

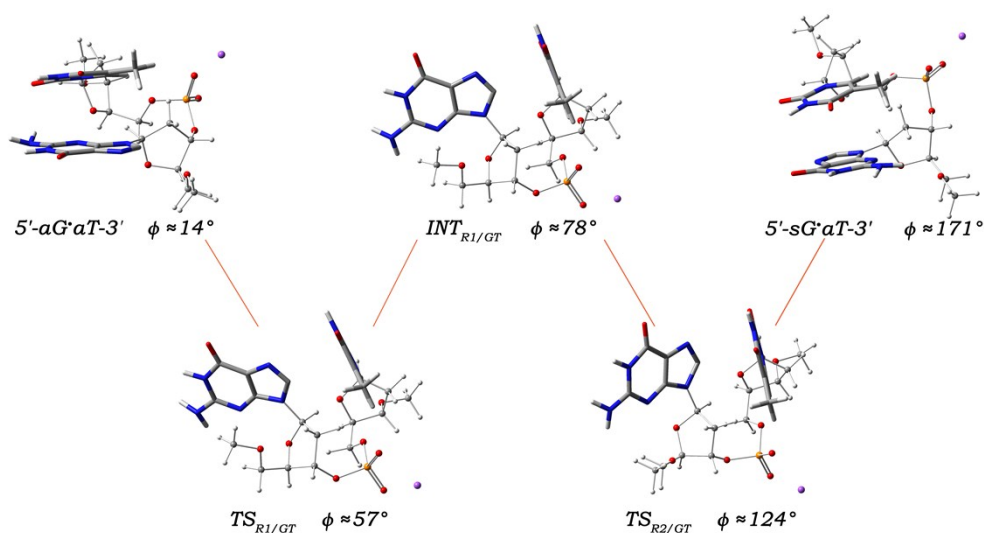
## Electronic Supplementary Information

### DNA Intrastrand Cross-Links Induced by the Purine-Type Deoxyguanosine-8-yl Radical: A DFT Study

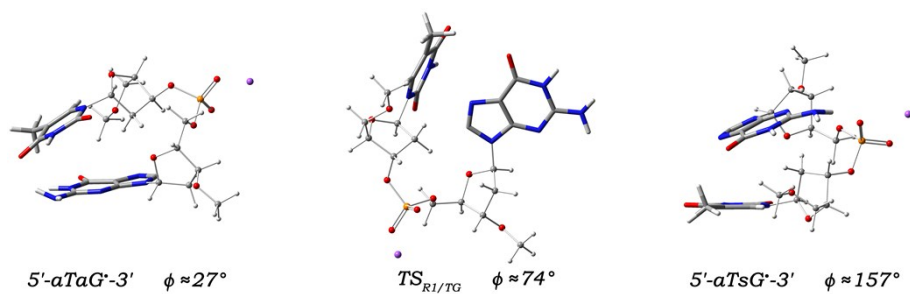
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<sup>a</sup>Guangdong Engineering and Technology Research Center for Advanced Nanomaterials, School of Environment and Civil Engineering, Dongguan University of Technology, Dongguan 523808, People's Republic of China.

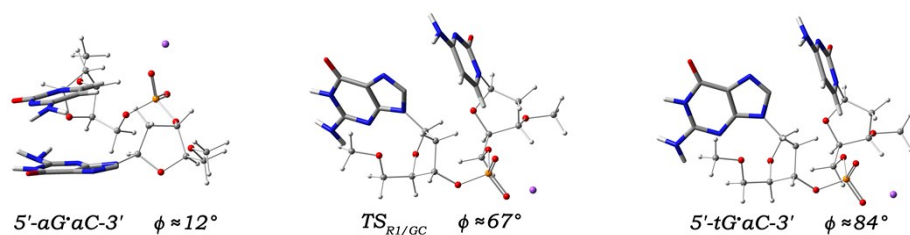
<sup>b</sup>School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510641, People's Republic of China.



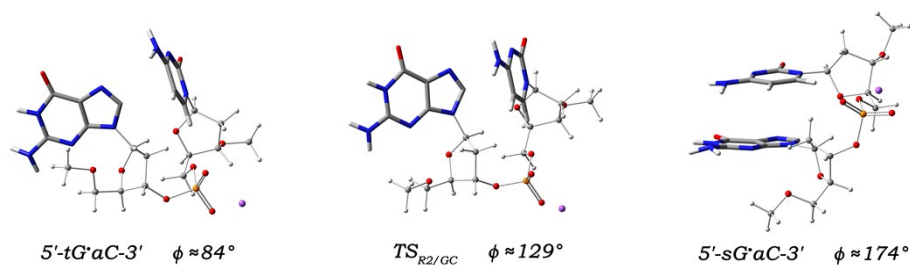
**Figure S1.** Optimized structures for stationary points along the conformation transformation pathway of the canonical 5'-aG\*aT-3' sequence to the non-canonical 5'-sG\*aT-3' sequence.



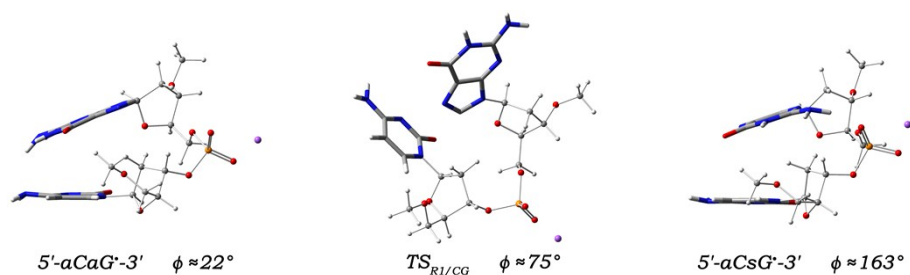
**Figure S2.** Optimized structures for stationary points along the conformation transformation pathway of the canonical 5'-aTaG\*-3' sequence to the non-canonical 5'-aTsG\*-3' sequence.



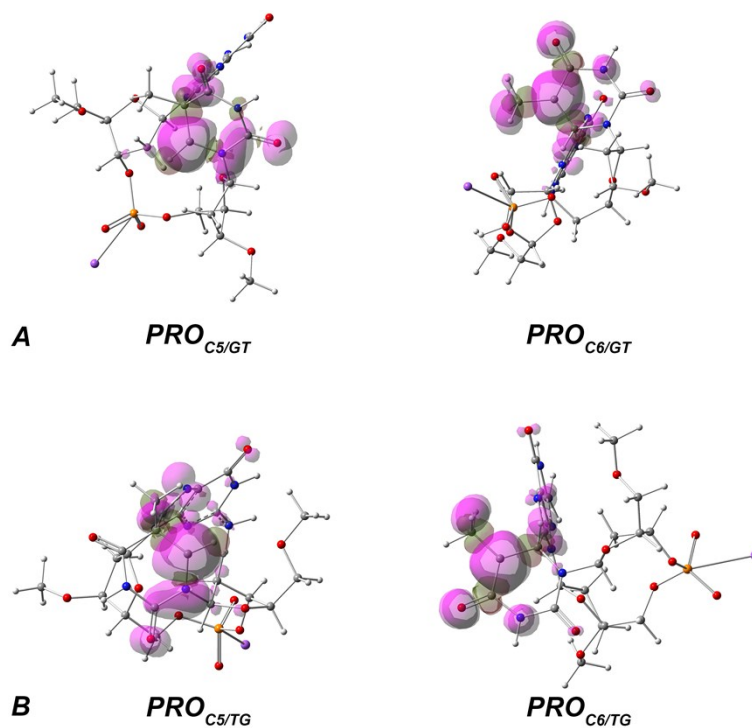
**Figure S3.** Optimized structures for stationary points along the conformation transformation pathway of the canonical 5'-aG\*aC-3' sequence to the non-canonical 5'-tG\*aC-3' sequence.



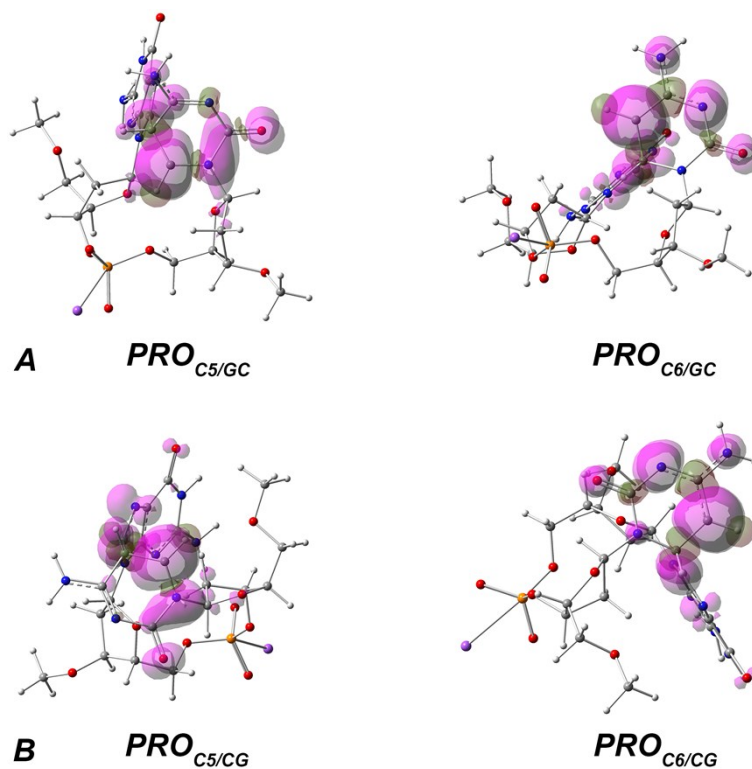
**Figure S4.** Optimized structures for stationary points along the conformation transformation pathway of the non-canonical 5'-tG\*aC-3' sequence to the non-canonical 5'-sG\*aC-3' sequence.



**Figure S5.** Optimized structures for stationary points along the conformation transformation pathway of the canonical 5'-aCaG\*-3' sequence to the non-canonical 5'-aCsG\*-3' sequence.



**Figure S6.** Spin density distributions of the reaction products formed by the deoxyguanosine-8-yl radical addition in the 5'-G<sup>\*</sup>T-3' (A) and 5'-TG<sup>\*</sup>-3' (B) sequences, respectively.



**Figure S7.** Spin density distributions of the reaction products formed by the deoxyguanosine-8-yl radical addition in the 5'-G<sup>\*</sup>C-3' (A) and 5'-CG<sup>\*</sup>-3' (B) sequences, respectively.

**Table S1.** Kinetic ( $\Delta G^\ddagger$ ) and thermodynamic ( $\Delta G$ ) characteristics for conformation transformations of the G moiety from the anti configuration to the syn configuration in the four sequences studied herein. Energies are in kcal/mol.

Initial sequence	$\Delta G_1^\ddagger$	$\Delta G_1$	$\Delta G_2^\ddagger$	$\Delta G_2$	$\Delta G_t^a$
5'-aG <sup>*</sup> aT-3'	10.13	8.89	0.19	-4.06	4.83
5'-aTaaG <sup>*</sup> -3'	9.97	-0.84	-	-	-0.84
5'-aG <sup>*</sup> aC-3'	10.74	9.04	2.01	-2.93	6.11
5'-aCaG <sup>*</sup> -3'	8.39	-1.29	-	-	-1.29

<sup>a</sup> Total reaction free energy for the complete conformation transformation process.

**Table S2.** Cartesian coordinates of stationary points along the reaction paths of deoxyguanosine-8-yl radical addition to the C5 and C6 sites of its 3' flanking deoxythymidine started from the canonical 5'-aG<sup>\*</sup>aT-3' sequence, respectively.

5'-aG <sup>*</sup> aT-3'			
O	0.00601800	0.01652500	-0.02221700
C	-0.01733600	0.01753800	1.39561800
C	1.40642800	0.01213300	1.93558800
O	2.04551800	-1.26644900	1.75422500
C	2.34410000	1.02999000	1.26497900
O	3.25285400	1.51014400	2.27917200
C	2.96315000	0.21188400	0.12729600
C	2.88932800	-1.24711000	0.60465200
N	2.38302100	-2.13245400	-0.44046200
C	1.49017800	-1.84479800	-1.45076400
N	1.18248000	-2.82060500	-2.21647200
C	1.93917500	-3.89192600	-1.71689900
C	2.05246100	-5.24248500	-2.17372800
N	2.95405800	-5.96355000	-1.33946500
C	3.64386800	-5.46061200	-0.26223400
N	3.53678600	-4.20543800	0.13890700
C	2.68164800	-3.48012800	-0.61043600
P	4.87050500	1.69985000	2.10797900
O	5.34035800	2.42815900	3.34628500
O	5.26334700	2.27456100	0.76504700
O	5.40071300	0.14312500	2.10905900
C	5.16064600	-0.64666400	3.28906400
C	6.15457400	-1.78966500	3.31086300
O	5.91221500	-2.64389900	2.17795400

C	7. 62989500	-1. 35127300	3. 22410300
O	8. 37421400	-2. 24224700	4. 04906600
C	7. 95314500	-1. 53139500	1. 73589400
C	7. 09560600	-2. 74836000	1. 38493000
N	6. 69906200	-2. 86944700	-0. 01603300
C	6. 73174800	-4. 13972100	-0. 58453200
O	7. 17862500	-5. 13271100	-0. 01604400
N	6. 21583300	-4. 20149500	-1. 86239400
C	5. 57781300	-3. 18512000	-2. 58437400
O	5. 09235200	-3. 42031700	-3. 68738100
C	5. 55570900	-1. 89389500	-1. 90659300
C	6. 08871200	-1. 80920300	-0. 66546100
H	-0. 54051200	0. 91203600	1. 77061200
H	-0. 54256700	-0. 86934400	1. 78053600
H	1. 36184000	0. 19625800	3. 01274700
H	1. 80028400	1. 89618300	0. 88025200
H	3. 97491900	0. 52421800	-0. 11302700
H	2. 33972600	0. 34649200	-0. 75703500
H	3. 85486300	-1. 65670700	0. 90428800
H	5. 28571100	-0. 03231200	4. 18703300
H	4. 13880100	-1. 03999100	3. 25907500
H	6. 00843400	-2. 36420200	4. 23304600
H	7. 76571400	-0. 31316900	3. 55644000
H	7. 63741300	-0. 64144100	1. 19026700
H	9. 01182100	-1. 70913600	1. 54174300
H	7. 62198400	-3. 67295000	1. 62397100
H	6. 05038900	-0. 88960900	-0. 09431800
H	6. 23312800	-5. 11937600	-2. 29154300
C	4. 91564700	-0. 74134900	-2. 62341300
H	3. 83674500	-0. 89732600	-2. 73193600
H	5. 07916300	0. 19793400	-2. 09183900
H	5. 32748800	-0. 64630000	-3. 63266200
Na	6. 45207700	4. 04325400	1. 93269300
N	4. 43814100	-6. 32244900	0. 43348100
H	4. 76630800	-7. 15033100	-0. 04460000
H	3. 07492100	-6. 93550300	-1. 60193500
O	1. 50868700	-5. 80542500	-3. 12143600
H	5. 16103900	-5. 86881300	0. 97809700
C	-1. 28647100	-0. 07623400	-0. 60350600
H	-1. 14903500	-0. 09615300	-1. 68619100
H	-1. 80314100	-0. 99453900	-0. 29049800
H	-1. 90946300	0. 78756900	-0. 33105300
C	9. 71078400	-1. 82219600	4. 28857600
H	10. 15878200	-2. 55688400	4. 96101600

