Calculation of pKa Values of Nucleobases and the Guanine Oxidation Products Guanidinohydantoin and Spiroiminodihydantoin using Density Functional Theory and a Polarizable Continuum Model

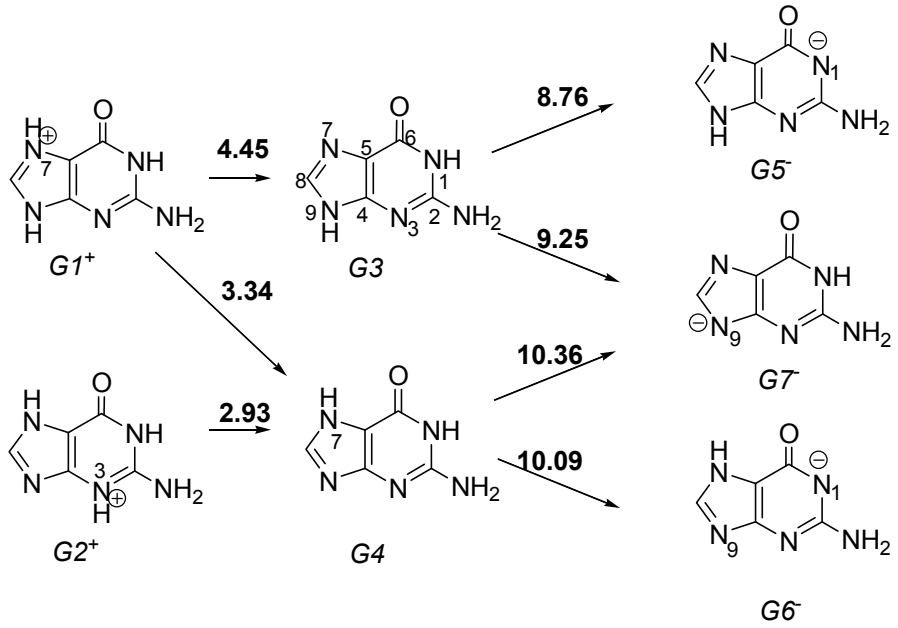
Vincenzo Verdolino,[‡] *Roberto Cammi,*[‡] *Barbara H. Munk*[†]*, H. Bernhard Schlegel*[†*]

[‡]Department o di Chimica Generale ed Inorganica, Università di Parma, Parco Area della Scienze 1, 43100 Parma, Italy [†]Department of Chemistry, Wayne State University, Detroit, Michigan, 48202.

Supporting Information

Table of Contents

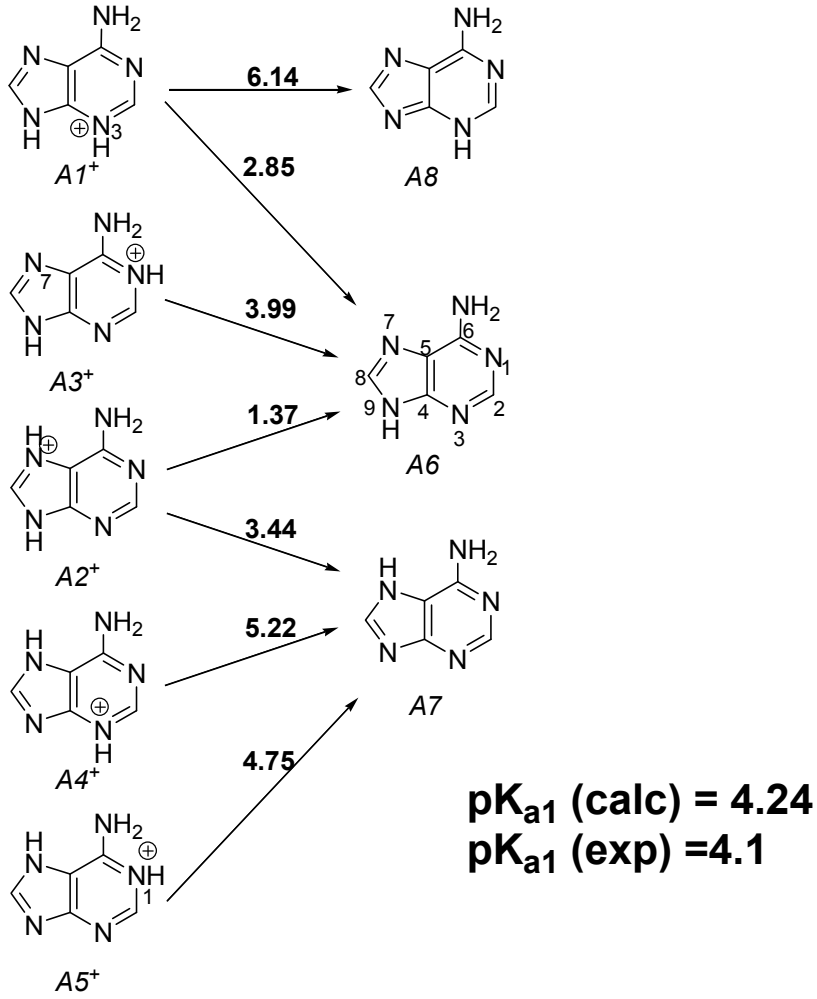
Scheme S1: Guanine tautomers and their local pK_a values



pK_{a1} (calc) = 3.45 **pK_{a2} (calc)=9.6**

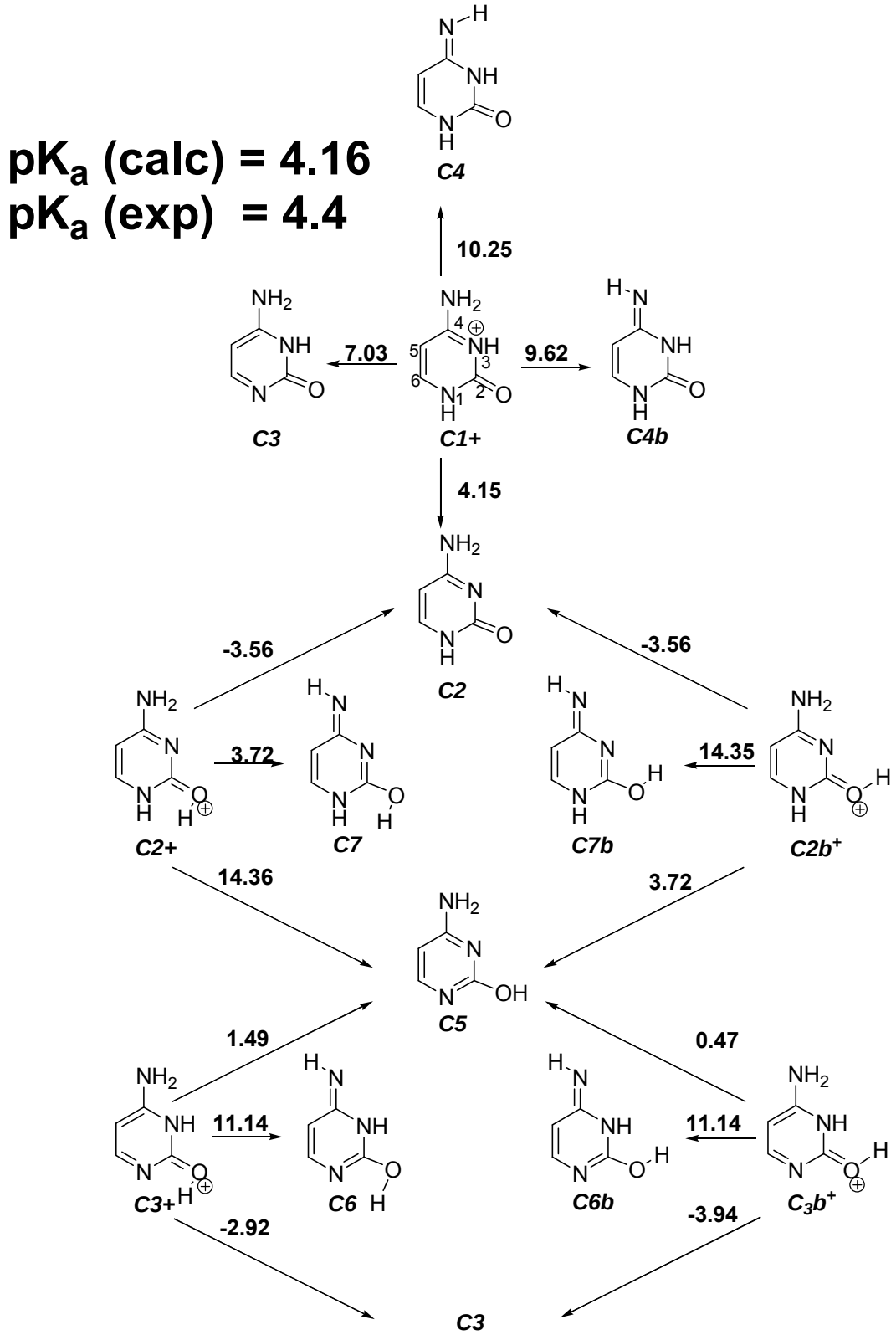
pK_{a1} (exp) =3.2-3.3 **pK_{a2} (exp)=9.2-9.6**

Scheme S2: Adenine tautomers and their local pK_a values

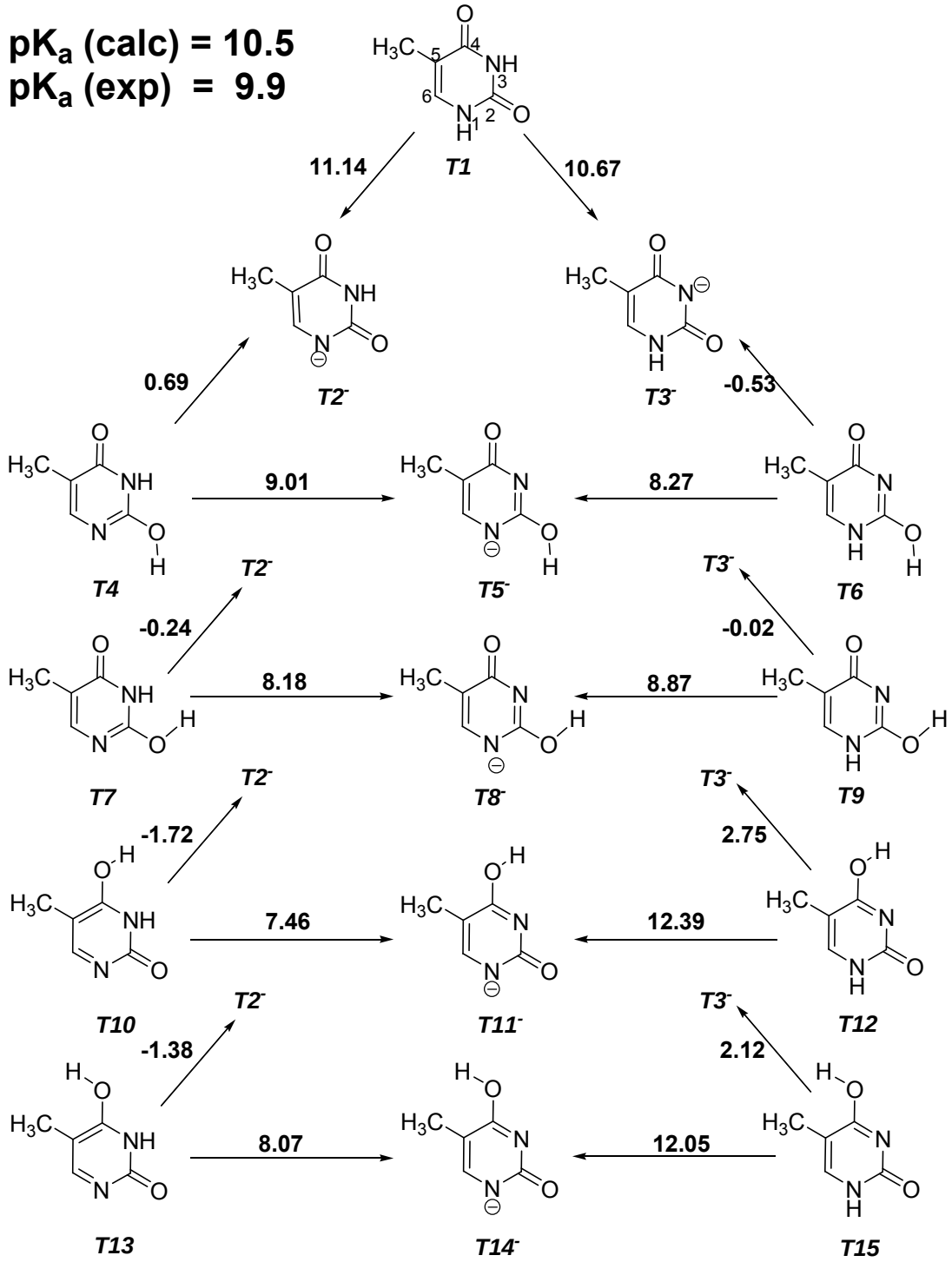


pK_{a1} (calc) = 4.24
pK_{a1} (exp) =4.1

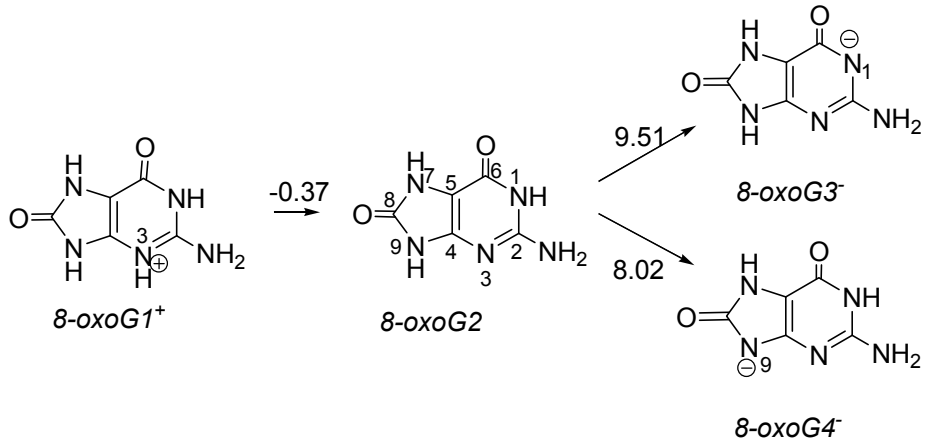
Scheme S3: Cytosine tautomers and their local pK_a values



Scheme S4: Thymine tautomers and their local pK_a values

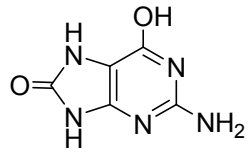


Scheme S5: 8-oxoguanine tautomers and their local pK_a values



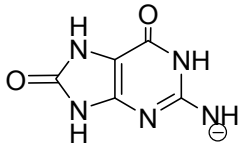
pK_{a1}(calc)=-0.37 pK_{a2}(calc)=8.00
pK_{a1}(exp)=~0.1 pK_{a2}(exp)=8.5-8.6

Other tautomers evaluated at UFF, α=0.91



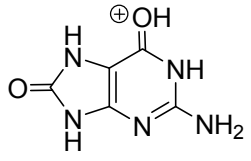
+ 8 kcal/mol

8-oxoG5



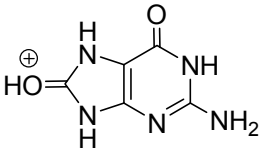
+ 14 kcal/mol

8-oxoG6-



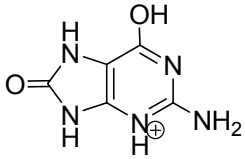
8-oxoG7+

+ ~5 kcal/mol



8-oxoG8+

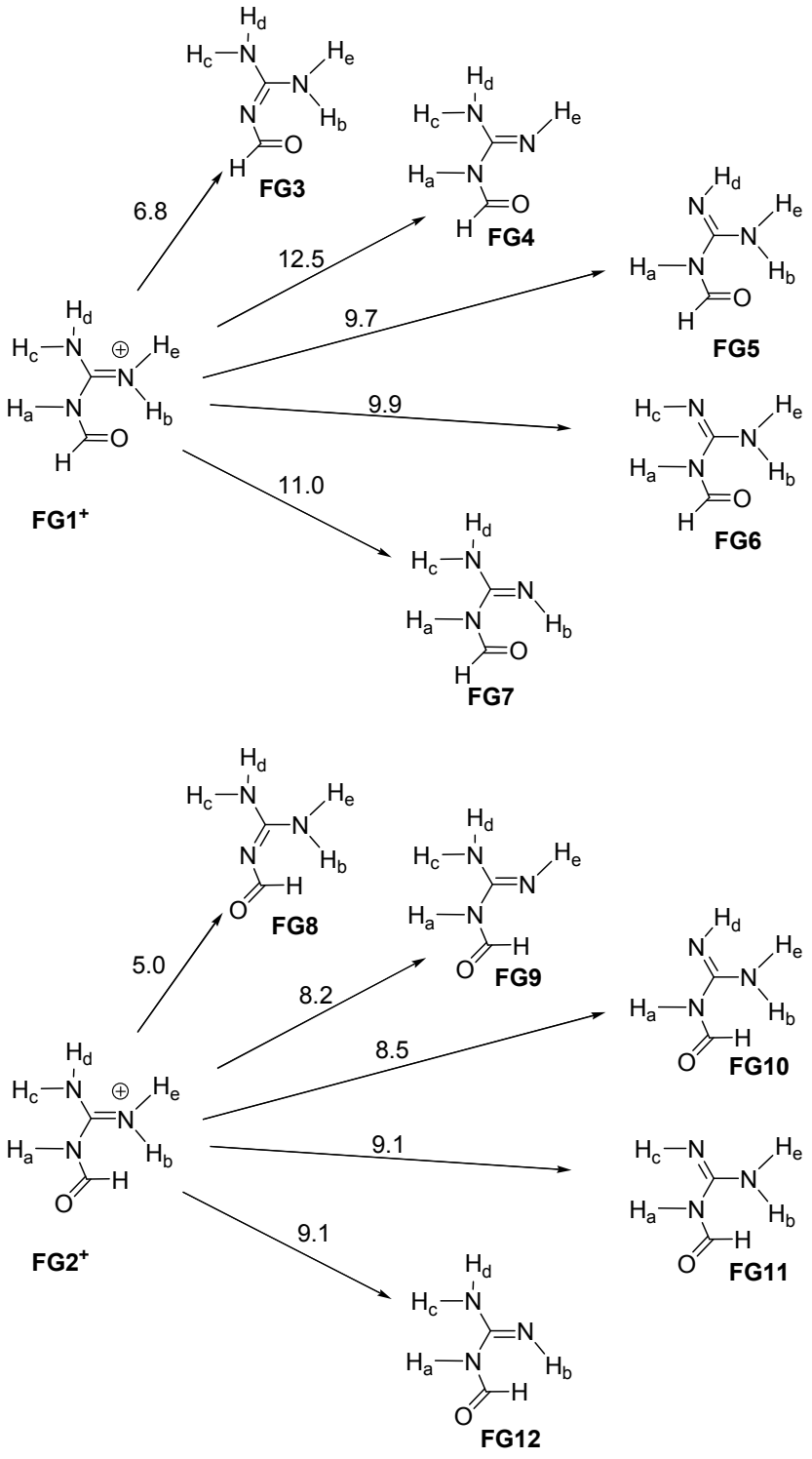
+ 10 kcal/mol



8-oxoG9+

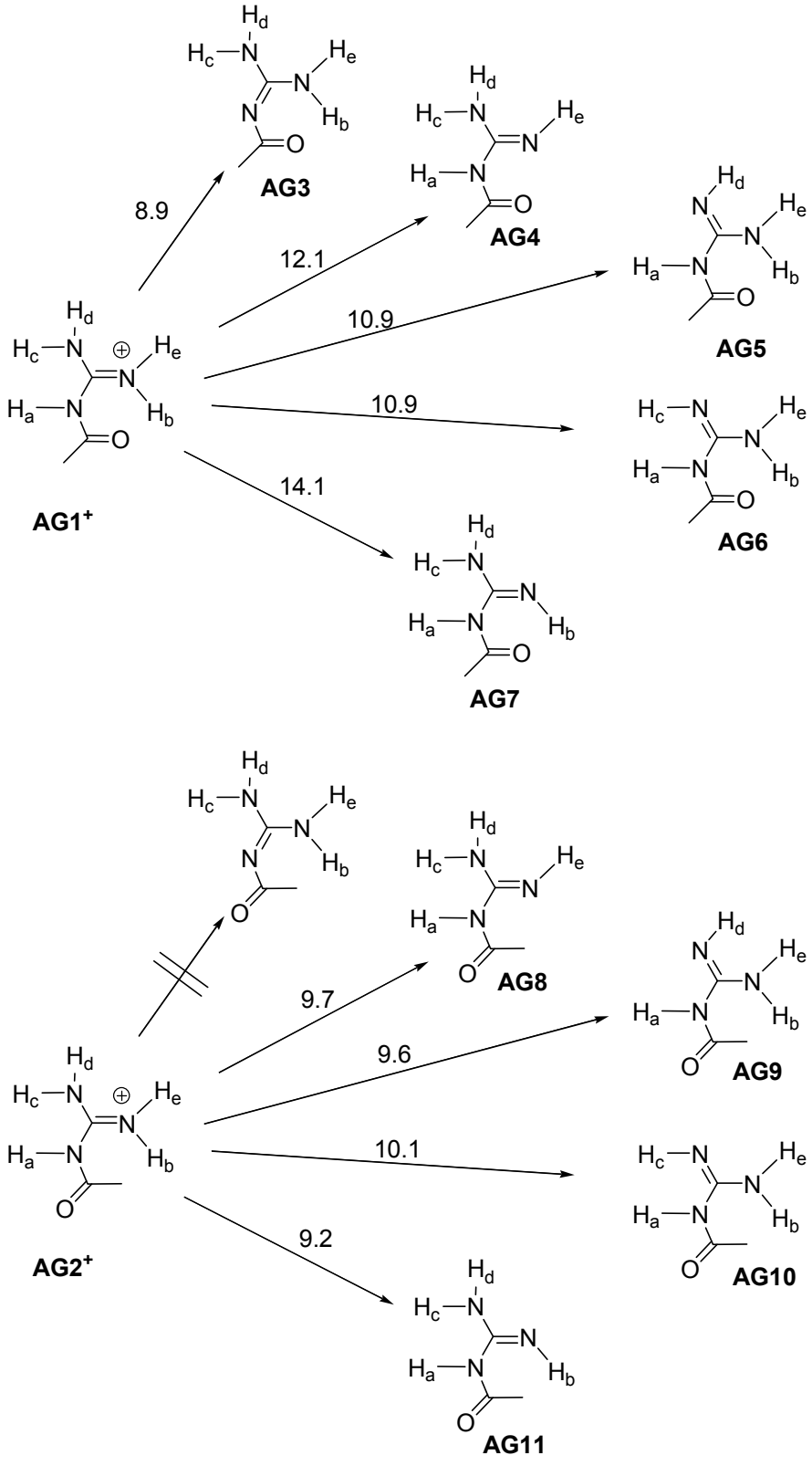
+ 5 kcal/mol

Scheme S6: N-formylguanidine tautomers and their local pK_a values



pK_{a1}(calc)=6.7
pK_{a1}(exp)=not published

Scheme S7: N-acetylguanidine tautomers and their local pK_a values



pK_{a1}(calc)=8.54
pK_{a1}(exp)=8.23

Table S-1: Calculation of the Local and Global pK_a for Guanine

Tautomer	$E^{\circ}_{(g)}(R)$[1] *(hartrees)*	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$ *(hartrees)*	$G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$E^{\circ}_{(g)}(R')$[1] *(hartrees)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'\ 3}_{(sol)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	$Rel\ G^{\circ}_{(g)}$ *(kcal/mol)*	*Boltzmann Pop. (g)*	$Rel\ G^{*}_{(aq)}$ *(kcal/mol)*	*Boltzmann Pop. (aq)*
$G1^{+}$	-543.1430	0.0967	-340766.70	-543.1421	0.59	-64.82	-340830.92	0	1.00	0	0.72
$G2^{+}$	-543.1353	0.0959	-340762.35	-543.1338	0.92	-68.93	-340830.36	4.35	0.64E-03	0.56	0.28
G3	-542.7640	0.0836	-340537.11	-542.7624	1.03	-18.51	-340554.59	0.65	0.25	1.52	0.07
G4	-542.7652	0.0837	-340537.75	-542.7640	0.71	-19.06	-340556.11	0	0.75	0	0.93
G5-	-542.2105	0.0701	-340198.25	-542.2084	1.31	-75.44	-340272.38	2.82	0.01	0	0.52
G6-	-542.2154	0.0705	-340201.08	-542.2138	1.02	-72.02	-340272.08	0	0.80	0.31	0.31
G7-	-542.2141	0.0704	-340200.25	-542.2114	1.66	-73.13	-340271.71	0.83	0.20	0.67	0.17

Reaction	*pKa Local*	*pKa Global*	*Exp*[4]	*Gas Phase Basicity*	*Literature Reference*[5]
$G1^{+}\rightarrow G3$	4.45	3.45	3.2-3.3	223.31	221.90
$G1^{+}\rightarrow G4$	3.34	3.45		222.66	221.60
$G2^{+}\rightarrow G4$	2.93	3.45		218.31	216.18
$G3\rightarrow G5^{-}$	8.76	9.62	9.2-9.6		
$G3\rightarrow G7^{-}$	9.25	9.62			
$G4\rightarrow G7^{-}$	10.36	9.62			
$G4\rightarrow G6^{-}$	10.09	9.62			

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species and 0.83 for anions on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

[4] References in manuscript 25, 86-92.

[5] Reference 25 in manuscript.

Table S-2: Calculation of the Local and Global pK_a for Adenine

Tautomer	$E^{\circ}_{(g)}(R)$[1] *(hartrees)*	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$ *(hartrees)*	$G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$E^{\circ}_{(g)}(R')$[1] *(hartrees)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'\ 3}_{(sol)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	$Rel\ G^{\circ}_{(g)}$ *(kcal/mol)*	*Boltzmann Pop. (g)*	$Rel\ G^{*}_{(aq)}$ *(kcal/mol)*	*Boltzmann Pop. (aq)*
A1+	-467.8671	0.09395	-293532.08	-467.8667	0.24	-60.43	-293592.27	1.74	0.04	1.55	0.04
A2+	-467.8561	0.093036	-293525.77	-467.8557	0.27	-65.56	-293591.06	8.04	0.85E-06	2.76	0.01
A3+	-467.8691	0.093977	-293533.34	-467.8688	0.21	-60.69	-293593.82	0.48	0.30	0.00	0.54
A4+	-467.8697	0.093788	-293533.82	-467.8694	0.17	-59.85	-293593.49	0.00	0.67	0.33	0.31
A5+	-467.8522	0.092461	-293523.70	-467.8517	0.34	-69.49	-293592.85	10.11	0.26E-07	0.97	0.11
A6	-467.4959	0.079134	-293308.48	-467.4955	0.29	-9.92	-293318.11	0.00	1.00	0.00	0.97
A7	-467.4834	0.080105	-293300.02	-467.4825	0.59	-16.68	-293316.11	8.46	0.6E-06	2.00	0.03
A8	-467.4834	0.080152	-293300.00	-467.4829	0.34	-13.98	-293313.64	8.48	0.6E-06	4.48	0.00

Reaction	*pKa Local*	*pKa Global*	*Exp*[4]
$A1^{+}\rightarrow A6$	2.85	4.24	4.15
$A2^{+}\rightarrow A6$	1.97	4.24	
$A2^{+}\rightarrow A7$	3.44	4.24	
$A3^{+}\rightarrow A6$	3.99	4.24	
$A4^{+}\rightarrow A7$	5.22	4.25	
$A5^{+}\rightarrow A7$	4.75	4.24	
$A1^{+}\rightarrow A8$	6.14	4.24	

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

[4] Reference 87 in manuscript.

