Supporting Information for

Eucalyptusdimers A–C, Dimeric Phloroglucinol-Phellandrene Meroterpenoids from *Eucalyptus robusta*

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Contents

Experimental Section

General Experiment Procedures

Optical rotations were determined on a Jasco P-1020 polarimeter. ECD spectra were recorded on an Applied Photophysics spectropolarimeter. UV spectra were taken on a Shimadzu UV2401 PC spectrophotometer. IR spectra were determined on a Bruker FT-IR Tensor-27 infrared spectrophotometer with KBr discs. HRESIMS were measured using an Agilent G6230 TOF-MS mass spectrometer. X-ray diffraction was conducted using Bruker APEX DUO diffractometer with graphite-monochromated CuKα radiation. 1D and 2D NMR spectra were obtained by Bruker DRX-500 or Avance III 600 spectrometers. Semi-preparative HPLC was performed on an Agilent 1260 instrument with a ZORBAX SBC18 column (9.4 × 250 mm, 5 μm) or an Agilent 1100 instrument with a CHIRALPAK IC column (10 × 250 mm, 5 μm). Sephadex LH-20 (GE Chemical Corporation), silica gel (200−300 mesh, Qingdao Marine Chemical Factory, Qingdao, People's Republic of China), and RP-18 (50 μm, Merck, Germany) were used for column chromatography (CC).

Plant Material

Eucalyptus robusta fruits identified by Dr. Rong Li (Kunming Institute of Botany, CAS) were collected from Kunming, Yunnan Province, China, in October 2015. A voucher specimen (HY0032) has been already deposited in the State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences.

Extraction and Isolation

The air-dried and powder fruits (5.0 kg) were extracted with PE-ethyl acetate (1:1 v/v, 15 L × 3, each 24 h) at room temperature to afford the crude extract after solvent evaporation under reduced pressure. This extract (230) was then chromatographed over silica gel and eluted with petroleum ether (PE)–EtOAC gradient solvent (100:1→1:1, v/v). Combination of similar fractions based on TLC analysis gave six fractions (Fr.A–Fr.F). Fr.E (10.5 g) was separated by column chromatography over Sephadex LH-20 ($CHCl_3$−MeOH, 3:2 v/v) to obtain four subfractions (Fr.E_1–Fr.E_4). Fr.E_1 (135 mg) was further purified by preparative HPLC (MeOH–H_2O, 5 mL/min) to give **1** (15.0 mg), **2** (12.0 mg), and **3** (2.5 mg). Fr.E_4 (1.2 g) was subjected to an RP-18 column (MeOH−H_2O, 40:60→80:20 v/v) to give **4** (35 mg) and three other subfractions. Compound **4** (3.0 mg) was then successively separated by chiral semi-preparative HPLC with *n*-hexane–2-propanol–CF_3COOH (98:2:0.05 v/v, 3.0 mL/min) to yield (+)-**4** (1.0 mg) and (–)-**4** (1.0 mg).

The physical data of 1–4

Eucalyptusdimer A (1): light yellow needle crystals ($CHCl_3$–MeOH, 1:3 v/v); $[\alpha]_D^{17}$ –56.2 (*c* 0.15, MeOH); UV (MeOH) λ_{max}(log ε) 204 (4.36), 219 (4.28), 305 (4.29) nm; ECD (MeOH) λ_{max} 237 ($\Delta\varepsilon$ –1.38), 251 ($\Delta\varepsilon$ –0.94), 267 ($\Delta\varepsilon$ +0.24), 321 ($\Delta\varepsilon$ –1.90), 339 ($\Delta\varepsilon$ –0.91), 345 ($\Delta\varepsilon$ –1.00) nm; IR (KBr) ν_{max} 3445, 2961, 1627, 1456, 1263, 1025 cm^{-1}; ^1H and ^{13}C NMR data, see Table 1; HRESIMS *m*/*z* 737.4028 $[M + Na]^+$ (calcd for $C_{44}H_{58}O_8Na$, 737.4029).

Eucalyptusdimer B (2): light yellow amorphous powder; $[\alpha]_D^{17}$ +45.4 (c 0.13, MeOH); UV (MeOH) λ_{max}(log ε) 204 (4.35), 219 (4.28), 305 (4.29) nm; ECD (MeOH) λ_{max} 231 ($\Delta\varepsilon$ +18.43), 260 ($\Delta\varepsilon$ +0.44), 296 ($\Delta\varepsilon$ +5.79), 344 ($\Delta\varepsilon$ +1.59) nm; IR (KBr) ν_{max} 3445, 2963, 1626, 1456, 1261, 1025 cm^{-1}; ^1H and ^{13}C NMR data, see Table 1; HRESIMS *m*/*z* 737.4023 $[M + Na]^+$ (calcd for $C_{44}H_{58}O_8Na$, 737.4029).

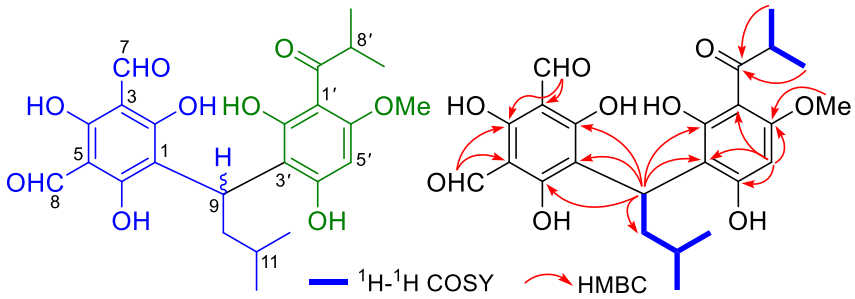
Eucalyptusdimer C (3): light yellow amorphous powder; $[\alpha]_D^{20}$ –100.6 (*c* 0.12, MeOH); UV (MeOH) λ_{max}(log ε) 203 (4.41), 219 (4.36), 305 (4.38) nm; ECD (MeOH) λ_{max} 243 ($\Delta\varepsilon$ +3.25), 251 ($\Delta\varepsilon$ –2.69), 267 ($\Delta\varepsilon$ +0.21), 318 ($\Delta\varepsilon$ –8.77) nm; IR (KBr) ν_{max} 3447, 2962, 1626, 1455, 1261, 1025 cm^{-1}; ^1H and ^{13}C NMR data, see Table S1; HRESIMS *m*/*z* 727.4208 $[M - H]^-$ (calcd for $C_{45}H_{59}O_8$, 727.4210).

Eucalyprobusone A (4): light yellow amorphous powder; $[\alpha]_D^{25}$ +119.3 (*c* 0.10, MeOH) for (+)-**4**, $[\alpha]_D^{25}$ –124.2 (*c* 0.10, MeOH) for (–)-**4**; UV (MeOH) λ_{max}(log ε) 205 (4.49), 295 (4.65) nm; ECD (MeOH) λ_{max} 230 ($\Delta\varepsilon$ –7.46), 267 ($\Delta\varepsilon$ –0.68), 298 ($\Delta\varepsilon$ +7.59), 352 ($\Delta\varepsilon$ –2.51) nm for (+)-**4**, ECD (MeOH) λ_{max} 230 ($\Delta\varepsilon$ +9.87), 267 ($\Delta\varepsilon$ –0.56), 299 ($\Delta\varepsilon$ –10.0), 350 ($\Delta\varepsilon$ +3.15) nm for (–)-**4**; ^1H and ^{13}C NMR data, see Table S2; HRESIMS *m*/*z* 499.1345 $[M + K]^+$ (calcd for $C_{24}H_{28}O_9K$, 499.1365).

Crystallographic Data of 1: $C_{44}H_{58}O_8$•$CHCl_3$, M = 834.27, orthorhombic, *a* = 11.7225(2) Å, *b* = 15.0056(2) Å, *c* = 24.7900(3) Å, α = 90 °, β = 90 °, γ = 90 °, *V* = 4360.64(11) $Å^3$, *Z* = 4, *T* = 100(2) K, μ(CuKα) = 2.315 mm^{-1}, Dcalc = 1.271 g/cm^3, 23721 reflections measured, 7653 independent reflections (R_{int} = 0.0423). The final R_1 values were 0.0659 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1794 ($I > 2\sigma(I)$). The final R_1 values were 0.0702 (all data). The final $wR(F^2)$ values were 0.1843 (all data). The goodness of fit on F^2 was 1.030. Flack parameter = 0.045(6).

Structure elucidation of 4

Eucalyprobusone A (**4**) had a molecular formula of $C_{24}H_{28}O_9$ as determined by the HRESIMS ion at *m*/*z* 499.1345 $[M + K]^+$ (calcd for $C_{24}H_{28}O_9K$, 499.1365), implying ten degrees of unsaturation. The gross structure of **4** was achieved to be a biogenetically related intermediate of **1**–**3** by the $^1H–^1H$ COSY and HMBC analyses. According to the fact that **1** and **2** were C-9 epimers, **4** was thus a racemic mixture as proved by chiral analysis. Finally, the ECD calculation allowed the establishment of the absolute configurations as 9*S* for (+)-**4** and 9*R* for (–)-**4**.



Structure and 2D NMR correlations of **4**

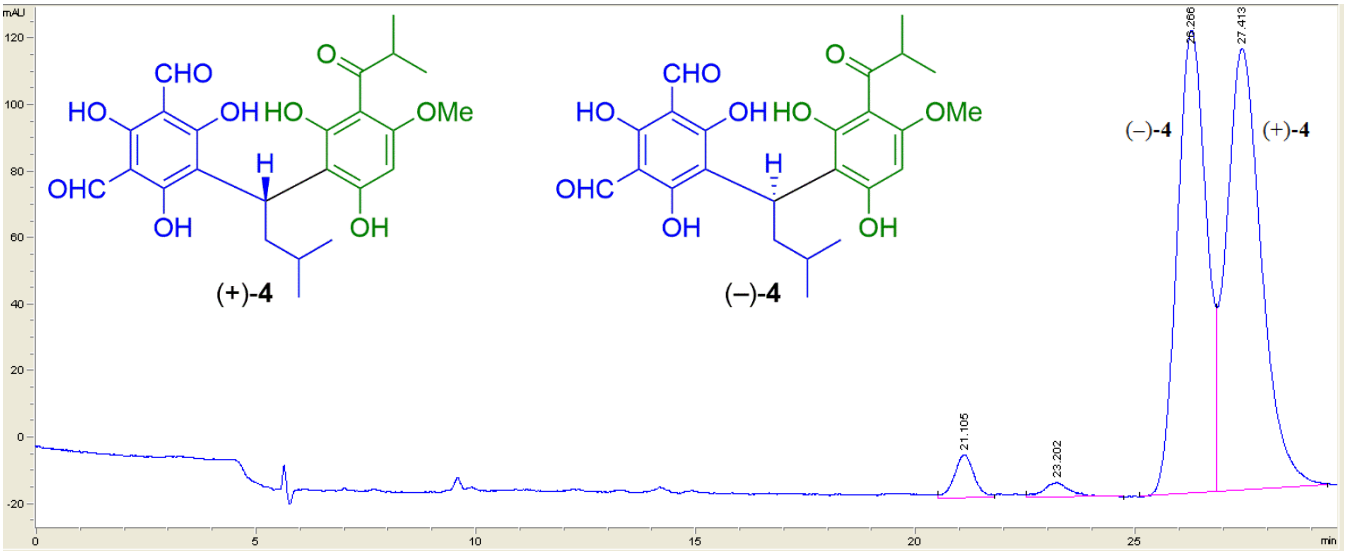


Table S1. ^1H (500 MHz) and ^{13}C (125 MHz) NMR data of Eucalyprobusone A (4) in Acetone-d_6

no.	δ_C	δ_H (mult., *J* in Hz)	no.	δ_C	δ_H (mult., *J* in Hz)
1	108.9		1′	104.6	
2/6	164.2 ×2		2′	166.3	
3/5	104.9 ×2		3′	110.1	
4	168.9		4′	162.8	
7/8	193.1	10.08 ×2 s	5′	92.9	6.22 s
9	26.7	5.27 t (8.4)	6′	162.8	
10a	41.2	2.20 ddd (15.2, 9.2, 6.1)	7′	211.8	
10b		1.79 dt (13.5, 6.8)	8′	40.0	3.82 sext. (6.8)
11	27.1	1.46 m	9′	19.5	1.13 d (6.8)
12	22.4	0.87 d (6.6)	10′	19.6	1.13 d (6.8)
13	23.2	0.93 d (6.6)	OMe-6′	56.2	3.90 s

Computational Methods and Results

Theoretical calculations of ECD spectra for compounds **1**–**4** were performed with the Gaussian 09 program package. The calculation of **1**–**4** were based on their crystal data, geometries and energy structures. The geometry was optimized with MM2 at the first time, and then reoptimized at the b3lyp/6-31g(d,p) level of theory. The ECD computation of compounds **1**–**4** were performed with DFT calculations at the B3LYP/6-311++G(2d,p) level. Their absolute configurations were determined as (7*S*,9*R*,1′*R*,4′*R*,6′*R*,1″*R*,4″*R*,6″*R*)-**1**, (7*S*,9*S*,1′*R*,4′*R*,6′*R*,1″*R*,4″*R*,6″*R*)-**2**, (7*S*,9*R*,1′*R*,4′*R*,6′*R*,1″*R*,4″*R*,6″*R*,8‴*S*)-**3**, (9*S*)-(+)-**4**, and (9*R*)-(–)-**4**, respectively.

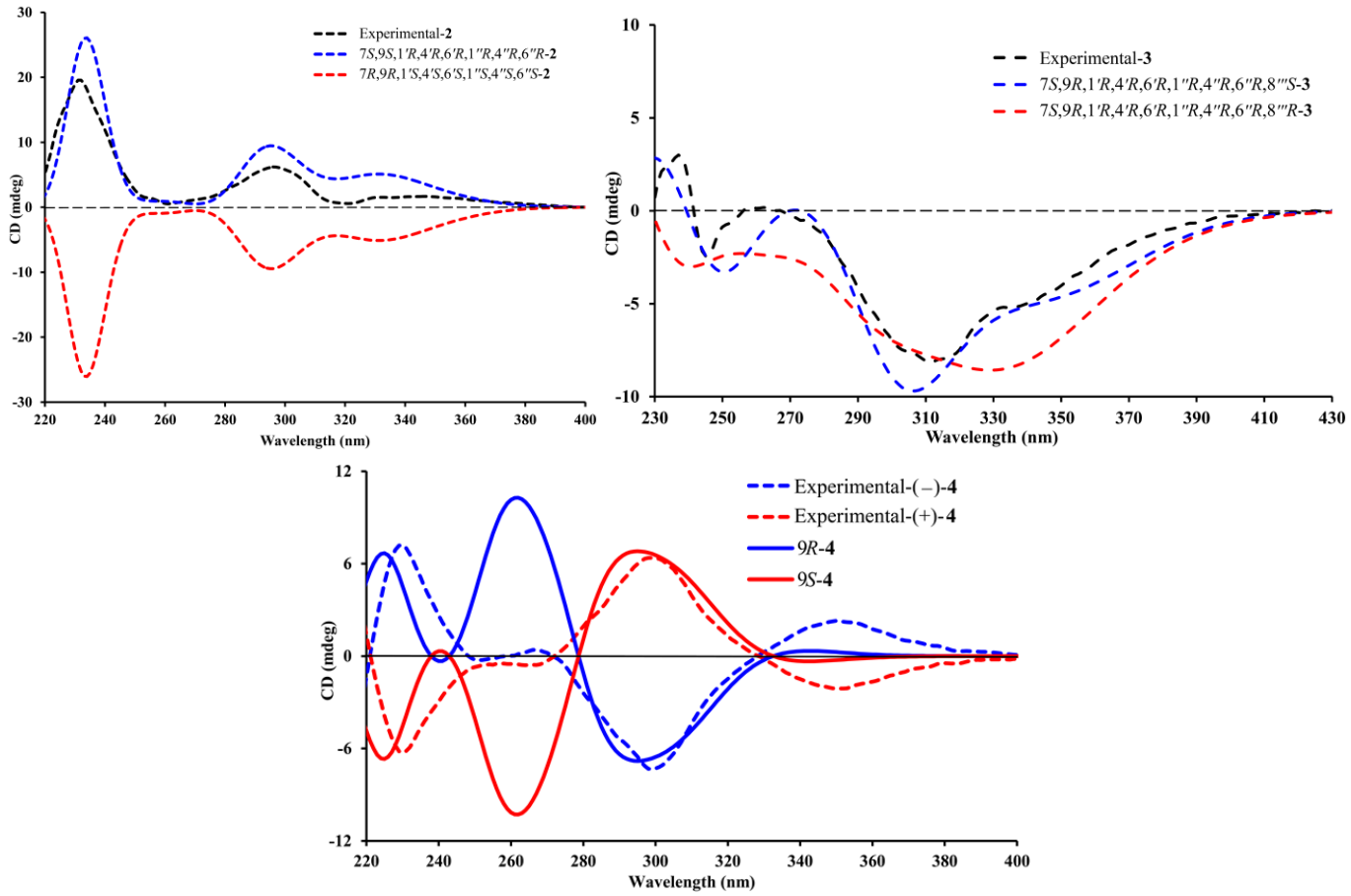


Figure S1. Calculated and experimental ECD spectra of **2**–**4**

Bioactivitiy Assays

Anti-inflammatory Assay

Murine monocytic RAW264.7 macrophages were dispensed into 96-well plates (2×10^5 cells/well) containing RPMI 1640 medium (HyClone) with 10% FBS under a humidified atmosphere with 5% CO_2 at 37 ℃. After 24 h of preincubation, cells were treated with serial dilutions of the test compounds, up to a maximum concentration of 50 μM, with the presence of 1.0 μg/mL LPS for 18 h. The compounds were dissolved in DMSO and further diluted in medium to produce different concentrations. NO production in each well was assessed by adding 100 μL of Griess reagent (reagent A and reagent B, Sigma) to 100 μL of each supernatant from the LPS (Sigma)-treated or LPS- and compound-treated cells in triplicate. After a 5 min incubation, the absorbance of samples was measured at 570 nm with a 2104 Envision multilabel plate reader (Perkin-Elmer Life Sciences, Inc., Boston, MA, USA). L-N^G-monomethyl arginine (L-NMMA) was used as a positive control.

PTP1B Inhibitory Assay

Briefly, 30 nM PTP1B (protein tyrosine phosphatase-1B), 50 mM 3-[*N*-morpholino]propanesulfonic acid (MOPs) buffer (pH 6.5), and 60 μM IR5 (insulin receptor) were successively added to each well of a 96-well plate with or without test compounds (50 μM, 100 μL for each well). The reaction was terminated with Red reagent (phosphoric acid test reagent) after incubation at 30 ℃ for 30 min, and then it was incubated for another 20 min at 30 ℃. The OD values were tested by a microplate reader at 620 nm. The percentage inhibition was calculated as follows: inhibition (%) = (1 – experimental OD/blank OD) × 100. Suramin, a known phosphatase inhibitor, was used as a positive control.

