Supporting Information

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Two New Sesquiterpenoids from Chloranthus henryi Hemsl

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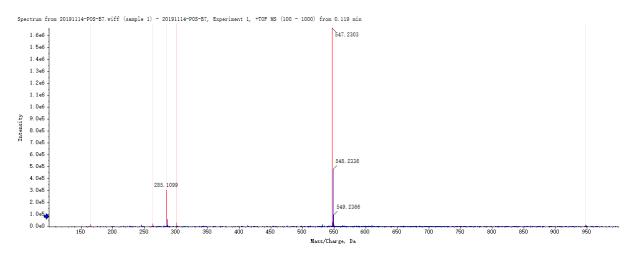


Figure S1: HR-ESI-MS Spectrum of 1 (Chloratene F)

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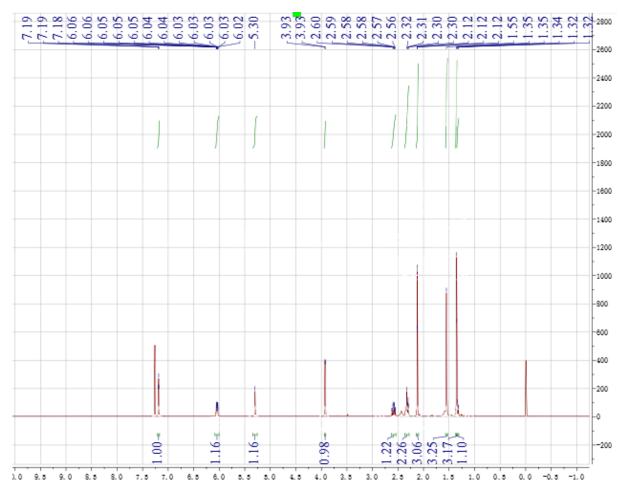


Figure S2: ¹H-NMR (600 MHz, CDCl₃) Spectrum of 1 (Chloratene F)

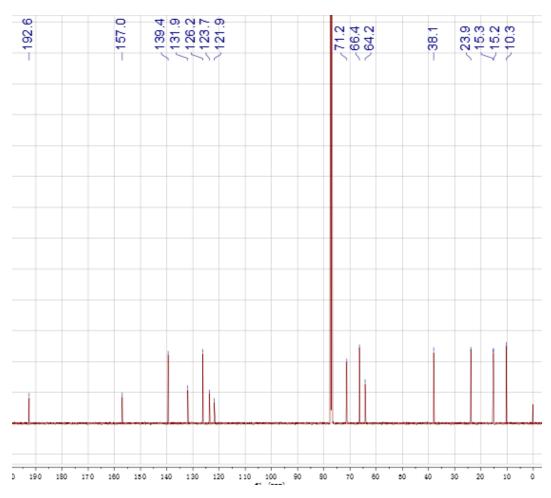


Figure S3: ¹³C-NMR (150MHz, CDCl₃) Spectrum of 1 (Chloratene F)

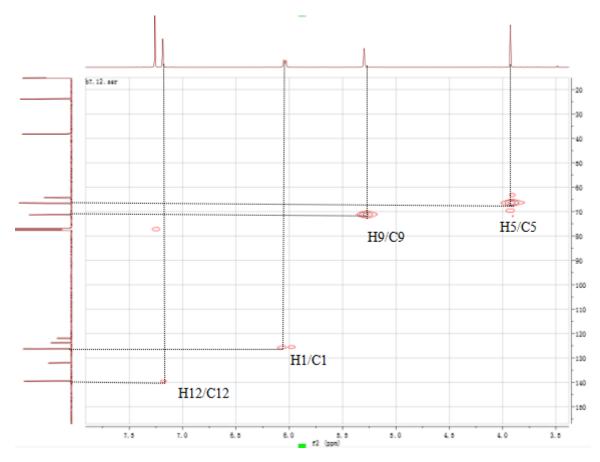


Figure S4: HSQC Spectrum of 1 (Chloratene F) (From $\delta_{\rm H}$ 3.5 ppm to $\delta_{\rm H}$ 7.5ppm)

