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Table S1. Selected minimum energy conformations for 5' d(TpTpGpApG^{AN}pGpCpCpG) 3' modified nonamers[a,b,c]

No	α_4	β_4	γ_4	P_4	χ_4	ε_4	ζ_4	α_5	β_5	γ_5	P_5	χ_5	α'	β'	ε_5	ζ_5	α_6	β_6	γ_6	P_6	χ_6	Me_6	ε_6	ζ_6	ΔE	Class
1	309	184	39	165	251	175	256	303	185	44	127	237	162	42	178	252	309	176	50	154	240		185	240	0.0	major
	299	178	53	160	238	186	239	296	177	55	159	236			183	252	298	189	44	149	240	80	187	241		

[a]Torsional angles and pseudorotation paremeters are in degrees. ΔE is in kcal/mol.

[b]Angles for the unmodified strand are given just below those for the modified strand. The residues on each strand are numbered from the 5' end.

[c]The angles are given for the central trimer of the nonamer.

Table S2. Selected minimum energy conformations for 5' d(GpApApTpG^{AN}pGpTpGpC) 3' modified nonamers[a,b,c]

No	α_4	β_4	γ_4	P_4	χ_4	Me_4	ε_4	ζ_{54}	α_5	β_5	γ_5	P_5	χ_5	α'	β'	ε_5	ζ_{55}	α_6	β_6	γ_6	P_6	χ_6	ε_6	ζ_{56}	ΔE	Class
1	306	184	53	153	235	51	177	257	307	185	51	116	230	188	39	173	258	314	171	57	147	232	178	249	0.0	major
	304	174	53	162	234		189	235	294	172	62	158	230			176	248	310	182	54	155	229	181	244		

[a]Torsional angles and pseudorotation paremeters are in degrees. ΔE is in kcal/mol.

[b]Angles for the unmodified strand are given just below those for the modified strand. The residues on each strand are numbered from the 5' end.

[c]The angles are given for the central trimer of the nonamer.

Table S3. Selected minimum energy conformations for 5' d(TpTpGpApG^{AF}pGpCpCpG) 3' modified nonamers[a,b,c]

No	α_4	β_4	γ_4	P_4	χ_4	ε_4	ζ_{54}	α_5	β_5	γ_5	P_5	χ_5	α'	β'	ε_5	ζ_{55}	α_6	β_6	γ_6	P_6	χ_6	Me_6	ε_6	ζ_{56}	ΔE	Class[d]
1	297	175	56	160	254	188	231	293	172	55	128	67	261	316	192	277	299	180	43	155	249		187	240	0.0	minor
	301	174	54	161	238	182	246	298	185	51	166	239			185	252	292	176	57	144	240	146	187	237		
2	304	177	52	163	252	182	239	294	179	53	127	67	249	141	189	273	304	176	44	155	248		186	241	0.8	minor
	301	176	54	161	237	181	248	298	187	50	166	239			188	243	298	169	57	145	237	145	185	243		
3	309	184	39	166	249	175	256	303	185	44	128	236	165	227	178	252	310	176	50	153	240		184	244	2.3	major
	300	177	53	160	238	186	240	297	177	55	160	236			182	253	298	189	43	148	240	81	187	241		
4	308	184	51	163	237	177	249	315	179	52	119	229	197	39	177	255	316	171	52	144	234		182	241	2.4	major
	303	173	53	160	238	184	234	300	170	61	160	230			178	249	309	184	52	157	228	44	182	241		
5	300	171	66	159	243	219	181	212	177	66	192	340	220	42	210	275	308	174	56	171	233		186	243	4.0	BD
	302	177	56	156	230	269	183	302	120	63	154	241			209	190	302	139	65	153	240	115	186	235		

[a]Torsional angles and pseudorotation paremeters are in degrees. ΔE is in kcal/mol.

[b]Angles for the unmodified strand are given just below those for the modified strand. The residues on each strand are numbered from the 5' end.

[c]The angles are given for the central trimer of the nonamer.

[d]BD = guanine base displaced

Table S4. Selected minimum energy conformations for 5' d(GpApApTpG^{AF}pGpTpGpC) 3' modified nonamers[a,b,c]

