Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Discovery and Photosynthesis of Sinuaustones A and B, Diterpenoids with Novel Carbon Scaffold isolated from Soft Coral *Sinularia australiensis* from Hainan

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Contents

1. Experiment section

1.1 General experimental procedures

Melting points were measured on an X-4 digital micro-melting point apparatus. The X-ray measurments were made on a Bruker D8 Venture X-ray diffractometer with Cu Kα radiation. Optical rotations were measured on a Perkin-Elmer 241MC polarimeter (PerkinElmer, Fremont, CA, USA). IR spectra was recorded on a Nicolet 6700 spectrometer (Thermo Scientific, Waltham, MA, USA); peaks are reported in cm^{-1}. CD&UV spectra were measured on a JASCO J-815-150s instrument (JASCO, Japan). The NMR spectra were measured at 300 K on Bruker DRX 400, DRX 500 and Avance 600 MHz NMR spectrometers (Bruker Biospin AG, Fallanden, Germany); Chemical shifts are reported in parts per million (δ) in $CDCl_3$ (δ_H reported referred to $CHCl_3$ at 7.26 ppm; δ_C reported referred to $CDCl_3$ at 77.16 ppm) and coupling constants (J) in Hz; assignments were supported by ^1H–^1H COSY, HSQC, HMBC, and NOESY experiments. LR-EIMS and HR-EIMS data were recorded on a Finnigan-MAT-95 mass spectrometer (Finnigan-MAT, San Jose, CA, USA), respectively. Semi-preparative HPLC was performed on an Agilent-1260 system equipped with a DAD G1315D detector using ODS-HG-5 (250 mm × 9.4 mm, 5 μm) by eluting with CH_3OH–H_2O or CH_3CN–H_2O system at 2.5 mL/min. Commercial silica gel (100−200, 200−300 and 300−400 mesh; Qingdao, China) was used for column chromatography (CC). Precoated SiO_2 plates (HSGF-254; Yantai, China) were used for analytical TLC. Spots were detected on TLC under UV light or by heating after spraying with anisaldehyde H_2SO_4 reagent. Sephadex LH-20 (Amersham Biosciences) was also used for CC. All solvents used for column chromatography and HPLC were of analytical grade (Shanghai Chemical Reagents Co., Ltd.) and chromatographic grade (Dikma Technologies Inc.), respectively.

1.2 Cytotoxicity assay

Table S1. Cytotoxicity assay of Compounds **1**-**5**.

	inhibitory ratio (%)								
Cell	H1975			MDA-MB-231			RAW264.7		
Conc.(μM)	20	4	0.8	20	4	0.8	20	4	0.8
1	9.59	10.03	14.22	3.63	3.30	6.32	15.03	14.9	8.80
2	8.62	5.30	5.20	-1.90	-0.51	3.58	11.97	3.71	-8.90
3	15.34	16.32	11.02	10.57	10.3	10.77	3.79	-8.18	-5.48
4	4.14	14.68	16.20	4.61	7.35	4.60	29.81	22.86	15.1
5	28.83	18.62	27.89	8.31	5.40	9.21	14.76	3.33	-6.10

1.3 Photosynthesis experiment

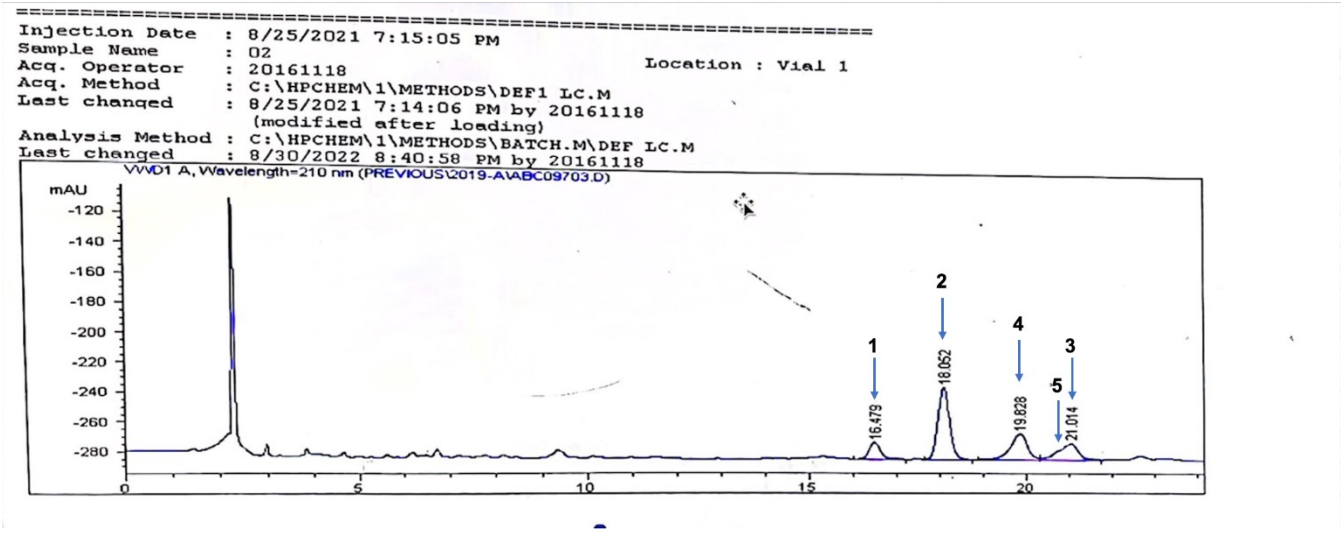

Figure S1. Reversed-Phase HPLC separation chromatography of the products of the photosynthesis experiment of compound **5**.

2. Original data for compounds 1–5

2.1 X-ray crystallographic analyses of 1

$C_{20}H_{30}O$ (M =286.44 g/mol), crystal size: 0.12 × 0.08 × 0.05 mm^3, trigonal, space group $P3_121$, a = 9.02720(10) Å, b = 9.02720(10) Å, c = 36.5504(11) Å, V = 2579.46(10) $Å^3$, Z = 6, μ(CuKα) = 0.494 mm^{-1}, D_{calc} = 1.106 g/cm^3, θ range = 7.256–149.162°, reflections collected

44959 [R_{int} = 0.0503], R_1 = 0.0310 [I > 2σ(I)], wR_2 = 0.0783 [all data], absolute structure parameter: –0.06(9). The single crystals of compound **1** were collected from a solvent system (CH_3OH-H_2O, 9:1) at 4°C. The X-ray measurements were made on a Bruker D8 Venture X-ray diffractometer with Cu Kα radiation (λ = 1.54178 Å). The crystal was kept at 110.0 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation. Crystallographic data for **1** has been deposited at the Cambridge Crystallographic Data Centre (Deposition nos. CCDC 2174239). Copies of these data can be obtained free of charge via ww.ccdc.cam.ac.uk/data request/cif or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, UK. [Fax: (+44) 1223-336-033. E-mail: deposit@ccdc.cam.ac.uk.]

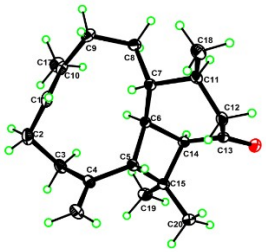

Figure S2. Perspective ORTEP drawing of X-ray structure of sinuaustone A (**1**) (displacement ellipsoids are drawn at the 50% probability level).

Table S2. X-ray crystallographic data for **1**.

Empirical formula	$C_{20}H_{30}O$
Formula weight	286.44
Temperature/K	110
Crystal system	trigonal
Space group	$P3_121$
a/Å	9.02720(10)
b/Å	9.02720(10)
c/Å	36.5504(11)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	2579.46(10)
Z	6
ϱ_{calc}g/cm^3	1.106
μ/mm^{-1}	0.494
F(000)	948.0
Crystal size/mm^3	0.12 × 0.08 × 0.05
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.256 to 149.162
Index ranges	-10 ≤ h ≤ 11, -11 ≤ k ≤ 11, -43 ≤ l ≤ 45
Reflections collected	44959
Independent reflections	3521 [R_{int} = 0.0503, R_{sigma} = 0.0185]
Data/restraints/parameters	3521/0/194
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0310, wR_2 = 0.0769
Final R indexes [all data]	R_1 = 0.0323, wR_2 = 0.0783
Largest diff. peak/hole / e Å^{-3}	0.19/-0.13
Flack parameter	-0.06(9)

2.2 X-ray crystallographic analyses of 2

$C_{20}H_{30}O$ (M =286.44 g/mol), crystal size: 0.15 × 0.08 × 0.03 mm^3, orthorhombic, space group $P2_12_12_1$, a = 6.3034(2) Å, b = 16.0980(5) Å, c = 16.7484(4) Å, V = 1699.50(9) Å^3, Z = 4, μ (CuKα) = 0.499 mm^{-1}, D_{calc} = 1.119 g/cm^3, θ range = 7.616–148.964°, reflections collected 39324 [R_{int} = 0.0651], R_1 = 0.0328 [I > 2σ(I)], wR_2 = 0.0773 [all data], absolute structure parameter: 0.00(15). The single crystals of compound **1** were collected from methanol solution at 4°C. The X-ray measurements were made on a Bruker D8 Venture X-ray diffractometer with Cu Kα radiation (λ = 1.54178 Å). The crystal was kept at 170.0 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation. Crystallographic data for **2** has been deposited at the Cambridge Crystallographic Data Centre (Deposition nos.

CCDC 2174244). Copies of these data can be obtained free of charge via ww.ccdc.cam.ac.uk/data request/cif or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, UK. [Fax: (+44) 1223-336-033. E-mail: deposit@ccdc.cam.ac.uk.]

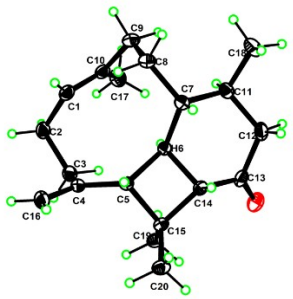

Figure S3. Perspective ORTEP drawing of X-ray structure of sinuaustone B (**2**) (displacement ellipsoids are drawn at the 50% probability level).

Table S3. X-ray crystallographic data for **2**.

Empirical formula	$C_{20}H_{30}O$
Formula weight	286.44
Temperature/K	170.0
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.3034(2)
b/Å	16.0980(5)
c/Å	16.7484(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1699.50(9)
Z	4
ϱ_{calc}g/cm^3	1.119
μ/mm^{-1}	0.499
F(000)	632.0
Crystal size/mm^3	0.15 × 0.08 × 0.03
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.616 to 148.964
Index ranges	-7 ≤ h ≤ 7, -20 ≤ k ≤ 20, -20 ≤ l ≤ 20
Reflections collected	39324
Independent reflections	3463 [R_{int} = 0.0651, R_{sigma} = 0.0242]
Data/restraints/parameters	3463/0/194
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0328, wR_2 = 0.0752
Final R indexes [all data]	R_1 = 0.0359, wR_2 = 0.0773
Largest diff. peak/hole / e Å^{-3}	0.17/-0.13
Flack parameter	0.00(15)

2.3 Detailed structural elucidation of compound 2

Sinuaustone B (**2**) was obtained as colorless crystals with the molecular formula determined to be $C_{20}H_{30}O$ by its HREIMS at *m/z* 286.2291 ([M]+, calcd 286.2291), indicating six DBEs. The IR absorptions indicative of the presence of a ketone carbonyl (ν_{max} 1717 cm^{-1}) of **2**. However, the ^{13}C NMR data of **2** were reminiscent of those of **1** (Table 1), especially the typical signals related to the four-membered ring ($\delta_{C/H}$ 59.9/2.18, C-5; $\delta_{C/H}$ 56.5/1.88, C-6; $\delta_{C/H}$ 58.3/2.21, C-14; δ_C 43.1, C-15) with the two methyls linked to a quaternary carbon ($\delta_{C/H}$ 30.8/0.99, C-19; $\delta_{C/H}$ 18.7/1.08, C-20) in **2**, suggesting the same skeleton of the two compounds, which was further confirmed by ^1H-^1H COSY and HMBC experiments (Figure S3). However, owing to the limited conformation caused by the existence of rigid four-membered ring, the ^1H and ^{13}C NMR of **2** showed numerous wide peaks with weak absorption, which brought great difficulties to determine the plane structure of **2**. After careful NMR data analysis, the 3-methyl-cyclohexanone moiety of **2** was deduced by the clear COSY correlations of H-11/H-12, H-11/H_3-18 and H-14/H-6, and the well resolved HMBC cross peaks from H_3-18 (δ_H 1.02) to C-7/C-11/C-12, from H_2-12 to C-7 and from H-14 to C-7 (Figure S3). Finally, the substituted 10-membered ring of **2** was inferred by the $^1H-^1H$ COSY correlations of H-1/H-2 and H-5/H-6, the HMBC cross peaks from H_3-17 to C-1/C-10 and H_2-16 to C-3/C-5. However, some 2D signals linked to C-8 and C-9 were missing. The attribution of C-8 and C-9 was supported by the ^1H and ^{13}C NMR data comparison of **1** and **2**.

However, the relative configuration of the five contiguous stereocenters was indistinct because they were heavily overlapped in the NOESY spectra, which made elucidating its stereochemistry a great challenge. Fortunately, we also obtained suitable single crystals of **2** in methanol, which allowed X-ray crystallography using Cu Kα radiation [λ = 1.54178 Å, Flack parameter of 0.00 (15)]. Analysis of the X-ray data confirmed the planar structure of **2** as the isomer of **1** with the same planar structure and addressed its absolute configuration as 5*S*, 6*R*, 7*R*, 11*S*, 14*S* (Figure S2, CCDC 2174244) with comparing the predicted ECD curves with the experimental one (Figure S40).

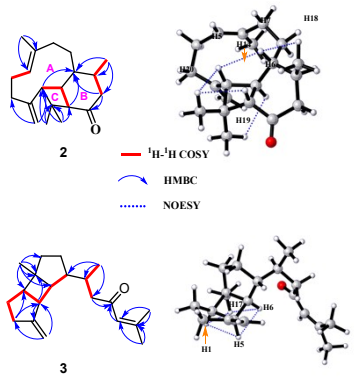

Figure S4. ^1H-^1H COSY, key HMBC and NOESY correlations of compounds **2** and **3**.

2.4 MS, NMR, IR, CD&UV spectra of compounds 1.

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EI202101295-1 A8-A8-FDA-2-c2#13 RT: 2.89
T: + c EI Full ms [49.50-800.50]
m/z= 48-803

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
69.0332	1646629.0	2.73	69.0335	-0.30	2.5	$C_4H_5O_1$
69.0695	2814100.0	4.66	69.0699	-0.34	1.5	C_5H_9
78.0120	1682964.0	2.79	78.0100	1.96	5.0	$C_5H_2O_1$
79.0180	9075712.0	15.04	79.0178	0.16	4.5	$C_5H_3O_1$
80.0237	1698294.0	2.81	80.0257	-2.01	4.0	$C_5H_4O_1$
81.0313	8289030.0	13.74	81.0335	-2.22	3.5	$C_5H_5O_1$
93.0701	7309204.0	12.11	93.0699	0.26	3.5	C_7H_9
95.0865	3061582.0	5.07	95.0855	1.01	2.5	C_7H_{11}
105.0721	10868480.0	18.01	105.0699	2.24	4.5	C_8H_9
106.0785	2202853.0	3.65	106.0777	0.80	4.0	C_8H_{10}
107.0883	5306386.0	8.79	107.0855	2.76	3.5	C_8H_{11}
115.0554	1589200.0	2.63	115.0542	1.12	6.5	C_9H_7
117.0704	3996664.0	6.62	117.0699	0.55	5.5	C_9H_9
118.0777	2136393.0	3.54	118.0777	0.02	5.0	C_9H_{10}
119.0853	10064384.0	16.68	119.0855	-0.25	4.5	C_9H_{11}
120.0930	6108131.0	10.12	120.0934	-0.30	4.0	C_9H_{12}
121.1007	7985961.0	13.23	121.1012	-0.49	3.5	C_9H_{13}
123.0801	1564719.0	2.59	123.0804	-0.31	3.5	$C_8H_{11}O_1$
125.0962	15427072.0	25.57	125.0961	0.09	2.5	$C_8H_{13}O_1$
129.0694	1492762.0	2.47	129.0699	-0.44	6.5	$C_{10}H_9$
131.0855	6107389.0	10.12	131.0855	-0.04	5.5	$C_{10}H_{11}$
132.0929	3590741.0	5.95	132.0934	-0.42	5.0	$C_{10}H_{12}$
133.1014	5459539.0	9.05	133.1012	0.21	4.5	$C_{10}H_{13}$
143.0851	1448049.0	2.40	143.0855	-0.40	6.5	$C_{11}H_{11}$
145.1007	5978835.0	9.91	145.1012	-0.45	5.5	$C_{11}H_{13}$
146.1077	3203297.0	5.31	146.1090	-1.29	5.0	$C_{11}H_{14}$
147.1162	2735399.0	4.53	147.1168	-0.59	4.5	$C_{11}H_{15}$
157.1016	2403602.0	3.98	157.1012	0.43	6.5	$C_{12}H_{13}$
159.1152	15476224.0	25.65	159.1168	-1.60	5.5	$C_{12}H_{15}$
160.1217	5436722.0	9.01	160.1247	-2.99	5.0	$C_{12}H_{16}$
161.1307	4749389.0	7.87	161.1325	-1.79	4.5	$C_{12}H_{17}$
171.1169	1644549.0	2.73	171.1168	0.11	6.5	$C_{13}H_{15}$
173.1325	16312064.0	27.03	173.1325	0.03	5.5	$C_{13}H_{17}$
186.1404	4328759.0	7.17	186.1403	0.13	6.0	$C_{14}H_{18}$
187.1475	2684833.0	4.45	187.1481	-0.63	5.5	$C_{14}H_{19}$
188.1566	60343808.0	100.00	188.1560	0.61	5.0	$C_{14}H_{20}$
230.1662	2252528.0	3.73	230.1665	-0.33	6.0	$C_{16}H_{22}O_1$
243.1747	1478947.0	2.45	243.1743	0.32	6.5	$C_{17}H_{23}O_1$
253.1956	2696539.0	4.47	253.1951	0.54	7.5	$C_{19}H_{25}$
271.2054	5544034.0	9.19	271.2056	-0.23	6.5	$C_{19}H_{27}O_1$
286.2297	1412338.0	2.34	286.2291	0.54	6.0	$C_{20}H_{30}O_1$

Figure S5. HREIMS spectrum of sinuaustone A (**1**).

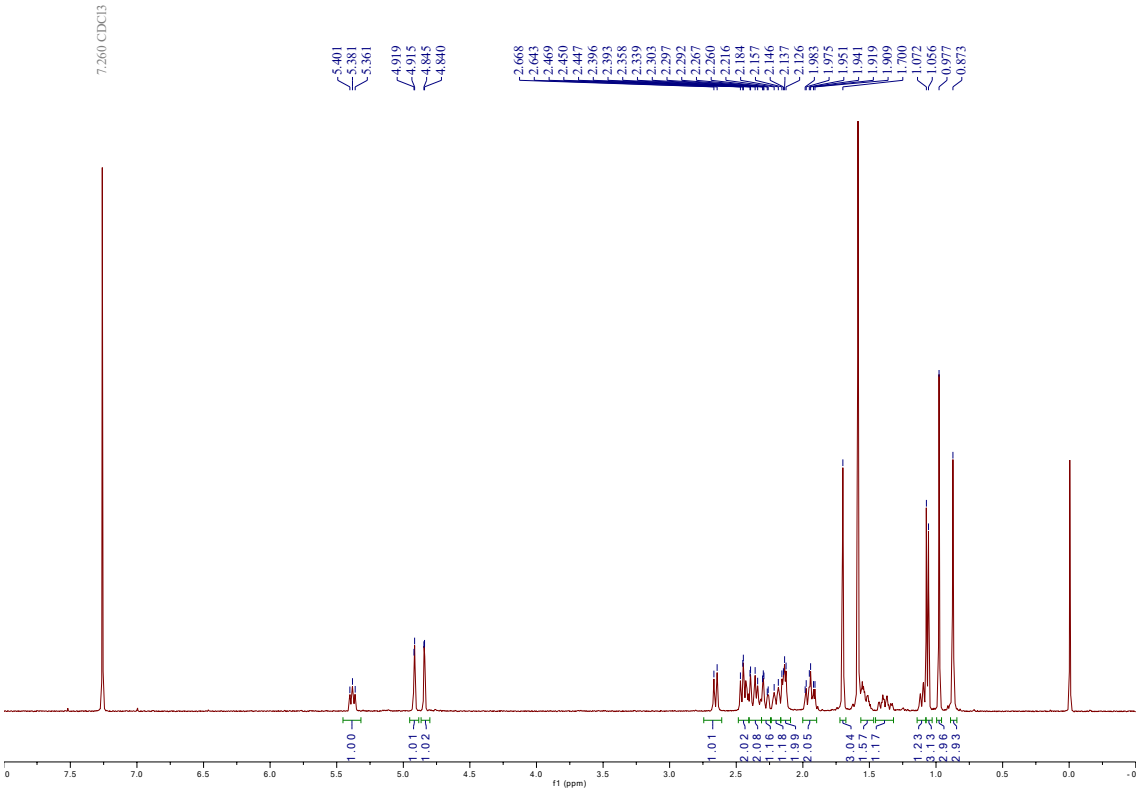

Figure S6. ^{1}H NMR spectrum (600 MHz) of sinuaustone A (**1**) in $CDCl_3$.

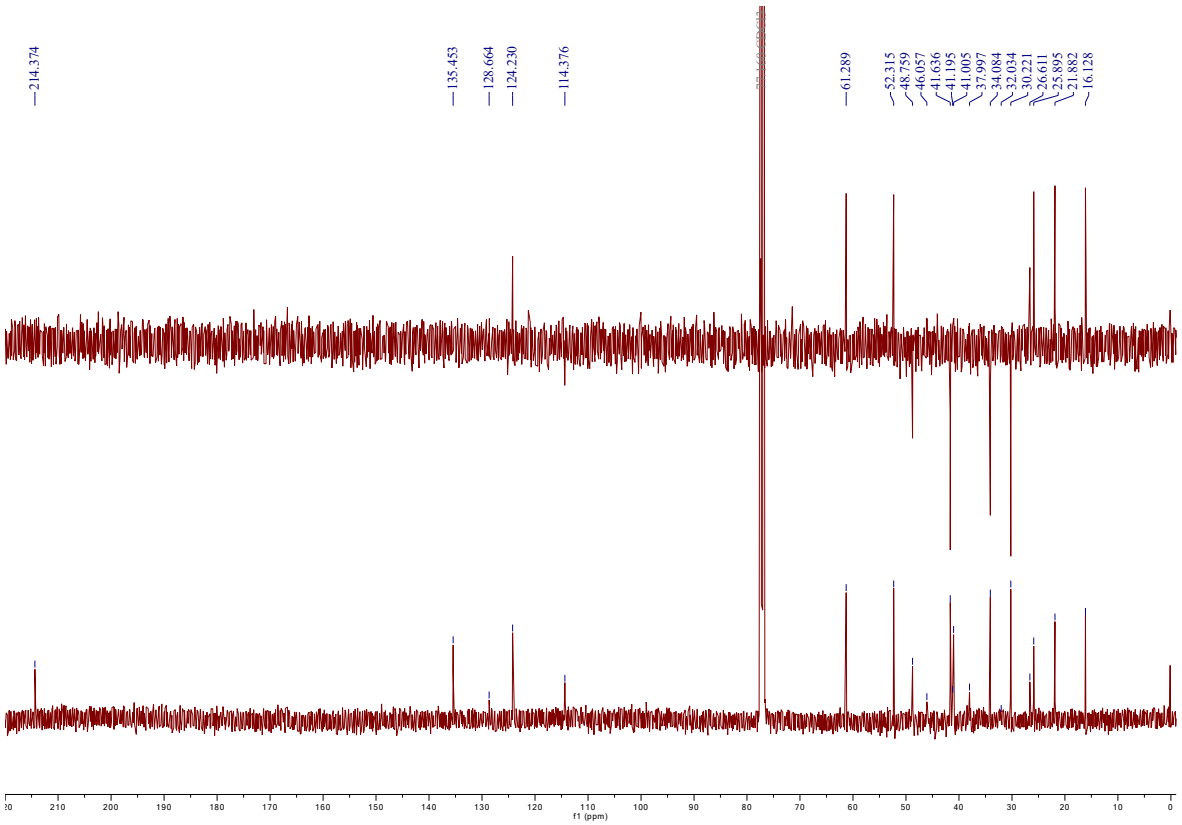

Figure S7. ^{13}C NMR spectrum (125 MHz) of sinuaustone A (**1**) in $CDCl_3$.

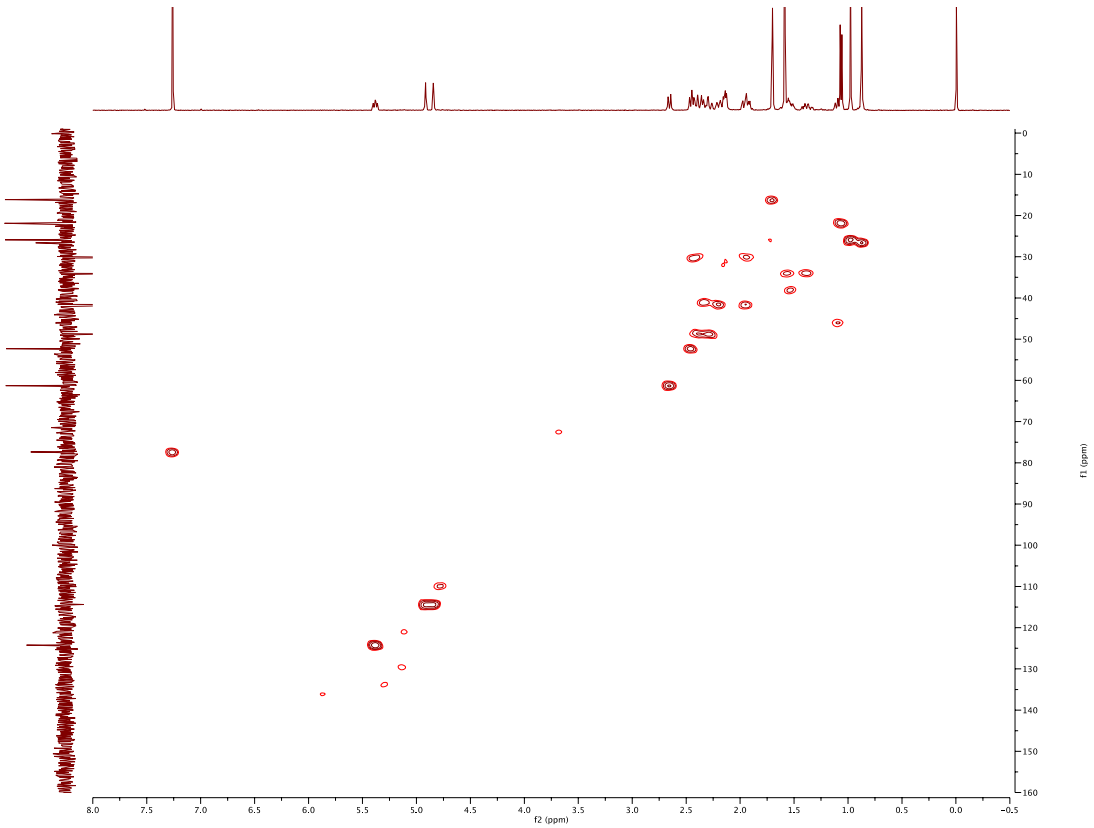

Figure S8. HSQC spectrum (500 MHz) of sinuaustone A (**1**) in $CDCl_3$.

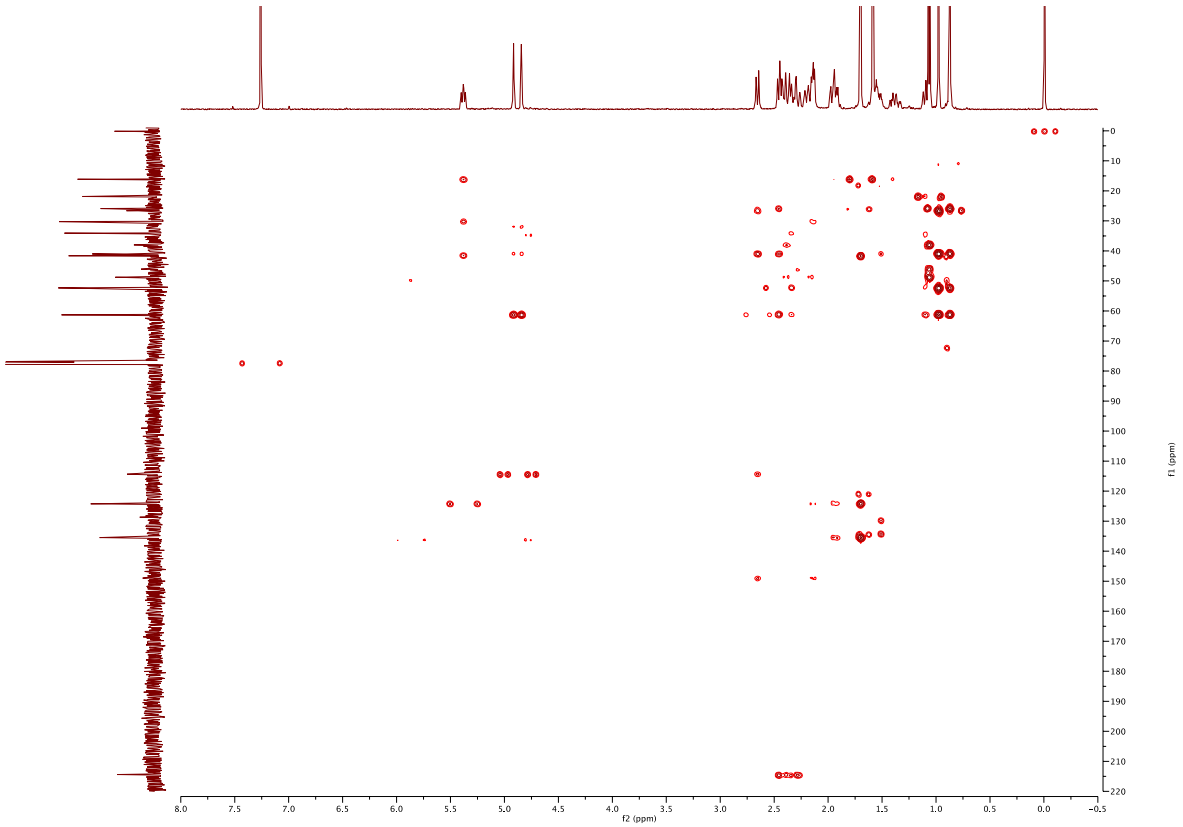

Figure S9. HMBC spectrum (500 MHz) of sinuaustone A (**1**) in $CDCl_3$.

