

Supplementary material

Figure 1. Pair-wise rmsds *versus* nucleotide for: 9-a-p-DACA compared with each structure, (a) sugar-phosphate atoms; (b) base atoms; and for all structures compared with all others, (c) sugar-phosphate atoms; (d) base atoms.

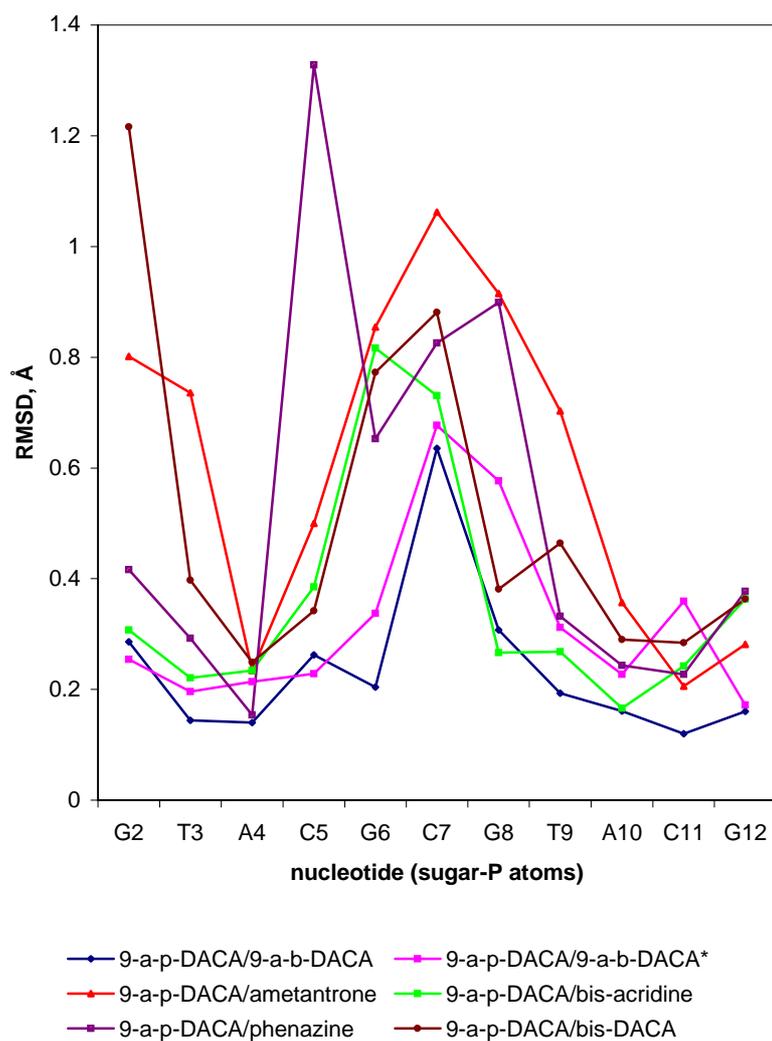


Fig. 1(a)