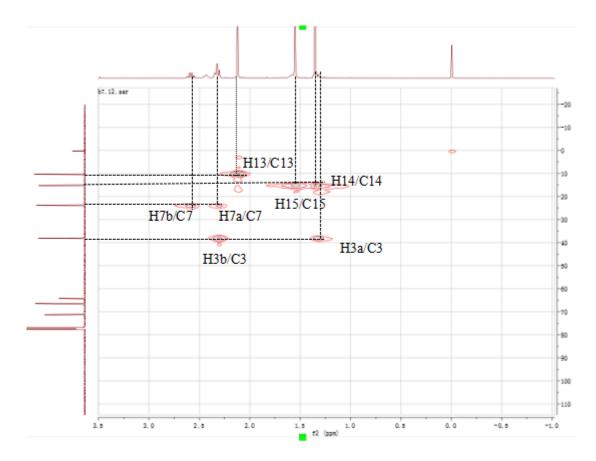


Figure S5: HSQC Spectrum of 1 (Chloratene F) (From $\delta_{\rm H}$ 0 ppm to $\delta_{\rm H}$ 3.5ppm)

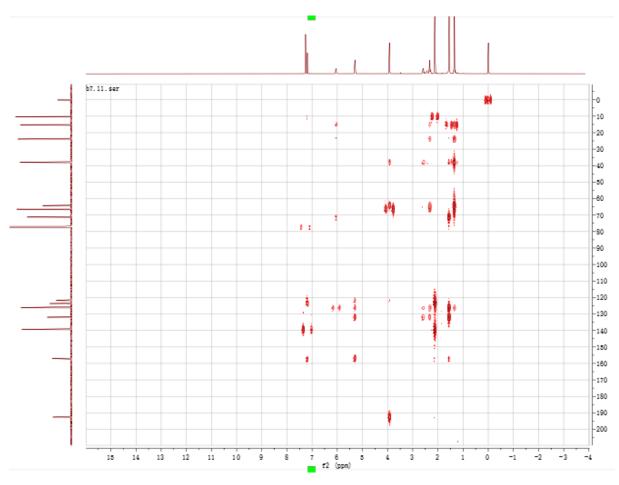


Figure S6: HMBC Spectrum of 1 (Chloratene F)

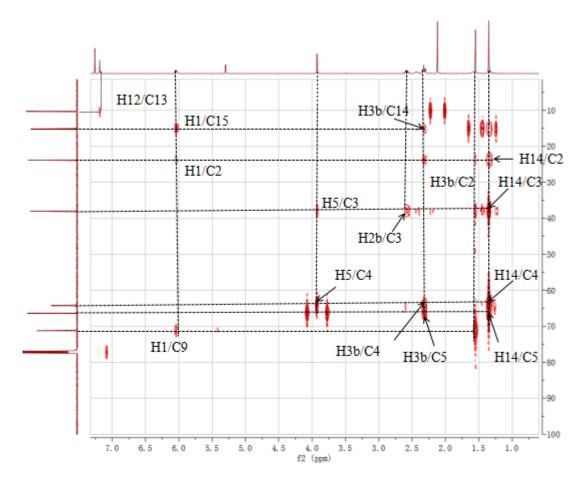


Figure S7: HMBC Spectrum of 1 (Chloratene F) (From δ_C 10 ppm to δ_C 100 ppm)

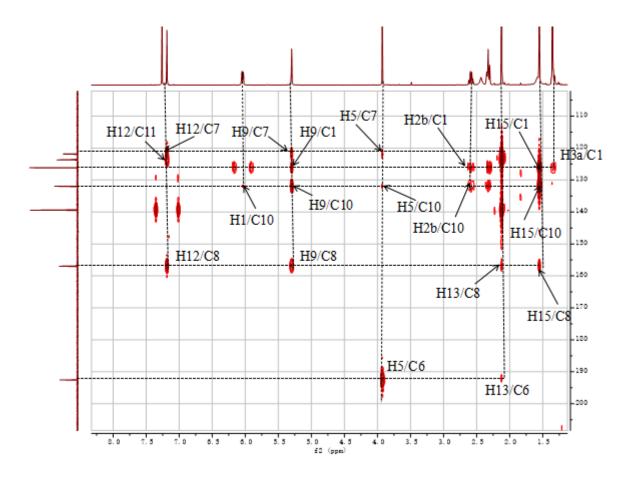


Figure S8: HMBC Spectrum of 1 (Chloratene F) (From δ_C 110 ppm to δ_C 200 ppm)