Table S-3: Calculation of the Local and Global pK_a for Cytosine

Tautomer	$E^{\circ}_{(g)}(R)$[1] *(hartrees)*	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$ *(hartrees)*	$G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$E^{\circ}_{(g)}(R')$[1] *(hartrees)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'\ 3}_{(sol)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	$Rel\ G^{\circ}_{(g)}$ *(kcal/mol)*	*Boltzmann Pop. (g)*	$Rel\ G^{*}_{(aq)}$ *(kcal/mol)*	*Boltzmann Pop. (aq)*
C1+	-395.4682	0.0819	-248108.67	-395.4670	0.74	-65.82	-248173.75	0.11	4.55E-01	0.00	1.00E+00
C2b+	-395.4686	0.0821	-248108.77	-395.4686	0.03	-56.09	-248164.83	0.00	5.45E-01	8.91	2.92E-07
C2+	-395.4562	0.0812	-248101.58	-395.4561	0.11	-61.75	-248163.22	7.20	2.88E-06	10.53	1.91E-08
C3b+	-395.4390	0.0800	-248091.52	-395.4386	0.21	-67.47	-248158.78	17.25	1.23E-13	14.97	1.07E-11
C3+	-395.4546	0.0814	-248100.41	-395.4544	0.11	-59.87	-248160.17	8.36	4.06E-07	13.58	1.11E-10
C2	-395.0913	0.0674	-247881.23	-395.0893	1.24	-17.83	-247897.82	0.00	8.71E-01	0.00	9.99E-01
C3	-395.0798	0.0668	-247874.42	-395.0774	1.50	-20.97	-247893.89	6.81	8.90E-06	3.93	1.32E-03
C4b	-395.0885	0.0685	-247878.79	-395.0877	0.51	-12.07	-247890.36	2.44	1.42E-02	7.46	3.37E-06
C4	-395.0856	0.0683	-247877.14	-395.0849	0.48	-12.84	-247889.51	4.09	8.76E-04	8.31	8.05E-07
C5	-395.0899	0.0679	-247880.03	-395.0894	0.32	-8.17	-247887.88	1.21	1.14E-01	9.94	5.17E-08
C6b	-395.0577	0.0673	-247860.26	-395.0571	0.39	-13.45	-247873.32	20.97	3.66E-16	24.50	1.09E-18
C6	-395.0695	0.0686	-247866.87	-395.0690	0.32	-8.16	-247874.71	14.36	2.57E-11	23.11	1.14E-17
C7b	-395.0566	0.0676	-247859.34	-395.0557	0.57	-15.6	-247874.37	21.89	7.77E-17	23.45	6.47E-18
C7	-395.0412	0.0660	-247850.75	-395.0401	0.75	-23.37	-247873.37	30.49	3.90E-23	24.45	1.19E-18

Reaction	*pKa Local*	*pKa Global*	*Exp*[4]	*Reaction*	*pKa Local*	*pKa Global*	*Exp*[4]
$C1^{+}\rightarrow C2$	4.15	4.15	4.45	$C3^{+}\rightarrow C3$	-2.92	4.16	4.45
$C1^{+}\rightarrow C3$	7.03	4.15		$C3^{+}\rightarrow C5$	1.49	4.15	
$C1^{+}\rightarrow C4$	10.25	4.15		$C3^{+}\rightarrow C6$	11.14	4.15	
$C1^{+}\rightarrow C4b$	9.62	4.15		$C3b^{+}\rightarrow C3$	-3.94	4.16	
$C2^{+}\rightarrow C2$	-3.56	4.16		$C3b^{+}\rightarrow C6b$	11.14	4.15	
$C2^{+}\rightarrow C5$	3.72	4.15		$C3b^{+}\rightarrow C5$	0.47	4.16	
$C2^{+}\rightarrow C7$	14.36	4.15					
$C2^{+}\rightarrow C2$	-2.38	4.16					
$C2^{+}\rightarrow C7b$	14.81	4.15					

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

[4] Reference 87 in manuscript.

Table S-4: Calculation of the Local and Global pK_a for Thymine

Tautomer	$E^{\circ}_{(g)}(R)$[1] (hartrees)	ZPE[2] + $\Delta G_{0\rightarrow 298}$ (hartrees)	$\Delta G^{\circ}_{(g)}(R)$ (kcal/mol)	$E^{\circ}_{(g)}(R')$[1] (hartrees)	$\Delta E^{\circ}_{(dis)}$ (kcal/mol)	$\Delta G^{R'\ 3}_{(sol)}$ (kcal/mol)	$G^{*}_{(aq)}$ (kcal/mol)	$Rel\ G^{\circ}_{(g)}$ (kcal/mol)	Boltzmann Population (g)	$Rel\ G^{*}_{(aq)}$ (kcal/mol)	Boltzmann Population (aq)
T1	-454.3178	0.0822	-285037.17	-454.3168	0.61	-11.10	-285047.67	0.00	1.00E+00	0.00	1.00E+00
T6	-454.2732	0.0794	-285010.94	-454.2714	1.13	-22.58	-285032.39	26.24	5.85E-20	15.28	6.33E-12
T9	-454.2884	0.0815	-285019.18	-454.2868	1.01	-14.91	-285033.08	18.00	6.40E-14	14.59	2.03E-11
T4	-454.3002	0.0820	-285026.23	-454.2995	0.47	-7.64	-285033.40	10.94	9.56E-09	14.27	3.48E-11
T7	-454.2884	0.0807	-285019.65	-454.2876	0.50	-12.98	-285032.14	17.52	1.43E-13	15.53	4.12E-12
T12	-454.2978	0.0820	-285024.73	-454.2963	0.93	-13.05	-285036.85	12.44	7.56E-10	10.81	1.18E-08
T15	-454.2871	0.0814	-285018.37	-454.2854	1.04	-18.68	-285036.01	18.80	1.64E-14	11.66	2.83E-09
T10	-454.2775	0.0797	-285013.42	-454.2757	1.15	-17.85	-285030.12	23.75	3.86E-18	17.54	1.38E-13
T13	-454.2817	0.0806	-285015.54	-454.2799	1.11	-16.15	-285030.58	21.63	1.38E-16	17.08	2.99E-13
T2-	-453.7706	0.0684	-284702.45	-453.7698	0.53	-60.28	-284762.21	0.00	1.00E+00	0.64	2.52E-01
T3-	-453.7522	0.0672	-284691.66	-453.7504	1.13	-72.32	-284762.85	10.79	1.22E-08	0.00	7.48E-01
T5-	-453.7485	0.0685	-284688.54	-453.7471	0.87	-63.17	-284750.84	13.91	6.35E-11	12.00	1.19E-09
T8-	-453.7503	0.0686	-284689.62	-453.7490	0.82	-61.92	-284750.72	12.83	3.92E-10	12.13	9.52E-10
T11-	-453.7399	0.0675	-284683.73	-453.7375	1.46	-67.42	-284749.68	18.73	1.87E-14	13.16	1.67E-10
T14-	-453.7294	0.0668	-284677.65	-453.7270	1.54	-73.20	-284749.31	24.80	6.58E-19	13.54	8.91E-11

Reaction	pKa Local	pKa Global	Exp[4]
T1→T2-	11.14	10.54	9.9
T1→T3-	10.67	10.54	
T6→T5-	8.27	10.54	
T6→T3-	-0.53	10.55	
T9→T8-	8.87	10.54	
T9→T3-	-0.02	10.55	
T4→T5-	9.01	10.54	
T4→T2-	0.69	10.55	
T12→T11-	12.39	10.54	
T12→T3-	2.75	10.55	
T15→T14-	12.05	10.54	
T15→T3-	2.12	10.55	
T10→T11-	7.46	10.54	
T10→T2-	-1.72	10.55	
T13→T14-	8.07	10.54	
T13→T2-	-1.38	10.55	
T7→T2-	-0.24	10.55	
T7→T8-	8.18	10.54	

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species and 0.83 for anions on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

[4] Reference 87 in manuscript.

Table S-5: Calculation of the Local and Global pK_a for 8-oxoguanine

Tautomer	$E^{\circ}_{(g)}(R)$[1] *(hartrees)*	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$ *(hartrees)*	$\Delta G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$E^{\circ}_{(g)}(R')$[1] *(hartrees)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'\ 3}_{(sol)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	$Rel\ G^{\circ}_{(g)}$ *(kcal/mol)*	*Boltzmann Pop. (g)*	$Rel\ G^{*}_{(aq)}$ *(kcal/mol)*	*Boltzmann Pop. (aq)*
8-oxoG1+	-618.3931	0.0973	-387986.53	-618.3899	2.02	-82.64	-388067.15	6.96	7.69E-06	0.00	1.00E+00
8-oxoG7+	-618.4007	0.0972	-387991.37	-618.3989	1.14	-70.94	-388061.17	2.12	2.69E-02	5.98	4.11E-05
8-oxoG8+	-618.3976	0.0983	-387988.72	-618.3965	0.68	-68.29	-388056.33	4.77	3.09E-04	10.82	1.17E-08
8-oxoG9+	-618.4053	0.0984	-387993.49	-618.4034	1.20	-69.28	-388061.57	0.00	9.73E-01	5.58	8.07E-05
8-oxoG2	-618.0483	0.0856	-387777.45	-618.0466	1.07	-21.01	-387797.39	0.00	7.80E-01	0.00	1.00E+00
8-oxoG5	-618.0474	0.0859	-387776.70	-618.0464	0.59	-13.16	-387789.27	0.75	2.20E-01	8.12	1.11E-06
8-oxoG3-	-617.5063	0.0725	-387445.55	-617.5047	1.02	-69.63	-387514.15	0.00	1.00E+00	2.04	3.09E-02
8-oxoG4-	-617.4934	0.0705	-387438.73	-617.4909	1.60	-79.06	-387516.19	6.82	1.00E-05	0.00	9.69E-01
8-oxoG6-	-617.4971	0.0721	-387440.11	-617.4965	0.42	-67.07	-387506.76	5.44	1.03E-04	9.43	1.18E-07

Reaction	*pKa Local*	*pKa Global*	*Calc*[4]	*Exp*[4]	*Gas Phase Basicity*	*Literature Reference*[5]
8-oxoG1$^{+}\rightarrow$2	-0.37	-0.37	0.22	0.1	202.80	200.80
8-oxoG8$^{+}\rightarrow$2	-8.30	-0.37			204.99	204.20
8-oxoG7$^{+}\rightarrow$2	-4.75	-0.37			207.64	208.50
8-oxoG7$^{+}\rightarrow$5	1.20	-0.37			208.39	208.8
8-oxoG9$^{+}\rightarrow$5	1.49	-0.37			210.51	201.9
8-oxoG2$\rightarrow$3^{-}	9.51	8.00	8.69	8.5		
8-oxoG2$\rightarrow$4^{-}	8.02	8.00				

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species and 0.83 for anions on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

[4] Reference 95 in manuscript.

[5] Reference 25 in manuscript.

Table S-6: Calculation of the Local and Global pK_a for Hydantoin and Phenyltoin

Tautomer	$E^{\circ}_{(g)}(R)$[1] *(hartrees)*	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$ *(hartrees)*	$\Delta G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$E^{\circ}_{(g)}(R')$[1] *(hartrees)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'\ 3}_{(sol)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	$Rel\ G^{\circ}_{(g)}$ *(kcal/mol)*	*Boltzmann Pop. (g)*	$Rel\ G^{*}_{(aq)}$ *(kcal/mol)*	*Boltzmann Pop. (aq)*
Hydantoin neutral	-376.8663	0.0498	-236455.95	-376.8653	0.66	-12.56	-236467.86	0.00	1.00E+00	0.00	1.00E+00
Hydantoin N3 anion	-376.3094	0.0381	-236113.82	-376.3076	1.12	-69.93	-236182.63	0.00	1.00E+00	0.00	1.00E+00
Hydantoin N1 anion	-376.3010	0.0371	-236109.19	-376.3000	0.59	-67.92	-236176.51	4.63	4.04E-04	6.12	3.28E-05
Phenytoin neutral	-839.1199	0.1982	-526431.34	-839.1190	0.56	-1.63	-526432.41	0	1.00E+00	0.00	1.00E+00
Phenytoin N3 anion	-838.5724	0.1849	-526096.13	-838.5698	1.67	-55.77	-526150.22	0.00	9.99E-01	0.00	1.00E+00
Phenytoin N1 anion	-838.5655	0.1844	-526092.11	-838.5619	2.29	-54.06	-526143.89	4.02	1.14E-03	6.34	2.26E-05

Reaction	*pKa Local*	*pKa Global*	*Exp*[4]
$H\rightarrow HN3^-$	10.97	10.97	9.1
$H\rightarrow HN1^-$	15.45	10.97	
$Ph\rightarrow PhN3^-$	8.72	8.72	8.31
$Ph\rightarrow PhN1^-$	13.36	8.72	

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species and 0.83 for anions on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

[4] Hydantoin reference: M. J. Bausch, D. Selmarten, R. Gostowski and P. Dobrowolski, J. Phys Org. Chem. (1991) 67. Phenytoin reference is de Oliveira, S. M.; da Silva, J. B. P.; Hernandes, M. Z.; de Lima, M. D. A.; Galdino, S. L.; Pitta, I. D. Structure, reactivity and biological properties of hidantoines. *Quim. Nova* **2008**, *31*, 614.

Table S-7: Calculation of the Local and Global pK_a for Guanidine, Formylguanidine, and Acetylguanidine

Tautomer	$E^{\circ}_{(g)}(R)$[1] *(hartrees)*	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$ *(hartrees)*	$\Delta G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$E^{\circ}_{(g)}(R')$[1] *(hartrees)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'\ 3}_{(sol)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	$Rel\ G^{\circ}_{(g)}$ *(kcal/mol)*	*Boltzmann Pop. (g)*	$Rel\ G^{*}_{(aq)}$ *(kcal/mol)*	*Boltzmann Pop. (aq)*
Guanidine cation	-205.8566	0.0615	-129138.37	-205.8567	-0.09	-62.52	-129200.98	0.00	1.00E+00	0.00	1.00E+00
Guanidine	-205.4660	0.0496	-128900.78	-205.4652	0.54	-10.66	-128910.90	0.00	1.00E+00	0.00	1.00E+00
$FG1^{+}$	-319.2230	0.0691	-200272.11	-319.2221	0.59	-66.97	-200338.49	0.00	1.00E+00	0.00	9.96E-01
$FG2^{+}$	-319.2101	0.0684	-200264.48	-319.2085	1.04	-71.73	-200335.17	7.63	2.55E-06	3.32	3.67E-03
FG3	-318.8520	0.0559	-200047.56	-318.8506	0.85	-12.18	-200058.89	0.00	9.74E-01	0.00	7.91E-01
FG4	-318.8305	0.0550	-200034.63	-318.8291	0.88	-17.33	-200051.08	12.93	3.26E-10	7.81	1.50E-06
FG5	-318.8488	0.0562	-200045.39	-318.8482	0.39	-9.96	-200054.96	2.17	2.51E-02	3.93	1.05E-03
FG6	-318.8454	0.0558	-200043.51	-318.8448	0.38	-11.55	-200054.68	4.05	1.05E-03	4.21	6.47E-04
FG7	-318.8410	0.0564	-200040.36	-318.8398	0.76	-13.60	-200053.21	7.20	5.17E-06	5.68	5.41E-05
FG8	-318.8381	0.0548	-200039.51	-318.8338	2.67	-21.26	-200058.10	8.05	1.21E-06	0.79	2.07E-01
FG9	-318.8416	0.0555	-200041.32	-318.8406	0.66	-13.06	-200053.73	6.23	2.62E-05	5.16	1.30E-04
FG10	-318.8411	0.0557	-200040.85	-318.8404	0.45	-12.90	-200053.30	6.71	1.18E-05	5.59	6.31E-05
FG11	-318.8410	0.0560	-200040.63	-318.8403	0.42	-12.32	-200052.53	6.93	8.06E-06	6.36	1.73E-05
FG12	-318.8409	0.0558	-200040.71	-318.8401	0.52	-12.24	-200052.44	6.85	9.30E-06	6.45	1.47E-05
$AG1^{+}$	-358.5693	0.0930	-224947.32	-358.5684	0.57	-61.63	-225008.38	0.00	1.00E+00	0.00	1.00E+00
$AG2^{+}$	-358.5514	0.0939	-224935.53	-358.5487	1.70	-67.03	-225000.86	11.79	2.29E-09	7.51	3.11E-06
AG3b	-358.1900	0.0807	-224717.00	-358.1887	0.81	-9.78	-224725.97	0.09	4.55E-01	0.08	4.60E-01
AG4	-358.1791	0.0810	-224709.96	-358.1778	0.81	-12.48	-224721.64	7.12	3.15E-06	4.42	3.05E-04
AG5	-358.1869	0.0808	-224715.09	-358.1865	0.36	-8.54	-224723.27	2.00	1.79E-02	2.79	4.82E-03
AG6	-358.1836	0.0801	-224713.37	-358.1831	0.34	-10.21	-224723.25	3.71	9.97E-04	2.81	4.63E-03
AG7	-358.1678	0.0796	-224703.75	-358.1663	0.93	-16.04	-224718.86	13.34	8.75E-11	7.20	2.81E-06
AG3a	-358.1900	0.0806	-224717.09	-358.1887	0.81	-9.78	-224726.06	0.00	5.26E-01	0.00	5.31E-01
AG8	-358.1761	0.0820	-224707.45	-358.1753	0.47	-10.42	-224717.40	9.63	4.56E-08	8.66	2.40E-07
AG9	-358.1735	0.0813	-224706.22	-358.1727	0.49	-11.72	-224717.45	10.87	5.68E-09	8.61	2.60E-07
AG10	-358.1742	0.0812	-224706.76	-358.1734	0.49	-10.52	-224716.80	10.32	1.42E-08	9.26	8.62E-08
AG11	-358.1768	0.0813	-224708.34	-358.1758	0.62	-10.31	-224718.03	8.75	2.03E-07	8.02	6.96E-07

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species and 0.83 for anions on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

Table S-7 (cont): Calculation of the Local and Global pK_a for Guanidine, Formylguanidine, and Acetylguanidine

Reaction	*pKa Local*	*pKa Global*	*Exp*[4]	*Reaction*	*pKa Local*	*pKa Global*	*Exp*[4]
$Guan^+ \rightarrow Guan$	14.53	14.53	13.7				
$FG1^+ \rightarrow FG3$	6.82	6.72	-----	$AG1^+ \rightarrow AG3b$	8.88	8.54	8.23
$FG1^+ \rightarrow FG4$	12.55	6.72		$AG1^+ \rightarrow AG4$	12.06	8.54	
$FG1^+ \rightarrow FG5$	9.70	6.72		$AG1^+ \rightarrow AG5$	10.86	8.54	
$FG1^+ \rightarrow FG6$	9.91	6.72		$AG1^+ \rightarrow AG6$	10.88	8.54	
$FG1^+ \rightarrow FG7$	10.99	6.72		$AG1^+ \rightarrow AG7$	14.09	8.54	
$FG2^+ \rightarrow FG8$	4.97	6.72		$AG2^+ \rightarrow AG3a$	3.31	8.54	
$FG2^+ \rightarrow FG9$	8.18	6.72		$AG2^+ \rightarrow AG8$	9.65	8.54	
$FG2^+ \rightarrow FG10$	8.49	6.72		$AG2^+ \rightarrow AG9$	9.62	8.54	
$FG2^+ \rightarrow FG11$	9.05	6.72		$AG2^+ \rightarrow AG10$	10.10	8.54	
$FG2^+ \rightarrow FG12$	9.12	6.72		$AG2^+ \rightarrow AG11$	9.19	8.54	

[4] Guanidine reference is A. Albert, R. Goldacre, and J. Phillips, J. Chem. Soc. (1948), 2240. No experimental pKa was found for formylguanidine. Acetylguanidine reference is Dean, J.A. (1999). Lange's Handbook of Chemistry (15th Edition). McGraw-Hill, 8.24.

Table S-8: Raw Data Used in the Calculation of the Local and Global pK_a for Guanidinohydantoin

Tautomer	$E^{\circ}_{(g)}(R)$[1]	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$	$\Delta G^{\circ}_{(g)}(R)$	$E^{\circ}_{(g)}(R')$[1]	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'}_{(sol)}$[3] *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*
Neutrals							
Gh1 (Gh N3H)	-581.1173	0.0999	-364593.92	-581.1157	0.99	-19.30	-364612.23
Gh2 (Gh N3imine)	-581.1297	0.1021	-364600.37	-581.1280	1.10	-15.24	-364614.51
Gh3 (Gh_neut_N3Henol_R)	-581.0829	0.0993	-364572.71	-581.0812	1.07	-19.82	-364591.47
Gh4 (Gh_N7C5enol_N3H)	-581.0894	0.1002	-364576.19	-581.0877	1.02	-20.78	-364595.95
Gh5 (Gh_N7C5enol_N3imine)	-581.0955	0.1013	-364579.41	-581.0930	1.60	-20.42	-364598.23
Gh6 (Gh_neut_enol_taut2_R)	-581.0934	0.1002	-364578.75	-581.0916	1.17	-18.89	-364596.47
Gh7 (Gh_N7C8enol_N3H)	-581.0892	0.0990	-364576.88	-	-	-	-
Gh8 (Gh_N7C8enol_N3imine)	-581.1019	0.1022	-364582.82	-581.0998	1.31	-16.65	-364598.16
Gh9 (Gh zwitter N7an N1H2)	-581.0865	0.1002	-364574.47	-581.0792	4.59	-43.90	-364613.78
Cations							
Gh10^{+} (Gh N3H N1H2cat)	-581.5113	0.1153	-364831.55	-581.5083	1.88	-68.41	-364898.08
Gh11^{+} (Gh N3H C5OHcat)	-581.4317	0.1118	-364783.78	-581.4288	1.86	-79.93	-364861.85
Gh12^{+} (Gh N3H C8OHcat)	-581.4414	0.1113	-364790.19	-581.4386	1.79	-77.44	-364865.84
Gh13+ (Gh enol N1H2 cat)	-581.4714	0.1120	-364808.57	-581.4684	1.91	-71.21	-364877.87
Gh14^{+} (Gh N3imine C5OHcat)	-581.4567	0.1117	-364799.46	-581.4540	1.65	-64.76	-364862.57
Gh15^{+} (Gh N3imine C8OHcat)	-581.4690	0.1127	-364806.58	-581.4674	0.97	-64.76	-364870.37

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species and 0.83 for anions on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

Table S-8: Raw Data Used in the Calculation of the Local and Global pK_a for Guanidinohydantoin

Tautomer	$E^{\circ}_{(g)}(R)$[1]	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$	$\Delta G^{\circ}_{(g)}(R)$	$E^{\circ}_{(g)}(R')$[1]	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'}_{(sol)}$[3] *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*
Anions							
Gh16$^-$ (Gh N3H N7-)	-580.5762	0.0881	-364261.83	-580.5712	3.15	-73.60	-364332.28
Gh17$^-$ (Gh N3H N9-)	-580.5644	0.0865	-364255.39	-580.5616	1.80	-73.00	-364326.60
Gh18$^-$ (Gh N3H-)	-580.5575	0.0865	-364251.01	-580.5552	1.41	-69.48	-364319.08
Gh19$^-$ (Gh N3H C2NH-)	-580.5327	0.0859	-364235.86	-580.5283	2.75	-82.33	-364315.44
Gh20$^-$ (Gh N3imine N7b-)	-580.5734	0.0888	-364259.62	-580.5697	2.32	-75.87	-364333.17
Gh21$^-$ (Gh N3imine N9b-)	-580.5586	0.0861	-364252.02	-580.5539	2.91	-75.65	-364324.76
Gh22$^-$ (Gh enol -)	-580.5439	0.0865	-364242.56	-580.5353	5.45	-80.06	-364317.17
Gh23$^-$ (Gh_enol_taut_anion)	-580.5576	0.0874	-364251.15	-580.5554	1.39	-70.96	-364320.15
Gh24$^-$ (Gh_N3Henol_N7anion_R)	-580.5209	0.0856	-364228.70	-580.5159	3.15	-82.80	-364308.35
Gh25$^-$ (Gh_N3Henol_N9anion_R)	-580.5250	0.0854	-364231.37	-580.5208	2.64	-82.94	-364311.67
Gh26$^-$ (Gh_N3Henol_N3anion_R	-580.5600	0.0872	-364252.18	-580.5566	2.11	-70.27	-364320.34
Gh27$^-$ (Gh_N3Henol_C2NHanion_R)	-580.5134	0.0852	-364224.25	-580.5114	1.30	-71.23	-364294.18
Gh28$^-$ (Gh_enol_taut2_N7anion)	-580.5325	0.0874	-364234.85	-580.5267	3.64	-78.63	-364309.84
Gh29$^-$ (Gh_enol_taut2_N9anion)	-580.5296	0.0866	-364233.49	-580.5265	1.96	-76.62	-364308.15
Gh 30a$^-$ (Gh_enol_taut2_C2NHa_anion)	-580.5298	0.0868	-364233.47	-580.5265	2.02	-67.95	-364299.40
Gh 30b$^-$ (Gh_enol_taut2_C2NHb_anion)	-580.5168	0.0860	-364225.79	-580.5120	2.99	-76.11	-364298.91
Gh 30c$^-$ (Gh_enol_taut2_C2NHc_anion)	-580.5341	0.0866	-364236.36	-580.5325	1.02	-64.86	-364300.20
Gh 30d$^-$ (Gh_enol_taut2_C2NHd_anion)	-580.5250	0.0869	-364230.41	-580.5212	2.39	-70.93	-364298.96

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species and 0.83 for anions on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