H	10.30887300	-1.77882700	3.36826000
H	9.73902000	-0.83254000	4.76753900
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TS <sub>C5/GT</sub>			
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O	2.03124700	-1.25066200	1.59623800
C	2.34678500	1.07653000	1.30211200
O	3.34142200	1.38523600	2.30543600
C	2.96351400	0.34293300	0.11814700
C	3.07852100	-1.08528400	0.63187500
N	2.95214500	-2.11007300	-0.39501100
C	2.42854400	-2.05596400	-1.69018600
N	2.24404300	-3.23322700	-2.20654200
C	2.58901300	-4.13811200	-1.20795700
C	2.55818900	-5.56894300	-1.19232700
N	3.03403300	-6.05555400	0.05867500
C	3.46779200	-5.28868300	1.11436600
N	3.49109000	-3.96859600	1.08553000
C	3.04455300	-3.45716800	-0.08322900
P	4.35573200	2.65718000	2.06815100
O	5.04514500	2.91176800	3.38892600
O	3.64003200	3.81004400	1.40291800
O	5.43186400	2.07576300	0.96197700
C	6.33154900	1.03856200	1.38133500
C	7.03474200	0.45618900	0.17215100
O	6.10799900	-0.32925800	-0.60441600
C	7.65100000	1.50472500	-0.79233000
O	9.00931900	1.13214300	-0.99421300
C	6.80545000	1.34597600	-2.06694100
C	6.44926800	-0.13617000	-1.98047900
N	5.34736100	-0.61331400	-2.80827700
C	5.53487600	-1.80911900	-3.52005100
O	6.57934400	-2.44344200	-3.51372100
N	4.44400000	-2.18861100	-4.27721100
C	3.16780400	-1.62867600	-4.28812400
O	2.32371300	-2.00023700	-5.08751800
C	2.96537100	-0.55696100	-3.28196600
C	4.12497200	0.01544900	-2.78126900
H	-0.51966900	0.95547000	1.70303600
H	-0.55450900	-0.82459200	1.70390200
H	1.35152000	0.12443900	2.97751800
H	1.82515500	1.99169500	1.01313200
H	3.92562600	0.75008300	-0.16946500

H	2.25536100	0.37570200	-0.70545300
H	4.03610400	-1.26770300	1.12738000
H	7.08009300	1.45122600	2.06673200
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H	7.34612600	1.60204500	-2.97902200
H	7.31305000	-0.74770700	-2.25012200
H	4.10089700	0.96241700	-2.26552400
H	4.59250200	-2.99353300	-4.87428800
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H	0.84000700	-0.42444800	-3.49216700
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H	1.72854900	0.84696300	-4.34015400
Na	4.38518300	5.22281200	3.24772400
N	3.83736100	-5.94299700	2.25098200
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PRO<sub>C5/GT</sub>

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C	2.30697100	1.06191300	1.23604600
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C	3.06141900	0.27572200	0.16585700
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N	3.50471700	-2.27994000	0.11222700
C	3.52456300	-2.67912100	-1.23549600
N	3.89214500	-3.93297300	-1.36885000
C	4.11177900	-4.40382200	-0.09198200
C	4.53602600	-5.69491600	0.36408100
N	4.65060500	-5.70001400	1.78172200

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N	4. 01392300	-3. 45046000	2. 18036500
C	3. 88395800	-3. 39695500	0. 83620300
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O	4. 78323800	2. 97756500	3. 51633000
O	3. 35340700	3. 90091200	1. 55982200
O	5. 24360000	2. 30214600	1. 04621600
C	6. 31355900	1. 42678000	1. 43795900
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O	6. 30127800	-0. 13631100	-0. 41977200
C	7. 29785800	1. 99987000	-0. 88950100
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C	6. 42747000	1. 50658200	-2. 05823000
C	6. 50440400	-0. 00155700	-1. 83383500
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N	5. 06545000	-2. 67315500	-3. 90560800
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O	2. 93706000	-3. 30375500	-4. 38579600
C	3. 26829500	-1. 80257000	-2. 46258600
C	4. 18195600	-0. 61155200	-2. 48480200
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H	-0. 71347600	-0. 68485100	1. 44134700
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H	4. 03726600	0. 68772200	-0. 06182600
H	2. 43082900	0. 24625900	-0. 71676700
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H	6. 80224000	1. 81613700	-3. 03489500
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H	3. 83561900	0. 40843700	-2. 45472100
H	5. 42151600	-3. 36719000	-4. 55152000
C	1. 77781600	-1. 44735100	-2. 61167000
H	1. 23061300	-2. 34787500	-2. 89383100
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H	1. 64328800	-0. 70155100	-3. 40015800
Na	3. 87734000	5. 22856100	3. 51471000
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H	4.51916600	-4.01321200	4.52371800
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H	-1.07775300	0.54053900	-1.94051400
H	-1.89430300	-0.43290100	-0.68713200
H	-1.81117600	1.34258300	-0.52333300
C	9.13488700	3.06780400	-1.96721600
H	10.21332400	2.95167700	-2.09458200
H	8.66615300	3.10498800	-2.96005400
H	8.93378100	4.01894600	-1.45306600

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$TS_{R1/GT}$

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O	0.04881900	-0.09635400	-0.12283700
C	0.08197700	0.23628900	1.25436400
C	1.52430500	0.32563100	1.73624000
O	2.14959600	-0.97388400	1.78058400
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O	3.48363000	1.69889100	1.75178800
C	2.97132600	0.13106000	-0.15454100
C	2.84877600	-1.21728100	0.58309500
N	2.14284300	-2.20929500	-0.26505000
C	2.38510100	-2.38293000	-1.60377900
N	1.67656700	-3.26240400	-2.20010100
C	0.84211900	-3.74891900	-1.18575200
C	-0.19805500	-4.72831200	-1.24809200
N	-0.79390000	-4.89010800	0.03210800
C	-0.43089800	-4.22479500	1.17954800
N	0.53044200	-3.32235300	1.22252500
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P	5.09622700	1.77011400	1.47607800
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O	5.57954300	0.22149200	1.74244700
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C	6.00550600	-1.74749600	3.04712900
O	5.58358600	-2.57308100	1.94380100
C	7.53972500	-1.66536100	2.95764600
O	8.05193200	-2.71850100	3.76880100
C	7.80992200	-1.89729000	1.46780200
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N	6.25332800	-2.80892700	-0.30804200
C	6.00938500	-4.01675700	-0.96764100
O	6.18368200	-5.11904700	-0.46295100

N	5. 55605000	-3. 86524700	-2. 26408300
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C	5. 97837700	-1. 59347300	-0. 91372300
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H	-0. 42009000	-0. 53761700	1. 85198200
H	1. 51860100	0. 70452400	2. 76177800
H	1. 97443800	2. 00271900	0. 38385000
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H	2. 29790800	0. 15057700	-1. 01086500
H	3. 81198400	-1. 65322400	0. 85022100
H	5. 59992200	0. 21653500	3. 83248500
H	4. 19900700	-0. 58204300	3. 06550700
H	5. 73491700	-2. 24724300	3. 98415100
H	7. 91915100	-0. 69457800	3. 30445000
H	7. 72162800	-0. 94948600	0. 93644900
H	8. 79634600	-2. 31806700	1. 26786200
H	6. 99923000	-3. 90478100	1. 24923000
H	6. 12520200	-0. 72411300	-0. 28651700
H	5. 37967300	-4. 73033100	-2. 76137800
C	5. 27908100	-0. 14140100	-2. 84350000
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N	-1. 15280700	-4. 48831300	2. 30588200
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H	-1. 56245400	-5. 55088500	0. 05541700
O	-0. 60615300	-5. 38503800	-2. 20504300
H	-0. 74769900	-4. 12785700	3. 15828100
C	-1. 22063900	-0. 55711700	-0. 55667600
H	-2. 00146500	0. 20409800	-0. 41331200
H	-1. 13308700	-0. 78388700	-1. 62136100
H	-1. 51496700	-1. 47038200	-0. 02031800
C	9. 45132000	-2. 63554800	4. 00306200
H	9. 71098300	-3. 46195700	4. 66805400
H	10. 03852900	-2. 73130500	3. 07972300
H	9. 72018600	-1. 68589200	4. 48819500

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INT<sub>R1/GT</sub>

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O	-0. 05334400	-0. 18967500	0. 11180000
C	0. 05584000	0. 10110300	1. 49412900
C	1. 52118800	0. 17472800	1. 90019700
O	2. 15534700	-1. 12459900	1. 90600200

C	2. 40888600	1. 02489100	0. 98068800
O	3. 44757600	1. 59430800	1. 81101500
C	2. 86597300	0. 00174900	-0. 06027400
C	2. 85282400	-1. 33604300	0. 70267600
N	2. 22867900	-2. 41265200	-0. 10651100
C	2. 76478000	-2. 84671100	-1. 29367700
N	2. 10361600	-3. 74226600	-1. 92048400
C	0. 99063600	-3. 95948400	-1. 09889100
C	-0. 11800400	-4. 84480200	-1. 28065800
N	-1. 02280100	-4. 72596300	-0. 19182900
C	-0. 86579600	-3. 90045300	0. 89638900
N	0. 16732600	-3. 09894900	1. 05735800
C	1. 05179200	-3. 14128100	0. 03707200
P	5. 04108600	1. 71160100	1. 45920400
O	5. 62662100	2. 66880300	2. 47203400
O	5. 31468900	1. 98851800	-0. 00372100
O	5. 58214500	0. 18175700	1. 72073500
C	5. 34720800	-0. 45759800	2. 98482900
C	6. 13716800	-1. 75621300	3. 01692800
O	5. 73813100	-2. 59238800	1. 91231600
C	7. 66425400	-1. 59700900	2. 90521100
O	8. 24067700	-2. 62591400	3. 70445100
C	7. 92250800	-1. 81095900	1. 41123800
C	6. 85080800	-2. 84221900	1. 04711500
N	6. 40002000	-2. 80374900	-0. 34505500
C	6. 28827200	-4. 01583400	-1. 03117500
O	6. 57182400	-5. 10483500	-0. 54740300
N	5. 83619900	-3. 88375200	-2. 32997600
C	5. 44766500	-2. 71794600	-3. 00151400
O	5. 05809300	-2. 77355000	-4. 16437500
C	5. 55157200	-1. 50412500	-2. 19846500
C	6. 00788200	-1. 60960400	-0. 92686000
H	-0. 42531900	1. 06532400	1. 72825900
H	-0. 42576200	-0. 68441300	2. 09121400
H	1. 57107700	0. 54731600	2. 92683800
H	1. 86226600	1. 85353600	0. 52403300
H	3. 83538600	0. 23934100	-0. 48463400
H	2. 12290500	-0. 02615800	-0. 85638000
H	3. 85453100	-1. 69364600	0. 94670400
H	5. 66523500	0. 19069400	3. 80961000
H	4. 27890100	-0. 67193100	3. 09051300
H	5. 90603500	-2. 27517600	3. 95406300
H	7. 99941800	-0. 60961600	3. 25079600
H	7. 77216500	-0. 86988900	0. 88125100

H	8.92652900	-2.17787000	1.19364200
H	7.21170900	-3.85793800	1.20873900
H	6.07009400	-0.74293700	-0.28165000
H	5.75111500	-4.75193800	-2.84546500
C	5.15574900	-0.19966600	-2.82704600
H	4.09973200	-0.21679000	-3.11775200
H	5.31609900	0.63259100	-2.13762300
H	5.73441400	-0.02459300	-3.74014100
Na	6.61193100	3.94259900	0.68443600
N	-1.87610600	-3.88078800	1.81415500
H	-2.46087300	-4.69824200	1.91759500
H	-1.85262100	-5.30278900	-0.27178200
O	-0.35929100	-5.62584200	-2.20033200
H	-1.64477800	-3.41263500	2.67908900
C	-1.39132700	-0.42769300	-0.29388900
H	-2.01907500	0.46576000	-0.15848800
H	-1.36501400	-0.68844900	-1.35425600
H	-1.83731200	-1.25906000	0.26896600
C	9.63830400	-2.47563400	3.91519500
H	9.94916400	-3.29019900	4.57278100
H	10.21331900	-2.54023700	2.98157400
H	9.86900900	-1.51533100	4.39899900

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$TS_{R2/GT}$

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O	-0.14344700	0.36581900	0.26136700
C	-0.16724600	0.09232200	1.65187200
C	1.24897200	-0.13092300	2.18041200
O	1.67156700	-1.51075700	2.05449000
C	2.31779200	0.69332500	1.44599400
O	3.34207700	0.99092500	2.41923300
C	2.76301900	-0.28455600	0.36337500
C	2.70972100	-1.62370700	1.09756500
N	2.47142800	-2.77465200	0.22405900
C	3.46979300	-3.57053100	-0.28412700
N	3.11351700	-4.45048300	-1.13612200
C	1.72739000	-4.26662600	-1.23756200
C	0.76383200	-4.97212700	-2.02587100
N	-0.53746900	-4.45629900	-1.77832300
C	-0.85259400	-3.44619800	-0.90023300
N	0.04895000	-2.79154500	-0.19340400
C	1.30891800	-3.22798000	-0.39942100
P	4.83073800	1.55989300	2.02675900
O	5.25615300	2.50145900	3.12994100
O	4.89343500	2.07039400	0.60386400
O	5.73287600	0.18274100	2.06062700

C	5. 65969800	-0. 67255700	3. 21010800
C	6. 47903400	-1. 92545800	2. 94576400
O	6. 00414100	-2. 57045000	1. 74767200
C	7. 98829300	-1. 69104300	2. 74633100
O	8. 65400200	-2. 80713100	3. 33033700
C	8. 12768400	-1. 66560600	1. 22298700
C	7. 06660300	-2. 68175600	0. 79422200
N	6. 53093100	-2. 47841900	-0. 54916800
C	6. 50463200	-3. 56434300	-1. 42537600
O	6. 93100400	-4. 67911600	-1. 14901400
N	5. 96201600	-3. 26906700	-2. 66080500
C	5. 38956600	-2. 06732100	-3. 09350300
O	4. 90247700	-1. 98346100	-4. 21848100
C	5. 43784500	-0. 99244100	-2. 10900400
C	4. 85956300	0. 34175800	-2. 48254100
C	5. 98673300	-1. 25365800	-0. 89965900
H	1. 25788900	0. 10443200	3. 24868100
H	1. 92329500	1. 62440900	1. 03527400
H	3. 74323600	-0. 05864400	-0. 03934100
H	2. 02419900	-0. 27280300	-0. 43914800
H	3. 66383500	-1. 84622700	1. 58400500
H	6. 04704400	-0. 15943900	4. 09854900
H	4. 61646700	-0. 94676800	3. 39801200
H	6. 34345300	-2. 60452300	3. 79542200
H	8. 32433000	-0. 75666800	3. 21576100
H	9. 12266500	-1. 94188700	0. 87131900
H	7. 88958600	-0. 66616900	0. 85469700
H	7. 46465800	-3. 69668100	0. 80476400
H	5. 35906300	0. 74119800	-3. 37175600
H	4. 96093200	1. 05706200	-1. 66293500
H	3. 79707000	0. 24479500	-2. 73210900
H	6. 00956600	-0. 50696400	-0. 11579800
O	0. 92117200	-5. 89341300	-2. 82484100
H	-1. 27343200	-4. 90615200	-2. 31115600
N	-2. 16678100	-3. 09301400	-0. 80525700
H	-2. 39283100	-2. 54045100	0. 00943900
H	-2. 87217000	-3. 76840900	-1. 06417200
H	-0. 61122000	0. 94419100	2. 19286700
H	-0. 76634800	-0. 80348200	1. 86776900
H	5. 91373900	-4. 04961200	-3. 30478000
Na	5. 63547700	4. 21165600	1. 42062700
C	-1. 43203900	0. 58404800	-0. 28039700
H	-1. 93882300	1. 43223800	0. 20451400
H	-1. 30389600	0. 80551600	-1. 34233700

H	-2.07079700	-0.30403800	-0.18103500
C	10.06035400	-2.64026100	3.45189900
H	10.44222300	-3.52978000	3.95740900
H	10.55897200	-2.55027600	2.47734500
H	10.30760300	-1.75236800	4.05180600

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5'-sG<sup>a</sup>T-3'

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O	-0.46692000	0.19576000	1.03735500
C	-0.22567200	0.25715600	2.43087900
C	1.24029200	-0.04224000	2.69902000
O	1.50426800	-1.43998100	2.43957800
C	2.21405400	0.75852400	1.80750400
O	3.34108500	1.12445700	2.63721800
C	2.55952500	-0.24934700	0.72147800
C	2.58876700	-1.54718100	1.51564900
N	2.46653200	-2.76682300	0.73710500
C	3.09965600	-3.94782200	1.05800600
N	2.95497500	-4.90910200	0.23479200
C	2.13586600	-4.36523300	-0.76789400
C	1.73735200	-4.91943700	-2.02498800
N	0.93473800	-3.99116100	-2.73898500
C	0.67050100	-2.69965000	-2.35788800
N	1.08836000	-2.18425300	-1.21407500
C	1.81957700	-3.03888500	-0.47175300
P	4.77275300	1.63841200	2.01403500
O	5.36711100	2.61058700	3.00721000
O	4.64240100	2.09183800	0.57648100
O	5.64686800	0.24129600	1.97844500
C	5.79292400	-0.49775300	3.20015300
C	6.56164600	-1.77736600	2.92026400
O	5.87403800	-2.54208400	1.91117600
C	8.00405500	-1.57638400	2.41546400
O	8.79236400	-2.60262400	3.01139200
C	7.86412500	-1.75841000	0.90259400
C	6.75645100	-2.81040800	0.81574900
N	5.98931100	-2.79909600	-0.42602200
C	5.79235200	-4.00851000	-1.09611100
O	6.27337400	-5.07579600	-0.73895700
N	5.00606500	-3.89536500	-2.22716500
C	4.37081900	-2.75475400	-2.73030900
O	3.65550300	-2.83568400	-3.72709600
C	4.62670300	-1.53723900	-1.97077400
C	3.98651000	-0.26372600	-2.44120100
C	5.39490500	-1.62614000	-0.86040300
H	1.45329800	0.17088300	3.75297600

