Supporting Information

Isolation and Photo-induced Conversion of 6-*epi*-Stephacidins from *Aspergillus taichungensis*

Shengxin Cai, Yepeng Luan, Xianglan Kong, Tianjiao Zhu, Qianqun Gu, and Dehai Li *

Key Laboratory of Marine Drugs, Chinese Ministry of Education, School of Medicine and
Pharmacy, Ocean University of China, Qingdao 266003, P. R. China

*To whom correspondence should be addressed. Tel: 0086-532-82032065. Fax:
0086-532-82033054. E-mail: dehaili@ouc.edu.cn

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Experimental details

General Experimental Procedures: Specific rotations were obtained on a JASCO P-1020 digital polarimeter. IR spectra were recorded on a NICOLET NEXUS 470 spectrophotometer in KBr discs. UV spectra were recorded on Beckman DU[®]640 spectrophotometer. CD spectra were measured on JASCO J-715 spectropolarimeter. ¹H, ¹³C NMR, DEPT and 2D NMR spectra were recorded on a JEOL JNM-ECP 600 spectrometer and a Bruker 400 spectrometer using TMS as internal standard and chemical shifts are recorded as δ values. ESI-MS was measured on a Micromass Q-TOF ULTIMA GLOBAL GAA076 LC Mass spectrometer a Thermo Scientific LTQ Orbitrap XL mass spectrometer. Semipreparative HPLC was performed using an ODS column [YMC-Pack ODS-A, 10×250 mm, 5 μ m, 4 mL/min].

Fungal Material: The fungal strain *A.taichungensis* ZHN-7-07 was isolated from the root soil of the mangrove plant *Acrostichum aureum*. The voucher specimen is deposited in our laboratory at -20°C. Working stocks were prepared on Potato Dextrose agar slants stored at 4°C.

Fermentation, Extraction and Purification: Fermentation was carried out as follows. *A.taichungensis* ZHN-7-07 was cultured under static conditions at room temperature in 1000-mL Erlenmeyer flasks containing rice media (rice 80 g, sea water 120 mL). After 30 days of cultivation, the fermentation of 20 flasks was extracted with methanol. The methanol extract was evaporated under reduced pressure to afford an aqueous solution, and then extracted with ethyl acetate. The ethyl acetate solution was concentrated under reduced pressure to give a crude extract (10.0 g). The crude extract (10.0 g) was applied on a C-18 ODS column using a step gradient elution of MeOH/H₂O and was separated into five subfractions (Fr.1-Fr.5). Fr. 3 was separated by Sephadex LH-20 column using CHCl₃/MeOH (50:50) and further purified by semi-preparative HPLC (70:30 MeOH/H₂O, 4 mL/min) to afford compounds **5** (20 mg, *t_R* 12.0 min), **6** (30 mg, *t_R* 13.5 min), and **7** (10 mg, *t_R* 20.5 min).

Photo-induced conversion of N-hydroxy-6-*epi*-stephacidin A (6**).** Compound **6** was unstable in DMSO with drops of methanol and in the condition of atmosphere and daylight, after fifteen days, several peaks with similar UV absorptions with **6** were obtained in the HPLC profile of the conversion product. Interestingly, the process of the conversion could be accelerated under radiation of UV lamp. In order to get enough compounds from the photo-induced conversion products as soon as possible, we dissolved all N-hydroxy-6-*epi*-stephacidin A (**6**) (28 mg) in 2 mL DMSO with drops of methanol and put it radiation of UV lamp for three days. Finally, compounds **7-15** were purified from the conversion mixture using semi-preparative HPLC (65:35 MeOH/H₂O, 4 mL/min, **7** (2.0 mg, yield: 7.1%), **8** (1.5 mg, yield: 5.3%), **9** (1.7 mg, yield: 6.1%), **10** (1.0 mg, yield: 3.6%), **11** (1.2 mg, yield: 4.3%), **12** (1.8 mg, yield: 6.4%), **13** (2.1 mg, yield: 7.5%), **14** (1.5 mg, yield: 5.3%), **15** (0.5 mg, yield: 1.8%)).