Table S-9: Local pK_a for Deprotonation of Various Guanidinohydantoin Tautomers

Reaction		*pKa Local*	*pKa Global*
$Gh10^+ \rightarrow Gh1$	Gh+,N3H	11.42	9.63
$Gh10^+ \rightarrow Gh2$	Gh+,N3imine	9.75	9.64
$Gh10^+ \rightarrow Gh3$	Gh+,Gh enol tauto	22.40	9.63
$Gh13^+ \rightarrow Gh3$	Gh_cat_N3Henol_R,Gh_neut_N3Henol_R	11.83	9.63
$Gh13^+ \rightarrow Gh6$	Gh_cat_N3Henol_R,Gh_neut_enol_taut2_R	8.16	9.63
$Gh11^+ \rightarrow Gh4$	Gh_C5OHcat_N3H,Gh_N7C5enol_N3H	-3.20	9.63
$Gh15^+ \rightarrow Gh8$	Gh_C8OHcat_N3imine,Gh_N7C8enol_N3imine	1.43	9.64
$Gh14^+ \rightarrow Gh5$	Gh_C5OHcat_N3imine,Gh_N7C5enol_N3imine	-4.34	9.64
$Gh10^+ \rightarrow Gh9$	Gh+,Ghzwitter	10.29	9.63
$Gh1 \rightarrow Gh19^-$	N3HC2NH-,N3H	19.45	8.14
$Gh1 \rightarrow Gh16^-$	N3HN7-,N3H	7.10	8.15
$Gh1 \rightarrow Gh17^-$	N3HN9-,N3H	11.27	8.14
$Gh1 \rightarrow Gh18^-$	N3H-,N3H	16.78	8.15
$Gh2 \rightarrow Gh18^-$	N3H-,N3imine	18.45	8.15
$Gh2 \rightarrow Gh20^-$	N3imineN7b-,N3imine	8.12	8.15
$Gh2 \rightarrow Gh21^-$	N3imineN9b-,N3imine	14.29	8.15
$Gh6 \rightarrow Gh26^-$	GhenolN3-,Ghenoltaut	4.88	8.15
$Gh6 \rightarrow Gh29^-$	GhenoltautN9-,Ghenoltaut	13.78	8.15
$Gh6 \rightarrow Gh23^-$	Ghenoltaut-,Ghenoltaut	5.02	8.15
$Gh3 \rightarrow Gh22^-$	Gh_enol_anion,Gh_neut_N3Henol_R	2.96	8.15
$Gh3 \rightarrow Gh27^-$	Gh_N3Henol_C2NHanion_R,Gh_neut_N3Henol_R	19.81	8.14
$Gh3 \rightarrow Gh24^-$	Gh_N3Henol_N7anion_R,Gh_neut_N3Henol_R	9.42	8.14
$Gh3 \rightarrow Gh25^-$	Gh_N3Henol_N9anion_R,Gh_neut_N3Henol_R	6.99	8.15
$Gh3 \rightarrow Gh26^-$	Gh_N3Henol_N3anion_R,Gh_neut_N3Henol_R	0.63	8.15
$Gh6b \rightarrow Gh26^-$	Gh_N3Henol_N3anion_R,Gh_neut_enol_taut2_R	4.30	8.15
$Gh6b \rightarrow Gh29^-$	Gh_enol_taut2_N9anion,Gh_neut_enol_taut2_R	13.23	8.15
$Gh6b \rightarrow Gh24^-$	Gh_enol_taut2_N7anion,Gh_neut_enol_taut2_R	12.00	8.15
$Gh6b \rightarrow Gh27a^-$	Gh_enol_taut2_C2NHa_anion,Gh_neut_enol_taut2_R	19.65	8.15
$Gh6b \rightarrow Gh27b^-$	Gh_enol_taut2_C2NHb_anion,Gh_neut_enol_taut2_R	20.01	8.15
$Gh6b \rightarrow Gh27c^-$	Gh_enol_taut2_C2NHc_anion,Gh_neut_enol_taut2_R	19.06	8.15
$Gh6b \rightarrow Gh27d^-$	Gh_enol_taut2_C2NHd_anion,Gh_neut_enol_taut2_R	19.97	8.15
$Gh4 \rightarrow Gh16^-$	Gh_N7C5enol_N3H,Gh_N3H_N7an	-4.83	8.16
$Gh8 \rightarrow Gh20^-$	Gh_N7C8enol_N3imine,Gh_N3imine_N7b_anion	-3.86	8.15

Gh5→Gh20^{-}	Gh_N7C5enol_N3imine,Gh_N3imine_N7b_anion	-3.82	8.15
Gh9→Gh16^{-}	GhZwitter,Gh N3H_N7an	8.24	8.15

Table S-10: Raw Data Used in the Calculation of the Local and Global pK_a for Spiroiminodihydantoin

Tautomer	$E^{\circ}_{(g)}(R)$[1]	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$	$\Delta G^{\circ}_{(g)}(R)$	$E^{\circ}_{(g)}(R')$[1]	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'\ 3}_{(sol)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*
Neutrals							
Sp1 (Sp_neut_N3H)	-693.2972	0.0880	-434995.33	-693.2933	2.40	-26.18	-435019.10
Sp2 (Sp_neut_N1H)	-693.2940	0.0871	-434993.95	-693.2921	1.20	-22.63	-435015.38
Sp3 (Sp_neut_C2imina_b)	-693.2939	0.0880	-434993.28	-693.2927	0.77	-19.56	-435012.07
Sp4 (Sp_neut_C2imina_a)	-693.2953	0.0883	-434993.98	-693.2936	1.03	-19.37	-435012.32
Sp5 (Sp_neut_N1H_N7C5_R2)	-693.2654	0.0873	-434975.82	-693.2628	1.60	-24.98	-434999.20
Sp6 (Sp_neut_N1H_N7C8_R2)	-693.2650	0.0872	-434975.64	-693.2621	1.80	-25.56	-434999.40
Sp7 (Sp_neut_N1H_N9C8_R2)	-693.2648	0.0871	-434975.6	-693.2630	1.14	-22.59	-434997.05
Sp8 (Sp_neut_N1H_N1C6_R)	-693.2777	0.0880	-434983.09	-693.2765	0.72	-17.68	-435000.05
Sp9 (Sp_neut_N3H_N7C5_R2)	-693.2674	0.0879	-434975.42	-693.2635	1.20	-28.68	-435002.90
Sp10 (Sp_neut_N3H_N7C8_R)	-693.2699	0.0881	-434975.05	-693.2643	0.40	-28.53	-435003.17
Sp11 (Sp_neut_N3H_N9C8_R)	-693.2678	0.0877	-434977.13	-693.2644	2.18	-26.62	-435001.57
Sp12 (Sp_neut_C2imine_N7C5_R)	-693.2648	0.0875	-434975.34	-693.2629	1.18	-21.85	-434996.01
Sp13 (Sp_neut_C2imine_N7C8_R)	-693.2663	0.0883	-434975.8	-693.2642	1.33	-21.77	-434996.24
Sp14 (Sp_neut_C2imine_N9C8_R)	-693.2658	0.0874	-434976.04	-693.2645	0.80	-19.67	-434994.92
Sp15 (Sp_neut_C2imine_N1C6_R)	-693.2715	0.0871	-434979.76	-693.2701	0.86	-18.10	-434997.00
Cations							
Sp16^{+} (Spiro_cation)	-693.6567	0.1005	-435213.15	-693.6531	2.27	-79.19	-435290.07
Sp17^{+} (Spiro C5OH cat)	-693.6216	0.0989	-435192.09				
Sp18^{+} (Spiro C8OHcat)	-693.6299	0.0987	-435197.43	-693.6283	1.04	-71.35	-435267.74
Sp19^{+} (Spiro C6OH cat)	-693.6128	0.0990	-435186.51	-693.6103	1.61	-79.13	-435264.03

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species and 0.83 for anions on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

Table S-10 (cont): Raw Data Used in the Calculation of the Local and Global pK_a for Spiroiminodihydantoin

Tautomer	$E^{\circ}_{(g)}(R)$[1]	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$	$\Delta G^{\circ}_{(g)}(R)$	$E^{\circ}_{(g)}(R')$[1]	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	*Dipole Moment in Solution*	$\Delta G^{R'}_{(sol)}$[3] *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*
Anions								
Sp20^{-} (Sp_N7_anion)	-692.7564	0.0756	-434663.78	-692.7492	4.51	19.3	-83.07	-434742.33
Sp21^{-} (Sp_N9a_anion)	-692.7445	0.0744	-434657.09	-692.7396	3.06	15.2	-83.04	-434737.07
Sp22^{-} (Sp_N3H_anion)	-692.7627	0.0751	-434668.07	-692.7606	1.31	6.2	-70.94	-434737.69
Sp23a^{-} (Sp_C210a_anion)	-692.7579	0.0752	-434664.98	-692.7548	1.94	12.4	-72.05	-434735.09
Sp23b^{-} (Sp_C210b_anion)	-692.7646	0.0756	-434668.93	-692.7624	1.43	8.5	-67.44	-434734.94
Sp24^{-} (Sp_N1H_N7b_anion)	-692.7442	0.0743	-434656.93	-692.7387	3.46	20.9	-84.33	-434737.80
Sp25^{-} (Sp_N1H_N9b_anion)	-692.7338	0.0738	-434650.7	-692.7296	2.63	15.2	-83.80	-434731.87
Sp26^{-} (Sp_C2N10_N7c_anion_a)	-692.7617	0.0754	-434667.24	-692.7586	1.99	12.4	-71.17	-434736.42
Sp27^{-} (Sp_C2N10_N9c_a_anion)	-692.7528	0.0747	-434662.07	-692.7509	1.18	7.3	-70.07	-434730.96
Sp28^{-} (Sp_C2N10_N3d_anion)	-692.7443	0.0738	-434657.32	-692.7431	0.75	5.6	-71.24	-434727.81
Sp29^{-} (Sp_C2N10_N7c_anion_b)	-692.7589	0.0752	-434665.63	-692.7561	1.76	13.7	-72.46	-434736.33
Sp30^{-} (Sp_C2N10_N9c_b_anion)	-692.7498	0.0743	-434660.45	-692.7482	1.02	8.1	-71.64	-434731.08
Sp31^{-} (Sp_C2N10_N3c_anion)	-692.7534	0.0746	-434662.51	-692.7519	0.90	4.6	-66.33	-434727.94

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.
[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.
[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 0.91 for cation and neutral species and 0.83 for anions on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

Table S-11: Local pK_a for Deprotonation of Various Spiroiminodihydantoin Tautomers

Reaction		*pKa Local*	*pKa Global*
$Sp16^+ \rightarrow Sp4$	C2imA,Cat	5.49	0.52
$Sp16^+ \rightarrow Sp3$	C2imB,Cat	5.67	0.52
$Sp16^+ \rightarrow Sp2$	N1H,Cat	3.25	0.52
$Sp16^+ \rightarrow Sp1$	N3H,Cat	0.52	0.52
$Sp1 \rightarrow Sp20^-$	N7_anion,neut_N3H	4.77	4.77
$Sp1 \rightarrow Sp21^-$	N9a_anion,neut_N3H	8.62	4.77
$Sp1 \rightarrow Sp23a^-$	C210a,neut_N3H	10.08	4.77
$Sp1 \rightarrow Sp23b^-$	C210b,neut_N3H	10.19	4.76
$Sp1 \rightarrow Sp22^-$	N3H_anion,neut_N3H	8.17	4.77
$Sp2 \rightarrow Sp22^-$	N3H_anion,neut_N1H	5.44	4.77
$Sp2 \rightarrow Sp24^-$	N1H_N7b_anion,neut_N1H	5.37	4.77
$Sp2 \rightarrow Sp25^-$	N1H_N9b_anion,neut_N1H	9.71	4.77
$Sp2 \rightarrow Sp28^-$	C2N10_N3c_anion,neut_N1H	12.59	4.77
$Sp4 \rightarrow Sp28^-$	C2N10_N3c_anion,neut_C2imine_a	10.35	4.77
$Sp4 \rightarrow Sp29^-$	C2N10_N7c_anion_a,neut_C2imine_a	4.13	4.77
$Sp3 \rightarrow Sp26^-$	C2N10_N7c_anion_b,neut_C2imine_b	4.02	4.77
$Sp4 \rightarrow Sp28^-$	C2N10_N9c_anion_a,neut_C2imine_a	8.13	4.77
$Sp3 \rightarrow Sp27^-$	C2N10_N9c_anion_b,neut_C2imine_b	7.87	4.77
$Sp4 \rightarrow Sp23a^-$	C210a_anion_a,neut_C2imine_a	5.11	4.77
$Sp3 \rightarrow Sp23b^-$	C210a_anion_b,neut_C2imine_b	5.04	4.76
$Sp5 \rightarrow Sp24^-$	N1H_N7b_anion,neut_N1H_N7C5_R2	-6.49	4.77
$Sp6 \rightarrow Sp24^-$	N1H_N7b_anion,neut_N1H_N7C8_R2	-6.34	4.77
$Sp7 \rightarrow Sp25^-$	N9a_anion,neut_N1H_N9C8_R2	-7.54	4.77
$Sp8 \rightarrow Sp22^-$	N3H_anion,neut_N1H_N1C6_R	-5.80	4.77
$Sp9 \rightarrow Sp20^-$	N7_anion,neut_N3H_N7C5_R2	-7.11	4.77
$Sp10 \rightarrow Sp20^-$	N7_anion,neut_N3H_N7C8_R	-6.91	4.77
$Sp11 \rightarrow Sp21^-$	N9a_anion,neut_N3H_N9C8_R	-4.22	4.77
$Sp12 \rightarrow Sp26^-$	C2N10_N7c_anion_b,neut_C2imine_N7C5_R_b	-7.75	4.77
$Sp14 \rightarrow Sp27^-$	C2N10_N9c_anion_b,neut_C2imine_N9C8_R	-4.70	4.77
$Sp15 \rightarrow Sp28^-$	C210b_anion,neut_C2imine_N1C6_R	-6.01	4.77
$Sp13 \rightarrow Sp29^-$	C2N10_N7c_anion_b,neut_C2imine_N7C8_R	-7.58	4.77

Table S-12: Selection of Cavity Model – Raw Data for Deprotonation of Guanine with Various Alpha Values for UFF Cavity

Tautomer	**G5$^-$**					
α=	$\Delta G^{R'}_{(sol)}$ *(kcal/mol)*	$\Delta G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	G3→G5$^-$ pKa local	Global pKa
1.25	-51.25	-340198.25	1.31	-340248.19	26.98	27.84
1.20	-53.69			-340250.63	25.19	26.09
1.15	-56.31			-340253.25	23.27	24.24
1.10	-59.15			-340256.09	21.19	22.25
1.05	-62.13			-340259.07	19.01	20.10
1.00	-65.19			-340262.13	16.76	17.92
0.95	-68.39			-340265.33	14.42	15.63
0.90	-71.45			-340268.39	12.18	13.42
0.85	-74.33			-340271.27	10.07	11.37
0.80	-76.89			-340273.83	8.19	9.51
0.75	-78.65			-340275.59	6.90	8.26

Tautomer	**G6$^-$**				3-->12-	
α=	$\Delta G^{R'}_{(sol)}$ *(kcal/mol)*	$\Delta G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	G3→G6$^-$ pKa local	Global pKa
1.25	-48.58	-340201.08	1.02	-340248.64	27.80	27.42
1.20	-50.96			-340251.02	26.05	25.67
1.15	-53.51			-340253.57	24.18	23.81
1.10	-56.23			-340256.29	22.19	21.82
1.05	-59.14			-340259.20	20.06	19.68
1.00	-62.11			-340262.17	17.88	17.49
0.95	-65.21			-340265.27	15.61	15.21
0.90	-68.19			-340268.25	13.42	12.99
0.85	-70.92			-340270.98	11.42	10.93
0.80	-73.44			-340273.50	9.58	9.07
0.75	-75.13			-340275.19	8.34	7.82

Table S-12 (cont.): Selection of Cavity Model – Raw Data for Deprotonation of Guanine with Various Alpha Values for UFF Cavity

Tautomer	**G7$^-$**							
α=	$\Delta G^{R'}_{(sol)}$ *(kcal/mol)*	$\Delta G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	G3→G7$^-$ pKa local	G4→G7$^-$ pKa local	G3→G7$^-$ Global pKa	G4→G7$^-$ Global pKa
1.25	-50.09	-340200.25	1.66	-340248.67	26.63	27.77	27.42	27.42
1.20	-52.42			-340251.00	24.92	26.06	25.69	25.68
1.15	-54.94			-340253.52	23.07	24.21	23.80	23.80
1.10	-57.55			-340256.13	21.16	22.30	21.83	21.82
1.05	-60.43			-340259.01	19.05	20.19	19.67	19.67
1.00	-63.35			-340261.93	16.91	18.05	17.48	17.48
0.95	-66.36			-340264.94	14.70	15.84	15.21	15.21
0.90	-69.39			-340267.97	12.48	13.62	12.98	12.98
0.85	-72.14			-340270.72	10.47	11.61	10.92	10.92
0.80	-74.62			-340273.20	8.65	9.79	9.08	9.08
0.75	-76.18			-340274.76	7.51	8.65	7.83	7.83

Tautomer	**G1$^+$**					
α=	$\Delta G^{R'}_{(sol)}$ *(kcal/mol)*	$\Delta G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	G1$^+$→G3 pKa local	Global pKa
1.25	-42.24	-340766.70	0.59	-340808.35	-1.80	-2.33
1.20	-44.38			-340810.49	-1.19	-1.80
1.15	-46.84			-340812.95	-0.51	-1.13
1.10	-49.42			-340815.53	0.15	-0.55
1.05	-52.59			-340818.70	0.97	0.20
1.00	-56.32			-340822.43	1.96	1.11
0.95	-60.74			-340826.85	3.20	2.27
0.90	-65.93			-340832.04	4.77	3.76
0.85	-71.66			-340837.77	6.36	5.42
0.80	-79.11			-340845.22	8.77	7.83
0.75	-88.22			-340854.33	12.11	11.11

Table S-12 (cont.): Selection of Cavity Model – Raw Data for Deprotonation of Guanine with Various Alpha Values for UFF Cavity

Tautomer	$G2^+$					
α=	$\Delta G_{(sol)}^{R'}$ *(kcal/mol)*	$\Delta G_{(g)}^{\circ}(R)$ *(kcal/mol)*	$\Delta E_{(dis)}^{\circ}$ *(kcal/mol)*	$G_{(aq)}^{*}$ *(kcal/mol)*	$G2^+ \rightarrow G4$ pKa local	Global pKa
1.25	-45.42	-340762.35	0.92	-340806.85	-3.32	-2.32
1.20	-47.72			-340809.15	-2.69	-1.78
1.15	-50.37			-340811.80	-1.95	-1.22
1.10	-52.97			-340814.40	-1.35	-0.61
1.05	-56.36			-340817.79	-0.47	0.23
1.00	-60.23			-340821.66	0.52	1.14
0.95	-64.75			-340826.18	1.70	2.28
0.90	-70.14			-340831.57	3.29	3.76
0.85	-76.48			-340837.91	5.20	5.43
0.80	-84.12			-340845.55	7.65	7.83
0.75	-93.54			-340854.97	11.00	11.12

Tautomer	G3			
α=	$\Delta G_{(sol)}^{R'}$ *(kcal/mol)*	$\Delta G_{(g)}^{\circ}(R)$ *(kcal/mol)*	$\Delta E_{(dis)}^{\circ}$ *(kcal/mol)*	$G_{(aq)}^{*}$ *(kcal/mol)*
1.25	-4.46	-340537.11	1.03	-340540.54
1.20	-5.77			-340541.85
1.15	-7.30			-340543.38
1.10	-8.99			-340545.07
1.05	-11.04			-340547.12
1.00	-13.41			-340549.49
0.95	-16.14			-340552.22
0.90	-19.19			-340555.27
0.85	-22.75			-340558.83
0.80	-26.91			-340562.99
0.75	-31.46			-340567.54

Table S-12 (cont.): Selection of Cavity Model – Raw Data for Deprotonation of Guanine with Various Alpha Values for UFF Cavity

Tautomer	G4					
α=	$\Delta G_{(sol)}^{R'}$ *(kcal/mol)*	$\Delta G_{(g)}^{\circ}(R)$ *(kcal/mol)*	$\Delta E_{(dis)}^{\circ}$ *(kcal/mol)*	$G_{(aq)}^{*}$ *(kcal/mol)*	$G1^{+} \rightarrow G4$ pKa local	Global pKa
1.25	-4.08	-340537.75	0.71	-340541.12	-2.23	-2.33
1.20	-5.52			-340542.56	-1.71	-1.78
1.15	-7.15			-340544.19	-1.10	-1.13
1.10	-8.93			-340545.97	-0.52	-0.53
1.05	-11.13			-340548.17	0.19	0.21
1.00	-13.65			-340550.69	1.08	1.13
0.95	-16.55			-340553.59	2.19	2.28
0.90	-19.78			-340556.82	3.63	3.77
0.85	-23.51			-340560.55	5.10	5.43
0.80	-27.80			-340564.84	7.41	7.83
0.75	-32.65			-340569.69	10.53	11.12

Table S-13: Selection of Cavity Model – Raw Data for Deprotonation of Guanine with Test Set1 Parameters, UFF Radii, α=0.89 for all Ionic Species

Tautomer	$E^{\circ}_{(g)}(R)$[1] (hartrees)	ZPE[2] + $\Delta G_{0\rightarrow 298}$ (hartrees)	$\Delta G^{\circ}_{(g)}(R)$ (kcal/mol)	$E^{\circ}_{(g)}(R')$[1] (hartrees)	$\Delta E^{\circ}_{(dis)}$ (kcal/mol)	$\Delta G^{R'\ 3}_{(sol)}$ (kcal/mol)	$G^{*}_{(aq)}$ (kcal/mol)	$Rel\ G^{\circ}_{(g)}$ (kcal/mol)	Boltzmann Pop. (g)	$Rel\ G^{*}_{(aq)}$ (kcal/mol)	Boltzmann Pop. (aq)
G1+	-543.1430	0.0967	-340766.70	-543.1421	0.59	-66.71	-340832.81	0.00	9.96E-01	0.00	5.25E-01
G2+	-543.1353	0.0959	-340762.35	-543.1338	0.92	-71.32	-340832.75	4.35	0.64E-03	0.06	4.75E-01
G3	-542.7640	0.0836	-340537.11	-542.7624	1.03	-19.87	-340555.95	0.65	2.40E-01	1.62	6.10E-02
G4	-542.7652	0.0837	-340537.75	-542.7640	0.71	-20.52	-340557.57	0.00	7.19E-01	0.00	9.39E-01
G5-	-542.2105	0.0701	-340198.25	-542.2084	1.31	-72.02	-340268.96	2.82	0.64E-02	0.00	4.36E-01
G6-	-542.2154	0.0705	-340201.08	-542.2138	1.02	-68.78	-340268.84	0.00	7.50E-01	0.13	3.50E-01
G7-	-542.2141	0.0705	-340200.25	-542.2114	1.66	-69.96	-340268.54	0.83	1.85E-01	0.42	2.14E-01
G17--	-541.5191	0.0575	-339772.26	-541.5171	1.22	-202.37	-339973.41	0	1.00	0.00	1.00

Reaction	pKa Local	pKa Global	Exp[4]		Gas Phase Basicity	Literature Reference[5]
$G1^{+}\rightarrow G3$	4.84	3.90	3.2-3.3	$G1^{+}\rightarrow G3$	223.31	221.90
$G1^{+}\rightarrow G4$	3.65	3.91		$G1^{+}\rightarrow G4$	222.66	221.60
$G2^{+}\rightarrow G4$	3.61	3.90		$G2^{+}\rightarrow G4$	218.31	216.18
$G3\rightarrow G5^{-}$	12.26	13.11	9.2-9.6			
$G3\rightarrow G7^{-}$	12.57	13.11				
$G4\rightarrow G7^{-}$	13.75	13.11				
$G4\rightarrow G6^{-}$	13.54	13.11				
$G5^{-}\rightarrow G17^{--}$	18.53	18.90				
$G7^{-}\rightarrow G17^{--}$	18.23	18.90				
$G6^{-}\rightarrow G17^{--}$	18.44	18.90				

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.
[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.
[3] Free energy of solvation calculated on geometries optimized at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 1.0 for all species.
[4] References in manuscript 25, 86-92.
[5] Reference 25 in manuscript.

Table S-14: Selection of Cavity Model – Raw Data for Deprotonation of Guanine with UFF Radii and Alpha=0.915

Tautomer	$E^{\circ}_{(g)}(R)$[1] (hartrees)	ZPE[2] + $\Delta G_{0\rightarrow 298}$ (hartrees)	$\Delta G^{\circ}_{(g)}(R)$ (kcal/mol)	$E^{\circ}_{(g)}(R')$[1] (hartrees)	$\Delta E^{\circ}_{(dis)}$ (kcal/mol)	$\Delta G^{R'\ 3}_{(sol)}$ (kcal/mol)	$G^{*}_{(aq)}$ (kcal/mol)	$Rel\ G^{\circ}_{(g)}$ (kcal/mol)	Boltzmann Pop. (g)	$Rel\ G^{*}_{(aq)}$ (kcal/mol)	Boltzmann Pop. (aq)
G1+	-543.1430	0.0967	-340766.70	-543.1421	0.59	-64.27	-340830.37	0.00	9.96E-01	0.00	7.30E-01
G2+	-543.1353	0.0959	-340762.35	-543.1338	0.92	-68.35	-340829.78	4.35	0.64E-03	0.59	2.70E-01
G23+	-543.1336	0.0961	-340761.17	-543.1334	0.15	-51.62	-340812.64	5.52	0.89E-04	17.73	0.11E-07
G19+	-543.1380	0.0972	-340763.24	-543.1376	0.25	-51.74	-340814.73	3.46	0.29E-02	15.64	0.36E-06
G3	-542.7640	0.0836	-340537.11	-542.7624	1.03	-18.3	-340554.38	0.65	2.40E-01	1.39	8.74E-02
G4	-542.7652	0.0837	-340537.75	-542.7640	0.71	-18.72	-340555.77	0.00	7.19E-01	0.00	9.13E-01
G7a	-542.7625	0.0838	-340536.05	-542.7620	0.32	-7.84	-340543.57	1.70	4.08E-02	10.81	0.15E-05
G5-	-542.2105	0.0701	-340198.25	-542.2084	1.31	-70.49	-340267.43	2.82	0.64E-02	-0.10	1.09E-01
G6-	-542.2154	0.0705	-340201.08	-542.2138	1.02	-67.28	-340267.34	0.00	7.50E-01	0.00	5.34E-01
G7-	-542.2141	0.0705	-340200.25	-542.2114	1.66	-68.48	-340267.06	0.83	1.85E-01	0.27	3.56E-01
G34-	-542.2041	0.0695	-340194.61	-542.2031	0.60	-65.81	-340259.82	6.47	0.14E-04	7.52	0.15E-05
G15a-	-542.2106	0.0709	-340197.78	-542.2093	0.78	-61.09	-340258.09	3.30	0.29E-02	9.25	0.38E-06
G15b-	-542.2136	0.0712	-340199.53	-542.2123	0.83	-58.88	-340257.58	1.54	5.58E-02	9.76	0.16E-06
G16-	-542.2036	0.0700	-340194.01	-542.1998	2.41	-72.64	-340264.24	7.07	0.49E-05	3.10	0.16E-02

Reaction	pKa Local	pKa Global	Exp[4]		Gas Phase Basicity	Literature Reference[5]
$G1^{+}\rightarrow G3$	4.20	3.28	3.2-3.3	$G1^{+}\rightarrow G3$	223.31	221.90
$G1^{+}\rightarrow G4$	3.18	3.28		$G1^{+}\rightarrow G4$	222.66	221.60
$G2^{+}\rightarrow G4$	2.75	3.28		$G2^{+}\rightarrow G4$	218.31	216.18
$G3\rightarrow G5^{-}$	12.23	12.33	9.2-9.6	$G23^{+}\rightarrow G3$	217.79	216.40
$G3\rightarrow G7^{-}$	12.50	13.11		$G23^{+}\rightarrow G7a$	218.84	217.00
$G4\rightarrow G7^{-}$	13.52	13.11		$G19^{+}\rightarrow G7a$	220.91	219.70
$G4\rightarrow G6^{-}$	13.32	13.08				

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.
[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.
[3] Free energy of solvation calculated on geometries optimized at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 1.0 for all species.
[4] References in manuscript 25, 86-92.
[5] Reference 25 in manuscript.