H	1. 75800500	1. 66636400	1. 40653600
H	3. 49255400	-0. 02509200	0. 22016000
H	1. 74687800	-0. 27871200	-0. 00176800
H	3. 53544500	-1. 65865100	2. 05052600
H	6. 32992100	0. 09773600	3. 94787400
H	4. 80403500	-0. 74371300	3. 60208700
H	6. 60005900	-2. 35866800	3. 84908600
H	8. 39735800	-0. 58674200	2. 68397400
H	8. 78245800	-2. 09118800	0. 41687800
H	7. 55203000	-0. 81439000	0. 45234600
H	7. 16318100	-3. 81816100	0. 90588400
H	4. 26675500	-0. 05358700	-3. 47843300
H	4. 28452800	0. 58193600	-1. 81667200
H	2. 89556200	-0. 35449500	-2. 41076400
H	5. 57324800	-0. 76784000	-0. 22424400
O	2. 00603900	-6. 01366500	-2. 51856600
H	0. 66218900	-4. 30322400	-3. 66393200
N	-0. 01736300	-1. 91499600	-3. 22643700
H	-0. 35543000	-1. 04169800	-2. 84878000
H	-0. 59012100	-2. 33702100	-3. 94234900
H	-0. 46637000	1. 25713800	2. 82826500
H	-0. 84464500	-0. 47639900	2. 97101500
H	4. 79375600	-4. 77023200	-2. 69309000
Na	5. 54927300	4. 23124700	1. 17943600
C	-1. 82627000	0. 40957900	0. 69842800
H	-2. 17063100	1. 40880800	1. 00504700
H	-1. 90505400	0. 32354300	-0. 38789100
H	-2. 48254100	-0. 34048300	1. 16456900
C	10. 19278300	-2. 41751800	2. 85232100
H	10. 68304800	-3. 23525900	3. 38475600
H	10. 50369600	-2. 44876100	1. 79933800
H	10. 52122700	-1. 46037400	3. 28296000

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$TS_{C6/GT}$

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O	-0. 18200200	-0. 06393600	0. 55452900
C	0. 11349700	0. 09849100	1. 92929200
C	1. 61712100	0. 02754200	2. 15759300
O	2. 07050300	-1. 34585600	2. 16328300
C	2. 45849500	0. 75061700	1. 08285800
O	3. 56087600	1. 41271200	1. 75451000
C	2. 82960200	-0. 39921100	0. 15018600
C	3. 07391600	-1. 51578300	1. 15818900
N	3. 06218300	-2. 86548900	0. 64664400
C	4. 13426400	-3. 73359300	0. 76568100
N	3. 91261700	-4. 91564000	0. 28999600

C	2. 57284900	-4. 88313500	-0. 10359200
C	1. 74409900	-5. 91446300	-0. 65115100
N	0. 44119400	-5. 40795200	-0. 92028600
C	0. 00959100	-4. 12261800	-0. 69122000
N	0. 77967600	-3. 18328300	-0. 17302900
C	2. 03143800	-3. 60995600	0. 09323200
P	5. 17976900	1. 27391700	1. 58464400
O	5. 77516000	2. 51000300	2. 21854000
O	5. 61891200	0. 93327800	0. 17670600
O	5. 55521600	-0. 06061000	2. 47972600
C	5. 01059300	-0. 27950200	3. 78883900
C	5. 77572500	-1. 42095500	4. 43796900
O	5. 64279500	-2. 61163800	3. 63069200
C	7. 28559900	-1. 16916100	4. 61108300
O	7. 65801400	-1. 74177400	5. 86103100
C	7. 89138300	-1. 91973800	3. 42422600
C	6. 93127900	-3. 10351100	3. 26973900
N	6. 87886800	-3. 63569500	1. 90363300
C	7. 41879300	-4. 88871100	1. 64046900
O	7. 87655100	-5. 63130600	2. 50013400
N	7. 41994100	-5. 22882700	0. 29695400
C	7. 00844400	-4. 45788800	-0. 79664100
O	7. 12990800	-4. 88525000	-1. 94243200
C	6. 45302400	-3. 16038900	-0. 43806500
C	5. 93581800	-2. 25900900	-1. 51390200
C	6. 30250600	-2. 87130600	0. 90367200
H	1. 83206600	0. 46311400	3. 13928500
H	1. 89084400	1. 53311600	0. 57730500
H	3. 69322200	-0. 19042500	-0. 47715700
H	1. 95241100	-0. 64116500	-0. 45223100
H	4. 05702600	-1. 41471900	1. 61063100
H	5. 09904200	0. 62177700	4. 40608800
H	3. 95386000	-0. 55360400	3. 70759300
H	5. 33649500	-1. 61098200	5. 42387700
H	7. 52380000	-0. 09693200	4. 59408200
H	8. 92046300	-2. 24271400	3. 58870200
H	7. 85624200	-1. 28767300	2. 53365400
H	7. 21515700	-3. 94049600	3. 90990800
H	6. 64334900	-2. 22853100	-2. 34732800
H	5. 77964900	-1. 24595500	-1. 13437300
H	4. 98694900	-2. 63750100	-1. 91491300
H	5. 97805800	-1. 89029000	1. 22642400
O	2. 00737000	-7. 09089000	-0. 89677200
H	-0. 19312000	-6. 08587200	-1. 32756600



N	-1.25856800	-3.80870000	-1.07530800
H	-1.60358600	-2.92831600	-0.72090000
H	-1.94870700	-4.54049800	-1.16228500
H	-0.25592500	1.07280000	2.28984100
H	-0.36589800	-0.68682600	2.53384100
H	7.81150600	-6.13913100	0.08631600
Na	7.14193200	2.82903800	0.25857600
C	-1.56915000	-0.17888400	0.29933200
H	-1.69278500	-0.29409600	-0.78030700
H	-2.00406200	-1.05179700	0.81117100
H	-2.12215800	0.71501000	0.62518600
C	8.96291500	-1.37865500	6.29201100
H	9.11162200	-1.83522100	7.27283400
H	9.74581000	-1.74316500	5.61334200
H	9.06429700	-0.28743500	6.38452400

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PRO<sub>C6/GT</sub>

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O	0.11793400	0.01257500	-0.17035300
C	0.01556000	0.04164800	1.24084700
C	1.39851500	0.03617000	1.87632300
O	1.96945600	-1.29462200	1.87633700
C	2.42686400	0.94142200	1.16432200
O	3.25224600	1.55098400	2.18796900
C	3.13053000	-0.05525700	0.24764600
C	3.20014100	-1.27319000	1.16178100
N	3.44445900	-2.54544400	0.50420500
C	4.66521700	-3.21812300	0.51415200
N	4.61722200	-4.35882700	-0.13766500
C	3.31680100	-4.45798100	-0.58301000
C	2.68564600	-5.49428200	-1.34939800
N	1.33170300	-5.15768900	-1.61233100
C	0.68997000	-4.01212900	-1.19939000
N	1.27432700	-3.06900900	-0.48555800
C	2.57077100	-3.33443400	-0.21387400
P	4.87830900	1.60067900	2.36393100
O	5.16284200	2.74324000	3.31105500
O	5.63088900	1.58221300	1.05065400
O	5.22275100	0.15629800	3.08331200
C	4.46463200	-0.31067300	4.21092600
C	5.11225000	-1.58282700	4.73046400
O	5.07935700	-2.60445800	3.70784300
C	6.58710400	-1.41344000	5.14691000
O	6.77589200	-2.18958700	6.32715100
C	7.33800900	-1.98776800	3.94616600
C	6.39917300	-3.11219700	3.49780500

N	6.54911800	-3.49226500	2.09676600
C	7.41423800	-4.51083500	1.79022200
O	7.83599500	-5.32877300	2.60481200
N	7.83862700	-4.55012500	0.46079700
C	7.77265800	-3.50588800	-0.46547400
O	8.43545300	-3.54781100	-1.50628600
C	6.89088000	-2.41973600	-0.09631100
C	6.74367100	-1.21677700	-0.95615400
C	5.96111100	-2.63149300	1.06439600
H	1.29241200	0.35620900	2.91817900
H	1.94826100	1.75336700	0.61442500
H	4.10616100	0.28167500	-0.09666900
H	2.46919200	-0.26759500	-0.59421200
H	4.01575000	-1.16928900	1.86933500
H	4.45017100	0.44337000	5.00621200
H	3.43453700	-0.52251100	3.90575800
H	4.53865200	-1.92924900	5.59787500
H	6.83539400	-0.36070900	5.33801000
H	8.33671200	-2.35659300	4.18545400
H	7.41361600	-1.23047200	3.16156500
H	6.55939200	-4.01621300	4.09009100
H	7.59004500	-1.12853800	-1.63939400
H	6.64430000	-0.30956300	-0.34727900
H	5.83040900	-1.28527900	-1.56706200
H	5.76227600	-1.66604200	1.52920300
O	3.15175500	-6.55051900	-1.77221700
H	0.83176200	-5.83866300	-2.17274000
N	-0.59837800	-3.84038600	-1.60589200
H	-1.09439900	-3.09719000	-1.13532400
H	-1.15606200	-4.64804700	-1.84378900
H	-0.51546800	0.95068900	1.56908300
H	-0.54505900	-0.82867600	1.61496500
H	8.48254000	-5.30097000	0.24614500
Na	6.77784700	3.61210400	1.73207100
C	-1.14378000	-0.02894000	-0.80999200
H	-0.96245600	-0.09796400	-1.88471700
H	-1.73442500	-0.90099900	-0.48854500
H	-1.73717400	0.87439700	-0.60219900
C	8.01346700	-1.94440200	6.98139100
H	8.02080000	-2.55552300	7.88649800
H	8.87753600	-2.22280400	6.36309200
H	8.11464000	-0.88577500	7.26216400

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**Table S3.** Cartesian coordinates of stationary points along the reaction paths of deoxyguanosine-8-yl radical addition to the C5 and C6 sites of its 5' flanking deoxythymidine started from the canonical 5'-*aTaG*<sup>\*</sup>-3' sequence, respectively.

5'- <i>aTaG</i> <sup>*</sup> -3'			
O	0.80898900	-0.23440800	-0.54823700
C	0.59494100	-0.38162300	0.84449600
C	1.94776500	-0.40371500	1.54274400
O	2.66790500	-1.61646900	1.21230300
C	2.86691200	0.76049300	1.13916400
O	3.66521900	1.12343900	2.28527900
C	3.72146100	0.14826700	0.03816300
C	3.82438600	-1.32209800	0.45191600
N	3.87568600	-2.21736900	-0.73302900
C	5.12848400	-2.47954500	-1.26850700
O	6.18212300	-2.14633400	-0.73920400
N	5.08489600	-3.14540500	-2.48443600
C	3.95932000	-3.44141900	-3.25441100
O	4.09533300	-3.85876700	-4.41405500
C	2.69290900	-3.17032500	-2.60611500
C	1.42076600	-3.47238300	-3.34487200
C	2.71812900	-2.55409500	-1.39731500
P	4.14776900	2.68734700	2.43729600
O	4.76483800	2.81439800	3.81112000
O	3.03268700	3.63949000	2.06910900
O	5.28482100	2.83702900	1.25973600
C	6.53292200	2.14810600	1.41438900
C	7.34312600	2.30990600	0.14015500
O	6.69484600	1.61639300	-0.94510300
C	7.52608200	3.76518300	-0.32656900
O	8.82453500	3.85426700	-0.90438200
C	6.41548400	3.92944200	-1.37010500
C	6.34202900	2.53266800	-1.98308400
N	5.02351600	2.20021100	-2.48888700
C	3.79643100	2.70950700	-2.12031200
N	2.78131800	2.13316600	-2.63252200
C	3.32879900	1.09152800	-3.40046300
C	2.70260000	0.03525600	-4.13507100
O	1.50850200	-0.21923000	-4.29556500
N	3.69141800	-0.79812300	-4.72439500
C	5.05485000	-0.67250600	-4.58594600
N	5.82294000	-1.58129000	-5.24482400
N	5.61874000	0.29134400	-3.87710700
C	4.72139300	1.12496500	-3.31751700

H	-0.00064300	0.45567200	1.24229100
H	0.05615800	-1.31619000	1.06414900
H	1.78565500	-0.39698200	2.62495900
H	2.29805300	1.62767000	0.79749700
H	4.68883600	0.63040600	-0.08757300
H	3.16745400	0.20741200	-0.89809800
H	4.72431300	-1.54096300	1.02952100
H	1.27742300	-2.76360500	-4.16757900
H	0.55771900	-3.38885500	-2.68004300
H	1.44323400	-4.48099400	-3.76726200
H	1.81418200	-2.24904800	-0.89026600
H	7.08951900	2.56070300	2.26345900
H	6.35911800	1.08077200	1.59566100
H	8.32972500	1.86117700	0.30177800
H	7.42329200	4.47726700	0.50293700
H	5.47486400	4.16005000	-0.86418900
H	7.03684000	2.40689700	-2.81911000
H	6.80403700	-1.55014700	-5.00332400
H	6.62569200	4.70088300	-2.11182500
H	3.32915800	-1.59326300	-5.24026600
H	5.43501900	-2.51348300	-5.36676700
H	5.98879500	-3.31374200	-2.91033200
Na	3.20884100	4.61195100	4.28433400
C	-0.38192800	-0.21141900	-1.32372400
H	-0.06960300	-0.09840100	-2.36377500
H	-0.95150900	-1.14539900	-1.21008400
H	-1.02953000	0.62943300	-1.03647200
C	9.25395900	5.18757500	-1.14688800
H	10.26717200	5.12641500	-1.54960200
H	8.61774000	5.70758600	-1.87583800
H	9.27093500	5.77717700	-0.21870400

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$TS_{R1/TG}$

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O	0.00556400	0.02443800	0.08977700
C	0.01343200	-0.01497400	1.50890600
C	1.45141100	-0.03053300	2.00597200
O	2.07191000	-1.28647300	1.66422300
C	2.33556700	1.07048000	1.39533100
O	3.28976900	1.47859600	2.40062200
C	3.02860700	0.34797700	0.24724500
C	3.18735700	-1.07161000	0.80166400
N	3.19846300	-2.11481300	-0.22694800
C	4.36340800	-2.84613600	-0.42511800
O	5.37334400	-2.73161300	0.26343100
N	4.28920300	-3.73542600	-1.47928200

C	3. 26505500	-3. 86438300	-2. 42382500
O	3. 40223500	-4. 61893800	-3. 38565100
C	2. 07964200	-3. 06846200	-2. 13606500
C	0. 92776000	-3. 14899800	-3. 09375700
C	2. 10185200	-2. 25229700	-1. 05832700
P	4. 11574000	2. 88456800	2. 18077100
O	4. 75152400	3. 23203700	3. 50715800
O	3. 22846300	3. 91919700	1. 52485800
O	5. 26784300	2. 48511300	1. 07342600
C	6. 51630800	1. 92789200	1. 51224400
C	7. 53985500	2. 01084100	0. 39011200
O	7. 31638000	0. 95955800	-0. 57789700
C	7. 51759500	3. 33503800	-0. 39702900
O	8. 86873200	3. 65389400	-0. 71472300
C	6. 70067100	2. 96216400	-1. 64150000
C	7. 14781300	1. 51751300	-1. 86983600
N	6. 17806200	0. 67800200	-2. 55995800
C	5. 25789300	-0. 15735200	-1. 97712200
N	4. 50358900	-0. 79612900	-2. 78558800
C	4. 92536500	-0. 37284000	-4. 05045900
C	4. 45947200	-0. 72994100	-5. 35320800
O	3. 56570500	-1. 50559600	-5. 68835500
N	5. 20807700	-0. 02960600	-6. 34264800
C	6. 22634800	0. 86702500	-6. 11219200
N	6. 85189300	1. 39326800	-7. 19759600
N	6. 64135600	1. 19378000	-4. 89874400
C	5. 96927300	0. 54635800	-3. 92502300
H	-0. 50409800	0. 86446400	1. 92384800
H	-0. 50103300	-0. 91588900	1. 87583800
H	1. 44109300	0. 06876000	3. 09714400
H	1. 75651200	1. 93788400	1. 07224600
H	3. 98422200	0. 79909800	-0. 01378200
H	2. 37877500	0. 34662200	-0. 62876600
H	4. 12084800	-1. 18713900	1. 35414300
H	1. 24026500	-2. 78782000	-4. 08047800
H	0. 08621500	-2. 54132900	-2. 75197700
H	0. 58693200	-4. 18158800	-3. 22198000
H	1. 25550500	-1. 63303000	-0. 77972700
H	6. 88289800	2. 48837400	2. 37761700
H	6. 38343900	0. 87835500	1. 80093800
H	8. 53517700	1. 86516300	0. 82387000
H	7. 05252300	4. 14425900	0. 18011000
H	5. 63521400	2. 97788500	-1. 40193800
H	8. 08018500	1. 47600400	-2. 44613600

