Naphthomycins-Derived Macrolactams with Two New Carbon Skeletons from an Endophytic *Streptomyces*

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Compounds			$IC_{50} \pm SD \ (\mu M)$		
Compounds	HL-60	A549	SMMC-7721	MCF-7	SW480
1	19.82 ± 1.65	16.98 ± 2.40	20.35 ± 1.38	16.49 ± 0.45	18.70 ± 0.50
2	15.85 ± 1.05	16.86 ± 1.22	22.47 ± 1.31	10.68 ± 0.16	18.71 ± 0.57
3	18.38 ± 1.14	32.55 ± 1.16	>40	>40	>40
cisplatin	1.81 ± 0.35	9.62 ± 0.19	8.58 ± 0.19	13.93 ± 0.29	13.73 ± 0.51

Table S1. Cytotoxic activity of compounds 1-3 (μ M).



Figure S1. The chemical structures of compounds 1-3 and 1a-3a.

No.	δ_{C} (mult.) ^b	δ_{H} (mult., J in Hz)	COSY	HMBC	ROESY
1	168.2, C				
2	131.2, C				
2-Me	21.1, CH ₃	2.16, s	3	1, 2, 3, 4	3, 4, NH
3	130.1, CH	6.73, d (11.9)	2-Me, 4	1, 2, 4, 5	2-Me, 5, 6, 7
4	123.5, CH	6.59, overlap	3, 5	2, 3, 6	2-Me, NH
5	133.4, CH	6.13, t (11.2)	4,6	3, 4, 6, 7	3, 15
6	125.9, CH	6.58, overlap	5,7	4, 5, 8	3, 8, 8-Me
7	139.7, CH	5.90, dd (15.3, 7.0)	6, 8	5, 8-Me, 9	8, 8-Me, 9
8	43.0, CH	2.57, m	7, 8-Me, 9	5, 6, 9	6, 7, 8-Me, 9
8-Me	15.1, CH ₃	1.09, d (6.9)	8	7, 8, 9	6, 8
9	72.7, CH	3.86, m	8, 10a, 10b	7, 8, 10, 11	8
10a	29 6 CH	2.87, overlap	9, 10b	8, 9, 11	10, 13
10b	$58.0, CH_2$	2.60, dd (15.6, 5.8)	9, 10a	8, 9, 11	10
11	202.9, C				
12	140.1, C				
12-Me	11.6, CH ₃	1.68, s	13	11, 12, 13	14a, 14b
13	143.6, CH	6.43, dd (8.7, 5.0)	12-Me, 14a 14b	11, 14, 15	10a, 14b, 15
14a	38.0 CH	2.37, m	13, 14b, 15	12, 13, 15	12-Me, 13
14b	$50.0, C\Pi_2$	2.20, m	13, 14a, 15	12, 13, 15	12-Me, 14, 15
15	74.3, CH	3.91, m	14a, 14b, 16	13, 16, 17	5, 7, 13, 14b, 17
16	132.7, CH	5.25, overlap	15, 17	17, 18	14a, 14b, 18, 18a
17	137.8, CH	5.24, overlap	16, 18	16, 18	15
18	42.1, CH	1.84, m	17, 18-Me, 19	16, 17, 19	16, 18-Me, 20-Me
18-Me	16.2, CH ₃	1.07, d (7.0)	18	17, 18, 19	19, 20
19	74.0, CH	3.82, d (8.9)	18, 20	17, 18, 20, 20-Me, 21	16, 20, 21, 30
20	31.3, CH	2.88, overlap	19, 20-Me, 21	21, 22, 31	18-Me, 19, 20-Me, 21, 22-Me, 30
20-Me	10.2, CH ₃	0.80, d (6.6)	20	19, 20, 21, 31	20, 21, 22-Me
21	72.5, CH	3.32, d (11.8)	20	19, 20, 22, 23, 31, 31a	19, 20, 20-Me, 22-Me, 30
22	88.0, C				
22-Me	16.3, CH ₃	1.60, s		21, 22, 23	20, 20-Me
23	202.7, C				
24	117.2, C				
25	164.7, C				
26	129.0, C				
26-Me	15.3, CH ₃	2.34, s	27	25, 26, 27, 31a,	27
27	134.0, CH	7.99, s	26-Me	25, 27a, 31, 31a, 26-Me	26-Me
27a	110.5, C				
28	177.1, C				
29	133.0, C				
30	121.6, CH	8.16, s		21, 24, 25, 27a, 28, 29, 31, 31a	18-Me, 19, 20, 21, NH
31	77.8, C				
31a	150.2, C				
25-ОН		11.14, s			
NH		8.59, s		1, 28, 30, 31	2-Me, 4, 30

Table S2. NMR spectral data for naphthomycin O (1) in CDCl_{3^a} .