Detailed observation and analysis of *A. taichungensis* fermentation The fungal strain was cultured on rice medium, and the metabolites profiles was analyzed daily by HPLC and then HPLC-MS from the fourth day, N-hydroxy-6-*epi*-stephacidin A (**6**) appeared from the fourth day, and 6-*epi*-stephacidin A (**5**) and 6-*epi*-avrainvillamide (**7**) appeared from the ninth day. And after ten days, there was no obvious change in the HPLC profile. We tried to find compounds **8-15** that obtained from the chemical transformation and any other analogues through the HPLC and HPLC-MS data, but unfortunately, no peaks with related PDA profiles and MS data was detected.

Figure S1. Detailed observation and analysis of *A. taichungensis* fermentation

Physicochemical constants (5-15)

6-*epi*-Stephacidin A (5): colorless block crystal; $[\alpha]_D^{25} +27.0$ (c 0.26, $\text{CH}_2\text{Cl}_2\text{:MeOH}$ 1:1); IR (KBr) ν_{max} 3443, 3262, 2972, 2936, 1692, 1668, 1456, 1406, 1253, 1187, 1117, 1058, 729 cm^{-1} ; ^1H -NMR and ^{13}C -NMR (see **Table S1** and **S2**); HRESIMS $[M+\text{H}]^+$ m/z 432.2299 (calcd. for $\text{C}_{26}\text{H}_{28}\text{N}_3\text{O}_3$, 432.2287).

N-hydroxy-6-*epi*-stephacidin A (6): colorless block crystal; $[\alpha]_D^{25} +28.6$ (*c* 0.2, CH₂Cl₂:MeOH 1:1); IR (KBr) $\nu_{\max}$ 3439, 3192, 2972, 2923, 1680, 1668, 1438, 1409, 1360, 1205, 1117, 1021, 726 cm⁻¹; ¹H-NMR and ¹³C-NMR (see **Table S1** and **S2**); HRESIMS $[M-H]^-$ *m/z* 446.2085 (calcd. for C₂₆H₂₈N₃O₄, 446.2080).

6-*epi*-avrainvillamide (7): pale yellow amorphous solid; $[\alpha]_D^{25} +97.8$ (*c* 0.1, MeOH); IR (KBr) $\nu_{\max}$ 3416, 3241, 2988, 2925, 2875, 1692, 1406, 1265, 1191, 1112 cm⁻¹; ¹H-NMR and ¹³C-NMR (see **Table S1** and **S2**); HRESIMS $[M+H]^+$ *m/z* 446.2076 (calcd. for C₂₆H₂₈N₃O₄, 446.2080).

(+)-versicolamide B (8): colorless amorphous solid; $[\alpha]_D^{25} +5.8$ (*c* 0.1, MeOH); IR (KBr) $\nu_{\max}$ 3416, 3241, 2988, 2925, 2875, 1692, 1406, 1265, 1191, 1112 cm⁻¹; ¹H-NMR and ¹³C-NMR (see **Table S1** and **S2**); HRESIMS $[M+H]^+$ *m/z* 448.2235 (calcd. for C₂₆H₃₀N₃O₄, 448.2231).

(+)-versicolamide C (9): colorless amorphous solid; $[\alpha]_D^{25} +8.5$ (*c* 0.1, MeOH); IR (KBr) $\nu_{\max}$ 3365, 2980, 2933, 2863, 1692, 1374, 1209, 1127 cm⁻¹; ¹H-NMR and ¹³C-NMR (see **Table S1** and **S2**); HRESIMS $[M+H]^+$ *m/z* 464.2186 (calcd. for C₂₆H₃₀N₃O₅, 464.2185).

6-*epi*-notoamide R (10): colorless amorphous solid; $[\alpha]_D^{25} +30.0$ (*c* 0.1, MeOH); IR (KBr) $\nu_{\max}$ 3392, 3276, 2968, 2925, 2886, 1688, 1398, 1192, 1120 cm⁻¹; ¹H-NMR and ¹³C-NMR (see **Table S1** and **S2**); HRESIMS $[M+Na]^+$ *m/z* 470.2058 (calcd. for C₂₆H₂₉N₃O₄Na, 470.2050).

6-*epi*-notoamide F (11): colorless amorphous solid; $[\alpha]_D^{25} +30.1$ (*c* 0.1, MeOH); IR (KBr) $\nu_{\max}$ 3404, 2988, 2929, 2894, 1686, 1396, 1190, 1116 cm⁻¹; ¹H-NMR and ¹³C-NMR (see **Table S1** and **S2**); HRESIMS $[M+Na]^+$ *m/z* 484.2214 (calcd. for C₂₇H₃₁N₃O₄Na, 484.2207).