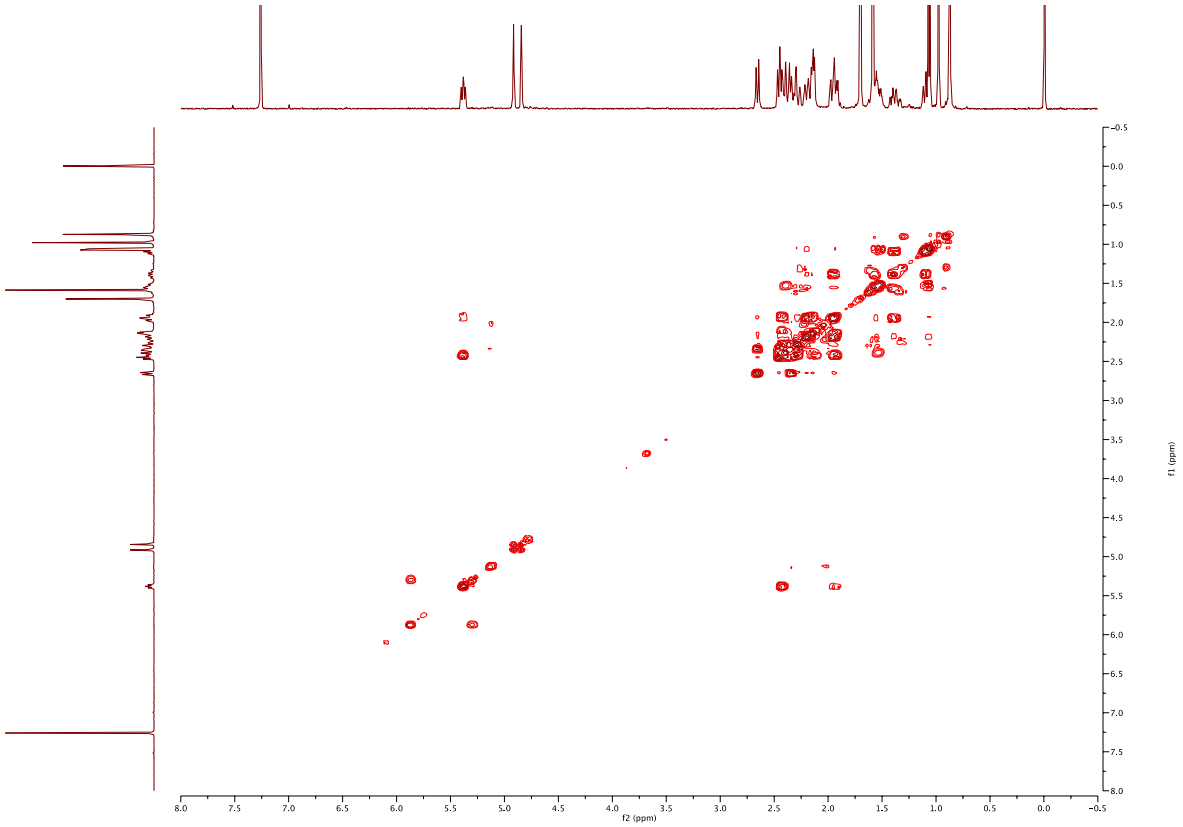

Figure S10. ^{1}H-^{1}H COSY spectrum (500 MHz) of sinuaustone A (**1**) in $CDCl_3$.

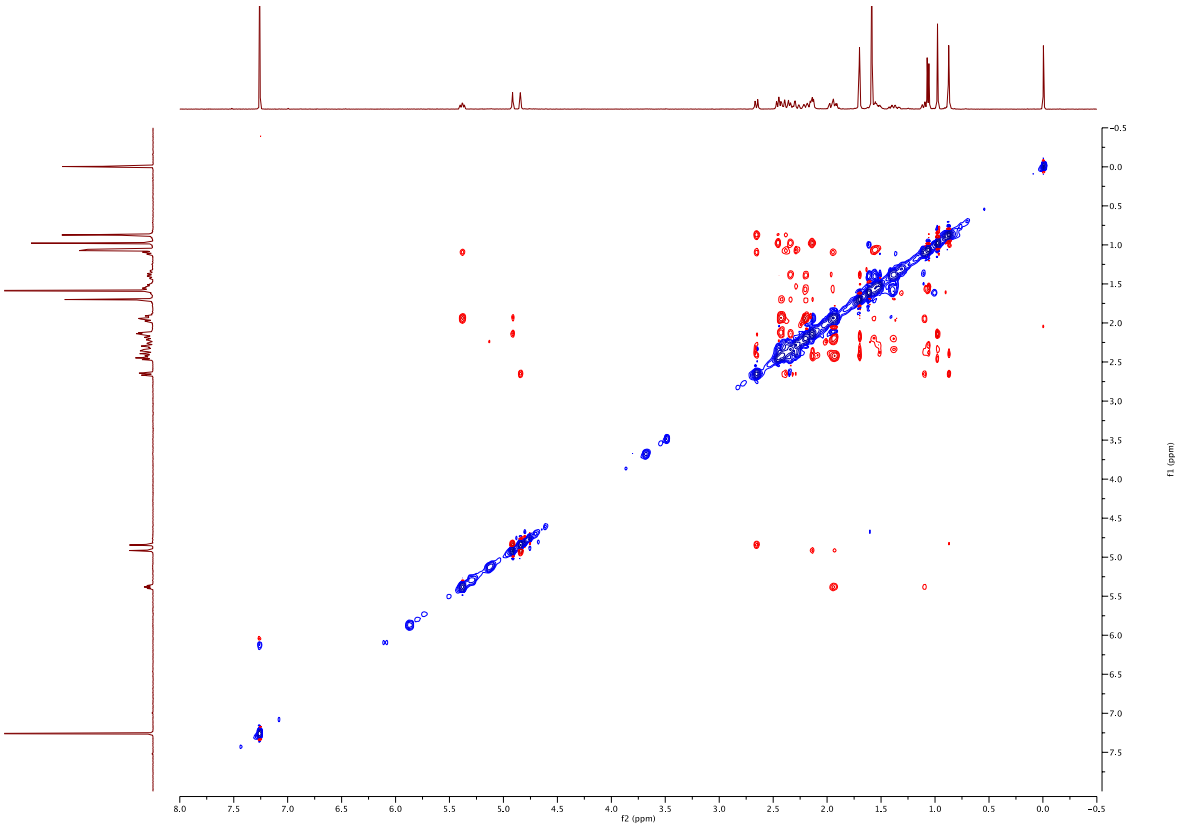

Figure S11. NOESY spectrum (500 MHz) of sinuaustone A (**1**) in $CDCl_3$.

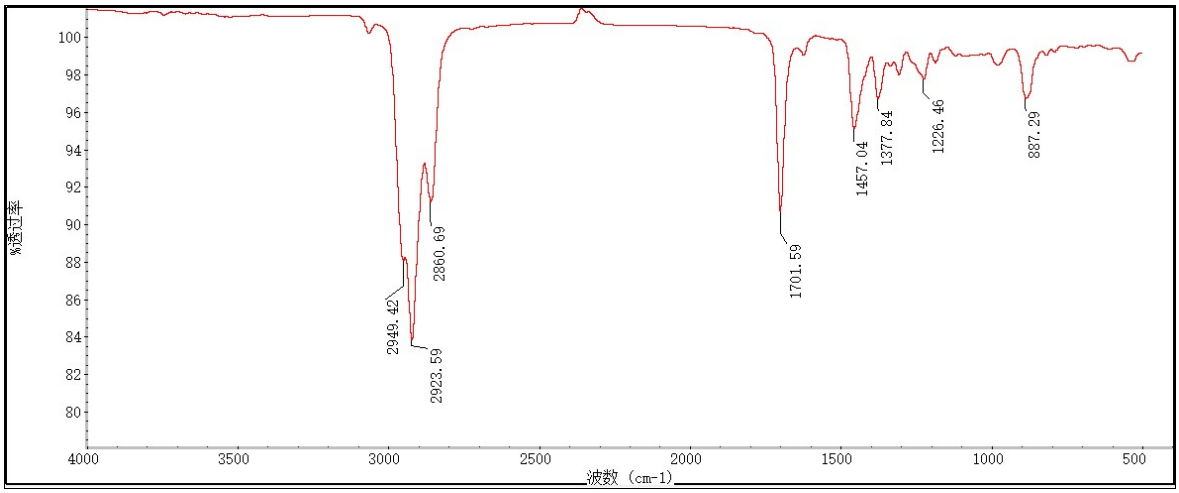

Figure S12. IR spectrum of sinuaustone A (**1**).

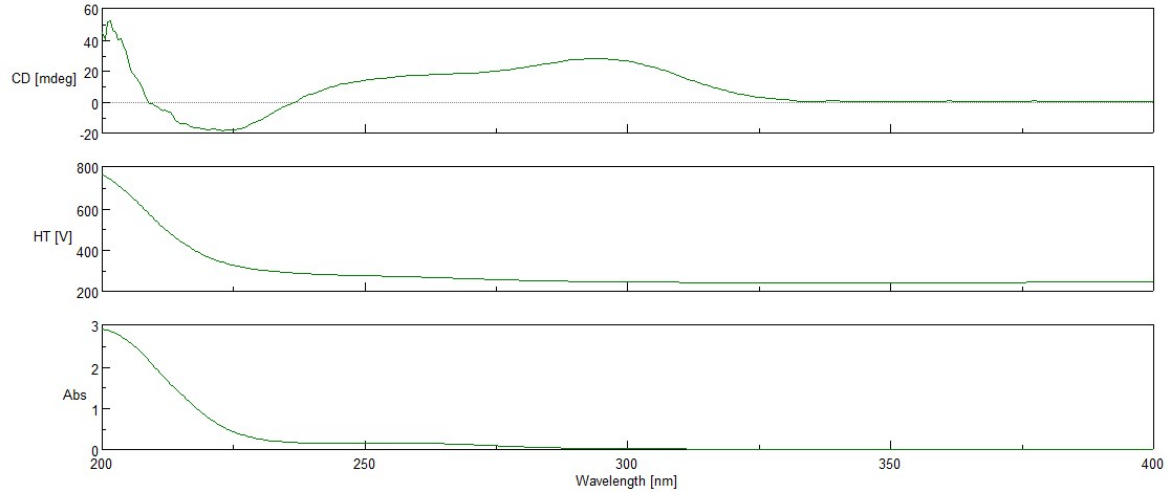

Figure S13. CD&UV spectrum of sinuaustone A (**1**).

2.5 MS, NMR, IR, CD&UV spectra of compounds 2.

D:\data\2021\EI202101474_A8-10FDA-4-c1 8/17/2021 2:02:45 PM

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T: + c EI Full ms [49.50-800.50]
m/z= 48-803

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
52.9992	7817345.0	6.60	53.0022	-3.00	3.5	$C_3H_1O_1$
81.0308	14909440.0	12.59	81.0335	-2.69	3.5	$C_5H_5O_1$
119.0863	22624000.0	19.11	119.0855	0.81	4.5	C_9H_{11}
131.0861	14881536.0	12.57	131.0855	0.53	5.5	$C_{10}H_{11}$
132.0945	8011756.0	6.77	132.0934	1.11	5.0	$C_{10}H_{12}$
143.0851	3307385.0	2.79	143.0855	-0.40	6.5	$C_{11}H_{11}$
229.1602	3016846.0	2.55	229.1587	1.52	6.5	$C_{16}H_{21}O_1$
230.1665	7530822.0	6.36	230.1665	0.02	6.0	$C_{16}H_{22}O_1$
231.1724	3230276.0	2.73	231.1743	-1.90	5.5	$C_{16}H_{23}O_1$
243.1737	3124541.0	2.64	243.1743	-0.66	6.5	$C_{17}H_{23}O_1$
253.1947	18896640.0	15.96	253.1951	-0.36	7.5	$C_{19}H_{25}$
271.2057	12158208.0	10.27	271.2056	0.09	6.5	$C_{19}H_{27}O_1$
286.2291	3205409.0	2.71	286.2291	-0.03	6.0	$C_{20}H_{30}O_1$

Figure S14. HREIMS spectrum of sinuaustone B (**2**).

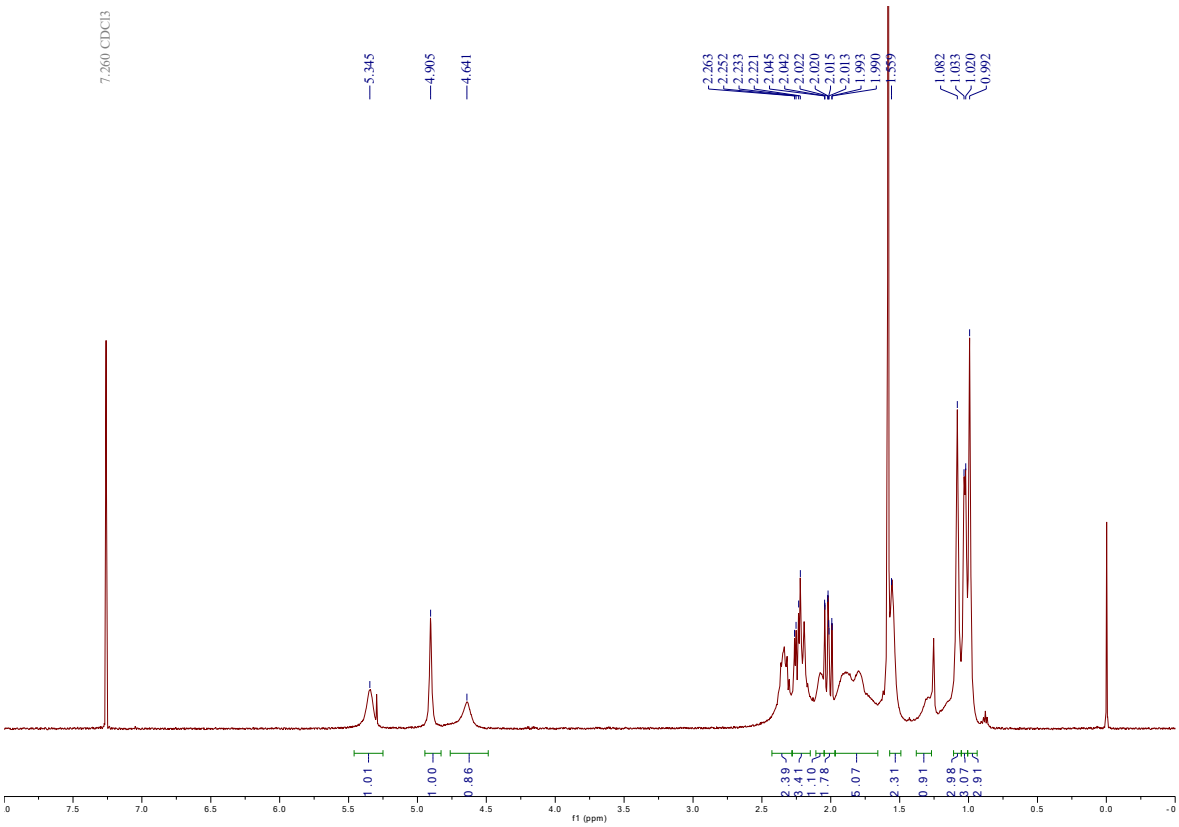

Figure S15. ^{1}H NMR spectrum (600 MHz) of sinuaustone B (**2**) in $CDCl_3$.

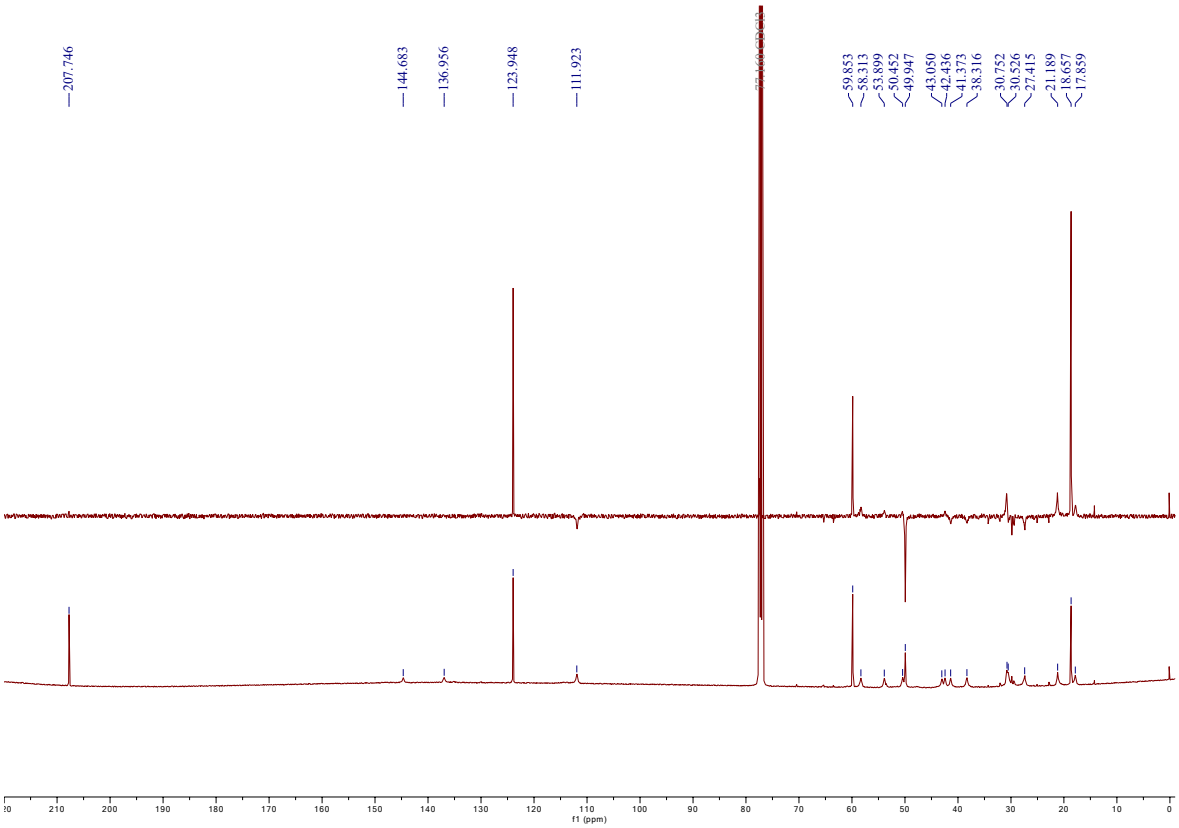

Figure S16. ^{13}C NMR spectrum (125 MHz) of sinuaustone B (**2**) in $CDCl_3$.

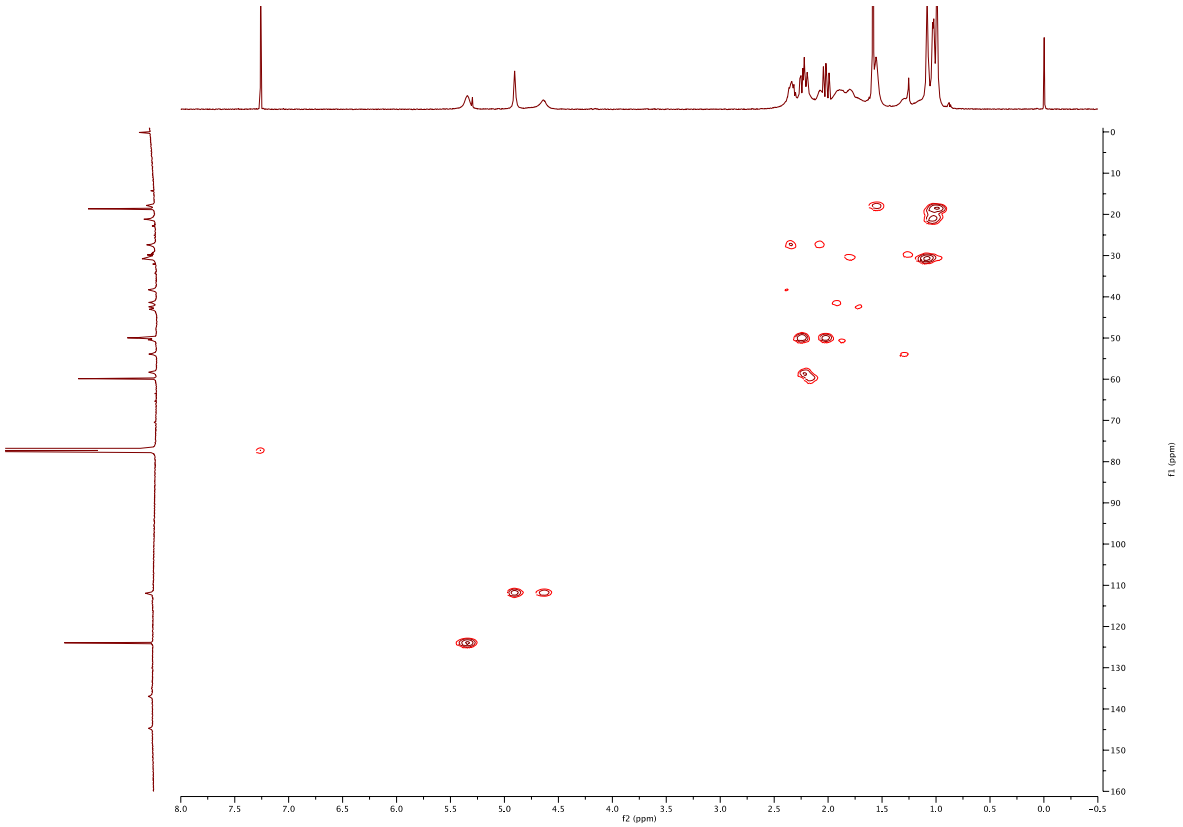

Figure S17. HSQC spectrum (500 MHz) of sinuaustone B (**2**) in $CDCl_3$.

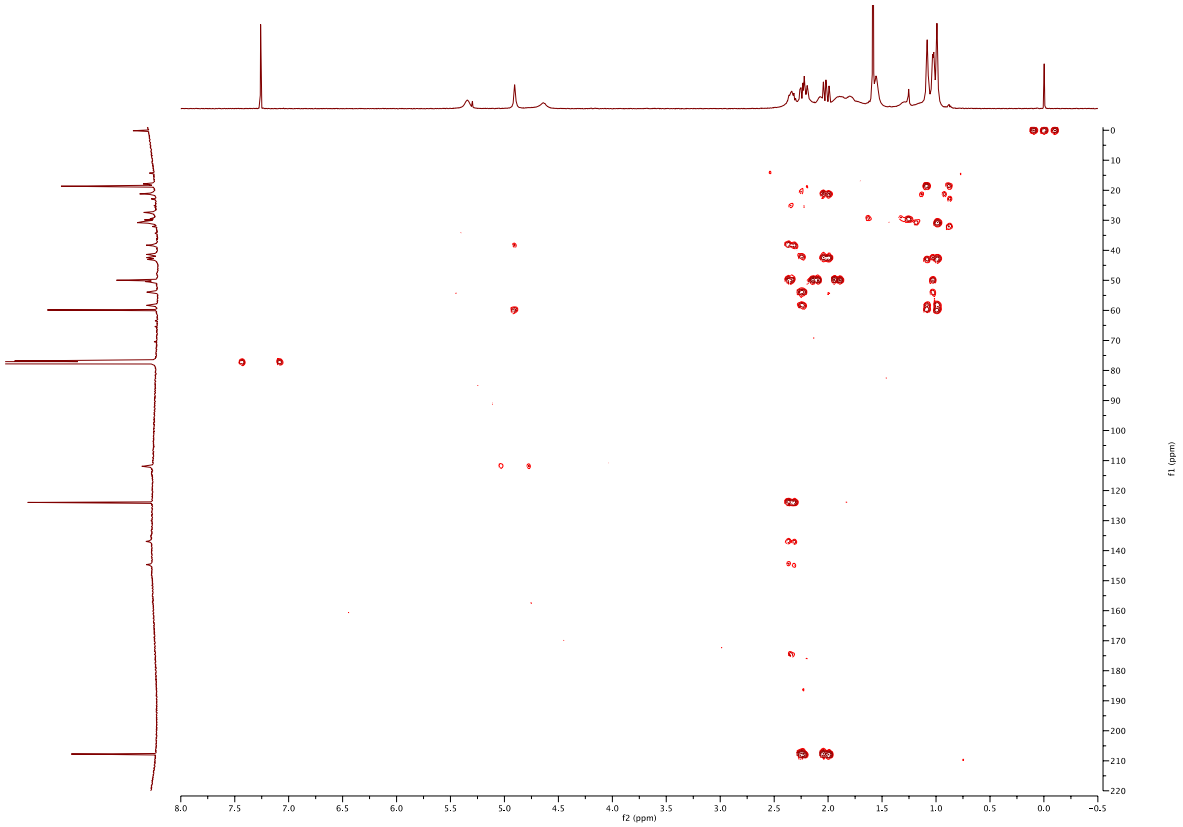

Figure S18. HMBC spectrum (500 MHz) of sinuaustone B (**2**) in $CDCl_3$.

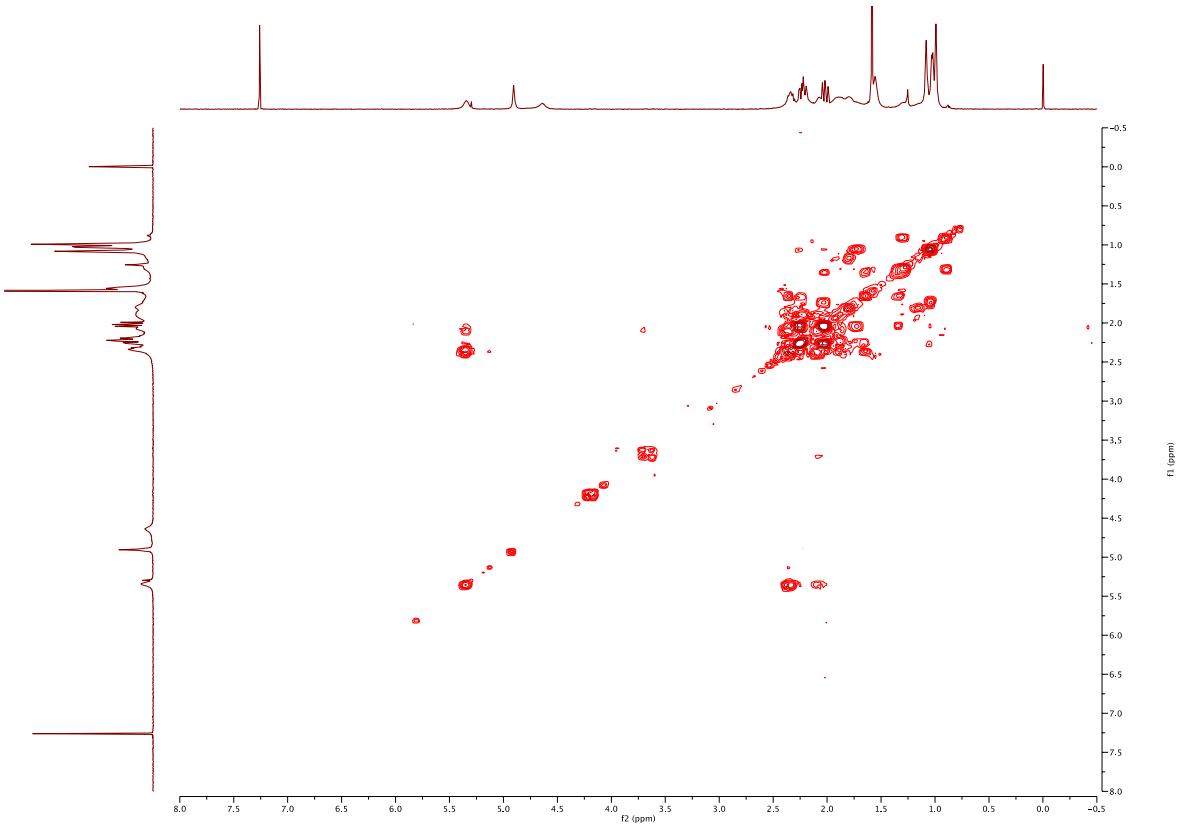

Figure S19. ^{1}H-^{1}H COSY spectrum (500 MHz) of sinuaustone B (**2**) in $CDCl_3$.

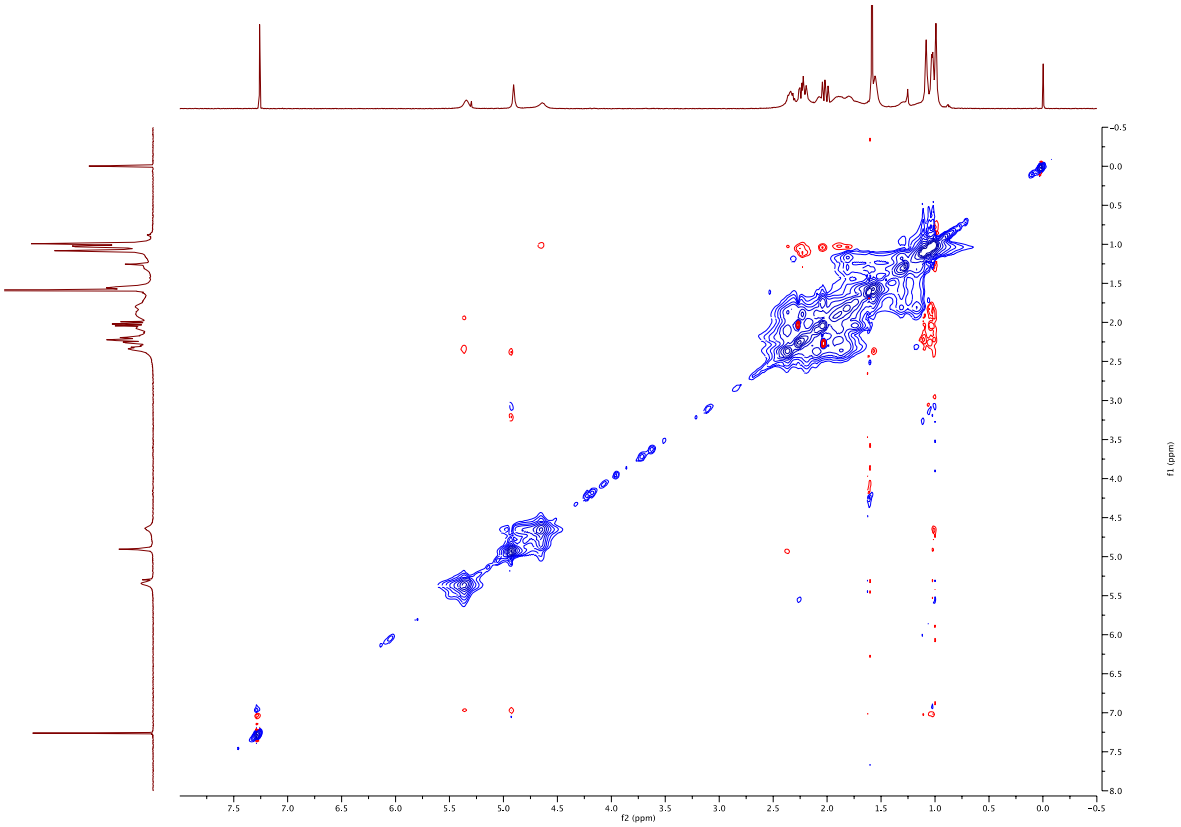

Figure S20. NOESY spectrum (500 MHz) of sinuaustone B (**2**) in $CDCl_3$.

