Supporting Information

Unique Hydrogen-Bonding of Adenine with the Oxidatively Damaged Base 8-oxoguanine Enables Specific Recognition and Repair by DNA Glycosylase MutY

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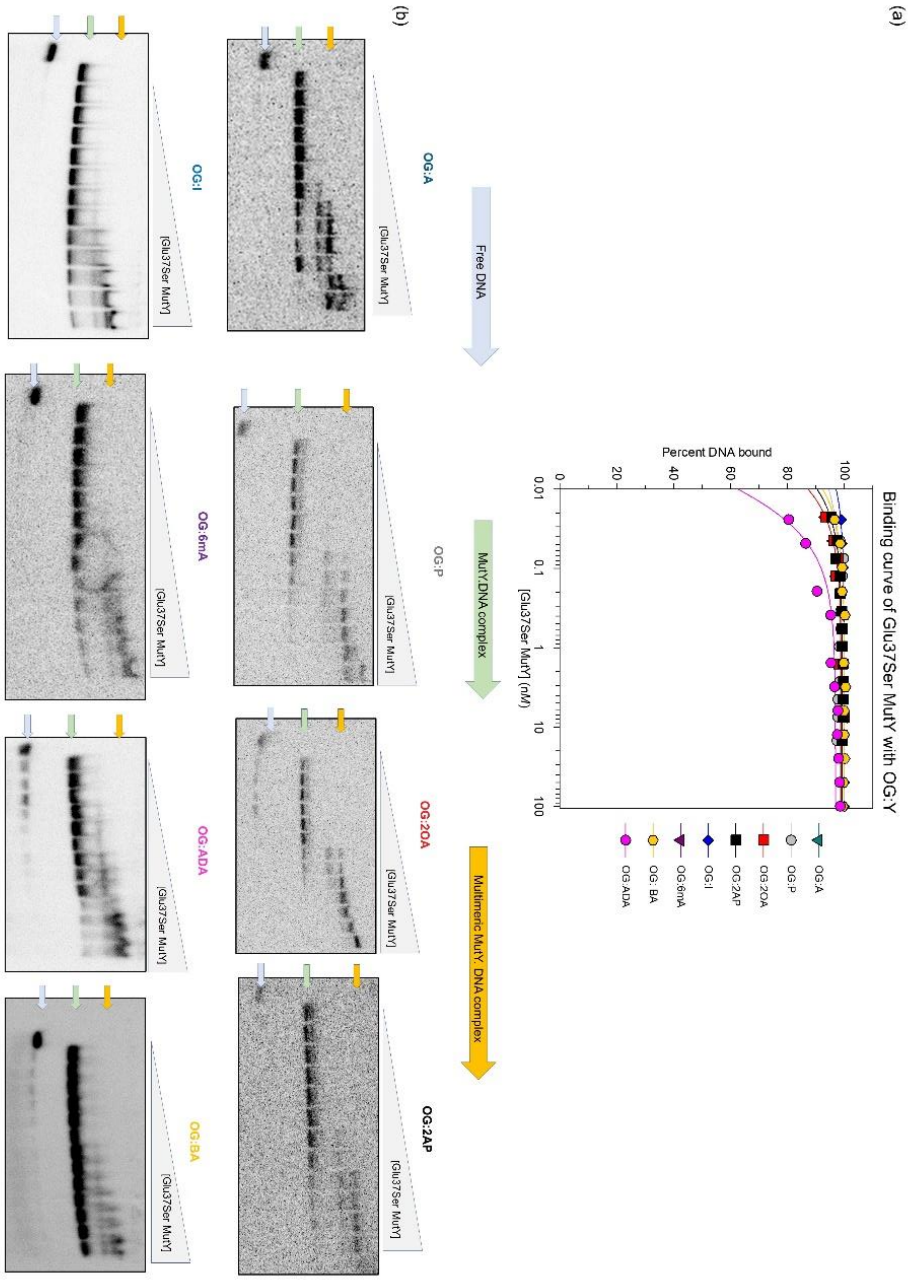


Figure S1: Dissociation constant measurement of A analogue substrates with Glu37Ser MutY (a) Representative plots for the titration of the catalytically inactive Glu37Ser MutY against the A analogues studied in this paper. When base paired opposite OG, all the analogues were almost completely bound even at the lowest enzyme concentration of 20 pM, and [DNA] = 5 pM. Note all "bound" species are quantitated to determine % bound versus unbound. **(b)** Representative EMSA gels for the titration of Glu37Ser MutY with a 30 bp duplex containing OG:Y (Y = A analogue). Slower migrating bands in EMSA titrated contain more than one MutY per duplex; of note, these are usually observed at concentrations well above where the 1:1 complex is fully saturated. With OG:Y duplexes, at the lowest enzyme concentration the duplex is almost already fully bound.

