Supporting Information

Rec. Nat. Prod. 16:1 (2022) 98-103

Two New Sesquiterpenoids from Chloranthus henryi Hemsl

Yuting Bian¹, Fangyou Chen¹, Weiming Huang¹, Zhichao Chen¹, Pengcheng Shuang² and Yongming Luo^{1*}

¹School of Pharmacy, Jiangxi University of Traditional Chinese Medicine,

Nanchang, Jiangxi 330004, P. R.China

²School of Chinese Materia Medica, Beijing University of Chinese Medicine,

Beijing, 100029, P. R.China

Table of Contents	Page
Figure S1: HR-ESI-MS Spectrum of 1 (Chloratene F)	2
Figure S2: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of 1 (Chloratene F)	3
Figure S3: ¹³ C-NMR (125 MHz, CDCl ₃) Spectrum of 1 (Chloratene F)	4
Figure S4: HSQC Spectrum of 1 (Chloratene F) (From $\delta_{\rm H}$ 3.5 ppm to $\delta_{\rm H}$ 7.5ppm)	5
Figure S5: HSQC Spectrum of 1 (Chloratene F) (From $\delta_H 0$ ppm to $\delta_H 3.5$ ppm)	6
Figure S6: HMBC Spectrum of 1 (Chloratene F)	7
Figure S7: HMBC Spectrum of 1 (Chloratene F) (From $\delta_{\rm C}$ 10 ppm to $\delta_{\rm C}$ 100 ppm)	8
Figure S8: HMBC Spectrum of 1 (Chloratene F) (From δ_C 110 ppm to δ_C 200 ppm)	9
Figure S9: ¹ H- ¹ H COSY Spectrum of 1 (Chloratene F)	10
Figure S10: ORTEP Spectrum of 1 (Chloratene F)	11
Figure S11 : CD Spectra of 2 (Chloratene F)	12
Figure S12: HR-ESI-MS Spectrum of 2 (Chlomultin G)	13
Figure S13: ¹ H-NMR (600 MHz, CDCl ₃) Spectrum of 2 (Chlomultin G)	14
Figure S14: ¹³ C-NMR (150 MHz, CDCl ₃) Spectrum of 2 (Chlomultin G)	15
Figure S15: HSQC Spectrum of 2 (Chlomultin G)	16
Figure S16: HMBC Spectrum of 2 (Chlomultin G)	17
Figure S17: HMBC Spectrum of 2 (Chlomultin G) (From $\delta_{\rm C}$ 100ppm to 180 ppm)	18
Figure S18: HMBC Spectrum of 2 (Chlomultin G) (From δ_C 10 ppm to 80 ppm)	19
Figure S19: ¹ H- ¹ H COSY Spectrum of 2 (Chlomultin G)	20
Figure S20: ORTEP Spectrum of 2 (Chlomultin G)	21
Figure S21 : CD Spectra of 2 (Chlomultin G)	22
Table 1. The most similar compound data to compound 1	23
Table 2. The most similar compound data to compound 2	24

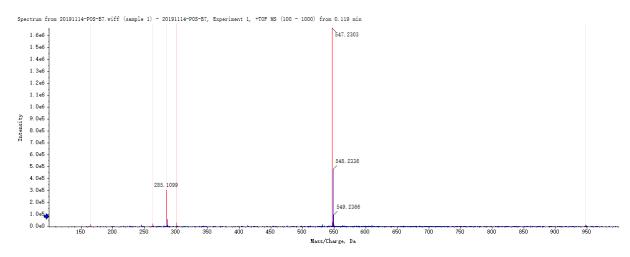


Figure S1: HR-ESI-MS Spectrum of 1 (Chloratene F)

© 2021 ACG Publications. All rights reserved.

