

Theoretical studies on the purine radical induced purine-purine type intrastrand cross-links

Shoushan Wang^{a,§}, Jie Ding^{b,§}, Peng Liu^a, Shilei Xie^a, Dong Xie^a, Min Zhang^{a,*}, Faliang Cheng^{a,*}

^a Guangdong Engineering and Technology Research Center for Advanced Nanomaterials, School of Environment and Civil Engineering, Dongguan University of Technology, Dongguan 523808, People's Republic of China.

^b Guangdong Provincial Key Laboratory of Medical Molecular Diagnostics, China-America Cancer Research Institute, Guangdong Medical University, Dongguan 523808, China.

Table S1 Mulliken spin density distributions of closely related atoms along the reaction path of the guanine-8-yl radical adding to the C₈ site of its 5' neighboring deoxyguanosine.

Atom	5'-aG(aG [•])-3'	5'-aG(sG [•])-3'	5'-•G _{N7} (8-8)G-3'
5' N ₇	0	0	0.51
5' C ₈	0	0	-0.04
3' N ₇	0.04	0.03	0
3' C ₈	0.86	0.87	0.03

Table S2 Mulliken spin density distributions of closely related atoms along the reaction path of the guanine-8-yl radical adding to the C₈ site of its 3' neighboring deoxyguanosine.

Atom	5'-(aG [•])aG-3'	5'-G(8-8)(•G _{N7})-3'
5' N ₇	0.02	0
5' C ₈	0.86	0.04
3' N ₇	0	0.52
3' C ₈	0	-0.04

Table S3 Mulliken spin density distributions of closely related atoms along the reaction path of the guanine-8-yl radical adding to the C₈ site of its 5' neighboring deoxyadenosine.

Atom	5'-aA(aG [•])-3'	5'-aA(sG [•])-3'	5'-•A _{N7} (8-8)G-3'
5' N ₇	0	0	0.48
5' C ₈	0	0	-0.03
3' N ₇	0.04	0.03	0
3' C ₈	0.86	0.87	0.03

Table S4 Mulliken spin density distributions of closely related atoms along the reaction path of the guanine-8-yl radical adding to the C₈ site of its 3' neighboring deoxyadenosine.

Atom	5'-(aG*)aA-3'	5'-G(8-8)(*A _{N7})-3'
5' N ₇	0.02	0
5' C ₈	0.86	0.04
3' N ₇	0	0.48
3' C ₈	0	-0.03

Table S5 Cartesian coordinates of stationary points along the reaction path of the guanine-8-yl radical addition to the C₈ site of its 5' neighboring deoxyguanosine.

5'-aG(aG*)-3'			
O	-40.07509500	22.77201300	9.17518900
C	-41.21419600	23.46718100	8.69115300
C	-42.48085000	22.76782500	9.16228600
O	-42.64828500	21.50545400	8.48687800
C	-42.49785000	22.45629200	10.66633800
O	-43.86210300	22.59463400	11.11638000
C	-42.01970600	21.00715300	10.72232500
C	-42.52450500	20.41869900	9.39857000
N	-41.62590200	19.42669900	8.82088900
C	-40.35068000	19.65468700	8.32470900
N	-39.77358300	18.56585000	7.87409100
C	-40.71061400	17.56515700	8.08079900
C	-40.62375700	16.15285900	7.87135000
N	-41.83113000	15.51823800	8.26904200
C	-42.91189800	16.12695600	8.86221600
N	-42.98152200	17.42755600	9.06656200
C	-41.86850700	18.08447700	8.66745300
P	-44.16741400	22.72118900	12.72679400
O	-45.55494000	23.30606900	12.86105100
O	-43.03238300	23.41535100	13.44479100
O	-44.14930500	21.15243500	13.21945600
C	-45.20029100	20.29499800	12.74812600
C	-44.92547400	18.87784200	13.20739000
O	-43.79986100	18.35113100	12.47722300
C	-44.58381100	18.74924000	14.71027000
O	-45.29973600	17.62155000	15.20451800
C	-43.06918500	18.51038200	14.69303800
C	-42.91451700	17.71574400	13.40117400

N	-41.58230300	17.71201700	12.84799400
C	-40.66911000	18.74304400	12.79946700
N	-39.60584500	18.50911300	12.13774800
C	-39.78164200	17.20148500	11.65633900
C	-38.95016600	16.39230500	10.81693100
O	-37.85690500	16.63614100	10.31779100
N	-39.58141100	15.13440900	10.57735300
C	-40.80241600	14.73563400	11.06051800
N	-41.27974600	13.52249200	10.64626000
N	-41.55527500	15.49305700	11.83635900
C	-41.00866700	16.70058700	12.08343300
H	-41.22138700	24.50352600	9.06522100
H	-41.21046000	23.50396200	7.59130200
H	-43.33536300	23.40376300	8.90789200
H	-41.85863900	23.13239800	11.23766200
H	-42.40911800	20.46292900	11.58216000
H	-40.92919600	20.98775100	10.74173600
H	-43.48826700	19.91401800	9.51741500
H	-39.93694400	20.65327500	8.33506900
H	-46.16361700	20.63066600	13.14806700
H	-45.24639400	20.31893200	11.65311900
H	-45.81247800	18.26693000	12.99904300
H	-44.85615600	19.65350500	15.26877200
H	-42.69928300	17.97827100	15.57031100
H	-42.54526300	19.46578400	14.59710700
H	-43.19684000	16.66600900	13.53745500
H	-42.04984900	13.17298600	11.20110000
C	-38.85068000	23.39481000	8.81023300
H	-38.04440500	22.78093800	9.21672800
H	-38.74041800	23.45698500	7.71822200
H	-38.77809600	24.40901800	9.22813800
O	-39.68767500	15.46815300	7.45349900
H	-41.80667700	14.50627900	8.21137800
N	-43.96045100	15.32710500	9.20949500
H	-44.61159700	15.75712800	9.85198900
H	-43.76744600	14.35312400	9.39981300
Na	-44.60232000	25.06661600	14.23529600
C	-45.31401700	17.52790400	16.62303200
H	-45.75759100	18.42522600	17.07850300
H	-45.92506900	16.65929400	16.87753200
H	-44.30956100	17.38592500	17.04425300
H	-39.11495000	14.57144100	9.87329400
H	-40.61204400	12.81249900	10.37626200

O	-39.74173600	22.42406000	9.28494200
C	-40.77214400	23.36189200	9.01676700
C	-42.11421500	22.78959600	9.44851100
O	-42.48775300	21.68216000	8.60439200
C	-42.14056300	22.25334500	10.88724500
O	-43.47409800	22.47807800	11.39341100
C	-41.84998700	20.76635700	10.69926900
C	-42.50395500	20.46591300	9.34379900
N	-41.81078400	19.44381600	8.57242400
C	-40.56709700	19.55383800	7.97118000
N	-40.17409700	18.43848300	7.40097500
C	-41.20191100	17.54195500	7.64802500
C	-41.31941400	16.15022200	7.33098700
N	-42.53888600	15.62605200	7.84723300
C	-43.49364700	16.32727400	8.54647100
N	-43.38453100	17.61242400	8.82070200
C	-42.22659700	18.15173200	8.37311100
P	-43.76386500	22.34419500	13.00506200
O	-45.08153200	23.03710900	13.26845100
O	-42.56161000	22.77191600	13.81499700
O	-43.91251200	20.71945400	13.21388400
C	-45.04958600	20.05644400	12.64359000
C	-45.01054200	18.58821500	13.02332600
O	-43.94244200	17.92604900	12.30929700
C	-44.75751500	18.32741500	14.51955000
O	-45.55151900	17.20301900	14.88704200
C	-43.25599500	18.01744900	14.55650900
C	-43.07736700	17.28311300	13.22893600
N	-41.72747400	17.36588600	12.67351300
C	-41.39336100	17.49354900	11.34569400
N	-40.14247100	17.46731500	11.08243300
C	-39.54181300	17.25886700	12.33132500
C	-38.16421900	17.11152400	12.68887400
O	-37.15749600	17.13870700	11.98424100
N	-38.04433900	16.90160000	14.09267600
C	-39.07816900	16.83825700	14.99667500
N	-38.76357000	16.56883900	16.29163200
N	-40.34658800	16.97863900	14.65155500
C	-40.51626600	17.18459100	13.32866100
H	-40.59393500	24.30150900	9.56399100
H	-40.81254900	23.59882000	7.94270400
H	-42.87001900	23.57413000	9.33493400