No	α_4	β_4	γ_4	P_4	χ_4	Me_4	ε_4	ζ_{4}	α_5	β_5	γ_5	P_5	χ_5	α'	β'	ε_5	ζ_{5}	α_6	β_6	γ_6	P_6	χ_6	ε_6	ζ_{6}	ΔE	Class[d]
1	302	172	54	146	239	40	189	239	294	174	54	130	67	248	137	188	273	305	176	43	153	249	188	244	0.0	minor
	302	173	53	161	239		187	243	296	181	52	162	240			181	243	297	178	58	169	247	182	241		
2	307	184	52	154	234	48	177	256	307	185	53	111	228	203	212	174	259	315	170	56	144	230	177	250	0.1	major
	308	173	53	162	233		187	235	297	172	61	159	228			177	249	312	183	53	152	230	181	244		
3	309	185	49	158	234	35	180	249	317	178	49	127	232	191	45	177	252	308	170	60	147	232	179	247	0.7	major
	307	174	54	161	232		188	236	295	173	61	159	230			176	248	310	181	56	154	229	181	245		
4	302	173	55	149	240	36	189	240	290	173	57	132	68	259	314	192	275	306	177	38	155	251	185	246	1.2	minor
	300	172	55	162	238		185	247	295	187	49	166	243			182	241	294	177	60	170	249	181	237		
5	303	170	60	143	232	160	216	189	218	178	65	193	341	218	40	205	280	302	181	57	172	232	183	233	3.2	BD
	309	170	56	156	228		273	190	313	108	62	141	241			211	180	303	136	59	162	233	183	233		
6	305	171	59	149	229	33	178	257	303	219	26	151	235	160	233	189	280	295	172	47	146	252	178	251	3.5	major
	301	176	52	164	242		193	279	284	166	49	42	239			181	254	297	159	73	168	247	177	245		

[a]Torsional angles and pseudorotation paremeters are in degrees. ΔE is in kcal/mol.

[b]Angles for the unmodified strand are given just below those for the modified strand. The residues on each strand are numbered from the 5' end.

[c]The angles are given for the central trimer of the nonamer.

[d]BD = guanine base displaced

Table S5. Selected minimum energy conformations for 5' d(TpTpGpApG^{AP}pGpCpCpG) 3' modified nonamers[a,b,c]

No	α_4	β_4	γ_4	P_4	χ_4	ε_4	ζ_4	α_5	β_5	γ_5	P_5	χ_5	α'	β'	ε_5	ζ_5	α_6	β_6	γ_6	P_6	χ_6	Me_6	ε_6	ζ_6	ΔE	Class[d]
1	309	184	39	165	249	175	256	304	185	44	129	236	161	228	178	252	310	176	49	153	240		184	240	0.0	major
	300	177	53	160	238	185	240	297	177	55	159	236			182	254	298	190	43	148	240	81	187	241		
2	299	172	64	160	240	221	180	213	177	66	193	336	218	220	208	275	308	171	62	173	230		186	239	0.5	BD
	304	175	57	157	226	268	184	301	129	60	156	236			212	184	300	134	69	157	243	81	185	237		
3	305	179	51	166	251	181	240	294	179	54	123	64	243	139	187	274	307	174	44	150	244		184	240	4.6	minor
	301	180	51	162	239	183	246	297	184	51	163	237			189	237	299	167	58	147	237	144	185	245		

[a]Torsional angles and pseudorotation paremeters are in degrees. ΔE is in kcal/mol.

[b]Angles for the unmodified strand are given just below those for the modified strand. The residues on each strand are numbered from the 5' end.

[c]The angles are given for the central trimer of the nonamer.

[d]BD = guanine base displaced

Table S6. Selected minimum energy conformations for 5' d(GpApApTpG^{AP}pGpTpGpC) 3' modified nonamers[a,b,c]

No	α_4	β_4	γ_4	P_4	χ_4	Me_4	ε_4	ζ_4	α_5	β_5	γ_5	P_5	χ_5	α'	β'	ε_5	ζ_5	α_6	β_6	γ_6	P_6	χ_6	ε_6	ζ_6	ΔE	Class[d]
1	309	173	55	149	229	43	179	258	308	186	49	121	230	191	223	176	255	316	172	52	145	232	182	247	0.0	major
	300	176	53	158	240		187	234	298	169	60	158	230			176	252	307	188	51	158	231	180	246		
2	309	184	50	159	234	38	180	247	316	176	50	131	231	151	73	177	252	309	173	57	148	232	179	246	1.7	major
	305	173	56	160	232		185	240	296	177	60	158	229			177	249	308	182	55	152	229	180	244		
3	305	172	55	146	235	159	219	188	218	179	65	194	340	214	222	203	273	307	174	63	172	227	184	244	2.8	BD
	308	163	64	152	224		275	194	315	112	59	137	237			212	179	302	133	64	162	237	184	239		
4	300	175	54	145	240	47	187	244	288	178	57	127	66	247	137	187	274	305	175	44	150	245	185	244	3.1	minor
	302	173	53	162	239		180	252	294	190	50	165	242			184	238	295	177	58	170	248	182	241		
5	304	171	59	149	231	31	180	255	302	221	24	150	235	164	232	187	280	294	173	50	150	254	180	250	3.7	major
	299	175	52	165	245		189	279	285	169	49	53	237			184	257	297	160	73	165	248	176	245		

[a]Torsional angles and pseudorotation paremeters are in degrees. ΔE is in kcal/mol.

[b]Angles for the unmodified strand are given just below those for the modified strand. The residues on each strand are numbered from the 5' end.

[c]The angles are given for the central trimer of the nonamer.

[d]BD = guanine base displaced