Bisindole Alkaloids from a New Zealand Deep

Sea Marine Sponge Lamellomorpha strongylata

Kavita Ragini, Andrew M. Piggott and Peter Karuso*

Department of Chemistry and Biomolecular Sciences, Macquarie University, Sydney, NSW 2109, Australia.

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Characterization of Compounds

Coscinamide B (7):¹ orange amorphous powder (3.2 mg); UV (MeOH) λ_{max} 208, 268, 346 nm; IR (neat film) v_{max} 3437, 3195, 2987, 2939, 1647, 1594, 1541, 1489, 1236, 1130, 924, 738 cm⁻¹; ¹H NMR (DMSO-*d*₆, 600MHz) δ 12.30 (d, J = 2.4 Hz, NH), 11.20 (br s, J = 2.0 Hz, NH), 10.83 (d, J = 10.0 Hz, H-10), 8.83 (d, J = 3.3 Hz, H-2'), 8.28 (m, H-4'), 7.68 (d, J = 7.9 Hz, H-4), 7.55 (m, H-7'), 7.49 (d, J = 2.4 Hz, H-2), 7.42 (m, J = 10 Hz, H-9), 7.39 (m, J = 7.3 Hz, H-7), 7.28 (m, H-6'), 7.27 (m, H-5'), 7.14 (dt, J = 7.3 Hz, H-6), 7.10 (dt, J = 7.8 Hz, H-5), 6.84 ((d, J = 14.8 Hz, H-8). ¹³C-NMR (DMSO-*d*₆, 150MHz) δ 181.2 (C-8'), 160.4 (C-9'), 138.7 (C-2'), 136.9 (C-7a), 136.3 (C-7a'), 126.2 (C-3a'), 124.8 (C-3a), 124.4 (C-2), 123.6 (C-6'), 122.7 (C-5'), 121.6 (C-4'), 121.3 (C-6), 119.5 (C-5), 119.1 (C-4), 118.6 (C-9), 112.6 (C-7'), 112.3(C-3') 112.0 (C-3), 111.6 (C-7) 110.0 (C-8); Mass spectrum (ESI+) *m/z*: 330 [M + H]⁺ for C₂₀H₁₅N₃O₂.

(Z)-Coscinamide B (8):² yellow amorphous powder (8.5 mg); UV (MeOH) λ_{max} 208, 260, 265, 348 nm; IR (neat film) v_{max} 3265, 2976, 1675, 1622, 1438, 1417, 1203, 1132, 995, 801, 746 cm⁻¹; ¹H NMR (DMSO-*d*₆, 600MHz) δ 12.37 (br s, NH), 11.45 (br s, NH), 9.68 (d, *J* = 11.3 Hz, H-10), 8.92 (d, *J* = 3.3 Hz, H-2'), 8.23 (m, *J* = 6.5, 1.9 Hz H-4'), 7.64 (m, H-2), 7.63 (m, H-7), 7.55 ((m, H-7'), 7.44 (td, *J* = 8.1 Hz, H-4), 7.28 (m, H-6'), 7.27 (m, H-5'), 7.16 (m, H-5), 7.07 (m, H-6), 6.81 (dd, *J* = 9.2, 11.3 Hz, H-9), 6.23 (d, *J* = 9.2 Hz, H-8); ¹³C-NMR (DMSO-*d*₆, 150MHz) δ 179.8 (C-8'), 159.8 (C-9'), 139.2 (C-2'), 136.3 (C-7a'), 135.8 (C-7a), 126.4 (C-3a), 126.2 (C-3a'), 123.7 (C-2), 123.7 (C-6'), 122.8 (C-5'), 122.0 (C-5), 121.4 (C-4'), 119.4 (C-6'), 118.4 (C-7), 117.3 (C-9), 112.7 (C-7'), 111.9(C-3') 111.7 (C-4), 109.7 (C-3), 105.9 (C-8); Mass spectrum (ESI+) *m/z*: 330 [M + H]⁺ for C₂₀H₁₅N₃O₂.

Deoxytopsentin (9):³ yellow amorphous powder (282.7 mg); UV (MeOH) λ_{max} 208, 252, 274, 375 nm; IR (neat film) v_{max} 3363, 3263, 1682, 1627, 1522, 1415, 1239, 1104, 855, 738 cm⁻¹; ¹H NMR (MeOD, 600MHz) δ 9.01 (s, H-2'), 8.40 (m, H-4'), 7.94 (d, *J* = 7.5 Hz, H-4), 7.77 (s, H-2), 7.57 (s, H-4''), 7.52 (m, H-7'), 7.28 (m, H-6'), 7.26 (m, H-5'), 7.46 (d, *J* = 7.5 Hz, H-7), 7.21 (dt, *J* = 6.9, 1.2 Hz, H-6), 7.17 (dt, *J* = 6.9, 1.2 Hz, H-5); Mass spectrum (ESI+) *m/z*: 327 [M + H]⁺; HRESIMS *m/z* 327.1237 [M + H]⁺ (calcd. for C₂₀H₁₄N₄O, 327.1168)