H	-41.41604200	22.75150000	11.53496100
H	-42.25280400	20.14604500	11.49903300
H	-40.77220000	20.61536300	10.62501700
H	-43.53202700	20.10752300	9.45918400
H	-40.02895100	20.49022500	8.00765000
H	-45.97378600	20.50758300	13.02114400
H	-45.03364000	20.14971900	11.55126200
H	-45.96222500	18.12978100	12.73223400
H	-45.01585400	19.19933700	15.13451100
H	-42.94556200	17.42480100	15.41537000
H	-42.68716600	18.94878400	14.53458400
H	-43.34782200	16.22303500	13.32150900
H	-39.51083800	16.71172300	16.95567900
C	-38.45091300	22.90785100	8.93938800
H	-37.73808400	22.11316400	9.16857700
H	-38.38571900	23.15239700	7.86949900
H	-38.19084200	23.80462800	9.51980100
Na	-43.99330100	24.34631300	14.98519100
C	-45.61762300	16.98234800	16.28967600
H	-46.02053100	17.86105500	16.81427700
H	-46.28846700	16.13495900	16.44640200
H	-44.63809300	16.73910800	16.72297700
H	-37.09147600	16.76392100	14.41037100
H	-37.83406800	16.76641700	16.63284400
O	-40.54559900	15.40961000	6.72515700
H	-42.66240600	14.63196300	7.69374500
N	-44.56462300	15.62772700	9.01645900
H	-45.31565700	16.19786100	9.37863900
H	-44.85435900	14.78661600	8.53821800

5'-*a*G(*s*G^{*})-3'

O	0.18094200	0.47517200	-0.36497700
C	0.06995200	0.55487800	1.04798900
C	1.45365800	0.41785800	1.67150200
O	1.95721400	-0.92254000	1.48046600
C	2.49205000	1.36449800	1.04832500
O	3.43162500	1.75735300	2.07446300
C	3.14975300	0.48210800	0.00047200
C	3.10079200	-0.90619800	0.63463900
P	4.35245100	3.09710700	1.84718400
O	4.97642000	3.42933100	3.18055500
O	3.55384100	4.19721700	1.16688300
O	5.47726300	2.62403700	0.75764100

C	6.42272100	1.60260800	1.10268300
C	7.19958200	1.21315700	-0.14325900
O	6.32508000	0.54246400	-1.07215400
C	7.82854200	2.39686000	-0.90890700
O	9.12133000	1.97107800	-1.33343600
C	6.86230100	2.59614700	-2.08149100
C	6.43019400	1.15818100	-2.35855100
N	5.17118600	0.99262500	-3.06262700
C	4.85937300	-0.09710200	-3.84983400
N	3.64949400	-0.18828100	-4.23470400
C	3.02039300	0.90966400	-3.62267300
C	1.63865700	1.28097300	-3.58193900
O	0.66362000	0.74622800	-4.11021700
N	1.46296500	2.42769700	-2.76139200
C	2.44706600	3.08274800	-2.05675600
N	2.09063200	4.12903600	-1.27036100
N	3.72290300	2.73526300	-2.12871000
C	3.94846700	1.65172900	-2.88986700
H	-0.36141500	1.52279200	1.34939200
H	-0.58274800	-0.24265400	1.43356000
H	1.37089200	0.60287900	2.74773200
H	2.02322500	2.25558900	0.62934800
H	4.15497000	0.79057500	-0.26888400
H	2.52407000	0.47335800	-0.89070600
H	4.00314000	-1.13564500	1.21095400
H	7.11619900	1.97088000	1.86754200
H	5.90411900	0.72024900	1.49552000
H	7.99940300	0.52510200	0.15625700
H	7.90826200	3.29337300	-0.28026500
H	6.00120400	3.17780600	-1.75507000
H	7.17897200	0.62940500	-2.95946900
H	2.71118700	4.28493300	-0.46407500
H	7.32354500	3.06904800	-2.94980900
H	0.49668300	2.71036600	-2.64433200
H	1.10723100	4.25406400	-1.07423900
Na	4.04555900	5.68257600	3.01348800
C	-1.05249100	0.67338600	-1.04311600
H	-1.80017800	-0.07635600	-0.74756800
H	-1.46270700	1.67332000	-0.83821600
H	-0.84232100	0.57741000	-2.11060300
C	9.93691700	3.02372800	-1.82986100
H	10.90623500	2.58522700	-2.07673600
H	9.52106000	3.48671100	-2.73503600
H	10.08066000	3.80935500	-1.07360200

N	2.98135500	-1.96190400	-0.36303000
C	1.89014200	-2.21234400	-1.18060100
N	2.12963300	-3.13307000	-2.08554400
C	3.45009900	-3.49643100	-1.86984400
C	4.28483500	-4.43013800	-2.56557200
N	5.59287400	-4.43875000	-2.00237000
C	6.02778500	-3.67570900	-0.94356000
N	5.25166300	-2.82164600	-0.30493100
C	3.99491100	-2.77524600	-0.80521500
O	4.02632000	-5.16360200	-3.51868900
H	6.23064300	-5.09144700	-2.44355600
N	7.30938300	-3.86599100	-0.51970700
H	7.99308000	-4.22558300	-1.17033800
H	7.65420700	-3.15502400	0.10986700
H	0.97024200	-1.66250800	-1.04076900

TS_{2/GG}

O	-0.00724300	-0.14303500	0.01429100
C	0.03811100	-0.08603800	1.42964300
C	1.48712100	-0.04172300	1.88736500
O	2.11757700	-1.30990800	1.59345500
C	2.33428900	1.03622800	1.17552300
O	3.30551100	1.52120500	2.13630800
C	3.01633000	0.22956900	0.08142000
C	3.32028900	-1.04214900	0.86386300
P	4.34341000	2.73249100	1.73133600
O	4.92651500	3.24507000	3.02899300
O	3.67951800	3.72969100	0.80910800
O	5.50218000	1.98204800	0.83149900
C	6.29323800	0.93762000	1.41393300
C	6.99170600	0.14481200	0.31703600
O	6.02346100	-0.44032100	-0.57971500
C	7.94526200	0.96822000	-0.56452200
O	9.07364800	0.14083000	-0.83899700
C	7.10018000	1.23725300	-1.81123100
C	6.31992100	-0.07093100	-1.92481500
N	5.06307000	0.01950200	-2.66732100
C	4.03337200	-0.91671200	-2.63652000
N	3.05436400	-0.64554500	-3.43766400
C	3.44347500	0.52123900	-4.09172000
C	2.77051200	1.27255600	-5.10669900
O	1.67949500	1.07385200	-5.64045800
N	3.55628200	2.39211300	-5.49561300

