Computational Study of the Formation of C8, C5 and C4 Guanine:Lysine Adducts via Oxidation of Guanine by Sulfate Radical Anion

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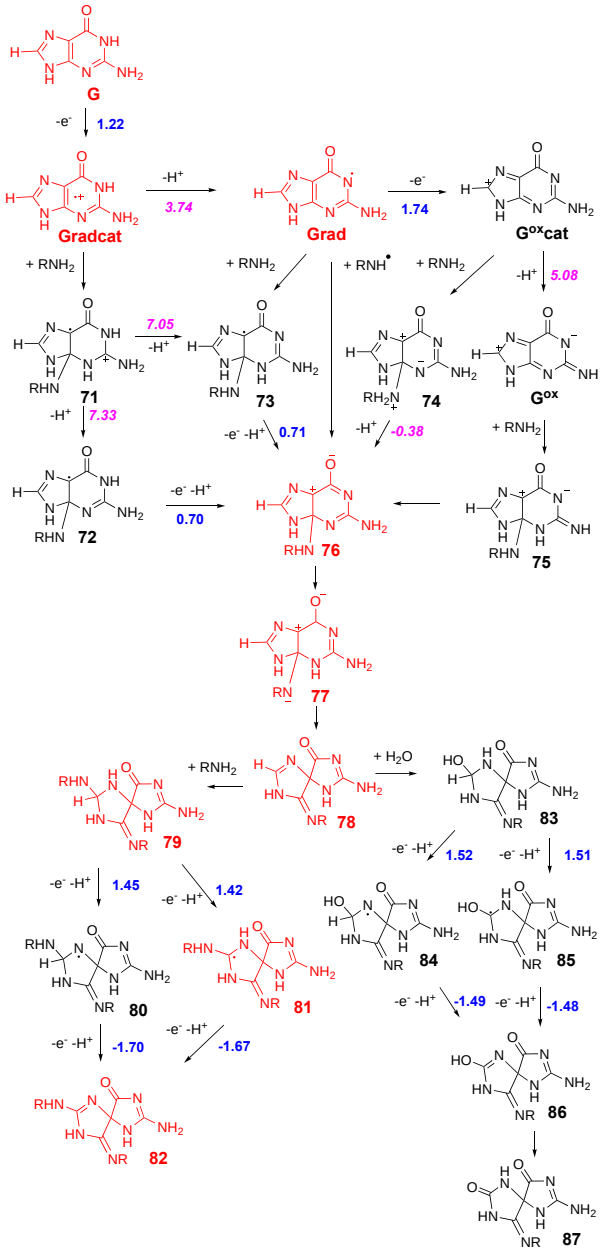
Supporting Information

C4 addition of methylamine

C4 lysine:guanine adducts were not isolated in any of the reported experimental studies, indicating that the barriers for key reactions are higher than for C8 and C5 addition. Possible pathways for methylamine addition to C4 are shown in **Scheme S1** and **Figure S1**. Water-assisted methylamine addition to guanine radical cation (**Gradcat**) has a barrier of 24.4 kcal/mol to form **71** and is endothermic by 10.5 kcal/mol. Deprotonation of **71** yields two neutral radical tautomers **72** (pK_a = 7.33) and **73** (pK_a = 7.05) of comparable energy. **72** and **73** can undergo proton-coupled oxidation reactions to form a common zwitterionic intermediate, **76** (E^o = 0.70 V and 0.71 V, resp.). It is also possible to form a neutral diradical rather than a zwitterion, but the singlet diradical is higher in energy than the zwitterionic species. Addition of methylamine to the guanine radical (**Grad**) has a barrier of 30.6 kcal/mol to form **73**. Addition to the oxidized guanine cation, **G^{ox}cat,** is barrierless and forms **74** (ΔH = –11.1 kcal/mol) which deprotonates (pK_a = –0.38) to give the zwitterionic species, **76**. **76** also be formed by methylamine addition across C4-N3

bond of $\mathbf{G^{ox}}$ (8.2 kcal/mol) followed by tautomerization. **76** can tautomerize and undergo acyl migration to form the 4-methylamine substituted spirocyclic intermediate, **78**. In a second nucleophilic addition step, methylamine or water can add across the C8-N7 double bond. The ring rearrangement reaction can also occur after the addition of second nucleophile but the barriers are calculated to be 4-8 kcal/mol higher. The methylamine addition (barrier height of 17.1 kcal/mol) is calculated to be more favored than water addition (barrier height of 21.4 kcal/mol). Both the methylamine adduct (**79**) and the water adduct (**83**) can undergo subsequent two proton-coupled oxidation reactions to produce the final products, **4,8-diNR-Sp** (**82**) and **4-NR,8-oxo-Sp** (**87**), respectively.

Scheme S1. Possible pathways for the formation of guanine:methylamine adducts via sequential one-electron oxidations of guanine and nucleophilic attack of methylamine ($R=CH_3$) at C4. Numbers next to the arrow correspond to pK_a's (pink, italics) and standard redox potentials (E^o) (blue, regular). The structures shown in red represent the thermodynamically favored pathway.


G
-e⁻
1.22
Gradcat
-H⁺
3.74
Grad
-e⁻
1.74
Gᵒˣcat
+ RNH₂
+ RNH₂
+ RNH•
+ RNH₂
-H⁺
5.08
7.05
-H⁺
71
73
74
Gᵒˣ
-H⁺
7.33
-e⁻ -H⁺
0.71
-H⁺
-0.38
+ RNH₂
72
-e⁻ -H⁺
0.70
76
75
77
+ RNH₂
+ H₂O
79
78
83
-e⁻ -H⁺
1.52
-e⁻ -H⁺
1.51
-e⁻ -H⁺
1.45
-e⁻ -H⁺
1.42
84
85
80
81
-e⁻ -H⁺
-1.49
-e⁻ -H⁺
-1.48
-e⁻ -H⁺
-1.70
-e⁻ -H⁺
-1.67
86
82
87

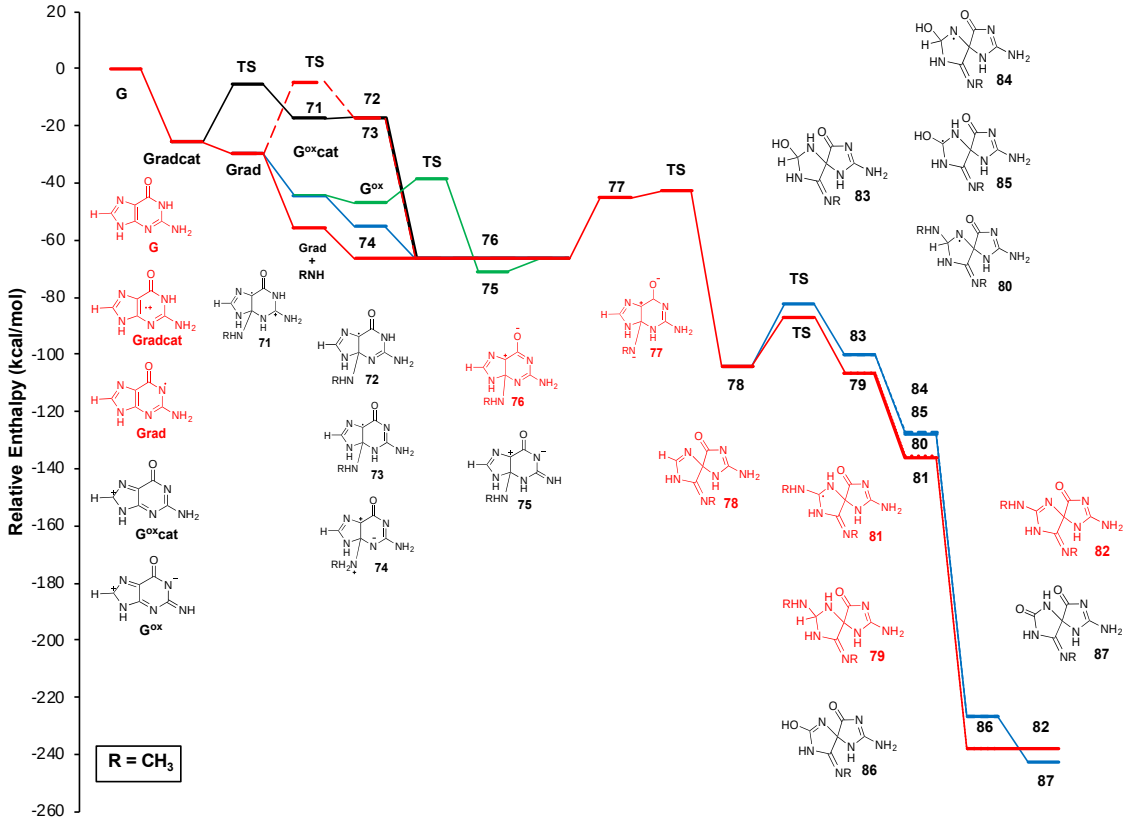


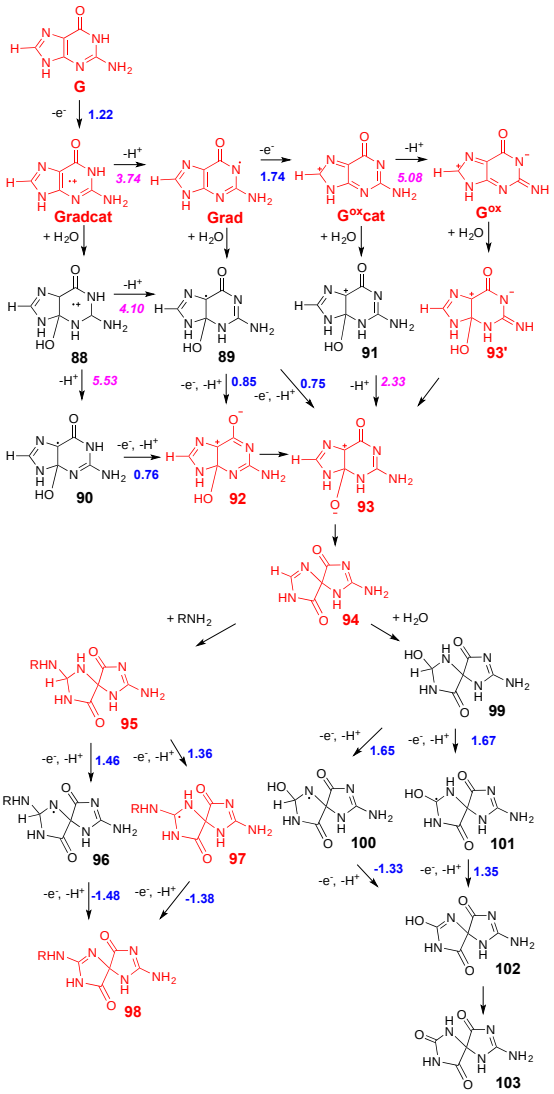
Figure S1. Comparison of the relative enthalpies (kcal/mol) of adducts resulting from the addition of methylamine at the C4 position of guanine radical cation (**Gradcat**, red), guanine radical (**Grad**, black), oxidized guanine cation (**G^{ox}cat**, green) and neutral oxidized guanine (**G^{ox}**, blue) calculated at the SMD/B3LYP/aug-cc-pVTZ//SMD/B3LYP/6-31+G(d,p) level of theory. On the right side of the figure, the red line corresponds to the addition of a second methylamine and the blue line corresponds to the addition of water. The solid red line represents the most favored pathway.

C4 addition of water

Scheme S2 shows the various possible pathways for water addition to an oxidized guanine intermediate at the C4 position and **Figure S2** summarizes the thermodynamics. Water addition to C4 follows almost the same pattern as for methylamine addition. In comparison to the water addition to the guanine radical cation (**Gradcat**), guanine radical (**Grad**), and oxidized guanine neutral (**G^{ox}**) (barriers of 33.4, 30.1, and 33.7 kcal/mol, resp.), addition of water to the oxidized guanine cation (**G^{ox}cat**) has smaller barriers (8.5 kcal/mol). Loss of a proton from **88** (pK_a = 4.10 for N1 and pK_a = 5.53 for N3) produces neutral radicals, **89** and **90**, respectively. Proton-coupled oxidation of **89** (E^o = 0.86, PCET)

or **90** (E^o = 0.76, PCET) forms a zwitterionic species, **92**. **92** can then tautomerize to form **93. 93** can also be formed by deprotonation of **91** (pK_a = 2.33) or tautomerization of **93'**. **93** can undergo acyl migration to form the spirocyclic intermediate **94**. Addition of methylamine across the C8-N7 double bond of **94** has a barrier of 13.8 kcal/mol while water addition has a barrier of 24.0 kcal/mol and forms **95**. Two sequential proton coupled electron transfer reactions form the final products, **4-oxo,8-NHR-Sp**, **98** and **4,8-dioxo-Sp**, **103**, respectively.

Scheme S2. Possible pathways for the formation of guanine:water adduct at the C4 position of guanine via sequential one-electron oxidation of guanine and nucleophilic attack of water at C4. Numbers next to the arrow correspond to pK_a's (pink, italics) and standard redox potentials (E^o) (blue, regular). The structures shown in red represent the thermodynamically favored pathway.



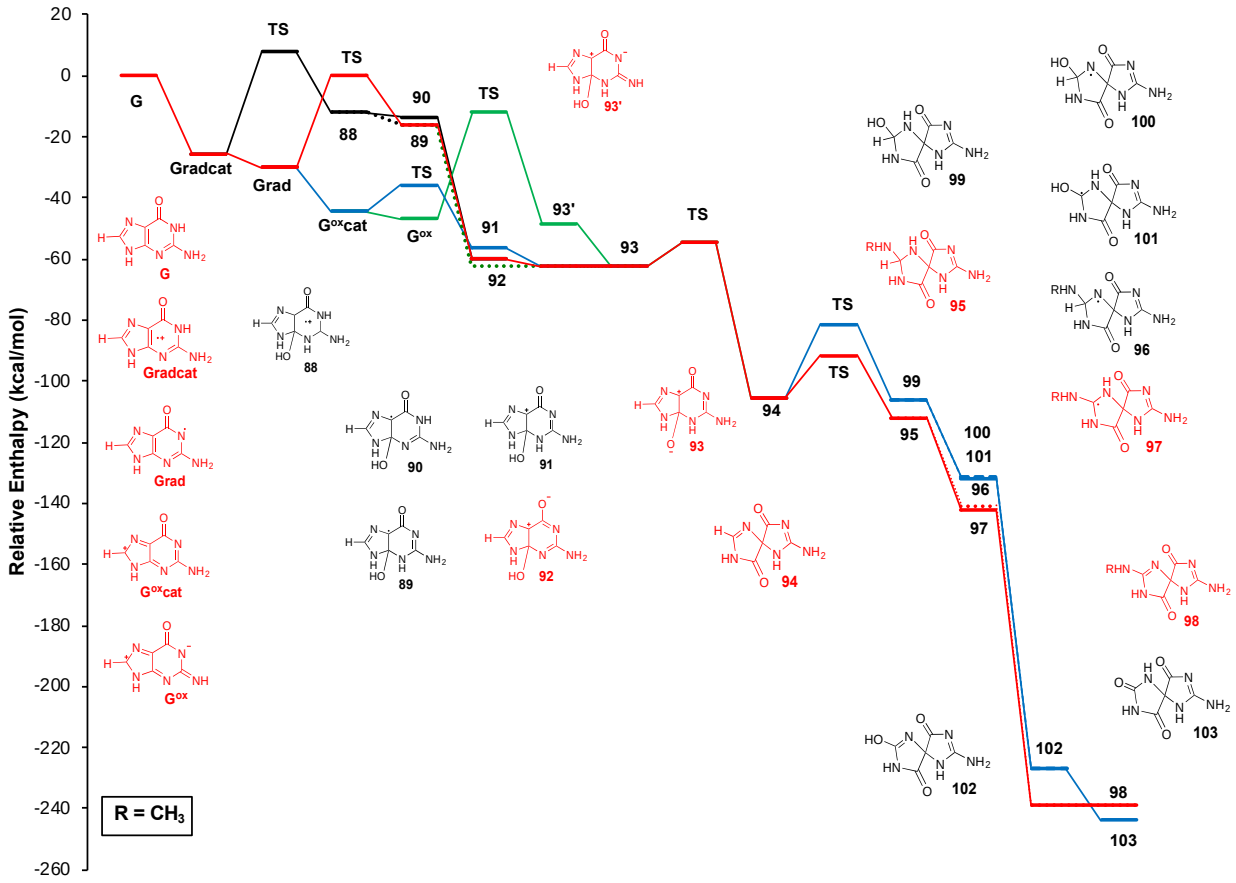


Figure S2. Comparison of the relative enthalpies (kcal/mol) of adducts resulting from the addition of water at the C4 position of guanine radical cation (**Gradcat**, black), guanine radical (**Grad**, red), oxidized guanine cation (**G^{ox}cat**, blue) and neutral oxidized guanine (**G^{ox}**, green) calculated at the SMD/B3LYP/aug-cc-pVTZ//SMD/B3LYP/6-31+G(d,p) level of theory. On the right side of the figure, the red line corresponds to the addition of a second methylamine and the blue line corresponds to the addition of water.

Geometry Coordinates (SMD/B3LYP/6-31+G(d,p) optimized in water)

Sulfate radical anion

SCF Done: E(UB3LYP) = -699.161202188 a.u.

-1 2

S	0.00000000	0.00000000	0.07978600
O	0.00000000	1.24114200	0.88832500
O	0.00000000	-1.24114200	0.88832500
O	1.13082200	0.00000000	-0.96811100
O	-1.13082200	0.00000000	-0.96811100

Sulfate dianion (with alpha=0.90)

SCF Done: E(RB3LYP) = -699.394742999 a.u.

-2 1

S	0.00005700	-0.00011400	0.00020000
O	1.31957900	-0.21302700	0.72497400
O	-1.01414300	0.60511200	0.95735700
O	-0.51931300	-1.33484300	-0.51010100
O	0.21376400	0.94298500	-1.17263000

Sulfate radical anion (8 explicit waters)

SCF Done E(RB3LYP) =: -1310.78071329 a.u.

-1 2

O	-1.801529	0.208494	1.052681
S	-0.635967	-0.221409	1.965837
O	-0.533198	0.644366	3.163446
O	0.630977	-0.365061	1.211925
O	-1.256163	-1.592723	2.304644
O	2.339263	1.973824	0.687084
H	3.246763	1.786986	0.969781
H	1.858002	1.135905	0.818063
O	0.943033	3.289868	2.778208
H	0.378302	2.544873	3.042002
H	1.483489	2.919379	2.047669
O	1.775548	0.510440	4.991502
H	2.138878	1.405436	5.065165
H	0.970914	0.612692	4.450634
O	3.133503	-0.856017	2.905540
H	2.436281	-0.784830	2.233017
H	2.751500	-0.391526	3.680954
O	-1.749197	-3.719025	0.218590
H	-2.530547	-4.219517	0.497050
H	-1.524638	-3.160041	0.982387
O	-2.458301	-1.512524	-1.423219
H	-2.249289	-2.331330	-0.924690
H	-2.257911	-0.803037	-0.792241
O	-3.995439	-1.615712	3.811031
H	-3.086520	-1.795875	3.524419
H	-4.249650	-0.820594	3.294666
O	-4.514973	0.694084	2.248869
H	-3.668401	0.664287	1.770115
H	-5.189372	0.517872	1.576247

Sulfate dianion (8 explicit waters)

SCF Done E(RB3LYP) =: -1311.02927194 a.u.

-2 1

O	-1.649051	0.413316	1.110619
S	-0.593771	-0.205536	2.012943
O	-0.421384	0.667389	3.245231
O	0.716568	-0.303692	1.248578
O	-1.022496	-1.597714	2.446477
O	2.089054	2.006014	0.492878
H	3.015725	1.825915	0.708027
H	1.607822	1.180244	0.731729
O	0.836984	3.188043	2.777023
H	0.352065	2.364530	2.992672
H	1.348658	2.936986	1.980115
O	1.663028	0.255028	5.049149
H	2.018630	1.140306	5.214261
H	0.907741	0.395732	4.432628
O	3.042087	-0.863685	2.809350
H	2.276697	-0.724133	2.214046
H	2.721567	-0.506868	3.663612
O	-1.952651	-3.466880	0.594845
H	-2.771348	-3.808635	0.982523
H	-1.610326	-2.821136	1.255135
O	-2.548178	-1.212414	-1.054764
H	-2.421335	-2.084244	-0.626324
H	-2.231406	-0.586852	-0.370411
O	-3.663830	-1.763154	3.516721
H	-2.730522	-1.753432	3.218742
H	-4.063194	-1.029138	3.005821
O	-4.337965	0.462489	1.847419
H	-3.387322	0.469391	1.589067
H	-4.806490	0.141416	1.063267

Water

SCF Done: E(RB3LYP) = -76.4480563420 A.U.

0 1

O	0.00000000	0.00000000	0.11849700
H	0.00000000	0.76563900	-0.47398800
H	0.00000000	-0.76563900	-0.47398800

O_2 (4 explicit waters)

SCF Done: E(RB3LYP) = -456.131708532 A.U.

0 3

O	-0.800942	0.511823	-0.232404
O	-0.019553	0.738064	-1.133793
O	-3.036074	3.150615	-0.140315

H	-2.603309	3.171909	-1.021873
H	-2.646443	2.385728	0.306536
O	0.599209	-2.550854	0.627944
H	1.092299	-2.572100	1.461709
H	-0.032976	-1.823561	0.732686
O	-1.799598	3.280671	-2.664565
H	-1.172661	2.541929	-2.692656
H	-2.453886	3.075691	-3.349177
O	2.284542	-1.775671	-1.487741
H	2.001726	-0.879633	-1.719717
H	1.703575	-2.033224	-0.738652

$O_2^{\bullet-}$ (4 explicit waters)

SCF Done: E(RB3LYP) = -456.298582075 A.U.
-1 2

O	-0.805643	0.329723	-0.300646
O	-0.177825	0.701872	-1.421092
O	-2.725468	2.335004	0.004265
H	-2.475214	2.808953	-0.811174
H	-2.095177	1.576813	0.002397
O	0.320175	-1.982434	0.712658
H	0.817819	-1.739065	1.506427
H	-0.091769	-1.139570	0.394147
O	-1.303578	3.014126	-2.434287
H	-0.891623	2.171259	-2.115798
H	-1.801144	2.770783	-3.228113
O	1.741947	-1.303471	-1.726047
H	1.111698	-0.545247	-1.724189
H	1.491709	-1.777358	-0.910567

O_2^{2-} (4 explicit waters)

SCF Done: E(RB3LYP) = -456.434814942 A.U.
-2 1

O	-1.418453	-0.351725	-0.869754
O	-0.659094	0.191273	-2.050972
O	-2.209312	1.838446	0.259408
H	-1.856836	2.471542	-0.392387
H	-1.916656	0.942828	-0.149986
O	0.191514	-1.344933	0.819282
H	0.408604	-0.643579	1.448935
H	-0.455971	-0.909063	0.117465
O	-0.791109	2.717683	-2.125098
H	-0.762654	1.667658	-2.090397
H	-1.418477	2.942947	-2.825798
O	1.689156	-0.794467	-1.628217
H	0.771306	-0.383557	-1.841616
H	1.543892	-1.123665	-0.722885

$HOO^{\bullet}$ (4 explicit waters)

SCF Done: E(RB3LYP) = -456.745721154 A.U.
0 2

O	-0.760275	0.255310	-0.233702
O	-0.133795	0.635651	-1.340746
O	-2.756459	2.415186	-0.130497
H	-2.435192	2.813309	-0.963867
H	-2.168827	1.644709	-0.018904
O	0.545371	-2.246650	0.585776
H	1.074554	-2.180983	1.394363
H	0.021189	-1.423082	0.549719
O	-1.356855	3.100386	-2.550079
H	-0.870428	2.280476	-2.353810
H	-1.867313	2.904541	-3.349576
O	1.694644	-1.106096	-1.615071
H	0.621528	-0.070183	-1.510253
H	1.442140	-1.710627	-0.874790
H	1.605538	-1.619143	-2.432908

HOO^- (4 explicit waters)

SCF Done: E(RB3LYP) = -456.923002688 A.U.
-1 1

O	-0.255588	0.834337	0.369962
O	0.512118	1.307008	-0.811410
O	-2.716918	1.141159	-0.549784
H	-2.544801	1.754378	-1.285147
H	-1.795432	0.995832	-0.164739
O	0.202114	-1.707127	0.555332
H	0.954538	-1.852065	1.146391
H	0.043227	-0.696510	0.540905
O	-1.159572	2.862428	-2.387208
H	-0.529612	2.304850	-1.868340
H	-1.081602	2.551415	-3.300218
O	1.100395	-1.212429	-1.995348
H	0.698900	0.474544	-1.304130
H	0.787680	-1.590226	-1.137535
H	0.440372	-1.474790	-2.653075

HOOH (4 explicit waters)

SCF Done: E(RB3LYP) = -457.395079057 A.U.
0 1

O	0.000176	0.942397	0.283690
O	0.719363	1.254314	-0.944613
O	-2.532773	1.540726	-0.479118
H	-2.239227	2.099323	-1.235362
H	-0.947198	1.143141	0.036168
O	0.209832	-1.867392	0.593162
H	0.938840	-2.104616	1.184759
H	0.138578	-0.889663	0.643753
O	-1.097789	2.833020	-2.462557
H	-0.371058	2.302572	-2.070737
H	-1.242450	2.461558	-3.345126
O	1.087309	-1.235443	-1.960636
H	0.833793	0.353893	-1.362308
H	0.784027	-1.685084	-1.138681
H	0.436766	-1.463197	-2.641051
H	-2.945124	2.148925	0.151977

Imidazole

SCF Done: E(RB3LYP) = -226.250742195 A.U.

0 1

C	0.58186900	1.00111700	0.00000100
C	1.15110400	-0.24822900	0.00000000
C	-0.97795900	-0.56347700	0.00000000
N	-0.77915100	0.78086700	0.00000000
H	-1.50247800	1.48966800	0.00000600
H	1.00186600	1.99529800	-0.00000900
H	2.20203000	-0.49963600	0.00000000
H	-1.96525800	-1.00151700	-0.00000400
N	0.16968700	-1.22662100	0.00000000

Imidazole Cation

SCF Done: E(RB3LYP) = -226.708382892 A.U.

1 1

C	-0.68136700	0.97742000	0.00000000
C	0.68185200	0.97705300	0.00000000
C	-0.00029300	-1.13937400	-0.00000100
N	-1.07515700	-0.34813100	0.00000100
H	-2.03354000	-0.68315400	-0.00000200
H	-1.39361200	1.78661300	0.00000100
H	1.39460800	1.78579700	-0.00000200
H	-0.00065500	-2.21803800	0.00000100
N	1.07498500	-0.34868800	0.00000100
H	2.03325000	-0.68407200	0.00000000

Methylamine

SCF Done: E(RB3LYP) = -95.8787924904 A.U.

0 1

C	0.05417800	0.70777000	0.00000000
H	0.58702800	1.07242200	0.88249200
H	0.58702800	1.07242200	-0.88249200
H	-0.94856400	1.15759500	0.00000000
N	0.05417800	-0.76525800	0.00000000
H	-0.46490200	-1.09612300	0.81122000
H	-0.46490200	-1.09612300	-0.81122000

Lysine

SCF Done: E(RB3LYP) = -497.104960135 a.u.

0 1

N	2.67004200	-1.56767100	-0.09236800
H	3.39378600	-1.67224900	-0.80044000
C	1.68279000	-0.55669200	-0.50997100
H	1.57957500	-0.48889600	-1.59896200
C	0.30091600	-0.87844800	0.10517100
C	2.17885700	0.80545200	-0.02364700
H	0.08742900	-1.92470800	-0.14891600
H	0.37693800	-0.82578500	1.19883000
C	-0.85552600	-0.00177600	-0.38771600
O	1.79911800	1.88349000	-0.46306500
H	-0.65567000	1.05145500	-0.15873500
H	-0.92441100	-0.07781500	-1.48148000
C	-2.19774900	-0.40329600	0.23825600
H	-2.40346100	-1.46289100	0.02867600
H	-2.13702500	-0.30381000	1.33149700
C	-3.37062000	0.44008400	-0.27266500
H	-3.17287400	1.49996500	-0.07463000
H	-3.44940600	0.33479100	-1.36089000
N	-4.68394000	0.11034500	0.30900900
H	-4.62656700	0.20561600	1.32243700
H	-4.87943500	-0.87564100	0.13821800
O	3.07514500	0.74320000	0.97359400
H	3.25823400	-0.23020000	1.08343200
H	2.22406100	-2.47402100	0.0236940

Guanine (G)

SCF Done: E(RB3LYP) = -542.635312440 A.U.

0 1

C	0.84037200	0.50174100	-0.00108800
C	0.53428300	-0.86081900	-0.00033800
C	-1.67911500	-0.57244700	-0.00152500
C	-0.23166300	1.43701200	-0.00001700
C	2.71457000	-0.51704900	0.00145400
H	-2.29150700	1.40185700	-0.00721000
H	3.76579100	-0.76603700	0.00224900
H	1.90601200	-2.49717200	0.00142100
N	-1.47936200	0.78962800	-0.00224600
N	-0.68458000	-1.44658000	0.00262400
O	-0.18191800	2.68443800	0.00305300
N	2.21470300	0.69896200	0.00031400
N	1.74649000	-1.49602000	0.00137900
N	-2.96350300	-1.00278200	-0.05224700
H	-3.71104600	-0.36536300	0.19091700
H	-3.12082700	-1.98187400	0.14852100

Guanine Radical Cation (Gradcat)

SCF Done: E(UB3LYP) = -542.430288212 A.U.

1 2

C	0.83864300	0.51782300	-0.00000600
C	0.54038100	-0.88447400	-0.00000600
C	-1.67640700	-0.56630300	0.00001200
C	-0.27049400	1.45586100	0.00000300
C	2.69815600	-0.49842500	-0.00002100
H	-2.32930000	1.39054000	0.00001900
H	3.75874000	-0.70616300	-0.00002900
H	1.96739700	-2.48744200	-0.00002000
N	-1.50408300	0.79116600	0.00000900
N	-0.64200500	-1.45462400	0.00000200
O	-0.20390700	2.68053300	0.00000600
N	2.16140200	0.73625100	-0.00001500
N	1.77377000	-1.48901700	-0.00001800
N	-2.90253500	-1.05273100	0.00002500
H	-3.71756600	-0.44667500	0.00003700
H	-3.03553700	-2.05873400	0.00002800

Guanine Radical (Grad)

SCF Done: E(UB3LYP) = -541.980639737 A.U.
0 2

C	0.79835600	0.50991400	-0.00000100
C	0.50498900	-0.88773200	0.00000100
C	-1.69332500	-0.46944700	0.00000300
C	-0.33195300	1.43722100	0.00000000
C	2.66600200	-0.50735000	-0.00000200
H	3.72628300	-0.71649500	-0.00000200
H	1.93570900	-2.49679500	-0.00000100
N	-1.57072200	0.86220800	0.00000100
N	-0.68447500	-1.43440500	0.00000600
O	-0.17131700	2.67956600	-0.00000100
N	2.13117100	0.72397400	-0.00000200
N	1.74172900	-1.50014900	-0.00000200
N	-2.92691000	-0.98780500	0.00001900
H	-3.73208800	-0.37500200	-0.00007500
H	-3.05933000	-1.99063800	-0.00008800

8-NH_2CH_3 Guanine Radical Cation (1)

SCF Done: E(UB3LYP) = -638.334177484 a.u.
1 2

C	0.13758700	0.75444100	-0.17122900
C	0.11714500	-0.67209500	-0.20754200
C	2.33035400	-0.88191900	0.08789600
C	1.39938500	1.40019200	0.03844100
H	-1.47990700	-1.94598000	-0.70758200
N	2.45468200	0.47970600	0.16270500
N	1.15170600	-1.49891200	-0.08934200
O	1.62865600	2.62249000	0.11052400
N	-1.17862000	-1.03432600	-0.38234900

8-$NHCH_3$-N7H Guanine Radical Cation (2)

SCF Done: E(UB3LYP) = -638.335763215 a.u.
1 2

C	-4.21621000	0.19731500	0.40941500
H	-4.91867900	-0.04192800	1.20954700
H	-4.69842400	-0.01989500	-0.54735800
N	-3.02408700	-0.65467000	0.55678500
H	-2.59712500	-0.51546800	1.47194000
C	0.03945400	0.57950700	-0.20900000
C	0.24265500	-0.83626100	-0.21975300
C	2.45688800	-0.62510900	0.11772000
C	1.15411600	1.45673200	-0.02273000
H	3.18870500	1.30377200	0.26630000
H	-1.11739100	-2.41366500	-0.42741900
N	2.35055200	0.74351300	0.12354400
N	1.41122800	-1.44915200	-0.06261000
O	1.13046000	2.69573400	0.01025700
N	-0.95213000	-1.41401500	-0.40382400
N	3.66673500	-1.14833500	0.30204100
H	4.48167000	-0.56635800	0.45213400

Oxidized Guanine Cation (G^{ox}cat)

SCF Done: E(RB3LYP) = -541.758118396 A.U.
1 1

C	0.79677300	0.54523000	0.00037100
C	0.51637100	-0.89742100	0.00035500
C	-1.69417300	-0.47385000	-0.00011500
C	-0.38193000	1.46021300	-0.00000100
C	2.65908300	-0.49607800	0.00002000
H	3.73045900	-0.65315800	0.00018200
H	2.01679400	-2.48129000	0.00012700
N	-1.59705200	0.84611100	-0.00008100
N	-0.62981000	-1.44908000	-0.00051500
O	-0.22687900	2.68464900	-0.00008800
N	2.07515900	0.77748400	-0.00013500
N	1.79318700	-1.48427800	-0.00003300
N	-2.87541400	-1.06143400	0.00018900
H	-3.72178900	-0.49946600	0.00072700
H	-2.94965400	-2.07346500	-0.00008500

N	3.44022600	-1.61797500	0.20169200
H	4.34905400	-1.19147000	0.32573500
H	3.36968600	-2.62487300	0.14271200
C	-1.96416300	0.17324700	-0.53948500
H	-2.49773800	0.20323600	-1.49407500
N	-1.07674600	1.29851900	-0.36271900
H	-3.44221000	1.19367000	0.48558800
H	3.37826700	0.88434800	0.29878100
N	-3.05886400	0.24191300	0.52098600
C	-4.17198800	-0.74219800	0.34692500
H	-3.77293700	-1.75206800	0.43111600
H	-4.90242600	-0.56198700	1.13491700
H	-4.62214900	-0.58413800	-0.63287700
H	-2.62549400	0.12685400	1.44464600
H	3.77252900	-2.15458400	0.31072900
H	-3.99834500	1.27278500	0.45617800
C	-2.04526200	-0.44221100	-0.46732500
H	-2.54929600	-0.47754600	-1.43758100
N	-1.26571900	0.82627400	-0.38964000
H	-1.70322100	1.74187300	-0.37057500

8-$NHCH_3$-N7H Guanine Radical (3)

SCF Done: E(UB3LYP) = -637.876679870 a.u.
0 2

C	-4.14475500	0.20511400	0.45774600
H	-4.82657600	-0.01351700	1.28175400
H	-4.66310600	-0.01149900	-0.48044200
N	-2.96310000	-0.66506300	0.57353900
H	-2.50329700	-0.51368400	1.47110500
C	0.07494400	0.56814000	-0.22304600
C	0.28073400	-0.84181000	-0.23277900
C	2.47094500	-0.52677900	0.13693100
C	1.20529700	1.43960600	-0.01746300
H	-1.08748600	-2.42793700	-0.41926200
N	2.40710000	0.81788600	0.15886800

N	1.45185900	-1.42588100	-0.05802500
O	1.08339100	2.69975400	-0.00275500
N	-0.91766000	-1.43082400	-0.44889400
N	3.68657000	-1.08167000	0.32499500
H	4.48662800	-0.49669500	0.51726100
H	3.78414300	-2.08588600	0.36263400
H	-3.90960100	1.27802300	0.48620600
C	-2.00926400	-0.46028300	-0.48556400
H	-2.55123200	-0.50493800	-1.43489000
N	-1.23403000	0.80806000	-0.43642300
H	-1.67918200	1.71661800	-0.37569200

8-NHCH$_3$-N1H Guanine Radical (4)

SCF Done: E(UB3LYP) = -637.876771635 a.u.

0 2

C	-4.24630200	0.20938900	0.34153500
H	-4.95699200	0.01190500	1.14731700
H	-4.71965300	-0.07162200	-0.60395900
N	-3.04765500	-0.62036100	0.55192200
H	-2.64782700	-0.39482000	1.46290900
C	-0.01071500	0.58852500	-0.20061200
C	0.22705900	-0.82294300	-0.20389600
C	2.44387300	-0.62000400	0.10775900
C	1.11420100	1.45098000	-0.03159100
H	3.15767100	1.31157400	0.22974000
H	-1.13476800	-2.40713500	-0.38649300
N	2.32409300	0.74296000	0.10308800
N	1.40389000	-1.44482100	-0.05220000
O	1.12770000	2.70287200	0.00407900
N	-0.96582700	-1.40963800	-0.37283500
N	3.67550300	-1.13388700	0.26182800
H	4.46679200	-0.54390200	0.48195400
H	3.77446300	-2.13520300	0.35724300
H	-4.04479800	1.28824000	0.31989700
C	-2.02090900	-0.38434800	-0.45236700
H	-2.51702200	-0.43615900	-1.42906800
N	-1.31039200	0.89782700	-0.34567900

8-NH$_2$CH$_3$ oxidized Guanine Cation (5)

SCF Done: E(RB3LYP) = -637.719150058 a.u.

