Supplementary Information

Secopaxilline A, an Indole-Diterpenoid Alkaloid from an Aciduric Penicillium fungus, its Identification and Semisynthesis

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Figure S1. ECD spectrum of secopaxilline A (1)

![ECD spectrum of secopaxilline A (1)](image)

Figure S2. HPLC traces for reaction mixtures of paxilline

paxilline
Pure paxilline

Paxilline treated with Oxone for 50 min

2 in acetone/H₂O (20:1) for 30 min

2 in acetone/H₂O/acetic acid (20:1:6) for 30 min
Figure S3. ESIMS spectrum of compound 2

Figure S4. HPLC traces for one-pot synthesis of deacetylsocopaxilline A (4) from paxilline

<table>
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<th>2 equiv</th>
<th>5 equiv</th>
<th>10 equiv</th>
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<tr>
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<td>1 h</td>
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</tr>
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<td>2 h</td>
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Figure S5. HRESIMS spectrum of secopaxilline A (I)

C_{29}H_{38}O_{7}N = 512.2643

-1.9978 ppm
Figure S6. $^1$H-NMR spectrum of secopaxilline A (1) in DMSO-$d_6$. 
Figure S7. $^{13}$C-NMR spectrum of secopaxilline A (1) in DMSO-$d_6$.
Figure S8. DEPT spectrum of secopaxilline A (1) in DMSO-$d_6$. 
Figure S9. HSQC spectrum of secopaxilline A (1) in DMSO-\(d_6\).
Figure S10. $^1$H-$^1$H COSY spectrum of secopaxilline A (1) in DMSO-$d_6$. 

![COSY Spectrum of Secopaxilline A](image)
Figure S11. HMBC spectrum of secopaxilline A (1) in DMSO-$d_6$. 
Figure S12. NOESY spectrum of secopaxilline A (1) in DMSO-$d_6$.
Figure S13. HRESIMS spectrum of deacetylsecopaxilline A (4)

20180521-FYQ-10-2-2_180521110353 #10  RT: 0.08  AV: 1  NL: 4.29E8
T: FTMS + ESI Full 2 MS [170.00-2000.00]

470.2525
C_{27}H_{36}O_{6}N = 470.2537
-2.5770 ppm

Relative Abundance

m/z

191.0921 337.1138 510.2832 554.3042 704.8762 781.4993 884.4573 939.4999
Figure S14. $^1$H-NMR spectrum of deacetylsocopaxilline A (4) in DMSO-$d_6$.  

![NMR spectrum of deacetylsocopaxilline A (4) in DMSO-$d_6$.]
Figure S15. $^{13}$C-NMR spectrum of deacetyllecopaxilline A (4) in DMSO-$d_6$. 

![C-NMR spectrum of deacetyllecopaxilline A (4) in DMSO-$d_6$.]
Figure S16. HSQC spectrum of deacetylsecopaxilline A (4) in DMSO-$d_6$. 
Figure S17. $^1$H–$^1$H COSY spectrum of deacetylsecopaxilline A (4) in DMSO-$d_6$. 
Figure S18. HMBC spectrum of deacetylsecopaxilline A (4) in DMSO-\(d_6\)
Figure S19. NOESY spectrum of deacetylsecopaxilline A (4) in DMSO-$d_6$. 
**Figure S20.** Comparison of the $^1$H-NMR of the isolated and synthetic secopaxilline A (1)

$^1$H-NMR spectrum of the isolated secopaxilline A (1)

$^1$H-NMR spectrum of the synthetic secopaxilline A (1)
Figure S21. UV spectrum of secopaxilline A (1) and deacetylsecopaxilline A (4)
Figure S22. IR spectrum of secopaxilline A (1)
Figure S23. IR spectrum of deacetyleneopaxilline A (4)