Figure S1. Calculated electrostatic charges on O^6-[4-oxo[3-pyridyl)butyl]guanine

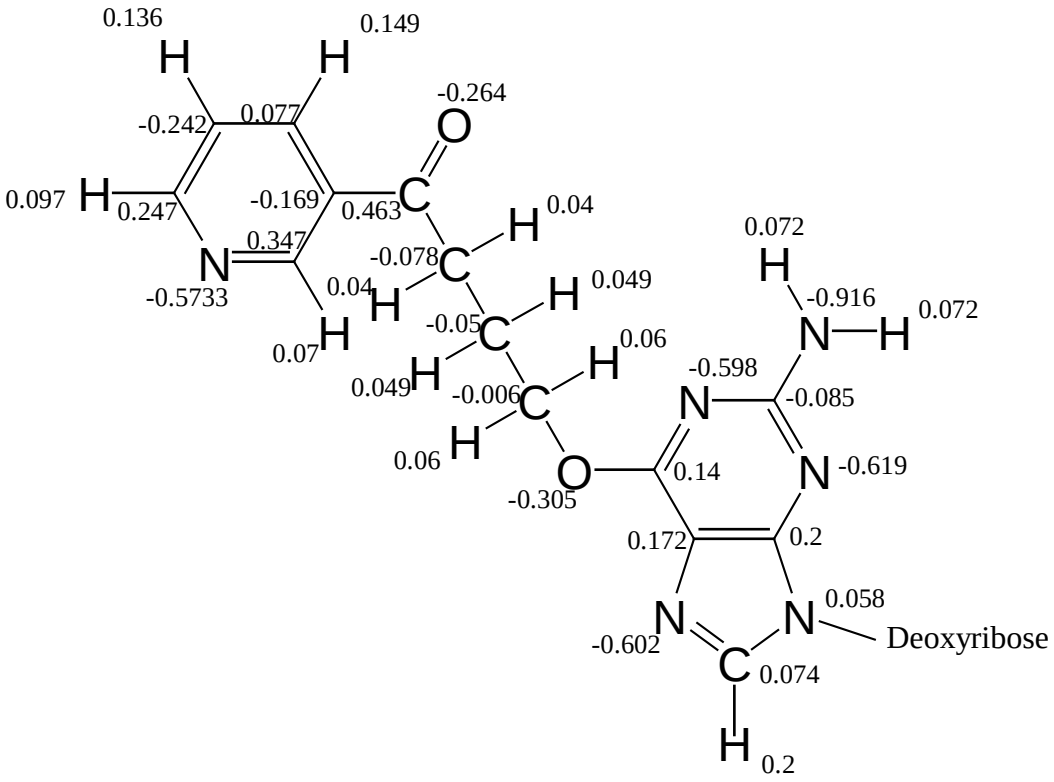

Table S1. Bond, angle, and torsion parameters for O^6-[4-oxo[3-pyridyl)butyl]guanine

Bond	Kcal/mol (Å)^2	Å		
CA-OS	450.0	1.364		
Angle	Kcal/mol rad^2	degrees		
NC-CA-CA	70.0	120.00		
NC-CA-OS	80.0	120.00		
NC-CA-H4	35.0	120.00		
CA-NC-CA	70.0	120.00		
CA-C -CT	70.0	120.00		
CA-C -O	80.0	120.00		
CT-OS-CA	60.0	120.00		
CA-CA-OS	80.0	120.00		
NC-CA-NC	70.0	129.10		
CB-CA-OS	80.0	120.00		
Torsion		Kcal/mol	degrees	
CT-CT-CT-OS	1	1.25	0.0	2
C –CT-CT-CT	1	1.25	0.0	-3
C -CT-CT-CT	1	0.15	180	-2
C -CT-CT-CT	1	0.25	180	1
X -CA-OS-X	3	1.5	0.0	3

Figure S2 Root mean square deviations (RMSD) from the starting structure for the POB- and Me- guanine containing duplex DNA. POB-duplex values are shown as a solid line and Me-duplex as a dotted line.