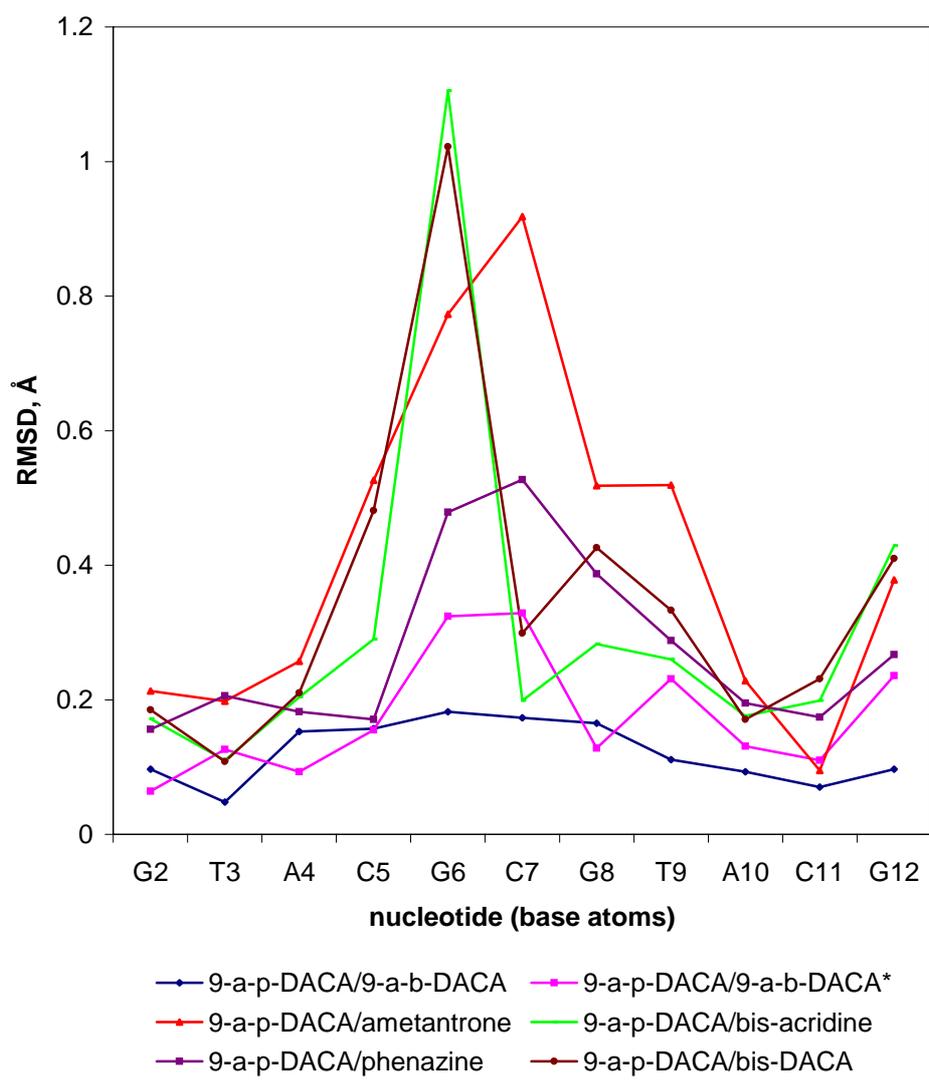
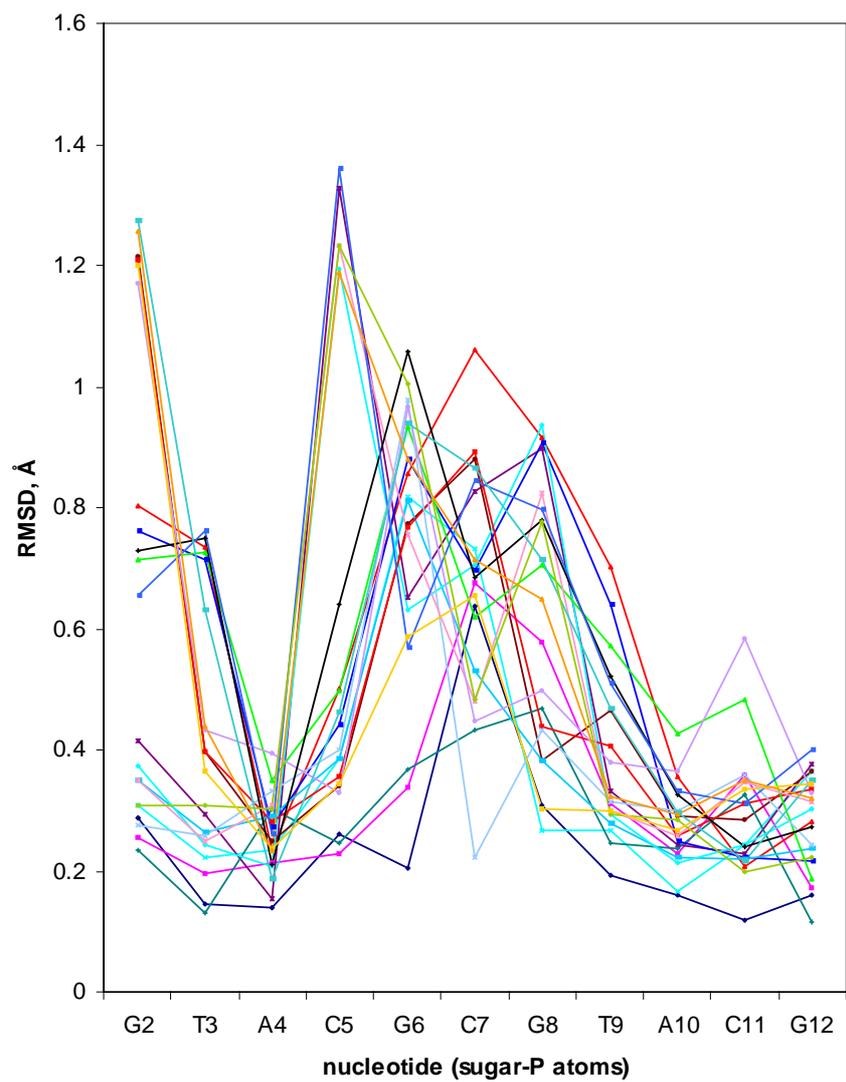