1 1

C	-0.17100300	0.73672500	0.15072200
C	-0.13777300	-0.73889700	0.16823700
C	-2.36232900	-0.79680700	-0.08660900
C	-1.50462300	1.38422400	-0.04257400
C	1.91561500	0.15808000	0.50808300
H	2.35947600	0.21544900	1.50535500
H	1.51615000	-1.98763500	0.52800200
N	-2.55244900	0.53688100	-0.14562900
N	-1.17573000	-1.51060400	0.05776800
O	-1.61027700	2.62300200	-0.09589900
N	0.98617100	1.26548400	0.31604400
N	1.15860400	-1.06031100	0.31986700
N	-3.44425300	-1.56299400	-0.18044700
H	-4.35690900	-1.13915200	-0.28815200
H	-3.36039400	-2.57076300	-0.14428100
N	3.03899200	0.28249400	-0.47626600
H	3.42519100	1.23056800	-0.37930700
H	2.66455300	0.20505700	-1.43106900
C	4.14970300	-0.71037500	-0.28485900
H	4.52955100	-0.60660600	0.73079900
H	3.76318400	-1.71312900	-0.45957700
H	4.92453100	-0.47215400	-1.01193200

8-NHCH$_3$-N7H oxidized Guanine Cation (6)

SCF Done: E(RB3LYP) = -637.699239779 a.u.

1 1

C	0.18495300	0.70126700	-0.12440300
C	0.13560400	-0.77039100	-0.16385000
C	2.37275400	-0.79386000	0.07769800
C	1.50796400	1.38259000	0.03500600
C	-2.02265800	0.09677300	-0.41174600
H	-2.41436100	0.16597300	-1.43213800
H	-1.51525300	-2.03624000	-0.39730300
N	2.55568500	0.54902500	0.12737300
N	1.19746200	-1.51675900	-0.06500100
O	1.55464800	2.62300000	0.06931900
N	-1.00233200	1.16725800	-0.24999600
N	-1.14868400	-1.09261800	-0.31212600
N	3.46284200	-1.54115600	0.17410800
H	4.37015600	-1.10384300	0.28066800
H	3.39319400	-2.55106000	0.14151300
N	-3.08116400	0.24208900	0.51714000
H	-2.74497800	0.06951100	1.46385800
C	-4.25467100	-0.60439700	0.22605200
H	-4.64272100	-0.35556300	-0.76441600
H	-4.03368800	-1.67837300	0.26346300
H	-5.02518800	-0.38088600	0.96519100
H	-1.25467900	2.15971500	-0.24842000

8-NHCH$_3$ oxidized Guanine neutral (7)

SCF Done: E(RB3LYP) = -637.273431877 a.u.

0 1

C	-4.22987900	0.25566800	0.16468700
H	-5.02749800	0.04076000	0.87896100
H	-4.58943200	-0.00257300	-0.83515100
N	-3.06961100	-0.58588000	0.50000000
H	-2.76334100	-0.37611100	1.44983600
C	0.01763000	0.56455400	-0.14015400
C	0.26890500	-0.88845100	-0.10436400
C	2.47046000	-0.51632300	0.07767900
C	1.20588500	1.45734000	0.00142400
H	-1.11393900	-2.44901500	-0.26460300
N	2.40167600	0.83456600	0.09408900
N	1.45083900	-1.44403300	-0.00383300
O	1.07883700	2.69898400	0.02570200
N	-0.93162700	-1.45414300	-0.19358100

N	3.69353600	-1.04351100	0.15350600
H	4.50050000	-0.43768300	0.21901700
H	3.81895000	-2.04682200	0.14706800
H	-4.02080500	1.33208500	0.19338800
C	-1.95940500	-0.42412400	-0.39651600
H	-2.33363000	-0.47985800	-1.42481600
N	-1.22239500	0.85519700	-0.29101800

8-NH_2CH_3 oxidized Guanine neutral (7')

SCF Done: E(RB3LYP) = -637.241528765 a.u.

0 1

C	0.09730700	0.53929300	-0.14382800
C	0.36343200	-0.90585900	-0.08835800
C	2.60537500	-0.52624300	0.10269100
C	1.27041300	1.44567500	0.00310600
C	-1.83139700	-0.46158800	-0.47632200
H	-2.25709700	-0.55936000	-1.47836300
H	-0.99750800	-2.44792600	-0.50234300
N	2.45886500	0.85336000	0.10564600
N	1.52361300	-1.45225900	0.02605500
O	1.09815300	2.69898400	0.01371800
N	-1.14474700	0.81785100	-0.33837400
N	-0.86536500	-1.49468200	-0.18083100
N	3.80925000	-1.00594700	0.18160600
H	3.74816800	-2.02551200	0.16922800
N	-2.99538400	-0.53192100	0.48142400
H	-3.36657200	-1.48900800	0.44154900
C	-4.11290000	0.42499000	0.18860200
H	-4.91543200	0.21638900	0.89479100
H	-3.74999900	1.44218700	0.31536600
H	-4.45147500	0.25518300	-0.83296500
H	-2.65231300	-0.38625400	1.43896300

8-$NHCH_3$ oxidized Guanine neutral (8)

SCF Done: E(RB3LYP) = -637.317515832 a.u.

0 1

C	4.14533600	-0.82149600	0.28004200
H	5.19626700	-0.55424300	0.16618500
H	3.96623900	-1.72101300	-0.31448100
N	3.33539100	0.29543000	-0.21913100
H	3.69387600	1.20717300	0.04343900
C	-0.10927900	0.76646500	-0.04750400
C	-0.06559400	-0.62528500	-0.07343300
C	-2.27814100	-0.90922900	0.00862300
C	-1.37570700	1.39480200	0.03517800
C	1.96976700	0.25201800	-0.11247500
H	-3.36109900	0.84723200	0.10650600
H	1.66191600	-1.87761900	-0.14063200
N	-2.42442300	0.45527000	0.05272300
N	-1.09423500	-1.50034800	-0.04756600
O	-1.64352400	2.61855200	0.09397100
N	1.17397600	1.30735800	-0.06818700
N	1.27046400	-0.94361000	-0.11679400
N	-3.41726100	-1.65363500	-0.02536100
H	-4.27734800	-1.23176400	0.30300400
H	-3.30727600	-2.63942300	0.17551300
H	3.94993200	-1.04566800	1.33632000

8-$NHCH_3$ Oxidized Guanine Radical Neutral(9)

SCF Done: E(UB3LYP) = -636.682639940 a.u.

0 2

C	-0.00908800	0.54542700	0.00326600
C	-0.27906300	-0.85687300	0.00430600
C	-2.47851800	-0.49386000	-0.00142500
C	-1.15259000	1.44420800	0.00135100
C	1.88917100	-0.43580800	0.00215100
H	1.15846200	-2.44886400	0.00310300
N	-2.37983600	0.84525500	-0.00151900
N	-1.46050000	-1.42794400	0.00258900
O	-1.02339400	2.69776300	0.00165000
N	1.31749400	0.79396500	0.00265900
N	0.95764400	-1.45435600	0.00571800
N	-3.71647700	-1.01960200	-0.00555100
H	-4.52243900	-0.41037100	-0.01156000
H	-3.84426200	-2.02180000	-0.00825700
N	3.19561900	-0.66796400	-0.00571900
H	3.50111200	-1.63471000	0.01130700
C	4.20930800	0.38451600	-0.00517900
H	4.05522600	1.06690400	-0.84369500
H	4.18452200	0.95080800	0.92968600
H	5.18159400	-0.09521100	-0.10784600

8-NCH_3 Oxidized Guanine Neutral (10)

SCF Done: E(RB3LYP) = -636.054805514 a.u.

0 1

C	0.05562400	0.53390600	-0.00408200
C	-0.23268000	-0.90946300	-0.00173800
C	-2.42918200	-0.47977500	0.00121300
C	-1.11120200	1.45824100	-0.00022700
C	1.96389300	-0.48555800	-0.00337100
H	1.17275300	-2.49097900	-0.00046600
N	-2.32727600	0.86439000	0.00220100
N	-1.42114600	-1.43874700	-0.00028400
O	-0.94873500	2.69370600	0.00161900
N	1.32196300	0.78568800	-0.00799800
N	0.97736600	-1.49538400	-0.00206100
N	-3.65861600	-0.98905100	0.00236000
H	-4.46046300	-0.37168100	0.00408400
H	-3.79634300	-1.99152700	0.00185200
N	3.21070800	-0.74797700	0.00405800
C	4.18013600	0.33175700	0.00366100
H	3.74753000	1.33166300	-0.06279000
H	4.77898600	0.25330900	0.91690900
H	4.86688300	0.17247900	-0.83320200

8-NCH_3-5-$NHCH_3$ Oxidized Guanine Neutral (11)

SCF Done: E(RB3LYP) = -731.949850307 a.u.

0 1

C	0.13813800	0.56959800	-0.00871200
C	-0.05315800	-0.91710300	-0.20525400
C	2.15699700	-1.24962100	0.00527600
C	1.38894000	0.76677900	0.86153500
C	-2.09114500	-0.01665000	0.24487900
H	-1.78770300	-2.08119200	-0.27836500
N	2.40947300	-0.10622500	0.65864100
N	0.90654800	-1.78082600	-0.30758400
O	1.47789200	1.74389800	1.62409100
N	-1.12817300	0.92643800	0.60581300
N	-1.37665100	-1.15633800	-0.20275700
N	3.18654900	-2.03283000	-0.31124300
H	4.12788800	-1.75224300	-0.06950900
H	3.02988500	-2.93380900	-0.74255600
N	-3.35238300	0.13217800	0.36259700
C	-4.21502300	-0.99006100	-0.00530500
H	-4.17758900	-1.78575800	0.74912100
H	-5.24686400	-0.63955000	-0.06023200
H	-3.95880600	-1.42784300	-0.97796800
H	-1.41455800	1.89822800	0.56189900
N	0.30596000	1.19635900	-1.34366600
C	0.63734600	2.63270800	-1.31913000
H	1.59852800	2.86496000	-0.84352400
H	0.67483900	2.98092300	-2.35398500
H	-0.15085300	3.19331400	-0.81032900
H	1.05027000	0.70658800	-1.83962100

5,8-NCH$_3$ Oxidized Guanine Anion (11AN)

SCF Done: E(RB3LYP) = -731.452350959 a.u.

-1 1

C	-0.14802700	0.59956800	0.06663200
C	0.05129900	-0.88527700	0.21770600
C	-2.15109500	-1.26902400	0.00749100
C	-1.41010800	0.79279100	-0.76507500
C	2.08191000	-0.00032900	-0.27475600
N	-2.42868200	-0.10327200	-0.58988300
N	-0.89385600	-1.77380100	0.31257500
O	-1.57669900	1.82236800	-1.46212800
N	1.37433100	-1.13062300	0.19672400
N	-3.16638800	-2.09516400	0.28400000
H	-4.10990500	-1.83774200	0.02543000
H	-2.98343000	-3.02126500	0.64772700
N	1.13275300	0.94944100	-0.63599500
H	1.78410400	-2.05831300	0.25419600
C	-0.57992200	2.63778200	1.28168900
H	-0.59065700	3.03832100	2.30221700
H	-1.54031300	2.94354100	0.82378800
N	-0.35257600	1.19550600	1.36036900
C	4.17001400	-1.02458300	0.01986000
H	3.96778800	-1.91876900	-0.58398500
H	4.01183200	-1.28339600	1.07418500
N	3.35179300	0.11803000	-0.39856000
H	5.22425000	-0.77235100	-0.10746200
H	0.20714400	3.19474800	0.73780700
H	1.43673900	1.90989500	-0.50277300

8-NCH$_3$-5-NHCH$_3$ Oxidized Guanine Anion (11'AN)

SCF Done: E(RB3LYP) = -731.478253296 a.u.

-1 1

C	-0.09415800	0.60542400	0.02404000
C	0.12476600	-0.87135100	0.26551400
C	-2.05261100	-1.30557200	-0.02999900
C	-1.30460600	0.71214600	-0.91730600
C	2.08902100	0.14979300	-0.20061200
H	1.89106200	-1.96189200	0.36999500
N	-2.29913300	-0.20047800	-0.76327300
N	-0.81750000	-1.77295500	0.37994800
O	-1.41320000	1.66049400	-1.72566500
N	1.17185700	1.10146200	-0.45668400
N	1.44091700	-1.05636000	0.28529100
N	-3.08723300	-2.09753600	0.25848300
H	-4.01497500	-1.85547900	-0.06499400
H	-2.93941500	-2.97316800	0.74368900
N	3.38152300	0.23527000	-0.36905000
C	4.18011700	-0.94752400	-0.04735600
H	3.95717200	-1.80927500	-0.69473000
H	5.23796300	-0.71154000	-0.18891700
H	4.06263600	-1.28149600	0.99414200
N	-0.46738900	1.21058000	1.35598700
C	-0.91516600	2.61425000	1.27984200
H	-1.84168000	2.75362500	0.70743000
H	-1.08795600	2.97087500	2.29897100
H	-0.13400600	3.23410700	0.83565600
H	-1.25066900	0.66741200	1.72442500

5,8-diNCH$_3$ Sp Anion (12AN)

SCF Done: E(RB3LYP) = -731.511346788 a.u.

-1 1

C	3.47918400	-2.01350600	-0.32203300
H	4.54401500	-2.20332700	-0.17342000
H	3.21325800	-2.37314300	-1.32515500
N	3.22170100	-0.58009000	-0.16536600
C	0.19995300	1.22582500	-0.13206800
C	1.98763600	-0.22199600	-0.23214200
N	0.85149700	-0.98006200	-0.45085100
H	0.87048600	-1.93971300	-0.11888300
N	1.57043700	1.10231300	-0.12163000
C	-0.36390800	-0.19994900	-0.18708700
N	-1.42783000	-0.39877400	-1.15151500
C	-1.02315000	-0.58891700	1.17306700
O	-0.40205900	-0.59440100	2.26630900
N	-2.30236900	-0.90629600	0.95940600
C	-2.46262600	-0.76347700	-0.41727200
N	-3.69927700	-0.96990100	-0.93672300
H	-4.36165800	-1.48751200	-0.37351900
H	-3.77674300	-1.07793700	-1.94027900

C	0.23796300	3.55517400	-0.02008900
H	-0.46297200	4.39172800	-0.02456800
H	0.91694900	3.67638600	-0.87470400
N	-0.50567900	2.29410500	-0.08717600
H	0.83907300	3.62210300	0.89640400
H	2.92664000	-2.62209800	0.40676100
H	2.21775800	1.88073300	-0.10037200

5-NCH$_3$-8-NCH$_3$ Oxidized Guanine Anion (12AN')

SCF Done: E(RB3LYP) = -731.519959370 a.u.

-1 1

C	3.64891700	-1.73211000	-0.31526500
H	4.72761100	-1.84650400	-0.18856200
H	3.38558900	-2.13571100	-1.30277000
N	3.29207300	-0.31970400	-0.18234700
C	0.23031700	1.17122700	-0.13000700
C	2.03190800	-0.04547600	-0.25587700
N	0.98299000	-0.94162700	-0.48002300
H	1.09486300	-1.88234400	-0.11264900
N	1.54190500	1.26310800	-0.15394000
C	-0.28025700	-0.26867800	-0.19829200
N	-1.34691200	-0.49589600	-1.15773500
C	-0.91127800	-0.70667200	1.16154400
O	-0.28029800	-0.70668400	2.24845600
N	-2.18073300	-1.06553200	0.95351800
C	-2.36058400	-0.90754800	-0.41807200
N	-3.59530000	-1.15107800	-0.92841200
H	-4.22462200	-1.71049800	-0.36682200
H	-3.67361500	-1.25929300	-1.93210400
C	-0.18496900	3.59022500	0.03658400
H	-1.07397400	4.20907700	0.15844200
H	0.33809800	3.89365300	-0.87619700
N	-0.61031500	2.19775100	-0.04220000
H	0.48083300	3.74564100	0.89067300
H	3.15849600	-2.36340500	0.43954800
H	-1.60118000	1.98790600	-0.04292600

5-NCH$_3$, 8-NHCH$_3$ Sp Neutral (12)

SCF Done: E(RB3LYP) = -731.960852955

0 1

C	3.65538200	-1.90495000	-0.22014700
H	4.74061200	-2.00070500	-0.27419500
H	3.22836300	-2.46496900	-1.06234300
N	3.29334400	-0.48858300	-0.26863600
C	0.23272300	1.14060400	-0.11360100
C	2.04954900	-0.22706200	-0.14368700
N	0.95003300	-1.02491900	0.06505200
H	0.96061400	-1.98776100	-0.24961300
N	1.56148200	1.10517200	-0.17024600
C	-0.30783800	-0.28000400	-0.01633900
N	-1.17235100	-0.63732000	-1.11593800
C	-1.21051600	-0.47333500	1.26144600
O	-0.80442700	-0.26593600	2.42501400
N	-2.41801800	-0.87554200	0.85775800
C	-2.32058400	-0.94032800	-0.52494500
N	-3.42258700	-1.28693800	-1.22555400
H	-4.19620700	-1.70328200	-0.72673700
H	-3.32341800	-1.51153800	-2.20611300
H	3.31852300	-2.38504800	0.70765500
H	2.17694400	1.90799100	-0.26075200
N	-0.50786800	2.21591600	-0.14895900
H	-1.51445500	2.08036400	-0.11700200
C	0.01156700	3.58024500	-0.28073900
H	0.53171700	3.69682800	-1.23530500
H	-0.83307900	4.26539000	-0.24319200
H	0.69586200	3.80470500	0.54122800

5,8-diNCH$_3$-Sp Tautomer (13)

SCF Done: E(RB3LYP) = -731.969319702 a.u.

0 1

C	3.66622600	-1.78333800	-0.36428900
H	4.75089100	-1.88167000	-0.29539100
H	3.36056300	-2.17148700	-1.34472600
N	3.29964300	-0.37906300	-0.18392100
C	0.16277400	1.21093900	-0.08345100
C	2.04953800	-0.10754100	-0.23163200
N	0.95952400	-0.94383400	-0.45102600
H	1.04489800	-1.90833000	-0.14798000
N	1.53854500	1.18231000	-0.09123000
C	-0.28472400	-0.25514200	-0.16055600
N	-1.36161200	-0.51439600	-1.09363600
H	-1.43163100	-0.00916400	-1.97141800
C	-0.96684100	-0.72326600	1.16857300
O	-0.35245200	-0.79168200	2.23980400
N	-2.26730700	-1.02944100	0.94475500
C	-2.47403900	-0.83148200	-0.37286200
N	-3.66423400	-0.96689300	-0.94006000
H	-4.46340900	-1.20587900	-0.36794900
H	-3.79185100	-0.81868300	-1.93302000
C	-0.04668300	3.53168800	0.08299000
H	-0.83917500	4.28088400	0.11264500
H	0.59871300	3.75516900	-0.77665200
N	-0.64286200	2.19937600	-0.01058600
H	0.55723600	3.64064400	0.99329000
H	3.22748500	-2.43298400	0.40511500
H	2.13649900	1.99740300	-0.04506300

5,8-diNHCH$_3$-Sp (14)

SCF Done: E(RB3LYP) = -731.977115787 a.u.

0 1

C	4.28077600	-0.55410100	-0.21230500
H	5.05278100	-1.32340400	-0.20469000
H	4.32294900	-0.00110000	0.72881100
N	2.98960200	-1.21847400	-0.36624200
H	2.98034000	-2.19952100	-0.61408700
C	0.33601000	0.97621400	-0.02342300
C	1.82398200	-0.57355300	-0.32100500
N	0.63922200	-1.25251000	-0.55449100
H	0.57695300	-2.22348000	-0.26133500
N	1.69448500	0.72864000	-0.08780800
C	-0.43912800	-0.35429200	-0.19384800
N	-1.54822100	-0.30800100	-1.12778700
H	-1.50686700	0.28694500	-1.94935100
C	-1.19797700	-0.77123800	1.10081300
O	-0.61284100	-1.07680600	2.14841500
N	-2.53752500	-0.74177400	0.89048300
C	-2.69921000	-0.39867200	-0.40273600
N	-3.89036500	-0.19186600	-0.94890600

H	-4.72188500	-0.27275400	-0.37922100
H	-3.98307300	0.05410200	-1.92599000
C	0.54963900	3.27982700	0.32024400
H	-0.09419900	4.14047800	0.51393700
H	1.13901600	3.49447600	-0.58008900
N	-0.27800600	2.08604000	0.16053400
H	1.25235400	3.18398500	1.15725800
H	4.47545900	0.13521800	-1.03948200

5-NHCH$_3$-8-NCH$_3$ Sp (A14')

SCF Done: E(RB3LYP) = -731.974058335 a.u.

0 1

C	4.23293500	-0.64763500	-0.20774900
H	5.06433600	-1.35585100	-0.18515000
H	4.25786400	-0.07564000	0.72738400
N	2.98491000	-1.38784400	-0.38991900
C	0.44149000	0.88231800	-0.06004800
C	1.89300600	-0.71596600	-0.34973700
N	0.63818800	-1.33005700	-0.55122200
H	0.54397500	-2.27802200	-0.20204300
N	1.73043900	0.65978000	-0.14746600
C	-0.39768900	-0.39599600	-0.19217900
N	-1.51656400	-0.30963100	-1.11503100
H	-1.46317000	0.20097200	-1.99060700
C	-1.17447100	-0.75152200	1.12177200
O	-0.59251600	-1.02192000	2.17910800
N	-2.51106500	-0.72628200	0.90101900
C	-2.66971000	-0.40360800	-0.39982300
N	-3.85956400	-0.21485200	-0.95363200
H	-4.69358900	-0.30911600	-0.38947200
H	-3.95063800	0.00947700	-1.93622300
C	0.64213800	3.30235600	0.29321800
H	-0.05833200	4.11326500	0.49035200
H	1.20883100	3.53100600	-0.61400000
N	-0.12403500	2.07010400	0.13203500
H	1.33884400	3.21717300	1.13184900
H	4.42231300	0.05260500	-1.03081200
H	-1.13266200	2.12128100	0.20264900

8-NCH$_3$-5-OH Oxidized Guanine Neutral (15)

SCF Done: E(R3LYP) = -712.508992331 a.u.

0 1

C	-0.14999000	0.73010800	0.30475400
C	-0.02361200	-0.76678400	0.08591700
C	-2.25095700	-0.93863100	-0.13194900
C	-1.44399400	1.23326500	-0.34989700
C	2.03619300	0.15427600	-0.15349100
H	1.67828800	-1.96644600	-0.14907900
N	-2.47543200	0.35909900	-0.40170800
N	-1.02113200	-1.58439500	-0.01858800
O	-1.52878900	2.41514800	-0.72279600
N	1.09758500	1.19081800	-0.22956500
N	1.29026900	-1.04055800	-0.00128700
N	-3.30348800	-1.74653300	-0.04626400
H	-4.23813000	-1.37353900	-0.15065700
H	-3.17363200	-2.73646500	0.11729700
N	3.29775000	0.29570400	-0.26050900
C	4.13065400	-0.90659500	-0.19454300
H	3.94531000	-1.49629800	0.71138300
H	3.97190200	-1.55648800	-1.06385100
H	5.17992900	-0.60925900	-0.19120000
H	1.41127300	2.11198300	0.05987900
H	-1.04649900	0.77780900	2.09345300
O	-0.18584500	1.02184400	1.71198200

8-NCH$_3$-5-O Oxidized Guanine Anion (15AN)

SCF Done: E(R3LYP) = -712.054851148 a.u.

-1 1

C	0.16028100	0.74706900	0.37153100
C	0.02128200	-0.73813800	0.09102300
C	2.24504100	-0.93694800	-0.11691800
C	1.44201000	1.23773600	-0.30023200
C	-2.03242000	0.18467600	-0.15243600
H	-1.68430000	-1.93623600	-0.16411900
N	2.48058800	0.36522500	-0.36405200
N	1.01287300	-1.57299500	-0.01745800
O	1.56195000	2.43128200	-0.65881800
N	-1.10855600	1.22727600	-0.22000800
N	-1.28979700	-1.01157600	-0.02039400
N	3.29651100	-1.75229300	-0.04009300
H	4.23332000	-1.38380400	-0.14715100
H	3.16152200	-2.74669300	0.09081500
N	-3.30271400	0.30590800	-0.24477000
C	-4.10571900	-0.91867800	-0.17542100
H	-5.16266900	-0.64719700	-0.16830500
H	-3.93384300	-1.56823000	-1.04294200
H	-3.90099700	-1.50220800	0.73067700
O	0.27829900	0.98021000	1.73091000
H	-1.44020200	2.10733300	0.16643900

8-NCH$_3$-5-OH Oxidized Guanine Anion (15AN')

SCF Done: E(R3LYP) = -712.043634566 a.u.

-1 1

C	0.11305300	0.74888100	0.32317500
C	-0.01623700	-0.74899900	0.15742400
C	2.19441100	-0.94831800	-0.15403800
C	1.37277100	1.21561100	-0.41157500
C	-2.02285400	0.25831400	-0.07665200
H	-1.72641100	-1.91618600	-0.07034400
N	2.40175100	0.33954800	-0.50085200
N	0.97993400	-1.58417700	0.04385100
O	1.46893000	2.39228900	-0.82547300
N	-1.14486200	1.28974100	-0.04511800
N	-1.32227400	-1.00050600	0.09720800
N	3.26312000	-1.74148300	-0.08235200
H	4.18703800	-1.36247000	-0.24781300
H	3.15617500	-2.72377400	0.13617100
N	-3.30527500	0.33793700	-0.27100600
C	-4.06982500	-0.90962700	-0.30935200
H	-5.11468800	-0.67790100	-0.52950900
H	-3.72253800	-1.60357900	-1.08837300
H	-4.05379000	-1.45166200	0.64657300
O	0.43871600	0.93922400	1.74995100
H	0.47836500	1.90087300	1.89147300

8-NCH$_3$ Sp Anion (16AN)

SCF Done: E(R3LYP) = -712.087371678 a.u.
-1 1

C	-0.16370400	1.50907100	-0.09374800
C	0.32947000	0.05428300	-0.18716500
C	2.42189900	-0.51324600	-0.43077900
C	0.98465900	-0.37075800	1.16738100
C	-2.01205700	0.16358100	-0.24011700
N	2.26139400	-0.68668400	0.94133700
N	1.38460000	-0.13433700	-1.15815700
O	0.36212500	-0.39584500	2.25734300
N	-0.92051900	-0.65325100	-0.46256500
N	3.65403700	-0.71178400	-0.95729400
H	4.32662200	-1.22745700	-0.40481900
H	3.73465700	-0.78572500	-1.96355000
N	-1.51641900	1.47089800	-0.11347600
H	-0.99859200	-1.61884800	-0.15698900
N	-3.26197600	-0.11337900	-0.17517400
O	0.54432700	2.51640700	-0.00924600
C	-3.60661200	-1.52728100	-0.34210300
H	-3.08382500	-2.17179400	0.37719500
H	-4.67940000	-1.65560300	-0.18817800
H	-3.36580500	-1.88876000	-1.35033900
H	-2.11502600	2.28955100	-0.06160000

8-NCH$_3$, 5-OH Sp Anion (16AN')

SCF Done: E(R3LYP) = -712.067594694 a.u.
-1 1

C	-0.24685400	1.43808900	-0.08267500
C	0.29623800	0.02574600	-0.18598400
C	2.39119800	-0.53788600	-0.43970900
C	0.95531900	-0.41905300	1.16259400
C	-2.01940900	0.21263400	-0.24804200
N	2.23077900	-0.73493400	0.92926400
N	1.35531400	-0.14673900	-1.16103900
O	0.33563000	-0.45564000	2.25351200
N	-0.95880000	-0.66025200	-0.47103700
N	3.62534400	-0.72472800	-0.96885000
H	4.29318700	-1.25896800	-0.42810300
H	3.70265700	-0.78601800	-1.97635300
N	-1.53255900	1.53658500	-0.11484700
H	-1.06036600	-1.61903100	-0.15127600
N	-3.27570100	-0.05566400	-0.19004600
O	0.61114200	2.44128900	0.03746100
C	-3.63336700	-1.46588900	-0.34826500
H	-3.14208200	-2.10720500	0.39648300
H	-4.71211600	-1.58172100	-0.22811500
H	-3.36366100	-1.84757300	-1.34219800
H	0.13881300	3.29360100	0.09014800

8-NCH$_3$ Sp Tautomer (16)

SCF Done: E(R3LYP) = -712.495731564 a.u.
0 1

C	3.67782200	-1.49338600	-0.36265800
H	4.76454500	-1.55928100	-0.30264400
H	3.36855800	-1.87264300	-1.34474200
N	3.27006300	-0.10258400	-0.16451300
C	0.19201500	1.44210000	-0.08662400
O	-0.50613000	2.52684700	0.01265300
C	2.01879900	0.12851200	-0.23499500
N	0.92436900	-0.66804400	-0.48828000
H	0.98475300	-1.65451200	-0.25855100
N	1.49939000	1.45022100	-0.07598800
C	-0.33119900	0.03257600	-0.20486000
N	-1.39391800	-0.11586400	-1.15725500
C	-0.98209900	-0.42456600	1.17918300
O	-0.34351200	-0.44945900	2.24844600
N	-2.24542000	-0.76642200	0.93222900
C	-2.41724500	-0.55038500	-0.42711100
N	-3.61785200	-0.82604900	-0.96755400
H	-4.39876200	-1.03442900	-0.36260700
H	-3.80392400	-0.57784500	-1.92890100
H	3.25601800	-2.15575200	0.40378900
H	2.08887800	2.27624400	0.01448600
H	-1.46792200	2.35119300	-0.03768900

8-NCH$_3$ Sp (17)

SCF Done: E(R3LYP) = -712.543583366 a.u.
0 1

C	3.73284400	-1.35337900	-0.52248800
H	4.82197800	-1.40625600	-0.49194100
H	3.41176000	-1.64167800	-1.53148400
N	3.30965000	0.00392600	-0.17640800
C	0.14558400	1.47709600	0.10293500
O	-0.61855100	2.42194500	0.27457400
C	2.05241900	0.22708900	-0.19020800
N	0.98581300	-0.61033400	-0.49796800
H	1.09755000	-1.60034100	-0.30260800
N	1.49840100	1.48693500	0.09747500
C	-0.27285300	0.01113000	-0.14784700
N	-1.34102200	-0.12542800	-1.11180900
H	-1.38972500	0.47155200	-1.93224700
C	-0.97594000	-0.58757700	1.12164500
O	-0.36815100	-0.80067400	2.17521800
N	-2.28369800	-0.81540700	0.85774700
C	-2.47340200	-0.47008700	-0.43077900
N	-3.66215900	-0.49134100	-1.01312000
H	-4.47662000	-0.74546200	-0.46958500
H	-3.77683300	-0.23048700	-1.98434700
H	3.34374700	-2.10050900	0.18165500
H	2.06094200	2.31890900	0.24125700

8-NHCH$_3$ Sp (18)

SCF Done: E(R3LYP) = -712.555158014 a.u.
0 1

C	-4.32700500	0.00564100	-0.11406300
H	-5.13675900	0.58271700	-0.55898700
H	-4.31663100	0.17990900	0.96427200
N	-3.07699000	0.45457700	-0.72660100
H	-3.12024500	1.17959000	-1.43316300
C	-0.32616200	-1.07546800	0.65576400
O	0.30021100	-1.88073600	1.35422500
C	-1.87933300	0.00673600	-0.38447100
N	-0.74124500	0.49951300	-0.98211100
H	-0.73808600	1.46537000	-1.29888600
N	-1.67089300	-0.96628000	0.52299500
C	0.38103900	-0.00209300	-0.22513600
N	1.50423500	-0.50198300	-0.98291500
H	1.50238300	-1.45065100	-1.34676700
C	1.09262700	1.07047600	0.65458600

O	0.46947500	1.86475600	1.36827500
N	2.43594700	0.97519900	0.49973800
C	2.63766700	0.00529400	-0.41240400
N	3.84297100	-0.41586000	-0.76678900
H	4.66117800	-0.01815600	-0.32476300
H	3.95890200	-1.13510500	-1.46936700
H	-4.49940700	-1.05550700	-0.30821200

8-OH Guanine Radical Cation (19)

SCF Done: E(UB3LYP) = -618.892521252 a.u.

1 2

C	0.34760600	0.62362900	-0.13487900
C	0.21313900	-0.80151800	-0.16249900
C	-2.02319000	-0.69467500	0.05473500
C	-0.81687300	1.44761800	0.00113600
C	2.47380800	-0.28027000	-0.33206500
H	-2.85488600	1.19401200	0.17840500
N	-1.98298400	0.67659300	0.08399000
N	-0.92846300	-1.46771300	-0.06945200
O	-0.85017900	2.68398200	0.04335200
N	1.44457700	-1.31647000	-0.30388600
N	-3.21165100	-1.27979400	0.15610100
H	-4.06474500	-0.74316400	0.25905600
H	-3.26363100	-2.29046100	0.14246500
N	1.64728700	0.93238300	-0.25567000
H	1.66889300	-2.30384600	-0.35967300
O	3.41498400	-0.38419000	0.69755700
H	2.96021400	-0.40364000	1.55829500
H	3.04567500	-0.30227200	-1.26157200
H	2.04174100	1.86732700	-0.28040500

8-OH Guanine Radical (20)

SCF Done: E(UB3LYP) = -618.404822321 a.u.

0 2

C	0.35007800	0.62310600	-0.05243300
C	0.21823500	-0.76311600	-0.05368800
C	-2.02338100	-0.70890800	0.02743400
C	-0.79447500	1.43179300	0.01099600
C	2.42794500	-0.26740000	-0.32353600
H	-2.84859700	1.18085100	0.07059700
N	-1.97742400	0.65754900	0.04273900
N	-0.93208500	-1.46621600	-0.01477100
O	-0.87387900	2.68804400	0.03452600
N	1.47304900	-1.29727600	-0.10458200
N	-3.24729900	-1.29159300	0.00829600
H	-4.05389900	-0.74537600	0.28419400
H	-3.27894700	-2.28014500	0.22091200
N	1.72157400	0.93617600	-0.05315000
H	1.66710800	-2.27270500	-0.29720200
O	3.68742600	-0.43023300	0.24065800
H	3.62788700	-0.39700100	1.21817900
H	2.04295100	1.78855900	-0.50050700

8-OH Guanine Radical (21)

SCF Done: E(UB3LYP) = -618.435447844 a.u.

0 2

C	0.30690600	0.61323900	-0.14253100
C	0.17604500	-0.80661100	-0.17184900
C	-2.04564500	-0.60396500	0.06227300
C	-0.87685000	1.42578500	0.00491800
C	2.43971900	-0.28834800	-0.33135400
N	-2.05224500	0.74069400	0.10134100
N	-0.96910000	-1.44992900	-0.07379600
O	-0.81851300	2.68770100	0.04273100
N	1.41873700	-1.32557700	-0.32350500
N	-3.23800900	-1.22283600	0.16243000
H	-4.07796600	-0.68120100	0.30695900
H	-3.28526100	-2.23142400	0.17357400
N	1.61303600	0.92077300	-0.27350600
H	1.64950600	-2.31042200	-0.36430000
O	3.36430800	-0.38687400	0.72441600
H	2.88534500	-0.40739700	1.57144300
H	3.04343100	-0.31155700	-1.24079700
H	2.01060300	1.85290600	-0.26354200

8-OH Guanine Radical (22)

SCF Done: E(UB3LYP) = -618.438556671 a.u.

0 2

C	0.39837500	0.63221200	-0.12428500
C	0.23080200	-0.78941200	-0.12344100
C	-2.00673700	-0.69014600	0.05304600
C	-0.77392800	1.44274500	-0.00437800
C	2.44596700	-0.23039600	-0.34695000
N	-1.95181400	0.67732800	0.07643000
N	-0.91886100	-1.46481700	-0.03970600
O	-0.84491600	2.68979500	0.02584300
N	1.46393900	-1.31919300	-0.20800200
N	-3.21651000	-1.26355800	0.11685700
H	-4.05449600	-0.71517500	0.25971700
H	-3.27592800	-2.27109100	0.16985000
N	1.68349000	1.00512600	-0.23448500
H	1.66799800	-2.29230100	-0.40092400
O	3.49679300	-0.32504900	0.59354600
H	3.13286900	-0.18268100	1.48384900
H	2.94508200	-0.29445000	-1.31903100
H	-2.81912500	1.20350300	0.14982200

8-oxo Guanine (23)

SCF Done: E(RB3LYP) = -617.890026992 a.u.

0 1

C	0.39399600	0.60806100	-0.00409200
C	0.24855200	-0.77083200	-0.00172900
C	-1.98722300	-0.69904300	-0.00164200
C	-0.74455000	1.43700700	-0.00023900
C	2.46991900	-0.29179500	0.00121700
H	-2.79485300	1.20137200	0.00067900

N	-1.92676300	0.67091900	0.00050700
N	-0.90224700	-1.46695700	0.00090100
O	-0.80393200	2.68721900	0.00360600
N	1.51619900	-1.30620800	0.00166500
N	-3.21485700	-1.26550600	-0.05083800
H	-4.02754900	-0.70774600	0.18032000
H	-3.26956800	-2.25519000	0.15092900
O	3.70345400	-0.44283300	0.00314300
N	1.76446100	0.88219700	-0.00168300
H	2.19929500	1.79595700	-0.00362600
H	1.75477700	-2.29099800	0.00275100

8-OH oxidized Guanine (24)

SCF Done: E(RB3LYP) = -617.871619027 a.u.

0 1

C	0.39824700	0.62128500	-0.00275900
C	0.22859900	-0.76233500	-0.00103300
C	-2.00031600	-0.70125100	-0.00167500
C	-0.75780500	1.44072800	-0.00010700
C	2.35493400	-0.20468900	0.00078300
N	-1.93715700	0.67068900	-0.00012600
N	-0.92016400	-1.46905700	0.00193300
O	-0.83681800	2.68939200	0.00316300
N	1.50201900	-1.28107600	0.00141500
N	-3.23523600	-1.26194900	-0.05704300
H	-4.03664900	-0.70119600	0.20507800
H	-3.28987100	-2.24764600	0.16445900
N	1.75517400	0.95764800	-0.00131200
H	1.77210100	-2.25832300	0.00254300
O	3.67538800	-0.44752200	0.00223700
H	4.15763600	0.39675100	0.00209800
H	-2.80618900	1.19923900	-0.00269800

8-H_2O oxidized Guanine Cation (25)

SCF Done: E(RB3LYP) = -618.226895332 a.u.