No.	$\delta_{ m C}$ (mult.) ^b	$\delta_{\rm H}$ (mult., J in Hz)	COSY	HMBC	ROESY
1	167.6, C				
2	129.3, C				
2-Me	12.9, CH ₃	2.15, s	3	1, 2, 3	4, 16, NH
3	136.1, CH	7.19, d (11.4)	2-Me, 4	1, 2-Me, 5	
4	126.3, CH	6.52, dd (14.7, 11.3)	3, 5	5, 6	2-Me, 6
5	139.4, CH	6.63, dd (14.9, 10.7)	4, 6	3, 4, 6, 7	7
6	131.5, CH	6.32, dd (15.4, 10.6)	5,7	4, 5, 8	8, 8-Me
7	141.0, CH	5.81, dd (15.2, 8.6)	6, 8	5, 8-Me, 9	5, 8, 9
8	44.0, CH	2.43, overlap	7, 8-Me, 9	6, 7, 8-Me, 9, 10	
8-Me	16.1, CH ₃	1.13, d (6.6)	8	7, 8, 9	9
9	73.4, CH	3.45, m	8, 10a, 10b	7, 8, 8-Me, 11	7, 8-Me
10a	40.0 CU	2.41, overlap	9, 10b	9, 11	
10b	$40.0, CH_2$	3.15, brd (13.9)	9, 10a	9, 11	
11	202.7, C				
12	139.5, C				
12-Me	11.4, CH ₃	1.74, s	13, 14a	11, 12, 13	14b
13	142.2, CH	6.47, dd (9.3, 4.3)	12-Me, 14a, 14b	11, 12-Me, 15	9, 15
14a	377 CH	2.22, brd (16.2)	12-Me, 13, 14b, 15	13, 15	15
14b	$57.7, CH_2$	2.46, overlap	13, 14a, 15	15	12-Me
15	73.4, CH	3.89, t (9.4)	14a, 14b, 16	13, 14, 16, 17	6, 14a, 16
16	133.2, CH	5.47, dd (15.3, 8.0)	15, 17	14, 15, 17, 18, 18-Me	15, 18, 18-Me
17	137.3, CH	5.34, dd (15.3, 9.0)	16, 18	15, 16, 18, 18-Me	15, 18, 18-Me
18	42.0, CH	2.11, m	17, 18-Me, 19	18-Me, 19	
18-Me	16.3, CH ₃	1.17, d (6.7)	18	17, 18, 19	20
19	73.5, CH	4.01, d (9.0)	18, 20	17, 18, 20, 20-Me	16, 21, 30
20	31.4, CH	2.93, m	19, 20-Me, 21	20-Me, 21, 22	19, 20-Me, 22-Me, 30
20-Me	10.3, CH ₃	0.91, d (6.5)	20	20, 21	18, 20, 21,22-Me
21	73.0, CH	3.28, d (11.7)	20	20, 20-Me, 23, 31, 31a	19, 20-Me, 22-Me, 30
22	87.7, C				
22-Me	15.7, CH ₃	1.63, s		21, 22, 23	20, 20-Me, 21
23	202.3, C				
24	116.9, C				
25	164.7, C				
26	128.9, C				
26-Me	15.2, CH ₃	2.35, s	27	25, 26, 27	27
27	133.9, CH	7.99, s	26-Me	25, 26-Me, 28, 31, 31a	26-Me
27a	110.3, C				
28	177.0, C				
29	133.1, C				
30	121.1, CH	8.24, s		21, 27a, 28, 29, 31a	19, 20
31	78.1, C				
31a	149.9, C				
NH		8.78, s		1, 28, 30, 31	18
^a 600 MHz	for ¹ H NMR and 1	50 MHz for ¹³ C NMR. ^b Number	rs of attached protons were de	termined by analysis of 2D NMR s	pectra.

Table S3. NMR spectral data for 1a in CDCl₃^a.

No.	$\delta_{\rm C}$ (mult.) ^b	$\delta_{\rm H}$ (mult., J in Hz)	COSY	НМВС	ROESY
1	169.1. C	•11 ()			
2	133.8, C				
2-Me	21.2, CH ₃	2.12, s	3	1, 2, 3	3, 4
3	125.7, CH	6.64, d (12.2)	2-Me, 4	1, 2, 2-Me	2-Me, 5, NH
4	123.6, CH	6.25, t (12.6)	3, 5	2, 3	2-Me, 7, NH
5	131.5, CH	6.06, t (11.6)	4, 6, 7	6, 7	3, 7, 8
6	125.1, CH	6.38, dd (14.9, 11.5)	5,7	4, 5	3, 7, 8
7	140.8, CH	5.57, dd (14.9, 10.3)	6, 8	5, 8, 8-Me, 9	5, 8-Me, 9, 10
8	44.7, CH	2.55, m	7, 8-Me, 9	6, 7, 9	6, 7, 8-Me
8-Me	18.2, CH ₃	1.22, d (6.5)	8	7, 8, 9	7,8
9	74.6, CH	3.57, m	8, 10a, 10b	8-Me, 11	7
10a		2.72, overlap	9, 10b	8, 11, 12	10b, 12-Me
10b	$40.0, CH_2$	3.18. dd (17.6. 3.3)	9. 10a	11	7. 10a. 13
11	203.5, C		- ,		.,, -
12	141.3, C				
12-Me	11.1, CH ₃	1.86, s		11, 12, 13	14a
13	138.5, CH	6.54, dd (9.4, 4.2)	14	11, 12-Me	10b, 14a, 14b, 15
14a		2.72, overlap	13, 14b, 15	12, 13, 15	16
14b	39.1, CH ₂	2.36, d (14.5, 4.2)	13, 14a, 15	12, 13, 15	8-Me, 13, 15
15	74.9, CH	4.27, t (9.3)	14a, 14b, 16	13, 16, 17	13, 14b, 16
16	131.2, CH	5.88, dd (15.5, 8.2)	15, 17	15, 18	15, 18, 20
17	135.8, CH	5.85, dd (15.3, 9.5)	15, 18	15, 18, 18-Me	15, 18, 20
18	39.0, CH	2.95, m	1.19, 5.85	16, 17, 18-Me	18-Me. 19. 22
18-Me	19.1, CH ₃	1.19, d (6.7)	18	17, 18, 19	18, 19
19	77.1, CH	4.10, d (10.3)	18, 20	17, 18-Me, 20, 20-Me	18, 18-Me, 20, 22
20	47.9, CH	1.72, m	19, 20-Me	20-Me, 21, 22, 31	20-Me, 22, 30
20-Me	11.8, CH ₃	0.76, d (6.6)	20	19, 20, 21	19, 20
21	76.0, C				
21-Me	30.9, CH ₃	1.30, s		21, 22, 23	22
22	49.2, CH	3.55, s		20, 20-Me, 21, 21-Me, 23, 30, 31, 31a	18, 19, 20, 21-Me, 30
23	206.1, C				
24	106.2, C				
25	162.0, C				
26	127.5, C				
26-Me	16.0, CH ₃	2.43, s		25, 26, 27	27
27	133.7, C	8.42, s		25, 26-Me, 28, 31a	26-Me
27a	119.9, C				
28	142.9, C				
29	120.2, C				
30	123.3, CH	7.23, s		22, 27a, 28, 29, 31a	20, 22, NH
31	126.4, C				
31a	128.7, C				
25-OH		12.41, s		23, 24, 25, 26	
28-OH		9.90, s		29	
NH		8.82, s		1, 28, 29, 30	3, 4,30
^a 600 MHz	for ¹ H NMR and	1 150 MHz for ¹³ C NMR. ^b Nur	nbers of attached pr	otons were determined by analysis of 2D NMR spec	tra.