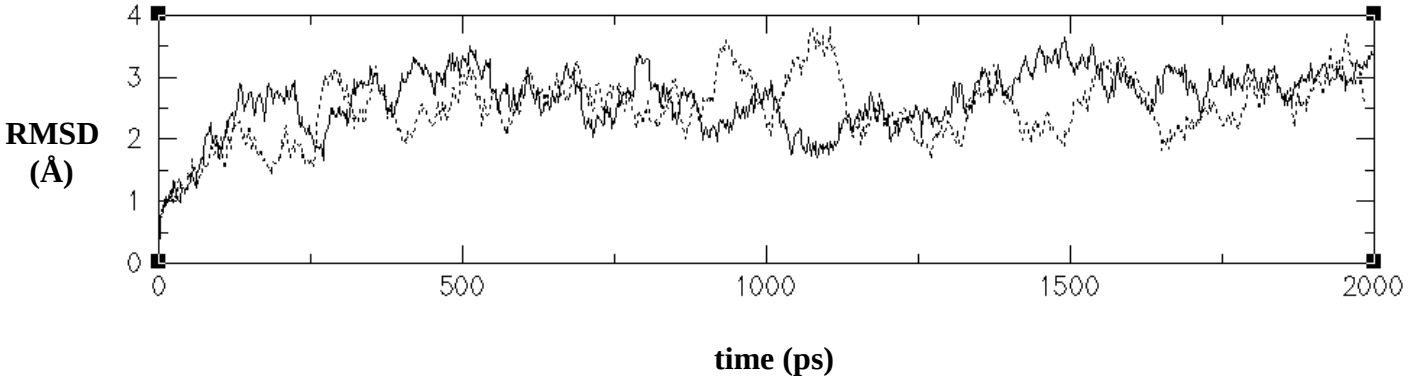

Figure S3. MALDI-TOF MS analysis of *E. Coli* Polymerase I digests of single-stranded DNA substrates containing O^6-guanine lesions d(AACAGCCATATGXCCC): (A) X = O^6-POB-dG, (B) X = O^6-Me-dG. Both incubations were performed at identical conditions. Arrows indicate the portion of the sequence represented in the spectra, and doubly charged ions are marked with #.