Fig. 1(b)



- | | |
|----------------------------|-----------------------------|
| — 9-a-p-DACA/9-a-b-DACA | — 9-a-p-DACA/9-a-b-DACA* |
| — 9-a-p-DACA/ametrantrone | — 9-a-p-DACA/bis-acridine |
| — 9-a-p-DACA/phenazine | — 9-a-p-DACA/bis-DACA |
| — 9-a-b-DACA/9-a-b-DACA* | — 9-a-b-DACA/ametrantrone |
| — 9-a-b-DACA/bis-acridine | — 9-a-b-DACA/phenazine |
| — 9-a-b-DACA/bis-DACA | — 9-a-b-DACA*/ametrantrone |
| — 9-a-b-DACA*/bis-acridine | — 9-a-b-DACA*/phenazine |
| — 9-a-b-DACA*/bis-DACA | — ametrantrone/bis-acridine |
| — ametrantrone/phenazine | — ametrantrone/bis-DACA |
| — bis-acridine/phenazine | — bis-acridine/bis-DACA |
| — phenazine/bis-DACA | |

Fig. 1(c)

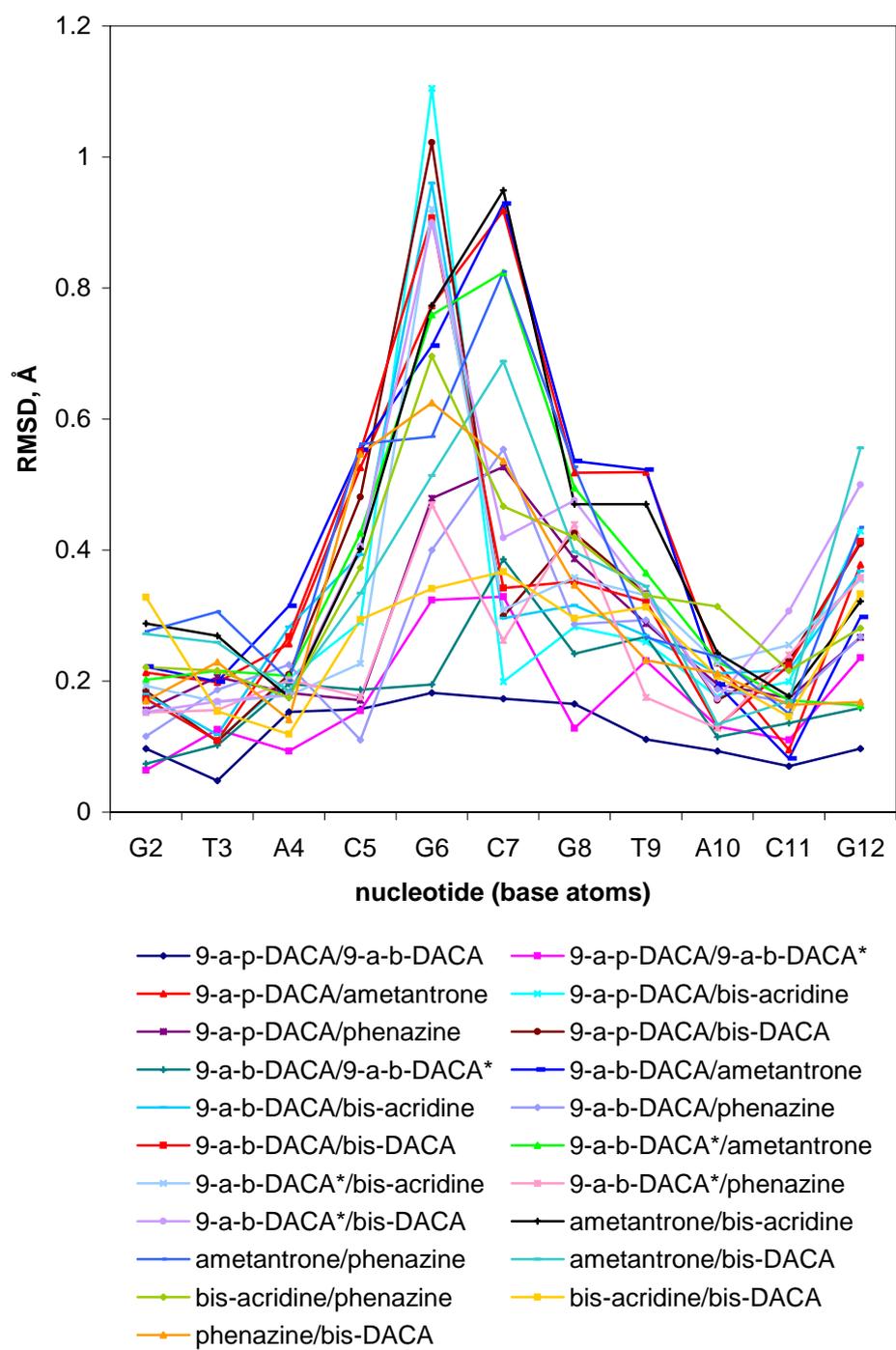


Fig. 1(d)

Table 1 α (P-O5')

	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2							
T3	-60	-48	-50	-108	-45	61	-63
A4	-68	-53	-69	-46	-65	-49	-62
C5	-57	-67	-61	-49	-136	-33	-62
G6	-66	-64	-79	-99	46	25	-76
C7							
G8							
T9	-61	-66	-70	-66	-52	-13	-64
A10	-73	-71	-64	-38	-74	-82	-65
C11	-63	-54	-63	-66	-57	-72	-69
G12	-59	-57	-60	-88	-42	-52	-56

using CG^{5Br}UACG in place of CGTACG

Table 2 β (O5'-C5')

	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2							
T3	173	164	168	180	155	-141	168
A4	-167	-172	-171	178	-163	174	-175
C5	177	165	170	-178	42	167	173
G6	-144	-150	-150	-138	138	162	-136
C7							
G8							
T9	-176	-179	-171	-171	-175	162	-179
A10	-157	-165	-168	-173	-172	-161	-166
