0.622	-0.2219	0.5397	H	0.4116	0.0505	0.7697
C	3.9943	-3.7199	1.0574	C	3.607	-1.8799	2.8493	C	3.5932	-4.0511	1.1375
C	5.3441	-3.8364	1.6964	C	3.8241	-1.0533	4.0791	C	4.9413	-4.2761	1.7503
O	3.3621	-4.6621	0.6037	O	4.014	-3.0233	2.7055	O	2.8606	-4.9427	0.7351
H	0.1344	-1.2602	-1.935	H	0.3851	-0.9415	-2.3874	H	-0.0758	-1.3293	-1.8667
O	-1.9216	0.2566	1.2173	O	-1.8036	-0.3517	0.9594	O	-1.929	0.4838	1.2618
C	-2.2906	-0.3494	2.3699	C	-2.1972	-1.1358	1.9898	C	-2.3321	-0.0455	2.4405
C	0.1402	0.9666	5.6447	C	-0.1324	-0.0973	5.6003	C	0.2685	1.1464	5.6315
C	-0.6906	-0.1455	5.7777	C	-0.9002	-1.2592	5.529	C	-0.6655	0.1277	5.8179
C	-1.4804	-0.5595	4.7034	C	-1.5697	-1.5825	4.3472	C	-1.5092	-0.2464	4.7703
C	-1.4396	0.137	3.4885	C	-1.4705	-0.7452	3.2283	C	-1.4197	0.3965	3.5288
C	-0.6071	1.2586	3.3639	C	-0.6987	0.4231	3.308	C	-0.4828	1.4247	3.3503
C	0.1818	1.6691	4.4406	C	-0.0314	0.7434	4.4922	C	0.3597	1.7953	4.4004
O	-3.169	-1.186	2.5026	O	-3.0147	-2.0404	1.9412	O	-3.2823	-0.791	2.6148
H	-4.3634	0.4413	-1.047	H	-4.1788	0.0345	-1.3627	H	-4.3668	0.8059	-0.9989
H	-3.1246	-1.0886	0.1615	H	-2.8235	-1.5983	-0.3791	H	-3.2639	-0.7852	0.2716
H	-2.7438	2.8898	-1.0256	H	-2.8118	2.5587	-0.6632	H	-2.5291	3.1006	-1.0336
H	-3.3431	1.8866	-2.3577	H	-3.3047	1.8755	-2.222	H	-3.2224	2.1366	-2.351
H	1.2395	0.4511	-2.8817	H	1.424	0.9484	-2.9051	H	1.1616	0.2472	-2.8985
H	-0.9126	0.6442	-3.6069	H	-0.745	1.0772	-3.6434	H	-1.0214	0.6257	-3.563
H	-4.829	1.031	1.3259	H	-4.8435	0.0389	1.0338	H	-4.7772	1.4987	1.3568
H	-3.5751	2.2864	1.2667	H	-3.74	1.3947	1.3457	H	-3.4207	2.64	1.2643
H	-5.0092	2.4178	0.2425	H	-5.1184	1.6057	0.2608	H	-4.8397	2.8657	0.2354
H	-0.3595	-3.9171	1.1141	H	0.3652	-4.2967	-0.1272	H	-0.7539	-3.8266	1.2807
H	0.951	-1.5866	2.1389	H	0.6318	-2.1355	1.6577	H	0.7942	-1.5984	2.1988
H	1.5238	-3.226	2.1762	H	1.6135	-3.542	1.5903	H	1.2085	-3.2831	2.2837
H	2.1896	-2.7953	-0.3985	H	3.3913	-2.5193	0.4263	H	1.8545	-3.0053	-0.3175
H	1.4999	1.9921	-0.4837	H	1.4906	1.9545	-0.2328	H	1.6237	1.8211	-0.551
H	-1.5924	-4.291	-0.7377	H	-0.7571	-4.375	-2.0871	H	-2.0557	-4.1418	-0.5342
H	-2.5903	-2.8683	-1.0177	H	-1.9314	-3.0613	-2.1536	H	-2.919	-2.6412	-0.8515
H	-1.2933	-3.2914	-2.1542	H	-0.4929	-3.0334	-3.1991	H	-1.6887	-3.2253	-1.9905
H	1.2967	3.4921	-2.5722	H	1.1769	3.8427	-1.9673	H	1.4926	3.2812	-2.6982
H	1.6229	2.5902	-4.0687	H	1.5979	3.3157	-3.6121	H	1.7661	2.2845	-4.1448
H	2.691	2.4158	-2.6721	H	2.6661	2.9382	-2.2565	H	2.7936	2.0899	-2.7252
H	-2.4633	4.787	-4.1516	H	-2.6711	5.0906	-3.4056	H	-2.1583	4.5397	-4.8284
H	-1.0772	4.5841	-5.278	H	-1.2636	5.2343	-4.5144	H	-0.3867	4.8215	-4.9448
H	-2.7254	4.1893	-5.8042	H	-2.8648	4.807	-5.1489	H	-1.2958	4.2155	-6.3455
H	3.3052	0.3751	-1.7022	H	2.8413	-0.6691	-2.6149	H	3.2348	-0.002	-1.7563
H	4.1067	-1.0945	-1.1876	H	3.9771	-1.6732	-1.7271	H	3.9038	-1.5248	-1.2079

H	2.6329	-1.2087	-2.1484	H	2.3714	-2.2796	-2.0567	H	2.4022	-1.5266	-2.132
H	2.5009	0.2644	1.9345	H	3.2332	0.9466	0.7439	H	2.5125	0.0872	1.8981
H	4.047	-0.0753	1.1453	H	4.492	-0.0584	0.0185	H	3.9995	-0.4289	1.091
H	3.0959	1.2875	0.6213	H	3.5868	1.0658	-0.9868	H	3.1736	1.0017	0.5372
H	5.6665	-4.8813	1.6747	H	4.2761	-0.0953	3.8091	H	5.1606	-5.3476	1.7605
H	6.0699	-3.237	1.1412	H	2.8727	-0.8987	4.5925	H	5.7072	-3.7702	1.1571
H	5.2903	-3.5094	2.7378	H	4.5086	-1.5777	4.7519	H	4.9462	-3.9091	2.7797
H	0.7536	1.289	6.4828	H	0.3847	0.1554	6.5229	H	0.924	1.4378	6.4487
H	-0.7254	-0.6904	6.7179	H	-0.9813	-1.9129	6.394	H	-0.7385	-0.3754	6.779
H	-2.1259	-1.4287	4.8148	H	-2.1682	-2.4904	4.3003	H	-2.235	-1.0428	4.9235
H	-0.5659	1.8223	2.4339	H	-0.6125	1.0945	2.4558	H	-0.401	1.946	2.3985
H	0.826	2.539	4.3397	H	0.5634	1.6517	4.5493	H	1.0848	2.5928	4.2576
3F-4				**3F-5**							
C	-3.5303	0.4427	-0.7628	C	-3.4457	0.8959	-0.2611				
C	-2.4626	-0.5985	-0.361	C	-2.4995	-0.3201	-0.0691				
C	-1.4108	-0.4195	-1.4736	C	-1.5736	-0.2851	-1.3059				
C	-1.3263	1.1139	-1.6146	C	-1.4164	1.219	-1.5822				
C	-2.7694	1.5961	-1.4582	C	-2.8222	1.764	-1.3762				
C	-0.0266	-1.0952	-1.29	C	-0.2089	-1.0234	-1.2313				
C	0.9193	1.572	-2.3714	C	0.7869	1.5608	-2.5133				
C	-0.5508	1.5792	-2.854	C	-0.7077	1.5315	-2.9093				
C	-4.4248	0.9371	0.3648	C	-3.7309	1.7169	0.9925				
C	-0.1306	-2.5896	-0.993	C	-0.3482	-2.4972	-0.8569				
C	0.4227	-3.2321	0.0509	C	0.2973	-3.1297	0.1389				
C	1.189	-2.644	1.1877	C	1.2236	-2.5454	1.1514				
C	2.4692	-1.8347	0.8926	C	2.4939	-1.8117	0.6793				
C	0.9483	-0.2187	-0.4287	C	0.8913	-0.1599	-0.5154				
C	0.8183	1.2738	-0.8631	C	0.78	1.3233	-0.9945				
C	-0.861	-3.4073	-2.0379	C	-1.2434	-3.3131	-1.7663				
C	1.6757	2.8786	-2.6169	C	1.4994	2.8697	-2.8616				
O	-0.9862	2.9031	-3.218	O	-1.1096	2.8109	-3.4336				
H	-1.8576	-0.8113	-2.4006	H	-2.148	-0.7082	-2.1445				
O	-0.5369	1.6468	-0.5374	O	-0.5317	1.7764	-0.5969				
C	-0.9756	3.1966	-4.5457	C	-2.0516	2.7919	-4.4143				
C	-1.4606	4.5968	-4.7627	C	-2.3584	4.1887	-4.8579				
O	-0.6185	2.4415	-5.4381	O	-2.5895	1.7896	-4.8624				
C	2.4132	-0.7974	-0.2996	C	2.34	-0.8006	-0.5269				
C	2.9194	-1.4978	-1.5859	C	2.673	-1.5628	-1.8353				
C	3.4491	0.3254	-0.0211	C	3.4422	0.286	-0.401				
O	2.7532	-1.1001	2.1191	O	2.976	-1.0722	1.8402				
H	0.5476	-0.2087	0.592	H	0.6087	-0.0921	0.5419				
C	3.4332	-1.7642	3.092	C	3.7218	-1.7652	2.7439				
C	3.6163	-0.8747	4.2829	C	4.1431	-0.8613	3.8612				
O	3.8319	-2.9175	3.024	O	4.0198	-2.9482	2.6642				
H	0.4107	-1.0784	-2.2993	H	0.1232	-1.07	-2.2792				
O	-1.9076	-0.3022	0.9242	O	-1.7549	-0.216	1.1489				
C	-2.3491	-1.0308	1.9757	C	-2.2172	-0.9251	2.2074				
C	-0.41	0.1633	5.6078	C	0.3304	-0.4006	5.6055				
C	-1.1895	-0.9922	5.5642	C	-0.4917	-1.5224	5.5017				
C	-1.8179	-1.3664	4.3748	C	-1.3283	-1.674	4.3948				
C	-1.6657	-0.5866	3.2207	C	-1.3344	-0.7075	3.3811				
C	-0.8826	0.5756	3.2726	C	-0.5099	0.4206	3.492				
C	-0.2564	0.9469	4.4644	C	0.3194	0.5716	4.6048				
O	-3.174	-1.9292	1.939	O	-3.1905	-1.6608	2.2228				
H	-4.1747	-0.022	-1.5225	H	-4.4075	0.5235	-0.6388				
H	-2.8797	-1.6113	-0.3903	H	-3.0776	-1.2517	-0.0896				
H	-2.8216	2.5253	-0.8797	H	-2.8203	2.8288	-1.1196				
H	-3.2369	1.7767	-2.4333	H	-3.4247	1.6318	-2.2818				
H	1.4768	0.7838	-2.8833	H	1.3244	0.7625	-3.0293				
H	-0.7093	0.8791	-3.6825	H	-0.8731	0.7443	-3.6546				
H	-4.9513	0.102	0.8373	H	-4.1982	1.1017	1.7673				
H	-3.8541	1.4659	1.1352	H	-2.8172	2.1599	1.4028				
H	-5.1787	1.6308	-0.0224	H	-4.4206	2.5367	0.7637				
H	0.2816	-4.3107	0.1305	H	0.1126	-4.1953	0.2809				
H	0.5004	-2.0581	1.8075	H	0.6468	-1.9028	1.8226				
H	1.4709	-3.4733	1.8517	H	1.5404	-3.366	1.8099				

H	3.299	-2.5276	0.6984	H	3.2554	-2.5534	0.4024				
H	1.4629	1.9179	-0.2603	H	1.4954	1.9582	-0.4657				
H	-0.7695	-4.4848	-1.8628	H	-1.1733	-4.3877	-1.5652				
H	-1.9283	-3.1684	-2.0445	H	-2.2913	-3.0263	-1.6404				
H	-0.4504	-3.2061	-3.033	H	-0.9608	-3.1621	-2.8134				
H	1.1987	3.7263	-2.1136	H	1.05	3.7263	-2.3479				
H	1.7396	3.099	-3.6869	H	1.467	3.0553	-3.9404				
H	2.7006	2.8055	-2.2384	H	2.553	2.8232	-2.567				
H	-2.4785	4.7002	-4.3785	H	-2.8437	4.7355	-4.0459				
H	-0.7883	5.302	-4.2677	H	-1.4381	4.692	-5.1653				
H	-1.4697	4.8154	-5.8343	H	-3.035	4.1555	-5.7167				
H	2.8714	-0.8335	-2.4529	H	2.5658	-0.9265	-2.7169				
H	3.9698	-1.7956	-1.4754	H	3.7143	-1.9088	-1.8252				
H	2.3723	-2.4106	-1.8284	H	2.0607	-2.454	-1.9852				
H	3.1603	0.952	0.8295	H	3.2731	0.9459	0.4568				
H	4.4355	-0.0983	0.2038	H	4.4312	-0.1708	-0.2738				
H	3.5769	0.9777	-0.8911	H	3.4962	0.9094	-1.2994				
H	4.0974	0.0589	3.9799	H	3.2644	-0.4495	4.358				
H	2.6481	-0.6757	4.7473	H	4.7162	-1.4359	4.5927				
H	4.2623	-1.373	5.0113	H	4.7753	-0.0617	3.471				
H	0.0753	0.4556	6.5359	H	0.9795	-0.2831	6.4701				
H	-1.3114	-1.6014	6.4565	H	-0.4826	-2.2795	6.282				
H	-2.4255	-2.269	4.3496	H	-1.9668	-2.552	4.3178				
H	-0.7552	1.2029	2.3924	H	-0.5066	1.1849	2.7176				
H	0.3476	1.8502	4.4996	H	0.9578	1.4476	4.6894				

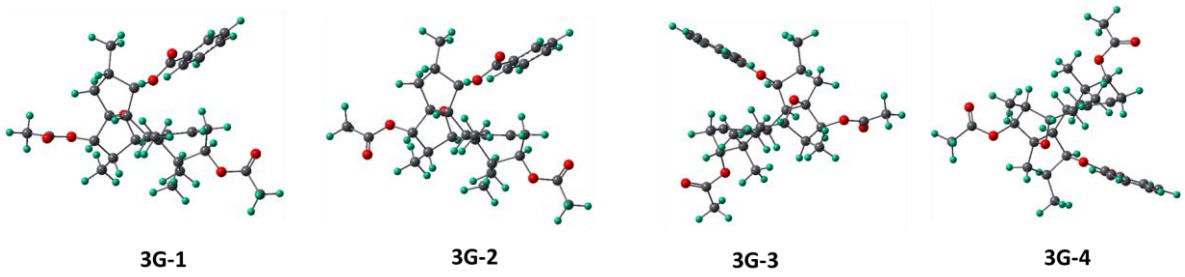


Figure S20. Key conformers of isomer **3G**.

Table S23. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **3G** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
3G-1	-1731.980373	0.139048368	41.06%	0
3G-2	-1731.980595	0	51.93%	0
3G-3	-1731.977906	1.687035272	3.01%	0
3G-4	-1731.978176	1.517728714	4.00%	0

Table S24. Optimized Z-matrixes of isomer **3G** in the gas phase (Å) at B3LYP/6-31G* level.

3G-1				**3G-2**				**3G-3**			
C	-2.7971	-1.7775	-1.6026	C	-2.2058	-2.2206	-2.0326	C	-3.3083	-1.07	-0.9121
C	-1.6401	-1.8493	-0.5848	C	-1.2073	-2.1332	-0.8583	C	-2.016	-1.3877	-0.1333
C	-0.4593	-1.2944	-1.4069	C	-0.054	-1.325	-1.485	C	-0.8996	-0.9994	-1.1375
C	-1.09	-0.0915	-2.1412	C	-0.7995	-0.2194	-2.2621	C	-1.4522	0.3084	-1.7361
C	-2.5043	-0.5535	-2.5007	C	-2.0351	-0.9131	-2.8399	C	-2.9552	0.0723	-1.8869
C	0.8498	-0.9417	-0.6509	C	1.0537	-0.7795	-0.545	C	0.5687	-0.8963	-0.5888
C	0.731	1.4543	-2.4919	C	0.7282	1.6448	-2.331	C	0.4907	1.5843	-2.3377
C	-0.2076	0.4901	-3.2548	C	0.0907	0.5643	-3.2347	C	-0.6798	0.7988	-2.9639
C	-4.1987	-1.7373	-1.0114	C	-3.656	-2.4773	-1.6494	C	-4.5257	-0.7494	-0.0562
C	1.3731	-2.091	0.2089	C	1.6638	-1.857	0.3496	C	0.9004	-2.1673	0.2009
C	1.6549	-2.0372	1.5233	C	1.7536	-1.8194	1.6915	C	1.4003	-2.2259	1.4483
C	1.4582	-0.8864	2.4577	C	1.2238	-0.7712	2.6171	C	1.9861	-1.0979	2.2406
C	2.2029	0.4249	2.1386	C	1.749	0.6668	2.4376	C	2.966	-0.2486	1.4107
C	0.8054	0.4988	-0.0323	C	0.6603	0.5961	0.0964	C	0.8182	0.5128	0.0645

C	0.1666	1.4805	-1.0611	C	-0.0095	1.496	-0.9862	C	0.1659	1.6226	-0.829
C	1.6681	-3.3737	-0.5404	C	2.2916	-3.0242	-0.3831	C	0.7039	-3.4771	-0.5391
C	0.805	2.8621	-3.0851	C	0.6083	3.0741	-2.8614	C	0.6656	2.9963	-2.9027
O	-0.9968	1.2292	-4.2074	O	-0.7299	1.1494	-4.264	O	-1.4886	1.6781	-3.7695
H	-0.2162	-2.0522	-2.1679	H	0.4274	-1.9818	-2.2263	H	-0.9089	-1.7542	-1.9389
O	-1.1905	1.0175	-1.2267	O	-1.2244	0.8032	-1.3439	O	-1.2505	1.3729	-0.7895
C	-1.2569	0.6121	-5.3904	C	-0.1666	1.2541	-5.4972	C	-2.0139	1.1504	-4.9068
C	-2.0682	1.5132	-6.2694	C	-1.1417	1.8692	-6.4531	C	-2.8104	2.1907	-5.6322
O	-0.8973	-0.5152	-5.6978	O	0.9681	0.9083	-5.7924	O	-1.8735	-0.0033	-5.2857
C	2.1557	0.954	0.6494	C	1.7997	1.2537	0.9702	C	2.2811	0.8738	0.5564
C	2.2427	2.5007	0.7519	C	1.5818	2.7831	1.1237	C	2.1768	2.1165	1.4942
C	3.4203	0.5267	-0.1369	C	3.2135	1.1042	0.3549	C	3.2257	1.2725	-0.596
O	3.5841	0.3158	2.564	O	3.0591	0.786	3.0458	O	3.7709	-1.0959	0.5489
H	0.0618	0.4795	0.7732	H	-0.1665	0.4011	0.7899	H	0.2137	0.5101	0.9794
C	3.8473	0.5473	3.8779	C	3.1015	0.9936	4.3891	C	4.7845	-1.7841	1.1387
C	5.3142	0.3901	4.1373	C	4.5255	1.0906	4.8432	C	5.4726	-2.6424	0.1224
O	3.0229	0.8393	4.7317	O	2.1332	1.0876	5.129	O	5.1008	-1.721	2.3178
H	1.6036	-0.874	-1.449	H	1.8803	-0.5356	-1.2286	H	1.2311	-0.935	-1.4651
O	-1.9048	-1.0293	0.5576	O	-1.7758	-1.4392	0.2561	O	-1.9301	-0.6067	1.0634
C	-2.3495	-1.6503	1.6754	C	-2.2403	-2.1915	1.2814	C	-2.1469	-1.2412	2.239
C	-3.0082	1.1623	4.8404	C	-3.8296	0.2746	4.4046	C	-1.5386	1.4127	5.5483
C	-2.7958	1.6327	3.5448	C	-3.5359	0.8476	3.1675	C	-1.6365	1.9407	4.2612
C	-2.5854	0.7314	2.4992	C	-3.0231	0.059	2.1356	C	-1.8402	1.0923	3.1709
C	-2.5833	-0.6485	2.7497	C	-2.7985	-1.3099	2.3415	C	-1.943	-0.2926	3.3663
C	-2.8048	-1.1135	4.0526	C	-3.1028	-1.8796	3.5847	C	-1.8502	-0.8146	4.663
C	-3.0147	-0.2088	5.0949	C	-3.6154	-1.0875	4.6136	C	-1.6467	0.0371	5.7504
O	-2.5298	-2.849	1.8154	O	-2.2091	-3.4089	1.3586	O	-2.4446	-2.4152	2.3878
H	-2.7289	-2.6699	-2.2411	H	-1.8797	-3.0456	-2.6817	H	-3.5509	-1.9509	-1.5231
H	-1.4452	-2.8872	-0.2921	H	-0.86	-3.1318	-0.5701	H	-1.9793	-2.4577	0.0923
H	-3.2373	0.2469	-2.3494	H	-2.9222	-0.2736	-2.7705	H	-3.5295	0.9817	-1.6777
H	-2.5742	-0.8831	-3.5418	H	-1.8894	-1.1777	-3.8938	H	-3.2105	-0.2639	-2.8969
H	1.7487	1.059	-2.5012	H	1.7946	1.4428	-2.2131	H	1.4231	1.0464	-2.5256
H	0.3836	-0.2852	-3.7557	H	0.8469	-0.0982	-3.6718	H	-0.2921	-0.0328	-3.5638
H	-4.3597	-0.8401	-0.4051	H	-4.0681	-1.6627	-1.0452	H	-4.3777	0.1587	0.5374
H	-4.9492	-1.7356	-1.8091	H	-4.277	-2.5697	-2.5469	H	-5.4062	-0.5919	-0.6882
H	-4.381	-2.6156	-0.3843	H	-3.7486	-3.4089	-1.0826	H	-4.7479	-1.5752	0.627
H	2.0432	-2.9333	2.0085	H	2.2353	-2.6528	2.2039	H	1.5486	-3.2037	1.9079
H	0.3842	-0.6945	2.5446	H	0.1309	-0.7807	2.5575	H	1.2111	-0.5005	2.7293
H	1.7603	-1.2312	3.4552	H	1.449	-1.1053	3.6383	H	2.5557	-1.5577	3.0591
H	1.7156	1.1885	2.7622	H	1.0521	1.298	3.0079	H	3.6572	0.243	2.1093
H	0.0967	2.4912	-0.6514	H	-0.3192	2.4554	-0.5643	H	0.3178	2.615	-0.401
H	0.7449	-3.8363	-0.9007	H	1.5282	-3.6276	-0.8824	H	-0.3527	-3.7123	-0.6821
H	2.3171	-3.1713	-1.3989	H	3.0006	-2.6632	-1.1355	H	1.1854	-3.4265	-1.5217
H	2.1805	-4.1131	0.0847	H	2.8445	-3.6895	0.289	H	1.1545	-4.3237	-0.0091
H	-0.1666	3.3672	-3.0581	H	-0.437	3.3762	-2.9866	H	-0.2153	3.6205	-2.7169
H	1.1506	2.8289	-4.1236	H	1.1193	3.1789	-3.8234	H	0.8459	2.9631	-3.9823
H	1.5125	3.4783	-2.5205	H	1.0746	3.7804	-2.1665	H	1.5225	3.4957	-2.4396
H	-3.034	1.7159	-5.8	H	-2.0389	1.2484	-6.518	H	-3.6526	2.5098	-5.0131
H	-1.5241	2.4439	-6.4492	H	-1.3953	2.8798	-6.1235	H	-2.1706	3.0412	-5.8806
H	-2.2418	1.0215	-7.2308	H	-0.6874	1.9286	-7.4462	H	-3.1998	1.7661	-6.5619
H	2.3381	2.9671	-0.2339	H	1.7178	3.309	0.1732	H	1.8292	3.0099	0.9681
H	3.1179	2.8104	1.3357	H	2.2989	3.2164	1.8314	H	3.1546	2.3768	1.9174
H	1.3583	2.9181	1.2463	H	0.5775	3.0073	1.5007	H	1.4947	1.9299	2.3307
H	3.5811	-0.5538	-0.1267	H	3.5713	0.072	0.3605	H	3.2814	0.4939	-1.3633
H	3.3783	0.8533	-1.1784	H	3.2465	1.4687	-0.6745	H	2.9158	2.2053	-1.0736
H	4.3255	0.9807	0.2849	H	3.9546	1.6943	0.9079	H	4.244	1.4431	-0.2255
H	5.876	1.109	3.5356	H	5.0176	1.9286	4.3431	H	5.9015	-2.0151	-0.663
H	5.5185	0.5854	5.1939	H	4.5508	1.2658	5.9225	H	6.2807	-3.1991	0.6053
H	5.6238	-0.632	3.9053	H	5.047	0.1543	4.6295	H	4.7619	-3.3571	-0.3004
H	-3.1701	1.8657	5.6537	H	-4.2272	0.8907	5.2076	H	-1.3816	2.0749	6.3964
H	-2.7948	2.7019	3.3477	H	-3.7069	1.909	3.0054	H	-1.5574	3.0138	4.1055
H	-2.4266	1.1171	1.4941	H	-2.8048	0.523	1.1758	H	-1.9192	1.5224	2.1743
H	-2.8092	-2.1818	4.2601	H	-2.9365	-2.9412	3.7568	H	-1.9326	-1.8871	4.8289
H	-3.1814	-0.5741	6.1052	H	-3.8458	-1.5329	5.5782	H	-1.5735	-0.3734	6.7545
3G-4											
C	-3.5275	-0.65	-0.6572								

C	-2.1984	-1.2066	-0.1057								
C	-1.1627	-0.7222	-1.1522								
C	-1.6418	0.7165	-1.4248								
C	-3.1685	0.6358	-1.4301								
C	0.3599	-0.8429	-0.7882								
C	0.3336	1.9236	-2.0508								
C	-0.977	1.3653	-2.6405								
C	-4.6184	-0.4214	0.3795								
C	0.6456	-2.2618	-0.2843								
C	1.2734	-2.5924	0.8585								
C	2.0579	-1.6829	1.7533								
C	3.0215	-0.7769	0.9648								
C	0.826	0.3938	0.0637								
C	0.1946	1.7005	-0.527								
C	0.2364	-3.3898	-1.2125								
C	0.5884	3.4005	-2.3615								
O	-1.8257	2.4126	-3.148								
H	-1.3364	-1.3053	-2.0698								
O	-1.2253	1.5623	-0.3411								
C	-1.7936	2.6157	-4.4922								
C	-2.7306	3.7236	-4.8632								
O	-1.1019	1.9982	-5.2886								
C	2.3649	0.5365	0.4142								
C	2.4997	1.5892	1.5578								
C	3.2067	1.0614	-0.767								
O	3.633	-1.5124	-0.1276								
H	0.3322	0.2683	1.035								
C	4.63	-2.3779	0.1975								
C	5.1097	-3.0835	-1.0335								
O	5.0797	-2.5622	1.3191								
H	0.9117	-0.77	-1.7361								
O	-1.9105	-0.6709	1.19								
C	-2.0602	-1.4955	2.2526								
C	-0.828	0.4323	5.8763								
C	-1.0046	1.1977	4.7239								
C	-1.4111	0.5883	3.5351								
C	-1.6392	-0.7949	3.4952								
C	-1.4657	-1.5559	4.6586								
C	-1.0594	-0.9427	5.8453								
O	-2.4569	-2.6492	2.2269								
H	-3.9091	-1.372	-1.3929								
H	-2.2431	-2.2994	-0.0792								
H	-3.6205	1.525	-0.9764								
H	-3.5566	0.5423	-2.4514								
H	1.1774	1.3589	-2.4547								
H	-0.7877	0.6123	-3.4145								
H	-4.3289	0.3373	1.114								
H	-5.5395	-0.0794	-0.1043								
H	-4.8458	-1.3491	0.9141								
H	1.3724	-3.6476	1.1158								
H	1.4086	-1.1255	2.4347								
H	2.6649	-2.3317	2.3986								
H	3.8336	-0.4815	1.6434								
H	0.4968	2.5789	0.046								
H	-0.8479	-3.5076	-1.2615								
H	0.6112	-3.1956	-2.2234								
H	0.6524	-4.3544	-0.9006								
H	-0.2162	4.0404	-1.9835								
H	0.685	3.5623	-3.4395								
H	1.52	3.739	-1.8966								
H	-3.7487	3.4646	-4.5616								
H	-2.4118	4.6533	-4.3854								
H	-2.7145	3.8641	-5.9478								
H	2.1918	2.5904	1.2438								
H	3.5411	1.6842	1.8885								
H	1.9006	1.3095	2.4311								

H	3.0911	0.4358	-1.6576								
H	2.9431	2.0885	-1.0315								
H	4.2732	1.0763	-0.5108								
H	5.5097	-2.3567	-1.745								
H	5.906	-3.7828	-0.7635								
H	4.2874	-3.648	-1.4805								
H	-0.5128	0.9086	6.8016								
H	-0.8288	2.2703	4.7506								
H	-1.5485	1.2023	2.6471								
H	-1.6431	-2.6295	4.6423								
H	-0.9243	-1.5382	6.7448								

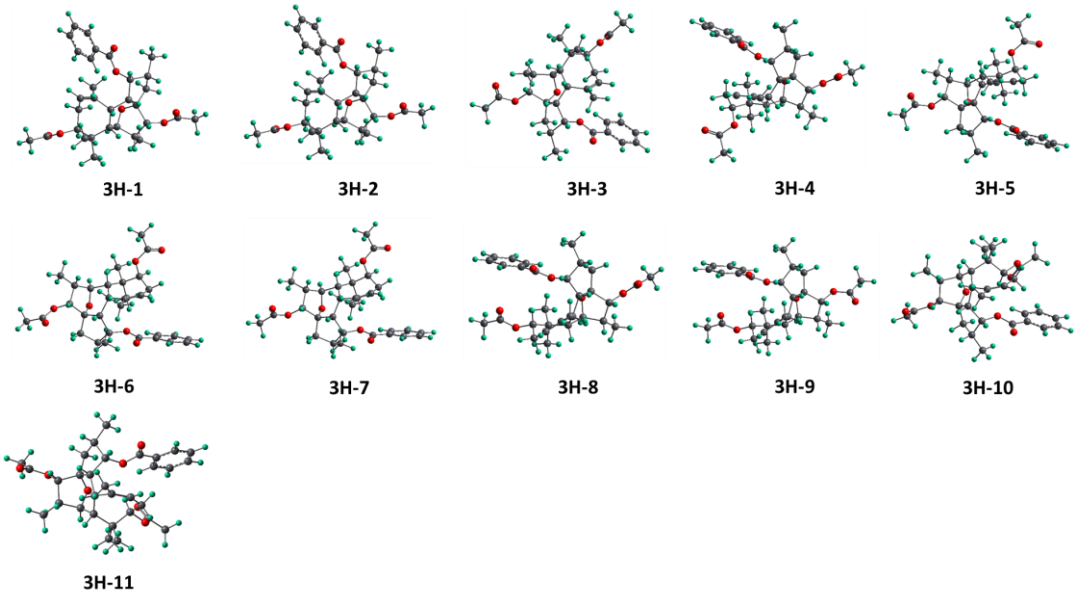


Figure S21. Key conformers of isomer **3H**.

Table S25. Important thermodynamic parameters and Boltzmann distributions of the optimized isomer **3H** at B3LYP/6-31G* level in the gas phase.

Conformations	Energy (a.u)	*Δ*G(kcal/mol)	%	Number of imaginary frequencies
3H-1	-1731.969699	0.576235913	12.49%	0
3H-2	-1731.969699	0.576348864	12.49%	0
3H-3	-1731.968529	1.310226055	3.62%	0
3H-4	-1731.970144	0.296771222	20.03%	0
3H-5	-1731.970617	0	33.06%	0
3H-6	-1731.967526	1.939875015	1.25%	0
3H-7	-1731.967514	1.946934423	1.23%	0
3H-8	-1731.968353	1.420628916	3.00%	0
3H-9	-1731.968832	1.120400153	4.98%	0
3H-10	-1731.968606	1.262015007	3.92%	0
3H-11	-1731.968606	1.262021282	3.92%	0

Table S26. Optimized Z-matrixes of isomer **3H** in the gas phase (Å) at B3LYP/6-31G* level.

3H-1				**3H-2**				**3H-3**			
C	-3.5587	-0.1899	-0.1371	C	-3.5845	0.0347	0.0036	C	-3.6015	-0.5877	-0.094
C	-2.3561	-0.8848	0.5223	C	-2.4084	-0.7299	0.633	C	-2.3094	-1.2793	0.3665
C	-1.4185	-1.0985	-0.691	C	-1.5175	-0.9995	-0.6041	C	-1.4042	-1.1019	-0.8777
C	-1.5712	0.2269	-1.4773	C	-1.6096	0.334	-1.3862	C	-1.7074	0.3543	-1.311
C	-2.9048	0.8562	-1.0465	C	-2.8936	1.04	-0.9245	C	-3.1037	0.6974	-0.7668

C	0.0785	-1.5291	-0.4699	C	-0.0441	-1.52	-0.4206	C	0.1315	-1.426	-0.7783
C	0.0427	0.7621	-3.1988	C	-0.0072	0.7781	-3.1438	C	-0.1831	1.4669	-2.8294
C	-1.2972	0.0394	-2.9964	C	-1.3818	0.1342	-2.9113	C	-1.4517	0.5992	-2.8246
C	-4.5658	0.4243	0.8236	C	-4.528	0.7076	0.9891	C	-4.6234	-0.3127	0.9991
C	0.4844	-1.8175	0.9745	C	0.3759	-1.8392	1.0131	C	0.601	-2.037	0.541
C	1.3018	-1.0502	1.7188	C	1.2528	-1.1247	1.7418	C	1.3607	-1.4102	1.458
C	1.9153	0.2404	1.2851	C	1.9332	0.1273	1.2964	C	1.8349	0.0036	1.3727
C	2.9914	0.1041	0.1949	C	2.9708	-0.0677	0.1808	C	2.8909	0.2608	0.2848
C	1.0995	-0.7481	-1.405	C	0.9996	-0.7974	-1.3775	C	1.0463	-0.335	-1.4779
C	0.6319	0.6933	-1.7869	C	0.6096	0.6705	-1.7462	C	0.431	1.1008	-1.4753
C	0.0021	-3.1348	1.5426	C	-0.1711	-3.1283	1.5871	C	0.2632	-3.4974	0.7479
C	-0.109	2.2124	-3.6689	C	-0.0849	2.2362	-3.6076	C	-0.4638	2.9717	-2.9113
O	-2.2965	0.5607	-3.879	O	-2.369	0.7144	-3.7704	O	-2.5524	1.2325	-3.4884
H	-1.8915	-1.8945	-1.2872	H	-2.0529	-1.7647	-1.1876	H	-1.8227	-1.7713	-1.6457
O	-0.4973	1.0637	-0.9947	O	-0.477	1.1047	-0.9269	O	-0.7178	1.1472	-0.6239
C	-3.3469	-0.2715	-4.121	C	-3.4717	-0.0545	-3.9882	C	-2.5563	1.1307	-4.8459
C	-4.301	0.3695	-5.0806	C	-4.4073	0.6416	-4.9272	C	-3.7515	1.836	-5.4086
O	-3.5024	-1.3747	-3.6176	O	-3.6809	-1.1465	-3.4797	O	-1.7109	0.5553	-5.5156
C	2.6301	-0.8172	-1.0217	C	2.533	-0.9575	-1.0323	C	2.5867	-0.3465	-1.1288
C	3.4799	-0.3286	-2.2354	C	3.3755	-0.5118	-2.2669	C	3.3512	0.5217	-2.1752
C	3.0828	-2.2893	-0.814	C	2.904	-2.4538	-0.8417	C	3.1848	-1.7692	-1.311
O	4.2315	-0.3621	0.7821	O	4.1709	-0.6124	0.7845	O	4.1846	-0.2161	0.7303
H	1.0643	-1.3202	-2.3468	H	0.9077	-1.3636	-2.319	H	1.041	-0.6475	-2.5353
C	5.0157	0.5718	1.3839	C	5.3256	0.089	0.6397	C	4.8905	0.6029	1.5551
C	6.2417	-0.08	1.9457	C	6.4426	-0.6269	1.3355	C	6.1891	-0.0454	1.9249
O	4.7715	1.767	1.4625	O	5.4564	1.1417	0.0324	O	4.5332	1.7049	1.9452
H	0.1148	-2.5392	-0.9148	H	-0.0789	-2.5283	-0.8697	H	0.2508	-2.2782	-1.4706
O	-1.7736	-0.001	1.4894	O	-1.75	0.1202	1.5815	O	-1.7852	-0.5892	1.5076
C	-1.9849	-0.2897	2.7954	C	-1.9373	-0.156	2.8936	C	-1.9213	-1.1969	2.7105
C	-0.1009	2.5839	5.3573	C	0.1534	2.6324	5.3884	C	-0.2555	1.1796	5.864
C	-0.1768	2.8381	3.9883	C	0.0383	2.8929	4.0232	C	-0.4097	1.7407	4.5966
C	-0.7918	1.9161	3.1386	C	-0.6417	1.9973	3.1951	C	-0.9557	0.9836	3.558
C	-1.3276	0.7291	3.6571	C	-1.2057	0.8313	3.7316	C	-1.343	-0.3446	3.7834
C	-1.2528	0.484	5.0347	C	-1.091	0.5798	5.1053	C	-1.191	-0.8991	5.0612
C	-0.6397	1.4094	5.8816	C	-0.4114	1.4782	5.9303	C	-0.6473	-0.1381	6.0979
O	-2.6133	-1.2401	3.2345	O	-2.5988	-1.0731	3.3541	O	-2.435	-2.2854	2.9164
H	-4.0846	-0.9217	-0.7655	H	-4.1689	-0.6649	-0.6096	H	-4.0781	-1.2168	-0.8588
H	-2.6608	-1.8414	0.9573	H	-2.7579	-1.6659	1.0789	H	-2.4979	-2.3382	0.5668
H	-2.7279	1.791	-0.4993	H	-2.6496	1.9639	-0.3846	H	-3.0436	1.5231	-0.0472
H	-3.5778	1.1019	-1.8703	H	-3.5717	1.3227	-1.7322	H	-3.8226	0.9916	-1.5363
H	0.6704	0.2403	-3.9303	H	0.5718	0.2229	-3.8907	H	0.4782	1.2052	-3.6631
H	-1.1397	-1.0212	-3.235	H	-1.292	-0.9334	-3.154	H	-1.2582	-0.3665	-3.3097
H	-4.9687	-0.3374	1.4986	H	-4.9569	-0.0288	1.6762	H	-5.5242	0.1412	0.5724
H	-4.124	1.2205	1.4311	H	-4.0243	1.4767	1.5832	H	-4.9178	-1.2432	1.4948
H	-5.4035	0.8603	0.269	H	-5.353	1.1918	0.4559	H	-4.2384	0.3736	1.76
H	1.5621	-1.3676	2.7275	H	1.5173	-1.4619	2.7429	H	1.6785	-1.9493	2.3492
H	2.3451	0.7168	2.1748	H	2.4273	0.5696	2.1715	H	2.2384	0.2763	2.3557
H	1.125	0.9181	0.9511	H	1.178	0.8565	0.9905	H	0.9745	0.6613	1.2233
H	3.1637	1.117	-0.1939	H	3.177	0.9454	-0.1867	H	2.9555	1.3516	0.172
H	1.4091	1.4458	-1.6393	H	1.4331	1.3753	-1.6156	H	1.1339	1.8627	-1.1322
H	-1.0826	-3.232	1.4736	H	-1.2608	-3.1618	1.5395	H	-0.8083	-3.6817	0.6546
H	0.4526	-3.9663	0.9903	H	0.219	-3.9824	1.0234	H	0.7784	-4.1089	-0.0006
H	0.2719	-3.2545	2.5974	H	0.1122	-3.2677	2.6359	H	0.5695	-3.8575	1.7359
H	0.8647	2.7137	-3.6813	H	0.9159	2.6799	-3.6418	H	0.4617	3.5407	-2.7711
H	-0.7759	2.7885	-3.0187	H	-0.7018	2.8481	-2.9411	H	-1.1785	3.299	-2.1487
H	-0.5112	2.251	-4.6867	H	-0.5076	2.3014	-4.6156	H	-0.8666	3.2432	-3.892
H	-4.7232	1.2731	-4.6339	H	-4.7665	1.5679	-4.472	H	-4.6666	1.3861	-5.0152
H	-3.785	0.6062	-6.0145	H	-3.8987	0.8486	-5.8722	H	-3.7059	2.8987	-5.1578
H	-5.1151	-0.3267	-5.3014	H	-5.2651	-0.0059	-5.1301	H	-3.7535	1.7334	-6.4975
H	3.2768	-0.9327	-3.1272	H	3.0916	-1.0774	-3.162	H	3.1829	0.1512	-3.193
H	4.5528	-0.4039	-2.0225	H	4.4457	-0.6799	-2.1006	H	4.4319	0.5023	-1.991
H	3.2811	0.7157	-2.4936	H	3.2533	0.5509	-2.4963	H	3.0453	1.5719	-2.1529
H	4.1762	-2.3759	-0.8135	H	3.9906	-2.6019	-0.8575	H	4.281	-1.7429	-1.3343
H	2.7438	-2.7233	0.127	H	2.5538	-2.8753	0.1009	H	2.9147	-2.4632	-0.5146
H	2.7152	-2.9278	-1.6257	H	2.489	-3.064	-1.6523	H	2.8586	-2.2099	-2.2603
H	5.956	-0.8222	2.6953	H	6.2152	-0.7228	2.4002	H	5.9978	-0.9816	2.4553

