

Table 2: ^1H and ^{15}N Assignments for gramicidin A in different environments.

Residue	DMPC (1/20 mol/mol)		SDS (1/100 mol/mol) ^a		TFE (10mM)		DMSO (50 mM)		MeOH/ CHCl_3 ^b	
	^1H	^{15}N	^1H	^{15}N	^1H	^{15}N	^1H ^c	^{15}N ^c	^1H	^{15}N
1 Val	9.15	130.0	8.99	130.1	8.56	129.8	8.71	129.0	8.41	120.9
2 Gly ^d	<u>8.83</u>	<u>114.2</u>	8.83	114.2	8.83	114.2	8.83	114.2	8.83	114.2
3 Ala	9.34	130.3	9.29	129.9	8.76	126.8	8.52	125.8	8.84	128.5
4 Leu	8.82	127.1	8.78	126.7	8.63	124.3	8.63	123.0	9.31	123.3
5 Ala	9.34	128.8	9.30	129.1	8.84	128.7	8.47	125.3	9.40	130.7
6 Val	8.45	124.1	8.42	124.2	8.59	128.9	8.31	117.6	8.36	132.1
7 Val	8.90	126.9	8.83	126.7	8.67	125.2	8.51	122.2	8.73	122.8
8 Val	8.43	126.4	8.22	126.4	8.69	125.5	8.42	122.2	9.12	125.2
9 Trp	9.08	132.5	9.02	131.8	8.82	127.5	8.66	127.7	9.18	132.0
10 Leu	7.96	132.1	7.97	132.0	8.59	120.7	8.52	126.8	9.02	128.4
11 Trp	8.80	128.6	8.70	128.6	9.00	126.7	8.73	125.7	9.47	129.5
12 Leu	8.29	127.8	8.14	127.5	8.73	129.1	8.52	126.9	9.25	127.9
13 Trp	8.70	126.8	8.61	126.3	8.95	126.1	8.73	126.1	9.85	131.4
14 Leu	8.58	126.6	8.35	126.2	8.41	129.6	8.61	127.7	7.71	130.8
15 Trp	8.83	128.5	8.83	127.8	8.53	125.7	8.78	126.5	8.77	132.4
16 Eth	8.67	117.2	8.33	116.9	8.58	118.6	8.36	115.4	8.62	123.3
Trp-indoles ^e	10.38	130.7	9.87	130.3	10.24	129.4	N/A	N/A	10.47	132.6
	10.49	132.7	9.96	129.9	10.28	129.4	N/A	N/A	10.76	133.5
	10.35	132.4	9.73	130.0	10.26	129.4	N/A	N/A	10.60	132.7
	10.41	132.2	9.85	130.5	10.26	129.4	N/A	N/A	10.40	131.9

^a Sample: 5 mM gA, 500 mM SDS- d_{25} in 50 mM potassium phosphate buffer at pH = 6.0.^b Sample: 20 mM gA, 20 mM CsCl in MeOH/ CHCl_3 (1/1 vol/vol)^c Chemical shift results from reference 10.^d For comparison, the chemical shifts were corrected for all environments to match those of glycine in DMPC, referenced against the external references $^{15}\text{NH}_4$, $^{15}\text{NO}_3$ and TMS (^1H).^e The chemical shifts for the four tryptophan indole NH groups were not assigned specifically with residue position.