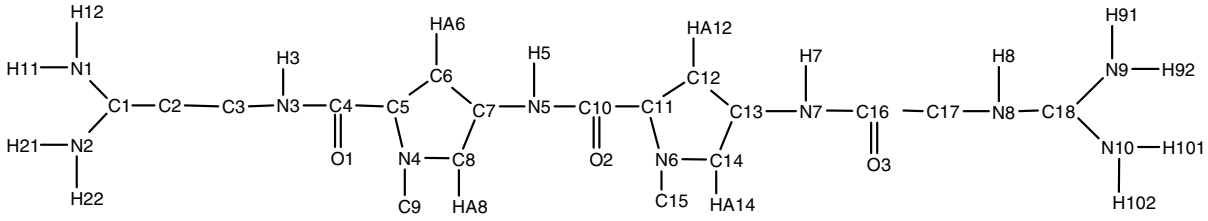
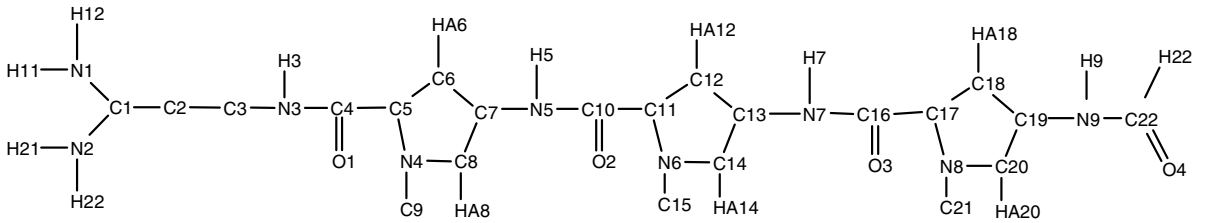
Supplementary material



(A)



(B)

Figure 1. The atomic numbering scheme used in the force field parameter tables for netropsin (A) and distamycin (B).

Netropsin 45A4 force field parameters

Table 1. Atom names, masses, van der Waals parameters and charges for Netropsin. Atom names according to Figure 1A. Charges in brackets are from the 45B4 force field.

Atom name	Mass (a.u.)	$C_6^{1/2}$ $(kJ\ mol^{-1}\ nm^6)^{1/2}$	$C_{12}^{1/2}$ $10^{-3}\ (kJ\ mol^{-1}\ nm^{12})^{1/2}$	Charge (*e*)	
N1	14.0067	0.04936	1.301 (2.148)[a]	-0.26	
H11	1.008	0.0	0.0	0.28	
H12	1.008	0.0	0.0	0.28	
N2	14.0067	0.04936	1.301 (2.148)[a]	-0.26	
H21	1.008	0.0	0.0	0.28	
H22	1.008	0.0	0.0	0.28	
C1	12.011	0.04838	1.837	0.40	
C2	14.027	0.08642 (0.06873)[b]	5.828 (2.178)[b]	0.00	
C3	14.027	0.08642 (0.06873)[b]	5.828 (2.178)[b]	0.00	
N3	14.0067	0.04936	1.301 (1.943)[a]	-0.28	
H3	1.008	0.0	0.0	0.28	
C4	12.011	0.04838	1.837	0.38	
O1	15.9994	0.04756	0.8611 (1.125)[a]	-0.38	
C5	12.011	0.04838	1.837	0.00	
C6	12.011	0.04838	1.837	-0.10	
HA6	1.008	0.0092	0.123	0.10	
C7	12.011	0.04838	1.837	0.00	
C8	12.011	0.04838	1.837	-0.10	
HA8	1.008	0.0092	0.123	0.10	
N4	14.0067	0.04936	1.301 (1.841)[a]	-0.20	
C9	15.035	0.09805 (0.08278)[b]	5.162 (2.456)[b]	0.20	
N5	14.0067	0.04936	1.301 (1.943)[a]	-0.28	
H5	1.008	0.0	0.0	0.28	
C10	12.011	0.04838	1.837	0.38	
O2	15.9994	0.04756	0.8611 (1.125)[a]	-0.38	
C11	12.011	0.04838	1.837	0.00	
C12	12.011	0.04838	1.837	-0.10	
HA12	1.008	0.0092	0.123	0.10	
C13	12.011	0.04838	1.837	0.00	
C14	12.011	0.04838	1.837	-0.10	
HA14	1.008	0.0092	0.123	0.10	
N6	14.0067	0.04936	1.301 (1.841)[a]	-0.20	
C15	15.035	0.09805 (0.08278)[b]	5.162 (2.456)[b]	0.20	
N7	14.0067	0.04936	1.301 (1.943)[a]	-0.28	
H7	1.008	0.0	0.0	0.28	
C16	12.011	0.04838	1.837	0.38	
O3	15.9994	0.04756	0.8611 (1.125)[a]	-0.38	
C17	14.027	0.08642 (0.06873)[b]	5.828 (2.178)[b]	0.09	(0.00)
N8	14.0067	0.04936	1.301 (1.984)[a]	-0.11	(-0.24)
H8	1.008	0.0	0.0	0.24	(0.24)
C18	12.011	0.04838	1.837	0.34	(0.00)
N9	14.0067	0.04936	1.301 (2.148)[a]	-0.26	(-0.48)
H91	1.008	0.0	0.0	0.24	(0.24)
H92	1.008	0.0	0.0	0.24	(0.24)
N10	14.0067	0.04936	1.301 (2.148)[a]	-0.26	(-0.48)
H101	1.008	0.0	0.0	0.24	(0.24)
H102	1.008	0.0	0.0	0.24	(0.24)