H	6.8154	-0.5462	1.1408	H	6.5904	-1.6105	0.8828	H	6.7823	-0.2265	1.0251
H	6.8673	0.6777	2.426	H	7.3657	-0.0503	1.2277	H	6.7518	0.6208	2.5851
H	0.3788	3.3033	6.0167	H	0.6822	3.3316	6.0316	H	0.1705	1.7713	6.6707
H	0.2442	3.7538	3.5801	H	0.477	3.7941	3.6018	H	-0.103	2.768	4.4149
H	-0.8419	2.132	2.0733	H	-0.7229	2.2176	2.1326	H	-1.0684	1.4387	2.576
H	-1.6699	-0.4307	5.4514	H	-1.5295	-0.3183	5.5358	H	-1.493	-1.927	5.2516
H	-0.5823	1.2132	6.9493	H	-0.3242	1.2774	6.9951	H	-0.5289	-0.5738	7.0868
3H-4				**3H-5**				**3H-6**			
C	-2.8749	1.4649	0.9199	C	-3.2651	0.6924	0.6138	C	-2.3289	2.252	0.1708
C	-1.7656	0.4925	1.3586	C	-2.0061	0.0013	1.1686	C	-1.8088	1.0562	1.0023
C	-1.6488	-0.4131	0.1127	C	-1.5253	-0.7877	-0.0693	C	-1.6808	-0.1554	0.0331
C	-1.8235	0.5501	-1.0842	C	-1.7818	0.1685	-1.2544	C	-1.9919	0.4109	-1.3639
C	-2.5104	1.8067	-0.5303	C	-2.8417	1.1736	-0.7806	C	-2.8857	1.6175	-1.1046
C	-0.4699	-1.4388	0.0021	C	-0.1267	-1.4928	-0.0489	C	-0.4572	-1.1341	0.0897
C	-1.2903	-0.9241	-2.8911	C	-0.6867	-1.0203	-3.015	C	-1.2661	-1.3224	-2.8586
C	-2.4651	-0.1256	-2.307	C	-2.0823	-0.5613	-2.5725	C	-2.5389	-0.628	-2.3564
C	-3.0426	2.7062	1.7832	C	-3.8316	1.817	1.4673	C	-1.3057	3.3486	-0.117
C	-0.1567	-2.1042	1.3369	C	0.1728	-2.1365	1.2997	C	-0.0842	-1.5553	1.5072
C	0.9679	-2.0128	2.0623	C	1.1432	-1.8193	2.1696	C	1.0819	-1.4003	2.1541
C	2.2497	-1.3267	1.7415	C	2.2492	-0.8316	2.0365	C	2.3783	-0.8115	1.7157
C	2.7731	-1.5268	0.3181	C	2.9762	-0.8256	0.6904	C	2.8214	-1.0576	0.2765
C	0.6064	-1.1669	-1.1317	C	0.9803	-0.9072	-1.0235	C	0.5941	-0.9978	-1.0884
C	-0.0481	-0.2799	-2.2364	C	0.2684	-0.1362	-2.1788	C	-0.1254	-0.4162	-2.3473
C	-1.2726	-2.9776	1.8897	C	-0.7556	-3.2801	1.6791	C	-1.207	-2.2443	2.2703
C	-1.2011	-0.9151	-4.4161	C	-0.3997	-0.8995	-4.51	C	-1.196	-1.5193	-4.3729
O	-2.9016	0.8556	-3.2695	O	-2.6395	0.3742	-3.5184	O	-3.2039	0.0191	-3.4607
H	-2.5695	-1.0206	0.1463	H	-2.2672	-1.5986	-0.1683	H	-2.5604	-0.7722	0.2849
O	-0.5276	0.9046	-1.5813	O	-0.5647	0.8567	-1.5586	O	-0.7559	0.8132	-1.9619
C	-4.2429	1.0476	-3.3789	C	-3.5969	-0.1061	-4.3555	C	-4.5625	0.0433	-3.4231
C	-4.5275	2.073	-4.4327	C	-4.0751	0.9854	-5.2626	C	-5.0949	0.741	-4.6365
O	-5.0989	0.4832	-2.7133	O	-4.0104	-1.2561	-4.3792	O	-5.257	-0.4235	-2.5321
C	2.0726	-0.6811	-0.7842	C	2.2335	-0.1105	-0.4747	C	2.0035	-0.3325	-0.8346
C	2.1504	0.8109	-0.4236	C	1.9068	1.3365	-0.0729	C	1.9196	1.1721	-0.5458
C	2.9658	-0.8598	-2.0588	C	3.2921	-0.0058	-1.6248	C	2.8769	-0.4773	-2.1257
O	2.7192	-2.9253	-0.0585	O	3.307	-2.1748	0.2776	O	2.8469	-2.4794	-0.0049
H	0.765	-2.1516	-1.6012	H	1.4276	-1.797	-1.4958	H	0.8428	-2.0354	-1.3635
C	3.6935	-3.7326	0.4381	C	4.3778	-2.756	0.8804	C	3.9269	-3.1767	0.4374
C	3.4623	-5.142	-0.013	C	4.5501	-4.1533	0.3694	C	3.7709	-4.6256	0.0915
O	4.6267	-3.3785	1.1439	O	5.1035	-2.2314	1.7126	O	4.8898	-2.7079	1.0267
H	-0.9885	-2.2813	-0.4916	H	-0.3588	-2.4059	-0.6277	H	-0.9382	-2.0722	-0.244
O	-0.5647	1.2125	1.6425	O	-1.0637	0.9792	1.6115	O	-0.6299	1.4081	1.7239
C	-0.2719	1.3798	2.9588	C	-0.981	1.1547	2.9564	C	-0.7393	1.4615	3.0765
C	3.1279	3.9186	3.5122	C	1.5913	4.42	3.9718	C	2.8833	2.8301	4.8945
C	2.3733	4.0332	2.3445	C	0.978	4.3982	2.7191	C	2.5744	3.2387	3.5971
C	1.2602	3.2136	2.1484	C	0.135	3.3409	2.3719	C	1.3951	2.8033	2.9894
C	0.9059	2.2681	3.1195	C	-0.0881	2.2956	3.2775	C	0.5256	1.9488	3.6787
C	1.6588	2.1672	4.2961	C	0.5192	2.3298	4.539	C	0.8333	1.5541	4.9867
C	2.7705	2.9889	4.4887	C	1.3608	3.389	4.8826	C	2.0132	1.9913	5.5907
O	-0.8662	0.8893	3.9058	O	-1.5454	0.4931	3.8135	O	-1.7103	1.1439	3.7452
H	-3.8296	0.9203	0.9145	H	-4.0482	-0.0689	0.4892	H	-3.1526	2.7331	0.7144
H	-2.1032	-0.0932	2.2203	H	-2.2838	-0.6899	1.9714	H	-2.6169	0.7916	1.6979
H	-1.8313	2.6674	-0.5705	H	-2.4241	2.1869	-0.7389	H	-2.8946	2.3254	-1.9399
H	-3.4178	2.0863	-1.0705	H	-3.7228	1.2066	-1.43	H	-3.9148	1.2936	-0.9103
H	-1.3735	-1.9757	-2.5942	H	-0.5471	-2.0765	-2.7589	H	-1.186	-2.3213	-2.4142
H	-3.283	-0.8006	-2.0321	H	-2.7612	-1.4052	-2.4068	H	-3.2022	-1.3573	-1.8775
H	-3.8807	3.3111	1.421	H	-4.0808	1.4537	2.4693	H	-1.7421	4.1206	-0.7599
H	-3.252	2.4292	2.8213	H	-3.1293	2.6503	1.569	H	-0.992	3.8389	0.8102
H	-2.1507	3.3403	1.7704	H	-4.7476	2.2129	1.0159	H	-0.4138	2.966	-0.6163
H	0.9982	-2.5269	3.0245	H	1.1799	-2.3633	3.115	H	1.1282	-1.7436	3.1899
H	2.9967	-1.755	2.4239	H	2.9882	-1.1057	2.8019	H	3.1407	-1.2564	2.3699
H	2.1939	-0.2714	2.0195	H	1.9049	0.1637	2.3284	H	2.3941	0.2548	1.9546
H	3.8293	-1.2192	0.3343	H	3.9172	-0.2791	0.853	H	3.8523	-0.6787	0.2141
H	0.6686	0.0256	-2.9995	H	0.9758	0.3802	-2.8287	H	0.5697	-0.1999	-3.1583
H	-2.1823	-2.3984	2.0672	H	-1.7932	-2.9442	1.752	H	-2.0356	-1.5554	2.456
H	-1.506	-3.7814	1.1832	H	-0.7004	-4.0748	0.9274	H	-1.584	-3.101	1.7017
H	-1.0034	-3.4529	2.8393	H	-0.495	-3.7312	2.6428	H	-0.8819	-2.627	3.2441

H	-0.3698	-1.545	-4.751	H	0.61	-1.2618	-4.7324	H	-0.2804	-2.0564	-4.6437
H	-1.0304	0.092	-4.8112	H	-0.4611	0.1372	-4.8572	H	-1.1888	-0.5646	-4.9097
H	-2.1209	-1.3093	-4.8602	H	-1.1037	-1.5029	-5.0915	H	-2.047	-2.1101	-4.7274
H	-5.6094	2.1931	-4.5389	H	-4.4948	1.8024	-4.6702	H	-6.1883	0.7293	-4.6109
H	-4.0952	3.0332	-4.1407	H	-3.2471	1.3428	-5.8799	H	-4.7561	1.78	-4.644
H	-4.1198	1.7423	-5.3914	H	-4.8574	0.5944	-5.9193	H	-4.7633	0.2209	-5.5387
H	1.9441	1.4573	-1.2829	H	1.6552	1.9609	-0.9364	H	1.5667	1.7364	-1.4145
H	3.1492	1.0822	-0.0621	H	2.7605	1.8158	0.4204	H	2.9033	1.5796	-0.2844
H	1.437	1.0599	0.355	H	1.0669	1.3682	0.6129	H	1.248	1.3824	0.281
H	4.0217	-0.6698	-1.8303	H	4.2347	0.4168	-1.2559	H	3.9234	-0.2134	-1.93
H	2.8947	-1.8761	-2.4618	H	3.5186	-0.9876	-2.0552	H	2.8621	-1.504	-2.5078
H	2.7029	-0.164	-2.8604	H	2.9687	0.6484	-2.4392	H	2.5526	0.1905	-2.9295
H	4.2433	-5.7874	0.3989	H	3.6568	-4.742	0.5928	H	4.6389	-5.1813	0.4575
H	2.4933	-5.4929	0.351	H	4.7392	-4.1334	-0.7068	H	2.874	-5.0262	0.5707
H	3.5059	-5.1937	-1.1037	H	5.4065	-4.6181	0.8661	H	3.7132	-4.7432	-0.9935
H	3.994	4.5584	3.6636	H	2.247	5.2447	4.2408	H	3.8021	3.1704	5.3665
H	2.6504	4.7624	1.5871	H	1.1549	5.2056	2.0127	H	3.251	3.8986	3.0596
H	0.6771	3.3182	1.2362	H	-0.3413	3.3398	1.394	H	1.163	3.1371	1.9819
H	1.3822	1.4463	5.063	H	0.3399	1.53	5.255	H	0.156	0.9027	5.5354
H	3.356	2.9051	5.401	H	1.8347	3.4105	5.8609	H	2.2522	1.6793	6.6044
3H-7				**3H-8**				**3H-9**			
C	-3.1277	1.0326	-0.0122	C	-2.9838	1.0694	0.5469	C	-3.1634	0.6898	-0.3485
C	-2.3065	-0.1616	0.5296	C	-1.8075	0.2567	1.1254	C	-2.1502	-0.3245	0.223
C	-1.4207	-0.6766	-0.6411	C	-1.7121	-0.8835	0.0947	C	-1.4265	-0.7645	-1.0632
C	-1.6345	0.3331	-1.7816	C	-1.9318	-0.1949	-1.2732	C	-1.2454	0.5406	-1.8708
C	-3.0197	0.9172	-1.5339	C	-2.7539	1.067	-0.9748	C	-2.3848	1.4676	-1.425
C	0.0679	-1.1177	-0.426	C	-0.5272	-1.8888	0.1286	C	-0.1595	-1.6619	-0.9971
C	0.1062	-0.1837	-3.3495	C	-1.1578	-1.8603	-2.8367	C	0.4015	-0.0699	-3.5193
C	-1.4172	-0.2527	-3.185	C	-2.4468	-1.1603	-2.3561	C	-1.0878	0.3062	-3.3828
C	-2.7015	2.4066	0.5015	C	-3.1639	2.4746	1.101	C	-3.8306	1.6124	0.6603
C	0.266	-1.9924	0.8073	C	-0.2566	-2.5483	1.4808	C	-0.2942	-2.9356	-0.1629
C	1.0523	-1.7798	1.8744	C	0.9435	-2.7982	2.031	C	0.6259	-3.4599	0.664
C	1.9939	-0.6708	2.1953	C	2.2905	-2.3933	1.5379	C	1.9382	-2.8842	1.0732
C	2.8092	-0.0763	1.0506	C	2.318	-0.9677	0.9871	C	1.8699	-1.3814	1.3438
C	1.1712	-0.1267	-0.9851	C	0.6168	-1.627	-0.928	C	1.2169	-0.9083	-1.1756
C	0.5641	0.6983	-2.165	C	-0.0237	-1.0191	-2.216	C	1.0028	0.2978	-2.1445
C	-0.551	-3.2768	0.8009	C	-1.4763	-3.1074	2.1929	C	-1.5431	-3.7601	-0.4231
C	0.5943	0.3815	-4.6829	C	-1.0158	-1.9572	-4.3562	C	1.1462	0.6361	-4.6524
O	-2.0897	0.5789	-4.152	O	-3.0404	-0.4381	-3.4537	O	-1.3804	1.5305	-4.0861
H	-1.9493	-1.5873	-0.971	H	-2.6208	-1.4832	0.2747	H	-2.1838	-1.3521	-1.6099
O	-0.6249	1.3388	-1.6818	O	-0.6626	0.2027	-1.8136	O	0.0122	1.1391	-1.5311
C	-2.624	-0.0557	-5.2292	C	-4.3974	-0.4616	-3.5346	C	-1.9933	1.4042	-5.2932
C	-3.2918	0.9392	-6.1277	C	-4.8506	0.3064	-4.7377	C	-2.2348	2.7579	-5.8865
O	-2.5682	-1.2571	-5.4474	O	-5.1473	-1.0125	-2.7418	O	-2.3006	0.3492	-5.8286
C	2.0209	0.766	0.0025	C	1.9608	-0.8683	-0.5258	C	2.1096	-0.5005	0.0818
C	1.1932	1.8541	0.6994	C	1.9777	0.6363	-0.9034	C	1.9519	0.9796	0.5194
C	3.1267	1.5179	-0.8116	C	3.1118	-1.4885	-1.3817	C	3.6039	-0.6086	-0.3619
O	3.5455	-1.119	0.3638	O	3.645	-0.4088	1.1868	O	2.8655	-1.036	2.3452
H	1.922	-0.7799	-1.458	H	0.9483	-2.6393	-1.2105	H	1.8392	-1.6286	-1.7309
C	4.695	-1.5499	0.9478	C	3.9388	0.0454	2.4354	C	2.5506	-1.3028	3.6418
C	5.3025	-2.6437	0.1245	C	5.2863	0.6985	2.4339	C	3.6229	-0.7742	4.5436
O	5.1763	-1.1189	1.9855	O	3.2269	-0.0635	3.4229	O	1.5529	-1.8926	4.0296
H	0.1582	-1.8982	-1.2042	H	-1.0041	-2.7611	-0.3544	H	-0.2157	-2.1435	-1.9904
O	-1.6161	0.1897	1.727	O	-0.6307	1.0613	1.2088	O	-1.2973	0.2995	1.1831
C	-2.0389	-0.4112	2.8692	C	-0.3603	1.5679	2.4439	C	-1.6368	0.0876	2.4851
C	0.049	1.0765	6.2937	C	2.8567	4.3855	2.3501	C	0.6921	2.4796	5.159
C	-0.1147	1.9031	5.1821	C	2.0317	4.2514	1.2332	C	0.4073	2.9615	3.8813
C	-0.7955	1.4344	4.0568	C	0.978	3.3353	1.2482	C	-0.3509	2.1919	2.9966
C	-1.3069	0.1307	4.0398	C	0.7569	2.54	2.3789	C	-0.8142	0.9296	3.3859
C	-1.1531	-0.6896	5.1645	C	1.575	2.6927	3.5038	C	-0.5426	0.4594	4.6755
C	-0.4717	-0.2174	6.2873	C	2.6274	3.6096	3.486	C	0.2153	1.2312	5.5578
O	-2.881	-1.2902	2.9645	O	-0.9414	1.297	3.4829	O	-2.502	-0.6701	2.8953
H	-4.1787	0.9051	0.2779	H	-3.9091	0.5095	0.7451	H	-3.9553	0.1214	-0.8573
H	-3.0282	-0.9659	0.7276	H	-2.0828	-0.1499	2.1035	H	-2.6828	-1.1763	0.6574
H	-3.1647	1.8854	-2.0248	H	-2.2138	1.9673	-1.2921	H	-1.9888	2.4088	-1.0255
H	-3.7903	0.2256	-1.897	H	-3.7275	1.0775	-1.4708	H	-3.0717	1.7149	-2.2415

H	0.537	-1.1879	-3.2623	H	-1.1187	-2.8882	-2.4594	H	0.5075	-1.1444	-3.7049
H	-1.7879	-1.2827	-3.2351	H	-3.145	-1.9018	-1.952	H	-1.7457	-0.5034	-3.7182
H	-3.2916	3.1951	0.0221	H	-3.2991	2.4485	2.1868	H	-4.5649	2.254	0.1614
H	-2.8702	2.4865	1.5802	H	-2.3081	3.1181	0.8752	H	-4.3576	1.0338	1.4254
H	-1.6476	2.6151	0.3069	H	-4.0517	2.9446	0.6645	H	-3.1087	2.2666	1.1585
H	1.0198	-2.5217	2.6753	H	0.9796	-3.345	2.9744	H	0.4135	-4.4198	1.1372
H	2.7076	-1.0893	2.9181	H	2.6571	-3.1337	0.8207	H	2.7018	-3.1495	0.336
H	1.464	0.1096	2.7472	H	2.9816	-2.4718	2.3866	H	2.2489	-3.4071	1.9865
H	3.5363	0.6001	1.5238	H	1.6142	-0.3385	1.5439	H	0.8892	-1.1205	1.758
H	1.2438	1.4729	-2.5195	H	0.7436	-0.7934	-2.9623	H	1.9289	0.8669	-2.267
H	-1.6216	-3.061	0.8549	H	-2.113	-2.3067	2.5755	H	-2.4335	-3.2641	-0.0305
H	-0.3542	-3.8487	-0.1121	H	-2.0662	-3.7279	1.5098	H	-1.6771	-3.9214	-1.498
H	-0.3117	-3.9328	1.6451	H	-1.2091	-3.7404	3.0464	H	-1.4957	-4.7505	0.0433
H	1.6894	0.3942	-4.7116	H	-0.1002	-2.4988	-4.618	H	2.1924	0.3118	-4.6786
H	0.2484	1.4081	-4.8431	H	-0.9593	-0.9692	-4.8256	H	1.142	1.7243	-4.5294
H	0.2509	-0.2364	-5.5184	H	-1.8608	-2.5007	-4.7914	H	0.7023	0.3929	-5.6227
H	-2.5537	1.6524	-6.5031	H	-4.5621	1.3556	-4.6368	H	-2.7458	2.6468	-6.8471
H	-3.738	0.4168	-6.9787	H	-4.4146	-0.1281	-5.6409	H	-2.8711	3.3463	-5.2205
H	-4.0854	1.4566	-5.5828	H	-5.9399	0.2479	-4.8159	H	-1.2808	3.2638	-6.0545
H	0.8261	2.6052	-0.0069	H	1.9282	0.7986	-1.985	H	2.2874	1.6834	-0.2492
H	1.7927	2.39	1.4447	H	2.8976	1.1321	-0.5729	H	2.5477	1.2101	1.4099
H	0.3331	1.4337	1.2118	H	1.1464	1.1659	-0.4467	H	0.9175	1.2111	0.7574
H	3.8617	1.9867	-0.1457	H	4.0723	-0.9952	-1.195	H	4.291	-0.3069	0.4364
H	3.6708	0.8364	-1.4747	H	3.2456	-2.5555	-1.1802	H	3.8725	-1.6265	-0.6596
H	2.721	2.3328	-1.4185	H	2.9077	-1.3886	-2.4536	H	3.811	0.0405	-1.2202
H	4.6076	-3.4845	0.0552	H	5.4989	1.0928	3.4317	H	3.3451	-0.9609	5.5849
H	5.5494	-2.2649	-0.8705	H	6.0536	-0.0354	2.1758	H	4.5668	-1.2838	4.3356
H	6.2221	-2.9907	0.6042	H	5.2937	1.5302	1.7247	H	3.7273	0.3045	4.4016
H	0.5793	1.4433	7.1694	H	3.6749	5.1014	2.3382	H	1.2801	3.0811	5.8479
H	0.2859	2.9138	5.1928	H	2.2051	4.8637	0.3517	H	0.7713	3.939	3.5746
H	-0.9236	2.0925	3.2018	H	0.3332	3.2497	0.3768	H	-0.5778	2.5841	2.008
H	-1.5604	-1.6986	5.1658	H	1.4049	2.083	4.3898	H	-0.9056	-0.5183	4.9883
H	-0.349	-0.8579	7.1573	H	3.2656	3.7155	4.3596	H	0.4316	0.8552	6.5547
3H-10				**3H-11**							
C	-3.0522	1.1096	0.0537	C	-3.3041	-0.3185	0.6276				
C	-2.1452	0.2264	0.933	C	-1.927	-0.7546	1.1656				
C	-1.754	-0.8877	-0.0704	C	-1.3485	-1.495	-0.0658				
C	-1.5631	-0.1318	-1.4074	C	-1.7259	-0.5666	-1.2245				
C	-2.2554	1.2289	-1.2494	C	-3.038	0.1189	-0.8238				
C	-0.6397	-1.9337	0.2977	C	0.156	-1.9322	-0.071				
C	-0.8533	-1.9465	-2.7648	C	-0.3637	-0.6937	-3.2128				
C	-2	-0.9458	-2.6342	C	-1.6281	-1.2925	-2.5875				
C	-3.4276	2.4692	0.6229	C	-4.0294	0.7517	1.429				
C	-0.5338	-2.1649	1.7949	C	0.6107	-2.2999	1.3366				
C	0.395	-1.6691	2.6284	C	1.4633	-1.6351	2.1347				
C	1.5978	-0.8263	2.3591	C	2.306	-0.4245	1.903				
C	2.0211	-0.4833	0.9234	C	2.4309	0.2127	0.5138				
C	0.6274	-2.0129	-0.6565	C	1.1058	-1.2284	-1.1389				
C	0.3036	-1.2703	-1.9843	C	0.3709	-0.1353	-1.9883				
C	-1.6345	-3.0301	2.3794	C	0.005	-3.5892	1.8697				
C	-0.4459	-2.3038	-4.1916	C	-0.655	0.4175	-4.2285				
O	-2.0587	-0.0825	-3.7876	O	-2.7589	-1.1249	-3.4506				
H	-2.6819	-1.4758	-0.1752	H	-1.9487	-2.4145	-0.1636				
O	-0.1588	0.0375	-1.6237	O	-0.6919	0.4382	-1.2357				
C	-3.0461	-0.3348	-4.6869	C	-3.7685	-2.0202	-3.2686				
C	-2.9757	0.6518	-5.8115	C	-4.8665	-1.7642	-4.254				
O	-3.8708	-1.2334	-4.6056	O	-3.7899	-2.8955	-2.4151				
C	2.0586	-1.6939	-0.0548	C	2.552	-0.7841	-0.6752				
C	3.0901	-1.4222	-1.1885	C	3.3235	-0.1245	-1.8627				
C	2.6141	-2.9744	0.636	C	3.4303	-2.0237	-0.3451				
O	3.3652	0.0591	1.0949	O	3.6361	1.0255	0.6081				
H	0.7102	-3.0715	-0.9536	H	1.3375	-2.0223	-1.8685				
C	3.66	1.2514	0.5131	C	3.5523	2.333	0.2443				
C	5.0548	1.6573	0.8794	C	4.8622	3.0127	0.5014				
O	2.9257	1.9067	-0.2105	O	2.5765	2.8867	-0.24				
H	-1.1293	-2.8725	-0.0207	H	0.0953	-2.9301	-0.5432				

O	-1.0249	0.9943	1.3842	O	-1.1419	0.3875	1.5279				
C	-1.1375	1.5111	2.6366	C	-1.1333	0.7188	2.8427				
C	1.9427	4.3614	3.4969	C	0.9307	4.4084	3.5498				
C	1.7084	3.986	2.1749	C	0.6464	4.0253	2.2399				
C	0.71	3.056	1.8757	C	-0.0275	2.8279	1.9886				
C	-0.056	2.4938	2.9031	C	-0.4149	2.0035	3.0521				
C	0.177	2.883	4.2291	C	-0.1319	2.3982	4.3672				
C	1.1767	3.8121	4.5243	C	0.5404	3.5969	4.6141				
O	-2.0072	1.2463	3.4526	O	-1.6452	0.0848	3.7525				
H	-3.9809	0.5592	-0.1525	H	-3.9481	-1.209	0.5947				
H	-2.7124	-0.2014	1.7673	H	-2.0485	-1.4433	2.0084				
H	-1.514	2.0352	-1.1893	H	-2.9435	1.2092	-0.8969				
H	-2.9351	1.4707	-2.0726	H	-3.8957	-0.1705	-1.4346				
H	-1.1392	-2.8872	-2.2794	H	0.2275	-1.4602	-3.7266				
H	-2.9633	-1.4372	-2.4583	H	-1.4476	-2.3667	-2.4465				
H	-2.5549	3.1142	0.7637	H	-5.0117	0.9557	0.9895				
H	-4.1103	2.9894	-0.0576	H	-4.1871	0.4228	2.4609				
H	-3.9354	2.3588	1.5861	H	-3.4761	1.6959	1.4481				
H	0.2993	-1.9106	3.6889	H	1.6316	-2.0462	3.1328				
H	2.4429	-1.3248	2.8567	H	3.3184	-0.694	2.2401				
H	1.494	0.1095	2.9199	H	1.9968	0.3528	2.6123				
H	1.3593	0.2909	0.5251	H	1.5614	0.8586	0.3555				
H	1.1666	-1.1599	-2.6406	H	1.0239	0.6819	-2.2863				
H	-2.6201	-2.6145	2.149	H	-1.0875	-3.549	1.865				
H	-1.5783	-4.0416	1.9632	H	0.3211	-4.4343	1.2488				
H	-1.5656	-3.1197	3.4688	H	0.3156	-3.8068	2.8973				
H	0.3657	-3.0394	-4.181	H	0.2784	0.8769	-4.5714				
H	-0.0911	-1.4303	-4.7484	H	-1.2817	1.2076	-3.8013				
H	-1.2866	-2.7441	-4.737	H	-1.1648	0.016	-5.1106				
H	-3.0963	1.6661	-5.4227	H	-5.3002	-0.7771	-4.076				
H	-2.0211	0.5501	-6.3337	H	-4.4754	-1.8354	-5.2721				
H	-3.7848	0.4524	-6.5199	H	-5.648	-2.5192	-4.1298				
H	3.0523	-2.2057	-1.9547	H	3.2182	-0.719	-2.7779				
H	4.1183	-1.4129	-0.8068	H	4.3973	-0.0527	-1.649				
H	2.9209	-0.4559	-1.6738	H	2.9898	0.8922	-2.0827				
H	3.5602	-2.7688	1.1499	H	4.3936	-1.7186	0.0801				
H	1.9248	-3.4087	1.3625	H	2.975	-2.7291	0.3487				
H	2.8122	-3.7611	-0.1027	H	3.6438	-2.5993	-1.2546				
H	5.1412	1.7479	1.9652	H	5.1246	2.9246	1.5588				
H	5.7672	0.9231	0.4954	H	5.6387	2.5693	-0.1268				
H	5.2785	2.63	0.4319	H	4.7741	4.0746	0.2548				
H	2.7193	5.0871	3.7254	H	1.4543	5.3419	3.74				
H	2.3017	4.4129	1.3692	H	0.9528	4.6528	1.4055				
H	0.545	2.7791	0.8358	H	-0.236	2.5506	0.9566				
H	-0.4206	2.4631	5.0359	H	-0.4349	1.7715	5.2038				
H	1.3539	4.1097	5.5548	H	0.7571	3.897	5.6361				

Table S27. Experimental chemical shifts of **3**, calculated shielding tensors and chemical shifts of isomers **3A**–**3D** in gas phase with TMS as reference at mPW1PW91/6-31G* level.

Nuclie	δ(exptl)	3A					3B					3C					3D				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
C-1	36.3	156.6	35.4	36.3	0.9	0.0	155.2	36.8	36.6	0.5	0.3	155.0	37.0	35.9	0.7	0.4	156.5	35.5	36.4	0.8	0.1
C-2	36.3	156.1	35.9	36.8	0.4	0.5	155.9	36.1	35.8	0.2	0.5	155.4	36.6	35.5	0.3	0.8	156.2	35.8	36.7	0.5	0.4
C-3	78.6	117.0	75.0	78.1	3.6	0.5	113.2	78.8	81.5	0.2	2.9	114.3	77.7	79.9	0.9	1.3	116.8	75.2	78.3	3.4	0.3
C-4	46.4	147.1	44.9	46.3	1.5	0.1	146.4	45.6	46.1	0.8	0.3	144.9	47.1	46.9	0.7	0.5	146.9	45.1	46.6	1.3	0.2
C-5	31.7	160.5	31.5	32.1	0.2	0.4	157.8	34.2	33.9	2.5	2.2	155.3	36.7	35.6	5.0	3.9	160.0	32.0	32.6	0.3	0.9
C-6	140.5	54.7	137.3	143.8	3.2	3.3	61.4	130.6	136.8	9.9	3.7	58.3	133.7	140.2	6.8	0.3	55.8	136.2	142.9	4.3	2.4
C-7	121.7	71.5	120.5	126.1	1.2	4.4	71.2	120.8	126.4	0.9	4.7	71.7	120.3	125.8	1.4	4.1	72.1	119.9	125.6	1.8	3.9
C-8	25.3	163.5	28.5	29.0	3.2	3.7	160.2	31.8	31.3	6.5	6.0	161.3	30.7	29.2	5.4	3.9	166.2	25.8	26.1	0.5	0.8
C-9	77.9	117.6	74.4	77.4	3.5	0.5	116.9	75.1	77.5	2.8	0.4	117.2	74.8	76.8	3.1	1.1	117.1	74.9	78.0	3.0	0.1
C-10	41.0	150.1	41.9	43.2	0.9	2.2	155.5	36.5	36.3	4.5	4.7	153.8	38.2	37.3	2.8	3.7	151.1	40.9	42.1	0.1	1.1
C-11	47.0	141.5	50.5	52.2	3.5	5.2	144.1	47.9	48.4	0.9	1.4	143.5	48.5	48.3	1.5	1.3	146.2	45.8	47.2	1.2	0.2
C-12	80.4	115.1	76.9	80.1	3.5	0.3	113.6	78.4	81.0	2.0	0.6	111.9	80.1	82.4	0.3	2.0	115.4	76.6	79.8	3.8	0.6
C-13	44.5	147.7	44.3	45.6	0.2	1.1	152.7	39.3	39.3	5.2	5.2	153.0	39.0	38.2	5.5	6.3	147.8	44.2	45.6	0.3	1.1
C-14	79.2	114.5	77.5	80.7	1.7	1.5	114.0	78.0	80.6	1.2	1.4	113.9	78.1	80.3	1.1	1.1	114.3	77.7	81.0	1.5	1.8
C-15	89.7	104.4	87.6	91.4	2.1	1.7	102.5	89.5	92.9	0.2	3.2	103.2	88.8	91.8	0.9	2.1	104.3	87.7	91.6	2.0	1.9
C-16	13.4	179.2	12.8	12.4	0.6	1.0	178.1	13.9	12.1	0.5	1.3	178.2	13.8	10.9	0.4	2.5	179.1	12.9	12.4	0.5	1.0
C-17	20.4	171.4	20.6	20.6	0.2	0.2	165.5	26.5	25.6	6.1	5.2	164.0	28.0	26.2	7.6	5.8	171.0	21.0	21.0	0.6	0.6
C-18	27.2	167.1	24.9	25.2	2.3	2.0	163.8	28.2	27.4	1.0	0.2	165.8	26.2	24.2	1.0	3.0	166.2	25.8	26.1	1.4	1.1
C-19	20.6	177.9	14.1	13.8	6.5	6.8	171.6	20.4	19.1	0.2	1.5	165.4	26.6	24.7	6.0	4.1	172.7	19.3	19.3	1.3	1.3
C-20	13.3	178.9	13.1	12.8	0.2	0.5	177.8	14.2	12.4	0.9	0.9	176.1	15.9	13.1	2.6	0.2	178.7	13.3	12.8	0.0	0.5
C-1'	165.4	35.2	156.8	164.4	8.6	1.0	33.6	158.4	166.5	7.0	1.1	34.5	157.5	166.0	7.9	0.6	35.2	156.8	164.7	8.6	0.7
C-2'	129.8	68.9	123.1	128.9	6.7	0.9	68.0	124.0	129.7	5.8	0.1	68.6	123.4	129.2	6.4	0.6	69.0	123.0	129.0	6.8	0.8
C-3',7'	129.5	66.0	126.0	131.9	3.5	2.4	67.7	124.3	130.1	5.2	0.6	68.5	123.5	129.2	6.0	0.3	65.9	126.1	132.2	3.4	2.7
C-3',7'	129.5	69.5	122.5	128.2	7.0	1.3	66.8	125.2	131.1	4.3	1.6	66.4	125.6	131.5	3.9	2.0	69.6	122.4	128.3	7.1	1.2
C-4',6'	128.5	70.5	121.5	127.1	7.0	1.4	70.5	121.5	127.1	7.0	1.4	70.8	121.2	126.7	7.3	1.8	70.5	121.5	127.4	7.0	1.1
C-4',6'	128.5	70.9	121.1	126.7	7.4	1.8	71.0	121.0	126.5	7.5	2.0	70.7	121.3	126.9	7.2	1.6	70.9	121.1	126.9	7.4	1.6
C-5'	133.2	66.4	125.6	131.5	7.6	1.7	66.3	125.7	131.6	7.5	1.6	66.3	125.7	131.6	7.5	1.6	66.3	125.7	131.8	7.5	1.4
C-1''	170.4	31.5	160.5	168.3	9.9	2.1	30.2	161.8	170.1	8.6	0.3	30.9	161.1	169.9	9.3	0.5	31.7	160.3	168.4	10.1	2.0
C-2''	21.0	172.6	19.4	19.4	1.6	1.6	173.0	19.0	17.6	2.0	3.4	171.4	20.6	18.2	0.4	2.8	172.6	19.4	19.3	1.6	1.7
C-1'''	171.3	30.1	161.9	169.8	9.4	1.5	30.3	161.7	170.0	9.6	1.3	30.5	161.5	170.2	9.8	1.1	30.1	161.9	170.1	9.4	1.2
C-2'''	20.9	172.8	19.2	19.2	1.7	1.7	172.8	19.2	17.8	1.7	3.1	172.8	19.2	16.7	1.7	4.2	172.7	19.3	19.2	1.6	1.7
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|; **3A**: Y = 0.9476X + 1.0201, R^2 = 0.9980, MAE = 3.5 ppm, CMAE = 1.7 ppm; **3B**: Y = 0.9361X + 2.5303, R^2 = 0.9974, MAE = 3.7 ppm, CMAE = 2.0 ppm; **3C**: Y = 0.927X + 3.6835, R^2 = 0.9974, MAE = 3.9 ppm, CMAE = 2.1 ppm; **3D**: Y = 0.9451X + 1.1367, R^2 = 0.9992, MAE = 3.2 ppm, CMAE = 1.2 ppm.																					