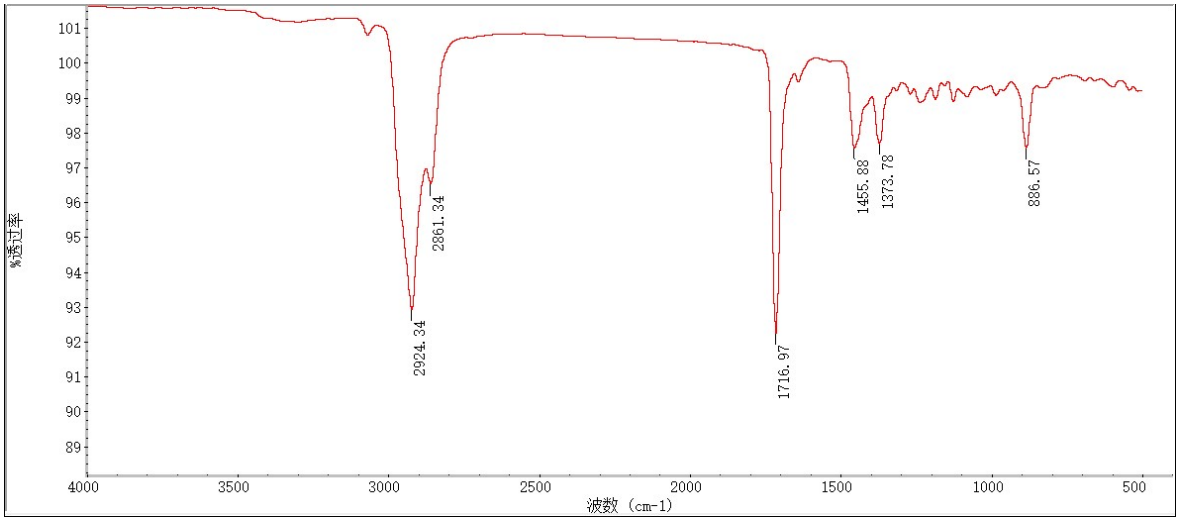

Figure S21. IR spectrum of sinuaustone B (**2**).

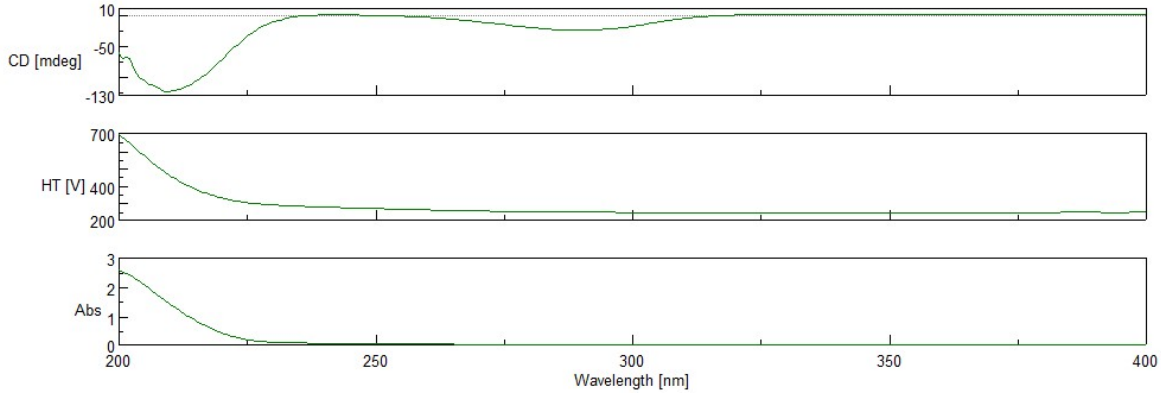

Figure S22. CD&UV spectrum of sinuaustone B (**2**).

2.6 MS, NMR, IR, CD&UV spectra of compounds 3

D:\data\2021\EI202101287_A8-EB16-4-1-c1 5/31/2021 1:39:13 PM

EI202101287_A8-EB16-4-1-c1#13 RT: 2.48
T: + c EI Full ms [49.50-800.50]
m/z= 48-803

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
79.0542	104028.0	1.26	79.0542	-0.04	3.5	C_6H_7
80.0622	76644.0	0.93	80.0621	0.11	3.0	C_6H_8
81.0696	162952.0	1.97	81.0699	-0.30	2.5	C_6H_9
83.0490	286129.0	3.45	83.0491	-0.10	2.5	$C_5H_7O_1$
91.0541	89367.0	1.08	91.0542	-0.15	4.5	C_7H_7
93.0699	83069.0	1.00	93.0699	-0.01	3.5	C_7H_9
105.0725	77817.0	0.94	105.0699	2.67	4.5	C_8H_9
125.0955	81718.0	0.99	125.0961	-0.57	2.5	$C_8H_{13}O_1$
159.1149	92325.0	1.11	159.1168	-1.96	5.5	$C_{12}H_{15}$
173.1329	165757.0	2.00	173.1325	0.37	5.5	$C_{13}H_{17}$
186.1405	225752.0	2.73	186.1403	0.23	6.0	$C_{14}H_{18}$
187.1452	94212.0	1.14	187.1481	-2.89	5.5	$C_{14}H_{19}$
188.1559	827537.0	9.99	188.1560	-0.01	5.0	$C_{14}H_{20}$
191.1436	103875.0	1.25	191.1430	0.52	4.5	$C_{13}H_{19}O_1$
203.1439	130392.0	1.57	203.1430	0.86	5.5	$C_{14}H_{19}O_1$
203.1802	233860.0	2.82	203.1794	0.80	4.5	$C_{15}H_{23}$
204.1516	141382.0	1.71	204.1509	0.77	5.0	$C_{14}H_{20}O_1$
205.1595	8282439.0	100.00	205.1587	0.79	4.5	$C_{14}H_{21}O_1$
207.1730	688093.0	8.31	207.1743	-1.37	3.5	$C_{14}H_{23}O_1$
211.1506	308031.0	3.72	211.1481	2.51	7.5	$C_{16}H_{19}$
212.1558	280137.0	3.38	212.1560	-0.15	7.0	$C_{16}H_{20}$
213.1645	415681.0	5.02	213.1638	0.74	6.5	$C_{16}H_{21}$
214.1691	119556.0	1.44	214.1716	-2.48	6.0	$C_{16}H_{22}$
215.1439	121570.0	1.47	215.1430	0.83	6.5	$C_{15}H_{19}O_1$
215.1779	112136.0	1.35	215.1794	-1.52	5.5	$C_{16}H_{23}$
217.1583	145308.0	1.75	217.1587	-0.39	5.5	$C_{15}H_{21}O_1$
225.1634	328021.0	3.96	225.1638	-0.36	7.5	$C_{17}H_{21}$
226.1691	132611.0	1.60	226.1716	-2.49	7.0	$C_{17}H_{22}$
227.1789	125446.0	1.51	227.1794	-0.54	6.5	$C_{17}H_{23}$
229.1594	122080.0	1.47	229.1587	0.70	6.5	$C_{16}H_{21}O_1$
230.1658	89393.0	1.08	230.1665	-0.67	6.0	$C_{16}H_{22}O_1$
231.1743	252677.0	3.05	231.1743	-0.05	5.5	$C_{16}H_{23}O_1$
253.1940	246022.0	2.97	253.1951	-1.12	7.5	$C_{19}H_{25}$
268.2179	88883.0	1.07	268.2186	-0.70	7.0	$C_{20}H_{28}$
271.2047	396915.0	4.79	271.2056	-0.91	6.5	$C_{19}H_{27}O_1$
286.2287	176823.0	2.13	286.2291	-0.37	6.0	$C_{20}H_{30}O_1$

Figure S23. HREIMS spectrum of isolobophytumin E (**3**).

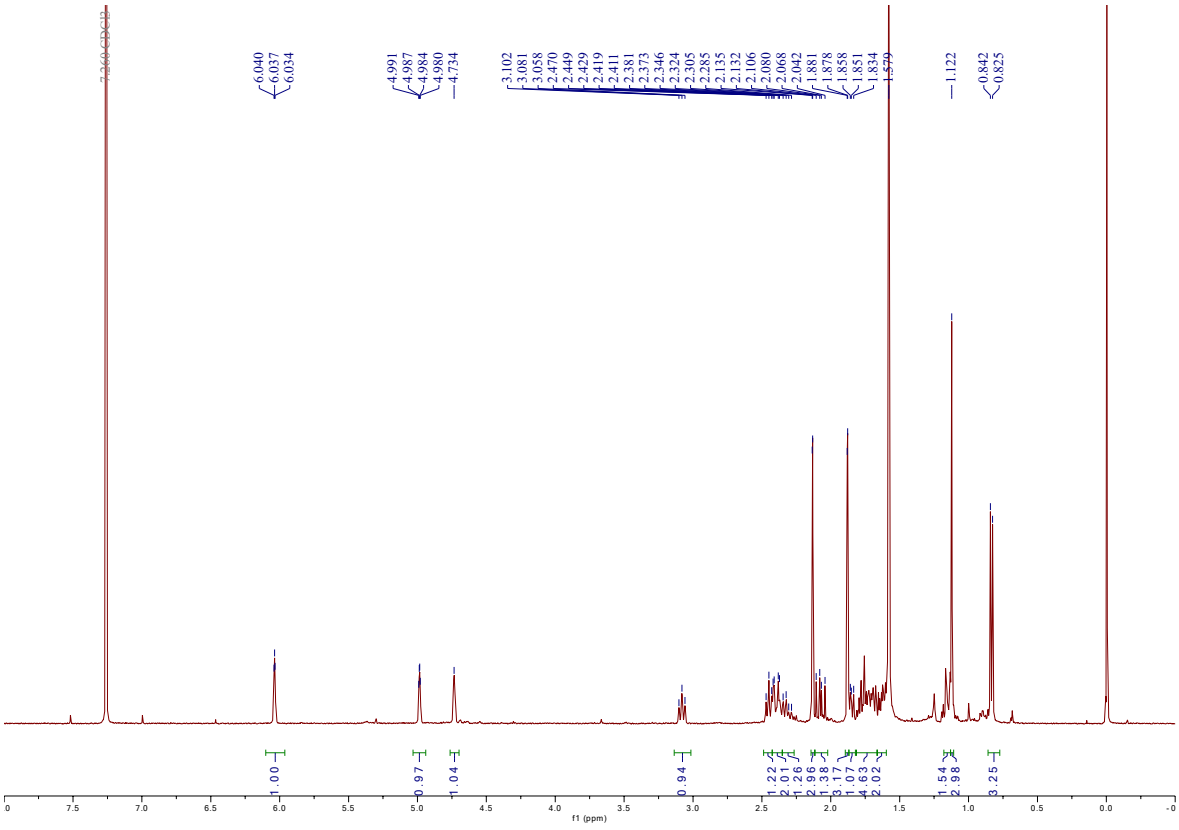

Figure S24. ^{1}H NMR spectrum (600 MHz) of isolobophytumin E (**3**) in $CDCl_3$.

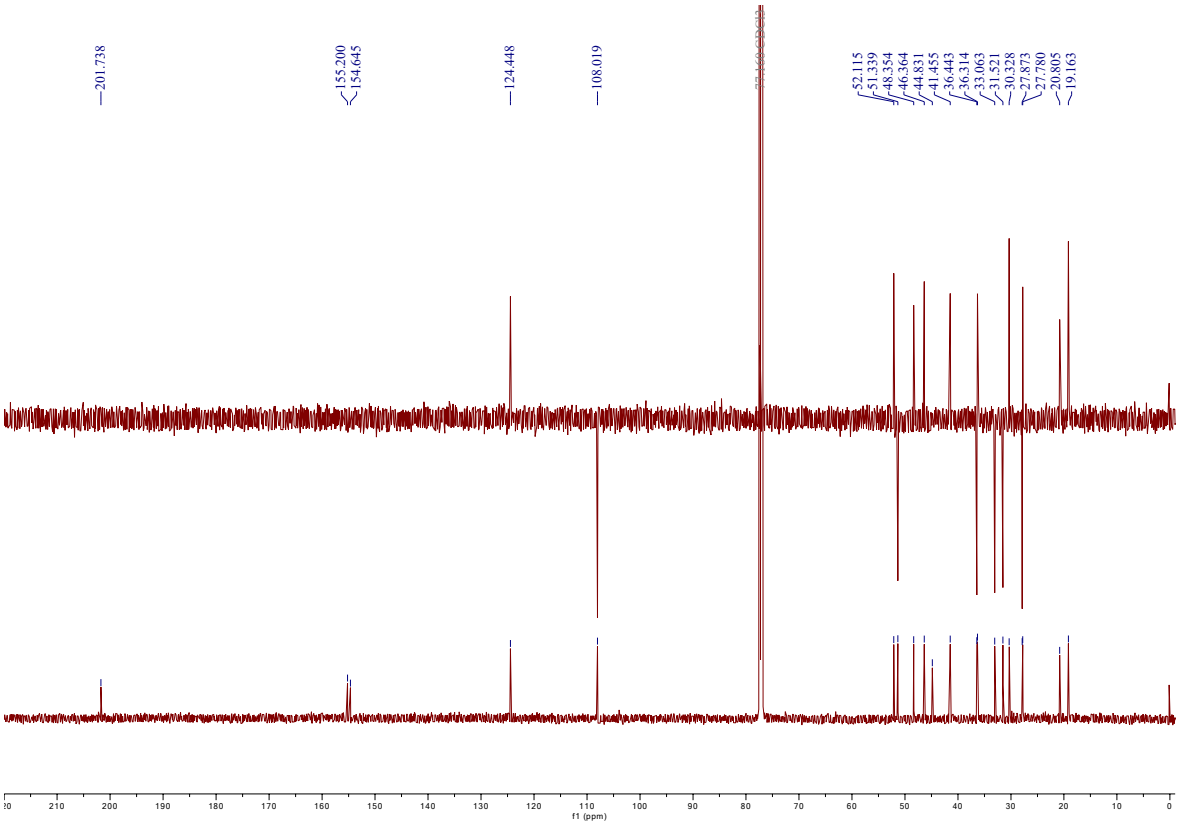

Figure S25. ^{13}C NMR spectrum (125 MHz) of isolobophytumin E (**3**) in $CDCl_3$.

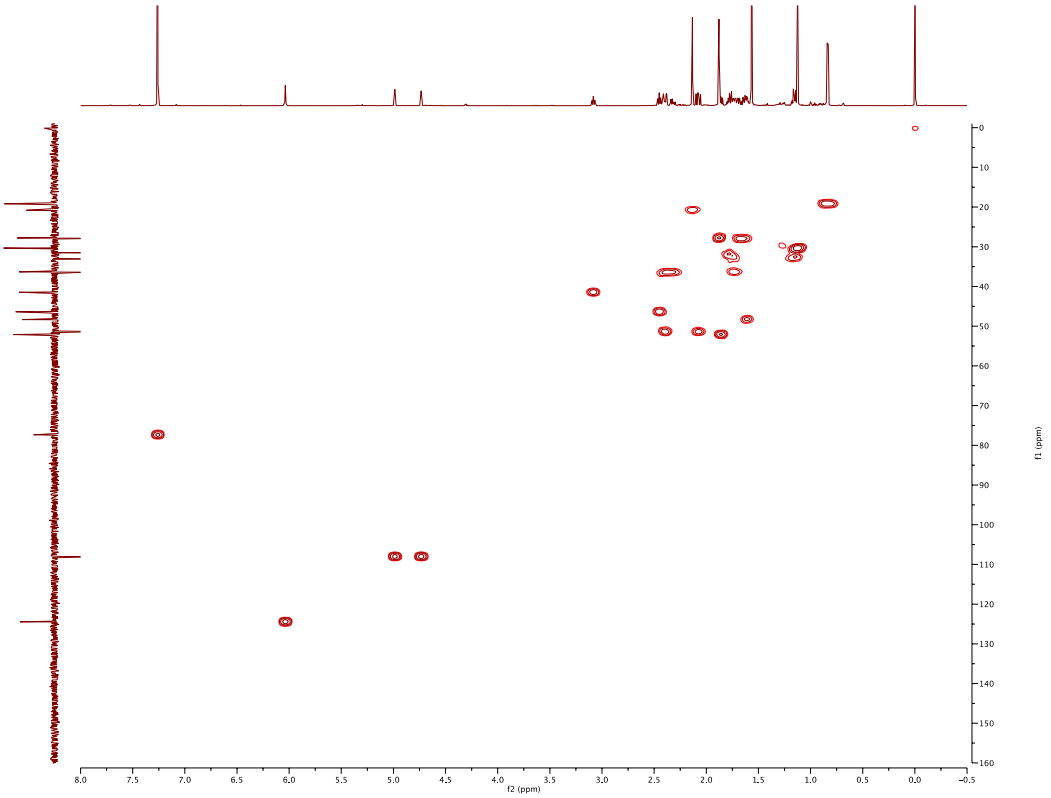

Figure S26. HSQC spectrum (500 MHz) of isolobophytumin E (**3**) in $CDCl_3$.

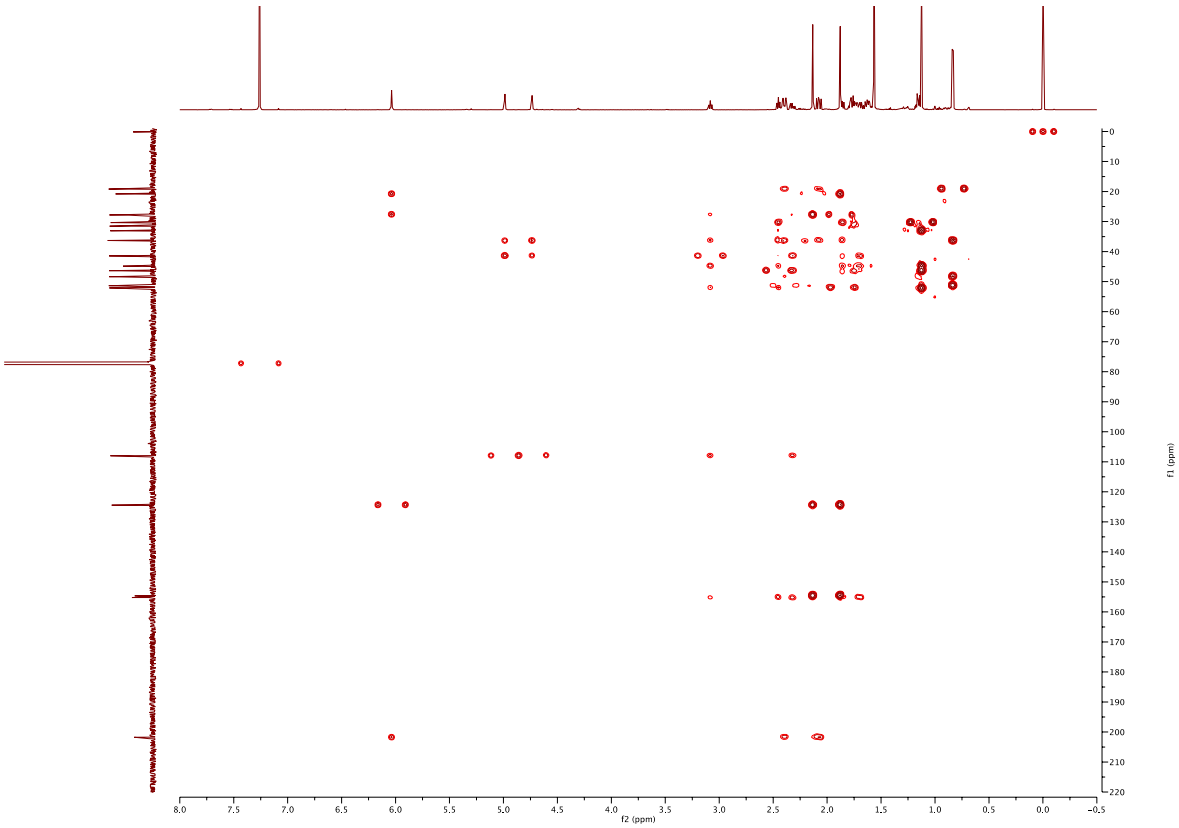

Figure S27. HMBC spectrum (500 MHz) of isolobophytumin E (**3**) in $CDCl_3$.

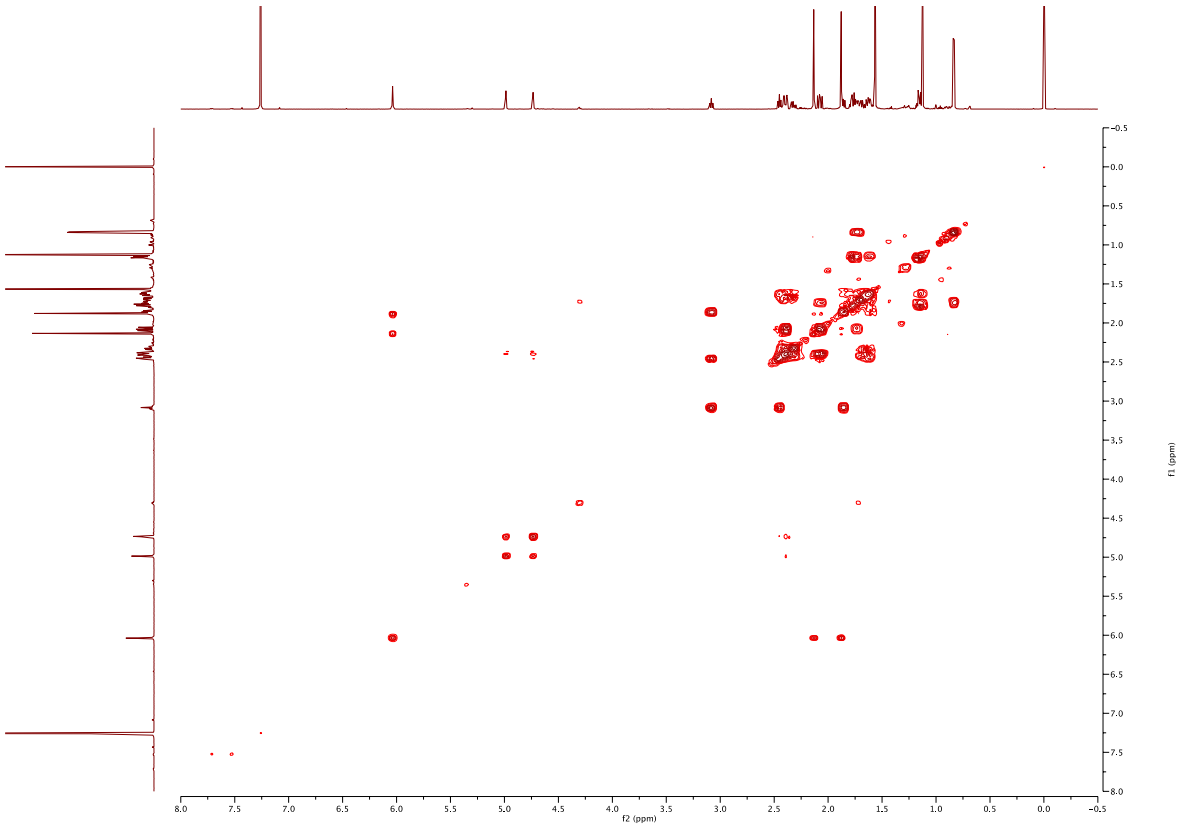

Figure S28. ^{1}H-^{1}H COSY spectrum (500 MHz) of isolobophytumin E (**3**) in $CDCl_3$.

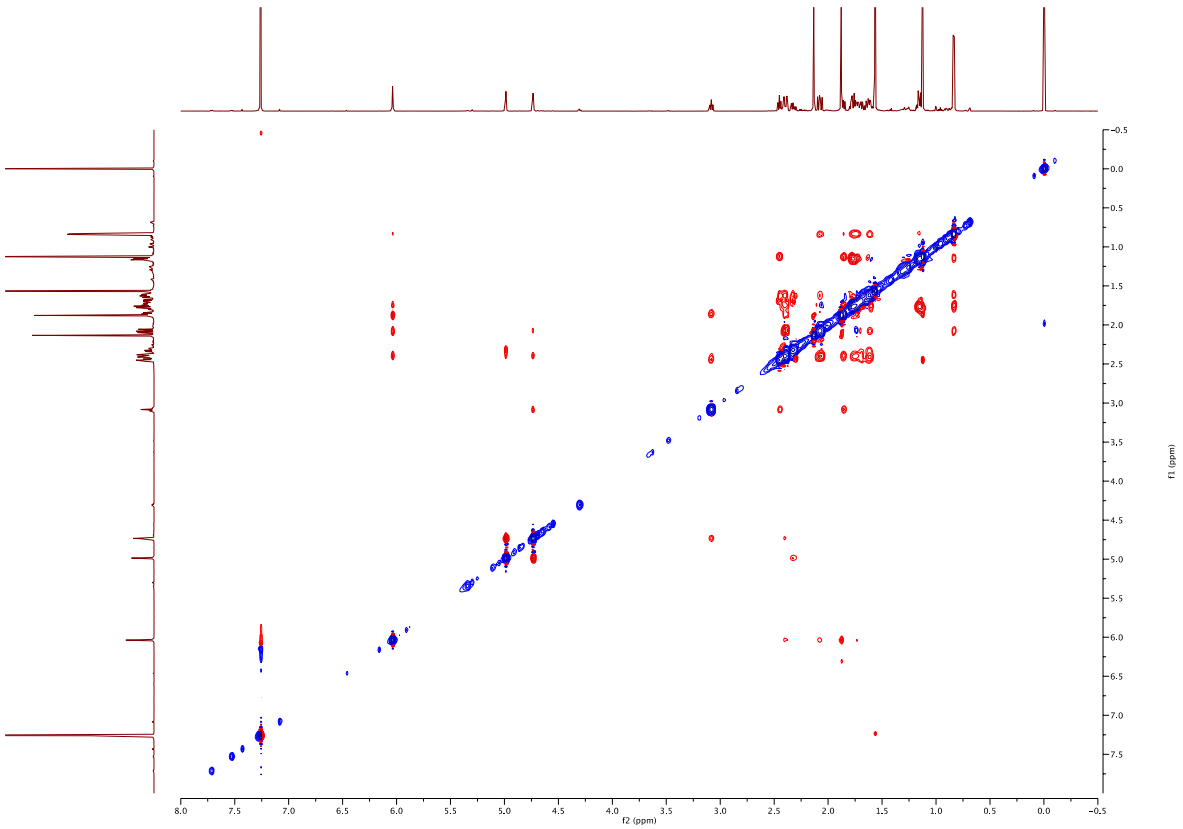

Figure S29. NOESY spectrum (500 MHz) of isolobophytumin E (**3**) in $CDCl_3$.

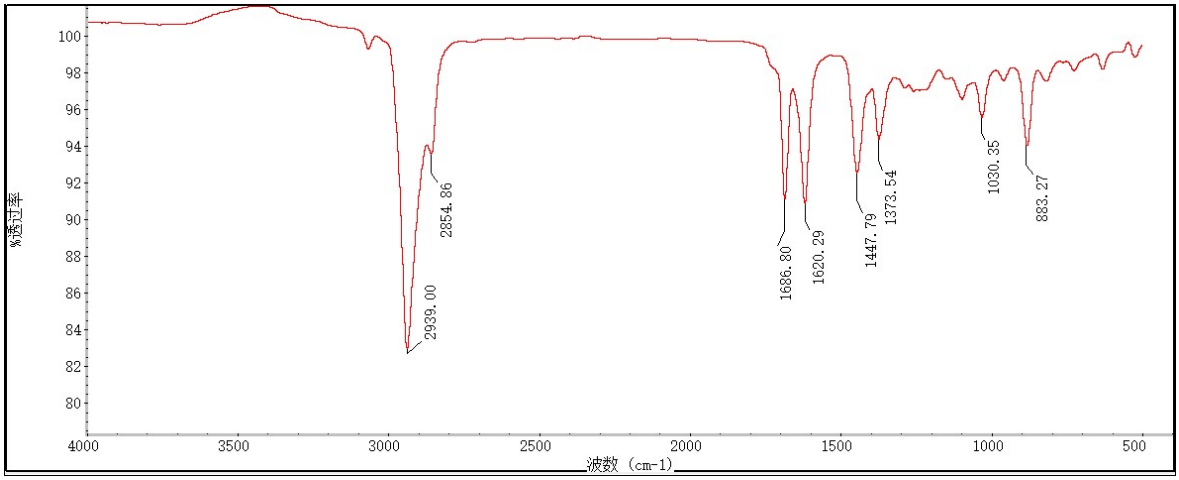

Figure S30. IR spectrum of isolobophytumin E (**3**).

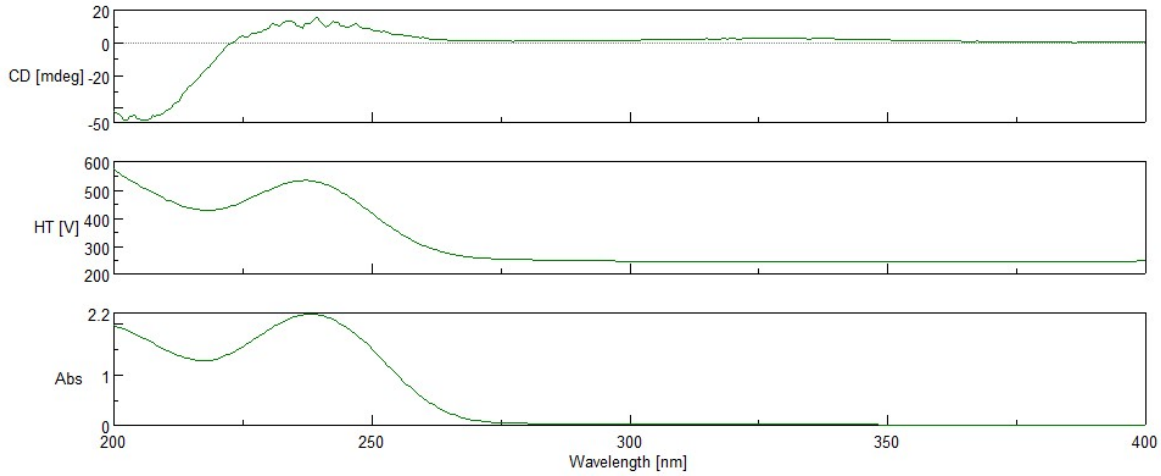

Figure S31. CD&UV spectrum of isolobophytumin E (**3**).

2.7 MS, NMR spectra of compounds 4

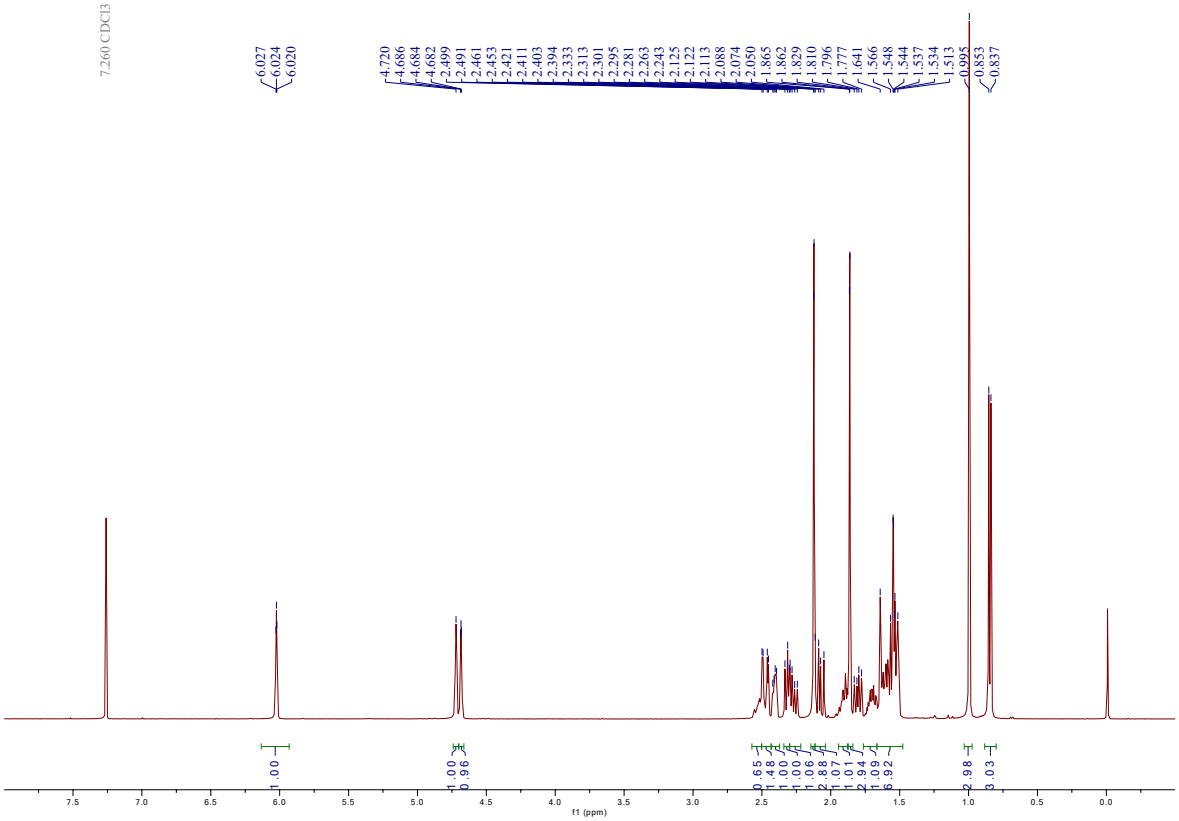

Figure S32. ^{1}H NMR spectrum (600 MHz) of lobophytumin E (**4**) in $CDCl_3$.