6-*epi*-notoamide G (12): colorless amorphous solid; ¹H-NMR and ¹³C-NMR (see **Table S1** and **S2**); HRESIMS $[M-H]^-$ *m/z* 476.2194 (calcd. for C₂₇H₃₀N₃O₅, 476.2180).

notoamide U (13): colorless amorphous solid; $[\alpha]_D^{25} +54.1$ (*c* 0.1, MeOH); IR (KBr) $\nu_{\max}$ 3373, 2968, 2921, 2879, 1689, 1400, 1183, 1111 cm⁻¹; ¹H-NMR and ¹³C-NMR (see **Table S1** and **S2**); HRESIMS $[M+H]^+$ *m/z* 464.2166 (calcd. for C₂₆H₃₀N₃O₅, 464.2180).

notoamide V (14): colorless amorphous solid; IR (KBr) $\nu_{\max}$ 3392, 2956, 2925, 2851, 1682, 1458, 1190, 1120 cm^{-1} ; ^1H -NMR and ^{13}C -NMR (see **Table S1** and **S2**); HRESIMS $[M-H]^-$ m/z 446.2084 (calcd. for $\text{C}_{26}\text{H}_{28}\text{N}_3\text{O}_4$, 446.2074).

notoamide W (15): colorless amorphous solid; ^1H -NMR and ^{13}C -NMR (see **Table S1** and **S2**).

X-ray analysis of 6-*epi*-stephacidin A (5): 6-*epi*-stephacidin A (5): colorless block crystal of $\text{C}_{27}\text{H}_{33}\text{N}_3\text{O}_4$, monoclinic, space group $\text{P}2_1$, $a = 10.8673$ (11), $b = 8.4827$ (7), $c = 13.5712$ (13) Å, $V = 1185.79$ (19) Å³, $Z = 2$, crystal size, $0.40 \times 0.30 \times 0.28$ mm³. Data were collected with a Bruker Smart-1000 CCD diffractometer and graphite monochromated Mo-K α radiation ($\lambda = 0.71073$ Å) at a temperature of 298 (2) K. The structure was solved by direct methods (SHELXS-97) and expanded using Fourier techniques (SHELXS-97). The final cycle of fullmatrix least squares refinement was based on 2231 unique reflections ($2\theta < 50.02^\circ$) and 312 variable parameters and converged with unweighted and weighted agreement factors of $R = 0.0760$, $wR = 0.1571$, and $R_1 = 0.0530$ for $I > 2\sigma(I)$ data. Crystallographic data (excluding structure factors) for structure 1 in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 886287. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax: +44 (0) 1223 336033 or e-mail: deposit@ccdc.cam.ac.uk].

X-ray analysis of N-hydroxy-6-*epi*-stephacidin A (6): N-hydroxy-6-*epi*-stephacidin A (6): colorless block crystal of $\text{C}_{27}\text{H}_{33}\text{N}_3\text{O}_5$, Orthorhombic, space group $\text{P}2_12_12_1$, $a = 9.1499$ (8), $b = 14.4705$ (13), $c = 18.7607$ (17) Å, $V = 2484.0$ (4) Å³, $Z = 4$, crystal size, $0.30 \times 0.28 \times 0.20$ mm³. Data were collected with a Bruker Smart-1000 CCD diffractometer and graphite monochromated Mo-K α radiation ($\lambda = 0.71073$ Å) at a temperature of 298 (2) K. The structure was solved by direct methods (SHELXS-97) and expanded using Fourier techniques (SHELXS-97). The final cycle of fullmatrix least squares refinement was based on 2497 unique reflections ($2\theta < 50.04^\circ$) and 321 variable parameters and converged with unweighted and weighted agreement factors of $R = 0.0614$, $wR = 0.0708$, and $R_1 = 0.0370$ for $I > 2\sigma(I)$ data. Crystallographic data (excluding structure factors) for structure 1 in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 886286. Copies of the data can be obtained,

free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax: +44 (0) 1223 336033 or e-mail: deposit@ccdc.cam.ac.uk].