a) In brackets, the value for $C_{12}(II)^{1/2}$ is given which is to be used in polar interactions. b) In brackets, the van der Waals parameters are given to be used in 1,4-interactions.

Table 2. Bond parameters for Netropsin. Atom names according to Figure 1A.

Bond	Force constant K_{b_n} (10^6 kJmol^{-1}nm^{-4})	Ideal bond length b_{0n} (nm)	Bond	Force constant K_{b_n} (10^6 kJmol^{-1}nm^{-4})	Ideal bond length b_{0n} (nm)
N1-H11	18.7	0.100	C10-O2	16.6	0.123
N1-H12	18.7	0.100	C10-C11	7.15	0.153
N2-H21	18.7	0.100	C11-C12	11.8	0.133
N2-H22	18.7	0.100	C12-HA12	12.3	0.109
N1-C1	10.5	0.134	C12-C13	11.8	0.133
N2-C1	10.5	0.134	C13-C14	11.8	0.133
C1-C2	7.15	0.153	C14-HA14	12.3	0.109
C2-C3	7.15	0.153	C14-N6	11.8	0.133
C3-N3	8.71	0.147	N6-C15	5.73	0.148
N3-H3	18.7	0.100	N6-C11	11.8	0.133
N3-C4	11.8	0.133	C13-N7	8.71	0.147
C4-O1	16.6	0.123	N7-H7	18.7	0.100
C4-C5	7.15	0.153	N7-C16	11.8	0.133
C5-C6	11.8	0.133	C16-O3	16.6	0.123
C6-HA6	12.3	0.109	C16-C17	7.15	0.153
C6-C7	11.8	0.133	C17-N8	8.71	0.147
C7-C8	11.8	0.133	N8-H8	18.7	0.100
C8-HA8	12.3	0.109	N8-C18	10.5	0.134
C8-N4	11.8	0.133	C18-N9	10.5	0.134
N4-C9	5.73	0.148	N9-H91	18.7	0.100
N4-C5	11.8	0.133	N9-H92	18.7	0.100
C7-N5	8.71	0.147	C18-N10	10.5	0.134
N5-H5	18.7	0.100	N10-H101	18.7	0.100
N5-C10	11.8	0.133	N10-H102	18.7	0.100

Table 3. Bond-angle parameters for Netropsin. Atom names according to Figure 1A.