C11	177	171	168	-178	168	177	175
G12	-167	-176	-166	-149	-175	-174	-172

using CG^{5Br}UACG in place of CGTACG

Table 3 γ (C5'-C4')

	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2	41	27	67	136	20	49	36
T3	43	34	43	79	44	-109	50
A4	41	28	46	35	42	32	43
C5	44	52	42	30	-163	29	43
G6	40	36	60	90	-38	-21	56
C7	81	180	169	-41	-74	-131	-99
G8	75	60	38	59	3.4	48	58
T9	62	60	68	65	54	26	63
A10	46	41	48	20	52	57	47
C11	43	33	45	51	46	52	44
G12	64	61	64	90	57	58	65

using CG^{5Br}UACG in place of CGTACG

Table 4 δ (C4'-C3')

	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2	147	153	139	35	151	147	145
T3	106	111	109	110	102	140	108
A4	134	138	132	123	128	118	132
C5	118	109	108	112	131	116	117
G6	80	81	93	-37	90	99	79
C7	123	133	151	164	147	141	153
G8	87	84	83	87	98	91	84
T9	134	136	144	160	139	130	137
A10	140	144	141	140	137	137	136
C11	134	131	128	125	123	135	128
G12	89	99	98	93	105	99	97

using CG^{5Br}UACG in place of CGTACG

Table 5 ϵ (C3'-O3')

	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2	-167	-167	-172	174	-169	-160	-176
T3	166	168	169	-171	161	-169	174
A4	-173	-172	-177	-177	165	-173	-175
C5	-164	-158	-165	-175	-131	-141	-162
G6							
C7	-129	-134	-131			-103	-130
G8	-163	-174	-169	176	170	-154	-176
T9	174	178	179	-166	177	163	178
A10	-166	-162	-171	-177	-159	-168	-171
C11	-156	-160	-160	-172	-156	-152	-161
G12							

using CG^{5Br}UACG in place of CGTACG

Table 6 ζ (O3'-P)