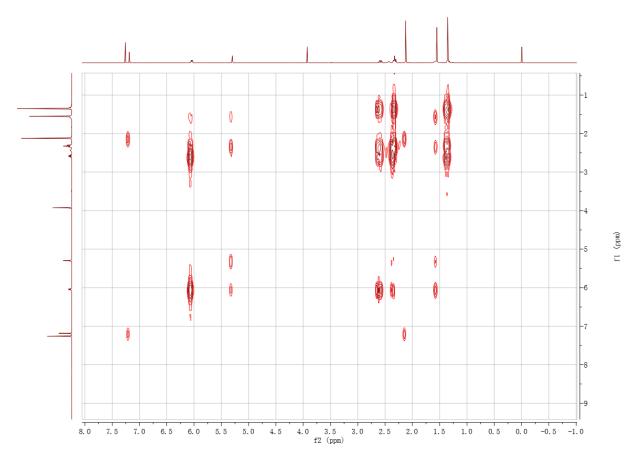


Figure S9: ¹H-¹H COSY Spectrum of 1 (Chloratene F)

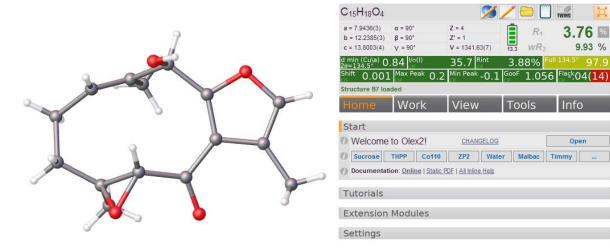


Figure S10: ORTEP Spectrum of 1 (Chloratene F)

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Tools

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Info

Open

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| | | [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 | |

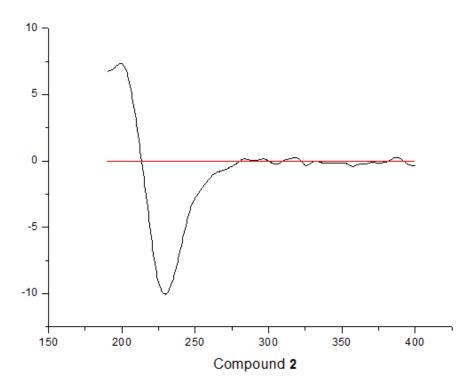


Figure S11: CD Spectra of 1 (Chlomultin G)

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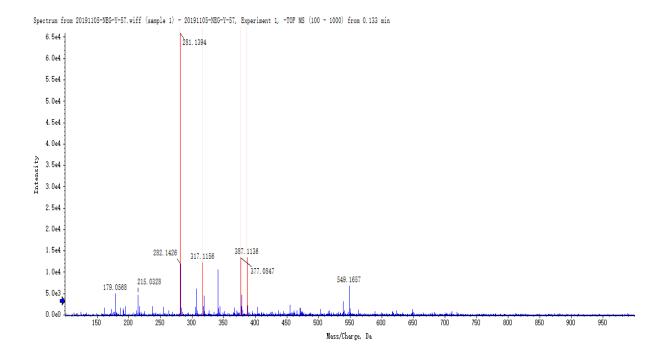


Figure S12: HR-ESI-MS Spectrum of 2 (Chlomultin G)

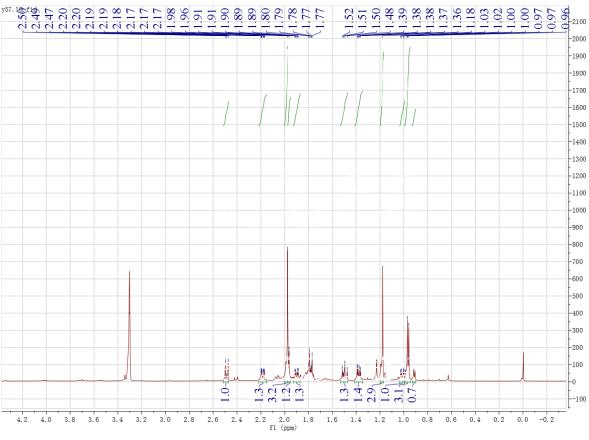


Figure S13: ¹H-NMR (600 MHz, CDCl₃) Spectrum of 2 (Chlomultin G)