H	7.46185700	2.17558400	-7.00879500
H	6.89202700	3.60437800	-2.50218000
H	4.94514700	-0.25004100	-7.29667700
H	6.37692100	1.41519300	-8.08821300
H	5.13852100	-4.25661500	-1.66086000
Na	3.64996500	5.38826400	3.40365800
C	-1.30357700	-0.01204600	-0.46107100
H	-1.19494500	0.00620700	-1.54750800
H	-1.83753200	-0.92731800	-0.16817300
H	-1.89693400	0.85701500	-0.14295700
C	9.04198600	4.97067000	-1.22146800
H	10.11360100	5.11257100	-1.37669200
H	8.52566900	5.12384400	-2.17890400
H	8.67947800	5.72445700	-0.50731700

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**5'- $\alpha$ TsG'-3'**

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O	0.69087800	0.01043700	-1.51546800
C	0.16472100	0.36894800	-0.24573500
C	1.31818400	0.57190100	0.72924100
O	1.93773100	-0.70063100	1.02522300
C	2.42524800	1.48264700	0.16797500
O	2.97916600	2.27046600	1.24612200
C	3.43237800	0.47866600	-0.36247500
C	3.29536600	-0.69861600	0.59657900
N	3.61435900	-1.97346000	-0.06391400
C	4.82397900	-2.58994300	0.23271100
O	5.55937700	-2.25671200	1.15560000
N	5.13623300	-3.63294400	-0.62193900
C	4.42034100	-4.08680700	-1.73873600
O	4.87102000	-4.99898900	-2.42923900
C	3.15415700	-3.40008300	-1.95679600
C	2.31462300	-3.79568300	-3.13621400
C	2.82460900	-2.38866700	-1.12246800
P	3.89068900	3.58635100	0.87619500
O	4.05560500	4.37366500	2.15333300
O	3.31663900	4.32737400	-0.32041200
O	5.31324300	2.95919600	0.36441000
C	6.13157400	2.19234500	1.25798100
C	7.26650000	1.56280700	0.46694300
O	6.74434600	0.55641900	-0.42363100
C	8.06851400	2.55039100	-0.40834300
O	9.44202100	2.19047700	-0.28085900
C	7.51992600	2.28393900	-1.81435700
C	7.24146100	0.78422300	-1.74530200
N	6.28167300	0.26442100	-2.70332100

C	6.26527000	-1.03953200	-3.15650500
N	5.24114400	-1.39158300	-3.82534400
C	4.41739200	-0.25357500	-3.80216800
C	3.07640900	-0.06901900	-4.26648800
O	2.32573700	-0.85542200	-4.84541100
N	2.61582700	1.23366700	-3.93333000
C	3.31190300	2.18805300	-3.22668300
N	2.69127000	3.35796300	-2.93296700
N	4.56305800	2.00534000	-2.83306600
C	5.04775500	0.78404100	-3.11198100
H	-0.41873400	1.30048300	-0.31655900
H	-0.49784300	-0.42065400	0.13862200
H	0.92173600	0.98888000	1.66121600
H	2.04065100	2.15154600	-0.60301800
H	4.44662000	0.85672500	-0.42744900
H	3.10808700	0.15954400	-1.35132400
H	3.96533500	-0.62922100	1.45499500
H	2.74353800	-3.39094100	-4.05855900
H	1.29969700	-3.40151200	-3.04450700
H	2.26578300	-4.88421400	-3.23059000
H	1.91259700	-1.81471400	-1.24118500
H	6.54563100	2.83898100	2.04028900
H	5.53931000	1.40216300	1.73355900
H	7.95353800	1.08950100	1.17879800
H	7.91515500	3.59115900	-0.09424800
H	6.58286500	2.82171300	-1.95304200
H	8.15894200	0.20458300	-1.89936200
H	3.02682600	3.81648400	-2.07498000
H	8.21888400	2.54420300	-2.61061400
H	1.64784300	1.40498900	-4.17968900
H	1.69181100	3.40877500	-3.07286100
H	6.02055500	-4.09105600	-0.43643400
Na	3.15404500	6.32474700	1.03695800
C	-0.30324300	-0.26386600	-2.49388400
H	0.22650200	-0.56510700	-3.40069600
H	-0.96748300	-1.07898800	-2.17334900
H	-0.91547000	0.62548800	-2.70146600
C	10.33890900	3.15390000	-0.81668400
H	11.35000200	2.79290400	-0.61624300
H	10.22072700	3.28065800	-1.90137200
H	10.20624800	4.13463400	-0.33678500

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TS<sub>C5/TG</sub>

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O	0.17759700	0.22129300	-0.27560000
C	0.00589100	0.18178800	1.13231800

C	1. 37334800	0. 09042500	1. 79795800
O	1. 94602900	-1. 21806300	1. 52385200
C	2. 37259200	1. 13127300	1. 24039700
O	3. 30061100	1. 51725000	2. 28879100
C	3. 09950800	0. 31228400	0. 20175900
C	3. 23114300	-1. 00800600	0. 94296400
N	3. 63803300	-2. 12050600	0. 07723100
C	4. 89976700	-2. 68182000	0. 32343300
O	5. 48954200	-2. 58567500	1. 38898600
N	5. 43151600	-3. 37868800	-0. 74707200
C	4. 92583900	-3. 49233000	-2. 03754300
O	5. 55587200	-4. 07882900	-2. 90683100
C	3. 58064600	-2. 89298800	-2. 22752900
C	2. 74695800	-3. 49565600	-3. 33221900
C	2. 97193500	-2. 35145800	-1. 09716400
P	4. 44859900	2. 66675500	2. 01442000
O	5. 09146600	2. 94134800	3. 35314300
O	3. 85527900	3. 85211200	1. 27289700
O	5. 52812300	1. 99257300	0. 97424500
C	6. 36640600	0. 90287200	1. 38627200
C	6. 93528900	0. 18185000	0. 16901600
O	5. 86901300	-0. 38833000	-0. 60639400
C	7. 77469000	1. 02598100	-0. 81107200
O	8. 91148300	0. 23469400	-1. 15265500
C	6. 82760300	1. 24415900	-1. 99540700
C	5. 97807300	-0. 03054300	-1. 98604500
N	4. 64730400	0. 09007100	-2. 56635700
C	3. 94765300	-0. 95165000	-3. 19236100
N	2. 79865100	-0. 56256900	-3. 66813900
C	2. 70936100	0. 79167600	-3. 37983900
C	1. 59202100	1. 67574300	-3. 52224300
O	0. 51006200	1. 48869900	-4. 08330900
N	1. 83465100	2. 89963000	-2. 84430600
C	2. 95354500	3. 20075900	-2. 10147300
N	2. 97571500	4. 36982700	-1. 40116400
N	4. 00162200	2. 39811300	-2. 03945400
C	3. 82423900	1. 21129400	-2. 65558300
H	-0. 50448400	1. 09111500	1. 48829900
H	-0. 60149600	-0. 68637600	1. 43057700
H	1. 25852500	0. 20777000	2. 88126800
H	1. 87488800	2. 01964500	0. 84552300
H	4. 04690100	0. 73487200	-0. 08618300
H	2. 45849200	0. 18614500	-0. 66907800
H	3. 98801800	-0. 96151300	1. 72482800



H	1. 95752500	-1. 97129400	-1. 13095200
H	7. 19278600	1. 27708900	2. 00149600
H	5. 79801000	0. 17892200	1. 97818800
H	7. 56740000	-0. 62977900	0. 54914100
H	8. 09602200	1. 97613900	-0. 36309600
H	6. 19053000	2. 10441000	-1. 79587200
H	6. 46693100	-0. 84828700	-2. 52744700
H	3. 49018400	4. 28801000	-0. 51512900
H	7. 34839500	1. 38872400	-2. 94328600
H	1. 04692900	3. 53779900	-2. 84508100
H	2. 09071500	4. 84802300	-1. 29622800
H	6. 34653000	-3. 78177800	-0. 58148400
Na	4. 61789500	5. 28680300	3. 09655600
H	3. 33700800	-3. 57368700	-4. 24554500
H	2. 42698700	-4. 50185000	-3. 04166500
H	1. 86980800	-2. 87935500	-3. 52732900
C	-1. 03408700	0. 39585600	-0. 99493100
H	-1. 71511100	-0. 45593400	-0. 85215300
H	-1. 55621500	1. 31330100	-0. 68499800
H	-0. 76596000	0. 47935200	-2. 05068100
C	9. 92417800	0. 95409000	-1. 84207000
H	10. 75259800	0. 26093100	-2. 00386100
H	9. 58457700	1. 32777200	-2. 81772700
H	10. 28214400	1. 80899500	-1. 24963900

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PRO<sub>C5/TG</sub>

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O	0. 00623600	-0. 01452800	0. 00740500
C	0. 00495700	-0. 01335700	1. 42631000
C	1. 44647900	-0. 00952700	1. 92303000
O	2. 04939400	-1. 29946200	1. 64099900
C	2. 30817700	1. 04921400	1. 19645700
O	3. 32792200	1. 55653000	2. 09861700
C	2. 95427900	0. 21270900	0. 11971200
C	3. 24306600	-1. 06872100	0. 88805800
N	3. 58804700	-2. 20241700	0. 02662800
C	4. 86667200	-2. 71898700	0. 14857400
O	5. 56014800	-2. 65016000	1. 15276000
N	5. 34511300	-3. 35496700	-1. 01018200
C	4. 96241000	-3. 06007500	-2. 30725100
O	5. 70102100	-3. 27431300	-3. 25533100
C	3. 52798700	-2. 55159800	-2. 46490900
C	2. 80627600	-3. 55641600	-3. 39138200
C	2. 84170000	-2. 48752600	-1. 11410400
P	4. 34183900	2. 76079900	1. 61159600
O	5. 09109300	3. 20298000	2. 84630000

O	3. 58575300	3. 82592300	0. 83721900
O	5. 36501400	2. 07169100	0. 52262600
C	6. 28743100	1. 05024300	0. 92544100
C	6. 78471600	0. 27689900	-0. 29133400
O	5. 68832400	-0. 40184700	-0. 92980000
C	7. 46921600	1. 09581000	-1. 39995500
O	8. 55020900	0. 29801400	-1. 87898200
C	6. 35831000	1. 27361000	-2. 43999900
C	5. 58596500	-0. 04193500	-2. 30915200
N	4. 17137000	-0. 01324700	-2. 69787100
C	3. 37175700	-1. 12880500	-3. 02288900
N	2. 17981100	-0. 76937300	-3. 45330800
C	2. 14714100	0. 60314000	-3. 36235300
C	1. 01897000	1. 48049200	-3. 48723100
O	-0. 11928700	1. 23460100	-3. 88742100
N	1. 33864200	2. 77493200	-3. 00262100
C	2. 53228700	3. 13966800	-2. 42257500
N	2. 62837300	4. 36899100	-1. 83970600
N	3. 58542800	2. 34368700	-2. 39846600
C	3. 34356300	1. 09337500	-2. 84366500
H	-0. 50940900	0. 88076100	1. 81402000
H	-0. 51365700	-0. 90039800	1. 82110800
H	1. 45599600	0. 16097100	3. 00571500
H	1. 71322800	1. 88258100	0. 81725500
H	3. 83779800	0. 67062700	-0. 29104500
H	2. 22514600	0. 01480900	-0. 66347400
H	4. 08665500	-0. 95215100	1. 56940600
H	1. 79991700	-2. 19740400	-1. 07315000
H	7. 14400000	1. 49796500	1. 44264900
H	5. 80463100	0. 34417600	1. 60840100
H	7. 49205700	-0. 47643800	0. 07406300
H	7. 84251800	2. 06049300	-1. 03027200
H	5. 72359600	2. 10862300	-2. 15320000
H	6. 05172700	-0. 82310800	-2. 91531700
H	3. 20688000	4. 33962200	-0. 99309700
H	6. 73405400	1. 43260900	-3. 45193200
H	0. 55233300	3. 41452900	-2. 97366700
H	1. 75777400	4. 86352300	-1. 69564500
H	6. 29488900	-3. 69763600	-0. 91225800
Na	4. 36641100	5. 47450600	2. 43426700
H	3. 29773400	-3. 57869400	-4. 36572900
H	2. 83943000	-4. 55434800	-2. 94745000
H	1. 76669700	-3. 25495100	-3. 51882400
C	-1. 28531100	0. 08718700	-0. 57080400

H	-1.90495900	-0.79103500	-0.33688900
H	-1.81344600	0.98705700	-0.22161600
H	-1.14105200	0.15723300	-1.65175900
C	9.44035300	0.99372100	-2.74082300
H	10.24478400	0.29956100	-2.99341000
H	8.95571300	1.32117200	-3.67062200
H	9.87050200	1.87612100	-2.24475700
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<b>TS<sub>C6/TG</sub></b>			
O	0.02831700	0.02444200	-0.00127900
C	0.01183000	0.01893500	1.41685400
C	1.43937400	0.00529600	1.94227100
O	2.06231700	-1.24744600	1.57628100
C	2.33865300	1.11728200	1.35690600
O	3.31179600	1.46428900	2.37475000
C	3.01291100	0.39116200	0.20417000
C	3.28579700	-0.94110500	0.89648200
N	3.68939600	-2.05682200	0.05936800
C	4.85403700	-2.74157700	0.41102700
O	5.48405900	-2.53788000	1.44082000
N	5.24640300	-3.69981100	-0.50435700
C	4.59948400	-4.09032000	-1.68129000
O	5.04880200	-5.00754300	-2.36572100
C	3.39655800	-3.33036500	-1.98379300
C	2.61037700	-3.67942400	-3.20664400
C	3.05612600	-2.28124700	-1.14603500
P	4.43209600	2.64152300	2.11300100
O	5.10495300	2.88014900	3.44576800
O	3.81714700	3.82576800	1.40264000
O	5.49566900	1.97314500	1.04401000
C	6.30828400	0.85902200	1.43996500
C	6.93416500	0.21145300	0.21326600
O	5.91392900	-0.31361600	-0.66916100
C	7.79375600	1.15814100	-0.64228900
O	8.95310200	0.42693400	-1.03457100
C	6.87769400	1.47584500	-1.82615200
C	6.14432900	0.14632000	-1.99646800
N	4.85531300	0.24209400	-2.68555100
C	3.79321700	-0.65314600	-2.60347400
N	2.81000700	-0.37532600	-3.39683400
C	3.22197300	0.75663800	-4.09219400
C	2.55293100	1.50092100	-5.11560300
O	1.44451900	1.32459100	-5.61906300
N	3.36962200	2.57867900	-5.55456200
C	4.62522100	2.88112300	-5.08490200