Bond angle	Force constant K_{θ_n} (kJmol^{-1})	Ideal bond angle θ_{0_n} (degree)	Bond angle	Force constant K_{θ_n} (kJmol^{-1})	Ideal bond angle θ_{0_n} (degree)
H11-N1-H12	445	120.0	O2-C10-C11	685	121.0
H21-N2-H22	445	120.0	N5-C10-C11	610	115.0
C1-N1-H11	390	120.0	C10-C11-C12	640	126.0
C1-N1-H12	390	120.0	N6-C11-C12	465	108.0
C1-N2-H21	390	120.0	N6-C11-C10	640	126.0
C1-N2-H22	390	120.0	C11-C12-HA12	575	126.0
N1-C1-N2	670	120.0	HA12-C12-C13	575	126.0
N1-C1-C2	670	120.0	C11-C12-C13	465	108.0
N2-C1-C2	670	120.0	C12-C13-C14	465	108.0
C1-C2-C3	530	111.0	C12-C13-N7	640	126.0
C2-C3-N3	530	111.0	C14-C13-N7	640	126.0
C3-N3-H3	460	115.0	C13-C14-HA14	575	126.0
H3-N3-C4	415	123.0	HA14-C14-N6	575	126.0
C3-N3-C4	700	122.0	C13-C14-N6	465	108.0
N3-C4-O1	730	124.0	C14-N6-C15	640	126.0
O1-C4-C5	685	121.0	C15-N6-C11	640	126.0
N3-C4-C5	610	115.0	C14-N6-C11	465	108.0
C4-C5-C6	640	126.0	C13-N7-H7	460	115.0
C6-C5-N4	465	108.0	H7-N7-C16	415	123.0
N4-C5-C4	640	126.0	C13-N7-C16	700	122.0
C5-C6-HA6	575	126.0	N7-C16-O3	730	124.0
C5-C6-C7	465	108.0	O3-C16-C17	685	121.0
HA6-C6-C7	575	126.0	N7-C16-C17	610	115.0
C6-C7-C8	465	108.0	C16-C17-N8	520	109.5
C6-C7-N5	640	126.0	C17-N8-H8	465	116.0
C8-C7-N5	640	126.0	H8-N8-C18	390	120.0
C7-C8-HA8	575	126.0	C17-N8-C18	730	124.0
HA8-C8-N4	575	126.0	N8-C18-N9	670	120.0
C7-C8-N4	465	108.0	N8-C18-N10	670	120.0
C8-N4-C9	640	126.0	N9-C18-N10	670	120.0
C9-N4-C5	640	126.0	H91-N9-H92	445	120.0
C8-N4-C5	465	108.0	C18-N9-H91	390	120.0
C7-N5-H5	460	115.0	C18-N9-H92	390	120.0
H5-N5-C10	415	123.0	C18-N10-H101	390	120.0
C7-N5-C10	700	122.0	C18-N10-H102	390	120.0
N5-C10-O2	730	124.0	H101-N10-H102	445	120.0

Table 4. Improper dihedral-angle parameters for Netropsin. Atom names according to Figure 1A.

Improper diheral angle	Force constant K_{ξ_n} ($kJmol^{-1}degree^{-2}$)	Ideal improper dihedral angle ξ_{0_n} (degree)
N1-H11-H12-C1	0.0510	0.0
N2-H21-H22-C1	0.0510	0.0
C1-N1-N2-C2	0.0510	0.0
N3-C3-H3-C4	0.0510	0.0
C4-N3-O1-C5	0.0510	0.0
C5-C4-C6-N4	0.0510	0.0
C6-C5-HA6-C7	0.0510	0.0
C7-C6-C8-N5	0.0510	0.0
C8-C7-HA8-N4	0.0510	0.0
N4-C5-C8-C9	0.0510	0.0
C5-C6-C7-C8	0.0510	0.0
C6-C7-C8-N4	0.0510	0.0
C7-C8-N4-C5	0.0510	0.0
C8-N4-C5-C6	0.0510	0.0
N4-C5-C6-C7	0.0510	0.0
N5-C7-H5-C10	0.0510	0.0
C10-N5-O2-C11	0.0510	0.0
C11-C10-C12-N6	0.0510	0.0
C12-C11-HA12-C13	0.0510	0.0
C13-C12-C14-N7	0.0510	0.0
C14-C13-HA14-N6	0.0510	0.0
N6-C11-C14-C15	0.0510	0.0
C11-C12-C13-C14	0.0510	0.0
C12-C13-C14-N6	0.0510	0.0
C13-C14-N6-C11	0.0510	0.0
C14-N6-C11-C12	0.0510	0.0
N6-C11-C12-C13	0.0510	0.0
N7-C13-H7-C16	0.0510	0.0
C16-N7-O3-C17	0.0510	0.0
N8-C17-H8-C18	0.0510	0.0
C18-N8-N9-N10	0.0510	0.0
N9-C18-H91-H92	0.0510	0.0
N10-C18-H101-H102	0.0510	0.0

Table 5. Dihedral-angle parameters for Netropsin. Atom names according to Figure 1A.