Nuclie	δ(exptl)	3A					3B					3C					3D				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
H-1a	1.90	30.20	1.80	1.88	0.10	0.02	29.93	2.07	2.07	0.17	0.17	29.96	2.04	2.01	0.14	0.11	30.17	1.83	1.89	0.07	0.01
H-1b	1.94	29.93	2.07	2.13	0.13	0.19	30.18	1.82	1.82	0.12	0.12	30.22	1.78	1.75	0.16	0.19	29.92	2.08	2.13	0.14	0.19
H-2	2.09	30.01	1.99	2.06	0.10	0.03	30.01	1.99	1.99	0.10	0.10	29.99	2.01	1.98	0.08	0.11	30.01	1.99	2.05	0.10	0.04
H-3	5.50	26.49	5.51	5.51	0.01	0.01	26.44	5.56	5.46	0.06	0.04	26.50	5.50	5.40	0.00	0.10	26.44	5.56	5.55	0.06	0.05
H-4	2.29	30.20	1.80	1.88	0.49	0.41	30.00	2.00	1.99	0.29	0.30	29.94	2.06	2.03	0.23	0.26	30.14	1.86	1.92	0.43	0.37
H-5	2.90	28.71	3.29	3.33	0.39	0.43	28.29	3.71	3.66	0.81	0.76	29.13	2.87	2.82	0.03	0.08	28.82	3.18	3.21	0.28	0.31
H-7	5.04	26.58	5.42	5.41	0.38	0.37	26.76	5.24	5.15	0.20	0.11	26.65	5.35	5.26	0.31	0.22	26.81	5.19	5.20	0.15	0.16
H-8a	1.92	30.53	1.47	1.55	0.45	0.37	29.96	2.04	2.04	0.12	0.12	29.77	2.23	2.19	0.31	0.27	30.00	2.00	2.05	0.08	0.13
H-8b	1.55	29.87	2.13	2.20	0.58	0.65	29.64	2.36	2.34	0.81	0.79	29.83	2.17	2.13	0.62	0.58	30.14	1.86	1.92	0.31	0.37
H-9	4.18	27.82	4.18	4.20	0.00	0.02	27.71	4.29	4.22	0.11	0.04	27.47	4.53	4.45	0.35	0.27	27.90	4.10	4.11	0.08	0.07
H-11	1.23	30.91	1.09	1.18	0.14	0.05	29.40	2.60	2.57	1.37	1.34	29.44	2.56	2.51	1.33	1.28	30.56	1.44	1.50	0.21	0.27
H-12	3.80	28.24	3.76	3.79	0.04	0.01	28.20	3.80	3.74	0.00	0.06	27.92	4.08	4.01	0.28	0.21	28.22	3.78	3.80	0.02	0.00
H-13	2.21	29.97	2.03	2.10	0.18	0.11	29.49	2.51	2.49	0.30	0.28	28.85	3.15	3.10	0.94	0.89	29.92	2.08	2.13	0.13	0.08

H-14	5.06	27.10	4.90	4.90	0.16	0.16	26.63	5.37	5.27	0.31	0.21	26.89	5.11	5.02	0.05	0.04	27.08	4.92	4.93	0.14	0.13
H-16	0.94	31.18	0.82	0.92	0.12	0.02	31.18	0.82	0.85	0.12	0.09	31.13	0.87	0.86	0.07	0.08	31.03	0.97	1.04	0.03	0.10
H-16	0.94	31.20	0.80	0.90	0.14	0.04	31.09	0.91	0.94	0.03	0.00	31.18	0.82	0.81	0.12	0.13	31.16	0.84	0.91	0.10	0.03
H-16	0.94	31.02	0.98	1.07	0.04	0.13	31.17	0.83	0.85	0.11	0.09	31.06	0.94	0.93	0.00	0.01	31.20	0.80	0.87	0.14	0.07
H-17	1.70	30.25	1.75	1.83	0.05	0.13	30.49	1.51	1.52	0.19	0.18	29.96	2.04	2.00	0.34	0.30	30.58	1.42	1.48	0.28	0.22
H-17	1.70	30.45	1.55	1.62	0.15	0.08	30.10	1.90	1.89	0.20	0.19	30.52	1.48	1.46	0.22	0.24	30.17	1.83	1.88	0.13	0.18
H-17	1.70	30.57	1.43	1.51	0.27	0.19	30.23	1.77	1.77	0.07	0.07	30.47	1.53	1.51	0.17	0.19	30.38	1.62	1.68	0.08	0.02
H-18	0.84	31.07	0.93	1.02	0.09	0.18	31.75	0.25	0.29	0.59	0.55	30.48	1.52	1.50	0.68	0.66	31.01	0.99	1.05	0.15	0.21
H-18	0.84	30.88	1.12	1.21	0.28	0.37	31.07	0.93	0.95	0.09	0.11	31.44	0.56	0.56	0.28	0.28	31.49	0.51	0.58	0.33	0.26
H-18	0.84	31.67	0.33	0.44	0.51	0.40	31.22	0.78	0.80	0.06	0.04	31.53	0.47	0.47	0.37	0.37	31.04	0.96	1.02	0.12	0.18
H-19	1.01	30.98	1.02	1.12	0.01	0.11	30.63	1.37	1.38	0.36	0.37	31.62	0.38	0.38	0.63	0.63	30.60	1.40	1.46	0.39	0.45
H-19	1.01	31.01	0.99	1.08	0.02	0.07	31.39	0.61	0.64	0.40	0.37	31.54	0.46	0.46	0.55	0.55	30.65	1.35	1.41	0.34	0.40
H-19	1.01	30.50	1.50	1.58	0.49	0.57	31.51	0.49	0.52	0.52	0.49	30.78	1.22	1.21	0.21	0.20	31.59	0.41	0.48	0.60	0.53
H-20	0.99	31.09	0.91	1.01	0.08	0.02	30.87	1.13	1.15	0.14	0.16	30.97	1.03	1.02	0.04	0.03	30.88	1.12	1.18	0.13	0.19
H-20	0.99	30.89	1.11	1.20	0.12	0.21	31.03	0.97	0.99	0.02	0.00	30.75	1.25	1.24	0.26	0.25	31.17	0.83	0.90	0.16	0.09
H-20	0.99	31.19	0.81	0.91	0.18	0.08	31.12	0.88	0.91	0.11	0.08	31.29	0.71	0.70	0.28	0.29	31.07	0.93	1.00	0.06	0.01
H-3',7'	7.99	23.81	8.19	8.12	0.20	0.13	23.53	8.47	8.29	0.48	0.30	23.63	8.37	8.21	0.38	0.22	23.81	8.19	8.15	0.20	0.16
H-3',7'	7.99	23.78	8.22	8.15	0.23	0.16	23.88	8.12	7.95	0.13	0.04	23.82	8.18	8.03	0.19	0.04	23.83	8.17	8.13	0.18	0.14
H-4',6'	7.37	24.65	7.35	7.30	0.02	0.07	24.63	7.37	7.22	0.00	0.15	24.65	7.35	7.22	0.02	0.15	24.63	7.37	7.34	0.00	0.03
H-4',6'	7.37	24.65	7.35	7.30	0.02	0.07	24.65	7.35	7.20	0.02	0.17	24.63	7.37	7.24	0.00	0.13	24.68	7.32	7.29	0.05	0.08
H-5'	7.49	24.57	7.43	7.38	0.06	0.11	24.55	7.45	7.30	0.04	0.19	24.56	7.44	7.30	0.05	0.19	24.57	7.43	7.40	0.06	0.09
H-2''	1.90	30.30	1.70	1.77	0.20	0.13	30.49	1.51	1.51	0.39	0.39	30.20	1.80	1.77	0.10	0.13	30.66	1.34	1.40	0.56	0.50
H-2''	1.90	30.40	1.60	1.67	0.30	0.23	30.68	1.32	1.34	0.58	0.56	30.36	1.64	1.62	0.26	0.28	30.26	1.74	1.79	0.16	0.11
H-2''	1.90	30.67	1.33	1.42	0.57	0.48	30.23	1.77	1.77	0.13	0.13	30.12	1.88	1.85	0.02	0.05	30.25	1.75	1.81	0.15	0.09
H-2'''	2.11	30.45	1.55	1.63	0.56	0.48	30.16	1.84	1.83	0.27	0.28	30.05	1.95	1.92	0.16	0.19	30.03	1.97	2.02	0.14	0.09
H-2'''	2.11	30.05	1.95	2.02	0.16	0.09	30.31	1.69	1.69	0.42	0.42	30.46	1.54	1.52	0.57	0.59	30.27	1.73	1.78	0.38	0.33
H-2'''	2.11	30.04	1.96	2.03	0.15	0.08	30.03	1.97	1.96	0.14	0.15	30.11	1.89	1.86	0.22	0.25	30.22	1.78	1.84	0.33	0.27
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|; **3A**: Y = 1.0228X – 0.116, R^2 = 0.9871, MAE = 0.20 ppm, CMAE = 0.19 ppm; **3B**: Y = 1.0276X – 0.0477, R^2 = 0.9738, MAE = 0.30 ppm, CMAE = 0.30 ppm; **3C**: Y = 1.0205X – 0.0098, R^2 = 0.9720, MAE = 0.30 ppm, CMAE = 0.30 ppm; **3D**: Y = 1.0153X – 0.0818, R^2 = 0.9898, MAE = 0.20 ppm, CMAE = 0.20 ppm;																				

Table S28. Experimental chemical shifts of **3**, calculated shielding tensors and chemical shifts of isomers **3E**–**3H** in gas phase with TMS as reference at mPW1PW91/6-31G* level.

Nuclie	δ(exptl)	**3E**					**3F**					**3G**					**3H**				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
C-1	36.3	155.4	36.6	35.3	0.3	1.0	155.1	36.9	36.8	0.6	0.5	155.0	37.0	36.9	0.7	0.6	155.0	37.0	36.3	0.7	0.0
C-2	36.3	154.2	37.8	36.6	1.5	0.3	154.6	37.4	37.3	1.1	1.0	154.6	37.4	37.4	1.1	1.1	154.7	37.3	36.6	1.0	0.3
C-3	78.6	116.3	75.7	77.7	2.9	0.9	116.8	75.2	77.8	3.4	0.8	116.9	75.1	77.7	3.5	0.9	117.0	75.0	77.1	3.6	1.5
C-4	46.4	138.7	53.3	53.5	6.9	7.1	145.0	47.0	47.7	0.6	1.3	145.0	47.0	47.6	0.6	1.2	142.9	49.1	49.3	2.7	2.9
C-5	31.7	153.8	38.2	37.1	6.5	5.4	151.9	40.1	40.3	8.4	8.6	151.7	40.3	40.5	8.6	8.8	153.4	38.6	38.0	6.9	6.3
C-6	140.5	56.8	135.2	142.1	5.3	1.6	59.3	132.7	139.2	7.8	1.3	60.7	131.3	137.7	9.2	2.8	61.1	130.9	137.4	9.6	3.1
C-7	121.7	74.9	117.1	122.6	4.6	0.9	72.4	119.6	125.2	2.1	3.5	71.8	120.2	125.9	1.5	4.2	72.3	119.7	125.3	2.0	3.6
C-8	25.3	163.1	28.9	27.0	3.6	1.7	163.6	28.4	27.8	3.1	2.5	163.0	29.0	28.3	3.7	3.0	164.0	28.0	26.5	2.7	1.2
C-9	77.9	118.5	73.5	75.3	4.4	2.6	113.8	78.2	81.0	0.3	3.1	113.6	78.4	81.2	0.5	3.3	115.7	76.3	78.5	1.6	0.6
C-10	41.0	152.2	39.8	38.8	1.2	2.2	154.7	37.3	37.3	3.7	3.7	154.7	37.3	37.3	3.7	3.7	151.7	40.3	39.8	0.7	1.2
C-11	47.0	145.3	46.7	46.3	0.3	0.7	151.2	40.8	41.0	6.2	6.0	150.0	42.0	42.3	5.0	4.7	147.2	44.8	44.7	2.2	2.3
C-12	80.4	114.7	77.3	79.4	3.1	1.0	111.0	81.0	84.0	0.6	3.6	111.1	80.9	83.8	0.5	3.4	112.7	79.3	81.8	1.1	1.4
C-13	44.5	147.4	44.6	44.0	0.1	0.5	153.4	38.6	38.7	5.9	5.8	153.4	38.6	38.6	5.9	5.9	148.8	43.2	42.9	1.3	1.6
C-14	79.2	110.5	81.5	84.0	2.3	4.8	114.1	77.9	80.7	1.3	1.5	113.9	78.1	80.9	1.1	1.7	112.6	79.4	81.9	0.2	2.7
C-15	89.7	106.7	85.3	88.0	4.4	1.7	101.0	91.0	94.7	1.3	5.0	101.2	90.8	94.5	1.1	4.8	104.0	88.0	91.2	1.7	1.5
C-16	13.4	178.5	13.5	10.3	0.1	3.1	177.9	14.1	12.4	0.7	1.0	178.0	14.0	12.4	0.6	1.0	178.6	13.4	10.8	0.0	2.6
C-17	20.4	165.7	26.3	24.2	5.9	3.8	168.5	23.5	22.5	3.1	2.1	168.5	23.5	22.5	3.1	2.1	165.4	26.6	25.0	6.2	4.6
C-18	27.2	164.2	27.8	25.8	0.6	1.4	168.1	23.9	22.9	3.3	4.3	173.5	18.5	17.1	8.7	10.1	166.1	25.9	24.3	1.3	2.9
C-19	20.6	165.5	26.5	24.4	5.9	3.8	168.5	23.5	22.6	2.9	2.0	164.5	27.5	26.7	6.9	6.1	168.0	24.0	22.3	3.4	1.7

C-20	13.3	178.3	13.7	10.5	0.4	2.8	177.3	14.7	13.1	1.4	0.2	177.5	14.5	12.9	1.2	0.4	177.8	14.2	11.7	0.9	1.6
C-1'	165.4	34.0	158.0	166.8	7.4	1.4	34.5	157.5	165.7	7.9	0.3	34.5	157.5	165.8	7.9	0.4	33.6	158.4	167.0	7.0	1.6
C-2'	129.8	69.0	123.0	129.0	6.8	0.8	67.8	124.2	130.2	5.6	0.4	68.2	123.8	129.7	6.0	0.1	68.5	123.5	129.4	6.3	0.4
C-3',7'	129.5	67.6	124.4	130.5	5.1	1.0	66.5	125.5	131.6	4.0	2.1	68.8	123.2	129.1	6.3	0.4	68.2	123.8	129.7	5.7	0.2
C-3',7'	129.5	66.5	125.5	131.7	4.0	2.2	68.0	124.0	130.0	5.5	0.5	66.6	125.4	131.4	4.1	1.9	66.1	125.9	132.0	3.6	2.5
C-4',6'	128.5	71.2	120.8	126.6	7.7	1.9	70.8	121.2	126.9	7.3	1.6	70.7	121.3	127.1	7.2	1.4	71.1	120.9	126.6	7.6	1.9
C-4',6'	128.5	71.2	120.8	126.6	7.7	1.9	71.1	120.9	126.6	7.6	1.9	70.6	121.4	127.2	7.1	1.3	70.9	121.1	126.9	7.4	1.6
C-5'	133.2	66.5	125.5	131.6	7.7	1.6	66.8	125.2	131.2	8.0	2.0	66.2	125.8	131.9	7.4	1.3	66.4	125.6	131.6	7.6	1.6
C-1''	170.4	32.2	159.8	168.8	10.6	1.6	32.2	159.8	168.2	10.6	2.2	31.4	160.6	169.1	9.8	1.3	31.4	160.6	169.3	9.8	1.1
C-2''	21.0	172.3	19.7	17.1	1.3	3.9	172.7	19.3	18.0	1.7	3.0	172.6	19.4	18.1	1.6	2.9	172.5	19.5	17.4	1.5	3.6
C-1'''	171.3	30.0	162.0	171.2	9.3	0.1	30.6	161.4	170.0	9.9	1.3	30.5	161.5	170.0	9.8	1.3	30.3	161.7	170.6	9.6	0.7
C-2'''	20.9	172.8	19.2	16.5	1.7	4.4	172.9	19.1	17.8	1.8	3.1	172.9	19.1	17.8	1.8	3.1	172.8	19.2	17.1	1.7	3.8
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|;																				
	3E: Y = 0.9232X + 3.9661, R^2 = 0.9973, MAE = 4.2 ppm, CMAE = 2.2 ppm; **3F**: Y = 0.9355X + 2.4288, R^2 = 0.9965, MAE = 4.1 ppm, CMAE = 2.5 ppm;																				
	3G: Y = 0.9355X + 2.4374, R^2 = 0.9951, MAE = 4.4 ppm, CMAE = 2.7 ppm; **3H**: Y = 0.9287X + 3.3127, R^2 = 0.9978, MAE = 3.8 ppm, CMAE = 2.0 ppm.																				

Nuclie	δ(exptl)	**3E**					**3F**					**3G**					**3H**				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
H-1a	1.90	30.09	1.91	1.92	0.01	0.02	30.29	1.71	1.77	0.19	0.13	30.27	1.73	1.77	0.17	0.13	29.98	2.02	2.04	0.12	0.14
H-1b	1.94	30.15	1.85	1.86	0.09	0.08	29.99	2.01	2.06	0.07	0.12	29.98	2.02	2.06	0.08	0.12	30.04	1.96	1.99	0.02	0.05
H-2	2.09	30.07	1.93	1.94	0.16	0.15	29.99	2.01	2.06	0.08	0.03	30.01	1.99	2.02	0.10	0.07	30.14	1.86	1.89	0.23	0.20
H-3	5.50	26.22	5.78	5.72	0.28	0.22	26.55	5.45	5.41	0.05	0.09	26.56	5.44	5.41	0.06	0.09	26.33	5.67	5.64	0.17	0.14
H-4	2.29	29.60	2.40	2.40	0.11	0.11	30.04	1.96	2.01	0.33	0.28	30.04	1.96	2.00	0.33	0.29	29.89	2.11	2.14	0.18	0.15
H-5	2.90	29.33	2.67	2.67	0.23	0.23	29.62	2.38	2.42	0.52	0.48	29.54	2.46	2.49	0.44	0.41	29.18	2.82	2.83	0.08	0.07
H-7	5.04	26.95	5.05	5.01	0.01	0.03	26.71	5.29	5.25	0.25	0.21	26.70	5.30	5.28	0.26	0.24	26.79	5.21	5.19	0.17	0.15
H-8a	1.92	29.01	2.99	2.99	1.07	1.07	30.36	1.64	1.70	0.28	0.22	30.58	1.42	1.46	0.50	0.46	29.90	2.10	2.13	0.18	0.21
H-8b	1.55	30.02	1.98	2.00	0.43	0.45	30.27	1.73	1.78	0.18	0.23	29.93	2.07	2.11	0.52	0.56	29.96	2.04	2.07	0.49	0.52
H-9	4.18	27.33	4.67	4.63	0.49	0.45	27.66	4.34	4.33	0.16	0.15	27.73	4.27	4.26	0.09	0.08	27.51	4.49	4.48	0.31	0.30
H-11	1.23	30.55	1.45	1.47	0.22	0.24	28.82	3.18	3.19	1.95	1.96	29.17	2.83	2.85	1.60	1.62	30.40	1.60	1.64	0.37	0.41
H-12	3.80	27.43	4.57	4.53	0.77	0.73	27.88	4.12	4.12	0.32	0.32	27.96	4.04	4.03	0.24	0.23	27.97	4.03	4.03	0.23	0.23
H-13	2.21	29.92	2.08	2.09	0.13	0.12	29.63	2.37	2.41	0.16	0.20	29.58	2.42	2.44	0.21	0.23	29.80	2.20	2.23	0.01	0.02
H-14	5.06	27.02	4.98	4.94	0.08	0.12	26.91	5.09	5.06	0.03	0.00	26.94	5.06	5.04	0.00	0.02	26.97	5.03	5.01	0.03	0.05
H-16	0.94	31.43	0.57	0.61	0.37	0.33	30.97	1.03	1.10	0.09	0.16	31.15	0.85	0.90	0.09	0.04	31.11	0.89	0.94	0.05	0.00
H-16	0.94	31.32	0.68	0.71	0.26	0.23	31.13	0.87	0.95	0.07	0.01	31.21	0.79	0.85	0.15	0.09	31.22	0.78	0.83	0.16	0.11
H-16	0.94	30.90	1.10	1.13	0.16	0.19	31.19	0.81	0.88	0.13	0.06	30.97	1.03	1.08	0.09	0.14	31.25	0.75	0.80	0.19	0.14
H-17	1.70	30.05	1.95	1.96	0.25	0.26	30.53	1.47	1.53	0.23	0.17	30.20	1.80	1.84	0.10	0.14	30.06	1.94	1.97	0.24	0.27
H-17	1.70	30.68	1.32	1.34	0.38	0.36	30.21	1.79	1.85	0.09	0.15	30.67	1.33	1.38	0.37	0.32	30.57	1.43	1.47	0.27	0.23
H-17	1.70	30.84	1.16	1.19	0.54	0.51	30.69	1.31	1.38	0.39	0.32	30.52	1.48	1.52	0.22	0.18	30.58	1.42	1.46	0.28	0.24
H-18	0.84	30.49	1.51	1.53	0.67	0.69	30.74	1.26	1.33	0.42	0.49	30.63	1.37	1.42	0.53	0.58	31.30	0.70	0.75	0.14	0.09
H-18	0.84	31.34	0.66	0.70	0.18	0.14	31.38	0.62	0.70	0.22	0.14	31.46	0.54	0.61	0.30	0.23	30.82	1.18	1.22	0.34	0.38
H-18	0.84	31.29	0.71	0.74	0.13	0.10	31.44	0.56	0.64	0.28	0.20	31.09	0.91	0.96	0.07	0.12	31.21	0.79	0.84	0.05	0.00
H-19	1.01	31.64	0.36	0.40	0.65	0.61	31.26	0.74	0.82	0.27	0.19	31.36	0.64	0.70	0.37	0.31	31.11	0.89	0.94	0.12	0.07
H-19	1.01	31.26	0.74	0.77	0.27	0.24	31.46	0.54	0.63	0.47	0.38	31.14	0.86	0.91	0.15	0.10	31.61	0.39	0.45	0.62	0.56
H-19	1.01	30.66	1.34	1.36	0.33	0.35	30.71	1.29	1.36	0.28	0.35	31.15	0.85	0.91	0.16	0.10	30.30	1.70	1.74	0.69	0.73
H-20	0.99	31.08	0.92	0.95	0.07	0.04	30.69	1.31	1.38	0.32	0.39	30.72	1.28	1.32	0.29	0.33	31.12	0.88	0.93	0.11	0.06
H-20	0.99	31.08	0.92	0.95	0.07	0.04	31.18	0.82	0.90	0.17	0.09	31.20	0.80	0.86	0.19	0.13	30.81	1.19	1.24	0.20	0.25
H-20	0.99	30.82	1.18	1.20	0.19	0.21	31.10	0.90	0.98	0.09	0.01	31.12	0.88	0.93	0.11	0.06	31.13	0.87	0.92	0.12	0.07
H-3',7'	7.99	23.90	8.10	8.00	0.11	0.01	23.83	8.17	8.07	0.18	0.08	23.62	8.38	8.30	0.39	0.31	23.90	8.10	8.04	0.11	0.05
H-3',7'	7.99	23.85	8.15	8.06	0.16	0.07	23.51	8.49	8.38	0.50	0.39	23.85	8.15	8.07	0.16	0.08	23.84	8.16	8.10	0.17	0.11
H-4',6'	7.37	24.76	7.24	7.16	0.13	0.21	24.64	7.36	7.28	0.01	0.09	24.64	7.36	7.30	0.01	0.07	24.71	7.29	7.24	0.08	0.13
H-4',6'	7.37	24.65	7.35	7.26	0.02	0.11	24.61	7.39	7.30	0.02	0.07	24.63	7.37	7.31	0.00	0.06	24.65	7.35	7.30	0.02	0.07
H-5'	7.49	24.61	7.39	7.31	0.10	0.18	24.59	7.41	7.32	0.08	0.17	24.54	7.46	7.39	0.03	0.10	24.59	7.41	7.35	0.08	0.14
H-2''	1.90	30.15	1.85	1.86	0.05	0.04	30.51	1.49	1.56	0.41	0.34	30.24	1.76	1.80	0.14	0.10	30.39	1.61	1.65	0.29	0.25
H-2''	1.90	30.52	1.48	1.50	0.42	0.40	30.67	1.33	1.39	0.57	0.51	30.67	1.33	1.38	0.57	0.52	30.27	1.73	1.76	0.17	0.14

H-2''	1.90	30.11	1.89	1.90	0.01	0.00	30.67	1.33	1.40	0.57	0.50	30.27	1.73	1.77	0.17	0.13	30.55	1.45	1.49	0.45	0.41
H-2'''	2.11	30.01	1.99	2.00	0.12	0.11	30.05	1.95	1.99	0.16	0.12	30.06	1.94	1.97	0.17	0.14	30.14	1.86	1.89	0.25	0.22
H-2'''	2.11	30.04	1.96	1.98	0.15	0.13	30.03	1.97	2.01	0.14	0.10	30.03	1.97	2.00	0.14	0.11	30.03	1.97	2.00	0.14	0.11
H-2'''	2.11	30.45	1.55	1.57	0.56	0.54	30.47	1.53	1.59	0.58	0.52	30.47	1.53	1.57	0.58	0.54	30.33	1.67	1.70	0.44	0.41
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|; **3E**: Y = 1.0182X – 0.0468, R^2 = 0.9765, MAE = 0.30 ppm, CMAE = 0.30 ppm; **3F**: Y = 1.0253X – 0.0994, R^2 = 0.9672, MAE = 0.30 ppm, CMAE = 0.30 ppm; **3G**: Y = 1.0189X – 0.0742, R^2 = 0.9739, MAE = 0.30 ppm, CMAE = 0.20 ppm; **3H**: Y = 1.0157X – 0.061, R^2 = 0.9869, MAE = 0.20 ppm, CMAE = 0.20 ppm;																				

Table S29. Experimental chemical shifts of **3**, calculated shielding tensors and chemical shifts of isomers **3A**–**3D** in chloroform with TMS as reference at mPW1PW91/6-31G** level.

Nuclie	δ(exptl)	3A					3B					3C					3D				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
C-1	36.3	158.1	33.9	36.1	2.4	0.2	156.4	35.6	36.6	0.7	0.3	156.4	35.6	35.8	0.7	0.5	157.9	34.1	36.3	2.2	0.0
C-2	36.3	157.0	35.0	37.3	1.3	1.0	157.0	35.0	36.0	1.3	0.3	156.5	35.5	35.7	0.8	0.6	157.0	35.0	37.2	1.3	0.9
C-3	78.6	117.1	74.9	78.6	3.7	0.0	113.2	78.8	82.0	0.2	3.4	114.4	77.6	80.3	1.0	1.7	117.0	75.0	78.8	3.6	0.2
C-4	46.4	148.1	43.9	46.5	2.5	0.1	147.0	45.0	46.5	1.4	0.1	145.5	46.5	47.4	0.1	1.0	147.8	44.2	46.8	2.2	0.4
C-5	31.7	161.2	30.8	32.9	0.9	1.2	158.2	33.8	34.7	2.1	3.0	156.0	36.0	36.2	4.3	4.5	160.8	31.2	33.3	0.5	1.6
C-6	140.5	53.2	138.8	144.8	1.7	4.3	60.9	131.1	137.0	9.4	3.5	57.9	134.1	140.3	6.4	0.2	54.7	137.3	143.6	3.2	3.1
C-7	121.7	73.3	118.7	124.0	3.0	2.3	72.3	119.7	125.0	2.0	3.3	72.8	119.2	124.5	2.5	2.8	73.7	118.3	123.8	3.4	2.1
C-8	25.3	165.0	27.0	29.0	1.7	3.7	161.5	30.5	31.2	5.2	5.9	162.6	29.4	29.2	4.1	3.9	167.6	24.4	26.3	0.9	1.0
C-9	77.9	118.0	74.0	77.7	3.9	0.2	116.9	75.1	78.1	2.8	0.2	117.5	74.5	77.0	3.4	0.9	117.5	74.5	78.3	3.4	0.4
C-10	41.0	150.5	41.5	44.0	0.5	3.0	155.9	36.1	37.2	4.9	3.8	154.2	37.8	38.2	3.2	2.8	151.5	40.5	42.9	0.5	1.9
C-11	47.0	142.5	49.5	52.3	2.5	5.3	144.5	47.5	49.1	0.5	2.1	144.1	47.9	48.9	0.9	1.9	147.1	44.9	47.5	2.1	0.5
C-12	80.4	115.9	76.1	79.8	4.3	0.6	114.5	77.5	80.6	2.9	0.2	112.7	79.3	82.2	1.1	1.8	116.3	75.7	79.6	4.7	0.8
C-13	44.5	149.1	42.9	45.5	1.6	1.0	153.6	38.4	39.6	6.1	4.9	153.9	38.1	38.4	6.4	6.1	149.1	42.9	45.5	1.6	1.0
C-14	79.2	115.2	76.8	80.6	2.4	1.4	114.6	77.4	80.5	1.8	1.3	114.6	77.4	80.1	1.8	0.9	115.1	76.9	80.8	2.3	1.6
C-15	89.7	104.6	87.4	91.6	2.3	1.9	102.7	89.3	93.0	0.4	3.3	103.4	88.6	92.0	1.1	2.3	104.5	87.5	91.8	2.2	2.1
C-16	13.4	181.2	10.8	12.2	2.6	1.2	180.1	11.9	11.7	1.5	1.7	180.1	11.9	10.7	1.5	2.7	181.1	10.9	12.1	2.5	1.3
C-17	20.4	173.4	18.6	20.2	1.8	0.2	167.5	24.5	25.0	4.1	4.6	166.0	26.0	25.7	5.6	5.3	173.1	18.9	20.5	1.5	0.1
C-18	27.2	169.0	23.0	24.8	4.2	2.4	165.5	26.5	27.0	0.7	0.2	167.7	24.3	23.8	2.9	3.4	168.2	23.8	25.6	3.4	1.6
C-19	20.6	179.7	12.3	13.7	8.3	6.9	173.5	18.5	18.6	2.1	2.0	167.2	24.8	24.3	4.2	3.7	174.5	17.5	19.1	3.1	1.5
C-20	13.3	180.8	11.2	12.6	2.1	0.7	179.8	12.2	12.0	1.1	1.3	178.0	14.0	12.9	0.7	0.4	180.7	11.3	12.6	2.0	0.7
C-1'	165.4	34.1	157.9	164.6	7.5	0.8	32.9	159.1	166.5	6.3	1.1	33.5	158.5	166.1	6.9	0.7	34.1	157.9	165.0	7.5	0.4
C-2'	129.8	69.2	122.8	128.2	7.0	1.6	68.3	123.7	129.2	6.1	0.6	68.7	123.3	128.8	6.5	1.0	69.3	122.7	128.4	7.1	1.4
C-3',7'	129.5	67.2	124.8	130.4	4.7	0.9	68.4	123.6	129.1	5.9	0.4	68.9	123.1	128.6	6.4	0.9	67.1	124.9	130.7	4.6	1.2
C-3',7'	129.5	69.6	122.4	127.8	7.1	1.7	67.5	124.5	130.1	5.0	0.6	67.5	124.5	130.0	5.0	0.5	69.7	122.3	127.9	7.2	1.6
C-4',6'	128.5	70.6	121.4	126.8	7.1	1.7	70.5	121.5	126.9	7.0	1.6	70.7	121.3	126.7	7.2	1.8	70.6	121.4	127.0	7.1	1.5
C-4',6'	128.5	70.7	121.3	126.7	7.2	1.8	70.8	121.2	126.6	7.3	1.9	70.7	121.3	126.7	7.2	1.8	70.7	121.3	127.0	7.2	1.5
C-5'	133.2	65.7	126.3	131.9	6.9	1.3	65.7	126.3	132.0	6.9	1.2	65.7	126.3	132.0	6.9	1.2	65.7	126.3	132.2	6.9	1.0
C-1''	170.4	29.6	162.4	169.3	8.0	1.1	28.7	163.3	170.9	7.1	0.5	29.0	163.0	170.9	7.4	0.5	29.9	162.1	169.4	8.3	1.0
C-2''	21.0	174.0	18.0	19.6	3.0	1.4	174.2	17.8	17.9	3.2	3.1	173.0	19.0	18.2	2.0	2.8	174.1	17.9	19.4	3.1	1.6
C-1'''	171.3	28.4	163.6	170.5	7.7	0.8	28.7	163.3	170.9	8.0	0.4	28.8	163.2	171.1	8.1	0.2	28.5	163.5	170.8	7.8	0.5
C-2'''	20.9	174.3	17.7	19.4	3.2	1.5	174.3	17.7	17.8	3.2	3.1	174.3	17.7	16.8	3.2	4.1	174.2	17.8	19.4	3.1	1.5
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|; **3A**: Y = 0.9649X – 0.9534, R^2 = 0.9981, MAE = 4.0 ppm, CMAE = 1.7 ppm; **3B**: Y = 0.951X + 0.7786, R^2 = 0.9977, MAE = 3.8 ppm, CMAE = 1.9 ppm; **3C**: Y = 0.9428X + 1.8547, R^2 = 0.9976, MAE = 3.9 ppm, CMAE = 2.0 ppm; **3D**: Y = 0.9622X – 0.8335, R^2 = 0.9993, MAE = 3.8 ppm, CMAE = 1.2 ppm.																				

Nuclie	δ(exptl)	3A					3B					3C					3D				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
H-1a	1.90	29.65	2.35	1.90	0.45	0.00	29.36	2.64	2.11	0.74	0.21	29.35	2.65	2.10	0.75	0.20	29.63	2.37	1.91	0.47	0.01
H-1b	1.94	29.57	2.43	1.97	0.49	0.03	29.85	2.15	1.65	0.21	0.29	29.90	2.10	1.58	0.16	0.36	29.55	2.45	1.98	0.51	0.04
H-2	2.09	29.52	2.48	2.02	0.39	0.07	29.42	2.58	2.06	0.49	0.03	29.40	2.60	2.05	0.51	0.04	29.52	2.48	2.01	0.39	0.08
H-3	5.50	25.87	6.13	5.46	0.63	0.04	25.84	6.16	5.41	0.66	0.09	25.90	6.10	5.35	0.60	0.15	25.83	6.17	5.51	0.67	0.01
H-4	2.29	29.58	2.42	1.97	0.13	0.32	29.41	2.59	2.07	0.30	0.22	29.35	2.65	2.09	0.36	0.20	29.53	2.47	2.01	0.18	0.28

H-5	2.90	28.26	3.74	3.21	0.84	0.31	27.86	4.14	3.52	1.24	0.62	28.62	3.38	2.79	0.48	0.11	28.37	3.63	3.10	0.73	0.20
H-7	5.04	25.97	6.03	5.37	0.99	0.33	26.11	5.89	5.15	0.85	0.11	26.00	6.00	5.26	0.96	0.22	26.18	5.82	5.17	0.78	0.13
H-8a	1.92	30.13	1.87	1.45	0.05	0.47	29.34	2.66	2.13	0.74	0.21	29.32	2.68	2.13	0.76	0.21	29.60	2.40	1.94	0.48	0.02
H-8b	1.55	29.35	2.65	2.18	1.10	0.63	29.22	2.78	2.24	1.23	0.69	29.26	2.74	2.18	1.19	0.63	29.61	2.39	1.93	0.84	0.38
H-9	4.18	27.41	4.59	4.01	0.41	0.17	27.25	4.75	4.09	0.57	0.09	26.99	5.01	4.32	0.83	0.14	27.46	4.54	3.96	0.36	0.22
H-11	1.23	30.47	1.53	1.13	0.30	0.10	29.07	2.93	2.38	1.70	1.15	29.05	2.95	2.38	1.72	1.15	30.20	1.80	1.37	0.57	0.14
H-12	3.80	27.64	4.36	3.79	0.56	0.01	27.65	4.35	3.71	0.55	0.09	27.38	4.62	3.95	0.82	0.15	27.64	4.36	3.79	0.56	0.01
H-13	2.21	29.36	2.64	2.17	0.43	0.04	28.99	3.01	2.46	0.80	0.25	28.34	3.66	3.05	1.45	0.84	29.33	2.67	2.19	0.46	0.02
H-14	5.06	26.49	5.51	4.87	0.45	0.19	25.99	6.01	5.27	0.95	0.21	26.31	5.69	4.97	0.63	0.09	26.48	5.52	4.89	0.46	0.17
H-16	0.94	30.76	1.24	0.86	0.30	0.08	30.76	1.24	0.80	0.30	0.14	30.76	1.24	0.77	0.30	0.17	30.63	1.37	0.96	0.43	0.02
H-16	0.94	30.68	1.32	0.93	0.38	0.01	30.73	1.27	0.83	0.33	0.11	30.65	1.35	0.87	0.41	0.07	30.76	1.24	0.84	0.30	0.10
H-16	0.94	30.63	1.37	0.98	0.43	0.04	30.66	1.34	0.89	0.40	0.05	30.69	1.31	0.83	0.37	0.11	30.68	1.32	0.91	0.38	0.03
H-17	1.70	29.76	2.24	1.79	0.54	0.09	29.99	2.01	1.52	0.31	0.18	29.48	2.52	1.97	0.82	0.27	30.10	1.90	1.46	0.20	0.24
H-17	1.70	29.77	2.23	1.78	0.53	0.08	29.53	2.47	1.95	0.77	0.25	30.04	1.96	1.44	0.26	0.26	29.70	2.30	1.84	0.60	0.14
H-17	1.70	30.11	1.89	1.47	0.19	0.23	29.72	2.28	1.78	0.58	0.08	29.91	2.09	1.57	0.39	0.13	29.71	2.29	1.83	0.59	0.13
H-18	0.84	30.51	1.49	1.09	0.65	0.25	31.32	0.68	0.27	0.16	0.57	29.95	2.05	1.52	1.21	0.68	30.47	1.53	1.11	0.69	0.27
H-18	0.84	30.42	1.58	1.17	0.74	0.33	30.54	1.46	1.01	0.62	0.17	31.03	0.97	0.51	0.13	0.33	31.09	0.91	0.53	0.07	0.31
H-18	0.84	31.20	0.80	0.44	0.04	0.40	30.89	1.11	0.67	0.27	0.17	31.09	0.91	0.46	0.07	0.38	30.58	1.42	1.01	0.58	0.17
H-19	1.01	30.58	1.42	1.02	0.41	0.01	30.15	1.85	1.37	0.84	0.36	31.24	0.76	0.31	0.25	0.70	30.10	1.90	1.46	0.89	0.45
H-19	1.01	30.57	1.43	1.03	0.42	0.02	30.91	1.09	0.66	0.08	0.35	31.07	0.93	0.47	0.08	0.54	30.29	1.71	1.29	0.70	0.28
H-19	1.01	29.99	2.01	1.58	1.00	0.57	31.01	0.99	0.57	0.02	0.44	30.29	1.71	1.21	0.70	0.20	31.11	0.89	0.50	0.12	0.51
H-20	0.99	30.53	1.47	1.07	0.48	0.08	30.43	1.57	1.11	0.58	0.12	30.40	1.60	1.10	0.61	0.11	30.49	1.51	1.09	0.52	0.10
H-20	0.99	30.49	1.51	1.11	0.52	0.12	30.62	1.38	0.93	0.39	0.06	30.42	1.58	1.08	0.59	0.09	30.74	1.26	0.86	0.27	0.13
H-20	0.99	30.75	1.25	0.86	0.26	0.13	30.58	1.42	0.97	0.43	0.02	30.84	1.16	0.69	0.17	0.30	30.52	1.48	1.06	0.49	0.07
H-3',7'	7.99	23.18	8.82	7.99	0.83	0.00	22.89	9.11	8.18	1.12	0.19	22.96	9.04	8.13	1.05	0.14	23.17	8.83	8.02	0.84	0.03
H-3',7'	7.99	23.01	8.99	8.16	1.00	0.17	23.20	8.80	7.89	0.81	0.10	23.16	8.84	7.93	0.85	0.06	23.06	8.94	8.13	0.95	0.14
H-4',6'	7.37	23.85	8.15	7.36	0.78	0.01	23.84	8.16	7.28	0.79	0.09	23.84	8.16	7.29	0.79	0.08	23.85	8.15	7.38	0.78	0.01
H-4',6'	7.37	23.84	8.16	7.37	0.79	0.00	23.84	8.16	7.28	0.79	0.09	23.83	8.17	7.31	0.80	0.06	23.87	8.13	7.36	0.76	0.01
H-5'	7.49	23.73	8.27	7.47	0.78	0.02	23.72	8.28	7.39	0.79	0.10	23.73	8.27	7.40	0.78	0.09	23.74	8.26	7.48	0.77	0.01
H-2''	1.90	29.61	2.39	1.94	0.49	0.04	29.93	2.07	1.58	0.17	0.32	29.55	2.45	1.91	0.55	0.01	30.12	1.88	1.44	0.02	0.46
H-2''	1.90	29.73	2.27	1.83	0.37	0.07	30.05	1.95	1.46	0.05	0.44	29.80	2.20	1.67	0.30	0.23	29.59	2.41	1.94	0.51	0.04
H-2''	1.90	30.12	1.88	1.46	0.02	0.44	29.64	2.36	1.84	0.46	0.06	29.46	2.54	2.00	0.64	0.10	29.54	2.46	1.99	0.56	0.09
H-2'''	2.11	29.89	2.11	1.67	0.00	0.44	29.53	2.47	1.95	0.36	0.16	29.37	2.63	2.08	0.52	0.03	29.34	2.66	2.18	0.55	0.07
H-2'''	2.11	29.39	2.61	2.15	0.50	0.04	29.72	2.28	1.77	0.17	0.34	29.89	2.11	1.58	0.00	0.53	29.67	2.33	1.87	0.22	0.24
H-2'''	2.11	29.36	2.64	2.18	0.53	0.07	29.36	2.64	2.11	0.53	0.00	29.43	2.57	2.02	0.46	0.09	29.61	2.39	1.93	0.28	0.18
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|; **3A**: Y = 1.0619X + 0.3311, R^2 = 0.9887, MAE = 0.50 ppm, CMAE = 0.20 ppm; **3B**: Y = 1.0669X + 0.3886, R^2 = 0.9796, MAE = 0.60 ppm, CMAE = 0.20 ppm; **3C**: Y = 1.0598X + 0.4289, R^2 = 0.9745, MAE = 0.60 ppm, CMAE = 0.30 ppm; **3D**: Y = 1.0558X + 0.3555, R^2 = 0.9918, MAE = 0.50 ppm, CMAE = 0.10 ppm;																				

Table S30. Experimental chemical shifts of **3**, calculated shielding tensors and chemical shifts of isomers **3E**–**3H** in chloroform with TMS as reference at mPW1PW91/6-31G** level.