Table S4. NMR spectral data for naphthomycin P (2) in $CDCl_3^{a}$

No.	$\delta_{ m C}$ (mult.) ^b	δ_{H} (mult., J in Hz)	COSY	HMBC	ROESY
1	170.7, C				
2	131.8, C				
2-Me	13.6, CH ₃	2.05, s		1, 2, 3	4
3	133.2, CH	6.69, d (8.8)	2-Me, 4	1, 2-Me, 5	5, 7, NH
4	126.4, CH	6.38, overlap	3, 5	2	2-Me, NH
5	138.2, CH	6.37, overlap	4,6	7	7
6	130.8, CH	6.05, dd (15.2, 9.5)	5,7	4, 5, 8	8
7	140.9, CH	5.58, dd (15.1, 10.1)	6, 8	2, 8, 8-Me	3, 9, 8-Me, 10b
8	45.3, CH	2.41, overlap	7, 8-Me, 9	7, 8-Me, 9	6
8-Me	18.3, CH ₃	1.22, d (6.6)	8	7, 8, 9	8
9	75.3, CH	3.68, m	8, 9-OH, 10a, 10b	8-Me	7, 8
10a	41.1 CH	2.79, dd (16.8, 4.3)	9, 10b	8, 9, 11	10b
10b	$41.1, CH_2$	2.99, dd (16.8, 4.1)	9, 10a	11	10a, 13
11	202.6, C				
12	140.2, C				
12-Me	11.8, CH ₃	1.79, s		11, 12 , 13	14b
13	138.4, CH	6.58, t (7.2)	14a, 14b	11, 14, 15, 12-Me	15, 18
14a	20.4. CH	2.42, overlap	13, 14b	12, 15	13, 15, 27
14b	39.4, CH ₂	2.63, dt (16.8, 4.3)	13, 14a, 15	12, 13, 15, 16	12-Me, 16
15	75.2, CH	4.38, brs	14b, 16	16	13, 14a, 17
16	135.1, CH	5.88, overlap	15, 17	15, 18	13-Me, 22
17	132.4, CH	5.89, overlap	16, 18	15, 18	14b, 15, 18, 30
18	39.2, CH	2.95, overlap	17, 18-Me, 19	16, 17, 18-Me	16, 18-Me, 19, 22
18-Me	19.4, CH ₃	1.18, d (6.7)	18	16, 18, 19	17, 19, 22
19	77.4, CH	4.08, d (9.9)	18, 20	16, 18-Me, 20, 20-Me	18, 20
20	48.5, CH	1.70, m	19, 20-Me	21, 22, 31	20-Me, 22, 30
20-Me	12.0, CH ₃	0.73, d (6.9)	20	21, 22	19, 20
21	76.1, CH				
21-Me	31.3, CH ₃	1.29, s		21, 22 ,23	22
22	49.7, CH	3.59, s		20, 20-Me, 21, 23, 30, 31, 31a	16, 18, 19, 20, 21-Me, 30
23	206.1, C				
24	106.3, C				
25	162.1, C				
26	127.6, C				
26-Me	16.1, CH ₃	2.43, s	27	25, 26, 27	27
27	133.9, CH	8.41, s	26-Me	25, 26-Me, 31a	26-Me
27a	120.3, C				
28	142.9, C				
29	120.1, C				
30	123.6, CH	7.15, s		22, 28, 29, 31a	17, 20, 22, NH
31	126.4, C				
31a	128.8, C				
9-OH		3.41, d (9.0)	9	8, 9, 10	8
21-OH		3.97, s		21, 22, 23	21-Me
25-OH		12.37, s		23, 24, 25, 26	26-Me
28-OH		10.03, s		27a, 28	
NH		8.40, s		1, 28, 30	3, 17, 28-OH, 30
^a 600 MHz	for ¹ H NMR an	d 150 MHz for ¹³ C NMR. ^b N	Jumbers of attached protons	were determined by analysis of 2D NMR	spectra.