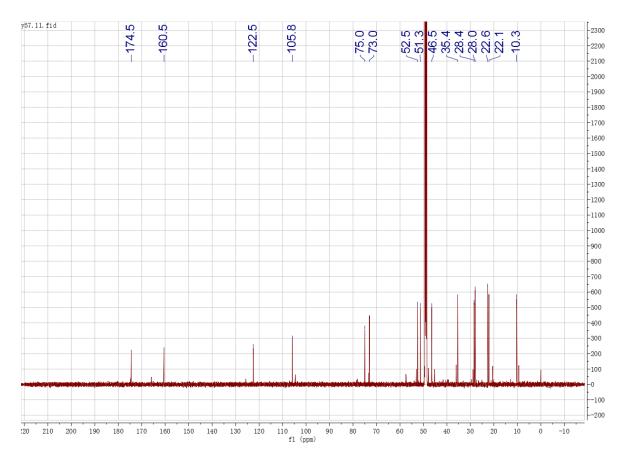


Figure S14: ¹³C-NMR (150 MHz, CDCl₃) Spectrum of 2 (Chlomultin G)

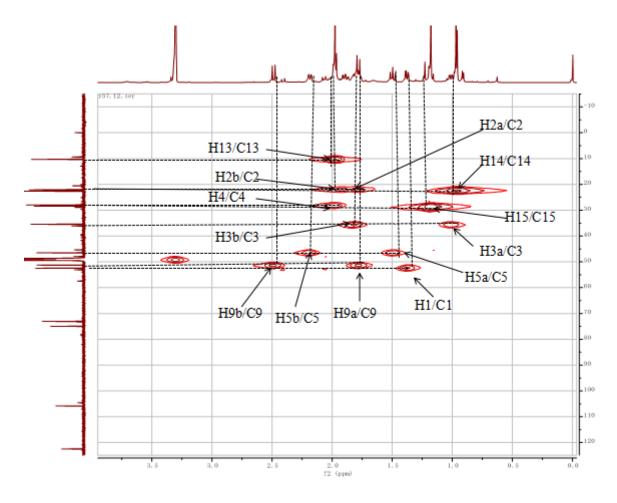


Figure S15: HSQC Spectrum of 2 (Chlomultin G)

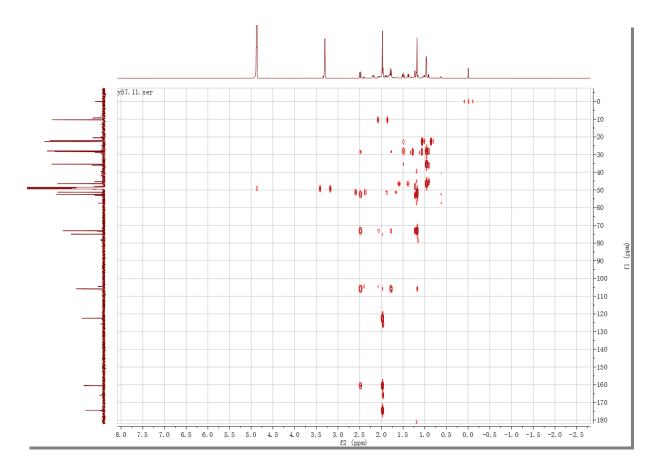


Figure S16: HMBC Spectrum of 2 (Chlomultin G)

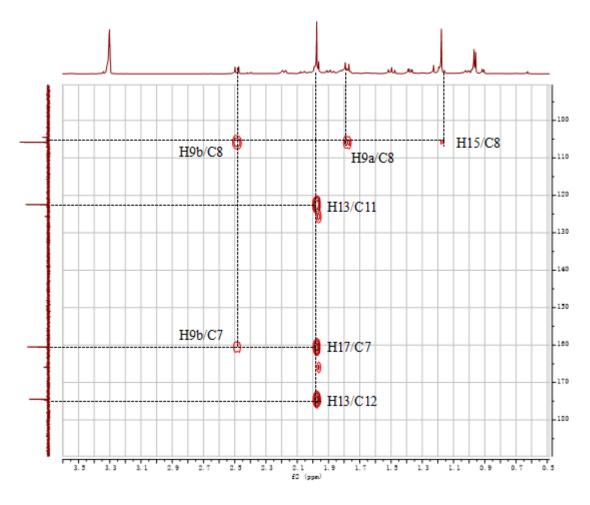


Figure S17: HMBC Spectrum of **2** (Chlomultin G) (From δ_{C} 100ppm to 180 ppm)