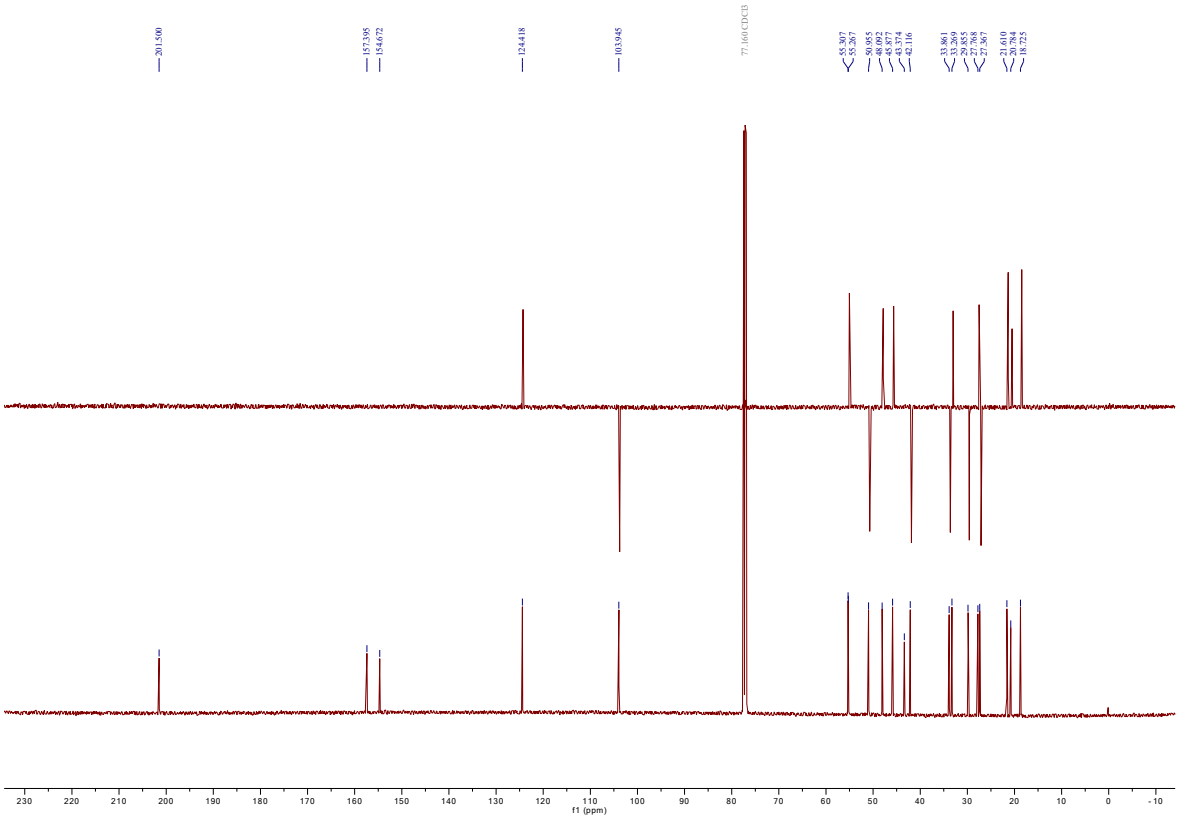

Figure S33. ^{13}C NMR spectrum (125 MHz) of lobophytumin E (**4**) in $CDCl_3$.

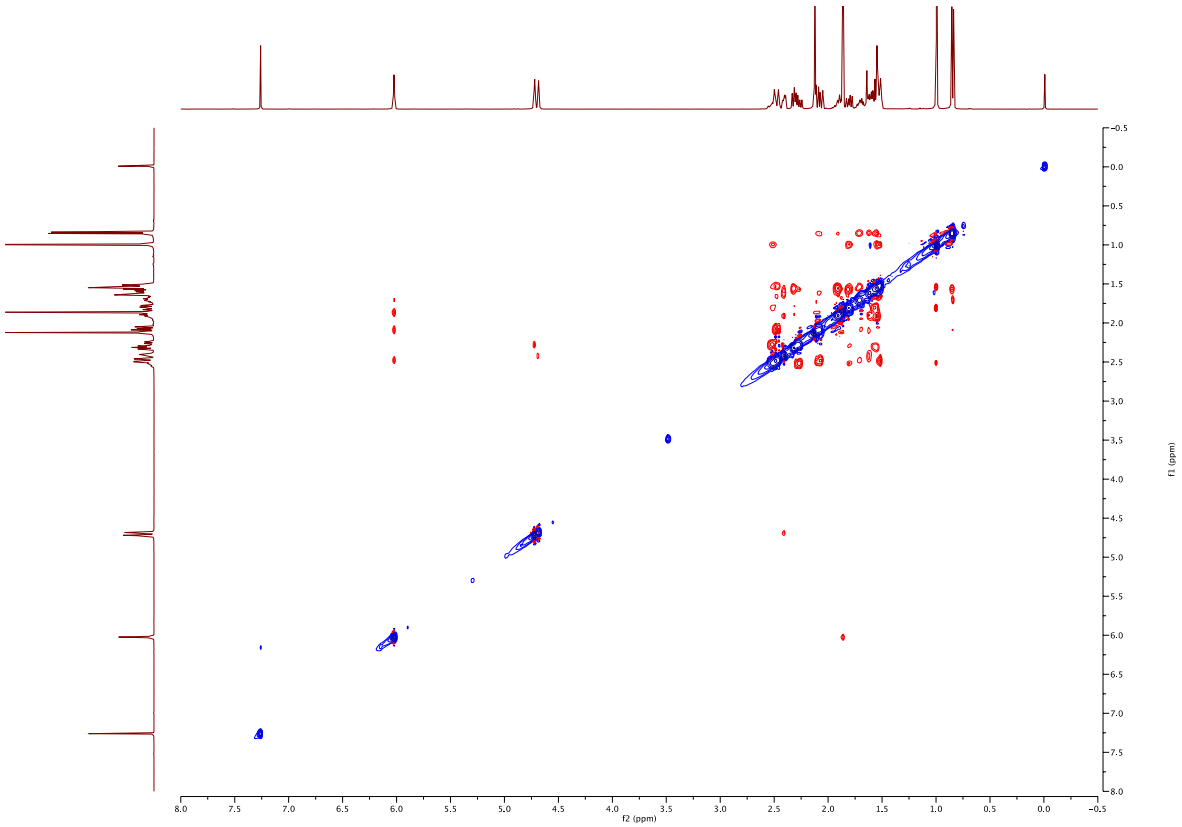

Figure S34. NOESY spectrum (500 MHz) of lobophytumin E (**4**) in $CDCl_3$.

2.8 MS, NMR spectra of compounds 5

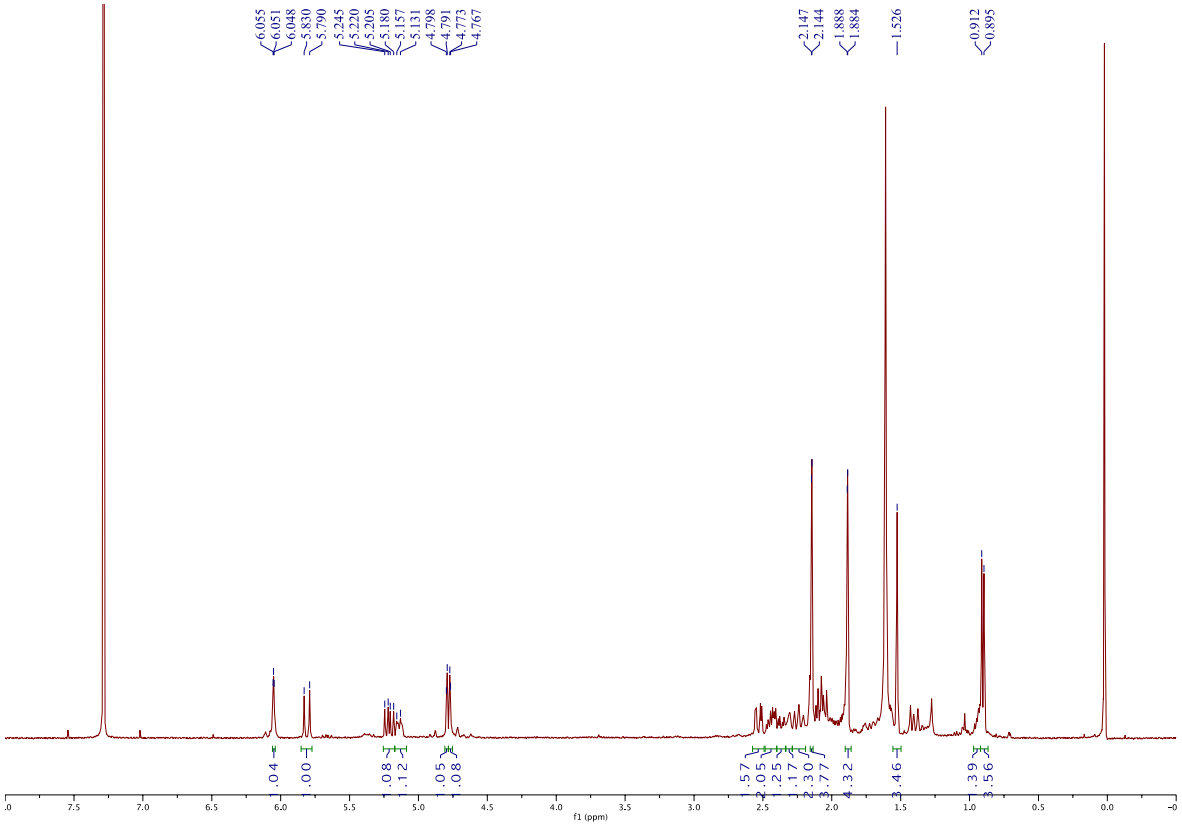

Figure S35. ^1H NMR spectrum (600 MHz) of lobophytumin A (**5**) in $CDCl_3$.

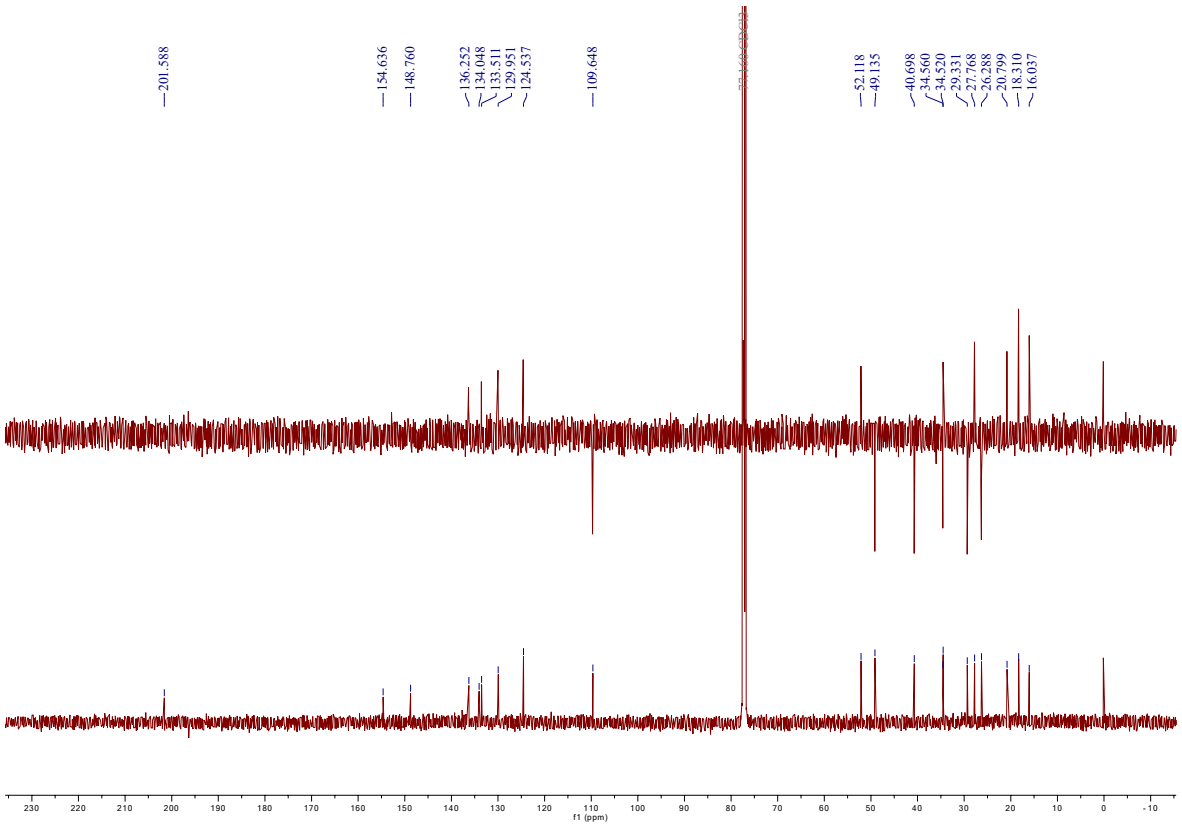

Figure S36. ^{13}C NMR spectrum (125 MHz) of lobophytumin A (**5**) in $CDCl_3$.

3. Computational Section

3.1 QM-NMR calculation for compounds 3

Theoretical calculation of all theoretical stereoisomers was carried out to determine the relative configuration at C-11 of **3**, based on the alignment of its 1D NMR chemical shifts (^{13}C NMR chemical shifts herein) and calculation-generated chemical shifts. Confab was used to search the conformational space of **3a**–**3b**. Conformational searches were carried out using the torsional sampling (MCMM) method and OPLS_2005 force field in the Macromodel 9.9.223 software applying an energy window of 21 kJ/mol. Conformers above 1% population were re-optimized with Gaussian 09 at the B3LYP/6-311G(d,p) level with IEFPCM (Polarizable Continuum Model using the Integral Equation Formalism variant) solvent model for acetonitrile. The initial torsional sampling (MCMM) and OPLS_2005 force field conformational searches of **3a**–**3b**, afforded 125 and 48 conformers within the 21 kJ/mol energy window. The Boltzmann populations of the conformers were obtained based on the potential energy provided by the OPLS_2005 force field, leading to 15 and 11 conformers above 1% population for further re-optimization, respectively. The obtained conformers were subjected to optimization and frequency calculations on B3LYP/6-311G(d,p) ($CHCl_3$) level of theory. GIAO DFT ^{13}C NMR calculations were calculated on mPW1PW91/6-31G* ($CHCl_3$) level of theory, and the calculated shielding tensors were Boltzmann averaged according to Gibbs free energy and then converted into chemical shifts following MSTD protocol.[4-8] The experimental ^{13}C NMR data of **3** were compared with the calculated NMR chemical shifts of **3a**–**3b** using the correlation coefficient (R^2), and DP4+ probability analysis.

3a 1*R**,5*S**,6*S**,7*R**,10*R**,11*S** **3b** 1*R**,5*S**,6*S**,7*R**,10*R**,11*R**

Figure S37. Structures of two possible C-11 epimeric structures **3a** and **3b**.

Table S4. Cartesian coordinates of all conformers of isomers **3a**–**3b** used after optimization at the B3LYP/6-311G(d,p) level of theory as required for DP4+ analysis.

3a-conf.1 Imaginary Freq =0				C	-3.1858	-1.7423	0.2819	C	-2.7729	-3.1349	-1.6478	
C	-4.4088	-1.6255	-0.5861	C	-2.0769	-2.4598	-0.4335	C	-4.2716	-2.8378	-1.5183	

C	-1.8736	-2.3162	-2.6084
C	-1.1443	-1.6789	-1.3893
C	-1.2640	-0.1535	-1.5171
C	-1.5511	0.0393	-3.0186
C	-2.4516	-1.1415	-3.4048
C	-3.1074	-1.2875	1.5387
C	-0.9513	-3.1986	-3.4605
H	-0.0902	-2.0362	-1.3623
H	-2.5561	-4.2288	-1.7089
H	-1.5366	-3.1884	0.2153
C	-0.0358	0.6437	-1.0219
C	-0.2647	2.1565	-1.2159
C	0.2958	0.3707	0.4616
C	1.0719	-0.9136	0.7246
C	0.6349	-1.7112	1.8911
O	2.0154	-1.2151	0.0293
C	0.7164	-3.0513	1.9805
C	0.2409	-3.7677	3.2247
C	1.2467	-3.9753	0.9091
H	-2.1566	0.2005	-0.9532
H	-4.3671	-0.6661	-1.1482
H	-5.3574	-1.6422	0.0003
H	-4.7469	-3.7135	-1.0144
H	-4.7833	-2.7128	-2.5006
H	-2.0374	1.0163	-3.2500
H	-0.5977	-0.0247	-3.5945
H	-2.4528	-1.3277	-4.5041
H	-3.4990	-0.9093	-3.1188
H	-2.1910	-1.4168	2.1334
H	-3.9593	-0.7743	2.0114
H	-0.1732	-2.5874	-3.9719
H	-0.4244	-3.9672	-2.8496
H	-1.5416	-3.7316	-4.2400
H	0.8478	0.3637	-1.6447
H	0.6164	2.7496	-0.8787
H	-0.4247	2.4217	-2.2852
H	-1.1507	2.5059	-0.6380
H	0.9534	1.1801	0.8555
H	-0.6441	0.4053	1.0588
H	0.1920	-1.1480	2.7281
H	1.0711	-4.3657	3.6641
H	-0.1258	-3.0728	4.0139
H	-0.5970	-4.4568	2.9732
H	2.1967	-4.4457	1.2495
H	0.5106	-4.7864	0.7087
H	1.4363	-3.4883	-0.0706

3a-conf.2 Imaginary Freq =0

C	-4.6457	-1.1176	-1.0485
C	-3.6571	-1.2231	0.0802
C	-2.5886	-2.2348	-0.2223
C	-3.1417	-3.0344	-1.4345
C	-4.5530	-2.5014	-1.7074
C	-1.9313	-2.5708	-2.2844
C	-1.3533	-1.8152	-1.0527
C	-1.1533	-0.3464	-1.4517
C	-1.0889	-0.4222	-2.9892
C	-2.1034	-1.5073	-3.3744
C	-3.7290	-0.5157	1.2147
C	-1.0396	-3.7337	-2.7407
H	-0.4126	-2.3135	-0.7270
H	-3.1258	-4.1374	-1.2598
H	-2.3379	-2.8838	0.6498
C	0.0788	0.3361	-0.8165
C	0.2102	1.7877	-1.3200
C	0.0328	0.3449	0.7274
C	0.3499	-0.9793	1.4101
C	1.6334	-1.6116	1.0314
O	-0.3896	-1.4286	2.2557
C	1.8617	-2.9375	1.0053
C	3.2151	-3.4763	0.5980
C	0.8547	-4.0134	1.3387
H	-2.0561	0.2462	-1.1802
H	-4.3215	-0.3093	-1.7412
H	-5.6769	-0.8793	-0.6967
H	-5.2750	-3.1772	-1.1889
H	-4.8244	-2.5058	-2.7884
H	-1.3216	0.5494	-3.4858
H	-0.0693	-0.7452	-3.3070
H	-1.9209	-1.9094	-4.3982
H	-3.1228	-1.0677	-3.3800
H	-2.9804	-0.6420	2.0116
H	-4.5392	0.2116	1.3800
H	-0.0727	-3.3606	-3.1489
H	-0.8015	-4.4327	-1.9064
H	-1.5501	-4.3195	-3.5384
H	0.9939	-0.2085	-1.1509
H	1.1011	2.2928	-0.8807
H	0.3392	1.8374	-2.4246
H	-0.6884	2.3889	-1.0509
H	0.7795	1.0691	1.1284
H	-0.9648	0.7124	1.0619
H	2.4398	-0.9270	0.7224
H	3.1178	-4.1110	-0.3119
H	3.9522	-2.6740	0.3677
H	3.6428	-4.0976	1.4172
H	1.1880	-4.5816	2.2363
H	-0.1730	-3.6439	1.5363
H	0.7684	-4.7256	0.4871

3a-conf.3 Imaginary Freq =0

C	-4.8831	-1.2453	-0.9441
C	-3.8594	-2.2173	-0.4232
C	-3.0747	-2.8322	-1.5459
C	-3.8834	-2.4891	-2.8275
C	-5.1533	-1.7659	-2.3633
C	-2.6642	-1.7063	-3.3800
C	-1.8475	-2.0803	-2.1088
C	-1.3804	-0.7677	-1.4604
C	-1.4112	0.2197	-2.6400
C	-2.6708	-0.1735	-3.4253
C	-3.6737	-2.5051	0.8712
C	-2.0893	-2.3219	-4.6626
H	-1.0069	-2.7646	-2.3738
H	-4.1077	-3.3929	-3.4442
H	-2.8983	-3.9267	-1.4158
C	-0.0123	-0.8825	-0.7568
C	0.4707	0.4852	-0.2405
C	-0.0857	-1.8914	0.4079
C	1.2610	-2.1395	1.0736
C	1.2925	-2.0251	2.5484
O	2.2244	-2.4420	0.4065
C	2.3489	-1.5844	3.2556
C	2.2962	-1.5264	4.7660
C	3.6575	-1.1094	2.6686
H	-2.1257	-0.4155	-0.7118
H	-4.4424	-0.2235	-0.9638
H	-5.8041	-1.2137	-0.3160
H	-5.9695	-2.5252	-2.2992
H	-5.4980	-0.9801	-3.0745
H	-1.4428	1.2870	-2.3164
H	-0.5102	0.0698	-3.2808
H	-2.6589	0.2256	-4.4663
H	-3.5625	0.2586	-2.9234
H	-2.9077	-3.2313	1.1854
H	-4.2794	-2.0217	1.6535
H	-1.0967	-1.8809	-4.9088
H	-1.9528	-3.4240	-4.5740
H	-2.7747	-2.1331	-5.5199
H	0.7310	-1.2510	-1.5051
H	1.4513	0.4062	0.2817
H	0.6156	1.2125	-1.0709
H	-0.2600	0.9238	0.4768
H	-0.8249	-1.5230	1.1560
H	-0.4487	-2.8809	0.0462
H	0.3714	-2.3056	3.0845
H	2.4220	-0.4770	5.1166
H	1.3351	-1.9046	5.1828
H	3.1146	-2.1438	5.2010
H	4.4655	-1.8404	2.8982
H	3.6351	-0.9470	1.5699
H	3.9395	-0.1288	3.1143

3a-conf.4 Imaginary Freq =0

C	-2.8632	-3.8575	-0.0011
C	-1.6924	-3.7526	-0.9403
C	-2.1049	-3.0071	-2.1721
C	-3.4779	-2.3671	-1.8093
C	-3.6178	-2.5503	-0.2891
C	-2.9968	-1.0398	-2.4537
C	-1.5399	-1.5976	-2.4493
C	-0.8111	-0.8178	-1.3453
C	-1.4902	0.5599	-1.4102
C	-2.9802	0.2515	-1.6259
C	-0.4743	-4.2650	-0.7306
C	-3.5549	-0.8366	-3.8678
H	-1.0775	-1.4951	-3.4568
H	-4.3162	-2.8593	-2.3590
H	-2.1712	-3.6518	-3.0811
C	0.7312	-0.8128	-1.4088
C	1.3221	-0.3706	-2.7602
C	1.3502	0.0426	-0.2827
C	0.7995	-0.2357	1.1085
C	0.9015	-1.6309	1.5894

O	0.3590	0.6670	1.7841
C	0.0145	-2.2091	2.4197
C	0.2227	-3.6233	2.9120
C	-1.2351	-1.5477	2.9520
H	-1.0966	-1.2608	-0.3651
H	-2.5658	-3.9688	1.0672
H	-3.4842	-4.7326	-0.3050
H	-4.6843	-2.5942	0.0344
H	-3.1283	-1.7366	0.2896
H	-1.3245	1.1771	-0.4961
H	-1.1062	1.1268	-2.2897
H	-3.4867	1.0963	-2.1486
H	-3.5121	0.1259	-0.6573
H	0.3205	-4.1544	-1.4843
H	-0.2388	-4.8167	0.1920
H	-3.0156	-0.0159	-4.3937
H	-3.4589	-1.7548	-4.4911
H	-4.6348	-0.5685	-3.8207
H	1.0649	-1.8669	-1.2528
H	2.4358	-0.3641	-2.7238
H	1.0478	-1.0594	-3.5900
H	0.9976	0.6564	-3.0404
H	2.4549	-0.1066	-0.2440
H	1.1883	1.1206	-0.5168
H	1.7588	-2.2178	1.2223
H	-0.6395	-4.2680	2.6291
H	1.1433	-4.0952	2.4998
H	0.3109	-3.6285	4.0220
H	-2.1016	-2.2412	2.8658
H	-1.1031	-1.2913	4.0273
H	-1.5330	-0.6299	2.4008

3a-conf.5 Imaginary Freq =0

C	-4.8862	-0.5514	-1.4209
C	-4.1616	-1.3641	-0.3826
C	-3.3986	-2.4932	-1.0123
C	-3.9588	-2.5904	-2.4584
C	-5.0916	-1.5618	-2.5589
C	-2.5446	-2.2911	-3.0194
C	-1.9817	-2.2283	-1.5696
C	-1.3243	-0.8507	-1.3911
C	-1.0087	-0.4378	-2.8393
C	-2.2212	-0.9283	-3.6435
C	-4.1959	-1.1207	0.9336
C	-1.9657	-3.4548	-3.8350
H	-1.2816	-3.0777	-1.3867
H	-4.2954	-3.6236	-2.7163
H	-3.4758	-3.4512	-0.4446
C	-0.0999	-0.8740	-0.4529
C	0.6098	0.4914	-0.4151
C	-0.5172	-1.2963	0.9709
C	0.6524	-1.4240	1.9367
C	1.6825	-2.4179	1.5629
O	0.6818	-0.7786	2.9599
C	2.9923	-2.3036	1.8475
C	3.9671	-3.3854	1.4395
C	3.6321	-1.1396	2.5672
H	-2.0576	-0.1169	-0.9864
H	-4.2387	0.2952	-1.7414
H	-5.8470	-0.1296	-1.0431
H	-6.0523	-2.0987	-2.3703
H	-5.1750	-1.0951	-3.5676
H	-0.8523	0.6608	-2.9566
H	-0.0909	-0.9662	-3.1906
H	-2.0026	-0.9965	-4.7346
H	-3.0537	-0.2026	-3.5253
H	-3.6446	-1.7589	1.6418
H	-4.7732	-0.2758	1.3404
H	-0.8800	-3.3044	-4.0330
H	-2.0775	-4.4311	-3.3101
H	-2.4889	-3.5350	-4.8148
H	0.6239	-1.6228	-0.8562
H	1.4920	0.4777	0.2648
H	0.9933	0.7864	-1.4178
H	-0.0795	1.2920	-0.0618
H	-1.2386	-0.5491	1.3762
H	-1.0464	-2.2769	0.9574
H	1.3335	-3.2922	0.9899
H	4.4957	-3.7816	2.3360
H	3.4742	-4.2470	0.9344
H	4.7260	-2.9752	0.7353
H	4.5176	-0.7808	1.9954
H	2.9705	-0.2554	2.6876
H	3.9766	-1.4588	3.5768

3a-conf.6 Imaginary Freq =0

C	-4.8897	-1.3589	-0.9604
C	-3.7999	-2.2519	-0.4325
C	-2.9745	-2.8199	-1.5508
C	-3.8066	-2.5460	-2.8342
C	-5.1239	-1.9101	-2.3744
C	-2.6462	-1.6839	-3.3950
C	-1.8036	-1.9888	-2.1223
C	-1.4285	-0.6414	-1.4854
C	-1.5319	0.3320	-2.6726
C	-2.7612	-0.1559	-3.4528
C	-3.5938	-2.5149	0.8641
C	-2.0306	-2.2680	-4.6734
H	-0.9177	-2.6148	-2.3833
H	-3.9670	-3.4687	-3.4426
H	-2.7215	-3.8981	-1.4113
C	-0.0533	-0.6536	-0.7862
C	0.3334	0.7487	-0.2829
C	-0.0498	-1.6570	0.3850
C	1.3187	-1.8177	1.0344
C	1.4306	-1.3925	2.4480
O	2.2493	-2.2272	0.3782
C	2.3197	-1.8810	3.3322
C	2.3683	-1.3492	4.7477
C	3.3358	-2.9635	3.0525
H	-2.1943	-0.3369	-0.7367
H	-4.5217	-0.3090	-0.9896
H	-5.8102	-1.3864	-0.3312
H	-5.8845	-2.7244	-2.3023
H	-5.5239	-1.1569	-3.0920
H	-1.6393	1.3968	-2.3573
H	-0.6236	0.2418	-3.3142
H	-2.7786	0.2345	-4.4970
H	-3.6807	0.2164	-2.9531
H	-2.7786	-3.1828	1.1837
H	-4.2317	-2.0685	1.6428
H	-1.0716	-1.7603	-4.9246
H	-1.8167	-3.3570	-4.5760
H	-2.7282	-2.1350	-5.5312
H	0.7124	-0.9742	-1.5339
H	1.3240	0.7441	0.2260
H	0.4148	1.4803	-1.1182
H	-0.4188	1.1363	0.4416
H	-0.8095	-1.3495	1.1399
H	-0.3509	-2.6696	0.0302
H	0.7164	-0.6251	2.7875
H	3.3817	-0.9438	4.9689
H	1.6348	-0.5317	4.9319
H	2.1485	-2.1641	5.4742
H	4.3602	-2.5273	3.0322
H	3.3028	-3.7325	3.8571
H	3.1718	-3.5143	2.1022