Isobromodeoxytopsentin (**10**):⁴ yellow amorphous powder (6.2 mg); UV (MeOH) λ_{max} 213, 254, 280, 372 nm; ¹H NMR (DMSO-*d*₆, 600MHz) **10a** δ 13.25 (br s, H-1"), 12.17 (s, H-1'), 11.45 (br s, H-1), 9.38 (br s, H-2'), 8.33 (s, H-4'), 8.16 (d, *J* = 8.0 Hz, H-4), 8.11 (d, *J* = 2.4 Hz, H-2), 7.75 (d, *J* = 1.6 Hz, H-7'), 7.70 (br s, H-4"), 7.45 (d, 8.0 Hz, H-7), 7.39 (m, H-5'), 7.18 (m, H-6), 7.13 (m, H-5); **10b** δ 13.17 (br s, H-1"), 12.11 (s, H-1'), 11.23 (br s, H-1), 9.18 (br s, H-2'), 8.31 (s, H-4'), 7.91 (d, *J* = 8.0 Hz, H-4), 7.84 (d, *J* = 2.4 Hz, H-2), 7.74 (d, *J* = 1.6 Hz, H-7'), 7.38 (m, H-5'), 7.16 (d, *J* = 8.0 Hz, H-6), 7.13 (t, *J* = 7.2 Hz, H-5); Mass spectrum (ESI+) *m/z*: isotopic cluster 405:407 (in ratio 1:1) [M + H]⁺ for C₂₀H₁₃BrN₄O

Bromodeoxytopsentin (**11**):⁴ yellow amorphous powder (2.4 mg); UV (MeOH) λ_{max} 208, 250, 274, 370 nm; ¹H NMR (DMSO-*d*₆, 600MHz) δ 12.08 (s, H-1'), 11.47 (br s, H-1), 9.25 (br s, H-2'), 8.39 (m, H-4'), 8.02 (br, H-4), 7.98 (br, H-2), 7.69 (br, H-4''), 7.63 (m, H-7), 7.54 (m, H-7'), 7.23 (m, H-5), 7.23 (m, H-5'), 7.23 (m, H-6'); Mass spectrum (ESI+) *m/z*: isotopic cluster 405:407 (in ratio 1:1) [M + H]⁺ for C₂₀H₁₃BrN₄O

Dibromodeoxytopsentin (12):⁴ yellow amorphous powder (5.8 mg); UV (MeOH) λ_{max} 212, 254, 280, 370 nm; ¹H NMR (DMSO-*d*₆, 600MHz) δ 13.24 (br s, H-1"), 12.13 (s, H-1'), 11.46 (br s, H-1), 9.27 (br, H-2'), 8.42 (m, H-4'), 8.08 (br, H-4), 7.92 (br, H-2), 7.74 (d, *J* = 1.8 Hz, H-7'), 7.69 (br, H-4"), 7.63 (s, H-7), 7.39 (dd, 1.8, 8.5 Hz, H-5'), 7.23 (d, 7.7 Hz, H-5); Mass spectrum (ESI+) *m/z*: isotopic cluster 483:485:487 (in ratio 1:2:1) [M + H]⁺ for C₂₀H₁₂N₄OBr₂

6-bromoindole-3-carboxylic acid (13):⁵ light brown amorphous powder (1.9 mg); UV

(MeOH) λ_{max} 212, 250, 275, 330 nm; IR (neat film) v_{max} 3323, 3126, 2973, 1645, 1525, 1446, 1227, 1184, 1131, 1021, 805 cm⁻¹; ¹H NMR (DMSO-*d*₆, 600MHz) δ 12.08 (br s, OH), 11.91 (br s, NH), 8.01 (d, *J* = 2.9 Hz H-2), 7.92 (d, *J* = 8.5 Hz H-4), 7.64 (d, *J* = 1.7 Hz H-7), 7.28 (dd, *J* = 1.8, 8.5 Hz H-5); ¹³C-NMR (DMSO-*d*₆, 150MHz) δ 165.6 (C-8), 137.3 (C-3a), 133.2 (C-2), 125.0 (C-7a), 124.0 (C-5), 122.3 (C-4), 114.9 (C-7), 114.9 (C-3), 107.6 (C-6); Mass spectrum (ESI+) *m/z*: isotopic cluster 240:242 (in ratio 1:1) [M + H]⁺; HRESIMS *m/z* 237.95070 [M – H]⁻ (calcd. for C₉H₅BrNO₂, 237.95037).

(6-bromo-1*H*-indol-3-yl) oxoacetamide (**14**):⁶ yellow amorphous powder (1.9 mg); UV (MeOH) λ_{max} 210, 325 nm; IR (neat film) v_{max} 3384, 3184, 1662, 1616, 1591, 1513, 1404, 1135, 993, 925 cm⁻¹; ¹H NMR (DMSO-*d*₆, 600MHz) δ 12.25 (br s, NH), 8.69 (d, *J* = 3.17 Hz, H-2), 8.13 (d, *J* = 8.4 Hz, H-4), 8.09 (br s, H-10a), 7.74 (br s, H-10b), 7.72 (m, *J* = 1.8 Hz, H-7), 7.38 (dd, *J* = 1.8, 8.4 Hz, H-5); ¹³C-NMR (DMSO-*d*₆, 150MHz) δ 183.0 (C-8), 165.7 (C-9), 139.1 (C-2), 137.3 (C-7a), 125.4 (C-5), 125.2 (C-3a), 122.9 (C-4), 115.9 (C-6), 115.3 (C-7), 112.0 (C-3); Mass spectrum (ESI+) *m/z*: isotopic cluster 267:269 (in ratio 1:1) [M + H]⁺ for C₁₀H₇N₂O₂.