	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine #	ametantrone	bis-acridine
G2	-94	-97	-97	20	-117	-114	-88
T3	-84	-87	-83	-115	-80	-100	-94
A4	-95	-88	-92	-83	-9.9	-91	-89
C5	-110	-87	-94	-92	-96	-117	-102
G6							
C7	65	75	68	84		59	69
G8	-77	-55	-70	-72	-78	-100	-70
T9	-86	-82	-102	-131	-101	-75	-99
A10	-92	-90	-88	-89	-103	-94	-86
C11	-82	-76	-84	-72	-94	-91	-87
G12							

using CG^{5Br}UACG in place of CGTACG

Table 7 χ (C1'-N)

	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2	-110	-117	-118	-119	-101	-100	-108
T3	-115	-120	-122	-117	-112	-121	-126
A4	-109	-117	-113	-106	-102	-110	-108
C5	-106	-128	-126	-100	-142	-121	-112
G6	-80	-88	-88	-83	-67	-64	-70
C7	-115	-117	-119	-99	-97	-123	-113
G8	-159	-161	-162	-158	-136	-176	-163
T9	-121	-128	-127	-101	-116	-116	-121
A10	-112	-119	-117	-107	-122	-113	-114
C11	-97	-106	-110	-91	-90	-100	-94
G12	-57	-65	-60	-49	-55	-54	-55

using CG^{5Br}UACG in place of CGTACG

Table 8

P

	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2	178	180	160	179	188	175	164
T3	112	111	112	125	101	163	104
A4	149	146	140	135	176	117	132
C5	125	110	99	138	222	124	110
G6	14	20	19	66	9.0	36	14
C7	135	149	156	209	195	146	164
G8	29	21	14	33	66	45	36
T9	159	150	158	183	170	142	150
A10	165	164	162	188	162	158	156
C11	147	132	134	155	146	132	130
G12	339	335	347	341	332	349	335

using CG^{5Br}UACG in place of CGTACG

Table 9

Shift (Å)

base pair	step	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2-C11								
	2	-0.2	-0.3	-0.3	-0.4	-0.4	-0.1	0.0
T3-A10								
	3	-0.3	-0.2	-0.3	-0.2	-0.6	-0.4	-0.5
A4-T9								
	4	0.8	0.7	0.7	0.8	0.8	0.5	0.7
C5-G8								
	5 ^c	2.6	2.4	2.8	3.7	2.3	3.3	3.0
G6-C7*								
B DNA ^b		0						
A DNA ^b		-4.4						

using CG^{5Br}UACG in place of CGTACG

Table 10

Slide (Å)

base pair	step	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2-C11								
	2	-0.1	-0.1	0.0	-0.1	0.0	-0.1	-0.2
T3-A10								
	3	-0.1	-0.2	-0.1	0.1	-0.5	0.1	0.0
A4-T9								
	4	-0.3	-0.1	-0.4	-0.4	-0.2	-0.6	-0.3
C5-G8								
	5 ^c	2.1	2.0	2.4	2.3	1.3	1.2	2.3
G6-C7*								

using CG^{5Br}UACG in place of CGTACG

Table 11

Rise (Å)

base pair	step	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2-C11								
	2	3.0	3.0	3.1	2.9	3.2	3.0	3.1
T3-A10								
	3	3.2	3.2	3.0	3.2	3.3	3.1	2.9
A4-T9								
	4	2.9	2.8	3.2	2.8	2.9	2.7	2.7
C5-G8								
	5 ^c	7.2	7.3	6.9	8.0	7.3	6.9	8.5
G6-C7*								

using CG^{5Br}UACG in place of CGTACG

Table 12

Tilt (deg)

base pair	step	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2-C11								
	2	-4.3	-2.5	-5.5	-2.8	-2.0	-0.4	-6.0
T3-A10								
	3	0.3	0.3	-0.5	1.1	6.0	3.9	4.8
A4-T9								
	4	-6.6	-5.0	-6.0	-8.6	-1.5	-4.6	-3.8
C5-G8								
	5 ^c	-1.9	0.2	-2.0	-2.6	4.0	3.6	-0.4
G6-C7*								

using CG^{5Br}UACG in place of CGTACG

Table 13

Roll (deg)

base pair	step	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2-C11								
	2	-0.3	-0.9	-1.1	-2.0	1.0	2.7	1.6
T3-A10								
	3	-1.3	1.6	-0.9	-3.2	-1.8	-0.1	-2.8
A4-T9								
	4	2.2	-1.2	3.4	3.6	1.9	1.9	4.9
C5-G8								
	5 ^c	-5.5	-5.4	0.0	-9.4	-9.0	-17.7	-7.0
G6-C7*								