Dihedral angle	Force constant K_{φ_n} ($kJmol^{-1}$)	Phase shift $\cos(\delta_n)$	Multiplicity m_n
H11-N1-C1-C2	33.5	-1.0	2
H21-N2-C1-C2	33.5	-1.0	2
N1-C1-C2-C3	1.0	+1.0	6
C1-C2-C3-N3	5.92	+1.0	3
C2-C3-N3-C4	1.0	-1.0	6
C3-N3-C4-C5	33.5	-1.0	2
N3-C4-C5-C6	33.5	-1.0	2
C6-C7-N5-C10	33.5	-1.0	2
C7-N5-C10-C11	33.5	-1.0	2
N5-C10-C11-C12	33.5	-1.0	2
C12-C13-N7-C16	33.5	-1.0	2
C13-N7-C16-C17	33.5	-1.0	2
N7-C16-C17-N8	1.0	+1.0	6
C16-C17-N8-C18	1.0	-1.0	6
C17-N8-C18-N9	33.5	-1.0	2
N8-C18-N9-H91	33.5	-1.0	2
N8-C18-N10-H101	33.5	-1.0	2

Distamycin 45A4 force field parameters

Table 6. Atom names, masses, van der Waals parameters and charges for Distamycin. Atom names according to Figure 1B.

Atom name	Mass (a.u.)	$C_6^{1/2}$ (kJ mol^{-1} nm^{-6})$^{1/2}$	$C_{12}^{1/2}$ 10^{-3} (kJ mol^{-1} nm^{-12})$^{1/2}$	Charge (*e*)
N1	14.0067	0.04936	1.301 (2.148)[a]	-0.26
H11	1.008	0.0	0.0	0.28
H12	1.008	0.0	0.0	0.28
N2	14.0067	0.04936	1.301 (2.148)[a]	-0.26
H21	1.008	0.0	0.0	0.28
H22	1.008	0.0	0.0	0.28
C1	12.011	0.04838	1.837	0.40
C2	14.027	0.08642 (0.06873)[b]	5.828 (2.178)[b]	0.00
C3	14.027	0.08642 (0.06873)[b]	5.828 (2.178)[b]	0.00
N3	14.0067	0.04936	1.301 (1.943)[a]	-0.28
H3	1.008	0.0	0.0	0.28
C4	12.011	0.04838	1.837	0.38
O1	15.9994	0.04756	0.8611 (1.125)[a]	-0.38
C5	12.011	0.04838	1.837	0.00
C6	12.011	0.04838	1.837	-0.10
HA6	1.008	0.0092	0.123	0.10
C7	12.011	0.04838	1.837	0.00
C8	12.011	0.04838	1.837	-0.10
HA8	1.008	0.0092	0.123	0.10
N4	14.0067	0.04936	1.301 (1.841)[a]	-0.20
C9	15.035	0.09805 (0.08278)[b]	5.162 (2.456)[b]	0.20
N5	14.0067	0.04936	1.301 (1.943)[a]	-0.28
H5	1.008	0.0	0.0	0.28
C10	12.011	0.04838	1.837	0.38
O2	15.9994	0.04756	0.8611 (1.125)[a]	-0.38
C11	12.011	0.04838	1.837	0.00
C12	12.011	0.04838	1.837	-0.10
HA12	1.008	0.0092	0.123	0.10
C13	12.011	0.04838	1.837	0.00
C14	12.011	0.04838	1.837	-0.10
HA14	1.008	0.0092	0.123	0.10
N6	14.0067	0.04936	1.301 (1.841)[a]	-0.20
C15	15.035	0.09805 (0.08278)[b]	5.162 (2.456)[b]	0.20
N7	14.0067	0.04936	1.301 (1.943)[a]	-0.28
H7	1.008	0.0	0.0	0.28
C16	12.011	0.04838	1.837	0.38
O3	15.9994	0.04756	0.8611 (1.125)[a]	-0.38
C17	12.011	0.04838	1.837	0.00
C18	12.011	0.04838	1.837	-0.10
HA18	1.008	0.0092	0.123	0.10
C19	12.011	0.04838	1.837	0.00
C20	12.011	0.04838	1.837	-0.10
HA20	1.008	0.0092	0.123	0.10
N8	14.0067	0.04936	1.301 (1.841)[a]	-0.20
C21	15.035	0.09805 (0.08278)[b]	5.162 (2.456)[b]	0.20
N9	14.0067	0.04936	1.301 (1.943)[a]	-0.28
H9	1.008	0.0	0.0	0.28
C22	12.011	0.04838	1.837	0.28
H22	1.008	0.0092	0.123	0.10
O4	15.9994	0.04756	0.8611 (1.125)[a]	-0.38

Table 7. Bond parameters for Distamycin. Atom names according to Figure 1B.