Table S-15: Selection of Cavity Model – Raw Data for Deprotonation of Guanine with Test Set3 Parameters, UFF Radii, α=0.95 for all Ionic Species

Tautomer	$E^{\circ}_{(g)}(R)$[1] *(hartrees)*	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$ *(hartrees)*	$\Delta G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$E^{\circ}_{(g)}(R')$[1] *(hartrees)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'\ 3}_{(sol)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	$Rel\ G^{\circ}_{(g)}$ *(kcal/mol)*	*Boltzmann Pop. (g)*	$Rel\ G^{*}_{(aq)}$ *(kcal/mol)*	*Boltzmann Pop. (aq)*
G1+	-543.1430	0.0967	-340766.70	-543.1421	0.59	-60.72	-340826.82	0.00	9.96E-01	0.00	7.40E-01
G2+	-543.1353	0.0959	-340762.35	-543.1338	0.92	-64.77	-340826.20	4.35	0.64E-03	0.62	2.60E-01
G3	-542.7640	0.0836	-340537.11	-542.7624	1.03	-16.16	-340552.24	0.65	2.40E-01	1.38	8.87E-02
G4	-542.7652	0.0837	-340537.75	-542.7640	0.71	-16.57	-340553.62	0.00	7.19E-01	0.00	9.11E-01
G5-	-542.2105	0.0701	-340198.25	-542.2084	1.31	-68.41	-340265.35	2.82	0.64E-02	0.00	4.19E-01
G6-	-542.2154	0.0705	-340201.08	-542.2138	1.02	-65.23	-340265.29	0.00	7.50E-01	0.07	3.72E-01
G7-	-542.2141	0.0705	-340200.25	-542.2114	1.66	-66.36	-340264.94	0.83	1.85E-01	0.41	2.10E-01
G17--	-541.5191	0.0575	-339772.26	-541.5171	1.22	-198.14	-339969.18	0.00	1.00	0.00	1.00

Reaction	*pKa Local*	*pKa Global*	*Exp*[4]		*Gas Phase Basicity*	*Literature Reference*[5]
$G1^{+}\rightarrow G3$	3.17	2.25	3.2-3.3	$G1^{+}\rightarrow G3$	223.31	221.90
$G1^{+}\rightarrow G4$	2.16	2.25		$G1^{+}\rightarrow G4$	222.66	221.60
$G2^{+}\rightarrow G4$	1.70	2.25		$G2^{+}\rightarrow G4$	218.31	216.18
$G3\rightarrow G5^{-}$	12.18	12.86	9.2-9.6			
$G3\rightarrow G7^{-}$	12.48	12.86				
$G4\rightarrow G7^{-}$	13.49	12.86				
$G4\rightarrow G6^{-}$	13.24	12.85				
$G5^{-}\rightarrow G17^{--}$	18.99	19.37				
$G7^{-}\rightarrow G17^{--}$	18.69	19.37				
$G6^{-}\rightarrow G17^{--}$	18.94	19.37				

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated on geometries optimized at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 1.0 for all species.

[4] References in manuscript 25, 86-92.

[5] Reference 25 in manuscript.

Table S-16: Selection of Cavity Model – Raw Data for Deprotonation of Guanine with Test Set4 Parameters, UFF Radii, α=0.98 for all Ionic Species

Tautomer	$E^{\circ}_{(g)}(R)$[1] *(hartrees)*	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$ *(hartrees)*	$\Delta G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$E^{\circ}_{(g)}(R')$[1] *(hartrees)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'\ 3}_{(sol)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*	$Rel\ G^{\circ}_{(g)}$ *(kcal/mol)*	*Boltzmann Pop. (g)*	$Rel\ G^{*}_{(aq)}$ *(kcal/mol)*	*Boltzmann Pop. (aq)*
G1+	-543.1430	0.0967	-340766.70	-543.1421	0.59	-57.99	-340824.09	0.00	9.96E-01	0.00	7.71E-01
G2+	-543.1353	0.0959	-340762.35	-543.1338	0.92	-61.94	-340823.37	4.35	0.64E-03	0.72	2.29E-01
G3	-542.7640	0.0836	-340537.11	-542.7624	1.03	-14.45	-340550.53	0.65	2.40E-01	1.27	1.05E-01
G4	-542.7652	0.0837	-340537.75	-542.7640	0.71	-14.75	-340551.80	0.00	7.19E-01	0.00	8.95E-01
G5-	-542.2105	0.0701	-340198.25	-542.2084	1.31	-66.48	-340263.42	2.82	0.64E-02	0.00	3.87E-01
G6-	-542.2154	0.0705	-340201.08	-542.2138	1.02	-63.36	-340263.42	0.00	7.50E-01	0.01	3.80E-01
G7-	-542.2141	0.0705	-340200.25	-542.2114	1.66	-64.54	-340263.12	0.83	1.85E-01	0.30	2.33E-01
G17--	-541.5191	0.0575	-339772.26	-541.5171	1.22	-195.7	-339966.74	0.00	1.00	0.00	1.00

Reaction	*pKa Local*	*pKa Global*	*Exp*[4]		*Gas Phase Basicity*	*Literature Reference*[5]
$G1^{+}\rightarrow G3$	2.42	1.55	3.2-3.3	$G1^{+}\rightarrow G3$	223.31	221.90
$G1^{+}\rightarrow G4$	1.49	1.56		$G1^{+}\rightarrow G4$	222.66	221.60
$G2^{+}\rightarrow G4$	0.96	1.55		$G2^{+}\rightarrow G4$	218.31	216.18
$G3\rightarrow G5^{-}$	12.35	12.91	9.2-9.6			
$G3\rightarrow G7^{-}$	12.57	12.91				
$G4\rightarrow G7^{-}$	13.49	12.91				
$G4\rightarrow G6^{-}$	13.28	12.91				
$G5^{-}\rightarrow G17^{--}$	19.36	19.78				
$G7^{-}\rightarrow G17^{--}$	19.14	19.78				
$G6^{-}\rightarrow G17^{--}$	19.36	19.78				

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.
[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.
[3] Free energy of solvation calculated on geometries optimized at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model α= 1.0 for all species.
[4] References in manuscript 25, 86-92.
[5] Reference 25 in manuscript.

Table S-17: Raw Data for Evaluation of Through-Space Electronic Effects on the pKa of Sp

Tautomer	$E^{\circ}_{(g)}(R)$[1] *(hartrees)*	*ZPE*[2] + $\Delta G_{0\rightarrow 298}$ *(hartrees)*	$\Delta G^{\circ}_{(g)}(R)$ *(kcal/mol)*	$E^{\circ}_{(g)}(R')$[1] *(hartrees)*	$\Delta E^{\circ}_{(dis)}$ *(kcal/mol)*	$\Delta G^{R'\ 3}_{(sol)}$ *(kcal/mol)*	$G^{*}_{(aq)}$ *(kcal/mol)*
Sp_neut_N1H_CH2	-619.2369	0.1081	-388509.2	-619.2352	1.09	-17.69	-388525.80
Sp_neut_N3H_CH2	-619.2340	0.1068	-388508.21	-619.2324	1.00	-16.88	-388524.09
Sp_neut_C2imine_a_CH2	-619.2294	0.1070	-388505.22	-619.2288	0.38	-18.36	-388523.20
Sp_neut_C2imine_b_CH2	-619.2287	0.1075	-388504.44	-619.2273	0.85	-18.70	-388522.30
Sp_N7an_N1H_CH2	-618.6702	0.0916	-388163.95	-618.6671	1.95	-78.74	-388240.74
Sp_N7an_N3H_CH2	-618.6860	0.0951	-388171.66	-618.6824	2.27	-68.25	-388237.64
Sp_N7an_C2imine_a_CH2	-618.6882	0.0950	-388173.13	-618.6861	1.33	-65.89	-388237.69
Sp_N7an_C2imine_b_CH2	-618.6840	0.0945	-388170.78	-618.6822	1.18	-68.06	-388237.66
Sp_neut_N1H_C6CH2	-657.3378	0.1102	-412416.5	-657.3356	1.33	-17.65	-412432.83
Sp_neut_N3H_C6CH2	-657.3409	0.1111	-412417.98	-657.3393	1.04	-16.05	-412432.99
Sp_neut_C2imine_a_C6CH2	-657.3365	0.1104	-412415.64	-657.3354	0.71	-15.14	-412430.07
Sp_neut_C2imine_b_C6CH2	-657.3354	0.1101	-412415.16	-657.3344	0.66	-15.65	-412430.15
Sp_neut_N1H_C6CH2_N7an	-656.7810	0.0976	-412075.06	-656.7756	3.42	-80.43	-412152.07
Sp_neut_N3H_C6CH2_N7an	-656.7953	0.0986	-412083.44	-656.7911	2.62	-72.89	-412153.71
Sp_C2imine_a_C6CH2_N7an	-656.7972	0.0976	-412085.23	-656.7948	1.50	-67.81	-412151.54
Sp_C2imine_b_C6CH2_N7an	-656.7942	0.0974	-412083.5	-656.7923	1.18	-69.36	-412151.68
Sp_neut_C2imina_a	-693.2953	0.0883	-434993.98	-693.2936	1.03	-19.37	-435012.32
Sp_neut_C2imina_b	-693.2939	0.0880	-434993.28	-693.2927	0.77	-19.56	-435012.07
Sp_neut_N1H	-693.2940	0.0871	-434993.95	-693.2921	1.20	-22.63	-435015.38
Sp_neut_N3H	-693.2972	0.0880	-434995.33	-693.2933	2.40	-26.18	-435019.10
Sp_N1H_N7b_anion	-692.7442	0.0743	-434656.93	-692.7387	3.46	-84.33	-434737.80
Sp_N3H_N7_anion	-692.7564	0.0756	-434663.78	-692.7492	4.51	-83.07	-434742.34
Sp_C2N10_N7c_anion_a	-692.7617	0.0754	-434667.24	-692.7586	1.99	-71.17	-434736.42
Sp_C2N10_N7c_anion_b	-692.7589	0.0752	-434665.63	-692.7561	1.76	-72.46	-434736.33

[1] Gas phase calculations conducted at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p) and B3LYP/aug-cc-pVTZ//IEF-PCM/B3LYP/6-31+G(d,p) for the gas and solution phase optimized geometries, respectively.

[2] Frequency calculation conducted at B3LYP/6-31+G(d,p) on geometry optimized in the gas phase at the same level of theory.

[3] Free energy of solvation calculated at IEF-PCM/B3LYP/6-31+G(d,p) using UFF atom model = 0.91 for cation and neutral species and 0.83 for anions on the geometry optimized in solution with radii=UFF and α= 1.0 for all species.

Table S-18: Site-Specific pKa for Evaluation of Through-Space Electronic Effects on the pKa of Sp

	Reaction	pKa Local	pKa Global	$\Delta G^{\circ}_{(g)}(R)$ (kcal/mol)	$\Delta G^{R'}_{(sol)}$ (kcal/mol)	$\Delta E^{\circ}_{(dis)}$ (kcal/mol)
CH2	SpC2imAneut →C2imAN7an	11.18	10.87	325.815557	-47.53	0.94
CH2	SpC2imBneut →C2imBN7an	10.53	10.87	327.380412	-49.36	0.33
CH2	N1Hneut → N1HN7an	10.85	10.87	338.967689	-61.05	0.87
CH2	N3Hneut → N3HN7an	11.87	10.87	330.27017	-51.37	1.28
C6CH2	SpC2imAneut→ C2imAN7an	6.06	6.81	324.124657	-52.67	0.80
C6CH2	SpC2imBneut→ C2imBN7an	6.02	6.81	325.378856	-53.71	0.52
C6CH2	N1Hneut→ N1HN7an	7.69	6.81	335.166894	-62.78	2.09
C6CH2	N3Hneut→ N3HN7an	6.61	6.81	328.261209	-56.84	1.58
Sp	SpC2imAneut→ C2imAN7an	4.13	4.77	320.460112	-51.80	0.96
Sp	SpC2imBneut→ C2imBN7an	4.02	4.77	321.368854	-52.90	1.00
Sp	N1Hneut→ N1HN7an	5.37	4.77	330.74101	-61.70	2.26
Sp	N3Hneut→ N3HN7an	4.77	4.77	325.26364	-56.89	2.11

Cartesian Coordinates for Geometries Optimized in the Gas Phase at B3LYP/6-31+G(d,p)

SCF Energies were calculated at B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d,p)

Guanine Tautomers

G1$^+$ SCF Energy: -543.143007823

	X	Y	Z
C	0.019761	-0.002109	-0.005261
C	0.056290	-0.001731	1.351140
C	2.256426	-0.000425	1.485166
C	1.241179	-0.001588	-0.762435
C	-2.047139	-0.003098	0.692718
O	1.377060	-0.001805	-1.943557
N	2.328791	-0.000735	0.121074
H	3.221624	-0.000350	-0.328515
N	3.400829	0.000386	2.158569
H	4.290464	0.000879	1.716749
H	3.360221	0.000659	3.152840
N	1.124809	-0.000906	2.144408
N	-1.257942	-0.002367	1.763835
H	-1.566549	-0.002292	2.714328
N	-1.313426	-0.002964	-0.384073
H	-1.656492	-0.003414	-1.323527
H	-3.117221	-0.003701	0.717705

G2$^+$ SCF Energy: -543.135277360

	X	Y	Z
C	-0.018641	0.000003	-0.027184
C	-0.097229	0.000003	1.353168
C	2.261437	0.000016	1.563410
C	1.223010	0.000008	-0.739136
C	-2.095278	-0.000009	0.690210
O	1.460448	0.000008	-1.924142
N	2.329646	0.000017	0.214797
H	3.239939	0.000015	-0.236845
N	3.374675	0.000014	2.306842
H	4.291759	0.000056	1.883027
H	3.338316	0.000037	3.316759
N	1.047153	0.000011	2.144708
N	-1.364783	-0.000004	1.804536
N	-1.335008	-0.000007	-0.436223
H	-1.663534	-0.000011	-1.394746
H	-3.175899	-0.000016	0.663432
H	0.940385	0.000011	3.153645

G19$^+$ SCF Energy: -543.137954693

	X	Y	Z
C	0.016460	0.000001	0.012610
C	-0.005621	0.000007	1.409285
C	2.210874	0.000024	1.545298
C	1.295328	0.000009	-0.583720
C	-2.106881	-0.000009	0.643566
O	1.393459	0.000008	-1.911051
N	2.360054	0.000020	0.184922

N	3.340725	0.000020	2.266121
H	4.235942	0.000043	1.801394
H	3.294644	0.000040	3.274035
N	1.034797	0.000018	2.217784
N	-1.356315	-0.000001	1.760140
N	-1.304460	-0.000009	-0.420085
H	-3.186396	-0.000016	0.614428
H	-1.713721	-0.000001	2.709449
H	-1.619478	-0.000015	-1.384060
H	2.333253	0.000014	-2.166713

G23^{+} SCF Energy: -543.133589581

	X	Y	Z
C	-0.040785	0.000001	0.016926
C	-0.017921	0.000006	1.433104
C	2.213814	0.000022	1.576994
C	1.183637	0.000007	-0.617356
C	-2.073056	-0.000012	0.602764
O	1.436980	0.000004	-1.910365
N	2.289941	0.000018	0.188564
H	3.192222	0.000022	-0.279036
N	3.366833	0.000033	2.265006
H	4.278943	0.000037	1.834779
H	3.311620	0.000035	3.274262
N	1.057261	0.000016	2.222811
N	-1.332619	-0.000002	1.783759
N	-1.332174	-0.000010	-0.472514
H	-3.154647	-0.000020	0.617018
H	-1.697616	-0.000001	2.728881
H	0.612143	-0.000003	-2.428984

G3 SCF Energy: -542.764014543

	X	Y	Z
C	-0.018691	0.009591	-0.003630
C	0.047841	-0.016313	1.363365
C	2.247420	-0.049928	1.493157
C	1.207662	-0.001273	-0.750449
C	-2.019030	0.020584	0.654924
O	1.409567	0.005442	-1.928790
N	2.309850	-0.030696	0.135793
H	3.194260	-0.102858	-0.319056
N	3.435597	-0.125300	2.151555
H	4.246763	0.252400	1.717918
H	3.371572	0.016263	3.134442
N	1.144269	-0.035999	2.160409
N	-1.236957	-0.008055	1.785441
H	-1.540372	-0.022975	2.731520
N	-1.330737	0.031526	-0.423479
H	-3.087939	0.031783	0.713345

G4 SCF Energy: -542.765170509

	X	Y	Z
C	0.048366	0.003652	-0.010526
C	-0.040764	0.000970	1.383429
C	2.194857	-0.002321	1.616494
C	1.295092	-0.010568	-0.702727
C	-2.043220	-0.000252	0.646487

O	1.520808	-0.026639	-1.911844
N	2.351858	-0.014527	0.242552
H	3.276232	-0.102922	-0.163394
N	3.358058	-0.066163	2.357206
H	4.172423	0.413556	1.997957
H	3.198305	0.078662	3.345780
N	1.038535	0.013287	2.221975
N	-1.356770	0.000444	1.775732
N	-1.253114	0.001517	-0.466806
H	-3.122591	-0.001772	0.579576
H	-1.545637	-0.000590	-1.433352

G7a SCF Energy: -542.762512961

	X	Y	Z
C	0.019265	-0.007930	0.022633
C	-0.009369	0.000961	1.429385
C	2.204351	0.011255	1.603819
C	1.310343	0.000815	-0.527977
C	-2.042151	-0.014025	0.547122
O	1.497059	0.001747	-1.856354
N	2.381956	0.010728	0.258243
N	3.347313	-0.025617	2.357349
H	4.213748	0.203123	1.896148
H	3.259049	0.192086	3.337777
N	1.034778	0.013362	2.261350
N	-1.345480	-0.002440	1.747993
N	-1.264723	-0.016886	-0.503600
H	-3.123380	-0.019889	0.523616
H	2.456846	0.003105	-2.007268
H	-1.730258	-0.002397	2.681204

G5^{-} SCF Energy: -542.210535998

	X	Y	Z
N	-0.019485	-0.000530	-0.014013
C	-0.012749	0.001504	1.377818
C	1.298394	0.002413	1.857756
N	2.098765	0.000799	0.730844
C	1.243636	0.000618	-0.363243
N	1.715781	0.002059	3.137535
C	0.646767	0.003593	3.966133
N	-0.652019	-0.008608	3.680744
C	-1.096202	-0.008615	2.356484
N	0.968163	0.054302	5.336130
O	-2.307724	-0.022801	2.074163
H	0.213740	-0.297885	5.910860
H	1.870516	-0.354645	5.542275
H	3.106786	0.011015	0.729940
H	1.620353	0.001074	-1.378228

G6^{-} SCF Energy: -542.215439218

	X	Y	Z
N	-0.006475	0.002803	0.040197
C	-0.022379	0.008574	1.423862
C	1.314004	0.003244	1.815642
N	2.141439	-0.004124	0.697522
C	1.309663	-0.003858	-0.330702
N	1.698700	-0.000236	3.117322

C	0.643594	0.003693	3.945014
N	-0.675788	-0.006837	3.679887
C	-1.107712	-0.005608	2.372424
N	0.962676	0.054620	5.316471
O	-2.316304	-0.021325	2.027353
H	0.221881	-0.323520	5.892334
H	1.877834	-0.329642	5.513513
H	1.611089	-0.006678	-1.370760
H	-0.826414	0.002576	-0.546793

G7^{-} SCF Energy: -542.214076285

	X	Y	Z
N	-0.040670	-0.014967	-0.023076
C	-0.052148	-0.015964	1.352285
C	1.293185	-0.014922	1.821966
N	2.136655	-0.016897	0.768114
C	1.272399	-0.015633	-0.288432
N	1.670128	-0.033023	3.155083
C	0.678410	-0.011590	3.988082
N	-0.647323	0.002542	3.620467
C	-1.141298	0.006801	2.273218
N	0.914419	0.041828	5.382468
O	-2.370785	0.037215	2.113231
H	0.411917	-0.676640	5.896656
H	1.912345	-0.053431	5.540507
H	1.643233	-0.015779	-1.309716
H	-1.363143	0.137261	4.322812

G14^{-} SCF Energy: -542.204065201

	X	Y	Z
N	-0.029605	0.013615	-0.028395
C	-0.033389	-0.007518	1.361447
C	1.280148	-0.013436	1.877394
N	2.079041	0.004943	0.745487
C	1.235493	0.020519	-0.360364
N	1.731512	-0.031797	3.127848
C	0.749964	-0.047705	4.079543
N	-0.604481	-0.042811	3.623114
C	-1.109892	-0.023512	2.307146
N	1.033316	-0.066675	5.357088
O	-2.337222	-0.022464	2.119314
H	0.169791	-0.076263	5.903298
H	1.622263	0.036476	-1.371117
H	3.087057	0.006228	0.759045
H	-1.330252	-0.054538	4.327781

G15b^{-} SCF Energy: -542.213618406

	X	Y	Z
N	-0.069815	-0.045023	0.020823
C	-0.009311	0.011340	1.397269
C	1.345550	0.071066	1.823522
N	2.145429	0.053655	0.723673
C	1.239362	-0.014358	-0.290745
N	1.696270	0.124111	3.137171
C	0.659382	0.120070	3.967720
N	-0.666939	0.053760	3.676903
C	-0.984953	-0.001587	2.388060

N	0.949139	0.231667	5.341718
O	-2.315578	-0.078713	2.073801
H	0.233616	-0.185936	5.922572
H	1.568766	-0.042644	-1.325974
H	1.884776	-0.087785	5.557619
H	-2.349037	-0.113553	1.103753

G15a$^-$ SCF Energy: -542.210587550

	X	Y	Z
N	-0.048938	-0.060678	-0.012810
C	-0.030366	-0.003356	1.365883
C	1.329863	0.068712	1.818161
N	2.149810	0.056264	0.739977
C	1.261403	-0.020235	-0.292588
N	1.681562	0.128758	3.131535
C	0.651982	0.122621	3.964281
N	-0.667859	0.049884	3.660491
C	-0.996984	-0.013560	2.364644
N	0.938781	0.240267	5.340002
O	-2.333646	-0.091695	2.090337
H	0.240227	-0.205486	5.921012
H	1.613403	-0.047314	-1.320835
H	1.882268	-0.061857	5.548327
H	-2.762158	-0.069135	2.960903

G16$^-$ SCF Energy: -542.203600735

	X	Y	Z
N	-0.035081	0.035682	-0.010526
C	-0.014124	0.014127	1.371595
C	1.331908	0.010814	1.762091
N	2.166384	0.028929	0.711833
C	1.263001	0.043087	-0.325090
N	1.680164	-0.012420	3.109411
C	0.653255	-0.050798	4.011039
N	-0.610333	-0.036407	3.717538
C	-1.071926	-0.040025	2.360434
N	1.054010	-0.138454	5.364125
O	-2.288713	-0.076993	2.145425
H	0.230418	-0.050423	5.949227
H	1.605899	0.059641	-1.355099
H	1.751630	0.552996	5.622023
H	2.629311	-0.224719	3.383054

Adenine Tautomers

A1$^+$ SCF Energy: -467.867074150

	X	Y	Z
N	0.046232	0.005993	0.021495
C	0.024065	0.010499	1.415670
H	0.939353	-0.033472	1.989781
N	-1.186788	0.071711	1.902335
C	-2.008797	0.109883	0.798324
C	-3.421115	0.179982	0.680318
N	-4.234343	0.222514	1.726314
H	-5.235042	0.271478	1.582020
H	-3.865706	0.206028	2.668656
N	-3.974294	0.205107	-0.570782

C	-3.211726	0.164583	-1.626036
H	-3.664862	0.185192	-2.612385
N	-1.844313	0.096010	-1.600083
C	-1.253928	0.069560	-0.370162
H	0.874478	-0.036615	-0.559354
H	-1.320629	0.067603	-2.468597

A2$^+$ SCF Energy: -467.856112176

	X	Y	Z
N	0.025114	0.006806	0.021513
C	0.112658	0.004489	1.355423
H	1.028931	-0.039941	1.926192
N	-1.117068	0.065919	1.874660
C	-2.051244	0.110603	0.835415
C	-3.465226	0.181108	0.711316
N	-4.336517	0.226166	1.735778
H	-5.322014	0.274809	1.511086
H	-4.069413	0.216154	2.706703
N	-3.956533	0.203707	-0.537544
C	-3.135918	0.161112	-1.593462
H	-3.613557	0.183333	-2.568001
N	-1.795344	0.094451	-1.586520
C	-1.317746	0.072561	-0.353346
H	0.806717	-0.032579	-0.625376
H	-1.298808	0.076191	2.871029

A3$^+$ SCF Energy: -467.869109621

	X	Y	Z
N	-0.005367	0.008319	0.009283
C	-0.007232	0.011602	1.392271
H	0.910651	-0.032823	1.962513
N	-1.215448	0.072982	1.904787
C	-2.038434	0.111634	0.807786
C	-3.439610	0.181575	0.721561
N	-4.252967	0.224459	1.775644
H	-5.259585	0.273241	1.705931
H	-3.841322	0.205625	2.701159
N	-3.916889	0.202975	-0.564454
C	-3.103285	0.159602	-1.684692
H	-3.624619	0.183705	-2.635618
N	-1.805822	0.094521	-1.643890
C	-1.307076	0.072385	-0.388173
H	0.803944	-0.033548	-0.599586
H	-4.918480	0.252866	-0.722948

A4$^+$ SCF Energy: -467.869678455

	X	Y	Z
N	0.073476	0.006051	-0.016299
C	0.110398	0.006129	1.307372
H	1.015600	-0.037306	1.898122
N	-1.126957	0.067424	1.882143
C	-2.046047	0.111068	0.845365
C	-3.452165	0.180413	0.710667
N	-4.331897	0.225102	1.715632
H	-5.317474	0.273099	1.487763
H	-4.067199	0.213873	2.688613
N	-3.968192	0.204423	-0.550439

C	-3.183732	0.164233	-1.596808
H	-3.625700	0.184839	-2.587885
N	-1.830660	0.097303	-1.533994
C	-1.244851	0.070244	-0.300925
H	-1.258277	0.067978	-2.373480
H	-1.305537	0.077615	2.877560