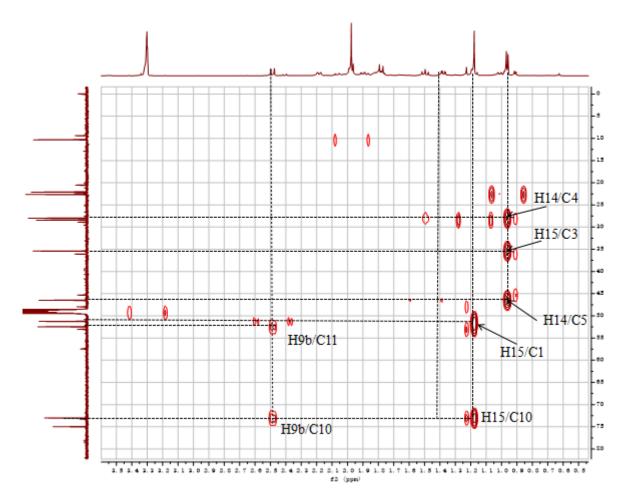


Figure S18: HMBC Spectrum of **2** (Chlomultin G) (From δ_C 10 ppm to 80 ppm)

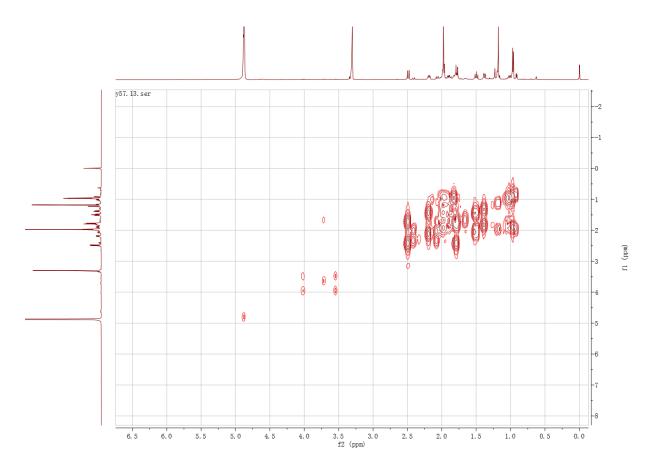
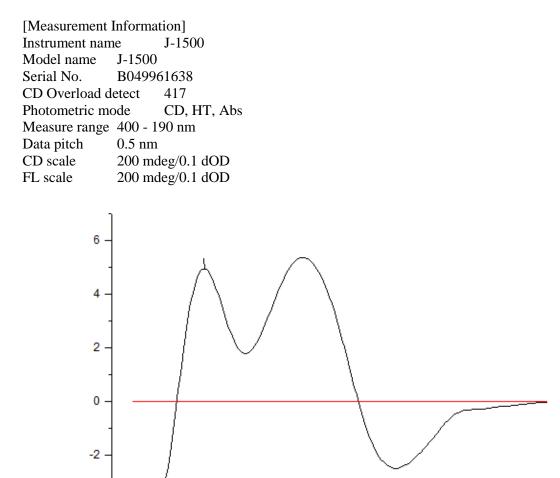


Figure S19: ¹H-¹H COSY Spectrum of 2 (Chlomultin G)

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| 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 | |
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| 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 | | | | |
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| C | | | | 3 |

Figure S20: ORTEP Spectrum of 2 (Chlomultin G)



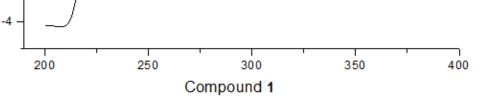
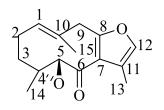


Figure S21: CD Spectra of 2 (Chlomultin G)



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

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

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