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TABLE 1. Chemical shift assignments for neuromodulin in CD₃OH.†

Residue	NH	α H	β H	other
Lys 1	8.47	4.03	1.82	
Ile 2	8.74	3.82	1.89	0.88, 1.19
Gln 3	8.54	4.04	2.20, 2.06	2.44, 2.49
Ala 4	8.39	4.11	1.48	
Ser 5	8.15	4.21	4.02	
Phe 6	8.58	4.36	3.23	7.58
Arg 7	8.51	3.91		
Gly 8	8.71	3.81		
His 9	8.31	4.34	3.26	7.96
Ile 10	8.17	3.63	1.92	0.84
Thr 11	8.12	4.27	3.75	1.18
Arg 12	7.98	3.91	1.85	1.37, 1.53
Lys 13	8.07	3.90	1.95	
Lys 14	8.11	4.00	1.96	1.08, 1.44, 0.67
Leu 15	7.93	4.19	1.86	1.54, 0.86
Lys 16	7.84	4.21	1.88	1.58, 1.47
Gly 17	7.98	3.90, 3.79		

† Chemical shifts are ± 0.01 PPM.

TABLE 2. Chemical shift assignments for neuromodulin in SDS.†

Residue	NH	α H	β H	other
Lys 1	8.30	4.20	1.82	
Ile 2	8.18	4.07	2.12	0.98, 1.71
Gln 3	8.38	4.16	2.18, 2.08	2.48, 2.40
Ala 4	7.94	4.29	1.43	
Ser 5	8.04	4.49		
Phe 6	8.16	4.19	3.23	7.28
Arg 7	8.09	4.32	1.95	1.84
Gly 8	8.23	3.94, 3.90		
His 9	8.23	3.98	3.41	
Ile 10	7.93	4.32	2.02	0.97
Thr 11	8.01	4.00	3.91	
Leu 15	8.09	4.38	1.67	1.27, 0.98
Lys 16	7.98	4.39	1.84	1.94
Gly 17	8.05	3.98		

† Chemical shifts for Arg 12, Lys 13, and Lys 14 could not be differentiated due to overlap in the NOE spectrum. Chemical shifts are ± 0.01 PPM.

Table 3. Chemical shifts of the neuromodulin peptide in aqueous solution.†

Residue	NH	α H	β H	other
Lys or Arg*	8.46	4.37	1.86	1.76, 1.65
Ile 2 or 10*	8.21	4.18	1.86	0.92, 1.50, 1.23
Gln 3	8.54	4.33	1.99, 2.11	2.40
Arg or Lys*	8.43	4.30	1.83	1.72, 1.39
Gly 8 or 17*	8.45	3.93		
Ile 10 or 2*	8.34	4.27	1.84	0.88, 1.46, 1.20
Thr 11	8.42	4.36	4.16	1.21
Arg or Lys*	8.39	4.28	1.77	1.69, 1.46
Lys or Arg*	8.33	4.34	1.83	1.80, 1.47
Lys or Arg*	8.29	4.27	1.80	1.76, 1.72
Leu 15	8.36	4.37	1.65	0.92, 0.88
Lys or Arg*	8.25	4.41	1.85	1.70, 1.58
Gly 17 or 8*	8.31	3.95, 3.94		

† Chemical shifts are ± 0.01 PPM. Spin systems for Ala 4, Ser 5, Phe 6, and His 9 could not be assigned due to a lack of NOEs. *These residues could not be differentiated due to a lack of NOEs.