3a-conf.7 Imaginary Freq =0

C	-2.6621	-3.6185	-0.1782
C	-1.5495	-3.6833	-1.1892
C	-1.8791	-2.8802	-2.4134
C	-3.3995	-2.5830	-2.2976
C	-3.8934	-3.3182	-1.0455
C	-3.0918	-1.0632	-2.2798
C	-1.5710	-1.3659	-2.4294
C	-0.8723	-0.7038	-1.2328
C	-1.8516	0.4076	-0.8223
C	-3.2287	-0.2538	-0.9830
C	-0.4103	-4.3682	-1.0294
C	-3.6701	-0.3194	-3.4910
H	-1.1941	-1.0291	-3.4218
H	-3.9625	-2.8783	-3.2158
H	-1.6058	-3.3957	-3.3651
C	0.5896	-0.2736	-1.4731
C	0.7614	0.8290	-2.5345
C	1.2750	0.1777	-0.1653
C	1.2899	-0.9032	0.9092
C	0.2922	-0.7608	1.9943
O	2.1118	-1.7894	0.8543
C	-0.2282	-1.7773	2.7062
C	-1.2529	-1.5125	3.7870
C	0.1028	-3.2405	2.5326
H	-0.8656	-1.4392	-0.3992
H	-2.4631	-2.7901	0.5380
H	-2.7660	-4.5627	0.4062
H	-4.3238	-4.2941	-1.3758
H	-4.7032	-2.7745	-0.5062
H	-1.6827	0.7814	0.2148
H	-1.7819	1.2708	-1.5231
H	-4.0541	0.4944	-1.0282
H	-3.4249	-0.9005	-0.1010
H	0.3647	-4.3664	-1.8118
H	-0.2191	-4.9485	-0.1136

H	-3.2500	0.7093	-3.5673
H	-3.4481	-0.8426	-4.4491
H	-4.7768	-0.2362	-3.3988
H	1.1307	-1.1791	-1.8440
H	1.8406	1.0157	-2.7405
H	0.2958	0.5630	-3.5091
H	0.3246	1.7969	-2.2013
H	2.3357	0.4554	-0.3701
H	0.7849	1.1031	0.2147
H	-0.0706	0.2587	2.2004
H	-0.8905	-1.9047	4.7642
H	-1.4744	-0.4296	3.9230
H	-2.2127	-2.0191	3.5369
H	0.6279	-3.6208	3.4377
H	-0.8331	-3.8296	2.4029
H	0.7363	-3.4697	1.6512

3a-conf.8 Imaginary Freq =0

C	-3.3779	-2.7935	0.1516
C	-2.1758	-3.4310	-0.4906
C	-2.1080	-3.1126	-1.9552
C	-3.5086	-2.5376	-2.3033
C	-4.3516	-2.6398	-1.0262
C	-2.8441	-1.2046	-2.7351
C	-1.4397	-1.7967	-2.4121
C	-0.7918	-0.8562	-1.3855
C	-1.5180	0.4779	-1.6218
C	-2.9741	0.0526	-1.8649
C	-1.2802	-4.1903	0.1521
C	-3.0302	-0.8975	-4.2271
H	-0.8489	-1.9342	-3.3454
H	-3.9811	-3.0614	-3.1691
H	-1.8273	-3.9910	-2.5843
C	0.7501	-0.8046	-1.4013
C	1.3666	-0.3508	-2.7379
C	1.3016	0.0904	-0.2709
C	0.7707	-0.2563	1.1131
C	1.2074	-1.5580	1.6647
O	0.0823	0.5345	1.7177
C	0.5211	-2.2719	2.5757
C	1.0830	-3.5659	3.1214
C	-0.8207	-1.8889	3.1548
H	-1.0952	-1.1977	-0.3712
H	-3.0914	-1.8026	0.5696
H	-3.7979	-3.4094	0.9811
H	-4.9541	-3.5774	-1.0946
H	-5.0746	-1.7999	-0.9072
H	-1.4255	1.1854	-0.7642
H	-1.1269	0.9797	-2.5364
H	-3.5720	0.8556	-2.3556
H	-3.4576	-0.1612	-0.8876
H	-0.4177	-4.6232	-0.3785
H	-1.3855	-4.3997	1.2272
H	-2.3638	-0.0659	-4.5511
H	-2.8005	-1.7789	-4.8684
H	-4.0833	-0.5967	-4.4291
H	1.1041	-1.8489	-1.2165
H	2.4796	-0.3785	-2.6895
H	1.0779	-1.0045	-3.5901
H	1.0791	0.6929	-2.9956
H	2.4149	0.0314	-0.2377
H	1.0560	1.1554	-0.4905
H	2.1603	-1.9576	1.2821
H	0.3973	-4.4153	2.9043
H	2.0772	-3.8238	2.6911
H	1.2058	-3.4898	4.2255
H	-1.4975	-2.7725	3.1747
H	-0.6955	-1.5268	4.2002
H	-1.3629	-1.1140	2.5718

3a-conf.9 Imaginary Freq =0

C	-2.2042	-4.3956	-0.8722
C	-1.2294	-3.6768	-1.7652
C	-1.9654	-2.6694	-2.5961
C	-3.3554	-2.5387	-1.9039
C	-3.2072	-3.2745	-0.5621
C	-3.2478	-0.9965	-2.0276
C	-1.7376	-1.1562	-2.3839
C	-0.9727	-0.6451	-1.1547
C	-1.9058	0.4428	-0.5991
C	-3.3228	-0.1265	-0.7660
C	0.0877	-3.9062	-1.8202
C	-4.0774	-0.4384	-3.1904
H	-1.4871	-0.6171	-3.3254
H	-4.1667	-2.9861	-2.5276
H	-2.0622	-2.9647	-3.6684
C	0.4875	-0.2105	-1.4072
C	0.6545	0.9688	-2.3835
C	1.2179	0.1213	-0.0885
C	1.1980	-1.0308	0.9068
C	0.3681	-0.8358	2.1163
O	1.8579	-2.0239	0.6999
C	-0.3088	-1.8179	2.7384
C	-1.1259	-1.5279	3.9772
C	-0.3489	-3.2628	2.3011
H	-0.9586	-1.4668	-0.4041
H	-1.7356	-4.8370	0.0377
H	-2.6998	-5.2037	-1.4598
H	-4.1809	-3.6636	-0.1819
H	-2.7646	-2.6345	0.2329
H	-1.6839	0.7110	0.4606
H	-1.8233	1.3651	-1.2187
H	-4.0714	0.6943	-0.8629
H	-3.6287	-0.7141	0.1270
H	0.7300	-3.3432	-2.5144
H	0.5597	-4.6663	-1.1783
H	-3.8001	0.6192	-3.4039
H	-3.9269	-1.0212	-4.1277
H	-5.1621	-0.4700	-2.9401
H	1.0087	-1.0840	-1.8679
H	1.7328	1.1673	-2.5831
H	0.1844	0.7755	-3.3729
H	0.2247	1.9114	-1.9771
H	2.2874	0.3630	-0.2934
H	0.7716	1.0374	0.3618
H	0.2840	0.1928	2.5023
H	-0.7729	-2.1581	4.8247
H	-1.0619	-0.4644	4.3016
H	-2.1999	-1.7557	3.7908
H	0.2161	-3.8955	3.0222
H	-1.4023	-3.6220	2.2773
H	0.0598	-3.4432	1.2844

3a-conf.10 Imaginary Freq =0

C	-3.1693	-3.5508	0.0975
C	-1.8936	-3.5989	-0.6990
C	-2.1361	-3.0408	-2.0679
C	-3.5202	-2.3336	-1.9652
C	-3.8367	-2.2852	-0.4614
C	-2.9287	-1.1229	-2.7340
C	-1.4997	-1.6977	-2.4876
C	-0.8641	-0.7737	-1.4387
C	-1.5033	0.5882	-1.7550
C	-2.9673	0.2722	-2.0976
C	-0.7250	-4.0851	-0.2655
C	-3.3217	-1.1170	-4.2164
H	-0.9250	-1.7632	-3.4388
H	-4.3067	-2.8889	-2.5312
H	-2.1228	-3.8155	-2.8718
C	0.6781	-0.7903	-1.3687
C	1.3925	-0.3776	-2.6691
C	1.2047	0.0809	-0.2088
C	0.6129	-0.2829	1.1459
C	1.0909	-1.5516	1.7392
O	-0.1559	0.4714	1.6980
C	0.3977	-2.2898	2.6251
C	0.9984	-3.5427	3.2229
C	-0.9914	-1.9726	3.1258
H	-1.2462	-1.0817	-0.4396
H	-3.0033	-3.5108	1.1992
H	-3.7801	-4.4496	-0.1531
H	-4.9336	-2.2567	-0.2612
H	-3.3799	-1.4079	0.0474
H	-1.4190	1.3174	-0.9152
H	-1.0187	1.0326	-2.6546
H	-3.3863	1.0403	-2.7890
H	-3.6103	0.2953	-1.1906
H	0.1604	-4.0973	-0.9196
H	-0.6243	-4.4929	0.7515
H	-2.7020	-0.3892	-4.7885
H	-3.1867	-2.1170	-4.6882
H	-4.3913	-0.8282	-4.3303
H	0.9797	-1.8451	-1.1601
H	2.4975	-0.4748	-2.5613
H	1.1086	-1.0157	-3.5348
H	1.1874	0.6820	-2.9401
H	2.3147	0.0008	-0.1364
H	0.9889	1.1539	-0.4201
H	2.0826	-1.9048	1.4136
H	0.3658	-4.4296	2.9936
H	2.0229	-3.7578	2.8429
H	1.0661	-3.4391	4.3295
H	-1.6060	-2.9001	3.1605
H	-0.9399	-1.5547	4.1565

H	-1.5552	-1.2667	2.4784

3a-conf.11 Imaginary Freq =0

C	-2.3138	-4.1492	-0.3454
C	-1.2360	-3.6537	-1.2711
C	-1.8537	-2.8559	-2.3796
C	-3.3127	-2.5890	-1.9030
C	-3.3378	-3.0074	-0.4234
C	-3.1617	-1.1109	-2.3498
C	-1.6221	-1.3308	-2.4673
C	-1.0136	-0.5728	-1.2793
C	-1.9832	0.6046	-1.0907
C	-3.3808	0.0121	-1.3275
C	0.0727	-3.8993	-1.1398
C	-3.8271	-0.8313	-3.7026
H	-1.2316	-1.0000	-3.4569
H	-4.0524	-3.1700	-2.5050
H	-1.8265	-3.3730	-3.3687
C	0.4784	-0.2057	-1.4214
C	0.7682	0.8627	-2.4916
C	1.0884	0.2412	-0.0756
C	1.1166	-0.8676	0.9716
C	-0.0182	-0.9008	1.9234
O	2.0566	-1.6287	1.0000
C	-0.3810	-1.9552	2.6772
C	-1.5730	-1.8573	3.6043
C	0.2959	-3.3053	2.7110
H	-1.1185	-1.2256	-0.3863
H	-1.9536	-4.3451	0.6911
H	-2.7475	-5.0845	-0.7708
H	-4.3547	-3.3219	-0.0901
H	-2.9958	-2.2000	0.2612
H	-1.8932	1.0894	-0.0903
H	-1.7998	1.3772	-1.8722
H	-4.0835	0.7925	-1.7028
H	-3.8255	-0.3677	-0.3818
H	0.7968	-3.5099	-1.8717
H	0.4563	-4.5032	-0.3030
H	-3.5048	0.1555	-4.1066
H	-3.5706	-1.6053	-4.4615
H	-4.9352	-0.8168	-3.5916
H	1.0135	-1.1334	-1.7374
H	1.8647	0.9684	-2.6613
H	0.3164	0.6095	-3.4765
H	0.3931	1.8657	-2.1875
H	2.1426	0.5704	-0.2321
H	0.5478	1.1353	0.3109
H	-0.6295	0.0135	1.9862
H	-1.2632	-2.0708	4.6524
H	-2.0528	-0.8523	3.5957
H	-2.3504	-2.5974	3.3071
H	0.7980	-3.4506	3.6941
H	-0.4585	-4.1145	2.5888
H	1.0510	-3.4705	1.9154

3a-conf.12 Imaginary Freq =0

C	-4.9244	-0.7669	-1.2808
C	-4.0351	-1.5045	-0.3171
C	-3.2024	-2.5333	-1.0256
C	-3.8591	-2.6764	-2.4265
C	-5.1039	-1.7811	-2.4198
C	-2.5350	-2.2133	-3.0872
C	-1.8714	-2.1042	-1.6836
C	-1.3597	-0.6633	-1.5266
C	-1.2058	-0.2011	-2.9862
C	-2.4148	-0.8155	-3.7060
C	-3.9936	-1.2808	1.0024
C	-1.8954	-3.2947	-3.9681
H	-1.0688	-2.8714	-1.5720
H	-4.0974	-3.7380	-2.6788
H	-3.1280	-3.5003	-0.4729
C	-0.0724	-0.5582	-0.6823
C	0.4802	0.8782	-0.6766
C	-0.3318	-1.0444	0.7584
C	0.9229	-1.1023	1.6205
C	1.7782	-2.2941	1.4175
O	1.1715	-0.1996	2.3867
C	2.7135	-2.7442	2.2742
C	3.5440	-3.9620	1.9307
C	3.0568	-2.1389	3.6153
H	-2.1370	-0.0219	-1.0529
H	-4.4024	0.1509	-1.6325
H	-5.8939	-0.4604	-0.8225
H	-5.9811	-2.4250	-2.1693
H	-5.3172	-1.3154	-3.4097
H	-1.1831	0.9093	-3.0935
H	-0.2649	-0.6186	-3.4164
H	-2.2753	-0.8457	-4.8118
H	-3.3114	-0.1897	-3.5104
H	-3.3212	-1.8604	1.6541
H	-4.6280	-0.5107	1.4684
H	-0.8519	-3.0207	-4.2448
H	-1.8569	-4.2835	-3.4566
H	-2.4809	-3.4214	-4.9070
H	0.6990	-1.2172	-1.1492
H	1.4165	0.9561	-0.0788
H	0.7382	1.2269	-1.7019
H	-0.2601	1.5914	-0.2476
H	-1.0733	-0.3720	1.2494
H	-0.7891	-2.0606	0.7569
H	1.6114	-2.8553	0.4840
H	3.3763	-4.7679	2.6807
H	3.3055	-4.3853	0.9286
H	4.6262	-3.6992	1.9319
H	4.0609	-1.6598	3.5695
H	2.3300	-1.3862	3.9859
H	3.0887	-2.9346	4.3937

3a-conf.13 Imaginary Freq =0

C	-3.8464	-2.1000	-0.1178
C	-2.5009	-2.7706	-0.1756
C	-2.0518	-2.9605	-1.5949
C	-3.3466	-2.7817	-2.4362
C	-4.4888	-2.5460	-1.4396
C	-2.6816	-1.6030	-3.1916
C	-1.3810	-1.7948	-2.3568
C	-1.0843	-0.4561	-1.6609
C	-1.8293	0.5570	-2.5490
C	-3.1306	-0.1600	-2.9325
C	-1.8115	-3.1863	0.8938
C	-2.4796	-1.8889	-4.6857
H	-0.5469	-2.1424	-3.0113
H	-3.5412	-3.6500	-3.1111
H	-1.5488	-3.9414	-1.7704
C	0.4219	-0.1594	-1.5082
C	0.7059	1.3027	-1.1184
C	1.1217	-1.1549	-0.5581
C	0.7674	-1.0902	0.9239
C	1.4535	-2.1035	1.7609
O	0.0120	-0.2551	1.3624
C	1.1185	-2.4528	3.0171
C	1.9233	-3.4987	3.7587
C	-0.0295	-1.8978	3.8280
H	-1.5592	-0.4285	-0.6555
H	-3.7097	-0.9963	-0.0822
H	-4.4432	-2.4046	0.7737
H	-4.9898	-3.5279	-1.2619
H	-5.2715	-1.8496	-1.8197
H	-2.0250	1.5270	-2.0332
H	-1.2354	0.7596	-3.4716
H	-3.6223	0.3034	-3.8194
H	-3.8479	-0.0843	-2.0878
H	-0.8405	-3.6925	0.7789
H	-2.1991	-3.0355	1.9133
H	-1.8112	-1.1300	-5.1524
H	-2.0239	-2.8900	-4.8627
H	-3.4577	-1.8630	-5.2177
H	0.8840	-0.2999	-2.5168
H	1.7874	1.4595	-0.9015
H	0.4414	2.0057	-1.9411
H	0.1273	1.6202	-0.2229
H	0.9190	-2.1942	-0.9073
H	2.2232	-0.9961	-0.6366
H	2.3051	-2.6196	1.2887
H	1.2775	-4.3675	4.0200
H	2.7830	-3.8897	3.1687
H	2.3343	-3.0692	4.7004
H	-0.6433	-2.7333	4.2343
H	0.3642	-1.3089	4.6870
H	-0.7340	-1.2496	3.2674

3a-conf.14 Imaginary Freq =0

C	-4.5899	-1.8675	-0.7012
C	-3.3366	-2.6025	-0.3110
C	-2.5270	-2.9748	-1.5193
C	-3.4966	-2.7798	-2.7177
C	-4.8538	-2.3850	-2.1228
C	-2.5364	-1.7174	-3.3121
C	-1.5533	-1.9388	-2.1256
C	-1.3437	-0.5783	-1.4421
C	-1.7022	0.4182	-2.5587
C	-2.8975	-0.2277	-3.2735
C	-2.9894	-2.9006	0.9471
C	-1.9444	-2.1362	-4.6644
H	-0.6043	-2.4006	-2.4873

H	-3.5614	-3.6871	-3.3656
H	-2.0957	-4.0028	-1.4641
C	0.0721	-0.3939	-0.8564
C	0.2727	1.0345	-0.3170
C	0.3398	-1.4246	0.2617
C	1.7687	-1.3810	0.7858
C	2.0243	-1.2421	2.2365
O	2.6982	-1.3673	0.0097
C	1.3902	-1.9112	3.2165
C	1.7097	-1.6315	4.6684
C	0.3572	-2.9931	3.0154
H	-2.0802	-0.4380	-0.6187
H	-4.3906	-0.7726	-0.6972
H	-5.4396	-2.0679	-0.0071
H	-5.4685	-3.3134	-2.0400
H	-5.4262	-1.6747	-2.7631
H	-1.9524	1.4351	-2.1737
H	-0.8483	0.5090	-3.2711
H	-3.0619	0.2010	-4.2895
H	-3.8205	-0.0326	-2.6873
H	-2.0604	-3.4514	1.1589
H	-3.6212	-2.6041	1.7989
H	-1.1018	-1.4690	-4.9568
H	-1.5540	-3.1794	-4.6461
H	-2.7229	-2.0796	-5.4587
H	0.8076	-0.5576	-1.6813
H	1.2856	1.1701	0.1256
H	0.1787	1.7978	-1.1220
H	-0.4758	1.2740	0.4725
H	-0.3802	-1.2288	1.0885
H	0.1616	-2.4548	-0.1231
H	2.8119	-0.5194	2.5055
H	2.1327	-2.5401	5.1539
H	2.4471	-0.8075	4.8012
H	0.7829	-1.3397	5.2125
H	-0.6571	-2.6111	3.2703
H	0.3467	-3.4057	1.9840
H	0.5756	-3.8600	3.6789

3a-conf.15 Imaginary Freq =0

C	-3.9680	-2.0290	-0.2243
C	-2.6527	-2.7589	-0.2572
C	-2.1746	-2.9470	-1.6676
C	-3.4349	-2.6925	-2.5410
C	-4.5924	-2.4210	-1.5716
C	-2.6941	-1.5342	-3.2567
C	-1.4293	-1.8001	-2.3880
C	-1.0959	-0.4893	-1.6569
C	-1.7614	0.5732	-2.5500
C	-3.0821	-0.0756	-2.9861
C	-2.0081	-3.2162	0.8234
C	-2.4610	-1.8058	-4.7489
H	-0.5916	-2.1714	-3.0246
H	-3.6507	-3.5390	-3.2368
H	-1.7125	-3.9471	-1.8474
C	0.4151	-0.2660	-1.4403
C	0.7434	1.1609	-0.9649
C	1.0419	-1.3322	-0.5164
C	0.6462	-1.3130	0.9560
C	1.3220	-2.3398	1.7845
O	-0.1807	-0.5432	1.3856
C	1.3768	-2.3563	3.1292
C	2.0664	-3.4929	3.8524
C	0.7858	-1.3217	4.0582
H	-1.6087	-0.4565	-0.6709
H	-3.7846	-0.9332	-0.1641
H	-4.6030	-2.3226	0.6444
H	-5.1433	-3.3813	-1.4265
H	-5.3310	-1.6822	-1.9600
H	-1.9285	1.5426	-2.0231
H	-1.1280	0.7627	-3.4487
H	-3.5233	0.4250	-3.8794
H	-3.8216	0.0196	-2.1627
H	-1.0577	-3.7632	0.7239
H	-2.4096	-3.0584	1.8366
H	-1.7445	-1.0717	-5.1828
H	-2.0471	-2.8241	-4.9297
H	-3.4204	-1.7257	-5.3087
H	0.9051	-0.3785	-2.4392
H	1.8257	1.2656	-0.7222
H	0.5185	1.9174	-1.7511
H	0.1615	1.4469	-0.0609
H	0.8038	-2.3447	-0.9177
H	2.1515	-1.2225	-0.5546
H	1.8204	-3.1533	1.2327
H	1.3501	-3.9990	4.5388
H	2.4709	-4.2686	3.1633
H	2.9194	-3.1065	4.4552
H	-0.1099	-1.7404	4.5704
H	1.5300	-1.0409	4.8374
H	0.4943	-0.3689	3.5690

3b-conf.1 Imaginary Freq =0

C	-18.4399	0.8234	-0.5146
C	-17.4734	-0.3265	-0.4255
C	-16.0581	0.1617	-0.3085
C	-16.1265	1.6584	-0.7209
C	-17.5783	1.9351	-1.1307
C	-15.5919	2.0601	0.6779
C	-15.5040	0.5582	1.0789
C	-16.3657	0.3694	2.3371
C	-16.3911	1.7865	2.9363
C	-16.5184	2.7069	1.7144
C	-17.8217	-1.6187	-0.4630
C	-14.2195	2.7441	0.6191
H	-14.4397	0.2571	1.2245
H	-15.3992	1.9114	-1.5298
H	-15.3330	-0.4298	-0.9170
C	-15.8445	-0.7197	3.2962
C	-15.7603	-2.0828	2.5853
C	-16.6853	-0.8316	4.5861
C	-18.1301	-1.2432	4.3386
C	-19.1119	-0.1459	4.2020
O	-18.4452	-2.4112	4.2996
C	-20.1004	-0.1392	3.2898
C	-21.0690	1.0179	3.2058
C	-20.3442	-1.2276	2.2714
H	-17.4044	0.1038	2.0425
H	-18.7841	1.0992	0.5070
H	-19.3391	0.5840	-1.1293
H	-17.6398	1.8391	-2.2414
H	-17.9202	2.9649	-0.8760
H	-17.2241	1.9490	3.6589
H	-15.4278	1.9915	3.4604
H	-16.2338	3.7591	1.9485
H	-17.5783	2.7237	1.3820
H	-17.0603	-2.4119	-0.4004
H	-18.8761	-1.9216	-0.5565
H	-13.7655	2.8197	1.6333
H	-13.5022	2.1893	-0.0279
H	-14.3209	3.7739	0.2074
H	-14.8065	-0.4361	3.5987
H	-15.3883	-2.8752	3.2745
H	-16.7543	-2.4047	2.2020
H	-15.0645	-2.0559	1.7162
H	-16.2248	-1.5861	5.2664
H	-16.6556	0.1288	5.1502
H	-18.9902	0.7216	4.8701
H	-20.9874	1.5144	2.2122
H	-22.1133	0.6536	3.3347
H	-20.8854	1.7944	3.9826
H	-21.2758	-1.7828	2.5231
H	-20.4710	-0.7811	1.2596
H	-19.5132	-1.9602	2.1825

3b-conf.2 Imaginary Freq =0

C	-18.4432	1.3763	-0.3603
C	-17.7289	0.0518	-0.3599
C	-16.2389	0.2392	-0.3412
C	-16.0267	1.7327	-0.7149
C	-17.4151	2.3119	-1.0125
C	-15.3280	1.9685	0.6491
C	-15.5198	0.4659	1.0081
C	-16.3132	0.4098	2.3222
C	-16.0095	1.7779	2.9563
C	-16.0304	2.7491	1.7671
C	-18.3376	-1.1404	-0.3873
C	-13.8525	2.3645	0.5041
H	-14.5315	-0.0485	1.0668
H	-15.3189	1.8613	-1.5692
H	-15.6950	-0.4651	-1.0149
C	-15.9644	-0.7967	3.2154
C	-16.2023	-2.1211	2.4672
C	-16.7075	-0.7652	4.5688
C	-18.2038	-0.4996	4.4744
C	-19.0332	-1.5895	3.9190
O	-18.6763	0.5365	4.8852
C	-20.0870	-1.3914	3.1065
C	-20.8881	-2.5610	2.5818
C	-20.5732	-0.0441	2.6262
H	-17.4025	0.3733	2.1007
H	-18.6579	1.6820	0.6877
H	-19.4097	1.3436	-0.9157
H	-17.5684	2.2708	-2.1177

H	-17.5212	3.3797	-0.7110
H	-16.7422	2.0711	3.7442
H	-14.9909	1.7650	3.4112
H	-15.5228	3.7134	2.0026
H	-17.0847	2.9907	1.5140
H	-17.7541	-2.0742	-0.3929
H	-19.4357	-1.2184	-0.4044
H	-13.3246	2.3099	1.4833
H	-13.3084	1.7010	-0.2064
H	-13.7704	3.4080	0.1239
H	-14.8703	-0.7517	3.4410
H	-15.9811	-3.0000	3.1151
H	-17.2526	-2.2128	2.1143
H	-15.5508	-2.2110	1.5685
H	-16.5429	-1.7163	5.1268
H	-16.2613	0.0329	5.2079
H	-18.7312	-2.6187	4.1718
H	-21.9563	-2.4573	2.8789
H	-20.8326	-2.5974	1.4703
H	-20.5264	-3.5416	2.9660
H	-20.7032	-0.0571	1.5207
H	-21.5589	0.1909	3.0874
H	-19.8798	0.7967	2.8419

3b-conf.3 Imaginary Freq =0

C	-17.2501	0.4473	-1.8146
C	-16.1007	-0.3623	-1.2791
C	-15.2175	0.4680	-0.3929
C	-15.6399	1.9353	-0.6813
C	-16.6932	1.8782	-1.7942
C	-16.0465	2.1034	0.8052
C	-15.5889	0.6445	1.0971
C	-16.7905	-0.1083	1.6916
C	-17.6521	1.0352	2.2525
C	-17.5235	2.1568	1.2124
C	-15.8830	-1.6526	-1.5626
C	-15.2039	3.1533	1.5416
H	-14.6961	0.6459	1.7662
H	-14.7709	2.5842	-0.9480
H	-14.1287	0.2833	-0.5553
C	-16.3881	-1.1934	2.7134
C	-15.5160	-2.2635	2.0270
C	-17.6048	-1.8818	3.3682
C	-18.3155	-1.0503	4.4279
C	-19.7934	-1.0251	4.3531
O	-17.6808	-0.4872	5.2908
C	-20.5627	0.0131	4.7290
C	-22.0695	-0.0680	4.6251
C	-20.0588	1.3327	5.2650
H	-17.3767	-0.5992	0.8822
H	-18.1231	0.3402	-1.1328
H	-17.5652	0.1242	-2.8345
H	-16.1693	2.0553	-2.7642
H	-17.4761	2.6660	-1.7012
H	-18.7174	0.7436	2.4056
H	-17.2286	1.3851	3.2231
H	-17.8206	3.1490	1.6253
H	-18.2044	1.9442	0.3610
H	-15.0164	-2.1862	-1.1420
H	-16.5651	-2.2127	-2.2212
H	-15.3629	3.0947	2.6425
H	-14.1136	3.0227	1.3539
H	-15.4854	4.1769	1.2049
H	-15.7691	-0.7199	3.5135
H	-15.1548	-3.0237	2.7572
H	-16.0896	-2.7999	1.2372
H	-14.6109	-1.8228	1.5512
H	-18.3136	-2.2045	2.5708
H	-17.2727	-2.8053	3.8973
H	-20.2787	-1.9214	3.9341
H	-22.5314	0.0967	5.6249
H	-22.4502	0.7126	3.9281
H	-22.4280	-1.0535	4.2502
H	-20.5116	2.1717	4.6897
H	-20.3508	1.4459	6.3335
H	-18.9598	1.4735	5.1923

3b-conf.4 Imaginary Freq =0

C	-17.2201	2.0871	-1.6581
C	-17.1674	0.6235	-1.3135
C	-15.8336	0.2494	-0.7344
C	-14.9102	1.4563	-1.0585
C	-15.7432	2.4322	-1.8980
C	-14.6863	1.6843	0.4588
C	-15.5829	0.4525	0.7771
C	-16.7203	0.9347	1.6911
C	-16.1280	2.2063	2.3234
C	-15.3449	2.8666	1.1796
C	-18.1741	-0.2387	-1.5025
C	-13.2254	1.4864	0.8844
H	-14.9728	-0.3664	1.2266
H	-13.9686	1.1460	-1.5728
H	-15.4405	-0.7219	-1.1190
C	-17.1845	-0.1286	2.7082
C	-17.7478	-1.3612	1.9761
C	-18.2379	0.4380	3.6818
C	-18.7106	-0.5871	4.7040
C	-20.1662	-0.8486	4.7496
O	-17.9134	-1.1178	5.4440
C	-20.7158	-2.0420	5.0397
C	-22.2183	-2.2087	5.0860
C	-19.9487	-3.3093	5.3364
H	-17.6025	1.2416	1.0849
H	-17.6343	2.6523	-0.7935
H	-17.8596	2.2963	-2.5476
H	-15.5154	2.2321	-2.9726
H	-15.4928	3.5016	-1.7082
H	-16.9046	2.8906	2.7399
H	-15.4249	1.9268	3.1434
H	-14.6023	3.6100	1.5527
H	-16.0526	3.4179	0.5247
H	-18.0682	-1.3007	-1.2311
H	-19.1330	0.0922	-1.9311
H	-13.1342	1.4362	1.9933
H	-12.7916	0.5474	0.4705
H	-12.6017	2.3355	0.5234
H	-16.2950	-0.4505	3.3028
H	-18.0150	-2.1780	2.6846
H	-18.6656	-1.0992	1.4023
H	-17.0107	-1.7909	1.2608
H	-17.8163	1.2911	4.2616
H	-19.0995	0.8331	3.0955
H	-20.8287	-0.0025	4.5059
H	-22.5482	-2.9481	4.3214
H	-22.5313	-2.5763	6.0896
H	-22.7678	-1.2597	4.8917
H	-20.0644	-3.5821	6.4098
H	-20.3474	-4.1468	4.7204
H	-18.8635	-3.2538	5.1056