Table S2. PTP1B Inhibitory Effects of 1–4 (50 μM)

Compounds	Suramin	**1**	**2**	**3**	**4**	(+)-**4**
Inhibitory rate (%)	90.79	10.95	21.16	22.34	17.08	4.25
SD	0.06	1.41	1.87	2.42	0.72	1.46

AChE Inhibitory Assay

AChE (acetylcholinesterase) inhibitory effects of **1**–**3** were evaluated by the spectrophotometric method[1] with slightly modification. All these meroterpenoids were dissolved in DMSO. The reaction mixture (totally 200 μL) containing phosphate buffer (pH = 8.0), **1**–**3** (50 μM), and acetyl cholinesterase (0.02 U/mL), was incubated for 20 min at 37 ℃. Then, the reaction was initiated by the addition of 40 μL of solution containing DTNB (0.625 mM) and acetylthiocholine iodide (0.625 mM) for AChE inhibitory activity assay, respectively. The hydrolysis of acetylthiocholine was monitored at 405 nm every 30 seconds for an hour. All the reactions were performed in triplicate. The percentage inhibition was calculated as follows: inhibition (%) = (E – S)/E × 100 (E is the activity of the enzyme without **1**–**3** and S is the activity of enzyme with **1**–**3**).

1. Ellman, G. L.; Courtney, K. D.; Andres, V. J.; Featherstone, R. M. *Biochem. Pharmacol.* **1961**, *7*, 88–95.

Table S3. AChE Inhibitory Effects of 1–4 (50 μM)

Compounds	**1**	**2**	**3**	**4**	(+)-**4**	(–)-**4**
Inhibitory rate (%)	75.85	43.79	38.16	84.21	75.73	78.06
SD	1.64	1.64	1.50	1.20	0.61	0.70

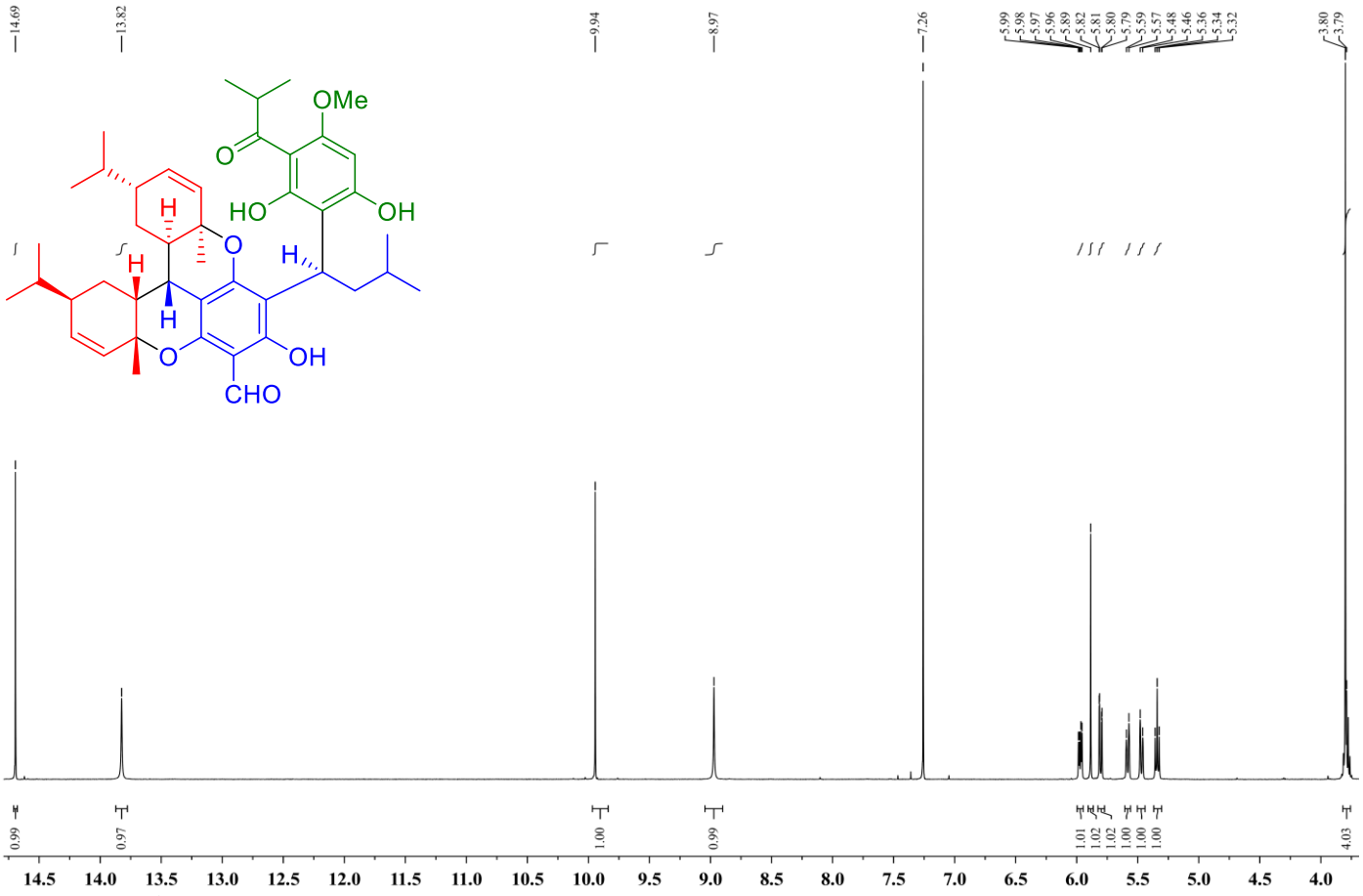


Figure S2 ^{1}H NMR Spetrum of Eucalyptusdimer A (**1**) in $CDCl_3$

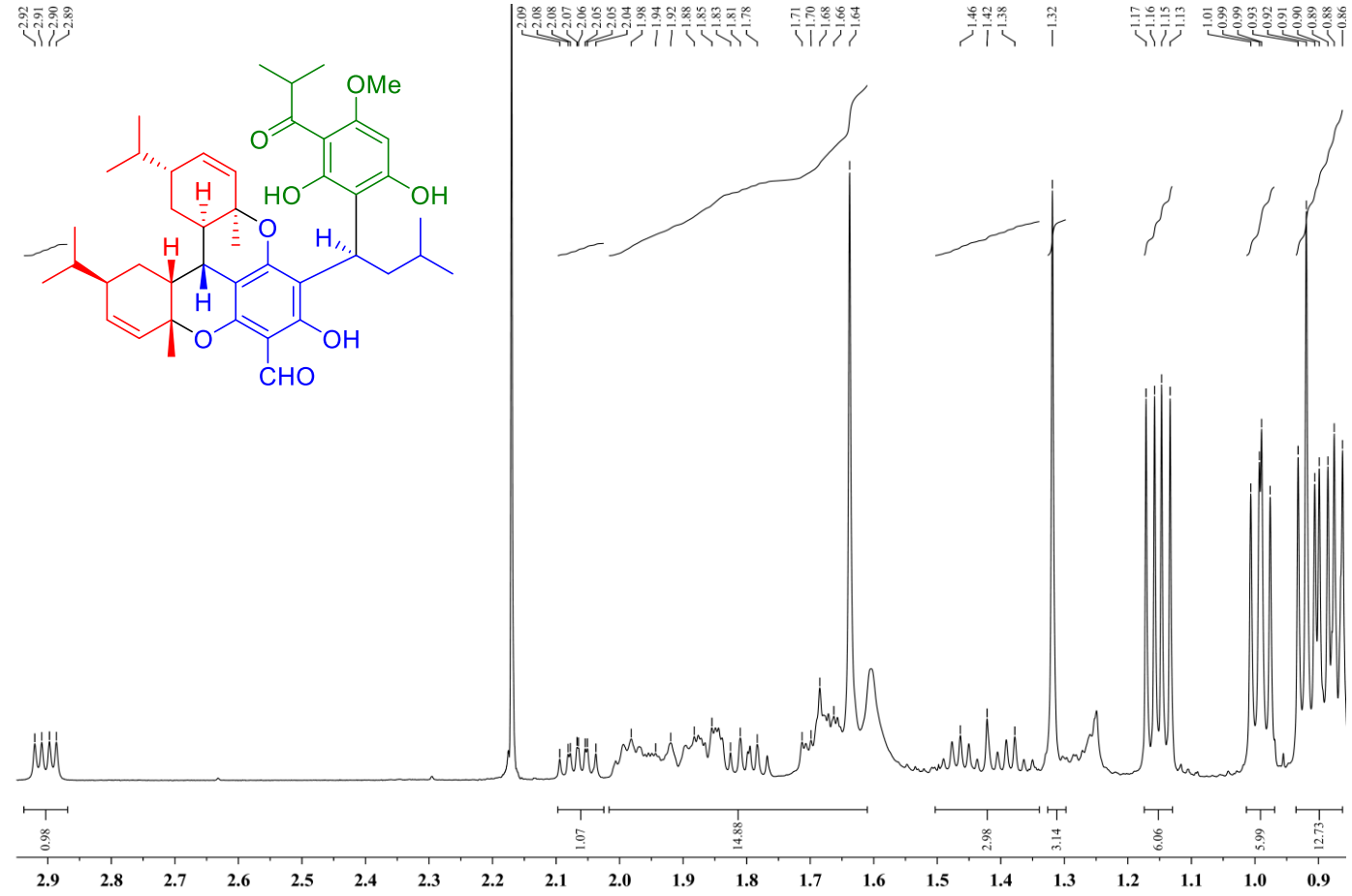


Figure S3 ^{1}H NMR Spetrum of Eucalyptusdimer A (**1**) in $CDCl_3$

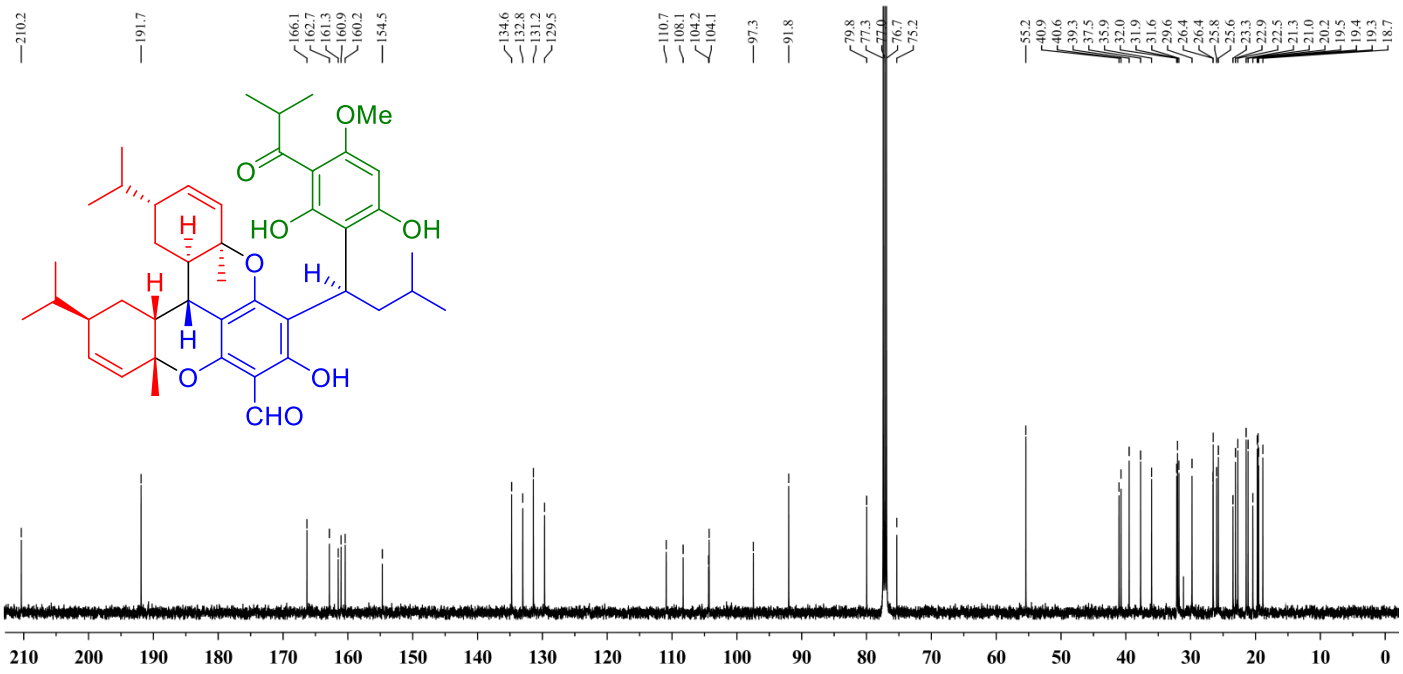


Figure S4 ^{13}C NMR Spetrum of Eucalyptusdimer A (**1**) in $CDCl_3$

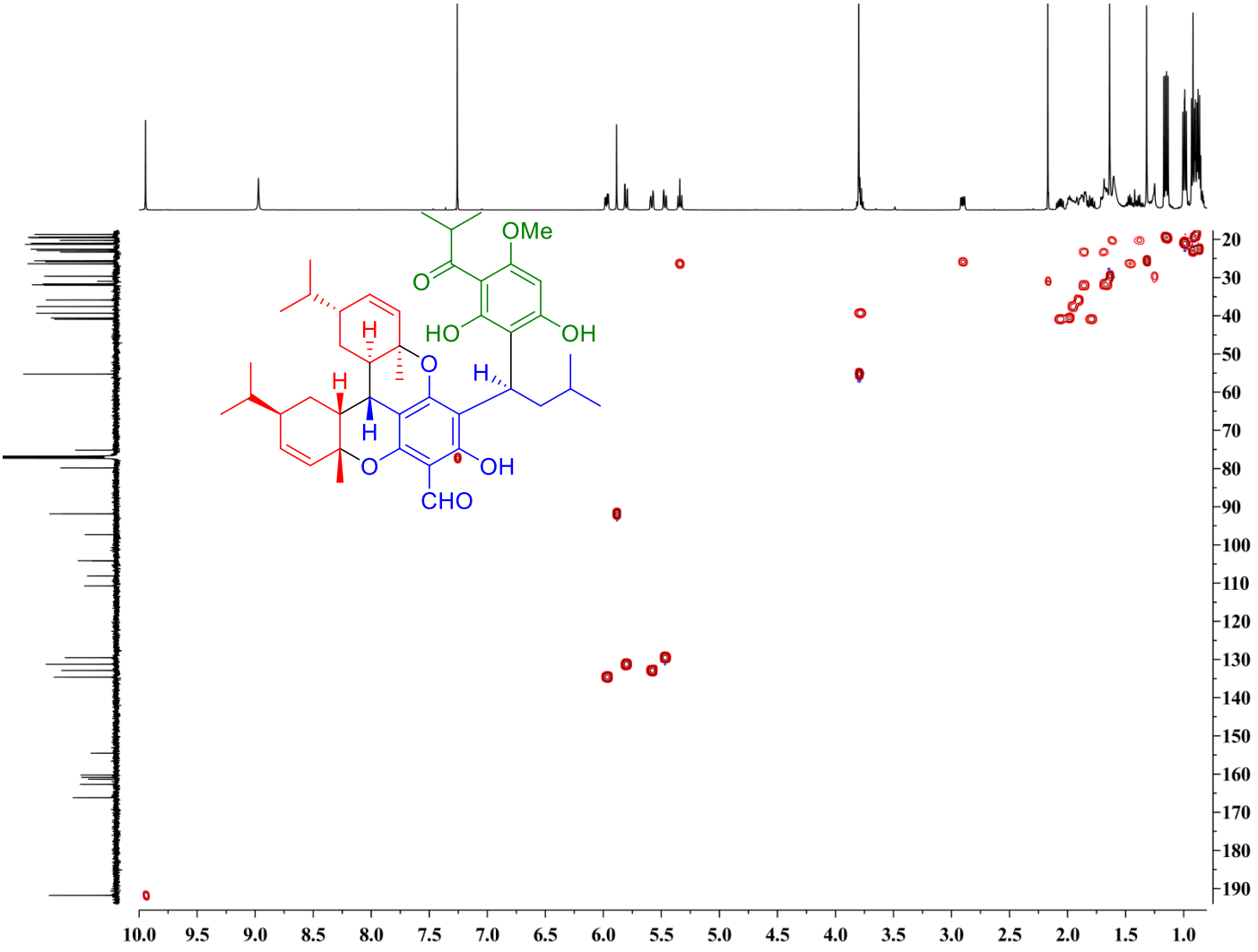


Figure S5 HSQC Spetrum of Eucalyptusdimer A (**1**)

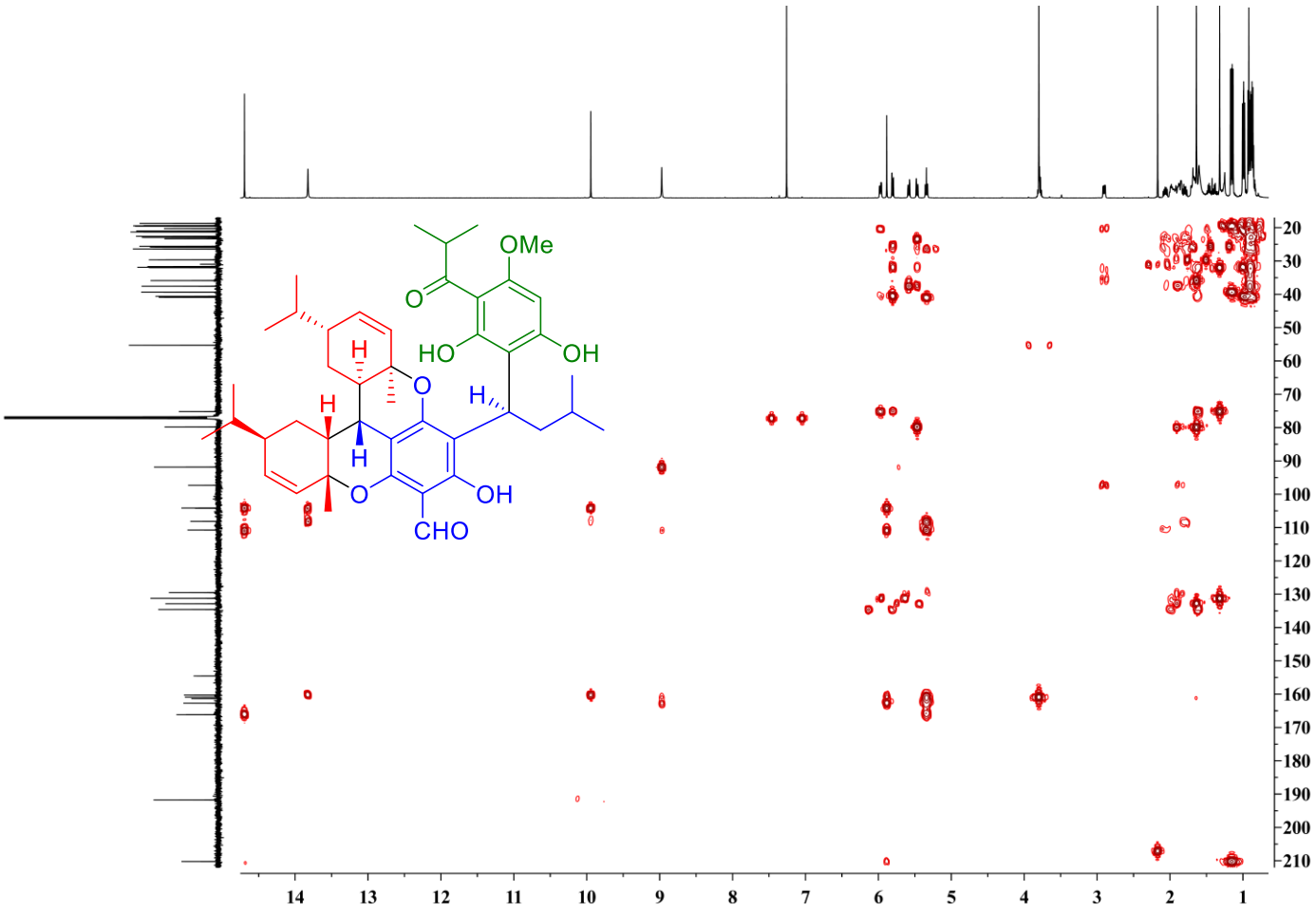


Figure S6 HMBC Spetrum of Eucalyptusdimer A (**1**)