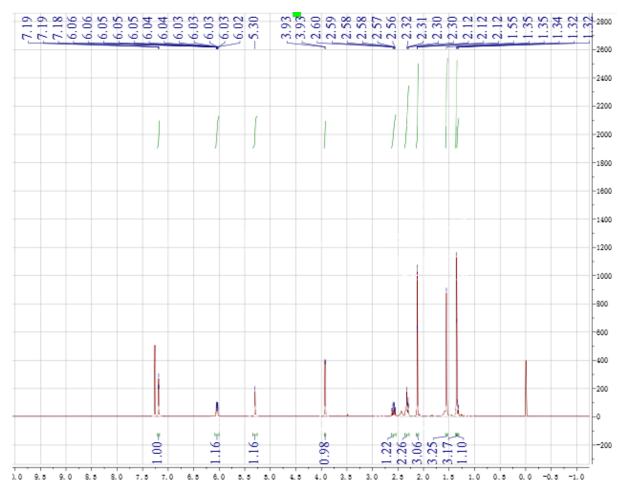


Figure S2: ¹H-NMR (600 MHz, CDCl₃) Spectrum of 1 (Chloratene F)

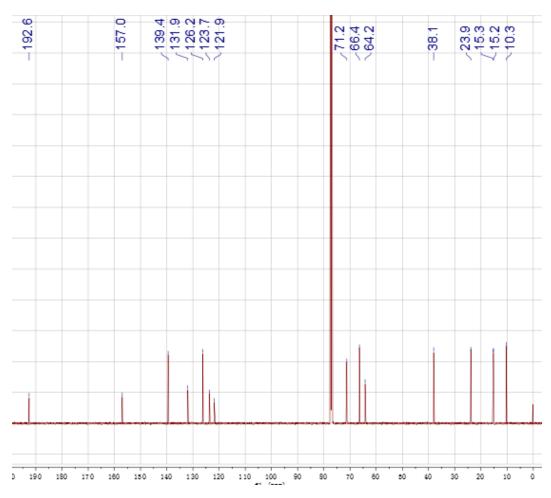


Figure S3: ¹³C-NMR (150MHz, CDCl₃) Spectrum of 1 (Chloratene F)

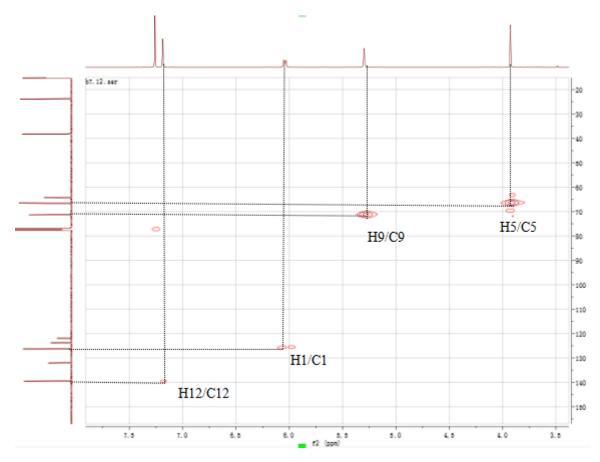


Figure S4: HSQC Spectrum of 1 (Chloratene F) (From $\delta_{\rm H}$ 3.5 ppm to $\delta_{\rm H}$ 7.5ppm)

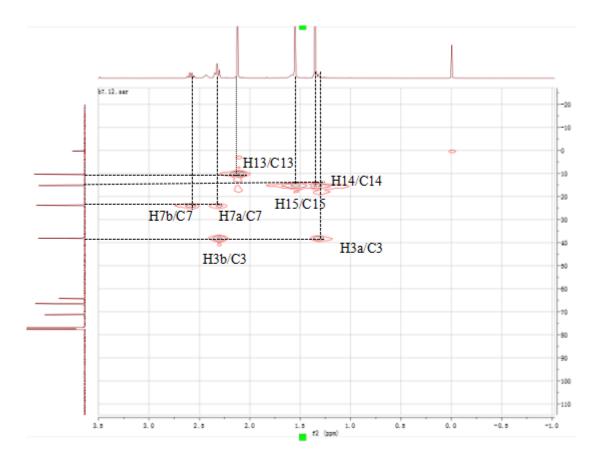


Figure S5: HSQC Spectrum of 1 (Chloratene F) (From $\delta_{\rm H}$ 0 ppm to $\delta_{\rm H}$ 3.5ppm)