3,4-Seco-(*R*)-6"-debromohamacanthin A (**15**): yellow amorphous solid (43.2 mg); $[\alpha]^{20}{}_{D}$ –31 (*c* 0.50, MeOH); UV (MeOH) λ_{max} (log ε) 326 (3.92), 304 (3.82), 280 (4.15), 246 (3.96) nm; ECD (*c* 0.06 mM, MeOH) λ_{max} ($\Delta \varepsilon$) 362 (+0.4), 330 (–2.74), 287 (–1.05) 241 (–2.75) nm; IR (neat film) v_{max} 3232, 1672, 1627, 1488, 1439, 1201, 1180, 1130, 997, 744 cm⁻¹; Mass spectrum (ESI+) *m/z*: isotopic cluster 425:427 (in ratio 1:1) [M + H]⁺ for C₂₀H₁₈BrN₄O₂⁺.

(*R*)-6"-debromohamacanthin A (22): $[\alpha]^{23}_{D}$ –82 (*c* 0.05, MeOH) Lit.⁷ –76 (*c* 0.05, MeOH).

3,4-Seco-(*R*)-6',6"-didebromohamacanthin A (**16**): yellow amorphous solid (14.9 mg); $[\alpha]^{20}_{D}$ –26 (*c* 0.40, MeOH); UV (MeOH) λ_{max} (log ε) 328 (3.70), 298 (3.52), 269 (3.89), 243 (3.70) nm; ECD (*c* 0.07 mM, MeOH) λ_{max} ($\Delta \varepsilon$) 363 (+0.2), 331 (–1.57), 280 (–0.83), 239 (–2.85) nm; IR (neat film) v_{max} 3246, 2980, 1672, 1620, 1490, 1430, 1240, 1130, 997, 745 cm⁻¹; Mass spectrum (ESI+) *m/z*: 347 [M + H]⁺ for C₂₀H₁₉N₄O₂⁺.

(*R*)-6',6''-didebromohamacanthin A (**23**): $[\alpha]^{23}_{D}$ -34 (*c* 0.05, MeOH) Lit.⁸+59 (*c* 0.72, MeOH)

3,4-Seco-(*S*)-Hamacanthin A (17): yellow amorphous solid (2.9 mg); $[\alpha]^{20}{}_{\rm D}$ –10 (*c* 0.10, MeOH); UV (MeOH) $\lambda_{\rm max}$ (log ε) 322 (4.20), 300 (4.08), 277 (4.37), 259 (4.33) nm; ECD (*c* 0.05 mM, MeOH) $\lambda_{\rm max}$ ($\Delta \varepsilon$) 360 (–0.05), 331 (+0.28), 289 (+0.20) 260 (–0.03) nm; IR (neat film) $v_{\rm max}$ 3157, 2975, 2901, 1670, 1615, 1489, 1440, 1131, 896, 799 cm⁻¹; Mass spectrum (ESI+) *m/z*: isotopic cluster 503:505:507 (in ratio 1:2:1) [M + H]⁺ for C₂₀H₁₇Br₂N₄O₂⁺.

(*S*)-Hamacanthin A (**24**) $[\alpha]^{23}_{D}$ +64 (*c* 0.05, MeOH) Lit.⁸⁻⁹ +83.7 (*c* 0.47, MeOH), +58 (*c* 0.05, MeOH)

3,4-Seco-(*S*)-Hamacanthin B (18): light brown amorphous solid (2.0 mg); $[\alpha]^{20}_{D}$ +7 (*c* 0.50, MeOH); UV (MeOH) λ_{max} (log ε) 330 (3.38), 311 (3.38), 280 (3.73), 245 (3.81) nm; ECD (*c* 0.05 mM, MeOH) λ_{max} ($\Delta \varepsilon$) 370 (-0.01), 339 (+0.26), 284 (+0.24) 230 (+0.71) nm; IR (neat film) v_{max} 3232, 1672, 1627, 1488, 1439, 1201, 1180, 1130, 997, 744 cm⁻¹; Mass spectrum (ESI+) *m/z*: isotopic cluster 503:505:507 (in ratio 1:2:1) [M + H]⁺ C₂₀H₁₇Br₂N₄O₂⁺.

(*S*)-Hamacanthin B (**25**): $[\alpha]^{23}_{D}$ +46 (*c* 0.05, MeOH) Lit.^{8, 10} +56 (*c* 0.2, MeOH), +172 (*c* 0.1, MeOH)

3,4-Seco-(*S*)-6"-debromohamacanthin B (**19**): orange amorphous solid (5.2 mg); $[\alpha]^{20}{}_{D}$ -27 (*c* 0.25, MeOH); UV (MeOH) λ_{max} (log ε) 326 (3.46), 306 (3.43), 268 (3.67), 242 (3.69) nm; ECD (*c* 0.12 mM, MeOH) λ_{max} ($\Delta \varepsilon$) 337 (+0.61), 278 (+0.55) 230 (+1.32) nm; IR (neat film) v_{max} 3141, 1670, 1616, 1498, 1418, 1199, 1128, 797, 743 cm⁻¹; Mass spectrum (ESI+) m/z: isotopic cluster 425:427 (in ratio 1:1) [M + H]⁺ for C₂₀H₁₈BrN₄O₂⁺.