Table S5. NMR spectral data for 2a in CDCl₃^a.

No.	$\delta_{ m C}$ (mult.) ^b	$\delta_{ m H}$ (mult., J in Hz)	COSY	HMBC	ROESY
1	170.1, C				
2	131.7, C				
2-Me	20.9, CH ₃	2.13, s	3	1, 2, 3	3
3	132.3, CH	6.94, d (12.0)	2-Me, 4	1, 2-Me, 5	2-Me, 6
4	124.0, CH	6.47, t (11.5)	3, 5	2,6	
5	135.5, CH	6.18, t (11.1)	4,6	3, 6, 7	7
6	126.7, CH	6.71, dd (15.0, 11.4)	5,7	4, 5, 8	3, 8, 8-Me
7	142.1, CH	5.80, dd (15.0, 8.5)	6, 8	5, 8, 8-Me, 9	5, 8, 8-Me, 9, 10
8	45.2, CH	2.38, m	7, 8-Me, 9	6, 7, 8-Me, 9	6, 7, 8-Me, 9, 10
8-Me	16.6, CH ₃	1.11, d (6.73)	8	7, 8, 9	7, 8, 9, 10
9	73.2, CH	3.97, m	8, 10		7, 8, 8-Me, 10, 13
10a	43.4 CH	2.79, dd (16.1, 5.1)	9, 10b	8, 9, 11	8-Me, 10, 13
10b	43.4, CH <u>2</u>	2.83, dd (16.1, 7.7)	9, 10a	8, 9, 11	7, 8
11	202.7, C				
12	139.8, C				
12-Me	11.8, CH ₃	1.75, s	13	11, 12, 13	14
13	141.4, CH	6.76, t (7.1)	12-Me, 14	11, 12-Me, 14, 15	10, 14, 15
14	38.0, CH ₂	2.47, m	13, 15	12, 13, 15, 16	12-Me, 13, 15, 16
15	72.5, CH	4.18, m	14, 16	13, 17	13, 14, 16, 17
16	134.6, CH	5.41, dd (15.5, 6.6)	15, 17	14, 15, 18	14, 15, 18, 18-Me
17	133.6, CH	5.65, dd (15.5, 8.6)	16, 18	15, 18, 18-Me, 19	14, 15, 18, 18-Me
18	41.9, CH	2.22, m	17, 18-Me, 19		16, 18-Me, 19
18-Me	19.1, CH3	1.05, d (6.9)	18	17, 18, 19	18, 19
19	79.9, CH	3.26, dd (8.5, 3.1)	18, 20	17, 18, 18-Me, 20, 20-Me, 21	16, 20, 21,
20	38.9, CH	2.59, m	19, 20-Me, 21	19, 20-Me, 21, 22	16, 20, 20-Me, 21, 22-Me
20-Me	16.4, CH ₃	1.03, d (6.7)	20	18, 19, 20, 21	4, 20
21	145.9, CH	6.57, d (10.2)	20	19, 20, 22, 22-Me, 23	
22	128.5, C				
22-Me	13.2, CH ₃	1.82, s		21, 22, 23	18-Me, 20
23	172.2, C				
24	116.8, CH	7.63, s		26, 28, 31a	
25	163.5, C				
26	133.9, C				
26-Me	16.3, CH ₃	2.26, s		25, 26, 27	
27	131.1, CH	7.79, s		24, 25, 26, 26-Me, 28, 31	
27a	123.4, C				
28	180.5, C				
29	132.2, C				
30	112.1, CH	7.29, s		25, 27a, 28, 29, 31	
31	187.4, C				
31a	142.0, C				

Table S6. NMR spectral data for naphthomycin Q (3) in CD₃OD^a.

^a 600 MHz for ¹H NMR and 150 MHz for ¹³C NMR. ^b Numbers of attached protons were determined by analysis of 2D NMR spectra.