Nuclie	δ(exptl)	**3E**					**3F**					**3G**					**3H**				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
C-1	36.3	156.8	35.2	35.3	1.1	1.0	156.4	35.6	36.8	0.7	0.5	156.4	35.6	36.9	0.7	0.6	156.4	35.6	36.2	0.7	0.1
C-2	36.3	155.0	37.0	37.2	0.7	0.9	155.7	36.3	37.5	0.0	1.2	155.7	36.3	37.6	0.0	1.3	155.6	36.4	37.1	0.1	0.8
C-3	78.6	116.4	75.6	78.2	3.0	0.4	116.9	75.1	78.3	3.5	0.3	117.0	75.0	78.3	3.6	0.3	117.1	74.9	77.7	3.7	0.9
C-4	46.4	139.4	52.6	53.8	6.2	7.4	145.8	46.2	48.0	0.2	1.6	145.8	46.2	47.9	0.2	1.5	143.8	48.2	49.5	1.8	3.1
C-5	31.7	154.8	37.2	37.4	5.5	5.7	152.7	39.3	40.7	7.6	9.0	152.6	39.4	40.9	7.7	9.2	154.5	37.5	38.2	5.8	6.5
C-6	140.5	55.7	136.3	142.9	4.2	2.4	57.6	134.4	140.6	6.1	0.1	59.0	133.0	139.1	7.5	1.4	59.5	132.5	138.7	8.0	1.8
C-7	121.7	76.6	115.4	120.6	6.3	1.1	74.7	117.3	122.7	4.4	1.0	74.0	118.0	123.3	3.7	1.6	74.4	117.6	123.0	4.1	1.3
C-8	25.3	164.3	27.7	27.3	2.4	2.0	164.8	27.2	28.0	1.9	2.7	164.4	27.6	28.4	2.3	3.1	165.3	26.7	26.8	1.4	1.5
C-9	77.9	119.0	73.0	75.5	4.9	2.4	114.1	77.9	81.2	0.0	3.3	114.0	78.0	81.4	0.1	3.5	116.1	75.9	78.8	2.0	0.9
C-10	41.0	152.6	39.4	39.7	1.6	1.3	155.1	36.9	38.2	4.1	2.8	155.1	36.9	38.2	4.1	2.8	152.1	39.9	40.8	1.1	0.2
C-11	47.0	146.4	45.6	46.4	1.4	0.6	151.7	40.3	41.7	6.7	5.3	150.6	41.4	42.9	5.6	4.1	148.2	43.8	44.9	3.2	2.1

C-12	80.4	115.3	76.7	79.5	3.7	0.9	111.8	80.2	83.7	0.2	3.3	111.9	80.1	83.6	0.3	3.2	113.5	78.5	81.6	1.9	1.2
C-13	44.5	148.5	43.5	44.1	1.0	0.4	154.5	37.5	38.8	7.0	5.7	154.5	37.5	38.8	7.0	5.7	150.0	42.0	43.0	2.5	1.5
C-14	79.2	111.4	80.6	83.6	1.4	4.4	114.8	77.2	80.6	2.0	1.4	114.6	77.4	80.7	1.8	1.5	113.4	78.6	81.7	0.6	2.5
C-15	89.7	107.0	85.0	88.2	4.7	1.5	101.2	90.8	94.9	1.1	5.2	101.3	90.7	94.6	1.0	4.9	104.2	87.8	91.4	1.9	1.7
C-16	13.4	180.5	11.5	10.1	1.9	3.3	179.8	12.2	12.2	1.2	1.2	179.9	12.1	12.2	1.3	1.2	180.6	11.4	10.6	2.0	2.8
C-17	20.4	167.6	24.4	23.8	4.0	3.4	170.6	21.4	21.9	1.0	1.5	170.6	21.4	21.9	1.0	1.5	167.5	24.5	24.5	4.1	4.1
C-18	27.2	166.0	26.0	25.5	1.2	1.7	170.0	22.0	22.5	5.2	4.7	175.4	16.6	16.9	10.6	10.3	168.0	24.0	23.9	3.2	3.3
C-19	20.6	167.4	24.6	23.9	4.0	3.3	170.3	21.7	22.2	1.1	1.6	166.4	25.6	26.3	5.0	5.7	169.7	22.3	22.2	1.7	1.6
C-20	13.3	180.3	11.7	10.3	1.6	3.0	179.2	12.8	12.8	0.5	0.5	179.4	12.6	12.7	0.7	0.6	179.8	12.2	11.5	1.1	1.8
C-1'	165.4	33.2	158.8	166.8	6.6	1.4	33.5	158.5	165.9	6.9	0.5	33.4	158.6	166.0	6.8	0.6	32.6	159.4	167.1	6.0	1.7
C-2'	129.8	69.2	122.8	128.5	7.0	1.3	68.2	123.8	129.5	6.0	0.3	68.4	123.6	129.3	6.2	0.5	68.7	123.3	128.9	6.5	0.9
C-3',7'	129.5	68.2	123.8	129.6	5.7	0.1	67.6	124.4	130.1	5.1	0.6	69.1	122.9	128.5	6.6	1.0	68.7	123.3	129.0	6.2	0.5
C-3',7'	129.5	67.5	124.5	130.3	5.0	0.8	68.6	123.4	129.0	6.1	0.5	67.7	124.3	129.9	5.2	0.4	67.2	124.8	130.6	4.7	1.1
C-4',6'	128.5	71.1	120.9	126.5	7.6	2.0	70.8	121.2	126.8	7.3	1.7	70.6	121.4	127.0	7.1	1.5	71.0	121.0	126.5	7.5	2.0
C-4',6'	128.5	71.1	120.9	126.5	7.6	2.0	70.8	121.2	126.8	7.3	1.7	70.7	121.3	126.8	7.2	1.7	70.8	121.2	126.7	7.3	1.8
C-5'	133.2	65.9	126.1	132.0	7.1	1.2	65.9	126.1	131.8	7.1	1.4	65.7	126.3	132.1	6.9	1.1	65.8	126.2	132.0	7.0	1.2
C-1''	170.4	30.2	161.8	170.0	8.6	0.4	30.4	161.6	169.2	8.8	1.2	29.5	162.5	170.1	7.9	0.3	29.6	162.4	170.3	8.0	0.1
C-2''	21.0	173.7	18.3	17.2	2.7	3.8	174.1	17.9	18.2	3.1	2.8	174.1	17.9	18.3	3.1	2.7	174.0	18.0	17.6	3.0	3.4
C-1'''	171.3	28.4	163.6	172.0	7.7	0.7	28.9	163.1	170.8	8.2	0.5	28.9	163.1	170.8	8.2	0.5	28.6	163.4	171.4	7.9	0.1
C-2'''	20.9	174.2	17.8	16.8	3.1	4.1	174.4	17.6	18.0	3.3	2.9	174.4	17.6	18.0	3.3	2.9	174.3	17.7	17.3	3.2	3.6

Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|;
3E: Y = 0.9395X + 2.0665, R^2 = 0.9974, MAE = 4.2 ppm, CMAE = 2.1 ppm; **3F**: Y = 0.9521X + 0.5352, R^2 = 0.9968, MAE = 4.0 ppm, CMAE = 2.2 ppm;
3G: Y = 0.9523X + 0.5187, R^2 = 0.9955, MAE = 4.3 ppm, CMAE = 2.5 ppm; **3H**: Y = 0.9456X + 1.3659, R^2 = 0.9981, MAE = 3.8 ppm, CMAE = 1.8 ppm.

Nuclie	δ(exptl)	3E					3F					3G					3H				
		σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2	σiso	δ(calcd)	δ(scaled)	Δ1	Δ2
H-1a	1.90	29.78	2.22	1.73	0.32	0.17	29.96	2.04	1.60	0.14	0.30	29.95	2.05	1.59	0.15	0.31	29.67	2.33	1.85	0.43	0.05
H-1b	1.94	29.50	2.50	2.00	0.56	0.06	29.39	2.61	2.13	0.67	0.19	29.36	2.64	2.15	0.70	0.21	29.43	2.57	2.08	0.63	0.14
H-2	2.09	29.59	2.41	1.92	0.32	0.17	29.38	2.62	2.14	0.53	0.05	29.40	2.60	2.11	0.51	0.02	29.60	2.40	1.92	0.31	0.17
H-3	5.50	25.61	6.39	5.68	0.89	0.18	25.99	6.01	5.33	0.51	0.17	26.00	6.00	5.33	0.50	0.17	25.74	6.26	5.58	0.76	0.08
H-4	2.29	29.09	2.91	2.39	0.62	0.10	29.46	2.54	2.07	0.25	0.22	29.46	2.54	2.06	0.25	0.23	29.33	2.67	2.18	0.38	0.11
H-5	2.90	28.78	3.22	2.69	0.32	0.21	29.10	2.90	2.41	0.00	0.49	29.03	2.97	2.46	0.07	0.44	28.61	3.39	2.86	0.49	0.04
H-7	5.04	26.41	5.59	4.93	0.55	0.11	26.12	5.88	5.20	0.84	0.16	26.11	5.89	5.23	0.85	0.19	26.23	5.77	5.11	0.73	0.07
H-8a	1.92	28.52	3.48	2.93	1.56	1.01	29.97	2.03	1.59	0.11	0.33	30.21	1.79	1.34	0.13	0.58	29.40	2.60	2.10	0.68	0.18
H-8b	1.55	29.63	2.37	1.88	0.82	0.33	29.83	2.17	1.72	0.62	0.17	29.45	2.55	2.07	1.00	0.52	29.54	2.46	1.98	0.91	0.43
H-9	4.18	26.89	5.11	4.48	0.93	0.30	27.21	4.79	4.18	0.61	0.00	27.27	4.73	4.13	0.55	0.05	27.07	4.93	4.32	0.75	0.14
H-11	1.23	30.06	1.94	1.47	0.71	0.24	28.49	3.51	2.98	2.28	1.75	28.79	3.21	2.69	1.98	1.46	29.95	2.05	1.58	0.82	0.35
H-12	3.80	26.96	5.04	4.41	1.24	0.61	27.35	4.65	4.05	0.85	0.25	27.42	4.58	3.98	0.78	0.18	27.43	4.57	3.98	0.77	0.18
H-13	2.21	29.38	2.62	2.11	0.41	0.10	29.02	2.98	2.48	0.77	0.27	28.98	3.02	2.51	0.81	0.30	29.23	2.77	2.27	0.56	0.06
H-14	5.06	26.43	5.57	4.91	0.51	0.15	26.28	5.72	5.05	0.66	0.01	26.32	5.68	5.03	0.62	0.03	26.36	5.64	5.00	0.58	0.06
H-16	0.94	31.05	0.95	0.53	0.01	0.41	30.63	1.37	0.96	0.43	0.02	30.79	1.21	0.79	0.27	0.15	30.70	1.30	0.88	0.36	0.06
H-16	0.94	30.76	1.24	0.81	0.30	0.13	30.76	1.24	0.84	0.30	0.10	30.67	1.33	0.91	0.39	0.03	30.83	1.17	0.75	0.23	0.19
H-16	0.94	30.56	1.44	1.00	0.50	0.06	30.66	1.34	0.94	0.40	0.00	30.64	1.36	0.94	0.42	0.00	30.76	1.24	0.81	0.30	0.13
H-17	1.70	29.63	2.37	1.88	0.67	0.18	30.07	1.93	1.49	0.23	0.21	29.63	2.37	1.89	0.67	0.19	29.52	2.48	1.99	0.78	0.29
H-17	1.70	30.10	1.90	1.43	0.20	0.27	29.64	2.36	1.90	0.66	0.20	30.07	1.93	1.48	0.23	0.22	29.98	2.02	1.55	0.32	0.15
H-17	1.70	30.45	1.55	1.10	0.15	0.60	30.09	1.91	1.47	0.21	0.23	30.06	1.94	1.48	0.24	0.22	30.16	1.84	1.39	0.14	0.31
H-18	0.84	30.04	1.96	1.48	1.12	0.64	30.31	1.69	1.27	0.85	0.43	30.20	1.80	1.36	0.96	0.52	30.91	1.09	0.67	0.25	0.17
H-18	0.84	30.82	1.18	0.75	0.34	0.09	30.96	1.04	0.66	0.20	0.18	30.87	1.13	0.72	0.29	0.12	30.35	1.65	1.20	0.81	0.36
H-18	0.84	30.89	1.11	0.68	0.27	0.16	30.92	1.08	0.70	0.24	0.14	30.66	1.34	0.91	0.50	0.07	30.66	1.34	0.91	0.50	0.07
H-19	1.01	31.13	0.87	0.45	0.14	0.56	30.71	1.29	0.89	0.28	0.12	30.87	1.13	0.72	0.12	0.29	30.68	1.32	0.89	0.31	0.12
H-19	1.01	30.84	1.16	0.73	0.15	0.28	31.04	0.96	0.59	0.05	0.42	30.73	1.27	0.85	0.26	0.16	31.18	0.82	0.41	0.19	0.60
H-19	1.01	30.18	1.82	1.36	0.81	0.35	30.23	1.77	1.35	0.76	0.34	30.69	1.31	0.89	0.30	0.12	29.83	2.17	1.70	1.16	0.69
H-20	0.99	30.60	1.40	0.96	0.41	0.03	30.35	1.65	1.23	0.66	0.24	30.38	1.62	1.18	0.63	0.19	30.56	1.44	1.00	0.45	0.01
H-20	0.99	30.52	1.48	1.03	0.49	0.04	30.71	1.29	0.89	0.30	0.10	30.75	1.25	0.84	0.26	0.15	30.45	1.55	1.11	0.56	0.12

H-20	0.99	30.49	1.51	1.06	0.52	0.07	30.53	1.47	1.06	0.48	0.07	30.55	1.45	1.02	0.46	0.03	30.69	1.31	0.88	0.32	0.11
H-3',7'	7.99	23.27	8.73	7.91	0.74	0.08	23.19	8.81	7.96	0.82	0.03	22.92	9.08	8.25	1.09	0.26	23.22	8.78	7.98	0.79	0.01
H-3',7'	7.99	23.19	8.81	7.98	0.82	0.01	22.84	9.16	8.29	1.17	0.30	23.21	8.79	7.97	0.80	0.02	23.20	8.80	7.99	0.81	0.00
H-4',6'	7.37	23.96	8.04	7.25	0.67	0.12	23.84	8.16	7.34	0.79	0.03	23.83	8.17	7.38	0.80	0.01	23.92	8.08	7.31	0.71	0.06
H-4',6'	7.37	23.86	8.14	7.35	0.77	0.02	23.79	8.21	7.40	0.84	0.03	23.84	8.16	7.37	0.79	0.00	23.86	8.14	7.37	0.77	0.00
H-5'	7.49	23.77	8.23	7.43	0.74	0.06	23.73	8.27	7.45	0.78	0.04	23.72	8.28	7.48	0.79	0.01	23.76	8.24	7.46	0.75	0.03
H-2''	1.90	29.46	2.54	2.04	0.64	0.14	29.85	2.15	1.71	0.25	0.19	29.54	2.46	1.98	0.56	0.08	29.77	2.23	1.76	0.33	0.14
H-2''	1.90	29.99	2.01	1.53	0.11	0.37	30.07	1.93	1.49	0.03	0.41	30.13	1.87	1.42	0.03	0.48	29.58	2.42	1.94	0.52	0.04
H-2''	1.90	29.41	2.59	2.09	0.69	0.19	30.06	1.94	1.51	0.04	0.39	29.60	2.40	1.92	0.50	0.02	29.96	2.04	1.57	0.14	0.33
H-2'''	2.11	29.31	2.69	2.18	0.58	0.07	29.38	2.62	2.15	0.51	0.04	29.38	2.62	2.13	0.51	0.02	29.48	2.52	2.03	0.41	0.08
H-2'''	2.11	29.34	2.66	2.15	0.55	0.04	29.35	2.65	2.17	0.54	0.06	29.35	2.65	2.15	0.54	0.04	29.36	2.64	2.15	0.53	0.04
H-2'''	2.11	29.89	2.11	1.63	0.00	0.48	29.91	2.09	1.64	0.02	0.47	29.91	2.09	1.62	0.02	0.49	29.74	2.26	1.78	0.15	0.33
	Δ1 = |δ(calcd) – δ(exptl)|, Δ2 = |δ(scaled) – δ(exptl)|; **3E**: Y = 1.0549X + 0.3859, R^2 = 0.9803, MAE = 0.60 ppm, CMAE = 0.20 ppm; **3F**: Y = 1.0641X + 0.3399, R^2 = 0.9737, MAE = 0.50 ppm, CMAE = 0.20 ppm; **3G**: Y = 1.0569X + 0.3699, R^2 = 0.9774, MAE = 0.50 ppm, CMAE = 0.20 ppm; **3H**: Y = 1.0531X + 0.382, R^2 = 0.9897, MAE = 0.50 ppm, CMAE = 0.20 ppm;																				

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	Gas Phase	6-31G(d)	Shielding Tensors

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
sDP4+ (H data)	2.81%	0.00%	0.00%	97.09%	0.00%	0.00%	0.00%	0.09%
sDP4+ (C data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%
sDP4+ (all data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%
uDP4+ (H data)	37.43%	0.00%	0.00%	60.04%	0.00%	0.00%	0.00%	2.53%
uDP4+ (C data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%
uDP4+ (all data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%
DP4+ (H data)	1.77%	0.00%	0.00%	98.22%	0.00%	0.00%	0.00%	0.00%
DP4+ (C data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%
DP4+ (all data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%

Figure S22. Detailed DP4+ probability of **3** calculated at mPW1PW91/6-31G* level in gas phase.

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-31G(d,p)	Shielding Tensors

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8
sDP4+ (H data)	2.06%	0.00%	0.00%	96.60%	0.00%	0.00%	0.00%	1.33%
sDP4+ (C data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%
sDP4+ (all data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%
uDP4+ (H data)	11.69%	0.00%	0.00%	61.48%	0.00%	0.00%	0.00%	26.84%
uDP4+ (C data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%
uDP4+ (all data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%
DP4+ (H data)	0.40%	0.00%	0.00%	99.00%	0.00%	0.00%	0.00%	0.60%
DP4+ (C data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%
DP4+ (all data)	0.00%	0.00%	0.00%	100.00%	0.00%	0.00%	0.00%	0.00%

Figure S23. Detailed DP4+ probability of compound **3** calculated at mPW1PW91/6-31G** level in chloroform with PCM model.

Experimental		mPW1PW91/6-31G* gas phase		mPW1PW91/6-31G** PCM		
δ ^{13}C	δ ^{1}H	σ ^{13}C	σ ^{1}H	sp2	σ ^{13}C	σ ^{1}H
36.3	1.90	156.6	30.20		158.074	29.6523
	1.94		29.93			29.5717
36.3	2.09	156.1	30.01		156.978	29.5215
78.6	5.50	116.964	26.485		117.119	25.8661
46.4	2.29	147.067	30.198		148.059	29.5789
31.7	2.90	160.534	28.709		161.221	28.2552
140.5		54.740		x	53.2122	
121.7	5.04	71.464	26.582	x	73.3495	25.9676
25.3	1.92	163.490	30.532		165.008	30.1277
	1.55		29.869			29.3518
77.9	4.18	117.642	27.824		117.987	27.4123
41.0		150.088			150.459	
47.0	1.23	141.498	30.912		142.484	30.4729
80.4	3.80	115.091	28.238		115.934	27.6416
44.5	2.21	147.747	29.970		149.072	29.3642
79.2	5.06	114.470	27.100		115.159	26.4922
89.7		104.364			104.583	
13.4	0.94	179.199	31.176		181.174	30.7602
20.4	1.70	171.413	30.248		173.45	29.7648
27.2	0.84	167.073	31.072		168.993	30.5141
20.6	1.01	177.893	30.975		179.709	30.5823
13.3	0.99	178.874	31.085		180.835	30.5335
165.4		35.214		x	34.1337	
129.8		68.861		x	69.22	
129.5	7.99	65.975	23.815	x	67.1546	23.1809
129.5	7.99	69.500	23.778	x	69.6467	23.008
128.5	7.37	70.518	24.647	x	70.5994	23.8545
128.5	7.37	70.912	24.653	x	70.6724	23.8398
133.2	7.49	66.360	24.570	x	65.6764	23.7345
170.4		31.519		x	29.569	
21.0	1.90	172.581	30.303		174.049	29.6051
171.3		30.053		x	28.3934	
20.9	2.11	172.820	30.451		174.283	29.8921

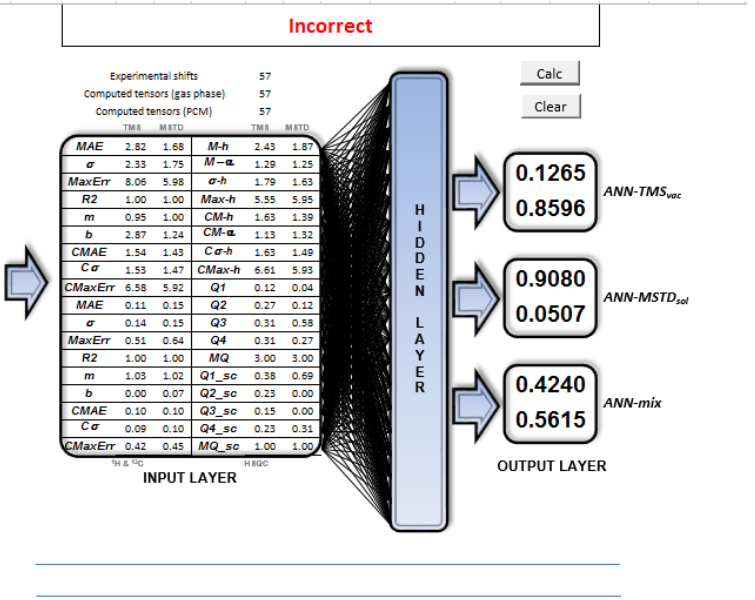


Figure S24. The result of ANN-PRA statistical analysis between compound **3** and isomer **3A**.

Experimental		mPW1PW91/6-31G* gas phase		mPW1PW91/6-31G** PCM		
δ ^{13}C	δ ^{1}H	σ ^{13}C	σ ^{1}H	sp2	σ ^{13}C	σ ^{1}H
36.3	1.90	156.5	30.17		157.938	29.6302
	1.94		29.92			29.554
36.3	2.09	156.2	30.01		157.041	29.5206
78.6	5.50	116.834	26.442		116.984	25.826
46.4	2.29	146.852	30.136		147.807	29.5265
31.7	2.90	160.018	28.820		160.779	28.3718
140.5		55.842		x	54.6965	
121.7	5.04	72.146	26.807	x	73.7033	26.1809
25.3	1.92	166.215	29.998		167.558	29.5989
	1.55		30.136			29.606
77.9	4.18	117.117	27.904		117.516	27.4598
41.0		151.110			151.515	
47.0	1.23	146.240	30.558		147.133	30.1951
80.4	3.80	115.408	28.222		116.261	27.6422
44.5	2.21	147.756	29.920		149.077	29.3276
79.2	5.06	114.349	27.078		115.061	26.4784
89.7		104.257			104.495	
13.4	0.94	179.133	31.027		181.145	30.632
20.4	1.70	170.995	30.575		173.138	30.1007
27.2	0.84	166.223	31.014		168.166	30.4695
20.6	1.01	172.668	30.597		174.484	30.1002
13.3	0.99	178.734	30.880		180.725	30.4914
165.4		35.172		x	34.0911	
129.8		68.975		x	69.278	
129.5	7.99	65.917	23.806	x	67.1207	23.1744
129.5	7.99	69.648	23.831	x	69.7396	23.0559
128.5	7.37	70.460	24.633	x	70.5922	23.8479
128.5	7.37	70.893	24.680	x	70.6699	23.8693
133.2	7.49	66.252	24.568	x	65.6545	23.743
170.4		31.747		x	29.8714	
21.0	1.90	172.634	30.657		174.133	30.1204
171.3		30.115		x	28.4562	
20.9	2.11	172.718	30.033		174.196	29.3449

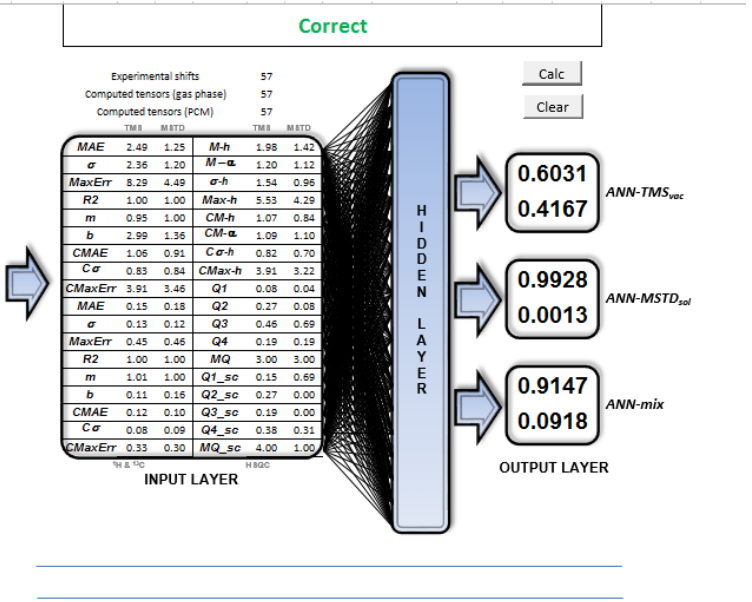


Figure S25. The result of ANN-PRA statistical analysis between compound **3** and isomer **3D**.

NMR, HRESIMS, IR, UV, CD spectra and OR report of compound 1

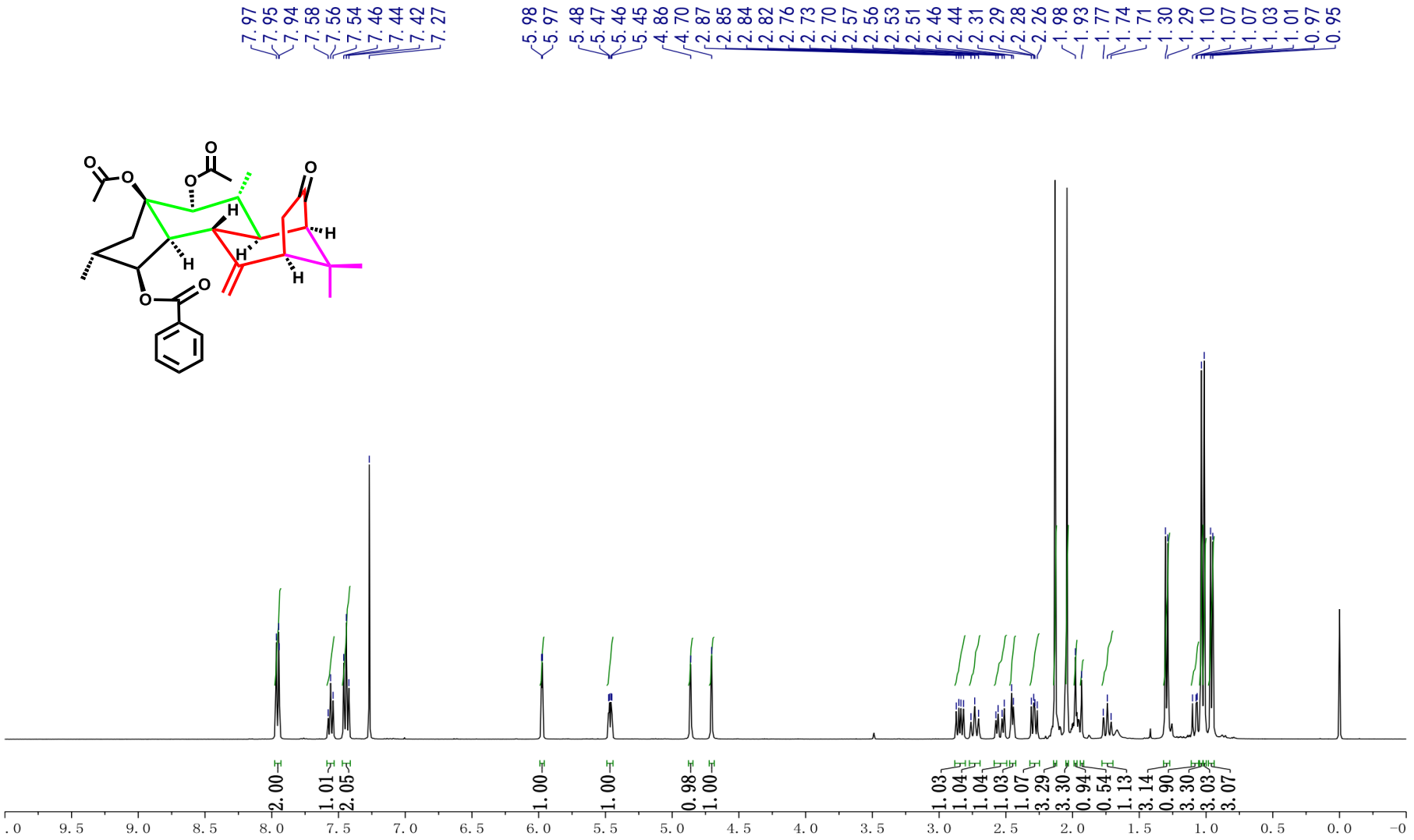


Figure S26. ^{1}H NMR spectrum of euphopia D (**1**) in chloroform-d (400 MHz)

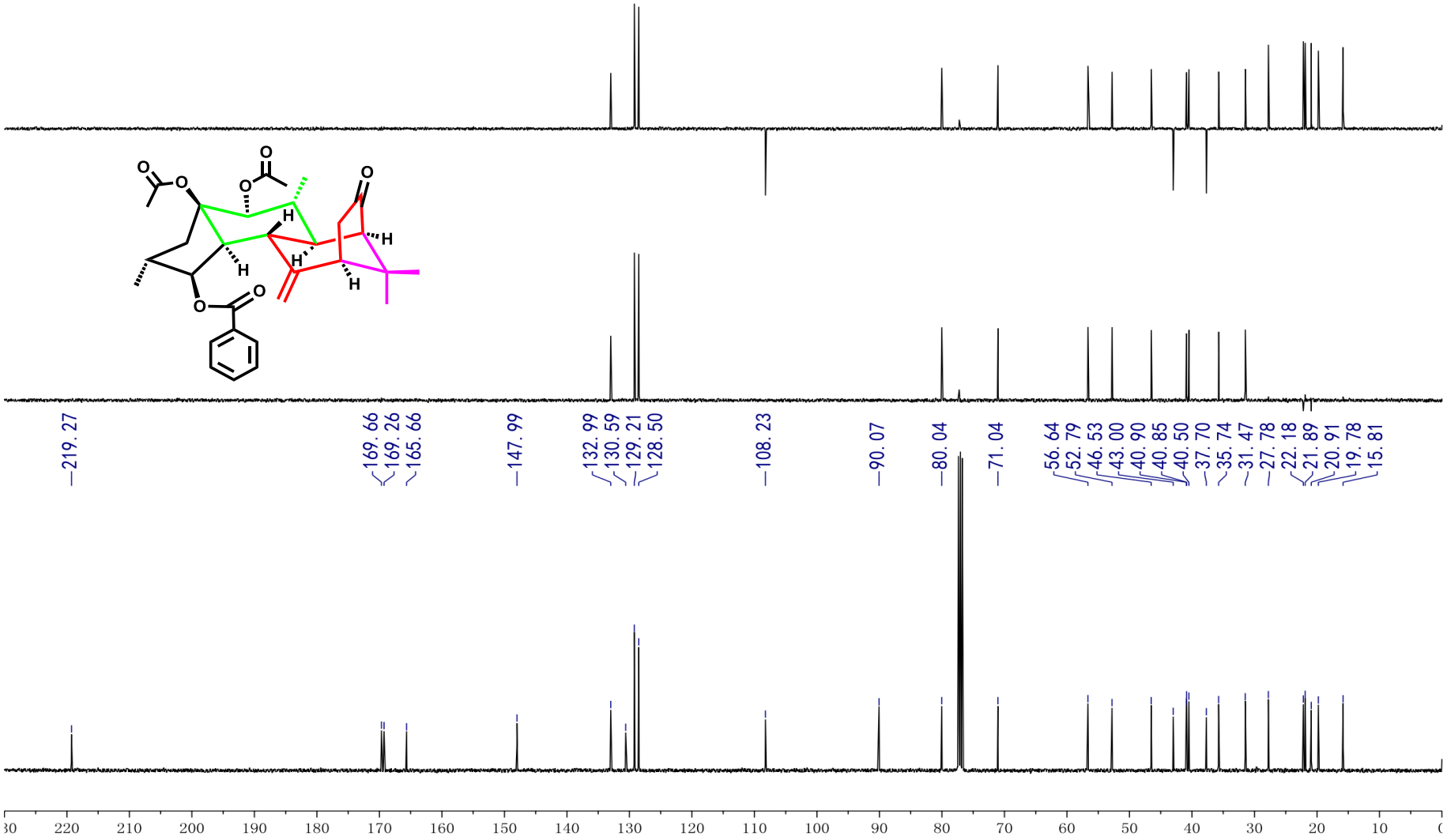


Figure S27. ^{13}C and DEPT NMR spectra of euphopia D (**1**) in chloroform-d (100 MHz)