1 1

C	-0.31660100	0.63019500	-0.13693000
C	-0.16417300	-0.84003400	-0.11906800
C	2.05798500	-0.60857800	0.06765700
C	0.93174100	1.44363800	0.00200100
C	-2.30730000	-0.21904700	-0.42064100
H	-2.87297100	-0.25100300	-1.35069200
H	-1.66065600	-2.28087600	-0.47730100
N	2.08158000	0.73582900	0.08532100
N	0.95902100	-1.47060400	-0.02321300
O	0.88010100	2.68428100	0.03045600
N	-1.53540900	1.00441000	-0.28189700
N	-1.42071900	-1.32392800	-0.23477900
N	3.22036200	-1.24231900	0.15379500
H	4.08124400	-0.71619800	0.23921700
H	3.25033500	-2.25401400	0.14844500
O	-3.38142100	-0.16016200	0.61481700
H	-4.07597300	-0.84350300	0.48286900
H	-3.05517900	-0.20812000	1.54257200

8-OH N7H oxidized Guanine Cation (26)

SCF Done: E(RB3LYP) = -618.252065906 a.u.

1 1

C	0.30692500	0.60506900	0.11071400
C	0.17693200	-0.86390800	0.09660000
C	-2.05375200	-0.60439500	-0.05502500
C	-0.92655500	1.44607600	-0.01494700
C	2.41754400	-0.30493500	0.33116300
H	2.87725100	-0.30279800	1.32381300
H	1.66977500	-2.33316700	0.25580900
N	-2.07132800	0.74754400	-0.08197600
N	-0.96554100	-1.47126900	0.01723200
O	-0.82127400	2.68113300	-0.04913300
N	1.54296100	0.91326400	0.23561400
N	1.41994400	-1.35006400	0.19375500
N	-3.22567700	-1.21651300	-0.10543300
H	-4.07909100	-0.67351300	-0.16633500
H	-3.27608400	-2.22804200	-0.08692600
H	1.92092300	1.86475000	0.27267200
O	3.35185100	-0.34377800	-0.68615900
H	4.21353400	-0.05423300	-0.34207500

8-OH oxidized Guanine (27)

SCF Done: E(RB3LYP) = -617.829850696 a.u.

0 1

C	0.36785700	0.62475300	-0.12360800
C	0.20774200	-0.84519700	-0.11593800
C	-2.01518300	-0.60710200	0.05460500
C	-0.87737300	1.44130600	0.00124500
C	2.40074500	-0.22528000	-0.34462100
N	-2.03235600	0.74374100	0.07626300
N	-0.93555400	-1.47036500	-0.03384800
O	-0.82529800	2.68630800	0.03162900
N	1.44496400	-1.33202200	-0.20597400
N	-3.19711800	-1.21655200	0.13226700
H	-4.04406300	-0.66998600	0.21627800
H	-3.25108500	-2.22636200	0.12671600
N	1.58937900	0.99806200	-0.22943300
H	1.70125000	-2.30989400	-0.28991900
O	3.45589500	-0.27613600	0.56898100
H	3.10749100	-0.22324600	1.47573500
H	2.85370300	-0.24281300	-1.33871600

8-oxoguanine Radical Neutral (27')

SCF Done: E(RB3LYP) = -617.753086017 a.u.

0 1

C	-0.26532200	0.60429300	-0.16167700
C	-0.11174400	-0.85774700	-0.12654600
C	2.14783600	-0.64973600	0.09872900
C	0.97054500	1.41786900	-0.00095400

C	-2.25150000	-0.25095800	-0.44953100
H	-2.91257200	-0.30001300	-1.31147400
H	-1.61036600	-2.28411900	-0.58631600
N	2.10912100	0.73340400	0.10785400
N	0.99508200	-1.49255700	0.00029600
O	0.89291500	2.67828200	0.01884500
N	-1.48848800	0.97264200	-0.34284000
N	-1.38714000	-1.34622300	-0.27189600
N	3.30350300	-1.23024000	0.19337500
H	3.15793700	-2.24132500	0.17396700
O	-3.22860700	-0.18022400	0.76485000
H	-3.91438600	-0.88306900	0.71584900
H	-3.69851100	0.68255600	0.77077200

8-oxoguanine Radical Neutral (28)

SCF Done: E(UB3LYP) = -617.252869287 a.u.

0 2

C	0.45936400	0.62558900	0.00001100
C	0.28771300	-0.79901100	0.00008800
C	-1.94767100	-0.69270200	0.00003200
C	-0.72423400	1.44795100	0.00003400
C	2.45234400	-0.22157500	-0.00002500
H	-2.77027800	1.20062900	0.00016900
N	-1.89611100	0.67835500	0.00021500
N	-0.85182400	-1.47392700	0.00005200
O	-0.78283500	2.68396400	-0.00006600
N	1.54616800	-1.30141200	0.00023600
N	-3.14739400	-1.26845800	-0.00045700
H	-4.00196900	-0.72461300	0.00060800
H	-3.20697200	-2.27853000	0.00029700
O	3.68212500	-0.35465500	-0.00014800
N	1.74995300	0.97772800	-0.00006600
H	1.81425900	-2.27947700	-0.00006700

8-oxoguanine Radical Neutral (29)

SCF Done: E(U3LYP) = -617.244600648 a.u.

0 2

C	0.35856100	0.59984700	0.00005700
C	0.22127700	-0.81734600	0.00000000
C	-2.00811500	-0.59712000	0.00000900
C	-0.83346800	1.42855700	0.00001600
C	2.42693800	-0.30692500	-0.00000900
N	-2.01055300	0.74484800	0.00001100
N	-0.91804000	-1.45737900	-0.00002600
O	-0.76429200	2.68194700	-0.00004400
N	1.49450100	-1.33348100	-0.00003200
N	-3.19389000	-1.21901900	0.00003200
H	-4.04868600	-0.67851100	-0.00025500
H	-3.23967500	-2.22888500	0.00011000
O	3.64768500	-0.39980000	-0.00000200
N	1.68102600	0.88195300	0.00001700
H	1.75198800	-2.31493100	-0.00002800
H	2.10675800	1.80461300	0.00009800

8-oxoguanine Oxidized Neutral (30)

SCF Done: E(R3LYP) = -616.616781166 a.u.

0 1

C	0.42536000	0.63010100	0.00010400
C	0.26702700	-0.84320000	0.00002000
C	-1.96507800	-0.59976300	-0.00004000
C	-0.82816000	1.44385700	0.00001100
C	2.41855300	-0.24242200	0.00001900
N	-1.98644100	0.73955000	-0.00004300
N	-0.85588700	-1.47015800	-0.00005300
O	-0.77756900	2.68354000	-0.00006900
N	1.53651200	-1.32391600	0.00004900
N	-3.12349700	-1.24248000	0.00008600
H	-3.99299700	-0.72211900	-0.00026600
H	-3.14600400	-2.25485600	0.00005900
O	3.62859200	-0.29982000	-0.00009400
N	1.65778400	0.99320000	0.00012400
H	1.82531300	-2.29759300	-0.00030800

5-NHCH$_3$, 8-oxoguanine Neutral (31)

SCF Done: E(R3LYP) = -712.530904635 a.u.

0 1

C	-0.31934400	0.41046700	-0.05024800
C	-0.09722100	-1.07860800	-0.23950100
C	2.10632700	-0.76844100	0.02007900
C	0.78146300	0.90768500	0.90949800
C	-2.30490000	-0.77997500	0.20603300
N	2.00648200	0.35420900	0.74632300
N	1.06360600	-1.63474600	-0.31848100
O	0.53804800	1.81597100	1.71764500
N	-1.30839500	-1.67573200	-0.24579800
N	3.31448400	-1.19567100	-0.33041300
H	4.13376100	-0.65280100	-0.08983000
H	3.42196300	-2.07682800	-0.81574000
O	-3.48909300	-1.07277000	0.33914600
N	-1.68449000	0.40276800	0.48345500
H	-1.47129200	-2.67660000	-0.30788100
H	-2.23278600	1.25226800	0.55758400
N	-0.14630900	1.08203900	-1.33844800

H	-0.82236900	0.67711400	-1.98572200
C	-0.33635200	2.54484800	-1.31290400
H	0.49865700	3.02830600	-0.80143400
H	-0.34357400	2.89286800	-2.34779500
H	-1.27349200	2.86413200	-0.83773000

5-NHCH$_3$, 8-oxoguanine Anion (31 AN)

SCF Done: E(R3LYP) = -712.034039288 a.u.

-1 1

C	0.33778200	0.42395000	0.10304500
C	0.08018000	-1.05258800	0.26845100
C	-2.12762800	-0.75154700	-0.01039200
C	-0.77168300	0.96247500	-0.79491200
C	2.27768200	-0.82995100	-0.22976800
N	-2.01829300	0.42102600	-0.64759900
N	-1.08766200	-1.61077200	0.33697200
O	-0.58436100	1.96627500	-1.51975200
N	1.27412100	-1.68668100	0.26714400
N	-3.34808500	-1.22080400	0.25796700
H	-4.16578200	-0.69029100	-0.01461600
H	-3.45998800	-2.14069300	0.66443800
O	3.46093300	-1.16647500	-0.35987500
N	1.69349400	0.35388800	-0.55064700
H	1.39931500	-2.69457600	0.31007300
H	2.28110500	1.18210900	-0.54109500
N	0.29741800	1.08439400	1.37438500
C	0.47841700	2.53143500	1.26026000
H	-0.36372500	3.07982000	0.79699400
H	0.58681400	2.94068100	2.27152600
H	1.38423400	2.83455300	0.70204600

5-NHCH$_3$, 8-oxoguanine Anion (31AN')

SCF Done: E(R3LYP) = -712.071236811 a.u.

-1 1

C	0.39111500	0.40795700	0.04164600
C	0.14662000	-1.06590600	0.28786000
C	-2.05559600	-0.79945900	-0.03306800
C	-0.70865600	0.87504900	-0.92513500
C	2.31605600	-0.68291800	-0.20268300
N	-1.93996700	0.32104000	-0.77641800
N	-1.02867200	-1.62625900	0.39358800
O	-0.49555100	1.79861900	-1.73858800
N	1.34768200	-1.63966800	0.30793900
N	-3.28388200	-1.23417000	0.24684700
H	-4.09166600	-0.71772400	-0.07768200
H	-3.41121600	-2.10617100	0.74456000
O	3.50488400	-1.06058200	-0.39084900
N	1.76233800	0.49571200	-0.42302400
H	1.52483900	-2.63828700	0.36775000
N	0.22908400	1.10544000	1.35393800
C	0.26469800	2.57784500	1.28082700
H	-0.54403700	3.01353100	0.67951900
H	0.17674100	2.96230000	2.30056900
H	1.22149000	2.91113400	0.87447700
H	-0.68231800	0.84085600	1.72953800

5-NHCH$_3$-Sp Anion (32AN)

SCF Done: E(R3LYP) = -712.093130102 a.u.

-1 1

C	0.87877900	0.77414500	-0.09330200
C	1.88667200	-1.26420200	-0.40841800
N	0.55041600	-1.46979000	-0.56176400
H	0.17264800	-2.39950800	-0.41163900
N	2.07931600	0.08335100	-0.16324300
C	-0.23153400	-0.28041500	-0.20906700
N	-1.28816900	0.03958800	-1.14409900
C	-0.98133300	-0.47361700	1.14918700
O	-0.40293900	-0.78811200	2.21882200
N	-2.28446100	-0.26014200	0.95338000
C	-2.38308300	0.03489000	-0.40426500
N	-3.60657200	0.34452600	-0.90082000
H	-4.41355500	0.06898200	-0.35587900
H	-3.71963200	0.34034400	-1.90691000
C	1.88227000	2.87457700	0.12992600
H	1.58023700	3.92269900	0.15804500
H	2.54521300	2.73231300	-0.73307500
O	2.78982500	-2.11127400	-0.49593200
N	0.68770700	2.02953500	0.04442400
H	2.46121700	2.66200500	1.03727600
H	3.00049600	0.50653100	-0.15044600

5-NHCH$_3$-Sp Anion (32AN')

SCF Done: E(R3LYP) = -712.102588649 a.u.

-1 1

C	0.89989800	0.71678800	-0.08777000
C	2.02126200	-1.10413300	-0.43232500
N	0.70851100	-1.46612700	-0.65091900
H	0.43862800	-2.42174300	-0.43913000
N	2.13968200	0.25606500	-0.17457100
C	-0.16328000	-0.37182700	-0.24699900
N	-1.24021700	-0.04003100	-1.15625700
C	-0.89272700	-0.65424000	1.10845500
O	-0.29677400	-1.02532000	2.14864900
N	-2.20002900	-0.43964700	0.94097800

C	-2.32248200	-0.08009600	-0.39818200
N	-3.55476700	0.25159600	-0.85858000
H	-4.35137300	-0.05400100	-0.31417100
H	-3.68509600	0.29169900	-1.86197400
C	1.51855400	3.07741700	0.22353500
H	0.95409100	4.00588000	0.30517400
H	2.15850700	3.12233400	-0.66203400
O	2.98193100	-1.89637100	-0.49434900
N	0.56362700	1.97779800	0.11006600
H	2.14655700	2.95937100	1.11117800
H	-0.42757100	2.18896300	0.15125300

5-NHCH$_3$-Sp Tautomer (32)

SCF Done: E(R3LYP) = -712.540279529 a.u.

0 1

C	0.85550300	0.72628300	-0.11486700
C	1.94766900	-1.24224500	-0.42098900
N	0.63044200	-1.48523300	-0.62242800
H	0.27783400	-2.43434600	-0.56356600
N	2.06097300	0.14753200	-0.15159600
C	-0.21224900	-0.34440200	-0.25356300
N	-1.28021600	-0.01691600	-1.15060000
C	-0.93417800	-0.58788600	1.14223300
O	-0.31778700	-0.92068200	2.17352200
N	-2.23883600	-0.38576200	0.96009100
C	-2.36307800	-0.05343500	-0.38177400
N	-3.59027400	0.24441400	-0.85147200
H	-4.39557300	0.04474000	-0.27585100
H	-3.72939500	0.34229700	-1.84752600
C	1.63441700	3.03492900	0.19563300
H	1.13579700	4.00117300	0.15375400
H	2.37396600	2.97436500	-0.60640500
O	2.90278600	-2.00875500	-0.47248700
N	0.61297200	1.99686600	0.02052300
H	-0.36654900	2.27146100	0.00933100
H	2.12825500	2.91834700	1.16353900
H	2.96174000	0.61167900	-0.07322700

5-NHCH3 Sp Neutral (33)

SCF Done: E(R3LYP) = -712.550508700

0 1

C	0.82743300	0.81118700	-0.05003000
C	2.04670400	-1.10173000	-0.43472600
N	0.72930300	-1.43640300	-0.62126600
H	0.45545100	-2.40406800	-0.48805700
N	2.09324900	0.25088800	-0.14115200
C	-0.15435800	-0.35934400	-0.21340000
N	-1.26716000	-0.10578500	-1.09804400
H	-1.16496200	0.47443600	-1.92479100
C	-0.92944600	-0.66643000	1.11586900
O	-0.35738100	-1.05720200	2.13840300
N	-2.25458100	-0.45070300	0.93946600
C	-2.40404000	-0.06933100	-0.34444600
N	-3.57143300	0.29066700	-0.85547500
H	-4.39071900	0.30410300	-0.26246300
H	-3.65937300	0.55746100	-1.82785800
C	1.54422600	3.01140800	0.28728100
H	1.10092000	3.99681200	0.43584500
H	2.18114600	3.05560000	-0.60513800
O	3.01955200	-1.85187200	-0.52782500
N	0.47704200	2.02052100	0.14031500
H	2.18413100	2.79181500	1.15081000
H	2.96798400	0.75758200	-0.07317200

5-NHCH3 Sp Neutral (33')

SCF Done: E(R3LYP) = -712.557448563

0 1

C	0.90531600	0.73268700	-0.08614700
C	2.09025100	-1.05195700	-0.43010900
N	0.78003000	-1.46398200	-0.63908600
H	0.54622600	-2.42888200	-0.42771800
N	2.15223400	0.31566300	-0.17670200
C	-0.11318200	-0.40745000	-0.22962400
N	-1.23867200	-0.14539800	-1.09541700
H	-1.15676700	0.36178100	-1.97079100
C	-0.87501800	-0.70195800	1.11448900
O	-0.28883300	-1.07979300	2.13298400
N	-2.20233500	-0.49203900	0.94922000
C	-2.37005900	-0.12289400	-0.33697600
N	-3.54654800	0.21715000	-0.84089500
H	-4.36316400	0.21308400	-0.24408600
H	-3.64639600	0.47044000	-1.81582800
C	1.45331400	3.09596100	0.29096500
H	0.86968800	4.01163500	0.37626100
H	2.12159400	3.17467900	-0.56984200
O	3.06710400	-1.80798000	-0.49255100
N	0.52334700	1.98189500	0.11872400
H	-0.46923400	2.17520200	0.18539800
H	2.05176400	2.96488800	1.19665200

5-OH, 8-oxoguanine Neutral (34)

SCF Done: E(R3LYP) = -693.088689197 a.u.

0 1

C	0.32955100	0.55522000	0.36062700

C	0.16664700	-0.91941500	0.01844100
C	-2.04866100	-0.60855100	-0.14798300
C	-0.79988200	1.33434900	-0.33929700
C	2.36305300	-0.39829100	-0.21171000
N	-1.99594900	0.70678500	-0.40797300
N	-0.97241900	-1.50375400	-0.12341500
O	-0.60177400	2.49763400	-0.71740400
N	1.40530400	-1.43493900	-0.13731400
N	-3.23717200	-1.17974300	0.00212900
H	-4.08016300	-0.62048700	-0.03288600
H	-3.30844900	-2.17950400	0.14103200
O	3.55926300	-0.56944500	-0.40548900
N	1.68633300	0.78375000	-0.06910600
H	1.62075800	-2.39031800	-0.40776500
O	0.11831000	0.81048000	1.74157900
H	0.71209600	0.25413100	2.27540900
H	2.18243200	1.64227700	0.14401400

5-OH, 8-oxoguanine Anion (34AN)

SCF Done: E(R3LYP) = -692.635293394

-1 1

C	-0.33328600	0.57830600	0.40510400
C	-0.17351600	-0.89713400	0.06578100
C	2.04273700	-0.62060600	-0.12837800
C	0.80132200	1.33589700	-0.28971400
C	-2.35797900	-0.38982300	-0.21090000
N	1.99960700	0.70110100	-0.37529200
N	0.96414900	-1.50323700	-0.06321900
O	0.65829500	2.52911500	-0.63366600
N	-1.40686700	-1.42307500	-0.08495200
N	3.23539100	-1.20098200	-0.02537500
H	4.08022100	-0.64667400	-0.08806300
H	3.30445900	-2.20246300	0.10492700
O	-3.56325300	-0.58566600	-0.38951700
N	-1.69662700	0.79807400	-0.13600700
H	-2.21947500	1.61708600	0.16102700
H	-1.61889700	-2.38776500	-0.32445600
O	-0.23148400	0.80365100	1.75932300

5-OH, 8-oxoguanine Anion (34AN')

SCF Done: E(R3LYP) = -692.634062226 a.u.

-1 1

C	-0.38985500	0.55642500	0.34947100
C	-0.19734000	-0.92260100	0.06856200
C	2.01215900	-0.61838700	-0.15088600
C	0.74241200	1.31909700	-0.35517300
C	-2.35303000	-0.31641400	-0.19745700
N	1.94170000	0.69783900	-0.44248400
N	0.95659000	-1.51347800	-0.05018100
O	0.57208800	2.49733000	-0.73208200
N	-1.42117000	-1.42681600	-0.07780200
N	3.22141600	-1.16376700	-0.04459000
H	4.05044000	-0.59147900	-0.14490800
H	3.31789800	-2.15862500	0.11559600
O	-3.55464300	-0.55853700	-0.47215300
N	-1.74886400	0.84955200	-0.01124500
H	-1.64059100	-2.37364500	-0.37297600
O	-0.14689200	0.71700400	1.76979800
H	-0.22594700	1.66534100	1.97479300

Spiroiminodihydantion Anion (35AN)

SCF Done: E(R3LYP) = -692.666606338

-1 1

C	0.77176800	1.15179200	0.42481400
O	0.31792400	2.11880500	1.03056900
C	2.25315700	-0.29330300	-0.55000200
O	3.34426000	-0.80059300	-0.82897500
N	1.01725200	-0.71492500	-0.92108400
H	0.88775800	-1.68425800	-1.19299200
N	2.08833900	0.86930800	0.21044000
H	2.86858800	1.43829700	0.52662100
C	-0.03815200	0.01745000	-0.22652700
N	-1.13144600	0.47983400	-1.04523200
C	-0.72985600	-0.84590000	0.88337200
O	-0.09688100	-1.46801100	1.76864400
N	-2.04961800	-0.78732900	0.69693000
C	-2.20656000	0.00329700	-0.43696800
N	-3.46492100	0.27908800	-0.85243600
H	-4.21385600	-0.30544900	-0.50448600
H	-3.58430100	0.66793100	-1.77949900

Spiroiminodihydantion Anion (35 AN')

SCF Done: E(R3LYP) = -692.646828663 a.u.

-1 1

C	0.85183100	1.11594500	0.24679100
O	0.26533800	2.16377300	0.78684700
C	2.26385700	-0.32601700	-0.51381600
O	3.35448800	-0.87467000	-0.72469000
N	1.03927700	-0.82890800	-0.85505500
H	0.92418800	-1.82877100	-0.98721700
N	2.12857600	0.94094200	0.10178500
C	-0.01187800	-0.02959800	-0.24274300
N	-1.11331600	0.34800000	-1.09680600
C	-0.70073900	-0.75886800	0.96613600

O	-0.06297400	-1.26966300	1.91559500
N	-2.02033800	-0.72907500	0.77375500
C	-2.18330900	-0.06695500	-0.43833100
N	-3.44451100	0.15605100	-0.87964900
H	-4.18466200	-0.40525800	-0.47816000
H	-3.56092800	0.43270300	-1.84666900
H	0.92020400	2.82969600	1.07359100

Spiroiminodihydantion Tautomer (35)

SCF Done: E(R3LYP) = -693.071278512

0 1

C	0.77829700	1.12661700	0.29288200
O	0.32675100	2.20548400	0.83346500
C	2.25635600	-0.36859900	-0.53815000
O	3.35375200	-0.86035900	-0.74391600
N	1.02210000	-0.77896400	-0.90442500
H	0.86977900	-1.73905600	-1.19602700
N	2.05974100	0.86887100	0.17415600
H	2.82704500	1.46161300	0.48836300
C	-0.03922600	-0.00246800	-0.26418400
N	-1.14497600	0.41285500	-1.06583700
C	-0.70880500	-0.82701100	0.94053700
O	-0.03740400	-1.36907000	1.83360300
N	-2.02369900	-0.80958900	0.73766300
C	-2.20624800	-0.07162300	-0.42126200
N	-3.45908200	0.13600300	-0.85457400
H	-4.23260200	-0.31887800	-0.39233100
H	-3.61768000	0.59500400	-1.74023500
H	-0.65215400	2.24715600	0.78718300

Spiroiminodihydantion (36)

SCF Done: E(R3LYP) = -693.121945447

0 1

C	0.75023000	1.05890700	0.62171200
O	0.22638700	1.89993600	1.33525700
C	2.31571800	-0.15764400	-0.53726700
O	3.42292000	-0.56067600	-0.87743400
N	1.09741200	-0.56679500	-1.00075700
H	1.01415500	-1.47412200	-1.44829900
N	2.08065200	0.85240900	0.40653100
H	2.82820100	1.39868100	0.82414000
C	0.01392700	-0.00592200	-0.22398400
N	-1.10817300	0.50518500	-0.96687600
H	-1.08933400	1.42949300	-1.38807400
C	-0.71678200	-1.04467600	0.70459100
O	-0.09842800	-1.81571900	1.44167200
N	-2.05550400	-0.93537600	0.54195600
C	-2.24799900	0.01701400	-0.39026100
N	-3.44664700	0.43824200	-0.75836400
H	-4.26942500	0.05011000	-0.31563300
H	-3.55537600	1.14578300	-1.47426900

5-NHCH$_3$ N7H Guanine Radical Cation (37)

SCF Done: E(UB3LYP) = -638.297456244 a.u.

1 2

C	-0.70112700	-0.08044800	0.06894300
C	0.10300900	1.18193000	0.25276400
C	2.08227900	0.14259800	0.12248600
C	0.13156800	-1.00861400	-0.82008800
C	-1.88722200	1.81588100	-0.52056500
N	1.48276100	-0.90023700	-0.57779300
N	1.41807000	1.24543800	0.44029600
O	-0.33331000	-1.78878100	-1.65139300
N	-0.72867000	2.25250700	-0.01661200
N	3.38260000	-0.00103300	0.44024000
H	3.92908800	-0.75205400	0.03828500
H	3.87794400	0.81555800	0.77468500
N	-1.89003900	0.48654700	-0.60761400
H	-0.46711200	3.23240800	0.04545500
H	-2.70105200	2.46125300	-0.81782700
N	-0.96452900	-0.75267800	1.33750600
H	-1.36309400	-0.06465100	1.97620300
C	-1.84414700	-1.93431100	1.26157300
H	-1.35268300	-2.73494200	0.70496500
H	-2.01398900	-2.29079700	2.27940100
H	-2.82097100	-1.73270900	0.80222900
H	2.08030400	-1.58613300	-1.03441200
H	-2.70946700	-0.05370300	-0.86067500

5-NHCH$_3$ N7H Guanine Radical (38)

SCF Done: E(UB3LYP) = -637.835037644

0 2

C	0.66329300	-0.09168300	-0.06353300
C	-0.11481000	1.18064400	-0.25690400
C	-2.05520500	0.09306600	-0.06173700
C	-0.19685500	-0.98213700	0.85661900
C	1.91089000	1.79827700	0.44819600
N	-1.52572700	-0.92338100	0.66990500
N	-1.43182100	1.24395000	-0.40445100
O	0.35597800	-1.72462800	1.71074900
N	0.74007000	2.24166100	-0.03278100
N	-3.36039100	-0.03572400	-0.43432400
H	-3.91328700	-0.73988300	0.03529600
H	-3.84400100	0.79952400	-0.73694700
N	1.88527900	0.46546300	0.56381100
H	0.49044300	3.22306400	-0.10284200
H	2.74321600	2.43545300	0.70622000
N	0.90385300	-0.78131300	-1.33729300
H	1.38060800	-0.12213400	-1.95205100

C	1.69790000	-2.01922200	-1.24177700
H	1.11929400	-2.79997200	-0.74291400
H	1.91729500	-2.36205900	-2.25534200
H	2.65215100	-1.89890300	-0.70990300
H	2.69634400	-0.08633000	0.81324500

5-NHCH$_3$ N1H Guanine Radical (39)

SCF Done: E(UB3LYP) = -637.836524252 a.u.

0 2

C	0.66329300	-0.09168300	-0.06353300
C	-0.11481000	1.18064400	-0.25690400
C	-2.05520500	0.09306600	-0.06173700
C	-0.19685500	-0.98213700	0.85661900
C	1.91089000	1.79827700	0.44819600
N	-1.52572700	-0.92338100	0.66990500
N	-1.43182100	1.24395000	-0.40445100
O	0.35597800	-1.72462800	1.71074900
N	0.74007000	2.24166100	-0.03278100
N	-3.36039100	-0.03572400	-0.43432400
H	-3.91328700	-0.73988300	0.03529600
H	-3.84400100	0.79952400	-0.73694700
N	1.88527900	0.46546300	0.56381100
H	0.49044300	3.22306400	-0.10284200
H	2.74321600	2.43545300	0.70622000
N	0.90385300	-0.78131300	-1.33729300
H	1.38060800	-0.12213400	-1.95205100
C	1.69790000	-2.01922200	-1.24177700
H	1.11929400	-2.79997200	-0.74291400
H	1.91729500	-2.36205900	-2.25534200
H	2.65215100	-1.89890300	-0.70990300
H	2.69634400	-0.08633000	0.81324500

5-NH$_2$CH$_3$ oxidized Guanine Cation (40)

SCF Done: E(RB3LYP) = -637.703587907 a.u.

1 1

C	-0.77756100	0.31762900	-0.08277500
C	-0.36212200	-1.11745000	0.19603100
C	1.78903500	-0.62270100	-0.19130300
C	0.28781300	0.96327800	-1.00803300
C	-2.50768700	-0.99773200	-0.32744400
H	-3.49535700	-1.39871900	-0.51950000
H	-1.58372300	-2.84221200	0.24737100
N	1.54651000	0.48819600	-0.90699200
N	0.84461700	-1.56250800	0.23026600
O	-0.03943100	1.92498300	-1.71305900
N	-2.15722900	0.22448700	-0.55202400
N	-1.51665500	-1.83064100	0.18390700
N	3.04633700	-0.95203900	0.06085000
H	3.80182800	-0.35214800	-0.24724900
H	3.25911100	-1.81101100	0.55269100
C	0.38458500	1.55636700	1.93527000
H	0.91506700	0.66280700	2.25935200
H	0.04751900	2.11828100	2.80640400
H	1.00453900	2.18797400	1.30354100
N	-0.86031100	1.16553200	1.18845700
H	-1.49389200	0.68248000	1.83937700
H	-1.34690800	2.02515600	0.90076000

5-NHCH3 oxidized Guanine Cation (41)

SCF Done: E(RB3LYP) = -637.700130771 a.u.

1 1

C	-0.72990200	0.38831200	0.02232400
C	-0.36522700	-1.07888700	0.17490200
C	1.79064900	-0.62429900	-0.22695100
C	0.30623100	1.01863000	-0.93610600
C	-2.52371500	-0.98720600	-0.30231900
H	-3.53203100	-1.32821200	-0.50230300
H	-1.64115000	-2.80465000	0.25310100
N	1.56071600	0.51473600	-0.88847100
N	0.81857000	-1.56290600	0.17258600
O	-0.03085500	1.98207100	-1.63258400
N	-2.10179100	0.23688500	-0.48759200
N	-1.54879600	-1.79590000	0.15708400
N	3.03731400	-1.01207100	-0.01359700
H	3.80972100	-0.42346700	-0.30180700
H	3.22519100	-1.90566400	0.42378600
C	0.44602000	1.50059800	1.95521700
H	1.06677100	0.63297400	2.21172700
H	0.16782400	1.99872800	2.88590400
H	1.03201400	2.20265500	1.35992600
N	-0.81170700	1.16386000	1.26621400
H	-1.40442400	0.63960800	1.91145700
H	-2.70155300	1.01632700	-0.74709300

5-NHCH3 oxidized Guanine (42)

SCF Done: E(RB3LYP) = -637.258775155 a.u.

0 1

C	-0.70418700	-0.09500500	0.01395900
C	0.01227100	1.23209600	0.17322400
C	1.98102000	0.19722800	0.02242700
C	0.19127900	-0.94686300	-0.91183700
C	-2.10612300	1.55107700	-0.39699500
N	1.52598600	-0.83478300	-0.70641000
N	1.29150400	1.37590700	0.30430100
O	-0.30885100	-1.73533000	-1.72842600
N	-0.93464700	2.18531500	0.04890800
N	3.25074200	0.18047800	0.41711100
H	3.83450100	-0.61900600	0.20895100
H	3.64558200	0.97510800	0.90267300
N	-2.04298100	0.27213300	-0.49671000
H	-0.77337200	3.18741100	0.04201600
C	-1.33896300	-2.12165300	1.29816300
H	-1.52944600	-2.41828400	2.33197700
H	-0.62173800	-2.82899000	0.87504800
N	-0.76200200	-0.76456900	1.32435000
H	-1.34420300	-0.17912900	1.92284300
H	-2.97353200	2.15743500	-0.62949400
H	-2.27896800	-2.19455200	0.73890000

5-NHCH3 oxidized Guanine (42')

SCF Done: E(RB3LYP) = -637.231345318

0 1

C	0.65246000	-0.04112600	-0.04432600
C	-0.11945900	1.24909800	0.17216600
C	-2.09309300	0.12470900	0.03938500
C	-0.22978000	-0.93803100	-0.95503100
C	1.98815200	1.65605000	-0.38323800
H	2.84025400	2.28016100	-0.62473500
H	0.62274900	3.23643400	0.05479900
N	-1.53933900	-0.86954200	-0.75069300
N	-1.39094900	1.35413000	0.26791600
O	0.33735700	-1.70444300	-1.77207200
N	1.97256400	0.36765400	-0.50736200
N	0.82383600	2.24248600	0.08278300
N	-3.30174300	-0.00359500	0.47970000
H	-3.55807300	0.84825300	0.98146700
N	0.83796000	-0.76262000	1.29381600
H	1.46209700	-0.18201700	1.86844300
C	1.40058200	-2.15494400	1.22999700
H	1.59110000	-2.46519800	2.25728300
H	0.66577700	-2.81132600	0.76886800
H	2.32825100	-2.13978700	0.66306300
H	-0.06047500	-0.80510500	1.79055000

5, 8-diNHCH$_3$ Guanine Neutral (43)

SCF Done: E(R3LYP) = -733.151728686

0 1

C	0.09464600	0.47660400	-0.10943300
C	0.21784200	-1.00111300	-0.39758100
C	2.39389400	-0.95721600	0.16089200
C	1.15140100	0.84332100	0.94277600
C	-2.03916200	-0.47762000	-0.38129800
N	2.33094800	0.17567000	0.88560000
N	1.34225100	-1.66823200	-0.38659100
O	0.95108600	1.78188700	1.73758400
N	-0.99701500	-1.47030800	-0.64930700
N	3.59373600	-1.52688500	0.01367800
H	4.40948100	-1.10507200	0.43628200
H	3.68280800	-2.40935000	-0.47094000
N	-1.28957800	0.56216600	0.34069600
H	-1.20188000	-2.44370400	-0.85003500
C	0.47388700	2.66625400	-1.26157000
H	0.59522400	3.07436200	-2.26817300
H	1.32564100	2.99649200	-0.65275600
N	0.34919100	1.20324800	-1.38430900
C	-4.23522400	-0.14263100	0.57378000
H	-4.59100800	0.25614500	-0.38830200
H	-3.96037100	0.69797000	1.21571900
N	-3.09563300	-1.06713900	0.43007200
H	-3.43599000	-1.87419700	-0.09471200
H	-5.05821400	-0.67511300	1.05453400
H	-0.44075600	3.09211600	-0.84089500
H	-2.44307800	-0.10039800	-1.33336200
H	1.21388200	0.84769700	-1.79102200
H	-1.68543100	1.48272200	0.16872800

5,8-diNHCH$_3$ guanine radical Neutral (44)

SCF Done: E(U3LYP) = -732.493378426

0 2

C	0.08638000	0.49588300	-0.13966700
C	0.17105300	-0.98195300	-0.46207000
C	2.31766800	-1.01563500	0.16338300
C	1.08768400	0.77262200	1.00455400
C	-2.06111800	-0.37858900	-0.42094500
N	2.23799300	0.06680800	0.96323000
N	1.27252500	-1.68508900	-0.43888200
O	0.85574300	1.64991600	1.85313700
N	-1.05518700	-1.40181700	-0.73922100
N	3.51900300	-1.57609600	0.00946600
H	4.32700300	-1.17714100	0.46798000
H	3.62012100	-2.42551300	-0.52928100
N	-1.31464200	0.75612500	0.11349400
H	-1.29004800	-2.36369800	-0.96540100
C	0.77321200	2.70151800	-1.15476400
H	0.94361100	3.12121900	-2.14886800
H	1.67649700	2.86078700	-0.56207800
N	0.53181900	1.25946900	-1.32964600
H	-0.15564200	1.11422000	-2.06801700
C	-4.29215300	-0.16290800	0.53050800
H	-4.71361100	-0.08318000	-0.48230800
H	-4.16732400	0.84477300	0.93215900
N	-3.01227300	-0.89304800	0.56114100
H	-3.20614100	-1.85889100	0.29734300
H	-5.00724000	-0.68963400	1.16551200
H	-0.05550600	3.24646500	-0.69024800
H	-2.56869300	-0.05883100	-1.34496200

5,8-diNHCH$_3$ Guanine Radical Neutral (45)

SCF Done: E(U3LYP) = -732.524775965

0 2

C	0.06518700	0.43948800	-0.17207400

C	0.29047400	-1.01743200	-0.41206800
C	2.45252100	-0.85947500	0.13111300
C	1.06822400	0.85242500	0.91387000
C	-1.91221100	-0.75667200	-0.05383600
N	2.28104200	0.27467700	0.86214200
N	1.46813000	-1.62705700	-0.38445900
O	0.75328600	1.73388900	1.77036000
N	-0.96449500	-1.63534500	-0.46304400
N	3.75357200	-1.27244100	-0.07594500
H	4.42595500	-0.92419600	0.59655700
H	3.86516000	-2.25220000	-0.30819900
N	-1.34069700	0.42483900	0.25953700
H	-1.12036300	-2.63551400	-0.52736000
C	0.28632600	2.68205600	-1.25161600
H	0.35119200	3.14582600	-2.23914500
H	1.14980600	3.01412600	-0.66000100
N	0.20725200	1.22107000	-1.43113900
C	-4.20558800	-0.07459800	0.50446900
H	-4.15211100	0.85210900	-0.07329000
H	-4.06861200	0.14913700	1.56692700
N	-3.20956100	-1.03278100	0.02692800
H	-3.48991300	-1.99529800	-0.11912600
H	-5.18955000	-0.51846900	0.35926600
H	-0.62462300	3.04767700	-0.76992900
H	-1.88017400	1.27519600	0.36612800
H	1.07065400	0.90501100	-1.87200200

5-NHCH$_3$-8-NCH$_3$ guanine radical Neutral (44a)