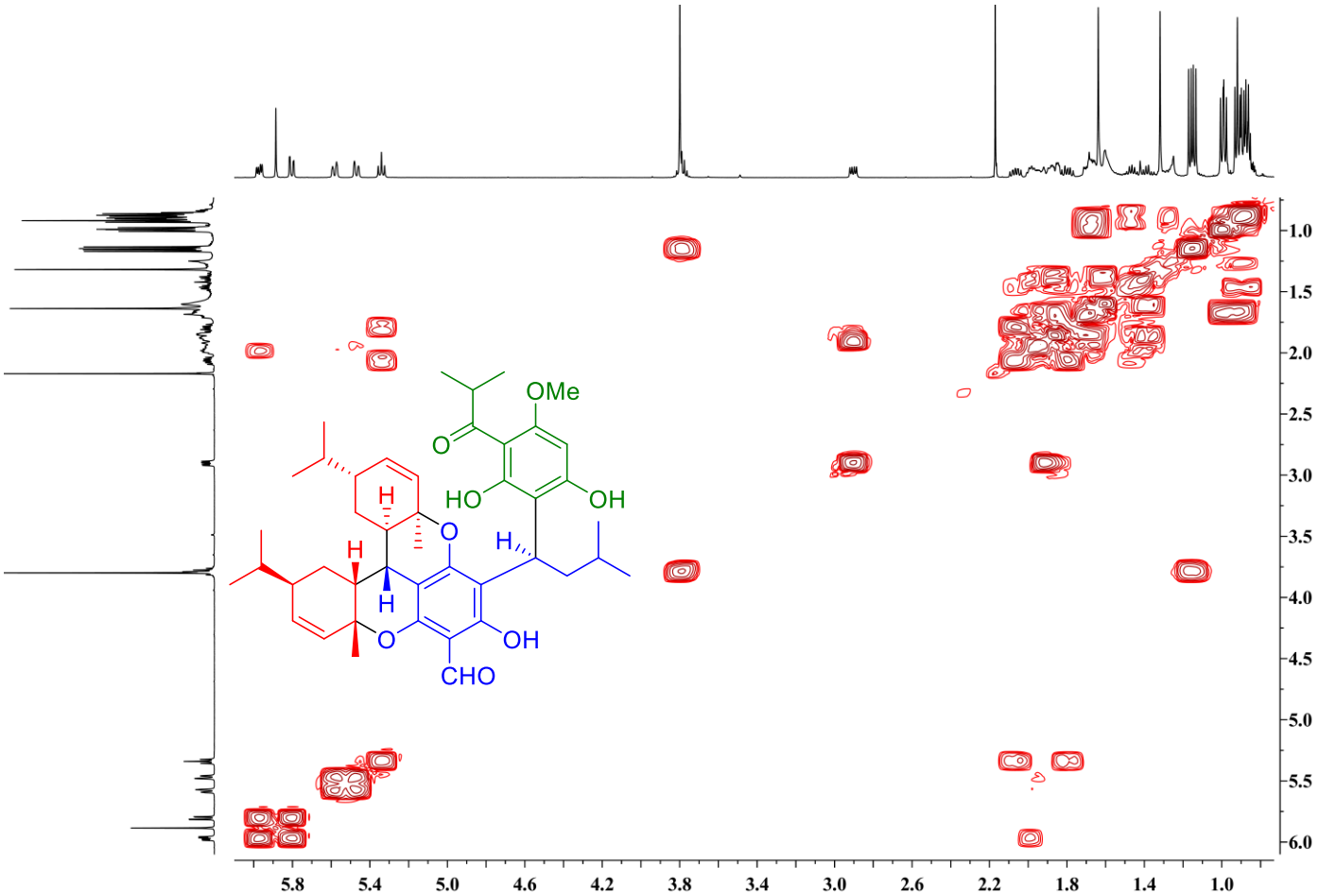


Figure S7 ^{1}H–^{1}H COSY Spetrum of Eucalyptusdimer A (**1**)

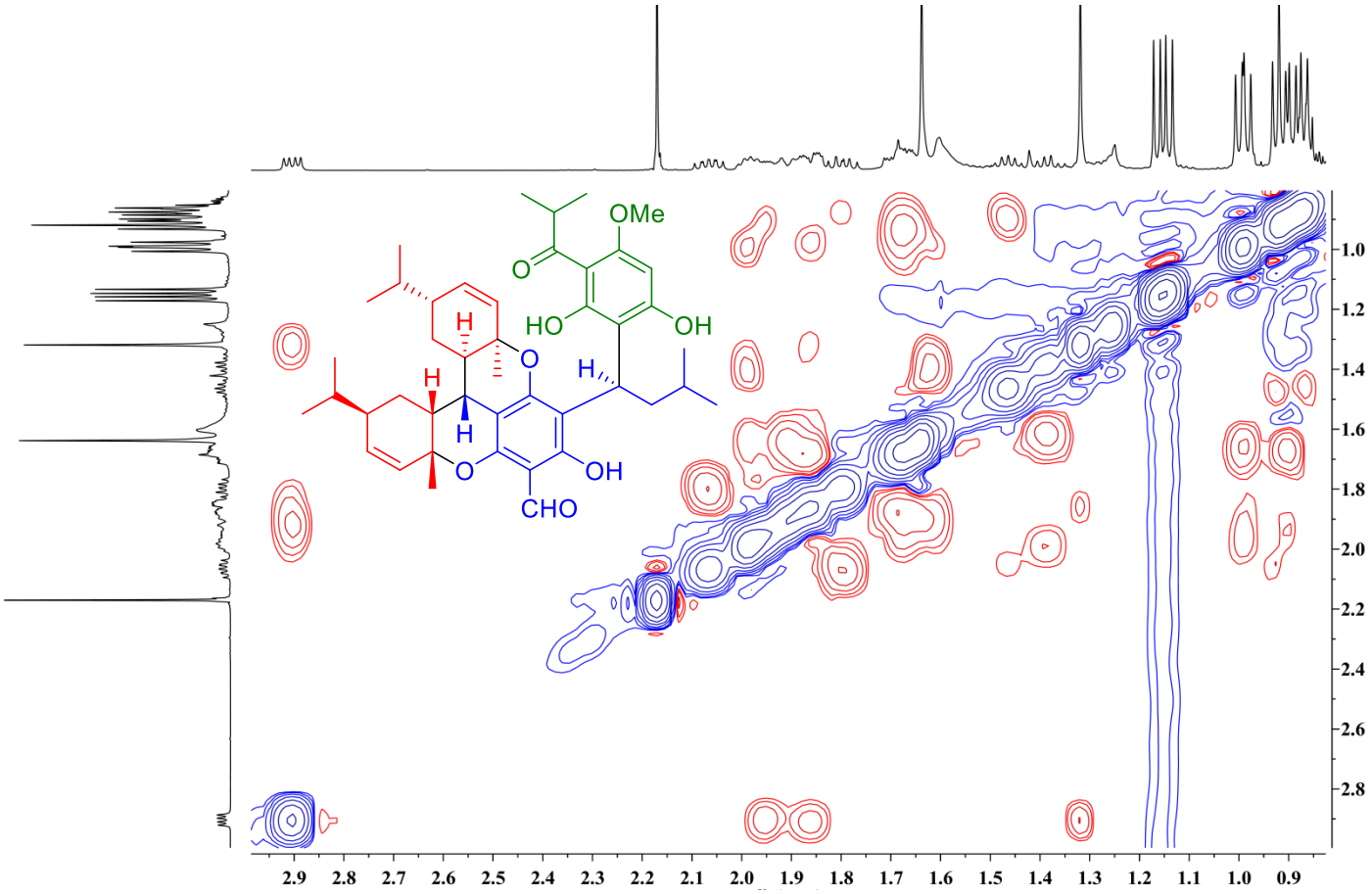


Figure S8 ROESY Spetrum of Eucalyptusdimer A (**1**)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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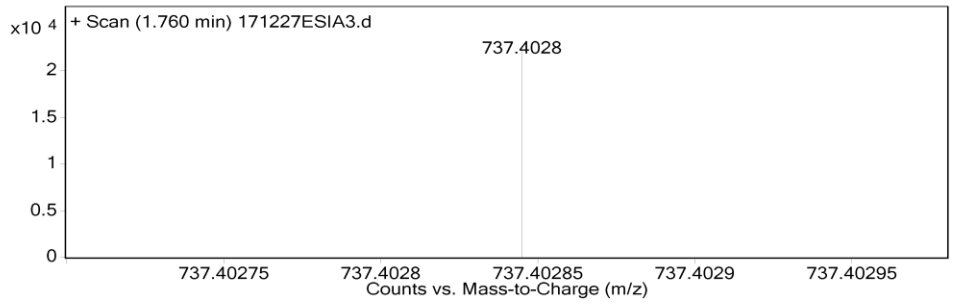

Peak List

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391.1896	1	10453.85		
437.1953	1	27722.77		
438.1987	1	6109.48		
527.3138	1	8758.85		
619.5266	1	6440.91		
647.5589	1	5551.11		
737.4028	1	22277.34	C44 H58 Na O8	M+
738.4055	1	9167.02	C44 H58 Na O8	M+
922.0098	1	60144.13		
923.0121	1	8105.51		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	4	10
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C44 H58 Na O8	737.4029	737.4028	0.1	0.2	15.5

Figure S9 ROESY Spetrum of Eucalyptusdimer A (**1**)

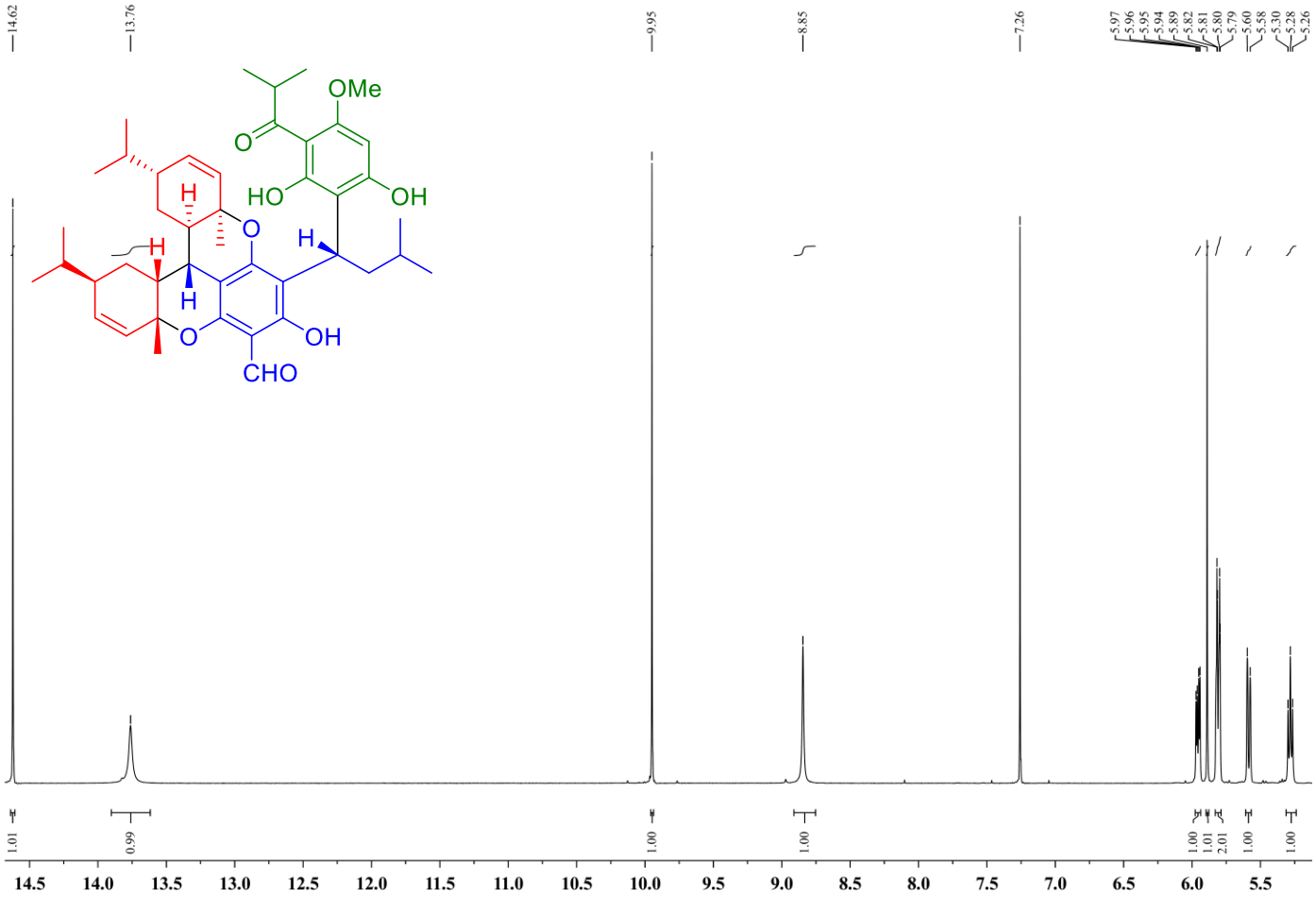


Figure S11 ^{1}H NMR Spetrum of Eucalyptusdimer B (**2**)

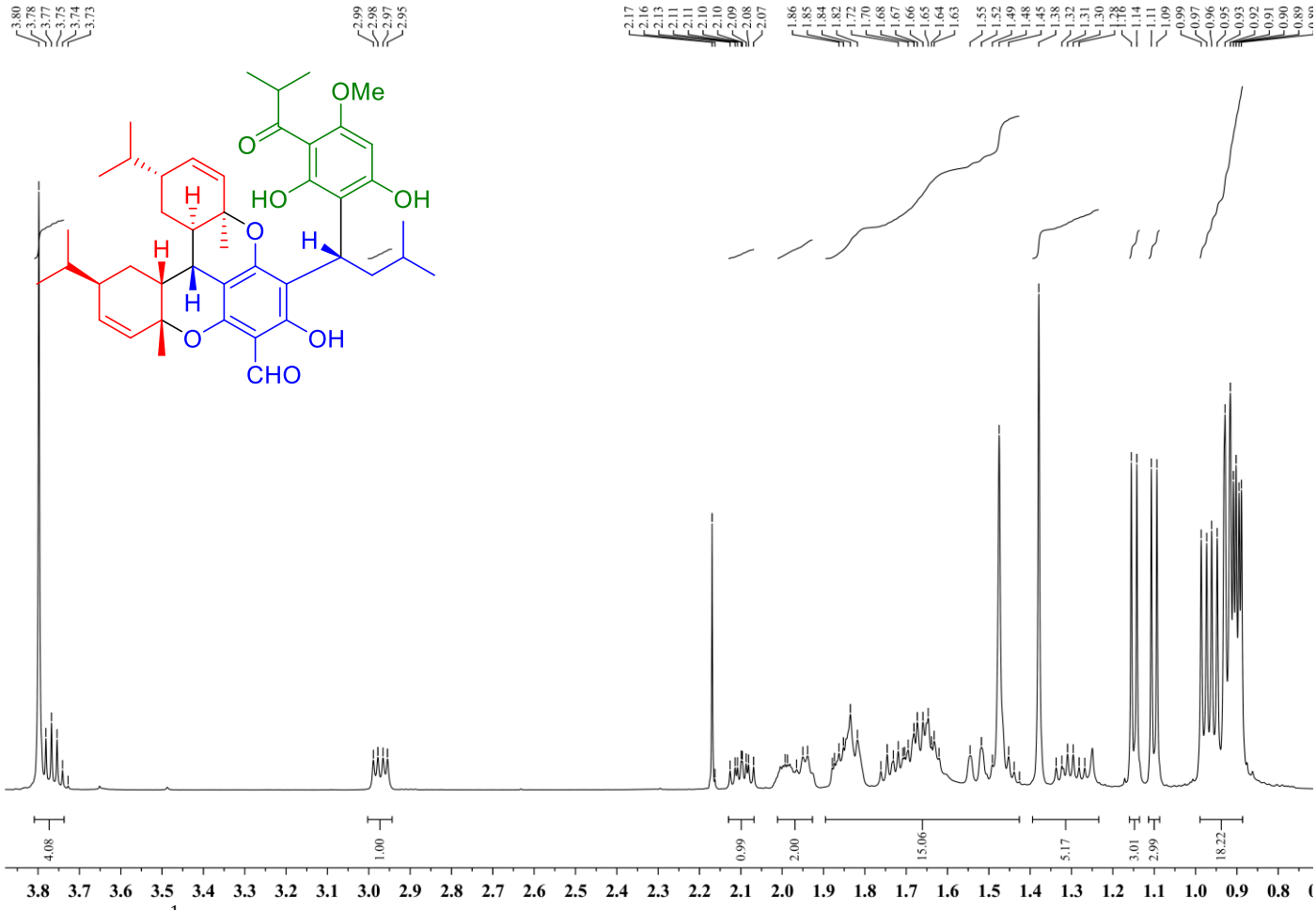


Figure S12 ^{1}H NMR Spetrum of Eucalyptusdimer B (**2**)

