

Supplementary Material

Chemical shifts (ppm) of the [TAGGGTTA]₄-distamycin complex

DNA	H6/H8	H1/H2/CH ₃	H1', H2'	Distamycin	
T1	7.22	1.65	6.06, 1.81	CH ₃ -1	3.51
A2	8.23	7.96	6.18	CH ₃ -2	3.49
G3	7.94	11.51	5.99	CH ₃ -3	3.59
G4	7.67	11.19	5.97	H3-1	6.34
G5	7.59	10.80	6.18	H3-2	6.34
T6	7.46	1.79	6.07, 2.19	H3-3	6.51
T7	7.28	1.68	5.86, 1.85	H5-1	6.77
A8	8.12	7.89	6.16	H5-2	6.71
				H5-3	6.80
				HF	7.84

Chemical shifts (ppm) of [TAGGGTTA]₄

DNA	H6/H8	H1/H2/CH ₃	H1', H2'
T1	7.15	1.54	5.87, 1.72
A2	8.24	7.97	6.15
G3	7.99	11.52	5.99
G4	7.67	11.26	5.96
G5	7.63	10.82	6.18
T6	7.40	1.71	6.05, 2.20
T7	7.29	1.66	5.86, 1.83
A8	8.07	7.82	6.13

Chemical shifts (ppm) of the [TAGGGTT]₄-distamycin complex

DNA	H6/H8	H1/H2/ CH ₃	H1', H2'	Distamycin	
T1	7.24	1.69	6.12, 1.83	CH ₃ -1	3.59
A2	8.25	7.91	6.20	CH ₃ -2	3.58
G3	7.90	11.42	5.96	CH ₃ -3	3.64
G4	7.64	11.06	6.06	H3-1	6.48
G5	7.75	10.97	6.05	H3-2	6.54
G6	7.59	10.96	6.18	H3-3	6.58
T7	7.49	1.81	6.09, 2.25	H5-1	6.87
T8	7.45	1.68	6.04, 2.16	H5-2	6.82
				H5-3	6.88
				HF	7.97

Chemical shifts (ppm) of [TAGGGGTT]₄

DNA	H6/H8	H1/H2/ CH ₃	H1', H2'
T1	7.14	1.55	5.87, 1.72
A2	8.23	7.97	6.16
G3	8.04	11.42	5.98
G4	7.64	11.06	6.05
G5	7.76	10.98	6.04
G6	7.59	10.93	6.16
T7	7.26	1.68	5.90, 2.14
T8	7.40	1.63	5.99, 2.12

Chemical shifts (ppm) of the [TAGGGGT]₄-distamycin complex

DNA	H6/H8	H1/H2/ CH ₃	H1', H2'	Distamycin	
T1	7.20	1.68	6.13, 1.84	CH ₃ -1	3.54
A2	8.20	7.93	6.19	CH ₃ -2	3.51
G3	7.84	11.37	5.95	CH ₃ -3	3.61
G4	7.51	10.91	6.00	H3-1	6.44
G5	7.63	10.74	6.06	H3-2	6.36
G6	7.69	10.78	6.02	H3-3	6.49
G7	7.58	10.69	6.17	H5-1	6.78
T8	7.50	1.80	6.18, 2.29	H5-2	6.70
				H5-3	6.80
				HF	7.86

Chemical shifts (ppm) of [TAGGGGT]₄

DNA	H6/H8	H1/H2/ CH ₃	H1', H2'
T1	7.08	1.52	5.85, 1.70
A2	8.17	7.92	6.13
G3	7.89	11.35	5.97
G4	7.53	10.96	6.00
G5	7.65	10.77	6.06
G6	7.72	10.82	6.00
G7	7.58	10.82	6.19
T8	7.26	1.61	6.03, 2.16