3b-conf.5 Imaginary Freq =0

C	-16.8422	1.1839	-2.1708
C	-16.5270	-0.0741	-1.4082
C	-15.4474	0.1625	-0.3922
C	-14.8305	1.5338	-0.7836
C	-15.5306	1.9767	-2.0738
C	-15.2442	2.1064	0.5968
C	-15.8284	0.7205	0.9978
C	-17.3048	0.9332	1.3678
C	-17.3482	2.4266	1.7357
C	-16.4115	3.0932	0.7181
C	-17.1251	-1.2550	-1.6095
C	-14.0431	2.5203	1.4574
H	-15.2273	0.2692	1.8223
H	-13.7203	1.4851	-0.8946
H	-14.6957	-0.6613	-0.3447
C	-17.8021	-0.0123	2.4812
C	-17.7134	-1.4788	2.0197
C	-19.2435	0.3280	2.9117
C	-19.8053	-0.6071	3.9737
C	-19.0399	-0.6724	5.2381
O	-20.8412	-1.2037	3.7850
C	-18.9396	-1.7670	6.0137
C	-18.1475	-1.7294	7.3014
C	-19.5638	-3.1098	5.7152
H	-17.9542	0.7886	0.4749
H	-17.6782	1.7181	-1.6666
H	-17.1449	0.9827	-3.2252
H	-14.8827	1.6722	-2.9307
H	-15.6642	3.0809	-2.1460
H	-18.3764	2.8578	1.6939
H	-16.9440	2.5727	2.7654
H	-16.0848	4.1067	1.0484
H	-16.9529	3.2255	-0.2426
H	-16.8442	-2.1399	-1.0171
H	-17.9138	-1.3705	-2.3693
H	-14.3520	2.7134	2.5100
H	-13.2528	1.7354	1.4796
H	-13.5844	3.4517	1.0544
H	-17.1291	0.1159	3.3633
H	-17.9842	-2.1869	2.8357
H	-18.4003	-1.6698	1.1641
H	-16.6832	-1.7492	1.6953
H	-19.3026	1.3623	3.3221

H	-19.9084	0.2964	2.0170
H	-18.5018	0.2433	5.5323
H	-18.8005	-2.0055	8.1602
H	-17.3016	-2.4522	7.2550
H	-17.7172	-0.7254	7.5182
H	-18.8007	-3.9141	5.8190
H	-20.3865	-3.3163	6.4366
H	-19.9696	-3.2081	4.6857

3b-conf.6 Imaginary Freq =0

C	-16.6134	-0.0269	-1.9724
C	-15.4916	-0.4408	-1.0593
C	-15.1310	0.6627	-0.1072
C	-15.8152	1.9282	-0.6945
C	-16.4672	1.5012	-2.0151
C	-16.6479	2.0731	0.6052
C	-15.9343	0.8258	1.2033
C	-17.0203	-0.1956	1.5806
C	-18.2641	0.6939	1.7427
C	-18.1425	1.7335	0.6199
C	-14.8836	-1.6332	-1.0950
C	-16.3398	3.3645	1.3747
H	-15.2936	1.1255	2.0662
H	-15.1013	2.7772	-0.8245
H	-14.0304	0.7829	0.0345
C	-16.6534	-1.0472	2.8146
C	-15.3750	-1.8612	2.5304
C	-17.7755	-2.0187	3.2398
C	-18.9912	-1.3854	3.9023
C	-18.7169	-0.5004	5.0558
O	-20.1075	-1.6619	3.5250
C	-19.4534	0.5750	5.3893
C	-19.0905	1.4122	6.5954
C	-20.6653	1.0766	4.6397
H	-17.2133	-0.8873	0.7297
H	-17.5843	-0.3308	-1.5212
H	-16.5397	-0.4931	-2.9829
H	-15.7573	1.7541	-2.8390
H	-17.4186	2.0400	-2.2314
H	-19.2200	0.1251	1.6664
H	-18.2285	1.2148	2.7281
H	-18.7849	2.6264	0.8025
H	-18.4825	1.2804	-0.3354
H	-14.0622	-1.8708	-0.4011
H	-15.1902	-2.4060	-1.8171
H	-16.7781	3.3355	2.3983
H	-15.2445	3.5358	1.4847
H	-16.7679	4.2421	0.8392
H	-16.4251	-0.3581	3.6625
H	-15.0484	-2.4324	3.4297
H	-15.5421	-2.5933	1.7077
H	-14.5199	-1.2106	2.2384
H	-18.1032	-2.6077	2.3516
H	-17.3812	-2.7558	3.9777
H	-17.8250	-0.7436	5.6556
H	-18.8502	2.4535	6.2824
H	-19.9447	1.4463	7.3090
H	-18.2082	1.0182	7.1492
H	-21.5755	0.9684	5.2717
H	-20.5375	2.1553	4.3947
H	-20.8569	0.5645	3.6732

3b-conf.7 Imaginary Freq =0

C	-17.0525	1.5969	-1.9312
C	-16.7500	0.2201	-1.4053
C	-15.4606	0.2036	-0.6362
C	-14.7671	1.5457	-0.9998
C	-15.6584	2.2308	-2.0426
C	-14.8050	1.9624	0.4932
C	-15.4668	0.6014	0.8572
C	-16.7933	0.9100	1.5693
C	-16.5651	2.3352	2.1028
C	-15.7834	3.0367	0.9829
C	-17.5236	-0.8551	-1.6004
C	-13.4070	2.1296	1.1034
H	-14.7703	-0.0174	1.4710
H	-13.7206	1.4000	-1.3615
H	-14.8285	-0.6912	-0.8505
C	-17.1665	-0.1259	2.6503
C	-17.3578	-1.5162	2.0164
C	-18.4365	0.2890	3.4198
C	-18.8279	-0.7018	4.5089
C	-20.0993	-1.4328	4.3074
O	-18.0841	-0.8870	5.4454
C	-20.8635	-1.9391	5.2925
C	-22.1306	-2.6998	4.9690
C	-20.5803	-1.8285	6.7724
H	-17.6277	0.9572	0.8334
H	-17.6878	2.1387	-1.1954
H	-17.5932	1.5750	-2.9064
H	-15.2493	1.9824	-3.0514
H	-15.6599	3.3423	-1.9592
H	-17.5145	2.8710	2.3403
H	-15.9392	2.2960	3.0256
H	-15.2663	3.9564	1.3434
H	-16.4917	3.3548	0.1887
H	-17.2415	-1.8373	-1.1901
H	-18.4615	-0.7840	-2.1731
H	-13.4609	2.2079	2.2131
H	-12.7384	1.2723	0.8608
H	-12.9260	3.0553	0.7136
H	-16.3214	-0.1870	3.3786
H	-17.5446	-2.2989	2.7863
H	-18.2223	-1.5187	1.3141
H	-16.4572	-1.8402	1.4475
H	-18.2791	1.2671	3.9298
H	-19.2769	0.4374	2.7028
H	-20.4354	-1.5526	3.2647
H	-22.0772	-3.7284	5.3924
H	-23.0140	-2.1834	5.4083
H	-22.3126	-2.7989	3.8748
H	-21.4946	-1.4889	7.3097
H	-20.2890	-2.8232	7.1792
H	-19.7869	-1.0975	7.0361

3b-conf.8 Imaginary Freq =0

C	-18.5241	0.6030	-0.8582
C	-17.4534	-0.3881	-0.4866
C	-16.1293	0.3013	-0.3316
C	-16.4753	1.8143	-0.4519
C	-17.9957	1.9047	-0.2441
C	-15.4871	2.1006	0.7052
C	-15.4967	0.5811	1.0563
C	-16.3206	0.4419	2.3465
C	-16.1432	1.8144	3.0273
C	-16.0088	2.8683	1.9215
C	-17.6457	-1.7096	-0.4008
C	-14.1255	2.6006	0.2088
H	-14.4575	0.1908	1.1652
H	-16.1654	2.2356	-1.4387
H	-15.3802	-0.0155	-1.0964
C	-15.8867	-0.7189	3.2714
C	-15.9028	-2.0785	2.5544
C	-16.7196	-0.7978	4.5704
C	-18.1739	-1.1880	4.3434
C	-19.1052	-0.0894	4.0084
O	-18.5352	-2.3357	4.4766
C	-20.0840	-0.1943	3.0918
C	-20.9966	0.9739	2.7971
C	-20.3700	-1.4286	2.2695
H	-17.3885	0.3011	2.0711
H	-19.5370	0.3215	-0.4873
H	-18.5498	0.6915	-1.9696
H	-18.4358	2.8139	-0.7171
H	-18.2840	1.9109	0.8304
H	-16.9738	2.0657	3.7271
H	-15.1940	1.8071	3.6138
H	-15.3085	3.6773	2.2359
H	-16.9750	3.3762	1.7063
H	-16.8089	-2.3917	-0.1893
H	-18.6418	-2.1504	-0.5624
H	-13.3722	2.5781	1.0291
H	-13.7310	1.9783	-0.6265
H	-14.2094	3.6488	-0.1578
H	-14.8258	-0.5282	3.5678
H	-15.5552	-2.8945	3.2289
H	-16.9285	-2.3419	2.2145
H	-15.2299	-2.0856	1.6674
H	-16.2652	-1.5554	5.2516
H	-16.6727	0.1623	5.1330
H	-18.9486	0.8732	4.5205
H	-20.8857	1.2886	1.7345
H	-22.0577	0.6847	2.9716
H	-20.7810	1.8633	3.4315
H	-19.5665	-2.1954	2.3056
H	-21.3209	-1.8987	2.6076
H	-20.4828	-1.1559	1.1966

3b-conf.9 Imaginary Freq =0

C	-16.5178	0.8255	-2.2656
C	-16.0115	-0.2791	-1.3785
C	-15.0863	0.2528	-0.3225
C	-14.7358	1.6916	-0.7931
C	-15.4088	1.8822	-2.1577
C	-15.3651	2.2623	0.5040

C	-15.6810	0.8170	0.9877
C	-17.1939	0.7380	1.2473
C	-17.5723	2.2113	1.4799
C	-16.7165	2.9857	0.4673
C	-16.3365	-1.5710	-1.5127
C	-14.3459	2.9822	1.3971
H	-15.0658	0.5644	1.8836
H	-13.6341	1.8706	-0.8311
H	-14.1874	-0.3880	-0.1576
C	-17.5706	-0.2093	2.4058
C	-17.1387	-1.6510	2.0810
C	-19.0799	-0.1503	2.7169
C	-19.5163	-1.0942	3.8308
C	-19.2231	-0.6334	5.2073
O	-20.0410	-2.1490	3.5554
C	-19.7956	-1.1023	6.3316
C	-19.3807	-0.5638	7.6838
C	-20.8620	-2.1697	6.4095
H	-17.7280	0.3949	0.3324
H	-17.4827	1.2060	-1.8621
H	-16.6892	0.4892	-3.3151
H	-14.6471	1.6600	-2.9432
H	-15.7603	2.9251	-2.3339
H	-18.6605	2.4117	1.3371
H	-17.2887	2.5139	2.5157
H	-16.6324	4.0666	0.7274
H	-17.1968	2.9305	-0.5327
H	-15.9270	-2.3316	-0.8297
H	-17.0227	-1.9049	-2.3066
H	-14.7693	3.1818	2.4078
H	-13.4154	2.3858	1.5364
H	-14.0584	3.9576	0.9430
H	-17.0126	0.1219	3.3148
H	-17.3053	-2.3356	2.9435
H	-17.7082	-2.0518	1.2118
H	-16.0548	-1.7137	1.8345
H	-19.3829	0.8805	3.0123
H	-19.6578	-0.3957	1.7952
H	-18.4770	0.1722	5.2988
H	-20.2495	-0.0890	8.1936
H	-19.0048	-1.3922	8.3262
H	-18.5734	0.2009	7.6211
H	-20.4355	-3.1008	6.8466
H	-21.6931	-1.8284	7.0674
H	-21.3347	-2.4274	5.4388

3b-conf.10 Imaginary Freq =0

C	-17.8992	1.4370	-1.0120
C	-17.2687	0.0906	-0.7803
C	-15.7983	0.2199	-0.5050
C	-15.4427	1.6696	-0.9365
C	-16.7212	2.2772	-1.5262
C	-14.9935	1.9841	0.5138
C	-15.3230	0.5220	0.9345
C	-16.3401	0.5946	2.0845
C	-16.0952	1.9998	2.6611
C	-15.8486	2.8745	1.4237
C	-17.9280	-1.0741	-0.8181
C	-13.4985	2.3135	0.6187
H	-14.3888	-0.0250	1.2043
H	-14.5850	1.7031	-1.6510
H	-15.1815	-0.5563	-1.0177
C	-16.1976	-0.5486	3.1089
C	-16.4257	-1.9144	2.4366
C	-17.1169	-0.3917	4.3383
C	-18.6081	-0.3831	4.0227
C	-19.3327	-1.6538	4.2557
O	-19.1259	0.6186	3.5842
C	-20.6627	-1.7759	4.4224
C	-21.2886	-3.1400	4.6168
C	-21.6641	-0.6446	4.4315
H	-17.3736	0.5703	1.6743
H	-18.2892	1.8320	-0.0474
H	-18.7456	1.3958	-1.7371
H	-16.6724	2.1550	-2.6349
H	-16.8237	3.3688	-1.3259
H	-16.9477	2.3794	3.2721
H	-15.1802	1.9908	3.2995
H	-15.3450	3.8353	1.6812
H	-16.8250	3.1342	0.9620
H	-17.4042	-2.0267	-0.6424
H	-19.0095	-1.1087	-1.0228
H	-13.1620	2.3153	1.6805
H	-12.8676	1.5779	0.0693
H	-13.2960	3.3210	0.1894
H	-15.1446	-0.5325	3.4841
H	-16.2964	-2.7492	3.1631
H	-17.4511	-1.9890	2.0096
H	-15.7055	-2.0931	1.6063
H	-16.8968	-1.2025	5.0717
H	-16.8770	0.5538	4.8776
H	-18.7166	-2.5659	4.3030
H	-21.7962	-3.1947	5.6065
H	-22.0450	-3.3298	3.8218
H	-20.5479	-3.9707	4.5763
H	-22.2760	-0.6718	3.5015
H	-22.3515	-0.7525	5.3008
H	-21.2189	0.3680	4.5269

3b-conf.11 Imaginary Freq =0

C	-18.4168	1.7045	-0.0594
C	-17.9865	0.2696	0.0795
C	-16.5021	0.1294	-0.0904
C	-16.0637	1.4598	-0.7644
C	-17.3406	2.2787	-0.9926
C	-15.1255	1.7470	0.4353
C	-15.5508	0.4014	1.0972
C	-16.0942	0.7477	2.4906
C	-15.4424	2.1088	2.7969
C	-15.4740	2.8437	1.4499
C	-18.8209	-0.7583	0.2763
C	-13.6422	1.7740	0.0421
H	-14.6909	-0.3049	1.1066
H	-15.4900	1.2919	-1.7079
H	-16.2128	-0.7730	-0.6806
C	-15.8783	-0.2959	3.6086
C	-14.4621	-0.8985	3.6612
C	-16.9227	-1.4286	3.5300
C	-18.3513	-0.9998	3.8434
C	-19.4109	-1.8962	3.3300
O	-18.5781	-0.0144	4.5080
C	-20.6589	-1.5042	3.0147
C	-21.6795	-2.5058	2.5229
C	-21.1779	-0.0874	3.0954
H	-17.1864	0.9469	2.4144
H	-18.3971	2.1962	0.9386
H	-19.4463	1.8084	-0.4755
H	-17.6711	2.1019	-2.0444
H	-17.1873	3.3772	-0.8841
H	-15.9757	2.6704	3.6007
H	-14.3829	1.9732	3.1146
H	-14.7619	3.7010	1.4191
H	-16.4909	3.2610	1.2900
H	-18.4434	-1.7903	0.3493
H	-19.9061	-0.5971	0.3654
H	-12.9885	1.7589	0.9438
H	-13.3599	0.9012	-0.5900
H	-13.4142	2.6982	-0.5360
H	-16.0274	0.2326	4.5820
H	-14.3098	-1.4721	4.6047
H	-14.2800	-1.6125	2.8270
H	-13.6703	-0.1170	3.6286
H	-16.8800	-1.8878	2.5149
H	-16.6696	-2.2220	4.2716
H	-19.1298	-2.9520	3.1858
H	-22.5737	-2.4972	3.1866
H	-22.0042	-2.2490	1.4891
H	-21.2894	-3.5486	2.5001
H	-21.7406	0.1666	2.1688
H	-21.8713	0.0160	3.9604
H	-20.3841	0.6852	3.1814

Table S5. SCF energies (Hartree) computed at the PCM/ mPW1PW91/6-31G* level of theory of isomers **3a** and **3b** using coordinate files incorporated in Table S10.

3a_1_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.193566
3a_2_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.192640
3a_3_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.195336
3a_4_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.188848
3a_5_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.194024
3a_6_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.195335
3a_7_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.191597
3a_8_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.191828
3a_9_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.187601
3a_10_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.188848
3a_11_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.187710
3a_12_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.194025
3a_13_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.191428
3a_14_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.189653
3a_15_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.191428
3b_1_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.191006
3b_2_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.192328
3b_3_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.193515
3b_4_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.194803
3b_5_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.193759
3b_6_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.192214
3b_7_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.194803
3b_8_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.185862
3b_9_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.193759
3b_10_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.192330
3b_11_DP4+	SCF Energy (PCM/mPW1PW91/6-31G*)=	-855.192524

Table S6. Absolute energy values of all conformers of isomers **3a** and **3b** used after optimization at the B3LYP/6-311G(d,p) level of theory as required for DP4+.

Conformers	**Zero-point correction**	**Thermal correction to Energy**	**Thermal correction to Enthalpy**	**Thermal correction to Gibbs Free Energy**	**Sum of electronic and zero-point Energies**	**Sum of electronic and thermal Energies**	**Sum of electronic and thermal Enthalpies**	**Sum of electronic and thermal Free Energies**
	Hartree/ Particle	**Hartree/ Particle**	**Hartree/ Particle**	**Hartree**	**Hartree**	**Hartree**	**Hartree**	**Energies/ Hartree**
3a_1_DP4+	0.453419	0.475588	0.476532	0.400400	-855.143294	-855.121125	-855.120181	-855.196313
3a_2_DP4+	0.453792	0.475779	0.476723	0.402840	-855.141712	-855.119725	-855.118781	-855.192663
3a_3_DP4+	0.453264	0.475401	0.476345	0.401108	-855.145377	-855.123240	-855.122296	-855.197534
3a_4_DP4+	0.453808	0.475984	0.476928	0.401526	-855.138281	-855.116105	-855.115161	-855.190563
3a_5_DP4+	0.453491	0.475687	0.476631	0.400934	-855.143774	-855.121578	-855.120633	-855.196331
3a_6_DP4+	0.453264	0.475402	0.476346	0.401107	-855.145377	-855.123240	-855.122295	-855.197534
3a_7_DP4+	0.453605	0.475679	0.476623	0.402073	-855.141677	-855.119604	-855.118660	-855.193210
3a_8_DP4+	0.453889	0.475957	0.476901	0.401920	-855.141371	-855.119303	-855.118359	-855.193340
3a_9_DP4+	0.453676	0.475978	0.476567	0.401212	-855.141770	-855.119387	-855.118540	-855.193540
3a_10_DP4+	0.453807	0.475983	0.476927	0.401524	-855.138282	-855.116106	-855.115162	-855.190565
3a_11_DP4+	0.453681	0.475836	0.476780	0.401297	-855.137596	-855.115441	-855.114497	-855.189980
3a_12_DP4+	0.453491	0.475687	0.476631	0.400938	-855.143774	-855.121578	-855.120634	-855.196327
3a_13_DP4+	0.453661	0.475690	0.476634	0.401648	-855.141128	-855.119099	-855.118155	-855.193141
3a_14_DP4+	0.453604	0.475722	0.476666	0.401466	-855.139210	-855.117092	-855.116148	-855.191347

3a_15_DP4+	0.453657	0.475688	0.476632	0.401616	-855.141132	-855.119101	-855.118157	-855.193173
3b_1_DP4+	0.454020	0.475965	0.476909	0.402327	-855.140178	-855.118233	-855.117289	-855.191871
3b_2_DP4+	0.453921	0.475933	0.476877	0.401647	-855.141519	-855.119507	-855.118563	-855.193793
3b_3_DP4+	0.453325	0.475462	0.476406	0.400890	-855.143528	-855.121391	-855.120447	-855.195963
3b_4_DP4+	0.453209	0.475416	0.476361	0.400873	-855.144993	-855.122786	-855.121842	-855.197329
3b_5_DP4+	0.453476	0.475670	0.476614	0.400740	-855.143517	-855.121324	-855.120380	-855.196253
3b_6_DP4+	0.453632	0.475683	0.476627	0.401742	-855.141646	-855.119594	-855.118650	-855.193536
3b_7_DP4+	0.453210	0.475416	0.476360	0.400875	-855.144992	-855.122786	-855.121842	-855.197327
3b_8_DP4+	0.453736	0.475875	0.476819	0.401220	-855.135389	-855.113250	-855.112305	-855.187904
3b_9_DP4+	0.453475	0.475669	0.476613	0.400733	-855.143519	-855.121324	-855.120380	-855.196261
3b_10_DP4+	0.453822	0.475882	0.476826	0.401243	-855.141612	-855.119553	-855.118608	-855.194191
3b_11_DP4+	0.453390	0.475540	0.476484	0.401442	-855.142439	-855.120289	-855.119345	-855.194387

Table S7. Experiment and calculated ^{13}C NMR chemical shifts of stereoisomers **3a**–**3b**.

	3	3a	3b
Labels	*δ*exp.	*δ*calc.	*δ*calc.
1	36.4	41.2	40.2
2	152.2	151.1	150.3
3	41.5	45.9	46.0
4	46.4	50.1	49.1
5	27.9	33.3	32.7
6	44.8	48.8	48.3
7	52.1	54.2	55.5
8	48.4	50.6	48.4
9	31.5	35.2	36.9
10	33.1	37.3	36.6
11	108	107.3	107.3
12	30.3	32.7	32.2
16	36.3	38.2	43.8
17	19.2	23.2	23.4
18	51.3	55.3	51.2
19	201.7	192.5	193.2
20	124.4	120.7	121.8
22	154.6	155.1	155.2
23	27.8	31.8	31.0
24	20.8	23.0	22.4

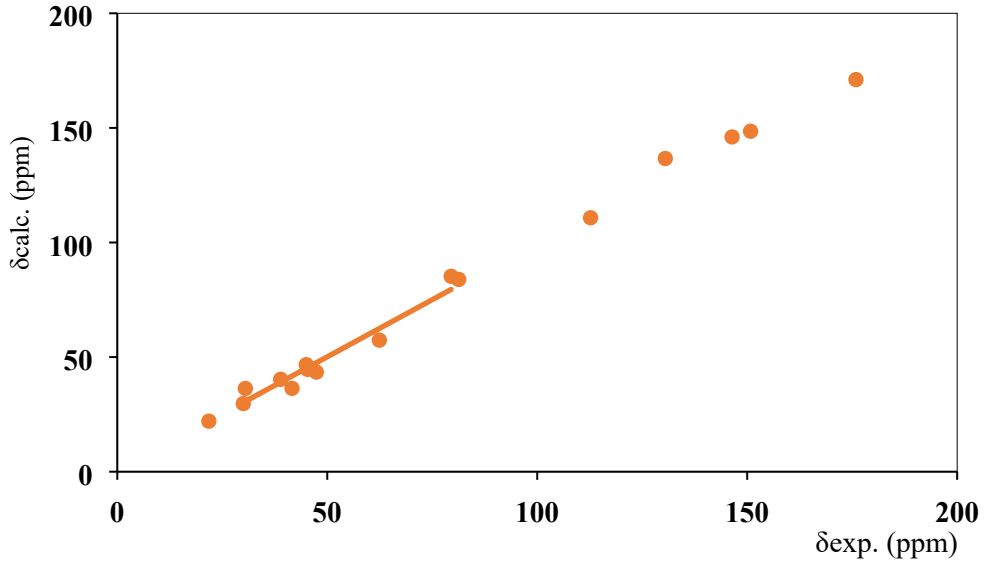

Figure S38. Regression analysis of experimental *versus* calculated ^{13}C NMR **c**hemical shifts at mPW1PW91/6-31G* level using GIAO method of **3a**; linear fitting is shown as a line (orange).

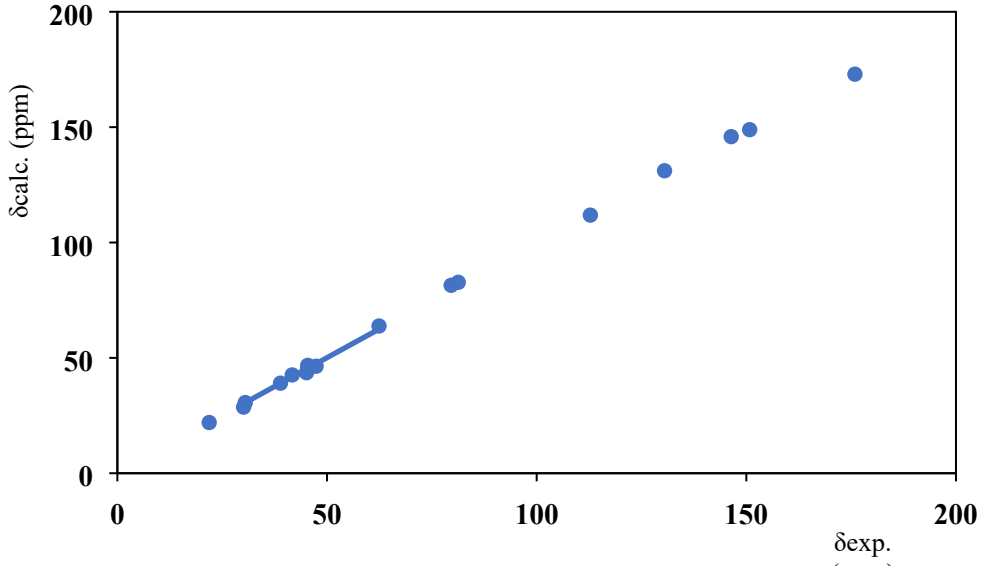

Figure S39. Regression analysis of experimental *versus* calculated ^{13}C NMR **c**hemical shifts at mPW1PW91/6-31G* level using GIAO method of **3b**; linear fitting is shown as a line (blue).

Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-31+G(d,p)

		DP4+	99.98%	0.02%	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3
C		36.4	156.521201	156.763843	
C	x	152.2	43.3714728	43.5502591	
C		41.5	151.626153	150.764556	
C		46.4	147.314211	147.648979	
C		27.9	164.678924	164.521795	
C		44.8	148.684553	148.466739	
C		52.1	143.126377	141.042538	
C		48.4	146.847153	148.302363	
C		31.5	162.687742	160.220954	
C		33.1	160.511347	160.524245	
C	x	108	88.4133262	87.7552455	
C		30.3	165.283877	165.018252	
C		36.3	159.554943	153.043952	
C		19.2	175.084154	174.100121	
C		51.3	142.018847	145.468509	
C	x	201.7	0.66312068	-0.627892	
C	x	124.4	74.6240214	72.8433294	
C	x	154.6	39.2183133	38.4600428	
C		27.8	166.244641	166.227533	
C		20.8	175.305669	175.078481	

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

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	-	-	-	-	-	-
sDP4+ (C data)	97.53%	2.47%	-	-	-	-
sDP4+ (all data)	97.53%	2.47%	-	-	-	-
uDP4+ (H data)	-	-	-	-	-	-
uDP4+ (C data)	99.41%	0.59%	-	-	-	-
uDP4+ (all data)	99.41%	0.59%	-	-	-	-
DP4+ (H data)	-	-	-	-	-	-
DP4+ (C data)	99.98%	0.02%	-	-	-	-
DP4+ (all data)	99.98%	0.02%	-	-	-	-

Figure S40. DP4+ evaluation of theoretical and experimental data of **3**.

3.2 Computational details (TDDFT-ECD) of 1-3

Torsional sampling (MCMM) conformational searches using OPLS_2005 force field were carried out by means of the conformational search module in the Macromodel [9] applying an energy window of 21 kJ/mol, which afforded the conformers for **1**-**3**. The Boltzmann populations of the conformers were obtained based on the potential energy provided by the OPLS_2005 force field, which afforded the conformers for **1**-**3** above 1% population for re-optimization. The re-optimization and the following TDDFT calculations of the re-optimized geometries were all performed with Gaussian 09 [4] at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile. Frequency analysis was performed as well to confirm that the re-optimized geometries were at the energy minima. Finally, the SpecDis1.62 [10] software was used to obtain the Boltzmann-averaged ECD spectra of **1**-**3** and visualize the results.

Table S8. Cartesian coordinates for the re-optimized conformers of **1**-**3** at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for methanol.