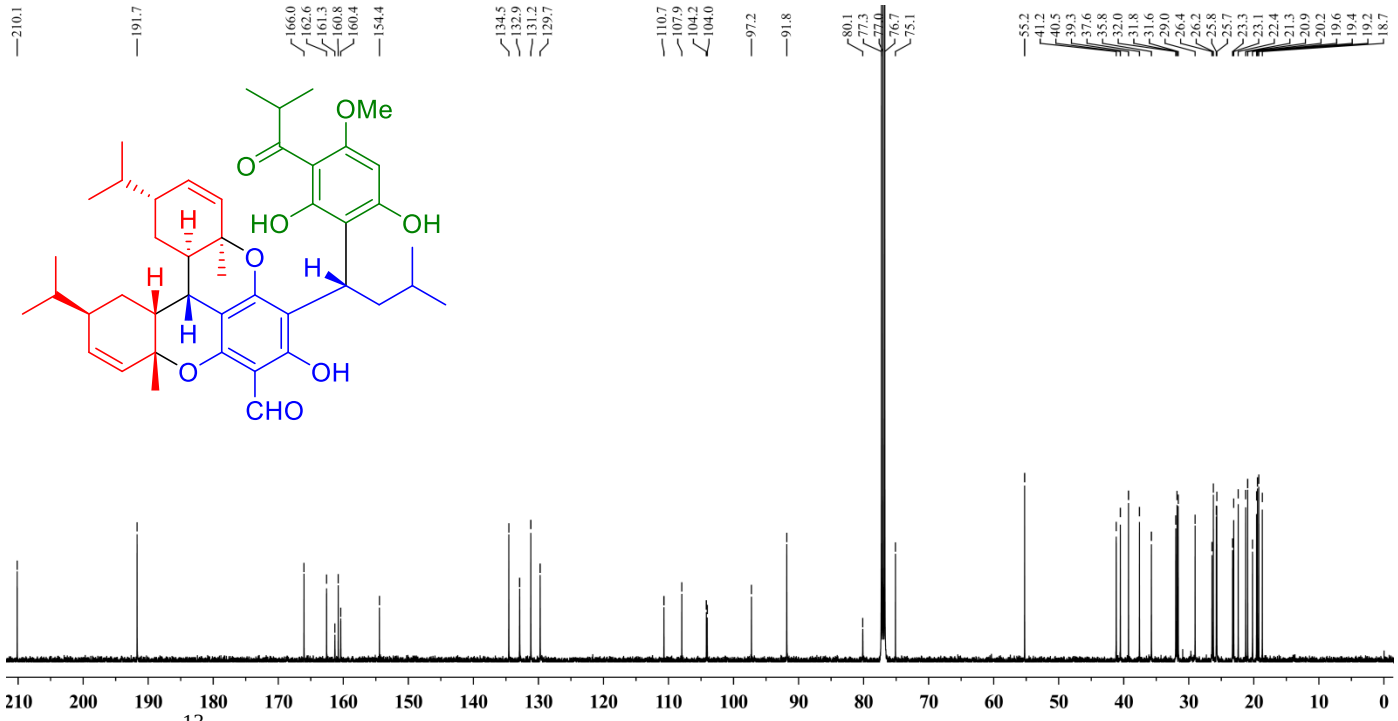


Figure S13 ^{13}C NMR Spetrum of Eucalyptusdimer B (**2**)

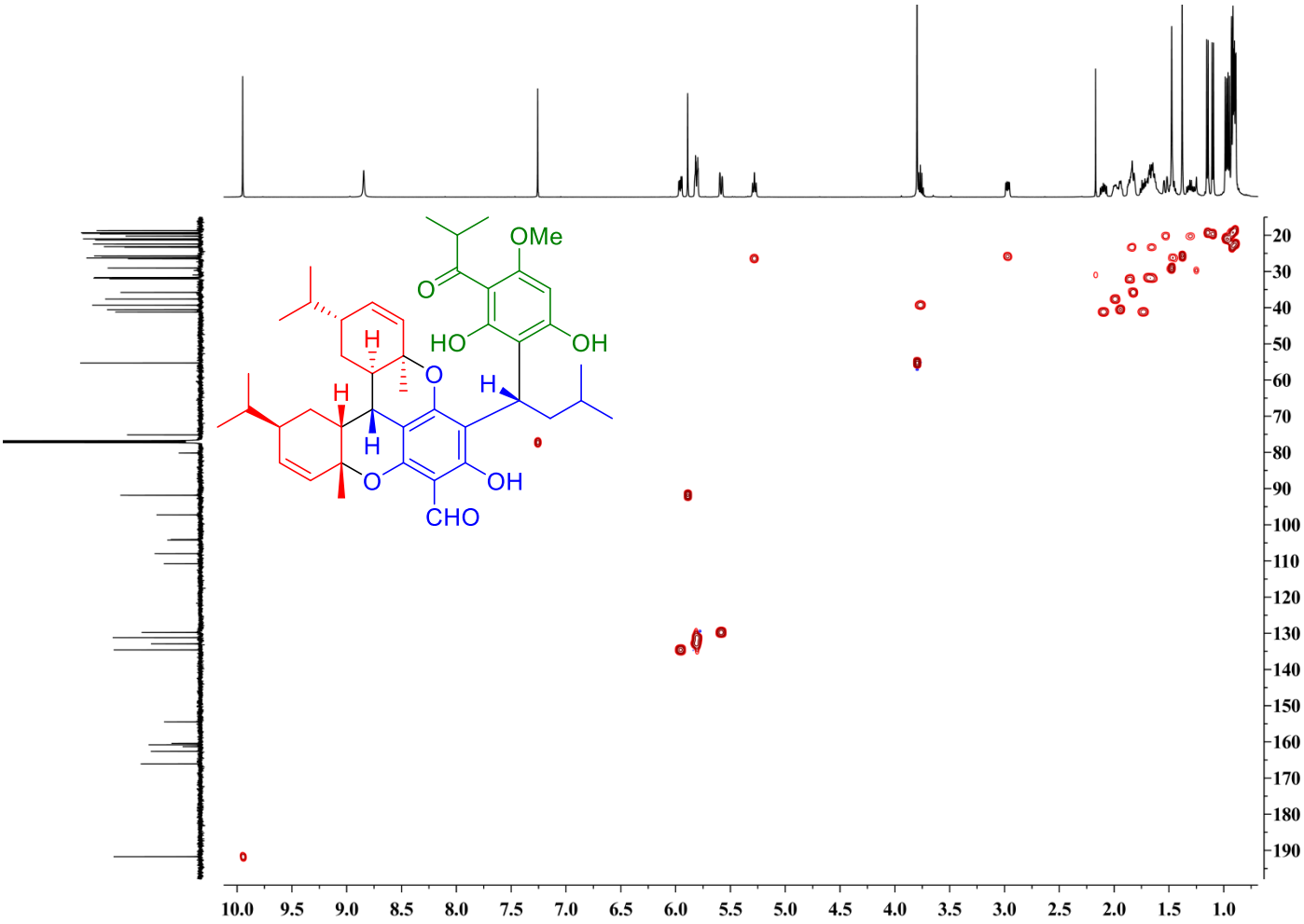


Figure S14 HSQC Spetrum of Eucalyptusdimer B (**2**)

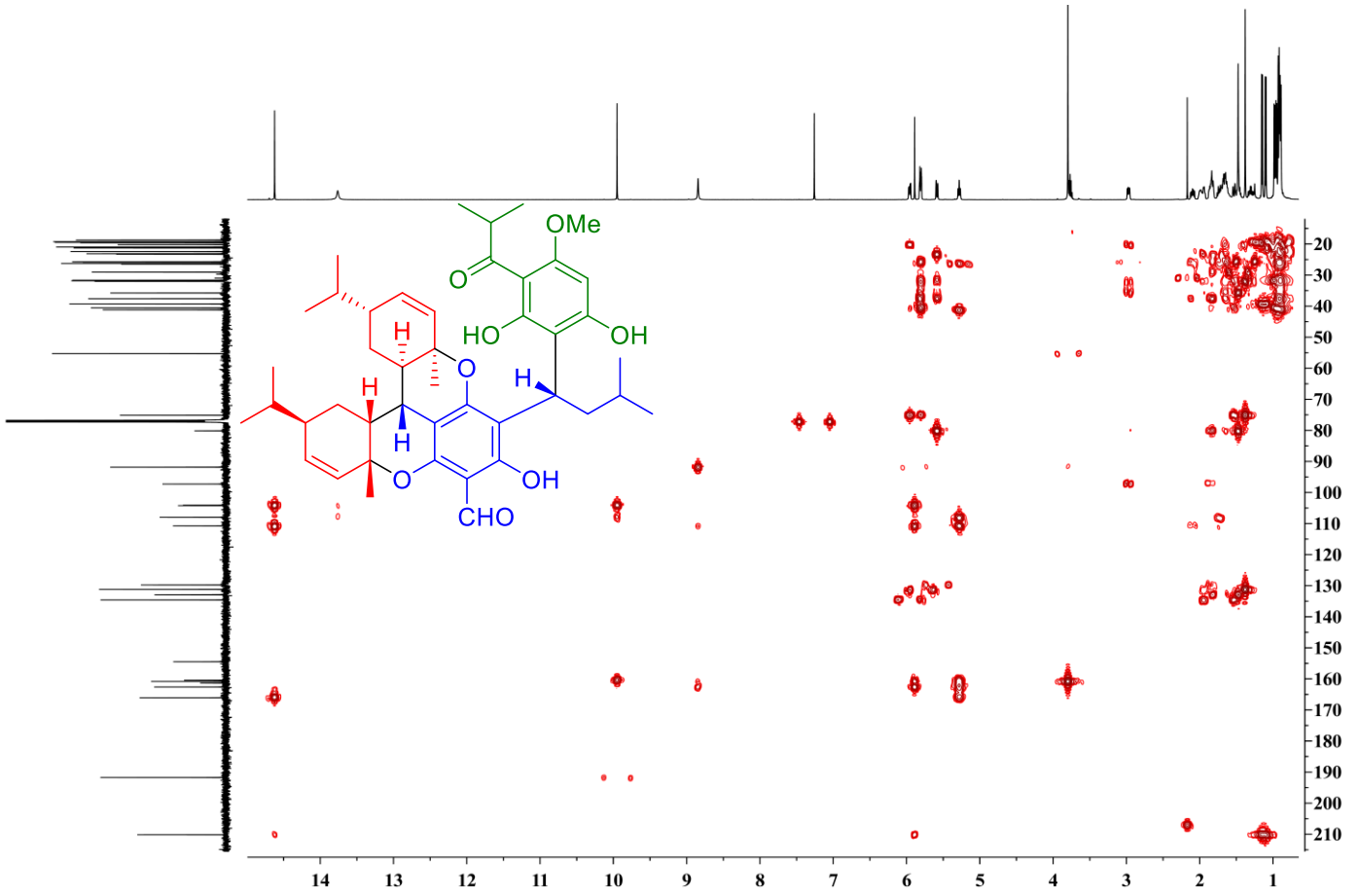


Figure S15 HMBC Spetrum of Eucalyptusdimer B (**2**)

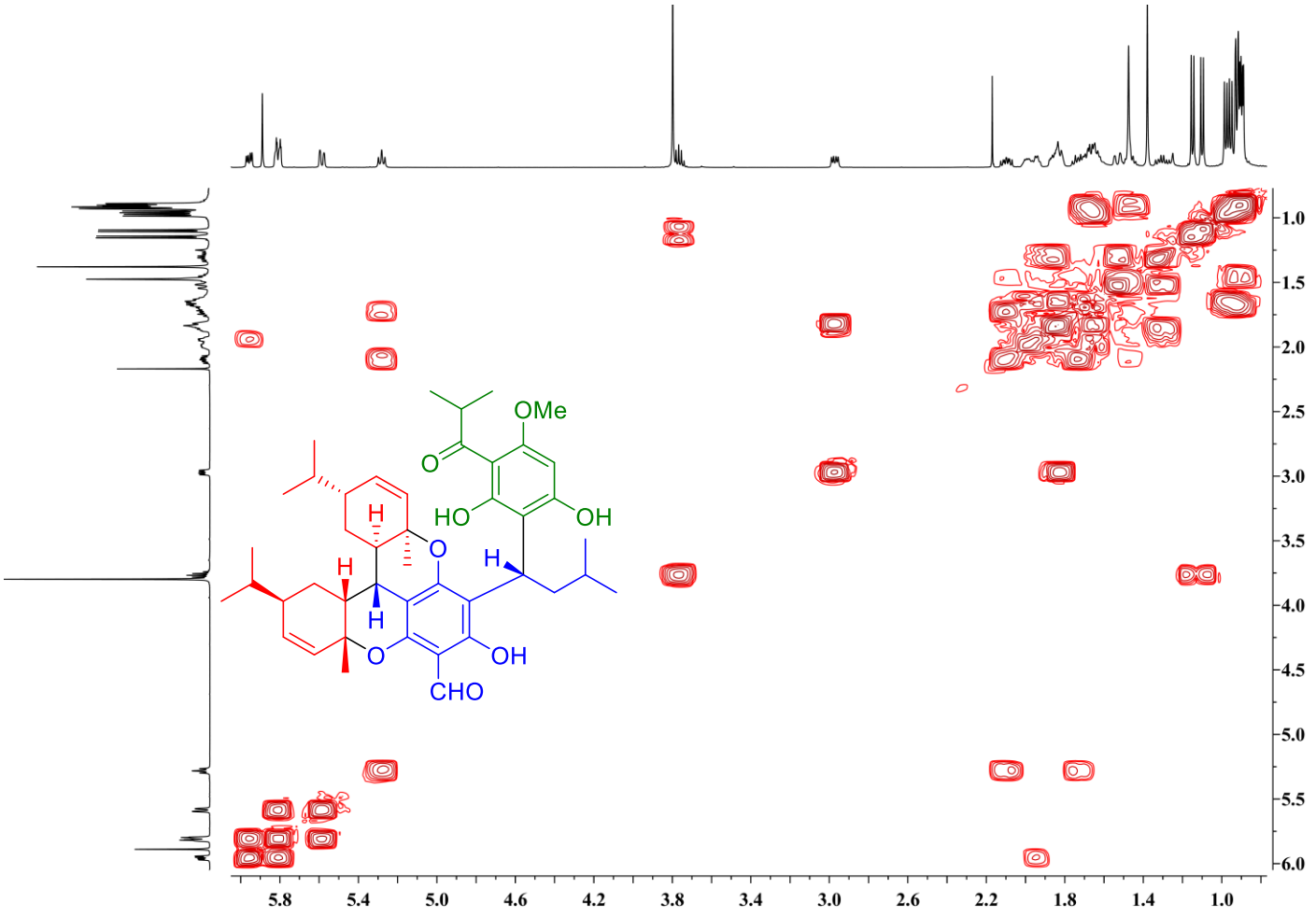


Figure S16 ^{1}H–^{1}H COSY Spetrum of Eucalyptusdimer B (**2**)

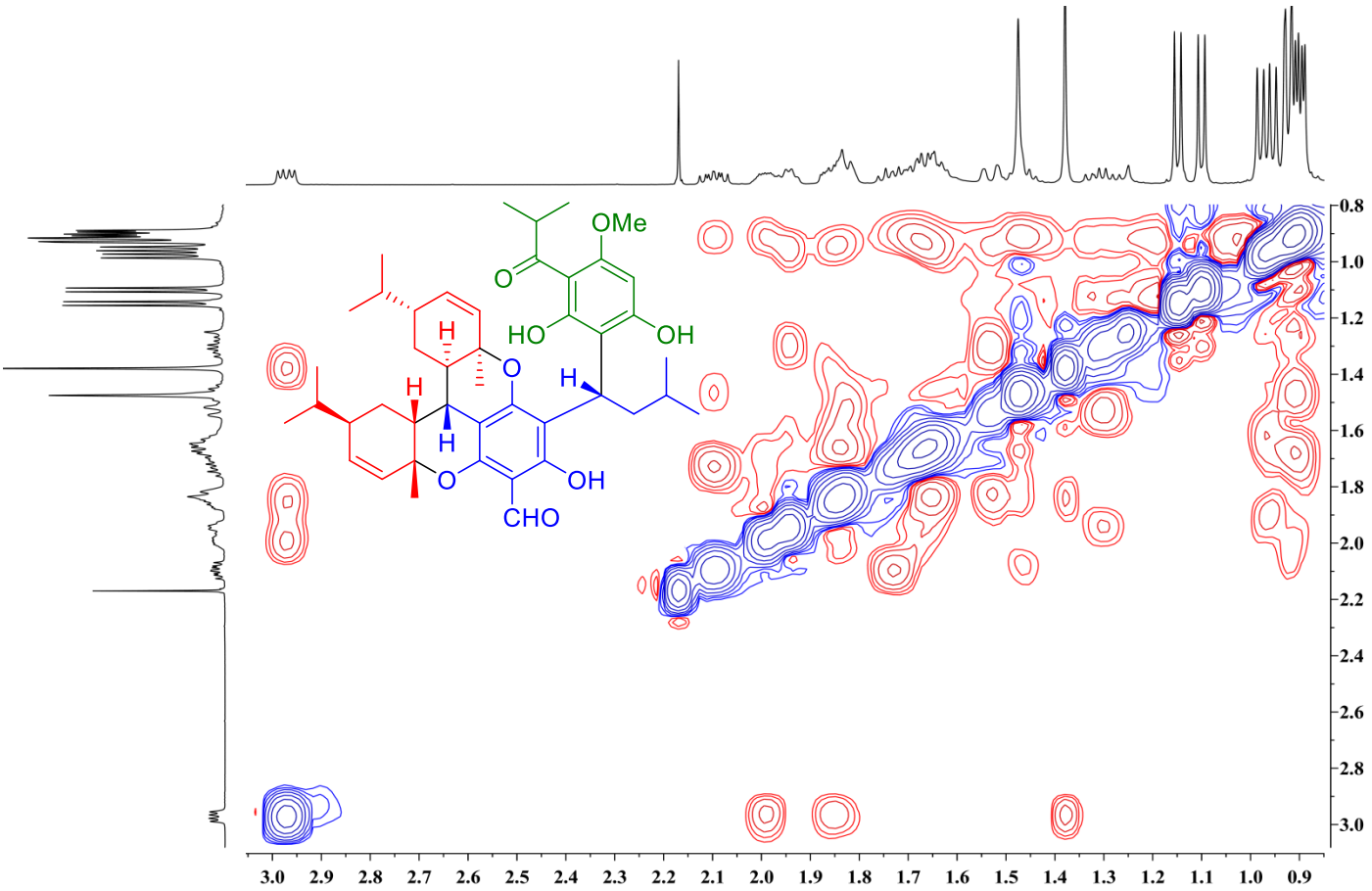
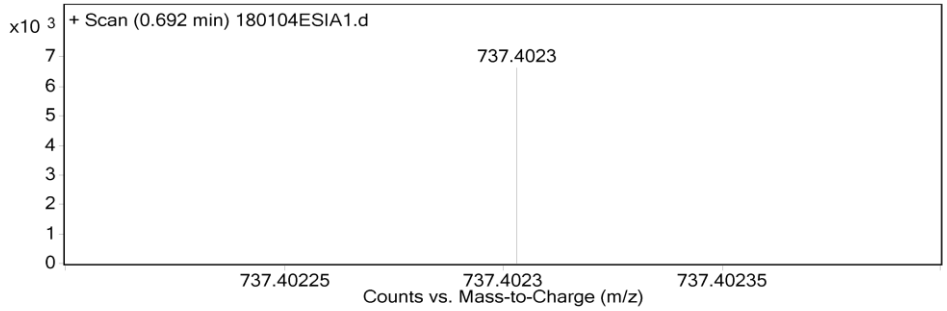


Figure S17 ROESY Spetrum of Eucalyptusdimer B (**2**)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

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121.0509		5352.75		
341.2666	1	6515.15		
385.2925	1	22730.14		
429.3189	1	27147.9		
430.3224	1	5150.71		
473.3454	1	12832.58		
517.3708	1	5177.51		
737.4023	1	6633.85	C44 H58 Na O8	M+
1452.8161	1	4019.75		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	4	10
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C44 H58 Na O8	737.4029	737.4023	0.6	0.9	15.5

Figure S18 HRESIMS Spetrum of Eucalyptusdimer B (**2**)