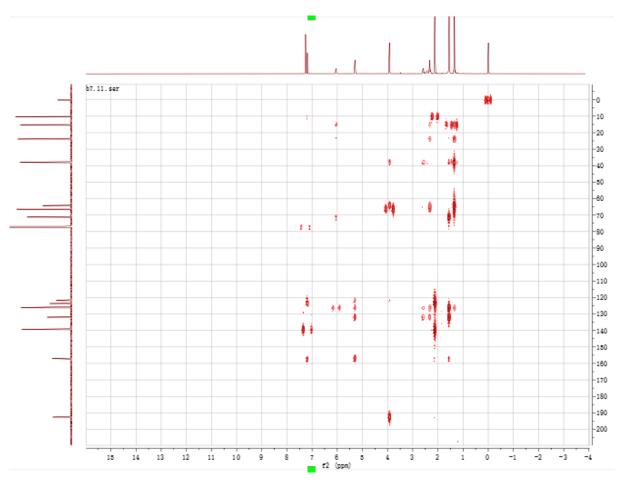


Figure S6: HMBC Spectrum of 1 (Chloratene F)

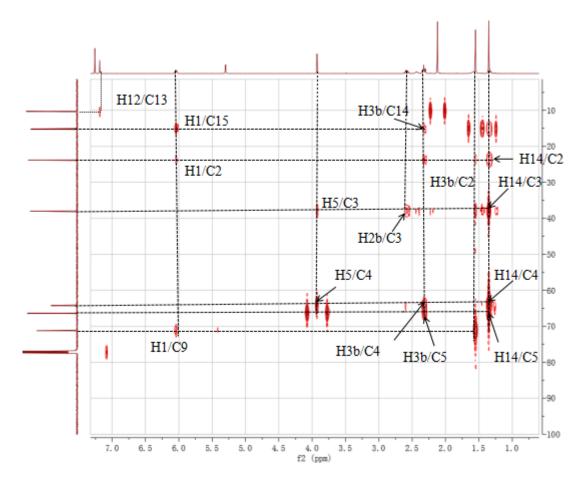


Figure S7: HMBC Spectrum of 1 (Chloratene F) (From δ_C 10 ppm to δ_C 100 ppm)

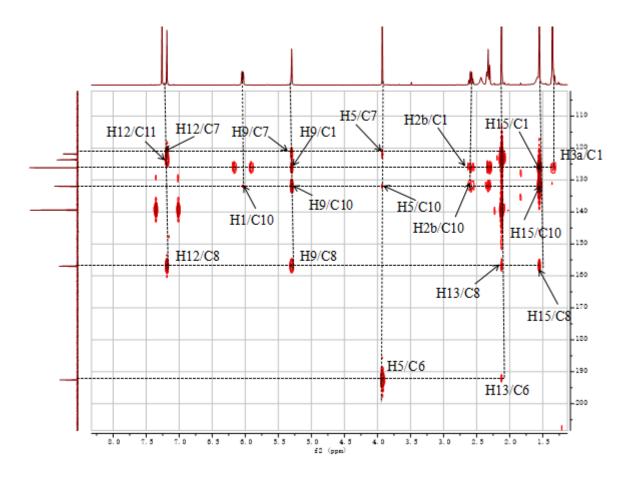


Figure S8: HMBC Spectrum of 1 (Chloratene F) (From δ_C 110 ppm to δ_C 200 ppm)

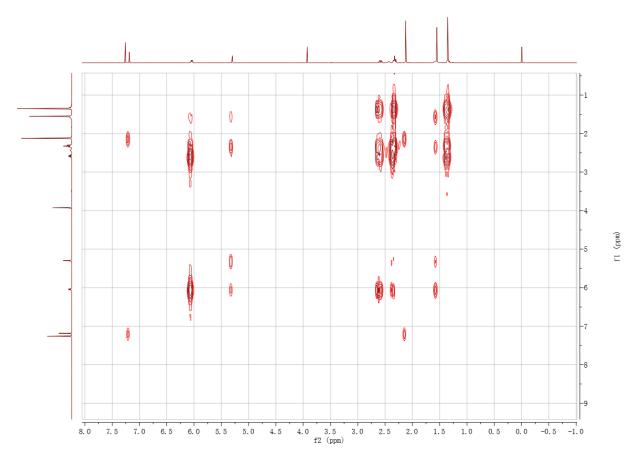


Figure S9: ¹H-¹H COSY Spectrum of 1 (Chloratene F)