Cell Proliferation/Viability Assays: In the MTT assay, the cell line (HL-60) was grown in RPMI-1640 supplemented with 10% FBS under a humidified atmosphere of 5% CO₂ and 95% air at 37°C. Cell suspensions (200 µL) at a density of 5×10⁴ cells/mL were plated in 96-well microtiter plates and incubated for 24 h. The test compound solutions (2 µL in MeOH) at different concentrations were added to each well and further incubated for 72 h under the same conditions. MTT solution (20 µL of a 5 mg/mL solution in RPMI-1640 medium) was added to each well and incubated for 4 h. Old medium (150 µL) containing MTT was then gently replaced by DMSO and pipetted to dissolve any formazan crystals formed. Absorbance was then determined on a SPECTRA MAX PLUS plate reader at 540 nm.

In the SRB assay, cell (A-549) suspensions (200 µL) were plated in 96-cell plates at a density of 2×10⁵ cells/mL. Then the test compound solutions (2 µL in MeOH) at different concentrations were added to each well and further incubated for 24h. Following drug exposure, the cells were fixed with 12% aqueous trichloroacetic acid and the cell layer was stained with 0.4% SRB. The absorbance of SRB solution was measured at 515 nm. Dose response curves were generated and the IC₅₀ values were calculated from the linear portion of log dose response curves

Table S1. ^1H NMR data for compounds **5-15** in $\text{DMSO-}d_6$

Position	5	6	7	8	9	10	11	12	13	14	15
1	3.42 m; 3.34 m	3.40 m; 3.33 m	3.35 m	3.30 m	3.30 m	3.44 m; 3.32 m	3.50 m; 3.34 m	3.50 m; 3.36 m	3.35 m; 3.28 m	3.42 m	3.44 m
2	2.00 m; 1.84 m	1.95 m; 1.85 m	1.99 m; 1.85 m	1.98 m; 1.80 m	1.96 m; 1.80 m	1.98 m; 1.85 m	2.02 m; 1.89 m	2.01 m; 1.89 m	1.98 m; 1.82 m	2.00 m; 1.81 m	2.00 m; 1.85 m
3	2.53 m; 1.81 m	2.53 m; 1.85 m	2.52 m; 1.84 m	2.46 m; 1.78 m	2.46 m; 1.78 m	2.52 m; 1.80 m	2.52 m; 1.83 m	2.52 m; 1.83 m	2.50 m; 1.81 m	2.51 m; 1.81 m	2.51 m; 1.81 m
5	2.14 m; 1.90 dd (12.6, 3.3)	2.15 m; 1.95 m	2.22 dd (13.3, 9.9); 1.85 m	1.93 m; 1.64 m	1.95 m; 1.65 m	2.15 m; 1.93 m	2.15 m; 1.89 m	2.15 m; 1.89 m	2.13 m; 1.86 m	2.56 dd (10.3, 2.8); 2.05 dd (13.6, 3.0)	2.15 m; 1.93 m
6	2.10 m	2.15 m	2.29 dd (10.1, 5.4)	3.09 dd (8.8, 8.6)	3.09 dd (8.8, 8.6)	2.15 m	2.15 m	2.17 m	2.14 m	2.10 dd (10.3, 13.7)	2.15 m
9-NH/OH	10.47 br s	10.82 br s		10.66 s	10.91 br s	10.59 s	10.58 s	11.01 br s		10.72 s	10.31 s
12	6.97 d (9.4)	7.24 d (9.9)	7.74 d (10.1)	6.58 d (10.1)	7.05 d (10.1)	6.96 d (9.9)	6.97 d (9.9)	7.23 d (9.9)	7.83 d (9.9)	6.99 d (9.4)	5.72 d (9.9)
13	5.73 d (9.9)	5.68 d (9.9)	5.95 d (10.2)	5.74 d (10.1)	5.74 d (10.1)	5.72 d (9.4)	5.73 d (9.4)	5.68 d (9.5)	5.90 d (10.4)	5.74 d (9.3)	4.87 d (9.9)
17	6.47 d (8.2)	6.49 d (8.3)	6.87 d (8.1)	6.38 d (8.0)	6.46 d (8.0)	6.48 d (8.8)	6.51 d (8.8)	6.53 d (8.3)	6.85 d (7.7)	6.50 d (8.3)	5.69 d (8.8)
18	7.14 d (8.3)	7.17 d (8.3)	7.79 d (8.1)	7.13 d (8.2)	7.20 d (8.2)	7.42 d (8.3)	7.23 d (8.3)	7.24 d (7.7)	7.32 d (8.3)	7.22 d (8.2)	6.92 d (8.8)
21	3.58 d (17.6); 2.72 d (17.6)	3.53 d (17.6); 2.74 d (17.6)	7.05 s	2.79 d (15.2); 2.08 d (15.4)	2.78 d (15.2); 2.12 d (15.4)	5.75 d (8.8)	5.61 d (8.8)	5.60 s	2.6 d (15.3); 2.0 dd (15.3, 2.2)	5.19 s	6.99 s
25-NH	8.56 br s	8.56 br s	8.83 s	8.77 s	8.80 br s	7.73 s	7.91 s	7.98 s	7.49 s	8.58 s	8.10 br s
27	1.29 s	1.39 s	1.54 s	0.97 s	0.96 s	1.26 s	1.26 s	1.35 s	1.54 s	1.32 s	1.24 s
28	1.19 s	1.27 s	1.22 s	0.69 s	0.67 s	1.23 s	1.21 s	1.27 s	1.34 s	1.20 s	1.21 s
29	1.37 s	1.37 s	1.41 s	1.37 s	1.37 s	1.36 s	1.36 s	1.38 s	1.39 s	1.38 s	1.38 s
30	1.36 s	1.38 s	1.40 s	1.36 s	1.35 s	1.36 s	1.38 s	1.38 s	1.39 s	1.37 s	1.37 s
21-OH/OMe						5.07 d (8.8)	3.47 s	3.48 s	6.30 d (2.2)	5.90 s	

