Supplementary Material

New 4-Methylidene Sterols from the Marine Sponge *Theonella swinhoei*

Fan Yang\(^a,^1\), Yan-Yun Li\(^a,^1\), Jie Tang\(^a,^1\), Fan Sun\(^a,^1\), Hou-Wen Lin\(^a\)\(^*\)

\(^a\) Research Center for Marine Drugs, State Key Laboratory of Oncogenes and Related Genes, Department of Pharmacy, Ren Ji Hospital, School of Medicine, Shanghai Jiao Tong University, Shanghai 200127, China

\(^*\) Corresponding author. Tel./fax: +86 21 68383346 (H.-W. Lin); E-mail: franklin67@126.com (H.-W. Lin)

\(^1\) These authors contributed equally to this paper.
Content

Figure S1. HRESIMS of compound 1

Figure S2. IR spectrum of compound 1

Figure S3. $^1$H NMR Spectrum of compound 1

Figure S4. $^{13}$C NMR Spectrum of compound 1

Figure S5. DEPT spectrum of compound 1

Figure S6. COSY spectrum of compound 1

Figure S7. HSQC spectrum of compound 1

Figure S8. HMBC spectrum of compound 1

Figure S9. NOESY spectrum of compound 1

Figure S10. HRESIMS of compound 2

Figure S11. IR spectrum of compound 2

Figure S12. $^1$H NMR spectrum of compound 2

Figure S13. $^{13}$C NMR spectrum of compound 2

Figure S14. DEPT spectrum of compound 2

Figure S15. HSQC spectrum of compound 2

Figure S16. COSY spectrum of compound 2

Figure S17. HMBC spectrum of compound 2

Figure S18. NOESY spectrum of compound 2

Figure S19. HRESIMS of compound 3

Figure S20. IR spectrum of compound 3

Figure S21. $^1$H NMR spectrum of compound 3

Figure S22. $^{13}$C NMR spectrum of compound 3

Figure S23. DEPT spectrum of compound 3

Figure S24. HSQC spectrum of compound 3
Figure S25. COSY spectrum of compound 3
Figure S26. HMBC spectrum of compound 3
Figure S27. NOESY spectrum of compound 3
Figure S28. $^1$H NMR spectrum of compound 4
Figure S29. $^{13}$C NMR spectrum of compound 4
Figure S1. HRESIMS of compound 1

Figure S2. IR spectrum of compound 1
Figure S3. $^1$H NMR spectrum of compound 1

Figure S4. $^{13}$C NMR spectrum of compound 1
Figure S5. DEPT spectrum of compound 1

Figure S6. COSY spectrum of compound 1
Figure S7. HSQC spectrum of compound 1

Figure S8. HMBC spectrum of compound 1
Figure S9. NOESY spectrum of compound 1

Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -0.5, max = 20.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-30  H: 0-100  O: 3-3  23Na: 0-1
Minimum:
-0.5
Maximum:
200.0  10.0  20.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>433.3508</td>
<td>433.3525</td>
<td>-1.7</td>
<td>-3.8</td>
<td>6.5</td>
<td>C29 H47 O3</td>
</tr>
</tbody>
</table>

Figure S10. HRESIMS of compound 2
**Figure S11.** IR spectrum of compound 2

**Figure S12.** $^1$H NMR spectrum of compound 2
Figure S13. $^{13}$C NMR spectrum of compound 2

Figure S14. DEPT spectrum of compound 2
Figure S15. HSQC spectrum of compound 2

Figure S16. COSY spectrum of compound 2
Figure S17. HMBC spectrum of compound 2

Figure S18. NOESY spectrum of compound 2
Figure S19. HRESIMS of compound 3

Figure S20. IR spectrum of compound 3
Figure S21. $^1$H NMR spectrum of compound 3

Figure S22. $^{13}$C NMR spectrum of compound 3
Figure S23. DEPT spectrum of compound 3

Figure S24. HSQC spectrum of compound 3
Figure S25. COSY spectrum of compound 3

Figure S26. HMBC spectrum of compound 3
Figure S27. NOESY spectrum of compound 3
Figure S28. $^1$H NMR spectrum of compound 4 (conicasterol)

Figure S29. $^{13}$C NMR spectrum of compound 4 (conicasterol)