Bond	Force constant K_{b_n} (10^6 kJmol^{-1}nm^{-4})	Ideal bond length b_{0n} (nm)	Bond	Force constant K_{b_n} (10^6 kJmol^{-1}nm^{-4})	Ideal bond length b_{0n} (nm)
N1-H11	18.7	0.100	C11-C12	11.8	0.133
N1-H12	18.7	0.100	C12-HA12	12.3	0.109
N2-H21	18.7	0.100	C12-C13	11.8	0.133
N2-H22	18.7	0.100	C13-C14	11.8	0.133
N1-C1	10.5	0.134	C14-HA14	12.3	0.109
N2-C1	10.5	0.134	C14-N6	11.8	0.133
C1-C2	7.15	0.153	N6-C15	5.73	0.148
C2-C3	7.15	0.153	N6-C11	11.8	0.133
C3-N3	8.71	0.147	C13-N7	8.71	0.147
N3-H3	18.7	0.100	N7-H7	18.7	0.100
N3-C4	11.8	0.133	N7-C16	11.8	0.133
C4-O1	16.6	0.123	C16-O3	16.6	0.123
C4-C5	7.15	0.153	C16-C17	7.15	0.153
C5-C6	11.8	0.133	C17-C18	11.8	0.133
C6-HA6	12.3	0.109	C18-HA18	12.3	0.109
C6-C7	11.8	0.133	C18-C19	11.8	0.133
C7-C8	11.8	0.133	C19-C20	11.8	0.133
C8-HA8	12.3	0.109	C20-HA20	12.3	0.109
C8-N4	11.8	0.133	C20-N8	11.8	0.133
N4-C9	5.73	0.148	N8-C21	5.73	0.148
N4-C5	11.8	0.133	N8-C17	11.8	0.133
C7-N5	8.71	0.147	C19-N9	8.71	0.147
N5-H5	18.7	0.100	N9-H9	18.7	0.100
N5-C10	11.8	0.133	N9-C22	11.8	0.133
C10-O2	16.6	0.123	C22-H22	12.3	0.109
C10-C11	7.15	0.153	C22-O4	16.6	0.123

Table 8. Bond-angle parameters for Distamycin. Atom names according to Figure 1B.

Bond angle	Force constant K_{θ_n} (kJmol^{-1})	Ideal bond angle θ_{0_n} (degree)	Bond angle	Force constant K_{θ_n} (kJmol^{-1})	Ideal bond angle θ_{0_n} (degree)
H11-N1-H12	445	120.0	N6-C11-C10	640	126.0
H21-N2-H22	445	120.0	C11-C12-HA12	575	126.0
C1-N1-H11	390	120.0	HA12-C12-C13	575	126.0
C1-N1-H12	390	120.0	C11-C12-C13	465	108.0
C1-N2-H21	390	120.0	C12-C13-C14	465	108.0
C1-N2-H22	390	120.0	C13-C14-HA14	575	126.0
N1-C1-N2	670	120.0	HA14-C14-N6	575	126.0
N1-C1-C2	670	120.0	C13-C14-N6	465	108.0
N2-C1-C2	670	120.0	C14-N6-C15	640	126.0
C1-C2-C3	530	111.0	C15-N6-C11	640	126.0
C2-C3-N3	530	111.0	C14-N6-C11	465	108.0
C3-N3-H3	460	115.0	C12-C13-N7	640	126.0
H3-N3-C4	415	123.0	C14-C13-N7	640	126.0
C3-N3-C4	700	122.0	C13-N7-H7	460	115.0
N3-C4-O1	730	124.0	H7-N7-C16	415	123.0
O1-C4-C5	685	121.0	C13-N7-C16	700	122.0
N3-C4-C5	610	115.0	N7-C16-O3	730	124.0
C4-C5-C6	640	126.0	O3-C16-C17	685	121.1
C6-C5-N4	465	108.0	N7-C16-C17	610	115.0
N4-C5-C4	640	126.0	C16-C17-C18	640	126.0
C5-C6-HA6	575	126.0	C18-C17-N8	465	108.0
C5-C6-C7	465	108.0	N8-C17-C16	640	126.0
HA6-C6-C7	575	126.0	C17-C18-HA18	575	126.0
C6-C7-C8	465	108.0	HA18-C18-C19	575	126.0
C6-C7-N5	640	126.0	C17-C18-C19	465	108.0
C8-C7-N5	640	126.0	C19-C20-HA20	575	126.0
C7-C8-HA8	575	126.0	HA20-C20-N8	575	126.0
HA8-C8-N4	575	126.0	C19-C20-N8	465	108.0
C7-C8-N4	465	108.0	C20-N8-C21	640	126.0
C8-N4-C9	640	126.0	C21-N8-C17	640	126.0
C9-N4-C5	640	126.0	C20-N8-C17	465	108.0
C8-N4-C5	465	108.0	C18-C19-N9	640	126.0
C7-N5-H5	460	115.0	C20-C19-N9	640	126.0
H5-N5-C10	415	123.0	C18-C19-C20	465	108.0
C7-N5-C10	700	122.0	C19-N9-H9	460	115.0
N5-C10-O2	730	124.0	H9-N9-C22	415	123.0
O2-C10-C11	685	121.0	C19-N9-C22	700	122.0
N5-C10-C11	610	115.0	N9-C22-H22	610	115.0
C10-C11-C12	640	126.0	N9-C22-O4	730	124.0
N6-C11-C12	465	108.0	O4-C22-H22	685	121.0