(S)-6"-debromohamacanthin B (26): $[\alpha]^{23}_{D}$ +36 (c 0.05, MeOH) Lit.⁷ +43 (c 0.3, MeOH)

3,4-Seco-(*R*)-6'-debromohamacanthin B (**20**): yellow amorphous solid (43.2 mg); $[\alpha]^{20}_{D}$ +19 (*c* 0.95, MeOH); UV (MeOH) λ_{max} (log ε) 329 (3.49), 305 (3.46), 280 (3.75), 245 (3.73) nm; ECD (*c* 0.06 mM, MeOH) λ_{max} ($\Delta \varepsilon$) 365 (+0.05), 332 (-0.55), 287 (-0.57) 234 (-1.90) nm; IR (neat film) v_{max} 3216, 2935, 1671, 1617, 1492, 1429, 1201, 1180, 1131, 997, 800, 750 cm⁻¹; Mass spectrum (ESI+) *m/z*: isotopic cluster 425:427 (in ratio 1:1) [M + H]⁺ for C₂₀H₁₈BrN₄O₂⁺.

6'-debromohamacanthin B (27): $[\alpha]^{23}_{D}$ +38 (c 0.05, MeOH) Lit.⁸ –194 (c 0.25, MeOH);

3,4-Seco-(*R*)-6',6"-didebromohamacanthin B (**21**): yellow amorphous solid (14.9 mg); $[\alpha]^{20}_{D}$ –16 (*c* 0.50, MeOH); UV (MeOH) λ_{max} (log ε) 329 (3.59), 300 (3.50), 267 (3.81), 242 (3.73) nm; ECD (*c* 0.07 mM, MeOH) λ_{max} ($\Delta \varepsilon$) 370 (+0.05), 332 (-0.65), 277 (-0.59) 230 (-1.51) nm; IR (neat film) v_{max} 3243, 2976, 1670, 1617, 1490, 1429, 1200, 1128, 1000, 744 cm⁻¹; Mass spectrum (ESI+) *m/z*: 347 [M + H]⁺ for C₂₀H₁₉N₄O₂⁺.

(*R*)-6',6''-didebromohamacanthin B (**28**): $[\alpha]^{20}_{D}$ -36 (*c* 0.04, MeOH) Lit.⁸ –288 (*c* 0.4, MeOH)



Table S1. NMR data (600 MHz) for (Z)-coscinamide D (1) in DMSO-d₆

Position	δ _C , type	$\delta_{\rm H} (J \text{ in Hz})$	COSY	HMBC	ROESY
1-NH		11.45, s	2	2,3,3a,7a	2,7,9
2	123.8, CH	7.64, m	1	3,3a,7a,8	1,8,9
3	109.6, C				
3a	126.4, C				
4	111.7, CH	7.43, d (8.1)	5	3a,6	5,8
5	122.0, CH	7.16, td (7.4, 1.0)	4,6	7,7a	4
6	119.4, CH	7.07, td (7.4, 1.0)	5,7	3a,4,7a	7
7	118.4, CH	7.63, m	6	5,7a	1,6
7a	135.8, C				
8	106.1, CH	6.24, d (9.2)	9	2,3a,9	2,4,9
9	117.2, CH	6.80, dd (11.0, 9.2)	8,10	3,8,9′	1,8,10
10-NH		9.66, d (11.0)	9	8,9′	2,9
1'-NH		12.43, br	2'	2',3',3a'	7',2'
2'	139.9, CH	8.92, d (3.3)	1'	3′,3a′,7a′	1'
3'	111.8, C				
3a′	125.3, C				
4′	123.0, CH	8.16, d (8.4)	5'	3',6',7a'	5'
5'	125.6, CH	7.41, dd (8.4, 1.8)	4'	3a',7'	4'
6'	116.1, C				
7'	115.4, CH	7.76, d (1.8)		3a',6',7a'	1'
7a′	137.2, C				
8'	180.0, C				
9′	159.7, C				



Table S2. NMR data (600 MHz) for (E)-coscinamide D (2) in DMSO- d_6

Position	δ _C , type	$\delta_{\rm H} (J \text{ in Hz})$	COSY	HMBC	ROESY
1-NH		11.21, s	2	3,3a,7a	2,7
2	124.4, CH	7.49, d (2.4)	1	3,3a,7a	1,8
3	111.6, C				
3a	124.8, C				
4	119.0, CH	7.68, d (7.8)	5	3,3a,6,7a	5,9
5	119.5, CH	7.09, t (7.4)	4,6	3a,7	4
6	121.6, CH	7.14, t (7.4)	5,7	4,7a	7
7	111.9, CH	7.39, m	6	3a,5	1,6
7a	136.9, C				
8	110.2, CH	6.85, d (14.7)	9	2,3a,9	2,10
9	118.5, CH	7.40, m	8,10	3,8	4,10
10-NH		10.85, d (9.9)	9	8, 9'	8,9
1'-NH		12.36, br	2'	3′,3a′	7',2'
2'	139.4, CH	8.85, d (3.2)	1′	3',3a',7a'	1'
3'	112.2, C				
3a′	125.3, C				
4'	122.9, CH	8.19, d (8.5)	5'	6′,7a′	5'
5'	125.5, CH	7.43, m	4′	3a',7'	4'
6'	116.0, C				
7′	115.4, CH	7.75, d (1.8)		3a',6'	1'
7a′	137.3, C				
8'	181.3, C				
9′	160.0, C				