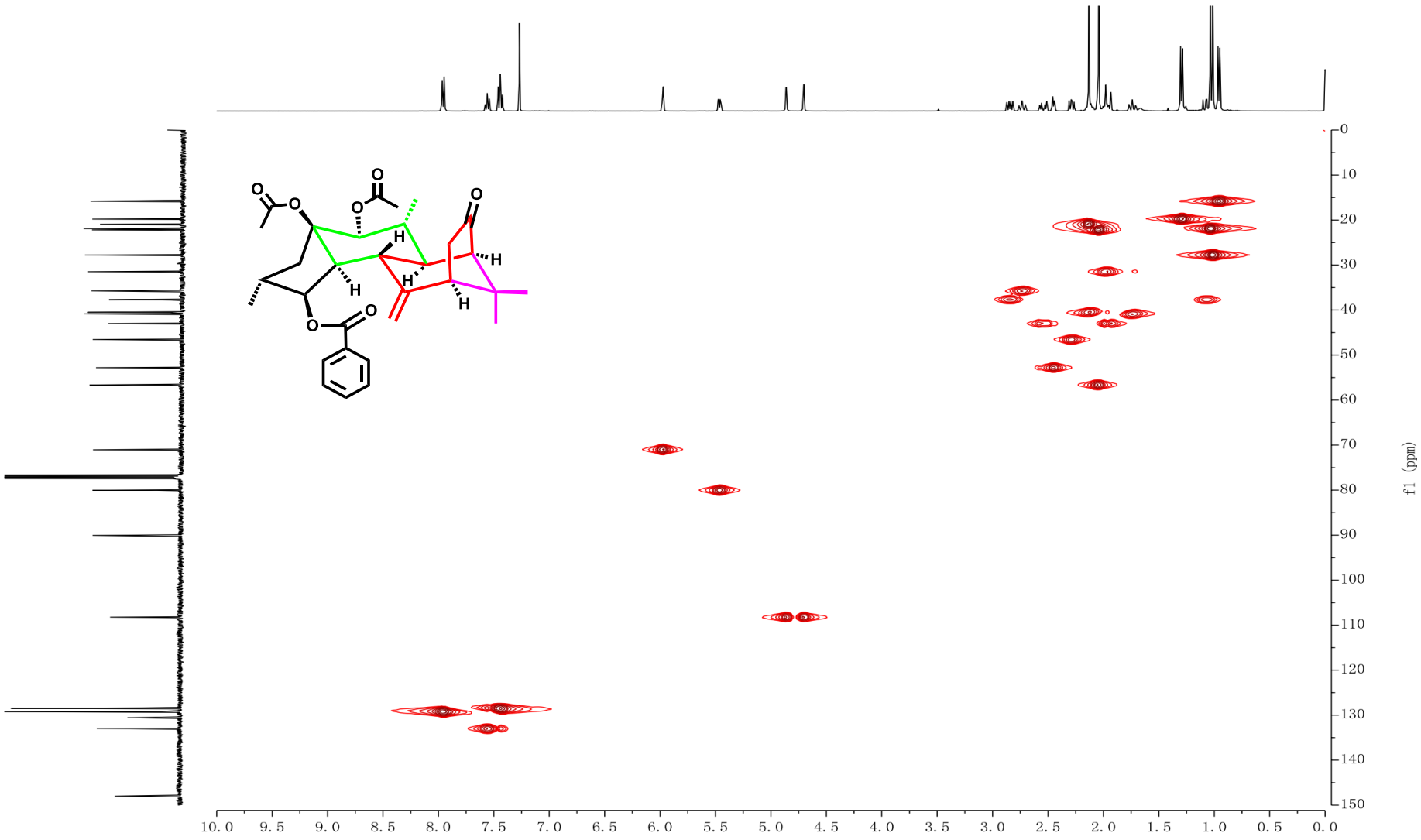


Figure S28. HSQC spectrum of euphopia D (**1**) in chloroform-d

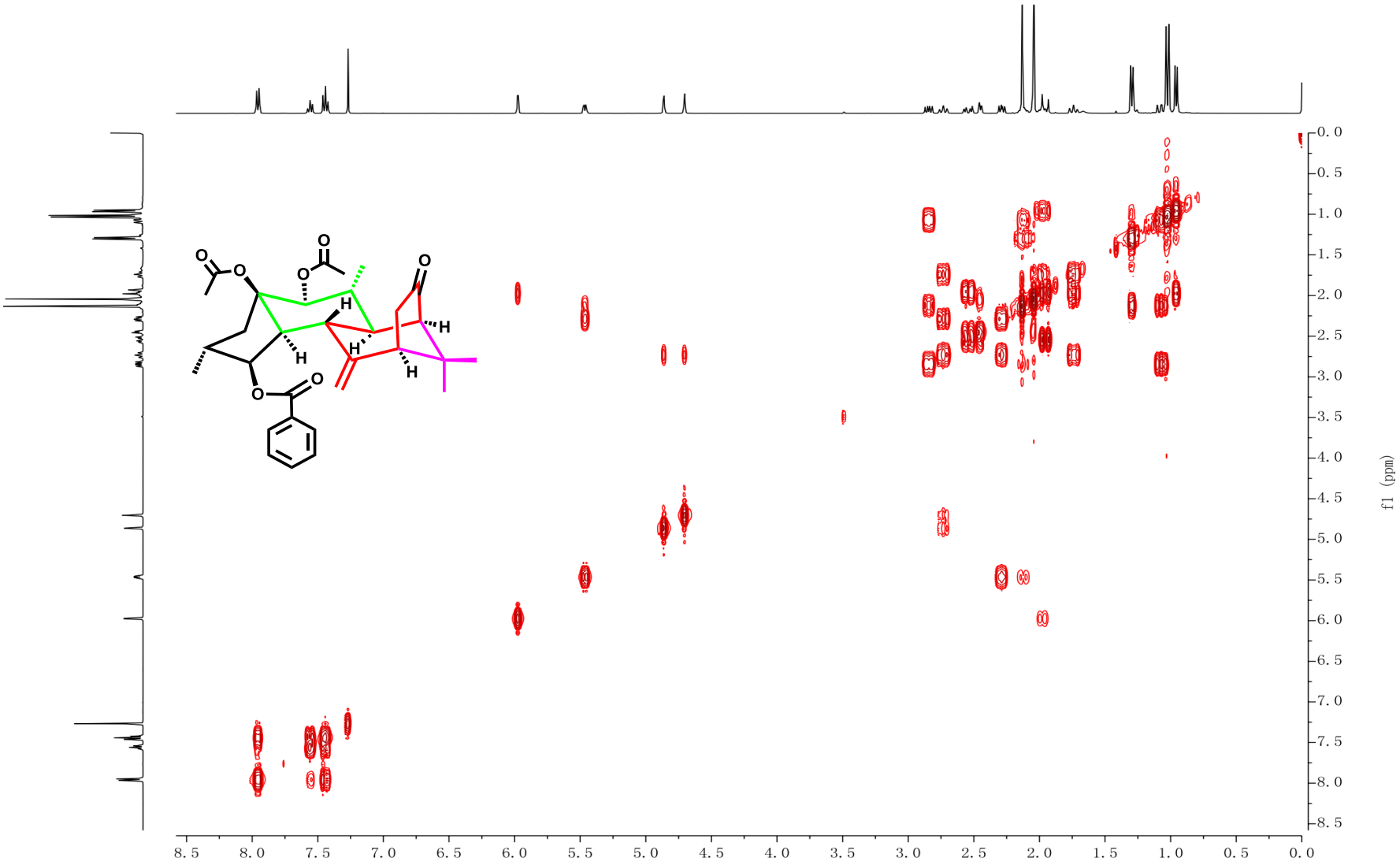


Figure S29. ^{1}H-^{1}H COSY spectrum of euphopia D (**1**) in chloroform-d

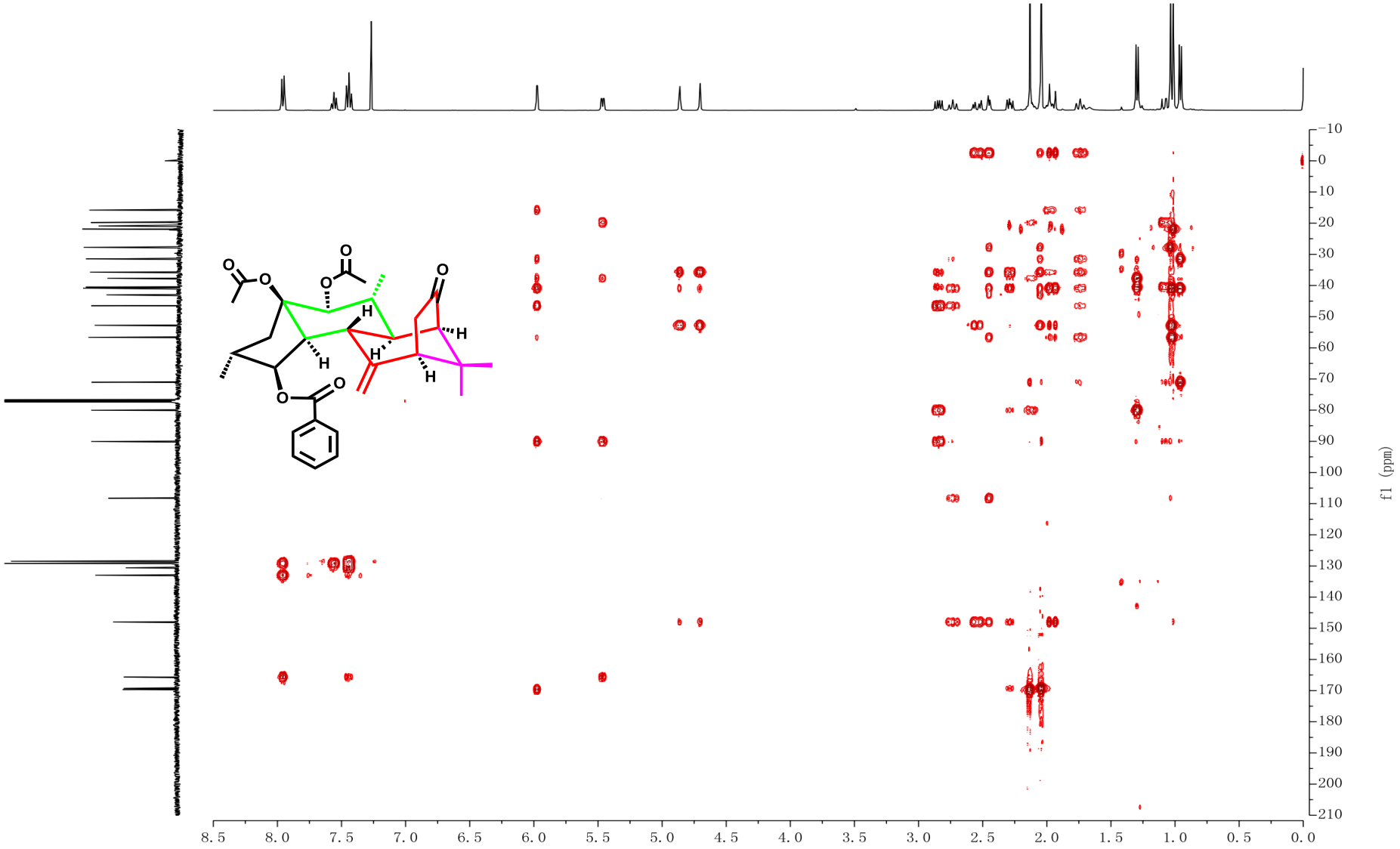


Figure S30. HMBC spectrum of euphopia D (**1**) in chloroform-d

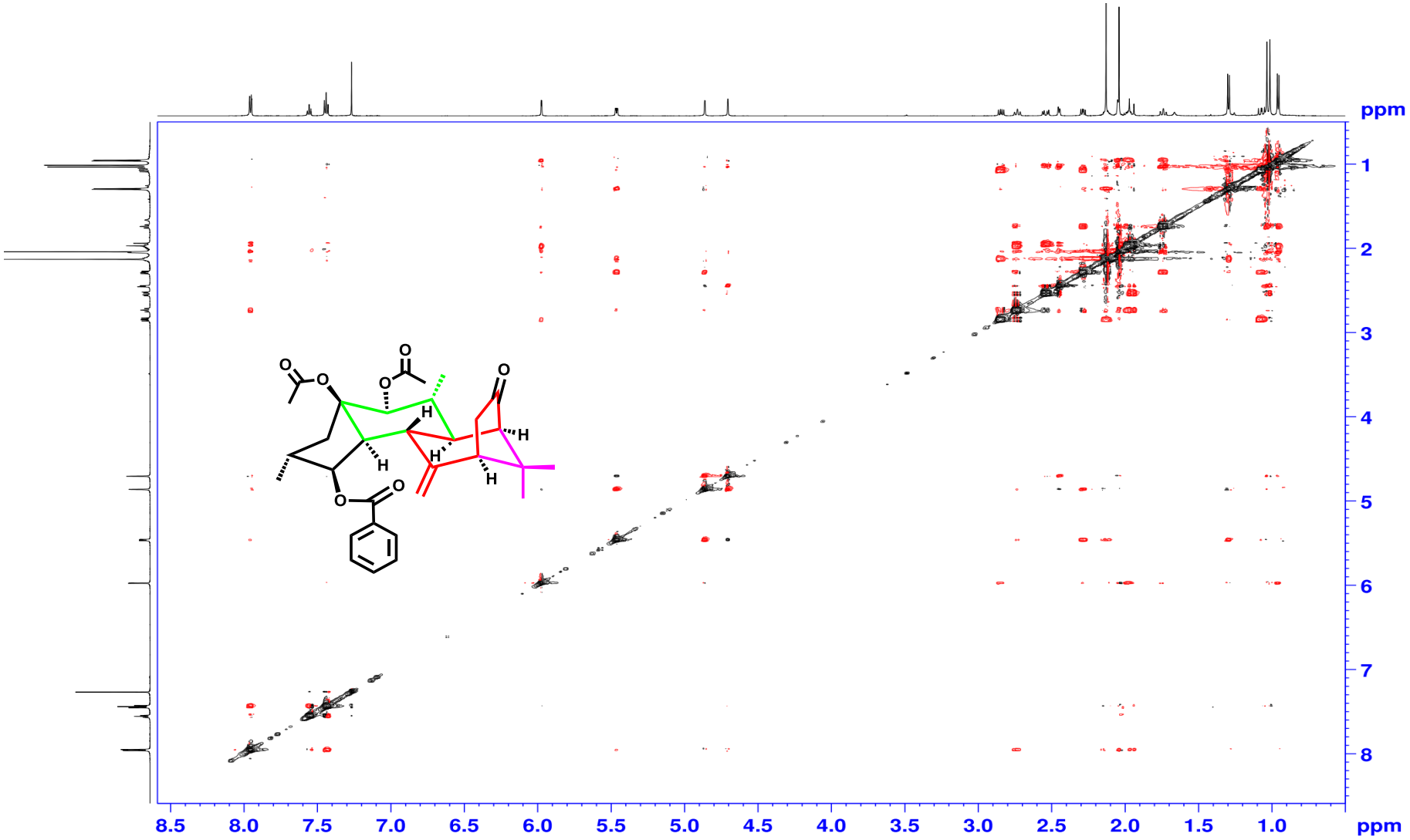


Figure S31. ROESY spectrum of euphopia D (**1**) in chloroform-d

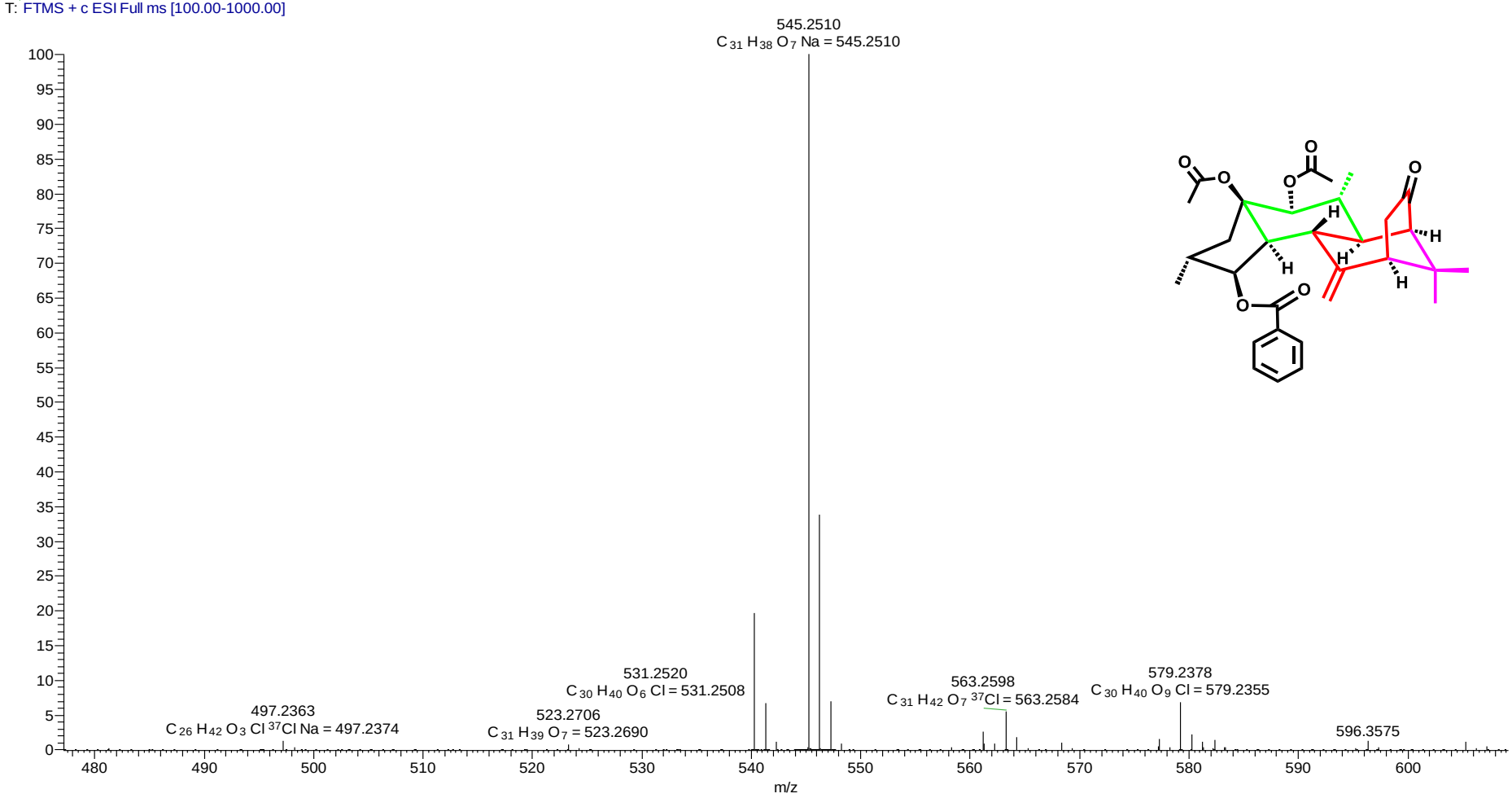
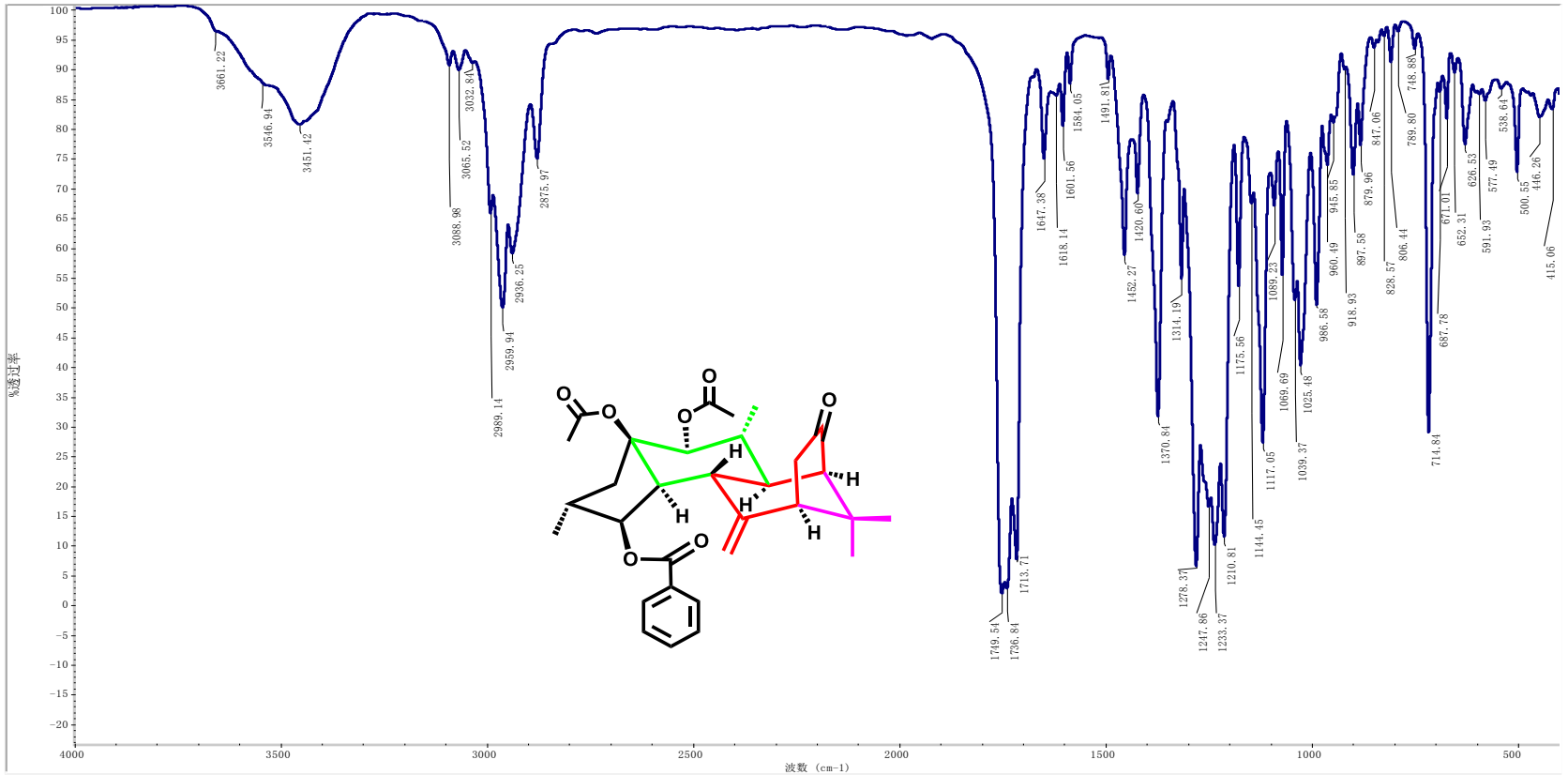


Figure S32. HRESIMS spectrum of euphopia D (**1**)



Sample Name: SEH-3
KBr压片
采集时间: 星期五 10月 09 15:51:28 2020 (GMT+08:00)
仪器型号: NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.4747
光阑: 80.00

Figure S33. IR spectrum of euphopia D (**1**)

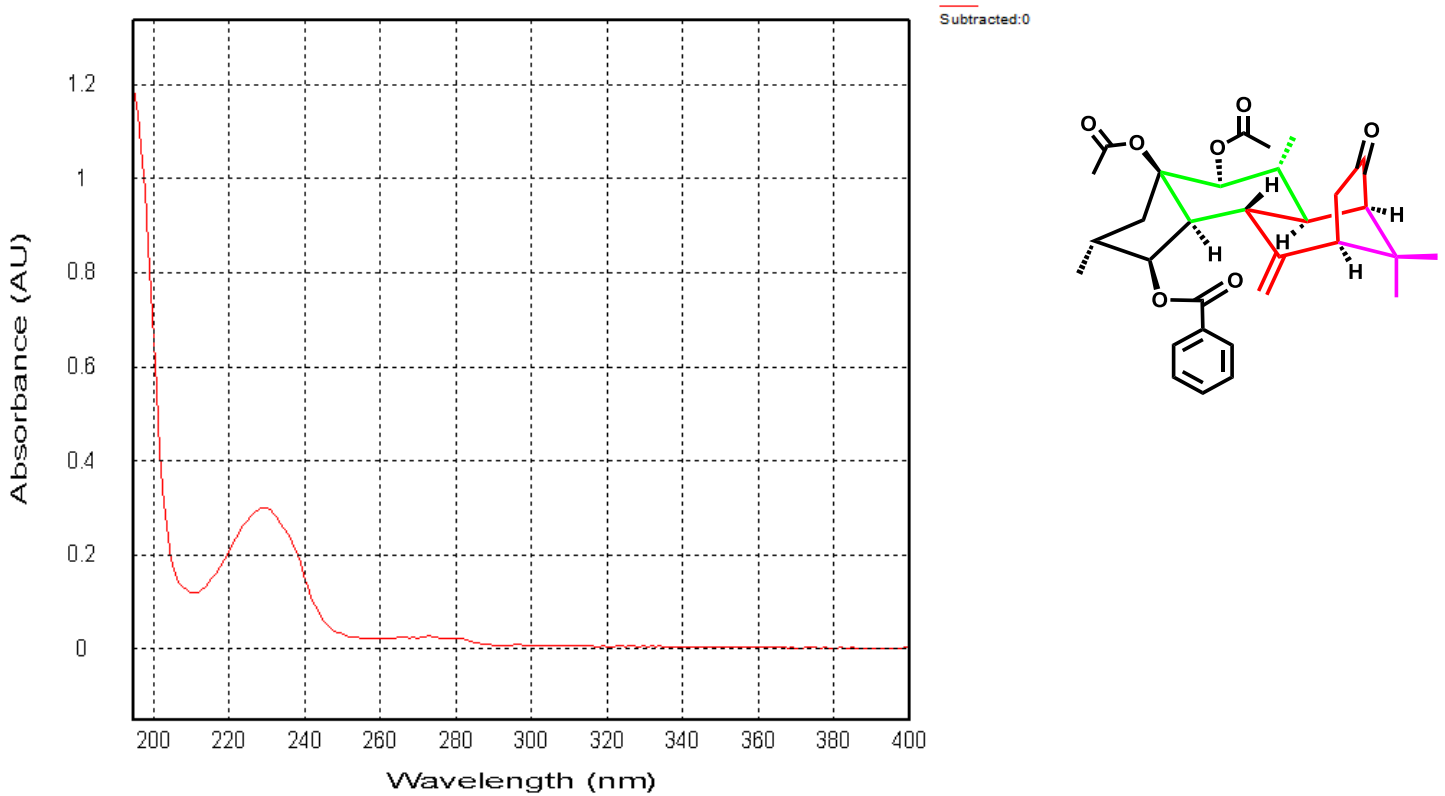


Figure S34. UV spectrum of euphopia D (**1**)

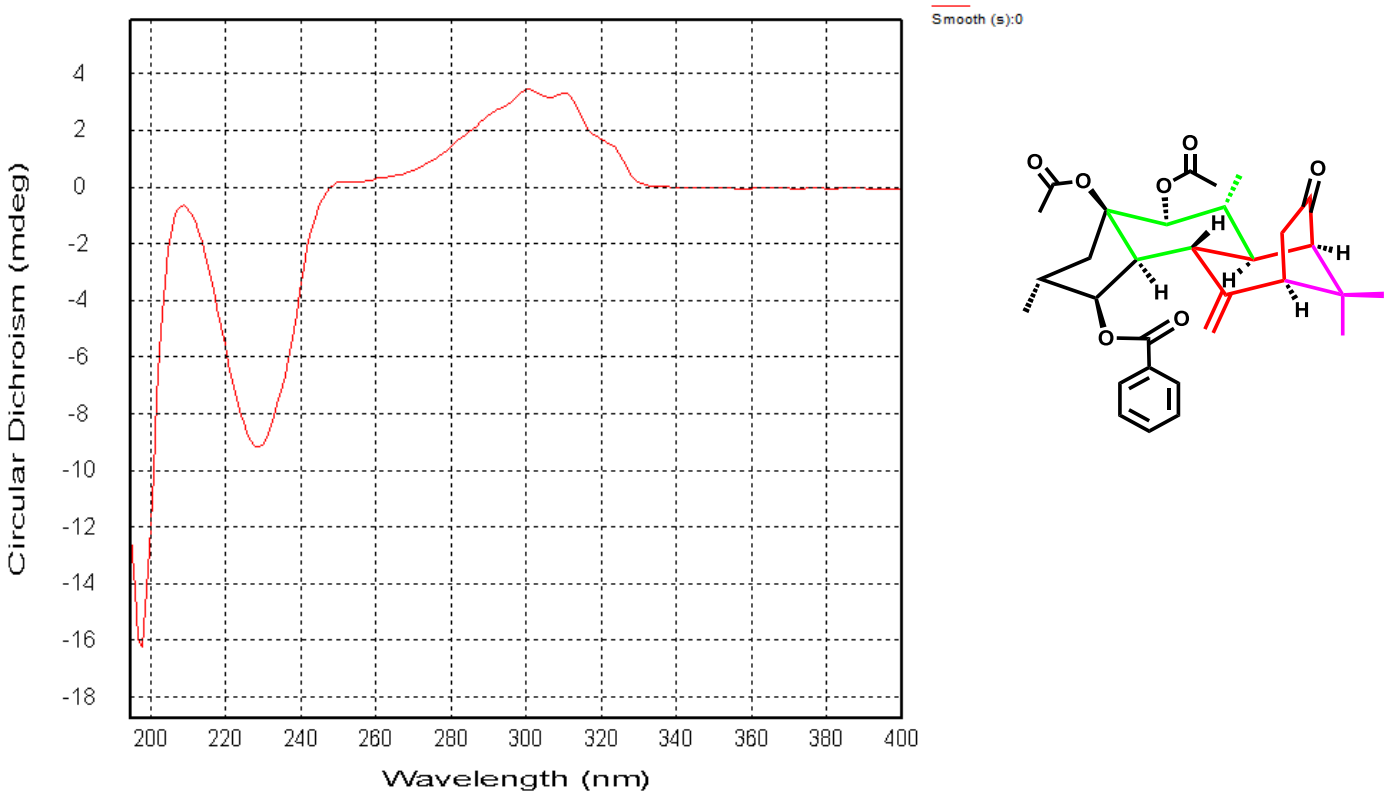


Figure S35. CD spectrum of euphopia D (**1**)

Rudolph Research Analytical

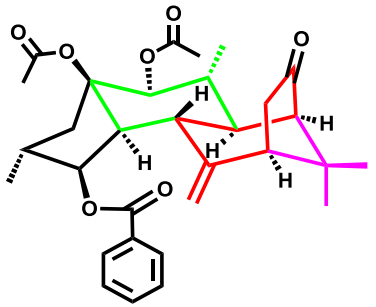
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 14-OCT-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-12.36	1.04	-8.41	-11.20	-13.30

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	SEH-3	07:37:25 PM	-13.30	SR	-0.0133	589	100.00	0.100	24.0
2	SEH-3	07:37:34 PM	-12.70	SR	-0.0127	589	100.00	0.100	24.0
3	SEH-3	07:37:42 PM	-13.30	SR	-0.0133	589	100.00	0.100	24.0
4	SEH-3	07:37:59 PM	-11.20	SR	-0.0112	589	100.00	0.100	24.0
5	SEH-3	07:38:07 PM	-11.30	SR	-0.0113	589	100.00	0.100	24.0

Figure S36. OR report of euphopia D (**1**)

NMR, HRESIMS, IR, UV, CD spectra and OR report of compound 2

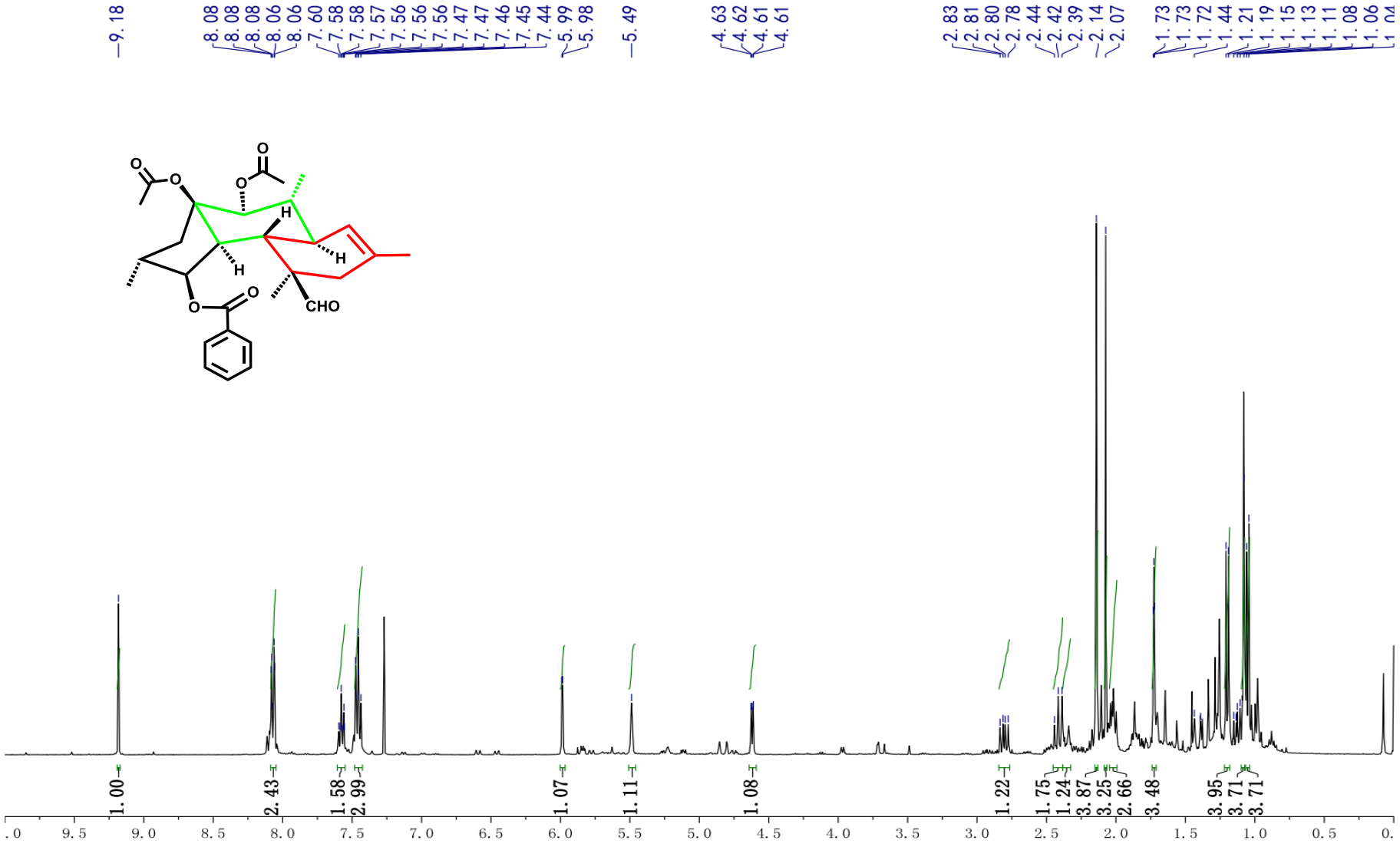


Figure S37. ^{1}H NMR spectrum of euphopia E (**2**) in chloroform-d (400 MHz)

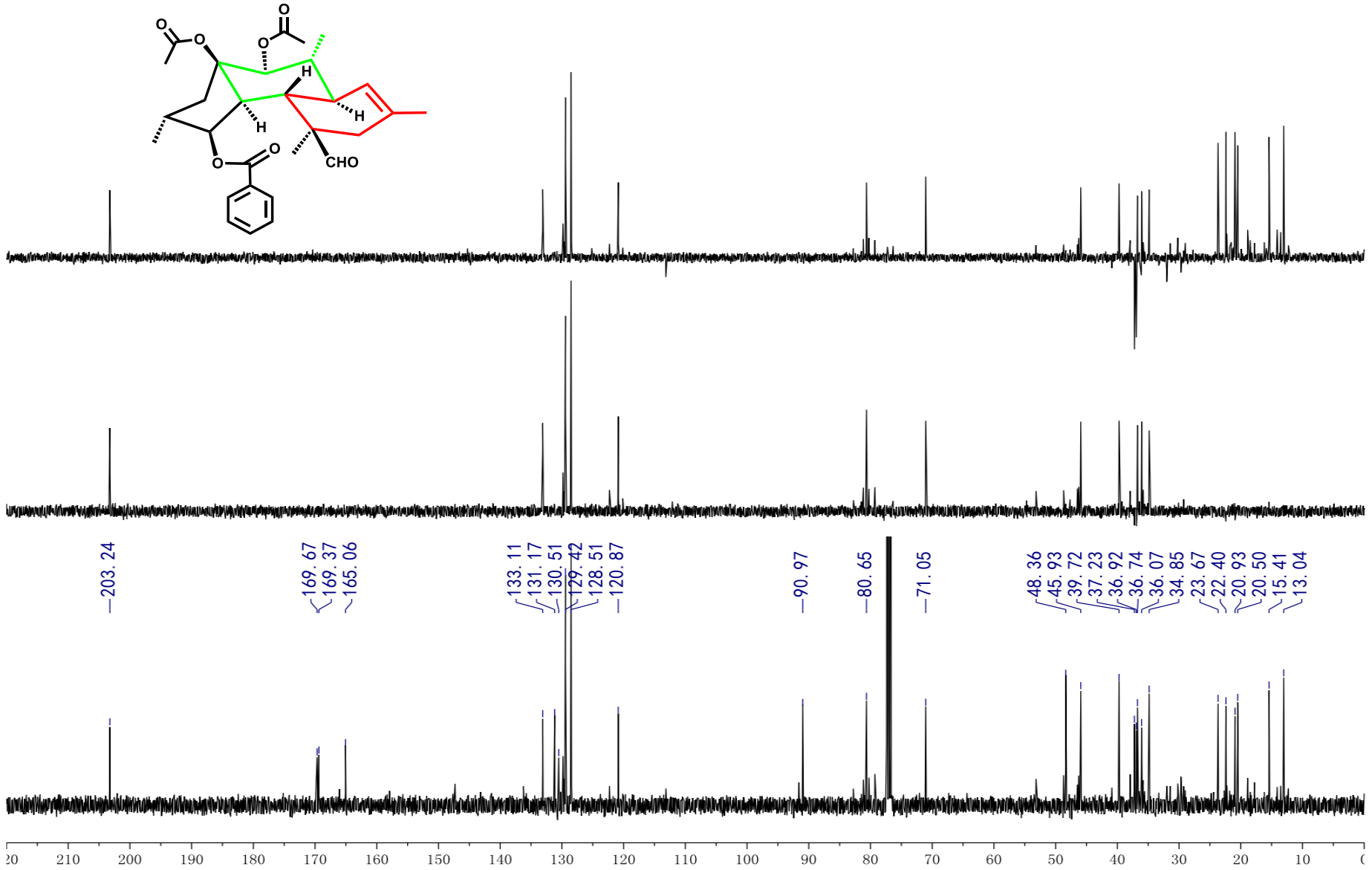


Figure S38. ^{13}C and DEPT NMR spectra of euphopia E (**2**) in chloroform-d (100 MHz)