N	5.28119600	3.91882900	-5.67565800
N	5.22826200	2.18697100	-4.13802600
C	4.49292600	1.15047500	-3.67516300
H	-0.50861600	0.90873600	1.80677400
H	-0.51435600	-0.87099200	1.79597100
H	1.41249100	0.09206900	3.03500000
H	1.77925800	2.00763600	1.06202500
H	3.91266000	0.87302400	-0.15753200
H	2.29288000	0.27858500	-0.60484800
H	4.08299300	-0.83115200	1.62674700
H	3.28300000	-3.86636700	-4.04863000
H	1.92398300	-2.87407800	-3.47088400
H	2.03538800	-4.59961300	-3.04542400
H	2.09805800	-1.78663400	-1.24659200
H	7.11185900	1.19740600	2.10467700
H	5.71684300	0.11292000	1.97545000
H	7.55562900	-0.62052900	0.56236400
H	8.08147400	2.06243300	-0.08976600
H	6.16207700	2.24935800	-1.54090700
H	6.76561700	-0.58340600	-2.53174500
H	6.10659700	4.23275900	-5.18519500
H	7.40676200	1.79645800	-2.72085400
H	2.96546800	3.13168300	-6.30168200
H	4.74771600	4.64840500	-6.12679500
H	6.08507100	-4.21137000	-0.25672300
Na	4.58591800	5.22314900	3.23862400
C	-1.27190900	0.02129700	-0.56886000
H	-1.84004300	-0.87307200	-0.27311500
H	-1.84628000	0.91112900	-0.27134800
H	-1.14883200	0.02270800	-1.65406000
C	9.96716100	1.23106000	-1.62219000
H	10.81176400	0.57192900	-1.83414400
H	9.64188900	1.69746500	-2.56187900
H	10.29556500	2.02570400	-0.93629200

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**PRO<sub>C6/TG</sub>**

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O	-0.20244700	0.08433100	0.28844000
C	-0.04644000	-0.07231900	1.68885900
C	1.43354400	-0.11158500	2.02937400
O	2.00765400	-1.33406400	1.51880000
C	2.24464300	1.04964000	1.40019000
O	3.25160200	1.44757300	2.36491900
C	2.87692000	0.36692500	0.19546600
C	3.22891300	-0.96811500	0.84684400
N	3.71105500	-2.04002800	0.01073400

C	4. 79832000	-2. 73927800	0. 48966600
O	5. 25100200	-2. 62236000	1. 62418600
N	5. 38638100	-3. 63879600	-0. 39664400
C	4. 85979800	-4. 10492400	-1. 59765200
O	5. 36490000	-5. 07273000	-2. 17389100
C	3. 70790400	-3. 37155200	-2. 07402800
C	2. 95433800	-3. 84890900	-3. 26158600
C	3. 29341500	-2. 09600700	-1. 38582200
P	4. 31760500	2. 65167700	2. 01706900
O	4. 94999000	3. 05106100	3. 33132900
O	3. 66472000	3. 73242400	1. 18578800
O	5. 43337600	1. 93188100	1. 03800700
C	6. 24269800	0. 86851600	1. 55776900
C	6. 87728200	0. 09503800	0. 41318100
O	5. 84629600	-0. 48022500	-0. 41391800
C	7. 77320600	0. 91400000	-0. 53197000
O	8. 94951200	0. 14138400	-0. 75927000
C	6. 91532800	1. 05548700	-1. 79148000
C	6. 12856600	-0. 26110300	-1. 78198900
N	4. 85127500	-0. 22021200	-2. 52453400
C	3. 64767800	-0. 91846900	-2. 31172000
N	2. 71656700	-0. 56810700	-3. 17292300
C	3. 29991900	0. 35732800	-4. 00201400
C	2. 74481000	1. 05767900	-5. 12432400
O	1. 61055100	1. 00381400	-5. 59438200
N	3. 72129400	1. 90367300	-5. 71008800
C	5. 02085600	2. 04275800	-5. 28292700
N	5. 83547700	2. 84770700	-6. 01487300
N	5. 51359600	1. 39902200	-4. 24136200
C	4. 62337300	0. 58205000	-3. 63337900
H	-0. 51719200	0. 76436600	2. 23090100
H	-0. 52089800	-1. 00455900	2. 03374200
H	1. 54440400	-0. 07789100	3. 12072700
H	1. 62533200	1. 91136000	1. 14491500
H	3. 73734200	0. 89258100	-0. 20519300
H	2. 10896600	0. 24129000	-0. 56823100
H	4. 00184000	-0. 80983700	1. 59529900
H	3. 49278400	-4. 65874500	-3. 75467200
H	2. 77221500	-3. 03281300	-3. 96812700
H	1. 96557000	-4. 21993800	-2. 95443600
H	2. 19838200	-2. 06073000	-1. 39195800
H	7. 03717800	1. 27326200	2. 19572600
H	5. 63971500	0. 18019700	2. 15682300
H	7. 47354200	-0. 71427400	0. 85046300

H	8.03592300	1.89147000	-0.10602200
H	6.21899600	1.88746600	-1.66853000
H	6.72692000	-1.09089200	-2.18126700
H	6.71569400	3.08353600	-5.57987400
H	7.49358600	1.21239100	-2.69779500
H	3.40142400	2.41572900	-6.52441300
H	5.43595900	3.55913200	-6.60912200
H	6.15862100	-4.16472600	-0.00704800
Na	4.27929500	5.33443400	2.89332300
C	-1.56234600	0.13316300	-0.11037700
H	-2.09594000	-0.79169800	0.15539200
H	-2.09076400	0.98142400	0.35024600
H	-1.57737600	0.25230600	-1.19607300
C	9.99340800	0.86074400	-1.40174200
H	10.84759700	0.18402900	-1.47356300
H	9.71803200	1.18645400	-2.41396800
H	10.28564500	1.74715900	-0.81985400

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**Table S4.** Cartesian coordinates of stationary points along the reaction paths of deoxyguanosine-8-yl radical addition to the C5 and C6 sites of its 3' flanking deoxycytidine started from the canonical 5'- $\alpha$ G $\cdot$  $\alpha$ C-3' sequence, respectively.

	5'- $\alpha$ G $\cdot$ $\alpha$ C-3'		
O	-0.41886800	0.44404900	0.05438400
C	-0.39715800	0.68766000	1.45112300
C	1.04053600	0.66483000	1.95189300
O	1.58409900	-0.66747700	1.92725900
C	2.01023900	1.51519100	1.12173000
O	3.03677700	1.97360200	2.02642900
C	2.54183700	0.51847800	0.09059300
C	2.44191100	-0.83952400	0.80302800
N	1.93988900	-1.89994600	-0.06342100
C	0.85614700	-1.87883800	-0.91416900
N	0.63923300	-2.96057600	-1.56333500
C	1.66746900	-3.81946000	-1.14263500
C	2.05896800	-5.10691200	-1.62075900
N	3.20430500	-5.56614500	-0.92187400
C	3.94623700	-4.83748200	-0.02546400

N	3. 60502000	-3. 62534400	0. 37213300
C	2. 47951400	-3. 17089200	-0. 21221300
P	4. 18150000	3. 02983700	1. 49879100
O	4. 74158000	3. 70840800	2. 72832600
O	3. 64924800	3. 90464500	0. 38713200
O	5. 30165100	2. 03032000	0. 82413500
C	5. 92071900	1. 06114200	1. 68492600
C	6. 66143000	0. 04100300	0. 84927000
O	5. 71999900	-0. 74317100	0. 10228100
C	7. 67454700	0. 62668200	-0. 17240500
O	8. 95177600	0. 09792200	0. 16559500
C	7. 15237600	0. 11336600	-1. 52507600
C	6. 38438900	-1. 14053100	-1. 10367400
N	5. 39779800	-1. 65470100	-2. 03725300
C	5. 40102300	-3. 05334000	-2. 35102700
O	6. 30247100	-3. 77018500	-1. 90797200
N	4. 38902900	-3. 53010700	-3. 12923400
C	3. 41999700	-2. 72700400	-3. 55532400
C	3. 40166000	-1. 31910700	-3. 27950500
C	4. 40564800	-0. 84132000	-2. 50371000
H	-0. 84487400	1. 66871300	1. 67863200
H	-0. 97077100	-0. 08034100	1. 99150300
H	1. 04286200	1. 00020800	2. 99381600
H	1. 52681600	2. 37781100	0. 65777500
H	3. 56913800	0. 72951400	-0. 19644400
H	1. 90030500	0. 53294500	-0. 79079400
H	3. 41553000	-1. 19296600	1. 14765200
H	6. 62846500	1. 55696400	2. 35895600
H	5. 16009200	0. 55323600	2. 28817400
H	7. 22627700	-0. 61094900	1. 53046700
H	7. 69622900	1. 72309700	-0. 13544700
H	6. 47758400	0. 85154800	-1. 96606600
H	7. 95098400	-0. 10047400	-2. 23739600
H	7. 06958100	-1. 96853300	-0. 90897700
H	4. 45847400	0. 19756600	-2. 20759800
Na	4. 12539800	5. 84164500	1. 75766800
N	5. 05329000	-5. 43342100	0. 50573700
H	5. 53689800	-6. 10033600	-0. 08146400
H	3. 54561000	-6. 46851800	-1. 23257500
O	1. 56933000	-5. 79428400	-2. 52126300
H	5. 68146500	-4. 77111100	0. 94179300
H	2. 61296000	-0. 67210300	-3. 63904100
N	2. 42194200	-3. 28087500	-4. 29072800
H	2. 30753200	-4. 28338000	-4. 18901900

H	1. 55306700	-2. 76812900	-4. 34556000
C	-1. 73230600	0. 33279000	-0. 47370000
H	-1. 63171400	0. 12783400	-1. 54117900
H	-2. 28760100	-0. 48970900	-0. 00105700
H	-2. 29888100	1. 26452400	-0. 33394200
C	10. 03206400	0. 76683000	-0. 47094700
H	10. 95189800	0. 30219400	-0. 10921300
H	9. 99660600	0. 67093600	-1. 56491000
H	10. 04589700	1. 83700800	-0. 21754800

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TS<sub>C5/GC</sub>

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O	-0. 00149300	-0. 03324600	0. 03280900
C	-0. 00361200	-0. 03320000	1. 45137300
C	1. 43048600	-0. 04998800	1. 96760000
O	2. 05233500	-1. 34547300	1. 85512100
C	2. 37363700	0. 89529000	1. 21636800
O	3. 32651300	1. 39060500	2. 18049600
C	3. 01547400	-0. 01168600	0. 15028200
C	2. 71985600	-1. 45321300	0. 62481900
N	1. 89747500	-2. 19196500	-0. 37146300
C	2. 01159800	-2. 03657000	-1. 73734700
N	1. 09726000	-2. 65343100	-2. 42360200
C	0. 28331800	-3. 24288900	-1. 46091300
C	-0. 91202100	-4. 00980500	-1. 62495800
N	-1. 42639700	-4. 39783100	-0. 35899300
C	-0. 86124400	-4. 10546900	0. 85972100
N	0. 24216900	-3. 39823100	0. 99799600
C	0. 76845200	-2. 97394400	-0. 17663700
P	4. 42251900	2. 52873200	1. 73104700
O	4. 87721800	3. 22485100	2. 99387900
O	3. 89643000	3. 38424100	0. 60121200
O	5. 63981500	1. 61196000	1. 10659600
C	6. 27549700	0. 67370200	1. 98978600
C	7. 13343000	-0. 27232400	1. 17822200
O	6. 28441900	-1. 14882600	0. 41306600
C	8. 08826600	0. 41996000	0. 17051800
O	9. 38062900	-0. 14221300	0. 36990000
C	7. 48779000	0. 03928900	-1. 19222100
C	6. 91123500	-1. 33501500	-0. 86162800
N	5. 93604200	-1. 90918800	-1. 77513000
C	6. 01765800	-3. 31969100	-2. 04932300
O	6. 91902900	-3. 97747500	-1. 53291700
N	5. 08799700	-3. 86357800	-2. 88814800
C	4. 08286600	-3. 13848600	-3. 34721800
C	3. 88842100	-1. 73763200	-2. 99197900



C	4.92025400	-1.16088000	-2.28011400
H	-0.51095400	0.86681100	1.83608500
H	-0.52409900	-0.91895700	1.84120900
H	1.41264700	0.18954300	3.03407500
H	1.85019700	1.74165200	0.76822600
H	4.08865500	0.15483900	0.09421300
H	2.56562600	0.17633100	-0.82382500
H	3.63261900	-2.03148000	0.79036900
H	6.90356900	1.20725800	2.71212700
H	5.51977000	0.09813100	2.53584400
H	7.74532300	-0.86555900	1.87012400
H	8.11591200	1.50649800	0.31907700
H	6.70141300	0.75327600	-1.44740200
H	8.22377300	0.01135200	-1.99706900
H	7.71352000	-2.07111300	-0.78415200
H	4.94045100	-0.10068900	-2.07307500
Na	4.26486200	5.34063200	1.96345200
N	-1.53033400	-4.53285800	1.97198300
H	-2.10824200	-5.35906500	1.90215700
H	-2.29397300	-4.92015900	-0.39976800
O	-1.50268200	-4.33632000	-2.65533100
H	-0.99691200	-4.46514900	2.82758300
H	3.24287600	-1.11176800	-3.59236000
N	3.20564500	-3.70944300	-4.20077100
H	3.28706100	-4.71276900	-4.30407000
H	2.25654800	-3.34505200	-4.17569000
C	-1.29233900	-0.21471900	-0.52491800
H	-1.17504800	-0.21395600	-1.61045400
H	-1.73023000	-1.17525100	-0.21738000
H	-1.97830900	0.59418700	-0.23260300
C	10.42524200	0.58707600	-0.26096700
H	11.36179800	0.08831500	-0.00259100
H	10.32496400	0.60124900	-1.35476900
H	10.46029500	1.62607000	0.09767800

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**PRO<sub>C5/GC</sub>**

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O	-0.15517300	0.07931400	0.11824200
C	0.01753200	0.16167500	1.52179100
C	1.49302200	0.30063500	1.86944500
O	2.23041900	-0.91943300	1.64059200
C	2.26261100	1.36010500	1.06980600
O	3.31094700	1.84477800	1.93914500
C	2.72606800	0.55884700	-0.14882200
C	2.91061900	-0.86418400	0.40887400
N	2.42359000	-1.90128200	-0.53782900

C	3.04385400	-2.19745000	-1.75036300
N	2.44622000	-3.16708500	-2.40495100
C	1.38779500	-3.53415000	-1.60233800
C	0.39679000	-4.54599600	-1.82208600
N	-0.51732600	-4.58743200	-0.73928300
C	-0.46483400	-3.78892200	0.37952900
N	0.45805800	-2.87395100	0.58067800
C	1.34984600	-2.76410100	-0.43449500
P	4.85427400	2.18450700	1.51032300
O	5.45343600	2.95146600	2.66743600
O	4.95880600	2.79824700	0.13214700
O	5.53397500	0.68883800	1.39759200
C	5.56842500	-0.13825100	2.57507600
C	6.49858300	-1.31388500	2.33050300
O	5.97302100	-2.15103000	1.28480800
C	7.92648500	-0.92366000	1.90502400
O	8.80945800	-1.85756800	2.52148000
C	7.88263200	-1.08096500	0.38281900
C	6.91126300	-2.25339900	0.20269600
N	6.17650900	-2.25621500	-1.05487900
C	6.27146200	-3.36594600	-1.92270600
O	6.87016000	-4.38751200	-1.57695900
N	5.74190900	-3.22013600	-3.19223400
C	4.85634800	-2.29235900	-3.43230700
C	4.24614500	-1.44184400	-2.31793400
C	5.37530400	-1.18026800	-1.37789000
H	-0.52567700	1.03061500	1.92958200
H	-0.36039800	-0.74638500	2.00922900
H	1.56695500	0.51081100	2.94006400
H	1.63889400	2.21194000	0.78709900
H	3.62404100	0.97068600	-0.60367700
H	1.91697100	0.56057800	-0.87905400
H	3.95452500	-1.11078400	0.59559500
H	5.93038100	0.44241200	3.43088300
H	4.55852900	-0.50368700	2.79261200
H	6.55500200	-1.89736700	3.25734600
H	8.17722700	0.10054500	2.21347700
H	7.48384600	-0.16958700	-0.06532600
H	8.85820900	-1.29108700	-0.05854200
H	7.42935500	-3.21175900	0.25254900
H	5.47255900	-0.27765000	-0.79691800
Na	6.17516600	4.65351700	1.12777800
N	-1.47653100	-3.93078900	1.28854400
H	-1.94622600	-4.82295800	1.35498300

H	-1.26687200	-5.26206000	-0.84293700
O	0.26060200	-5.31538100	-2.77351700
H	-1.29920800	-3.48280700	2.17676200
H	3.89496400	-0.48565700	-2.72220000
N	4.47349000	-2.03045100	-4.69061300
H	4.81517100	-2.62265100	-5.43475600
H	3.65365300	-1.47305400	-4.87306600
C	-1.48267500	-0.25755100	-0.24963900
H	-1.50566500	-0.33593600	-1.33900600
H	-1.78436900	-1.21979200	0.18575800
H	-2.19892800	0.51474400	0.06910900
C	10.18000800	-1.49290900	2.43650000
H	10.74561000	-2.25325400	2.97950300
H	10.54293800	-1.45992400	1.40021300
H	10.36264400	-0.51153400	2.89863600