Table S3. NMR data (600 MHz) for Lamellomorphamide A (3) in DMSO-d₆

Position	$\delta_{\rm C}$, type	$\delta_{\rm H} (J \text{ in Hz})$	COSY	HMBC	ROESY
1-NH		12.07, br	2	3,3a	2,7
2	133.8, CH	8.50, d (3.2)	1	3,3a,7a	1,9
3	113.9, C				
3a	125.4, C				
4	121.1, CH	8.16, m	5	6,7a	5,9
5	121.9, CH	7.20, td (7.1, 1.1)	4	3a,7	4
6	122.6, CH	7.23, td (7.1, 1.1)	7	4,7a	7
7	112.6, CH	7.49, m	6	3a,5	1,6
7a	136.3, C				
8	189.2 C				
9	45.7, CH ₂	4.63, d (5.9)	10	8,9′	2,10
10-NH		8.91, t (5.9)	9	8,9′	9
1'-NH		12.26, br	2'	3',3a',7a'	2',7'
2'	138.7, CH	8.82, d (3.2)	1'	3',3a',7a'	1'
3'	112.3, C				
3a′	126.2, C				
4'	121.3, CH	8.26, m	5'	6′,7a′	5',6'
5'	122.9, CH	7.27, m	4'	3a',7'	4′, ⁴ 7′
6'	123.5, CH	7.28, m	7'	4'	4'
7'	112.2, CH	7.54, m	6'	3a',5'	1′,5′
7a′	136.4, C				
8'	181.9, C				
9′	163.8, C				



Table S4. NMR data (600 MHz) for Lamellomorphamide B (4) in DMSO- d_6

Position	δ _C , type	$\delta_{\rm H} (J \text{ in Hz})$	COSY	HMBC	ROESY
1-NH		12.17, br	2	2,3,3a,7a	2,7
2	134.7, CH	8.53, d (3.0)	1	3,3a,7a	1,9
3	113.9, C				
3a	124.5, C				
4	122.7, CH	8.09, d (8.5)	5	6,7a	5,9
5	124.9, CH	7.35, dd (8.5,1.8)	4	3a,7	4
6	115.0, C				
7	115.6, CH	7.69, d (1.8)		3a,5,6,7a	1
7a	137.4, C				
8	189.4, C				
9	45.7, CH ₂	4.62, d (6.0)	10	8,9′	2,4,10
10-NH		8.93, t (5.3)	9	9,9′	9
1'-NH		12.25, br	2'	2',3',3a',7a'	2',7'
2'	138.6, CH	8.80, d (3.3)	1'	3',3a',7a'	1'
3'	112.3, C				
3a'	126.2, C				
4'	121.3, CH	8.25, m	5'	6′,7a′	5′,6′
5'	122.9, CH	7.27, m	4'	3a',7'	4′,7′
6'	123.6, CH	7.28, m	7'	4',5',7a'	4'
7'	112.7, CH	7.53, m	6'	3a',5'	1′,5′
7a′	136.3, C				
8'	181.8, C				
9'	163.8, C				

^a Obscured by H₂O signal



Table S5. NMR data (600 MHz) for Lamellomorphamide C (5) in DMSO-d₆

Position	$\delta_{\rm C}$, type	$\delta_{\rm H} (J \text{ in Hz})$	COSY	HMBC	ROESY
1-NH		12.06, br	2	2,3,3a,7a	2,7
2	133.8, CH	8.50, d (3.2)	1	3,3a,7a	1,9
3	113.9, C				
3a	125.2, C				
4	121.1, CH	8.16, m (7.6)	5	6,7a	5,9
5	121.9, CH	7.20, td (7.1, 1.1)	4,6	3a,7	4
6	122.9, CH	7.23, td (7.1, 1.1)	5,7	4,7a	7
7	112.2, CH	7.49, m	6	3a,5	1,6
7a	136.4, C				
8	189.1, C				
9	45.7, CH ₂	4.63, d (5.8)	10	8,9′	2,4,10
10-NH		8.94, t (5.8)	9	8,9,9′	9
1'-NH		12.32, br	2'	2',3',3a'	2',7'
2'	139.4, CH	8.83, d (3.2)	1′	3',3a',7a'	1'
3'	112.2, C				
3a'	125.3, C				
4'	123.0, CH	8.18, d (8.4)	5'	3',3a',6',7a'	5'
5'	125.5, CH	7.42, dd (8.4, 1.8)	4′	3a',7'	4'
6'	116.0, C				
7′	115.3, CH	7.75, dd (1.8)		3a',6',7a'	1'
7a′	137.2, C				
8'	181.9, C				
9′	163.4, C				