No.	δ_{C} (mult.) ^b	δ_{H} (mult., J in Hz)	COSY	HMBC	ROESY
1	169.3, C				
2	129.9, C				
2-Me	12.8, CH ₃	2.07, s		1, 2, 3	4
3	138.1, CH	7.09, d (11.1)	4	1, 2, 5	5
4	127.3, CH	6.57, overlap	3, 5	6	2-Me, 6
5	142.1, CH	6.65, dd (14.7, 10.5)	4, 6	3, 4, 7	2-Me, 3, 7
6	132.1, CH	6.32, dd (15.2, 10.5)	5,7	4, 5, 8	4, 8, 8-Me
7	142.8, CH	5.92, dd (15.2, 8.3)	6, 8	5, 8-Me, 9	5, 8, 8-Me, 9, 10
8	45.1, CH	2.36, m	7, 8-Me, 9	7, 8-Me, 9	6, 7, 8-Me, 9, 10
8-Me	16.4, CH ₃	1.11, d (6.8)	8	7, 8, 9	6, 7, 8, 9, 10
9	73.1, CH	3.97, m	8, 10		13, 7, 8, 8-Me, 10
10a	43.3 CH	2.79, dd (16.1, 4.4)	9, 10b	8, 9, 11	8, 9, 13
10b	45.5, CH ₂	2.83, dd (16.1, 8.4)	9, 10a	8, 9, 11	7, 8-Me,13
11	202.7, C				
12	139.8, C				
12-Me	11.8, CH ₃	1.75, s		11, 12, 13	14
13	141.4, CH	6.76, t (7.0)	14	11, 12-Me, 14, 15	9, 10, 14, 15, 16, 18-Me
14	38.0, CH ₂	2.47, m	13, 15	12, 13, 15, 16	12-Me, 13, 15, 16, 17
15	72.5, CH	4.18, dt (6.5, 6.5)	14, 16	13, 17	13, 14, 16, 17
16	134.6, CH	5.41, dd (15.6, 6.5)	15, 17	15, 18	13, 14, 15, 18, 18-Me, 22-Me
17	133.6, CH	5.66, dd (15.5, 8.6)	16, 18	15, 18, 18-Me	13, 15, 18, 18-Me, 19, 20
18	41.8, CH	2.24, m	17, 18-Me, 19	18-Me	16, 18-Me, 19, 21
18-Me	19.1, CH ₃	1.05, d (6.9)	18	17, 18, 19	7, 13, 16, 17, 20
19	80.0, CH	3.26, dd (8.5, 3.0)	18, 20	17, 18, 20, 21	17, 18, 18-Me, 20, 20-Me, 21
20	38.9, CH	2.58, dq (7.1, 7.0)	19, 20-Me, 21	19, 20-Me, 21, 22	20-Me, 22-Me
20-Me	16.4, CH ₃	1.03, d (6.7)	20	19, 20, 21	12-Me, 18, 19, 20, 21
21	145.1, CH	6.53, dd (11.0, 3.9)	20	19, 20, 22-Me, 23	3, 6, 18, 19, 20
22	129.3, C				
22-Me	13.4, CH ₃	1.82, s		21, 22, 23	18-Me, 20
23	173.1, C				
24	116.2, CH	7.57, s		26, 28, 31a	2-Me
25	163.6, C				
26	133.9, C				
26-Me	16.4, CH ₃	2.26, s		25, 29	27
27	131.1, CH	7.80, s		25, 26, 26-Me, 28, 31	15, 26-Me
27a	123.3, C				
28	180.7, C				
29	132.2, C				
30	112.1, CH	7.28, s		25, 27a, 28, 29, 31	
31	187.4, C				
31a	142.2, C				
^a 600 MHz f	for ¹ H NMR and 15	0 MHz for ¹³ C NMR. ^b Number	s of attached protons w	vere determined by analysis of 2E	ONMR spectra.

Table S7. NMR spectral data for 3a in CD₃OD^a.



Figure S3. Key ROESY correlations of naphthomycin O (1).



Figure S4. Key COSY and HMBC correlations of 1a.



Figure S5. Key ROESY correlations of 1a.





Figure S7. Key ROESY correlations of naphthomycin P (2).



Figure S8. Energy minimized model of simplified naphthomycin P (2) a) model of 21S*, 22R*, b) model of 21R*, 22S* (calculated by Chem3D ver 15.0, red = oxygen, blue = nitrogen, white = hydrogen, gray = carbon, pink = lone pair, double solid arrow = ROESY correlation).



H-19-H-22: 4.819 Å

H-19-H-22: 2.250 Å

Figure S9. Key COSY and HMBC correlations of 2a.



Figure S10. Key ROESY correlations of 2a.



Figure S11. Key COSY and HMBC correlations of naphthomycin Q (3).



Figure S12. Key ROESY correlations of naphthomycin Q (3).





Figure S14. Key ROESY correlations of 3a.



Figure S15. HPLC analysis of retro-Friedel-Crafts acylation reaction of naphthomycin E (**4**), with the aid of a Lewis acid, SnCl4. (I) reaction time of 10 min; (II) reaction time of 20 min; (III) reaction time of 35 min; (IV) reaction time of 50 min; (V) reaction time of 80 min; (VI) reaction time of 110 min; (VII) standard **3a**; (VIII) standard **3**; (IX)

standard 4.



2. NMR and HRESIMS spectra of compounds 1-3 and 1a-3a

Figure S16. ¹H NMR spectrum (600 MHz) of naphthomycin O (1) in CDCl₃.











Figure S19. HSQC spectrum (600 MHz) of naphthomycin O (1) in CDCl₃







Figure S22. HRESIMS spectrum of naphthomycin O (1).



S22

Figure S23. ¹H NMR spectrum (600 MHz) of 1a in CDCl₃.







Figure S25. COSY spectrum (600 MHz) of 1a in CDCl₃







Figure S27. HMBC spectrum (600 MHz) of 1a in CDCl₃





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Figure S36. HRESIMS spectrum of naphthomycin P (2).













