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Supplementary Material for Microfilm Edition

Table 1 *Assignments of the non-exchangeable ^1H DNA resonances of the free and bound d(CACGTG)$_2$ duplex.*

	H6/H8	H2/CH_3/H5	H1'	H2'	H2''	H3'	H4'	H5'	H5''
				Free d(CACGTG)$_2$ duplex					
C1	7.81	6.04	5.70	2.09	2.51	4.80	4.14	3.80	3.80
A2	8.48	8.01	6.33	2.87	3.00	5.12	4.50	4.22	4.07
C3	7.42	5.40	5.67	2.14	2.45	4.92	4.28	4.30	4.23
G4	8.02	-----	6.05	2.72	2.83	5.05	4.46	4.21	4.14
T5	7.30	1.62	5.93	2.01	2.44	4.93	4.24	4.31	4.18
G6	8.01	-----	6.23	2.70	2.41	4.76	4.26	4.19	4.14
				hedamycin:d(CACGTG)$_2$ complex					
C1	7.73	5.96	5.60	1.74	2.34	4.71	4.08	3.81	3.77
A2	8.43	7.94	6.27	2.82	2.95	5.09	4.50	4.19	4.07
C3	7.53	5.45	5.91	2.47	2.39	5.15	4.31	4.38	4.28
G4	8.31	-----	6.16	2.90	2.98	5.17	4.86	4.31	4.24
T5	7.31	1.45	5.86	2.18	2.44	5.01	4.35	4.12	4.32
G6	7.99	-----	6.23	2.71	2.43	4.77	4.25	4.22	4.16
C7	7.75	5.99	5.63	1.99	2.41	4.73	4.08	3.79	3.79
A8	8.34	7.93	6.27	2.75	2.94	5.09	4.47	4.19	4.05
C9	7.48	5.10	6.23	2.27	2.40	5.09	3.95	4.20	n.d.
G10	n/a	-----	6.02	2.48	2.67	4.86	4.53	n.d	n.d.
T11	7.29	1.41	5.73	n.d.	2.43	4.91	4.08	3.53	n.d.
G12	7.93	-----	6.17	2.61	2.44	4.67	4.19	4.14	n.d.

Table 2 *Assignments of the exchangeable ^1H DNA resonances of the free and bound d(CACGTG)$_2$ duplex.*

	NH_2 (1)	NH_2 (2)	NH	H8
	Free d(CACGTG)$_2$ duplex			
C1	7.08	8.20	--------	-----
A2	n.d.	n.d.	--------	-----
C3	6.68	8.25	--------	-----
G4	n.d.	n.d.	12.83	-----
T5	--------	--------	14.02	-----
G6	n.d.	n.d.	13.03	-----
	hedamycin:d(CACGTG)$_2$ complex			
C1	6.86	8.26	-----	-----
A2	n.d.	n.d.	-----	-----
C3	6.46	7.75	-----	-----
G4	n.d.	n.d.	13.58	-----
T5	-----	-----	14.08	-----
G6	n.d.	n.d.	n.d.	-----
C7	6.99	8.16	-----	-----
A8	n/a	n/a	-----	-----
C9	6.91	7.30	-----	-----
G10	6.47	7.25	11.87	9.76
T11	-----	-----	14.08	-----
G12	n.d.	n.d.	n.d.	-----

Table 3 Assignments of ^{1}H *hedamycin resonances arising from free and bound hedamycin.*

Epoxide	Free	Bound	Ring E	Free	Bound	Ring F	Free	Bound
$CH_3{}^{19}$	1.42	1.92	$CH_3{}^{7'}$	1.42	1.68	$CH_3{}^{7''}$	1.42	1.57
H^{18}	3.30	5.27	$H^{2'}$	3.66	3.96	$H^{2''}$	4.22	4.31
H^{17}	3.25	3.92	$H^{3'}$	3.70	3.73	$H^{3''}$	3.85	4.31
H^{16}	3.52	3.52	$H^{4'}$	3.70	3.85	$H^{5a''}$	2.38	3.22
$CH_3{}^{15}$	1.79	1.27	$H^{5a'}$	1.88	2.11	$H^{5b''}$	2.91	2.65
Ring A-D			$H^{5b'}$	2.62	1.45	$H^{6''}$	5.35	5.65
H^{3}	6.23	6.23	$H^{6'}$	5.35	5.64	$CH_3{}^{8''}$	1.12	1.18
$CH_3{}^{13}$	2.54	2.44	N-CH_3a	----	2.90	N-CH_3a	----	2.93
H^{6}	7.52	6.79	N-CH_3b	----	2.97	N-CH_3b	----	3.02
H^{9}	8.08	8.27	N-$(CH_3)_2$	2.94	----	N-$(CH_3)_2$	2.79	----