Sinuausone A (1) Conf. 1 P = 85.640%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5880477

I	atom	X	Y	Z
1	C	3.775008	-0.595666	-0.701302
2	C	2.83872	-1.829458	-0.517393
3	C	1.674512	-1.532786	0.413857
4	C	0.431589	-0.960139	-0.236307
5	C	2.97614	0.637455	-1.014066
6	C	-0.430933	0.077717	0.564885
7	C	-0.792656	1.424963	-0.125578
8	C	0.210224	2.56472	0.199341
9	C	1.553472	2.611939	-0.573635
10	C	2.591822	1.594817	-0.159622
11	C	1.779368	-1.77007	1.724563
12	C	3.111325	1.741644	1.250508
13	C	-1.566876	-0.983394	0.683177
14	C	-2.996708	-0.616586	0.400773
15	C	-3.251973	0.755502	-0.174106
16	C	-2.245347	1.837344	0.264785
17	C	-0.837427	-1.91628	-0.359896
18	C	-1.419273	-1.868473	-1.777745
19	C	-0.716732	-3.369532	0.088384
20	O	-3.90518	-1.404492	0.609321
21	C	-2.707725	3.180991	-0.32329
22	H	0.70341	-0.583861	-1.221398
23	H	-0.792486	1.281796	-1.215507
24	H	-0.005282	0.307495	1.544021
25	H	-1.552427	-1.470047	1.661673
26	H	4.356145	-0.468576	0.214487
27	H	4.48605	-0.816963	-1.50527
28	H	2.454634	-2.135396	-1.496494
29	H	3.432986	-2.663003	-0.131956
30	H	2.545644	0.662471	-2.014868
31	H	-0.277499	3.514886	-0.019741
32	H	0.399266	2.573839	1.278859
33	H	1.963754	3.619709	-0.423249
34	H	1.348111	2.515047	-1.64491
35	H	0.985195	-1.53874	2.426285
36	H	2.680219	-2.205026	2.146119
37	H	3.964212	1.096304	1.456769
38	H	3.419547	2.778449	1.42877
39	H	2.339838	1.510685	1.99132
40	H	-4.277858	1.037494	0.076812
41	H	-3.215983	0.65946	-1.268909
42	H	-2.288667	1.915488	1.360326
43	H	-2.40729	-2.33727	-1.816363
44	H	-1.511858	-0.848481	-2.158006
45	H	-0.762402	-2.413875	-2.462275
46	H	-1.710026	-3.829217	0.110317
47	H	-0.095138	-3.944494	-0.605882
48	H	-0.278732	-3.456491	1.083397
49	H	-2.190498	4.036683	0.111869
50	H	-2.554707	3.206461	-1.407809
51	H	-3.775897	3.322865	-0.136956

Sinuausone A (2) Conf. 1 P = 4.789%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5851837

1	C	3.790193	-0.49459	-0.673881
2	C	2.894156	-1.752669	-0.455055
3	C	1.725648	-1.478063	0.477968
4	C	0.470488	-0.935922	-0.172161
5	C	2.951516	0.695647	-1.041451
6	C	-0.436695	0.057229	0.637632
7	C	-0.850497	1.371034	-0.076721
8	C	0.12287	2.566166	0.116581
9	C	1.442892	2.622586	-0.690542
10	C	2.530136	1.676739	-0.232933
11	C	1.83734	-1.710267	1.78915
12	C	3.050211	1.914743	1.164541
13	C	-1.54749	-1.041725	0.662598
14	C	-2.957393	-0.571757	0.43222
15	C	-3.18301	0.803368	1.009622
16	C	-2.279545	1.877179	0.339798
17	C	-0.767675	-1.931366	-0.352376
18	C	-1.293553	-1.892757	-1.792529
19	C	-0.595306	-3.383629	0.087517
20	O	-3.818912	-1.224178	-0.130138
21	C	-2.998273	2.496269	-0.868237
22	H	0.739471	-0.521891	-1.141928
23	H	-0.900187	1.150367	-1.150793
24	H	-0.045348	0.28958	1.630486
25	H	-1.566986	-1.525142	1.6477
26	H	4.356166	-0.314047	0.242384
27	H	4.516868	-0.721722	-1.462183
28	H	2.514152	-2.091648	-1.425095

29	H	3.517962	-2.558008	-0.056559
30	H	2.518796	0.655928	-2.040894
31	H	-0.43061	3.471548	-0.153402
32	H	0.335784	2.666105	1.187096
33	H	1.810223	3.654956	-0.61295
34	H	1.221685	2.44759	-1.748552
35	H	1.037384	-1.497418	2.490163
36	H	2.748297	-2.123668	2.210753
37	H	3.923185	1.307144	1.399685
38	H	3.328911	2.968313	1.284491
39	H	2.289993	1.703392	1.9226
40	H	-2.930086	0.742532	2.074857
41	H	-4.237264	1.074757	0.927834
42	H	-2.143789	2.665658	1.087107
43	H	-2.245846	-2.420122	-1.876533
44	H	-1.44623	-0.871852	-2.151101
45	H	-0.570162	-2.37349	-2.45907
46	H	-1.564802	-3.892018	0.064221
47	H	0.081777	-3.922016	-0.583699
48	H	-0.194668	-3.460831	1.099591
49	H	-2.373182	3.244583	-1.362947
50	H	-3.248649	1.729744	-1.608774
51	H	-3.927622	2.985812	-0.56384

Sinuausone A (1) Conf. 3 P = 3.183%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5903136

1	C	-3.375046	-1.152122	0.514549
2	C	-2.167665	-2.032804	0.092425
3	C	-0.954092	-1.878167	1.001352
4	C	0.281666	-1.126633	0.549964
5	C	-2.984979	0.298555	0.611221
6	C	0.271926	0.125238	-0.386212
7	C	0.217515	1.553255	0.23044
8	C	-0.702173	2.519958	-0.562645
9	C	-2.197684	2.504769	-0.163573
10	C	-2.873218	1.172976	-0.39588
11	C	-0.962497	-2.444268	2.21436
12	C	-3.303586	0.895516	-1.814815
13	C	1.597839	-0.38623	-1.038749
14	C	2.872879	0.246257	-0.537175
15	C	2.743558	1.186321	0.636952
16	C	1.619493	2.21197	0.389857
17	C	1.308388	-1.821033	-0.429335
18	C	2.453087	-2.561859	0.259676
19	C	0.685858	-2.729562	-1.494822
20	O	3.942413	0.024471	-1.079489
21	C	1.627239	3.272053	1.498823
22	H	0.841813	-0.873318	1.454709
23	H	-0.198166	1.444206	1.240251
24	H	-0.526486	0.021264	-1.119701
25	H	1.640099	-0.382652	-2.130134
26	H	-4.182904	-1.308472	-0.206725
27	H	-3.746316	-1.501046	1.482639
28	H	-2.483794	-3.080931	0.087644
29	H	-1.911146	-1.779071	-0.936866
30	H	-2.639524	0.62282	1.590466
31	H	-0.348873	3.54613	-0.423112
32	H	-0.594403	2.315213	-1.63432
33	H	-2.70977	3.292463	-0.729355
34	H	-2.271474	2.774008	0.895192
35	H	-0.131049	-2.331648	2.902769
36	H	-1.802012	-3.040546	2.559652
37	H	-3.75699	-0.088045	-1.939052
38	H	-4.030107	1.648094	-2.142619
39	H	-2.457405	0.963255	-2.507972
40	H	3.704911	1.682117	0.789293
41	H	2.522377	0.609071	1.543425
42	H	1.854774	2.714985	-0.55825
43	H	3.220399	-2.858667	-0.461245
44	H	2.933371	-1.957845	1.033337
45	H	2.071001	-3.469715	0.7373
46	H	1.460456	-3.058769	-2.194026
47	H	0.24404	-3.620612	-1.038928
48	H	-0.088173	-2.225853	-2.076478
49	H	0.845163	4.021016	1.350698
50	H	1.463324	2.805496	2.475751
51	H	2.586502	3.796145	1.533096

Sinuausone A (1) Conf. 4 P = 2.349%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5845249

1	C	-3.487	-0.780647	-0.390462
2	C	-2.312897	-1.768142	-0.673944
3	C	-1.415062	-1.99763	0.536463
4	C	-0.069326	-1.303275	0.663606
5	C	-2.957358	0.468788	0.254415
6	C	0.255138	0.036158	-0.078312
7	C	0.596397	1.273291	0.778713
8	C	-0.632108	1.98979	1.393799
9	C	-1.679243	2.595518	0.432097
10	C	-2.531445	1.589439	-0.336907
11	C	-1.80923	-2.83842	1.499829
12	C	-2.770793	1.927664	-1.786467
13	C	1.46291	-0.637679	-0.786341
14	C	2.822553	0.009535	-0.695419
15	C	2.889967	1.458009	-0.237656
16	C	1.545455	2.185605	-0.044972
17	C	1.186589	-1.99399	-0.037903
18	C	2.2444	-2.420087	0.982669
19	C	0.888261	-3.154304	-0.987202
20	O	3.837308	-0.595369	-0.997134
21	C	1.807099	3.563529	0.577428
22	H	0.142129	-1.204626	1.731775
23	H	1.185142	0.928214	1.642858
24	H	-0.504587	0.311656	-0.804445
25	H	1.284406	-0.756909	-1.861118
26	H	-4.010236	-0.58286	-1.329509
27	H	-4.200554	-1.27464	0.276986
28	H	-2.73315	-2.724125	-1.000959
29	H	-1.7315	-1.376138	-1.512228
30	H	-2.726432	0.342509	1.308484
31	H	-1.12735	1.292569	2.074864
32	H	-0.260795	2.793781	2.035937
33	H	-1.176983	3.245955	-0.292012
34	H	-2.329238	3.263781	1.011733
35	H	-1.21914	-2.996744	2.396944
36	H	-2.73771	-3.396407	1.422814
37	H	-1.824865	1.959364	-2.341126
38	H	-3.433943	1.221858	-2.28737
39	H	-3.212263	2.927299	-1.874515
40	H	3.538888	1.992803	-0.938918
41	H	3.431414	1.445811	0.718793
42	H	1.095682	2.343786	-1.03423
43	H	3.163437	-2.743306	0.48782
44	H	2.501446	-1.608812	1.669628

45	H	1.863623	-3.254456	1.580603
46	H	1.800247	-3.434881	-1.523632
47	H	0.534468	-4.031427	-0.437948
48	H	0.130983	-2.894513	-1.730518
49	H	0.907089	4.180238	0.612175
50	H	2.189455	3.46681	1.599348
51	H	2.556024	4.10745	-0.005762

Sinuausone A (1) Conf. 5 P = 1.248%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5873318

1	C	3.366978	1.164748	0.388285
2	C	2.154214	2.014073	-0.08944
3	C	0.946397	1.968204	0.840216
4	C	-0.27772	1.143047	0.497972
5	C	3.001725	-0.278771	0.617976
6	C	-0.191308	-0.206583	-0.271434
7	C	-0.124461	-1.54434	0.507503
8	C	0.709336	-2.608044	-0.256995
9	C	2.228967	-2.559553	0.056821
10	C	2.881512	-1.242158	-0.304743
11	C	0.957599	2.684581	1.971023
12	C	3.266974	-1.081374	-1.754308
13	C	-1.490683	0.177697	-1.053483
14	C	-2.74396	-0.609684	-0.74271
15	C	-2.509835	-2.033132	-0.281886
16	C	-1.52335	-2.100304	0.904099
17	C	-1.337684	1.666558	-0.562245
18	C	-2.53698	2.368956	0.072355
19	C	-0.766412	2.549536	-1.677105
20	O	-3.861988	-0.154895	-0.907284
21	C	-2.127693	-1.44913	2.159288
22	H	-0.827036	0.987407	1.428771
23	H	0.404669	-1.343014	1.446025
24	H	0.645101	-0.168322	-0.965434
25	H	-1.384371	0.0825	-2.141431
26	H	4.161362	1.265164	-0.357822
27	H	3.753066	1.597203	1.316115
28	H	2.485593	3.052253	-0.191904
29	H	1.879313	1.676745	-1.089957
30	H	2.691218	-0.521835	1.631969
31	H	0.359327	-3.610325	0.011262
32	H	0.550322	-2.510666	-1.336839
33	H	2.717368	-3.383194	-0.477121
34	H	2.359016	-2.751425	1.126812
35	H	0.131576	2.654006	2.674258
36	H	1.794362	3.3262	2.231412
37	H	3.689864	-0.101737	-1.977562
38	H	4.004292	-1.842147	-2.035608
39	H	2.404123	-1.231901	-2.413499
40	H	-2.094376	-2.590515	-1.131463
41	H	-3.473631	-2.481363	-0.029863
42	H	-1.385296	-3.159537	1.144051
43	H	-3.304033	2.598904	-0.670938
44	H	-3.002669	1.767334	0.854968
45	H	-2.205093	3.310508	0.523429
46	H	-1.545992	2.758751	-2.416471
47	H	-0.415943	3.506877	-1.280009
48	H	0.064921	2.076014	-2.203354
49	H	-1.430315	-1.503839	2.999537
50	H	-2.386998	-0.397734	2.012037
51	H	-3.045518	-1.969121	2.449763

Sinuausone B (2) Conf. 1 P = 41.688%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5814690

I	atom	X	Y	Z
1	C	3.723198	-0.715943	-0.720139
2	C	2.769139	-1.904017	-0.37145
3	C	1.594212	-1.46957	0.492465
4	C	0.342584	-1.085477	-0.262032
5	C	2.944127	0.531392	-1.028805
6	C	-0.654141	0.030197	0.18779
7	C	-0.751151	1.501751	-0.245625
8	C	0.336884	2.456391	0.306814
9	C	1.645425	2.583853	-0.522958
10	C	2.692468	1.545525	-0.19099
11	C	1.695867	-1.442873	1.823656
12	C	3.366352	1.740151	1.146134
13	C	-1.769036	-0.833643	-0.461218
14	C	-3.091998	-0.471099	0.125345
15	C	-3.352837	1.014527	-0.098563
16	C	-2.173659	1.993107	0.211373
17	C	-0.894226	-2.104336	-0.314176
18	C	-0.904417	-3.055333	-1.509733
19	C	-1.139044	-2.880891	0.980891
20	O	-3.860048	-1.201994	0.722757
21	C	-2.558612	3.36374	-0.368879
22	H	-0.757521	-0.012732	1.279055
23	H	-1.804226	-0.558566	-1.522859
24	H	0.608031	-0.888489	-1.303574
25	H	-0.718252	1.539397	-1.343708
26	H	4.391438	-0.555823	0.127613
27	H	4.350649	-1.010854	-1.568419
28	H	2.391299	-2.344405	-1.299559
29	H	3.350997	-2.679807	0.134451
30	H	2.414778	0.527853	-1.98085
31	H	-0.088068	3.459255	0.371958
32	H	0.572279	2.17346	1.33804
33	H	1.397525	2.544456	-1.588531
34	H	2.059639	3.581872	-0.333029
35	H	0.89088	-1.098661	2.462741
36	H	2.607748	-1.755761	2.322809
37	H	3.819288	2.73786	1.189907
38	H	2.64812	1.686447	1.970288
39	H	4.146519	1.007259	1.345154
40	H	-4.233489	1.306953	0.478114
41	H	-3.615863	1.11598	-1.160671
42	H	-2.124473	2.087518	1.304474
43	H	-1.864818	-3.576303	-1.584129
44	H	-0.737574	-2.518761	-2.448227
45	H	-0.122362	-3.815069	-1.410905
46	H	-2.102548	-3.392327	0.925933
47	H	-0.357211	-3.629452	1.133455
48	H	-1.159509	-2.238601	1.862939
49	H	-1.876452	4.160249	-0.068366
50	H	-2.574561	3.327059	-1.463283
51	H	-3.5587	3.651229	-0.032274

Sinuausone B (2) Conf. 2 P = 28.638%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5799537

1	C	-3.249079	-1.198436	0.640389
2	C	-2.78579	0.279251	0.758754
3	C	-2.302551	0.870444	-0.561883

4	C	-0.834813	1.141295	-0.814518
5	C	-2.181932	-2.009853	-0.038563
6	C	0.359883	0.266223	-0.301266
7	C	1.188891	-0.806759	-1.030761
8	C	0.482833	-2.113968	-1.464269
9	C	0.015375	-3.099147	-0.371917
10	C	-1.10778	-2.579249	0.516651
11	C	-3.195046	1.208197	-1.500326
12	C	-0.890448	-2.718535	2.001591
13	C	1.168793	1.588006	-0.199964
14	C	2.306595	1.411567	0.752693
15	C	3.192261	0.257219	0.283872
16	C	2.450363	-1.05093	-0.138637
17	C	-0.146261	2.40261	-0.104597
18	C	-0.194432	3.687665	-0.928209
19	C	-0.606046	2.686972	1.328918
20	O	2.515542	2.039317	1.773884
21	C	3.46971	-2.000165	-0.783386
22	H	0.124302	-0.085419	0.707799
23	H	1.610542	1.764451	-1.188397
24	H	-0.704746	1.294951	-1.890737
25	H	1.53681	-0.348831	-1.968134
26	H	-3.485734	-1.570936	1.641008
27	H	-4.17527	-1.238328	0.05879
28	H	-1.991145	0.318825	1.504064
29	H	-3.612483	0.883365	1.146104
30	H	-2.2259	-1.978401	-1.12405
31	H	-0.371553	-1.839657	-2.089522
32	H	1.164218	-2.652498	-2.130833
33	H	-0.304925	-4.022694	-0.869895
34	H	0.863879	-3.389879	0.254505
35	H	-2.889894	1.60777	-2.462077
36	H	-4.262703	1.093861	-1.337442
37	H	-0.697712	-3.766598	2.259546
38	H	-0.006101	-2.156066	2.324482
39	H	-1.74074	-2.376816	2.592352
40	H	3.918408	0.033689	1.068961
41	H	3.755433	0.63316	-0.581522
42	H	2.099209	-1.516569	0.790269
43	H	0.42669	4.466343	-0.473467
44	H	0.16214	3.52152	-1.948724
45	H	-1.218567	4.070541	-0.986644
46	H	0.007349	3.482518	1.758102
47	H	-1.648471	3.018534	1.341679
48	H	-0.514841	1.821493	1.986565
49	H	3.058616	-2.9982	-0.94587
50	H	3.804817	-1.611069	-1.750775
51	H	4.350872	-2.108041	-0.144637

Sinuausone B (2) Conf. 3 P = 18.387%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5787587

1	C	3.704258	-0.829077	-0.74198
2	C	2.68466	-1.989487	-0.520342
3	C	1.538848	-1.57643	0.391187
4	C	0.297087	-1.063068	-0.301675
5	C	3.001205	0.476112	-0.988282
6	C	-0.576409	0.113523	0.241561
7	C	-0.598518	1.580651	-0.210453
8	C	0.475021	2.558429	0.319429
9	C	1.833036	2.587726	-0.425506
10	C	2.771924	1.44977	-0.097186
11	C	1.662199	-1.668076	1.717988
12	C	3.37825	1.511223	1.283855
13	C	-1.798206	-0.626011	-0.343014
14	C	-3.076357	-0.258388	0.339977
15	C	-3.021152	1.18086	0.849348
16	C	-2.045983	2.154423	0.123269
17	C	-1.023738	-1.973055	-0.341606
18	C	-1.179683	-2.837202	-1.59123
19	C	-1.278722	-2.806597	0.914676
20	O	-4.034519	-0.986961	0.517545
21	C	-2.697161	2.747433	-1.135585
22	H	-0.598329	0.061581	1.335635
23	H	-1.913639	-0.297265	-1.385874
24	H	0.541694	-0.842605	-1.343967
25	H	-0.510046	1.568896	-1.305086
26	H	4.345175	-0.765724	0.139295
27	H	4.350869	-1.0907	-1.58707
28	H	2.284434	-2.306171	-1.488599
29	H	3.219144	-2.846665	-0.10064
30	H	2.521356	0.568559	-1.962263
31	H	0.058802	3.568158	0.233687
32	H	0.628774	2.39429	1.392154
33	H	1.638889	2.611854	-1.503098
34	H	2.321588	3.537627	-0.172528
35	H	0.888016	-1.339578	2.401442
36	H	2.565499	-2.065918	2.170159
37	H	3.906585	2.463216	1.415327
38	H	2.608134	1.47157	2.060563
39	H	4.082109	0.704239	1.480549
40	H	-2.724007	1.091638	1.90256
41	H	-4.034345	1.591013	0.858391
42	H	-1.902987	2.98064	0.825949
43	H	-2.185099	-3.267904	-1.641991
44	H	-1.015644	-2.254707	-2.502347
45	H	-0.463031	-3.664861	-1.585243
46	H	-2.287923	-3.224541	0.875737
47	H	-0.566076	-3.631912	0.986948
48	H	-1.200689	-2.221107	1.833084
49	H	-2.033058	3.476084	-1.60967
50	H	-2.918722	1.972818	-1.87684
51	H	-3.634688	3.25661	-0.893219

Sinuausone B (2) Conf. 4 P = 5.883%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5794143

1	C	-3.582174	-0.515224	0.392273
2	C	-2.968457	-1.749657	-0.348606
3	C	-1.571033	-1.525675	-0.904499
4	C	-0.492369	-1.108534	0.070362
5	C	-3.051008	0.774194	-0.170496
6	C	0.605383	-0.079317	-0.330404
7	C	0.640623	1.442499	-0.172086
8	C	-0.385729	2.193419	-1.066329
9	C	-1.610703	2.779979	-0.322523
10	C	-2.380184	1.735676	0.475801
11	C	-1.345232	-1.684666	-2.212807
12	C	-2.263368	1.837108	1.976849
13	C	1.55508	-0.815599	0.641186
14	C	2.968067	-0.520898	0.251446
15	C	3.195278	0.992743	0.23899
16	C	2.114811	1.864744	-0.48022
17	C	0.687952	-2.103095	0.513962
18	C	0.436787	-2.856433	1.818862
19	C	1.15882	-3.070607	-0.572665

20	O	3.830623	-1.32319	-0.052824
21	C	2.390064	3.338234	-0.149415
22	H	0.91401	-0.308896	-1.35773
23	H	1.398055	-0.386622	1.638956
24	H	-0.959659	-0.769878	0.997877
25	H	0.447298	1.687489	0.879319
26	H	-4.672375	-0.578702	0.29463
27	H	-3.366668	-0.583683	1.45944
28	H	-2.960706	-2.597265	0.347304
29	H	-3.621834	-2.033961	-1.177613
30	H	-3.098	0.846814	-1.256469
31	H	0.105495	3.013804	-1.598363
32	H	-0.745712	1.507912	-1.838816
33	H	-1.27649	3.58301	0.343058
34	H	-2.266993	3.247444	-1.064896
35	H	-0.372429	-1.527199	-2.662893
36	H	-2.143825	-1.977314	-2.886804
37	H	-1.21973	1.789899	2.306499
38	H	-2.644672	2.809755	2.30981
39	H	-2.822617	1.065996	2.506713
40	H	4.17888	1.190972	-0.193441
41	H	3.239013	1.299993	1.293122
42	H	2.258952	1.724238	-1.559923
43	H	1.349459	-3.354782	2.162121
44	H	0.102337	-2.181003	2.61149
45	H	-0.330816	-3.625337	1.683542
46	H	2.067218	-3.580682	-0.244095
47	H	0.392438	-3.824362	-0.772575
48	H	1.387735	-2.571847	-1.515644
49	H	1.727068	4.014378	-0.693232
50	H	2.256129	3.523675	0.921483
51	H	3.417808	3.608325	-0.408374

Sinuausone B (2) Conf. 5 P = 4.875%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5794142

1	C	-3.582263	-0.515095	0.392283
2	C	-2.968649	-1.749322	-0.348878
3	C	-1.571095	-1.525463	-0.904581
4	C	-0.492451	-1.108472	0.070357
5	C	-3.051296	0.774449	-0.170414
6	C	0.605353	-0.07928	-0.330326
7	C	0.640693	1.442567	-0.171988
8	C	-0.385603	2.193603	-1.066149
9	C	-1.61073	2.780035	-0.32244
10	C	-2.380172	1.735725	0.475864
11	C	-1.345194	-1.684446	-2.212873
12	C	-2.262861	1.836711	1.976915
13	C	1.555042	-0.815672	0.641214
14	C	2.968017	-0.521124	0.251277
15	C	3.195371	0.992483	0.238765
16	C	2.114904	1.864688	-0.480216
17	C	0.687818	-2.103106	0.513999
18	C	0.436597	-2.856363	1.818942
19	C	1.158644	-3.070685	-0.572577
20	O	3.830464	-1.323494	-0.053069
21	C	2.390422	3.338087	-0.14924
22	H	0.913915	-0.308799	-1.357686
23	H	1.39816	-0.386701	1.638996
24	H	-0.959756	-0.769843	0.997867
25	H	0.447466	1.687534	0.87944
26	H	-4.672478	-0.578612	0.294781
27	H	-3.366593	-0.583646	1.459408
28	H	-2.96112	-2.597201	0.346709
29	H	-3.621948	-2.033234	-1.178076
30	H	-3.098651	0.847249	-1.256366
31	H	0.105624	3.014133	-1.597945
32	H	-0.745478	1.508247	-1.838827
33	H	-1.276662	3.583154	0.343107
34	H	-2.266985	3.247341	-1.064935
35	H	-0.372318	-1.527123	-2.66285
36	H	-2.143745	-1.976952	-2.886978
37	H	-1.219169	1.788889	2.306308
38	H	-2.643584	2.80945	2.310246
39	H	-2.822342	1.065722	2.506713
40	H	4.178926	1.190613	-0.193818
41	H	3.239344	1.299699	1.292903
42	H	2.258926	1.724298	-1.559949
43	H	1.349235	-3.35476	2.16221
44	H	0.102204	-2.18086	2.611526
45	H	-0.331062	-3.625218	1.683663
46	H	2.066966	-3.580876	-0.243976
47	H	0.392177	-3.824344	-0.772514
48	H	1.387666	-2.571967	-1.515548
49	H	1.727494	4.014411	-0.692908
50	H	2.256623	3.523405	0.921693
51	H	3.418187	3.608026	-0.408261

Isolobophytumin E (3) Conf. 1 P = 22.602%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5983840

I	atom	X	Y	Z
1	C	2.743259	-1.848181	-1.452695
2	C	1.243973	-1.832352	-1.217377
3	C	0.983748	-1.403425	0.207225
4	C	2.347512	-1.566923	0.961375
5	C	3.349904	-2.137176	-0.060533
6	C	2.345256	-0.034513	1.316344
7	C	0.977726	0.133131	0.573878
8	C	1.143526	1.235434	-0.501119
9	C	2.398998	2.002394	-0.016226
10	C	3.317997	0.927873	0.594037
11	C	0.320057	-2.229940	-2.092924
12	C	2.305119	0.230066	2.820528
13	H	0.153351	0.372527	1.246545
14	H	2.306164	-2.185516	1.860250
15	H	0.127753	-1.932671	0.628752
16	C	-0.096210	2.131478	-0.728270
17	C	0.188708	3.223013	-1.773051
18	C	-1.334555	1.312983	-1.141300
19	C	-2.280855	0.888516	-0.018820
20	C	-3.326088	-0.069704	-0.441898
21	O	-2.180104	1.350533	1.111718
22	C	-4.272384	-0.667486	0.313685
23	C	-5.242112	-1.627321	-0.321637
24	C	-4.462067	-0.466729	1.790495
25	H	1.380608	0.766815	-1.465072
26	H	3.069155	-0.866053	-1.814781
27	H	3.037478	-2.578177	-2.210077
28	H	3.422222	-3.219883	0.083090
29	H	4.359047	-1.732314	0.054380
30	H	2.889742	2.567264	-0.812507
31	H	2.104580	2.723392	0.756852
32	H	4.060971	1.352972	1.275095

33	H	3.875490	0.425246	-0.200276
34	H	-0.736373	-2.227723	-1.844005
35	H	0.588155	-2.576143	-3.086441
36	H	2.122396	1.289176	3.031305
37	H	1.510627	-0.348025	3.303061
38	H	3.255124	-0.047289	3.291022
39	H	-0.333185	2.620745	0.223222
40	H	-0.687720	3.862055	-1.916049
41	H	1.019926	3.864435	-1.472254
42	H	0.441431	2.782141	-2.743909
43	H	-1.962517	1.898223	-1.828019
44	H	-1.048600	0.424829	-1.715320
45	H	-3.302510	-0.318959	-1.499055
46	H	-6.272123	-1.299025	-0.143678
47	H	-5.086538	-1.723891	-1.396759
48	H	-5.149951	-2.618451	0.136322
49	H	-5.447579	-0.022276	1.973872
50	H	-4.465525	-1.437699	2.297990
51	H	-3.699844	0.173192	2.222389

Isolobophytumin E (3) Conf. 2 P = 8.343%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5972311

1	C	-3.466242	-0.892089	1.148646
2	C	-2.016546	-1.213625	1.465136
3	C	-1.246571	-1.321223	0.168279
4	C	-2.321882	-1.429645	-0.964901
5	C	-3.697539	-1.458968	-0.270570
6	C	-1.778074	-0.106438	-1.619177
7	C	-0.677870	-0.015235	-0.507768
8	C	-0.786052	1.369650	0.173827
9	C	-1.599854	2.198749	-0.853052
10	C	-2.589654	1.203214	-1.484581
11	C	-1.521793	-1.442049	2.682007
12	C	-1.256831	-0.304914	-3.041140
13	H	0.329251	-0.184250	-0.896838
14	H	-2.199367	-2.283327	-1.634769
15	H	-0.503007	-2.116471	0.216839
16	C	0.555856	2.025359	0.572534
17	C	0.340245	3.438890	1.140595
18	C	1.355285	1.190058	1.608477
19	C	2.106552	-0.038402	1.106267
20	C	3.150917	0.231472	0.091297
21	O	1.874277	-1.145086	1.582253
22	C	3.963247	-0.647165	-0.534912
23	C	4.975582	-0.151163	-1.532282
24	C	3.958354	-2.135459	-0.330443
25	H	-1.383803	1.274002	1.088891
26	H	-3.608770	0.195155	1.153433
27	H	-4.154358	-1.302220	1.891496
28	H	-4.031783	-2.498544	-0.194883
29	H	-4.469429	-0.915664	-0.822714
30	H	-2.104371	3.057603	-0.404285
31	H	-0.921435	2.589022	-1.622229
32	H	-2.976100	1.551900	-2.446534
33	H	-3.452760	1.077756	-0.827330
34	H	-0.470196	-1.666147	2.824154
35	H	-2.149040	-1.395987	3.567473
36	H	-0.725702	0.584826	-3.396209
37	H	-0.563961	-1.150692	-3.094028
38	H	-2.081496	-0.502936	-3.734978
39	H	1.158790	2.121847	-0.339455
40	H	1.296542	3.908195	1.388197
41	H	-0.173704	4.087532	0.428655
42	H	-0.260456	3.402765	2.055968
43	H	2.119554	1.845046	2.046793
44	H	0.696872	0.868704	2.418508
45	H	3.271604	1.280560	-0.161617
46	H	4.792785	-0.602370	-2.513936
47	H	4.956468	0.934113	-1.638448
48	H	5.984538	-0.457109	-1.234367
49	H	4.942233	-2.457558	0.030524
50	H	3.198268	-2.451863	0.375809
51	H	3.805849	-2.639295	-1.291596

Isolobophytumin E (3) Conf. 3 P = 8.311%

B3LYP/6-326G(d,p) Energy / Hartree = -855.6004695

1	C	3.282502	1.896357	1.123066
2	C	1.970623	2.116016	0.391425
3	C	1.944674	1.228451	-0.830686
4	C	3.424578	0.770958	-1.063433
5	C	4.274950	1.462040	0.020048
6	C	2.992660	-0.734011	-0.909886
7	C	1.510641	-0.282496	-0.687783
8	C	1.019465	-0.876451	0.654788
9	C	2.022353	-2.029738	0.908712
10	C	3.370218	-1.515969	0.370832
11	C	1.043052	3.015016	0.721118
12	C	3.241174	-1.561481	-2.169771
13	H	0.845779	-0.577007	-1.505095
14	H	3.817543	0.973773	-2.061763
15	H	1.451259	1.723728	-1.668434
16	C	-0.459958	-1.317051	0.656074
17	C	-0.849952	-2.013379	1.970108
18	C	-1.396859	-0.132856	0.383058
19	C	-2.821009	-0.502376	-0.025533
20	C	-3.759700	0.641473	-0.055843
21	O	-3.115191	-1.654204	-0.322824
22	C	-5.078770	0.639614	-0.343866
23	C	-5.855353	1.928479	-0.307002
24	C	-5.887138	-0.573049	-0.709318
25	H	1.145183	-0.131241	1.450749
26	H	3.161297	1.097462	1.864326
27	H	3.608106	2.785431	1.667647
28	H	4.743492	2.350939	-0.413886
29	H	5.081819	0.830540	0.401745
30	H	2.076045	-2.325896	1.959043
31	H	1.706369	-2.912929	0.339493
32	H	4.075614	-2.326793	0.167555
33	H	3.841673	-0.870771	1.115961
34	H	0.139361	3.139947	0.133219
35	H	1.155445	3.657142	1.589326
36	H	2.768714	-2.546827	-2.095716
37	H	2.837672	-1.063936	-3.057417
38	H	4.314202	-1.714821	-2.330142
39	H	-0.592717	-2.036835	-0.160834
40	H	-1.902952	-2.301918	1.959048
41	H	-0.260806	-2.917836	2.136877
42	H	-0.689021	-1.346188	2.824406
43	H	-1.442972	0.532147	1.254077
44	H	-1.008780	0.494370	-0.430257
45	H	-3.307262	1.595787	0.199219
46	H	-6.667203	1.861467	0.425777
47	H	-5.227389	2.783645	-0.054438
48	H	-6.328775	2.114678	-1.277360

49	H	-6.308695	-0.442050	-1.712859
50	H	-5.299091	-1.484494	-0.685286
51	H	-6.741288	-0.665161	-0.029029

Isolobophytumin E (3) Conf. 4 P = 8.224%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5940797