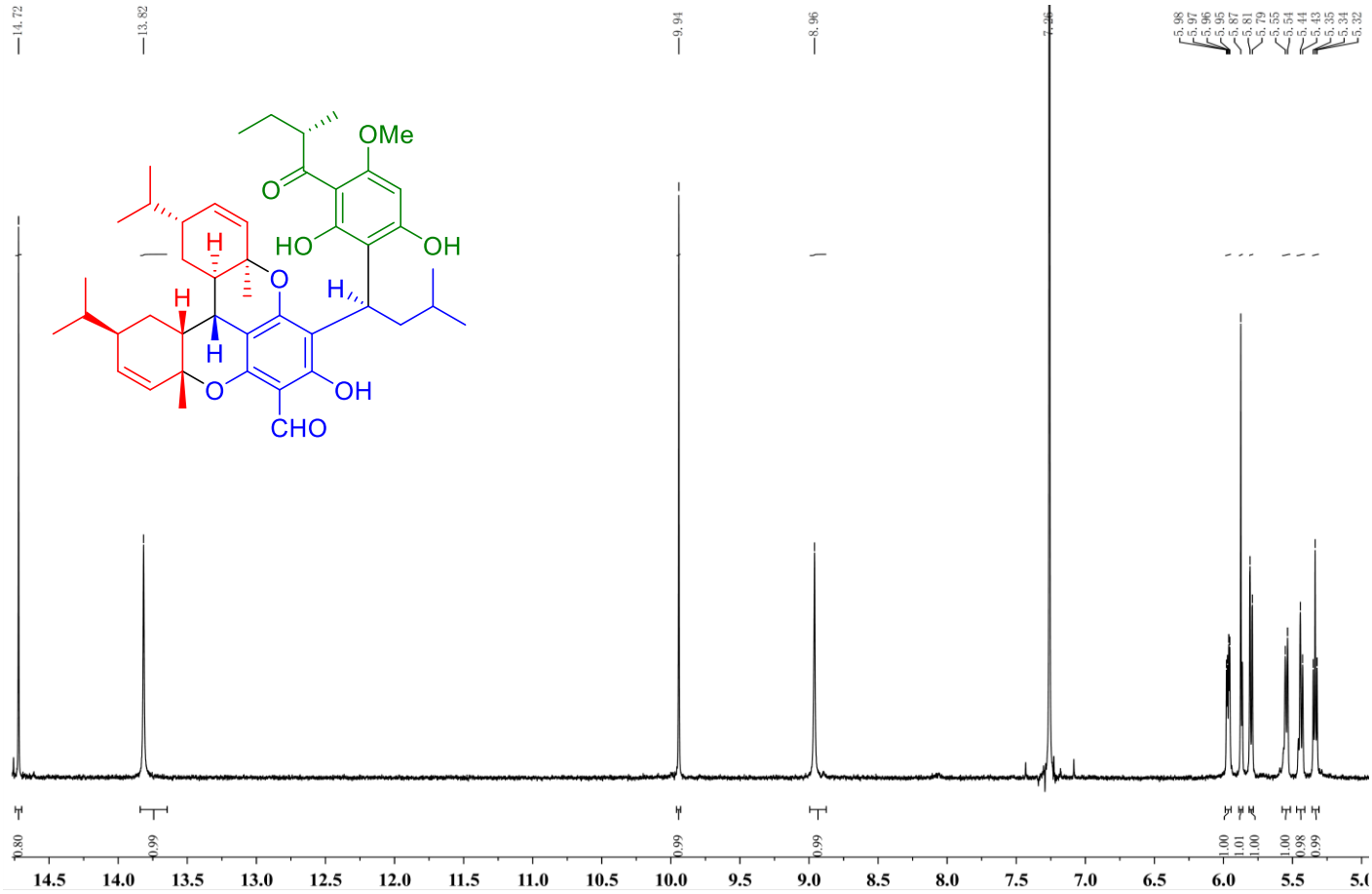


Figure S20. ^{1}H NMR Spetrum of Eucalyptusdimer C (**3**) in $CDCl_3$

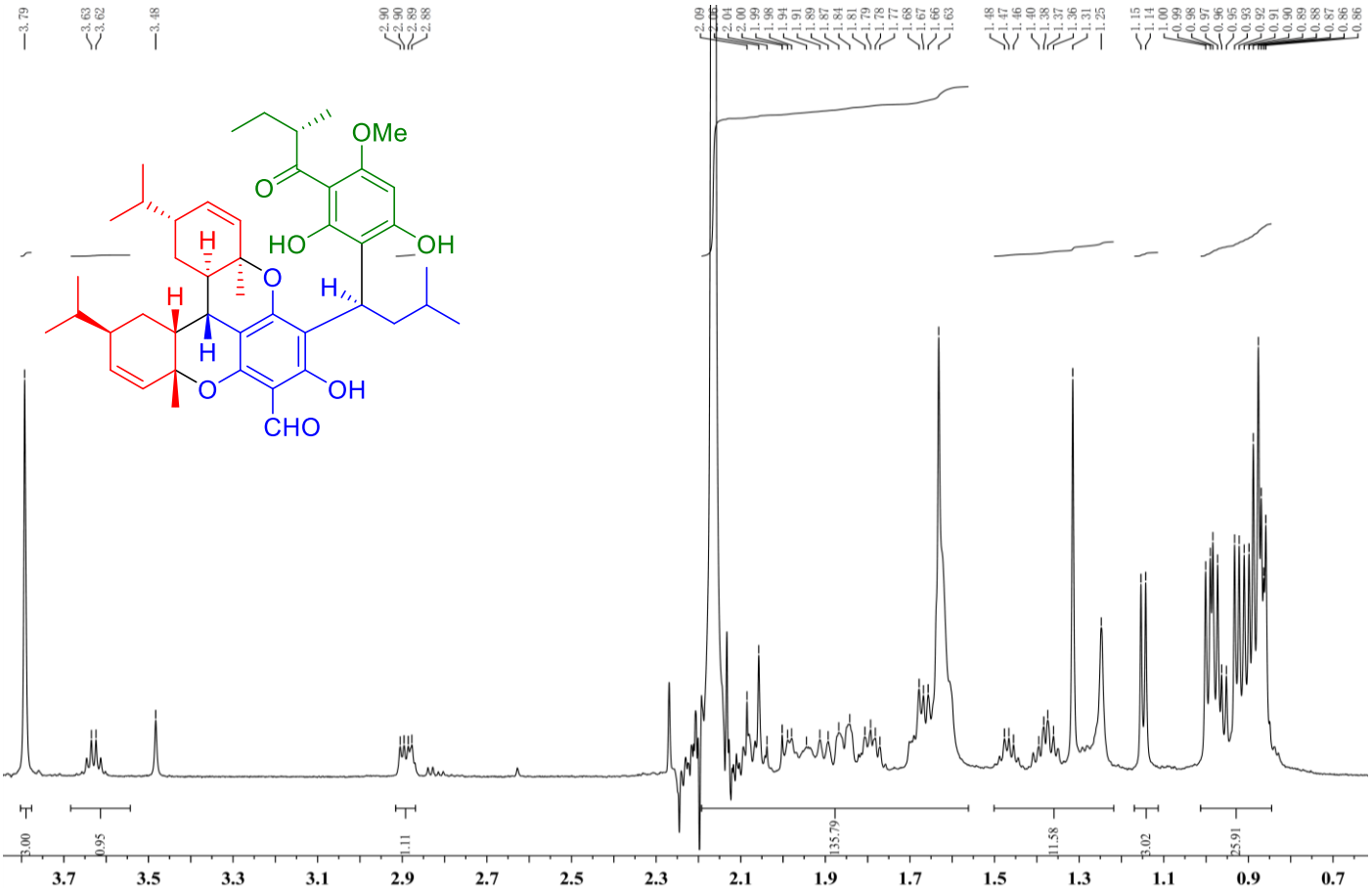


Figure S21. ^{1}H NMR Spetrum of Eucalyptusdimer C (**3**) in $CDCl_3$

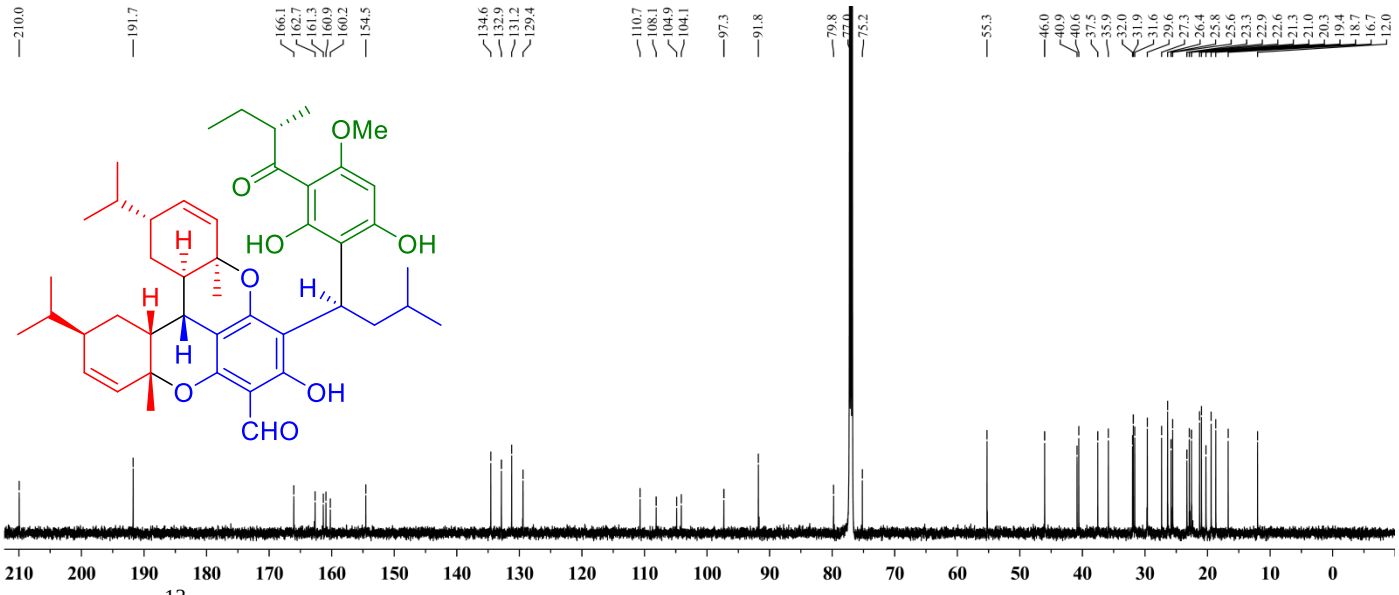


Figure S22. ^{13}C NMR Spetrum of Eucalyptusdimer B (**2**) in $CDCl_3$

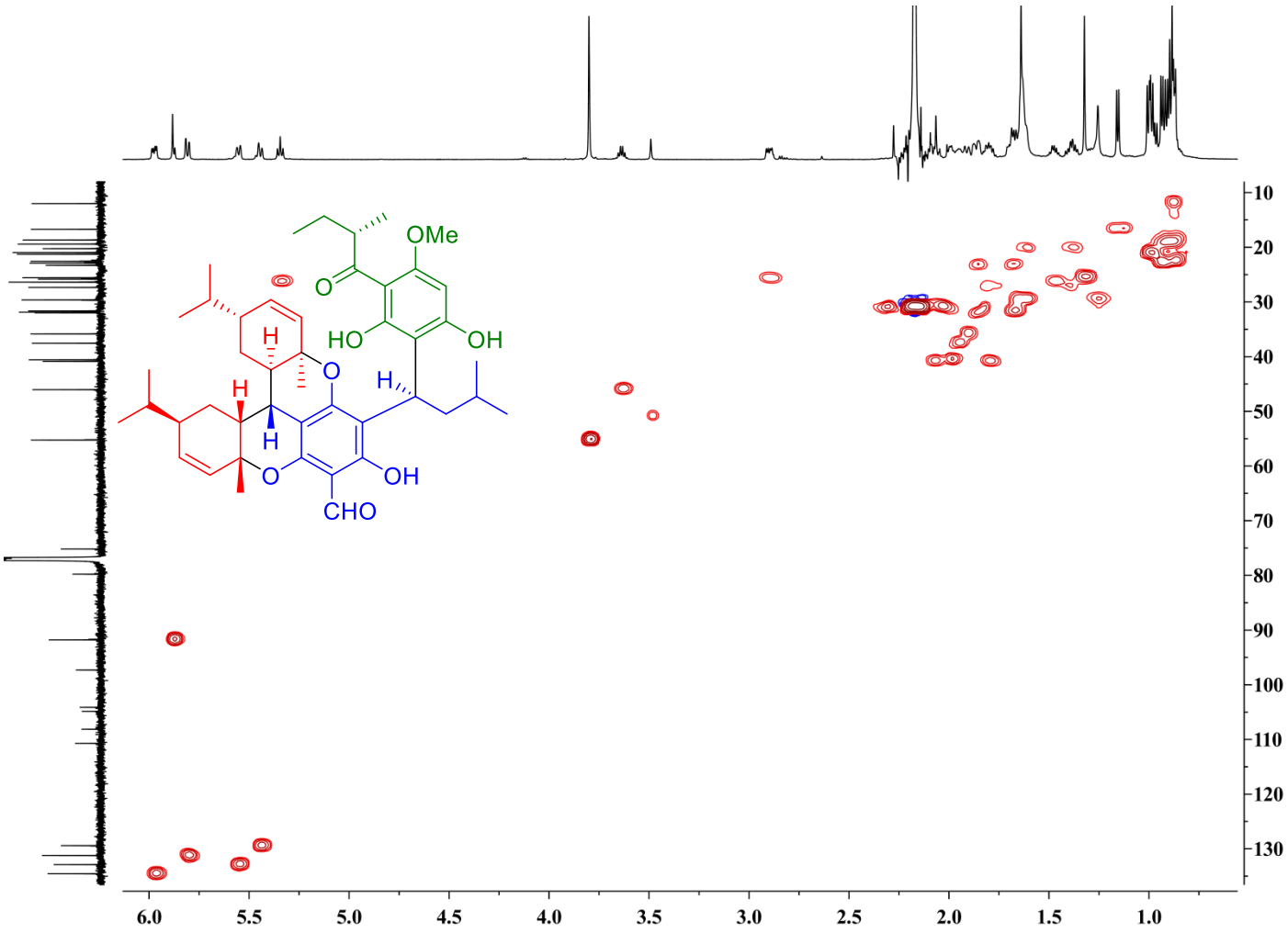


Figure S23. HSQC Spetrum of Eucalyptusdimer C (**3**)

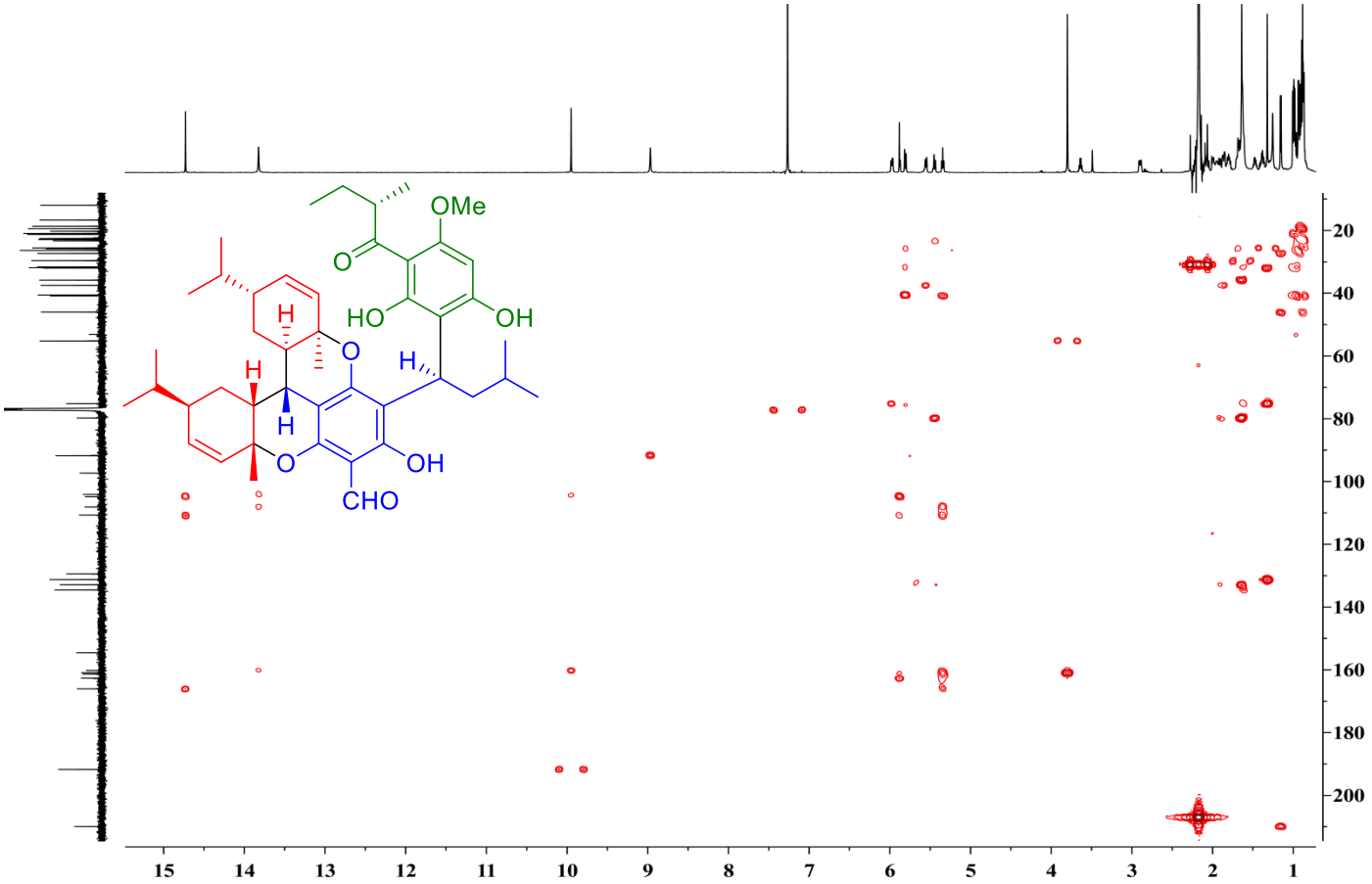


Figure S24. HMBC Spetrum of Eucalyptusdimer C (**3**)