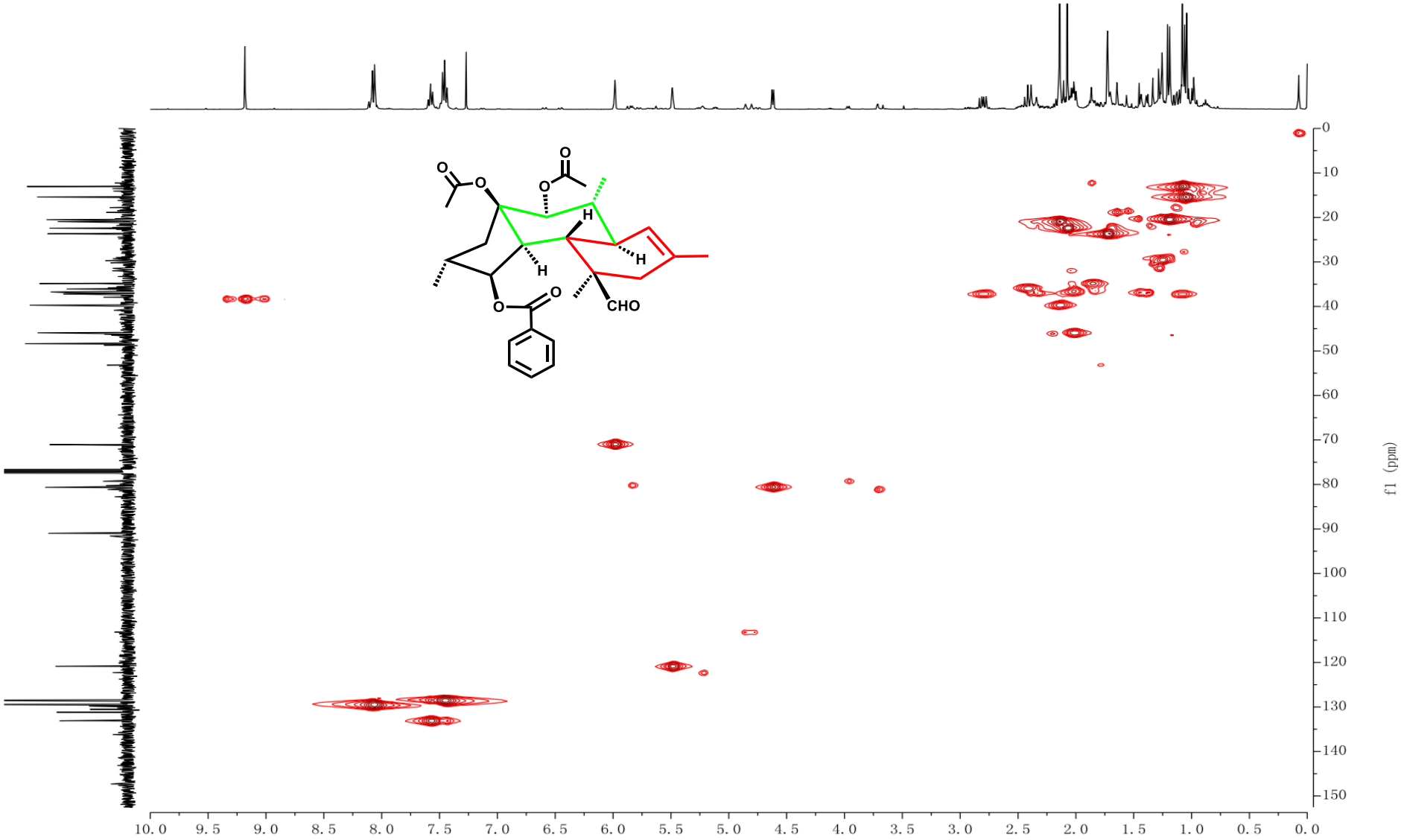


Figure S39. HSQC spectrum of euphopia E (**2**) in chloroform-d

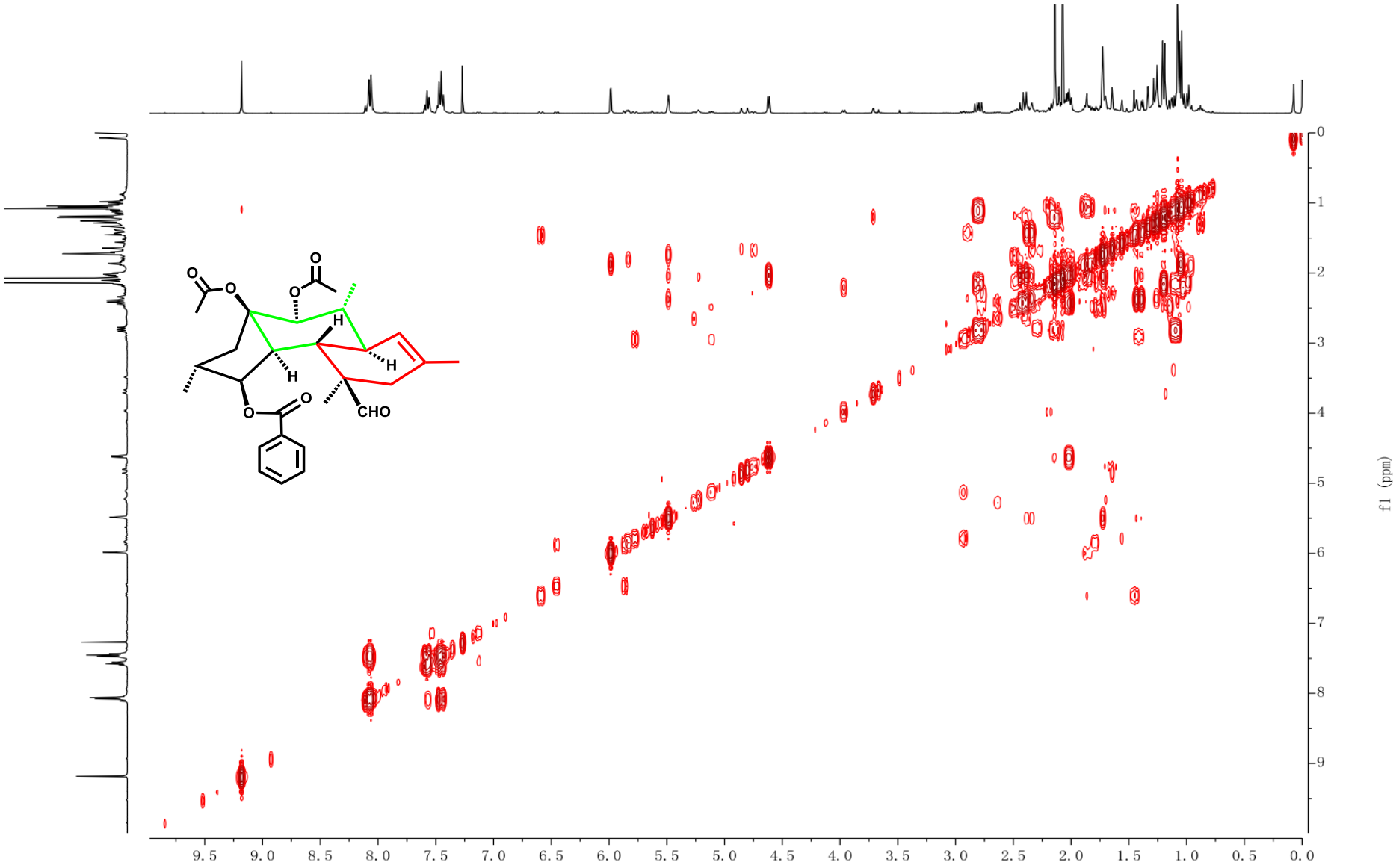


Figure S40. ^{1}H-^{1}H COSY NMR spectrum of euphopia E (**2**) in chloroform-d

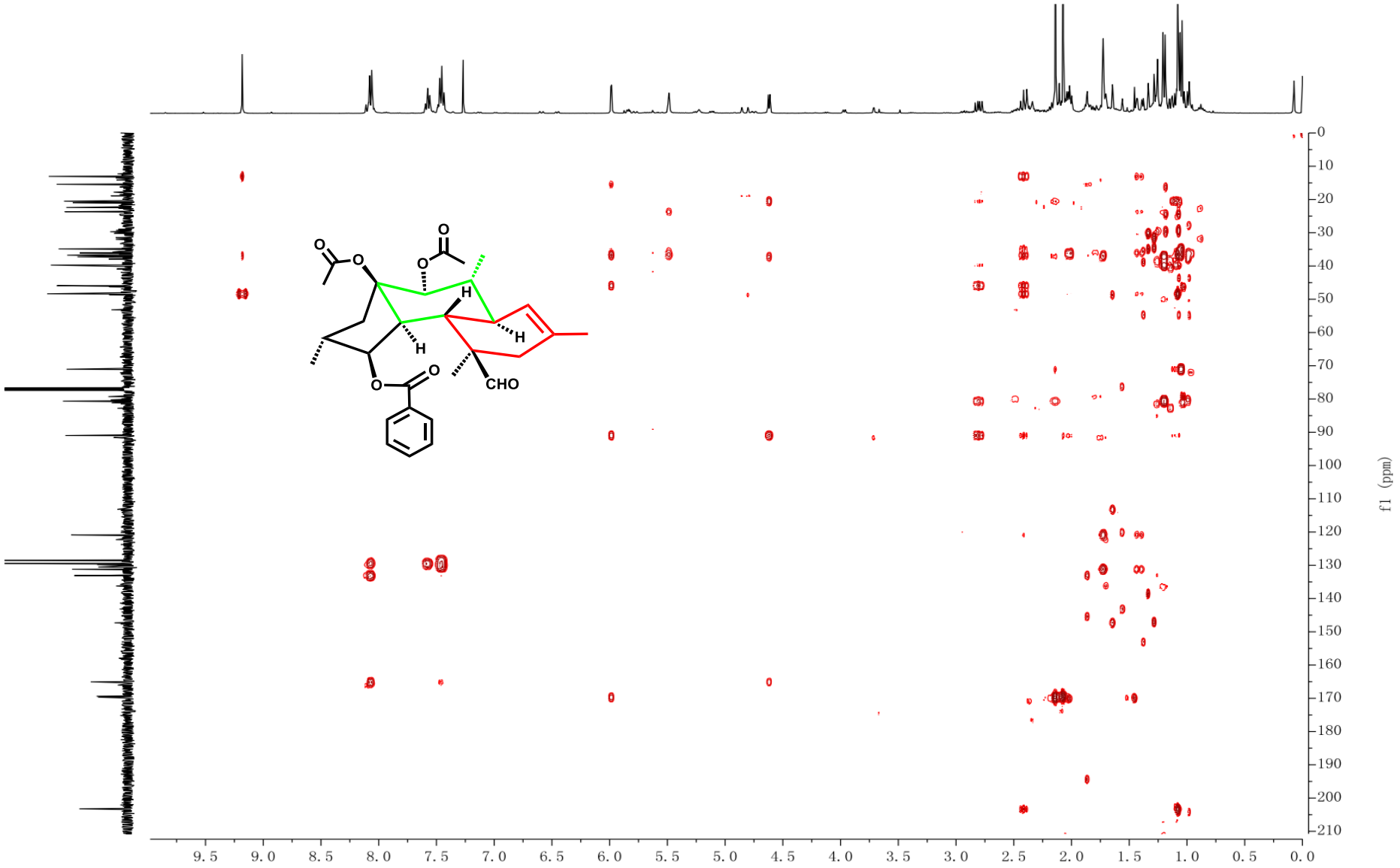


Figure S41. HMBC spectrum of euphopia E (**2**) in chloroform-d

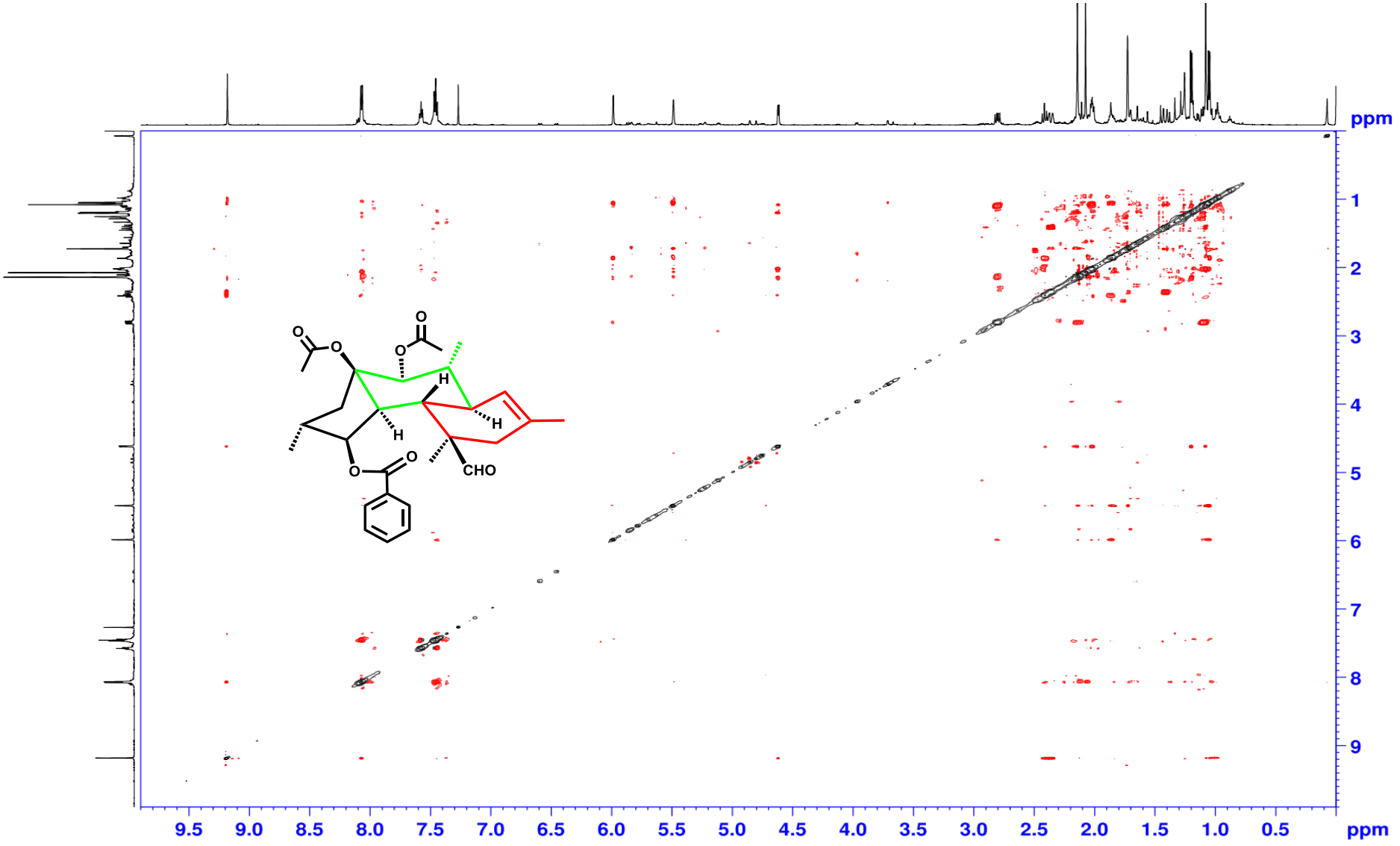


Figure S42. ROESY spectrum of euphopia E (**2**) in chloroform-d

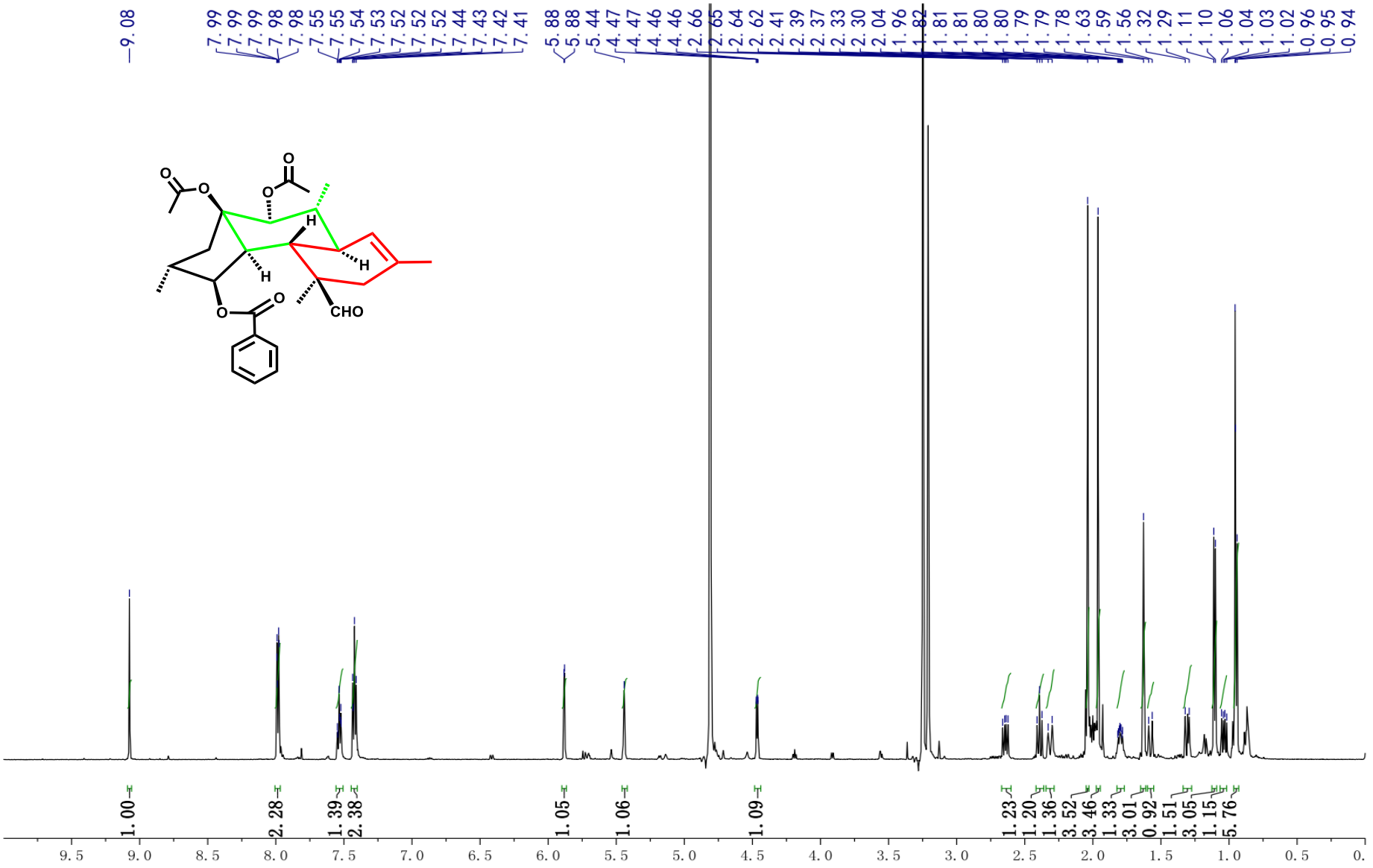


Figure S43. ^{1}H NMR spectrum of euphopia E (**2**) in methanol-d_4 (600 MHz)

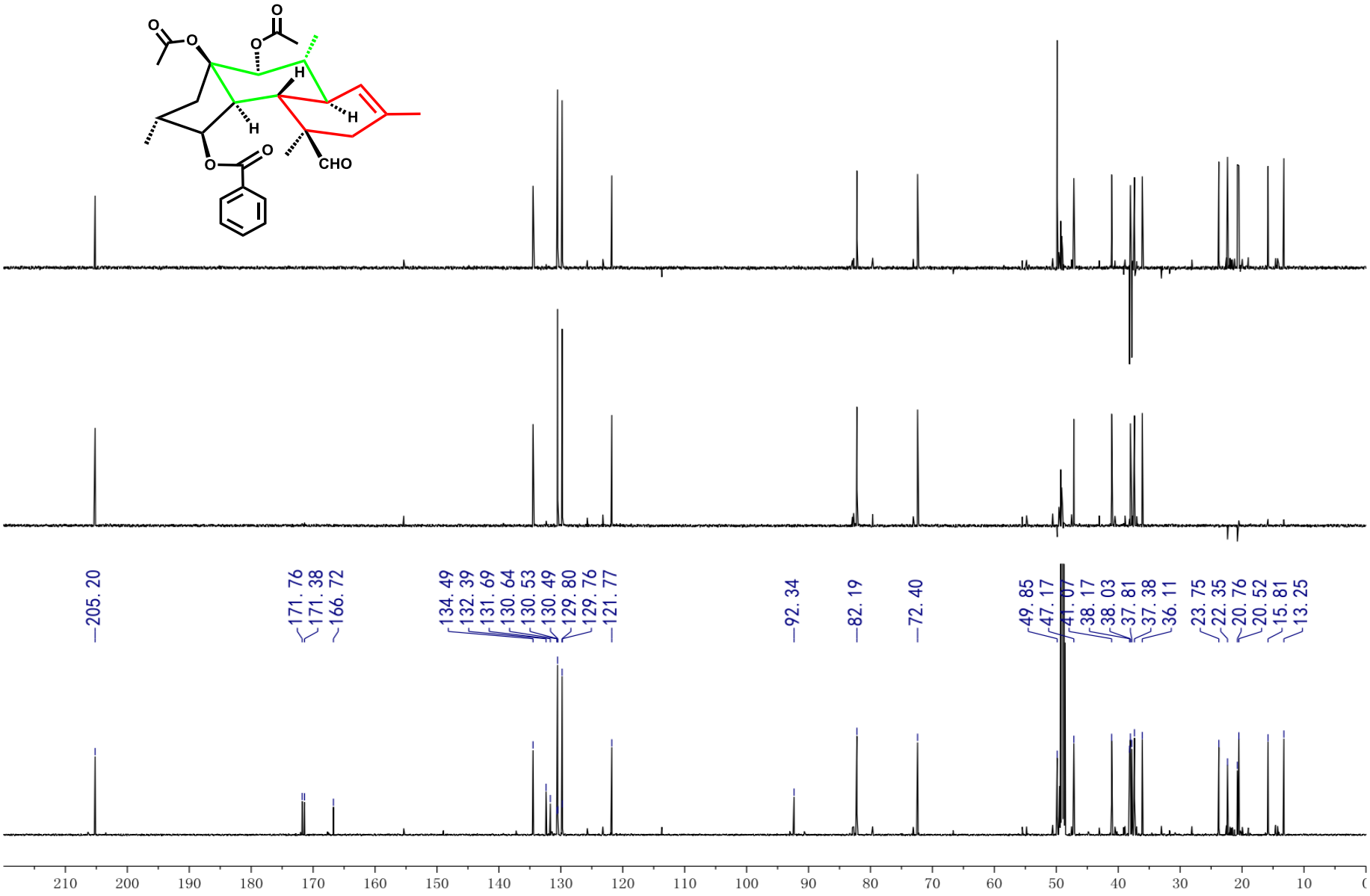


Figure S44. ^{13}C and DEPT NMR spectra of euphopia E (**2**) in methanol-d_4 (150 MHz)

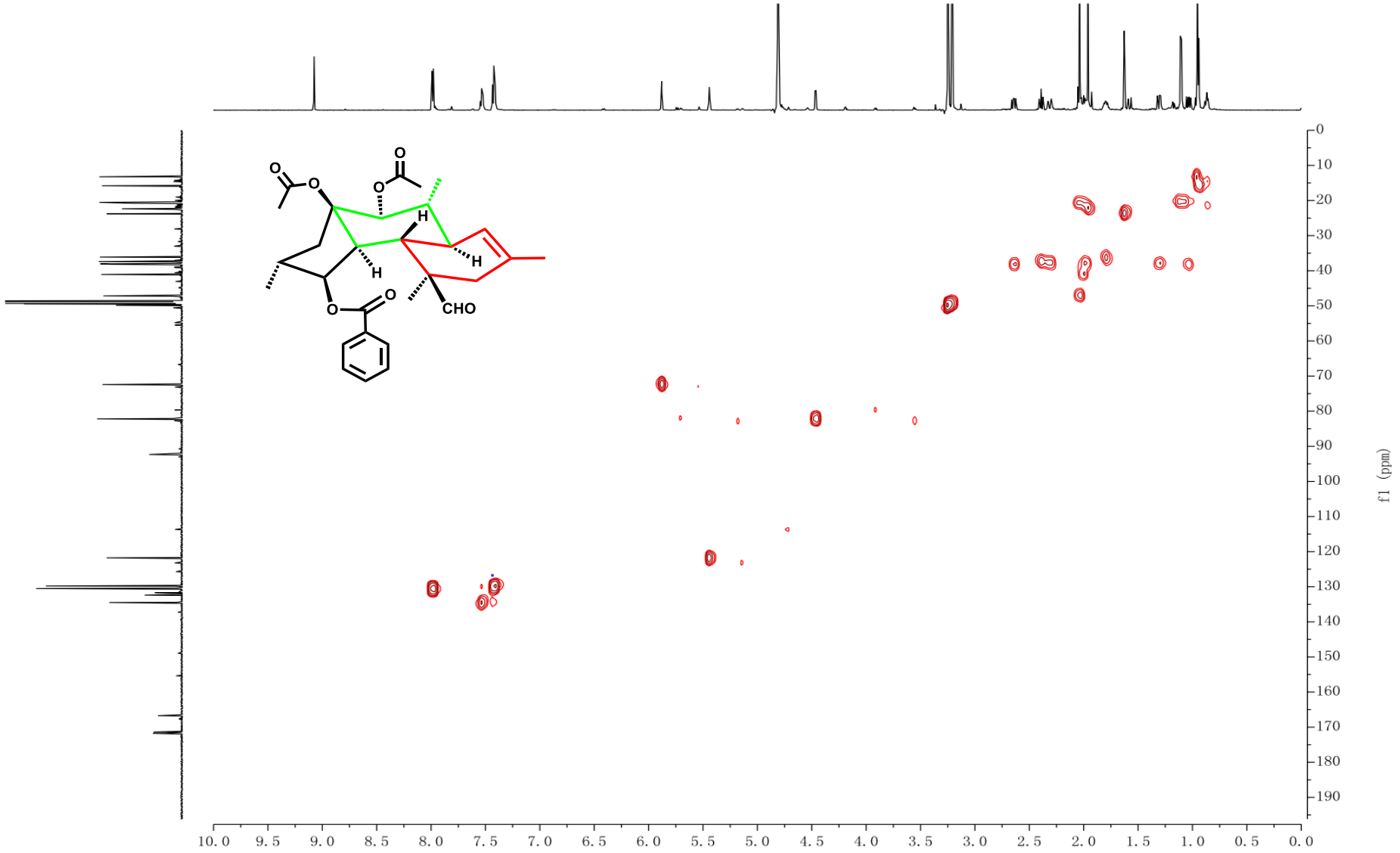


Figure S45. HSQC spectrum of euphopia E (**2**) in methanol-d_4

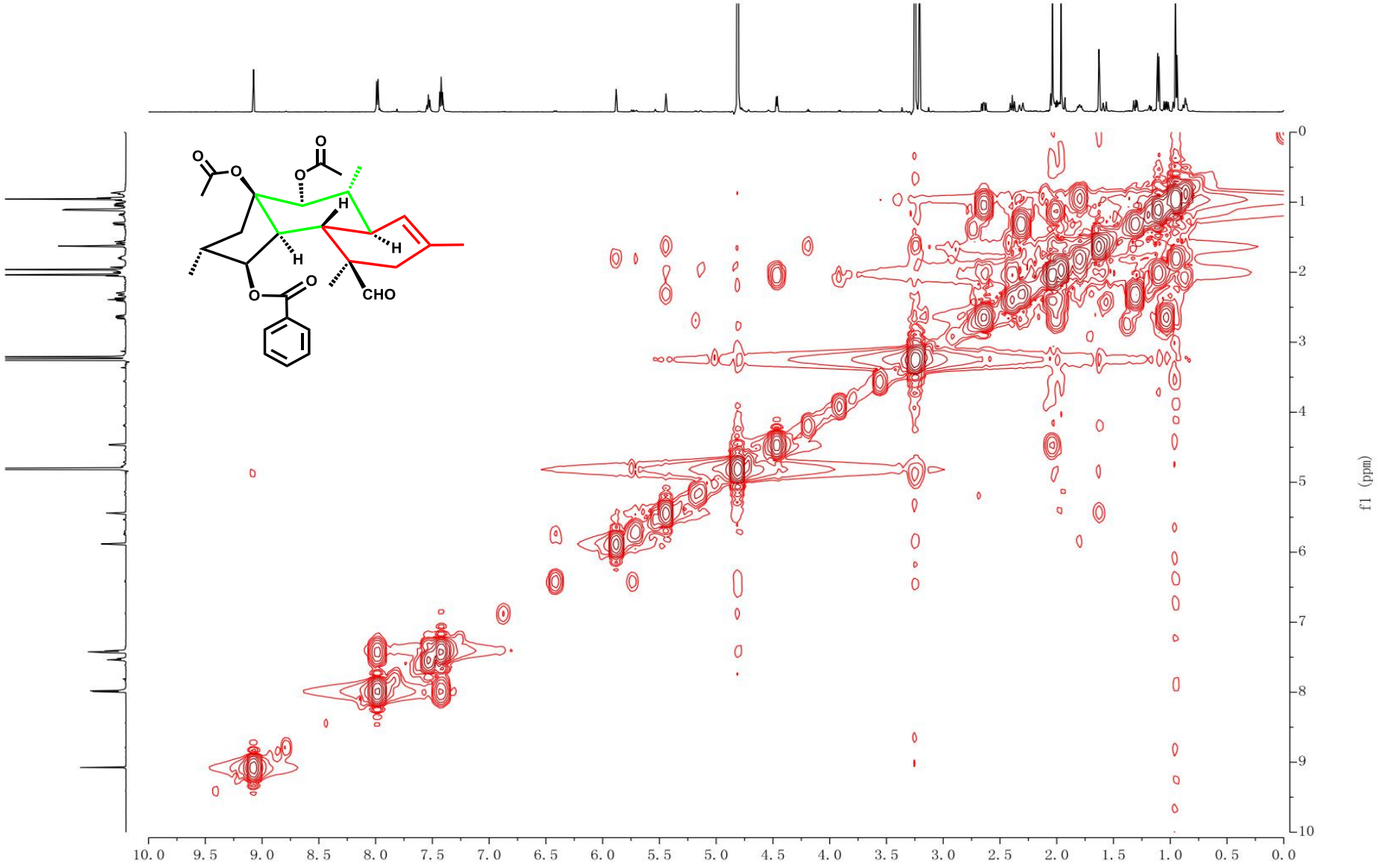


Figure S46. ^{1}H-^{1}H COSY NMR spectrum of euphopia E (**2**) in methanol-d_4

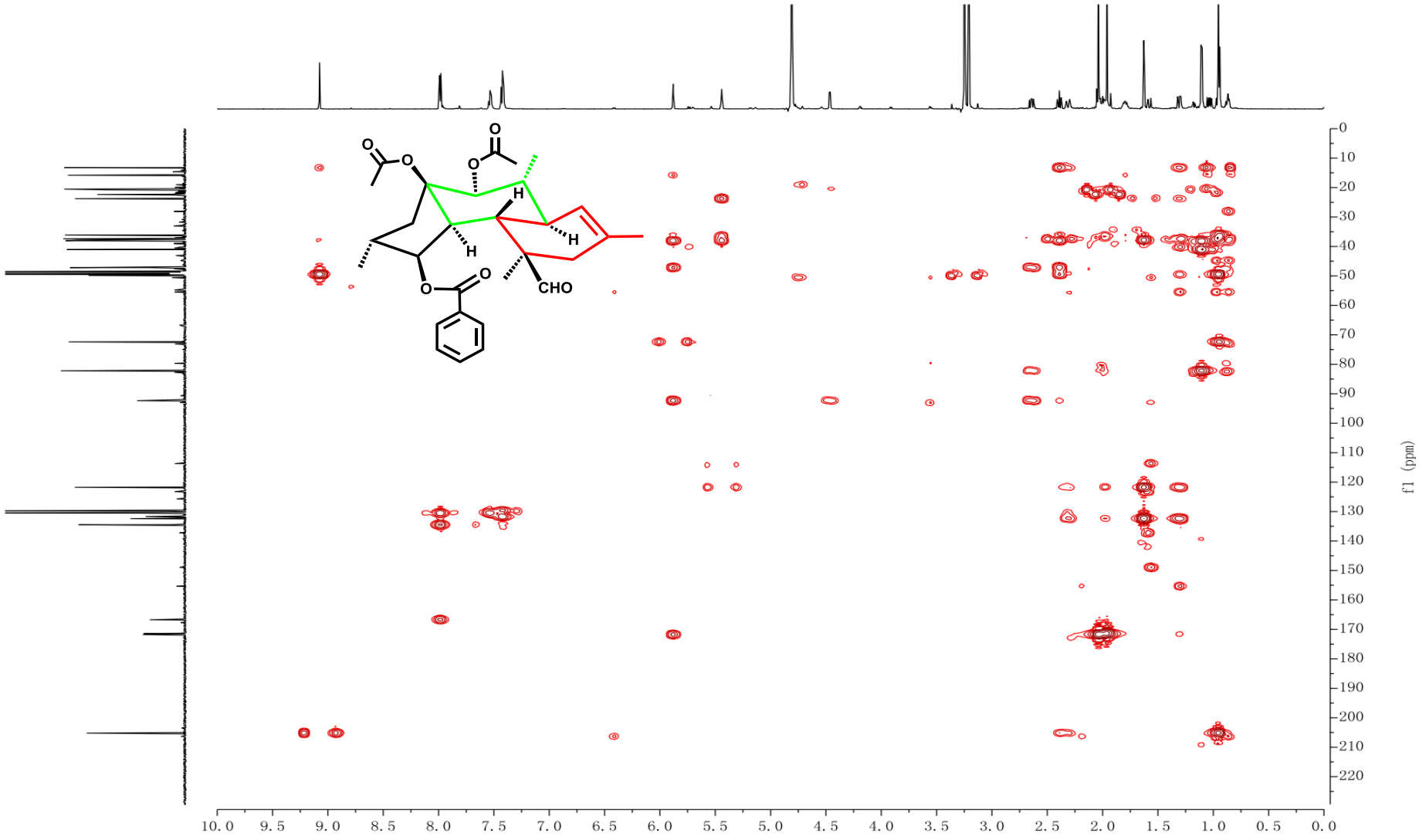


Figure S47. HMBC spectrum of euphopia E (**2**) in methanol-d_4

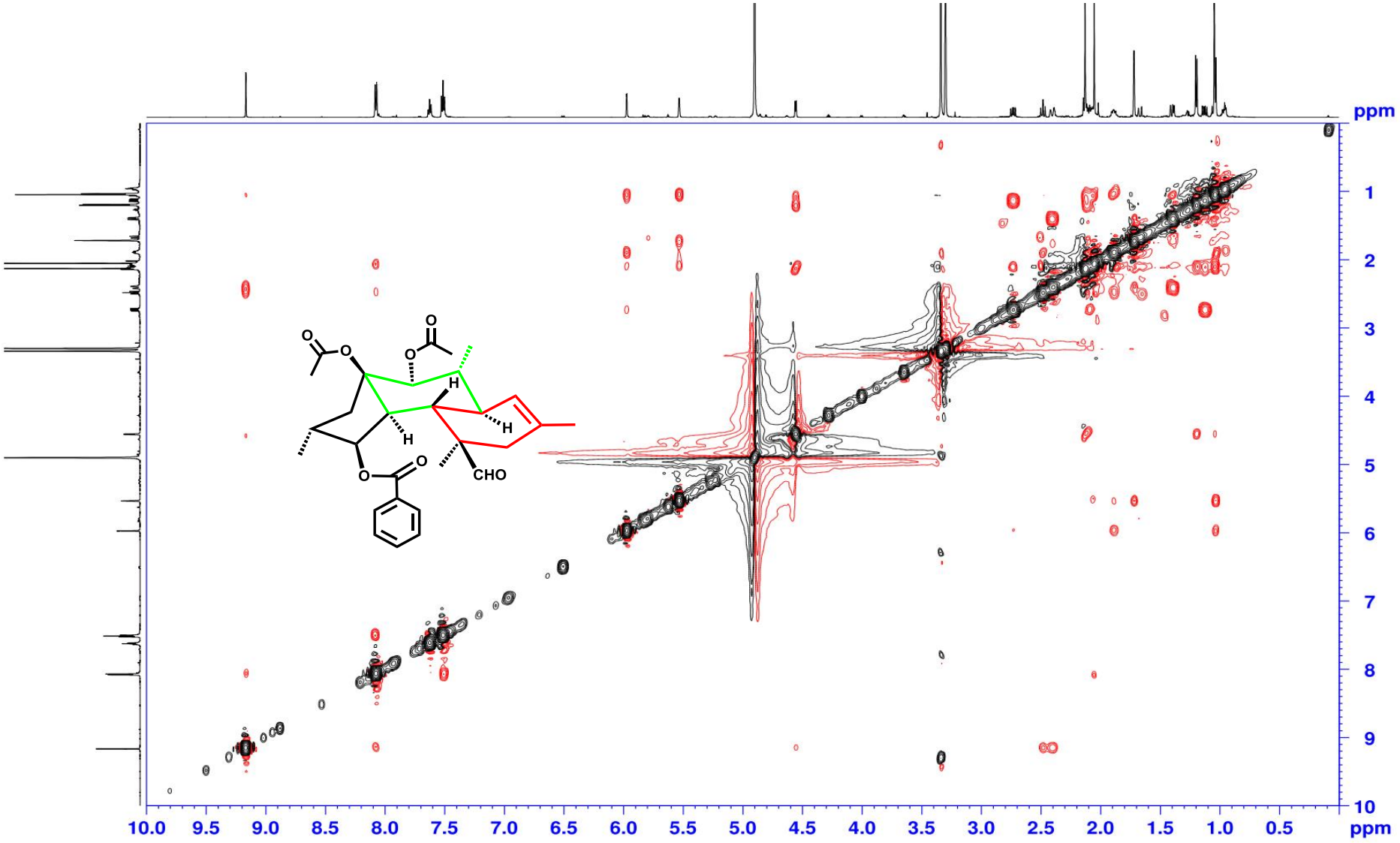


Figure S48. ROESY spectrum of euphopia E (**2**) in methanol-d_4

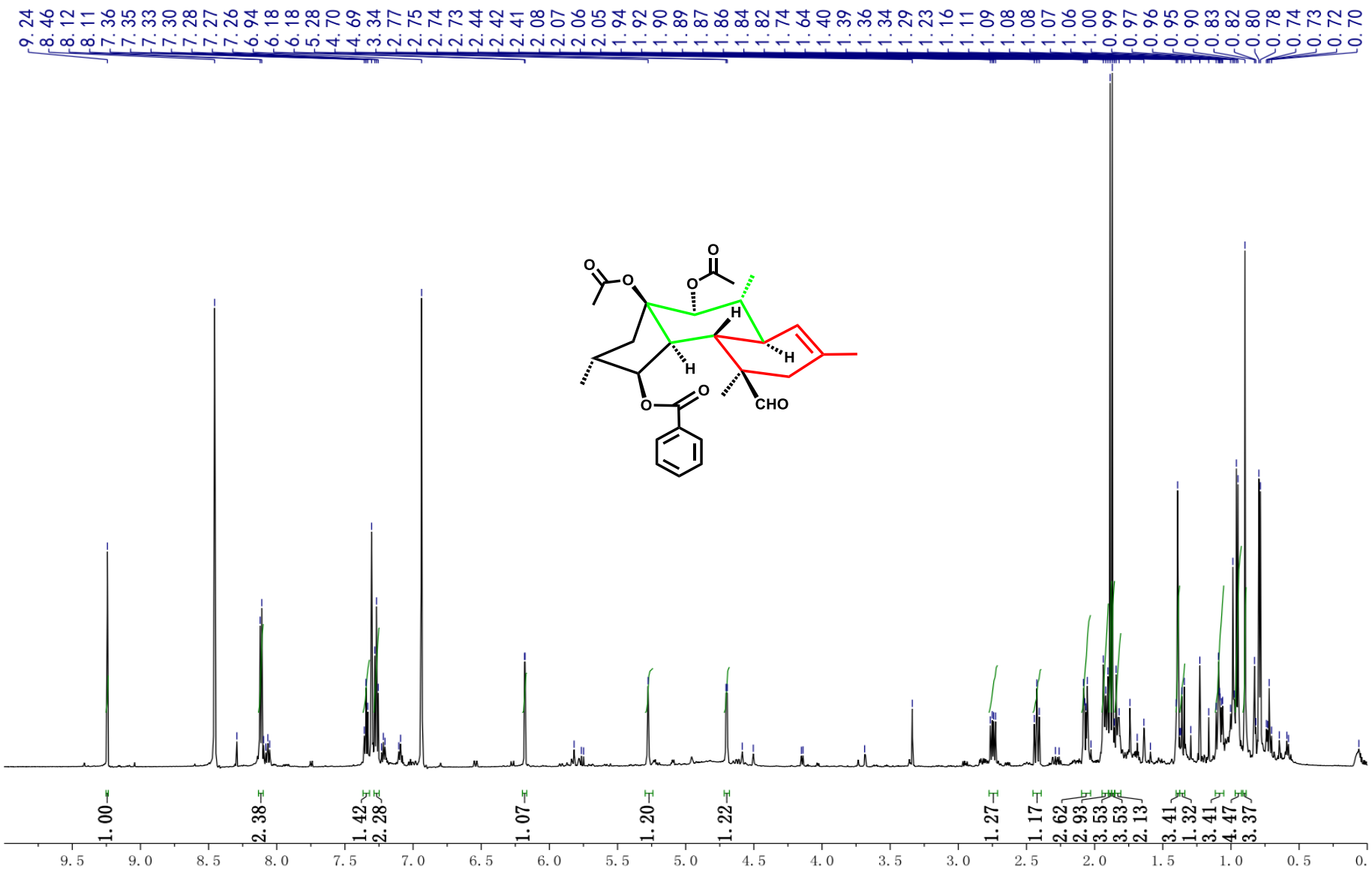


Figure S49. ^{1}H NMR spectrum of euphopia E (**2**) in pyridine-d_5 (600 MHz)