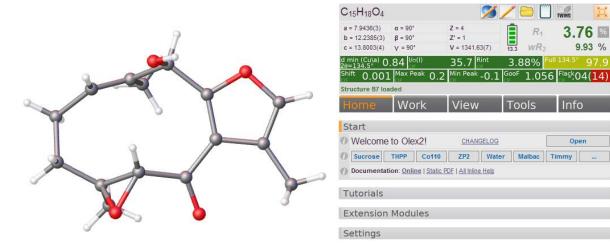


Figure S10: ORTEP Spectrum of 1 (Chloratene F)

💋 🥖 😑 🛄 🐖

3.88%

Tools

wR₂

3.76 9.93 %

Info

Open

13.3 R_1

		[Measurement Information]
Instrument name	J-1500	
Model name	J-1500	
Serial No.	B049961638	
Photometric me	ode CD, HT, Abs	
Measure range	500 - 200 nm	
Data pitch	1 nm	
CD scale	200 mdeg/0.1 dOD	
FL scale	200 mdeg/0.1 dODD	

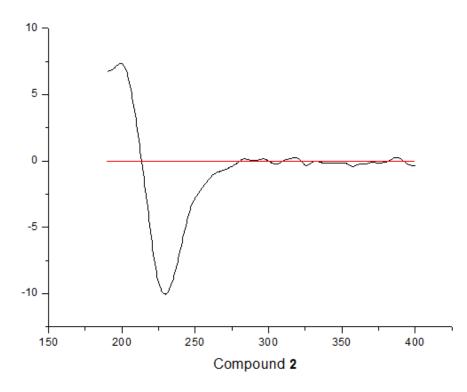


Figure S11: CD Spectra of 1 (Chlomultin G)

© 2021 ACG Publications. All rights reserved.

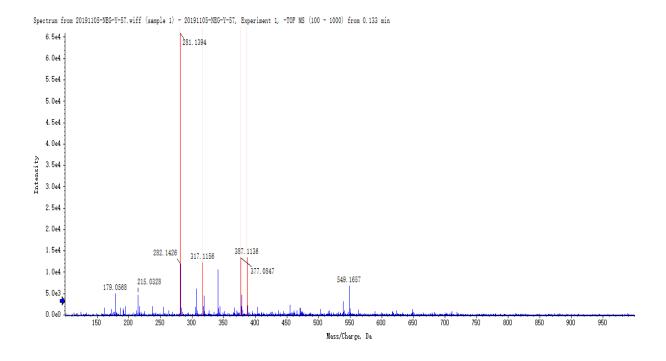


Figure S12: HR-ESI-MS Spectrum of 2 (Chlomultin G)

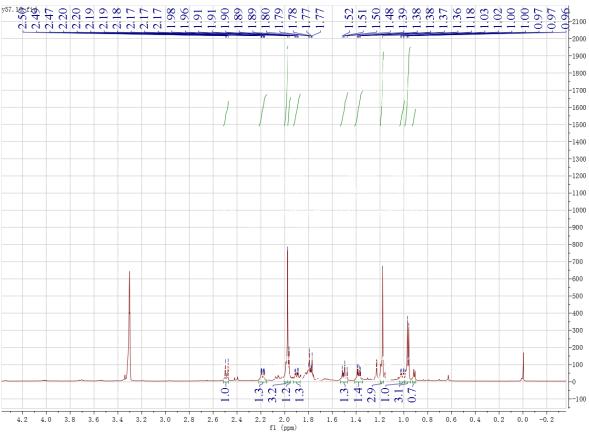


Figure S13: ¹H-NMR (600 MHz, CDCl₃) Spectrum of 2 (Chlomultin G)