C	4.79111900	2.72233800	-4.99185800
N	5.42450400	3.79654100	-5.54309900
N	5.39750600	2.02348100	-4.05142600
C	4.69028700	0.94772700	-3.63414900
H	-0.48388000	0.81007400	1.80342800
H	-0.45056600	-0.96799400	1.87275100
H	1.50876400	0.13179000	2.96989500
H	1.73778300	1.87158200	0.80421600
H	3.90734600	0.69698700	-0.32159300
H	2.29936900	0.02598100	-0.71415700
H	4.13989100	-0.87613300	1.56467400
H	7.05190800	1.36295800	2.08180100
H	5.66584200	0.26237600	2.00184800
H	7.55605600	-0.66030400	0.80129600
H	8.26407300	1.89655800	-0.07174700
H	6.40929200	2.05680500	-1.61076700
H	6.93083300	-0.85790900	-2.38490100
H	6.22527900	4.12758600	-5.02388500
H	7.68120900	1.47360500	-2.70069500
H	3.14756000	2.95405300	-6.23346400
H	4.87416500	4.51874500	-5.98565500
Na	4.21483600	5.47314500	2.39198500
C	-1.33109900	-0.18855300	-0.49272800
H	-1.87228800	-1.07601600	-0.13223300
H	-1.90549600	0.70603600	-0.20905600
H	-1.25845600	-0.23423200	-1.58158500
C	10.15711400	0.83081200	-1.44708000
H	10.97033000	0.11023200	-1.55778300
H	9.90048000	1.22498900	-2.43958200
H	10.50138700	1.66666700	-0.82050600
N	3.71679100	-2.19380700	0.09177200
C	3.26077500	-2.59653300	-1.16122400
N	3.93359800	-3.65178300	-1.62716900
C	4.92255300	-3.86331000	-0.70679700
C	6.01465800	-4.79859800	-0.71760600
N	6.83013600	-4.62222800	0.43326900
C	6.63708800	-3.69182100	1.42756800
N	5.62195900	-2.84108300	1.43621200
C	4.81434700	-2.96585800	0.36798400
O	6.29873300	-5.65879600	-1.54648500
H	7.61781900	-5.25797900	0.48779400
N	7.51438600	-3.68360600	2.45755200
H	8.41487800	-4.13096900	2.37655600
H	7.44954600	-2.90343100	3.09452800

H	2. 29897200	-2. 27294000	-1. 52906100
5'-*G _{N7} (8-8)G-3'			
O	-0. 01461400	-0. 03565000	0. 03864900
C	0. 00580700	-0. 01553400	1. 45588600
C	1. 44675300	0. 00209300	1. 93677200
O	2. 05782700	-1. 27571100	1. 65837900
C	2. 31881300	1. 06854900	1. 22812500
O	3. 20813300	1. 63478600	2. 22361300
C	3. 08656500	0. 22744200	0. 21819200
C	3. 35065800	-1. 00166300	1. 08155900
P	4. 28244700	2. 81141400	1. 81325700
O	4. 72046800	3. 45662000	3. 10899600
O	3. 72542000	3. 70462200	0. 72806200
O	5. 53682100	1. 98405200	1. 13106600
C	6. 26679600	1. 04608300	1. 93283800
C	7. 05276400	0. 09747000	1. 03857000
O	6. 14905400	-0. 61671400	0. 17466200
C	8. 09237000	0. 74840700	0. 11321300
O	9. 21787500	-0. 12645300	0. 08323600
C	7. 35695300	0. 80823200	-1. 22664800
C	6. 53983300	-0. 48545700	-1. 18571200
N	5. 32755800	-0. 48417900	-2. 02206300
C	4. 24188400	-1. 36749100	-1. 94093100
N	3. 33365300	-1. 13477500	-2. 86105000
C	3. 81863600	-0. 07587600	-3. 59106100
C	3. 24329000	0. 58737500	-4. 72537300
O	2. 17726000	0. 37196900	-5. 29820300
N	4. 10136400	1. 62085500	-5. 18151600
C	5. 31874800	1. 95133200	-4. 63471300
N	6. 03213300	2. 93416600	-5. 24909300
N	5. 83573800	1. 33385300	-3. 58976100
C	5. 05602300	0. 34161200	-3. 10027200
H	-0. 51143000	0. 87858200	1. 84126800
H	-0. 50293900	-0. 90103700	1. 86842500
H	1. 45532200	0. 19065700	3. 01809200
H	1. 72872100	1. 86631400	0. 77421100
H	3. 99004900	0. 70769000	-0. 14151100
H	2. 42197000	-0. 02417900	-0. 60835700
H	4. 03443500	-0. 73314600	1. 89064500
H	6. 96066900	1. 57332200	2. 59812100
H	5. 58030800	0. 45949700	2. 55171700
H	7. 56383600	-0. 62305000	1. 68810900

H	8.39223900	1.74571700	0.46246100
H	6.68259200	1.66418900	-1.22180000
H	7.13699700	-1.35848800	-1.47493000
H	6.82204100	3.27996400	-4.72311400
H	8.01234700	0.88172600	-2.09195600
H	3.76580300	2.11545100	-6.00012700
H	5.55023200	3.62399400	-5.80764300
Na	4.05297300	5.60115500	2.18983700
C	-1.32950500	-0.03448000	-0.49171700
H	-1.89880200	-0.91821100	-0.16656700
H	-1.88794100	0.86529800	-0.19218700
H	-1.23963900	-0.05081800	-1.58023100
C	10.36188700	0.42895100	-0.55155500
H	11.16374500	-0.30685800	-0.45998600
H	10.19360800	0.63284500	-1.61752200
H	10.67554100	1.36382700	-0.06452100
N	3.92020700	-2.17204100	0.47317100
C	4.05163100	-2.51442800	-0.97660800
N	5.13245400	-3.49216000	-1.07862700
C	5.54580500	-3.69912700	0.18027900
C	6.61910200	-4.54062100	0.64092700
N	6.79293700	-4.43505800	2.04913100
C	6.06973200	-3.62571900	2.88020300
N	5.07728600	-2.84654900	2.45146500
C	4.85159300	-2.90982100	1.13452300
O	7.35679400	-5.28046400	-0.01272100
H	7.54764400	-4.99982700	2.42195700
N	6.40122300	-3.59278600	4.18861800
H	6.98851300	-4.30203900	4.60002500
H	5.76933200	-3.10255600	4.80378400
H	3.10878100	-2.96901400	-1.31371000

Table S6 Cartesian coordinates of stationary points along the reaction path of the guanine-8-yl radical addition to the C₈ site of its 3' neighboring deoxyguanosine.

5'-(aG*)aG-3'			
O	-4.00469800	0.93148600	-1.35303900
C	-4.62867300	1.25086100	-0.12095200
C	-3.57581500	1.35368400	0.97443400
O	-3.01175200	0.06173200	1.26907000

C	-2.37861300	2.24755600	0.62600000
O	-1.87812300	2.77544700	1.87456600
C	-1.40018000	1.26563600	-0.01368300
C	-1.71836100	-0.06231600	0.68428100
N	-1.67296900	-1.20078500	-0.22293100
C	-2.15735300	-1.30574700	-1.50933200
N	-1.98400900	-2.43738000	-2.07593800
C	-1.31572400	-3.20393000	-1.10787000
C	-0.73513100	-4.50311600	-1.18137700
N	-0.15361800	-4.85496100	0.06611500
C	-0.05187500	-4.04292200	1.17167300
N	-0.52504800	-2.80887600	1.19956000
C	-1.13044000	-2.44815700	0.05275500
P	-0.67790000	3.89841400	1.86992900
O	-0.72658200	4.58795200	3.21482200
O	-0.73002000	4.75816200	0.62832100
O	0.68248100	2.98000200	1.73761600
C	0.93968500	1.98909200	2.74304200
C	2.05982500	1.08180000	2.26983800
O	1.61731700	0.33373400	1.11960100
C	3.34972500	1.82048600	1.84932600
O	4.44476300	1.06090600	2.35102500
C	3.27260300	1.79003400	0.31864700
C	2.60530000	0.43739900	0.08673700
N	1.96582100	0.26375200	-1.19810000
C	1.29129300	1.20192400	-1.96895300
N	0.71236000	0.68256100	-3.02314000
C	1.00480000	-0.67027100	-2.95101200
C	0.61306400	-1.75127500	-3.80985200
O	-0.06253800	-1.73437300	-4.83558600
N	1.13260900	-2.97848300	-3.31910300
C	1.90082000	-3.14307100	-2.19165600
N	2.34089300	-4.40936700	-1.92943100
N	2.25492700	-2.14430100	-1.40425600
C	1.77620500	-0.95022600	-1.82562900
H	-5.17245200	2.20658900	-0.19658400
H	-5.35177500	0.47166100	0.16404700
H	-4.06446600	1.71626800	1.88438700
H	-2.64288800	3.07461300	-0.03674200
H	-0.36153300	1.54443300	0.13913300
H	-1.60329200	1.19120600	-1.08181000
H	-0.99723500	-0.29836600	1.46935000
H	1.23264600	2.47076000	3.68346700
H	0.03872000	1.39247700	2.92317900