Table S6. NMR data (600 MHz) for Lamellomorphamide D (6) in DMSO-d₆

Position	δ _C , type	$\delta_{\rm H} (J \text{ in Hz})$	COSY	HMBC	ROESY
1-NH		12.17, br	2	3,3a	2,7
2	134.6, CH	8.53, d (3.1)	1	3,3a,7a	1,9
3	113.9, C				
3a	124.4, C				
4	122.8, CH	8.09, d (8.5)	5	6,7a	5,9
5	124.9, CH	7.35, dd (8.5,1.8)	4	3a,7	4
6	115.5, C				
7	114.9, CH	7.69, d (1.8)		3a,6,7a	1
7a	137.2, C				
8	189.1, C				
9	45.7, CH ₂	4.62, d (5.9)	10	8,9′	2,4,10
10-NH		8.96, t (5.9)	9	8,9,9′	9
1'-NH		12.32, br	2'	3′,3a′	2',7'
2'	139.4, CH	8.81, d (3.2)	1'	3',3a',7a'	1'
3'	112.2, C				
3a′	125.2, C				
4'	123.0, CH	8.18, d (8.4)	5'	6′,7a′	5'
5'	125.5, CH	7.42, dd (8.4,1.8)	4'	3a',7'	4′
6'	116.0, C				
7'	115.4, CH	7.75, d (1.8)		3a',6',7a'	1'
7a′	137.3, C				
8′	181.9, C				
9'	163.5, C				



Table S7. NMR data (600 MHz) for 15-17 in DMSO-d₆

		15		16		17
Position	δc, Type	δ_{H} , (J in Hz)	δc, Type	$\delta_{\rm H}$, (J in Hz)	δc, Type	$\delta_{\rm H}$, (J in Hz)
1		9.13, d (9.2)		9.11, d (9.3)		9.18, d (9.2)
2	162.8, C		163.1, C		162.9, C	
3	181.1, C		181.2, C		181.3, C	
4		8.05, br, s		7.97, br		7.94, br
5	42.12, CH ₂	3.51, 3.37 ^a	42.2, CH ₂	3.49, 3.36 ^a	42.1, CH ₂	3.48, 3.35 ^a
6	43.8, CH	5.59, td (9.2, 4.2)	43.8, CH	5.58, m	43.6, CH	5.54, m
1'		12.44, d (2.8)		12.27, br		12.32, s, d
2'	139.4, CH	8.84, d (3.1)	138.7, C	8.82, d (3.2)	139.4, CH	8.82, d (3.2)
3'	112.1, C		111.8, C		112.1, C	
3a′	125.6, C		126.4, C		125.4, C	
4′	122.9, CH	8.14, d (8.4)	121.3, CH	8.22, m	122.9, CH	8.13, d (8.4)
5'	125.5, CH	7.39 (m)	123.5, CH	7.26, m	125.6, CH	7.39, dd (1.6, 8.4)
6'	116.0, C		122.7, C	7.24, m	116.1, C	
7'	115.4, CH	7.75, d (1.6)	112.7, CH	7.54, m	115.4, CH	7.75, d (1.6)
7a′	137.2, C		136.2, C		137.2, C	
1″		11.17, d (2.0)		11.15, br		11.28, s
2''	123.3, CH	7.40, m	123.4, CH	7.40, m	124.6, CH	7.42, d (2.6)
3″	112.1, C		112.2, C		112.6, C	
3a″	125.4, C	7.39	125.6, C		124.7, C	
4''	111.8, CH	7.10, t (7.4)	111.8, CH	7.39, m	120.3, CH	7.62, d (8.5)
5″	121.5, CH	7.02, t (7.4)	121.5, CH	7.10, m	121.9, CH	7.18, dd (1.7, 8.5)
6''	119.0, CH	7.67, d (8.0)	119.0, CH	7.02, m	114.3, C	
7''	118.4, CH		118.5, CH	7.67, d (8.0)	114.4, CH	7.58, d (1.6)
7a″	136.1, C		136.2, C		137.1, C	

^a Obscured by H₂O signal



18 $R^1 = R^2 = Br$ **20** $R^1 = H, R^2 = Br$

Table S8.	NMR data	(600 MHz)	for 18 and	20 in DMS	$O-d_6$

		18		20
Position	δ _C , Type	$\delta_{\rm H}$, (J in Hz)	δ _c , Type	$\delta_{\rm H}$, (J in Hz)
1		8.98, t (5.8)		8.95, t (5.9)
2	163.2, C		163.6, C	
3	181.0, C		180.8, C	
4		8.30, br, s		8.34, br, d (3.8)
5	46.9, CH	4.81, br, s	46.8, CH	4.83, m
6	42.1, CH ₂	3.81, m; 3.67, m	42.1, CH ₂	3.82, m; 3.69, m
1'		12.31, d (2.9)		12.27, br, d (2.3)
2'	139.4, CH	8.78, d (2.9)	138.6, CH	8.76, d (3.3)
3'	112.0, C		112.0, C	
3a′	125.3, C		126.2, C	
4′	122.9, CH	8.13, d (8.4)	121.2, CH	8.21, m
5'	125.3, CH	7.40, dd (8.4, 1.8)	122.6, CH	7.25, m
6'	116.0, C		123.5, CH	7.26, m
7'	115.4, CH	7.75, d (1.8)	112.6, CH	7.54, m
7a′	137.1, C		136.7, C	
1″				11.46, s
2''	125.2, CH	11.44, d (2.6)	125.2, CH	7.57, d (2.4)
3″	109.6, C	7.56, d (2.6)	109.5, C	
3a''	124.7, C		124.7, C	
4''	120.3, CH	7.69, d (8.5)	120.3, CH	7.70, d (8.4)
5″	122.1, CH	7.22, dd (8.5, 1.7)	122.1, CH	7.22, dd (8.4, 1.7)
6''	114.4, C		114.5, C	. ,
7''	114.6, CH	7.62, d (1.7)	114.4, CH	7.63, d (1.7)
7a″	136.8, C		136.8, C	