Table S2. ^{13}C NMR data for compounds **5-14** in $\text{DMSO-}d_6$

Position	5	6	7	8	9	10	11	12	13	14
1	44.2 CH ₂	43.6 CH ₂	43.8 CH ₂	43.8 CH ₂	43.4 CH ₂	44.1 CH ₂	44.3 CH ₂ ^a	44.3 CH ₂	44.1 CH ₂	44.2 CH ₂
2	24.5 CH ₂	24.0 CH ₂	24.0 CH ₂	25.0 CH ₂	24.6 CH ₂	24.4 CH ₂	24.7 CH ₂	24.3 CH ₂	24.4 CH ₂	24.6 CH ₂
3	29.1 CH ₂	28.6 CH ₂	28.5 CH ₂	29.0 CH ₂	28.5 CH ₂	28.9 CH ₂	28.9 CH ₂	28.9 CH ₂	29.0 CH ₂	29.0 CH ₂
4	67.0 C	66.4 C	66.1 C	69.1 C	68.6 C	66.9 C	66.9 C	66.9 C	66.9 C	67.2 C
5	32.2 CH ₂	31.6 CH ₂	30.1 CH ₂	28.5 CH ₂	28.0 CH ₂	33.0 CH ₂	32.7 CH ₂	32.8 CH ₂	31.9 CH ₂	32.0 CH ₂
6	46.2 CH	46.2 CH	45.8 CH	50.5 CH	50.4 CH	46.5 CH	47.5 CH	47.7 CH	48.7 CH	41.1 CH
7	34.8 C	34.8 C	35.2 C	47.4 C	47.1 C	34.7 C	34.5 C	35.0 C	38.7 C	35.4 C
8	140.2 C	137.7 C	145.0 C	183.3 C	176.9 C	141.3 C	142.5 C	139.8 C	151.2 C	142.3 C
10	133.4 C	130.4 C	139.1 C	139.0 C	137.4 C	133.6 C	133.4 C	130.8 C	140.1 C	133.4 C
11	105.5 C	104.6 C	111.0 C	104.9 C	104.8 C	105.5 C	105.5 C	105.1 C	112.4 C	105.5 C
12	118.8 CH	118.4 CH	115.3 CH	117.3 CH	116.7 CH	118.7 CH	118.7 CH	118.8 CH	116.4 CH	118.7 CH
13	129.5 CH	128.3 CH	133.3 CH	130.7 CH	130.0 CH	129.5 CH	129.6 CH	128.9 CH	133.3 CH	129.6 CH
14	75.6 C	74.8 C	76.6 C	76.3 C	75.6 C	75.6 C	75.6 C	75.4 C	76.6 C	75.6 C
16	148.1 C	148.6 C	154.6 C	152.7 C	152.9 C	148.1 C	148.1 C	149.1 C	154.4 C	148.1 C
17	109.2 CH	109.3 CH	115.9 CH	108.7 CH	109.1 CH	109.5 CH	109.7 CH	110. CH	116.8 CH	109.6 CH
18	118.3 CH	118.1 CH	121.2 CH	126.9 CH	126.1 CH	120.3 CH	119.7 CH	120.2 CH	122.0 CH	118.8 CH
19	122.5 C	117.3 C	117.1 C	122.1 C	118.2 C	122.0 C	122.1 C	117.4 C	131.3 C	121.9 C
20	103.7 C	100.1 C	132.3 C	62.5 C	59.6 C	108.6 C	106.8 C	103.1 C	75.9 C	107.6 C
21	23.1 CH ₂	22.4 CH ₂	121.3 C	34.3 CH ₂	33.8 CH ₂	62.1 CH	70.7 CH	70.5 CH	36.1 CH ₂	63.3 CH
22	61.1 C	60.4 C	59.9 C	67.6 C	67.0 C	65.1 C	63.1 C	63.1 C	61.8 C	62.9 C
23	169.7 C	169.0 C	167.7 C	169.7 C	169.1 C	169.0 C	169.6 C	169.6 C	168.4 C	171.9 C
26	173.0 C	172.4 C	171.7 C	173.1 C	172.6 C	172.4 C	172.3 C	172.3 C	172.5 C	172.7 C
27	28.4 CH ₃	27.2 CH ₃	23.0 CH ₃	23.5 CH ₃	23.1 CH ₃	28.7 CH ₃	27.8 CH ₃	27.5 CH ₃	27.1 CH ₃	29.9 CH ₃
28	24.5 CH ₃	22.0 CH ₃	17.1 CH ₃	20.9 CH ₃	20.6 CH ₃	25.0 CH ₃	24.3 CH ₃	22.7 CH ₃	21.3 CH ₃	25.0 CH ₃
29	27.6 CH ₃	26.9 CH ₃	27.5 CH ₃	28.2 CH ₃	27.7 CH ₃	27.6 CH ₃	27.6 CH ₃	27.4 CH ₃	27.8 CH ₃	27.6 CH ₃
30	27.5 CH ₃	26.8 CH ₃	27.4 CH ₃	28.1 CH ₃	27.4 CH ₃	27.6 CH ₃	27.7 CH ₃	27.4 CH ₃	27.8 CH ₃	27.5 CH ₃
21- OMe							58.8 CH ₃	58.7 CH ₃		