A5^{+} SCF Energy: -467.852232820

	X	Y	Z
N	0.041586	0.007771	-0.017160
C	0.077030	0.007437	1.299151
H	0.978989	-0.036389	1.895767
N	-1.163233	0.069150	1.883498
C	-2.070036	0.112920	0.844892
C	-3.463177	0.181894	0.750801
N	-4.342562	0.226710	1.766050
H	-5.340776	0.273855	1.615647
H	-4.035372	0.213146	2.726636
N	-3.917182	0.203162	-0.541040
C	-3.085554	0.160530	-1.649156
H	-3.597039	0.184754	-2.606130
N	-1.794464	0.096595	-1.587201
C	-1.279299	0.072636	-0.331596
H	-1.335801	0.078670	2.879942
H	-4.916449	0.252712	-0.712630

A6 SCF Energy: -467.495929692

	X	Y	Z
N	0.016497	0.005528	0.009407
C	0.018107	0.011282	1.390548
H	0.939017	-0.034372	1.955801
N	-1.185065	0.076062	1.910239
C	-2.026301	0.115451	0.809769
C	-3.430205	0.187380	0.679742
N	-4.256489	0.242001	1.751407
H	-5.252832	0.258887	1.601401
H	-3.882912	0.193554	2.685586
N	-3.964265	0.207760	-0.555150
C	-3.138540	0.160451	-1.615112
H	-3.625839	0.180184	-2.586464
N	-1.803008	0.092189	-1.628730
C	-1.301925	0.072347	-0.386760
H	0.817191	-0.038724	-0.604127

A7 SCF Energy: -467.483423153

	X	Y	Z
N	0.070764	0.071440	-0.004814
C	0.093885	0.020238	1.304697
H	0.991085	-0.027480	1.907909
N	-1.153892	0.035515	1.885467
C	-2.059827	0.086156	0.837070
C	-3.456808	0.127889	0.708333
N	-4.330107	0.085902	1.776083
H	-5.291472	0.275562	1.521827
H	-4.038530	0.508169	2.646064
N	-3.971466	0.155376	-0.524852
C	-3.126721	0.155781	-1.578565

H	-3.606339	0.175044	-2.553693
N	-1.797859	0.145373	-1.569357
C	-1.273361	0.108698	-0.331571
H	-1.347720	-0.077249	2.868855

A8 SCF Energy: -467.483427109

	X	Y	Z
N	0.073387	0.006460	-0.023784
C	0.014477	0.012420	1.349675
H	0.922571	-0.030908	1.938525
N	-1.195259	0.073179	1.920504
C	-2.024685	0.111664	0.830822
C	-3.415118	0.179928	0.686449
N	-4.261003	0.224126	1.735416
H	-5.255016	0.269716	1.576390
H	-3.892006	0.206074	2.673782
N	-3.968367	0.204699	-0.567037
C	-3.182551	0.163578	-1.615830
H	-3.626131	0.183424	-2.606202
N	-1.828086	0.096592	-1.565579
C	-1.219043	0.069431	-0.333950
H	-1.272988	0.067198	-2.413082

Cytosine Tautomers

$C1^+$ SCF Energy: -395.468166638

	X	Y	Z
N	0.013325	0.000000	0.007274
C	-0.000727	0.000000	1.363836
H	0.967021	0.000000	1.853484
C	-1.169967	0.000000	2.071027
H	-1.168410	0.000000	3.152382
C	-2.392528	0.000000	1.345600
N	-3.583340	0.000000	1.940637
H	-4.454382	0.000000	1.425847
H	-3.649210	0.000000	2.949771
N	-2.324800	0.000000	-0.012097
C	-1.138955	0.000000	-0.781081
O	-1.147166	0.000000	-1.984313
H	0.887449	0.000000	-0.509588
H	-3.166292	0.000000	-0.582560

$C2^+$ SCF Energy:-395.456224630

	X	Y	Z
C	0.027089	0.000000	1.410842
H	1.001393	0.000000	1.884139
C	-1.144405	0.000000	2.094439
H	-1.153652	0.000000	3.177272
C	-2.355076	0.000000	1.321115
N	-3.556245	0.000000	1.893085
H	-4.382007	0.000000	1.306546
H	-3.675206	0.000000	2.896124
N	-2.326010	0.000000	-0.029667
C	-1.172713	0.000000	-0.639297
O	-1.188816	0.000000	-1.961442
H	0.904062	0.000000	-0.462029
H	-0.317908	0.000000	-2.387521

C2b$^+$ SCF Energy: -395.468616183

	X	Y	Z
N	-0.012434	0.000000	0.007002
C	0.015669	0.000000	1.377244
H	0.995209	0.000000	1.839578
C	-1.149587	0.000000	2.077364
H	-1.144313	0.000000	3.160102
C	-2.372904	0.000000	1.327357
N	-3.563992	0.000000	1.921110
H	-4.403322	0.000000	1.355166
H	-3.661497	0.000000	2.926505
N	-2.363594	0.000000	-0.028082
C	-1.208550	0.000000	-0.640963
O	-1.107867	0.000000	-1.955866
H	0.842423	0.000000	-0.541167
H	-1.993669	0.000000	-2.359989

C3$^+$ SCF Energy: -395.454552567

	X	Y	Z
N	0.060898	0.000000	-0.007781
C	0.003668	0.000000	1.345896
H	0.962498	0.000000	1.855673
C	-1.171933	0.000000	2.071274
H	-1.170286	0.000000	3.154031
C	-2.388254	0.000000	1.360462
N	-3.597548	0.000000	1.928634
H	-4.458210	0.000000	1.398418
H	-3.681367	0.000000	2.935899
N	-2.297830	0.000000	-0.006643
C	-1.080441	0.000000	-0.637806
O	-1.181996	0.000000	-1.952845
H	-3.128379	0.000000	-0.593897
H	-0.292778	0.000000	-2.351411

C3b$^+$ SCF Energy: -395.438964846

	X	Y	Z
N	0.031401	0.000000	-0.040343
C	-0.010235	0.000000	1.308577
H	0.955702	0.000000	1.805528
C	-1.175862	0.000000	2.053993
H	-1.160258	0.000000	3.136709
C	-2.395294	0.000000	1.359264
N	-3.600891	0.000000	1.939686
H	-4.469220	0.000000	1.422778
H	-3.672102	0.000000	2.948005
N	-2.323280	0.000000	-0.015051
C	-1.107949	0.000000	-0.671537
O	-1.086445	0.000000	-1.993028
H	-3.186264	0.000000	-0.550778
H	-1.949927	0.000000	-2.433455

C2 SCF Energy: -395.091253241

	X	Y	Z
N	0.000227	0.000000	0.027518
C	0.018700	0.000000	1.383622
H	0.992514	-0.000001	1.862016

C	-1.150503	0.000000	2.079372
H	-1.164404	0.000000	3.161736
C	-2.358169	0.000000	1.291320
N	-3.561434	0.000000	1.923825
H	-4.397277	0.000000	1.358921
H	-3.639265	0.000000	2.926695
N	-2.376452	0.000000	-0.030287
C	-1.203550	0.000002	-0.739326
O	-1.110445	-0.000001	-1.959789
H	0.854642	0.000000	-0.513726

C3 SCF Energy: -395.079794581

	X	Y	Z
N	0.078700	0.000000	-0.020156
C	-0.003339	0.000000	1.297393
H	0.951127	-0.000001	1.824575
C	-1.182894	0.000000	2.067869
H	-1.160064	0.000000	3.149958
C	-2.382027	0.000000	1.367916
N	-3.613292	0.000000	1.947777
H	-4.461353	0.000000	1.404839
H	-3.695815	-0.000001	2.950967
N	-2.309824	0.000001	0.011361
C	-1.088838	0.000003	-0.744061
O	-1.184622	-0.000002	-1.962798
H	-3.145440	0.000000	-0.561841

C4 SCF Energy: -395.085623028

	X	Y	Z
N	-0.001763	0.000000	-0.001293
C	-0.018690	0.000000	1.383630
H	0.953957	0.000000	1.861417
C	-1.174757	0.000000	2.075929
H	-1.192603	0.000000	3.156718
C	-2.453651	0.000000	1.375641
N	-3.570521	0.000000	2.008647
H	-4.375813	0.000000	1.379198
N	-2.323085	0.000000	-0.033689
C	-1.153008	0.000000	-0.774715
O	-1.132608	0.000000	-1.997174
H	-3.162253	0.000000	-0.600421
H	0.865122	0.000000	-0.518913

C4b SCF Energy: -395.088494808

	X	Y	Z
N	-0.001500	0.000000	0.004696
C	-0.002581	0.000000	1.383896
H	0.974789	0.000000	1.853195
C	-1.152866	0.000000	2.090587
H	-1.138739	0.000000	3.172723
C	-2.437787	0.000000	1.395580
N	-3.625110	0.000000	1.885220
N	-2.321319	0.000000	-0.007517
C	-1.167978	0.000000	-0.759658
O	-1.147028	0.000000	-1.981532
H	-3.189086	0.000000	-0.530812
H	0.858693	0.000000	-0.524070

H	-3.595180	0.000000	2.903998

C5 SCF Energy: -395.089862908

	X	Y	Z
N	0.047984	0.000000	-0.014268
C	0.017004	0.000000	1.330616
H	0.983456	0.000000	1.829462
C	-1.154885	0.000000	2.064823
H	-1.149170	0.000000	3.148842
C	-2.357623	0.000000	1.319010
N	-3.580373	0.000000	1.915456
H	-4.401987	0.000000	1.331359
H	-3.682146	0.000000	2.915962
N	-2.350870	0.000000	-0.023644
C	-1.153596	0.000000	-0.601906
O	-1.167369	0.000000	-1.949903
H	-0.239819	0.000000	-2.234228

C6 SCF Energy: -395.069532834

	X	Y	Z
N	0.050720	0.000000	-0.027242
C	-0.004251	0.000000	1.352439
H	0.963347	0.000000	1.845968
C	-1.154418	0.000000	2.080081
H	-1.133348	0.000000	3.163636
C	-2.443595	0.000000	1.407728
N	-3.643054	0.000000	1.871135
H	-3.633784	0.000000	2.889998
N	-2.305835	0.000000	0.000721
C	-1.106452	0.000000	-0.622113
O	-1.191569	0.000000	-1.962893
H	-0.281069	0.000000	-2.300342
H	-3.161505	0.000000	-0.543326

C6b SCF Energy: -395.057718205

	X	Y	Z
N	0.039733	0.000000	-0.050651
C	-0.012344	0.000000	1.326031
H	0.958450	0.000000	1.813880
C	-1.155341	0.000000	2.066813
H	-1.125971	0.000000	3.150173
C	-2.444077	0.000000	1.402453
N	-3.646389	0.000000	1.860314
H	-3.644586	0.000000	2.878994
N	-2.312103	0.000000	-0.008037
C	-1.109534	0.000000	-0.649659
O	-1.114438	0.000000	-1.998066
H	-3.195659	0.000000	-0.506386
H	-2.011214	0.000000	-2.359624

C7 SCF Energy: -395.041247149

	X	Y	Z
N	0.008205	0.000000	0.004343
C	0.010840	0.000000	1.395728
H	0.987027	0.000000	1.865892
C	-1.154258	0.000000	2.068401
H	-1.153013	0.000000	3.152605

C	-2.435600	0.000000	1.337976
N	-3.605951	0.000000	1.874404
H	-3.519791	0.000000	2.892750
N	-2.353629	0.000000	-0.068030
C	-1.216256	0.000000	-0.645738
O	-1.181103	0.000000	-2.001564
H	0.882749	0.000000	-0.498119
H	-0.278997	0.000000	-2.347589

C7b SCF Energy: -395.056629980

	X	Y	Z
N	0.006709	0.000000	0.000757
C	0.008874	0.000000	1.388300
H	0.983363	0.000000	1.861561
C	-1.159052	0.000000	2.060298
H	-1.159209	0.000000	3.144390
C	-2.443085	0.000000	1.333674
N	-3.614717	0.000000	1.867324
H	-3.531861	0.000000	2.885715
N	-2.357013	0.000000	-0.074350
C	-1.206141	0.000000	-0.638645
O	-1.077272	0.000000	-1.981997
H	-1.979744	0.000000	-2.341677
H	0.857942	0.000000	-0.541017

Thymine Tautomers

T1 SCF Energy: -454.170239

	X	Y	Z
N	-0.013287	0.146637	-0.014734
C	-0.007076	0.150873	1.366550
H	0.975138	0.228916	1.820641
C	-1.139208	0.064468	2.104084
C	-1.162661	0.066826	3.605473
H	-0.151411	0.146117	4.014270
H	-1.760269	0.902505	3.984498
H	-1.625165	-0.848500	3.989360
C	-2.419031	-0.037385	1.391267
O	-3.517367	-0.121906	1.926454
N	-2.315860	-0.032749	-0.012015
H	-3.186463	-0.102350	-0.527185
C	-1.167169	0.054836	-0.780465
O	-1.159358	0.052411	-2.001892
H	0.847059	0.212942	-0.540087

T4 SCF Energy: -454.152849

	X	Y	Z
N	0.033457	0.185962	-0.040320
C	-0.014699	0.182391	1.336037
H	0.954150	0.276497	1.820254
C	-1.149095	0.073369	2.092625
C	-1.157588	0.074181	3.594040
H	-0.142984	0.171309	3.990121
H	-1.766232	0.898604	3.981425
H	-1.599915	-0.849314	3.983425
C	-2.426692	-0.050756	1.403877
O	-3.536547	-0.157803	1.915392

N	-2.302431	-0.039636	-0.006875
C	-1.110967	0.074934	-0.642615
O	-1.200316	0.065279	-1.984128
H	-0.296341	0.152458	-2.327857
H	-3.159489	-0.123209	-0.543291

T6 SCF Energy: -454.123007

	X	Y	Z
N	0.008901	0.116986	-0.002537
C	0.029262	0.148841	1.389343
H	1.010769	0.258614	1.837178
C	-1.116573	0.053988	2.096033
C	-1.165998	0.091834	3.594106
H	-0.168023	0.208636	4.027507
H	-1.800529	0.916829	3.934564
H	-1.619670	-0.825345	3.983679
C	-2.392213	-0.110292	1.351658
O	-3.461166	-0.230074	1.939264
N	-2.333097	-0.114758	-0.052081
C	-1.198992	-0.017496	-0.644531
O	-1.174267	-0.057156	-1.998758
H	0.882360	0.077832	-0.507609
H	-0.322787	0.224662	-2.360145

T7 SCF Energy: -454.139550

	X	Y	Z
N	0.006722	0.227100	-0.046800
C	-0.034617	0.203517	1.325837
H	0.938077	0.295881	1.803383
C	-1.158847	0.078235	2.097570
C	-1.149228	0.058558	3.598903
H	-0.129968	0.154628	3.982912
H	-1.755730	0.875328	4.005508
H	-1.582186	-0.872196	3.981571
C	-2.436836	-0.042668	1.420051
O	-3.547751	-0.163349	1.928086
N	-2.322712	-0.010951	0.004112
C	-1.131749	0.119567	-0.652218
O	-1.139264	0.137570	-2.001689
H	-2.031587	0.053805	-2.364120
H	-3.208005	-0.095496	-0.484771

T9 SCF Energy: -454.140118

	X	Y	Z
N	-0.017473	0.154775	-0.010147
C	0.016710	0.163307	1.377717
H	1.001786	0.259650	1.820165
C	-1.124424	0.056477	2.094327
C	-1.156978	0.059273	3.593768
H	-0.152933	0.157499	4.017423
H	-1.780209	0.881204	3.961339
H	-1.612781	-0.863224	3.968349
C	-2.413009	-0.069811	1.364885
O	-3.480521	-0.170042	1.959481
N	-2.362522	-0.069737	-0.041001
C	-1.221806	0.037513	-0.632164
O	-1.122122	0.042625	-1.976696

H	0.823167	0.234104	-0.564256
H	-2.026903	-0.045248	-2.319292

T10 SCF Energy: -454.128949

	X	Y	Z
N	0.067646	0.190839	-0.018433
C	-0.017528	0.172515	1.295332
H	0.935435	0.228210	1.824511
C	-1.193001	0.089651	2.087113
C	-1.176615	0.076187	3.593102
H	-0.146569	0.136877	3.955295
H	-1.731059	0.921448	4.015700
H	-1.621421	-0.839162	3.998953
C	-2.359124	0.022180	1.355905
O	-3.554546	-0.060207	1.975274
N	-2.305860	0.039009	0.000366
C	-1.088801	0.124211	-0.757764
O	-1.176635	0.130578	-1.975796
H	-4.291688	-0.104069	1.349734
H	-3.143615	-0.008774	-0.569092

T12 SCF Energy: -454.149907005

	X	Y	Z
N	-0.010847	0.121793	0.006761
C	0.020191	0.136188	1.367653
H	1.000831	0.198887	1.828463
C	-1.131160	0.074451	2.097289
C	-1.179935	0.085523	3.600134
H	-0.171049	0.149992	4.018198
H	-1.759818	0.936148	3.973906
H	-1.654532	-0.821104	3.990400
C	-2.318577	-0.003532	1.289284
O	-3.484782	-0.066711	1.960892
N	-2.368818	-0.018387	-0.016557
C	-1.204024	0.044306	-0.753799
O	-1.139342	0.037463	-1.974037
H	0.842257	0.168049	-0.535330
H	-4.190114	-0.114740	1.292501

T13 SCF Energy: -454.097625

	X	Y	Z
N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.370000
H	0.935308	0.000000	1.910000
C	-1.144672	0.053981	2.064557
C	-1.155394	0.054487	3.564519
H	-0.602923	0.919245	3.932036
H	-2.184307	0.103010	3.921008
H	-0.686753	-0.858424	3.932036
C	-2.414707	0.113875	1.388522
O	-3.512815	0.165660	1.940225
N	-2.320234	0.109420	0.011766
C	-1.158037	0.054612	-0.730322
O	-1.175693	0.055444	-1.950193
H	-3.392980	0.160009	2.892700
H	-3.179133	0.149924	-0.498774

T15 SCF Energy: -454.149907

	X	Y	Z
N	-0.010873	0.122025	0.006752
C	0.020170	0.136539	1.367638
H	1.000793	0.199550	1.828442
C	-1.131164	0.074547	2.097287
C	-1.179925	0.085709	3.600133
H	-0.171051	0.150487	4.018175
H	-1.760044	0.936198	3.973848
H	-1.654269	-0.821023	3.990466
C	-2.318560	-0.003830	1.289298
O	-3.484744	-0.067275	1.960913
N	-2.368808	-0.018809	-0.016546
C	-1.204042	0.044137	-0.753799
O	-1.139353	0.037202	-1.974035
H	0.842216	0.168464	-0.535348
H	-4.190063	-0.115596	1.292532

T2^{-} SCF Energy: -453.625490

	X	Y	Z
N	0.056432	0.226452	-0.033083
C	-0.038172	0.202298	1.308038
H	0.921231	0.296981	1.827738
C	-1.177494	0.075032	2.090377
C	-1.156910	0.061746	3.594089
H	-0.129153	0.162196	3.965291
H	-1.754399	0.879382	4.020913
H	-1.577290	-0.867591	4.002976
C	-2.431244	-0.048532	1.398053
O	-3.562184	-0.172146	1.918080
N	-2.297658	-0.019784	0.009654
C	-1.105793	0.112523	-0.738785
O	-1.195107	0.116256	-1.980316
H	-3.151619	-0.103580	-0.527643

T3^{-} SCF Energy: -453.605342

	X	Y	Z
N	-0.007079	0.133475	0.006323
C	0.022585	0.159986	1.377612
H	1.003478	0.269950	1.838257
C	-1.122639	0.052769	2.089654
C	-1.162087	0.074090	3.590465
H	-0.155064	0.187649	4.014731
H	-1.792047	0.894229	3.956621
H	-1.608457	-0.846503	3.986498
C	-2.398314	-0.092454	1.328872
O	-3.465458	-0.192967	1.977020
N	-2.370526	-0.111473	-0.039381
C	-1.221444	-0.003135	-0.732324
O	-1.100256	-0.009454	-1.975182
H	0.831613	0.213909	-0.548222

T5^{-} SCF Energy: -453.602500

	X	Y	Z
N	0.028596	0.181975	-0.046015
C	-0.006475	0.193737	1.314834
H	0.961197	0.320067	1.806897

C	-1.149431	0.060452	2.062516
C	-1.155949	0.078212	3.565049
H	-0.141208	0.211311	3.963784
H	-1.792016	0.885628	3.951494
H	-1.572702	-0.852003	3.973602
C	-2.417900	-0.105772	1.347346
O	-3.503113	-0.233453	1.959951
N	-2.362891	-0.115057	-0.040306
C	-1.182053	0.025121	-0.600815
O	-1.169382	0.010571	-1.981829
H	-0.233225	0.123553	-2.205625

T8^{-} SCF Energy: -453.604640

	X	Y	Z
N	0.047719	0.231773	-0.041882
C	-0.006745	0.216131	1.318948
H	0.956729	0.332702	1.821911
C	-1.151671	0.069133	2.063785
C	-1.160122	0.059424	3.566617
H	-0.145811	0.184908	3.968244
H	-1.795881	0.860103	3.967500
H	-1.577183	-0.878010	3.958146
C	-2.417646	-0.083459	1.345387
O	-3.509996	-0.222970	1.944085
N	-2.342833	-0.064797	-0.039424
C	-1.150789	0.086887	-0.599143
O	-1.156250	0.095824	-1.978704
H	-2.094069	-0.018044	-2.198360

T11^{-} SCF Energy: -453.594419

	X	Y	Z
N	0.041654	0.185244	-0.014781
C	-0.012240	0.176977	1.308278
H	0.953411	0.250012	1.823479
C	-1.170599	0.085289	2.095394
C	-1.169009	0.081339	3.599834
H	-0.139986	0.160525	3.974346
H	-1.740920	0.918648	4.025158
H	-1.604167	-0.836534	4.020827
C	-2.330647	-0.001711	1.309056
O	-3.549661	-0.097535	1.951939
N	-2.369796	-0.000633	-0.002805
C	-1.166068	0.094418	-0.717699
O	-1.180621	0.097318	-1.961965
H	-4.185600	-0.143790	1.217911

T14^{-} SCF Energy: -453.582512011

	X	Y	Z
N	0.049336	0.188826	-0.008515
C	-0.010595	0.187453	1.311336
H	0.950187	0.277401	1.834544
C	-1.174510	0.083157	2.087718
C	-1.158986	0.089423	3.594095
H	-0.126404	0.184199	3.953288
H	-1.719979	0.929529	4.037970
H	-1.559792	-0.835137	4.043615
C	-2.340211	-0.026415	1.294951

O	-3.583208	-0.138313	1.909427
N	-2.369127	-0.033252	-0.008967
C	-1.159625	0.075664	-0.712428
O	-1.162852	0.071609	-1.955754
H	-3.447440	-0.122823	2.865577

8-oxoG Tautomers

8-oxoG1$^+$ SCF Energy: -618.393148

	X	Y	Z
C	-0.000219	0.000000	-0.000880
C	-0.000173	0.000000	1.370289
C	2.366644	0.000000	1.485762
C	1.211214	0.000000	-0.755144
C	-2.180024	0.000000	0.689107
O	1.396014	0.000000	-1.950202
N	2.369645	0.000000	0.145021
H	3.254851	0.000000	-0.355218
N	3.503273	0.000000	2.193924
H	4.404635	0.000000	1.736571
H	3.506827	0.000000	3.204415
N	1.166908	0.000000	2.118668
N	-1.283913	0.000000	1.813639
H	-1.635691	0.000000	2.761973
O	-3.383156	0.000000	0.739515
N	-1.325085	0.000000	-0.407980
H	-1.655875	0.000000	-1.363837
H	1.128860	0.000000	3.130581

8-oxoG7$^+$ SCF Energy: -618.400745

	X	Y	Z
C	0.038546	0.000000	-0.024836
C	0.058961	0.000000	1.398982
C	2.305368	0.000000	1.514065
C	1.241368	0.000000	-0.668723
C	-2.125562	0.000000	0.697356
O	1.332729	0.000000	-1.997419
N	2.374542	0.000000	0.133490
H	3.285141	0.000000	-0.312160
N	3.451302	0.000000	2.212721
H	4.369361	0.000000	1.795204
H	3.383613	0.000000	3.221631
N	1.147057	0.000000	2.161667
N	-1.226084	0.000000	1.809247
H	-1.550385	0.000000	2.769125
O	-3.326501	0.000000	0.742587
N	-1.286174	0.000000	-0.420590
H	-1.646324	0.000000	-1.364931
H	2.232241	0.000000	-2.357460

8-oxoG8$^+$ SCF Energy: -618.397613

	X	Y	Z
C	0.032300	0.000000	0.009430
C	0.086266	0.000000	1.385585
C	2.307915	0.000000	1.492037
C	1.237725	0.000000	-0.768017
C	-2.058286	0.000000	0.742891

O	1.367317	0.000000	-1.977504
N	2.357947	0.000000	0.116112
H	3.253256	0.000000	-0.363648
N	3.466783	0.000000	2.171930
H	4.370566	0.000000	1.725072
H	3.426572	0.000000	3.181090
N	1.163120	0.000000	2.173066
N	-1.245761	0.000000	1.826352
H	-1.532574	0.000000	2.798720
O	-3.372082	0.000000	0.693559
N	-1.315026	0.000000	-0.361813
H	-1.680793	0.000000	-1.308641
H	-3.810121	0.000000	1.559143

8-oxoG9^{+} SCF Energy: -618.405345

	X	Y	Z
C	0.025738	0.000000	0.022335
C	-0.007197	0.000000	1.409978
C	2.352587	0.000000	1.457498
C	1.279972	0.000000	-0.591372
C	-2.167442	-0.000001	0.667043
O	1.355555	0.000000	-1.912925
N	2.406232	0.000000	0.135843
N	3.488562	0.000000	2.172781
H	4.364240	0.000000	1.667905
H	3.517830	0.000000	3.181076
N	1.146186	0.000000	2.137351
N	-1.294813	0.000000	1.815959
H	-1.668735	0.000000	2.756459
O	-3.369506	0.000000	0.695193
N	-1.292648	0.000000	-0.413294
H	-1.613709	0.000000	-1.371831
H	2.286489	0.000000	-2.198249
H	1.119455	0.000000	3.151012

8-oxoG2 SCF Energy: -618.048254

	X	Y	Z
C	0.026704	0.000000	-0.013609
C	0.058250	0.000000	1.369857
C	2.290120	0.000000	1.494087
C	1.229367	-0.000001	-0.763859
C	-2.140296	0.000000	0.710123
O	1.405586	0.000000	-1.981282
N	2.354347	0.000000	0.125024
H	3.247755	0.000000	-0.353351
N	3.463477	0.000000	2.185529
H	4.363788	0.000001	1.737547
H	3.413571	0.000000	3.191718
N	1.153323	0.000000	2.162581
N	-1.247559	0.000000	1.801980
H	-1.560456	0.000000	2.761250
O	-3.359896	0.000001	0.760081
N	-1.314457	0.000000	-0.402124
H	-1.663642	0.000000	-1.347986

8-oxoG5 SCF Energy: -618.047377

	X	Y	Z

C	0.039855	0.000000	-0.001518
C	0.053475	0.000000	1.400675
C	2.287094	0.000000	1.456099
C	1.280761	0.000000	-0.614088
C	-2.134932	0.000000	0.703118
O	1.381801	0.000000	-1.961228
N	2.401361	0.000000	0.112000
N	3.447065	0.000000	2.170101
H	4.330080	0.000000	1.688780
H	3.409133	0.000000	3.175373
N	1.137129	0.000000	2.165769
N	-1.261761	0.000000	1.807790
H	-1.591881	0.000000	2.761292
O	-3.353899	0.000000	0.730912
N	-1.298189	0.000000	-0.404956
H	-1.651562	0.000000	-1.348642
H	2.328513	0.000000	-2.177356