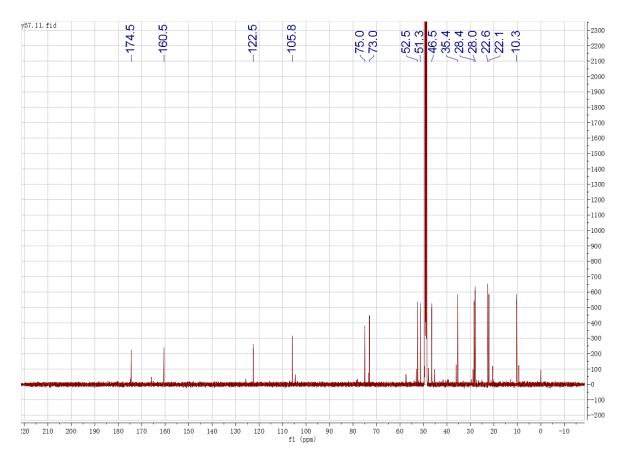


Figure S14: ¹³C-NMR (150 MHz, CDCl₃) Spectrum of 2 (Chlomultin G)

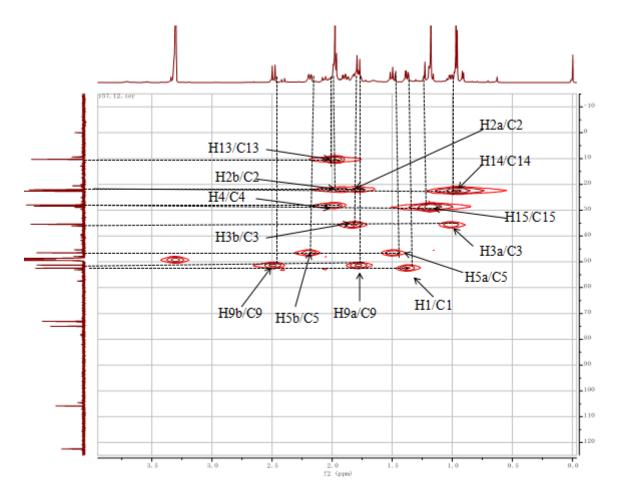


Figure S15: HSQC Spectrum of 2 (Chlomultin G)

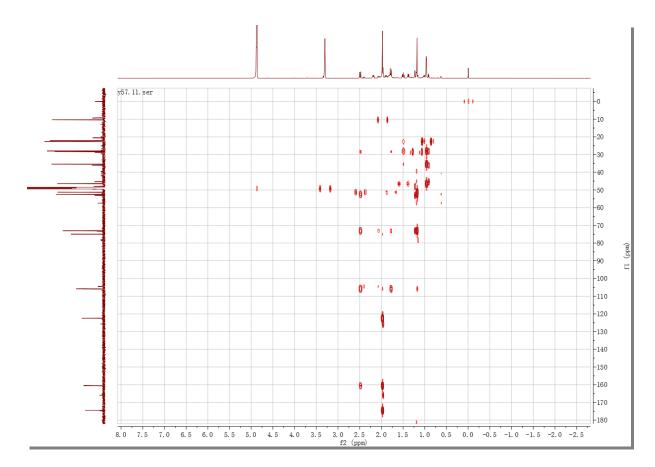


Figure S16: HMBC Spectrum of 2 (Chlomultin G)

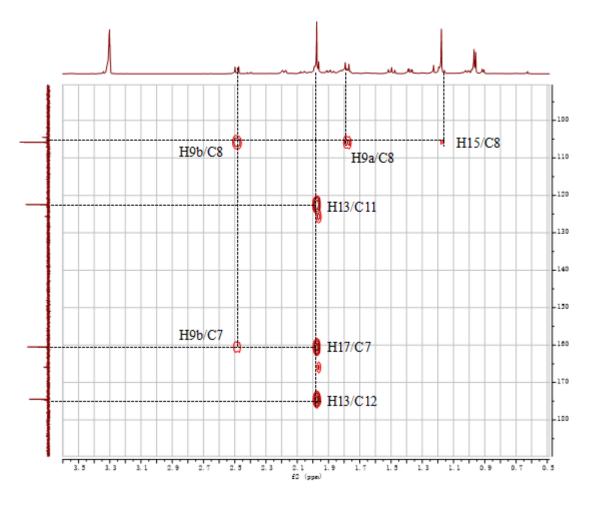


Figure S17: HMBC Spectrum of **2** (Chlomultin G) (From δ_{C} 100ppm to 180 ppm)