1	C	0.870084	-2.983433	-0.242261
2	C	0.719244	-2.085513	0.974655
3	C	1.969156	-1.237792	1.070052
4	C	2.801260	-1.492677	-0.223854
5	C	1.828289	-2.218128	-1.179780
6	C	3.063226	0.056663	-0.351024
7	C	1.976079	0.302974	0.752156
8	C	0.784321	0.965438	0.027164
9	C	1.467724	1.752377	-1.116880
10	C	2.601793	0.829301	-1.611134
11	C	-0.317906	-2.072026	1.811366
12	C	4.483822	0.423248	0.074589
13	H	2.317809	0.911340	1.592045
14	H	3.715087	-2.078174	-0.091947
15	H	2.510922	-1.437211	1.997666
16	C	-0.190828	1.766995	0.924528
17	C	0.459070	2.925199	1.699323
18	C	-1.396750	2.328054	0.118906
19	C	-2.228282	1.271008	-0.593713
20	C	-3.167664	0.520185	0.267307
21	O	-2.091299	1.092107	-1.800616
22	C	-4.041472	-0.448151	-0.084987
23	C	-4.923506	-1.077571	0.959173
24	C	-4.232770	-0.980153	-1.476661
25	H	0.192832	0.171039	-0.440649
26	H	-0.085271	-3.239129	-0.706919
27	H	1.339464	-3.925403	0.070853
28	H	2.342994	-2.877671	-1.882243
29	H	1.251210	-1.507203	-1.776022
30	H	0.768503	2.019538	-1.912114
31	H	1.895921	2.683752	-0.730596
32	H	3.421768	1.397337	-2.059329
33	H	2.230657	0.153682	-2.385831
34	H	-0.345933	-1.413115	2.673416
35	H	-1.175696	-2.721078	1.665486
36	H	4.588210	1.506360	0.197605
37	H	4.750494	-0.049057	1.025542
38	H	5.212507	0.097269	-0.675693
39	H	-0.587499	1.060795	1.663964
40	H	-0.273274	3.390873	2.364617
41	H	1.293433	2.587465	2.317386
42	H	0.832357	3.702343	1.026552
43	H	-2.043861	2.876416	0.811877
44	H	-1.039294	3.031997	-0.635880
45	H	-3.143228	0.809281	1.314032
46	H	-4.751602	-2.158993	0.998539
47	H	-4.752967	-0.660569	1.952329
48	H	-5.978774	-0.941520	0.697584
49	H	-4.047954	-2.060526	-1.484865
50	H	-5.277387	-0.846695	-1.780551
51	H	-3.580381	-0.495976	-2.195458

Isolobophytumin E (3) Conf. 5 P = 6.455%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5993168

1	C	3.767010	1.660605	0.034382
2	C	2.495698	1.798923	-0.783380
3	C	2.117826	0.439440	-1.323748
4	C	3.393116	-0.456857	-1.168353
5	C	4.496865	0.445448	-0.582536
6	C	2.593087	-1.450949	-0.247065
7	C	1.313326	-0.565017	-0.410614
8	C	0.812609	-0.172525	0.999912
9	C	1.493494	-1.221327	1.915197
10	C	2.869936	-1.479702	1.275084
11	C	1.874061	2.945990	-1.057199
12	C	2.490680	-2.859084	-0.829921
13	H	0.519629	-1.059342	-0.978548
14	H	3.727909	-0.945280	-2.085700
15	H	1.696204	0.515956	-2.327144
16	C	-0.723866	-0.113785	1.143026
17	C	-1.154699	0.154381	2.593071
18	C	-1.321591	0.952295	0.187576
19	C	-2.842841	0.940421	0.144288
20	C	-3.443600	-0.185425	-0.604406
21	O	-3.481410	1.821885	0.711269
22	C	-4.750323	-0.495284	-0.750480
23	C	-5.150009	-1.693784	-1.568254
24	C	-5.896414	0.269683	-0.151898
25	H	1.201187	0.819184	1.262870
26	H	3.511622	1.461742	1.081898
27	H	4.368138	2.572524	0.024485
28	H	5.141373	0.787531	-1.398368
29	H	5.139054	-0.071847	0.135338
30	H	1.571257	-0.893755	2.954497
31	H	0.900936	-2.144757	1.910962
32	H	3.308482	-2.428100	1.598078
33	H	3.567545	-0.694408	1.575283
34	H	0.981275	2.975273	-1.673659
35	H	2.235323	3.895119	-0.673211
36	H	1.782395	-3.471872	-0.262056
37	H	2.150900	-2.833245	-1.870147
38	H	3.463788	-3.362075	-0.807116
39	H	-1.115624	-1.095940	0.845600
40	H	-2.241851	0.216148	2.683847
41	H	-0.812024	-0.637084	3.262675
42	H	-0.739067	1.102532	2.951042
43	H	-1.005341	1.948107	0.507306
44	H	-0.941733	0.782603	-0.824590
45	H	-2.722400	-0.834926	-1.092134
46	H	-5.816367	-1.391396	-2.383715
47	H	-4.289622	-2.211581	-1.993755
48	H	-5.716299	-2.401573	-0.952740
49	H	-6.524357	-0.408204	0.437077
50	H	-5.562393	1.095006	0.467968
51	H	-6.534835	0.657886	-0.954287

Isolobophytumin E (3) Conf. 6 P = 5.966%

B3LYP/6-326G(d,p) Energy / Hartree = -855.6004694

1	C	3.282626	1.896128	1.123183
2	C	1.970970	2.116063	0.391247
3	C	1.945063	1.228359	-0.830768
4	C	3.424944	0.770615	-1.063233
5	C	4.275211	1.461650	0.020351
6	C	2.992763	-0.734272	-0.909631
7	C	1.510790	-0.282509	-0.687756
8	C	1.019368	-0.876280	0.654814
9	C	2.022043	-2.029708	0.908939
10	C	3.370054	-1.516216	0.371164
11	C	1.043577	3.015398	0.720533

12	C	3.241299	-1.561837	-2.169458
13	H	0.845985	-0.577027	-1.505114
14	H	3.818137	0.973299	-2.061501
15	H	1.451843	1.723606	-1.668651
16	C	-0.460097	-1.316689	0.655932
17	C	-0.850376	-2.012767	1.970019
18	C	-1.396896	-0.132459	0.382617
19	C	-2.820962	-0.502065	-0.026267
20	C	-3.759734	0.641728	-0.056735
21	O	-3.115073	-1.653901	-0.323545
22	C	-5.079019	0.639498	-0.343728
23	C	-5.855760	1.928283	-0.307179
24	C	-5.887523	-0.573535	-0.707662
25	H	1.145080	-0.131023	1.450731
26	H	3.161095	1.097213	1.864374
27	H	3.608294	2.785108	1.667877
28	H	4.743885	2.350497	-0.413550
29	H	5.081983	0.830109	0.402192
30	H	2.075576	-2.325787	1.959301
31	H	1.705967	-2.912893	0.339759
32	H	4.075305	-2.327200	0.168007
33	H	3.841586	-0.871080	1.116304
34	H	0.140103	3.140493	0.132335
35	H	1.155906	3.657646	1.588658
36	H	2.768662	-2.547102	-2.095430
37	H	2.837996	-1.064255	-3.057172
38	H	4.314323	-1.715360	-2.329681
39	H	-0.592834	-2.036576	-0.160886
40	H	-1.903420	-2.301154	1.958873
41	H	-0.261404	-2.917297	2.137020
42	H	-0.689468	-1.345469	2.824238
43	H	-1.443302	0.532538	1.253627
44	H	-1.008591	0.494754	-0.430589
45	H	-3.307213	1.596224	0.197500
46	H	-6.667226	1.861601	0.426048
47	H	-5.227778	2.783691	-0.055478
48	H	-6.329692	2.113827	-1.277418
49	H	-6.741722	-0.664701	-0.027319
50	H	-6.308979	-0.443769	-1.711412
51	H	-5.299548	-1.485004	-0.682581

Isolobophytumin E (3) Conf. 7 P = 5.675%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5976712

1	C	-1.772497	-2.509378	0.734915
2	C	-1.558077	-2.105070	-0.712789
3	C	-2.468548	-0.942249	-1.030529
4	C	-3.538946	-0.909423	0.112241
5	C	-3.232932	-2.101838	1.038941
6	C	-3.091984	0.546995	0.503354
7	C	-2.038103	0.529703	-0.653817
8	C	-0.651727	0.854626	-0.046660
9	C	-1.007805	1.519175	1.308438
10	C	-2.265541	0.774126	1.793391
11	C	-0.777959	-2.741595	-1.586150
12	C	-4.208868	1.579507	0.361863
13	H	-2.285845	1.213340	-1.468541
14	H	-4.576284	-0.930256	-0.228098
15	H	-2.850147	-1.010259	-2.050437
16	C	0.296532	1.663033	-0.971783
17	C	-0.217684	3.069376	-1.323114
18	C	1.713421	1.767389	-0.383819
19	C	2.568593	0.504979	-0.458492
20	C	3.794815	0.549392	0.369279
21	O	2.253996	-0.428149	-1.187163
22	C	4.756022	-0.390258	0.498327
23	C	5.932120	-0.139137	1.403265
24	C	4.771013	-1.720985	-0.199071
25	H	-0.141437	-0.089516	0.169852
26	H	-1.078892	-1.955803	1.378615
27	H	-1.579592	-3.571343	0.902370
28	H	-3.899791	-2.930318	0.780266
29	H	-3.398375	-1.877077	2.096153
30	H	-0.190755	1.473335	2.033385
31	H	-1.247373	2.576905	1.158560
32	H	-2.822796	1.340395	2.545220
33	H	-1.978163	-0.169719	2.262623
34	H	-0.694981	-2.413504	-2.617475
35	H	-0.188911	-3.607103	-1.298943
36	H	-3.822237	2.598656	0.468458
37	H	-4.693790	1.506987	-0.616869
38	H	-4.977493	1.430860	1.128643
39	H	0.380388	1.094104	-1.904099
40	H	0.413005	3.519036	-2.095466
41	H	-1.240376	3.049289	-1.706451
42	H	-0.200967	3.738415	-0.457690
43	H	2.285478	2.533791	-0.926771
44	H	1.686482	2.121324	0.652369
45	H	3.916394	1.466670	0.938597
46	H	6.868039	-0.209628	0.837954
47	H	5.885508	0.839820	1.881670
48	H	5.982810	-0.908176	2.182105
49	H	5.671494	-1.797946	-0.819601
50	H	4.842013	-2.524463	0.542825
51	H	3.893562	-1.872824	-0.818671

Isolobophytumin E (3) Conf. 8 P = 5.464%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5973684

1	C	-1.263884	-2.510704	0.792434
2	C	-0.775944	-2.090487	-0.583114
3	C	-1.801928	-1.170079	-1.201485
4	C	-3.106577	-1.339638	-0.351768
5	C	-2.805164	-2.415636	0.709121
6	C	-3.076861	0.190469	0.017028
7	C	-1.782018	0.366523	-0.843661
8	C	-0.686761	0.965487	0.067774
9	C	-1.495776	1.600511	1.225564
10	C	-2.671593	0.628826	1.446522
11	C	0.332466	-2.531077	-1.178775
12	C	-4.303750	0.952239	-0.480472
13	H	-1.937887	0.973096	-1.738333
14	H	-3.999862	-1.592735	-0.926424
15	H	-1.894904	-1.345190	-2.274393
16	C	0.334893	1.882289	-0.649060
17	C	-0.268759	3.167322	-1.237686
18	C	1.521040	2.264159	0.279427
19	C	2.351914	1.075914	0.741306
20	C	3.297053	0.542097	-0.263586
21	O	2.206436	0.625943	1.874270
22	C	4.166790	-0.484138	-0.138351
23	C	5.057401	-0.857197	-1.292431
24	C	4.345472	-1.323978	1.094057
25	H	-0.112597	0.137509	0.494337
26	H	-0.876954	-1.817101	1.548288
27	H	-0.911054	-3.506381	1.070420

28	H	-3.208072	-3.372965	0.364025
29	H	-3.268113	-2.205435	1.677076
30	H	-0.896952	1.746241	2.128018
31	H	-1.881251	2.581460	0.928615
32	H	-3.501526	1.091413	1.988104
33	H	-2.338174	-0.219893	2.048103
34	H	0.608092	-2.207243	-2.177548
35	H	1.002280	-3.230998	-0.688817
36	H	-4.170978	2.033775	-0.369545
37	H	-4.496269	0.746650	-1.538371
38	H	-5.197167	0.664515	0.084915
39	H	0.744078	1.299608	-1.484095
40	H	0.470257	3.683885	-1.856319
41	H	-1.137473	2.960611	-1.866948
42	H	-0.581343	3.860301	-0.451754
43	H	2.171239	2.960200	-0.261250
44	H	1.144649	2.774926	1.168605
45	H	3.281973	1.065935	-1.215060
46	H	4.884187	-1.899279	-1.583124
47	H	4.897077	-0.220258	-2.163100
48	H	6.110368	-0.789417	-0.997086
49	H	4.176890	-2.378280	0.846916
50	H	5.383551	-1.253025	1.438974
51	H	3.676367	-1.026880	1.894553

Isolobophytumin E (3) Conf. 9 P = 4.975%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5934597

1	C	1.056321	-2.963815	0.453291
2	C	1.143329	-1.825161	1.456358
3	C	2.294813	-0.937623	1.033508
4	C	2.776347	-1.441178	-0.361525
5	C	1.653610	-2.384612	-0.846630
6	C	2.859596	0.050283	-0.863777
7	C	2.090066	0.500382	0.426387
8	C	0.699990	0.976112	-0.050723
9	C	0.990144	1.508025	-1.475935
10	C	2.010728	0.516479	-2.071895
11	C	0.357451	-1.660356	2.519342
12	C	4.303886	0.542139	-0.938698
13	H	2.594002	1.279389	1.003027
14	H	3.740132	-1.957399	-0.372067
15	H	3.077044	-0.917700	1.796147
16	C	-0.038133	1.947777	0.904811
17	C	0.671884	3.295003	1.110049
18	C	-1.497249	2.202017	0.450006
19	C	-2.399546	0.975931	0.571456
20	C	-3.017294	0.482810	-0.676469
21	O	-2.572800	0.474841	1.678541
22	C	-3.935778	-0.498785	-0.823117
23	C	-4.442802	-0.850483	-2.195187
24	C	-4.528802	-1.306756	0.295275
25	H	0.058416	0.092980	-0.157256
26	H	0.042345	-3.353333	0.333747
27	H	1.682154	-3.794632	0.805309
28	H	2.018234	-3.159804	-1.524550
29	H	0.874488	-1.834633	-1.380329
30	H	0.089240	1.600265	-2.088367
31	H	1.442404	2.503573	-1.416909
32	H	2.627298	0.983727	-2.844723
33	H	1.494251	-0.320826	-2.547490
34	H	0.487849	-0.825650	3.200306
35	H	-0.449477	-2.350891	2.743465
36	H	4.340713	1.628393	-1.072857
37	H	4.857671	0.298889	-0.026118
38	H	4.830445	0.080513	-1.781206
39	H	-0.100066	1.450232	1.878708
40	H	0.171223	3.867534	1.895877
41	H	1.714531	3.168693	1.410290
42	H	0.657861	3.904242	0.201759
43	H	-1.934890	2.962423	1.106596
44	H	-1.512523	2.605739	-0.565202
45	H	-2.689646	0.993817	-1.576461
46	H	-5.524493	-0.685607	-2.253590
47	H	-3.957803	-0.267682	-2.978986
48	H	-4.281421	-1.915195	-2.397103
49	H	-5.620512	-1.315739	0.208183
50	H	-4.204864	-2.350341	0.200010
51	H	-4.233564	-0.938836	1.272292

Isolobophytumin E (3) Conf. 10 P = 4.176%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5940796

1	C	-0.870335	-2.983465	0.242312
2	C	-0.719675	-2.085625	-0.974683
3	C	-1.969530	-1.237792	-1.069865
4	C	-2.801388	-1.492528	0.224228
5	C	-1.828278	-2.218025	1.179988
6	C	-3.063181	0.056853	0.351356
7	C	-1.976224	0.302988	-0.752042
8	C	-0.784265	0.965383	-0.027315
9	C	-1.467408	1.752498	1.116764
10	C	-2.601423	0.829534	1.611328
11	C	0.317302	-2.072261	-1.811610
12	C	-4.483821	0.423582	-0.073984
13	H	-2.318044	0.911346	-1.591900
14	H	-3.715303	-2.077936	0.092548
15	H	-2.511501	-1.437201	-1.997361
16	C	0.190869	1.766758	-0.924901
17	C	-0.459048	2.924806	-1.699904
18	C	1.396819	2.327871	-0.119460
19	C	2.228355	1.270982	0.593432
20	C	3.167402	0.519643	-0.267509
21	O	2.091680	1.092662	1.800451
22	C	4.041523	-0.448310	0.085069
23	C	4.923308	-1.078184	-0.959029
24	C	4.233488	-0.979349	1.477014
25	H	-0.192786	0.170954	0.440467
26	H	0.085098	-3.239208	0.706787
27	H	-1.339848	-3.925420	-0.070644
28	H	-2.342906	-2.877491	1.882581
29	H	-1.251008	-1.507131	1.776078
30	H	-0.768032	2.019722	1.911838
31	H	-1.895631	2.683842	0.730432
32	H	-3.421262	1.397624	2.059704
33	H	-2.230125	0.153935	2.385963
34	H	0.345191	-1.413399	-2.673701
35	H	1.175073	-2.721372	-1.665880
36	H	-4.588102	1.506702	-0.197026
37	H	-4.750746	-0.048735	-1.024860
38	H	-5.212387	0.097723	0.676464
39	H	0.587428	1.060382	-1.664228
40	H	0.273292	3.390390	-2.365267
41	H	-1.293386	2.586934	-2.317922
42	H	-0.832368	3.702061	-1.027279
43	H	2.044020	2.876011	-0.812538

44	H	1.039488	3.032056	0.635165
45	H	3.142512	0.808064	-1.314409
46	H	4.751914	-2.159720	-0.997414
47	H	4.752061	-0.662070	-1.952435
48	H	5.978646	-0.941402	-0.698094
49	H	4.048853	-2.059747	1.486007
50	H	5.278194	-0.845513	1.780430
51	H	3.581271	-0.494844	2.195744

Isolobophytumin E (3) Conf. 11 P = 3.114%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5934592

1	C	-1.055673	-2.963683	-0.454068
2	C	-1.142703	-1.824774	-1.456845
3	C	-2.294407	-0.937530	-1.033968
4	C	-2.776080	-1.441520	0.360869
5	C	-1.653282	-2.384928	0.845896
6	C	-2.859595	0.049804	0.863492
7	C	-2.089946	0.500345	-0.426449
8	C	-0.699996	0.976129	0.050965
9	C	-0.990356	1.507584	1.476302
10	C	-2.010961	0.515800	2.071855
11	C	-0.356648	-1.659530	-2.519630
12	C	-4.303966	0.541441	0.938331
13	H	-2.593925	1.279426	-1.002953
14	H	-3.739802	-1.957860	0.371139
15	H	-3.076519	-0.917536	-1.796726
16	C	0.038058	1.948197	-0.904208
17	C	-0.672087	3.295425	-1.109003
18	C	1.497140	2.202438	-0.449275
19	C	2.399536	0.976457	-0.571053
20	C	3.016550	0.482450	0.676854
21	O	2.573431	0.476138	-1.678385
22	C	3.935138	-0.499090	0.823248
23	C	4.441358	-0.851897	2.195328
24	C	4.529005	-1.305994	-0.295469
25	H	-0.058306	0.093057	0.157278
26	H	-0.041639	-3.353032	-0.334450
27	H	-1.681284	-3.794529	-0.806405
28	H	-2.017935	-3.160360	1.523529
29	H	-0.874349	-1.834987	1.379903
30	H	-0.089529	1.599684	2.088872
31	H	-1.442654	2.503127	1.417524
32	H	-2.627699	0.982837	2.844676
33	H	-1.494499	-0.321561	2.547364
34	H	-0.487083	-0.824663	-3.200389
35	H	0.450441	-2.349863	-2.743799
36	H	-4.340965	1.627659	1.072732
37	H	-4.857591	0.298317	0.025621
38	H	-4.830573	0.079548	1.780662
39	H	0.100058	1.451006	-1.878280
40	H	-0.171536	3.868213	-1.894713
41	H	-1.714754	3.169119	-1.409172
42	H	-0.658017	3.904406	-0.200541
43	H	1.934740	2.963088	-1.105604
44	H	1.512309	2.605838	0.566065
45	H	2.688265	0.992659	1.577067
46	H	5.522944	-0.686642	2.254616
47	H	3.955597	-0.270039	2.979358
48	H	4.280272	-1.916868	2.396108
49	H	5.620621	-1.315494	-0.207275
50	H	4.204534	-2.349552	-0.201781
51	H	4.234912	-0.936843	-1.272375

Isolobophytumin E (3) Conf. 12 P = 3.094%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5993168

1	C	3.767258	1.660434	0.034369
2	C	2.495951	1.798802	-0.783385
3	C	2.117979	0.439340	-1.323712
4	C	3.393156	-0.457089	-1.168206
5	C	4.496996	0.445135	-0.582424
6	C	2.593000	-1.451026	-0.246900
7	C	1.313304	-0.564993	-0.410604
8	C	0.812509	-0.172378	0.999845
9	C	1.493262	-1.221156	1.915258
10	C	2.869737	-1.479651	1.275280
11	C	1.874294	2.945885	-1.057106
12	C	2.490516	-2.859225	-0.829578
13	H	0.519657	-1.059308	-0.978613
14	H	3.727902	-0.945607	-2.085521
15	H	1.696476	0.515837	-2.327164
16	C	-0.723976	-0.113533	1.142812
17	C	-1.154968	0.154735	2.592795
18	C	-1.321595	0.952530	0.187316
19	C	-2.842850	0.940674	0.143869
20	C	-3.443534	-0.185277	-0.604705
21	O	-3.481510	1.822237	0.710595
22	C	-4.750235	-0.495381	-0.750404
23	C	-5.149970	-1.693943	-1.568059
24	C	-5.896269	0.269298	-0.151357
25	H	1.201153	0.819319	1.262752
26	H	3.511857	1.461715	1.081908
27	H	4.368492	2.572281	0.024350
28	H	5.141560	0.787083	-1.398271
29	H	5.139121	-0.072187	0.135488
30	H	1.570965	-0.893502	2.954538
31	H	0.900645	-2.144547	1.911058
32	H	3.308246	-2.428027	1.598390
33	H	3.567347	-0.694341	1.575445
34	H	0.981478	2.975193	-1.673518
35	H	2.235596	3.894996	-0.673113
36	H	1.782130	-3.471890	-0.261705
37	H	2.150834	-2.833510	-1.869841
38	H	3.463579	-3.362299	-0.806622
39	H	-1.115762	-1.095686	0.845408
40	H	-2.242128	0.216617	2.683416
41	H	-0.812493	-0.636738	3.262492
42	H	-0.739280	1.102855	2.950781
43	H	-1.005349	1.948351	0.507037
44	H	-0.941667	0.782862	-0.824833
45	H	-2.722337	-0.834642	-1.092619
46	H	-5.817013	-1.391756	-2.383027
47	H	-4.289657	-2.211339	-1.994205
48	H	-5.715509	-2.402064	-0.952231
49	H	-6.523748	-0.408743	0.437937
50	H	-5.562230	1.094746	0.468341
51	H	-6.535158	0.657345	-0.953444

Isolobophytumin E (3) Conf. 13 P = 2.027%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5967944

1	C	1.752913	-2.264784	-1.296951
2	C	0.787248	-2.038146	-0.149118
3	C	1.500107	-1.264117	0.933950
4	C	3.029860	-1.412641	0.627531
5	C	3.143986	-2.306028	-0.622724
6	C	3.167018	0.148840	0.508939

7	C	1.642706	0.305179	0.830956
8	C	0.988313	1.146296	-0.296395
9	C	2.208811	1.827416	-0.967168
10	C	3.350371	0.799257	-0.882619
11	C	-0.441604	-2.546084	-0.061321
12	C	4.119481	0.749908	1.541177
13	H	1.461922	0.767867	1.805825
14	H	3.629279	-1.806173	1.451100
15	H	1.170484	-1.581420	1.924624
16	C	-0.068302	2.153369	0.216536
17	C	-0.499462	3.182895	-0.843470
18	C	-1.282943	1.478440	0.880189
19	C	-2.281363	0.735909	-0.005183
20	C	-3.454336	0.215201	0.737844
21	O	-2.110080	0.597611	-1.209979
22	C	-4.536263	-0.431945	0.255257
23	C	-5.627949	-0.870792	1.194364
24	C	-4.775015	-0.771366	-1.188891
25	H	0.506595	0.488977	-1.026157
26	H	1.693631	-1.425763	-2.000031
27	H	1.522502	-3.170046	-1.863056
28	H	3.359583	-3.331301	-0.305739
29	H	3.950985	-2.003132	-1.295521
30	H	2.007255	2.148021	-1.992260
31	H	2.479996	2.724653	-0.396311
32	H	4.336175	1.259378	-0.997196
33	H	3.251018	0.068823	-1.688747
34	H	-1.066940	-2.374878	0.809040
35	H	-0.868539	-3.144856	-0.859913
36	H	4.058328	1.843463	1.546803
37	H	3.884321	0.397105	2.550432
38	H	5.156866	0.472918	1.322447
39	H	0.423084	2.717243	1.022384
40	H	-1.266463	3.850726	-0.437558
41	H	0.342694	3.804807	-1.154919
42	H	-0.913754	2.693875	-1.725641
43	H	-0.952056	0.765830	1.646887
44	H	-1.857827	2.231594	1.435102
45	H	-3.422702	0.398348	1.808403
46	H	-5.777337	-1.953900	1.123331
47	H	-5.409935	-0.615594	2.232083
48	H	-6.580319	-0.408108	0.912317
49	H	-4.863233	-1.858508	-1.299410
50	H	-5.734759	-0.352315	-1.511837
51	H	-3.981672	-0.409367	-1.834065

Isolobophytumin E (3) Conf. 14 P = 1.523%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5949948

1	C	2.878439	2.055882	1.154743
2	C	1.572946	2.134099	0.384643
3	C	1.665225	1.227566	-0.820950
4	C	3.188197	0.909649	-1.002379
5	C	3.937981	1.702518	0.085228
6	C	2.899574	-0.625484	-0.818820
7	C	1.372164	-0.316928	-0.669778
8	C	0.871753	-0.940840	0.656023
9	C	1.989930	-1.956447	1.008174
10	C	3.298486	-1.322598	0.503644
11	C	0.559650	2.952907	0.667637
12	C	3.283809	-1.463066	-2.036978
13	H	0.781716	-0.680454	-1.515677
14	H	3.587743	1.124804	-1.995500
15	H	1.153144	1.663205	-1.680424
16	C	-0.529591	-1.584013	0.569980
17	C	-0.919344	-2.283387	1.882377
18	C	-1.608187	-0.560197	0.175321
19	C	-2.898861	-1.188769	-0.342533
20	C	-4.177320	-0.445567	-0.416568
21	O	-2.909507	-2.361293	-0.704989
22	C	-4.493138	0.858566	-0.274852
23	C	-5.936340	1.276727	-0.395801
24	C	-3.554472	2.002507	-0.001695
25	H	0.842281	-0.169549	1.436255
26	H	2.815341	1.262837	1.908912
27	H	3.100231	2.982343	1.689053
28	H	4.326625	2.625888	-0.355593
29	H	4.793278	1.161293	0.498829
30	H	2.026379	-2.198738	2.072978
31	H	1.801023	-2.894211	0.470960
32	H	4.090649	-2.062550	0.357870
33	H	3.670863	-0.607850	1.240470
34	H	-0.331491	2.988932	0.049596
35	H	0.587880	3.619652	1.524012
36	H	2.911104	-2.488930	-1.945626
37	H	2.870021	-1.037857	-2.956909
38	H	4.372713	-1.510278	-2.149370
39	H	-0.495020	-2.341655	-0.220695
40	H	-1.917027	-2.722239	1.810429
41	H	-0.223662	-3.087096	2.132750
42	H	-0.921874	-1.570669	2.714747
43	H	-1.830933	0.099952	1.018498
44	H	-1.237482	0.090834	-0.625953
45	H	-4.991317	-1.127522	-0.649754
46	H	-6.066084	1.958171	-1.243864
47	H	-6.603951	0.424757	-0.526996
48	H	-6.245864	1.831160	0.497247
49	H	-3.619625	2.293908	1.053315
50	H	-2.515691	1.787274	-0.230044
51	H	-3.860337	2.876181	-0.584117

Isolobophytumin E (3) Conf. 15 P = 1.027%

B3LYP/6-326G(d,p) Energy / Hartree = -855.5967944

1	C	1.752604	-2.264739	-1.296992
2	C	0.787056	-2.038160	-0.149057
3	C	1.500004	-1.264131	0.933954
4	C	3.029743	-1.412745	0.627436
5	C	3.143731	-2.306076	-0.622871
6	C	3.166983	0.148728	0.508889
7	C	1.642700	0.305146	0.830939
8	C	0.988330	1.146341	-0.296370
9	C	2.208862	1.827409	-0.967140
10	C	3.350362	0.799177	-0.882649
11	C	-0.441724	-2.546245	-0.061076
12	C	4.119504	0.749695	1.541139
13	H	1.461963	0.767846	1.805813
14	H	3.629192	-1.806351	1.450946
15	H	1.170416	-1.581395	1.924652
16	C	-0.068214	2.153443	0.216627
17	C	-0.499322	3.183052	-0.843321
18	C	-1.282878	1.478516	0.880236
19	C	-2.281283	0.736041	-0.005197
20	C	-3.454228	0.215228	0.737811
21	O	-2.110020	0.597894	-1.210011
22	C	-4.536118	-0.431961	0.255207

23	C	-5.627861	-0.870755	1.194279	38	H	5.156865	0.472633	1.322384
24	C	-4.774789	-0.771436	-1.188937	39	H	0.423197	2.717241	1.022515
25	H	0.506558	0.489082	-1.026158	40	H	-1.266284	3.850904	-0.437368
26	H	1.693310	-1.425646	-1.999985	41	H	0.342872	3.804928	-1.154734
27	H	1.522117	-3.169937	-1.863168	42	H	-0.913658	2.694097	-1.725507
28	H	3.359303	-3.331374	-0.305954	43	H	-0.952018	0.765883	1.646923
29	H	3.950686	-2.003178	-1.295721	44	H	-1.857764	2.231668	1.435147
30	H	2.007311	2.148078	-1.992213	45	H	-3.422611	0.398375	1.808372
31	H	2.480119	2.724601	-0.396245	46	H	-5.777458	-1.953823	1.123134
32	H	4.336193	1.259240	-0.997230	47	H	-5.409803	-0.615688	2.232023
33	H	3.250942	0.068769	-1.688793	48	H	-6.580141	-0.407847	0.912287
34	H	-1.066938	-2.375123	0.809391	49	H	-4.863526	-1.858545	-1.299349
35	H	-0.868710	-3.145055	-0.859612	50	H	-5.734304	-0.351991	-1.512077
36	H	4.058432	1.843254	1.546807	51	H	-3.981200	-0.409821	-1.834021
37	H	3.884326	0.396868	2.550382					

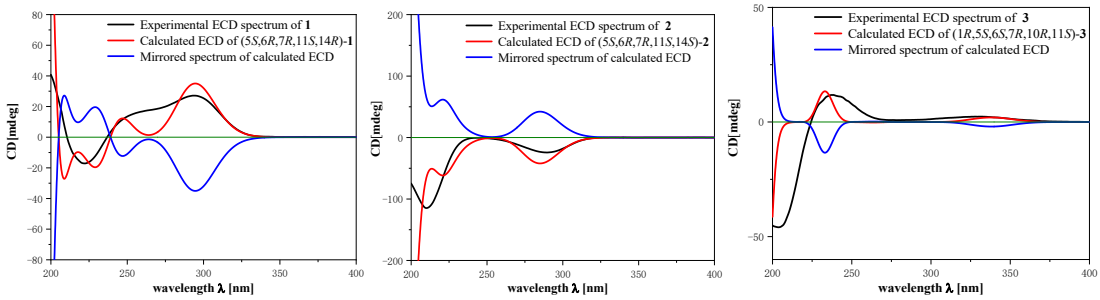

Figure S41. Experimental ECD spectrum (black), calculated spectrum (red) and its enantiomer (blue) of compounds **1**-**3**.

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