

Supplementary

Table S1. NCTC 7096 Gramicidins Mass Spectrometric peptide fragmentation. For GS-1141, GS-1155 and GS-1169, where (■) represent the presence of each fragment, (■) represent the absence and (■) represents the actual mass.

	Nterm_mod	aa1	aa2	aa3	aa4	aa5	aa6	aa7	aa8	aa9	aa10	adduct
	Term	L	F	P	V	K	L	F	P	V	K	[M+H] ⁺
Mass	1.007825	113.0841	147.0684	97.05276	99.06841	128.095	113.0841	147.0684	97.05276	99.06841	128.09496	1169.745
b-series	1.007825	114.0919	261.1603	358.2131	457.2815	585.3764	698.4605	845.5289	942.5817	1041.65	1169.745	
Actual mass		-	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A		
y-series	1.007825	1169.745	1056.661	909.5926	812.5398	713.4714	585.3764	472.2924	325.224	228.1712	129.102785	
Actual mass		-	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A		
	Nterm_mod	aa1	aa2	aa3	aa4	Orn	aa6	aa7	aa8	aa9	aa10	adduct
	Term	L	F	P	V	K	L	F	P	V	K	[M+H] ⁺
Mass	1.007825	113.0841	147.0684	97.05276	99.06841	114.0793	113.0841	147.0684	97.05276	99.06841	128.09496	1155.729
b-series	1.007825	114.0919	261.1603	358.2131	457.2815	571.3608	684.4448	831.5132	928.566	1027.634	1155.7294	
Actual mass		-	261.1609	358.2117	457.2812	N/A	684.4443	831.5142	928.5631	1027.6298		
y-series	1.007825	1155.729	1042.645	895.5769	798.5241	699.4557	585.3764	472.2924	325.224	228.1712	129.102785	
Actual mass			1042.6567	895.5766	798.5254	699.4559	585.3770	472.2921	325.2238	228.1710		
	Nterm_mod	aa1	aa2	aa3	aa4	Orn	aa6	aa7	aa8	aa9	Orn	adduct
	Term	L	F	P	V	K	L	F	P	V	K	[M+H] ⁺
Mass	1.007825	113.0841	147.0684	97.05276	99.06841	114.0793	113.0841	147.0684	97.05276	99.06841	113.93846	1141.573
b-series	1.007825	114.0919	261.1603	358.2131	457.2815	571.3608	684.4448	831.5132	928.566	1027.634	1141.5729	
Actual mass			261.1603	358.2106	457.2800	571.3608	684.4446	831.5139	928.5666	1027.6351		
y-series	1.007825	1141.714	1028.63	881.5613	784.5085	685.4401	571.3608	458.2767	311.2083	214.1555	115.087135	
Actual mass			1028.6406	881.5610	784.5090	685.4408	571.3608	458.2781	311.2081	214.1550		

Table S2. E-1 mutant (non-Gramicidin's producer) Gramicidins Mass Spectrometric peptide fragmentation. For GS-1141, GS-1155 and GS-1169, where (■) represent the presence of each fragment, (■) represent the absence and (■) represents the actual mass.

	Nterm_mod	aa1	aa2	aa3	aa4	aa5	aa6	aa7	aa8	aa9	aa10	adduct
	Term	L	F	P	V	K	L	F	P	V	K	[M+H] ⁺
Mass	1.007825	113.0841	147.0684	97.05276	99.06841	128.095	113.0841	147.0684	97.05276	99.06841	128.09496	1169.745
b-series	1.007825	114.0919	261.1603	358.2131	457.2815	585.3764	698.4605	845.5289	942.5817	1041.65	1169.745	
Actual mass		-	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A		
y-series	1.007825	1169.745	1056.661	909.5926	812.5398	713.4714	585.3764	472.2924	325.224	228.1712	129.102785	
Actual mass		-	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A		
	Nterm_mod	aa1	aa2	aa3	aa4	Orn	aa6	aa7	aa8	aa9	aa10	adduct
	Term	L	F	P	V	K	L	F	P	V	K	[M+H] ⁺
Mass	1.007825	113.0841	147.0684	97.05276	99.06841	114.0793	113.0841	147.0684	97.05276	99.06841	128.09496	1155.729
b-series	1.007825	114.0919	261.1603	358.2131	457.2815	571.3608	684.4448	831.5132	928.566	1027.634	1155.7294	
Actual mass		-	N/A	N/A	457.2799	N/A	684.4435	N/A	N/A	N/A		
y-series	1.007825	1155.729	1042.645	895.5769	798.5241	699.4557	585.3764	472.2924	325.224	228.1712	129.102785	
Actual mass			N/A	895.5762	N/A	N/A	N/A	N/A	325.2242	N/A		
	Nterm_mod	aa1	aa2	aa3	aa4	Orn	aa6	aa7	aa8	aa9	Orn	adduct
	Term	L	F	P	V	K	L	F	P	V	K	[M+H] ⁺
Mass	1.007825	113.0841	147.0684	97.05276	99.06841	114.0793	113.0841	147.0684	97.05276	99.06841	113.93846	1141.573
b-series	1.007825	114.0919	261.1603	358.2131	457.2815	571.3608	684.4448	831.5132	928.566	1027.634	1141.5729	
Actual mass			261.1600	358.2123	457.2805	571.3610	684.4446	831.5131	928.5654	1027.6370		
y-series	1.007825	1141.714	1028.63	881.5613	784.5085	685.4401	571.3608	458.2767	311.2083	214.1555	114.946285	
Actual mass			1028.6334	881.5617	784.5094	685.4408	571.3610	458.2766	311.2082	214.1550		