SCF Done: E(U3LYP) = -732.498789947

0 2

C	0.04652900	0.45330200	-0.11062000
C	0.21137600	-1.02314600	-0.38935300
C	2.38528500	-0.91021600	0.17082600
C	1.09241900	0.86032300	0.93793400
C	-2.05850200	-0.55425600	-0.39318900
N	2.29009400	0.22729300	0.88473000
N	1.35445000	-1.65695700	-0.36902800
O	0.86396800	1.80055500	1.72273700
N	-0.98994700	-1.52441600	-0.64238900
N	3.60100500	-1.44525700	0.02783100
H	4.40397300	-0.99567500	0.44633900
H	3.71555300	-2.32975200	-0.44762800
N	-1.33827000	0.50071500	0.34637300
H	-1.17921700	-2.50261700	-0.83264600
C	0.36964300	2.63967600	-1.28749900
H	0.47341500	3.03752800	-2.30009000
H	1.22198100	2.99129700	-0.69182200
N	0.26980100	1.17322400	-1.39133600
C	-4.19104700	-0.22746600	0.63286300
H	-4.53444700	0.28172800	-0.27993100
H	-3.85312500	0.55911100	1.32303800
N	-3.13216400	-1.16311000	0.34132400
H	-5.03062800	-0.75015600	1.09176200
H	-0.54812200	3.05367800	-0.86214500
H	-2.46734300	-0.19569700	-1.35053400
H	1.13086800	0.82589700	-1.81217800
H	-1.76366600	1.41047000	0.18562500

8-NHCH$_3$-5-NCH$_3$ Guanine Radical Neutral (44b)

SCF Done: E(U3LYP) = -732.497843524

0 2

C	-0.12538300	0.52258800	0.11777200
C	-0.31618100	-0.94474100	0.43912900
C	-2.49212100	-0.82523700	-0.10482500
C	-1.20619500	0.92753300	-0.92601500
C	1.96526800	-0.54071300	0.34395100
N	-2.38885100	0.28308100	-0.86633900
N	-1.46857200	-1.55825600	0.45777100
O	-0.96494500	1.86098900	-1.70943700
N	0.87964700	-1.46077700	0.69111800
N	-3.71215700	-1.33955600	0.05963200
H	-4.51196100	-0.89647900	-0.37189300
H	-3.83510600	-2.20378600	0.56960300
N	1.24619200	0.51942400	-0.37897900
H	1.04163000	-2.43916000	0.90702000
C	0.29162700	2.51174500	1.46241600
H	-0.13946400	3.11156400	2.26543300
H	0.31518400	3.11002600	0.53978200
N	-0.47358300	1.29668900	1.30944500
C	4.13904400	-0.36782200	-0.69350900
H	4.55158200	0.02301700	0.24885000
H	3.89413500	0.47788000	-1.34068700
N	2.94932500	-1.21704100	-0.49255300
H	3.25699200	-2.03246700	0.03958600
H	4.91166400	-0.95661700	-1.19142500
H	1.33664100	2.29153600	1.72802600
H	2.43174700	-0.15793500	1.26544800
H	1.70617000	1.41943900	-0.27842500

5,8 diNHCH$_3$-Guanine Neutral (46)

SCF Done: E(R3LYP) = -731.951822781

0 1

C	0.03726900	0.43355500	-0.11463900
C	0.26160100	-1.05368000	-0.32313300

C	2.43380300	-0.82338000	0.12685000
C	1.07165300	0.87075000	0.94462000
C	-1.89833100	-0.62280200	-0.00308000
N	2.29345200	0.28345500	0.87277200
N	1.41330200	-1.64852800	-0.33502400
O	0.80815300	1.76952600	1.76080900
N	-0.95862900	-1.60965100	-0.41077600
N	3.66561100	-1.27001300	-0.11424200
H	4.46682800	-0.76206600	0.23601900
H	3.80150800	-2.14303100	-0.60615200
N	-1.37875500	0.54597200	0.24344700
H	-1.14721500	-2.60648700	-0.46439600
C	0.22763600	2.58837400	-1.33190200
H	0.37325000	2.96989300	-2.34540600
H	0.99140600	3.04016400	-0.69439400
N	0.39674600	1.12485300	-1.37382500
H	-0.23209700	0.75691300	-2.08749100
C	-4.24595500	-0.05474400	0.45183200
H	-4.32425200	0.75245200	-0.28335600
H	-4.07517900	0.38203500	1.43984700
N	-3.18390600	-0.98963300	0.10182000
H	-3.43536300	-1.93184000	-0.16572100
H	-5.18481000	-0.60775600	0.47167900
H	-0.76010100	2.90990100	-0.97959400

5-NHCH$_3$-8-NCH$_3$ Guanine Neutral (46')

SCF Done: E(R3LYP) = -731.952607922

0 1

C	-0.02568300	0.40736200	0.08947200
C	-0.26844000	-1.07924500	0.26647500
C	-2.45589200	-0.77073400	-0.10586000
C	-1.08929400	0.92729800	-0.89657900
C	1.96825700	-0.79387800	-0.02234700
N	-2.31855700	0.37029600	-0.80189200
N	-1.44170000	-1.63160500	0.29489400
O	-0.81854100	1.85808700	-1.67363000
N	0.92713400	-1.68045600	0.34469800
N	-3.68852700	-1.20476300	0.14983300
H	-4.48880200	-0.66289600	-0.14826000
H	-3.82749800	-2.09206600	0.61460100
N	1.35550200	0.39075300	-0.40646400
H	1.07243800	-2.68082400	0.43776000
C	-0.02473300	2.52634900	1.38560400
H	-0.04873100	2.86021500	2.42505300
H	-0.83284000	3.03134200	0.85204500
N	-0.23832600	1.06749000	1.38149100
H	0.40608500	0.64458900	2.04913500
C	4.16246400	-0.14288900	-0.45056000
H	4.12486800	0.76847700	0.16087700
H	4.00378600	0.14860000	-1.49657300
N	3.19542200	-1.14822900	-0.01110800
H	5.16903700	-0.55546700	-0.36782100
H	0.93404000	2.83900900	0.95020100
H	1.89922700	1.24434700	-0.34537400

5,8-diNHCH$_3$ Guanine Anion (46AN)

SCF Done: E(R3LYP) = -731.449182317 a.u.

-1 1

C	-0.03422000	0.46153700	0.17303200
C	-0.24299600	-1.01729600	0.37452100
C	-2.41795100	-0.86549100	-0.13263200
C	-1.07850900	0.89639600	-0.85024900
C	1.90732200	-0.60741600	-0.00244500
N	-2.30155100	0.28098300	-0.81701100
N	-1.38531900	-1.64441000	0.36973800
O	-0.88834800	1.89242600	-1.58970800
N	0.97769200	-1.57069600	0.48406900
N	-3.64143300	-1.38676100	0.02224400
H	-4.44402200	-0.92241900	-0.38236600
H	-3.75467400	-2.29853200	0.44540400
N	1.38965600	0.55115600	-0.27494100
H	1.15875500	-2.57088900	0.50564900
C	-0.27706200	2.60231600	1.29905000
H	-0.40436700	3.02818500	2.30210800
H	-1.06649900	3.06453800	0.67346000
N	-0.33849400	1.14796600	1.41671900
C	4.25511000	-0.06974100	-0.46835600
H	4.34618800	0.70396800	0.30303800
H	4.07931200	0.41319700	-1.43289800
N	3.18563500	-1.01569900	-0.16667900
H	3.44696800	-1.86668200	0.31766500
H	5.19022100	-0.62778800	-0.52520700
H	0.68144300	2.99740700	0.91431900

5,8-diNCH$_3$-Sp Anion (47AN)

SCF Done: E(R3LYP) = -731.517040673 a.u.

-1 1

C	4.19486900	-0.77873000	-0.16426000
H	4.92055700	-1.59187600	-0.16302500
H	4.26689300	-0.23728000	0.78314100
N	2.86856700	-1.36474100	-0.33141600
H	2.79583000	-2.35914900	-0.50698500
C	0.35101200	1.00217900	-0.10719500

C	1.74191500	-0.65092100	-0.32941900
N	0.52330100	-1.25461000	-0.54940500
H	0.40514500	-2.20689800	-0.21407000
N	1.69458100	0.67112300	-0.15445800
C	-0.51351300	-0.27483400	-0.22139300
N	-1.61068500	-0.21252100	-1.17054500
C	-1.21457500	-0.59699400	1.12919700
O	-0.59309000	-0.79963700	2.20496300
N	-2.53646400	-0.62119600	0.93771900
C	-2.68569700	-0.38654600	-0.42718700
N	-3.95163800	-0.30810500	-0.92133500
H	-4.68073100	-0.74128400	-0.36824700
H	-4.06054900	-0.37662500	-1.92594400
C	0.77058000	3.29117600	0.15575600
H	0.20831400	4.22587100	0.21934200
H	1.44685900	3.36072600	-0.70550500
N	-0.16604200	2.17159900	0.04001600
H	1.39182900	3.21292100	1.05743000
H	4.43168500	-0.09213900	-0.98287100

5-NHCH$_3$-8-NCH$_3$ Sp Anion (47ANa)

SCF Done: E(R3LYP) = -731.517491016 a.u.

-1 1

C	4.18161300	-0.70194900	-0.16281700
H	5.00697200	-1.41776100	-0.14374900
H	4.19796300	-0.15257000	0.78665800
N	2.92863800	-1.42871900	-0.37967100
C	0.41723200	0.89035900	-0.10874700
C	1.84212100	-0.73421400	-0.36840900
N	0.58597000	-1.31726900	-0.61352700
H	0.46850700	-2.26023800	-0.25478000
N	1.71113800	0.64394300	-0.17021200
C	-0.44970600	-0.36198300	-0.24180000
N	-1.55734700	-0.23077100	-1.17339200
C	-1.14945900	-0.70335400	1.11232000
O	-0.52167300	-0.94161300	2.17497600
N	-2.47259700	-0.70074300	0.92845600
C	-2.62958800	-0.40778800	-0.42410400
N	-3.89260700	-0.37988900	-0.92656800
H	-4.64710800	-0.24536500	-0.26534200
H	-4.01955100	0.04347600	-1.83773600
C	0.64695700	3.31568900	0.23353200
H	-0.05175900	4.13062800	0.42215400
H	1.22608100	3.54134800	-0.66734600
N	-0.12461100	2.08836400	0.06712300
H	1.33385300	3.22825300	1.08040700
H	4.38978800	0.01716300	-0.96536900
H	-1.13647700	2.14299100	0.07998900

5,8-NCH$_3$ Sp anion (47'ANb)

SCF Done: E(R3LYP) = -731.510043693 a.u.

-1 1

C	4.08956300	-0.87161500	-0.15194700
H	4.89386500	-1.60943100	-0.13243300
H	4.10647400	-0.33418100	0.80564600
N	2.81680100	-1.55758700	-0.38971600
C	0.35838600	0.97997200	-0.09771700
C	1.76280200	-0.82292700	-0.37664800
N	0.47463100	-1.28020900	-0.63270700
H	0.28986000	-2.23219700	-0.33137700
N	1.66826100	0.54617800	-0.15596000
C	-0.51701200	-0.27113200	-0.24036600
N	-1.63021800	-0.13049100	-1.15963400
C	-1.20411200	-0.61766600	1.11737500
O	-0.56564000	-0.85859100	2.17366600
N	-2.52857800	-0.62026900	0.94530200
C	-2.69579700	-0.32343000	-0.40584100
N	-3.96162000	-0.30474600	-0.90141000
H	-4.71284400	-0.17522100	-0.23537500
H	-4.09533900	0.12269400	-1.80980000
C	0.92997800	3.22572500	0.19299200
H	0.43464100	4.18889500	0.32707800
H	1.56248300	3.29118900	-0.70180500
N	-0.07962000	2.17100300	0.06613000
H	1.58689200	3.05785500	1.05661000
H	4.32171100	-0.14823900	-0.94489100
H	2.47693500	1.14666000	-0.05410900

5-NHCH$_3$-8-NCH$_3$ Sp (47'a)

SCF Done: E(R3LYP) = -731.974058272 a.u.

0 1

C	4.23309300	-0.64691100	-0.20776300
H	5.06462000	-1.35497200	-0.18491100
H	4.25779000	-0.07474600	0.72727100
N	2.98521700	-1.38736000	-0.38999500
C	0.44131300	0.88221000	-0.05992100
C	1.89318300	-0.71572800	-0.34979300
N	0.63847800	-1.33009300	-0.55125300
H	0.54448200	-2.27807700	-0.20206100
N	1.73030400	0.65999100	-0.14743100
C	-0.39759300	-0.39626700	-0.19220200
N	-1.51640100	-0.30998100	-1.11518300
C	-1.17442700	-0.75196900	1.12163700
O	-0.59252600	-1.02259500	2.17894500

N	-2.51100800	-0.72649400	0.90086700
C	-2.66956900	-0.40362800	-0.39993000
N	-3.85937100	-0.21440100	-0.95368800
H	-4.69341500	-0.30848600	-0.38952400
H	-3.95040100	0.01008100	-1.93624800
C	0.64144300	3.30225400	0.29359900
H	-0.05928300	4.11328200	0.48934000
H	1.20923800	3.53027400	-0.61307700
N	-0.12451000	2.06989400	0.13216400
H	1.33714100	3.21764600	1.13313900
H	4.42248500	0.05320400	-1.03093000
H	-1.46296500	0.20122800	-1.99041100
H	-1.13309300	2.12067200	0.20373200

5,8-diNCH$_3$ Sp Neutral (47'b)

SCF Done: E(R3LYP) = -731.968207137 a.u.

0 1

C	4.18628000	-0.68477300	-0.16900200
H	5.01909800	-1.38988500	-0.15519900
H	4.17746600	-0.16460600	0.79803100
N	2.94521800	-1.41500300	-0.43024400
C	0.33893400	0.96355600	-0.04612200
C	1.85879900	-0.74074300	-0.38150700
N	0.59332700	-1.26821800	-0.64675400
H	0.46647200	-2.24429900	-0.39963300
N	1.67357100	0.61218300	-0.10064700
C	-0.44225200	-0.34459100	-0.22735000
N	-1.58388700	-0.25461800	-1.11590100
C	-1.17030500	-0.76404300	1.09387600
O	-0.55180700	-1.08552300	2.11577100
N	-2.51376000	-0.72405200	0.92317700
C	-2.71251000	-0.35773500	-0.35938000
N	-3.91823600	-0.14130500	-0.86576100
H	-4.73248500	-0.23689100	-0.27369700
H	-4.04018000	0.11585300	-1.83691500
C	0.69351700	3.24448000	0.32308100
H	0.10187100	4.15250800	0.44658300
H	1.35953100	3.38726400	-0.53794700
N	-0.20294900	2.10391200	0.13725600
H	1.31961400	3.12365800	1.21642600
H	4.39893500	0.05811100	-0.94910600
H	2.43765300	1.26725700	0.00251000
H	-1.56128100	0.32802400	-1.94668200

5-NCH3, 8-NHCH3-Sp Neutral (47')

SCF Done: E(R3LYP) = -731.962989797

0 1

C	4.17467000	-0.84991500	-0.18589900
H	4.90570900	-1.65640200	-0.19282600
H	4.26378600	-0.29795700	0.75331600
N	2.84544600	-1.45672600	-0.30485800
H	2.77485100	-2.46053600	-0.42769500
C	0.31213700	1.00628400	-0.10277700
C	1.71764100	-0.77156900	-0.28335600
N	0.48459300	-1.28010100	-0.41342500
H	0.29874600	-2.26889100	-0.28885500
N	1.64874700	0.57712500	-0.13526000
C	-0.54997300	-0.25905800	-0.17891700
N	-1.59704800	-0.23694300	-1.16666500
C	-1.30356100	-0.50884200	1.17711200
O	-0.71709500	-0.62006000	2.27770000
N	-2.61164600	-0.57102300	0.92003500
C	-2.70078200	-0.40153900	-0.45660800
N	-3.93031200	-0.45537700	-1.02471400
H	-4.73180000	-0.33361700	-0.42137600
H	-4.02596400	-0.13240700	-1.97791100
C	0.86050700	3.27830400	0.05878000
H	0.34461000	4.23795100	0.01265700
H	1.57664200	3.23877100	-0.77147300
N	-0.12441300	2.19756600	-0.00731400
H	1.42555100	3.24495300	0.99833500
H	4.37502900	-0.18144500	-1.02755200
H	2.45820200	1.18642800	-0.12281400

5,8-diNHCH$_3$-Sp Neutral (47)

SCF Done: E(R3LYP) = -731.979241407

0 1

C	4.21801600	-0.69616700	-0.16774100
H	4.97175800	-1.48262400	-0.16011800
H	4.26901800	-0.14466300	0.77318700
N	2.91206500	-1.33878800	-0.32498900
H	2.88591500	-2.33740700	-0.49379500
C	0.37276600	0.92493800	-0.11463500
C	1.76201700	-0.68444600	-0.32654200
N	0.56313500	-1.28704300	-0.53807900
H	0.43363100	-2.27312800	-0.33463800
N	1.67883900	0.66331600	-0.14765000
C	-0.49582500	-0.32375200	-0.22943800
N	-1.58126800	-0.24311300	-1.17032300
C	-1.19825900	-0.64981300	1.14395100
O	-0.56719600	-0.83192200	2.20798800
N	-2.51524100	-0.69534500	0.93223100
C	-2.65865000	-0.44487900	-0.42663100

N	-3.90690900	-0.46116000	-0.94931600
H	-4.69022100	-0.39858900	-0.31451600
H	-4.03940100	-0.10110600	-1.88444500
C	0.64603700	3.34964500	0.17357400
H	-0.04234600	4.17436700	0.35315800
H	1.22329400	3.55266700	-0.73246900
N	-0.14332600	2.12821000	0.02300700
H	1.33064100	3.26014100	1.02016800
H	4.42229100	-0.01480200	-0.99734500
H	-1.15470400	2.20482400	0.01751100

5-NHCH$_3$-8-OH Guanine Neutral (48)

SCF Done: E(R3LYP) = -713.716829346 a.u.

0 1

C	-0.25414600	0.47349900	-0.06649500
C	-0.09333300	-0.99856200	-0.38168000
C	2.10899700	-0.86743800	0.02751900
C	0.85231800	0.86006200	0.93104400
C	-2.36870700	-0.59554100	-0.11752900
N	2.04443200	0.23404900	0.79730000
N	1.05342100	-1.61699600	-0.45610800
O	0.65193300	1.75964600	1.76805600
N	-1.30645000	-1.51208600	-0.55828600
N	3.31952400	-1.36582600	-0.23489800
H	4.14407700	-0.91314300	0.13533400
H	3.41270100	-2.22855400	-0.75350600
N	-1.61638100	0.49445200	0.47702500
H	-1.49239900	-2.49328800	-0.73914900
C	-0.20128100	2.68476800	-1.20608200
H	-0.11805800	3.10568700	-2.21061300
H	0.58629300	3.12616200	-0.59200000
N	-0.01589100	1.22675000	-1.31208900
H	-0.67085000	0.87190900	-2.00814000
H	-1.17548000	2.98472500	-0.79496600
O	-3.18405300	-1.20099100	0.86294100
H	-3.96956900	-1.57174000	0.43107400
H	-2.99508400	-0.30280900	-0.96550300
H	-2.07835000	1.38868800	0.33822000

5-NHCH$_3$-8-OH Guanine Radical Neutral (49)

SCF Done: E(U3LYP) = -713.069393688 a.u.

0 2

C	0.27233500	0.45593900	0.15033900
C	0.01880100	-0.99548800	0.44938400
C	-2.16416900	-0.77763900	0.00529100
C	-0.77709600	0.86686900	-0.90186900
C	2.16061300	-0.85029600	-0.17716900
N	-1.99625700	0.32150600	-0.77965600
N	-1.18187400	-1.56364400	0.49149200
O	-0.46446700	1.68892100	-1.80916100
N	1.23752200	-1.68288300	0.32192600
N	-3.45894500	-1.13841800	0.28836000
H	-4.16645100	-0.77166700	-0.33552900
H	-3.59927100	-2.09646100	0.58461600
N	1.65857300	0.36372100	-0.38676900
H	1.37546200	-2.68013500	0.45271500
C	0.43979100	2.72722100	1.13759200
H	0.42742100	3.22094400	2.11168700
H	-0.33790500	3.18295700	0.52105200
N	0.15277700	1.29675600	1.34161400
H	0.78750300	0.92034200	2.04575800
H	1.41492600	2.92432800	0.67023200
O	3.42192500	-1.12889200	-0.43883400
H	3.63073800	-2.07174700	-0.30893800
H	2.22368400	1.15231400	-0.67782200

5-NHCH$_3$-8-OH Oxidized Guanine Radical Neutral (50)

SCF Done: E(U3LYP) = -713.055428672 a.u.

0 2

C	0.31199100	0.38957100	-0.08843200
C	0.08277800	-1.09931200	0.07691900
C	-2.13040500	-0.78045700	0.08369600
C	-0.90381200	0.95975400	-0.85439600
C	2.26980500	-0.78221900	-0.57108000
N	-2.09803000	0.39695800	-0.57027300
N	-1.07855700	-1.65517600	0.27853800
O	-0.76667900	1.92736000	-1.61985900
N	1.26003000	-1.70298100	-0.06568500
N	-3.31562700	-1.21786600	0.50798000
H	-4.14735200	-0.66469200	0.35086100
H	-3.39315900	-2.12401700	0.95002300
N	1.61283200	0.51573200	-0.70333900
H	1.38179100	-2.71050500	-0.09155500
C	0.30809300	2.47594600	1.33480100
H	0.46357200	2.74562400	2.38179100
H	-0.67429000	2.84587200	1.03359200
N	0.34363200	1.00695300	1.25627400
H	1.16908200	0.65605100	1.74130700
H	1.07568100	2.97562100	0.73434400
H	2.62454700	-1.10459600	-1.55534800
O	3.34927300	-0.74879100	0.34095900
H	4.13871800	-0.43294700	-0.12731000

5-NHCH$_3$-8-OH Guanine Neutral (51)

SCF Done: E(R3LYP) = -712.502743197 a.u.

0 1

C	-0.31842800	0.43088400	-0.06955200
C	-0.11690100	-1.06056900	-0.28532900
C	2.07657900	-0.82858800	0.04008900
C	0.76410200	0.85755800	0.94396500
C	-2.23045100	-0.61095300	0.16008200
N	1.98018200	0.27377100	0.79743100
N	1.02529500	-1.65872900	-0.35291100
O	0.53382200	1.74142500	1.78318700
N	-1.35173300	-1.60799400	-0.29496200
N	3.28712400	-1.27378700	-0.28398900
H	4.10977200	-0.75903600	0.00151900
H	3.39072000	-2.14475900	-0.78787600
N	-1.72167600	0.54990600	0.36770500
H	-1.57118800	-2.59942500	-0.32510700
C	-0.09078200	2.59358700	-1.26702200
H	-0.02416400	2.97549100	-2.28833900
H	0.77006800	2.97514500	-0.71300200
N	-0.03967900	1.12203600	-1.33785900
H	-0.75128400	0.81107000	-1.99877800
H	-1.00724000	2.98516000	-0.80922300
O	-3.49002500	-1.00496600	0.32493300
H	-4.02836200	-0.26323400	0.65453700

5-OH N7H Guanine Radical Cation (55)

SCF Done: E(UB3LYP) = -618.857401231 a.u.

1 2

C	0.75686900	0.38524100	0.34551000
C	0.32448200	-1.01689600	0.05149400
C	-1.84823500	-0.48897600	-0.05991400
C	-0.23296700	1.34269800	-0.30452700
C	2.47767700	-0.87917700	-0.48327400
N	-1.51311800	0.83604100	-0.32096300
N	-0.93004200	-1.44775600	0.01684900
O	0.05128900	2.46235800	-0.72994000
N	1.45090100	-1.72145800	-0.32279200
N	-3.15164600	-0.77392700	0.06934800
H	-3.86223000	-0.06728000	-0.07039100
H	-3.43417200	-1.74297100	0.13544300
N	2.09883300	0.37212900	-0.21008900
H	1.47862600	-2.70873300	-0.56313400
H	3.46551300	-1.17364700	-0.80567600
H	-2.24937900	1.47755100	-0.60940800
H	2.72403000	1.17084300	-0.21109000
O	0.75064000	0.60974100	1.76292500
H	0.91073200	1.55491000	1.93817700

5-OH Guanine Radical (56)

SCF Done: E(UB3LYP) = -618.398040924 a.u.

0 2

C	0.71415800	0.38755700	0.32678800
C	0.29551100	-1.01676300	0.04956800
C	-1.84891900	-0.40426900	-0.08462600
C	-0.30049900	1.32845400	-0.32653700
C	2.46180200	-0.88409400	-0.45201400
N	-1.57210400	0.89717500	-0.36440400
N	-0.96061500	-1.42798100	-0.02000600
O	0.07499800	2.45635700	-0.74324900
N	1.42884900	-1.72590800	-0.29462800
N	-3.15642100	-0.72060600	0.09236200
H	-3.85508500	-0.03702900	-0.16366600
H	-3.42387300	-1.69532200	0.09267900
N	2.06459200	0.37327100	-0.20899700
H	1.46177600	-2.71504300	-0.52147200
H	3.45630100	-1.18149700	-0.74717100
H	2.68159200	1.17637300	-0.22000000
O	0.71735800	0.62285700	1.76013400
H	0.77802100	1.58183700	1.91519500

5-OH Guanine Radical (57)

SCF Done: E(UB3LYP) = -618.402504741 a.u.

0 2

C	0.80743400	0.38137800	0.31432400
C	0.35200700	-1.01041400	0.02447200
C	-1.82078700	-0.48827000	-0.05732900
C	-0.19338500	1.33729900	-0.30098300
C	2.49132300	-0.78020100	-0.48601200
N	-1.48082600	0.83365400	-0.30086700
N	-0.90529100	-1.44751800	0.00131700
O	0.05737300	2.47206100	-0.73891300
N	1.48194700	-1.70433100	-0.33851500
N	-3.14006200	-0.76769300	0.12611200
H	-3.82573200	-0.10250300	-0.21149000
H	-3.39964200	-1.74278700	0.04082100
N	2.17630100	0.44846600	-0.18344100
H	1.50661200	-2.65690000	-0.68364900
H	3.46376900	-1.09465000	-0.84333700
O	0.77130600	0.58473400	1.76650700
H	1.09849800	1.48344700	1.94756600
H	-2.21697400	1.48223400	-0.56973700

5-H$_2$O oxidized Guanine Cation (58)

SCF Done: E(RB3LYP) = -618.213821116 a.u.

1 1

C	-0.75384200	0.39046300	0.17434900
C	-0.31100400	-1.05019500	-0.00799100
C	1.83641000	-0.39911400	-0.08241200
C	0.32348200	1.35171800	-0.37218900
C	-2.44985200	-0.78110400	-0.48116300
H	-3.43333100	-1.09758600	-0.80609900

H	-1.52125200	-2.70878900	-0.53053000
N	1.59275000	0.88898700	-0.36628300
N	0.90541300	-1.45213900	-0.05822100
O	-0.00519700	2.49220800	-0.71424100
N	-2.10736700	0.45566100	-0.28821800
N	-1.45901900	-1.72913800	-0.26821700
N	3.08862400	-0.78404700	0.09727600
H	3.83739400	-0.10262900	0.06370200
H	3.30564500	-1.76106900	0.25423300
O	-0.85792200	0.61964300	1.68293800
H	-1.28243100	1.48531800	1.88361600
H	-0.01504100	0.56407800	2.18756900

5-HO oxidized Guanine Cation (59)

SCF Done: E(RB3LYP) = -618.256309567

1 1

C	-0.69151700	0.39603100	0.33665100
C	-0.29693800	-1.02691600	-0.00231900
C	1.84838900	-0.38210500	-0.10229100
C	0.31949400	1.34532300	-0.34695700
C	-2.46604100	-0.81936000	-0.40917300
H	-3.46952500	-1.09561100	-0.70901400
H	-1.52900500	-2.68925300	-0.55788500
N	1.59806000	0.90317700	-0.36750900
N	0.90489700	-1.43580600	-0.12963600
O	-0.05027900	2.46289600	-0.71870100
N	-2.07732400	0.40259100	-0.14736300
N	-1.46284700	-1.71135600	-0.28269400
N	3.09255500	-0.78052700	0.09295000
H	3.84531100	-0.10242100	0.10246700
H	3.30151000	-1.76371300	0.22013600
O	-0.62883500	0.56253700	1.73290200
H	-2.69219800	1.21283400	-0.13454300
H	-0.69088300	1.51031100	1.94954200

5-OH oxidized Guanine (60)

SCF Done: E(RB3LYP) = -617.816766599 a.u.

0 1

C	0.74842800	0.39270500	0.30144600
C	0.33479900	-1.02850300	-0.02692800
C	-1.80753900	-0.39788500	-0.09395500
C	-0.28247700	1.33912100	-0.34590200
C	2.49544700	-0.72036400	-0.40001100
N	-1.56263900	0.89452100	-0.36078200
N	-0.88312200	-1.44632800	-0.10808500
O	0.05008900	2.47912600	-0.70465800
N	1.48132200	-1.68495100	-0.30886400
N	-3.06660100	-0.77550600	0.09523700
H	-3.80792300	-0.08698800	0.08422700
H	-3.29030000	-1.75210600	0.23708400
N	2.14902400	0.48554800	-0.11575000
H	1.55101600	-2.64017400	-0.64548400
H	3.48862200	-1.02917900	-0.70299600
O	0.63311700	0.54731800	1.71393800
H	0.83510200	1.47345700	1.93273100

5-H_2O oxidized Guanine neutral (60')

SCF Done: E(RB3LYP) = -617.744059287 a.u.

0 1

C	-0.68859500	0.39564800	0.18633100
C	-0.29705000	-1.04163900	-0.07178000
C	1.90470700	-0.46204300	-0.09322600
C	0.39271600	1.33159500	-0.39391400
C	-2.45422300	-0.70317400	-0.41601800
H	-3.46537200	-0.96922200	-0.69864000
H	-1.59594300	-2.64293600	-0.62241400
N	1.62989400	0.85702900	-0.40758000
N	0.89732300	-1.48088500	-0.17349300
O	0.04629700	2.48674000	-0.74706600
N	-2.06763100	0.51573200	-0.16445500
N	-1.48961900	-1.68092900	-0.31891900
N	3.11748500	-0.81668200	0.17625300
H	3.13776700	-1.82851500	0.31613800
O	-0.54196000	0.62674600	1.71662900
H	-0.70021200	1.56901900	1.95401000
H	-1.16841800	0.08159100	2.24340000

5-OH-8-$NHCH_3$ Guanine Neutral (61)

SCF Done: E(R3LYP) = -713.718581875 a.u.

0 1

C	-0.11511800	0.57749000	0.40460000
C	-0.26592200	-0.91132900	0.18631500
C	-2.45042800	-0.63749600	-0.25577500
C	-1.21244200	1.32637600	-0.36151700
C	2.01074000	-0.43758700	0.30042900
N	-2.38340600	0.67940000	-0.54064800
N	-1.40792700	-1.51152100	-0.02011400
O	-1.02710300	2.51181200	-0.70202700
N	0.94415300	-1.44853300	0.24977100
N	-3.65990800	-1.20058200	-0.27881800
H	-4.47489900	-0.63770000	-0.48145900
H	-3.76467900	-2.19080500	-0.10412600
N	1.24442800	0.79452000	-0.01132500
O	-0.36093500	0.78918200	1.81277400
H	-0.41577600	1.74705600	1.96846000
N	3.06535500	-0.76586200	-0.61829300
H	2.71296200	-0.62599100	-1.56519100
C	4.26751500	0.06319900	-0.42274600
H	5.02140800	-0.22633500	-1.15736100
H	4.08299100	1.14097900	-0.52983100
H	4.67714900	-0.11949200	0.57458100
H	1.14234100	-2.43394500	0.11395200
H	2.44417900	-0.39873500	1.30505500
H	1.65369600	1.62114500	0.41808000

5-OH-8-NHCH$_3$ Guanine Radical Neutral (62)

SCF Done: E(U3LYP) = -713.055396092

0 2

C	-0.10552400	0.56730800	0.48537400
C	-0.25276900	-0.91637500	0.23334100
C	-2.40621200	-0.61845300	-0.30595900
C	-1.12728500	1.32631800	-0.38284500
C	2.01002400	-0.41824100	0.36020600
N	-2.29736400	0.69295600	-0.60511600
N	-1.38685900	-1.50793700	-0.03349000
O	-0.89889900	2.49498300	-0.74419100
N	0.95612700	-1.45021400	0.31832700
N	-3.62578400	-1.15363900	-0.36526000
H	-4.42047300	-0.57381900	-0.59947600
H	-3.75978300	-2.13942200	-0.18435200
N	1.30538900	0.85877400	0.32612100
H	1.16659200	-2.42432200	0.12561500
C	4.25540000	-0.00872800	-0.53080500
H	4.72084400	-0.48032100	0.33916100
H	4.24702700	1.07749200	-0.37472800
N	2.92510200	-0.59256100	-0.74186100
H	2.50571300	-0.23343800	-1.59900800
H	4.87084100	-0.22267600	-1.40723700
O	-0.44920700	0.78283700	1.86172600
H	-0.50353500	1.74135000	2.02040600
H	2.57953900	-0.49002400	1.29242200

5-OH-8-NHCH$_3$ Guanine Radical Neutral (63)

SCF Done: E(U3LYP) = -713.089781225 a.u.