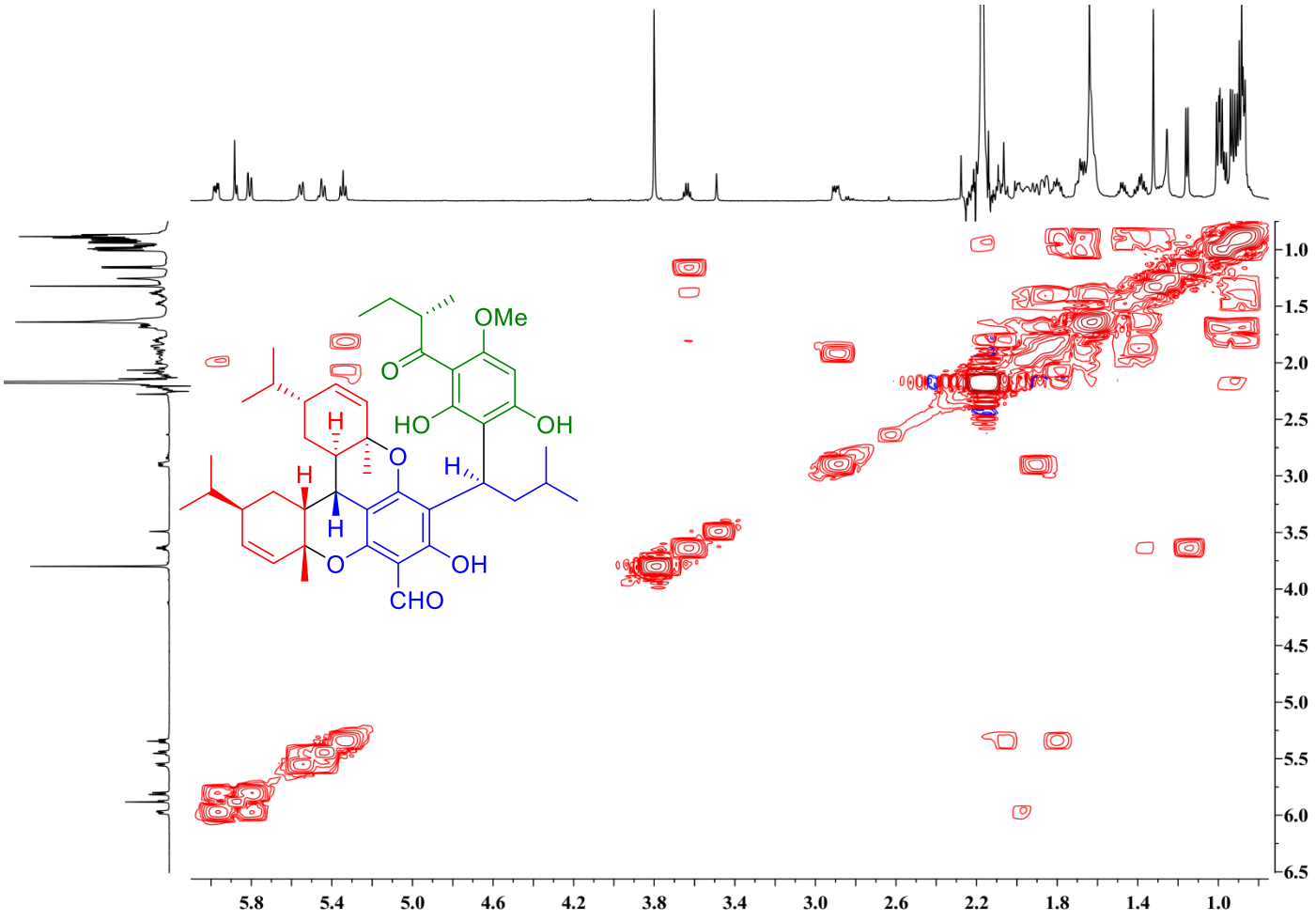


Figure S25. ^{1}H–^{1}H COSY Spetrum of Eucalyptusdimer B (**2**)

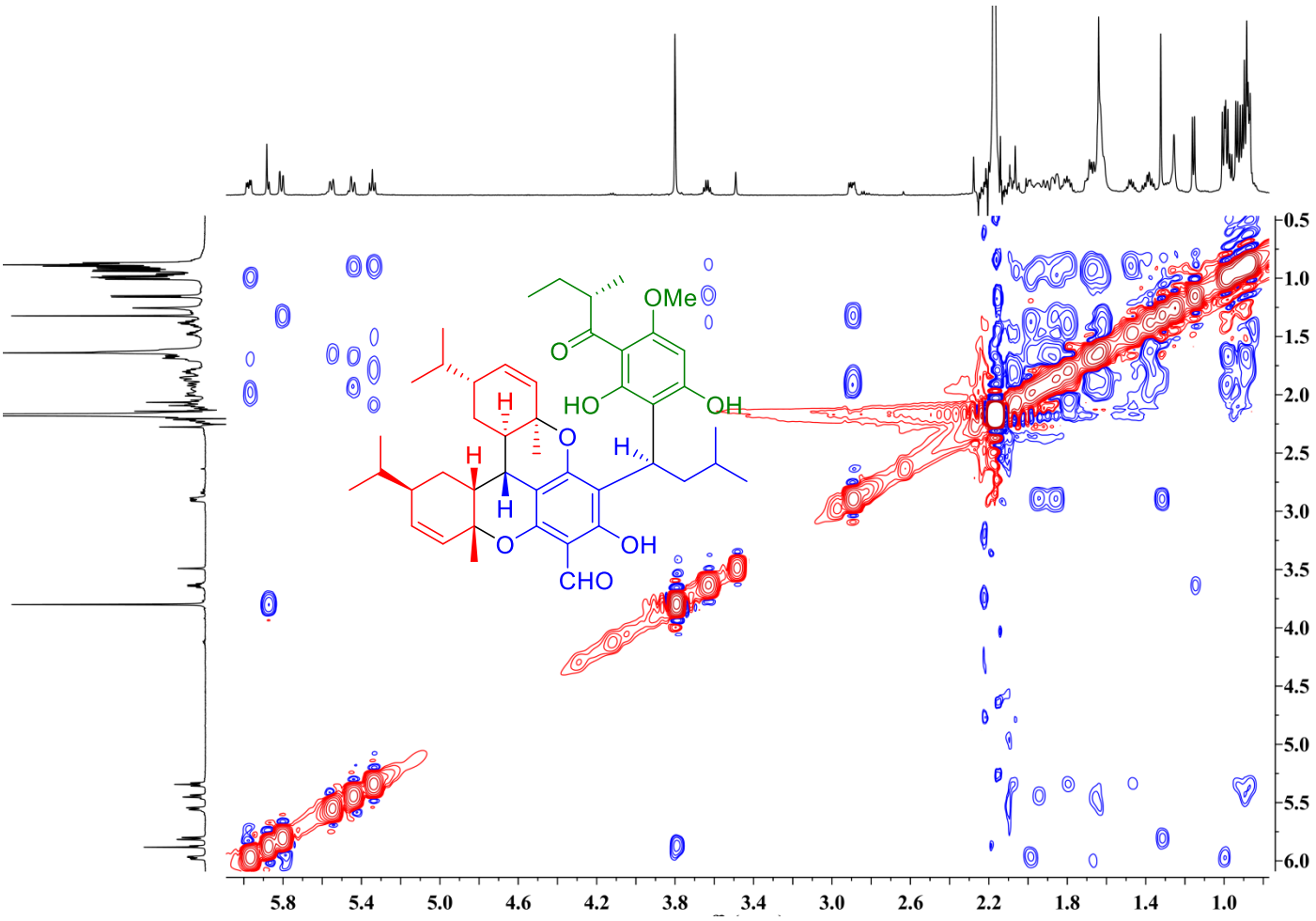
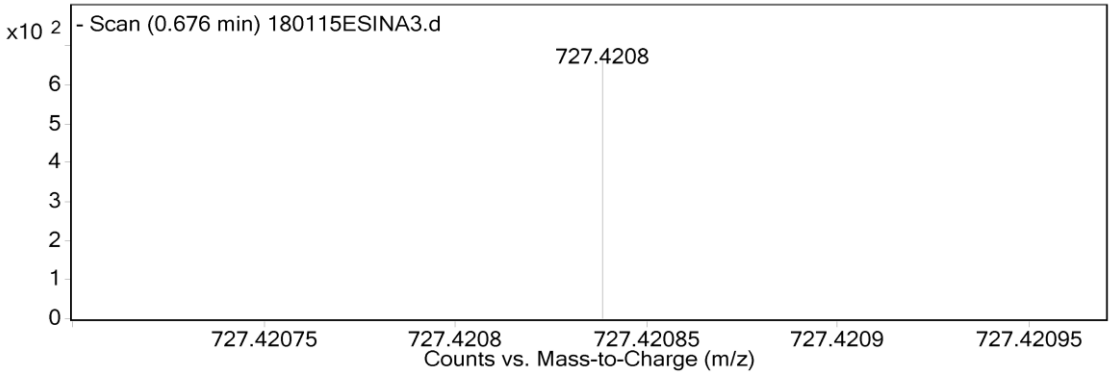


Figure S26. ROESY Spetrum of Eucalyptusdimer C (**3**)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
300	0	ESI



Peak List

m/z	Abund	Formula	Ion
112.9856	5847.54		
183.0118	221.24		
727.4208	667.38	C45 H59 O8	M-

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	4	10

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C45 H59 O8	727.4210	727.4208	0.2	0.3	16.5

Figure S27. HRESIMS Spetrum of Eucalyptusdimer C (**3**)

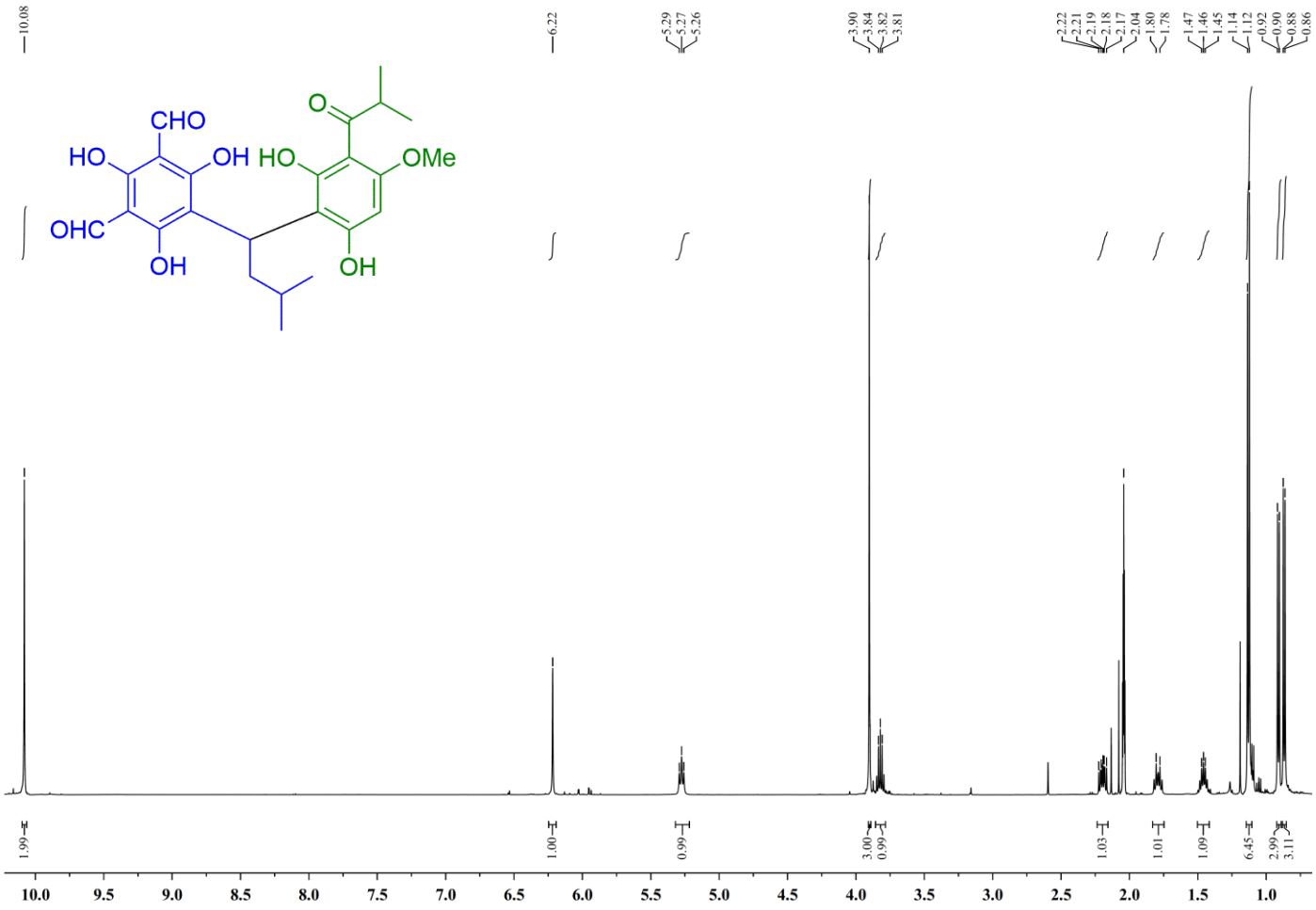


Figure S25. ^{1}H NMR Spetrum of Eucalyprobusone A (**4**) in Acetone-d_6

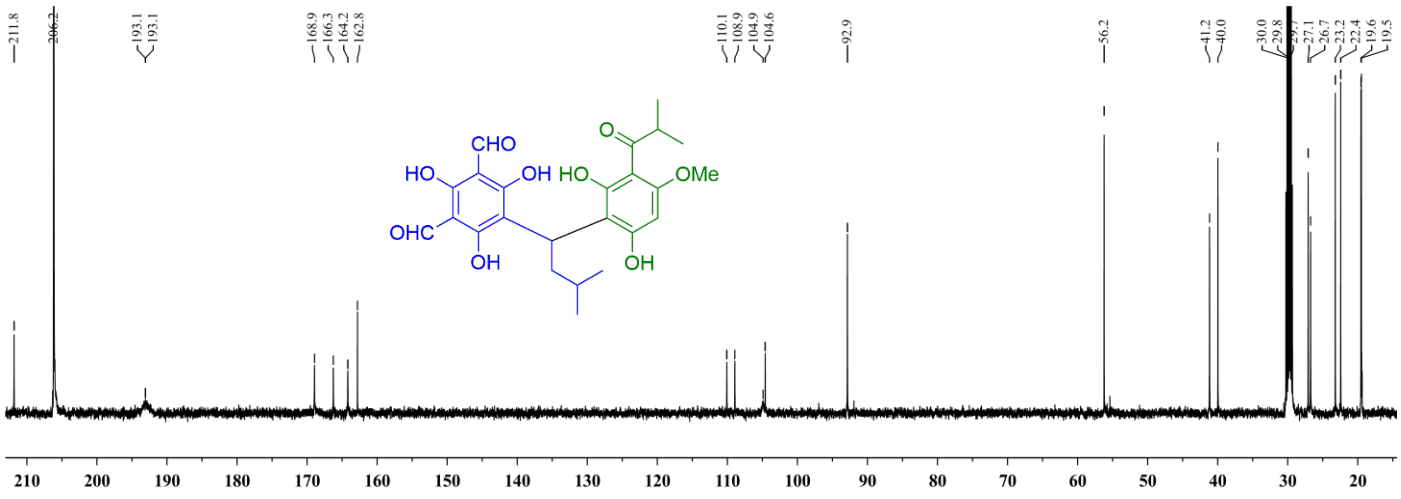


Figure S26. ^{13}C NMR Spetrum of Eucalyprobusone A (**4**) in Acetone-d_6

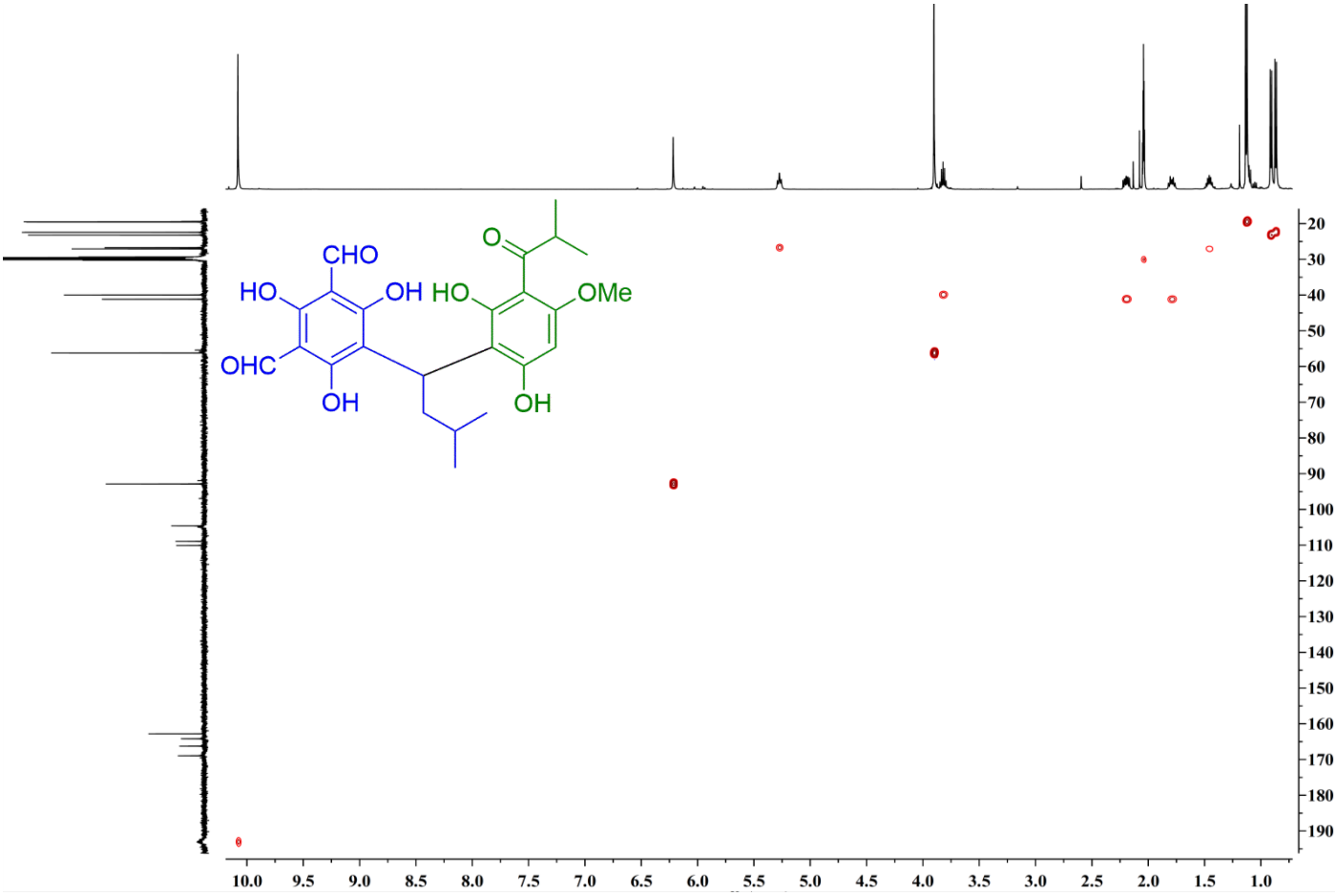


Figure S27. HSQC Spetrum of Eucalyprobusone A (**4**)