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$TS_{R1/GC}$

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O	-0.00239400	-0.07073200	0.01883900
C	0.00441300	-0.07630300	1.43603200
C	1.43679100	-0.06060600	1.95553500
O	2.10199800	-1.32179300	1.73826600
C	2.37909700	0.96102200	1.30413400
O	3.35453900	1.31116600	2.31118700
C	2.91797100	0.18632300	0.09479700
C	2.80149100	-1.29530900	0.51712800
N	2.09333500	-2.07799700	-0.52534100
C	2.28461200	-1.91345100	-1.87386300
N	1.56662900	-2.64328500	-2.64069400
C	0.77232700	-3.37150600	-1.74603600
C	-0.26873000	-4.31633900	-2.00754200
N	-0.81853300	-4.78915900	-0.78505600
C	-0.41712200	-4.41675800	0.47612000
N	0.54404500	-3.54228200	0.70321200
C	1.09371200	-3.03834000	-0.42435500
P	4.96213400	1.51745800	2.07746100
O	5.49118400	2.13700900	3.35117100
O	5.28678000	2.20678200	0.77132700
O	5.50343500	-0.02809300	1.91486300
C	5.29029300	-0.95298700	2.99612200
C	6.14013000	-2.18794800	2.75616000
O	5.73854400	-2.82073000	1.52633800
C	7.65225100	-1.91972900	2.63558300
O	8.31493400	-3.02348900	3.24594800
C	7.87199200	-1.87475500	1.12053200
C	6.84669800	-2.89478200	0.61850900

N	6.35258400	-2.67248400	-0.73767500
C	6.30678200	-3.77408700	-1.65399000
O	6.77851500	-4.86074900	-1.31236800
N	5.73908400	-3.56166600	-2.87622200
C	5.23312700	-2.37449500	-3.19135300
C	5.24424200	-1.25718300	-2.28707800
C	5.81363700	-1.46486800	-1.07168900
H	-0.53679700	0.79790000	1.83319600
H	-0.47846900	-0.98535900	1.82201500
H	1.40405200	0.09013900	3.03769100
H	1.86639800	1.87787100	1.00262600
H	3.92850300	0.48098300	-0.17095700
H	2.26176500	0.38369200	-0.75199500
H	3.76593600	-1.77763900	0.68409900
H	5.57254900	-0.49282400	3.94977800
H	4.23190900	-1.23088200	3.03140000
H	5.97237700	-2.88399000	3.58647000
H	7.94053800	-0.98059700	3.12728400
H	7.64903300	-0.87099700	0.75477700
H	8.88781600	-2.13860200	0.82253000
H	7.25645900	-3.90450700	0.61943400
H	5.84677700	-0.69932600	-0.30620800
Na	6.51049400	3.88512200	2.07476600
N	-1.09975200	-4.95096100	1.52919900
H	-1.55324100	-5.84672900	1.41660100
H	-1.58692900	-5.44085600	-0.89637100
O	-0.71202800	-4.72516900	-3.08033800
H	-0.66384300	-4.80504500	2.42884300
C	-1.25993800	-0.41766600	-0.53735300
H	-2.04438900	0.29725400	-0.24871100
H	-1.14360000	-0.40501400	-1.62307000
H	-1.56947300	-1.42511900	-0.22451400
C	9.70698500	-2.81893200	3.44554000
H	10.08708400	-3.70357600	3.96097700
H	10.25484400	-2.70198000	2.50060600
H	9.89598900	-1.93199800	4.06792900
H	4.83360600	-0.29377700	-2.55722500
N	4.70643300	-2.22568100	-4.42601500
H	4.14120600	-1.42063300	-4.64627900
H	4.57828800	-3.05368000	-4.98893400

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5'-tG<sup>\*</sup>aC-3'

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O	-0.08802300	-0.22964000	0.20767700
C	-0.01759000	-0.23030800	1.62267300
C	1.43652800	-0.22709100	2.07296200

O	2. 10038400	-1. 48120900	1. 80082000
C	2. 33237500	0. 82163000	1. 39943000
O	3. 33633000	1. 18456600	2. 37274300
C	2. 83537700	0. 07242200	0. 16034000
C	2. 78949200	-1. 41372100	0. 57743600
N	2. 13071400	-2. 23813400	-0. 46660500
C	2. 56509100	-2. 27229200	-1. 77020900
N	1. 87335800	-2. 99347000	-2. 57283300
C	0. 84550800	-3. 49037900	-1. 76295300
C	-0. 25861500	-4. 33192000	-2. 10559400
N	-1. 06567000	-4. 57317500	-0. 96109600
C	-0. 83279200	-4. 08464400	0. 30249800
N	0. 19487000	-3. 31876300	0. 60775000
C	0. 99137100	-3. 03308500	-0. 44669300
P	4. 92325100	1. 45461400	2. 07802600
O	5. 47874100	2. 08812600	3. 33364100
O	5. 17207000	2. 16013000	0. 76433500
O	5. 51106200	-0. 07136100	1. 89024200
C	5. 35601700	-1. 00630600	2. 97300700
C	6. 27306900	-2. 19030500	2. 72679300
O	5. 89842300	-2. 84276100	1. 49844400
C	7. 76604100	-1. 83206000	2. 59668300
O	8. 49778100	-2. 88622100	3. 21541800
C	7. 97682800	-1. 78852200	1. 08061000
C	7. 00653000	-2. 86663500	0. 59000100
N	6. 49617200	-2. 67189500	-0. 76548800
C	6. 60278800	-3. 73719200	-1. 71828700
O	7. 21551600	-4. 76096700	-1. 40877100
N	6. 01447300	-3. 56102200	-2. 93670700
C	5. 36269500	-2. 43917900	-3. 21796100
C	5. 23822000	-1. 35272200	-2. 28284400
C	5. 82850800	-1. 52446700	-1. 06957100
H	-0. 52055500	0. 65814800	2. 03930400
H	-0. 50029900	-1. 12804600	2. 03145100
H	1. 45474200	-0. 09770500	3. 15825100
H	1. 78612200	1. 72894700	1. 12952600
H	3. 82077900	0. 40179800	-0. 15803500
H	2. 12721900	0. 24521400	-0. 64920000
H	3. 78078900	-1. 84648300	0. 72827100
H	5. 61835000	-0. 53105400	3. 92489500
H	4. 31432100	-1. 34108700	3. 01644100
H	6. 15245200	-2. 89611400	3. 55699500
H	7. 99736300	-0. 87154600	3. 07719300
H	7. 69444100	-0. 80344100	0. 70431400

H	9.00459900	-1.99715800	0.77966100
H	7.46992300	-3.85316100	0.59165400
H	5.77741700	-0.78074100	-0.28354100
Na	6.38269600	3.87528100	2.03865700
N	-1.76310000	-4.37012300	1.26040300
H	-2.32237500	-5.20604900	1.16457800
H	-1.88768700	-5.13916700	-1.13822500
O	-0.56769400	-4.82385400	-3.19092900
H	-1.46717800	-4.16430000	2.20426900
C	-1.40515700	-0.42940000	-0.27867500
H	-2.07430600	0.39303500	0.01488400
H	-1.34341900	-0.46925900	-1.36839300
H	-1.82736700	-1.37420300	0.09066200
C	9.87516200	-2.59318600	3.40675500
H	10.31157500	-3.44652700	3.93024500
H	10.41104500	-2.45295600	2.45814600
H	10.01076900	-1.68911900	4.01835000
H	4.73335000	-0.43074600	-2.53619800
N	4.81491700	-2.32144200	-4.44693900
H	4.13266200	-1.60170300	-4.62907600
H	4.78266200	-3.14662100	-5.02781900

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TS<sub>C6/GC</sub>

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O	-0.03668500	-0.00966300	0.07198200
C	0.00316100	-0.03305300	1.48772100
C	1.44373000	-0.02538400	1.98801100
O	2.05290100	-1.33440700	1.91708300
C	2.39756500	0.88991000	1.20618200
O	3.41061700	1.30986300	2.14881000
C	2.89299600	-0.05214000	0.10925200
C	2.96303000	-1.39900900	0.83840500
N	2.68730600	-2.55388600	-0.02480400
C	3.68199700	-3.16165400	-0.76543100
N	3.28512200	-4.17350200	-1.46876800
C	1.94037600	-4.30990100	-1.13245400
C	0.98816900	-5.28841300	-1.56218800
N	-0.27603500	-5.04451500	-0.96075300
C	-0.56277400	-4.03413000	-0.07370900
N	0.31918600	-3.13556700	0.31369300
C	1.54107000	-3.30325000	-0.24316400
P	4.97137100	1.64319800	1.77686300
O	5.52624200	2.43476700	2.93937700
O	5.12875200	2.22096900	0.38956600
O	5.65196700	0.13880500	1.73753300
C	5.61674500	-0.63960600	2.94672700

C	6. 51940700	-1. 84822400	2. 78323700
O	6. 05532400	-2. 66476700	1. 68632000
C	7. 99603000	-1. 50365700	2. 49427100
O	8. 78827700	-2. 39480100	3. 27390700
C	8. 11675200	-1. 77435200	0. 99431900
C	7. 14623400	-2. 94273600	0. 80699100
N	6. 64779200	-3. 07869000	-0. 56150900
C	7. 18605300	-4. 09677300	-1. 39813800
O	7. 99139400	-4. 90105000	-0. 92362800
N	6. 79490700	-4. 12781500	-2. 70850600
C	6. 00326200	-3. 17997300	-3. 20084800
C	5. 47566500	-2. 11560300	-2. 40020300
C	5. 73078700	-2. 18200400	-1. 03996700
H	1. 43242200	0. 25664900	3. 04478100
H	1. 90146500	1. 77678900	0. 80482500
H	3. 84310400	0. 25806500	-0. 32235900
H	2. 13343900	-0. 09728900	-0. 67077100
H	3. 96240200	-1. 59039700	1. 22580700
H	5. 96768100	-0. 03981900	3. 79380300
H	4. 58792100	-0. 95771100	3. 15096700
H	6. 47546700	-2. 43459500	3. 70870800
H	8. 22668600	-0. 46126000	2. 75235300
H	9. 12936800	-2. 01754500	0. 66924700
H	7. 75970300	-0. 90511500	0. 43527500
H	7. 61339300	-3. 89617700	1. 05817700
H	5. 47834500	-1. 37613300	-0. 36262300
O	1. 12862200	-6. 23828900	-2. 33258800
H	-1. 00269900	-5. 69557700	-1. 23550400
N	-1. 85257000	-3. 94377500	0. 37154700
H	-1. 96910500	-3. 35071700	1. 18143900
H	-2. 42158400	-4. 77905800	0. 38094300
H	-0. 51865000	0. 84789100	1. 89736400
H	-0. 48287700	-0. 93767800	1. 87709000
Na	6. 30386600	4. 10893700	1. 40633200
H	4. 80885700	-1. 36390600	-2. 80076200
N	5. 70781500	-3. 22670000	-4. 51716400
H	5. 01130600	-2. 62061700	-4. 92010300
H	6. 02791200	-4. 01581800	-5. 05803700
C	-1. 34026300	-0. 21733200	-0. 44462500
H	-2. 04497800	0. 54807900	-0. 08576300
H	-1. 27020600	-0. 15072300	-1. 53293500
H	-1. 72410400	-1. 20938200	-0. 17272500
C	10. 16514100	-2. 04559400	3. 32124900
H	10. 65306500	-2. 76686000	3. 98032900

H	10.64463500	-2.09241400	2.33410400
H	10.30755100	-1.03375000	3.72823400
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PRO <sub>C6/GC</sub>			
O	-0.03517500	0.03339000	0.04866200
C	-0.00398200	-0.01487100	1.46361800
C	1.43191200	-0.01723600	1.97429100
O	2.05686500	-1.31286500	1.83614300
C	2.38781600	0.94685400	1.25726400
O	3.39749000	1.29908800	2.23063500
C	2.89176600	0.07716500	0.10546400
C	2.96993200	-1.30655800	0.76041300
N	2.70904300	-2.42216700	-0.16767600
C	3.68983500	-2.96397000	-0.99082100
N	3.26316400	-4.00605100	-1.67335900
C	1.96020300	-4.17727400	-1.27045400
C	1.00792600	-5.16956000	-1.67954600
N	-0.22912200	-4.97160800	-1.01563700
C	-0.49739200	-3.98193500	-0.09802100
N	0.38110400	-3.07332900	0.27266200
C	1.58231300	-3.20012200	-0.33902800
P	4.96392600	1.63954500	1.88775300
O	5.53007500	2.30849400	3.11964100
O	5.12441300	2.34779200	0.56217900
O	5.62336000	0.13878900	1.69663700
C	5.65537700	-0.73639700	2.83837900
C	6.48531700	-1.96109000	2.50088300
O	5.84448300	-2.73420600	1.46224900
C	7.90953100	-1.62701900	2.00347700
O	8.80042500	-2.52642800	2.65874300
C	7.80950000	-1.89532600	0.50142300
C	6.81599400	-3.06014100	0.46028500
N	6.15342000	-3.25736300	-0.82033900
C	6.77578100	-4.08550000	-1.75034500
O	7.66116400	-4.86954700	-1.39084700
N	6.42186200	-4.00991200	-3.09151800
C	5.72564600	-2.97090900	-3.52250800
C	5.15256400	-1.99727900	-2.64502000
C	5.07392200	-2.34612900	-1.19771100
H	1.40770700	0.20510100	3.04505400
H	1.89601800	1.85963800	0.91231400
H	3.84353800	0.41697000	-0.29968200
H	2.13632500	0.07390800	-0.67974600
H	3.96470900	-1.50795700	1.14643100
H	6.10884800	-0.22197800	3.69253700



H	4.63485600	-1.03031500	3.11146700
H	6.56821300	-2.57621200	3.40518100
H	8.18245300	-0.58772100	2.23019500
H	8.76264300	-2.14942300	0.03496100
H	7.38406700	-1.02322400	-0.00335400
H	7.31622900	-3.99923800	0.70660600
H	5.16137000	-1.44588400	-0.58734100
O	1.13816600	-6.09445900	-2.47984900
H	-0.95467000	-5.63105000	-1.27272600
N	-1.76788900	-3.92548400	0.39926900
H	-1.87043300	-3.34378100	1.21896700
H	-2.33088300	-4.76451000	0.40310500
H	-0.52980100	0.85688500	1.88762800
H	-0.49049400	-0.92754200	1.83286100
Na	6.32973200	4.11042800	1.73912400
H	4.60318700	-1.13975200	-3.01567100
N	5.57744900	-2.80822400	-4.86257700
H	4.86294600	-2.19733200	-5.22692300
H	5.89941600	-3.55387900	-5.46246600
C	-1.33161000	-0.18989000	-0.47978700
H	-2.05136800	0.55994500	-0.11803700
H	-1.25484700	-0.11065700	-1.56677100
H	-1.70088800	-1.19094700	-0.22030400
C	10.17098400	-2.18305400	2.50828900
H	10.74640700	-2.90960500	3.08612500
H	10.50179100	-2.22587300	1.46176500
H	10.37545100	-1.17379800	2.89521500

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TS<sub>R2/GC</sub>

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O	-0.08065800	0.08565000	0.09338800
C	-0.00688100	-0.05965200	1.50204900
C	1.44985100	-0.06031400	1.97031600
O	2.02378500	-1.38947400	2.01373500
C	2.38886500	0.75589700	1.06956400
O	3.40977600	1.28689500	1.94094800
C	2.87999200	-0.31679800	0.09872300
C	3.01932100	-1.53456500	1.01309400
N	2.86151200	-2.82592200	0.34454000
C	3.90058600	-3.65561500	-0.00513200
N	3.58675800	-4.71521800	-0.64191700
C	2.18971800	-4.64285200	-0.73376900
C	1.25911800	-5.56147900	-1.31429500
N	-0.06850700	-5.08243700	-1.14213800
C	-0.43177000	-3.92150000	-0.50156300
N	0.43908000	-3.07620100	0.01686900