8-oxoG3$^-$ SCF Energy: -617.506285

	X	Y	Z
C	0.054378	0.000001	0.025047
C	0.058186	0.000001	1.400999
C	2.273113	0.000000	1.440078
C	1.289925	0.000002	-0.706149
C	-2.134930	0.000000	0.703474
O	1.352106	-0.000003	-1.958820
N	2.412099	0.000001	0.113136
N	3.452553	0.000000	2.168838
H	4.325074	-0.000001	1.671057
H	3.415723	-0.000001	3.172644
N	1.143264	0.000001	2.191639
N	-1.278587	0.000000	1.808045
H	-1.614856	-0.000001	2.757316
O	-3.374236	-0.000001	0.726868
N	-1.294080	0.000000	-0.384019
H	-1.614908	0.000000	-1.338419

8-oxoG4$^-$ SCF Energy: -617.493412

	X	Y	Z
C	0.042162	0.000000	-0.033511
C	0.005888	0.000000	1.384379
C	2.269674	0.000000	1.490832
C	1.229045	0.000000	-0.769394
C	-2.087607	-0.000002	0.762407
O	1.450783	0.000000	-2.002573
N	2.359361	0.000000	0.122770
N	3.465914	0.000000	2.188735
H	4.362430	0.000000	1.736790
H	3.407322	0.000000	3.192866
N	1.150273	0.000000	2.158138
N	-1.246104	0.000000	1.865262
O	-3.330132	0.000001	0.737725
N	-1.296560	0.000000	-0.405773
H	-1.666570	0.000001	-1.341831
H	3.253016	0.000000	-0.350615

8-oxoG6$^-$ SCF Energy: -617.497145

	X	Y	Z
C	0.044618	0.000002	-0.014008
C	0.083150	0.000001	1.380913
C	2.348922	0.000000	1.562958
C	1.247797	0.000003	-0.744572
C	-2.129091	-0.000001	0.703563
O	1.418548	-0.000002	-1.983513
N	2.349682	0.000001	0.136660
N	3.461241	-0.000001	2.248072
H	4.261328	-0.000002	1.612365
N	1.127348	0.000002	2.192949
N	-1.252162	0.000000	1.792124
O	-3.365182	-0.000002	0.748129
N	-1.313530	0.000000	-0.401597
H	-1.663497	-0.000001	-1.345007
H	3.245581	-0.000001	-0.332414
H	-1.566387	0.000000	2.749415

Guanidinohydantoin Tautomers

Gh1 SCF Energy: -581.117266346

	X	Y	Z
C	-0.001314	0.001963	-0.000458
C	-0.000329	0.002235	1.553794
O	0.973148	0.005864	2.274740
C	-2.219278	0.089280	0.836001
O	-3.430165	0.103599	0.916758
N	0.872605	0.996302	-0.534162
H	0.807837	1.922055	-0.129342
C	1.343569	0.941103	-1.850443
N	-1.430488	0.164372	-0.283581
H	-1.843887	0.100976	-1.202502
N	-1.323762	-0.002334	1.926557
H	-1.644869	0.001737	2.885348
N	2.155305	2.028442	-2.152934
H	2.829098	2.284567	-1.441446
H	2.563184	1.947329	-3.075744
H	0.357349	-0.979420	-0.336233
N	1.099554	0.051075	-2.743846
H	0.394035	-0.623659	-2.457011

Gh2 SCF Energy: -581.129718991

	X	Y	Z
C	-0.600621	0.013644	-0.560330
C	-0.038752	-0.510945	0.783631
O	1.036908	-1.070248	0.945693
C	-2.114633	0.434040	1.201873
O	-3.042439	0.862603	1.857947
N	0.138570	1.115341	-1.123169
C	1.255635	0.863843	-1.731596
N	-1.940253	0.436076	-0.158079
H	-2.442136	1.119314	-0.708496
N	-0.972726	-0.217703	1.735636
H	-0.870223	-0.400302	2.724915
N	1.814316	1.848692	-2.532370
H	1.302633	2.720527	-2.492963
H	2.817760	1.965337	-2.474128
H	-0.655318	-0.839145	-1.256950
N	1.918283	-0.341303	-1.732033
H	1.871184	-0.892990	-0.879189
H	2.751476	-0.434047	-2.293786

Gh3 SCF Energy: -581.082856208

	X	Y	Z
C	0.941778	0.948053	-0.854635
C	0.073215	0.139453	-0.202634
C	-2.201129	-0.570094	0.409846
C	2.144433	-0.246706	0.692236
N	-1.855514	-0.865225	1.613599
N	-1.269626	-0.092990	-0.498789
N	0.803734	-0.620547	0.712695
N	-3.483632	-0.640313	-0.145004
H	-4.166561	-1.100862	0.440710
H	-3.532353	-0.952928	-1.107410
O	3.042596	-0.612998	1.441808

N	2.229200	0.655850	-0.363966
H	0.353148	-1.053354	1.511213
O	0.727381	1.678242	-1.992591
H	0.744355	2.625448	-1.791918
H	3.065563	1.191422	-0.536995
H	-2.619899	-1.286257	2.136655
H	-1.619584	0.430538	-1.289285

Gh4 SCF Energy: -581.089359086

	X	Y	Z
C	-0.025271	-0.001043	-0.015128
C	-0.114194	-0.003136	1.508612
O	1.011728	-0.090272	2.210489
C	-2.195554	0.147579	0.880010
O	-3.403045	0.173656	0.954215
N	0.871704	0.999544	-0.524368
H	0.682803	1.943524	-0.205405
C	1.370718	0.927816	-1.835454
N	-1.441150	0.184525	-0.286217
H	-1.872424	0.061274	-1.190576
N	-1.292949	0.076757	1.999714
N	2.139042	2.043117	-2.147705
H	2.775709	2.355841	-1.425131
H	2.575184	1.959558	-3.057207
H	0.340598	-0.978833	-0.354961
N	1.190489	0.005625	-2.709450
H	0.505175	-0.690727	-2.425942
H	0.779296	-0.093024	3.155248

Gh5 SCF Energy: -581.095524377

	X	Y	Z
C	-0.542844	0.068137	-0.478904
C	-0.103041	-0.299437	0.934549
O	1.123002	-0.815886	1.108590
C	-2.112620	0.464944	1.220167
O	-3.095746	0.877228	1.794881
N	0.170688	1.176470	-1.069840
H	1.249459	-0.984355	2.058240
C	1.259531	0.941712	-1.725236
N	-1.915846	0.415996	-0.154203
H	-2.431320	1.052323	-0.746429
N	-0.947871	-0.092671	1.868249
N	1.782977	1.935970	-2.539144
H	1.262124	2.801426	-2.477309
H	2.786213	2.066068	-2.509284
H	-0.501395	-0.829686	-1.119503
N	1.934752	-0.262828	-1.778177
H	1.969913	-0.821185	-0.936833
H	2.731624	-0.338996	-2.392806

Gh6 SCF Energy: -581.09344321

	X	Y	Z
C	0.725381	0.668427	0.346534
C	0.322013	-0.603030	0.061387
C	-1.913567	-1.031132	0.695561
C	2.619017	-0.473015	-0.269454
N	-2.034381	-0.095167	1.698179

N	-0.861821	-1.301384	-0.011951
N	1.496094	-1.276814	-0.336018
N	-3.066849	-1.766049	0.451301
H	-3.640292	-1.978547	1.257970
H	-2.894742	-2.568178	-0.140757
O	3.790325	-0.771808	-0.483948
N	2.106959	0.765267	0.109528
H	1.529937	-2.258410	-0.563627
O	0.008078	1.765428	0.757120
H	-0.270009	2.294005	-0.007163
H	2.702315	1.510724	0.437077
H	-2.972731	0.190048	1.941216
H	-1.357382	0.659055	1.708050

Gh7 SCF Energy: -581.089203529

	X	Y	Z
C	-0.080899	0.091065	-0.065206
C	-0.069777	0.181862	1.505575
O	0.945775	0.360365	2.145248
C	-2.130508	0.027004	0.911164
O	-3.451651	-0.099272	0.952064
N	0.695427	1.124200	-0.657184
H	0.999179	1.871663	-0.047679
C	1.329793	0.985678	-1.888534
N	-1.536693	0.141883	-0.294968
H	-2.004749	-0.083289	-1.161273
N	-1.368115	0.063701	1.979357
N	2.337457	1.922304	-2.084790
H	2.967387	2.073059	-1.306358
H	2.818060	1.778151	-2.963584
H	0.300087	-0.890472	-0.378022
N	1.043022	0.145426	-2.819651
H	0.197543	-0.385520	-2.621089
H	-3.711748	-0.155055	1.886865

Gh8 SCF Energy: -581.101855837

	X	Y	Z
C	-0.595731	-0.018986	-0.697656
C	-0.045752	-0.580898	0.659193
O	1.047199	-1.120694	0.766841
C	-1.994854	0.204654	1.069207
O	-3.074378	0.628451	1.717985
N	0.089270	1.124807	-1.234050
H	-2.936768	0.439108	2.660997
C	1.234447	0.936407	-1.812078
N	-1.949726	0.355977	-0.271330
H	-2.442719	1.110028	-0.732256
N	-0.976677	-0.378797	1.663056
N	1.772913	1.962807	-2.577525
H	1.224100	2.811223	-2.527779
H	2.767115	2.122968	-2.475736
H	-0.642727	-0.850086	-1.419486
N	1.946757	-0.237916	-1.812659
H	1.880712	-0.812681	-0.972775
H	2.804947	-0.283081	-2.341347

Gh9 SCF Energy: -581.086542157

	X	Y	Z
C	-0.109592	0.459060	0.640845
C	-0.954392	0.840928	-0.630294
O	-0.665635	1.885623	-1.227250
C	-1.677266	-1.144771	-0.012770
O	-2.315929	-2.168353	0.143668
N	1.302513	0.709502	0.229889
H	1.315222	1.559313	-0.339012
C	2.282365	-0.167807	0.047775
N	-0.488967	-0.903371	0.863892
H	-0.704675	-1.154958	1.824647
N	-1.840773	-0.123316	-0.898804
H	2.921100	-2.084906	0.388557
N	3.485033	0.266217	-0.422498
H	3.584821	1.238087	-0.676987
H	4.068636	-0.382726	-0.929859
H	-0.315084	1.128690	1.482298
N	2.134037	-1.456331	0.363562
H	1.170795	-1.757352	0.571662

$Gh10^{+}$ SCF Energy: -581.511324776

	X	Y	Z
C	-0.607336	0.208674	-0.519435
C	-0.063372	-0.628677	0.669764
O	0.989048	-1.245084	0.652745
C	-2.084412	0.301903	1.305359
O	-3.063519	0.507002	1.968070
N	0.344734	1.256750	-0.939318
H	0.127795	2.195417	-0.624354
C	1.459311	1.048646	-1.668217
N	-1.791193	0.801492	0.031441
H	-2.573915	1.088578	-0.544134
N	-0.975097	-0.506636	1.666759
H	-0.906499	-0.951273	2.575889
N	2.009800	2.079799	-2.326208
H	1.496261	2.933180	-2.494425
H	2.962110	2.035933	-2.661069
H	-0.791663	-0.451868	-1.376404
N	1.985944	-0.172944	-1.740356
H	1.807624	-0.834257	-0.973570
H	2.702556	-0.385618	-2.420979

$Gh11^{+}$ SCF Energy: -581.431731249

	X	Y	Z
C	-0.072596	0.055076	-0.030062
C	-0.071961	-0.009157	1.495118
O	1.049060	-0.089969	2.132787
C	-2.290700	0.134917	0.842342
O	-3.466607	0.174411	1.043565
N	0.764974	1.071344	-0.545880
H	0.488216	2.028547	-0.349427
C	1.415732	0.894024	-1.813747
N	-1.519809	0.172502	-0.270354
H	-1.933119	0.217657	-1.193883
N	-1.290970	0.021296	1.955858
H	-1.606613	-0.020426	2.923156
N	2.191864	1.986946	-2.112004

H	2.732303	2.406272	-1.366527
H	2.682047	1.908770	-2.994335
H	0.308143	-0.911132	-0.394409
N	1.309232	-0.095032	-2.611997
H	0.581743	-0.772588	-2.398637
H	0.981755	-0.146384	3.104190

$Gh12^{+}$ SCF Energy: -581.441409611

	X	Y	Z
C	0.026764	0.046480	0.005462
C	0.032727	0.027513	1.554697
O	0.961614	0.056680	2.301932
C	-2.151657	0.061007	0.868981
O	-3.455332	0.098462	0.870349
N	0.814585	1.050860	-0.559865
H	0.797604	1.977617	-0.151263
C	1.355271	0.930482	-1.872186
N	-1.467571	0.128406	-0.249890
H	-1.902644	0.217331	-1.162231
N	-1.341584	-0.039703	1.948635
H	-1.631974	-0.052967	2.921004
N	2.207371	1.970741	-2.158072
H	2.856495	2.262216	-1.437928
H	2.617377	1.908875	-3.081846
H	0.362679	-0.933453	-0.357061
N	1.090622	0.020834	-2.730123
H	0.333990	-0.611311	-2.480698
H	-3.871913	0.037974	1.747048

$Gh13^{+}$ SCF Energy: -581.471406793

	X	Y	Z
C	0.727240	0.981558	-0.255043
C	0.179661	-0.257122	-0.201306
C	-2.257405	-0.269495	0.132822
C	2.432585	-0.483379	0.196371
N	-2.256793	0.841473	0.868314
N	-1.130035	-0.694738	-0.475860
N	1.225921	-1.169786	0.022063
N	-3.385574	-0.980240	-0.023685
H	-4.289642	-0.580099	0.183116
H	-3.364564	-1.942900	-0.329374
O	3.517255	-0.930401	0.495121
N	2.087337	0.864548	-0.033001
H	1.125032	-2.112644	0.372696
O	0.071765	2.158957	-0.407710
H	0.436445	2.700968	-1.126137
H	2.726978	1.616510	0.187407
H	-3.031796	1.053614	1.480755
H	-1.245765	-1.360841	-1.234099
H	-1.542145	1.549802	0.735194

$Gh14^{+}$ SCF Energy: -581.456663431

	X	Y	Z
C	-0.429702	0.025303	-0.355528
C	-0.112258	-0.275148	1.105657
O	1.065914	-0.715761	1.431898
C	-2.291078	0.479463	1.051613
O	-3.317639	0.832015	1.552492

N	0.326831	1.142828	-0.806091
H	1.223410	-0.820698	2.387628
C	1.294805	0.958503	-1.673142
N	-1.857500	0.345876	-0.222574
H	-2.365042	0.788017	-0.978843
N	-1.123408	0.013339	1.871905
H	-1.189527	-0.020228	2.886704
N	1.756764	2.039035	-2.350766
H	1.310536	2.925040	-2.160848
H	2.693600	2.062098	-2.724610
H	-0.306294	-0.896799	-0.949037
N	1.843310	-0.253289	-2.016935
H	1.962965	-0.966408	-1.314581
H	2.488747	-0.302666	-2.792925

$Gh15^{+}$ SCF Energy: -581.468963218

	X	Y	Z
C	-0.523436	0.024321	-0.591802
C	-0.031068	-0.507619	0.776415
O	1.027258	-1.005061	1.045755
C	-2.139380	0.290709	1.056532
O	-3.266186	0.676905	1.591820
N	0.171973	1.155895	-1.081409
H	-3.329866	0.543623	2.552164
C	1.272282	0.956721	-1.767105
N	-1.913081	0.421571	-0.228413
H	-2.506632	0.969861	-0.841650
N	-1.091022	-0.277966	1.700713
H	-1.033729	-0.491429	2.691019
N	1.754661	1.974819	-2.528824
H	1.228418	2.836628	-2.519079
H	2.743752	2.049441	-2.715626
H	-0.565281	-0.829007	-1.290168
N	1.945614	-0.236136	-1.834008
H	1.989502	-0.811497	-1.002324
H	2.729182	-0.323199	-2.466400

$Gh16^{-}$ SCF Energy: -580.576214181

	X	Y	Z
C	-0.105347	0.096446	-0.071449
C	-0.095779	0.276706	1.488929
O	0.959285	0.597567	2.063179
C	-2.187885	-0.102364	0.931086
O	-3.381960	-0.403533	0.971685
N	0.700583	1.154958	-0.649192
H	1.213936	1.660275	0.067452
C	1.283481	1.060459	-1.889126
N	-1.528054	0.125328	-0.318413
H	-1.919187	-0.402282	-1.088929
N	-1.323771	0.078374	1.986468
N	2.389549	1.909036	-2.060689
H	3.031465	1.933422	-1.277026
H	2.855487	1.711206	-2.937129
H	0.334432	-0.878920	-0.340009
N	0.900871	0.339469	-2.892981
H	0.019653	-0.125954	-2.683367

Gh17$^-$ SCF Energy: -580.564426427

	X	Y	Z
C	0.076001	-0.076647	0.084746
C	-0.003466	0.114535	1.623048
O	0.924668	0.318657	2.410674
C	-2.111174	-0.068557	0.618153
O	-3.348041	-0.098371	0.711079
N	0.956178	0.947504	-0.473918
H	1.028207	1.815746	0.040126
C	1.239493	1.006509	-1.822863
N	-1.282540	-0.100503	-0.414537
N	-1.322288	0.015637	1.876019
H	-1.746958	0.139480	2.783717
N	2.202987	1.996390	-2.121912
H	3.015097	1.962850	-1.515083
H	2.458827	1.938275	-3.100557
H	0.574542	-1.043341	-0.109344
N	0.753174	0.285397	-2.770205
H	-0.070956	-0.215208	-2.430821

Gh18$^-$ SCF Energy: -580.557453772

	X	Y	Z
C	-0.014754	-0.011454	0.580081
C	-0.785216	1.212014	0.015612
O	-0.397616	2.359291	-0.121740
C	-2.236987	-0.607521	-0.021141
O	-3.232982	-1.258394	-0.323651
N	1.007558	-0.512245	-0.257428
C	2.286248	-0.228595	0.083829
N	-1.131788	-1.000509	0.679980
H	-0.860518	-1.972165	0.591630
N	-2.048175	0.751220	-0.327457
H	-2.746396	1.294954	-0.814177
N	3.214626	-1.027778	-0.640414
H	2.808999	-1.356761	-1.507982
H	4.088680	-0.534740	-0.775976
H	0.322220	0.252033	1.600512
N	2.825958	0.598744	0.954839
H	2.108237	1.195058	1.363311

Gh19$^-$ SCF Energy: -580.532696064

	X	Y	Z
C	0.175436	-0.228608	0.062578
C	0.014553	-0.198685	1.595427
O	0.849994	-0.447231	2.447494
C	-2.044846	0.380022	0.638584
O	-3.212347	0.747729	0.624349
N	1.190613	0.671678	-0.408706
H	1.198671	1.536767	0.124406
C	1.173957	0.972788	-1.871895
N	-1.205596	0.072509	-0.377261
H	-1.378752	0.295559	-1.351955
N	-1.294326	0.166572	1.826820
H	-1.696749	0.286464	2.744949
N	1.498905	2.198657	-2.231170
H	1.633613	2.784165	-1.404773
H	0.422930	-1.252617	-0.241604
N	0.815533	-0.001356	-2.701158

H	0.798968	-0.897893	-2.214638

Gh20$^-$ SCF Energy: -580.573405762

	X	Y	Z
C	-0.578585	0.201420	-0.572060
C	-0.024649	-0.545240	0.697693
O	1.099484	-1.106252	0.673110
C	-2.021873	0.182121	1.261618
O	-3.090225	0.335053	1.862859
N	0.258960	1.238846	-1.153261
C	1.333437	0.898796	-1.769837
N	-1.795042	0.733968	-0.011246
H	-2.595226	0.970022	-0.579525
N	-0.906945	-0.513263	1.698368
N	2.015885	1.876597	-2.532557
H	1.576843	2.778559	-2.382356
H	3.008879	1.922842	-2.324222
H	-0.781539	-0.571396	-1.339253
N	1.869229	-0.373332	-1.840376
H	1.750144	-0.895833	-0.952121
H	2.756162	-0.465619	-2.315179

Gh21$^-$ SCF Energy: -580.558577508

	X	Y	Z
C	0.478561	-0.357638	0.303647
C	-0.004212	0.297296	1.633427
O	0.665518	0.759756	2.555286
C	-1.794942	-0.427473	0.316091
O	-3.013592	-0.569465	0.110326
N	1.459499	0.486655	-0.371835
C	1.292018	0.935477	-1.562432
N	-0.732927	-0.750101	-0.415907
N	-1.355162	0.192379	1.564115
H	-1.997939	0.521498	2.269572
N	2.317843	1.755057	-2.099082
H	3.160741	1.646383	-1.547049
H	2.494818	1.601845	-3.086259
H	1.041892	-1.258798	0.608644
N	0.184581	0.805364	-2.381222
H	-0.463811	0.088982	-2.008333
H	0.338799	0.845493	-3.379439

Gh22$^-$ SCF Energy: -580.543946796

	X	Y	Z
C	0.900152	0.844872	-1.021231
C	0.067179	0.214199	-0.099472
C	-2.250754	-0.458203	0.378504
C	2.207032	-0.326058	0.526547
N	-2.062253	-0.559353	1.660695
N	-1.237432	-0.177193	-0.482512
N	0.877118	-0.637076	0.722517
N	-3.509332	-0.616651	-0.268480
H	-4.150060	-1.178359	0.277438
H	-3.431969	-0.991264	-1.208222
O	3.180706	-0.676422	1.218240
N	2.221649	0.507641	-0.575124
H	0.569790	-0.876162	1.656473
O	0.656639	1.470659	-2.094111

H	3.067274	0.911350	-0.944929
H	-2.929991	-0.821959	2.127006
H	-1.476905	0.139494	-1.417247

Gh23$^-$ SCF Energy: -580.557649328

	X	Y	Z
C	0.568982	0.854909	0.448227
C	0.119992	-0.396714	0.033736
C	-2.219783	-0.407601	0.052918
C	2.430661	-0.423925	-0.182407
N	-2.377872	0.957835	-0.106392
N	-1.101023	-1.048416	0.096306
N	1.288519	-1.174946	-0.265977
N	-3.435647	-1.154864	0.038554
H	-4.074488	-0.859982	0.774452
H	-3.203841	-2.133737	0.173486
O	3.599462	-0.757317	-0.472165
N	1.990509	0.800114	0.279501
H	1.264144	-2.033019	-0.792853
O	-0.016784	1.885755	0.941399
H	2.608605	1.564244	0.499297
H	-3.318181	1.311144	0.001873
H	-1.613288	1.534531	0.302303

Gh24$^-$ SCF Energy: =-580.520943775

	X	Y	Z
C	0.934577	0.963062	-0.701466
C	0.050955	0.145135	-0.054570
C	-2.291784	-0.458397	0.418343
C	2.224624	-0.363790	0.436306
N	-2.113382	-0.593958	1.693660
N	-1.282412	-0.119116	-0.435328
N	0.880309	-0.812648	0.585913
N	-3.532855	-0.629976	-0.261424
H	-4.227566	-1.078669	0.321390
H	-3.438452	-1.124474	-1.142385
O	3.178635	-0.883886	1.051933
N	2.238512	0.700192	-0.432210
H	0.613628	-1.195258	1.484164
O	0.599671	1.903775	-1.655562
H	1.456227	2.216142	-1.983678
H	-2.962598	-0.943535	2.136528
H	-1.559141	0.232816	-1.343742

Gh25$^-$ SCF Energy: -580.525003057

	X	Y	Z
C	0.770304	1.005254	-0.105677
C	0.258278	-0.257304	-0.174889
C	-2.215673	-0.059363	0.038066
C	2.428898	-0.579623	-0.053102
N	-2.219872	1.177922	0.464904
N	-1.078921	-0.710705	-0.272352
N	1.247550	-1.235772	-0.138102
N	-3.404530	-0.797851	-0.202300
H	-4.151731	-0.517327	0.421456
H	-3.281163	-1.804382	-0.165214
O	3.609026	-1.015737	-0.029168

N	2.140007	0.816692	0.018360
O	0.224410	2.259027	-0.104502
H	-0.732080	2.108952	0.131006
H	2.839164	1.539976	-0.033370
H	-3.167956	1.522656	0.592602
H	-1.117736	-1.689377	-0.523998

$Gh26^-$ SCF Energy: -580.559963038

	X	Y	Z
C	0.788004	1.021221	-0.033236
C	0.226788	-0.255763	0.007978
C	-2.130955	-0.094576	0.092580
C	2.531795	-0.551307	0.032514
N	-2.261240	1.250474	0.440259
N	-1.049754	-0.781003	-0.030241
N	1.322219	-1.184162	0.001565
N	-3.385605	-0.745921	-0.088683
H	-4.004089	-0.588206	0.705667
H	-3.223055	-1.740290	-0.208564
O	3.673990	-1.055563	0.089068
N	2.200323	0.790157	-0.006618
H	1.221512	-2.172402	0.163148
O	0.300367	2.204447	-0.101604
H	-1.380556	1.788362	0.309420
H	2.884109	1.528898	-0.038661
H	-3.047541	1.692725	-0.024338

$Gh27^-$ SCF Energy: -580.513430725

	X	Y	Z
C	0.929824	0.973984	-0.891390
C	0.071630	0.131335	-0.238432
C	-2.173131	-0.792042	0.430792
C	2.106510	-0.124420	0.751350
N	-1.604918	-1.269481	1.533889
N	-1.233480	-0.200074	-0.506756
N	0.785238	-0.507890	0.766444
N	-3.453209	-0.819856	0.096690
H	-3.599591	-0.390770	-0.819276
O	2.998731	-0.390776	1.566981
N	2.234711	0.683811	-0.381320
H	0.208857	-1.028762	1.460511
O	0.770633	1.489387	-2.173187
H	0.641881	2.443975	-2.110376
H	2.982045	1.363064	-0.376177
H	-2.343780	-1.675716	2.103808
H	-1.646513	0.307715	-1.273994

$Gh28^-$ SCF Energy: -580.532520072

	X	Y	Z
C	0.736430	0.612124	0.347173
C	0.292987	-0.673813	0.104835
C	-1.982306	-1.071397	0.699163
C	2.544242	-0.399712	-0.341576
N	-2.247854	0.020699	1.539760
N	-0.878307	-1.402332	0.136919
N	1.466861	-1.290707	-0.408505
N	-3.130026	-1.896458	0.526640

H	-3.532173	-2.172888	1.421499
H	-2.860017	-2.720328	-0.000555
O	3.722853	-0.707364	-0.636788
N	2.050078	0.810404	0.090976
H	1.589543	-2.288621	-0.478597
O	-0.023913	1.695489	0.771193
H	0.636029	2.389565	0.923399
H	-3.171591	0.411034	1.386518
H	-1.532644	0.744411	1.511293

