Supporting Information for

Dicarabrol A, dicarabrone C and dipulchellin A, unique sesquiterpene lactone dimers from *Carpesium abrotanoides* †

Jie-Wei Wu,ab Chun-Ping Tang,a Chang-Qiang Ke,a Sheng Yao,a Li-Gen Lin*c and Yang Ye*ad

aState Key Laboratory of Drug Research, & Natural Products Chemistry Department, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, P. R. China

bUniversity of Chinese Academy of Sciences, Beijing 100049, P. R. China

cState Key Laboratory of Quality Research in Chinese Medicine, Institute of Chinese Medical Sciences, University of Macau, Macao 999078, R. R. China

dSchool of Life Science and Technology, ShanghaiTech University, Shanghai 201203, P. R. China
Experimental Section

X-ray crystallographic analyses.

Table S1. X-ray crystallographic data for dipulchellin A (3)

Figure S1. $^1$H NMR spectrum of dicarabrol A (1) in CDCl$_3$

Figure S2. $^{13}$C NMR spectrum of dicarabrol A (1) in CDCl$_3$

Figure S3. $^1$H-$^1$H COSY spectrum of dicarabrol A (1) in CDCl$_3$

Figure S4. HSQC spectrum of dicarabrol A (1) in CDCl$_3$

Figure S5. HMBC spectrum of dicarabrol A (1) in CDCl$_3$

Figure S6. ROESY spectrum of dicarabrol A (1) in CDCl$_3$

Figure S7. IR spectrum of dicarabrol A (1)

Figure S8. HRESI(+)MS spectrum of dicarabrol A (1)

Figure S9. $^1$H NMR spectrum of dicarabrone C (2) in CDCl$_3$

Figure S10. $^{13}$C NMR spectrum of dicarabrone C (2) in CDCl$_3$

Figure S11. $^1$H-$^1$H COSY spectrum of dicarabrone C (2) in CDCl$_3$

Figure S12. HSQC spectrum of dicarabrone C (2) in CDCl$_3$

Figure S13. HMBC spectrum of dicarabrone C (2) in CDCl$_3$

Figure S14. ROESY spectrum of dicarabrone C (2) in CDCl$_3$

Figure S15. IR spectrum of dicarabrone C (2)

Figure S16. HRESI(+)MS spectrum of dicarabrone C (2)

Figure S17. $^1$H NMR spectrum of dipulchellin A (3) in CDCl$_3$
Figure S18. $^{13}$C NMR spectrum of dipulchellin A (3) in CDCl$_3$

Figure S19. $^1$H-$^1$H COSY spectrum of dipulchellin A (3) in CDCl$_3$

Figure S20. HSQC spectrum of dipulchellin A (3) in CDCl$_3$

Figure S21. HMBC spectrum of dipulchellin A (3) in CDCl$_3$

Figure S22. ROESY spectrum of dipulchellin A (3) in CDCl$_3$

Figure S23. IR spectrum of dipulchellin A (3)

Figure S24. HRESI(+)MS spectrum of dipulchellin A (3)
Experimental Section

**X-ray crystallographic analyses.** Dipulchellin A (3) was crystallized from acetone at room temperature. The X-ray crystallographic data was obtained on a Bruker SMART CCD detector employing graphite monochromated Cu-Kα radiation (\(\lambda = 1.54178 \text{ Å}\)) (operated in the \(\varphi-\omega\) scan mode). The structure was solved by direct method using SHELXS-97 program and refined with full-matrix least-squares calculations on \(F^2\) using SHELXL-97. Crystallographic data for 3 (key parameters see Table S1) have been deposited at the Cambridge Crystallographic Data Centre (Deposition No.: CCDC 1479445). Copies of these data can be obtained free of charge via the internet at www.ccdc.cam.ac.uk/conts/retrieving.html or on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [Tel: (+44) 1223-336-408; Fax: (+44) 1223-336-033; E-mail: deposit@ccdc.cam.ac.uk].

### Table S1. X-ray crystallographic data for dipulchellin A (3)

<table>
<thead>
<tr>
<th>Crystal data</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C(<em>{34})H(</em>{44})O(_{7})</td>
<td></td>
</tr>
<tr>
<td>(M_r = 564.69)</td>
<td></td>
</tr>
<tr>
<td>Orthorhombic, (P_{2_1}2_12_1)</td>
<td></td>
</tr>
<tr>
<td>(a = 10.4583 (1) \text{ Å})</td>
<td>(F(000) = 1216)</td>
</tr>
<tr>
<td>(b = 13.3200 (2) \text{ Å})</td>
<td>(D_s = 1.221 \text{ Mg m}^{-3})</td>
</tr>
<tr>
<td>(c = 22.0536 (3) \text{ Å})</td>
<td>(\mu = 0.68 \text{ mm}^{-1})</td>
</tr>
<tr>
<td>(V = 3072.17 (7) \text{ Å}^3)</td>
<td>(T = 296 \text{ K})</td>
</tr>
<tr>
<td>(Z = 4)</td>
<td></td>
</tr>
<tr>
<td>Plate, colourless</td>
<td>0.15 × 0.1 × 0.05 mm</td>
</tr>
</tbody>
</table>

<p>| Data collection       |   |
| Radiation source: fine-focus sealed tube | (R_{int} = 0.034) |</p>
<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>graphite</td>
<td>$\theta_{\text{max}} = 67.7^\circ$, $\theta_{\text{min}} = 3.9^\circ$</td>
</tr>
<tr>
<td>40986 measured reflections</td>
<td>$h = -10 \rightarrow 12$</td>
</tr>
<tr>
<td>5469 independent reflections</td>
<td>$k = -15 \rightarrow 14$</td>
</tr>
<tr>
<td>5246 reflections with $I &gt; 2\sigma(I)$</td>
<td>$l = -26 \rightarrow 25$</td>
</tr>
</tbody>
</table>

**Refinement**

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma (F^2)] = 0.099$

$wR(F^2) = 0.308$

$S = 1.54$

$5469$ reflections

$377$ parameters

$22$ restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.179$

$\Delta\rho_{\text{max}} = 0.93$ e Å$^{-3}$

$\Delta\rho_{\text{min}} = -1.14$ e Å$^{-3}$


Flack parameter: 0.1 (4)
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