0 2

C	-0.21011600	0.73401100	0.38769500
C	-0.10047000	-0.74096000	0.26102200
C	-2.28933300	-0.95259000	-0.14274900
C	-1.41018900	1.19413000	-0.43513900
C	1.95657700	0.09179400	-0.06667800
N	-2.44731000	0.34525600	-0.51720300
N	-1.11850600	-1.57540000	0.11470300
O	-1.40503800	2.35010800	-0.95500500
N	1.25607000	-1.05030500	0.11749000
N	-3.43287400	-1.70738100	-0.04130000
H	-4.24342600	-1.35714400	-0.53546700
H	-3.30881000	-2.71175500	-0.06868000
N	1.10806700	1.15056100	-0.07220300
H	1.63433600	-1.98222400	-0.00839900
O	-0.41280300	1.10070700	1.78508800
H	-0.67281500	2.03782000	1.81959100
H	1.44022900	2.10262300	0.03213500
N	3.27213000	0.16215200	-0.22489700
H	3.67241500	1.08057300	-0.37359000
C	4.13227600	-1.01548800	-0.34295100
H	5.16357600	-0.67013400	-0.39241000
H	4.01957500	-1.66136900	0.53201600
H	3.90215600	-1.58445600	-1.24919800

5-OH-8-NHCH$_3$ Guanine Neutral (64)

SCF Done: E(R3LYP) = -712.513021707

0 1

C	-0.02895500	0.51948100	0.40259500
C	-0.27658900	-0.94720800	0.10534400
C	-2.45221600	-0.54329700	-0.21368500
C	-1.09414000	1.34083500	-0.34588900
C	1.88221700	-0.44678000	-0.05585700
N	-2.31587200	0.76535300	-0.47752300
N	-1.43607200	-1.48977600	-0.07840700
O	-0.85743800	2.50812200	-0.70052500
N	0.94125800	-1.50885300	0.00571200
N	-3.68278800	-1.04872500	-0.17441000
H	-4.48217800	-0.44570600	-0.31883500
H	-3.82199300	-2.04136100	-0.03889000
N	1.36415600	0.74418800	0.10065200
H	1.12807400	-2.46700300	-0.27611500
N	3.16072800	-0.75136100	-0.29232200
H	3.41538200	-1.72936400	-0.33985700
O	-0.31183700	0.68792800	1.80665300
H	-0.12502700	1.61570900	2.02851400
C	4.22247100	0.24919400	-0.31240800
H	4.36601400	0.69747400	0.67576200
H	5.14400400	-0.24718400	-0.61532300
H	3.99332800	1.03989900	-1.03078700

5-OH-8-NCH$_3$ Guanine Neutral (64')

SCF Done: E(R3LYP) = -712.509910521

0 1

C	-0.15450600	0.72385100	0.30865400
C	-0.01827900	-0.76702600	0.08127800
C	-2.24552100	-0.94252100	-0.13271500
C	-1.44040300	1.22283600	-0.36587200
C	2.04238400	0.16272600	-0.14233900
N	-2.47217900	0.35024600	-0.41580500
N	-1.01253700	-1.58490300	-0.03333000
O	-1.52192100	2.40540500	-0.73953600

N	1.29629200	-1.03524300	-0.00991800
N	-3.29515600	-1.75151100	-0.02215800
H	-4.23214400	-1.38083000	-0.11238000
H	-3.16077400	-2.73929200	0.15022500
N	1.10459500	1.19731500	-0.20668500
O	-0.30892100	0.90244000	1.72233900
H	-0.55571500	1.82828500	1.88960400
N	3.30523100	0.30215600	-0.24167600
C	4.13420100	-0.90362900	-0.18945700
H	5.18447700	-0.60980900	-0.18465600
H	3.94829300	-1.50143300	0.71103000
H	3.97258800	-1.54510400	-1.06461700
H	1.68260700	-1.95715200	-0.18473200
H	1.41641500	2.11873900	0.08280400

5-O-8-NHCH$_3$ Oxidized Guanine Anion (64AN)

SCF Done: E(R3LYP) = -712.053511377

-1 1

C	-0.04516200	0.54175700	0.48460900
C	-0.27233800	-0.92104800	0.14132500
C	-2.44750600	-0.54645400	-0.21026400
C	-1.09454700	1.34656600	-0.28747300
C	1.87841400	-0.41965900	-0.05034300
N	-2.31634300	0.77111800	-0.45605300
N	-1.43340400	-1.48172300	-0.04626700
O	-0.88066900	2.53250100	-0.62815100
N	0.94026600	-1.48535500	0.03960300
N	-3.68041400	-1.05571100	-0.21570400
H	-4.47488500	-0.45357200	-0.39126600
H	-3.81926700	-2.05221500	-0.10714800
N	1.37061900	0.76651200	0.12328800
H	1.13106300	-2.44173700	-0.24704900
N	3.15026400	-0.74329300	-0.34301500
H	3.39964600	-1.72263700	-0.27626800
O	-0.30266400	0.76318300	1.83795900
C	4.22769100	0.24002900	-0.31486100
H	4.37945900	0.64702100	0.69133400
H	5.14318700	-0.25470800	-0.64018500
H	4.01124400	1.06439800	-0.99880100

5-O-8-NCH$_3$ Oxidized Guanine Anion (64'aAN)

SCF Done: E(R3LYP) = -712.054851182

-1 1

C	-0.16028400	0.74706200	0.37155300
C	-0.02129400	-0.73814600	0.09104400
C	-2.24505100	-0.93693500	-0.11693100
C	-1.44199200	1.23773700	-0.30024000
C	2.03241700	0.18465400	-0.15241100
N	-2.48057800	0.36524000	-0.36407000
N	-1.01289300	-1.57299400	-0.01745900
O	-1.56191100	2.43128200	-0.65883900
N	1.28977700	-1.01159800	-0.02035800
N	-3.29653800	-1.75226500	-0.04014100
H	-4.23334700	-1.38374500	-0.14709400
H	-3.16158000	-2.74664900	0.09093200
N	1.10855700	1.22725200	-0.21998200
O	-0.27831400	0.98019700	1.73092500
N	3.30269800	0.30589900	-0.24475800
C	4.10576200	-0.91865100	-0.17546400
H	5.16269700	-0.64711500	-0.16784700
H	3.90073800	-1.50251300	0.73034900
H	3.93428900	-1.56793100	-1.04326800
H	1.68426300	-1.93626500	-0.16409800
H	1.44022500	2.10731900	0.16642200

5-OH-8-NCH$_3$ Oxidized Guanine Anion (64'bAN)

SCF Done: E(R3LYP) = -712.043629635

-1 1

C	-0.11285500	0.74807600	0.32160700
C	0.01592100	-0.74954400	0.15348000
C	-2.19540800	-0.94763200	-0.15378300
C	-1.37362400	1.21639300	-0.41017000
C	2.02297200	0.25783300	-0.07795500
N	-2.40305900	0.34077000	-0.49852900
N	-0.98068600	-1.58427400	0.04019400
O	-1.47012300	2.39357200	-0.82262300
N	1.32182800	-1.00127300	0.09227200
N	-3.26427600	-1.74037200	-0.08004300
H	-4.18852300	-1.36068100	-0.24211800
H	-3.15719500	-2.72284400	0.13762300
N	1.14471800	1.28921500	-0.04707200
O	-0.43637500	0.93536500	1.74957100
H	-0.47261000	1.89670400	1.89398200
N	3.30586800	0.33834800	-0.26796100
C	4.07202900	-0.90807100	-0.30650800
H	5.12413400	-0.67147200	-0.48273200
H	4.02133700	-1.47292800	0.63480900
H	3.75420300	-1.58225100	-1.11487000
H	1.72567500	-1.91724800	-0.07432800

5-OH-8-NHCH$_3$-Sp Neutral (65)

SCF Done: E(R3LYP) = -712.519420460

0 1

C	4.28089700	-0.11679300	-0.15947400
H	4.50407300	0.78652400	-0.73203400
H	5.06957300	-0.84922700	-0.32573300
N	3.02068500	-0.72008900	-0.60365900
H	3.06313900	-1.59273300	-1.11932000
C	0.37403200	1.16756600	0.32583700
O	-0.16545900	2.23181400	0.87309700
C	1.83427300	-0.18096700	-0.41693000
N	0.67371200	-0.71074500	-0.86100100
H	0.59098900	-1.69652500	-1.09006400
N	1.66694100	1.02145900	0.24366900
C	-0.43298300	0.01955100	-0.24010600
N	-1.53237300	0.40278300	-1.07504400
C	-1.10221000	-0.83354400	0.92273700
O	-0.44401100	-1.36734800	1.83668900
N	-2.41567900	-0.85733600	0.69671400
C	-2.59180300	-0.11623200	-0.46254400
N	-3.84704000	0.07115000	-0.91440700
H	-4.59924800	-0.46809500	-0.51095000
H	-3.98764300	0.48252800	-1.82634500
H	4.23722700	0.12493400	0.90333800
H	-1.13929500	2.20882600	0.80179000

5,8-diOH Guanine Neutral (67)

SCF Done: E(R3LYP) = -694.278042245

0 1

C	0.26351500	0.60414700	0.36474000
C	0.14274300	-0.89096200	0.17422300
C	-2.06523700	-0.68105500	-0.17923300
C	-0.88270100	1.30968400	-0.37309000
C	2.39999900	-0.34513400	0.12551100
N	-2.04350100	0.62972200	-0.49351600
N	-0.98802700	-1.52310000	0.02797300
O	-0.74242700	2.49211000	-0.74033500
N	1.37127100	-1.39318000	0.18891900
N	-3.25618100	-1.27995700	-0.14040700
H	-4.09825700	-0.74740900	-0.31189400
H	-3.32189900	-2.26966600	0.05541200
N	1.60393600	0.85202800	-0.10415100
H	1.59579800	-2.36965500	0.02679800
O	0.07120300	0.84229800	1.77211000
H	-0.01215700	1.80137200	1.90902200
O	3.26964900	-0.55794100	-0.96128400
H	4.08621200	-0.96388700	-0.63189300
H	2.02081600	1.68151800	0.31145400
H	2.97968100	-0.32268600	1.05254400

5-8-diOH guanine Radical Neutral (68)

SCF Done: E(U3LYP) = -693.632216958

0 2

C	0.28269400	0.57542400	0.41028200
C	0.11065500	-0.88988000	0.21403400
C	-2.08379100	-0.65523800	-0.14209900
C	-0.81487800	1.29298800	-0.37507900
C	2.25222000	-0.43078400	-0.20342500
N	-1.99514800	0.66159300	-0.47263000
N	-1.05123300	-1.50578900	0.05403600
O	-0.58677000	2.44256100	-0.84844700
N	1.37763700	-1.43282700	-0.03416100
N	-3.34462400	-1.17279200	-0.03280000
H	-4.09486600	-0.64145900	-0.45432400
H	-3.43557700	-2.17999700	-0.06234100
N	1.65345700	0.75581500	-0.06094400
H	1.58401600	-2.40972100	-0.22086300
O	0.17091200	0.91530700	1.81428600
H	0.05307800	1.87867600	1.88872500
O	3.53525000	-0.52514100	-0.47457500
H	3.82323400	-1.44461900	-0.62406400
H	2.15295300	1.63824200	-0.05402700

5-8-diOH Guanine Radical Neutral (69)

SCF Done: E(U3LYP) = -693.611350170

0 2

C	0.28651300	0.59190000	0.38310900
C	0.15050000	-0.89745400	0.15990900
C	-2.04966800	-0.65354100	-0.18281100
C	-0.83323800	1.32171600	-0.38002900
C	2.39681100	-0.35330700	0.13502200
N	-2.00243300	0.65799400	-0.49402500
N	-0.98467200	-1.51610600	0.00332900
O	-0.66736600	2.49554000	-0.75431600
N	1.37832900	-1.40276400	0.13742900
N	-3.25104000	-1.22654000	-0.13289400
H	-4.08361400	-0.67582400	-0.29483300
H	-3.33586400	-2.21622500	0.05677900
N	1.66352200	0.90721800	0.04356700
H	1.60405100	-2.37884000	-0.02837600
O	0.10507400	0.82011900	1.78343600
H	0.00131300	1.77641800	1.93330900
O	3.23236400	-0.54540300	-0.97755700
H	4.13965500	-0.30452100	-0.73337000
H	2.98243200	-0.35755900	1.06095200

5-8-diOH Guanine Neutral (70)

SCF Done: E(R3LYP) = -693.058891811

0 1

C	0.32326500	0.56882400	0.37254000
C	0.15797400	-0.91038300	0.07341400
C	-2.04601800	-0.62881300	-0.15957700
C	-0.79730700	1.31889700	-0.37482400
C	2.25942000	-0.27095100	-0.15510500
N	-1.99080300	0.67751600	-0.45474000
N	-0.96667400	-1.51768900	-0.07982200
O	-0.62481900	2.48346000	-0.76531400
N	1.41185500	-1.39353900	-0.08022300
N	-3.23682400	-1.20334300	-0.03131200
H	-4.08106500	-0.65117800	-0.11182000
H	-3.30704100	-2.19936500	0.13177100
N	1.70406200	0.87537200	0.03932600
H	1.65216000	-2.33155700	-0.39034700
O	0.07246300	0.72581800	1.77155800
H	0.11923300	1.67396400	1.98106400
O	3.54950400	-0.41889000	-0.42455800
H	3.80420800	-1.34864800	-0.55544900

4-NHCH$_3$ N3H Guanine Radical Cation (71)

SCF Done: E(UB3LYP) = -638.302227108 a.u.

1 2

C	0.31997300	1.13106800	0.14151000
C	0.76307000	-0.30524800	-0.05387500
C	-1.59225800	-0.78491400	-0.43488000
C	-1.04198300	1.43324000	0.45861600
C	2.19944800	1.26059900	-0.85341800
N	-1.90870500	0.32984500	0.28142600
N	-0.31631400	-0.99735800	-0.79220300
O	-1.50126700	2.52313500	0.82485400
N	1.93185600	-0.06020700	-0.89488000
N	-2.55527100	-1.62833800	-0.77789100
H	-3.52805700	-1.39807900	-0.61178900
H	-2.33650900	-2.48558300	-1.27182500
N	1.25929900	2.01118100	-0.28212500
H	2.64967300	-0.75898800	-1.06026300
H	3.10568200	1.66152500	-1.28819700
N	1.14894100	-0.93790500	1.19320600
H	0.37414100	-0.83407100	1.84760500
C	1.51034200	-2.36580300	1.09876500
H	1.80157700	-2.70451300	2.09463700
H	0.69156600	-3.00385100	0.74361100
H	2.37157200	-2.49641600	0.43898000
H	-0.10293500	-1.88611100	-1.23883700
H	-2.88677900	0.48682900	0.51422100

4-NHCH3-gua-mN3H-rad-smd (A24)

4-NHCH3 Guanine Radical (72)

SCF Done: E(UB3LYP) = -637.844803826 a.u.

0 2

C	0.20016300	1.12277000	0.11839000
C	0.73623400	-0.27619900	-0.09333700
C	-1.45726500	-0.94372100	-0.44675400
C	-1.17328500	1.29833600	0.48529300
C	2.04501600	1.41218700	-0.90603800
N	-1.91246700	0.12715300	0.33298900
N	-0.21520500	-1.13852200	-0.77249900
O	-1.71495000	2.35227800	0.88229100
N	1.88613800	0.07847900	-0.94076700
N	-2.43802100	-1.82411800	-0.81139200
H	-3.37392200	-1.45841800	-0.94208300
H	-2.15595200	-2.52873300	-1.48130700
N	1.05227300	2.08537800	-0.32059700
H	2.63628000	-0.56460300	-1.16575900
H	2.90242600	1.89086900	-1.36148000
N	1.23468800	-0.82631500	1.18403000
H	0.43268900	-0.86188800	1.81297800
C	1.81247100	-2.18080400	1.09829300
H	2.08551100	-2.49577700	2.10829300
H	1.13289000	-2.92981400	0.67577800
H	2.72975200	-2.16595600	0.50245300
H	-2.90192400	0.18629900	0.55536000

4-NHCH3 Guanine Radical (73)

SCF Done: E(UB3LYP) = -637.845666570 a.u.

0 2

C	0.30299300	1.11298400	0.13738600
C	0.72046700	-0.32333900	-0.08359200
C	-1.64294000	-0.68078700	-0.40657200
C	-1.07778600	1.42504600	0.43543900
C	2.21876700	1.22432800	-0.80073400
N	-2.00754500	0.43535800	0.22543300
N	-0.36769700	-0.96653400	-0.82498600
O	-1.43074100	2.56375300	0.84626100
N	1.91394600	-0.09470800	-0.89740400
N	-2.59248000	-1.59329900	-0.68157500
H	-3.56108600	-1.33573900	-0.55069500
H	-2.37870300	-2.42640100	-1.21353100
N	1.28268900	1.97976200	-0.23867100
H	2.63635400	-0.79795800	-1.00969100
H	3.14972200	1.61161400	-1.19383700
N	1.08380000	-0.97797300	1.17553900
H	0.28180800	-0.88704500	1.79881000
C	1.43081300	-2.40741600	1.06456400
H	1.65653100	-2.78048500	2.06553800
H	0.63053700	-3.02947500	0.64259200
H	2.32923400	-2.53301300	0.45465400
H	-0.20134200	-1.91465400	-1.15122000

4-NH2CH3 Oxidized Guanine Cation (74)

SCF Done: E(RB3LYP) = -637.663022525 a.u.

1 1

C	0.06884900	1.12424000	0.05415800
C	-0.72638000	-0.14925000	-0.11235100
C	1.37540000	-1.05811800	-0.46737800
C	1.45746200	1.00405900	0.59839900
C	-1.63334400	1.66325200	-1.11594300
H	-2.31297000	2.28852300	-1.68207600
H	-2.63028000	-0.13926500	-1.27638900
N	2.07820400	-0.13323900	0.27144400
N	0.05611100	-1.11768700	-0.74484700
O	1.94173800	1.93595200	1.27498600
N	-0.45643500	2.14481100	-0.55989200
N	-1.82633900	0.38926800	-0.93719600
N	2.12598800	-2.05236800	-0.96078300
H	3.11660500	-2.07646800	-0.76368800
H	1.70093500	-2.81070200	-1.47656700
N	-1.35566200	-0.64207600	1.21019200
H	-1.89296400	0.12336000	1.63977800
C	-2.21759800	-1.86770500	1.09593600
H	-1.64304300	-2.65432200	0.61267700
H	-2.48779100	-2.16275500	2.10919600
H	-3.11298600	-1.62368500	0.52645100
H	-0.57082200	-0.85212500	1.84138200

4-NHCH3 N3H Oxidized Guanine Cation (74')

SCF Done: E(RB3LYP) = -637.676885444 a.u.

1 1

C	0.36869200	0.85240200	-0.24060400
C	0.56723900	-0.65441300	-0.06006200
C	-1.85817700	-0.59194900	-0.16170200
C	-0.87810600	1.47547500	0.29977000
C	2.00382200	0.34258700	-1.51262100
H	2.82391700	0.48569700	-2.20613000
H	2.16273000	-1.68898600	-1.21264400
N	-1.96859600	0.68179800	0.24969300
N	-0.68307600	-1.22211900	-0.50254100
O	-0.87259400	2.64411800	0.71179700
N	1.21260500	1.39980700	-1.05745900
N	1.65574600	-0.81796400	-1.05286400
N	-2.97089300	-1.30984100	-0.26327100
H	-3.85701400	-0.86857000	-0.05372600
H	-2.95605900	-2.28455000	-0.53858900
N	0.98813700	-1.19479800	1.20763700
H	0.19394700	-1.13250500	1.84430400
H	-0.70665000	-2.23481800	-0.60735500
C	2.17059500	-0.57166900	1.83772800
H	3.05542000	-0.73213600	1.21935800
H	2.05073100	0.50228900	2.02370200
H	2.33187700	-1.07214600	2.79329600

4-NH_2CH3 Oxidized Guanine Neutral (75)

SCF Done: E(RB3LYP) = -637.181042987 a.u.

0 1

C	0.23056700	0.82781500	-0.30621100
C	0.48320800	-0.63858600	-0.15422800
C	-1.87931500	-0.73502100	-0.16546000
C	-1.00066700	1.37935500	0.31447900
C	1.89166800	0.40848700	-1.57718900
N	-2.01883700	0.53451400	0.40842700
N	-0.66766900	-1.29575000	-0.57264400
O	-0.99489600	2.58122500	0.71743800
N	1.61659000	-0.77188500	-1.07255000
N	-2.97687100	-1.42675500	-0.31784500
H	-2.73463900	-2.30872800	-0.77462000
N	1.05067400	1.40595300	-1.16420600
H	2.12456900	-1.63308000	-1.26354700
H	2.68551200	0.56208600	-2.29718800
N	0.97613100	-1.09424700	1.26207600
H	0.17322600	-0.97987100	1.89192500
C	2.16850400	-0.39710300	1.84486700
H	2.35049700	-0.81495200	2.83469400
H	3.03193800	-0.57037800	1.20524900
H	1.95068600	0.66724200	1.92714000
H	1.15346300	-2.10460200	1.19649000

4-$NHCH_3$ Oxidized Guanine Neutral (76)

SCF Done: E(R3LYP) = -637.221348808 a.u.

0 1

C	0.33893300	0.78096600	-0.32877300
C	0.52483900	-0.67474000	0.02481700
C	-1.79810500	-0.66417100	-0.08833700
C	-0.88180600	1.44963500	0.21519200
C	1.92926200	0.13568700	-1.60096000
N	-1.95120700	0.65881600	0.30149300
N	-0.68647000	-1.36238100	-0.30975900
O	-0.83822100	2.66358500	0.53369600
N	1.60050900	-0.96317100	-1.00027700
N	-2.97374700	-1.31067700	-0.24684000
H	-3.83347200	-0.83785300	-0.01070000
H	-2.98581600	-2.30420400	-0.42835700
N	1.11479900	1.21890600	-1.27769300
H	2.12150800	-1.83666200	-1.06137800
H	2.74182100	0.21163900	-2.31355500
N	0.95812000	-0.94700200	1.36778800
C	2.17631300	-0.26217500	1.82997700
H	2.39079900	-0.60276000	2.84431200
H	3.06135100	-0.45029000	1.20879700
H	1.99958100	0.81654400	1.86649800
H	1.03936300	-1.95774600	1.47033200

4-NCH_3 Oxidized Guanine Neutral (77)

SCF Done: E(R3LYP) = -637.185138615 a.u.

0 1

C	0.18614800	1.11580100	0.08287100
C	0.76540800	-0.28050500	0.07836600
C	-1.53818700	-0.84689000	-0.44726100
C	-1.22829800	1.25505300	0.53670900
C	2.00296400	1.34637700	-1.02306300
N	-2.03895500	0.22755100	0.20364000
N	-0.22505300	-1.03932400	-0.75940200
O	-1.60796500	2.26845900	1.15353100
N	1.96200500	0.06112500	-0.84220000
N	-2.41050100	-1.78211100	-0.83075000
H	-3.39768800	-1.63292800	-0.67116600
H	-2.10847900	-2.61866400	-1.31342200
N	0.87505100	2.01344800	-0.56018900
H	2.75999500	-0.54842600	-1.00750400
H	2.84742600	1.87106500	-1.45233000
N	1.13138000	-0.76323100	1.30220400
C	1.77689700	-2.07586500	1.25439300
H	2.02880800	-2.38170000	2.27359100
H	1.13024900	-2.86536300	0.83745800
H	2.71970700	-2.10371700	0.68352300
H	0.03662300	-1.97397300	-1.06360100

4-NCH_3 Sp Neutral (78)

SCF Done: E(R3LYP) = -637.280999745 a.u.

0 1

C	0.06718700	-0.48711700	-0.32704600
C	-1.19122100	0.36099000	-0.09408000
C	2.16049900	0.39484900	-0.24669200
C	0.82584100	-0.73880200	1.01865500
N	2.05741300	-0.17384000	0.96999200
N	1.11094500	0.16263800	-1.08378100
O	0.32785300	-1.36412300	1.96149400
N	-2.23291100	-0.51970900	-0.36323300
N	3.21487400	1.10786700	-0.61894300
H	3.97259300	1.25339400	0.03462000
H	3.26881900	1.52387700	-1.53979800
N	-1.21661100	1.58044000	0.27800100
H	0.89718600	0.79427600	-1.84871300
C	-2.53319500	2.19372600	0.45888700
H	-3.10902600	2.20062500	-0.47540600
H	-3.12583400	1.66637700	1.21713600
H	-2.40925500	3.22681000	0.78644300
C	-1.69751000	-1.69161100	-0.85450900
N	-0.40979200	-1.75357900	-0.90180500
H	-3.21727500	-0.28273400	-0.38092000
H	-2.35706200	-2.48857700	-1.17822400

4-NCH_3-8-$NHCH_3$ Sp Neutral (79)

SCF Done: E(R3LYP) = -733.169460842 a.u.

0 1

C	0.45742100	-0.36350300	-0.16722600
C	-0.24110100	0.99106000	-0.01029000
C	2.71615300	-0.45719600	-0.43768800
C	1.25561000	-0.72965500	1.12387400
N	2.58836300	-0.75006000	0.87247700
N	1.54770000	-0.36481400	-1.12838400
O	0.70027300	-0.97339500	2.20530600
N	-1.58095300	0.73395900	0.01861200
N	3.89589800	-0.30246800	-1.02596100
H	4.74196200	-0.38879300	-0.47912300
H	3.96601800	-0.09517500	-2.01370100
N	0.39698400	2.10166600	0.06584300
H	1.49230800	0.18348300	-1.98076300
C	-0.41673700	3.30474400	0.23019900
H	-1.11427600	3.44803100	-0.60682900
H	-1.01015600	3.28182200	1.15547000
H	0.23346600	4.18062800	0.27550500
C	-1.88677100	-0.70276300	0.03549800
C	-4.30728000	-0.68018000	-0.18399900
H	-4.42703700	-1.11347000	0.81325100
H	-4.41659300	0.41127500	-0.10096400
H	-5.11923100	-1.05276100	-0.81252900
N	-3.02125000	-1.10861700	-0.75487900
H	-2.91948700	-0.71645500	-1.69061400
N	-0.63767900	-1.26801000	-0.49165500
H	-2.24377900	1.39929100	0.39600600
H	-2.08566700	-1.02356500	1.06508900
H	-0.48692100	-2.19377800	-0.09783600

4-NCH_3-8-$NHCH_3$ Sp Radical Neutral (80)

SCF Done: E(U3LYP) = -732.512680935 a.u.

0 2

C	0.33333700	-0.19142800	-0.39310300
C	-0.10113200	1.25593400	-0.13939200
C	2.51242200	-0.83672800	-0.21790000
C	0.70909900	-0.89786300	0.97727200
N	2.02115100	-1.22358600	0.97602400
N	1.58831500	-0.35366300	-1.08943600
O	-0.11462400	-1.08881900	1.87622100
N	-1.42732100	1.29490000	-0.46573700
N	3.79556700	-0.94402400	-0.53364200
H	4.44685700	-1.30655400	0.14966200
H	4.14068400	-0.64680100	-1.43734800
N	0.67939000	2.17439300	0.29643000
H	1.84887400	0.25302800	-1.85965000
C	0.07283400	3.48902700	0.50374700
H	-0.32675500	3.90944500	-0.42933500
H	-0.75004600	3.45295300	1.23136700
H	0.82510700	4.18107700	0.88721800
C	-1.95355400	-0.02268100	-0.79670600
C	-3.66720800	-1.66581600	-0.10817400

H	-4.35269900	-1.31023300	-0.88278600
H	-3.15774700	-2.56284000	-0.48203600
H	-4.25928700	-1.95251300	0.76445800
N	-2.76321400	-0.57759200	0.28095300
H	-2.14966200	-0.86852100	1.04461000
N	-0.77456400	-0.83834500	-1.05064000
H	-2.04086100	2.03858900	-0.15616600
H	-2.57752600	0.01566500	-1.69187600

4-NCH$_3$-8-NHCH$_3$ Sp Radical (81)

SCF Done: E(U3LYP) = -732.512025366 a.u.

0 2

C	0.44997100	-0.34317600	-0.16908100
C	-0.26793800	1.00626900	-0.03849500
C	2.71267400	-0.46875000	-0.40104500
C	1.22373000	-0.71150900	1.14091200
N	2.55892300	-0.75382500	0.90800700
N	1.55663200	-0.35401400	-1.10984100
O	0.64704600	-0.93801700	2.21336400
N	-1.60543500	0.71743900	-0.03352200
N	3.90330800	-0.34216800	-0.97288300
H	4.73970300	-0.44249000	-0.41361100
H	3.99122200	-0.14094800	-1.96057900
N	0.34882600	2.12862800	0.06593500
H	1.52131400	0.18748400	-1.96765000
C	-0.48654000	3.31898700	0.20196600
H	-1.17375800	3.44149100	-0.64742800
H	-1.09361600	3.29470400	1.11799600
H	0.14865200	4.20569000	0.24745300
C	-1.86760200	-0.67136900	-0.11180500
C	-4.29004700	-0.76702700	-0.04113000
H	-4.28070500	-1.06480300	1.01064200
H	-4.46702800	0.31714100	-0.09404500
H	-5.12531400	-1.26905800	-0.53513900
N	-3.03820000	-1.19612200	-0.67811300
H	-3.07178400	-1.02321700	-1.68872400
N	-0.63459000	-1.25455800	-0.49840100
H	-2.33093100	1.40420300	0.12708900
H	-0.50585600	-2.20427100	-0.15912600

4-NCH$_3$-8-NHCH$_3$ Sp Neutral (82)

SCF Done: E(R3LYP) = -731.973058442 a.u.

0 1

C	0.30418600	-0.26443200	-0.09281600
C	-0.16378000	1.20131600	-0.10093400
C	2.48716500	-0.84394800	-0.41290700
C	1.09651600	-0.58494000	1.21805100
N	2.37800400	-0.92210700	0.92904400
N	1.33148200	-0.57131100	-1.07000100
O	0.58101200	-0.52953100	2.34288700
N	-1.54063700	1.10944300	-0.02850000
N	3.63498100	-1.04736200	-1.04886100
H	4.47051200	-1.24034000	-0.51323100
H	3.69855900	-0.97727100	-2.05593300
N	0.58676200	2.23386300	-0.13772500
H	1.32383000	-0.18374000	-2.00705700
C	-0.08970000	3.53210200	-0.10731100
H	-0.68298000	3.65810900	0.80755200
H	0.65324800	4.33035500	-0.13987400
H	-0.76307100	3.66190800	-0.96500100
C	-1.90668400	-0.23341100	-0.13891700
C	-3.68340300	-1.90753500	-0.40166900
H	-4.76791600	-1.91786300	-0.29113000
H	-3.42728600	-2.23504300	-1.41553400
H	-3.25583700	-2.61237700	0.31476500
N	-3.21566300	-0.55335200	-0.12610200
N	-0.90486400	-1.06834900	-0.21451900
H	-2.18408700	1.88828500	-0.10051600
H	-3.86931400	0.20353800	-0.28148100

4,8 diNCH$_3$ Sp (82')

SCF Done: E(R3LYP) = -731.973109698 a.u.

0 1

C	0.30015600	-0.26531700	-0.09763300
C	-0.15880000	1.20318500	-0.09214900
C	2.48378300	-0.84783900	-0.41316900
C	1.08418400	-0.60538000	1.21290800
N	2.36637800	-0.94217400	0.92718900
N	1.33299200	-0.56389400	-1.07348000
O	0.56316100	-0.56121200	2.33582000
N	-1.53901700	1.12191300	-0.04917700
N	3.63482900	-1.04734700	-1.04468900
H	4.46635300	-1.25046600	-0.50659100
H	3.70489100	-0.96352600	-2.05031100
N	0.60108300	2.22911700	-0.09852900
H	1.33119400	-0.16603300	-2.00624400
C	-0.05945100	3.53479000	-0.05788000
H	-0.66222800	3.65385500	0.85172300
H	0.69419000	4.32355500	-0.06864100
H	-0.72063500	3.68693900	-0.92118100
C	-1.90940100	-0.21734600	-0.19353800
C	-3.68757100	-1.90485400	-0.30297300
H	-4.77070800	-1.89107600	-0.42525500
H	-3.25244900	-2.45933800	-1.13750900
H	-3.44005400	-2.42130000	0.63102400
N	-3.21617500	-0.52428000	-0.30308000
H	-3.88039800	0.19663200	-0.05254400
N	-0.91197000	-1.06004800	-0.23741400
H	-2.16967300	1.90402100	-0.18016800

4-NCH3, 8-OH Sp Neutral (83)

SCF Done: E(R3LYP) = -713.729263572 a.u.

0 1

C	0.14102600	-0.38517400	0.26483000
C	-0.87956300	0.73403400	0.01390900
C	2.24182500	-0.20601000	-0.60715600
C	1.23922500	0.01784400	1.29245800
N	2.44907200	0.11451000	0.68519000
N	0.98617200	-0.64271000	-0.90281400
O	0.99558600	0.22038900	2.48944900
N	-2.12171500	0.16923200	0.18736800
N	3.19654300	-0.13111000	-1.52646900
H	4.11735200	0.19310300	-1.26216500
H	3.01826400	-0.37817000	-2.49136100
N	-0.54946600	1.93257900	-0.28967700
H	0.61327600	-0.55281300	-1.84294700
C	-1.64315000	2.86758300	-0.55080200
H	-2.29436900	2.52609600	-1.36728200
H	-2.27255900	3.01734400	0.33643100
H	-1.23084300	3.83697200	-0.83608200
C	-2.04579400	-1.27463500	0.23295300
N	-0.69532300	-1.48657700	0.71016000
H	-2.95934100	0.61183700	-0.17142300
H	-0.33370700	-2.39575800	0.43726300
O	-2.22977200	-1.88442000	-1.04880300
H	-3.17361300	-2.07388900	-1.16901300
H	-2.78935800	-1.68580600	0.91794900

4-NCH$_3$-8-OH-Sp Radical Neutral (84)

SCF Done: E(U3LYP) = -713.069291921 a.u.

0 2

C	0.17144700	-0.26109600	-0.38012200
C	-0.78498000	0.89495900	-0.07968000
C	2.44025400	-0.08791600	-0.21548800
C	0.79302400	-0.83369800	0.98313400
N	2.13526800	-0.67405900	0.95766000
N	1.39190100	0.08220400	-1.06325500
O	0.10426400	-1.31556100	1.87970400
N	-2.03679100	0.35861800	-0.22709300
N	3.67275100	0.27549300	-0.53950400
H	4.42334800	0.14596200	0.12559300
H	3.86911700	0.72399100	-1.42494200
N	-0.41698100	2.07440200	0.25233100
H	1.41057700	0.77593700	-1.80313000
C	-1.48451900	3.04530300	0.49494700
H	-2.14731100	3.15426400	-0.37435400
H	-2.10518100	2.76417400	1.35587000
H	-1.04531200	4.02233000	0.70382000
C	-2.01488600	-0.95351700	-0.81644400
N	-0.60536700	-1.25398000	-1.06734600
H	-2.88280700	0.91411500	-0.20681600
O	-2.57344600	-1.89961400	0.08385200
H	-2.91132600	-2.64983500	-0.43131500
H	-2.56514700	-0.99248700	-1.76081800

4-NCH$_3$-8-OH Sp Radical Neutral (85)

SCF Done: E(U3LYP) = -713.069572753 a.u.

0 2

C	0.15891000	-0.32649000	-0.28014300
C	-0.74364200	0.88839300	-0.02737100
C	2.42735200	-0.14178200	-0.28830400
C	0.85951200	-0.83369300	1.02254000
N	2.20299800	-0.67830700	0.92759700
N	1.33002400	-0.03418700	-1.08790000
O	0.22765300	-1.31607700	1.97109800
N	-2.03801200	0.44084200	-0.17909400
N	3.63329000	0.22678100	-0.69931100
H	4.42437200	0.12389500	-0.07800800
H	3.77690500	0.61421500	-1.62279100
N	-0.30165200	2.05589700	0.25626000
H	1.29308000	0.67052300	-1.81761500
C	-1.30442000	3.10348100	0.44515700
H	-1.95352400	3.21701700	-0.43408500
H	-1.94847300	2.89823400	1.31067700
H	-0.80633300	4.05914400	0.61684600
C	-2.09012800	-0.85036700	-0.74858500
N	-0.75999100	-1.28913000	-0.86948600
H	-2.82250900	1.07760200	-0.25424600
O	-2.95295500	-1.79703200	-0.19840600
H	-3.86180700	-1.58492700	-0.46481200
H	-0.61139200	-2.26135400	-0.61372500

4-NCH$_3$-8-OH Sp Neutral (86)

SCF Done: E(R3LYP) = -712.525179883 a.u.

0 1

C	0.15043600	-0.38994300	-0.15064100
C	-0.79569400	0.82315200	-0.05398000
C	2.39964400	-0.13449700	-0.39355700
C	0.97303600	-0.57372700	1.16679700
N	2.29588800	-0.39933400	0.92371600
N	1.23607100	-0.22318900	-1.09349200
O	0.44354400	-0.83880700	2.25274800
N	-2.06495700	0.26194200	-0.12169500
N	3.55220300	0.15976000	-0.98080600
H	4.39246700	0.22907400	-0.42239300
H	3.59951300	0.36132100	-1.97116900
N	-0.44325900	2.04030000	0.07764800
H	1.10814900	0.26100700	-1.97563100
C	-1.51159500	3.03656900	0.16813000
H	-2.11332800	3.06641200	-0.74921300
H	-2.18597300	2.83356500	1.00956400
H	-1.07269600	4.02432200	0.31530700
C	-1.91743400	-1.08675300	-0.36796700
N	-0.71176400	-1.54192400	-0.41648800
H	-2.94130200	0.76522700	-0.19633700

O	-3.04307200	-1.78075500	-0.53339200
H	-2.83022600	-2.71611800	-0.69984400

4-NCH_3-8-oxo-Sp Neutral (87)

SCF Done: E(R3LYP) = -712.550508666 a.u.

0 1

C	0.15428800	-0.35956700	-0.21346700
C	-0.82719500	0.81123300	-0.05022900
C	2.40396000	-0.06967400	-0.34444700
C	0.92928500	-0.66647000	1.11589600
N	2.25443300	-0.45079200	0.93952400
N	1.26714700	-0.10643900	-1.09820700
O	0.35715400	-1.05706400	2.13845900
N	-2.09315500	0.25125700	-0.14124000
N	3.57135100	0.29033600	-0.85543300
H	4.39052000	0.30422400	-0.26227300
H	3.65934600	0.55704000	-1.82783300
N	-0.47646800	2.02047700	0.14006300
H	1.16494100	0.47424600	-1.92462900
C	-1.54343300	3.01156600	0.28730600
H	-2.18039900	3.05614200	-0.60504800
H	-2.18335400	2.79184300	1.15078900
H	-1.09993300	3.99683700	0.43616900
C	-2.04695800	-1.10141500	-0.43466700
N	-0.72964500	-1.43643600	-0.62112700
H	-2.96775200	0.75815300	-0.07298200
O	-3.01998900	-1.85133400	-0.52765200
H	-0.45601600	-2.40417000	-0.48804700

4-OH N3H Guanine Radical Cation (88)

SCF Done: E(UB3LYP) = -618.862671574 a.u.

1 2

C	0.75509700	0.71615400	0.06489400
C	0.62156700	-0.77973900	0.24163400
C	-1.71865700	-0.49345200	-0.24012700
C	-0.40667700	1.54913000	0.13893000
C	2.59967400	-0.09777300	-0.62200200
N	-1.61339700	0.81171100	0.12598300
N	-0.59919700	-1.22478000	-0.40801700
O	-0.44169400	2.78360000	0.18807400
N	1.83871900	-1.19762000	-0.43617800
N	-2.91435300	-1.01950700	-0.44743000
H	-3.74382200	-0.43614900	-0.44698200
H	-3.01092800	-2.00299900	-0.67393900
N	1.98434100	1.06082200	-0.37808900
H	2.22556500	-2.13161500	-0.33524200
H	3.62056500	-0.17384800	-0.97223200
H	-0.71169400	-2.21985000	-0.59300300
H	-2.47092400	1.35287400	0.21663600
O	0.63041200	-1.11874300	1.61199800
H	0.60267100	-2.08757700	1.71033300

4-OH Guanine Radical (89)

SCF Done: E(UB3LYP) = -618.411872269 a.u.

0 2

C	0.72264600	0.70861500	0.04714600
C	0.59466100	-0.78334000	0.23065100
C	-1.64742400	-0.58899800	-0.23915500
C	-0.45741800	1.51592500	0.14990100
C	2.57201800	-0.07808400	-0.65906000
N	-1.62059300	0.74824700	0.16168700
N	-0.59005500	-1.35018500	-0.33895200
O	-0.51052000	2.76037700	0.20897700
N	1.83764800	-1.18198800	-0.44241000
N	-2.88902000	-1.07765300	-0.49310100
H	-3.62417700	-0.43512400	-0.76208700
H	-2.93643000	-2.00561400	-0.89319800
N	1.93732300	1.07688800	-0.42506400
H	2.22652400	-2.11633900	-0.37747200
H	3.58773800	-0.13540700	-1.02808500
O	0.68285000	-1.09651000	1.62832700
H	0.43074900	-2.03009500	1.73542200
H	-2.49705000	1.25975900	0.21496700

4-OH Guanine Radical (90)

SCF Done: E(UB3LYP) = -618.408269367 a.u.

0 2

C	0.72207600	0.70174900	0.06550800
C	0.57718100	-0.79107100	0.21470500
C	-1.73763600	-0.38238800	-0.23485000
C	-0.45675400	1.53942300	0.13795300
C	2.57705400	-0.11753700	-0.60670500
N	-1.67747100	0.91378000	0.06529200
N	-0.64586200	-1.19867800	-0.42689500
O	-0.37782600	2.79150800	0.24133700
N	1.79647400	-1.21915500	-0.45930900
N	-2.94346600	-0.94584400	-0.40464700
H	-3.76537200	-0.35807900	-0.39224400
H	-3.04446000	-1.92648400	-0.62977700
N	1.96887400	1.03842900	-0.35273400
H	2.18718700	-2.14633600	-0.32442700
H	3.60310500	-0.19881700	-0.94036400
H	-0.81994300	-2.19967200	-0.48076400
O	0.59526000	-1.15069300	1.59416000
H	0.51864500	-2.11790200	1.67197900

4-OH N3H oxidized Guanine Cation (91)

SCF Done: E(RB3LYP) = -618.231438860 a.u.