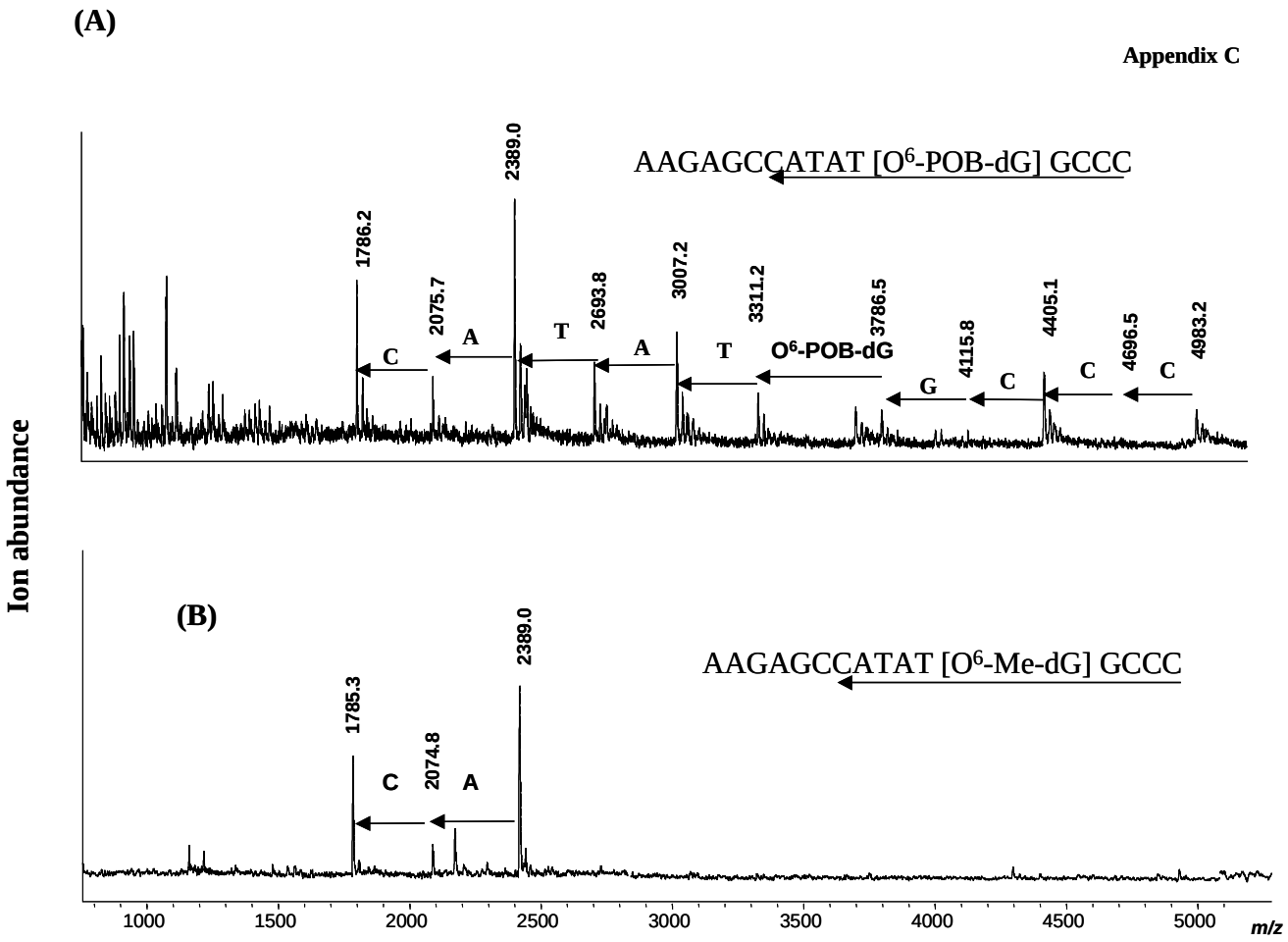

Figure S4. MALDI-TOF mass spectra of the time-controlled 3'-exonuclease digests of single-stranded DNA 16-mers containing O^6-guanine lesions d(AACAGCCATATGXCCC) in the presence of T4 DNA Polymerase: (A) X = O^6-POB-dG, (B) X = O^6-Me-dG. Arrows indicate the portion of the sequence represented in the spectra.