H	2.30666300	0.38813000	3.08288000
H	3.38067800	2.84475000	2.24280500
H	4.24277500	1.87400400	-0.17260600
H	2.62379800	2.60156900	-0.01571800
H	3.32838900	-0.37919100	0.18536300
H	2.73331700	-4.52148400	-1.00444300
C	5.69338900	1.73700300	2.27778200
H	5.66628800	2.68710900	2.83089200
H	6.43720300	1.07975600	2.73309500
H	5.99688800	1.94679500	1.24327800
C	-4.92904800	0.66821400	-2.39754800
H	-4.34578500	0.42197600	-3.28693000
H	-5.58296500	-0.18051500	-2.15097900
H	-5.55796100	1.54536200	-2.60758700
H	0.80488400	-3.80240300	-3.81080100
H	1.73584500	-5.16993100	-2.21823200
O	-0.63680100	-5.27767400	-2.14009400
H	0.24796200	-5.78526200	0.09154600
N	0.52546200	-4.56672300	2.28229800
H	1.13552600	-5.36703500	2.20476100
H	0.75660900	-3.90412400	3.00826500
Na	-0.81659300	6.71533300	2.08177800
H	1.26434300	2.24529900	-1.69398100

TS_{3/GG}

O	0.18113900	0.59891700	-1.25997400
C	-0.27723000	0.58366600	0.08076200
C	0.90632500	0.39506900	1.01591100
O	1.42302100	-0.94452100	0.87050400
C	2.08340200	1.34783300	0.72695700
O	2.66291100	1.71376600	2.00058100
C	3.02720500	0.46300800	-0.08009600
C	2.82945100	-0.87514700	0.61466200
N	3.24014300	-2.01760800	-0.16625700
C	3.77770800	-2.05590500	-1.44916400
N	4.06420300	-3.25777400	-1.84034300
C	3.70185500	-4.08682200	-0.78057600
C	3.78687600	-5.50733600	-0.63423000
N	3.32488900	-5.89632300	0.65632900
C	2.87018300	-5.05400800	1.64347900
N	2.78932200	-3.74529700	1.49399200
C	3.20421500	-3.32706900	0.27624400
P	3.85882100	2.83999700	2.05885700

O	4. 01223100	3. 22932700	3. 51112200
O	3. 63134200	3. 93774200	1. 04548500
O	5. 18053200	2. 00366300	1. 54005700
C	5. 67316700	0. 92777000	2. 35069100
C	6. 71422500	0. 14710100	1. 57602000
O	6. 09475700	-0. 60951400	0. 51166200
C	7. 81862300	1. 02336800	0. 92480300
O	9. 06839800	0. 52872800	1. 39355900
C	7. 61385100	0. 77366600	-0. 57530000
C	7. 04310100	-0. 64436200	-0. 55324300
N	6. 41892600	-1. 08423000	-1. 78180200
C	5. 25911200	-0. 59903000	-2. 40325900
N	5. 13365000	-1. 06497900	-3. 65453600
C	6. 12996100	-1. 97893500	-3. 78244400
C	6. 43405900	-2. 87246500	-4. 86987600
O	5. 86276400	-3. 00714800	-5. 94737900
N	7. 57043900	-3. 66635500	-4. 56049400
C	8. 29869000	-3. 61892100	-3. 39498000
N	9. 37400100	-4. 42943400	-3. 29235400
N	8. 01434000	-2. 79443600	-2. 39479000
C	6. 94314000	-2. 02008500	-2. 63160700
H	-0. 78488100	1. 52949300	0. 33219100
H	-0. 99566000	-0. 23553800	0. 24106200
H	0. 56411200	0. 54236800	2. 04734700
H	1. 77710600	2. 24957100	0. 19345100
H	4. 05826500	0. 80242900	-0. 06159100
H	2. 64967500	0. 39238200	-1. 10214500
H	3. 37126500	-0. 92058300	1. 56592200
H	6. 13812800	1. 32860100	3. 25856800
H	4. 85560700	0. 26260000	2. 64811500
H	7. 20571300	-0. 54816700	2. 26899800
H	7. 70240900	2. 08155400	1. 18827400
H	8. 53185300	0. 85711600	-1. 15878900
H	6. 86541700	1. 46169000	-0. 97871700
H	7. 83728000	-1. 37094100	-0. 34260100
H	9. 81049000	-4. 48639600	-2. 38426200
C	10. 16069500	1. 40124600	1. 13536700
H	10. 00293500	2. 38696800	1. 59682200
H	11. 04727700	0. 93896700	1. 57460700
H	10. 33577500	1. 54585500	0. 06052900
C	-0. 86792400	0. 77902600	-2. 19724800
H	-0. 41711100	0. 77691900	-3. 19212700
H	-1. 60766000	-0. 03321300	-2. 13773600
H	-1. 39036400	1. 73503900	-2. 04279400

H	7.84147400	-4.31032100	-5.29541100
H	9.49625700	-5.21855500	-3.90858700
O	4.17863400	-6.36409900	-1.42689800
H	3.33279800	-6.89698300	0.81824700
N	2.43653200	-5.62929000	2.80287700
H	2.82339700	-6.52152900	3.07689900
H	2.29410000	-4.98000100	3.56385500
Na	3.84008500	5.55122500	2.85129100
H	4.78777000	0.30192400	-2.04782900

5'-G(8-8)(*G_{N7})-3'

O	-4.30804700	1.56494700	-1.24417500
C	-4.81923900	1.52452000	0.07692200
C	-3.68053300	1.25793900	1.04589700
O	-3.22196200	-0.10068600	0.87385600
C	-2.44806100	2.15923800	0.81926200
O	-1.91985900	2.51154700	2.11689800
C	-1.50346800	1.22253500	0.06880800
C	-1.79592600	-0.07789300	0.80352200
N	-1.33720700	-1.32999100	0.21527300
C	-0.45163900	-1.62106800	-0.82922800
N	-0.21344700	-2.90731700	-0.93831300
C	-0.93643000	-3.50057800	0.07196900
C	-1.04127200	-4.88144100	0.44620400
N	-1.86730600	-5.01801100	1.59361400
C	-2.47127500	-3.99044400	2.28177500
N	-2.37632200	-2.72437200	1.92285500
C	-1.62120500	-2.54237300	0.81444500
P	-0.68000900	3.58807900	2.22298100
O	-0.56326300	3.96724500	3.68080300
O	-0.83136700	4.69487500	1.20529300
O	0.62229800	2.69892900	1.74595700
C	1.08181200	1.63412800	2.59103000
C	2.10986800	0.80424400	1.84928100
O	1.47250600	-0.00839000	0.83671400
C	3.21121000	1.63285800	1.13361300
O	4.46492500	1.15682100	1.61321900
C	2.98257700	1.29958700	-0.34717100
C	2.40502300	-0.11318300	-0.23378800
N	1.73604600	-0.62581400	-1.40987200
C	0.27511300	-0.62646800	-1.71898300
N	0.16069300	-1.02681600	-3.11975600
C	1.41549100	-1.26816700	-3.52786400