Figure S40. HSQC spectrum (600 MHz) of 2a in CDCl₃







Figure S42. ROESY spectrum (600 MHz) of 2a in CDCl₃

Qualitative Analysis Report

Instrument Acq Method IRM Calibra Comment	pe t Nam d ation :	e Statu	s	H2054-9.d Sample Instrument 1 SIBU.m Success	Sample Name Position User Name Acquired Time DA Method	H2054-9 P1-E1 4/6/2017 3:35:19 F Default.m	РМ		
Sample Gro	oup		6200 co	I	nfo.				
Version	1 5 W		Q-TOF I	B.05.01 (B5125.2)					
User Spe	ctra								
Fragme	entor V	oltage	1	Collision Energy	Ionization Mode				
	175			0	ESI				
×10 5 +ES	SI Scan	(0.15-	0.17 min,	2 Scans) Frag=175.0V H2	054-9.d				
1.8				([C4	710.3296 0 H49 N O91+Na)+				
1.6				ue.					
1.4 -									
1.2-									
1									
0.8									
0.01									
0.4-									
0.4-									
0.4- 0.2- 0									
0.4- 0.2- 0 70	9.4	709.	6 70	09.8 710 710 Counts vs	.2 710.4 710.6 Mass-to-Charge (m/z)	710.8 711	711.2		
0.4- 0.2- 0 709	9.4	709.	6 70	09.8 710 710 Counts vs	.2 710.4 710.6 6. Mass-to-Charge (m/z)	710.8 711	711.2		
0.4- 0.2- 0 703 Peak List m/z	9.4	709.	6 7(09.8 710 710 Counts vs	.2 710.4 710.6 6. Mass-to-Charge (m/z)	710.8 711	711.2		
0.4- 0.2- 0- 709 Peak List <i>m/z</i> 160.0496	9.4	709.	6 70 nd 9.38	09.8 710 710 Counts vs	2 710.4 710.6 6. Mass-to-Charge (m/z)	710.8 711	711.2		
0.4 0.2 0 703 Peak List <i>m/z</i> 160.0496 345.2387	9.4	709. Abu 1316 1034	6 70 nd 9.38 5.73	09.8 710 710 Counts vs	.2 710.4 710.6 b. Mass-to-Charge (m/z)	710.8 711	711.2		
0.4 0.2 0 703 Peak List m/z 160.0496 345.2387 710.3296	9.4 2 1 1 1	709. Abu 1316 1034 1895	6 70 nd 9.38 5.73 20.95	09.8 710 710 Counts vs Formula	2 710.4 710.6 . Mass-to-Charge (m/z) Ion (M+Na)+	710.8 711	711.2		
0.4 0.2 0 709 Peak List m/z 160.0496 345.2387 710.3296 711.3326	9.4 2 1 1 1 1	709. 1316 1034 1895 7921	6 70 nd 9.38 5.73 20.95 4.05	09.8 710 710 Counts vs Formula C40 H49 N O9 C40 H49 N O9	2 710.4 710.6 . Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+	710.8 711	711.2		
0.4 0.2 0 709 709 709 709 700 700 700 700 700 7	9.4 2 1 1 1 1 1 1	709. 1316 1034 1895 7921 1886	6 70 nd 9.38 5.73 20.95 4.05 0.33	09.8 710 710 Counts vs Formula C40 H49 N 09 C40 H49 N 09 C40 H49 N 09	.2 710.4 710.6 5. Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ (M+Na)+	710.8 7 ¹ 1	711.2		
0.4 0.2 0 70: 70: 70: 70: 70: 710: 710: 710: 71	9.4 2 1 1 1 1 1 1 1	709. 1316 1034 1895 7921 1886 5382	6 70 nd 9.38 5.73 20.95 4.05 0.33 4.31	09.8 710 710 Counts vs Formula C40 H49 N 09 C40 H49 N 09 C40 H49 N 09 C40 H49 N 09	2 710.4 710.6 Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ (M+Na)+	710.8 7 ¹ 1	711.2		
0.4 0.2 0 70 Peak List m/z 160.0496 345.2387 710.3296 711.3326 712.3356 726.3032 727.3066	9.4 2 1 1 1 1 1 1 1 1 1	709. Abu 1316 1034 1895 7921 1886 5382 2445	6 70 nd 9.38 5.73 20.95 4.05 0.33 4.31 8.73	09.8 710 710 Counts vs Formula C40 H49 N O9 C40 H49 N O9 C40 H49 N O9	2 710.4 710.6 5. Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ (M+Na)+	710.8 711	711.2		
0.4 0.2 0 70 Peak List <i>m/z</i> 160.0496 345.2387 710.3296 711.3326 712.3356 726.3032 727.3066 728.3053	9.4 2 1 1 1 1 1 1 1 1 1 1	709. 1316 1034 1895 7921 1886 5382 2445 9344	6 70 9.38 5.73 20.95 4.05 0.33 4.31 8.73 .27	09.8 710 710 Counts vs Formula C40 H49 N O9 C40 H49 N O9 C40 H49 N O9	2 710.4 710.6 Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ (M+Na)+	710.8 711	711.2		