$Gh29^-$ SCF Energy: -580.529593015

	X	Y	Z
C	0.796956	1.086571	-0.459909
C	0.099842	0.150229	0.242489
C	-1.903975	-0.927783	0.783420
C	2.215563	-0.092763	0.870869
N	-1.402257	-1.594716	1.891239
N	-1.261230	-0.083754	0.049745
N	0.973308	-0.586288	1.067406
N	-3.288691	-1.119107	0.540596
H	-3.592555	-2.079674	0.667588
H	-3.517401	-0.791255	-0.390814
O	3.305933	-0.374385	1.425783
N	2.136063	0.913575	-0.153893
O	0.389343	1.962007	-1.447878
H	-0.567137	1.816545	-1.515667
H	2.843859	1.628315	-0.231213
H	-1.801859	-2.504593	2.086420
H	-0.366548	-1.537196	1.913010

$Gh30a^-$ SCF Energy: -580.529754289

	X	Y	Z
C	0.823699	1.119086	-0.235940
C	0.133652	0.004688	0.127468
C	-1.868191	-1.018535	0.792439
C	2.412068	-0.451733	0.227044
N	-1.524253	-1.556437	1.946780
N	-1.200934	-0.209911	-0.063108
N	1.152222	-0.968405	0.406532
N	-3.184436	-1.308428	0.355772
H	-3.548712	-2.129827	0.821486
H	-3.251015	-1.353068	-0.653333
O	3.507572	-0.964599	0.507771
N	2.200468	0.821932	-0.299791
H	0.985854	-1.864206	0.838354
O	0.322764	2.237750	-0.860670
H	-0.626950	2.042363	-0.954711
H	2.929512	1.511944	-0.197994
H	-0.640778	-1.152864	2.257707

$Gh30b^-$ SCF Energy: -580.516763544

	X	Y	Z
C	0.659386	0.673780	0.479517
C	0.337304	-0.648569	0.168385
C	-1.938322	-1.058245	0.674455
C	2.614081	-0.352570	-0.198555
N	-1.816274	-0.467879	1.968788

N	-0.787929	-1.348237	0.002665
N	1.568336	-1.249723	-0.182499
N	-3.101733	-1.426739	0.204898
H	-3.820405	-1.216996	0.902605
O	3.819067	-0.597407	-0.363504
N	2.028336	0.871419	0.069659
H	1.668766	-2.233432	-0.378387
O	-0.214789	1.751009	0.363421
H	-0.655602	1.710119	-0.504241
H	2.617827	1.573116	0.495614
H	-2.605289	0.122078	2.201852
H	-0.946311	0.042660	2.090522

$Gh30c^-$ SCF Energy: -580.53413438

	X	Y	Z
C	0.823893	1.076797	-0.353611
C	0.125717	0.050661	0.204946
C	-1.796219	-1.148195	0.793652
C	2.376052	-0.376156	0.483158
N	-1.188464	-2.047361	1.554941
N	-1.225477	-0.147885	0.113774
N	1.109848	-0.838853	0.715096
N	-3.225286	-1.158337	0.664399
H	-3.591158	-2.100116	0.572937
H	-3.505036	-0.586613	-0.125802
O	3.465173	-0.821193	0.887898
N	2.197483	0.774826	-0.295622
H	0.818778	-1.634920	1.278914
O	0.358013	2.070421	-1.191339
H	-0.594376	1.889507	-1.260611
H	2.926147	1.472725	-0.292397
H	-1.877875	-2.644102	2.011841

$Gh30d^-$ SCF Energy: -580.525036686

	X	Y	Z
C	0.749237	0.659000	0.503516
C	0.356094	-0.629995	0.173127
C	-1.945454	-1.048917	0.697683
C	2.638849	-0.415316	-0.254878
N	-1.936979	-0.196691	1.822332
N	-0.785386	-1.319972	0.029997
N	1.556892	-1.263228	-0.245997
N	-3.093023	-1.618243	0.418620
H	-2.926089	-2.267086	-0.351283
O	3.828262	-0.698647	-0.466876
N	2.112435	0.823079	0.077870
H	1.611262	-2.246447	-0.461225
O	-0.061508	1.787627	0.551134
H	-0.477458	1.926355	-0.319145
H	2.737733	1.474140	0.533174
H	-2.884986	0.024491	2.099638
H	-1.343944	0.620584	1.745706

Spiroiminodihydantoin Tautomers

Sp1 SCF Energy: -693.297167677

	X	Y	Z
C	0.003933	0.031951	-0.000267
C	-0.013929	-0.011214	1.592252
O	1.004969	-0.046601	2.246560
C	0.490596	-1.306673	-0.605991
O	-0.128562	-2.350292	-0.623029
C	2.065447	0.330378	-1.070834
O	3.108139	0.821808	-1.442005
N	-1.394888	0.295499	-0.269459
C	-2.063620	0.149229	0.934165
N	-1.322053	0.042204	2.017254
N	0.957892	0.971615	-0.542308
H	1.119772	1.864171	-0.092913
N	1.727763	-1.037981	-1.131526
H	2.321633	-1.721840	-1.581397
N	-3.406104	0.144586	0.966482
H	-3.956673	0.412864	0.166270
H	-3.851561	0.097397	1.870722
H	-1.809986	-0.094544	-1.108236

Sp2 SCF Energy: -693.294026389

	X	Y	Z
C	0.093186	-0.035034	0.192788
C	0.062816	-0.128394	1.752521
O	0.980558	-0.249180	2.529276
C	0.640335	-1.378843	-0.393559
O	0.194005	-2.483893	-0.183194
C	1.942086	0.364233	-1.211774
O	2.777988	0.929601	-1.884945
N	-1.283620	0.198140	-0.217567
C	-2.002676	0.117614	0.852968
N	-1.289237	-0.059324	2.045761
N	1.048903	0.915138	-0.321548
H	0.863159	1.907148	-0.354646
N	1.703007	-1.025287	-1.186113
H	2.255140	-1.677242	-1.726468
N	-3.361728	0.167037	0.887524
H	-3.806592	0.408667	0.012746
H	-3.826864	0.481584	1.726055
H	-1.669164	-0.207210	2.970301

Sp3 SCF Energy: -693.293881848

	X	Y	Z
C	0.029780	0.043386	0.057563
C	0.057436	-0.017675	1.617867
O	1.047563	-0.077184	2.312731
C	0.517514	-1.322955	-0.532036
O	-0.068299	-2.378867	-0.445859
C	2.049755	0.320045	-1.123680
O	3.060464	0.808820	-1.576985
N	-1.353972	0.347381	-0.198689
C	-2.152942	0.175016	0.925721
N	-1.256105	0.021543	2.005596
N	0.992437	0.958494	-0.509349

H	1.118980	1.901957	-0.168985
N	1.706864	-1.049254	-1.155091
H	2.278084	-1.736532	-1.629057
N	-3.422764	0.189292	0.905590
H	-3.833597	0.048500	1.826186
H	-1.542094	-0.009241	2.974717
H	-1.778570	0.143680	-1.094056

Sp4 SCF Energy: -693.295252359

	X	Y	Z
C	0.024796	0.041862	0.033844
C	0.041570	-0.013393	1.596384
O	1.033240	-0.076008	2.290111
C	0.515815	-1.318480	-0.558129
O	-0.084876	-2.368848	-0.507558
C	2.065207	0.322044	-1.105518
O	3.087549	0.810903	-1.530872
N	-1.363918	0.337106	-0.238523
C	-2.160927	0.183369	0.901102
N	-1.268828	0.040315	1.973815
N	0.988448	0.962502	-0.523958
H	1.123724	1.894190	-0.154477
N	1.723707	-1.047324	-1.144963
H	2.302875	-1.733875	-1.610311
N	-3.420133	0.195118	1.065514
H	-3.924201	0.328154	0.190147
H	-1.590359	0.009832	2.932317
H	-1.760617	0.065737	-1.128786

Sp5 SCF Energy: -693.265376757

	X	Y	Z
C	-0.830198	-0.345320	-0.091431
C	-0.114815	-1.295739	0.928848
O	-0.593546	-1.997890	1.787251
C	-1.682558	0.706922	0.625587
O	-1.092256	1.481927	1.528615
C	-3.083262	-0.265994	-0.718226
O	-4.094732	-0.475444	-1.346363
N	0.238046	0.238562	-0.898243
C	1.349993	-0.218829	-0.427256
N	1.228833	-1.134296	0.625787
N	-1.886843	-0.976059	-0.836704
H	-1.700556	-1.504076	-1.677546
N	-2.912858	0.748141	0.284792
H	-1.758319	2.089112	1.893839
N	2.590544	0.152348	-0.851369
H	2.601155	0.714452	-1.691819
H	3.358394	-0.495020	-0.747588
H	1.976211	-1.544387	1.168438

Sp6 SCF Energy: -693.264969761

	X	Y	Z
C	-0.049621	-0.215142	-0.000504
C	0.675651	-1.173279	0.979539
O	0.214893	-1.947225	1.787110
C	-0.839496	0.902761	0.825269
O	-0.309836	1.617152	1.642966

C	-2.256793	-0.067053	-0.468404
O	-3.365756	-0.362842	-1.135199
N	0.981975	0.362483	-0.841492
C	2.110141	-0.004959	-0.328580
N	2.016040	-0.907218	0.737384
N	-1.152069	-0.813071	-0.720718
H	-1.030055	-1.312716	-1.590955
N	-2.169367	0.884785	0.423898
H	-4.057063	0.252193	-0.838822
N	3.334692	0.434216	-0.732409
H	3.332621	0.992823	-1.574694
H	4.141321	-0.156463	-0.594021
H	2.769362	-1.259856	1.310740

Sp7 SCF Energy: -693.264819279

	X	Y	Z
C	0.072502	-0.176296	-0.055104
C	0.750319	-1.209088	0.899819
O	0.243343	-1.941624	1.718350
C	-0.701002	0.890085	0.792771
O	-0.273306	1.668172	1.612345
C	-2.052163	-0.273468	-0.575601
O	-3.251963	-0.563253	-1.086193
N	1.153733	0.433570	-0.812730
C	2.247370	-0.090234	-0.378912
N	2.096213	-1.082717	0.600696
N	-0.940662	-0.823244	-0.888984
H	-3.127373	-1.277910	-1.732148
N	-2.016382	0.729105	0.383870
H	-2.806037	1.262595	0.719455
N	3.506164	0.274831	-0.767141
H	3.525644	0.897227	-1.564306
H	4.229220	-0.430772	-0.760682
H	2.829296	-1.520804	1.140667

Sp8 SCF Energy: -693.277696234

	X	Y	Z
C	0.052275	-0.202834	0.044815
C	0.871854	-1.102363	0.976831
O	0.285307	-1.840515	1.907454
C	-0.712070	0.895840	0.860557
O	-0.237815	1.636749	1.690860
C	-2.227766	-0.167171	-0.546397
O	-3.266537	-0.370453	-1.138478
N	1.073488	0.375246	-0.805737
C	2.193444	-0.089516	-0.330554
N	2.134315	-1.013772	0.757022
N	-1.037393	-0.857721	-0.652385
H	-0.861135	-1.372417	-1.504917
N	-2.011667	0.833431	0.421439
H	-2.748403	1.453017	0.730305
N	3.420883	0.202428	-0.809906
H	3.514017	0.952775	-1.476822
H	4.228736	-0.090144	-0.284229
H	0.967452	-2.299990	2.425800

Sp9 SCF Energy: -693.267373361

	X	Y	Z
C	0.028100	0.023950	-0.079900
C	0.771565	-0.996824	0.893995
O	0.174169	-1.681128	1.694439
C	-0.863320	1.021707	0.642246
O	-0.302041	1.880490	1.483272
C	-2.247936	-0.118864	-0.574822
O	-3.285201	-0.563591	-1.003966
N	1.174860	0.620799	-0.747781
C	2.295268	-0.063370	-0.330040
N	2.124036	-0.949077	0.630454
N	-0.961425	-0.562302	-0.946800
H	-0.881041	-1.526710	-1.245330
N	-2.112585	0.945801	0.369253
H	-1.003820	2.422155	1.883251
N	3.493687	0.178267	-0.895363
H	3.649522	1.014536	-1.436885
H	4.294398	-0.269838	-0.473914
H	1.076465	0.946629	-1.701497

Sp10 SCF Energy: -693.269942612

	X	Y	Z
C	-0.136157	-0.051124	-0.079967
C	0.572146	-1.108593	0.858284
O	-0.052517	-1.913559	1.517606
C	-0.884744	1.089078	0.704104
O	-0.303868	1.997018	1.259972
C	-2.373185	-0.128563	-0.239574
O	-3.529643	-0.678985	-0.577895
N	0.992018	0.437384	-0.840395
C	2.122613	-0.041688	-0.193818
N	1.935480	-0.965424	0.725757
N	-1.243455	-0.630308	-0.817533
H	-1.229989	-1.609866	-1.079454
N	-2.250978	0.882397	0.581720
H	-4.229309	-0.232100	-0.072706
N	3.338256	0.418454	-0.530083
H	3.482056	0.996876	-1.342288
H	4.138689	0.018264	-0.064476
H	0.984427	1.419492	-1.096897

Sp11 SCF Energy: -693.267842798

	X	Y	Z
C	-0.088173	0.069597	0.041542
C	0.635545	-0.980559	1.003205
O	0.036305	-1.640252	1.821598
C	-0.911161	1.079638	0.883814
O	-0.533506	1.935059	1.649439
C	-2.199698	-0.209664	-0.431891
O	-3.379244	-0.615644	-0.905017
N	1.055472	0.637989	-0.633700
C	2.162797	-0.088011	-0.240426
N	1.985961	-0.971817	0.716176
N	-1.044102	-0.596683	-0.834924
H	-3.209062	-1.307094	-1.565659
N	-2.225460	0.744443	0.571434

H	-3.051587	1.171590	0.966442
N	3.355886	0.126091	-0.834085
H	3.524666	0.989800	-1.327166
H	4.151963	-0.336861	-0.419878
H	0.951814	0.913857	-1.602591

Sp12 SCF Energy: -693.264778471

	X	Y	Z
C	-0.840383	-0.297666	-0.249258
C	-0.158885	-1.315952	0.726656
O	-0.726364	-2.077086	1.477224
C	-1.634284	0.769065	0.520435
O	-0.958478	1.588714	1.318570
C	-3.153672	-0.288874	-0.615065
O	-4.243670	-0.642775	-0.994484
N	0.297291	0.179535	-0.998588
C	1.511656	-0.213147	-0.463607
N	1.190501	-1.157065	0.537610
N	-1.930668	-0.829498	-1.018608
H	-1.900239	-1.735014	-1.466175
N	-2.893943	0.779778	0.312112
H	-1.586724	2.198614	1.742432
N	2.641598	0.218504	-0.855333
H	0.265527	1.012309	-1.569888
H	3.419483	-0.195744	-0.346106
H	1.879622	-1.699527	1.040307

Sp13 SCF Energy: -693.266297402

	X	Y	Z
C	-0.011751	-0.026882	-0.215093
C	0.611237	-1.081018	0.735350
O	0.007950	-1.886168	1.413112
C	-0.762253	1.114240	0.606016
O	-0.171377	1.931819	1.273026
C	-2.256178	0.010148	-0.469595
O	-3.419965	-0.453985	-0.897773
N	1.129865	0.416795	-0.967896
C	2.325088	0.034969	-0.363926
N	1.966499	-0.911510	0.620258
N	-1.128116	-0.551359	-0.980936
H	-1.140930	-1.489525	-1.361142
N	-2.125466	0.993354	0.384368
H	-4.122339	0.039707	-0.441778
N	3.466654	0.478148	-0.702270
H	1.130065	1.335384	-1.393518
H	4.221534	0.089145	-0.141019
H	2.633863	-1.464400	1.140395

Sp14 SCF Energy: -693.265812228

	X	Y	Z
C	0.076603	-0.060515	-0.027572
C	0.755372	-1.101211	0.917371
O	0.202844	-1.792093	1.744316
C	-0.770560	0.948548	0.821998
O	-0.397471	1.766103	1.627022
C	-2.037969	-0.292064	-0.561290
O	-3.211141	-0.653861	-1.080109

N	1.211040	0.526053	-0.683375
C	2.393474	-0.148539	-0.431389
N	2.087320	-1.071972	0.590984
N	-0.884169	-0.728117	-0.912152
H	-3.041172	-1.339002	-1.747759
N	-2.075294	0.667452	0.438872
H	-2.903512	1.129562	0.788285
N	3.491994	0.079143	-1.032228
H	1.118735	1.006246	-1.567110
H	4.249740	-0.512708	-0.698258
H	2.772523	-1.661749	1.041882

Sp15 SCF Energy: = -693.271476408

	X	Y	Z
C	0.075616	-0.131441	-0.051851
C	0.865621	-1.059237	0.876746
O	0.188413	-1.791223	1.755798
C	-0.678158	0.988213	0.752351
O	-0.160670	1.811128	1.472738
C	-2.253780	-0.206843	-0.478125
O	-3.338804	-0.517199	-0.920368
N	1.167357	0.320333	-0.869096
C	2.392670	-0.100255	-0.324287
N	2.133383	-1.042377	0.715633
N	-1.026969	-0.756453	-0.753682
H	-0.921072	-1.497281	-1.431456
N	-2.006205	0.833317	0.447079
H	-2.747224	1.423606	0.801460
N	3.517445	0.313830	-0.740327
H	1.140446	1.216999	-1.336135
H	4.268836	-0.127784	-0.211914
H	0.818836	-2.308967	2.284585

Sp16^{+} SCF Energy: -693.656726188

	X	Y	Z
C	-0.779892	-0.897395	0.784445
O	-0.183640	-1.581328	1.580393
C	-2.395002	0.079014	-0.567114
O	-3.479433	0.385299	-0.977122
N	-1.150463	0.466596	-1.083889
H	-1.120369	1.287645	-1.677236
N	-2.110421	-0.768170	0.529870
H	-2.841994	-1.250896	1.040296
C	-0.074498	0.062716	-0.253239
N	1.043172	-0.633486	-0.913315
H	0.916960	-1.517744	-1.392031
C	0.687893	1.188180	0.497938
O	0.232980	2.135698	1.066228
N	2.055843	0.856489	0.371989
C	2.223906	-0.221765	-0.437033
N	3.399429	-0.755663	-0.725547
H	4.253875	-0.407206	-0.310521
H	3.477444	-1.558491	-1.336942
H	2.798142	1.414857	0.780013

Sp17$^+$ SCF Energy: -693.621631026

	X	Y	Z
C	0.053952	-0.108081	-0.044252
C	0.734035	-1.098610	0.998385
O	0.191472	-1.770170	1.835358
C	-0.771536	0.931509	0.704060
C	-2.241884	-0.244748	-0.627180
O	-3.315122	-0.491896	-1.088838
N	1.122542	0.462542	-0.810803
C	2.230199	-0.066574	-0.361292
N	2.070814	-0.984268	0.686863
N	-0.999730	-0.752031	-0.812878
H	-0.815010	-1.432320	-1.538829
N	-2.030886	0.831032	0.389832
H	-2.817695	1.383096	0.724543
N	3.448940	0.213562	-0.833158
H	3.528536	0.868320	-1.599099
H	4.287135	-0.224592	-0.483999
H	2.794414	-1.525487	1.144588
O	-0.186879	1.746121	1.521154
H	-0.770942	2.383536	1.971033

Sp18$^+$ SCF Energy: -693.612842227

	X	Y	Z
C	0.018250	-0.318442	-0.103826
C	0.776278	-1.255763	0.829846
C	-0.672872	0.790062	0.830885
O	-0.089074	1.417107	1.677822
C	-2.268393	-0.122947	-0.594802
O	-3.319319	-0.250859	-1.160038
N	1.052778	0.289706	-0.910347
C	2.186358	-0.047811	-0.417191
N	2.058823	-1.024395	0.669045
N	-1.104651	-0.874913	-0.782875
H	-0.997312	-1.353926	-1.669644
N	-1.967160	0.815755	0.421462
H	-2.665009	1.456631	0.783101
N	3.412532	0.376208	-0.746715
H	3.487582	1.066742	-1.482731
H	4.258086	-0.086130	-0.448242
H	2.822354	-1.419551	1.212272
O	0.183729	-2.051928	1.653931
H	0.754457	-2.552071	2.266101

Sp19$^+$ SCF Energy: -693.62993008

	X	Y	Z
C	0.088355	-0.113098	-0.072479
C	0.717630	-1.173788	0.909781
O	0.140351	-1.920858	1.657247
C	-0.692982	0.953316	0.749626
O	-0.277936	1.740054	1.543138
C	-2.173545	-0.157883	-0.575794
N	1.159804	0.424702	-0.842480
C	2.257106	-0.088122	-0.350794
N	2.067328	-1.014638	0.685395
N	-1.008711	-0.697330	-0.866849
H	-0.886015	-1.391141	-1.595849

N	-2.063671	0.797477	0.370627
H	-2.813794	1.367355	0.747477
N	3.489726	0.197816	-0.783528
H	3.591895	0.905239	-1.498149
H	4.320571	-0.148594	-0.329575
H	2.776906	-1.565058	1.153392
O	-3.260733	-0.546602	-1.181808
H	-4.072984	-0.093589	-0.899224

Sp20$^-$ SCF Energy: -692.756358278

	X	Y	Z
C	0.035063	0.103253	0.047685
C	-0.018037	0.066706	1.601491
O	0.963013	0.117515	2.323904
C	0.495919	-1.256588	-0.655822
O	-0.239972	-2.249751	-0.608640
C	2.017628	0.259196	-1.148739
O	3.054904	0.807285	-1.515676
N	-1.391610	0.337267	-0.255055
C	-2.062051	0.112418	0.920562
N	-1.348290	0.030834	2.019970
N	0.975146	1.016240	-0.511866
H	1.320838	1.768149	0.073228
N	1.657258	-1.058137	-1.289060
N	-3.422972	-0.004998	0.918431
H	-3.935162	0.450017	0.177408
H	-3.849602	0.007955	1.833444
H	-1.744415	-0.158360	-1.068342

Sp21$^-$ SCF Energy: -692.744491941

	X	Y	Z
C	0.036388	-0.210172	0.085750
C	-0.070681	-0.244134	1.657149
O	0.869489	-0.411304	2.409019
C	0.730111	-1.492919	-0.461378
O	0.392568	-2.662535	-0.302420
C	1.766466	0.474479	-1.169533
O	2.637519	1.070714	-1.817390
N	-1.405524	-0.177252	-0.256465
C	-2.078779	0.049572	0.914680
N	-1.401921	-0.047491	2.035631
N	0.736557	0.922046	-0.450427
N	1.779849	-0.995353	-1.150931
H	2.456211	-1.547559	-1.657140
N	-3.422209	0.303462	0.900236
H	-3.850177	0.601203	0.036685
H	-3.792726	0.694791	1.753683
H	-1.613172	0.416649	-1.053152

Sp22$^-$ SCF Energy: -692.762722480

	X	Y	Z
C	-0.056800	-0.125024	0.023390
C	-0.035670	-0.131418	1.631355
O	1.008017	-0.190032	2.284824
C	0.580598	-1.411965	-0.537191
O	0.167281	-2.554312	-0.473371
C	1.970991	0.369642	-1.093207

O	2.964594	0.952424	-1.516996
N	-1.445051	0.047421	-0.312918
C	-2.037756	0.054829	0.864650
N	-1.319529	-0.027490	2.032391
N	0.848547	0.890734	-0.526214
H	0.876568	1.828427	-0.154797
N	1.764190	-1.018266	-1.140222
H	2.425639	-1.650205	-1.566271
N	-3.413132	0.133933	0.963332
H	-3.871505	0.496156	0.138907
H	-3.745459	0.488752	1.848554

Sp23a$^-$ SCF Energy: -692.757935184

	X	Y	Z
C	-0.048457	-0.000832	-0.042500
C	-0.026669	-0.007724	1.571798
O	1.055048	-0.086382	2.161567
C	0.472838	-1.309217	-0.639232
O	-0.104530	-2.380932	-0.716672
C	2.062129	0.337283	-1.028382
O	3.132943	0.829490	-1.356943
N	-1.421746	0.292595	-0.293062
C	-2.139133	0.222872	0.963633
N	-1.273702	0.130521	2.020551
N	0.932238	0.961526	-0.569934
H	1.060872	1.845158	-0.094597
N	1.739727	-1.028873	-1.110246
H	2.359638	-1.708415	-1.526242
N	-3.426317	0.278772	1.051108
H	-3.823757	0.388768	0.115195
H	-1.857828	-0.222558	-1.049815

Sp23b$^-$ SCF Energy: -692.764642967

	X	Y	Z
C	-0.043881	0.001818	-0.031565
C	-0.023511	-0.011980	1.581637
O	1.055570	-0.086186	2.177297
C	0.477601	-1.315476	-0.620998
O	-0.089187	-2.392987	-0.672159
C	2.063453	0.331046	-1.033634
O	3.132423	0.821127	-1.372343
N	-1.411293	0.309290	-0.274083
C	-2.131356	0.199002	0.949876
N	-1.276179	0.106265	2.026347
N	0.939798	0.957155	-0.565388
H	1.066660	1.848445	-0.104655
N	1.738332	-1.034259	-1.110495
H	2.357668	-1.716491	-1.523040
N	-3.421557	0.217256	0.929618
H	-3.745726	0.126709	1.892786
H	-1.878058	-0.085479	-1.080930

Sp24a$^-$ SCF Energy: -692.744215245

	X	Y	Z
C	0.026952	0.127932	0.106739
C	0.081920	0.056687	1.636340
O	1.033853	0.060909	2.399145

C	0.548831	-1.301329	-0.492798
O	-0.061585	-2.335512	-0.226804
C	1.949266	0.256191	-1.209630
O	2.935137	0.816143	-1.690153
N	-1.395084	0.296617	-0.224330
C	-2.041700	0.075067	0.857226
N	-1.255945	-0.053164	2.011199
N	0.938851	1.006377	-0.537497
H	1.248947	1.854749	-0.082644
N	1.637716	-1.079956	-1.235557
N	-3.423526	-0.036236	0.976888
H	-3.873291	0.174237	0.093004
H	-3.820734	0.499354	1.741630
H	-1.553418	-0.416864	2.904550

Sp25a$^-$ SCF Energy: -692.733789281

	X	Y	Z
C	0.079928	-0.102478	0.139051
C	0.067947	-0.150128	1.695958
O	0.973767	-0.328626	2.485246
C	0.664902	-1.436682	-0.432556
O	0.269270	-2.581051	-0.218291
C	1.823204	0.459403	-1.155353
O	2.733020	0.984281	-1.813758
N	-1.356639	0.005738	-0.234635
C	-2.019127	0.069732	0.853646
N	-1.267442	0.059749	2.039826
N	0.887569	0.973133	-0.364453
N	1.682067	-1.010888	-1.203511
H	2.294596	-1.607834	-1.739276
N	-3.408063	0.127083	0.962172
H	-3.822549	0.257745	0.045702
H	-3.735488	0.828172	1.619169
H	-1.628462	-0.150952	2.959445