C	1.87580000	-1.69523200	-4.82195300
O	1.21886300	-1.94605400	-5.83462700
N	3.29550500	-1.81616400	-4.85624800
C	4.14461400	-1.55510600	-3.81698900
N	5.47320600	-1.67396800	-4.02891600
N	3.72263900	-1.15288600	-2.61833800
C	2.39206000	-1.02964200	-2.51786200
H	-5.29598700	2.48223800	0.34233100
H	-5.57613600	0.73163300	0.18231900
H	-4.04670700	1.39451400	2.07067200
H	-2.68190400	3.06627700	0.25942100
H	-0.46517100	1.53553000	0.11589400
H	-1.86182000	1.14821200	-0.95982100
H	-1.38073700	-0.04463200	1.81831200
H	1.54842200	2.05113700	3.49035300
H	0.24654300	0.99661000	2.90073100
H	2.60373600	0.14390600	2.57360500
H	3.10604900	2.70480500	1.33927900
H	3.89136000	1.34052700	-0.94880000
H	2.22811700	1.96309100	-0.77988200
H	3.20988200	-0.81846800	0.02094500
H	6.06718600	-1.61475800	-3.21539400
C	5.55816100	2.00352500	1.28461700
H	5.41583900	3.01638500	1.68913500
H	6.44956400	1.56136400	1.73480700
H	5.71449700	2.08287300	0.20011300
C	-5.31119400	1.82236700	-2.21363200
H	-4.82192400	1.83518300	-3.19002300
H	-6.08564800	1.04106200	-2.21132400
H	-5.79888500	2.79406300	-2.04451700
H	3.66736200	-2.10116500	-5.75521900
H	5.83540700	-2.17196100	-4.82765700
O	-0.53799400	-5.87627900	-0.07253500
H	-2.00368900	-5.97473500	1.89982100
N	-3.24337700	-4.32950100	3.35207700
H	-3.05042800	-5.18920100	3.84609300
H	-3.52076700	-3.55347700	3.93634100
Na	-0.68008500	6.29522500	3.02122800
H	-0.11710900	0.38025800	-1.59247900

Table S7 Cartesian coordinates of stationary points along the reaction path of the guanine-8-yl radical

addition to the C₈ site of its 5' neighboring deoxyadenosine.

5'-aA(aG ⁺)-3'			
O	-40.33205500	22.71795800	9.06791700
C	-41.51229400	23.09261600	8.37303100
C	-42.70450100	22.32650300	8.92837600
O	-42.63218400	20.93505300	8.56005800
C	-42.80792100	22.35991600	10.46019800
O	-44.21203300	22.36057200	10.79507500
C	-42.11980200	21.06161100	10.87471000
C	-42.42720300	20.11479400	9.70853400
N	-41.35849000	19.16735100	9.42839300
C	-40.05559000	19.47446000	9.07822600
N	-39.31003000	18.41775800	8.84683800
C	-40.16723400	17.34805700	9.05134100
C	-39.98111100	15.95215800	9.00728300
N	-41.03959600	15.14968700	9.24132200
C	-42.22037500	15.72000300	9.53770300
N	-42.51652600	17.01875400	9.65433100
C	-41.45003700	17.79133600	9.40036400
P	-44.66543800	22.73540800	12.32992300
O	-46.14114700	23.06020700	12.28191100
O	-43.73297000	23.75549600	12.94273900
O	-44.40938400	21.32461300	13.13644000
C	-45.26417700	20.21312900	12.82812100
C	-44.74017900	18.97642400	13.52814400
O	-43.53882200	18.52657300	12.86993300
C	-44.38030500	19.18966900	15.02022200
O	-44.94723600	18.10191000	15.74398200
C	-42.84696300	19.14048400	15.00860100
C	-42.60286200	18.14470800	13.88017800
N	-41.27315500	18.14936100	13.32535300
C	-40.46601800	19.22461400	13.01911700
N	-39.35543000	18.94105000	12.46488800
C	-39.36494300	17.53883200	12.36798700
C	-38.41724400	16.62686200	11.80815000
O	-37.34927100	16.84026700	11.23450100
N	-38.87614300	15.28900100	11.96789400
C	-40.07949800	14.89765400	12.50477300
N	-40.37047900	13.57502100	12.49683200
N	-40.96257900	15.75833100	12.98575200
C	-40.55642100	17.03689500	12.89101200
H	-41.69898900	24.17235800	8.48713700

H	-41.41678700	22.87701600	7.29808800
H	-43.61424900	22.74757500	8.48717000
H	-42.33332500	23.24401100	10.89086200
H	-42.48493900	20.66469500	11.82013100
H	-41.04536100	21.23522200	10.94276500
H	-43.31726500	19.50780000	9.89968300
H	-39.74635300	20.50762900	8.99831600
H	-46.28363400	20.42309100	13.16982700
H	-45.28556800	20.03613700	11.74654400
H	-45.50446700	18.19138900	13.46711400
H	-44.76343900	20.14504400	15.39917600
H	-42.41212900	18.82980900	15.95946600
H	-42.44334000	20.11645800	14.72335800
H	-42.79361500	17.11697000	14.20917000
H	-41.17277200	13.29365200	13.04051300
C	-39.17978400	23.41656000	8.61551400
H	-38.33315500	23.05385000	9.20195100
H	-38.98711300	23.22725000	7.54986100
H	-39.28487600	24.50050600	8.76559200
Na	-45.65791900	25.12953300	13.44022400
C	-44.95468900	18.29320600	17.15262100
H	-45.51197400	19.19982600	17.42995000
H	-45.44948500	17.42274100	17.58866900
H	-43.94173500	18.36760800	17.57093000
H	-38.25780000	14.59186500	11.56969700
H	-39.63763500	12.89011800	12.39068500
H	-43.03904100	15.02676300	9.71888500
N	-38.77386500	15.39034500	8.71914900
H	-38.70032400	14.39763600	8.89486800
H	-37.95710400	15.93773000	8.96070600

TS_{1/AG}

O	-39.94402000	22.64001400	9.18468100
C	-41.04380400	23.44847500	8.79490400
C	-42.34377800	22.81029800	9.26229200
O	-42.60723700	21.60122200	8.52277700
C	-42.35087300	22.41242500	10.74575900
O	-43.70406600	22.57528000	11.22266500
C	-41.94213700	20.94266900	10.70283400
C	-42.54349400	20.46211100	9.37586100
N	-41.76063600	19.42706200	8.71832300
C	-40.47674200	19.55091300	8.22234300
N	-40.01249100	18.44305800	7.68677700

C	-41.04617500	17.53349900	7.84401600
C	-41.17779100	16.16795200	7.51499200
N	-42.33310800	15.53767800	7.81594200
C	-43.30964800	16.24482800	8.41034800
N	-43.31047800	17.53046400	8.77675200
C	-42.14606200	18.12564400	8.47550000
P	-43.99661400	22.54971500	12.83980500
O	-45.37323100	23.14003500	13.04280500
O	-42.84460600	23.14926000	13.61295800
O	-44.00237600	20.93960400	13.18148400
C	-45.06648500	20.13984900	12.64523500
C	-44.88539900	18.70397000	13.09461300
O	-43.76237100	18.11492500	12.39777800
C	-44.60314100	18.54167800	14.60367200
O	-45.36127000	17.42247800	15.05224200
C	-43.09331700	18.27279800	14.63463300
C	-42.92139900	17.47954600	13.34095300
N	-41.56768700	17.49405400	12.79789600
C	-41.14242100	17.93082300	11.56694600
N	-39.89281600	17.79360400	11.33331700
C	-39.39729700	17.18191300	12.49318700
C	-38.07449800	16.76007500	12.83918100
O	-37.02819000	16.83028800	12.19842800
N	-38.07395600	16.18052400	14.14147700
C	-39.16148200	16.03307200	14.96990600
N	-38.96293500	15.40328700	16.15768600
N	-40.37821000	16.43162100	14.63836000
C	-40.43160400	16.98633600	13.40950900
H	-40.96117400	24.45350000	9.23864200
H	-41.07396000	23.56302000	7.70075900
H	-43.15906800	23.51466200	9.06546300
H	-41.67644600	23.02526300	11.34755400
H	-42.31344000	20.37168600	11.55223100
H	-40.85446400	20.87083500	10.66301100
H	-43.54269500	20.03534500	9.50998600
H	-39.96067400	20.49913200	8.29069300
H	-46.03193000	20.51392600	13.00346000
H	-45.05890100	20.18356800	11.54988400
H	-45.79176500	18.14282200	12.83981200
H	-44.87653200	19.44345600	15.16604800
H	-42.75620300	17.72759700	15.51565700
H	-42.54659700	19.21524600	14.55267100
H	-43.21671300	16.43116400	13.48401400
H	-39.72473400	15.47264400	16.81698900