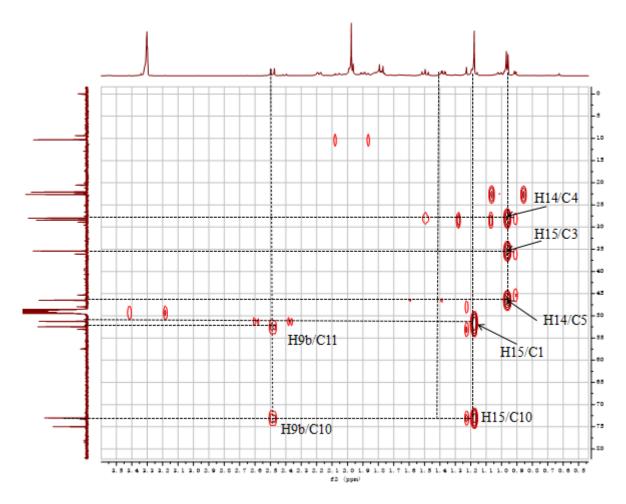


Figure S18: HMBC Spectrum of **2** (Chlomultin G) (From δ_C 10 ppm to 80 ppm)

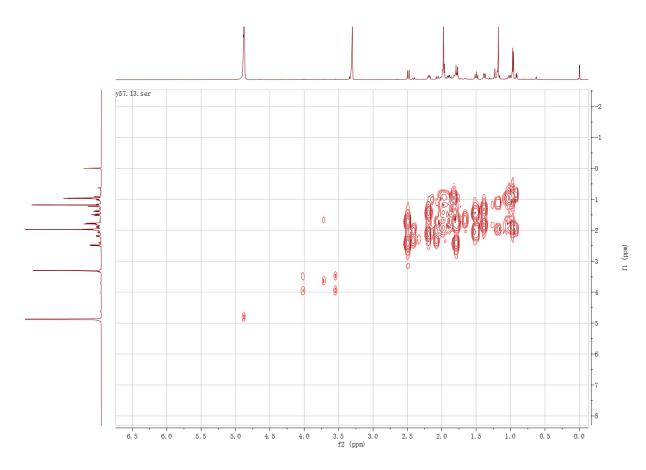
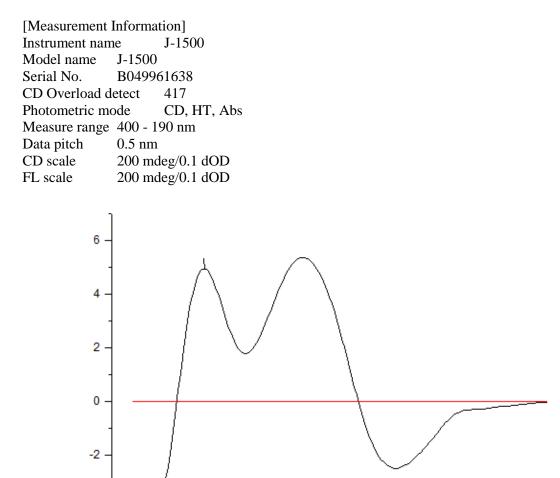


Figure S19: ¹H-¹H COSY Spectrum of 2 (Chlomultin G)

 $\ensuremath{\mathbb{C}}$ 2021 ACG Publications. All rights reserved.

C ₁₅ H ₂₂ O ₅	aha faha f		<u>/</u> 🖻	TWINS 🔀
a = 8.1067(1) b = 10.6992(1)	α = 90° β = 90°	Z = 4 Z' = 1		3.26 🛚
c = 16.1887(2) d min (Cu\a) 0 20=136.5°	γ = 90°	V = 1404.13(3) 39.1 Rint	13.6 WR ₂	8.92 %
$\frac{20=136.5}{5}$ 0.000		JJJ.L CIF		
Structure y57_a	CIF		ICIP	
Home	Work	View	Tools	Info
Start				
Welcome	to Olex2!	CHANGELOG		Open
Sucrose	THPP Co110	ZP2 Wat	er Malbac	Timmy
O Documentation	ion: <u>Online Static</u>	PDF <u>All Inline Help</u>		
Tutorials				
Extension	Modules			
Settings				
News				
C				3