1 1

C	-0.66661100	0.74283800	-0.03746200
C	-0.64924300	-0.72715000	0.36098200
C	1.67058600	-0.51282100	-0.26585400
C	0.59613300	1.52630600	0.13008900

C	-2.48428200	-0.08913100	-0.78775900
H	-3.45138700	-0.12394100	-1.27413600
H	-2.32341300	-2.06532300	-0.20359200
N	1.72726800	0.81024200	-0.04810900
N	0.51684500	-1.27356100	-0.26334600
O	0.55683800	2.73810100	0.37992500
N	-1.73518400	1.08555200	-0.68310700
N	-1.91317300	-1.13307700	-0.27276800
N	2.80344600	-1.15534300	-0.51620200
H	3.66649700	-0.62719400	-0.55830300
H	2.82861600	-2.15523600	-0.67819500
O	-0.79376100	-0.99958700	1.72336900
H	0.61744600	-2.28741300	-0.23632200
H	-0.03628700	-0.62594300	2.20893500

4-OH oxidized Guanine (92)

SCF Done: E(RB3LYP) = -617.780546516 a.u.

0 1

C	0.62326100	0.73534300	-0.04911100
C	0.63618800	-0.70821000	0.38980200
C	-1.58429000	-0.60474100	-0.26053900
C	-0.65771200	1.47948800	0.14956000
C	2.44843300	-0.05378200	-0.82826800
N	-1.75922600	0.73389200	0.03004300
N	-0.47004500	-1.35310300	-0.20776700
O	-0.62813300	2.70594400	0.40440600
N	1.93142900	-1.09320100	-0.25327200
N	-2.71105100	-1.23738500	-0.62949300
H	-3.57681600	-0.72296900	-0.70439800
H	-2.69496200	-2.22561700	-0.83980300
N	1.64265100	1.08290800	-0.77877800
H	2.38424700	-2.00051000	-0.15762800
H	3.40673800	-0.06518300	-1.33190600
O	0.74120700	-0.86599300	1.78206200
H	0.34461400	-1.72569400	2.00819600

4-O-Guanine neutral (93)

SCF Done: E(R3LYP) = -617.783844687 a.u.

0 1

C	0.67978400	0.72239100	-0.01190500
C	0.64706400	-0.72672000	0.49301200
C	-1.65711900	-0.52286900	-0.25386300
C	-0.57752800	1.51461300	0.12641800
C	2.50473600	-0.12085800	-0.75249200
N	-1.71431500	0.81042800	-0.05349300
N	-0.51546300	-1.27679500	-0.24972200
O	-0.53997900	2.73339100	0.37331700
N	1.93951300	-1.15808000	-0.23680900
N	-2.80891300	-1.15088300	-0.49179300
H	-3.66149000	-0.60946400	-0.54864800
H	-2.84741000	-2.15016400	-0.64754100
N	1.73246500	1.04961700	-0.69076500
H	2.39357500	-2.06213100	-0.11545300
H	3.49045800	-0.12929300	-1.20136000
O	0.69611300	-0.96876800	1.76931300
H	-0.63883900	-2.28529600	-0.17698600

4-OH (mN1N2H) Guanine neutral (93')

SCF Done: E(RB3LYP) = -617.761986247 a.u.

0 1

C	0.61255000	0.74534400	-0.03550200
C	0.59824300	-0.72097800	0.34865300
C	-1.74436600	-0.56976700	-0.30611400
C	-0.66093800	1.49769500	0.12303100
C	2.47777300	-0.04388900	-0.72056800
N	-1.77266300	0.78214900	-0.03548400
N	-0.50084800	-1.26234200	-0.36784500
O	-0.61874100	2.73114700	0.37014200
N	1.90459800	-1.10751500	-0.24156900
N	-2.85215200	-1.19293700	-0.54151100
H	-2.67855300	-2.18208200	-0.72946600
N	1.70449600	1.10836100	-0.64285300
H	2.33269900	-2.02960700	-0.16666900
H	3.46636000	-0.05401000	-1.16243300
O	0.60733300	-0.90105200	1.73569400
H	0.45183300	-1.84111800	1.93710400
H	-0.56466500	-2.27838500	-0.37739600

4-O-Sp Neutral (94)

SCF Done: E(R3LYP) = -617.852398718 a.u.

0 1

C	0.24804900	-0.14212300	-0.26144400
C	1.33167900	-0.52886100	0.76542600
C	-2.01444700	-0.25557300	-0.08712200
C	-0.44017500	1.20774000	0.16674400
C	2.20288700	-0.10212400	-1.25831100
N	-1.78085900	1.03346300	0.22899900
N	-0.89704800	-1.00454400	-0.29218200
O	0.20006300	2.23804400	0.39188600
N	2.50057400	-0.40462900	0.06537900
N	-3.23241200	-0.77009200	-0.16955600
H	-4.03429300	-0.18428900	0.02166600
H	-3.37381800	-1.74677100	-0.39433800
N	0.95247600	0.02273800	-1.53814600
H	3.42798600	-0.58113100	0.43727800
H	3.00664700	-0.00273500	-1.97824900
O	1.18891700	-0.83785600	1.94178600
H	-0.90544400	-1.89949300	-0.76896100

4-oxo 8-NHCH3-Sp Neutral (95)

SCF Done: E(R3LYP) = -713.748711100 a.u.

0 1

C	-0.40383700	0.01302800	-0.20431200
C	0.24328900	-0.81898100	0.92160300
C	-2.65363800	-0.16999700	-0.47299700
C	-1.22853900	1.19172800	0.40264500
C	1.95804800	0.33642400	-0.22014200
N	-2.55513100	0.98391800	0.21725400
N	-1.46814300	-0.70183600	-0.88814500
O	-0.69262000	2.16184000	0.95535500
N	1.55766400	-0.58960900	0.85683500
N	-3.81819400	-0.73400300	-0.76226500
H	-4.67186900	-0.31278300	-0.42039200
H	-3.86779900	-1.60130000	-1.28137000
N	0.73067000	0.39194800	-1.02558400
H	2.21717300	-0.97068100	1.52609800
O	-0.37332400	-1.54294900	1.71349800
H	-1.38917600	-1.69882400	-1.06613000
N	3.08725900	-0.07385500	-1.00654500
H	2.92098100	-1.01437500	-1.36269800
C	4.35877400	-0.03291400	-0.26636900
H	4.39346700	-0.70954400	0.59968800
H	5.17485200	-0.30578400	-0.93871400
H	4.53922600	0.98572500	0.08863800
H	2.20795100	1.30412100	0.22629900
H	0.61928700	1.32065800	-1.42565400

4-oxo-8-NHCH$_3$-Sp Radical Neutral (96)

SCF Done: E(U3LYP) = -713.090744221 a.u.

0 2

C	-0.39105300	-0.07659600	-0.22377600
C	0.26679900	-0.92255100	0.89027400
C	-2.65227900	-0.06418300	-0.47815000
C	-1.13592200	1.16254400	0.47438800
C	1.88418600	0.32293100	-0.27658600
N	-2.46315700	1.04779000	0.25950800
N	-1.51174900	-0.68189400	-0.88989500
O	-0.53009100	2.03059600	1.09869900
N	1.56583200	-0.60805700	0.83270400
N	-3.85453900	-0.51043500	-0.80735600
H	-4.67543000	-0.02449100	-0.47120900
H	-3.96675600	-1.34973900	-1.36190600
N	0.67013300	0.34624300	-1.07327600
H	2.25076700	-0.93888100	1.50386200
O	-0.31677900	-1.68746200	1.66370800
H	-1.50654300	-1.66150400	-1.15580800
N	3.03445300	-0.01896300	-1.06481700
H	2.94066600	-0.98215400	-1.38543300
C	4.30464800	0.13062500	-0.33460500
H	4.38862700	-0.51233600	0.55302300
H	5.12960000	-0.11482300	-1.00653900
H	4.42106500	1.17098500	-0.01871300
H	2.04787900	1.32846300	0.13612300

4-oxo-8-NHCH$_3$-Sp Radical Neutral (97)

SCF Done: E(U3LYP) = -713.092074836 a.u.

0 2

C	0.37711700	0.16801400	0.02110100
C	-0.30289800	-0.37782800	-1.24221400
C	2.51032100	-0.44131500	0.57300100
C	1.45933700	1.25068200	-0.26307100
C	-1.92341800	0.10971100	0.30944600
N	2.69290500	0.79556800	0.06838000
N	1.21227900	-0.81762500	0.74317900
O	1.18566300	2.36046900	-0.74120600
N	-1.68416000	-0.53875000	-0.83081900
N	3.52479900	-1.22708900	0.91475800
H	4.47247200	-0.91706900	0.74566400
H	3.36831200	-2.15723800	1.28026500
N	-0.76146300	0.64845700	0.78361300
H	-2.41067600	-0.87328000	-1.45277900
O	0.25484700	-1.18885400	-2.07515800
H	0.97379100	-1.80443000	0.69948500
N	-3.11749200	0.31796700	0.87156000
H	-3.11386300	0.72175700	1.80078700
C	-4.33123500	-0.36033500	0.41936900
H	-4.25549700	-1.44609000	0.54222600
H	-5.16323200	0.00900500	1.01741000
H	-4.52988800	-0.12684100	-0.63000900
H	-0.66890800	0.87799800	1.76737200

4-oxo-8-NHCH$_3$-Sp Neutral (98)

SCF Done: E(R3LYP) = -712.545521224 a.u.

0 1

C	0.37895300	-0.05913600	-0.07792000
C	-0.40219300	1.12263300	-0.69302900
C	2.60208200	-0.52801700	-0.23622200
C	1.23715600	0.43099800	1.13820300
C	-1.78321600	-0.47512800	0.08883200
N	2.53700900	0.09004100	0.96066200
N	1.43328500	-0.56171800	-0.92989200
O	0.74311100	1.02550000	2.10365400
N	-1.71096100	0.79465900	-0.50387400
N	3.72293700	-1.04697700	-0.71991400
H	4.57666100	-0.98076300	-0.18206800
H	3.74426500	-1.49177100	-1.62859700

N	-0.62222600	-1.03339000	0.31270900
H	-2.49428600	1.37012400	-0.79290700
O	0.04340900	2.14035900	-1.21182100
H	1.25762300	-1.22848200	-1.67371400
N	-2.97684700	-1.00252800	0.41317600
H	-2.93075700	-1.95926600	0.74318300
C	-4.25588400	-0.55462100	-0.14155900
H	-4.32618200	-0.73397900	-1.21980200
H	-5.04797600	-1.11124800	0.35892700
H	-4.41528000	0.50753100	0.06042100

4-oxo-8-OH-Sp Neutral (99)

SCF Done: E(R3LYP) = -694.308952624 a.u.

0 1

C	-0.01140300	0.02498400	-0.20806400
C	0.67056100	-0.56113300	1.04355700
C	-2.25123700	-0.31379000	-0.39960300
C	-0.89094100	1.25539200	0.18569300
C	2.35701400	0.24651700	-0.37778400
N	-2.20450700	0.94962200	0.06880100
N	-1.04418100	-0.85452000	-0.73291600
O	-0.39872900	2.33370300	0.54060300
N	1.98388200	-0.33639000	0.90163400
N	-3.38993600	-0.97134300	-0.56645200
H	-4.25938200	-0.53124500	-0.29560900
H	-3.40298200	-1.92023100	-0.91766200
N	1.09431900	0.32324800	-1.09493600
H	2.67870600	-0.64922300	1.57131000
O	0.08401300	-1.11101700	1.97987600
H	-0.91776100	-1.86250100	-0.73384200
O	3.26510200	-0.58379000	-1.07745800
H	4.16820600	-0.28837200	-0.88171400
H	0.99142400	1.22736200	-1.54678100
H	2.81769000	1.22691400	-0.23558300

4-oxo-8-OH-Sp Radical Neutral (100)

SCF Done: E(U3LYP) = -693.645711481 a.u.

0 2

C	-0.02306600	-0.13700700	-0.32386800
C	0.70879200	-1.16999400	0.55997300
C	-2.29298200	0.09419500	-0.28271700
C	-0.56350200	1.04876200	0.62126300
C	2.25694000	-0.07589600	-0.79716000
N	-1.91108400	1.07684100	0.55602300
N	-1.27286400	-0.57273200	-0.88074500
O	0.18599600	1.76195800	1.28191300
N	2.01256900	-1.02656600	0.26406200
N	-3.56287200	-0.19032500	-0.52739900
H	-4.29082700	0.33099900	-0.05690000
H	-3.82039000	-0.93637100	-1.16111900
N	0.93199500	0.30545000	-1.29333900
H	2.75294900	-1.55607200	0.71237300
O	0.18762300	-1.93483400	1.37135100
H	-1.38795400	-1.47264600	-1.33428800
O	2.94293800	1.04948500	-0.28443800
H	3.47770500	1.43458600	-0.99672300
H	2.83477100	-0.52240000	-1.60911800

4-oxo-8-OH-Sp Radical Neutral (101)

SCF Done: E(U3LYP) = -693.645442974 a.u.

0 2

C	-0.00642200	-0.06804000	-0.16272700
C	-0.70293200	0.75331000	0.94831500
C	2.23504500	0.21148900	-0.46034100
C	0.87667600	-1.21864900	0.42134200
C	-2.26746500	0.24702900	-0.66243400
N	2.18997200	-0.95284200	0.21457200
N	1.02305600	0.70872200	-0.84486300
O	0.39503600	-2.20397600	0.99115400
N	-2.00513500	0.83536700	0.59529200
N	3.37024100	0.82499500	-0.76270300
H	4.24767600	0.42674200	-0.45474100
H	3.37561600	1.69986500	-1.27154200
N	-1.12270300	-0.50391200	-0.96960800
H	-2.69070300	1.37806800	1.11095400
O	-0.14164600	1.27445400	1.91665000
H	0.90380000	1.70332600	-1.01495100
O	-3.46798400	-0.40961300	-0.85901000
H	-4.17920200	0.24669900	-0.94148800
H	-0.93785900	-0.67876400	-1.95234500

4-oxo-8-OH-Sp Neutral (102)

SCF Done: E(R3LYP) = -693.094586523 a.u.

0 1

C	0.00841400	-0.01151100	0.21927500
C	0.72586000	1.01351700	-0.69312300
C	-2.25435500	0.03784400	0.43269900
C	-0.75377400	-1.05185300	-0.67880900
C	2.16293700	-0.16216200	0.55928300
N	-2.08889600	-0.93424200	-0.48498700
N	-1.10024500	0.53519300	0.95891400
O	-0.16813800	-1.83205400	-1.43532900
N	2.05473100	0.79164700	-0.45477800
N	-3.44507000	0.46710200	0.82409100
H	-4.27840800	0.06872800	0.41215200
H	-3.53545100	1.19116700	1.52534100
N	1.05609600	-0.62944800	1.01846400

H	2.82474500	1.29689300	-0.88450200
O	0.22816000	1.81715500	-1.46802600
H	-1.05980600	1.44656500	1.40350100
O	3.35159200	-0.54783700	1.01369000
H	4.08520700	-0.06824300	0.59294300

4,8-oxoSp Neutral (103)

SCF Done: E(R3LYP) = -693.121945757 a.u.

0 1

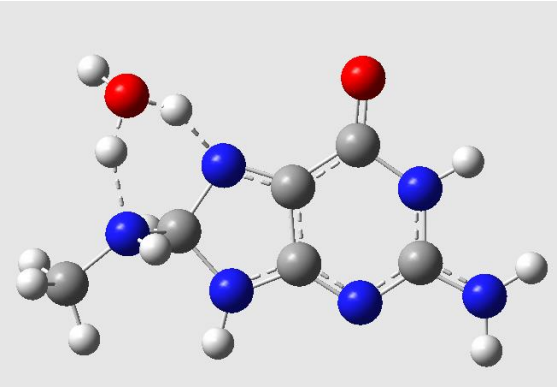
C	-0.01387600	-0.00585700	-0.22409500
C	-0.75019400	1.05937600	0.62106200
C	2.24811100	0.01667700	-0.39005100
C	0.71653100	-1.04419200	0.70497200
C	-2.31561600	-0.15794000	-0.53719100
N	2.05516900	-0.93523700	0.54256300
N	1.10842400	0.50478600	-0.96709300
O	0.09784700	-1.81484500	1.44226700
N	-2.08067100	0.85270500	0.40599700
N	3.44687000	0.43738200	-0.75824000
H	4.26948200	0.04913400	-0.31532100
H	3.55579600	1.14468700	-1.47433400
N	-1.09726600	-0.56698600	-1.00076000
H	-2.82835800	1.39858300	0.82387200
O	-0.22632000	1.90075000	1.33422600
H	1.08979600	1.42914400	-1.38822800
O	-3.42278900	-0.56137100	-0.87699600
H	-1.01403400	-1.47476900	-1.44741300

TS (NH_2CH_3 addition to at guanine)

SCF Done: E(UB3LYP) = -714.762904444 a.u.

1 2

C	3.77372800	-1.56239600	-0.20838900
H	4.50457100	-1.56117700	-1.01903100
H	3.34105500	-2.56591500	-0.12535100
N	2.75119700	-0.53121000	-0.49067800
H	2.32097000	-0.71301400	-1.39956400
C	-0.32674200	0.52950900	0.23735800
C	-0.56334800	-0.88236700	0.20362000
C	-2.77353700	-0.65233200	-0.13194600
C	-1.44101700	1.41024800	0.06602300
H	-3.47652200	1.28658700	-0.23751000
H	0.77774100	-2.47946600	0.46686500
N	-2.64731600	0.71155500	-0.10621200
N	-1.73729200	-1.48823600	0.02545700
O	-1.43182400	2.65569900	0.06123800
N	0.62797500	-1.48269500	0.36623100
N	-3.99584400	-1.15738000	-0.32283400
H	-4.80243200	-0.56156400	-0.45715300
H	-4.11463700	-2.16112100	-0.35066800
H	4.28479500	-1.31337700	0.72461300
C	1.67938900	-0.47572800	0.52049700
H	2.16202700	-0.57457200	1.49988100
N	0.97211900	0.80801700	0.42946800
H	1.98726600	1.78775900	0.05762300
O	2.97876700	2.00692800	-0.36393000
H	3.55930100	2.37105800	0.32810800
H	3.19361000	0.96182700	-0.49928700

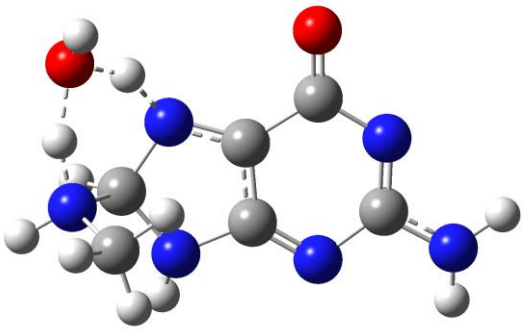


TS (Guanine radical + NH_2CH_3 at C8)

SCF Done: E(U3LYP) = -714.301195379 a.u.

0 2

C	-2.42984200	-1.23059700	1.49665800
H	-3.33325300	-1.15070200	2.10199400
H	-1.67764800	-0.53730700	1.87270100
N	-2.79450100	-0.85369200	0.10105300
H	-3.46696300	-1.52525100	-0.27801700
C	0.21307200	0.49092100	-0.33331900
C	0.58251100	-0.88386300	-0.37651700
C	2.69345200	-0.35824100	0.15330700
C	1.22182000	1.46261100	0.01944100
H	-0.53639500	-2.54466400	-1.04692900
N	2.47095400	0.96241700	0.25856300
N	1.79154000	-1.35199500	-0.15184100
O	0.96644000	2.69938100	0.10010500
N	-0.54152600	-1.59920400	-0.68348400
N	3.95307700	-0.78726900	0.37279500
H	4.67111100	-0.12854100	0.63754400
H	4.16545200	-1.77380300	0.33866800
H	-2.05375700	-2.25159800	1.52626000
C	-1.64308600	-0.69827400	-0.88948200
H	-2.10261200	-0.81630400	-1.87431700
N	-1.08084800	0.63194700	-0.69565800
H	-3.22087500	0.15693300	0.12780300
O	-3.19176900	1.72829800	0.04556500
H	-1.88190300	1.36758900	-0.35257100
H	-3.17896800	2.07144800	0.95099200

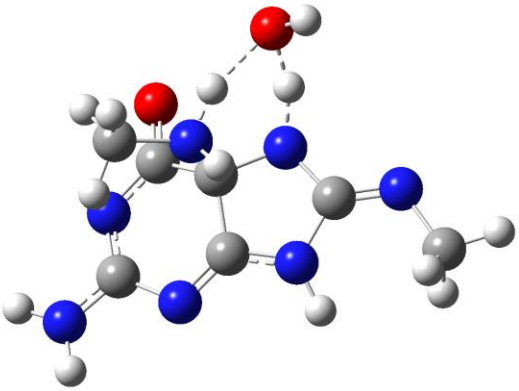


TS (C5 addition of NH_2CH_3 to 10)

SCF Done: E(R3LYP) = -808.368742364 a.u.

0 1

C	0.09844000	0.38871700	0.11391900
C	0.10546000	-1.08718800	-0.22401300
C	2.31733200	-1.20759200	0.13679400
C	1.31546900	0.70539600	1.00791200
C	-2.02062700	-0.43751600	0.24262000
H	-1.47915700	-2.42321800	-0.43627600
N	2.40039000	-0.08855600	0.87984000
N	1.16217700	-1.83392200	-0.31261100
O	1.27560900	1.69492600	1.75645600
N	-1.21230900	0.61178200	0.64588700
N	-1.17938600	-1.46365400	-0.29869500
N	3.44402300	-1.86091100	-0.12885800
H	4.32917200	-1.49920200	0.20209000
H	3.41741300	-2.73509200	-0.63763500
N	-3.29242400	-0.49439000	0.37351900
C	-3.97381700	-1.70265300	-0.09024800
H	-3.68521300	-2.58873200	0.49061600
H	-5.05021700	-1.57171400	0.03174700
H	-3.78489700	-1.91500300	-1.15037300
H	-1.53973100	1.76520800	0.41584500
N	0.21611400	1.26286600	-1.17725800
C	1.54703200	1.59909300	-1.76301800
H	2.07327600	0.68935700	-2.05144900
H	1.36072600	2.20752400	-2.64891700
H	2.12576300	2.17630800	-1.04373500
H	-0.35509200	0.80868400	-1.89808200
O	-1.51432400	2.97562200	-0.02946400
H	-0.32513100	2.14428300	-0.90010500
H	-2.28300800	3.09515600	-0.60622900

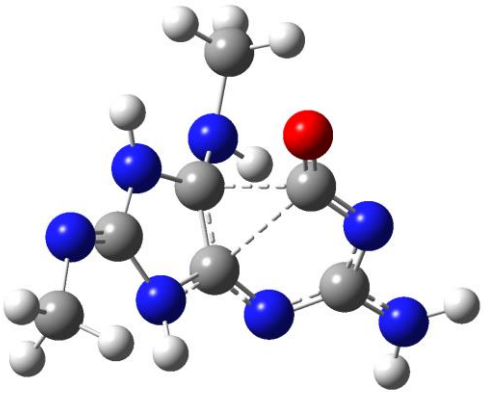


TS (Acyl Group Migration, 11→12)

SCF Done: E(R3LYP) = -731.909722031 a.u.

0 1

C	0.04952900	0.79698100	-0.54290900
C	0.03143700	-0.61026200	-0.68062000
C	2.06422800	-1.30708900	-0.03641100
C	0.93389500	0.19775900	1.26297400
C	-2.09027600	0.06605000	-0.19874300
N	1.98686000	-0.56122100	1.12155000
N	1.07773400	-1.42734000	-0.92137300
O	0.47187700	0.88996300	2.14956300
N	-1.27910000	-1.02184700	-0.55692700
N	3.21006500	-1.98078600	-0.21904000
H	3.91131400	-1.97778000	0.50765700
H	3.29129700	-2.63753600	-0.98276000
N	-1.27589400	1.18920500	-0.33720900
H	-1.52543500	-1.97724000	-0.32190600
N	-3.31479900	0.08527000	0.17559500
C	-3.99261400	-1.20831300	0.24870400
H	-3.47064700	-1.92293000	0.89999100
H	-4.99365500	-1.06378000	0.65876600
H	-4.10475700	-1.67387800	-0.73950900
N	0.96941200	1.67120400	-1.10779500
H	1.83832900	1.19205800	-1.32833500
C	1.22344800	2.95262600	-0.43251000
H	1.86792700	3.55269200	-1.07681900
H	0.28575800	3.49541100	-0.29413100
H	1.71089400	2.83228900	0.54326500
H	-1.52387300	2.05307900	0.13073900

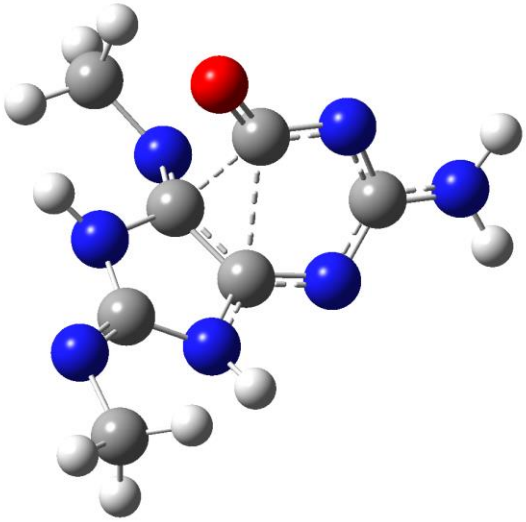


TS (Acyl Group Migration (11AN→12AN)

SCF Done: E(R3LYP) = -731.424705424 a.u.

-1 1

C	0.11499900	0.78764500	-0.52010400
C	0.05984700	-0.65012200	-0.65477300
C	2.11348700	-1.26037500	-0.01190800
C	0.93520500	0.32086800	1.11996100
C	-2.05109900	0.02557200	-0.15920700
N	2.04642200	-0.42138400	1.06268900
N	1.09243600	-1.48881900	-0.84800000
O	0.58193700	1.08782600	2.02863400
N	-1.25039000	-1.05778400	-0.55777900
N	3.27649300	-1.92461300	-0.20120700
H	3.95518900	-1.91654400	0.54955100
H	3.28192100	-2.71622800	-0.83198800
N	-1.25872800	1.15084700	-0.28700200
H	-1.48912500	-2.00619100	-0.28351200
N	-3.27327900	0.01076900	0.24070500
C	-3.93467900	-1.29638500	0.26816300
H	-4.07041200	-1.71190600	-0.73896200
H	-3.38286400	-2.03611100	0.86426300
H	-4.92451200	-1.18419000	0.71500500
N	1.02300600	1.61308800	-1.08483700
C	0.94176200	2.99484500	-0.62526200
H	1.61917800	3.61087800	-1.22515700
H	-0.06104000	3.44566800	-0.71674600
H	1.24827000	3.12120200	0.42939900
H	-1.50095200	1.98380100	0.23586400

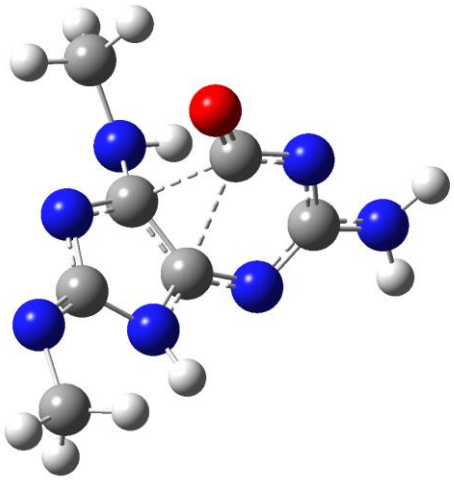


TS (Acyl Group Migration (11AN'→12AN')

SCF Done: E(R3LYP) = -731.446469687 a.u.

-1 1

C	-0.00916000	0.79355400	-0.48756200
C	-0.00687800	-0.63666900	-0.61067400
C	2.06039000	-1.29677400	-0.04364300
C	0.93063500	0.24951900	1.18444800
C	-2.07612800	0.13687000	-0.13577600
N	2.02006200	-0.49892100	1.07803900
N	1.03018800	-1.47048800	-0.87011400
O	0.55785700	0.95822000	2.12165900
N	-1.30161500	-1.01937200	-0.43980300
N	3.21170600	-1.96251200	-0.26438800
H	3.91087100	-1.97733700	0.46650600
H	3.22777500	-2.69642000	-0.96120200
N	-1.28698000	1.24647400	-0.23654100
H	-1.57203000	-1.96177600	-0.17924000
N	-3.34176600	0.12164600	0.18704500
C	-3.99053300	-1.18888200	0.17494700
H	-3.96092300	-1.67442600	-0.81206900
H	-3.54953800	-1.89434300	0.89651000
H	-5.04309200	-1.07226500	0.44481100
N	0.92319100	1.63560800	-1.12337300
C	1.14409800	2.96565200	-0.53484800
H	1.85433500	3.50173800	-1.16781400
H	0.20956200	3.52871500	-0.51619500
H	1.54791000	2.91824000	0.48532400
H	1.81424800	1.15545500	-1.22730700

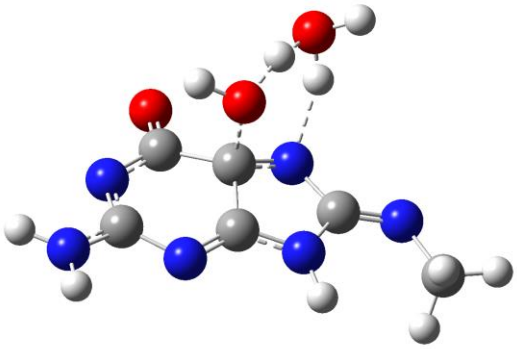


TS (C5 addition of H_2O to 10)

SCF Done: E(R3LYP) = -788.911187173 a.u.

0 1

C	-0.14438400	0.46626000	-0.11942900
C	-0.21401100	-1.00378700	0.17249600
C	-2.45256700	-0.95257900	0.06533900
C	-1.42921900	0.98030900	-0.75280100
C	1.89197000	-0.37318700	-0.33636100
H	1.34545500	-2.39209600	0.28344300
N	-2.54906300	0.24948800	-0.53424800
N	-1.30594300	-1.68791800	0.33826800
O	-1.43155100	2.04636900	-1.39406200
N	1.10234000	0.72772700	-0.63489200
N	1.05566800	-1.42767300	0.16714600
N	-3.58910700	-1.57413000	0.37623400
H	-4.47762600	-1.12763800	0.19236000
H	-3.56781400	-2.49659100	0.79040500
N	3.15886300	-0.44769600	-0.51350000
C	3.83100900	-1.69696100	-0.15818000
H	3.55962800	-2.51628800	-0.83663800
H	4.91009800	-1.55476000	-0.23693200
H	3.61523900	-2.02135700	0.86768400
H	1.55035700	2.17831600	0.07238900
O	1.34651000	2.83916000	0.83894700
H	0.54140500	2.13530300	1.29348300
H	2.12815600	2.88437000	1.41647100
O	-0.22460500	1.12988600	1.41595400
H	-1.13382300	1.38850200	1.65118400

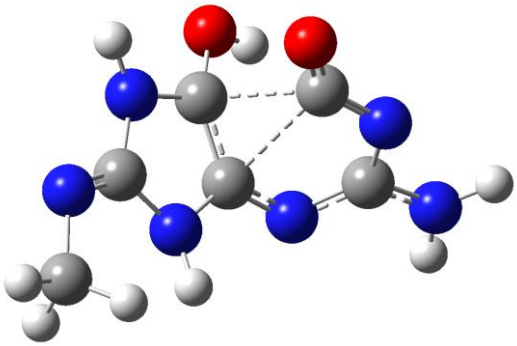


TS (Acyl Group Migration, 15→16)

SCF Done: E(R3LYP) = -712.460426100 a.u.

0 1

C	-0.00596500	0.91245000	-0.78136400
C	0.16161700	-0.47267300	-0.63674500
C	2.27248500	-0.83913700	0.05660300
C	1.07256300	0.82737400	1.09966500
C	-2.02575200	0.04105500	-0.20936100
N	2.15384600	0.11963500	1.04675200
N	1.28925800	-1.20791600	-0.75356200
O	0.56440300	1.66869900	1.80392500
N	-1.08890700	-0.99309900	-0.34543600
N	3.46529800	-1.44558500	-0.01465300
H	4.19547300	-1.20616300	0.64047800
H	3.60492100	-2.20567700	-0.66585700
N	-1.35270600	1.19427200	-0.61799400
H	-1.20514700	-1.88827600	0.11712700
N	-3.24244900	0.00248900	0.18998200
O	0.73725800	1.84080300	-1.43671100
C	-3.76259000	-1.31234100	0.56043500
H	-3.16149900	-1.80077800	1.34018300
H	-4.77520300	-1.19855200	0.95117500
H	-3.81486400	-1.99361800	-0.29927200
H	-1.69035800	2.11632200	-0.36452100
H	1.58886100	1.47179000	-1.72805100

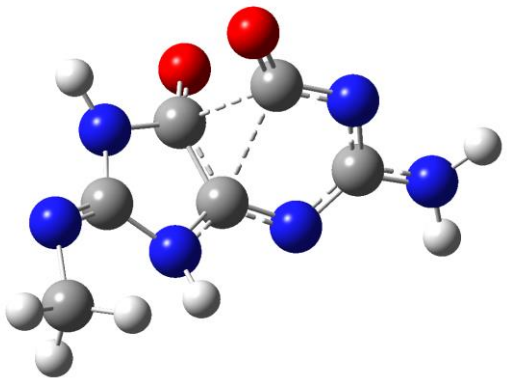


TS (Acyl Group Migration (15AN→16AN)

SCF Done: E(R3LYP) = -712.020526856 a.u.

-1 1

C	0.07910300	0.88211800	-0.83681900
C	0.16935600	-0.53216700	-0.59211000
C	2.28112000	-0.78294900	0.10574800
C	0.97421600	0.88926500	0.92455900
C	-1.99506900	0.06048600	-0.22650100
N	2.13501100	0.25756700	0.99434100
N	1.28642000	-1.28400900	-0.62844500
O	0.51038400	1.78337800	1.63503700
N	-1.08813800	-1.00933900	-0.30733200
N	3.50053000	-1.35071500	0.04023100
H	4.19302000	-1.10791500	0.73635100
H	3.60457800	-2.22311000	-0.46190400
N	-1.30955700	1.16939600	-0.69827300
H	-1.23336700	-1.86303100	0.22364100
N	-3.21311700	0.04845900	0.18422600
O	0.86595000	1.65304400	-1.51677700
C	-3.74521200	-1.25354400	0.59403600
H	-3.12608800	-1.74082800	1.35988000
H	-4.74345200	-1.11519300	1.01347200
H	-3.83410600	-1.94410400	-0.25483600
H	-1.63038900	2.10404200	-0.46941200

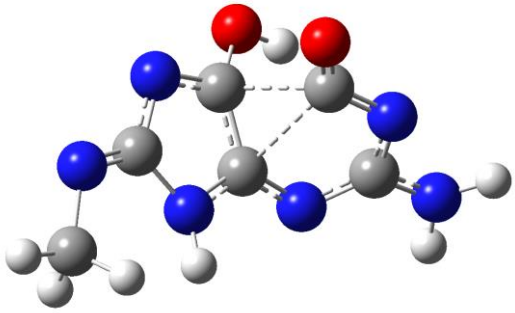


TS (Acyl Group Migration (15AN'→16AN')

SCF Done: E(R3LYP) = -712.003195831 a.u.

-1 1

C	-0.04718700	0.84662300	-0.77777500
C	0.10999200	-0.54700200	-0.50602200
C	2.25801200	-0.81544300	0.09796400
C	1.02490900	0.90040100	0.95280000
C	-2.02439100	0.13812000	-0.20453400
N	2.17474600	0.25089700	0.96826700
N	1.22353400	-1.31173700	-0.57815600
O	0.60547700	1.81152100	1.66290000
N	-1.13981600	-0.97562400	-0.17063400
N	3.46391500	-1.40513500	-0.00796400
H	4.19381200	-1.15111800	0.64437900
H	3.53410400	-2.28911000	-0.49547600
N	-1.34229500	1.24314100	-0.64714000
H	-1.32045900	-1.82237600	0.35855800
N	-3.28198500	0.10636100	0.13554800
O	0.77234600	1.62064200	-1.56689600
C	-3.80178400	-1.20162000	0.53132200
H	-3.29941900	-1.60828200	1.42238600
H	-4.86312100	-1.10927600	0.77405400
H	-3.71394400	-1.95537800	-0.26549300
H	1.64243700	1.19643900	-1.66841500

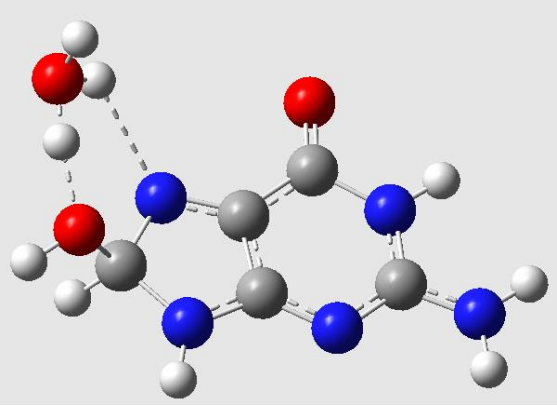


TS (H_2O addition to Guanine at C8)

SCF Done: E(UB3LYP) = -695.313778276 a.u.