using CG^{5Br}UACG in place of CGTACG

Table 14

Twist (deg)

base pair	step	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2-C11								
	2	31	30	34	26	29	29	28
T3-A10								
	3	36	36	37	40	34	36	37
A4-T9								
	4	27	29	26	24	33	27	28
C5-G8								
	5 ^c	57	54	57	58	51	60	57
G6-C7*								

using CG^{5Br}UACG in place of CGTACG

Table 15

Propeller twist (deg)

base pair	step	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2-C11		3.4	3.8	2.7	4.3	9.7	-10.0	-6.4
	2							
T3-A10		-1.2	-1.0	-4.1	4.9	-0.6	-11.7	-8.6
	3							
A4-T9		4.5	4.9	3.6	2.8	3.8	-7.7	-3.0
	4							
C5-G8		1.1	0.61	-1.6	5.3	2.3	8.3	-0.6
	5 ^c							
G6-C7*		-8.7	-8.4	-8.6	-9.6	-9.3	-23.6	-15.9

using CG^{5Br}UACG in place of CGTACG

Table 16

Buckle (deg)

base pair	step	9-a-p-DACA	9-a-b-DACA	9-a-b-DACA#	bis-DACA	phenazine#	ametantrone	bis-acridine
G2-C11		-11.8	-12.2	-10.5	-12	-10	-11	-10.2
	2							
T3-A10		1.7	2.6	0.2	4.3	3.2	-0.1	-2.6
	3							
A4-T9		-3.8	-6.2	2.0	-0.5	-3.9	-2.1	2.0
	4							
C5-G8		17.3	15.6	13.5	19.6	9.0	17.9	24.8
	5 ^c							
G6-C7*		0.5	-4.7	-2.5	-0.9	1.2	15.9	-1.7

using CG^{5Br}UACG in place of CGTACG

Table 17: Rmsds, Å, for base atoms

Structures	Nucleotide										
	G2	T3	A4	C5	G6	C7	G8	T9	A10	C11	G12
9-a-p-DACA/9-a-b-DACA	0.097	0.048	0.153	0.157	0.182	0.173	0.165	0.111	0.093	0.07	0.097
9-a-p-DACA/9-a-b-DACA*	0.064	0.126	0.093	0.155	0.324	0.329	0.128	0.231	0.131	0.11	0.236
9-a-p-DACA/ametrantrone	0.213	0.198	0.257	0.526	0.773	0.918	0.518	0.519	0.228	0.095	0.378
9-a-p-DACA/bis-acridine	0.172	0.11	0.204	0.29	1.105	0.199	0.283	0.26	0.176	0.199	0.429
9-a-p-DACA/phenazine	0.156	0.206	0.182	0.171	0.479	0.527	0.387	0.288	0.195	0.174	0.267
9-a-p-DACA/bis-DACA	0.185	0.108	0.21	0.481	1.022	0.299	0.426	0.333	0.171	0.231	0.41
9-a-b-DACA/9-a-b-DACA*	0.074	0.102	0.196	0.187	0.195	0.386	0.242	0.268	0.115	0.136	0.159
9-a-b-DACA/ametrantrone	0.222	0.199	0.315	0.553	0.712	0.929	0.536	0.523	0.195	0.082	0.298
9-a-b-DACA/bis-acridine	0.18	0.118	0.283	0.393	0.96	0.296	0.316	0.269	0.212	0.217	0.368
9-a-b-DACA/phenazine	0.116	0.187	0.225	0.11	0.4	0.554	0.287	0.293	0.188	0.167	0.268
9-a-b-DACA/bis-DACA	0.173	0.109	0.268	0.55	0.907	0.342	0.352	0.322	0.131	0.224	0.413
9-a-b-DACA*/ametrantrone	0.202	0.216	0.208	0.426	0.759	0.824	0.495	0.365	0.23	0.171	0.163