0.4 0.2 0 70 Peak List m/z 160.0496 345.2387 710.3296 711.3326 712.3356 726.3032 727.3066 728.3053 Formula Ca	9.4 z 1 1 1 1 1 1 1 1 1 1 1 1 1	709. 1316 1034 1895 7921 1886 5382 2445 9344 or Ele	6 70 9.38 5.73 20.95 4.05 0.33 4.31 8.73 .27 ment L	09.8 710 710 Counts vs Formula C40 H49 N O9 C40 H49 N O9 C40 H49 N O9 C40 H49 N O9	2 710.4 710.6 Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ (M+Na)+	710.8 711	711.2		
0.4 0.2 0 70 Peak List m/z 160.0496 345.2387 710.3296 711.3326 712.3356 726.3032 727.3066 728.3053 Formula Ca Element	9.4 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	709. 1316 1034 1895 7921 1886 5382 2445 9344 or Ele	6 70 9.38 5.73 20.95 4.05 0.33 4.31 8.73 .27 ment L Max	09.8 710 710 Counts vs Formula C40 H49 N O9 C40 H49 N O9 C40 H49 N O9 C40 H49 N O9	2 710.4 710.6 Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ (M+Na)+	710.8 711	711.2		
0.4- 0.2- 0-70 Peak List <i>m/z</i> 160.0496 345.2387 710.3296 711.3326 712.3356 726.3032 727.3066 728.3053 727.3066 Formula Ca Element	9.4 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	709. Abu 1316 1034 1895 7921 1886 5382 2445 9344 or Ele 3	6 70 9.38 5.73 20.95 4.05 0.33 4.31 8.73 .27 ment L Max 60	09.8 710 710 Counts vs Formula C40 H49 N 09 C40 H49 N 09 C40 H49 N 09 C40 H49 N 09	2 710.4 710.6 Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ (M+Na)+	710.8 711	711.2		
0.4 0.2 0 70 Peak List <i>m/z</i> 160.0496 345.2387 710.3296 711.3326 712.3356 726.3032 727.3066 728.3053 727.3066 728.3053 727.3066 728.3053 727.3066 728.3053 727.3066 728.3053	9.4 z 1 1 1 1 1 1 1 1 1 i i i i i i i i	709. Abu 1316 1034 1895 5382 2445 9344 or Ele 3 0	6 70 9.38 5.73 20.95 4.05 0.33 4.31 8.73 .27 ment L Max 60 120	09.8 710 710 Counts vs Formula C40 H49 N 09 C40 H49 N 09 C40 H49 N 09 C40 H49 N 09	2 710.4 710.6 Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ (M+Na)+	710.8 711	711.2		
0.4- 0.2- 0-70 Peak List <i>m/z</i> 160.0496 345.2387 710.3296 711.3326 712.3356 726.3032 727.3066 728.3053 Formula Ca Element 1 2 1 2 1 2 2 1 2 2 2 2 2 2 2 2 2 2 2 2 2	9.4 z 1 1 1 1 1 1 1 1 1 1 1 1 1	709. Abu 1316 1034 1895 5382 2445 9344 or Ele 3 0 0 0	6 70 9.38 5.73 20.95 4.05 0.33 4.31 8.73 .27 ment L Max 60 120 30	09.8 710 710 Counts vs Formula C40 H49 N 09 C40 H49 N 09 C40 H49 N 09 C40 H49 N 09 C40 H49 N 09	.2 710.4 710.6 b. Mass-to-Charge (m/z) (M+Na)+ (M+Na)+ (M+Na)+	710.8 711	711.2		
0.4 0.2 0 70 Peak List m/z 160.0496 345.2387 710.3296 711.3326 711.3326 712.3356 726.3032 727.3066 728.3053 Formula Ca Element 2 1 0	9.4 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	709. Abu 1316 1034 1895 7921 1886 53822 2445 9344 or Ele 3 0 0 0 0	6 70 9.38 5.73 20.95 4.05 0.33 4.31 8.73 .27 Max 60 120 30 3	09.8 710 710 Counts vs Formula C40 H49 N 09 C40 H49 N 09 C40 H49 N 09 C40 H49 N 09 C40 H49 N 09	2 710.4 710.6 Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ (M+Na)+	710.8 711	711.2		
0.4 0.2 0 70 Peak List m/z 160.0496 345.2387 710.3296 711.3326 712.3356 726.3032 727.3066 728.3053 Formula Ca Element	9.4 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	709. 1316 1034 18895 7921 18866 5382 24454 9344 0 r Ele 33 0 0 0 0 0 0 0 0 0 0 0 0 0	6 70 9.38 5.73 20.95 4.05 0.33 4.31 8.73 .27 Max 60 120 3 sults	09.8 710 710 Counts vs Formula C40 H49 N O9 C40 H49 N O9 C40 H49 N O9 C40 H49 N O9 C40 H49 N O9	2 710.4 710.6 Mass-to-Charge (m/z) Ion (M+Na)+ (M+Na)+ (M+Na)+	710.8 711	711.2	,	