1 2

C	-0.03272500	0.29379800	-0.40628000
C	0.44975300	-1.03593200	-0.18384300
C	2.56495800	-0.38069900	0.18228100
C	0.90599400	1.37133300	-0.31909800
H	-0.59033800	-2.86340600	-0.32351900
N	2.20320200	0.92575700	-0.01174200
N	1.69759600	-1.40062800	0.10583100
O	0.68897100	2.58812200	-0.48240900
N	-0.61327300	-1.85123600	-0.32152100
N	3.84559900	-0.63555600	0.46964800
H	4.53828400	0.09987600	0.51803900
H	4.13568400	-1.59499500	0.60121300
C	-1.78820400	-1.05387600	-0.62717700
H	-2.26367100	-1.37649800	-1.55717600
N	-1.34650900	0.32541600	-0.68182700
H	-2.93037400	1.53937200	0.24944300
O	-3.66659500	1.11689000	0.75090500
H	-3.63244800	1.43843800	1.67206300
H	-3.40454700	0.08801600	0.70142900
O	-2.78935200	-1.18044900	0.42545700
H	-3.44178500	-1.85734500	0.17416200
H	2.91409300	1.64981500	0.05882400

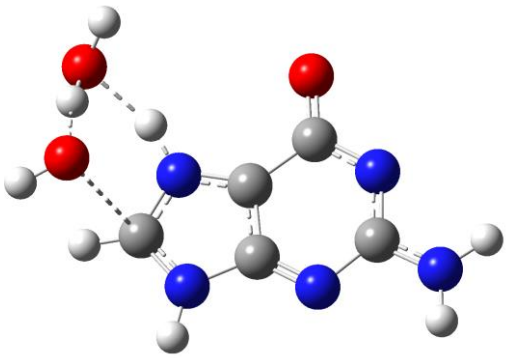


TS (Guanine radical + H_2O at C8)

SCF Done: E(U3LYP) = -694.839942476

0 2

C	0.51371500	0.33935400	-0.50649700
C	1.03529700	-0.94569400	-0.79011100
C	3.03982300	-0.31817900	-0.01651200
C	1.38958600	1.34217800	0.08984000
H	0.00253000	-2.62938700	-1.65533600
N	2.66875700	0.92771500	0.30620600
N	2.26321200	-1.33561900	-0.57314600
O	0.97845100	2.48929400	0.37051600
N	-0.02504600	-1.66982900	-1.32015500
N	4.30677700	-0.67808600	0.20848500
H	4.95840300	-0.01615300	0.61041000
H	4.61994100	-1.61166900	-0.02469800
C	-1.11017500	-0.88590900	-1.33596800
H	-2.05340500	-1.15496500	-1.77879000
N	-0.78835600	0.34630000	-0.87704700
H	-3.05689800	0.32071600	0.35088200
O	-3.04015600	1.34541900	0.07909400
H	-1.55380200	1.02286200	-0.58859900
H	-2.93834400	1.85092800	0.89855900
O	-2.83949200	-1.10417400	0.58433700
H	-3.51007700	-1.61535600	0.10724900

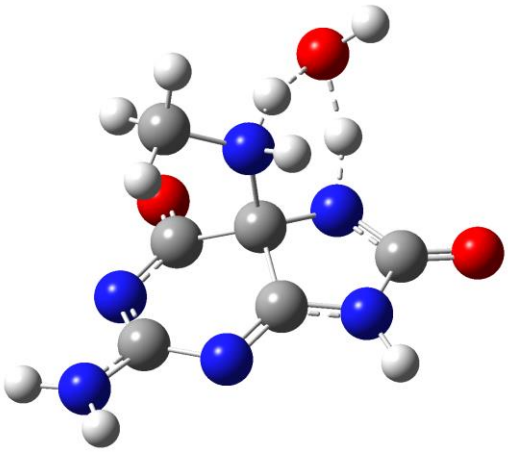


TS (C5 addition of NH_2CH_3 of 30)

SCF Done: E(R3LYP) = -788.950862804 a.u.

0 1

C	-0.27856100	0.15775500	0.09030900
C	0.27438000	-1.20075000	-0.29542200
C	2.36938400	-0.50664200	0.11854600
C	0.71828400	0.83936000	1.05476900
C	-1.93879900	-1.39902500	0.16486100
N	2.02229200	0.51796800	0.91634200
N	1.52856300	-1.49699500	-0.38479100
O	0.29776800	1.68510900	1.85714700
N	-0.78509600	-2.02374800	-0.39806900
N	3.65593300	-0.68165100	-0.15533000
H	4.34506500	-0.03620900	0.20903400
H	3.95572900	-1.47948300	-0.70105800
O	-3.02722700	-1.96527600	0.25317600
N	-1.60325600	-0.14778400	0.58427300
H	-0.73371700	-3.02302500	-0.57439600
H	-1.37139800	1.66431800	-0.82805800
H	-2.31481300	0.78050900	0.40442300
O	-2.66629800	1.99129700	-0.06346600
H	-3.41008800	1.88049900	-0.67417000
N	-0.48774500	1.06939200	-1.13131300
H	-0.81037600	0.47743200	-1.90404900
C	0.61978500	1.93323600	-1.63558800
H	0.22771100	2.46806900	-2.50158000
H	0.90443400	2.64940800	-0.86637800
H	1.47183400	1.32557000	-1.94125400

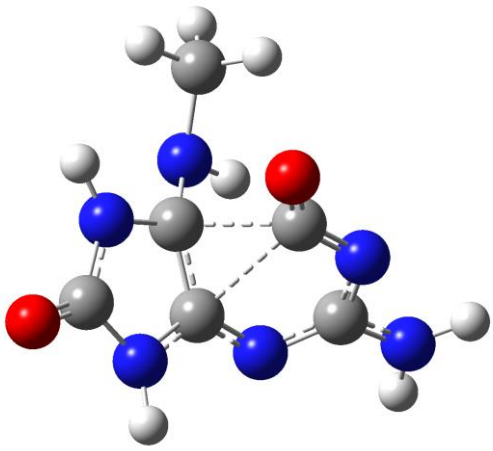


TS (Acyl Group Migration (31→32)

SCF Done: E(R3LYP) = -712.492775143

0 1

C	-0.51369000	0.48914200	-0.50713200
C	-0.07255500	-0.85378200	-0.56544100
C	2.11102900	-0.75344500	-0.04672000
C	0.63800900	0.44882200	1.25119800
C	-2.28012600	-0.87549000	-0.01287000
N	1.85840300	0.05488500	1.04315800
N	1.17151200	-1.30026200	-0.81419100
O	0.02806800	1.04168400	2.11318700
N	-1.16500400	-1.65399100	-0.30408300
N	3.40107500	-1.03495200	-0.26935200
H	4.10847300	-0.68685800	0.36190100
H	3.65817300	-1.68547100	-0.99886500
N	-1.88069400	0.42303600	-0.19975000
H	-1.11430000	-2.64017600	-0.07257500
O	-3.38779300	-1.28383200	0.35237700
N	-0.00362400	1.55928400	-1.23927300
H	0.95124900	1.36675100	-1.53039200
C	-0.12307000	2.91434200	-0.67748800
H	0.23452900	3.62163000	-1.42722900
H	-1.17061100	3.14362800	-0.46996000
H	0.45969900	3.04984600	0.24208100
H	-2.47867000	1.21429900	0.00567300

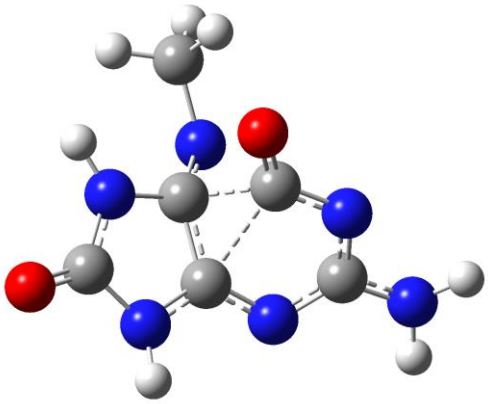


TS (Acyl Group Migration (31AN→32AN)

SCF Done: E(R3LYP) = -712.008207358

-1 1

C	-0.46819000	0.48463900	-0.48561000
C	0.01767200	-0.87774400	-0.51756800
C	2.18891500	-0.60973800	-0.04139300
C	0.58696100	0.53954500	1.10289300
C	-2.18384200	-0.98806000	0.02930100
N	1.88460900	0.26369600	0.96231500
N	1.27353300	-1.29342300	-0.74116000
O	0.03887600	1.21855200	1.97996600
N	-1.04514600	-1.72356100	-0.28992500
N	3.49883100	-0.81574300	-0.29778100
H	4.17794900	-0.46325000	0.36414500
H	3.76266500	-1.60217500	-0.87759600
N	-1.84965500	0.31747000	-0.11096000
H	-0.94403700	-2.69198000	-0.00182000
O	-3.27414700	-1.46927700	0.38463400
N	-0.00405100	1.52922900	-1.19919500
C	-0.59036800	2.81452900	-0.83693100
H	-0.31481600	3.14509900	0.18093000
H	-0.22306900	3.57945000	-1.52781700
H	-1.69233400	2.84173700	-0.88831300
H	-2.49793300	1.07421200	0.06645400

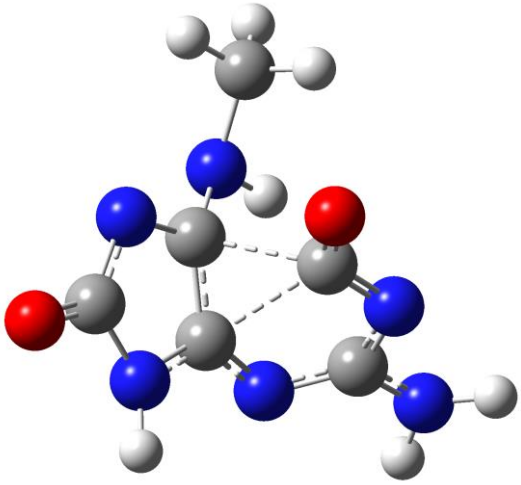


TS (Acyl Group Migration (31AN'→32AN')

SCF Done: E(R3LYP) = -712.036772644

-1 1

C	-0.57069800	0.50428800	-0.49731500
C	-0.06454100	-0.83231900	-0.55745300
C	2.11213600	-0.71065900	-0.05172100
C	0.53506300	0.35943900	1.19481100
C	-2.25693600	-0.81121900	-0.05101100
N	1.81129800	0.05716200	1.05318700
N	1.19327400	-1.25519200	-0.84434200
O	-0.07074600	0.89675200	2.11594600
N	-1.14346900	-1.63641700	-0.32285700
N	3.42107400	-0.92958000	-0.28835600
H	4.08666300	-0.69779900	0.43760400
H	3.67648600	-1.64187400	-0.96073000
N	-1.92506100	0.48404100	-0.19626500
H	-1.08990400	-2.61372000	-0.05541100
O	-3.37717000	-1.29521600	0.27757200
N	-0.01084600	1.59293000	-1.17295300
C	-0.20694800	2.93437000	-0.60312300
H	0.26716000	3.05025600	0.38060000
H	0.22755600	3.66216300	-1.29131200
H	-1.27271300	3.14765400	-0.50610300
H	0.97572900	1.42702800	-1.35680700

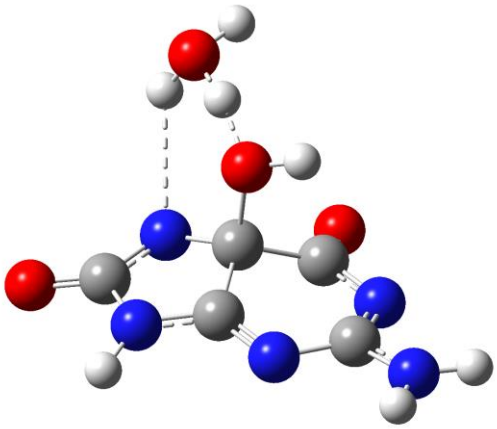


TS (C5 addition of H2O to 30)

SCF Done: E(R3LYP) = -769.496483299

0 1

C	0.29489700	-0.20897500	-0.04464700
C	-0.36047100	1.13007500	0.24977800
C	-2.39472000	0.20351200	0.09028000
C	-0.68855600	-1.08933900	-0.83364800
C	1.80488900	1.37992300	-0.34719500
H	0.53019600	3.02703500	0.31473200
N	-2.00748400	-0.88455700	-0.60359200
N	-1.63468600	1.31761900	0.42168200
O	-0.26522100	-1.99359700	-1.57406300
N	1.57932100	0.08244800	-0.57571900
N	0.63187400	2.02086000	0.23026900
N	-3.67832700	0.28692900	0.43305200
H	-4.31582700	-0.46067300	0.19254500
H	-4.02603000	1.10707600	0.91196600
O	2.56946200	-2.18130500	0.98959000
H	2.89455800	-1.72720400	0.18170300
H	2.44234900	-3.12548100	0.77752800
O	0.49809000	-0.88690100	1.27361900
H	1.61945500	-1.70700000	1.17716900
H	-0.30182500	-1.34893900	1.58396400
O	2.82092100	2.05941900	-0.58500200

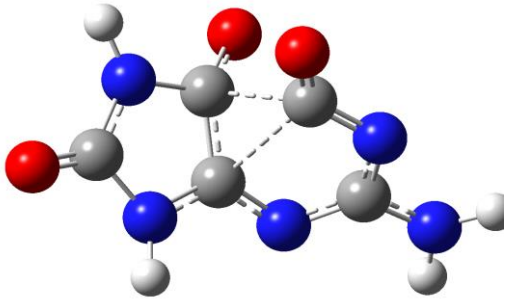


TS (Acyl Group Migration (34AN→35AN)

SCF Done: E(R3LYP) = -692.603338517

-1 1

C	0.47013500	0.44957400	0.87530500
C	0.07623400	-0.80296400	0.28372000
C	-2.10209700	-0.48078900	-0.12325100
C	-0.58424200	1.14081900	-0.65278600
C	2.28474700	-0.52619300	-0.16839900
N	-1.84040200	0.74137000	-0.69970900
N	-1.15799500	-1.33534900	0.27589300
O	-0.02701500	2.11469200	-1.15403200
N	1.18568200	-1.36853200	-0.30204700
N	-3.39556300	-0.83128700	-0.03252900
H	-4.09930300	-0.24744800	-0.46380000
H	-3.64049800	-1.76869800	0.25821000
N	1.86651400	0.53025100	0.57909200
H	1.15448000	-2.09901900	-1.00761200
O	-0.05029800	1.10321300	1.86195900
O	3.40879600	-0.72372000	-0.66031200
H	2.45713900	1.32382900	0.79984400

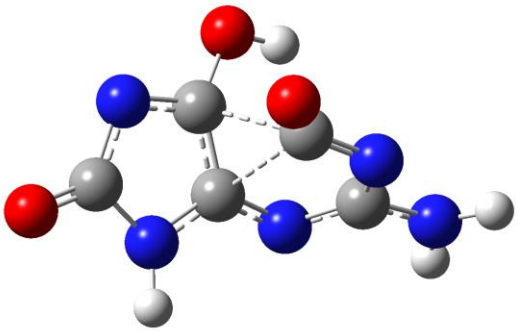


TS (Acyl Group Migration (34AN'→35AN')

SCF Done: E(R3LYP) = -692.592408687 a.u.

-1 1

C	0.57735900	0.40892400	0.84940800
C	0.10448700	-0.79618300	0.25639900
C	-2.08025600	-0.48921100	-0.14448300
C	-0.56593000	1.12640100	-0.71392800
C	2.29910400	-0.46661300	-0.13495900
N	-1.81434500	0.72740400	-0.74492600
N	-1.14063000	-1.32885700	0.27869400
O	0.02979600	2.06162400	-1.22741300
N	1.20827500	-1.33418400	-0.34699800
N	-3.37755600	-0.82566200	-0.04966200
H	-4.07440100	-0.24691100	-0.49857300
H	-3.63070800	-1.75583400	0.25703200
N	1.92229300	0.57411800	0.63959900
H	1.18756700	-2.05004500	-1.06678900
O	0.01524300	1.09902200	1.89107700
O	3.43602400	-0.68625600	-0.63624200
H	-0.92581500	0.86802400	1.97738100

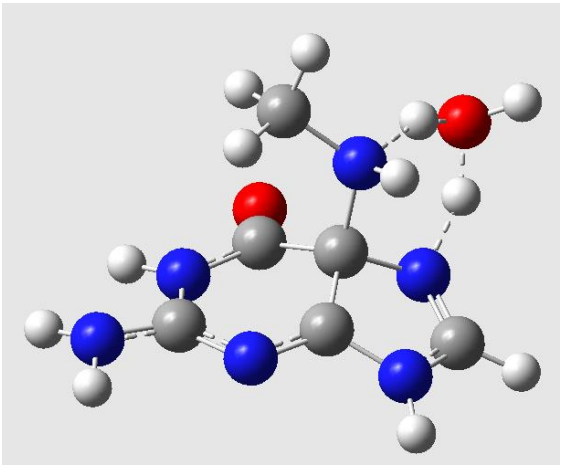


TS(NH_2CH_3 + Gradcat at C5)

SCF Done: E(UB3LYP) = -714.722412223 a.u.

1 2

C	-0.51057200	0.10924700	-0.02196700
C	0.43349800	1.22207900	0.32377600
C	2.31396100	0.05595500	-0.03391200
C	0.21949000	-0.84839200	-0.95697600
C	-1.48437200	2.10115900	-0.36900800
N	1.58641500	-0.85392400	-0.79194500
N	1.75974900	1.15545400	0.45047400
O	-0.33989700	-1.56959000	-1.79018300
N	-0.29951600	2.39255100	0.21893500
N	3.61888000	-0.23618000	0.18703200
H	4.07400700	-0.92149200	-0.40380800
H	4.20075200	0.51894600	0.52781200
N	-1.65739600	0.82291100	-0.62495600
H	0.06516900	3.32952800	0.35326500
H	-2.43815200	-1.04377800	0.61424900
H	-2.77935300	-0.00780200	-0.51033100
O	-3.28227400	-0.92292100	-0.07752800
H	-4.06747200	-0.65478200	0.43067200
N	-1.09511600	-0.67516700	1.15844500
H	-1.27190600	0.02150600	1.88669300
C	-0.27545200	-1.76050700	1.74100900
H	-0.82284500	-2.15914200	2.59768800
H	-0.14902600	-2.56490000	1.01357700
H	0.70492000	-1.41239300	2.08260200
H	-2.20289600	2.87411400	-0.60769300
H	2.09373900	-1.55647100	-1.32646900

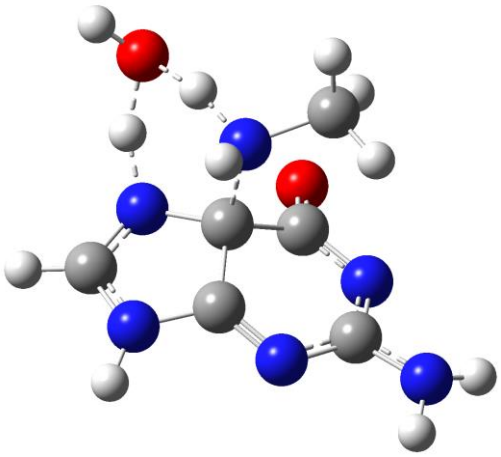


TS (Guanine radical + NH_2CH_3 at C5)

SCF Done: E(UB3LYP) = -714.264111042 a.u.

0 2

C	-0.27972700	-1.86082500	-1.67873500
H	-0.84194200	-2.27068600	-2.51955900
H	-0.18500500	-2.62322700	-0.90608600
N	-1.04855000	-0.70615500	-1.14680100
H	-1.19280700	-0.02617700	-1.89980700
C	-0.44792900	0.12223400	0.07893800
C	0.46871000	1.22635800	-0.29990500
C	2.29121800	-0.01046700	0.07742500
C	0.30519100	-0.83784100	1.00846900
H	0.06490500	3.32508500	-0.45534300
N	1.63797400	-0.90553500	0.86522300
N	1.78681800	1.14297600	-0.41775000
O	-0.34508500	-1.52343100	1.83937300
N	-0.28238800	2.39219000	-0.25545000
N	3.59370700	-0.28369300	-0.19830000
H	4.05447700	-0.99770400	0.34900900
H	4.16827100	0.45495000	-0.58109500
H	0.70320300	-1.53520300	-2.02146700
C	-1.48533400	2.12786600	0.27307400
H	-2.25033500	2.87503400	0.42605100
N	-1.60241400	0.83684500	0.60208300
H	-2.04314100	-0.98902600	-0.77473600
O	-3.35311700	-0.94733400	0.08560600
H	-2.52989100	0.25483400	0.57260500
H	-4.07091900	-0.64210600	-0.48804600

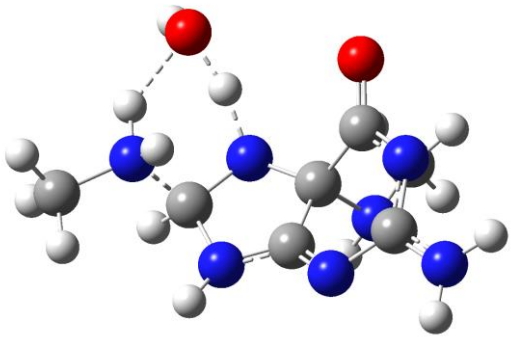


TS (C8 addition of NH_2CH_3 to 42)

SCF Done: E(R3LYP) = -809.566171640 a.u.

0 1

C	-0.35575600	0.47788500	0.40379200
C	-0.37689800	-1.03091600	0.55245100
C	-2.36824300	-1.12533200	-0.46051100
C	-1.12449800	0.77820700	-0.90433100
C	1.78646600	-0.35464800	0.76867500
N	-2.21493500	0.01034300	-1.16069200
N	-1.38815700	-1.79451300	0.25575400
O	-0.79062800	1.72805600	-1.63555300
N	0.82392900	-1.41945400	1.00152200
N	-3.54056200	-1.75878700	-0.53980300
H	-4.29216200	-1.36814700	-1.09132800
H	-3.66592900	-2.65298400	-0.08564200
N	1.05282500	0.82101500	0.47928200
H	1.09333100	-2.39481100	1.08984100
C	-1.38440100	2.49219000	1.44578400
H	-1.83039400	2.81419200	2.39019100
H	-2.07897700	2.75851800	0.64474300
N	-1.20242300	1.03215200	1.50178300
H	-0.69478100	0.81751800	2.35951500
C	3.78436000	-1.70278400	-0.17267900
H	3.36256100	-2.64439900	0.18133200
H	4.43393800	-1.26862500	0.58786600
N	2.68142600	-0.74571900	-0.45907100
H	2.06715400	-1.11723400	-1.19074400
H	4.34917400	-1.87425100	-1.08931400
H	-0.45193400	3.05393600	1.29913900
H	2.51267900	-0.27858100	1.58334100
H	3.03730700	0.16988700	-0.81240300
O	2.55437400	1.97206200	-1.13846500
H	3.06706300	2.63075000	-0.64828000
H	1.73009800	1.53042800	-0.37663500

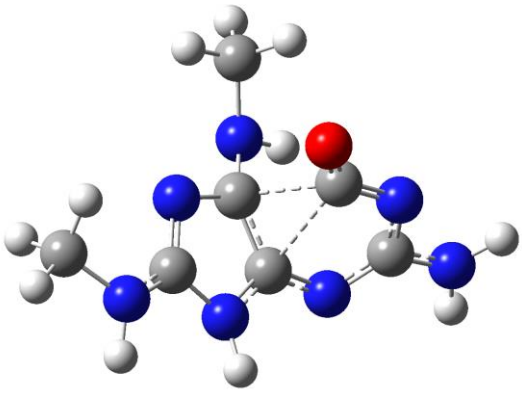


TS (Acyl Group Migration (46→47)

SCF Done: E(R3LYP) = -731.919831368 a.u.

0 1

C	-0.11836600	0.54210000	-0.53648300
C	0.28924300	-0.82341500	-0.59700100
C	2.44140600	-0.83226500	0.01265000
C	0.92215000	0.39371800	1.21385300
C	-1.88235600	-0.64726600	-0.16331100
N	2.16162600	-0.01728200	1.08644200
N	1.51853000	-1.33574500	-0.80346100
O	0.32299900	0.99106400	2.09046000
N	-0.85346500	-1.55432700	-0.38259300
N	3.73181700	-1.16479800	-0.15467200
H	4.41690800	-0.87022600	0.52605200
H	3.98809700	-1.84553300	-0.85620600
N	-1.49346900	0.60803400	-0.28998800
H	-0.87282000	-2.53928700	-0.13909300
N	-3.11285300	-1.07445600	0.18558400
H	-3.31683700	-2.04927800	0.00227700
C	-4.24653700	-0.15489700	0.22430000
H	-4.46813800	0.26696500	-0.76272300
H	-5.11776300	-0.70653800	0.57777900
H	-4.04528600	0.66306300	0.91910600
N	0.51543900	1.58978100	-1.21232500
H	1.48089000	1.35788600	-1.42729200
C	0.41472500	2.94380200	-0.65287200
H	0.83469700	3.64512400	-1.37657600
H	-0.63267100	3.20297300	-0.49412900
H	0.95396200	3.05723700	0.29740000

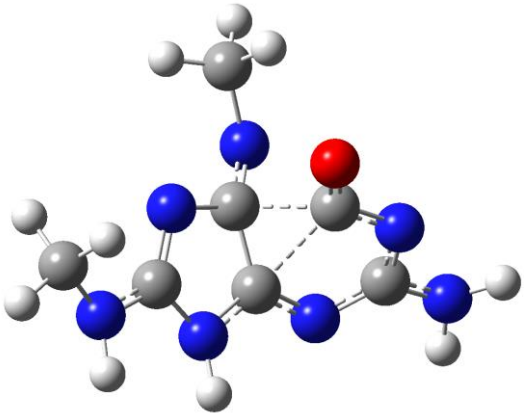


TS (Acyl Group Migration (46AN→47AN)

SCF Done: E(R3LYP) = -731.427380860 a.u.

-1 1

C	-0.05360700	0.56688900	-0.54167400
C	0.33979200	-0.83211100	-0.59029200
C	2.47707100	-0.77918900	0.06981600
C	0.89348700	0.50834000	1.09388000
C	-1.84572900	-0.67276700	-0.23208500
N	2.17528100	0.11280800	1.05220900
N	1.56781800	-1.36189800	-0.72079300
O	0.37868000	1.24055300	1.95501100
N	-0.80634400	-1.57292800	-0.47572400
N	3.78313600	-1.11730900	-0.07854700
H	4.41424600	-0.88217900	0.67714500
H	3.99658900	-1.94928900	-0.61480700
N	-1.47369100	0.58235800	-0.27044700
H	-0.82258400	-2.54432500	-0.17770900
N	-3.09705900	-1.14778100	-0.02614400
H	-3.15438600	-2.13184000	0.21078500
C	-4.14484700	-0.28594400	0.51672100
H	-4.34804800	0.54277700	-0.16547200
H	-5.05209800	-0.88253800	0.61729000
H	-3.87343200	0.12222500	1.49756300
N	0.59243100	1.56885000	-1.19169600
C	0.10947100	2.90572100	-0.87297700
H	0.65955500	3.63687900	-1.47491500
H	-0.96198800	3.06357100	-1.07778000
H	0.26787600	3.18596300	0.18547900

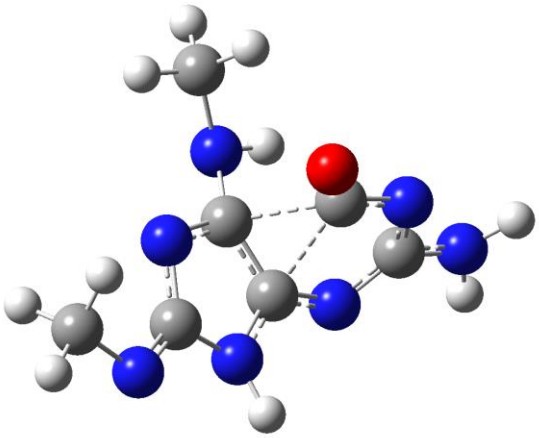


TS (Acyl Group Migration (46'ANa→47'ANa)

SCF Done: E(R3LYP) = -731.447910738 a.u.

-1 1

C	-0.18204300	0.53864800	-0.54608700
C	0.28536700	-0.81511900	-0.59898700
C	2.44079500	-0.77399400	0.02291200
C	0.84669900	0.35215200	1.19030900
C	-1.93435300	-0.73781700	-0.20813800
N	2.12185700	-0.00001800	1.11677600
N	1.54323700	-1.27771700	-0.81999200
O	0.23964300	0.92506200	2.09642600
N	-0.82259200	-1.58936600	-0.44925300
N	3.75065200	-1.04992700	-0.15495200
H	4.38998000	-0.85134300	0.60358500
H	4.00310900	-1.77795700	-0.81143000
N	-1.54509200	0.56425900	-0.33103600
H	-0.79189600	-2.55875000	-0.15158100
N	-3.09751200	-1.25612900	0.07932000
C	-4.15849000	-0.28497500	0.33147400
H	-4.41865400	0.30392000	-0.56079300
H	-5.06286300	-0.81371200	0.64506200
H	-3.90233700	0.43164700	1.12553700
N	0.45683600	1.61470700	-1.17643800
C	0.21738500	2.96094000	-0.63726500
H	0.72843400	3.68118400	-1.27933500
H	-0.85011300	3.18634900	-0.65357700
H	0.58753700	3.07971100	0.38992700
H	1.45579300	1.43876800	-1.25508500

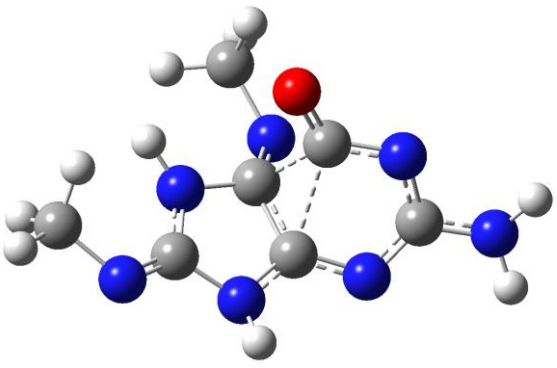


TS (Acyl Group Migration (46'ANb→47'ANb)

SCF Done: E(R3LYP) = -731.426307173 a.u.

-1 1

C	-0.05687000	0.58067700	-0.57806000
C	0.36966100	-0.79885900	-0.66095300
C	2.48152600	-0.70655800	0.07576200
C	0.81073300	0.43387500	1.11493100
C	-1.85931900	-0.84790100	-0.23989400
N	2.10327600	0.09139600	1.11788700
N	1.62818500	-1.25743000	-0.79506200
O	0.19476200	1.06776700	1.98606100
N	-0.73361600	-1.61123600	-0.59215000
N	3.80374900	-0.97453500	-0.04302400
H	4.40094700	-0.75356200	0.74350900
H	4.08201400	-1.74647700	-0.63609300
N	-1.48080400	0.46998800	-0.37432400
H	-0.66130200	-2.57770800	-0.28844600
N	-2.97672400	-1.37252300	0.12383600
C	-4.03445400	-0.42402200	0.47788300
H	-4.36970200	0.16056300	-0.38953100
H	-4.89568700	-0.97562700	0.85978100
H	-3.71762700	0.28558400	1.25480300
N	0.53660800	1.64595200	-1.15223000
C	-0.04089500	2.93034500	-0.77092400
H	0.42871400	3.72287900	-1.36170100
H	-1.12762900	3.00646600	-0.94439700
H	0.12835700	3.18417900	0.29129800
H	-2.01320000	1.20493600	0.07529000



TS (C8 addition of H_2O to 42)

SCF Done: E(R3LYP) = -790.121783382 a.u.

0 1

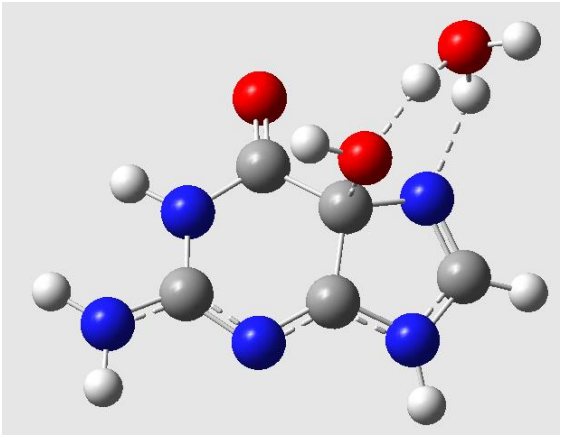
C	-0.15257600	0.46169900	0.40055000
C	-0.54419900	-0.95949400	0.75102900
C	-2.40475800	-0.72330900	-0.46493900
C	-0.67374600	0.70400800	-1.03755700
C	1.64408700	-0.78030400	1.09886900
N	-1.90065500	0.19360500	-1.29840700
N	-1.66416100	-1.50036700	0.44411200
O	-0.01828700	1.38961400	-1.82963200
N	0.54652400	-1.55603800	1.32716400
N	-3.68334000	-1.05683900	-0.55673500
H	-4.28724000	-0.58219200	-1.21664600
H	-4.05549900	-1.80513500	0.01440200
N	1.31221900	0.37299100	0.57124000
H	0.59476300	-2.52497200	1.63026900
C	-0.51839400	2.82363100	1.03217800
H	-0.94920100	3.40441500	1.84984700
H	-1.00099100	3.13873100	0.10461400
N	-0.80769000	1.40200100	1.29842200
H	-0.52734200	1.17211800	2.25125300
H	3.48150500	-0.37415400	-0.85665900
H	0.55323500	3.05258100	0.97293600
H	2.62366700	-1.04255600	1.45940100
O	3.72330500	0.63717300	-0.89406700
H	4.64785900	0.70640500	-0.61928200
H	2.02191300	1.01031700	0.20109000
O	3.01574100	-1.81537200	-0.71659500
H	2.40849500	-1.99173300	-1.45022900

TS(H_2O addition to Guanine Radical Cation at C5)

SCF Done: E(UB3LYP) = -695.279438386 a.u.

1 2

C	0.74243700	0.25660700	0.20461000
C	0.23224400	-1.10404800	-0.02523100
C	-1.92289200	-0.50601100	-0.07228100
C	-0.24243200	1.28027600	-0.27440000
C	2.37808500	-0.99535900	-0.53448600
N	-1.54485400	0.81045900	-0.27632900
N	-1.03772000	-1.49842200	-0.02663100
O	0.03282100	2.43615100	-0.61549600
N	1.33534400	-1.85751300	-0.35235300
N	-3.23827400	-0.75358600	0.05458300
H	-3.92358200	-0.02743000	-0.10990400
H	-3.54760400	-1.71649900	0.04636700
N	2.08798200	0.26583700	-0.30269700
H	1.33813700	-2.84109100	-0.60064300
H	3.34498700	-1.35124600	-0.86461100
H	-2.26562500	1.49485700	-0.49735900
H	2.97093500	1.48480900	0.63212200
O	0.92900200	0.51774100	1.77826600
H	0.08527400	0.80014000	2.17503100
O	2.89678400	1.98537800	1.51364100
H	3.66709400	1.75511800	2.06706800
H	2.03657400	1.48309900	1.87127000

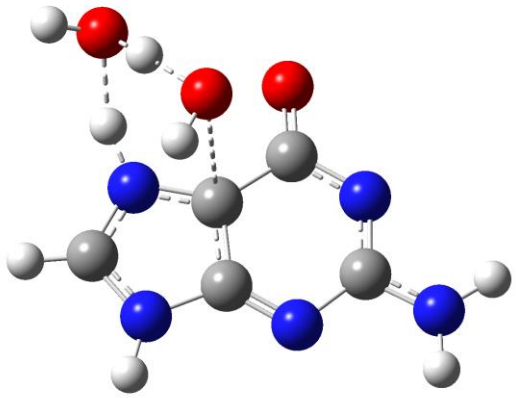


TS (Guanine radical + H_2O at C5)

SCF Done: E(U3LYP) = -694.836110423 a.u.

0 2

C	0.16037300	0.08133500	-0.32502500
C	-0.43074300	1.23314900	0.24776900
C	-2.42120800	0.21236600	0.30580500
C	-0.70746600	-1.03625100	-0.69720100
H	0.51724800	3.11752400	0.70738000
N	-2.00571500	-0.90466200	-0.30058400
N	-1.68722400	1.36751500	0.58301500
O	-0.29010800	-2.01597400	-1.34791800
N	0.58939300	2.17253000	0.33867200
N	-3.69873600	0.28508600	0.69323100
H	-4.32076600	-0.49660200	0.53161200
H	-4.05092700	1.12061300	1.14195400
C	1.70730500	1.62576700	-0.15167600
H	2.67062800	2.11416700	-0.17326400
N	1.46711600	0.38590200	-0.59671100
H	2.26879200	-1.70506500	0.67562500
O	2.94017700	-1.73972900	-0.14742100
H	2.21195500	-0.36656400	-0.70424200
H	3.82280400	-1.55262600	0.20332700
O	1.21410400	-1.55557600	1.67120400
H	1.37213500	-0.71586300	2.12848100

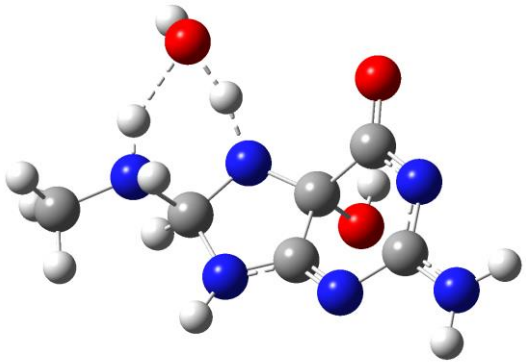


TS (C8 addition of NH_2CH_3 to 60)

SCF Done: E(R3LYP) = -790.132371310 a.u.