9-a-b-DACA*/bis-acridine	0.193	0.168	0.178	0.227	0.921	0.309	0.358	0.331	0.228	0.255	0.355
9-a-b-DACA*/phenazine	0.152	0.156	0.202	0.176	0.469	0.262	0.439	0.175	0.128	0.24	0.358
9-a-b-DACA*/bis-DACA	0.153	0.169	0.18	0.406	0.9	0.419	0.476	0.332	0.173	0.307	0.5
ametantrone/bis-acridine	0.288	0.269	0.175	0.402	0.773	0.949	0.47	0.47	0.243	0.177	0.322
ametantrone/phenazine	0.276	0.306	0.201	0.562	0.573	0.825	0.527	0.267	0.237	0.15	0.435
ametantrone/bis-DACA	0.272	0.259	0.185	0.334	0.514	0.688	0.397	0.345	0.134	0.17	0.556
bis-acridine/phenazine	0.221	0.216	0.175	0.373	0.696	0.467	0.42	0.331	0.314	0.216	0.281
bis-acridine/bis-DACA	0.328	0.154	0.119	0.294	0.341	0.367	0.296	0.313	0.207	0.146	0.333
phenazine/bis-DACA	0.17	0.229	0.141	0.547	0.625	0.536	0.347	0.232	0.212	0.164	0.168

* using CG^{5Br}UACG in place of CGTACG

Table 18: Rmsds, Å, for sugar and phosphate atoms

Structure	Nucleotide										
	G2	T3	A4	C5	G6	C7	G8	T9	A10	C11	G12
9-a-p-DACA/9-a-b-DACA	0.286	0.144	0.14	0.262	0.204	0.636	0.307	0.193	0.161	0.12	0.16
9-a-p-DACA/9-a-b-DACA*	0.254	0.196	0.214	0.228	0.337	0.677	0.577	0.312	0.227	0.359	0.172
9-a-p-DACA/ametatrone	0.802	0.736	0.234	0.5	0.855	1.062	0.915	0.703	0.357	0.206	0.281
9-a-p-DACA/bis-acridine	0.307	0.221	0.234	0.385	0.817	0.731	0.266	0.268	0.166	0.242	0.363
9-a-p-DACA/phenazine	0.416	0.292	0.154	1.328	0.653	0.826	0.899	0.332	0.243	0.227	0.377
9-a-p-DACA/bis-DACA	1.216	0.397	0.249	0.342	0.773	0.881	0.381	0.464	0.29	0.284	0.363
9-a-b-DACA/9-a-b-DACA*	0.234	0.131	0.303	0.246	0.366	0.434	0.469	0.246	0.236	0.326	0.115
9-a-b-DACA/ametatrone	0.761	0.713	0.273	0.442	0.88	0.697	0.908	0.641	0.25	0.222	0.216
9-a-b-DACA/bis-acridine	0.351	0.264	0.291	0.384	0.811	0.531	0.383	0.279	0.223	0.22	0.237
9-a-b-DACA/phenazine	0.373	0.242	0.206	1.193	0.632	0.704	0.937	0.293	0.214	0.242	0.303
9-a-b-DACA/bis-DACA	1.208	0.396	0.28	0.357	0.766	0.892	0.439	0.405	0.257	0.312	0.334
9-a-b-DACA*/ametatrone	0.713	0.726	0.351	0.497	0.933	0.618	0.706	0.571	0.426	0.482	0.187

9-a-b-DACA*/bis-acridine	0.277	0.259	0.331	0.399	0.978	0.223	0.434	0.314	0.299	0.359	0.244
9-a-b-DACA*/phenazine	0.351	0.25	0.307	1.232	0.755	0.481	0.825	0.298	0.257	0.347	0.315
9-a-b-DACA*/bis-DACA	1.17	0.432	0.393	0.328	0.967	0.446	0.499	0.379	0.363	0.584	0.328
ametantrone/bis-acridine	0.728	0.749	0.21	0.641	1.058	0.683	0.778	0.521	0.325	0.239	0.273
ametantrone/phenazine	0.656	0.761	0.261	1.36	0.568	0.845	0.796	0.51	0.333	0.311	0.399
ametantrone/bis-DACA	1.274	0.63	0.188	0.462	0.938	0.865	0.715	0.467	0.295	0.216	0.351
bis-acridine/phenazine	0.308	0.309	0.303	1.233	1.005	0.482	0.777	0.294	0.284	0.2	0.222
bis-acridine/bis-DACA	1.199	0.364	0.238	0.343	0.587	0.656	0.303	0.3	0.267	0.336	0.343
phenazine/bis-DACA	1.256	0.438	0.235	1.189	0.879	0.715	0.649	0.322	0.294	0.351	0.319

* using CG^{5Br}UACG in place of CGTACG