Sp26$^-$ SCF Energy: -692.761736868

	X	Y	Z
C	0.050256	0.122949	0.062062
C	0.048654	0.067315	1.595570
O	1.008533	0.074656	2.347608
C	0.506225	-1.263824	-0.613016
O	-0.212756	-2.260093	-0.494592
C	2.018395	0.241528	-1.173146
O	3.048005	0.779283	-1.573730
N	-1.370116	0.401950	-0.220261
C	-2.157008	0.154978	0.893967
N	-1.275714	0.034393	1.969772
N	0.997207	1.011029	-0.522873
H	1.333649	1.808141	0.003331
N	1.647586	-1.075737	-1.284304
N	-3.429608	0.084084	1.046715
H	-3.902111	0.217464	0.153019
H	-1.598631	-0.045179	2.922796
H	-1.724603	0.036712	-1.095601

Sp27^{-} SCF Energy: -692.752819413

	X	Y	Z
C	0.065194	-0.153948	0.086874
C	0.005961	-0.174386	1.639494
O	0.919650	-0.339835	2.424521
C	0.703777	-1.480483	-0.444182
O	0.325158	-2.629532	-0.240214
C	1.819419	0.431657	-1.185525
O	2.713853	0.977600	-1.842251
N	-1.376866	-0.071068	-0.250928
C	-2.148655	0.203566	0.864901
N	-1.314236	0.045535	1.971459
N	0.825367	0.935491	-0.452213
N	1.751298	-1.038891	-1.170059
H	2.396998	-1.626085	-1.677156
N	-3.387217	0.524859	0.988139
H	-3.831153	0.563248	0.070735
H	-1.657991	0.124638	2.917235
H	-1.560284	0.492477	-1.072437

Sp28^{-} SCF Energy: -692.744250545

	X	Y	Z
C	0.059845	-0.120179	0.181963
C	0.009998	-0.235913	1.739653
O	0.937044	-0.433209	2.518559
C	0.687425	-1.415266	-0.421487
O	0.315787	-2.562998	-0.278639
C	1.952191	0.391580	-1.163179
O	2.772481	0.995786	-1.844504
N	-1.261490	0.160169	-0.266859
C	-2.077877	0.184120	0.796035
N	-1.302696	-0.059978	2.012547
N	1.059404	0.886093	-0.256230
H	0.736830	1.836305	-0.383434
N	1.768434	-1.001869	-1.177417
H	2.336000	-1.613442	-1.746127
N	-3.362777	0.400913	0.823441
H	-1.680189	-0.073833	2.948868
H	-3.701155	0.360685	1.785476

Sp29^{-} SCF Energy: -692.758901185

	X	Y	Z
C	0.049276	0.131619	0.074459
C	0.060776	0.075485	1.604897
O	1.019297	0.098168	2.357941
C	0.501641	-1.272343	-0.577627
O	-0.201073	-2.272068	-0.412040
C	2.004832	0.225804	-1.184857
O	3.029997	0.755989	-1.607252
N	-1.366012	0.423291	-0.190364
C	-2.154074	0.154915	0.905411
N	-1.264903	0.010127	1.985716
N	0.996264	1.005406	-0.529451
H	1.335499	1.815531	-0.025849
N	1.630923	-1.092161	-1.271926
N	-3.437402	0.098891	0.902763
H	-3.793134	-0.127937	1.830404

H	-1.554853	-0.052943	2.950487
H	-1.751632	0.145078	-1.083351

Sp30$^-$ SCF Energy: -692.749800005

	X	Y	Z
C	0.061275	-0.168611	0.091136
C	0.016191	-0.216175	1.642847
O	0.932892	-0.384856	2.423049
C	0.719002	-1.478722	-0.462109
O	0.355790	-2.635847	-0.275770
C	1.814381	0.461007	-1.162153
O	2.708860	1.028023	-1.801012
N	-1.378930	-0.103847	-0.225487
C	-2.151864	0.154993	0.878735
N	-1.305817	-0.008701	1.989738
N	0.811328	0.939666	-0.425491
N	1.761118	-1.011135	-1.178061
H	2.416580	-1.580965	-1.692393
N	-3.398290	0.473235	0.858936
H	-3.746871	0.623780	1.805004
H	-1.618488	0.041040	2.948135
H	-1.629421	0.385163	-1.074668

Sp31$^-$ SCF Energy: -692.753370322

	X	Y	Z
C	0.055927	-0.107843	0.175743
C	0.009006	-0.194069	1.738887
O	0.939951	-0.394404	2.512193
C	0.669896	-1.413993	-0.413219
O	0.285315	-2.556425	-0.261374
C	1.951353	0.371937	-1.178132
O	2.777540	0.960494	-1.866681
N	-1.270998	0.174422	-0.267908
C	-2.066616	0.230241	0.817255
N	-1.296595	0.014044	2.014852
N	1.060885	0.884150	-0.280582
H	0.758780	1.841266	-0.402810
N	1.755129	-1.020035	-1.174374
H	2.318493	-1.644389	-1.733209
N	-3.340707	0.448991	0.966139
H	-3.741864	0.575510	0.035816
H	-1.703669	0.024356	2.938018

Hydantoin Tautomers

Hydantoin neutral SCF Energy: -376.866326772

	X	Y	Z
Structure from Gaussian File hydantoin_neut_gasopt.log			
C	0.200602	-0.027177	-0.242432
C	-0.506518	1.045275	0.597717
O	0.013523	1.869279	1.321412
C	-2.133367	-0.182167	-0.541568
O	-3.238861	-0.539078	-0.898591
N	-0.911397	-0.687112	-0.904188
H	-0.845945	-1.496958	-1.500514
N	-1.853005	0.872520	0.355846
H	-2.584164	1.432901	0.771634

H	0.768295	-0.694085	0.416838
H	0.895267	0.451094	-0.941928

Hydantoin N1 anion SCF Energy: -376.300986173

	X	Y	Z
C	0.146529	-0.027138	-0.253403
C	-0.515316	1.054391	0.612990
O	0.027271	1.884784	1.355465
C	-2.066042	-0.231933	-0.589212
O	-3.245312	-0.494468	-0.897997
N	-0.904665	-0.753931	-0.945172
N	-1.831538	0.880290	0.368688
H	-2.577066	1.425875	0.775816
H	0.756638	-0.674142	0.399601
H	0.854937	0.462125	-0.943363

Hydantoin N3 anion SCF Energy: -376.309411694

	X	Y	Z
C	0.201896	-0.017533	-0.285766
C	-0.562814	1.042352	0.557182
O	0.041623	1.848386	1.283060
C	-2.107580	-0.104109	-0.532066
O	-3.184870	-0.602445	-0.882146
N	-0.874153	-0.568775	-1.087594
H	-0.876233	-1.550561	-1.332576
N	-1.894506	0.912335	0.362664
H	0.674804	-0.749607	0.387095
H	0.989237	0.461428	-0.881027

Phenytoin Tautomers

Phenytoin neutral SCF Energy: -839.119876064

	X	Y	Z
C	0.338823	0.073024	-0.115633
C	-0.020773	1.259337	0.833448
O	0.748345	1.929122	1.490279
C	-2.005258	0.500283	-0.117111
O	-3.185035	0.488889	-0.411097
N	-1.006127	-0.328150	-0.561192
H	-1.153840	-0.848672	-1.414545
N	-1.388671	1.391752	0.781659
H	-1.911205	2.084286	1.300859
C	1.032490	-1.019329	0.714403
C	2.360379	-0.830583	1.126678
C	0.356468	-2.180840	1.104246
C	2.999351	-1.792677	1.908328
H	2.890645	0.071564	0.840702
C	1.001747	-3.148148	1.882230
H	-0.674597	-2.329475	0.802214
C	2.323669	-2.957700	2.286177
H	4.026667	-1.632060	2.222037
H	0.465606	-4.047318	2.171799
H	2.824599	-3.707890	2.891062
C	1.180443	0.519657	-1.322216
C	1.694144	-0.466032	-2.179907
C	1.388167	1.867224	-1.641314
C	2.386193	-0.112418	-3.338521

H	1.565829	-1.516301	-1.932293
C	2.089155	2.220976	-2.798640
H	1.025087	2.650281	-0.984623
C	2.586289	1.235269	-3.652189
H	2.776339	-0.889068	-3.989857
H	2.246669	3.270964	-3.027043
H	3.130527	1.512627	-4.550062

Phenytoin N1 anion SCF Energy: -838.565504738

	X	Y	Z
C	0.223017	0.085035	-0.147525
C	-0.180872	1.356186	0.675896
O	0.553527	2.163827	1.253628
C	-2.042891	0.216137	-0.155340
O	-3.273356	0.098740	-0.283942
N	-1.028495	-0.517561	-0.584383
N	-1.524809	1.361755	0.610826
H	-2.118207	2.051685	1.048629
C	1.030317	-0.879831	0.758285
C	2.190431	-0.473280	1.436578
C	0.600697	-2.205728	0.904763
C	2.899751	-1.369788	2.239990
H	2.523733	0.554967	1.356323
C	1.315857	-3.106048	1.700800
H	-0.306522	-2.498068	0.386601
C	2.469538	-2.694060	2.373355
H	3.789662	-1.030398	2.765632
H	0.965295	-4.131368	1.798421
H	3.024086	-3.392176	2.996465
C	1.096127	0.478423	-1.366302
C	0.927530	-0.229167	-2.566627
C	2.061128	1.496261	-1.321631
C	1.711892	0.060384	-3.685235
H	0.152546	-0.987087	-2.601313
C	2.839411	1.793281	-2.446066
H	2.182798	2.075095	-0.412343
C	2.674852	1.073947	-3.632247
H	1.563393	-0.501767	-4.604763
H	3.572444	2.595414	-2.392135
H	3.281229	1.304941	-4.505183

Phenytoin N3 anion SCF Energy: -838.572430107

	X	Y	Z
C	0.237821	-0.208562	-0.427652
C	-0.786741	0.855324	0.185085
O	-0.372468	1.873098	0.753109
C	-2.035453	-0.769186	-0.641301
O	-2.986624	-1.517949	-0.880195
N	-0.715467	-1.111705	-1.060260
H	-0.523907	-2.106265	-1.065464
N	-2.051731	0.440287	0.003455
C	1.026768	-0.936851	0.671465
C	2.081722	-1.794941	0.315416
C	0.682098	-0.841052	2.028037
C	2.759362	-2.547935	1.276698
H	2.379666	-1.865971	-0.727473
C	1.362361	-1.590494	2.993274
H	-0.111595	-0.166576	2.329963

C	2.401140	-2.448966	2.624780
H	3.570233	-3.206059	0.973076
H	1.077919	-1.497640	4.038558
H	2.928790	-3.029585	3.377536
C	1.162988	0.482319	-1.427084
C	1.014453	0.302211	-2.808628
C	2.163250	1.358158	-0.970647
C	1.851782	0.964704	-3.712849
H	0.227524	-0.356404	-3.161235
C	2.995957	2.022737	-1.871857
H	2.267220	1.530016	0.095137
C	2.848916	1.826641	-3.249920
H	1.718776	0.808263	-4.781051
H	3.758785	2.701358	-1.497168
H	3.499269	2.344053	-3.951311

Guanidine Tautomers

Guanidine cation SCF Energy: -205.856582136

	X	Y	Z
N	-0.321784	1.298096	-0.000227
H	0.366860	2.011305	-0.194580
H	-1.263569	1.607328	0.194951
N	1.284975	-0.370446	0.000436
H	2.023682	0.290821	0.194625
H	1.558391	-1.323091	-0.195423
C	-0.000070	0.000019	0.000069
N	-0.963324	-0.927741	0.000031
H	-0.760088	-1.897799	0.195838
H	-1.925127	-0.688437	-0.195718

Guanidine neutral SCF Energy: -205.466025278

	X	Y	Z
N	-0.256001	1.324471	0.170681
H	0.296209	1.932826	-0.420993
H	-1.244104	1.542511	0.151700
N	1.334540	-0.331171	-0.153902
H	1.967718	0.239995	0.392343
H	1.567252	-1.314005	-0.122085
C	-0.024137	-0.038970	0.005257
N	-1.007672	-0.864051	0.000548
H	-0.687735	-1.831842	-0.003855

N-Formyl guanidine Tautomers

$FG1^{+}$ SCF Energy: -319.223013153

	X	Y	Z
C	-0.529734	-0.338235	-0.524886
O	-1.218378	0.634902	-0.720741
N	0.823414	-0.265160	-0.128845
H	-0.874219	-1.375796	-0.631683
H	1.303302	-1.148169	0.005483
C	1.533008	0.889153	0.086633
N	0.945542	2.062151	-0.077419
H	1.444211	2.928636	0.075398
H	-0.033864	2.079028	-0.365437
N	2.810675	0.785757	0.460070

H	3.375153	1.607498	0.630479
H	3.263354	-0.108601	0.587194

FG2^{+} SCF Energy: -319.210137232

	X	Y	Z
C	-0.480788	-0.401246	-0.656063
O	-1.045505	-1.456788	-0.652319
N	0.757542	-0.241489	0.039673
H	-0.820188	0.499240	-1.189364
H	1.125559	-1.105020	0.432469
C	1.499796	0.889771	0.143156
N	0.920138	2.086620	0.035573
H	1.471472	2.927026	-0.080633
H	-0.074583	2.205609	0.170286
N	2.812107	0.788212	0.353612
H	3.365888	1.584625	0.641984
H	3.300202	-0.086745	0.212443

FG3 SCF Energy: -318.851957746

	X	Y	Z
C	-0.438574	-0.309987	-0.498913
O	-1.200171	0.655632	-0.668167
N	0.876040	-0.300616	-0.130967
H	-0.822076	-1.331588	-0.648214
C	1.496580	0.858655	0.052511
N	0.922769	2.077276	-0.036026
H	1.474151	2.921510	-0.050399
H	-0.055597	2.070858	-0.330108
N	2.831321	0.803789	0.337966
H	3.288890	1.581311	0.789143
H	3.187782	-0.119763	0.535897

FG4 SCF Energy: -318.830479093

	X	Y	Z
C	-0.437523	-0.397210	-0.645413
O	-0.947502	0.380216	-1.420106
N	0.716245	-0.200456	0.094764
H	-0.844158	-1.411094	-0.461265
H	1.032930	-0.986560	0.647927
C	1.462618	0.995165	0.229773
N	0.881773	2.127479	0.259468
H	1.560233	2.889505	0.284165
N	2.819382	0.705693	0.413606
H	3.421695	1.513746	0.499415
H	3.205509	-0.013295	-0.186618

FG5 SCF Energy: -318.848779275

	X	Y	Z
C	-0.501088	-0.334932	-0.531055
O	-1.248915	0.601559	-0.786220
N	0.791886	-0.239579	-0.102639
H	-0.825178	-1.384620	-0.630551
H	1.313332	-1.094754	0.046757
C	1.582448	0.915233	0.125654
N	0.911702	2.101233	0.021959
H	1.447438	2.953983	0.020965

H	-0.029744	2.099825	-0.356975
N	2.808720	0.686935	0.430682
H	3.324370	1.549308	0.599075

FG6 SCF Energy: -318.845415449

	X	Y	Z
C	-0.511246	-0.349381	-0.536486
O	-1.240747	0.588378	-0.821041
N	0.784632	-0.264197	-0.092918
H	-0.847070	-1.398018	-0.617199
H	1.255854	-1.143837	0.070685
C	1.592780	0.894718	0.124117
N	0.923940	2.076639	0.035340
H	1.494882	2.906954	0.060572
H	-0.004011	2.099654	-0.367092
N	2.841447	0.837655	0.415399
H	3.191528	-0.116234	0.471649

FG7 SCF Energy: -318.840977907

	X	Y	Z
C	-0.501722	-0.385445	-0.579557
O	-1.200418	0.527134	-0.981962
N	0.767648	-0.260361	-0.064863
H	-0.834206	-1.439352	-0.595456
H	1.181813	-1.100403	0.319444
C	1.482315	0.952209	0.143105
N	1.043764	2.138048	0.006526
H	0.058563	2.143939	-0.251623
N	2.777132	0.693583	0.600156
H	3.298081	1.556348	0.706023
H	3.297109	-0.000625	0.075059

FG8 SCF Energy: -318.838072336

	X	Y	Z
C	-0.414280	-0.356095	-0.545521
O	-1.212886	-1.255796	-0.353024
N	0.849608	-0.299693	-0.002829
H	-0.674398	0.465967	-1.255918
C	1.469206	0.840373	0.111699
N	0.885998	2.084633	0.151064
H	1.428469	2.888388	-0.130670
H	-0.109865	2.152512	0.008978
N	2.835704	0.847359	0.250178
H	3.253910	1.554071	0.839633
H	3.238830	-0.075989	0.333706

FG9 SCF Energy: -318.841629647

	X	Y	Z
C	-0.464493	-0.378139	-0.581826
O	-1.050739	-1.443450	-0.651791
N	0.794242	-0.262053	-0.022738
H	-0.859511	0.576585	-0.953397
H	1.179313	-1.111602	0.372816
C	1.475384	0.950613	0.168349
N	0.852453	2.061131	0.044674
H	1.481158	2.858354	0.125983
N	2.800686	0.743687	0.543432

H	3.365795	1.578401	0.615186
H	3.286093	-0.031686	0.109600

FG10 SCF Energy: -318.841088342

	X	Y	Z
C	-0.532669	-0.390664	-0.377963
O	-1.071123	-1.451557	-0.637652
N	0.832193	-0.242140	-0.276465
H	-1.098407	0.537866	-0.199047
H	1.382090	-1.094730	-0.296578
C	1.555462	0.899393	0.106870
N	0.863068	2.096848	-0.047993
H	1.404019	2.925907	0.155497
H	0.290153	2.193642	-0.876864
N	2.729707	0.718548	0.582017
H	3.209659	1.599732	0.760402

FG11 SCF Energy: -318.840978597

	X	Y	Z
C	-0.541628	-0.415404	-0.343829
O	-1.082780	-1.463973	-0.642694
N	0.830741	-0.258395	-0.322377
H	-1.093899	0.492708	-0.057313
H	1.361233	-1.107953	-0.479936
C	1.556183	0.884499	0.086866
N	0.861569	2.073552	-0.066710
H	1.423342	2.873280	0.197708
H	0.364031	2.200314	-0.939146
N	2.733411	0.869432	0.586984
H	3.058965	-0.077075	0.778045

FG12 SCF Energy: -318.840948315

	X	Y	Z
C	-0.429197	-0.432911	-0.650509
O	-1.050137	-1.479274	-0.678638
N	0.722888	-0.254444	0.080916
H	-0.725659	0.458977	-1.226785
H	1.059683	-1.069038	0.583435
C	1.452900	0.954017	0.188239
N	0.993010	2.143010	0.088918
H	-0.023772	2.165753	0.057526
N	2.786928	0.724565	0.480213
H	3.328012	1.578475	0.530127
H	3.244602	-0.025402	-0.022016

N-Acetyl guanidine Tautomers

AG1^{+} SCF Energy: -358.569345452

	X	Y	Z
C	-0.531997	-0.373217	-0.538861
O	-1.189792	0.631178	-0.719361
N	0.836485	-0.276486	-0.135546
H	1.335701	-1.147440	-0.001026
C	1.530219	0.881513	0.084508
N	0.936289	2.052186	-0.074392
H	1.428032	2.921038	0.083248

H	-0.043970	2.051439	-0.364352
N	2.810997	0.791460	0.460423
H	3.364671	1.619179	0.634227
H	3.273175	-0.097767	0.585120
C	-1.027894	-1.780779	-0.702408
H	-0.443450	-2.313700	-1.460956
H	-0.949595	-2.332408	0.241287
H	-2.071719	-1.745458	-1.012346

AG2^{+} SCF Energy: -358.551436278

	X	Y	Z
C	-0.613472	-0.310408	-0.373108
O	-1.029034	-1.435575	-0.282654
N	0.757499	-0.123346	0.079401
H	1.158731	-1.021265	0.339329
C	1.574716	0.951650	0.171283
N	1.100865	2.196443	0.240513
H	1.714978	2.994473	0.149628
H	0.130264	2.380361	0.446060
N	2.895181	0.743104	0.209820
H	3.538540	1.469530	0.494520
H	3.293111	-0.149082	-0.050883
C	-1.388142	0.855963	-0.923629
H	-1.798473	1.463641	-0.106951
H	-0.791450	1.488024	-1.586090
H	-2.234603	0.446739	-1.476178

AG3b SCF Energy: -358.190020918

	X	Y	Z
C	-0.597181	0.913075	-0.592963
O	-0.524320	1.595711	-1.631390
N	0.434204	0.645762	0.278566
C	1.651939	1.091198	0.020114
N	2.001771	1.885633	-1.016418
H	2.968960	2.007630	-1.274468
H	1.245133	2.067381	-1.679441
N	2.650277	0.699771	0.874323
H	3.477731	1.270831	0.964071
H	2.325129	0.243856	1.714790
C	-1.913475	0.290359	-0.178851
H	-2.201937	0.657899	0.811595
H	-2.688441	0.532889	-0.906921
H	-1.802428	-0.795829	-0.095468

AG3b SCF Energy: -358.190021033

	X	Y	Z
C	-0.452826	-0.346100	-0.495253
O	-1.192100	0.641054	-0.664589
N	0.870293	-0.315959	-0.116905
C	1.484116	0.842663	0.053567
N	0.909212	2.063543	-0.030479
H	1.470291	2.898148	-0.104937
H	-0.066327	2.046816	-0.335866
N	2.826855	0.799435	0.326470
H	3.257902	1.568559	0.817863
H	3.180742	-0.123084	0.535493
C	-0.989651	-1.746528	-0.701564

H	-0.412187	-2.254751	-1.481086
H	-0.867989	-2.330539	0.216611
H	-2.042525	-1.706607	-0.983279

AG4 SCF Energy: -358.179061686

	X	Y	Z
C	-0.445229	-0.413997	-0.704523
O	-1.040397	0.514237	-1.234668
N	0.769624	-0.262004	-0.059783
H	1.132171	-1.064114	0.437234
C	1.470938	0.957197	0.142945
N	1.075895	2.135312	-0.127832
H	0.129034	2.125627	-0.504260
N	2.700007	0.720823	0.769874
H	3.216188	1.586746	0.874567
H	3.268713	-0.006338	0.349973
C	-0.999724	-1.827363	-0.709901
H	-1.221675	-2.108029	-1.742752
H	-0.326666	-2.570247	-0.273133
H	-1.944111	-1.833199	-0.157566

AG5 SCF Energy: -358.186948240

	X	Y	Z
C	-0.512571	-0.356436	-0.537917
O	-1.239671	0.613732	-0.747327
N	0.795193	-0.249277	-0.127332
H	1.342101	-1.093207	-0.013807
C	1.577177	0.906706	0.109406
N	0.894853	2.090898	0.070423
H	1.430796	2.943567	0.049567
H	-0.051103	2.084342	-0.299828
N	2.816680	0.684564	0.368250
H	3.324515	1.548777	0.550794
C	-1.002466	-1.783310	-0.699199
H	-0.325626	-2.370789	-1.328471
H	-1.066775	-2.274107	0.278366
H	-1.993442	-1.761695	-1.151953

AG6 SCF Energy: -358.183605253

	X	Y	Z
C	-0.518655	-0.384087	-0.460447
O	-1.273854	0.579395	-0.554171
N	0.826695	-0.274512	-0.170959
H	1.358580	-1.132546	-0.152990
C	1.612145	0.896599	0.053940
N	0.901031	2.049831	0.178645
H	1.444987	2.898126	0.200654
H	-0.070101	2.061618	-0.107909
N	2.891503	0.870173	0.171163
H	3.275535	-0.067948	0.079426
C	-1.021698	-1.801286	-0.661780
H	-0.248770	-2.567103	-0.556824
H	-1.815070	-1.992721	0.066070
H	-1.465652	-1.873634	-1.658469

AG7 SCF Energy: -358.167761335

	X	Y	Z
C	-0.413577	-0.400864	-0.723689
O	-0.936613	0.501742	-1.347158
N	0.795043	-0.271919	-0.040647
H	1.199116	-1.108526	0.357603
C	1.476262	0.933285	0.250791
N	0.837892	1.980534	0.594022
H	1.465079	2.779889	0.691394
N	2.861314	0.737859	0.204420
H	3.418880	1.563095	0.381102
H	3.203319	0.185616	-0.572766
C	-1.025884	-1.789746	-0.622347
H	-0.280284	-2.585220	-0.521388
H	-1.679673	-1.822742	0.256609
H	-1.634982	-1.970241	-1.508908

AG8 SCF Energy: -358.176099863

	X	Y	Z
C	-0.580300	-0.313110	-0.305872
O	-1.111615	-1.410984	-0.212024
N	0.707585	-0.147409	0.194003
H	1.097627	-1.008923	0.561971
C	1.528125	1.001071	0.277915
N	1.168623	2.218678	0.438613
H	0.175456	2.301258	0.637912
N	2.872151	0.661864	0.237433
H	3.481654	1.468551	0.279682
H	3.149454	-0.033256	-0.443486
C	-1.267479	0.859834	-0.971886
H	-1.805594	1.450669	-0.221799
H	-0.574220	1.521759	-1.495255
H	-2.005139	0.454162	-1.665538

AG9 SCF Energy: -358.173453535

	X	Y	Z
C	-0.512688	-0.305839	-0.628002
O	-0.888268	-1.421336	-0.961338
N	0.843984	-0.113024	-0.372451
H	1.352098	-0.989719	-0.319952
C	1.586767	0.957443	0.158750
N	1.131446	2.226804	-0.178548
H	1.740688	2.983852	0.098567
H	0.747052	2.342713	-1.106875
N	2.593423	0.658017	0.893217
H	3.141387	1.481519	1.140306
C	-1.484029	0.849995	-0.497036
H	-1.267331	1.490453	0.359296
H	-1.460461	1.471443	-1.399954
H	-2.482846	0.420958	-0.413512

AG10 SCF Energy: -358.174223577

	X	Y	Z
C	-0.490244	-0.310384	-0.704185
O	-0.852858	-1.392106	-1.145600
N	0.871674	-0.114355	-0.465690
H	1.396192	-0.975027	-0.574541

C	1.587736	0.952558	0.134265
N	1.173118	2.215026	-0.247262
H	1.764898	2.945306	0.128093
H	0.929847	2.337642	-1.221179
N	2.553843	0.805048	0.962045
H	2.650346	-0.163811	1.262041
C	-1.469420	0.803992	-0.403351
H	-1.210503	1.363848	0.496639
H	-1.500457	1.514155	-1.236610
H	-2.455936	0.349529	-0.306822

AG10 SCF Energy: -358.176768292

	X	Y	Z
C	-0.555210	-0.302346	-0.383982
O	-1.017917	-1.435332	-0.370310
N	0.771882	-0.141152	0.027652
H	1.180352	-1.019012	0.327147
C	1.535635	1.012854	0.243350
N	0.999513	2.172458	0.329245
H	1.706804	2.900849	0.415848
N	2.883815	0.689425	0.416889
H	3.506917	1.479179	0.512707
H	3.257354	-0.041931	-0.175341
C	-1.339926	0.898271	-0.844685
H	-1.547312	1.559726	0.000143
H	-0.774669	1.494640	-1.565085
H	-2.269786	0.534648	-1.283046