C	1. 72000700	-3. 47419900	-0. 12671500
P	4. 85518700	1. 87111400	1. 43552400
O	5. 22613900	3. 01382200	2. 35348300
O	4. 88611400	2. 12909200	-0. 05398700
O	5. 83743300	0. 57626900	1. 70048000
C	5. 83434600	-0. 05354900	2. 99021700
C	6. 82066200	-1. 20893200	2. 97111500
O	6. 45204900	-2. 14103600	1. 93750100
C	8. 28291200	-0. 80638900	2. 70055700
O	9. 09700000	-1. 66503500	3. 49486500
C	8. 43676200	-1. 08076500	1. 20330800
C	7. 53280700	-2. 30060800	1. 00721900
N	6. 98470000	-2. 44581400	-0. 33694700
C	7. 22381800	-3. 65187900	-1. 06796200
O	7. 94558100	-4. 52313600	-0. 57478100
N	6. 64044000	-3. 77672100	-2. 29411800
C	5. 87196700	-2. 80666400	-2. 77986500
C	5. 62239800	-1. 58135800	-2. 07423800
C	6. 19784100	-1. 45610900	-0. 85204300
H	1. 48054500	0. 32520900	2. 99332000
H	1. 88060700	1. 57786000	0. 56273900
H	3. 79960300	-0. 04499500	-0. 41089200
H	2. 09237800	-0. 49682100	-0. 63471900
H	4. 01628300	-1. 58032600	1. 46280800
H	6. 11995300	0. 66335800	3. 76928500
H	4. 82931700	-0. 42701000	3. 21419300
H	6. 77219600	-1. 71319300	3. 94341300
H	8. 47181100	0. 24478800	2. 95777100
H	9. 46551000	-1. 28142800	0. 90034200
H	8. 06396900	-0. 22519900	0. 63625700
H	8. 06518200	-3. 22949000	1. 21134800
H	6. 05033800	-0. 58891100	-0. 21953800
O	1. 45959800	-6. 62693900	-1. 89462300
H	-0. 78328700	-5. 68649300	-1. 53218100
N	-1. 76256900	-3. 62801100	-0. 45186100
H	-2. 01113600	-2. 92653400	0. 23082400
H	-2. 43252400	-4. 37780700	-0. 54892700
H	-0. 52715700	0. 78109900	1. 98905600
H	-0. 48059700	-0. 99602400	1. 82831000
Na	5. 53960100	4. 40502000	0. 38413500
C	-1. 40878000	0. 16656000	-0. 38659400
H	-1. 95148100	1. 01389200	0. 05922300
H	-1. 35446600	0. 30755800	-1. 46838900
H	-1. 97643200	-0. 75150000	-0. 18080200

C	10.46110700	-1.27117000	3.55423800
H	10.96481100	-1.97206500	4.22340000
H	10.95305700	-1.30915500	2.57282600
H	10.56672700	-0.25270600	3.95581700
H	4.99721900	-0.79868700	-2.48350000
N	5.32249500	-2.99754100	-3.99756700
H	4.65251400	-2.34941900	-4.37885500
H	5.43475800	-3.89361300	-4.44669400

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5'-sG<sup>a</sup>C-3'

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O	-0.27764900	-0.15213200	0.69518900
C	-0.12618800	0.18330500	2.06187800
C	1.34635300	0.12737600	2.43785400
O	1.79824300	-1.24483100	2.45055400
C	2.27769600	0.87190700	1.46182700
O	3.33217600	1.45048100	2.26753500
C	2.76015400	-0.25460900	0.55596300
C	2.91529000	-1.38523400	1.56661700
N	2.94658700	-2.73713100	1.04230500
C	3.59629800	-3.77971400	1.66581400
N	3.48242500	-4.92496400	1.11881900
C	2.66036500	-4.67917600	0.00824800
C	2.22062400	-5.56840800	-1.02294800
N	1.44333400	-4.85824600	-1.98126800
C	1.17781200	-3.51134000	-1.96425300
N	1.58250000	-2.70796100	-0.99909300
C	2.31593000	-3.32895600	-0.05257100
P	4.73318800	2.02009700	1.62527400
O	5.23602900	3.09946700	2.55659900
O	4.58970500	2.35800400	0.15924500
O	5.71638900	0.69681100	1.70566800
C	5.97580800	0.13855200	3.00343100
C	6.85448500	-1.09295600	2.85951400
O	6.21504400	-2.04718900	1.99196600
C	8.25783700	-0.83239000	2.27625100
O	9.16095200	-1.66809000	2.99518500
C	8.10646000	-1.26236700	0.81624700
C	7.10176100	-2.41225400	0.92394500
N	6.31735500	-2.65763700	-0.28045800
C	6.27313300	-3.97357700	-0.84172700
O	6.95036300	-4.86951900	-0.33311600
N	5.47464800	-4.17003700	-1.93143800
C	4.76639000	-3.16839100	-2.44173400
C	4.79831100	-1.83763100	-1.90719400
C	5.58067400	-1.64260300	-0.81742100

H	1.46225000	0.54730800	3.44354200
H	1.76781300	1.66695200	0.91326100
H	3.67274900	-0.00375900	0.02771700
H	1.97406700	-0.49982200	-0.15581800
H	3.85142700	-1.28675700	2.11880900
H	6.47687800	0.87492600	3.64221400
H	5.02915600	-0.13968000	3.48028600
H	6.97644000	-1.53418300	3.85622000
H	8.55256800	0.22114400	2.37534900
H	9.04373100	-1.57801900	0.35547700
H	7.69308100	-0.43431600	0.23623100
H	7.59664100	-3.35607100	1.15354800
H	5.64631600	-0.69111400	-0.30420200
O	2.42378600	-6.77146000	-1.16604500
H	1.12197100	-5.42348000	-2.75917200
N	0.53040500	-2.98388400	-3.04133700
H	0.17997500	-2.04569000	-2.90591900
H	-0.05604000	-3.58191900	-3.60624000
H	-0.50993600	1.19736400	2.26255100
H	-0.68186000	-0.51808300	2.70402800
Na	5.38415200	4.59315700	0.64650700
C	-1.63206400	-0.21274300	0.28262900
H	-2.13808900	0.75747400	0.39932600
H	-1.63476100	-0.49107300	-0.77386800
H	-2.19510900	-0.96727000	0.85210900
C	10.53040900	-1.36816700	2.76187500
H	11.11451300	-2.03796100	3.39660600
H	10.82434500	-1.53164500	1.71615700
H	10.76304500	-0.32683600	3.02856900
H	4.20285000	-1.03686700	-2.32402700
N	3.99917800	-3.43403100	-3.52509800
H	3.28272900	-2.78679000	-3.81805900
H	3.88675900	-4.40053600	-3.79377600

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**Table S5.** Cartesian coordinates of stationary points along the reaction paths of deoxyguanosine-8-yl radical addition to the C5 and C6 sites of its 5' flanking deoxycytidine started from the canonical 5'-*α*CaG<sup>+</sup>-3' sequence, respectively.

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## 5'-αCaG'-3'

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O	0. 81939000	-0. 25208800	-0. 51419500
C	0. 63674500	-0. 46220800	0. 87531500
C	2. 00479100	-0. 55981400	1. 53586600
O	2. 68503400	-1. 76034300	1. 10473900
C	2. 93753900	0. 61286100	1. 18717700
O	3. 75812500	0. 89736700	2. 34108100
C	3. 76330300	0. 05371400	0. 03834100
C	3. 85455700	-1. 43719300	0. 36512200
N	3. 90955700	-2. 26970000	-0. 85464500
C	5. 18906300	-2. 63375300	-1. 35702900
O	6. 19978700	-2. 29110100	-0. 73744500
N	5. 23126800	-3. 34658200	-2. 52430900
C	4. 11189900	-3. 62313300	-3. 17834000
C	2. 81692500	-3. 23973200	-2. 71590300
C	2. 77161600	-2. 55081500	-1. 54260500
P	4. 28328800	2. 43782400	2. 56630400
O	4. 90577100	2. 48332400	3. 94322300
O	3. 19526800	3. 43813300	2. 24697200
O	5. 42420200	2. 61505000	1. 39570800
C	6. 64558600	1. 87209700	1. 50735400
C	7. 45697600	2. 06497900	0. 23807500
O	6. 78159400	1. 44899100	-0. 87646200
C	7. 69397500	3. 53158300	-0. 16163900
O	8. 98874400	3. 59523200	-0. 75123100
C	6. 58016700	3. 78981800	-1. 18241300
C	6. 44063800	2. 42745600	-1. 85949800
N	5. 09856800	2. 17124800	-2. 34935900
C	3. 90391200	2. 73272900	-1. 95160300
N	2. 85458100	2. 22724400	-2. 47003400
C	3. 33901900	1. 18371400	-3. 27709300
C	2. 65091600	0. 18717700	-4. 03950800
O	1. 44524400	-0. 00023900	-4. 19857500
N	3. 59043500	-0. 67504800	-4. 66832300
C	4. 95872100	-0. 62614200	-4. 54160400
N	5. 67701700	-1. 53552400	-5. 25441800
N	5. 57854500	0. 27894900	-3. 80243600
C	4. 73197200	1. 13953200	-3. 20683100
H	0. 07980600	0. 37326000	1. 32892200
H	0. 07142700	-1. 38820100	1. 06166500
H	1. 86736900	-0. 61803300	2. 62059900
H	2. 37774700	1. 50780300	0. 90787000
H	4. 73503400	0. 52806400	-0. 08047200
H	3. 18984800	0. 17238600	-0. 88007900

H	4. 74841100	-1. 68981400	0. 93759300
H	1. 85539300	-2. 17187100	-1. 10837300
H	7. 22120500	2. 21933600	2. 37297100
H	6. 43092600	0. 80448700	1. 63475900
H	8. 42602700	1. 57163700	0. 37343800
H	7. 62955000	4. 20707300	0. 70171100
H	5. 65546900	4. 03517600	-0. 65472700
H	7. 11191100	2. 31587400	-2. 71642800
H	6. 64203600	-1. 60817900	-4. 96127300
H	6. 81505600	4. 58605100	-1. 88953300
H	3. 17262400	-1. 41077300	-5. 22675300
H	5. 23381300	-2. 43261400	-5. 42872300
Na	3. 41348500	4. 30802400	4. 49721400
H	1. 91595000	-3. 45753700	-3. 27375900
N	4. 24395400	-4. 23724700	-4. 39795900
H	3. 43130400	-4. 69206500	-4. 79066600
H	5. 11875400	-4. 72397200	-4. 54802900
C	-0. 38965100	-0. 05853400	-1. 23610700
H	-0. 10443100	0. 09182400	-2. 27899800
H	-1. 05018100	-0. 93412800	-1. 15568500
H	-0. 93465500	0. 82357900	-0. 86986800
C	9. 46963700	4. 91978500	-0. 93823500
H	10. 47554400	4. 83626500	-1. 35505500
H	8. 84826500	5. 49789000	-1. 63562900
H	9. 51982500	5. 46535400	0. 01532900

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TS<sub>R1/CG</sub>

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O	0. 04209100	0. 03019900	0. 03396900
C	0. 01379700	0. 02362500	1. 45355100
C	1. 43671900	0. 02831200	1. 99189600
O	2. 07745200	-1. 23023200	1. 71054900
C	2. 33502100	1. 11713700	1. 38120000
O	3. 24268500	1. 55359100	2. 41654600
C	3. 07023300	0. 36747600	0. 27485300
C	3. 21570400	-1. 03840900	0. 86619500
N	3. 24804500	-2. 10893500	-0. 13148100
C	4. 41774400	-2. 91622400	-0. 26557000
O	5. 37681200	-2. 72452300	0. 48851200
N	4. 41888500	-3. 87013100	-1. 24113700
C	3. 34237500	-4. 06144100	-1. 99867000
C	2. 12931100	-3. 31312400	-1. 83734400
C	2. 13897000	-2. 34045100	-0. 89220900
P	4. 06541200	2. 96224800	2. 21555100
O	4. 63583900	3. 32537300	3. 56772400
O	3. 21829800	3. 99092700	1. 50232700

O	5. 26620900	2. 53947800	1. 17305800
C	6. 30791800	1. 67792700	1. 65604000
C	7. 30085900	1. 42058000	0. 54070100
O	6. 71989100	0. 51516500	-0. 42705700
C	7. 73061100	2. 68503600	-0. 23733900
O	9. 13994200	2. 60037300	-0. 42486900
C	6. 95876000	2. 54514000	-1. 55636300
C	6. 96366900	1. 02723700	-1. 72235100
N	5. 92924300	0. 50388700	-2. 60483700
C	4. 86644300	-0. 31395200	-2. 30460800
N	4. 13142100	-0. 64681300	-3. 29615100
C	4. 74338000	-0. 03034900	-4. 39611900
C	4. 40333900	-0. 03561600	-5. 78586700
O	3. 47453600	-0. 58711900	-6. 37189700
N	5. 34617700	0. 74217600	-6. 52009200
C	6. 43185800	1. 41034300	-6. 00433300
N	7. 25007400	2. 04960800	-6. 88094400
N	6. 72921000	1. 41311100	-4. 71533000
C	5. 86568100	0. 68526900	-3. 97753300
H	-0. 51776600	0. 91066400	1. 83338200
H	-0. 50784500	-0. 87021300	1. 82785400
H	1. 38993800	0. 16109600	3. 07871600
H	1. 76433000	1. 97310800	1. 01508000
H	4. 03242600	0. 81161500	0. 02437000
H	2. 44139300	0. 33861800	-0. 61681300
H	4. 13572400	-1. 14616900	1. 44165700
H	1. 28548200	-1. 70408400	-0. 68258800
H	6. 82204500	2. 15356000	2. 49811300
H	5. 88714100	0. 72360900	1. 99441300
H	8. 19307000	0. 95114800	0. 97106200
H	7. 46777500	3. 60249000	0. 30377600
H	5. 92914100	2. 88752600	-1. 42570200
H	7. 93371500	0. 68360400	-2. 10724100
H	7. 92338800	2. 67692600	-6. 46514100
H	7. 41710000	3. 06683600	-2. 39651600
H	5. 17554900	0. 76313100	-7. 51936300
H	6. 89854800	2. 32475800	-7. 78633300
Na	3. 52668900	5. 45948900	3. 42412100
H	1. 25259700	-3. 50183000	-2. 44305400
N	3. 40913800	-5. 02786700	-2. 94091500
H	2. 67704500	-5. 14350600	-3. 62288500
H	4. 29268000	-5. 48653000	-3. 10293000
C	-1. 25487100	0. 00779500	-0. 54615400
H	-1. 12207800	0. 00523100	-1. 62990800

H	-1.81263400	-0.89195200	-0.24951400
H	-1.83854000	0.89315000	-0.25618300
C	9.72777300	3.80792300	-0.89109700
H	10.80399500	3.63353500	-0.95360900
H	9.36050800	4.09677500	-1.88527600
H	9.53811700	4.63917100	-0.19639600

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5'- $\alpha$ CsG $\cdot$ -3'

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O	0.77281800	0.27620900	-1.62470700
C	0.24625200	0.72703800	-0.38469400
C	1.36832700	0.77374200	0.64498100
O	1.79361700	-0.56732900	0.96670800
C	2.61379900	1.52536100	0.14132600
O	3.20462900	2.24856100	1.24531800
C	3.50920000	0.39388800	-0.33255400
C	3.16309800	-0.75373400	0.61094100
N	3.33713300	-2.06466400	-0.02710200
C	4.45029200	-2.87463100	0.34191900
O	5.17245500	-2.52014700	1.27947200
N	4.67053400	-4.01371200	-0.37708000
C	3.86586300	-4.34271700	-1.38444000
C	2.73265600	-3.55246500	-1.76965400
C	2.52027300	-2.41358100	-1.06319700
P	4.24270400	3.47797000	0.91759500
O	4.44810200	4.23280500	2.20889100
O	3.77392200	4.28172300	-0.28417500
O	5.61316000	2.72290100	0.43874100
C	6.33726400	1.89730200	1.36097500
C	7.44653100	1.18085600	0.61004300
O	6.87605100	0.21688400	-0.29700500
C	8.35131000	2.10027900	-0.23807000
O	9.68666400	1.62941500	-0.07253500
C	7.82266200	1.88248500	-1.65997300
C	7.41653400	0.41138300	-1.60637900
N	6.43437500	-0.02013800	-2.58578100
C	6.30693400	-1.32047100	-3.03128500
N	5.26728300	-1.58394900	-3.71666100
C	4.55255100	-0.37351500	-3.71890300
C	3.24324600	-0.07137500	-4.21234900
O	2.43395900	-0.79529300	-4.79315300
N	2.90301600	1.27466100	-3.90890500
C	3.66651100	2.16447100	-3.18851200
N	3.15187000	3.39166400	-2.92240800
N	4.88312800	1.86846300	-2.75793200
C	5.26056100	0.60651400	-3.02030900