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Figure S49. ROESY spectrum (600 MHz) of naphthomycin Q (3) in CD₃OD



Figure S50. HRESIMS spectrum of naphthomycin Q (3).









Figure S54. HSQC spectrum (600 MHz) of 3a in CD₃OD



Figure S55. HMBC spectrum (600 MHz) of 3a in CD₃OD



Figure S56. ROESY spectrum (600 MHz) of 3a in CD₃OD



Qualitative Analysis Report

Acq Metho	pe t Nam d	e		Sample Instrument 1 SIBU.m	Position User Name Acquired Time	P1-E3 4/6/2017 3:43:35	PM		
IRM Calibr Comment	ation \$	Status	5	Success	DA Method	Default.m			
Sample Gro Acquisition Version	oup I SW		6200 sei Q-TOF E	ries TOF/6500 series 8.05.01 (B5125.2)	Info.				
User Spe	ctra							 	
Fragme	175	oltage		Collision Energy 0	Ionization Mode ESI				
10 4 +ES	SI Scan	(0 25 m	ain) Ereat	=175 0V H2054-17+ 4 S	ubtract				
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1.4									
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0.8- 0.6- 0.4- 0.2 0- 72	25.4	725.	6 7	25.8 726 7	26.2 726.4 726.6	726.8 727	727.2		
0.8 0.6 0.4 0.2 0 72	25.4	725.	6 7.	25.8 726 7 Counts	26.2 726.4 726.6 vs. Mass-to-Charge (m/z)	726.8 727	727.2		
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0.8- 0.6- 0.4- 0.2 0- 72 Peak List m/z 242.9485 256.9641	25.4 21	725.0 Abur 34088	6 7: 1 d 8.71 7.84	25.8 726 7 Counts	26.2 726.4 726.6 vs. Mass-to-Charge (m/2)	726.8 727	727.2		
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0.8- 0.6- 0.4- 0.2 0-72 Peak List m/z 242.9485 256.9641 338.9674 414.954	25.4 2 1 1	725.0 Abur 34080 9620 9093. 11080	6 7: nd 8.71 7.84 .67 6.17	25.8 726 7 Counts	26.2 726.4 726.6 vs. Mass-to-Charge (m/z)	726.8 727	727.2		
0.8- 0.6- 0.4- 0.2 0-72 Peak List m/z 242.9485 256.9641 338.9674 414.954 726.3242	z 1 1 1	725.0 34084 9620 9093. 11086 17080	6 7: nd 8.71 7.84 .67 6.17 0.63	25.8 726 7 Counts	26.2 726.4 726.6 vs. Mass-to-Charge (m/z)	726.8 727	727.2		
0.8- 0.6- 0.4- 0.2 72 Peak List <i>m/z</i> 242.9485 256.9641 338.9674 414.954 726.3242 742.2913	25.4 1 1 1 1 2	725.0 34080 96200 9093.0 11080 17080 30682	6 7: 8.71 7.84 67 6.17 0.63 2.53	25.8 726 7 Counts	26.2 726.4 726.6 vs. Mass-to-Charge (m/z)	726.8 727	727.2		
0.8- 0.6- 0.4- 0.2 0 72 242.9485 256.9641 338.9674 414.954 726.3242 726.3242 722.913 742.2913	25.4 1 1 1 2 2	725.1 34084 96201 9093 11086 17086 30682 11454	6 7: nd 8.71 7.84 .67 6.17 0.63 2.53 4.71	25.8 726 7 Counts Formula C40 H49 N O10	26.2 726.4 726.6 vs. Mass-to-Charge (m/z)	726.8 727	727.2		
0.8- 0.6- 0.4- 0.2 0 72 Peak List m/2 242.9485 256.9641 338.9674 414.954 726.3242 742.79427 742.7927 743.2939	25.4 1 1 1 2 2 2 2	725.0 34084 96200 9093.0 11086 11086 30682 11456 12712	6 7: nd 8.71 7.84 .67 6.17 0.63 2.53 4.71 2.34	25.8 726 7 Counts Formula C40 H49 N O10	26.2 726.4 726.6 vs. Mass-to-Charge (m/2)	726.8 727	727.2		
Peak List m/2 242.9485 256.9641 338.9674 414.954 726.3242 742.7927 743.2939 Formula Ca Element	25.4 2 1 1 1 2 2 2 1 1 1 1 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1	725.7 34084 96207 9093. 11084 17086 30683 11454 12717 00 Ele	6 7. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1	25.8 726 7 Counts	26.2 726.4 726.6 vs. Mass-to-Charge (m/2)	726.8 727	727.2		
Peak List m/2 242.9485 256.9641 338.9674 414.954 726.3242 742.2913 742.7927 743.2939 Formula Ca Element	25.4 z 1 1 1 2 2 2 1 c d l l l l l l l l	725. 3408/ 9620: 9093. 1108/ 1708/ 30682: 1271: or Ele	6 7. 10 10 10 10 10 10 10 10 10 10	25.8 726 7 Counts	26.2 726.4 726.6 vs. Mass-to-Charge (m/z)	726.8 727	727.2		
Peak List m/z 242.9485 256.9641 338.9674 414.954 742.2913 742.7927 743.2927 743.2927 743.2939 C H	25.4 1 1 1 2 2 2 1 Culat Min	725. 34088 9620: 9093. 11086 17086 30685 11456 12712 0 r Ele 3 3 0	6 7: http://www.secondensity.org/linearized-secondensity.	25.8 726 7 Counts	26.2 726.4 726.6 vs. Mass-to-Charge (m/2)	726.8 727	727.2		
Peak List m/2 242.9485 256.9641 338.9674 742.2913 742.2913 742.7927 743.2929 745.2929 745.2955.2929 745.29577 745.295777577777777777777777	25.4 1 1 1 2 2 2 2 1 cutat Min	725.0 Abur 3408: 9620: 9093. 1108: 1271: or Ele 3 0 0	6 7: hd 8.71 7.84 .67 6.17 0.63 2.53 4.71 2.53 4.71 2.34 ment Li Max 60 120 30	25.8 726 7 Counts	26.2 726.4 726.6 vs. Mass-to-Charge (m/z)	726.8 727	727.2		
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