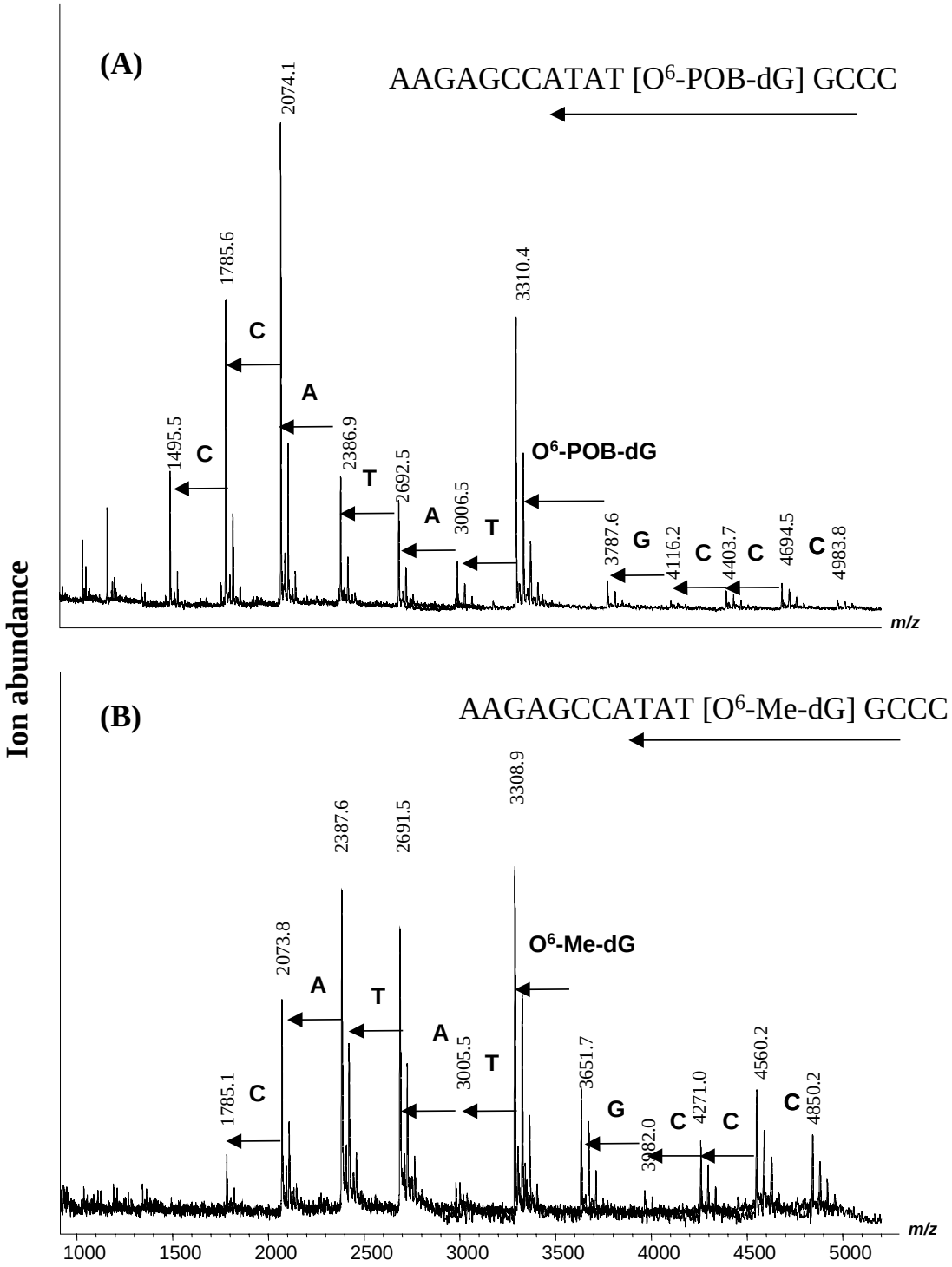

Table S2 Average sugar pucker, glycosidic and backbone torsions and the Watson-Crick base pairing distances for the last 200 ps of the 2 ns simulation, for the POB-adduct modified DNA duplex

	α°	β°	γ°	δ°	ε°	ζ°	χ°	Sugar pucker°	H-bond distance (Å)
	P-O5'	O5'-C5'	C5'-C4'	C4'-C3'	C3'-O3'	O3'-P			
C1							-125	134	3.0, 3.0, 2.9
A2	-72	175	55	117	-171	-97	-118	138	2.9, 3.0
T3	-70	167	63	116	-177	-100	-121	132	3.0, 3.0
A4	-67	175	60	122	-175	-90	-117	149	3.0, 3.0
T5	-73	173	60	119	-159	-82	-120	129	2.9, 3.1
G6	-114	171	59	123	-124	-180	-113	-7	7.5, 5.2, 3.7
G7	-69	179	60	127	-170	-91	-104	150	3.0, 2.9. 2.9
C8	-68	169	63	129	-176	-93	-131	125	3.0, 2.9, 2.9
C9	-70	170	60	115	-173	-92	-128	116	2.9, 3.0, 2.9
C10		176	56	123			-99	153	3.5, 3.1, 2.9
G11							-27	134	
G12	-69	172	60	113	-174	-97	-90	171	
G13	-75	174	59	106	-168	-88	-112	159	
C14	-71	172	58	99	-168	-85	-113	146	
C15	-63	173	60	129	-117	-87	-132	94	
A16	-70	168	61	112	-173	-90	-103	142	
T17	-72	174	58	117	-174	-88	-118	127	
A18	-69	174	54	115	-172	-89	-123	147	
T19	-76	167	59	119	-141	-137	-119	138	
G20		165	53	138			-120	143	
avg	-73	172	59	119	-163	-99	-112	131	

Table S3 Average standard deviations (σ) for the sugar pucker, glycosidic and backbone torsions and the Watson-Crick base pairing distances for the last 200 ps of the 2 ns simulation, for the POB-adduct modified DNA duplex

	α°	β°	γ°	δ°	ε°	ζ°	χ°	Sugar pucker°	H-bond distance (Å)
C1							**19**	**36**	**0.2, 0.1, 0.1**
A2	**11**	**12**	**9**	**15**	**9**	**15**	**15**	**20**	**0.1, 0.2**
T3	**11**	**10**	**9**	**16**	**12**	**19**	**15**	**17**	**0.1, 0.2**
A4	**9**	**11**	**9**	**15**	**9**	**10**	**12**	**24**	**0.1, 0.2**
T5	**10**	**9**	**9**	**14**	**13**	**12**	**12**	**16**	**0.1, 0.3**
G6	**38**	**9**	**9**	**16**	**44**	**64**	**9**	**20**	**0.4, 0.2, 0.4**
G7	**9**	**14**	**12**	**21**	**13**	**17**	**11**	**14**	**0.2, 0.1. 0.1**
C8	**10**	**9**	**9**	**9**	**9**	**9**	**13**	**20**	**0.2, 0.1, 0.1**
C9	**13**	**10**	**10**	**13**	**8**	**9**	**14**	**30**	**0.2, 0.1, 0.1**
C10		**10**	**10**	**15**			**18**	**19**	**1.0, 0.4, 0.3**
G11							**28**	**14**	
G12	**10**	**11**	**8**	**15**	**9**	**15**	**17**	**13**	
G13	**11**	**10**	**9**	**19**	**8**	**16**	**11**	**23**	
C14	**12**	**10**	**9**	**18**	**12**	**20**	**12**	**14**	
C15	**8**	**10**	**9**	**11**	**10**	**8**	**11**	**28**	
A16	**10**	**9**	**10**	**12**	**9**	**11**	**14**	**18**	
T17	**11**	**10**	**8**	**13**	**8**	**10**	**19**	**17**	
A18	**10**	**9**	**9**	**12**	**10**	**10**	**12**	**21**	
T19	**15**	**9**	**9**	**16**	**42**	**54**	**12**	**16**	
G20		**16**	**11**	**14**			**15**	**15**	