^a: Signals was observed in HMQC spectrum.

Figure S2. ^1H NMR spectrum of 6-*epi*-stephacidin A (5)

Figure S3. ^{13}C NMR spectrum of 6-*epi*-stephacidin A (5)

Figure S4. HMQC spectrum of 6-*epi*-stephacidin A (5)

Figure S5. COSY spectrum of 6-*epi*-stephacidin A (5)

Figure S6. HMBC spectrum of 6-*epi*-stephacidin A (**5**)

Figure S7. NOESY spectrum of 6-*epi*-stephacidin A (**5**)

Figure S8. HRESIMS spectrum of 6-*epi*-stephacidin A (**5**)

Figure S9. ^1H NMR spectrum of N-hydroxy-6-*epi*-stephacidin A (**6**)

Figure S10. ^{13}C NMR spectrum of N-hydroxy-6-*epi*-stephacidin A (6)

CSX-07-D-z-2-L-13-3-13C

Figure S12. COSY spectrum of N-hydroxy-6-*epi*-stephacidin A (**6**)

CSX-07-D-z-2-L-13-3-COS

Figure S13. HMBC spectrum of N-hydroxy-6-*epi*-stephacidin A (**6**)

CSX-07-D-z-2-L-13-3-HMBC

Figure S14. NOESY spectrum of N-hydroxy-6-*epi*-stephacidin A (**6**)

CSX-07-D-z-2-L-13-3-NOESY

Figure S15. HRESIMS spectrum of N-hydroxy-6-*epi*-stephacidin A (**6**)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

CSX-23HRESI

20110315-CSX-23HRESI 34 (1.217) AM (Cen.8, 80.00, H1.5000.0.0.00, 1.00); Sm (Md, 3.00)

TOF MS ES-
4.2963

Minimum:

Maximum:

200.0 5.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Score

Formula

446.2085

446.2080

0.5

1.2

14.5

1

C26 H28 N3 O4

Figure S16. ^1H NMR spectrum of 6-*epi*-avrainvillamide (7)

Figure S17. ^{13}C NMR spectrum of 6-*epi*-avrainvillamide (7)

Figure S18. HMQC spectrum of 6-*epi*-avrainvillamide (**7**)

Figure S19. COSY spectrum of 6-*epi*-avrainvillamide (**7**)

Figure S20. HMBC spectrum of 6-*epi*-avrainvillamide (7)

Figure S21. NOESY spectrum of 6-*epi*-avrainvillamide (7)

CSX-07-23b-NOESY

Figure S22. HRESIMS spectrum of 6-*epi*-avrainvillamide (7)

Figure S23. 1H NMR spectrum of (+)-versicolamide B (8)

Figure S24. ^{13}C NMR spectrum of (+)-versicolamide B (**8**)

Figure S25. CD spectrum of (+)-versicolamide B (**8**)

Figure S26. HRESIMS spectrum of (+)-versicolamide B (**8**)

Figure S27. 1H NMR spectrum of (+)-versicolamide C (**9**)

Figure S28. ^{13}C NMR spectrum of (+)-versicolamide C (**9**)

Figure S29. HMQC spectrum of (+)-versicolamide C (**9**)

Figure S30. COSY spectrum of (+)-versicolamide C (**9**)

Figure S31. HMBC spectrum of (+)-versicolamide C (**9**)

Figure S32. NOESY spectrum of (+)-versicolamide C (**9**)

Figure S33. CD spectrum of (+)-versicolamide C (**9**)

Figure S34. HRESIMS spectrum of (+)-versicolamide C (**9**)

Figure S35. ¹H NMR spectrum of 6-*epi*-notoamide R (**10**)

Figure S36. ^{13}C NMR spectrum of 6-*epi*-notoamide R (10)

Figure S37. HMQC spectrum of 6-*epi*-notoamide R (10)

Figure S38. HMBC spectrum of 6-*epi*-notoamide R (10)

Figure S39. NOESY spectrum of 6-*epi*-notoamide R (10)

Figure S40. HRESIMS spectrum of 6-*epi*-notoamide R (10)

Figure S41. ¹H NMR spectrum of 6-*epi*-notoamide F (11)

Figure S42. ^{13}C NMR spectrum of 6-*epi*-notoamide F (11)

Figure S43. HMQC spectrum of 6-*epi*-notoamide F (11)

Figure S44. HMBC spectrum of 6-*epi*-notoamide F (11)

Figure S45. NOESY spectrum of 6-*epi*-notoamide F (11)

CSX-07-23e-NOESY

Figure S46. HRESIMS spectrum of 6-*epi*-notoamide F (**11**)

Figure S47. ¹H NMR spectrum of 6-*epi*-notoamide G (**12**)

Figure S48. ^{13}C NMR spectrum of 6-*epi*-notoamide G (12)

Figure S49. HMQC spectrum of 6-*epi*-notoamide G (12)

Figure S50. COSY spectrum of 6-*epi*-notoamide G (12)

Figure S51. HMBC spectrum of 6-*epi*-notoamide G (12)

Figure S52. NOESY spectrum of 6-*epi*-notoamide G (12)

CSX-07-23g-NOESY

Figure S53. HRESIMS spectrum of 6-*epi*-notoamide G (12)

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CSX-23E

20111018-CSX-23E 111018141514 #246-278 RT: 2.22-2.51 AV: 33 NL: 1.80E5
T: FTMS - p ESI Full ms [150.00-1000.00]

Figure S54. ^1H NMR spectrum of notoamide U (13)

Figure S55. ^{13}C NMR spectrum of notoamide U (13)

Figure S56. HMQC spectrum of notoamide U (13)

Figure S57. HMBC spectrum of notoamide U (13)

Figure S58. NOESY spectrum of notoamide U (**13**)

CSX-07-23f-NOESY

Figure S59. HRESIMS spectrum of notoamide U (**13**)

Figure S60. ^1H NMR spectrum of notoamide V (14)

Figure S61. ^{13}C NMR spectrum of notoamide V (14)

Figure S62. HRESIMS spectrum of notoamide V (14)

Figure S63. ¹H NMR spectrum of notoamide W (15)