

Table of NMR Data for Bogorol A hexaacetate (**2**).

	δ		mult (<i>J</i> , Hz)	COSY ^b	HSQC-TOCSY ^b	HMBC ^{b,c}	TOCSY ^{b,c}	NOESY ^{b,c}
	¹³ C ^a	¹ H ^b						
2-Hydroxy-3-methyl-pentanoic acid, acetate (Hmp)								
CO	167.8							
1	76.8	4.75	d (5.6)	1.85	76.8, 36.1, 14.5	170.1, 167.8, 36.1, 23.8, 14.5	1.85, 1.50, 1.15, 0.88, 0.83	Hmp-CH ₃ Aba-2,NH
2	36.1	1.85		4.75, 0.88, 1.50, 1.15	36.1, 14.5, 23.8, 10.9			
3	23.8	1.50		4.75, 0.83	23.8, 10.9			
		1.15						
4	10.9	0.83		1.50, 1.15	10.9, 23.8, 36.1, 14.5, 76.8	36.1, 23.8		
5	14.5	0.88	d (7.2)	1.85	14.5, 36.1, 23.8, 10.9	76.8, 36.1, 23.8		Aba-2,NH
CH ₃	20.5	2.07				170.1		Hmp-1
CO'	170.1							
2-Amino-2-butenic acid (Aba)								
CO	163.9							
NH		9.54	s			167.8, 163.9, 120.7		Aba-2,3; Hmp-1,5
1	130.8							
2	120.7	5.66	q (7.2)	1.77	12.8	163.9, 130.8, 12.8	1.77	Aba-NH; Hmp-1,5; Leu1-NH
3	12.8	1.77		5.66	12.8	120.7, 130.8		
Leucine 1 (Leu1)								
CO	171.7							
NH		7.89	d (8.0)	4.30		163.9	4.30, 1.51, 1.63, 0.86, 0.84	Aba-2,NH; Orn-NH; Hmp-1
1	51.4	4.30	m	7.89, 1.51	51.4, 40.5,			
2	40.5	1.51		4.30, 1.63	40.5, 23.9, 23.0, 21.2			
3	23.9	1.63		0.86, 0.84, 1.51	23.9, 23.0, 21.2			
4	23.0	0.86		1.63	40.5	40.5, 23.9, 21.2		
5	21.2	0.84		1.63	40.5, 23.9	40.5, 23.9, 23.0		
Ornithine, acetate (Orn)								
CO	171.2							
NH		7.98	d (7.2)	4.29	52.4, 29.4	171.7	4.29, 1.63, 1.54, 1.39, 1.33	Leu1-NH; Ile-NH
1	52.4	4.29	m	7.98, 1.63, 1.54	52.4, 29.4			

2	29.4	1.63		4.29, 1.39,	37.9, 29.4, 25.4			
		1.54		1.33				
3	25.4	1.39		1.63, 1.54,	37.9, 29.4, 25.4			
		1.33		2.97				
4	37.9	2.97		1.39, 1.33	37.9, 29.4, 25.4			Orn-CH ₃
NH'		7.76		2.97	37.9, 25.4	168.9		
CO'	168.9							
CH ₃	22.4	1.76						Orn-NH'
				Isoleucine (Ile)				
CO	170.8							
NH		7.67	d (6.4)	4.23	56.5	171.2	4.23, 1.72, 1.37, 1.02, 0.77, 0.75	Orn-NH; Val1-NH
1	56.5	4.23		7.67, 1.72	56.5			
2	36.3	1.72		4.23, 0.77,	36.3, 24.0, 15.1			
				1.37				
3	24.0	1.37		1.72, 0.77	36.3, 24.0, 15.1, 10.7			
		1.02						
4	10.7	0.75	t (7.2)	1.37, 1.02	24.0, 10.7	36.3, 24.0		
5	15.1	0.77		1.72	56.4, 36.3, 24.0, 15.1	36.3, 24.0		
				Valine 1 (Val 1)				
CO	171.8							
NH		7.90	d (8.8)	4.17	57.8	170.8	4.17, 1.94, 0.81, 0.80	Ile-NH; Val2-NH
1	57.8	4.17	m	7.90, 1.94	57.8, 18.2, 17.8			
2	29.9	1.94		4.17, 0.81,	29.9, 18.2, 17.8			
				0.80				
3	17.8	0.81		1.94	57.8, 29.9, 18.2, 17.8	57.8, 29.9, 17.8		
4	18.2	0.80		1.94	57.8, 29.9, 18.2, 17.8	57.8, 29.9, 18.2		
				Valine 2 (Val 2)				
CO	170.7							
NH		7.76		4.18	57.8	171.8	4.18, 1.95, 0.81	Val1-NH; Lys1-NH
1	57.8	4.18	m	7.76, 1.95	57.8, 19.1, 19.0			
2	30.5	1.95		4.18, 0.81	30.5, 19.1, 19.0			
3	19.1	0.81		1.95	57.8, 30.5, 19.1, 19.0	57.8, 30.5, 19.0		
4	19.0	0.81		1.95	57.8, 30.5, 19.1, 19.0	57.8, 30.5, 19.1		
				Lysine 1 acetate (Lys 1)				
CO	171.5							
NH		7.97	d (7.2)	4.28	52.6	170.7	4.27, 1.63, 1.48, 1.24, 1.20	Val2-NH; Val3-NH