Table S4 Average sugar pucker, glycosidic and backbone torsions and the Watson-Crick base pairing distances over the course of the 2.0 ns simulation, for the O6-methyl guanine containing DNA duplex

	α°	β°	γ°	δ°	ε°	ζ°	χ°	Sugar pucker°	H-bond distance (Å)
	P-O5’	O5’-C5’	C5-C4’	C4’-C3’	C3’-O3’	O3’-P			
C1							-128	125	3.0, 3.0, 2.9
A2		173	60	126	-177	-95	-116	148	2.9, 3.0
T3	-68	170	62	111	-170	-87	-128	119	2.9, 3.1
A4	-72	175	55	115	-171	-91	-128	129	2.9, 3.0
T5	-71	175	56	119	-168	-85	-113	134	3.0, 3.0
G6	-74	165	57	120	-148	-134	-104	133	3.7, 3.6, 3.6
G7	-72	162	57	119	-174	-91	-130	136	3.0, 3.0, 2.9
C8	-71	173	60	117	-178	-93	-128	133	3.0, 2.9, 2.9
C9	-69	180	56	117	-165	-84	-130	131	2.9, 2.9, 2.9
C10	-74	169	55	128			-105	138	3.0, 3.0, 2.9
G11							-59	141	
G12		159	60	139	-179	-97	-107	169	
G13	-69	174	58	116	-176	-90	-127	131	
C14	-68	173	60	113	-170	-88	-130	126	
C15	-73	175	55	113	-174	-87	-127	126	
A16	-70	171	58	110	-173	-91	-127	125	
T17	-68	169	60	116	-174	-90	-120	130	
A18	-69	168	58	111	-176	-93	-130	125	
T19	-68	174	60	116	-174	-91	-126	129	
G20	-72	177	55	133			-113	146	
avg	-71	171	58	119	-172	-93	-119	134	

Table S5 Average standard deviations (σ) for the sugar pucker, glycosidic and backbone torsions and the Watson-Crick base pairing distances over the course of the 2.0 ns simulation, for the O6-methyl guanine containing DNA duplex

	α°	β°	γ°	δ°	ε°	ζ°	χ°	Sugar pucker°	H-bond distance (Å)
C1							**16**	**35**	**0.2, 0.1, 0.1**
A2		**11**	**10**	**13**	**9**	**10**	**12**	**21**	**0.1, 0.1**
T3	**10**	**9**	**8**	**17**	**9**	**13**	**14**	**32**	**0.1, 0.2**
A4	**10**	**9**	**9**	**13**	**9**	**12**	**14**	**21**	**0.1, 0.2**
T5	**10**	**10**	**8**	**13**	**9**	**10**	**12**	**19**	**0.1, 0.2**
G6	**11**	**9**	**10**	**15**	**46**	**57**	**20**	**19**	**0.3, 0.2, 0.3**
G7	**19**	**19**	**11**	**17**	**9**	**13**	**14**	**25**	**0.2, 0.1, 0.1**
C8	**10**	**11**	**9**	**12**	**8**	**12**	**13**	**17**	**0.1, 0.1, 0.1**
C9	**11**	**12**	**8**	**15**	**12**	**10**	**12**	**21**	**0.1, 0.1, 0.1**
C10	**13**	**10**	**9**	**20**			**20**	**29**	**0.1, 0.1, 0.1**
G11							**28**	**10**	
G12		**18**	**12**	**10**	**11**	**18**	**12**	**18**	
G13	**11**	**12**	**10**	**17**	**10**	**13**	**17**	**31**	
C14	**12**	**10**	**9**	**14**	**8**	**10**	**14**	**27**	
C15	**11**	**9**	**10**	**14**	**8**	**11**	**15**	**22**	
A16	**11**	**9**	**9**	**13**	**10**	**12**	**15**	**22**	
T17	**10**	**9**	**10**	**11**	**10**	**10**	**12**	**18**	
A18	**9**	**10**	**9**	**12**	**10**	**10**	**12**	**16**	
T19	**8**	**10**	**9**	**15**	**8**	**11**	**12**	**24**	
G20	**12**	**9**	**9**	**13**			**15**	**20**	