19 $R^1 = Br, R^2 = H$ **21** $R^1 = R^2 = H$

Table S9. NMR data (600 MHz) for 19	and 21 in DMSO- d_6
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		19		21
Position	δ _C , Type	$\delta_{\rm H}$, (<i>J</i> in Hz)	δ _C , Type	$\delta_{\rm H}$, (J in Hz)
1		8.99, t (6.0)		8.97, t (6.0)
2	163.3, C		163.7, C	
3	180.9, C		180.9, C	
4		8.30, br, s		8.30, br, s
5	47.0, CH	4.83, m	47.1, CH	4.83, m
6	42.2, CH ₂	3.84, m; 3.70, m	42.2, CH ₂	3.84, m; 3.71, m
1'		12.34, s		12.26, br
2'	139.4, CH	8.79, d (3.4)	138.7, CH	8.78, d (3.2)
3'	111.9, C		112.1, C	
3a'	125.5, C		126.3, C	
4′	122.9, CH	8.14, d (8.4)	121.3, CH	8.22, m
5'	125.5, CH	7.40, dd (1.8, 8.4)	122.7, CH	7.25, m
6'	116.0, C		123.6, CH	7.26, m
7'	115.3, CH	7.75, d (1.8)	112.7, CH	7.54, m
7a′	137.1, C		136.1, C	
1″		11.32, s		11.32, br
2''	124.0, CH	7.54, d (2.6)	125.6, CH	7.54, m
3″	109.1, C		109.2, C	
3a″	125.4, C		124.1, C	
4''	118.4, CH	7.72, d (8.0)	118.4, CH	7.73, d (8.0)
5″	119.2, CH	7.08, td (1.0, 7.5)	119.2, CH	7.08, t (7.5)
6''	121.8, C	7.15, td (1.0, 7.5)	121.9, C	7.15, t (7.5)
7''	111.8, CH	7.42, td (8.0)	111.9, CH	7.42, d (8.0)
7a''	135.9, C	· 、 、 /	136.0, C	· 、 /

	S. aureus (MRSA, ATTC 43300)		
Compound	Percentage inhibition (%)	Percentage inhibition (%)	
	10 µM (stdev)	20 µM (stdev)	
1	-8.3 (7.8)	14.3 (10.1)	
2	6.8 (4.1)	18.2 (6.1)	
3	11.0 (3.6)	16.6 (10.0)	
4	-2.8 (8.1)	14.0 (12.8)	
5	5.5 (2.1)	5.8 (8.1)	
6	9.3 (3.2)	14.9 (10.6)	
7	-0.1 (9.3)	9.2 (1.5)	
8	7.3 (3.9)	3.8 (7.6)	
9	8.6 (4.3)	3.3 (11.4)	
13	3.1 (3.2)	18.6 (13.2)	
14	8.4 (1.8)	4.7 (7.4)	
15	4.1 (1.7)	7.1 (6.2)	
16	7.3 (0.4)	3.8 (7.6)	
17	8.7 (2.9)	4.2 (6.7)	
18	10.7 (3.6)	18.9 (7.1)	
19	-10.0 (8.4)	4.1 (13.9)	
20	15.3 (7.9)	-4.5 (16.7)	
21	-5.4 (4.6)	18.9 (11.7)	

 Table S10. Bioassay results of compounds 1-9, 13-21

Antibacterial assay

Percentage growth inhibition of an individual sample was calculated based on negative controls (media only) and positive controls (bacterial media without inhibitors). Negative inhibition value meant that the growth rate (or OD_{600}) was higher compared to the negative control (Bacteria only, set to 0% inhibition).



Figure S1. HPLC chromatogram of compound 15

Run on an Agilent 6130B single quadrupole LCMS system using a C_{18} column with a gradient of 5-95% acetonitrile/water (0.025 % formic acid) at flowrate 0.25 mL/min with either A) UV detection at 254nm or B) TIC, positive ion mode.



Figure S2. UV-Vis and Mass spectra of peaks eluting in Figure S1. A) UV-Vis spectrum of the peak at 1.2 min. B) UV-Vis spectrum of the peak at 2.7 min. C) Mass spectrum of the peak eluting at 1.3 min. D) Mass spectrum of the peak 2.7 min.



Figure S3. HPLC chromatogram of *n*-butanol fraction with UV detection at 254 nm. Run on an Agilent 6130B single quadrupole LCMS system using a C18 column with a gradient of 5-95% acetonitrile/water (0.025 % formic acid) at flowrate 0.25 mL/min.