1	52.6	4.27	m	7.97, 1.63, 1.48	52.6, 31.7, 22.7			
2	31.7	1.63 1.48		4.27, 1.63, 1.48	31.7, 22.7			
3	22.7	1.24 1.20		1.63, 1.48, 1.33	38.2, 31.7, 28.6, 22.7			
4	28.6	1.33		1.24, 1.20, 2.95	38.2, 31.7, 28.6, 22.7			
5	38.2	2.95 7.73		1.33, 7.73 2.95	38.2, 28.6, 22.7 38.2, 28.6	168.8		Lys1-CH ₃
NH' CO' CH ₃	168.8 22.4	1.75						Lys1-NH'
CO	170.7				Valine 3 (Val 3)			
NH		7.75		4.16	57.8	171.5	4.16, 1.96, 0.79, 0.77	Lys1-NH; Leu2-NH
1	57.8	4.16	m	7.75, 1.96	57.8, 19.0, 17.8			Leu2-2,3
2	30.3	1.96		4.16, 0.79, 0.78	30.3, 19.0, 17.8			
3	19.0	0.79		1.96	57.8, 30.3, 19.0, 17.8	57.8, 30.3, 17.8		
4	17.8	0.78		1.96	57.8, 30.3, 19.0, 17.8	57.8, 30.3, 19.0		
CO	171.6				Leucine 2 (Leu 2)			
NH		8.05	d (7.2)	4.29	51.2, 40.7	170.7	4.29, 1.53, 1.43, 0.85, 0.80	Val3-NH; Lys2-NH
1	51.2	4.29	m	8.05, 1.43	51.2, 40.7			Tyr-NH; Lys2-,2,3
2	40.7	1.43		1.53, 4.29	51.2, 40.7, 24.1, 22.8, 21.3			Lys2-1?, Val3-1
3	24.1	1.53		1.43, 0.85, 0.80	22.8, 24.1, 21.3			Lys2-1?, Val3-1
4	22.8	0.85		1.53	40.7, 24.1, 22.8, 21.3	40.7, 24.1, 21.3		
5	21.3	0.80		1.53	40.7, 24.1, 22.8, 21.3	40.7, 24.1, 22.8		
CO	171.2				Lysine 2 acetate (Lys 2)			
NH		7.92	d (8.0)	4.20	52.2, 31.4	171.6	4.20, 1.39, 1.28, 0.99	Leu2-3,NH; Tyr-NH
1	52.2	4.20	m	7.92, 1.39, 1.28	52.2, 31.4, 22.3			Tyr-4,5,6,7; Leu3-NH
2	31.4	1.28 1.39		4.20	38.2, 31.4			Tyr-4,5,6,7

3	22.3	0.99		1.23	38.2, 31.4, 28.4, 22.3			Tyr-4,5,6,7
4	28.4	1.23		0.99	38.2, 28.4, 31.4, 22.3			Tyr-4,5,6,7
5	38.2	2.90		1.23, 7.68	38.2, 28.4, 22.3			Tyr-4,5,6,7
NH'		7.68		2.90	38.2, 28.4	168.7		Tyr-2; Lys2-CH ₃
CO'	168.7							
CH ₃	22.4	1.77						Lys2-NH'
Tyrosine (Try)								
CO	170.3							
NH		8.20	d (8.0)	4.57	54.0, 37.4	171.2	4.57, 2.98, 2.75	Lys2-NH; Leu3-NH;
1	54.0	4.57	m	8.20, 2.98, 2.75	54.0, 37.4	170.3		leu2-1
2	37.4	2.98	m	4.57	54.0, 37.4			Leu2-2,3
		2.75	dd (13.6, 10.4)					
3	134.8							
4,5	130.0	7.24		6.97		149.0, 130.0, 121.0, 37.4		Tyr-CH ₃ ; Lys2-1,2,3,4,5; Leu3-2,3,4,5
6,7	121.0	6.97		7.24		149.0, 134.8, 121.0		Tyr-CH ₃ ; Lys2-1,2,3,4,5; Leu3-2,3,4,5
8	149.0							
CO'	168.3							
CH ₃	20.7	2.23				168.3		
Leucine 3 (Leu 3)								
CO	170.7							
NH		8.14	d (8.8)	4.27	51.1, 41.0	170.3	4.27, 1.41, 1.36, 0.82, 0.77	Tyr-NH; Vol-NH; Lys2-1
1	51.1	4.27	m	8.14	51.1, 41.0			
2	41.0	1.41		4.27, 1.36	41.0, 23.9, 22.7, 21.7			Tyr-1,4,5,6,7
		1.36						
3	23.9	1.36		1.41, 0.82, 0.77	41.0, 23.9, 22.7, 21.7			Tyr-1,4,5,6,7
4	22.7	0.82		1.36	41.0, 23.9, 22.7, 21.7	41.0, 23.9, 21.7		Tyr-1,4,5,6,7
5	21.7	0.77		1.36	41.0, 23.9, 22.7, 21.7	41.0, 23.9, 22.7		Tyr-1,4,5,6,7
Valinol (Vol)								
NH		7.77		3.78	63.8, 52.4	170.7	3.78, 4.10, 3.85, 1.74, 0.86	Leu3-NH
1	52.4	3.78	m	7.77, 4.10, 3.85, 1.74	63.8, 52.4			

2	28.8	1.74		3.85, 0.86	28.8, 19.1, 18.3	
3	19.1	0.86		1.74	63.8, 28.8, 19.1, 18.3	52.4, 28.8, 18.3
4	18.3	0.84		1.74	63.8, 28.8, 19.1, 18.3	52.4, 28.8, 19.1
5	63.8	4.10	dd (11.2,4.8)	1.95, 3.78	63.8, 52.4	170.2, 52.4
		3.85	dd(11.2, 8.0)			
CO'	170.2					
CH ₃	20.4	1.95				170.2

^aSpectra acquired at 100 MHz in DMSO-d₆.

^bSpectra acquired at 800 MHz in DMSO-d₆.

^cSelected correlations reported.