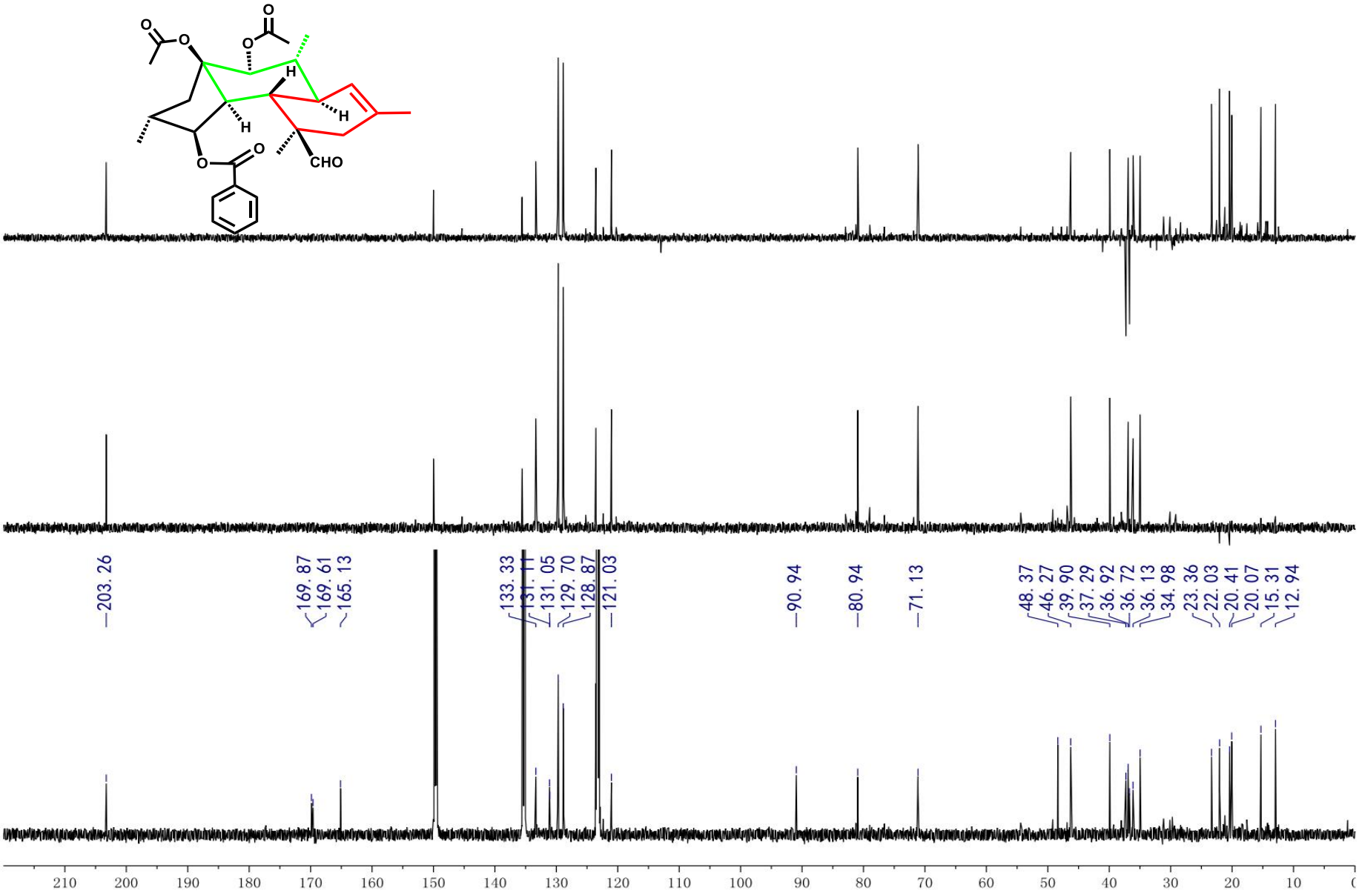


Figure S50. ^{13}C and DEPT NMR spectra of euphopia E (**2**) in pyridine-d_5 (150 MHz)

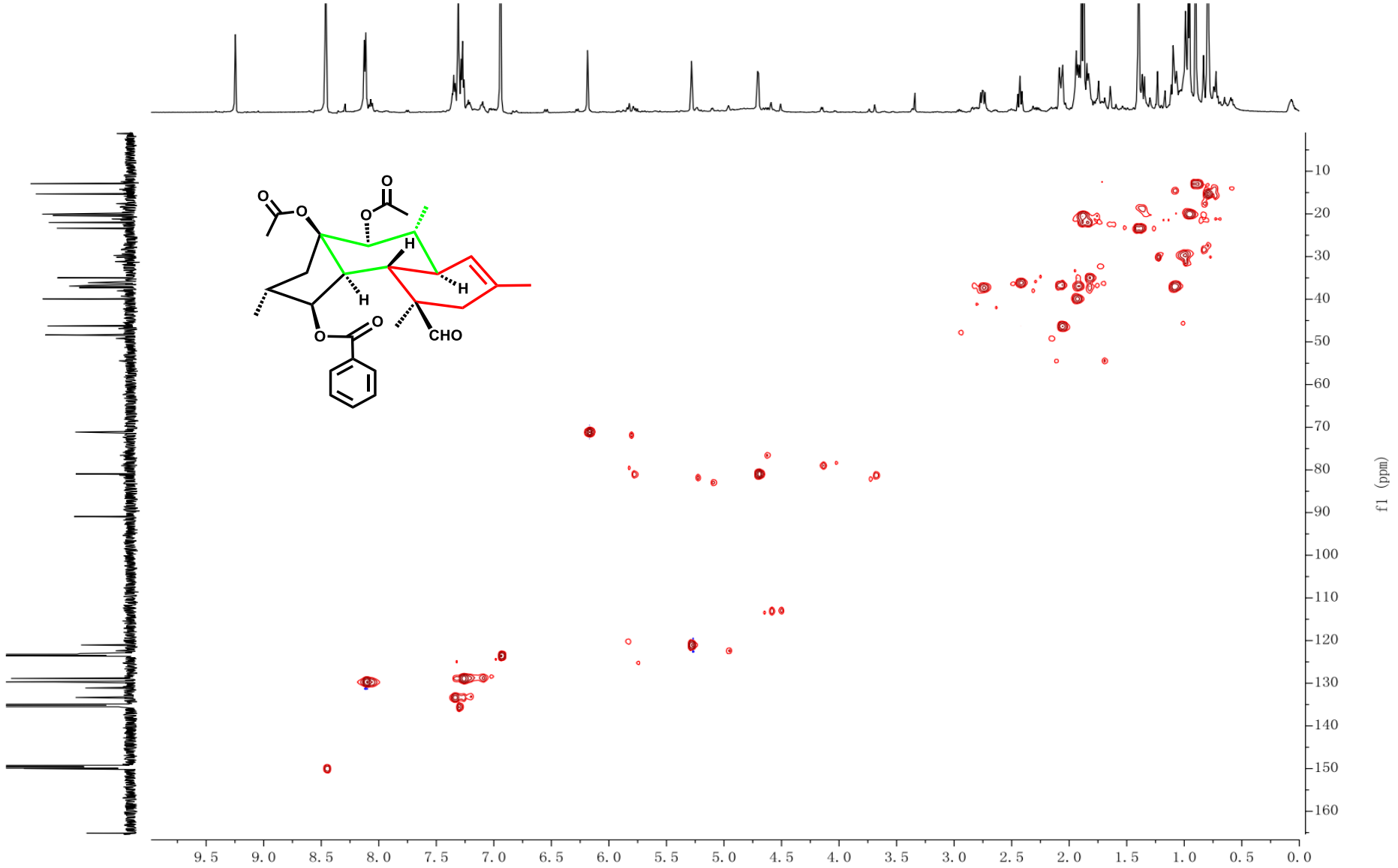


Figure S51. HSQC spectrum of euphopia E (**2**) in pyridine-d_5

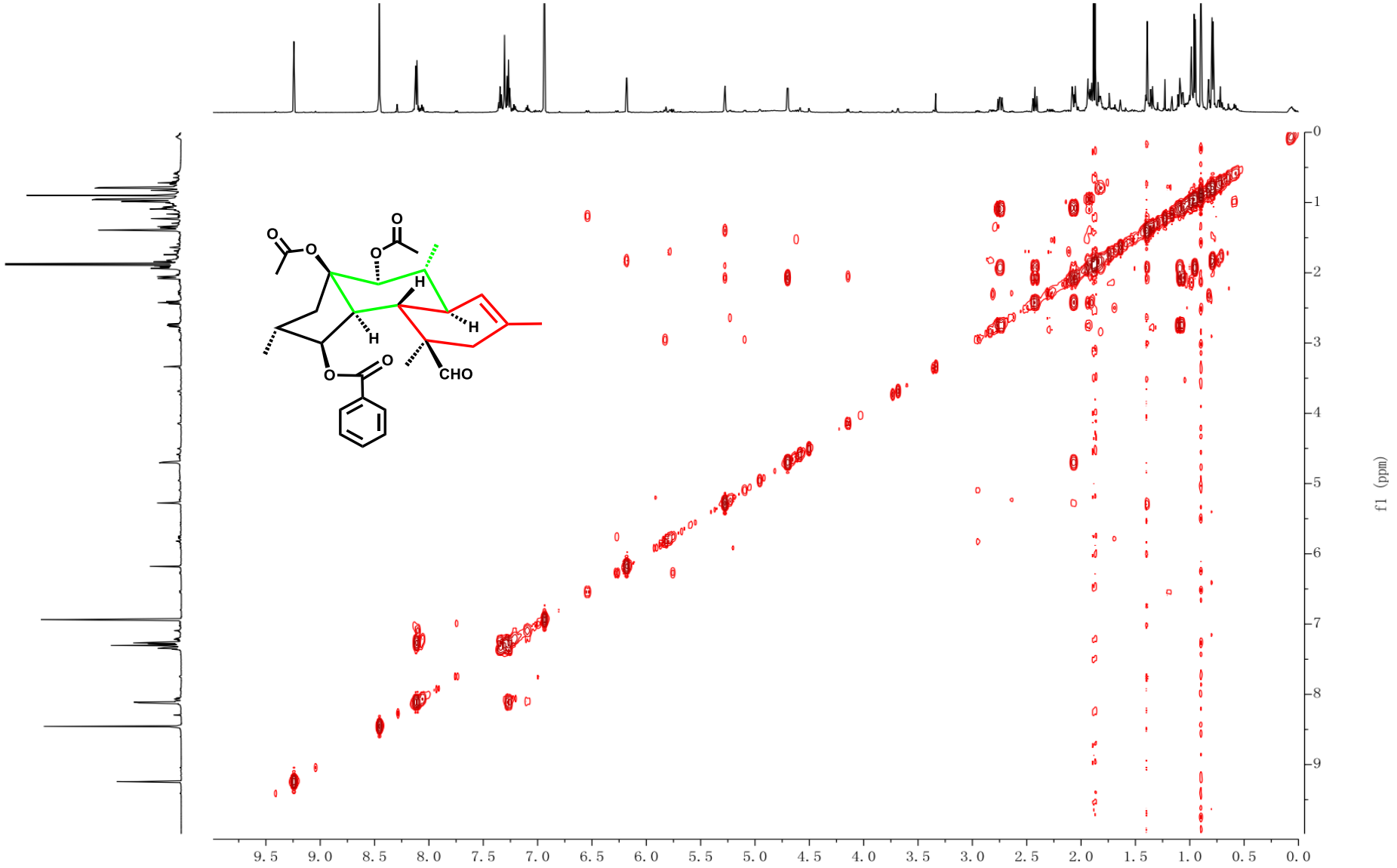


Figure S52. ^{1}H-^{1}H COSY NMR spectrum of euphopia E (**2**) in pyridine-d_5

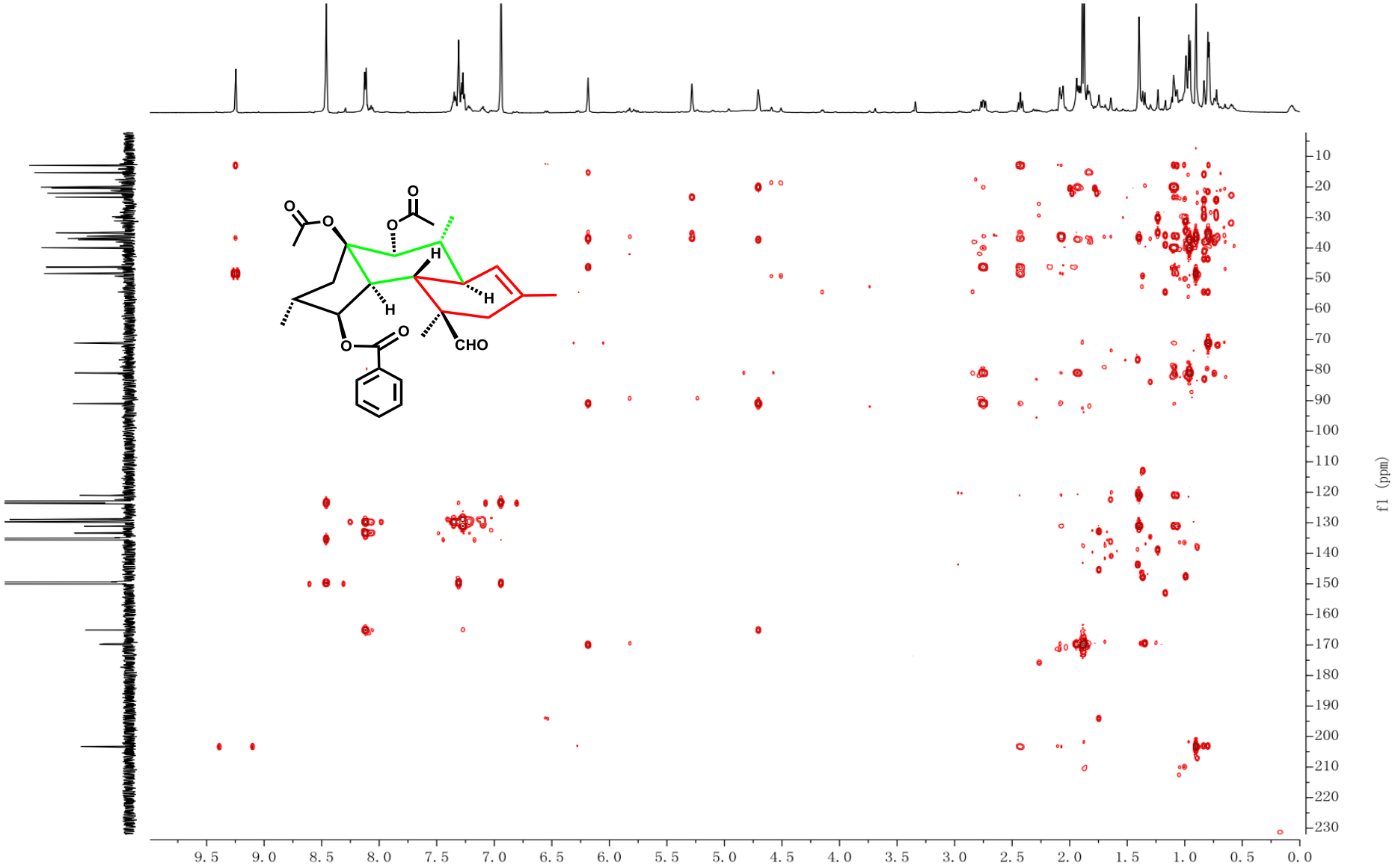


Figure S53. HMBC spectrum of euphopia E (**2**) in pyridine-d_5

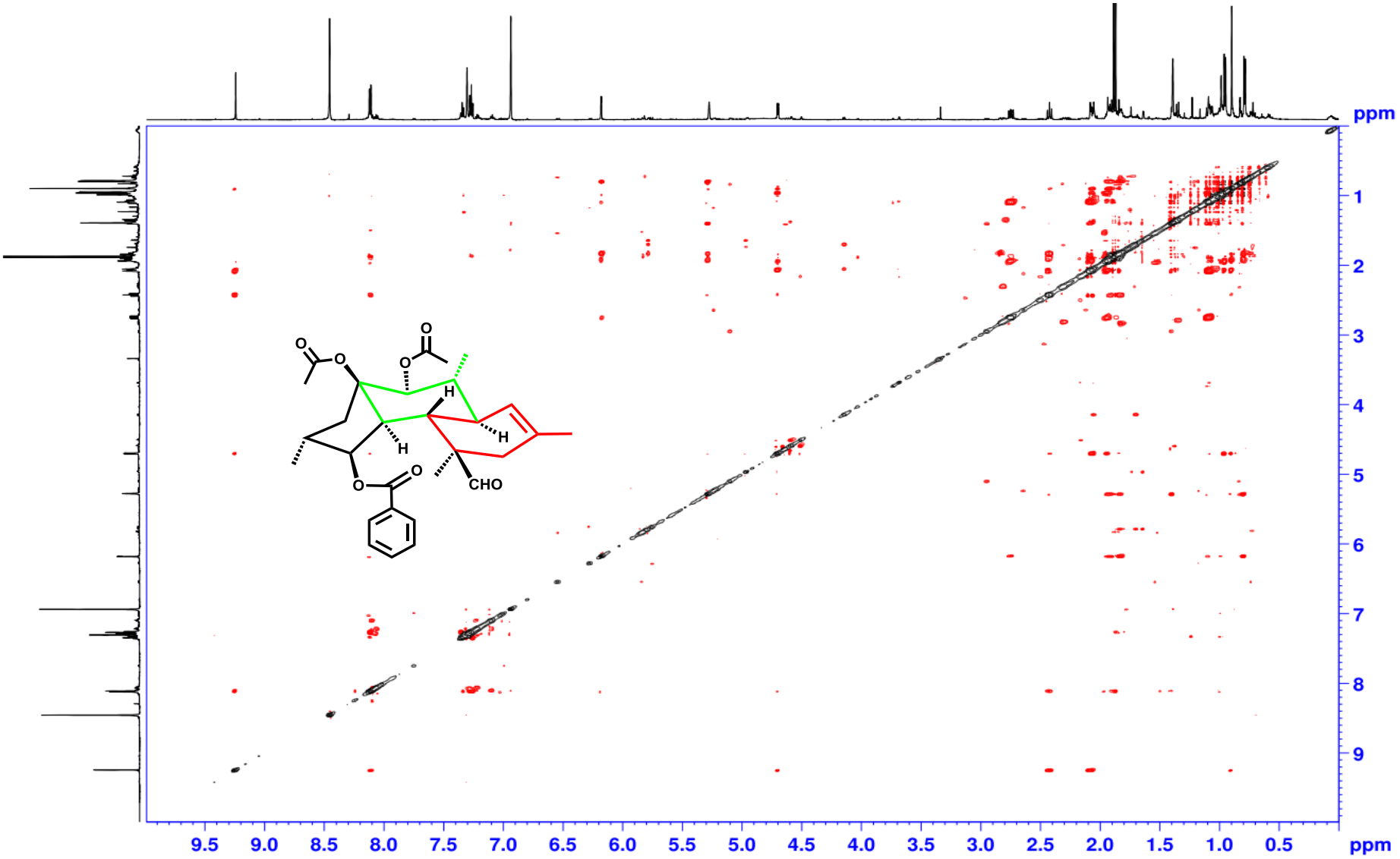
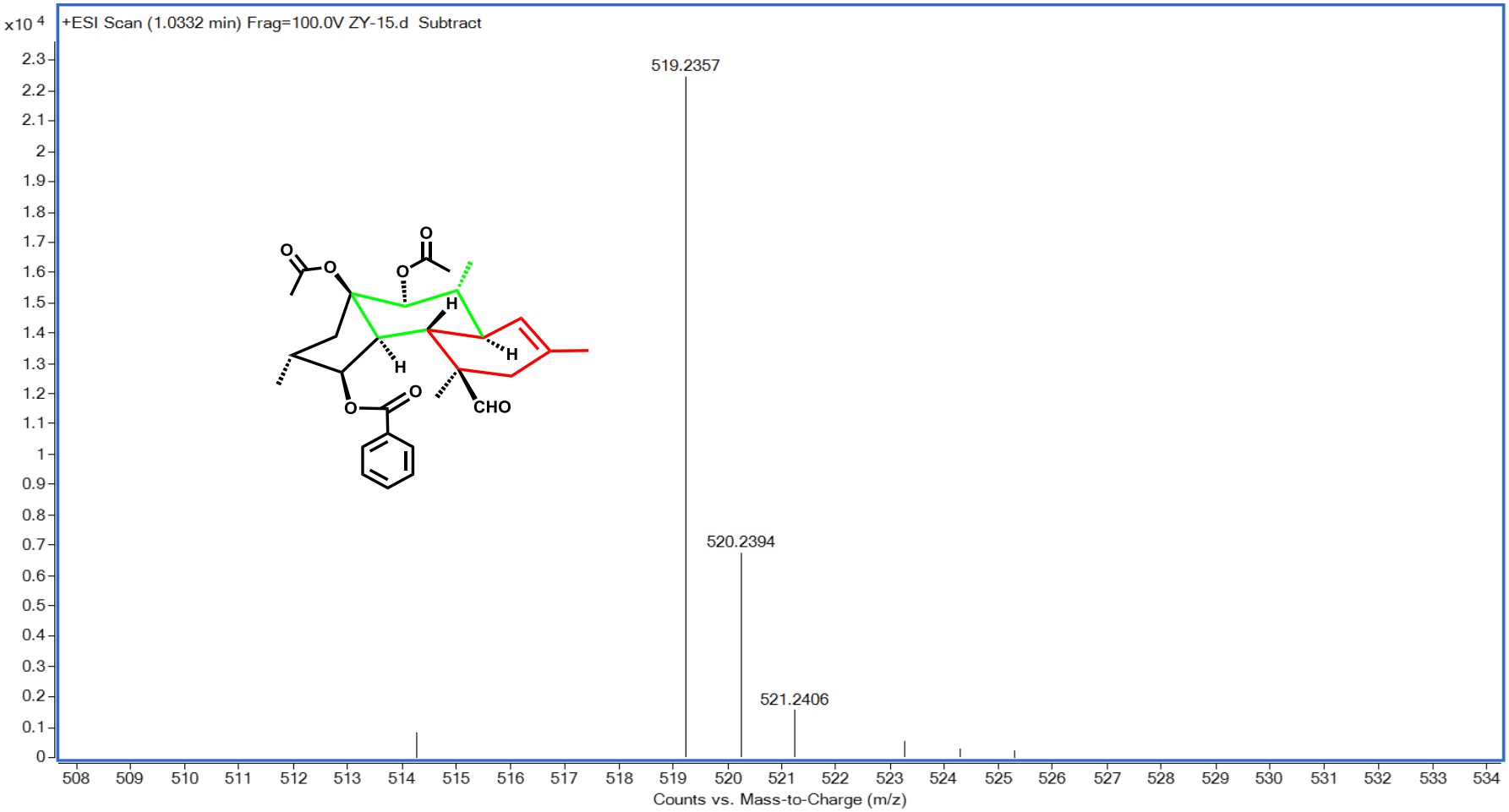


Figure S54. ROESY spectrum of euphopia E (**2**) in pyridine-d_5

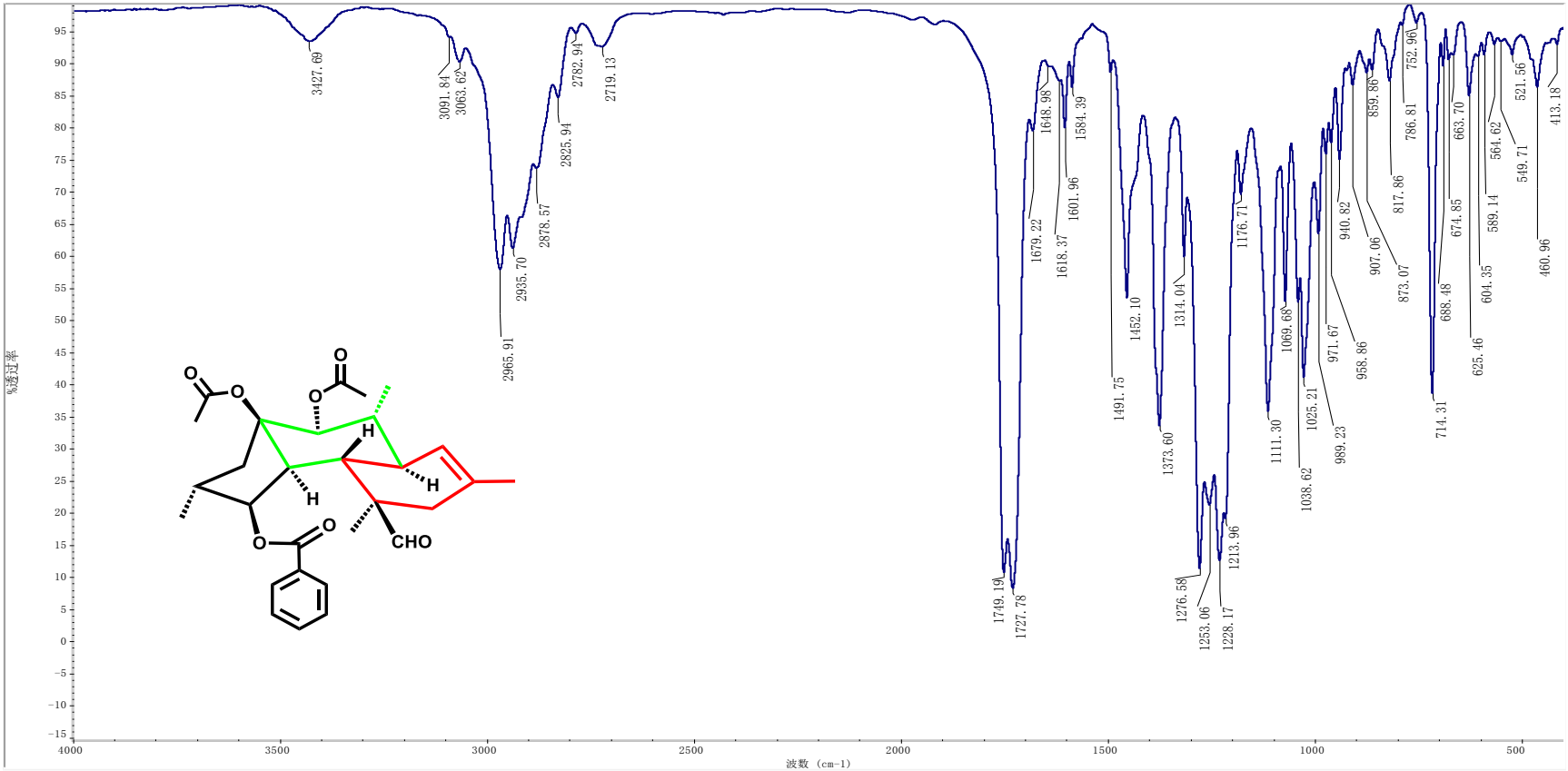


MS Formula Results: + Scan (1.0332 min) Sub (ZY-15.d)

m/z	Ion	Formula	Abundance
519.2357	(M+Na)+	C29 H36 Na O7	22485.9

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C29 H36 O7	C29 H36 Na O7	98.4		519.2353	-0.74	99.44	96.59	98.46

Figure S55. HRESIMS spectrum of euphopia E (**2**)



Sample Name: ZY-15
KBr压片
采集时间: 星期二 2月 02 13:51:53 2021 (GMT+08:00)
仪器型号：NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.4747
光阑: 80.00

Figure S56. IR spectrum of euphopia E (**2**)

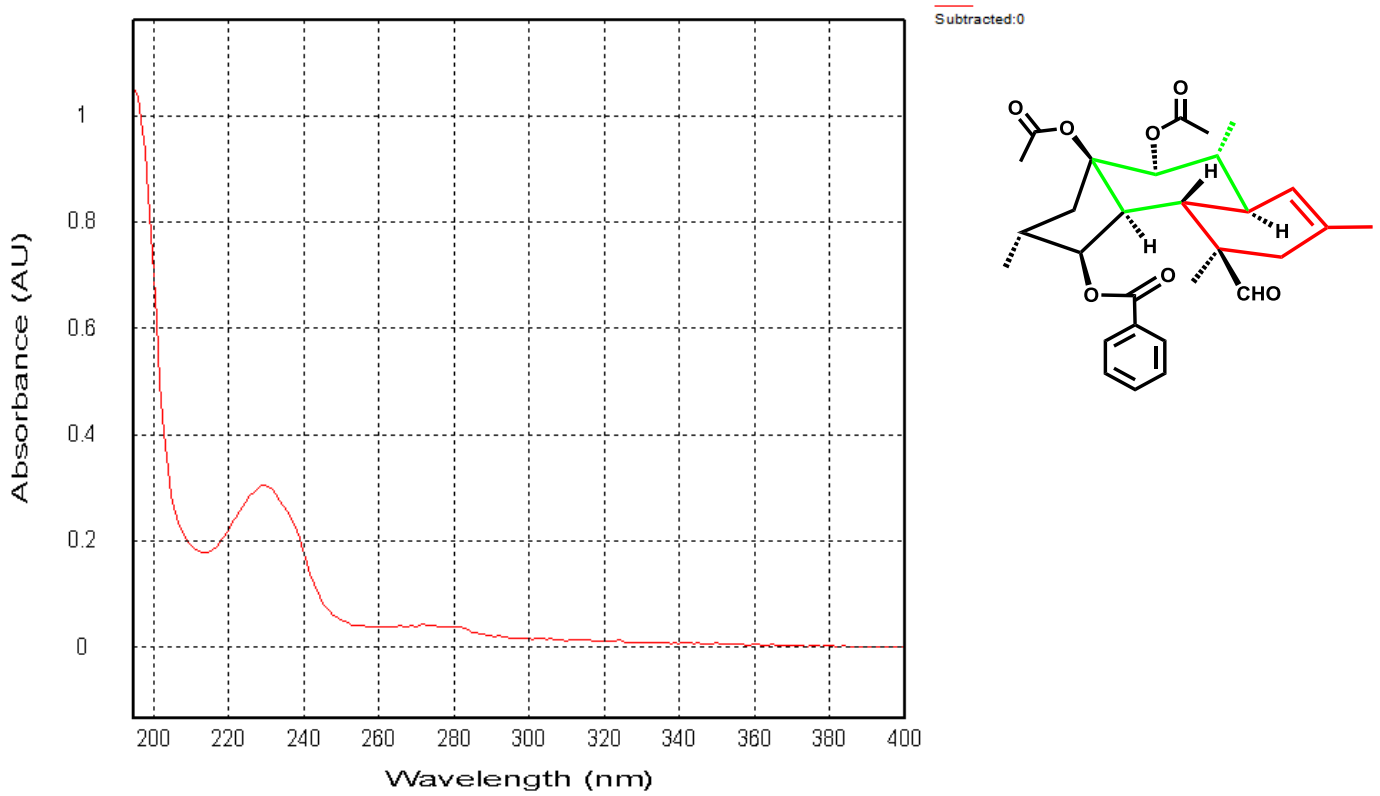


Figure S57. UV spectrum of euphopia E (**2**)

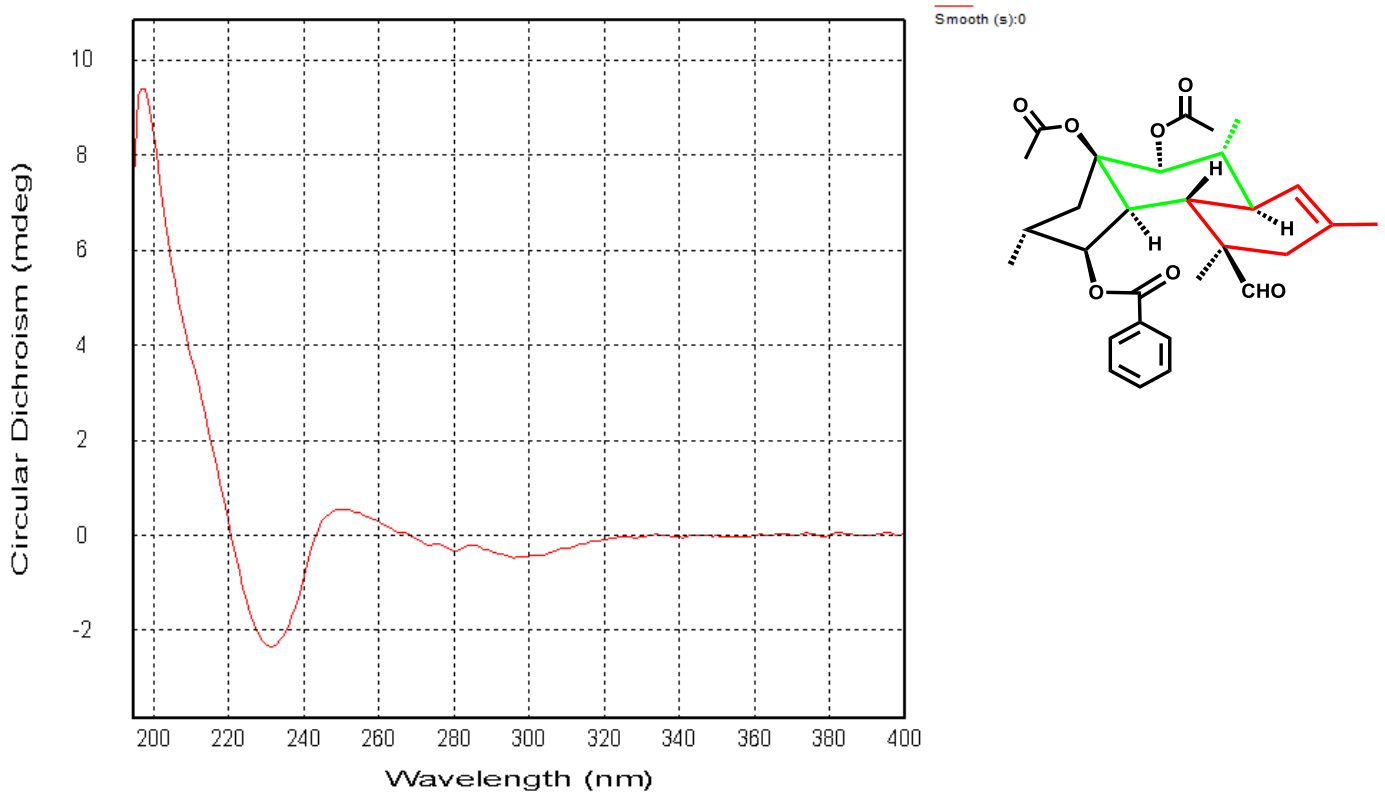
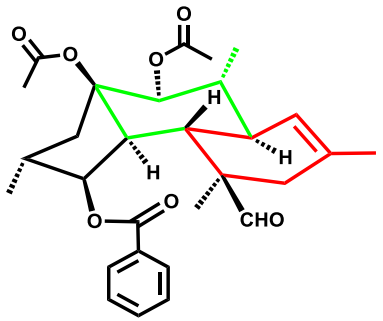


Figure S58. CD spectrum of euphopia E (**2**)

Rudolph Research Analytical



This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 02-FEB-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-13.56	0.44	-3.24	-13.10	-14.10

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	ZY-15	08:40:19 PM	-14.10	SR	-0.0141	589	100.00	0.100	20.7
2	ZY-15	08:40:28 PM	-13.80	SR	-0.0138	589	100.00	0.100	20.7
3	ZY-15	08:40:36 PM	-13.70	SR	-0.0137	589	100.00	0.100	20.7
4	ZY-15	08:40:48 PM	-13.10	SR	-0.0131	589	100.00	0.100	20.7
5	ZY-15	08:40:56 PM	-13.10	SR	-0.0131	589	100.00	0.100	20.7

Figure S59. OR report of euphopia E (**2**)