Figure S4. TIC and EIC of positive ion scan of *n*-butanol fraction (a) TIC of positive ion scan, under the same conditions as Figure S76. (b) EIC of open ring form (m/z 347) 3,4-seco-6',6"-didebromohamacanthin MA (16), and 3,4-seco-6',6"didebromohamacanthin B (21) (c) EIC of closed ring form (m/z 329) 6',6"didebromohamacanthin A (23) and 6',6"-didebromohamacanthin B (28) (d) EIC of open ring form (m/z 425) 3,4-seco-6"-debromohamacanthin A (15), 3,4-seco-6"-debromohamacanthin B (19), 3,4-seco-6'-debromohamacanthin B (20) (e) EIC of closed ring form (m/z 407) 6"debromohamacanthin A (22), 6"-debromohamacanthin B (26), 6'-debromohamacanthin B (27) (f) EIC of open ring form (m/z 503) 3,4-seco-hamacanthin A (17) and 3,4-seco-hamacanthin B (18) (g) EIC of closed ring form (m/z 485) Hamacanthins A (24) and B (25)



Figure S5. ECD and UV spectra of 15 (*c* 0.06 mM, MeOH) Cell path 10 mm (UV - orange trace, ECD - blue trace)







Figure S7. ECD and UV spectra of 17 (*c* 0.05 mM, MeOH) Cell path 10 mm (UV - orange trace, ECD - blue trace)



Figure S8. ECD and UV spectra of 18 (c 0.05 mM, MeOH) Cell path 10 mm (UV - orange trace, ECD - blue trace)



Figure S9. ECD and UV spectra of 19 (c 0.12 mM, MeOH) Cell path 10 mm (UV - orange trace, ECD - blue trace)



Figure S10. ECD and UV spectra of 20 (*c* 0.06 mM, MeOH) Cell path 10 mm (UV - orange trace, ECD - blue trace)



220 270 320 370 420 wavelength/nm

Figure S12. UV spectrum of 16 (*c* 0.07 mM, MeOH) compared to the calculated spectrum.







Figure S16. ¹H-¹³C HMBC spectrum (600 MHz) of (Z)-coscinamide D (1) in DMSO-d₆



Figure S18. ¹H-¹H ROESY spectrum (600 MHz) of (Z)-coscinamide D (1) in DMSO-d₆







Figure S21. ¹H-¹³C HSQC spectrum (600 MHz) of coscinamide D (2) in DMSO- d_6



Figure S22. ¹H-¹³C HMBC spectrum (600 MHz) of coscinamide D (2) in DMSO-*d*₆



Figure S24. ¹H-¹H ROESY spectrum (600 MHz) of coscinamide D (2) in DMSO-*d*





Figure S26. ¹³C NMR spectrum (150 MHz) of lamellomorphamide A (3) in DMSO-d₆



Figure S27. ¹H-¹³C HSQC spectrum (600 MHz) of lamellomorphamide A (3) in DMSO-*d*₆



Figure S28. ¹H-¹³C HMBC spectrum (600 MHz) of lamellomorphamide A (3) in DMSO-*d*₆



Figure S30. ¹H-¹H ROESY spectrum (600 MHz) of lamellomorphamide A (3) in DMSO-



Figure S31. ¹H NMR spectrum (600 MHz) of lamellomorphamide B (4) in DMSO-*d*₆




Figure S34. ¹H-¹³C HMBC spectrum (600 MHz) of lamellomorphamide B (4) in DMSO-d₆



Figure S36. ¹H-¹H ROESY spectrum (600 MHz) of lamellomorphamide B (4) in DMSO-*d*₆





Figure S38. ¹³C NMR spectrum (150 MHz) of lamellomorphamide C (5) in DMSO-*d*₆



Figure S40. ¹H-¹³C HMBC spectrum (600 MHz) of lamellomorphamide C (5) in DMSO-*d*₆



Figure S42. ¹H- ¹H ROESY spectrum (600 MHz) of lamellomorphamide C (5) in DMSO-*d*



Figure S43. ¹H NMR spectrum (600 MHz) of lamellomorphamide D (6) in DMSO-*d*₆



Figure S44. ¹³C NMR spectrum (150 MHz) of lamellomorphamide D (6) in DMSO-d₆



Figure S46. ¹H-¹³C HMBC spectrum (600 MHz) of lamellomorphamide D (6) in DMSO-*d*₆



Figure S48. ¹H-¹H ROESY spectrum (600 MHz) of lamellomorphamide D (6) in DMSO-d₆







Figure S51. ¹H NMR spectrum (600 MHz) of (Z)-coscinamide B (8) in DMSO-d₆









Figure S55. ¹H NMR spectrum (600 MHz) of isobromodeoxytopsentin (10) in DMSO-d₆



Figure S56. ¹H NMR spectrum (600 MHz) of bromodeoxytopsentin (11) in DMSO-*d*₆





Figure S58. ¹H NMR spectrum (600 MHz) of 6-bromoindole-3-carboxylic acid (13) in DMSO-*d*₆





Figure S60. ¹H NMR spectrum (600 MHz) of (6-bromo-1*H*-indol-3-yl) oxoacetamide (14) in DMSO-*d*₆





Figure S62. ¹H NMR spectrum (600 MHz) of 3,4-seco-6"-debromohamacanthin A (15) in DMSO-d₆













Figure S68. ¹H NMR spectrum (600 MHz) of 3,4-seco-hamacanthin B (18) in DMSO-*d*₆







Figure S71. ¹³C NMR spectrum (150 MHz) of 3,4-seco-6"-debromohamacanthin B (19) in DMSO-d₆







Figure S74. ¹H NMR spectrum (600 MHz) of 3,4-seco-6',6"-didebromohamacanthin B (21) in DMSO-d₆


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