0 1

C	-0.36651000	0.47208700	0.66558600
C	-0.50582200	-0.99266100	0.31787700
C	-2.57491600	-0.63999400	-0.46883400
C	-1.28480500	1.28373800	-0.26124100
C	1.71257900	-0.53730400	0.62577700
N	-2.42739600	0.67986200	-0.67576400
N	-1.59273300	-1.55617200	-0.12036900
O	-1.01938700	2.47108700	-0.52891200
N	0.68643300	-1.56386300	0.52522200
N	-3.77127400	-1.17755100	-0.71422700
H	-4.53901000	-0.59409100	-1.01776500
H	-3.90852900	-2.17486500	-0.62118000
N	1.02874800	0.71892500	0.66354900
H	0.89455100	-2.53702900	0.32232400
H	2.38878200	-0.73147500	1.46328600
O	-0.98716800	0.59414500	1.99438000
H	-0.88259100	1.52163500	2.26450400
H	2.93100800	0.41481800	-0.75410800
O	2.49057900	2.16447400	-0.72050300
H	1.65779500	1.57900500	-0.00935200
H	3.04674600	2.69575000	-0.13253400
N	2.62143000	-0.58247300	-0.61763600
H	2.03981600	-0.81117400	-1.43068600
C	3.77522900	-1.52093900	-0.53284800
H	3.40481100	-2.53697400	-0.39041300
H	4.33838400	-1.45737300	-1.46394400
H	4.40506700	-1.22653800	0.30681200

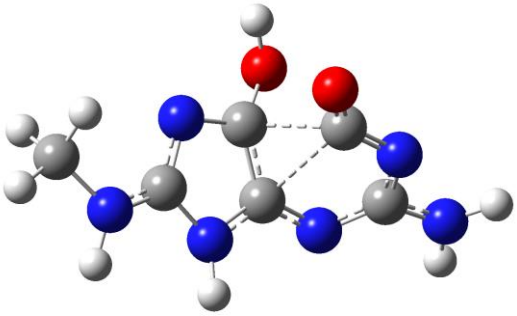


TS (Acyl Group Migration (64→65)

SCF Done: E(R3LYP) = -712.475394364 a.u.

0 1

C	0.12234100	0.40962700	0.85264900
C	-0.32399000	-0.82348500	0.31945000
C	-2.49000500	-0.50882200	-0.17519400
C	-1.01763300	1.18073500	-0.73187200
C	1.85323800	-0.50863300	-0.02081800
N	-2.22674200	0.70899100	-0.76908100
N	-1.56400800	-1.34407600	0.27889000
O	-0.42365000	2.13121800	-1.19362900
N	0.80194700	-1.39041700	-0.23064900
N	-3.78495000	-0.85904200	-0.13239800
H	-4.47654600	-0.27453700	-0.57924500
H	-4.04344700	-1.78419400	0.18197400
N	1.48903000	0.55932400	0.67414400
H	0.80250900	-2.15880800	-0.89330400
N	3.07391500	-0.74995200	-0.53373600
H	3.25890000	-1.69524700	-0.84465200
O	-0.52879000	1.05318100	1.87508600
C	4.21970000	0.09578200	-0.21569000
H	4.45772600	0.08214000	0.85383200
H	5.07819600	-0.27803000	-0.77366100
H	4.02648100	1.12678500	-0.52065700
H	-0.19053700	1.96168700	1.94271600

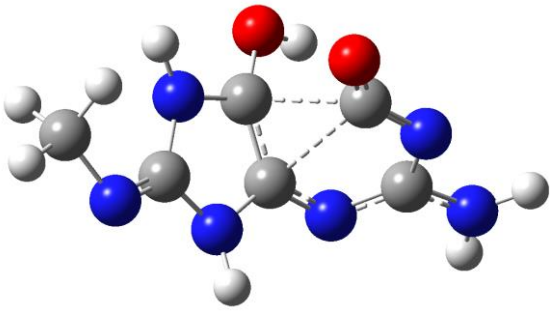


TS (Acyl Group Migration (64'→65')

SCF Done: E(R3LYP) = -712.460870867 a.u.

0 1

C	0.15518000	0.38793100	0.95002600
C	-0.33798900	-0.79104200	0.37724400
C	-2.48625500	-0.45393800	-0.20255800
C	-0.94151300	1.14694900	-0.79300800
C	1.89853600	-0.65541400	-0.06855700
N	-2.15897300	0.72093600	-0.85992800
N	-1.60783100	-1.26302800	0.37095900
O	-0.24256300	2.02233200	-1.24534900
N	0.74750600	-1.44135800	-0.18336400
N	-3.78837300	-0.77194900	-0.22229100
H	-4.44855600	-0.16887900	-0.69078700
H	-4.10548200	-1.63885700	0.18867500
N	1.52695800	0.41258700	0.75076400
H	0.65155700	-2.12451600	-0.92633900
N	3.02172400	-0.91956700	-0.62680100
O	-0.33921500	1.19214300	1.92284100
C	4.10245800	0.02920600	-0.36784500
H	3.85993800	1.04516200	-0.71057700
H	4.35661000	0.08733800	0.69930500
H	4.99701000	-0.29316800	-0.90338800
H	-1.26338900	0.96980500	2.12854000
H	2.07695900	1.26181300	0.81745700

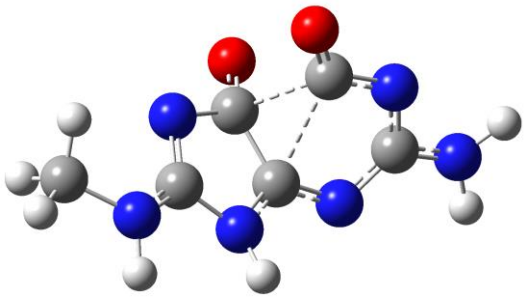


TS (Acyl Group Migration (64AN→65AN)

SCF Done: E(R3LYP) = -712.026078694 a.u.

-1 1

C	0.06682400	0.44886000	0.89457900
C	-0.33226600	-0.80660500	0.29203000
C	-2.49430600	-0.47457800	-0.16197900
C	-0.94586500	1.14009000	-0.62422000
C	1.83349300	-0.45310900	-0.03300500
N	-2.21241800	0.75535200	-0.70542900
N	-1.56646000	-1.34227600	0.24354300
O	-0.40027300	2.12786300	-1.12224700
N	0.79284600	-1.35192100	-0.25898900
N	-3.79686400	-0.82021400	-0.10139700
H	-4.47082700	-0.25176100	-0.59713600
H	-4.03676600	-1.78316900	0.09648600
N	1.47041900	0.59804400	0.66959000
H	0.80354000	-2.06922600	-0.97899200
N	3.05095600	-0.70047900	-0.56604400
H	3.21234200	-1.66675700	-0.82876400
O	-0.52487400	1.07341900	1.87838700
C	4.22573100	0.05437200	-0.13430500
H	4.42479000	-0.07463800	0.93617300
H	5.08438400	-0.30638400	-0.70142700
H	4.09268800	1.11795300	-0.34298000

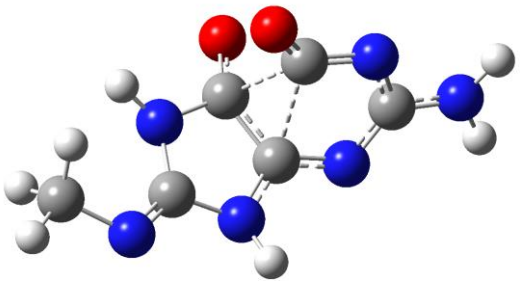


TS (Acyl Group Migration (64aAN→65aAN)

SCF Done: E(R3LYP) = -712.021778388 a.u.

-1 1

C	0.07502100	0.38294900	0.96656700
C	-0.35087300	-0.82579100	0.31422500
C	-2.48484700	-0.39986700	-0.20641900
C	-0.84469300	1.11542600	-0.63835600
C	1.88232100	-0.63302900	-0.05667700
N	-2.12374500	0.80581100	-0.76654000
N	-1.61383200	-1.30001700	0.25010600
O	-0.19776400	2.05305300	-1.10960100
N	0.75012400	-1.44579300	-0.22076200
N	-3.80188600	-0.67639800	-0.18914100
H	-4.43922200	-0.06204000	-0.67783900
H	-4.11391300	-1.60545200	0.06094000
N	1.48767500	0.39849300	0.77491800
H	0.68968700	-2.09245300	-1.00177500
N	3.01773000	-0.87996300	-0.60730900
O	-0.48599100	1.05500300	1.91625100
C	4.08304200	0.08097400	-0.31781000
H	4.32688700	0.11423900	0.75265100
H	4.98571600	-0.21335300	-0.85660000
H	3.82152100	1.10118600	-0.63140700
H	2.02708200	1.25451900	0.84275900

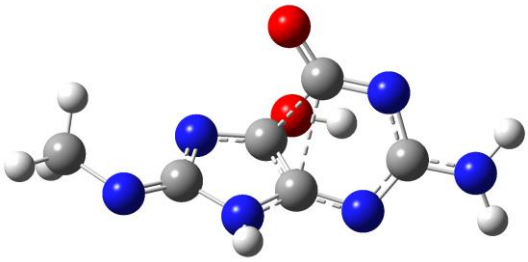


TS (Acyl Group Migration (64bAN→65bAN)

SCF Done: E(R3LYP) = -712.004368674 a.u.

-1 1

C	0.19849100	0.36970300	0.88402200
C	-0.29385200	-0.81488300	0.25710900
C	-2.46747700	-0.45770000	-0.19763800
C	-0.91500100	1.14150200	-0.68520800
C	1.92823300	-0.55781600	-0.05713400
N	-2.17523900	0.76466200	-0.76927100
N	-1.55276000	-1.31718000	0.24260500
O	-0.32330500	2.10829700	-1.15929000
N	0.80485500	-1.38912600	-0.30386900
N	-3.76745900	-0.80564500	-0.19019500
H	-4.46654000	-0.11717200	-0.43219100
H	-4.05386000	-1.65212900	0.28364400
N	1.54713800	0.49821700	0.72982800
H	0.77046500	-2.07197400	-1.05400000
N	3.08794500	-0.86220500	-0.56648000
O	-0.38273400	1.05200400	1.92463400
C	4.16668300	0.07262600	-0.25877200
H	4.40159100	0.11043800	0.81495700
H	5.07427500	-0.24474400	-0.77918200
H	3.94198600	1.10070800	-0.57785100
H	-1.33342700	0.85081300	1.96928600

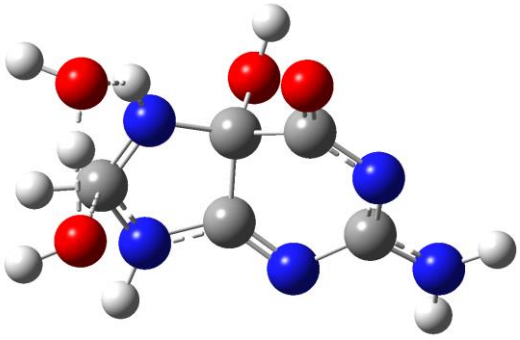


TS (C8 addition of H_2O to 60)

SCF Done: E(R3LYP) = -770.677313467 a.u.

0 1

C	-0.11627400	0.24214300	0.77067800
C	-0.60858100	-1.09658200	0.25905600
C	-2.44671500	-0.08515700	-0.52217100
C	-0.63438900	1.32568100	-0.20351100
C	1.57659200	-1.25968700	0.59091600
N	-1.89215900	1.12357800	-0.66491100
N	-1.75801700	-1.28995400	-0.26670700
O	0.03990700	2.33828400	-0.41793800
N	0.44349700	-1.97266400	0.35865800
N	-3.74087700	-0.23965000	-0.75017400
H	-4.31681500	0.56313800	-0.97315400
H	-4.15905800	-1.16137600	-0.71926900
N	1.32140800	0.00436600	0.85162700
H	0.43562800	-2.94550000	0.06279600
H	2.54781200	-1.72076800	0.66036600
O	-0.69204500	0.45491700	2.04441400
H	-0.56123700	1.38281200	2.30540100
O	2.81332400	-0.82027500	-1.60745900
H	3.49687100	-1.50476500	-1.64765800
H	3.32463300	0.32919400	-0.84679700
O	3.53135900	1.17763300	-0.25001800
H	2.07757000	0.71013700	0.74323700
H	4.37347700	1.00453100	0.19382700

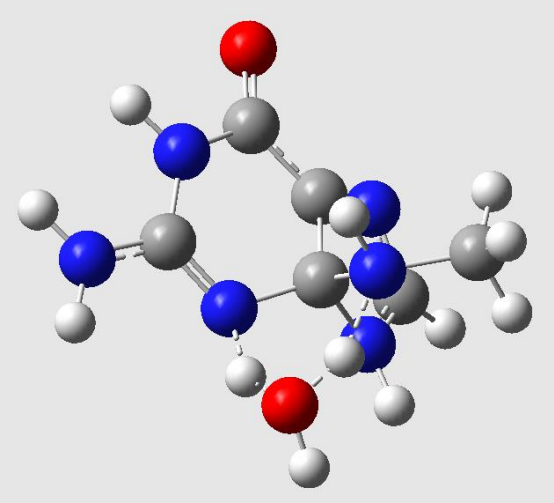


TS (Gradcat + NH_2CH_3 at C4)

SCF Done: E(UB3LYP) = -714.731056715 a.u.

1 2

C	0.10851600	-1.29112100	-0.06526500
C	-0.57562600	0.05058900	-0.19784900
C	1.57617200	1.01705400	-0.22924400
C	1.47505300	-1.35919200	0.36726700
C	-1.60390900	-1.67485000	-1.27326800
N	2.09913100	-0.10718400	0.38385100
N	0.32415600	1.10090700	-0.64754600
O	2.11038500	-2.38218100	0.67238500
N	-1.59745000	-0.33053900	-1.16821800
N	2.41722800	2.04674700	-0.38716000
H	3.39395100	1.97247800	-0.13595500
H	2.07580400	2.91505100	-0.77700100
N	-0.58913800	-2.28912300	-0.66540100
H	-2.40212700	0.24994300	-1.38093300
H	-2.36530300	-2.19048100	-1.84398400
N	-1.26117900	0.58050600	1.04126500
H	-0.52917400	0.67840700	1.74867900
C	-2.35354200	-0.23624700	1.61464400
H	-2.66098900	0.23904200	2.54840500
H	-3.20946200	-0.24894800	0.93827300
H	-2.04057400	-1.26294900	1.83090300
H	-0.43370700	2.33719500	-0.47041800
H	3.07860500	-0.09951800	0.65741100
O	-1.23045900	2.90656300	0.03914900
H	-1.92820500	3.13889600	-0.59960000
H	-1.52744400	2.02924100	0.59669200

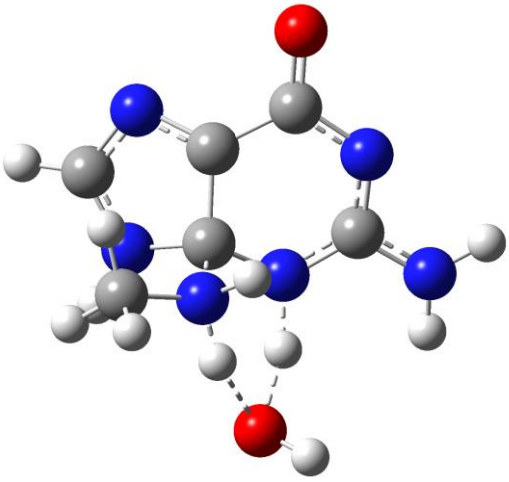


TS (Guanine radical + NH_2CH_3 at C4)

SCF Done: E(U3LYP) = -714.273671225 a.u.

0 2

C	-0.27474800	0.96287200	0.05341700
C	-0.53453900	-0.48813200	-0.22046600
C	1.81803000	-0.72871900	-0.14145800
C	1.03915700	1.37754900	0.51674200
H	-2.20435600	-1.15049400	-1.45171300
N	2.04697000	0.45702300	0.44870600
N	0.63417100	-1.19107200	-0.64378400
O	1.24677300	2.54892600	0.93114100
N	-1.62042800	-0.37152200	-1.16601300
N	2.86552300	-1.56306100	-0.26755700
H	3.78629400	-1.24424600	-0.00221500
H	2.76590000	-2.45426100	-0.73344300
C	-2.03968300	0.92106100	-1.15172100
H	-2.92693200	1.22822100	-1.68951400
N	-1.24855600	1.75002100	-0.47852500
H	-0.93356100	-2.30383300	0.73692200
N	-1.05901300	-1.28465000	1.03439800
H	-0.38474900	-1.10480100	1.78621800
C	-2.43218000	-0.99907400	1.53431600
H	-2.57178200	-1.57111600	2.45243400
H	-2.53641300	0.06500000	1.74813200
H	-3.16280200	-1.31643100	0.79222800
O	-0.23560900	-3.50684100	-0.25666800
H	0.41717500	-2.32998600	-0.58871700
H	0.35822400	-4.03710900	0.29459200

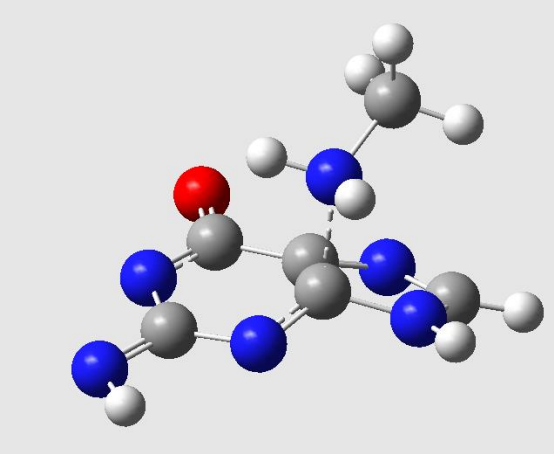


TS (G^{ox} + NH_2CH_3 at C4)

SCF Done: E(RB3LYP) = -637.176188760 a.u.

0 1

C	0.25759000	0.81217500	-0.35597100
C	0.30780400	-0.66202200	-0.38079500
C	-1.97131400	-0.67474700	-0.10850400
C	-0.94570300	1.43910300	0.23923200
C	1.98472000	0.28728000	-1.49303900
N	-2.01218600	0.64618200	0.33091400
N	-0.81485400	-1.33570500	-0.57402600
O	-0.90643000	2.64982900	0.60250500
N	1.46923400	-0.88259800	-1.21067400
N	-3.09407000	-1.33484500	-0.08472200
H	-2.92086000	-2.27434100	-0.44748300
N	1.25539600	1.35885200	-1.01342200
H	1.86757700	-1.78620600	-1.45895300
H	2.88749900	0.40459900	-2.07888800
N	1.06746300	-1.10708100	1.31538700
H	0.25301300	-1.00667200	1.92406100
C	2.23685400	-0.39786000	1.87422600
H	2.54615000	-0.86487000	2.81441400
H	3.06937600	-0.44769500	1.16933000
H	1.97358400	0.64369800	2.06239600
H	1.25851500	-2.10435000	1.19999800

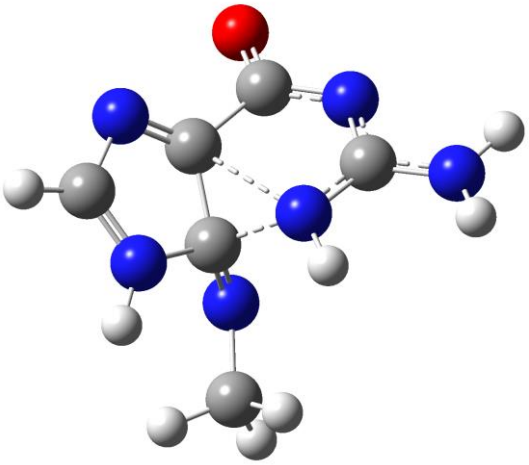


TS (77→78)

SCF Done: E(R3LYP) = -637.179768968 a.u.

0 1

C	-0.16460600	-1.09693400	0.09153600
C	-0.87660300	0.21386500	0.16719700
C	1.57340100	0.84572900	-0.49330800
C	1.24471300	-1.19845600	0.58246600
C	-1.92205800	-1.35411000	-1.09356300
N	2.06413800	-0.19345800	0.23869700
N	0.31452000	0.91237400	-0.96480500
O	1.58360500	-2.18847600	1.26712800
N	-1.99186400	-0.09650400	-0.76660900
N	2.44050100	1.84264900	-0.74159700
H	3.40526100	1.74831500	-0.45555600
H	2.17255900	2.63469400	-1.31010600
N	-0.77887900	-1.98850300	-0.64169200
H	-2.79624300	0.49945300	-0.94720500
H	-2.68396300	-1.86301400	-1.67100800
N	-1.09363900	0.84251100	1.30299000
C	-1.98834200	1.99994700	1.23113400
H	-2.00880000	2.49448400	2.20483000
H	-1.65519600	2.74432600	0.49336500
H	-3.02864300	1.73687100	0.99049000
H	0.04370200	1.81894800	-1.34350300

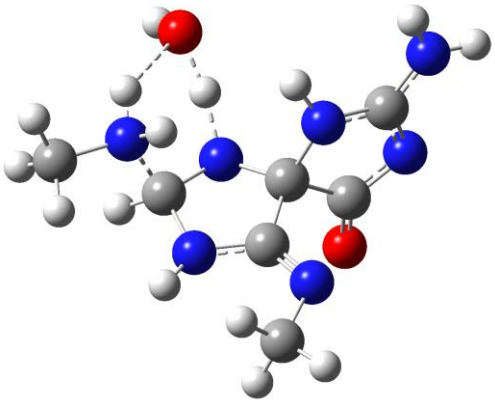


TS (C8 addition of NH_2CH_3 to 78)

SCF Done: E(R3LYP) = -809.586600270 a.u.

0 1

C	0.50487100	0.05659700	0.26407600
C	-0.23146700	1.37093500	-0.04664400
C	2.44111300	-0.72396600	-0.69760400
C	1.80037200	0.28769800	1.10135700
N	2.89222700	-0.20450800	0.46457700
N	1.12533700	-0.53015300	-0.94337100
O	1.79175000	0.84951200	2.20836800
N	-1.53445900	1.17064300	0.35447000
N	3.24013100	-1.36212000	-1.54884600
H	4.21590000	-1.48733400	-1.31672300
H	2.88219000	-1.74976400	-2.41186800
N	0.31057100	2.41078700	-0.56004400
H	0.60379000	-1.13018300	-1.57297900
C	-0.56827200	3.55210500	-0.81408700
H	-1.41371400	3.29047700	-1.46589900
H	-0.98007600	3.96557800	0.11646500
H	-0.00156200	4.34435000	-1.30687100
C	-1.75093400	-0.19619400	0.71383300
N	-0.47362800	-0.76809900	0.93364300
H	-2.29310000	1.79799500	0.11847400
H	-2.44500500	-0.31339700	1.54915000
N	-2.50467500	-0.95469900	-0.45770700
H	-2.27880500	-1.95640100	-0.29967200
H	-2.06099500	-0.68481200	-1.34130400
C	-3.97247000	-0.72540200	-0.52377000
H	-4.38777100	-1.31354200	-1.34270300
H	-4.41762400	-1.03872600	0.42124100
H	-4.16378000	0.33462600	-0.69705100
O	-0.84502600	-3.15142300	0.30460100
H	-0.54844700	-2.03239400	0.66248200
H	-1.01260700	-3.67476500	1.10149200

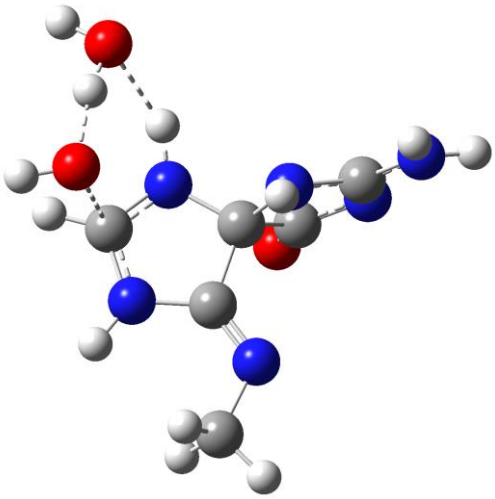


TS (C8 addition of H_2O to 78)

SCF Done: E(R3LYP) = -790.146443660 a.u.

0 1

C	0.26639100	-0.09239000	0.26364700
C	0.05231200	1.39457500	-0.06195000
C	1.96321200	-1.32359900	-0.60824700
C	1.45580400	-0.35298400	1.25501300
N	2.41612200	-1.07961600	0.63508000
N	0.68699200	-0.89939300	-0.85707400
O	1.45824400	0.07022100	2.41317800
N	-1.28489800	1.65866000	0.27962500
N	2.67381300	-1.95577800	-1.52791700
H	3.61852100	-2.24812200	-1.31419900
H	2.29967800	-2.12498900	-2.45310700
N	0.93228100	2.17316600	-0.54264300
H	0.38301900	-0.68516500	-1.80236700
C	0.54494100	3.55527100	-0.82772900
H	-0.25401700	3.59446400	-1.57748000
H	0.19440400	4.07026900	0.07429600
H	1.40823400	4.09496900	-1.21681500
C	-1.89845100	0.53665900	0.68923300
N	-1.02949300	-0.45858400	0.82932200
H	-1.75905300	2.54472000	0.14772900
H	-2.89577900	0.52653300	1.09501700
H	-3.05713200	-1.67039600	-0.41534400
O	-2.83058000	-2.54943100	0.08601200
H	-1.37901900	-1.42344100	0.84245100
H	-3.58277600	-2.73174200	0.66618600
O	-3.13194800	-0.32005600	-1.12454000
H	-4.01078900	0.07263700	-1.01810800

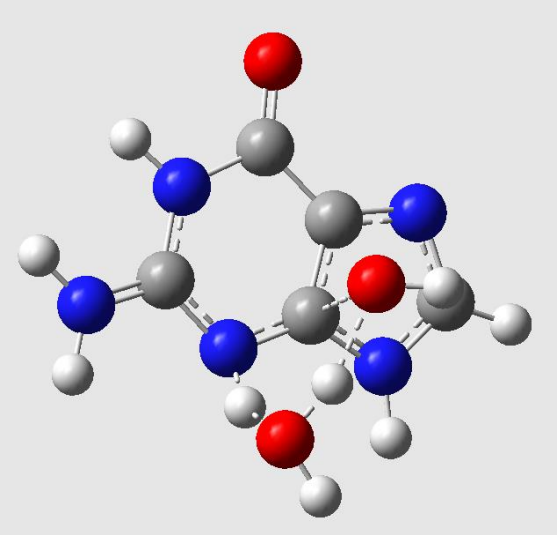


TS(Guanine Radical Cation at C4 + H_2O at C4)

SCF Done: E(UB3LYP) = -695.275237041 a.u.

1 2

C	0.64857200	1.15677200	-0.15375400
C	0.48575200	-0.00208900	-0.95059700
C	-1.75942600	0.31753800	-1.22853200
C	-0.51375300	1.97599400	0.12078600
C	2.58926700	0.36180600	-0.46675900
N	-1.66878300	1.46985700	-0.50300500
N	-0.66583100	-0.43315700	-1.51948300
O	-0.55877600	3.00835700	0.78212400
N	1.74504200	-0.47503800	-1.14768700
N	-2.94381700	-0.08006100	-1.65851400
H	-3.78740200	0.43165000	-1.42488100
H	-3.02175100	-0.92231000	-2.21745000
N	1.95996700	1.36572800	0.13351000
H	2.01013400	-1.30992800	-1.66290300
H	3.65571000	0.18965000	-0.44620300
H	-0.80134900	-1.64467700	-1.33270200
H	-2.52037700	2.01042200	-0.35406500
O	-0.04630000	-1.11981900	1.19324700
H	-0.44442900	-2.26592900	0.20847800
O	-0.81660400	-2.71788100	-0.64221200
H	-0.14427300	-3.33780500	-0.97082900
H	0.85934500	-1.22662200	1.53191700

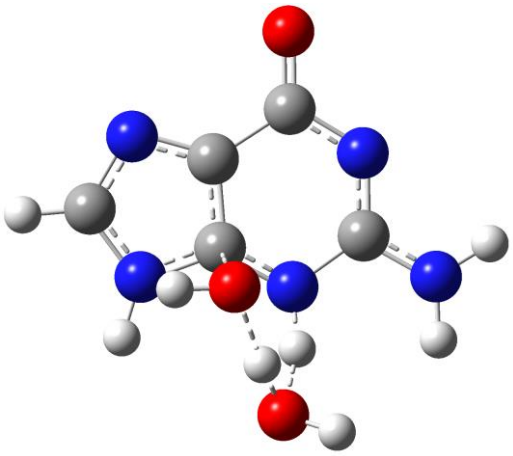


TS (Guanine radical + H_2O at C4)

SCF Done: E(U3LYP) = -694.830658427 a.u.

0 2

C	-0.01663800	1.25303800	-0.30880800
C	-0.26669600	-0.08479800	-0.73637900
C	1.93805900	-0.63114900	-0.31620100
C	1.34394200	1.60415700	0.11454800
H	-2.09016700	-0.90327300	-1.48546100
N	2.26650700	0.59169000	0.07203700
N	0.68790600	-1.01021200	-0.82498200
O	1.64231200	2.75577700	0.48135300
N	-1.56031300	-0.10136700	-1.15457000
N	2.83459500	-1.61467700	-0.25171800
H	3.75164000	-1.41856800	0.12903300
H	2.60913400	-2.56148800	-0.53281400
C	-2.04679300	1.15413900	-0.93433200
H	-3.07454800	1.40760000	-1.15199800
N	-1.13228500	1.99718400	-0.43502400
H	-0.75308100	-2.42414500	0.81235000
O	-0.47997000	-3.17000300	0.10951900
H	0.38113700	-2.02548700	-0.72770000
H	0.13229600	-3.77042300	0.55933300
O	-1.01756400	-1.24609500	1.63032800
H	-1.94972500	-0.99664200	1.54674900

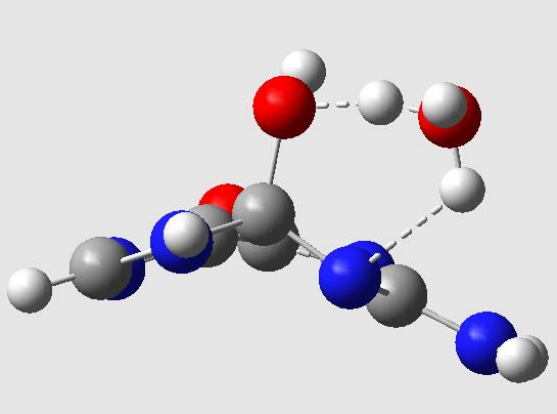


TS (G^{ox}cat + H_2O at C4)

SCF Done: E(RB3LYP) = -694.649829452 a.u.

1 1

C	-0.65665600	0.83645600	-0.01149700
C	-0.52867200	-0.64886000	0.22638000
C	1.65820500	-0.27888500	-0.44075000
C	0.56729400	1.67259000	0.19824000
C	-2.44057000	-0.02176800	-0.81129600
H	-3.41424200	-0.06887800	-1.28239500
H	-2.15302000	-2.02768700	-0.41407200
N	1.71861600	1.04025000	-0.05214200
N	0.61314700	-1.13202100	-0.43084700
O	0.45332800	2.86311900	0.56195100
N	-1.74993100	1.17323200	-0.63187000
N	-1.80029700	-1.07164000	-0.39680800
N	2.82260500	-0.77552200	-0.88326800
H	3.64582200	-0.19001700	-0.89519300
H	2.89755000	-1.75004800	-1.14084800
O	-0.63631500	-1.07209400	1.60636000
H	0.14994200	-2.39246300	1.74874600
H	-0.17602000	-0.43778500	2.18693100
O	0.82458700	-3.16902900	1.64801400
H	0.36335700	-4.03064100	1.67365000
H	1.20640600	-3.04516300	0.74909400

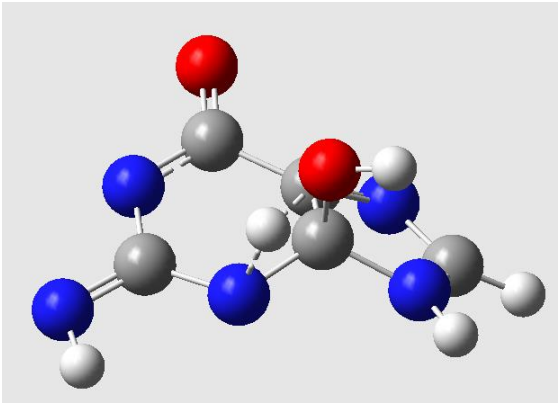


TS (G^{ox} + H_2O at C4)

SCF Done: E(RB3LYP) = -617.676413192 a.u.

0 1

C	0.60592000	0.76853400	-0.01832500
C	0.58873800	-0.71252100	0.20561400
C	-1.71597400	-0.57148300	-0.34800100
C	-0.66308500	1.50203700	0.17937500
C	2.47283300	0.03736100	-0.75414200
N	-1.75993500	0.78842200	-0.06539100
N	-0.55409700	-1.37791800	-0.23468900
O	-0.64333900	2.72247000	0.49881500
N	1.89141600	-1.06281700	-0.35391800
N	-2.83369900	-1.13769200	-0.69227500
H	-2.65467300	-2.12300200	-0.89467600
N	1.71671000	1.18124600	-0.57498400
H	2.28711900	-2.00144100	-0.39259000
H	3.45247500	0.04645100	-1.21541100
O	0.51642500	-1.14878400	1.65224200
H	1.29845300	-1.61316700	2.02632400
H	-0.32141200	-1.78057800	1.12956100

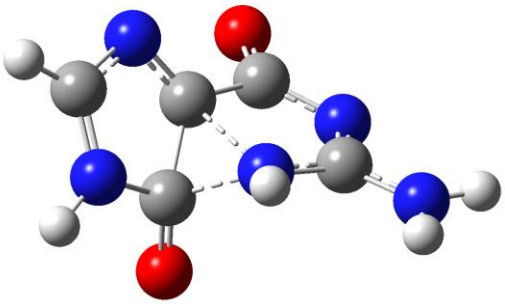


TS (93→94)

SCF Done: E(R3LYP) = -617.769088161 a.u.

0 1

C	0.56561300	0.65190800	-0.11047300
C	0.80424400	-0.62385200	0.67297600
C	-1.63565800	-0.54284200	-0.28629200
C	-0.69029700	1.43757500	0.13367900
C	2.45710200	-0.04254600	-0.78922700
N	-1.83926200	0.72499200	0.10360000
N	-0.36082200	-1.01649400	-0.46449300
O	-0.59595600	2.64391500	0.41046000
N	2.05752200	-1.02285100	0.00171900
N	-2.66627900	-1.34803000	-0.52110000
H	-3.60772300	-0.97906000	-0.47339500
H	-2.52808400	-2.31372500	-0.79112900
N	1.57091300	0.96735700	-0.93272200
H	2.64339700	-1.78892500	0.32368600
H	3.41231400	-0.06381900	-1.29871500
H	-0.20222200	-1.85915400	-1.01443500
O	0.58868000	-0.94536400	1.86716300

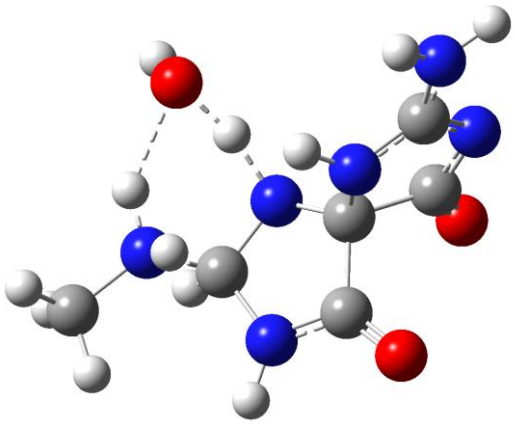


TS (C8 addition of NH_2CH_3 to 94)

SCF Done: E(R3LYP) = -790.164193539 a.u.

0 1

C	-0.48547200	-0.30905900	0.14143900
C	0.11874300	-1.57249000	-0.51506300
C	-2.35445500	0.81864700	-0.56379600
C	-1.79346300	-0.64873500	0.92118100
C	1.79712300	-0.38150300	0.53088600
N	-2.84234100	0.06924600	0.44640800
N	-1.05736700	0.58188600	-0.88656700
O	-1.82418800	-1.47536100	1.84451300
N	1.43585800	-1.55667200	-0.21370300
N	-3.09128700	1.71287200	-1.21403500
H	-4.05517900	1.85737600	-0.94540700
H	-2.70220000	2.25588900	-1.97359100
N	0.57779300	0.22275200	0.95019100
H	2.10017500	-2.24141800	-0.55815700
H	2.48883700	-0.60171200	1.34684400
O	-0.48095100	-2.41841900	-1.18101300
H	-0.48689200	1.29465000	-1.33021300
H	2.48163400	1.52812200	0.07692900
O	1.20594000	2.63110300	0.95951000
H	1.45230400	2.89729400	1.85714100
H	0.77576500	1.48714800	1.01976400
N	2.61072000	0.59704300	-0.37669800
H	2.13884600	0.65208800	-1.28572100
C	4.04945000	0.26313000	-0.56478200
H	4.52883200	0.21190700	0.41310600
H	4.13393600	-0.69589100	-1.07731200
H	4.51235200	1.04614200	-1.16582400



TS (C8 addition of H_2O to 94)

SCF Done: E(R3LYP) = -770.713489527 a.u.

0 1

C	0.27917000	-0.23838500	-0.09780800
C	-0.03015100	-1.53633400	0.68760500
C	2.09567600	1.03731800	0.35883200
C	1.48678400	-0.44643400	-1.09431800
C	-1.89081000	-0.87052400	-0.39039200
N	2.51198200	0.35313900	-0.72125400
N	0.78375500	0.83864300	0.70341900
O	1.43612400	-1.23416200	-2.03760900
N	-1.35188300	-1.83488300	0.39092300
N	2.86526400	1.86971700	1.03706300
H	3.83064000	1.99711400	0.76208700
H	2.50877900	2.37538300	1.83881100
N	-0.99100100	0.01242100	-0.76629400
H	-1.86585700	-2.62743400	0.76599000
H	-2.89405300	-0.92291400	-0.77927300
O	0.72359300	-2.16654000	1.39787800
H	0.45928600	0.99333600	1.65386400
O	-3.21915200	0.70163800	1.01447300
H	-4.14600000	0.42433000	0.97520300
H	-2.92578700	1.65452700	-0.07986800
O	-2.54145400	2.26402600	-0.84885500
H	-3.21770300	2.29384300	-1.54034700
H	-1.31303400	0.94500100	-1.09407700