NMR, HRESIMS, IR, UV, CD spectra and OR report of compound 3

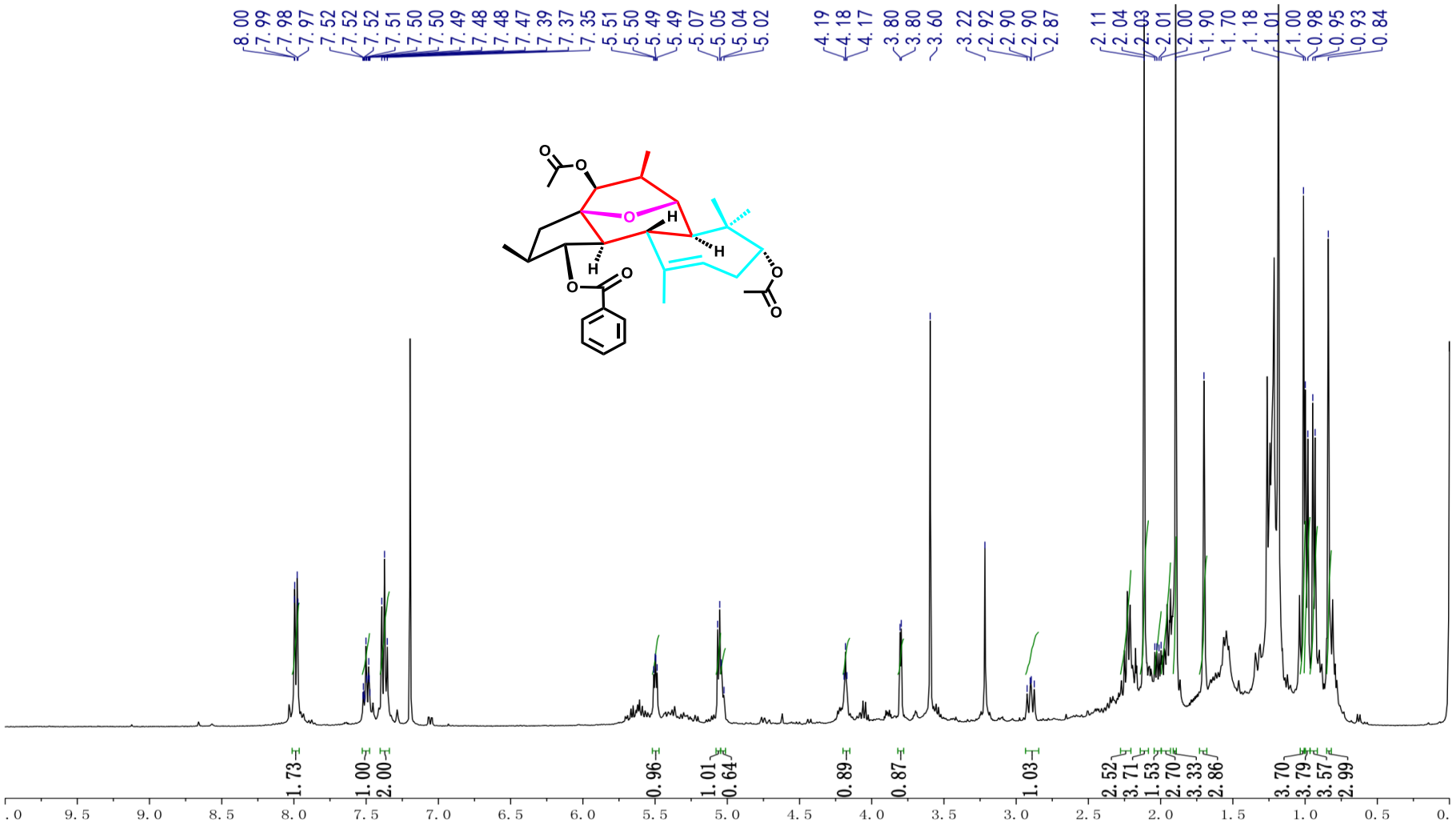


Figure S60. ^{1}H NMR spectrum of euphopia F (**3**) in chloroform-d (400 MHz)

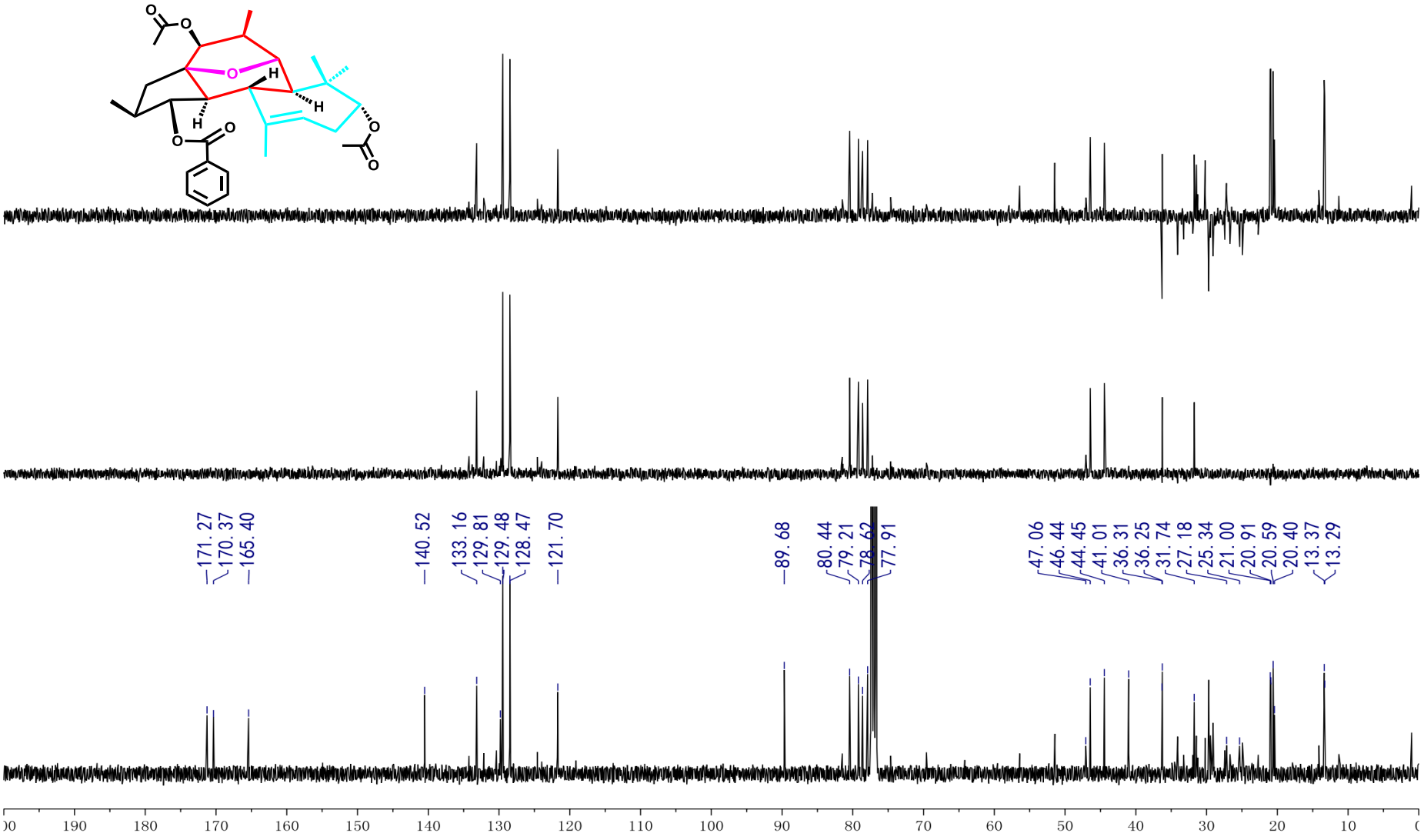


Figure S61. ^{13}C and DEPT NMR spectra of euphopia F (**3**) in chloroform-d (100 MHz)

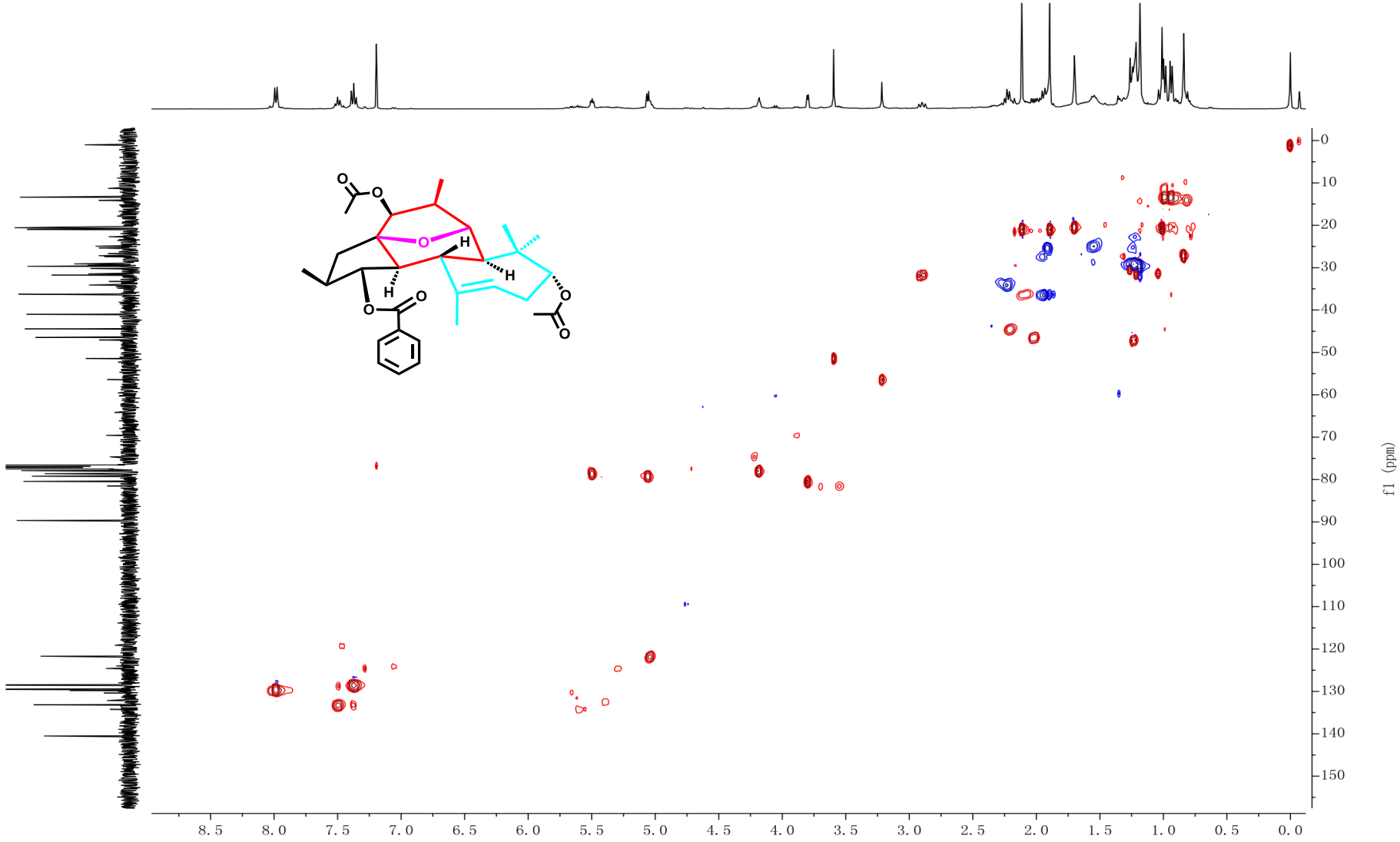


Figure S62. HSQC spectrum of euphopia F (**3**) in chloroform-d

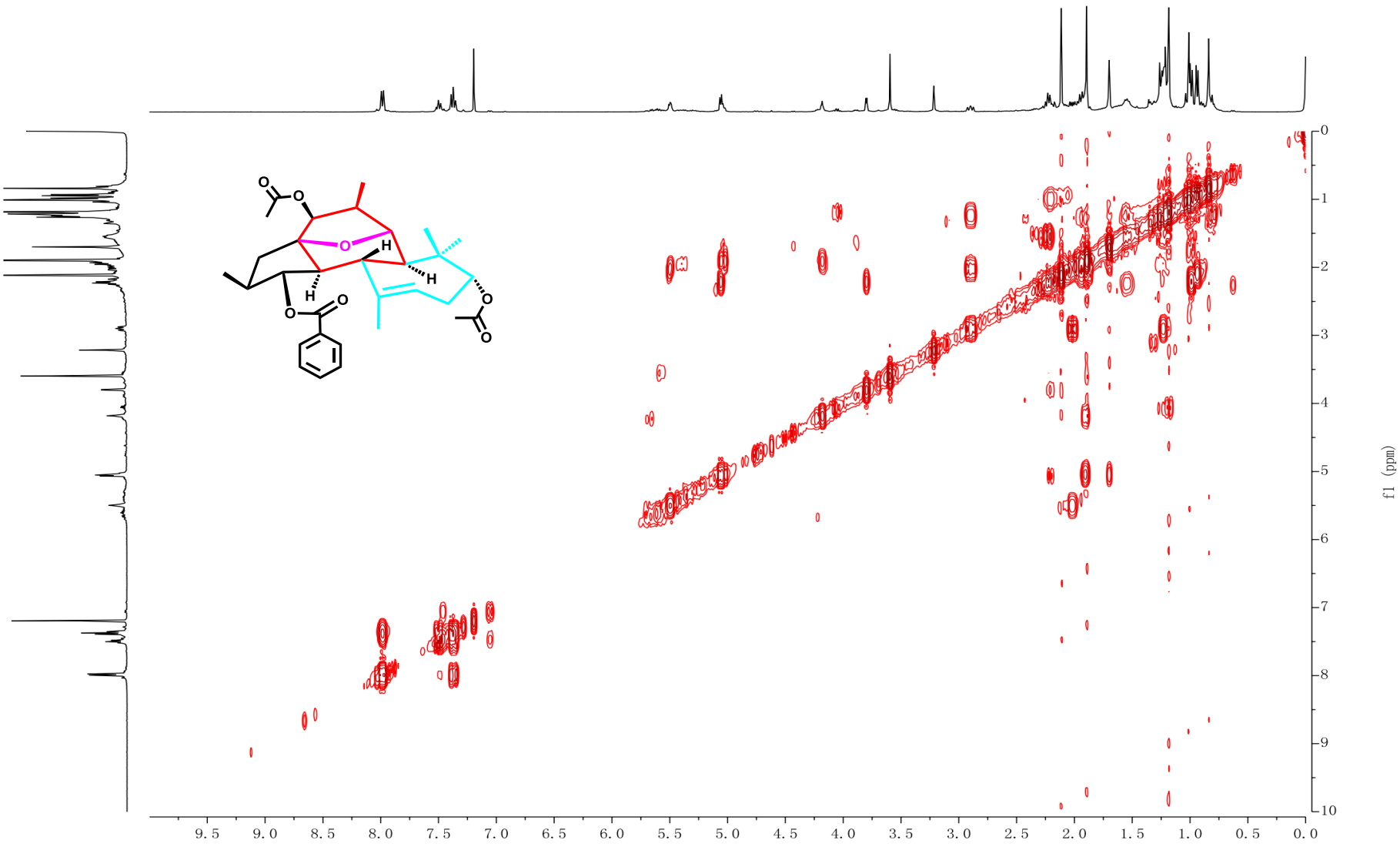


Figure S63. ^{1}H-^{1}H COSYspectrum of euphopia F (**3**) in chloroform-d

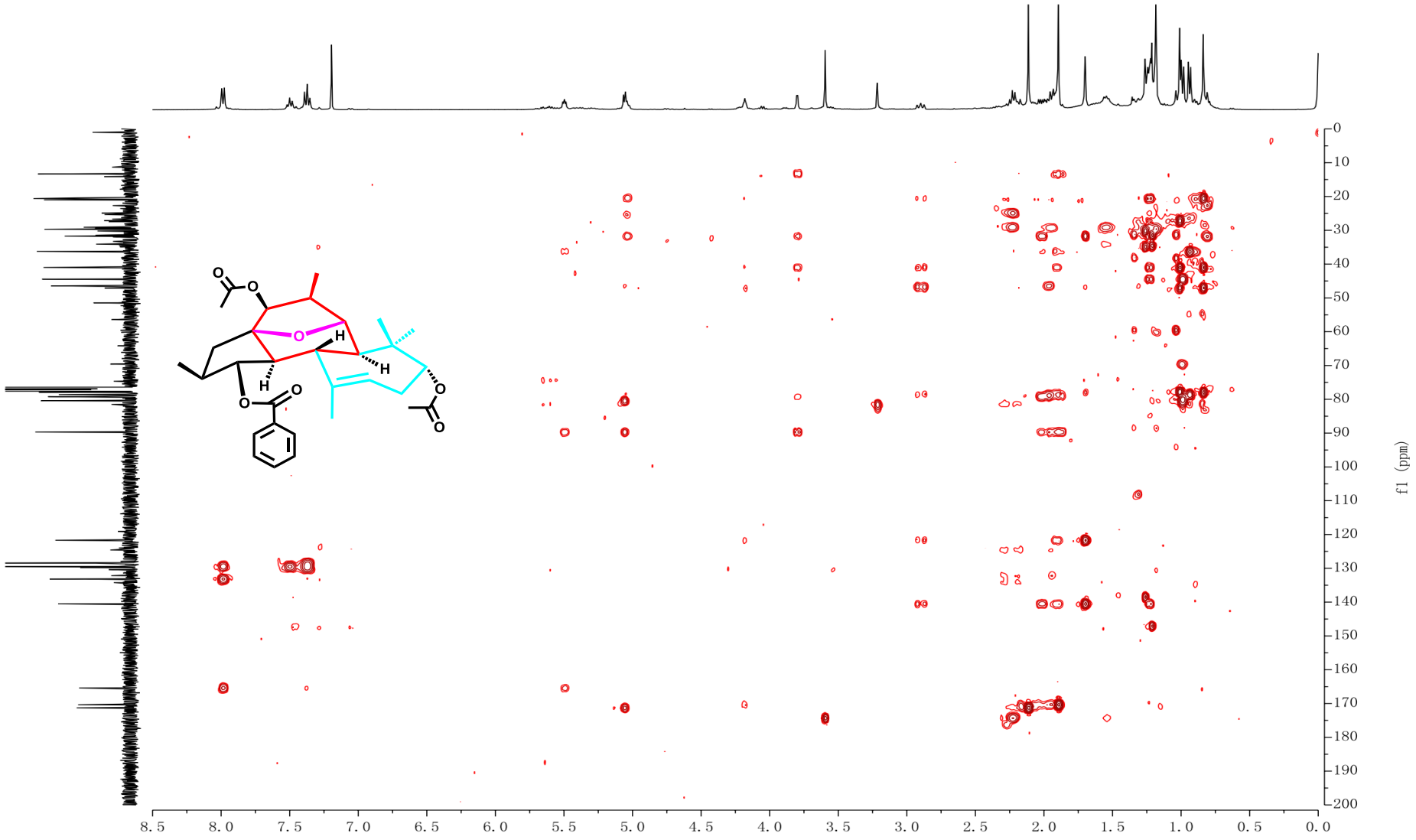


Figure S64. HMBC spectrum of euphopia F (**3**) in chloroform-d

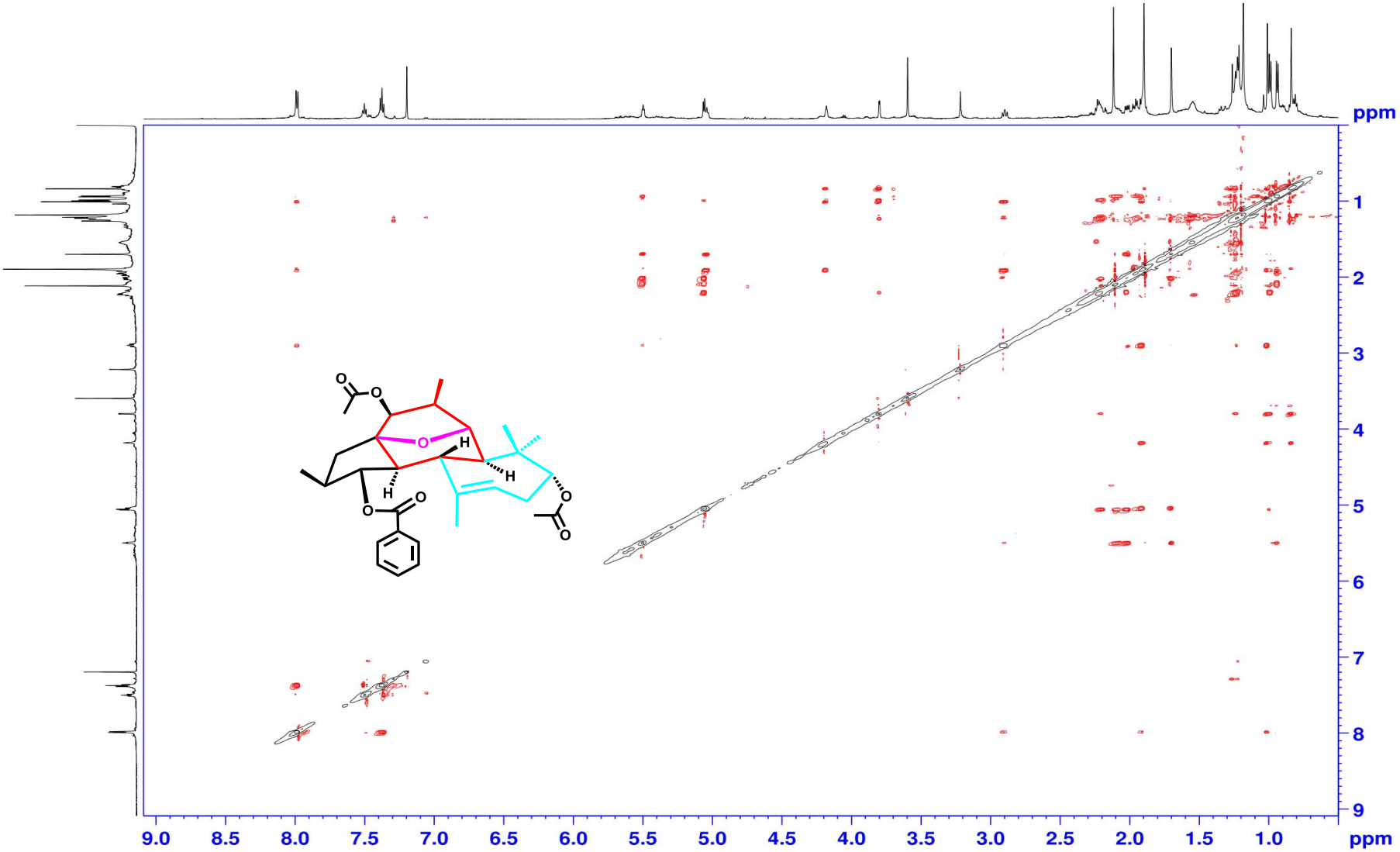
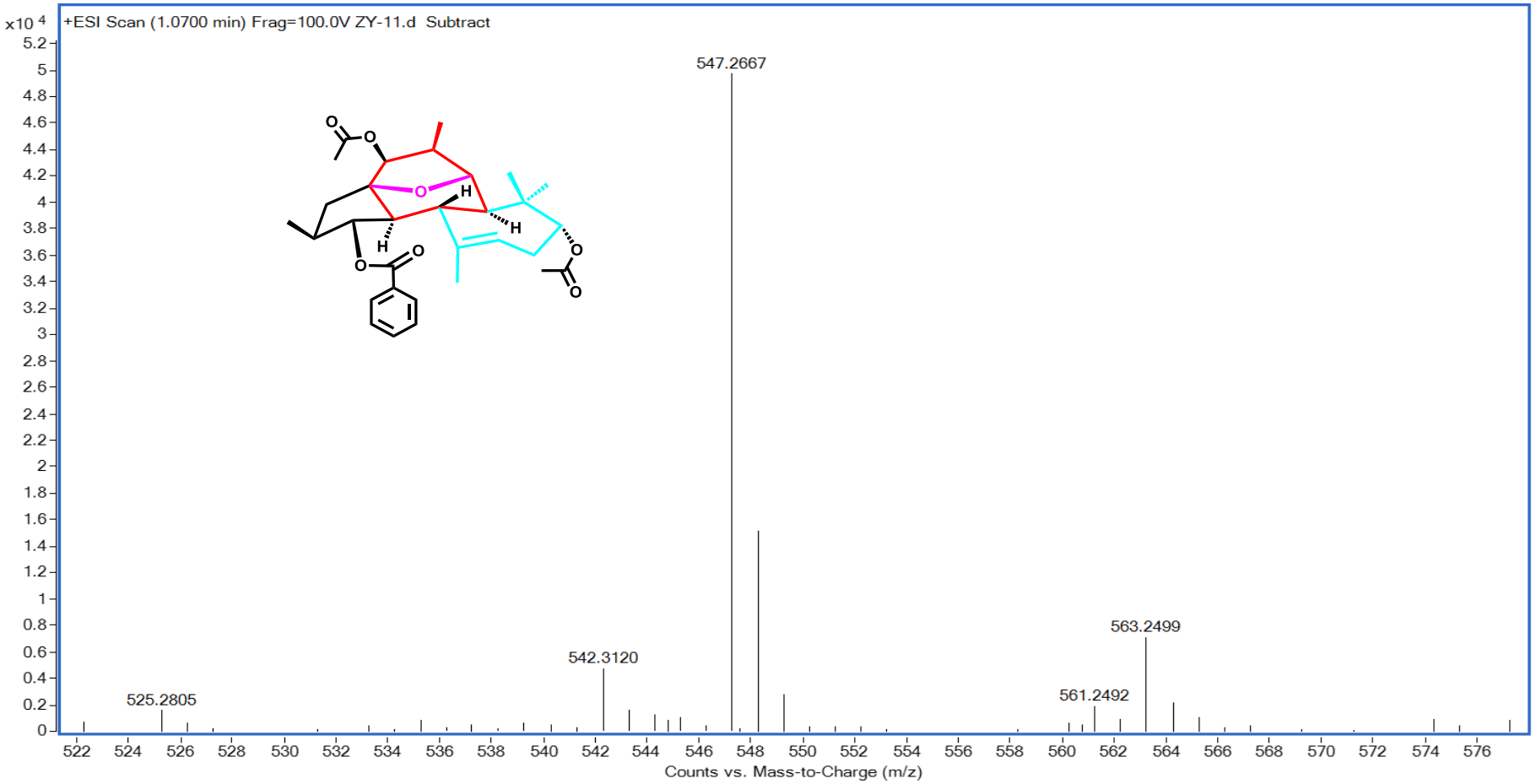


Figure S65. ROESY spectrum of euphopia F (**3**) in chloroform-d

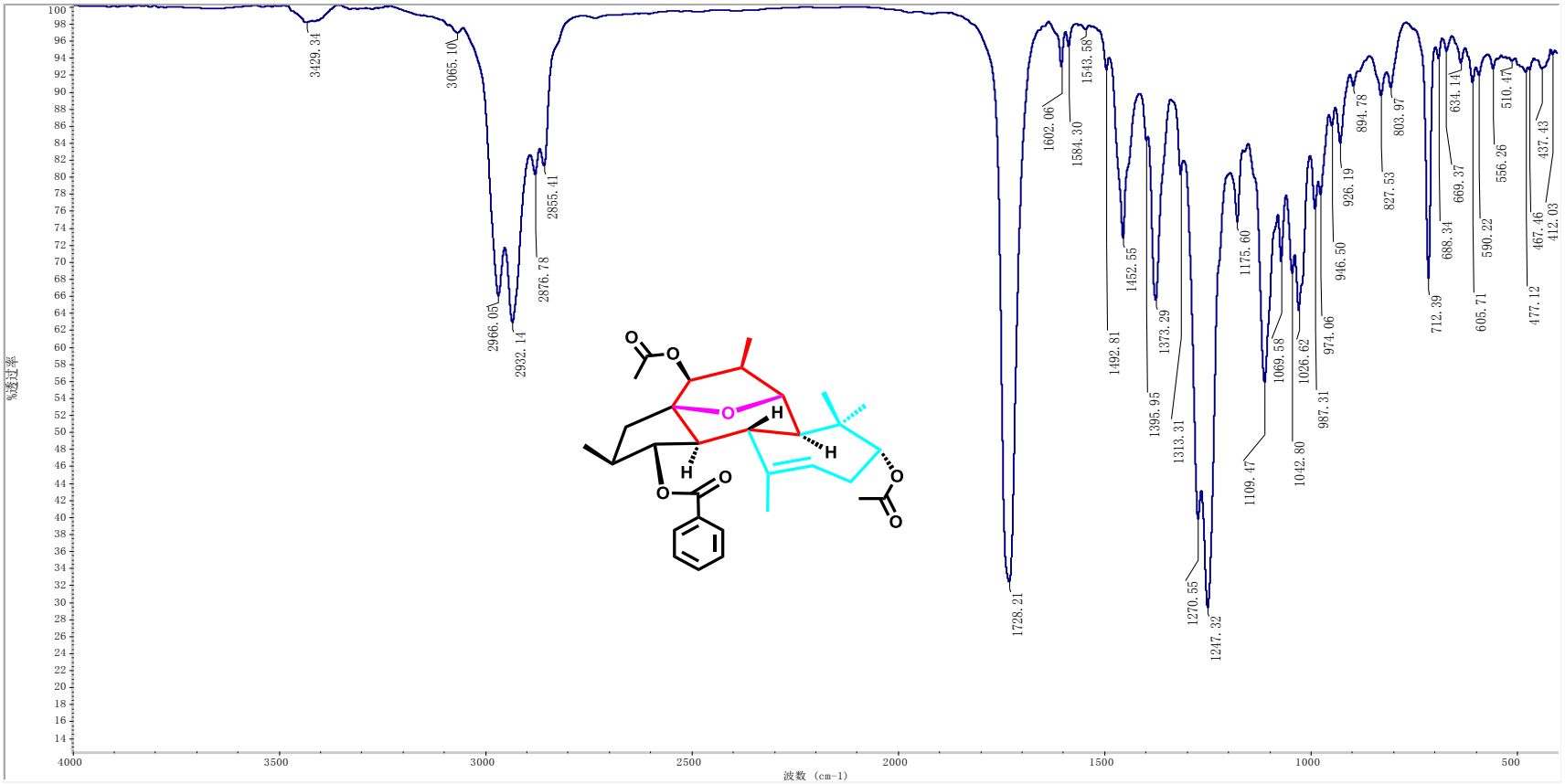


MS Formula Results: + Scan (1.0700 min) Sub (ZY-11.d)

m/z	Ion	Formula	Abundance
547.2667	(M+Na)+	C31 H40 Na O7	49741.1

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C31 H40 O7	C31 H40 Na O7	97.87		547.2666	-0.07	100	93.36	99.02

Figure S66. HRESIMS spectrum of euphopia F (**3**)



Sample Name: ZY-11
KBr压片
采集时间: 星期二 2月 02 13:24:21 2021 (GMT+08:00)
仪器型号: NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.4747
光阑: 80.00

Figure S67. IR spectrum of euphopia F (**3**)

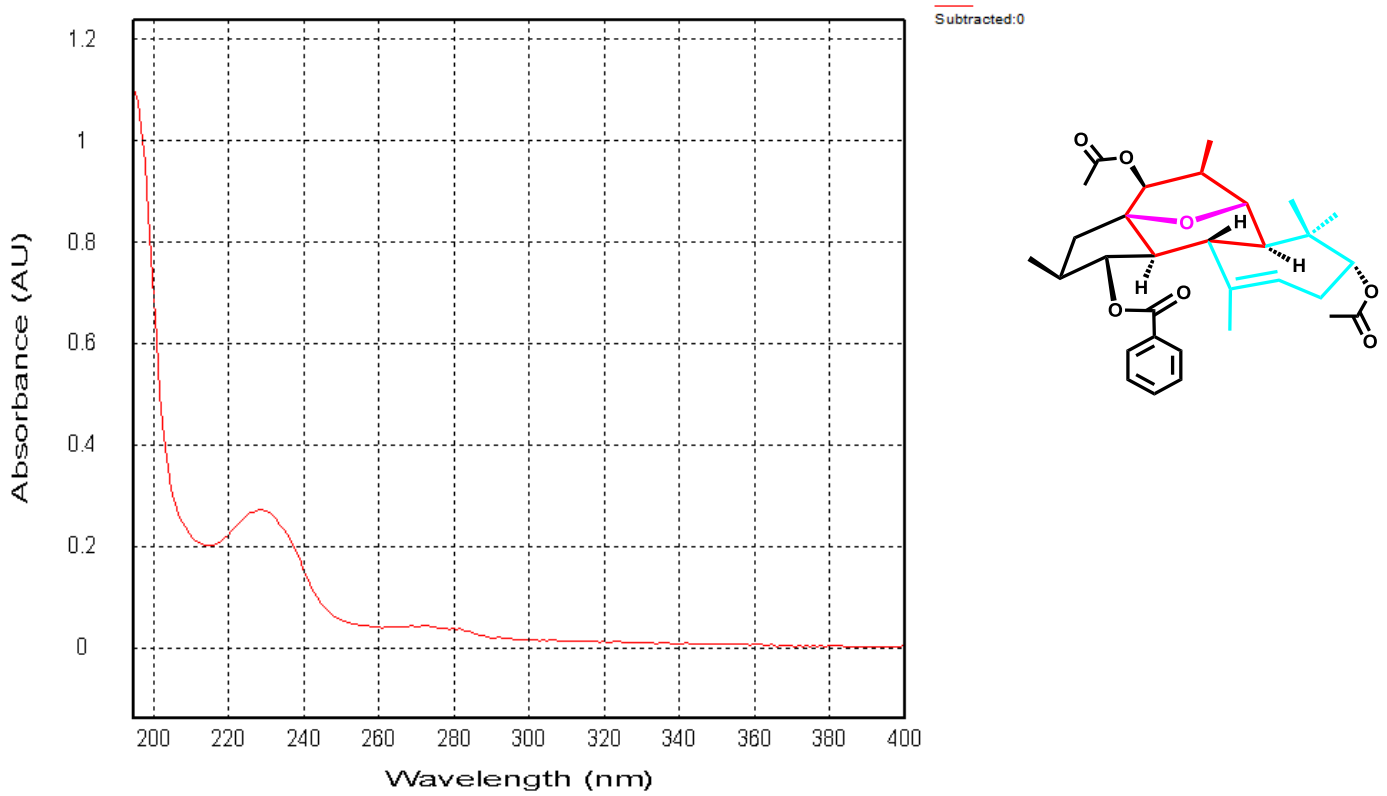


Figure S68. UV spectrum of euphopia F (**3**)

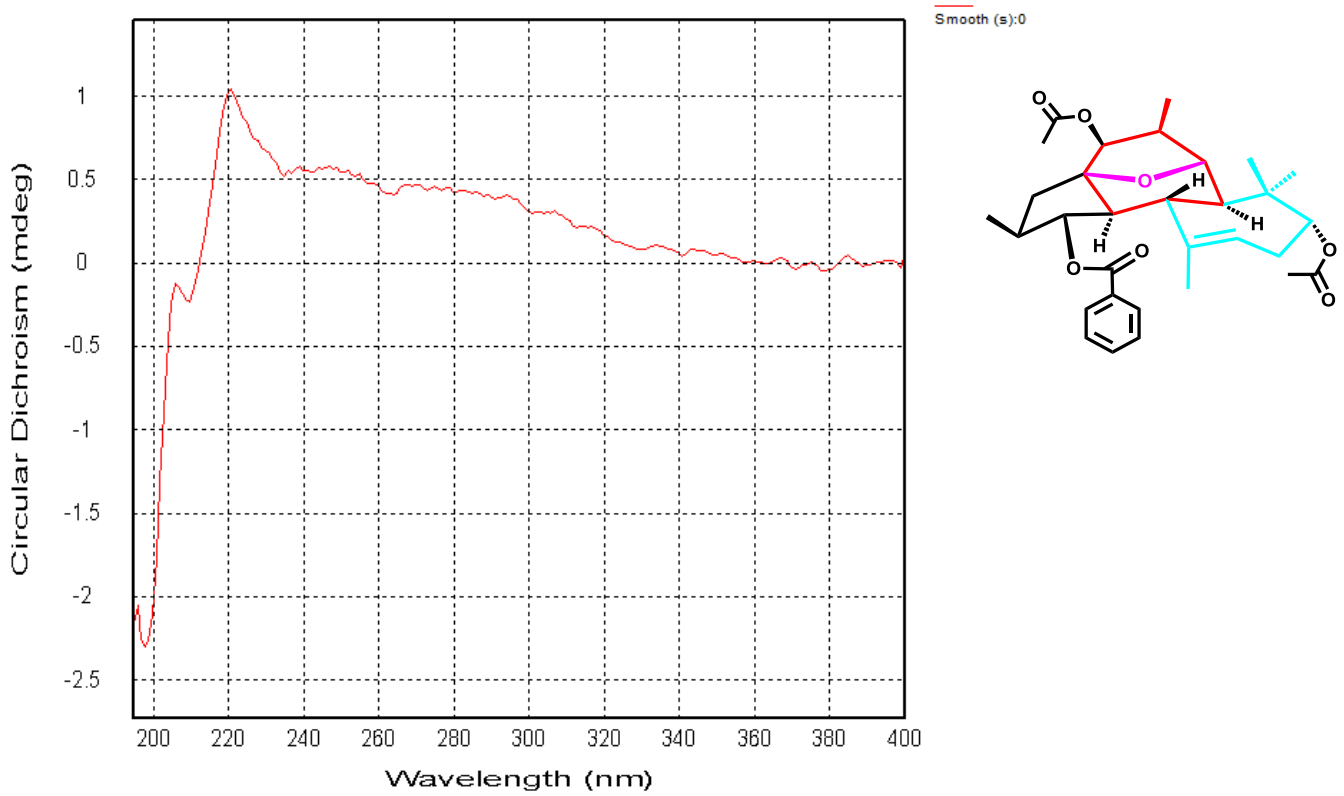


Figure S69. CD spectrum of euphopia F (**3**)

Rudolph Research Analytical

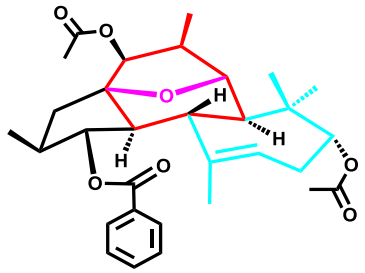
This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 02-FEB-2021

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled



n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	6.36	0.79	12.42	7.73	5.73

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	ZY-11	08:58:27 PM	7.73	SR	0.0085	589	100.00	0.110	20.3
2	ZY-11	08:58:35 PM	5.73	SR	0.0063	589	100.00	0.110	20.3
3	ZY-11	08:58:43 PM	6.27	SR	0.0069	589	100.00	0.110	20.3
4	ZY-11	08:58:51 PM	6.09	SR	0.0067	589	100.00	0.110	20.3
5	ZY-11	08:59:00 PM	6.00	SR	0.0066	589	100.00	0.110	20.3

Figure S70. OR report of euphopia F (**3**)