H	-0.18901600	1.73329600	-0.49153900
H	-0.54396400	0.04956400	-0.02840500
H	0.98712300	1.24737500	1.55643400
H	2.36019300	2.23064300	-0.65073200
H	4.56666600	0.63842900	-0.33736500
H	3.20299800	0.11527500	-1.33960900
H	3.78949000	-0.77316900	1.50352700
H	1.71305500	-1.72100700	-1.27547800
H	6.77048900	2.51143400	2.15888200
H	5.66914800	1.15469600	1.81263400
H	8.07049500	0.65683200	1.34402600
H	8.27436900	3.14962900	0.07558000
H	6.93972700	2.49905800	-1.82208400
H	8.28425200	-0.24329600	-1.74760600
H	3.50136500	3.81930700	-2.05401000
H	8.56385100	2.08380900	-2.43485600
H	1.96087400	1.53395600	-4.17688200
H	2.16477600	3.53141100	-3.08803300
Na	3.81602300	6.29245600	1.10860100
H	2.08678800	-3.83304000	-2.59125700
N	4.13829600	-5.48872800	-2.04779800
H	3.65465500	-5.72486700	-2.89933200
H	4.99515600	-5.97661800	-1.83495900
C	-0.20318800	0.16783500	-2.65288500
H	0.31274000	-0.22282400	-3.53296800
H	-1.01111200	-0.52131700	-2.36902800
H	-0.64592100	1.14688300	-2.88722200
C	10.67429000	2.51740200	-0.57807600
H	11.64635500	2.07516500	-0.34926000
H	10.59918700	2.65497200	-1.66534900
H	10.60774300	3.50509100	-0.09860300

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TS<sub>C5/CG</sub>

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O	0.22739600	0.16297100	-0.28832200
C	0.03366800	0.15920800	1.11768100
C	1.39115000	0.09053700	1.80647500
O	1.97183700	-1.22130200	1.57697700
C	2.39045900	1.12304100	1.23242000
O	3.28901700	1.56762500	2.28419100
C	3.15010500	0.27613800	0.24178600
C	3.27762200	-1.01789900	1.03042800
N	3.73442600	-2.14861800	0.22039500
C	5.00544500	-2.73947800	0.55071200
O	5.47057000	-2.56162300	1.67482700
N	5.64055300	-3.48306800	-0.40394000

C	5. 13719300	-3. 58489000	-1. 61966400
C	3. 86555300	-2. 98141000	-2. 01279900
C	3. 15223700	-2. 38991600	-0. 97626400
P	4. 40659600	2. 73508000	1. 96906600
O	4. 99807700	3. 12583900	3. 30252500
O	3. 79615600	3. 84703200	1. 13241900
O	5. 53591600	2. 03596300	1. 00348900
C	6. 36170000	0. 96051300	1. 47433800
C	6. 97515200	0. 21353700	0. 29533500
O	5. 94002800	-0. 39838300	-0. 48777300
C	7. 82490700	1. 05023200	-0. 68520300
O	9. 00991900	0. 29682000	-0. 93782200
C	6. 92737100	1. 17350100	-1. 92166500
C	6. 11916300	-0. 12679700	-1. 87888600
N	4. 82247700	-0. 09182000	-2. 53850400
C	4. 21719300	-1. 19160700	-3. 16371600
N	3. 05926200	-0. 89210400	-3. 69152400
C	2. 87567800	0. 46111400	-3. 43871800
C	1. 71166500	1. 27122000	-3. 63687700
O	0. 66000300	1. 00469000	-4. 22369200
N	1. 85567700	2. 52378000	-2. 98316200
C	2. 93186300	2. 91800100	-2. 22119800
N	2. 86047400	4. 10674400	-1. 55933900
N	4. 02557400	2. 18476300	-2. 10711800
C	3. 93650400	0. 97020700	-2. 68774000
H	-0. 48473300	1. 07603000	1. 44173200
H	-0. 57686500	-0. 70254500	1. 42807800
H	1. 25916100	0. 24078800	2. 88415800
H	1. 88949100	1. 98840000	0. 79335600
H	4. 09816500	0. 69678500	-0. 04874500
H	2. 52716900	0. 11576100	-0. 63651100
H	4. 00496500	-0. 93548000	1. 83636300
H	2. 15733000	-1. 98657500	-1. 12236100
H	7. 16533900	1. 35457900	2. 10729200
H	5. 77498400	0. 24904900	2. 06325600
H	7. 61468000	-0. 57243400	0. 71598900
H	8. 08407700	2. 03259000	-0. 26768700
H	6. 25393900	2. 02093200	-1. 80155400
H	6. 66510800	-0. 95819500	-2. 33925300
H	3. 37079500	4. 10100600	-0. 66673800
H	7. 48883800	1. 28392600	-2. 85084400
H	1. 03044300	3. 11053600	-3. 02706500
H	1. 94569600	4. 53226700	-1. 48895200
Na	4. 41122700	5. 43263600	2. 85262300

H	3.32850000	-3.38128400	-2.86287000
N	5.82085300	-4.28190000	-2.54213600
H	5.52504900	-4.30763800	-3.50506600
H	6.72847400	-4.65331000	-2.30403100
C	-0.97150600	0.33421800	-1.02895600
H	-1.47883900	1.27300800	-0.76072700
H	-0.69044900	0.37020900	-2.08420400
H	-1.67194000	-0.49753200	-0.86299800
C	10.02401000	1.03103200	-1.60871700
H	10.88757000	0.36870400	-1.70178500
H	9.71730700	1.34966400	-2.61443400
H	10.31713000	1.92424500	-1.03741500

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PRO<sub>C5/CG</sub>

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O	-0.00830100	-0.02035400	0.01441900
C	0.00215700	-0.00343400	1.43365800
C	1.44829100	-0.00090500	1.91811400
O	2.04476400	-1.28951200	1.63759400
C	2.30413100	1.05487200	1.18185300
O	3.32457200	1.56965000	2.08100500
C	2.94595300	0.21861200	0.10224000
C	3.23407400	-1.07283300	0.86132100
N	3.55352200	-2.21279300	0.00666100
C	4.84495800	-2.77443300	0.11205300
O	5.47616000	-2.70159400	1.16405500
N	5.38562400	-3.41192600	-0.99904600
C	4.85444400	-3.25041500	-2.17934900
C	3.51080700	-2.58765900	-2.43386200
C	2.78765600	-2.48190300	-1.11603600
P	4.33415500	2.77483300	1.59108200
O	5.03518300	3.26595500	2.83662900
O	3.58908200	3.80736000	0.76266800
O	5.40247500	2.07347700	0.55684300
C	6.29894500	1.05137700	1.01142500
C	6.79140200	0.22048800	-0.16851300
O	5.67510000	-0.41525600	-0.80475500
C	7.55036300	0.96357800	-1.28583300
O	8.64854100	0.12827800	-1.64881300
C	6.50736400	1.08970600	-2.40247100
C	5.66200600	-0.17344900	-2.20563100
N	4.27451600	-0.09888900	-2.67790200
C	3.46231500	-1.18787700	-3.04437900
N	2.31192100	-0.80177200	-3.55781000
C	2.31817700	0.57436100	-3.47787400
C	1.23195600	1.48901600	-3.68301400

O	0.11306100	1.27940200	-4.15174700
N	1.56742400	2.77852300	-3.19270000
C	2.73568900	3.11145000	-2.54597000
N	2.84072800	4.34708900	-1.97647500
N	3.75567900	2.27941400	-2.44549200
C	3.49520500	1.03173900	-2.88807000
H	-0.50665900	0.89666000	1.81504300
H	-0.51694900	-0.88445200	1.84125600
H	1.46407100	0.17761400	3.00000900
H	1.70600000	1.88699600	0.80466200
H	3.83285200	0.67662600	-0.30259800
H	2.21923600	0.03512700	-0.68739600
H	4.08728400	-0.96306700	1.53035900
H	1.76690500	-2.12335700	-1.09747500
H	7.15787800	1.50139600	1.52298600
H	5.79112000	0.38262700	1.71361300
H	7.45224100	-0.55458400	0.23797500
H	7.91485900	1.94567900	-0.95518700
H	5.89505400	1.97171900	-2.22771100
H	6.11035900	-1.02825000	-2.72287700
H	3.35840800	4.30826800	-1.09134600
H	6.94680000	1.14353300	-3.39961600
H	0.80396100	3.44529000	-3.22038200
H	1.98071000	4.87365800	-1.89614600
Na	4.25631700	5.50400200	2.35990100
H	2.93753500	-3.21739000	-3.12116300
N	5.49609300	-3.71829500	-3.26162900
H	5.09293100	-3.66189300	-4.18367800
H	6.38940100	-4.17599500	-3.14989000
C	-1.30371800	0.08058400	-0.55263100
H	-1.82263600	0.99095300	-0.21716100
H	-1.17076200	0.12708100	-1.63649200
H	-1.92857900	-0.78838000	-0.29865400
C	9.60122700	0.76464900	-2.48881200
H	10.40849800	0.04768100	-2.65377500
H	9.18031600	1.04801600	-3.46320400
H	10.01434500	1.66711900	-2.01465500

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TS<sub>C6/CG</sub>

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O	0.03442500	0.02058900	0.01548300
C	0.01495500	0.01370200	1.43355800
C	1.44085400	0.00188800	1.96232900
O	2.06099900	-1.25655200	1.61688700
C	2.34244500	1.10690200	1.36304300
O	3.29091900	1.49157900	2.39100300

C	3. 04502800	0. 35499900	0. 24392400
C	3. 31246600	-0. 95615200	0. 97662400
N	3. 76792100	-2. 08058300	0. 18705700
C	4. 94723400	-2. 77431800	0. 60519500
O	5. 47069000	-2. 48192100	1. 68217000
N	5. 44460100	-3. 75495100	-0. 20538300
C	4. 83812300	-4. 05913000	-1. 34813800
C	3. 66191900	-3. 38225700	-1. 80647500
C	3. 20823700	-2. 32263700	-1. 03382000
P	4. 40871500	2. 66782200	2. 12253800
O	5. 06356100	2. 93351800	3. 45964300
O	3. 79838800	3. 83836900	1. 38514800
O	5. 48842300	1. 98744600	1. 07930800
C	6. 30795700	0. 88793100	1. 50339500
C	6. 97521000	0. 24948000	0. 29542700
O	5. 98724600	-0. 32943900	-0. 59003900
C	7. 80492200	1. 22337400	-0. 56176000
O	9. 01875400	0. 55502000	-0. 89714300
C	6. 91111800	1. 45288300	-1. 78323000
C	6. 25219900	0. 08112600	-1. 92377900
N	4. 99101300	0. 08130500	-2. 66877600
C	3. 92087700	-0. 79469700	-2. 52649700
N	2. 98166800	-0. 62671200	-3. 40224200
C	3. 42961300	0. 41766600	-4. 20397700
C	2. 81390700	1. 03678100	-5. 33847300
O	1. 72989200	0. 80284800	-5. 87109400
N	3. 65625900	2. 05624700	-5. 86118000
C	4. 88946400	2. 41356700	-5. 37120900
N	5. 57759300	3. 37388300	-6. 04997400
N	5. 44328300	1. 83701400	-4. 32097300
C	4. 68087300	0. 86105200	-3. 77661900
H	-0. 50714100	0. 90320300	1. 82239800
H	-0. 51215900	-0. 87649000	1. 81112600
H	1. 41064300	0. 10850800	3. 05370800
H	1. 78047800	1. 98368000	1. 03413700
H	3. 94809100	0. 83312400	-0. 11562700
H	2. 34042500	0. 21397400	-0. 57513300
H	4. 07522400	-0. 81829900	1. 73775400
H	2. 23854600	-1. 87416300	-1. 20933000
H	7. 08874500	1. 24453900	2. 18553100
H	5. 71689700	0. 13165200	2. 02432700
H	7. 62838800	-0. 54968900	0. 66344000
H	8. 01905500	2. 15776500	-0. 02644300
H	6. 14568900	2. 19608300	-1. 54856100

H	6.93229700	-0.63594400	-2.40324000
H	6.37864400	3.74743400	-5.56088600
H	7.45157700	1.76824300	-2.67271500
H	3.28947600	2.52034200	-6.68419100
H	5.06870500	4.04184700	-6.61151100
Na	4.54337800	5.26614400	3.20791200
H	3.18037200	-3.62192700	-2.74436100
N	5.36054400	-5.05339000	-2.09432000
H	4.96124000	-5.31896000	-2.97984100
H	6.18447200	-5.53386300	-1.76670900
C	-1.26499000	0.01954900	-0.55307200
H	-1.83485500	-0.87442000	-0.25892400
H	-1.83922800	0.90956200	-0.25524900
H	-1.14198700	0.02196800	-1.63837000
C	10.00304600	1.40666800	-1.46785400
H	10.89286200	0.79596300	-1.63540300
H	9.68402900	1.83268900	-2.42870300
H	10.25830000	2.23404400	-0.78954800

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**PRO<sub>C6/CG</sub>**

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O	-0.00263400	-0.02103800	0.01243100
C	0.00313100	-0.00580300	1.43027000
C	1.43862800	0.00138500	1.92870200
O	2.04945700	-1.27122800	1.63924900
C	2.32276600	1.07773800	1.24910800
O	3.21201400	1.61134500	2.26337300
C	3.08583000	0.25113600	0.22354100
C	3.35089900	-0.99037900	1.07062900
N	3.91909600	-2.15593700	0.44988700
C	4.84795600	-2.87698800	1.20835600
O	5.03118300	-2.59758100	2.39621500
N	5.56272300	-3.92297300	0.64242500
C	5.31373300	-4.30105000	-0.60035100
C	4.36938900	-3.63693500	-1.43247800
C	3.73564200	-2.37125000	-0.97260700
P	4.32624900	2.75890400	1.88243700
O	4.78583900	3.35614400	3.19401900
O	3.80149700	3.69904700	0.82060200
O	5.55246600	1.90953200	1.17762200
C	6.25942500	0.92767100	1.94670600
C	7.04421000	0.01231200	1.01942400
O	6.14328800	-0.68365700	0.13399300
C	8.07164700	0.71091200	0.11531000
O	9.23585000	-0.11226100	0.09789700
C	7.36441400	0.74900100	-1.24045800

C	6.56811000	-0.56089000	-1.20979700
N	5.37987400	-0.57373800	-2.08945800
C	4.17114000	-1.28023200	-1.96721800
N	3.35311500	-1.04294400	-2.96924500
C	4.02243700	-0.17678000	-3.79836500
C	3.60438200	0.40661900	-5.04052600
O	2.54275000	0.27632900	-5.64627800
N	4.63105300	1.23052100	-5.56986000
C	5.86161800	1.44586500	-4.99544900
N	6.74878300	2.21018000	-5.68719400
N	6.22843800	0.90919100	-3.84707600
C	5.28334200	0.12020600	-3.28626200
H	-0.51564500	0.88861100	1.81301700
H	-0.51391400	-0.89113100	1.83292100
H	1.43189700	0.17575600	3.01281300
H	1.74165900	1.89245000	0.81347100
H	3.99112000	0.73157900	-0.13317700
H	2.41356000	0.02793200	-0.60547000
H	4.02547200	-0.73256100	1.88308000
H	2.65780300	-2.42879600	-1.17838600
H	6.95667200	1.41729000	2.63688800
H	5.56267500	0.32333400	2.53472500
H	7.56266500	-0.72535300	1.64251000
H	8.32102300	1.71786900	0.47584200
H	6.66884400	1.58987100	-1.26418600
H	7.19559100	-1.41960800	-1.48328000
H	7.55957500	2.50775000	-5.16378100
H	8.04112100	0.82701500	-2.08694700
H	4.40935100	1.65847200	-6.46182600
H	6.41200500	2.86585500	-6.37694900
Na	4.19033100	5.53991100	2.34207700
H	4.15941700	-3.96873500	-2.44219000
N	5.96401800	-5.39261600	-1.08206800
H	5.98374000	-5.58050300	-2.07237300
H	6.71372500	-5.77359300	-0.52343900
C	-1.31206600	-0.02205000	-0.53084700
H	-1.88226300	-0.90805000	-0.21332100
H	-1.87611900	0.87542400	-0.23486300
H	-1.21163900	-0.03569000	-1.61852000
C	10.36798400	0.50693200	-0.49779800
H	11.19920000	-0.19542600	-0.40534000
H	10.21387900	0.72942700	-1.56231100
H	10.62990600	1.44262000	0.01754700

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