C	-38.69049500	23.19624700	8.81117300
H	-37.91813600	22.49935400	9.14280300
H	-38.61598700	23.32502600	7.72192800
H	-38.52682400	24.17165900	9.29117600
Na	-44.40633000	24.68537900	14.64071800
C	-45.41247200	17.29647200	16.46735500
H	-45.84307400	18.19479700	16.93336500
H	-46.05243300	16.43917000	16.68655900
H	-44.42257400	17.11778000	16.90843300
H	-37.16769100	15.84036300	14.44284400
H	-38.03790400	15.37632200	16.56120700
H	-44.22087000	15.68940800	8.62384800
N	-40.19895200	15.47622900	6.88138000
H	-40.27483000	14.47027000	6.85315600
H	-39.27266400	15.87410400	6.84711900

5'-*aA(sG*)*-3'

O	-3.76338000	-0.05845800	-0.29184000
C	-4.12309800	0.41522000	0.99732900
C	-2.88461200	0.44523100	1.88465800
O	-2.44489200	-0.89993400	2.17642200
C	-1.69268900	1.16082200	1.22947900
O	-0.93593400	1.83852900	2.25688400
C	-0.91059500	0.00673200	0.62306200
C	-1.17762000	-1.15092800	1.58333500
P	0.08441300	3.05076100	1.82388300
O	0.46879400	3.77171900	3.09329500
O	-0.51296400	3.89283800	0.70832400
O	1.36404800	2.27298600	1.16415100
C	2.16792000	1.41107800	1.98121600
C	3.13743000	0.65431900	1.09053100
O	2.40987600	-0.26762500	0.25535600
C	3.97425800	1.54018200	0.14268700
O	5.29583700	1.00480000	0.14185900
C	3.26854700	1.36163100	-1.20572300
C	2.80073900	-0.08879600	-1.10821900
N	1.69111800	-0.46141600	-1.96713600
C	1.46346900	-1.74129100	-2.43035700
N	0.34516000	-1.94399000	-3.00345400
C	-0.31542700	-0.70807900	-2.89362900
C	-1.65634800	-0.34183800	-3.23455000
O	-2.55022400	-1.01407800	-3.74915400
N	-1.90885800	1.00393100	-2.85421200

C	-1.03574300	1.84302300	-2.20020000
N	-1.46962900	3.07941700	-1.84817400
N	0.20804300	1.48915700	-1.91437900
C	0.50376700	0.22286100	-2.25198000
H	-4.54105400	1.43258200	0.93456000
H	-4.88203400	-0.23688100	1.45480200
H	-3.14483100	0.93159700	2.83054100
H	-2.02046400	1.88896200	0.48663300
H	0.14693200	0.21261300	0.48865900
H	-1.35458800	-0.24291000	-0.33884200
H	-0.40710800	-1.24522800	2.35594600
H	2.72877400	1.99972100	2.71641200
H	1.53342800	0.69482500	2.51598900
H	3.82225600	0.09075800	1.73571000
H	3.98675500	2.58859200	0.46847300
H	2.40318000	2.02103900	-1.26048400
H	3.61279500	-0.78298100	-1.35302700
H	-1.00387000	3.47387600	-1.01948100
H	3.92089500	1.53351100	-2.06329900
H	-2.86052500	1.30944200	-3.02065400
H	-2.46337300	3.25841800	-1.89309700
Na	-0.25034400	5.86134200	2.11614400
C	-4.84553400	-0.07716600	-1.21380100
H	-5.66730900	-0.71411300	-0.85706600
H	-5.23928700	0.93521600	-1.38656600
H	-4.45243200	-0.48150900	-2.14932300
C	6.25664900	1.84972900	-0.47656300
H	7.22626700	1.35811700	-0.37180400
H	6.05534500	2.00325200	-1.54541200
H	6.29838500	2.83379100	0.01291800
N	-1.20979300	-2.43630200	0.89314900
C	-2.16871200	-2.86957900	-0.00348900
N	-1.85943500	-4.00407200	-0.59394800
C	-0.61612300	-4.32698900	-0.07398400
C	0.27981100	-5.38839300	-0.32306000
N	1.46042300	-5.40617000	0.33128300
C	1.72548600	-4.41271700	1.19741900
N	0.97123300	-3.35725900	1.52052900
C	-0.19136100	-3.36389500	0.84930600
H	-3.05963600	-2.28032200	-0.16851500
H	2.68955200	-4.47859000	1.69806400
N	-0.01438700	-6.40192000	-1.17355400
H	-0.78661900	-6.28672800	-1.81216500
H	0.73625200	-7.01480500	-1.45535800

TS _{2/AG}			
O	-0.02335200	-0.12320800	0.04546000
C	0.03252400	-0.08671400	1.46110200
C	1.48497500	-0.04980000	1.90762900
O	2.11064600	-1.31652100	1.59606600
C	2.32755500	1.03433100	1.19876800
O	3.29992300	1.51812100	2.15848500
C	3.00854400	0.23506200	0.09834600
C	3.31478300	-1.04139200	0.87233200
P	4.33253900	2.73461900	1.75491700
O	4.91870000	3.24371600	3.05246300
O	3.66284300	3.73317400	0.83856300
O	5.49042800	1.98986700	0.84868000
C	6.28389500	0.94527900	1.42750900
C	6.98385300	0.15738400	0.32846300
O	6.01609800	-0.43047900	-0.56840000
C	7.93251900	0.98694000	-0.55294700
O	9.06773700	0.16828000	-0.82437800
C	7.08835400	1.24723600	-1.80222800
C	6.31766700	-0.06678800	-1.91275900
N	5.06287200	0.01408300	-2.66082500
C	4.02471000	-0.90889700	-2.61600800
N	3.05301300	-0.65300100	-3.42847400
C	3.45444800	0.49565100	-4.10630400
C	2.79142400	1.23048500	-5.14012900
O	1.70145600	1.02865900	-5.67394700
N	3.58797800	2.33526600	-5.54826600
C	4.82233700	2.66768300	-5.04444200
N	5.46500500	3.72675800	-5.61217700
N	5.41932800	1.98349200	-4.08686400
C	4.70199900	0.92254200	-3.65156300
H	-0.48524400	0.80472400	1.85152400
H	-0.45398600	-0.97418200	1.89546100
H	1.51639300	0.11349500	2.99149200
H	1.72727600	1.86925900	0.83275900
H	3.89762400	0.70675100	-0.30424300
H	2.28896600	0.03496700	-0.69606600
H	4.13215100	-0.87845000	1.57723000
H	7.04225500	1.37001300	2.09605400
H	5.65785100	0.26791200	2.01450000
H	7.55149200	-0.64723600	0.80918400
H	8.24270500	1.91862700	-0.06110100

H	6.39054100	2.06222700	-1.60603500
H	6.93497000	-0.85184300	-2.36765200
H	6.26695800	4.06160700	-5.09728600
H	7.66983500	1.48463300	-2.69095000
H	3.18692700	2.88501000	-6.29942600
H	4.92283700	4.44322900	-6.07367700
Na	4.20297700	5.47237600	2.42838800
C	-1.35109500	-0.15581000	-0.45235800
H	-1.89328000	-1.04642300	-0.10124600
H	-1.91967700	0.73670000	-0.15096300
H	-1.28678200	-0.18531300	-1.54229800
C	10.14757700	0.86619700	-1.42996800
H	10.96622300	0.15150400	-1.53862300
H	9.89040400	1.25836600	-2.42314700
H	10.48423400	1.70455100	-0.80264000
N	3.72027500	-2.18547000	0.09379900
C	3.29350200	-2.56790300	-1.17319100
N	3.97801300	-3.61826400	-1.64899300
C	4.95012900	-3.83822900	-0.71183500
C	6.04363900	-4.73986800	-0.66248200
N	6.86726500	-4.69761600	0.40664400
C	6.61077700	-3.80118600	1.37259400
N	5.62073800	-2.90112000	1.44801600
C	4.81842900	-2.96224800	0.37913300
H	2.32865000	-2.25779800	-1.54588900
H	7.30693100	-3.80855800	2.20869600
N	6.27906100	-5.63587200	-1.63842300
H	5.72744900	-5.62578900	-2.48173800
H	7.11171400	-6.20336600	-1.60177500