Table 9. Improper dihedral-angle parameters for Distamycin. Atom names according to Figure 1B.

Improper diheral angle	Force constant K_{ξ_n} ($kJmol^{-1}degree^{-2}$)	Ideal improper dihedral angle ξ_{0_n} (degree)
N1-H11-H12-C1	0.0510	0.0
N2-H21-H22-C1	0.0510	0.0
C1-N1-N2-C2	0.0510	0.0
N3-C3-H3-C4	0.0510	0.0
C4-N3-O1-C5	0.0510	0.0
C5-C4-C6-N4	0.0510	0.0
C6-C5-HA6-C7	0.0510	0.0
C7-C6-C8-N5	0.0510	0.0
C8-C7-HA8-N4	0.0510	0.0
N4-C5-C8-C9	0.0510	0.0
C5-C6-C7-C8	0.0510	0.0
C6-C7-C8-N4	0.0510	0.0
C7-C8-N4-C5	0.0510	0.0
C8-N4-C5-C6	0.0510	0.0
N4-C5-C6-C7	0.0510	0.0
N5-C7-H5-C10	0.0510	0.0
C10-N5-O2-C11	0.0510	0.0
C11-C10-C12-N6	0.0510	0.0
C12-C11-HA12-C13	0.0510	0.0
C13-C12-C14-N7	0.0510	0.0
C14-C13-HA14-N6	0.0510	0.0
N6-C11-C14-C15	0.0510	0.0
C11-C12-C13-C14	0.0510	0.0
C12-C13-C14-N6	0.0510	0.0
C13-C14-N6-C11	0.0510	0.0
C14-N6-C11-C12	0.0510	0.0
N6-C11-C12-C13	0.0510	0.0
N7-C13-H7-C16	0.0510	0.0
C16-N7-O3-C17	0.0510	0.0
C17-C16-C18-N8	0.0510	0.0
C18-C17-HA18-C19	0.0510	0.0
C19-C18-C20-N9	0.0510	0.0
C20-C19-HA20-N8	0.0510	0.0
N8-C17-C20-C21	0.0510	0.0
C17-C18-C19-C20	0.0510	0.0
C18-C19-C20-N8	0.0510	0.0
C19-C20-N8-C17	0.0510	0.0
C20-N8-C17-C18	0.0510	0.0
N8-C17-C18-C19	0.0510	0.0
N9-C19-H9-C22	0.0510	0.0
C22-N9-O4-H22	0.0510	0.0

Table 10. Dihedral-angle parameters for Distamycin. Atom names according to Figure 1B.

Dihedral angle	Force constant K_{φ_n} ($kJmol^{-1}$)	Phase shift $\cos(\delta_n)$	Multiplicity m_n
H11-N1-C1-C2	33.5	-1.0	2
H21-N2-C1-C2	33.5	-1.0	2
N1-C1-C2-C3	1.0	+1.0	6
C1-C2-C3-N3	5.92	+1.0	3
C2-C3-N3-C4	1.0	-1.0	6
C3-N3-C4-C5	33.5	-1.0	2
N3-C4-C5-C6	33.5	-1.0	2
C6-C7-N5-C10	33.5	-1.0	2
C7-N5-C10-C11	33.5	-1.0	2
N5-C10-C11-C12	33.5	-1.0	2
C12-C13-N7-C16	33.5	-1.0	2
C13-N7-C16-C17	33.5	-1.0	2
N7-C16-C17-C18	33.5	-1.0	2
C18-C19-N9-C22	33.5	-1.0	2
C19-N9-C22-H22	33.5	-1.0	2