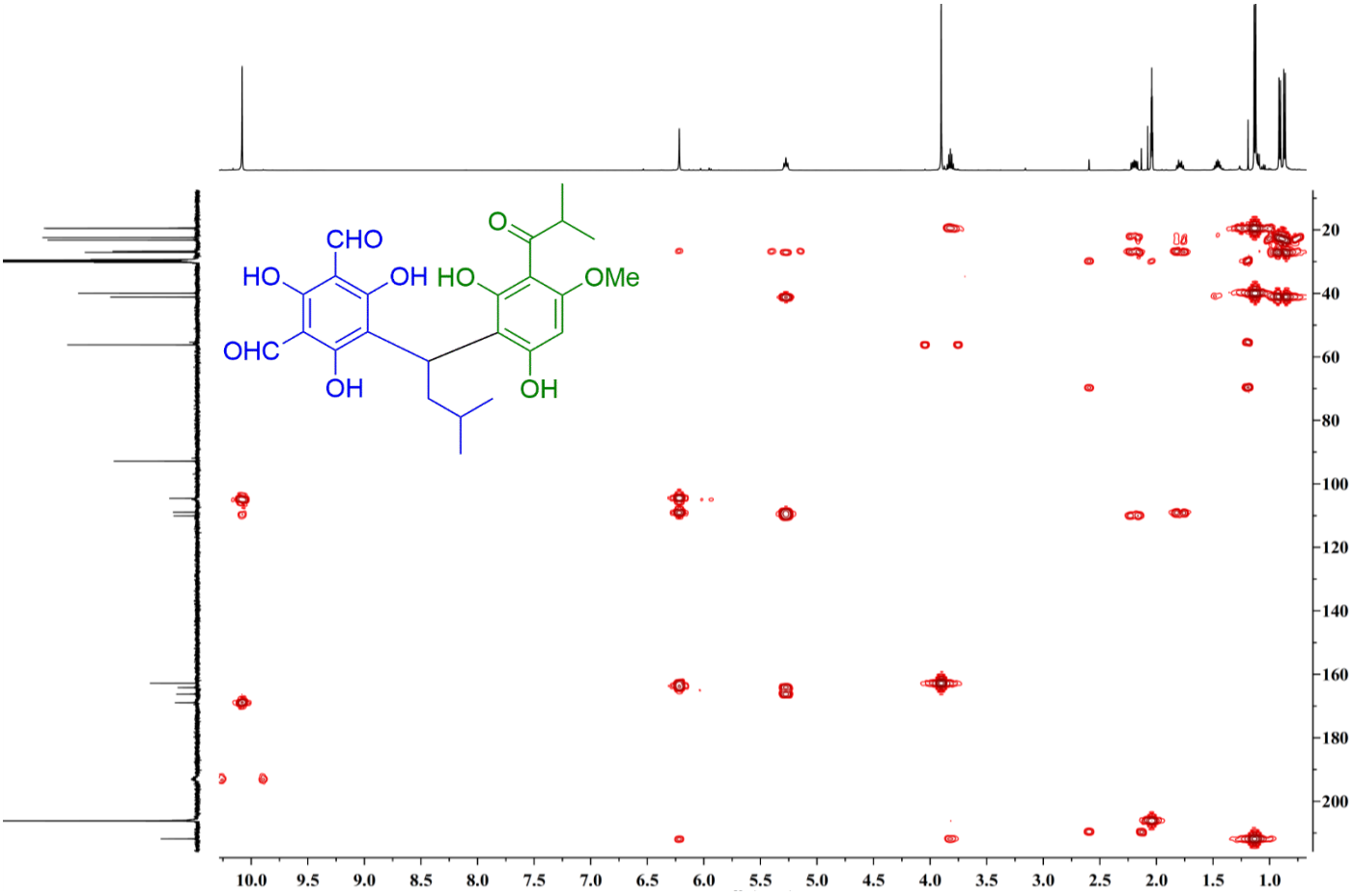


Figure S28. HMBC Spetrum of Eucalyprobusone A (**4**)

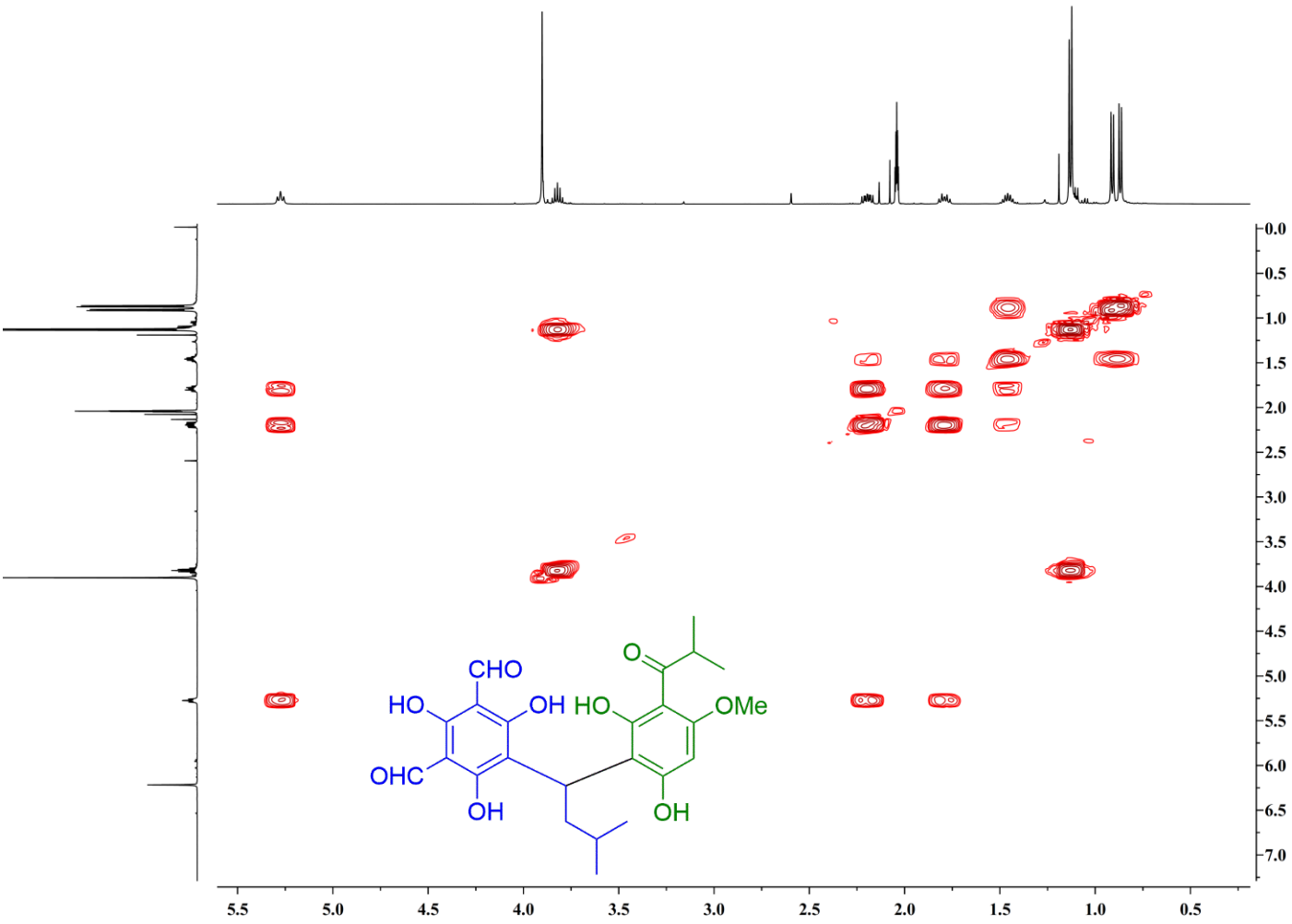
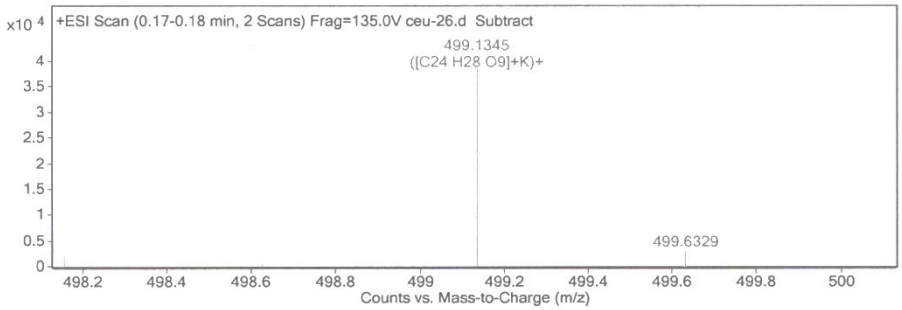


Figure S29. ^{1}H–^{1}H COSY Spetrum of Eucalyprobusone A (**4**)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
299.1114	1	56808.45		
301.1416	1	35021.72		
315.0855	1	90959.04		
317.1157	1	68790.2		
499.1345	1	38546.86	C24 H28 O9	(M+K)+
540.1553	1	19467.76		
575.233	1	21283.24		
658.433	1	26975.96		

Formula Calculator Element Limits

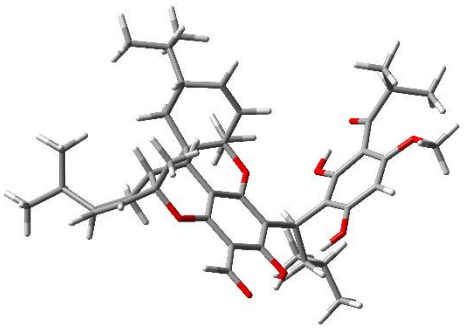
Element	Min	Max
C	3	60
H	0	120
O	0	10

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C24 H28 O9	460.1733	499.1365	499.1345	2.00	4.01	11.0000

Figure S30. HRESIMS Spetrum of Eucalyprobusone A (**4**)

Computational data for **1**



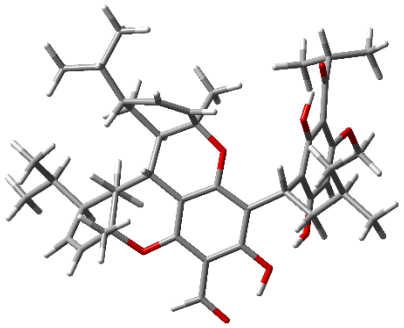
Optimized structure of **1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.682560	3.437189	-0.249510
2	6	0	3.220130	2.531260	0.884089
3	6	0	2.432497	1.209672	1.018974
4	6	0	0.966864	1.556601	1.321041
5	6	0	0.412827	2.521001	0.306158
6	6	0	1.171773	3.366312	-0.358377
7	6	0	2.515973	0.354465	-0.266528
8	6	0	1.520059	-0.786760	-0.244500
9	6	0	0.343167	-0.692720	0.486593
10	8	0	0.139135	0.355346	1.310585
11	1	0	2.812427	0.641333	1.857259
12	6	0	1.741885	-1.922604	-0.983629
13	6	0	0.800144	-2.948702	-1.006289
14	6	0	-0.398982	-2.791945	-0.292150
15	6	0	-0.663620	-1.666854	0.455571
16	6	0	3.151911	4.915292	-0.128627
17	6	0	4.687117	5.030131	-0.201396
18	6	0	2.619780	5.619429	1.133960
19	8	0	2.880268	-2.121365	-1.695625
20	6	0	3.878503	-1.053090	-1.852487
21	6	0	3.933793	-0.185852	-0.580917
22	6	0	4.538900	-1.001310	0.578428
23	6	0	5.950579	-1.571441	0.286370
24	6	0	6.089786	-1.982051	-1.158500
25	6	0	5.180142	-1.778707	-2.086975
26	1	0	2.233491	1.006546	-1.080851
27	6	0	3.493513	-0.259239	-3.105234
28	1	0	4.577663	0.648168	-0.816717
29	6	0	7.114606	-0.656435	0.770006
30	6	0	8.466851	-1.398368	0.703263
31	6	0	7.217476	0.677551	0.008233
32	8	0	-1.317438	-3.801910	-0.352507
33	6	0	-1.946805	-1.416290	1.258104
34	6	0	-3.139125	-0.975402	0.400414
35	6	0	-3.978603	-1.834668	-0.290143
36	6	0	-5.096121	-1.351427	-0.964193
37	6	0	-5.382634	-0.018359	-1.008823
38	6	0	-4.553072	0.913046	-0.357489
39	6	0	-3.466977	0.382076	0.385512
40	6	0	-2.254940	-2.556534	2.266117
41	6	0	-3.449091	-2.253207	3.196352
42	6	0	-3.220631	-0.978845	4.032953
43	8	0	-3.830484	-3.174632	-0.330490
44	8	0	-2.699976	1.196868	1.149631
45	1	0	-1.711161	-0.552595	1.847508
46	6	0	-3.686362	-3.457510	4.129133
47	6	0	-4.719834	2.378975	-0.372607

48	6	0	-5.515736	3.202188	-1.388608
49	8	0	-4.111004	3.066249	0.464536
50	6	0	-5.260585	2.826579	-2.858327
51	6	0	-7.012500	3.283454	-1.014718
52	6	0	0.734994	2.083483	2.741670
53	6	0	1.055973	-4.151723	-1.758730
54	8	0	0.272542	-5.102951	-1.825632
55	8	0	-6.492605	0.440944	-1.652877
56	6	0	-7.417486	-0.458246	-2.299672
57	1	0	3.086158	3.076361	-1.194516
58	1	0	3.164070	3.057697	1.826518
59	1	0	4.265864	2.313909	0.710657
60	1	0	-0.651828	2.482036	0.191079
61	1	0	0.721989	4.049398	-1.057533
62	1	0	2.742273	5.433906	-0.991604
63	1	0	4.983625	6.072832	-0.239038
64	1	0	5.074443	4.538040	-1.088069
65	1	0	5.152275	4.583815	0.670342
66	1	0	2.852314	6.678275	1.092222
67	1	0	1.545455	5.511034	1.219455
68	1	0	3.078650	5.218434	2.030291
69	1	0	3.869914	-1.825270	0.793639
70	1	0	4.594229	-0.390929	1.470135
71	1	0	6.042585	-2.483791	0.872116
72	1	0	6.985966	-2.513411	-1.419433
73	1	0	5.325672	-2.155491	-3.081950
74	1	0	2.512841	0.185628	-3.009275
75	1	0	4.223049	0.521012	-3.286334
76	1	0	3.475098	-0.926838	-3.957505
77	1	0	6.915798	-0.436821	1.815078
78	1	0	9.238237	-0.810760	1.189063
79	1	0	8.411445	-2.359644	1.203513
80	1	0	8.773925	-1.561308	-0.323534
81	1	0	8.093184	1.226772	0.337676
82	1	0	7.307238	0.501928	-1.057645
83	1	0	6.354153	1.305529	0.184696
84	1	0	-0.973553	-4.566663	-0.880450
85	1	0	-5.713779	-2.078293	-1.438240
86	1	0	-1.367209	-2.685488	2.879950
87	1	0	-2.434258	-3.491123	1.762304
88	1	0	-4.333874	-2.113914	2.586532
89	1	0	-4.047608	-0.825648	4.719235
90	1	0	-2.310655	-1.075931	4.618916
91	1	0	-3.135805	-0.098292	3.409541
92	1	0	-2.899072	-3.485108	-0.272105
93	1	0	-3.090672	2.104693	1.170016
94	1	0	-4.539878	-3.281070	4.775561
95	1	0	-3.874775	-4.359502	3.556397
96	1	0	-2.815545	-3.625743	4.756045
97	1	0	-5.104128	4.189865	-1.226909
98	1	0	-5.727248	3.570266	-3.496577
99	1	0	-4.197428	2.824483	-3.073307
100	1	0	-5.675401	1.863465	-3.091473
101	1	0	-7.477699	2.317792	-1.097034
102	1	0	-7.508106	3.980796	-1.682121
103	1	0	-7.122910	3.653199	-0.001113
104	1	0	1.123824	1.376515	3.464722
105	1	0	1.198722	3.048399	2.883208
106	1	0	-0.332171	2.175723	2.892374
107	1	0	1.996621	-4.184644	-2.282949
108	1	0	-8.181021	0.176423	-2.716968
109	1	0	-6.929691	-1.015785	-3.086993
110	1	0	-7.853418	-1.141119	-1.583838

Computational data for **2**



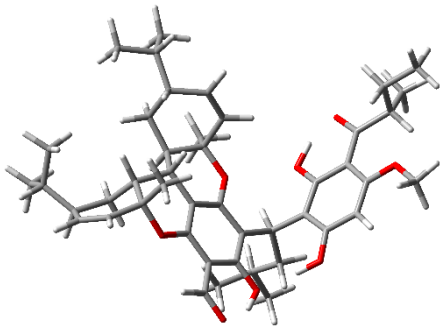
Optimized structure of **2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.349581	-2.606685	-2.120554
2	6	0	-2.926997	-2.509602	-0.642750
3	6	0	-1.954794	-1.347334	-0.355777
4	6	0	-0.679131	-1.546375	-1.196099
5	6	0	-1.021547	-1.820104	-2.641176
6	6	0	-2.193540	-2.301797	-3.039025
7	6	0	-2.581631	0.034608	-0.626485
8	6	0	-1.540695	1.120720	-0.516079
9	6	0	-0.196245	0.854879	-0.822153
10	8	0	0.201098	-0.378291	-1.176787
11	1	0	-1.657869	-1.393663	0.694925
12	6	0	-1.880023	2.406530	-0.125883
13	6	0	-0.900043	3.421217	-0.032964
14	6	0	0.440865	3.096150	-0.371703
15	6	0	0.829329	1.828913	-0.787286
16	6	0	-4.038036	-3.948942	-2.500321
17	6	0	-5.346875	-4.161071	-1.731256
18	6	0	-3.121801	-5.172125	-2.373245
19	8	0	-3.139509	2.758173	0.224628
20	6	0	-4.246840	1.832508	-0.037745
21	6	0	-3.810089	0.381767	0.249181
22	6	0	-3.586625	0.179397	1.757392
23	6	0	-4.793060	0.546683	2.652611
24	6	0	-5.581868	1.689540	2.079011
25	6	0	-5.334761	2.270722	0.911680
26	1	0	-2.932955	0.015391	-1.662499
27	6	0	-4.699847	2.054215	-1.483038
28	1	0	-4.643065	-0.246106	-0.073259
29	6	0	-5.678505	-0.667254	3.068907
30	6	0	-6.454782	-1.306621	1.912458
31	6	0	-6.632278	-0.306410	4.216093
32	8	0	1.374875	4.069568	-0.257762
33	6	0	2.249454	1.440804	-1.225685
34	6	0	3.098321	0.835894	-0.102084
35	6	0	3.482881	1.525472	1.050418
36	6	0	4.292067	0.928408	2.030854
37	6	0	4.705767	-0.376444	1.908877
38	6	0	4.327816	-1.165952	0.783620
39	6	0	3.579261	-0.481368	-0.238743
40	6	0	3.006333	2.525553	-2.038394
41	6	0	4.149506	1.979724	-2.914787
42	6	0	3.643393	1.139358	-4.093186
43	8	0	3.161507	2.801104	1.323525
44	8	0	3.306961	-1.110726	-1.384519
45	6	0	5.017427	3.140009	-3.418582
46	6	0	4.610768	-2.590379	0.589461
47	6	0	5.043399	-3.615435	1.653187
48	8	0	4.420220	-3.102940	-0.534527
49	6	0	6.562147	-3.623926	1.896312
50	6	0	4.204778	-3.631190	2.938599
51	6	0	0.219661	-2.652699	-0.631536
52	1	0	2.089123	0.616641	-1.912771
53	6	0	-1.228221	4.748504	0.409168
54	8	0	-0.403106	5.665631	0.522517
55	8	0	5.529067	-0.951276	2.824357
56	6	0	5.951595	-0.190383	3.948642
57	1	0	-4.111620	-1.836191	-2.309318