5'-•A_{N7}(8-8)G-3'

O	-4.61929700	-0.04152500	0.79643300
C	-4.43997500	-0.18767000	2.19510300
C	-2.95467100	-0.23972600	2.50761500
O	-2.40704700	-1.48318800	2.01886600
C	-2.14417100	0.89373200	1.82951100
O	-1.14639800	1.34565000	2.77968900
C	-1.50033900	0.16363100	0.65928200
C	-1.17272700	-1.15502100	1.35161500
P	-0.10604700	2.55642400	2.38228400
O	0.47695700	3.06397400	3.68227400
O	-0.76206300	3.55898900	1.46028300
O	1.05557300	1.80248000	1.48581200

C	1.84934000	0.77208600	2.08849600
C	2.52541700	-0.06086500	1.00855900
O	1.52816300	-0.67984100	0.17306000
C	3.45367000	0.70701700	0.05528200
O	4.56901200	-0.14145800	-0.20622100
C	2.57247000	0.91373500	-1.17841000
C	1.76446400	-0.38613800	-1.19674700
N	0.46459000	-0.30443700	-1.88453800
C	-0.61059200	-1.19668100	-1.77356900
N	-1.61443100	-0.87645600	-2.55809400
C	-1.20710800	0.25381200	-3.22554100
C	-1.89965600	1.02565200	-4.21693800
O	-3.02274300	0.86307600	-4.68870700
N	-1.09077200	2.10468800	-4.65693000
C	0.18167900	2.38442400	-4.21733000
N	0.82857900	3.42800700	-4.80232200
N	0.80730600	1.66595500	-3.30406100
C	0.08000900	0.62548800	-2.83561800
H	-4.88925700	0.66075700	2.73719300
H	-4.92015400	-1.10990000	2.55843500
H	-2.82026500	-0.17667800	3.59515700
H	-2.76611500	1.73819600	1.52848300
H	-0.63093100	0.67378500	0.25959600
H	-2.25265800	0.00831000	-0.11429400
H	-0.40801900	-0.98451700	2.11450300
H	2.61715500	1.21202400	2.73585200
H	1.22212300	0.11563700	2.69981800
H	3.10279500	-0.84736100	1.50866200
H	3.79005800	1.66043800	0.48435600
H	1.90378200	1.75590300	-1.00172800
H	2.32659800	-1.21087600	-1.65141400
H	1.67494400	3.72342100	-4.33723500
H	3.12900200	1.09193900	-2.09621300
H	-1.51165800	2.67750300	-5.37945300
H	0.29600700	4.16353900	-5.24410000
Na	-0.22327800	5.29501500	3.05159700
C	-5.98525100	0.03363300	0.42357100
H	-6.53353600	-0.87723200	0.70721100
H	-6.48632000	0.89677800	0.88728600
H	-6.01913000	0.14466400	-0.66258600
C	5.63822200	0.50809900	-0.88075100
H	6.44198400	-0.22448800	-0.98070600
H	5.35342700	0.85532600	-1.88304600
H	6.00786600	1.37039900	-0.30684300

N	-0.68210900	-2.25358800	0.56605000
C	-0.70095200	-2.43560300	-0.91675300
N	0.36329600	-3.39115900	-1.23400300
C	0.90098000	-3.72299800	-0.06186300
C	1.99785100	-4.58161000	0.24196300
N	2.40278500	-4.71235900	1.52550700
C	1.75203900	-4.01241100	2.45813900
N	0.70600900	-3.16784500	2.31205100
C	0.30982800	-3.05325300	1.04828500
H	-1.66926700	-2.86867800	-1.20371500
H	2.11190000	-4.13830900	3.47698000
N	2.63704900	-5.26714200	-0.72670700
H	2.41318900	-5.09381800	-1.69435600
H	3.47675700	-5.77848600	-0.50174500

Table S8 Cartesian coordinates of stationary points along the reaction path of the guanine-8-yl radical addition to the C₈ site of its 3' neighboring deoxyadenosine.

5'-(aG*)aA-3'			
O	-3.95245900	1.06438500	-1.29262600
C	-4.47349600	1.16537400	0.02287700
C	-3.33014700	1.26513600	1.02379500
O	-2.65509000	0.00689100	1.19930300
C	-2.23011300	2.25603900	0.62415000
O	-1.68642800	2.78350900	1.85177000
C	-1.23173100	1.37808800	-0.14044000
C	-1.47016400	-0.03722700	0.40979200
N	-1.59912600	-1.03776200	-0.64518300
C	-2.14037300	-0.90756100	-1.90447700
N	-2.25249100	-1.98925500	-2.57802300
C	-1.74357800	-2.97633400	-1.71609400
C	-1.49450100	-4.36430000	-1.93465800
N	-0.92773600	-4.95119700	-0.77227700
C	-0.55759800	-4.28509600	0.37148700
N	-0.75200100	-2.98826800	0.54462700
C	-1.33603700	-2.39591000	-0.51534600
P	-0.53779100	3.95780400	1.80091500
O	-0.58982600	4.67836200	3.12919200
O	-0.65107800	4.78533200	0.54113300
O	0.84935800	3.08227300	1.66728300

C	1. 15546200	2. 15286100	2. 71868500
C	2. 29003200	1. 25492400	2. 27181200
O	1. 81851800	0. 37294600	1. 23239100
C	3. 51528400	2. 00706000	1. 69692400
O	4. 67406600	1. 41890800	2. 27833000
C	3. 41267700	1. 72381600	0. 19161200
C	2. 82245900	0. 31798600	0. 21273100
N	2. 22266400	-0. 15203400	-1. 01208100
C	1. 49107700	0. 54892900	-1. 95703000
N	0. 97509300	-0. 21150000	-2. 89368600
C	1. 37833800	-1. 49510200	-2. 55319300
C	1. 11194400	-2. 76504600	-3. 10854700
N	1. 65735700	-3. 84997100	-2. 51980500
C	2. 40132600	-3. 67716500	-1. 41491100
N	2. 68958800	-2. 54123500	-0. 77032900
C	2. 14982500	-1. 48117200	-1. 38716100
H	-5. 11233100	2. 05868600	0. 11366800
H	-5. 08343900	0. 28439600	0. 27267500
H	-3. 75299900	1. 54033200	1. 99473500
H	-2. 60417100	3. 08065100	0. 01374100
H	-0. 20258000	1. 68724600	0. 02739200
H	-1. 45521600	1. 41873500	-1. 20673900
H	-0. 65110600	-0. 38113500	1. 04378500
H	1. 45411200	2. 69551200	3. 62296200
H	0. 27646500	1. 54064600	2. 94900800
H	2. 62305700	0. 66149200	3. 13246800
H	3. 47525100	3. 08047100	1. 92022800
H	4. 36837000	1. 78016100	-0. 33088300
H	2. 70883900	2. 42811100	-0. 25743800
H	3. 58752200	-0. 41932300	0. 48142300
C	5. 86397800	2. 16899200	2. 07029600
H	5. 77117100	3. 18651300	2. 47675700
H	6. 66481100	1. 64571700	2. 59698200
H	6. 13260300	2. 24319100	1. 00787000
C	-4. 95298000	0. 83768700	-2. 27496900
H	-4. 44433200	0. 76379900	-3. 23792200
H	-5. 49692700	-0. 09825700	-2. 08484100
H	-5. 67560800	1. 66535900	-2. 30663800
O	-1. 67935600	-5. 04975800	-2. 94335100
H	-0. 71211200	-5. 93687500	-0. 86902700
N	-0. 01239100	-5. 01923800	1. 37690100
H	0. 42326300	-5. 90597800	1. 16942600
H	0. 42267200	-4. 48281600	2. 11369600
Na	-0. 87512900	6. 75967200	1. 90657600