Table 4 *Intermolecular NOEs*

Chromophore	Epoxide Chain	Ring E	Ring F
H6/C3H6	$CH_3$15/C9H6	H2′/G4H1′	H5a″/C9H1′
H6/C3H5	$CH_3$15/C9H5	H2′/G4H4′	H5a″/G10H4′
H6/C3H1′	$CH_3$15/C9H1′	H3′/G4H4′	H6″/C9H1′
H6/C3H3′	$CH_3$15/C9H2′	H4′/G4H1′	H6″/G10H1′
H6/C3H2′	$CH_3$15/C9H2″	H4′/G4H4′	H6″/G10H4′
H6/C3H2″	$CH_3$15 /G10H1′	H5a′/G4H1′	H6″/G10H5′
H6/G4H8	$CH_3$15/G10H8	H5a′/T11H4′	H6″/G10H5″
H6/G10NH1	H16/G10H8	H5b′/T11H4′	$CH_3$7″/C9H4′
$CH_3$13/C3H5	H17/G10H8	H6′/G4H1′	$CH_3$7″/T11H4′
$CH_3$13/G10NH1	H18/G10H8	$CH_3$7′/G4H1′	$CH_3$8″/T5NH
H9/T11H4′	H18/T11CH_3	$CH_3$7′/T5H1′	$CH_3$8″/A8H2
H9/G10H5′	$CH_3$19/G10H8	$CH_3$7′/T5H4′	$CH_3$8″/C9H1′
H9/T11H5″	$CH_3$19/T11CH_3	N-CH_3/A2H2	$CH_3$8″/C9H4′
		N-CH_3/T11H1′	NCH3/A8H2
		N-CH_3/T3H1′	NCH_3/C9H1′
		N-CH_3/T11H4′	NCH_3/C9H2″
		N-CH_3/C3H4′	NCH_3/G10H2″
			NCH_3/C9H4′

Table 5 *AMBER potential types and partial charges of hedamycin, used in molecular modeling.*

Atom	Pot.	Par.Chg	Atom	Pot.	Par.Chg	Atom	Pot.	Par.Chg
C2	C	0.090	C16	CT	-0.058	H2N3	HC	0.084
C3	CA	-0.270	H16	HT	0.138	N	NT	-0.312
H3	HC	0.186	C17	CT	0.005	O1	OE	-0.296
C4	C	0.298	H17	HT	0.126	O6	OT	-0.314
C4A	CA	-0.170	C18	CT	0.000	HO6	HY	0.201
C5	CA	0.038	H18	HC	0.000	C6	CS	0.089
C13	CT	-0.177	C19	CT	-0.206	H6	HT	0.131
H131	HC	0.083	H191	HC	0.093	C2	CS	-0.009
H132	HC	0.112	H192	HC	0.074	H2	HT	0.080
H133	HC	0.114	H193	HC	0.084	C7	CT	-0.198
C6	CA	-0.116	O14	OE	-0.247	H71	HC	0.083
H6	HC	0.167	O17	OE	-0.318	H72	HC	0.085
C6A	CA	-0.060	HO17	HO	0.200	H73	HC	0.098
C7	C	0.305	C6	CS	0.084	C3	CS	0.018
C7A	CA	-0.082	H6	HT	0.103	H3	HT	0.116
C8	CA	-0.038	C5	CS	-0.220	C4	CS	0.050
C9	CA	-0.053	H51	HT	0.117	C4M	CT	-0.241
H9	HC	0.164	H52	HT	0.091	H4M1	HC	0.084
C10	CA	-0.098	C4	CS	0.028	H4M2	HC	0.078
C11	CA	0.149	H4	HT	0.111	H4M3	HC	0.084
C11A	CA	-0.194	C3	CT	0.013	C5	CS	-0.189
C12	C	0.329	H3	HT	0.080	HC	0.084	0.108
C12A	CA	-0.140	C2	CS	0.003	C1N	CT	-0.085
C12B	CA	0.149	H2	HT	0.089	H1N1	HC	0.079
O1	OE	-0.118	C7	CT	-0.210	H1N2	HC	0.092
O12	O	-0.315	H71	HC	0.094	H1N3	HC	0.036
O11	OH	-0.282	H72	HC	0.083	C2N	CT	-0.085
H11	HO	0.262	H73	HC	0.085	H2N1	HC	0.080
O7	O	-0.282	C1N	CT	-0.087	H2N2	HC	0.040
O4	O	-0.302	H1N1	HC	0.082	H2N3	HC	0.080
C14	CT	0.053	H1N2	HC	0.080	N1	NT	-0.326
C15	CT	-0.188	H1N3	HC	0.038	O9	OE	-0.280
H151	HC	0.085	C2N	CT	-0.086	O10	OT	-0.309

H152	HC	0.111	H2N1	HC	0.082	H10	HY	0.214
H153	HC	0.104	H2N2	HC	0.040			

Table 6 *AMBER potential types and partial charges of the adducted guanine, used in molecular modeling.*

Atom	Pot.	Par.Chg	Atom	Pot.	Par.Chg
P	P	1.385	H5'2	HC	0.021
O1P	O2	-0.847	O4'	OS	-0.368
O2P	O2	-0.847	N2	N2	-0.778
O5'	OS	-0.509	H21	H2	0.325
O3'	OS	-0.509	H22	H2	0.339
C1'	CT	0.376	O6	O	-0.458
H1'	HC	0.009	C6	C	0.690
C2'	CT	-0.307	C5	CB	-0.060
H2'1	HC	0.081	N7	NB	-0.543
H2'2	HC	0.081	C8	CK	0.266
C3'	CT	0.233	H8	HC	0.046
H3'	HC	0.025	N9	N*	-0.042
C4'	CT	0.036	C4	CB	0.391
H4'	HC	0.056	N3	NC	-0.709
C5'	CT	0.118	C2	CA	0.871
H5'1	HC	0.021	N1	NA	-0.729
			H1	H	0.336