Figure S20: ORTEP Spectrum of 2 (Chlomultin G)



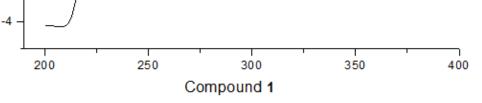
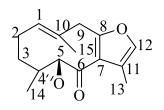


Figure S21: CD Spectra of 2 (Chlomultin G)



 $\begin{array}{c} 0H \\ 2 & 0H \\ 3 & 5' - 15 \\ 3 & 5' - 6 \\ 3 & 5' - 15 \\ 3 & 5' - 6 \\ 3 & 11 \\ 3 & 14 \\ 0 & 13 \end{array}$

similar compound

new compound

Table 1. The most	similar compound	data to compound 1
-------------------	------------------	---------------------------

NO.	similar compound		new compound	
	$\delta_{\rm H}$, mult. (<i>J</i> in Hz)	$\delta_{ m C}$	$\delta_{ m H}$, mult. (<i>J</i> in Hz)	δ_{C}
1	5.45 (1H, d, <i>J</i> = 9.1 Hz)	131.1	6.04 (1H, m)	126.2
2a	-	24.6	2.59 (1H, m)	22.0
2b	-	24.6	2.30 (1H, m)	23.9
3a	-	27.0	2.32 (1H, m)	20.1
3b	-	37.9	1.33 (1H, m)	38.1
4	-	63.9	-	64.2
5	3.81 (1H, d, <i>J</i> = 1.0 Hz)	66.5	3.93 (1H, d, <i>J</i> = 1.0 Hz)	66.4
6	-	192.1	-	192.0
7	-	131.0	-	123.7
8	-	157.0	-	157.0
9	3.71 (2H, m)	41.8	5.30 (1H, s)	71.2
10	-	122.2	-	131.9
11	-	123.2	-	121.9
12	7.08 (1H, s)	138.0	7.19 (1H, t, <i>J</i> = 1.2 Hz)	139.4
13	2.11 (3H, s)	10.2	2.12 (1H, d, <i>J</i> = 1.3 Hz)	10.3
14	1.34 (3H, s)	15.6	1.55 (3H, s)	15.3
15	1.60 (3H, s)	15.1	1.35 (3H, s)	15.2



NO.	similar compound		new compound	
	$\delta_{\rm H}$, mult. (<i>J</i> in Hz)	$\delta_{ m C}$	$\delta_{\rm H}$, mult. (<i>J</i> in Hz)	$\delta_{ m C}$
1	1.51 (1H, dd, <i>J</i> = 12.4, 3.6 Hz)	50.9	1.38 (1H, dd, <i>J</i> = 12.3, 3.7 Hz)	52.5
2a	1.72 (1H, m)	21.8	1.77 (1H, m)	22.1
2b	2.01 (1H, m)	21.8	1.90 (1H, m)	
3a	2.04 (1H, m)	33.8	1.01 (1H, m)	35.4
3b	2.33 (1H, m)	55.8	1.79 (1H, m)	
4	-	145.0	1.96 (1H, m)	28.0
5a	2.65 (1H, m)	44.9	2.18 (1H, m)	46.5
5b	2.53 (1H, m)	44.9	1.50 (1H, m)	
6	-	74.0	-	75.0
7	-	159.4	-	160.5
8	-	104.6	-	105.8
9a	1.73 (1H, m)	50.3	1.77 (1H, m)	51.3
9b	2.41 (1H, m)	50.5	2.49 (1H, m)	
10	-	71.6	-	73.0
11	-	120.5	-	122.5
12	-	172.5	-	174.5
13	1.90 (3H, s)	10.3	2.05 (3H, s)	10.3
14a	4.56 (1H, s)	110.7	0.96 (3H, d, <i>J</i> = 6.7 Hz)	22.6
14b	4.75 (1H, s)	110.7		
15	1.09 (3H, s)	28.7	1.98 (3H, s)	28.4

 Table 2. The most similar compound data to compound 2

© 2021 ACG Publications. All rights reserved.