H	1.38216000	1.62166100	-1.90237000
H	2.80903700	-4.58766200	-0.98074300
N	0.33188500	-2.93834300	-4.21165300
H	-0.09292700	-3.85735800	-4.27937600
H	-0.32088900	-2.18544500	-4.39116200

TS_{GA}

O	0.20657000	0.60724900	-1.29495300
C	-0.26509200	0.60617200	0.04128800
C	0.90711900	0.40721700	0.98799700
O	1.40412600	-0.94200200	0.85536400
C	2.10162800	1.33940500	0.70082600
O	2.67424000	1.71267300	1.97491700
C	3.04184500	0.42945700	-0.08268300
C	2.81528900	-0.89263100	0.63316700
N	3.23227300	-2.05645200	-0.11430500
C	3.84643500	-2.12993300	-1.35794200
N	4.14056700	-3.33697100	-1.71487500
C	3.70596600	-4.14310100	-0.66394400
C	3.76650900	-5.56198700	-0.48848600
N	3.21949200	-5.92251900	0.77658800
C	2.71166900	-5.05804000	1.71784400
N	2.65814600	-3.75052800	1.54232400
C	3.15391600	-3.35928700	0.34717100
P	3.87766500	2.83187600	2.03051600
O	4.03419800	3.22240500	3.48193000
O	3.65520000	3.92849400	1.01497300
O	5.19398600	1.98693400	1.51178900
C	5.69321200	0.92037500	2.33093000
C	6.74589300	0.14578600	1.56570400
O	6.13727800	-0.63006100	0.50840800
C	7.83925200	1.02926300	0.90595100
O	9.09535000	0.55052300	1.37406500
C	7.63306700	0.76801800	-0.59225700
C	7.08247000	-0.65759000	-0.55968800
N	6.45506600	-1.11621900	-1.77920500
C	5.26791300	-0.67744600	-2.37277300
N	5.10725800	-1.17243800	-3.61213600
C	6.12751000	-2.06117100	-3.75255300
C	6.46430600	-2.97315700	-4.78734000
N	7.56216400	-3.74401700	-4.63809600
C	8.28452900	-3.61323700	-3.51454800
N	8.07695500	-2.80406500	-2.46486000

C	6.98213600	-2.05536000	-2.63113400
H	-0.76171300	1.56040700	0.28250600
H	-0.99621700	-0.20207500	0.19951000
H	0.55973100	0.56727400	2.01572000
H	1.81476000	2.23804200	0.15160700
H	4.07660100	0.75696400	-0.05790700
H	2.67210500	0.34680200	-1.10696000
H	3.33458600	-0.92300800	1.59798900
H	6.14863700	1.33090100	3.23917200
H	4.88099100	0.24796500	2.62708300
H	7.24513100	-0.53629400	2.26599800
H	7.71273800	2.08781900	1.16294600
H	8.54787900	0.86086600	-1.17926900
H	6.87375900	1.44330100	-0.99697900
H	7.88806300	-1.37229500	-0.35013800
C	10.17772500	1.43298200	1.10774900
H	10.01077800	2.41960500	1.56402800
H	11.07029800	0.98253200	1.54710400
H	10.34827000	1.57321600	0.03161700
C	-0.83066300	0.79760800	-2.24345600
H	-0.37019600	0.78402900	-3.23380300
H	-1.58243900	-0.00367800	-2.18711300
H	-1.34071000	1.76177200	-2.09878100
O	4.19893600	-6.43543800	-1.23982500
H	3.20927300	-6.91997100	0.95752600
N	2.19510900	-5.60674500	2.85396000
H	2.53277000	-6.50792300	3.16044400
H	2.00988200	-4.94643000	3.59573100
Na	3.86901000	5.54389500	2.82113100
H	4.78076300	0.21568500	-2.01922000
H	9.15905400	-4.25694400	-3.44776800
N	5.73155300	-3.07973600	-5.90950800
H	5.96234700	-3.78778400	-6.58950100
H	4.86253500	-2.57684500	-5.99758100

5'-G(8-8)(*A_{N7})-3'

O	-4.19510700	1.47093100	-1.29820500
C	-4.69337600	1.41969600	0.02744900
C	-3.54189700	1.16657500	0.98485900
O	-3.06557100	-0.18493200	0.80373000
C	-2.32465500	2.08610600	0.75011600
O	-1.78892800	2.44015200	2.04394900
C	-1.37438200	1.16613600	-0.01401000

C	-1.64160500	-0.14206400	0.71687200
N	-1.17319700	-1.38445800	0.11466000
C	-0.29038400	-1.65553800	-0.93637800
N	-0.03362500	-2.93694600	-1.05780600
C	-0.74176000	-3.54818300	-0.04803200
C	-0.82304000	-4.93337200	0.31665300
N	-1.64006700	-5.09077500	1.46765000
C	-2.25583900	-4.07744100	2.16659300
N	-2.18201200	-2.80718900	1.81669300
C	-1.43607600	-2.60565600	0.70586200
P	-0.56087400	3.53098100	2.14324600
O	-0.43709800	3.90735100	3.60112200
O	-0.73238600	4.63819600	1.12933100
O	0.74782900	2.65816200	1.65360000
C	1.22521100	1.59531000	2.49102900
C	2.25757700	0.78092300	1.73845100
O	1.62251900	-0.02856000	0.72155400
C	3.34861800	1.62474700	1.02515600
O	4.60818000	1.15592000	1.49584200
C	3.11668400	1.30288600	-0.45783200
C	2.54884600	-0.11451300	-0.35535000
N	1.87663000	-0.61763700	-1.53347100
C	0.41362200	-0.64481300	-1.82321600
N	0.28941900	-1.04310600	-3.22729700
C	1.53439800	-1.25549700	-3.64842700
C	2.03012900	-1.67258600	-4.91796500
N	3.36483600	-1.79775200	-5.10302500
C	4.16970200	-1.51677300	-4.07514100
N	3.84577200	-1.11240800	-2.82571800
C	2.52974600	-1.00315000	-2.65243600
H	-5.18116200	2.36977400	0.30008300
H	-5.43789900	0.61582900	0.13765700
H	-3.90021800	1.29406100	2.01350700
H	-2.57672000	2.99205100	0.19641200
H	-0.34017100	1.49366900	0.02540500
H	-1.74200600	1.09248300	-1.03951100
H	-1.21409400	-0.10989500	1.72652500
H	1.69306900	2.01349900	3.38916900
H	0.39955200	0.94675200	2.80353700
H	2.75988300	0.11859600	2.45501700
H	3.23473200	2.69400700	1.24014200
H	4.02273700	1.35486000	-1.06273000
H	2.35630800	1.96522800	-0.88178700
H	3.35990100	-0.81810100	-0.11499200

C	5.69238900	2.01581900	1.17128500
H	5.54211000	3.02339200	1.58599900
H	6.58946700	1.57764000	1.61398300
H	5.84383100	2.10682300	0.08703000
C	-5.21057300	1.71753400	-2.25763900
H	-4.73053600	1.73967300	-3.23844300
H	-5.97437100	0.92584900	-2.25043900
H	-5.70965700	2.68209500	-2.08123100
O	-0.30717700	-5.91594200	-0.21251900
H	-1.75929000	-6.05158100	1.76832400
N	-3.01670200	-4.43546600	3.23811200
H	-2.81209100	-5.29725300	3.72355100
H	-3.30444000	-3.66839800	3.82909100
Na	-0.56807300	6.23774400	2.94693100
H	0.00255900	0.35405000	-1.69684400
H	5.23460000	-1.62769700	-4.26806200
N	1.19521000	-1.92389800	-5.94753400
H	1.56540800	-2.32576400	-6.79542000
H	0.20040900	-1.95809700	-5.78675000