58	1	0	-2.448338	-3.441692	-0.338546
59	1	0	-3.810045	-2.408628	-0.009804
60	1	0	-0.228312	-1.619439	-3.353253
61	1	0	-2.358679	-2.481099	-4.098638
62	1	0	-4.298086	-3.850848	-3.561493
63	1	0	-5.875655	-5.040236	-2.106255
64	1	0	-6.016419	-3.302884	-1.833272
65	1	0	-5.166968	-4.321807	-0.665365
66	1	0	-3.615792	-6.058296	-2.778146
67	1	0	-2.185437	-5.034565	-2.917385
68	1	0	-2.875722	-5.390184	-1.331136
69	1	0	-3.310480	-0.857933	1.956574
70	1	0	-2.729287	0.784308	2.062375
71	1	0	-4.375801	0.914827	3.598882
72	1	0	-6.389338	2.080818	2.690041
73	1	0	-5.923964	3.125959	0.595746
74	1	0	-3.899803	1.856857	-2.196146
75	1	0	-5.546326	1.405812	-1.719376
76	1	0	-5.015598	3.090433	-1.612705
77	1	0	-4.979932	-1.418376	3.456535
78	1	0	-7.135977	-0.589151	1.447869
79	1	0	-5.793596	-1.692487	1.135073
80	1	0	-7.053430	-2.146370	2.273307
81	1	0	-6.098752	0.150861	5.053156
82	1	0	-7.410298	0.389598	3.893364
83	1	0	-7.135373	-1.200339	4.591457
84	1	0	0.896274	4.891779	0.073661
85	1	0	4.580871	1.548880	2.863951
86	1	0	3.416616	3.287997	-1.377035
87	1	0	2.289009	3.044364	-2.683464
88	1	0	4.781292	1.338145	-2.290587
89	1	0	2.986425	1.732337	-4.737983
90	1	0	3.094705	0.258520	-3.759277
91	1	0	4.478416	0.788798	-4.705323
92	1	0	2.598423	3.230777	0.649972
93	1	0	3.760295	-2.011458	-1.312066
94	1	0	5.435848	3.714627	-2.588525
95	1	0	4.430828	3.828103	-4.035591
96	1	0	5.848483	2.776524	-4.028234
97	1	0	4.821030	-4.547271	1.127954
98	1	0	6.824354	-4.481220	2.521663
99	1	0	7.098413	-3.727932	0.950644
100	1	0	6.905465	-2.718606	2.389987
101	1	0	3.137226	-3.645616	2.706224
102	1	0	4.403673	-2.779188	3.582402
103	1	0	4.429600	-4.541915	3.499956
104	1	0	-0.275876	-3.621764	-0.669541
105	1	0	1.140350	-2.709202	-1.210234
106	1	0	0.485770	-2.423726	0.402431
107	1	0	-2.279174	4.939781	0.660592
108	1	0	5.101548	0.123413	4.560041
109	1	0	6.591147	-0.852856	4.528150
110	1	0	6.522146	0.688695	3.639230

Computational data for **3**−8‴*S*



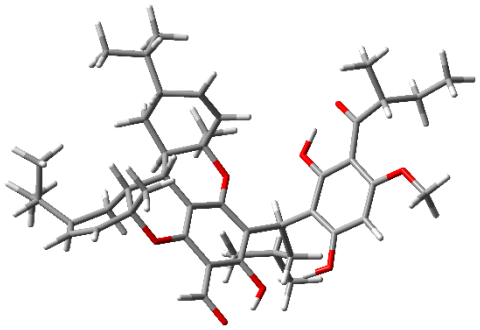
Optimized structure of **3**−8‴*S*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.812381	3.480572	0.087974
2	6	0	3.456260	2.385937	0.972327
3	6	0	2.638977	1.074902	0.995159
4	6	0	1.242244	1.395838	1.547846
5	6	0	0.599657	2.517588	0.777073
6	6	0	1.298454	3.450106	0.164728
7	6	0	2.509081	0.445746	-0.410869
8	6	0	1.495310	-0.681201	-0.420154
9	6	0	0.432533	-0.690916	0.475536
10	8	0	0.368228	0.227658	1.463783
11	1	0	3.104020	0.365950	1.667091
12	6	0	1.589818	-1.702436	-1.334486
13	6	0	0.640016	-2.721149	-1.359422
14	6	0	-0.438598	-2.670198	-0.463263
15	6	0	-0.579308	-1.658437	0.456315
16	6	0	3.350757	4.909104	0.388108
17	6	0	4.868200	5.008430	0.136843
18	6	0	3.008055	5.400646	1.807509
19	8	0	2.611000	-1.795889	-2.223560
20	6	0	3.578854	-0.699493	-2.382804
21	6	0	3.850051	-0.036635	-1.019989
22	6	0	4.607657	-1.015946	-0.101297
23	6	0	5.937756	-1.543967	-0.695573
24	6	0	5.848111	-1.710349	-2.192804
25	6	0	4.819194	-1.358675	-2.932612
26	1	0	2.128313	1.225716	-1.053774
27	6	0	2.999968	0.268216	-3.419642
28	1	0	4.467764	0.826663	-1.221260
29	6	0	7.216676	-0.741094	-0.312053
30	6	0	7.538708	-0.863290	1.190762
31	6	0	7.166431	0.739296	-0.729194
32	8	0	-1.368354	-3.671385	-0.515968
33	6	0	-1.760548	-1.551022	1.422443
34	6	0	-3.063893	-1.185276	0.702558
35	6	0	-3.987322	-2.099269	0.223770
36	6	0	-5.196862	-1.680495	-0.322300
37	6	0	-5.509480	-0.356271	-0.417836
38	6	0	-4.611879	0.625945	0.045877
39	6	0	-3.393785	0.167220	0.609392
40	6	0	-1.908533	-2.783557	2.370850
41	6	0	-1.160441	-2.637041	3.716848
42	6	0	0.371670	-2.644493	3.560022
43	8	0	-3.817316	-3.438147	0.277398
44	8	0	-2.502272	1.042407	1.119628
45	6	0	-1.586946	-3.782311	4.657841
46	6	0	-4.871368	2.073829	0.003626
47	6	0	-6.091940	2.656601	-0.695635
48	8	0	-4.096191	2.869423	0.556716
49	6	0	-6.354427	4.081564	-0.191225
50	6	0	-5.802710	2.633569	-2.221533
51	6	0	1.232029	1.698079	3.050186
52	1	0	-1.554429	-0.694523	2.039245
53	6	0	-7.043861	2.975835	-3.065351
54	6	0	0.761071	-3.811884	-2.293439
55	8	0	-0.028088	-4.759595	-2.342949
56	8	0	-6.680629	0.053955	-0.979267
57	6	0	-7.708868	-0.887711	-1.344710

58	1	0	3.075400	3.278010	-0.949159
59	1	0	3.548831	2.747089	1.986988
60	1	0	4.459237	2.179777	0.622935
61	1	0	-0.471685	2.503452	0.777916
62	1	0	0.788329	4.240359	-0.357748
63	1	0	2.857481	5.572468	-0.317444
64	1	0	5.198595	6.036833	0.235034
65	1	0	5.122598	4.667428	-0.861800
66	1	0	5.420578	4.412525	0.854445
67	1	0	3.269164	6.448704	1.908544
68	1	0	1.950522	5.292963	2.014719
69	1	0	3.563758	4.850812	2.558243
70	1	0	4.809838	-0.541563	0.846871
71	1	0	3.959386	-1.859744	0.097864
72	1	0	6.090930	-2.542169	-0.291022
73	1	0	6.698436	-2.174580	-2.661097
74	1	0	4.814307	-1.552371	-3.988587
75	1	0	2.050487	0.672994	-3.099169
76	1	0	3.693827	1.082024	-3.594742
77	1	0	2.840016	-0.262239	-4.349748
78	1	0	8.035646	-1.208314	-0.853262
79	1	0	8.489811	-0.389981	1.409549
80	1	0	7.603154	-1.903627	1.491827
81	1	0	6.781803	-0.378849	1.796169
82	1	0	8.130975	1.205663	-0.558627
83	1	0	6.920707	0.843805	-1.779176
84	1	0	6.432191	1.279749	-0.144054
85	1	0	-1.142971	-4.329160	-1.222082
86	1	0	-5.851270	-2.444341	-0.675216
87	1	0	-1.580079	-3.690438	1.884569
88	1	0	-2.960426	-2.905070	2.593741
89	1	0	-1.453840	-1.694070	4.169233
90	1	0	0.850254	-2.603542	4.533997
91	1	0	0.704676	-1.794776	2.985008
92	1	0	0.694339	-3.552611	3.060194
93	1	0	-2.886656	-3.716163	0.125551
94	1	0	-2.884608	1.952837	1.089346
95	1	0	-2.657144	-3.762967	4.833582
96	1	0	-1.083256	-3.702671	5.615661
97	1	0	-1.331568	-4.742513	4.219633
98	1	0	-6.940245	2.025854	-0.509402
99	1	0	-7.242174	4.485466	-0.662668
100	1	0	-6.509069	4.090269	0.881089
101	1	0	-5.513105	4.723183	-0.410079
102	1	0	-5.004224	3.337030	-2.431607
103	1	0	-5.459887	1.646853	-2.503110
104	1	0	1.666328	0.867105	3.592282
105	1	0	1.771041	2.606911	3.274370
106	1	0	0.203443	1.812738	3.363746
107	1	0	-6.807082	2.922205	-4.122777
108	1	0	-7.838527	2.266975	-2.859820
109	1	0	-7.408543	3.973779	-2.854666
110	1	0	1.614699	-3.776228	-2.949416
111	1	0	-8.580261	-0.289836	-1.554268
112	1	0	-7.421395	-1.440382	-2.228757
113	1	0	-7.914372	-1.574318	-0.535566

Computational data for **3**−8‴*R*



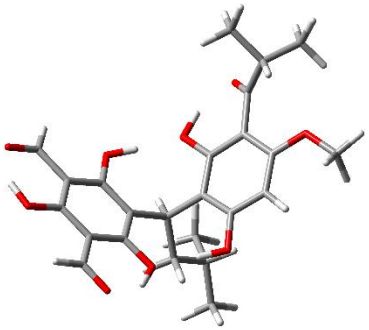
Optimized structure of **3**−8‴*R*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.048851	3.447053	0.270924
2	6	0	3.611028	2.254188	1.067909
3	6	0	2.712248	1.004710	1.019970
4	6	0	1.332809	1.359296	1.599165
5	6	0	0.780683	2.600320	0.935985
6	6	0	1.542973	3.524553	0.382859
7	6	0	2.559972	0.438324	−0.403868
8	6	0	1.498262	−0.637118	−0.433871
9	6	0	0.431453	−0.618186	0.469005
10	8	0	0.389884	0.294404	1.436231
11	1	0	3.141246	0.240757	1.659644
12	6	0	1.546675	−1.662346	−1.354481
13	6	0	0.562027	−2.661998	−1.392138
14	6	0	−0.499184	−2.579606	−0.467833
15	6	0	−0.607998	−1.560435	0.463762
16	6	0	3.710865	4.807105	0.610837
17	6	0	5.212646	4.805694	0.306219
18	6	0	3.449745	5.292200	2.041611
19	8	0	2.550130	−1.785493	−2.230189
20	6	0	3.509056	−0.729632	−2.413444
21	6	0	3.859663	−0.078975	−1.063204
22	6	0	4.670616	−1.049495	−0.188200
23	6	0	5.956933	−1.595637	−0.847193
24	6	0	5.780914	−1.767718	−2.332908
25	6	0	4.714152	−1.409643	−3.018283
26	1	0	2.212321	1.257695	−1.020575
27	6	0	2.921680	0.258387	−3.423675
28	1	0	4.479855	0.777648	−1.299120
29	6	0	7.278875	−0.846379	−0.526687
30	6	0	7.673210	−0.977484	0.948728
31	6	0	7.304631	0.621272	−0.963962
32	8	0	−1.442414	−3.528245	−0.475531
33	6	0	−1.786261	−1.446224	1.439929
34	6	0	−3.134727	−1.173270	0.739640
35	6	0	−4.111330	−2.114638	0.441466
36	6	0	−5.372851	−1.759896	−0.046084
37	6	0	−5.667886	−0.450010	−0.314930
38	6	0	−4.698583	0.563429	−0.121766
39	6	0	−3.466827	0.162046	0.452497
40	6	0	−1.854634	−2.561673	2.521329
41	6	0	−0.910390	−2.378951	3.727919
42	6	0	0.541836	−2.776410	3.440900
43	8	0	−3.953011	−3.427862	0.633925
44	8	0	−2.537443	1.064366	0.744961
45	6	0	−1.437076	−3.193083	4.916477
46	6	0	−4.889903	1.984644	−0.496657
47	6	0	−5.920188	2.446726	−1.525724
48	8	0	−4.174407	2.845929	−0.022539
49	6	0	−5.239164	3.409458	−2.508145
50	6	0	−7.100091	3.100559	−0.778476
51	6	0	1.359964	1.544474	3.119054

52	1	0	-1.602324	-0.539612	1.988259
53	6	0	-8.284903	3.451070	-1.679108
54	6	0	0.641249	-3.742413	-2.362038
55	8	0	-0.161899	-4.643113	-2.454392
56	8	0	-6.880506	-0.067323	-0.742215
57	6	0	-7.902438	-1.012974	-0.923250
58	1	0	3.269506	3.279601	-0.783936
59	1	0	3.749701	2.537258	2.103915
60	1	0	4.597491	2.002338	0.698189
61	1	0	-0.288619	2.707292	0.966927
62	1	0	1.076348	4.394863	-0.050820
63	1	0	3.250672	5.531482	-0.059436
64	1	0	5.624047	5.804758	0.412267
65	1	0	5.412042	4.473661	-0.708900
66	1	0	5.760374	4.157188	0.983398
67	1	0	3.821457	6.304779	2.165738
68	1	0	2.391272	5.298107	2.277878
69	1	0	3.953678	4.674094	2.778237
70	1	0	4.925551	-0.566535	0.745750
71	1	0	4.037511	-1.890855	0.072808
72	1	0	6.105995	-2.598677	-0.450160
73	1	0	6.594728	-2.247253	-2.853659
74	1	0	4.659069	-1.617053	-4.073598
75	1	0	1.980147	0.672779	-3.087366
76	1	0	3.615117	1.073125	-3.605000
77	1	0	2.739825	-0.249794	-4.363767
78	1	0	8.047458	-1.361683	-1.101123
79	1	0	8.663790	-0.565118	1.114809
80	1	0	7.691820	-2.016896	1.262565
81	1	0	6.989499	-0.445220	1.602845
82	1	0	8.301963	1.032156	-0.839841
83	1	0	7.028187	0.735963	-2.006515
84	1	0	6.632132	1.228807	-0.366754
85	1	0	-1.262190	-4.162687	-1.177484
86	1	0	-6.073633	-2.552814	-0.201014
87	1	0	-1.676082	-3.545820	2.102218
88	1	0	-2.869140	-2.573747	2.903348
89	1	0	-0.923790	-1.329448	4.015670
90	1	0	1.151737	-2.659850	4.332940
91	1	0	0.985596	-2.176887	2.658123
92	1	0	0.602412	-3.818506	3.136233
93	1	0	-3.037487	-3.661706	0.525397
94	1	0	-2.903267	1.942675	0.611612
95	1	0	-2.436195	-2.877583	5.201083
96	1	0	-0.793349	-3.081094	5.784307
97	1	0	-1.481238	-4.252171	4.673797
98	1	0	-6.288452	1.597774	-2.078085
99	1	0	-5.923683	3.685243	-3.302584
100	1	0	-4.375310	2.942988	-2.972006
101	1	0	-4.904662	4.309900	-2.009650
102	1	0	-6.740202	3.993774	-0.276350
103	1	0	-7.443632	2.423370	-0.003492
104	1	0	1.734729	0.647498	3.600294
105	1	0	1.973601	2.386868	3.407917
106	1	0	0.352190	1.724427	3.473974
107	1	0	-8.028964	4.201940	-2.418629
108	1	0	-8.647850	2.573597	-2.207307
109	1	0	-9.106795	3.844034	-1.088427
110	1	0	1.494146	-3.720099	-3.031770
111	1	0	-8.766140	-0.454480	-1.250848
112	1	0	-7.635608	-1.740416	-1.680319
113	1	0	-8.132777	-1.521624	0.004836

Computational data for **4**–*R*



Optimized structure of **4**–*R*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.749998	-0.303401	-1.190324
2	6	0	-4.022722	-1.507677	-0.542189
3	6	0	-3.218378	-1.908846	0.530574
4	6	0	-2.146559	-1.101391	0.950320
5	6	0	-1.871978	0.146429	0.341524
6	6	0	-2.681390	0.509868	-0.754782
7	8	0	-2.391427	1.682534	-1.412068
8	8	0	-5.074508	-2.269925	-0.986538
9	8	0	-1.383604	-1.580393	1.984845
10	6	0	-0.748452	1.053227	0.879582
11	6	0	-1.178282	2.525427	1.162218
12	6	0	-0.139938	3.382010	1.927087
13	6	0	0.569836	0.860202	0.123284
14	6	0	-0.652822	4.821063	2.046926
15	6	0	0.173725	2.836202	3.321257
16	6	0	0.933350	1.574818	-1.023673
17	6	0	2.191008	1.432428	-1.623194
18	6	0	3.127755	0.524038	-1.129886
19	6	0	2.769483	-0.271320	-0.034473
20	6	0	1.517085	-0.073072	0.596614
21	8	0	1.178284	-0.806187	1.718648
22	8	0	0.117141	2.472556	-1.647953
23	6	0	3.668513	-1.322429	0.522552
24	6	0	4.477498	-2.224470	-0.401824
25	8	0	3.644288	-1.493332	1.745796
26	6	0	4.075683	-3.678961	-0.156114
27	6	0	5.967331	-2.026030	-0.143321
28	6	0	-3.484486	-3.187439	1.224191
29	8	0	-4.406625	-3.911584	0.853353
30	6	0	-4.595390	0.106358	-2.331998
31	8	0	-4.381820	1.172755	-2.905901
32	8	0	4.389075	0.378431	-1.637988
33	6	0	4.796187	1.262497	-2.677082
34	1	0	-3.078247	1.826841	-2.110225
35	1	0	-5.129988	-3.086002	-0.433201
36	1	0	-0.458131	-1.263489	1.894800
37	1	0	-0.577339	0.706746	1.903466
38	1	0	-1.431771	3.060776	0.244804
39	1	0	-2.109851	2.503164	1.746174
40	1	0	0.794242	3.415800	1.354312
41	1	0	0.083130	5.456450	2.551111
42	1	0	-0.839669	5.251711	1.057467
43	1	0	-1.586266	4.864141	2.618440
44	1	0	0.827055	3.523680	3.869636
45	1	0	0.694895	1.876028	3.268128
46	1	0	-0.740220	2.699038	3.908666

47	1	0	2.399043	2.056114	-2.487932
48	1	0	2.020361	-1.155579	2.104657
49	1	0	-0.813383	2.201701	-1.505260
50	1	0	4.251572	-2.005268	-1.449168
51	1	0	4.298813	-3.991912	0.869965
52	1	0	3.000467	-3.815885	-0.315741
53	1	0	4.608636	-4.349546	-0.838199
54	1	0	6.234438	-2.298977	0.883835
55	1	0	6.259450	-0.980904	-0.287372
56	1	0	6.564917	-2.641972	-0.823293
57	1	0	-2.841173	-3.469291	2.073252
58	1	0	-5.412484	-0.562253	-2.648406
59	1	0	5.838416	1.033244	-2.919019
60	1	0	4.202019	1.103322	-3.582694
61	1	0	4.752293	2.306294	-2.349371