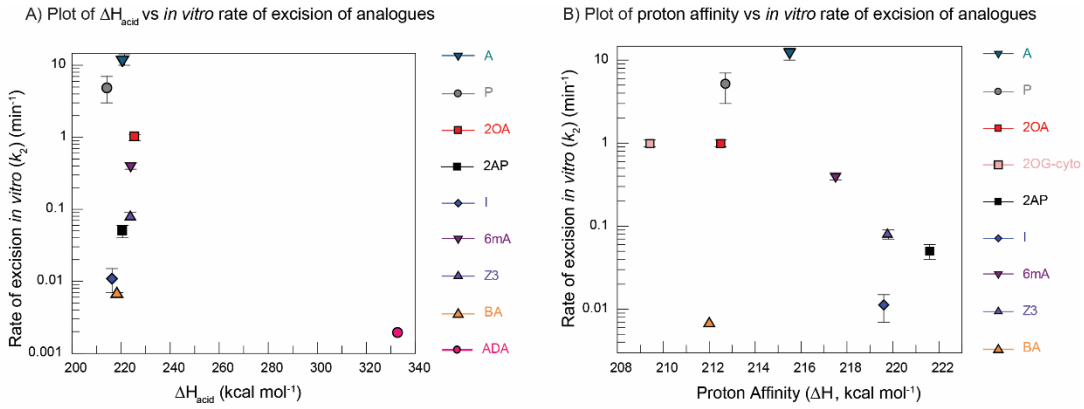


Figure S2 (A) Relationship between calculated gas phase N9-H acidities for N7 protonated and N3 hydrogen bonded analogs and the *in vitro* rate of base excision (k_2). (B) Relationship between calculated N7 proton affinities of analogues and the *in vitro* rate of base excision (k_2). ADA was not plotted as it lacks the N7.

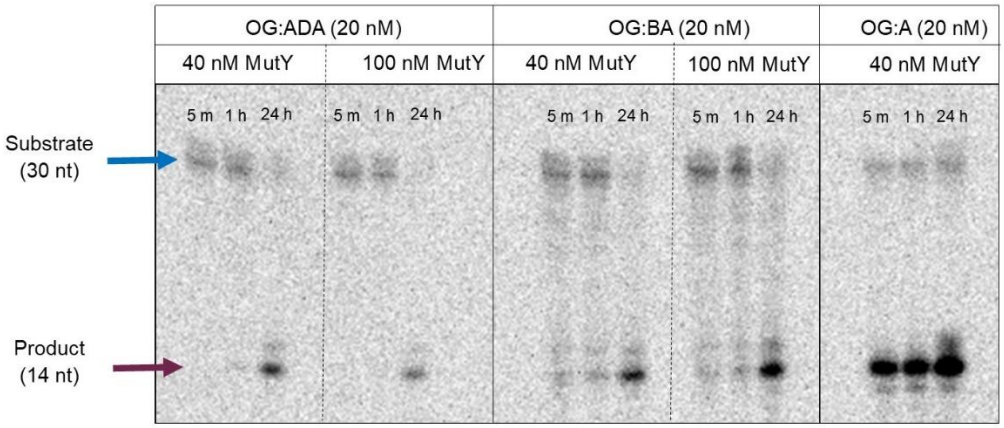


Figure S3 Cleavage assays for the analogues ADA and BA at extended timepoints (24 h) and MutY concentrations of 40 nM and 100 nM at 37 °C.

5'- $C_1T_2G_3$ $T_4A_5A_6$ $C_7G_8G_9$ $G_{10}A_{11}G_{12}$ $C_{13}G_{14}$**Y**$_{15}$ $T_{16}A_{17}G_{18}$ $C_{19}C_{20}T_{21}$ $C_{22}C_{23}A_{24}$ $T_{25}G_{26}A_{27}$ $T_{28}C_{29}G_{30}$-3'

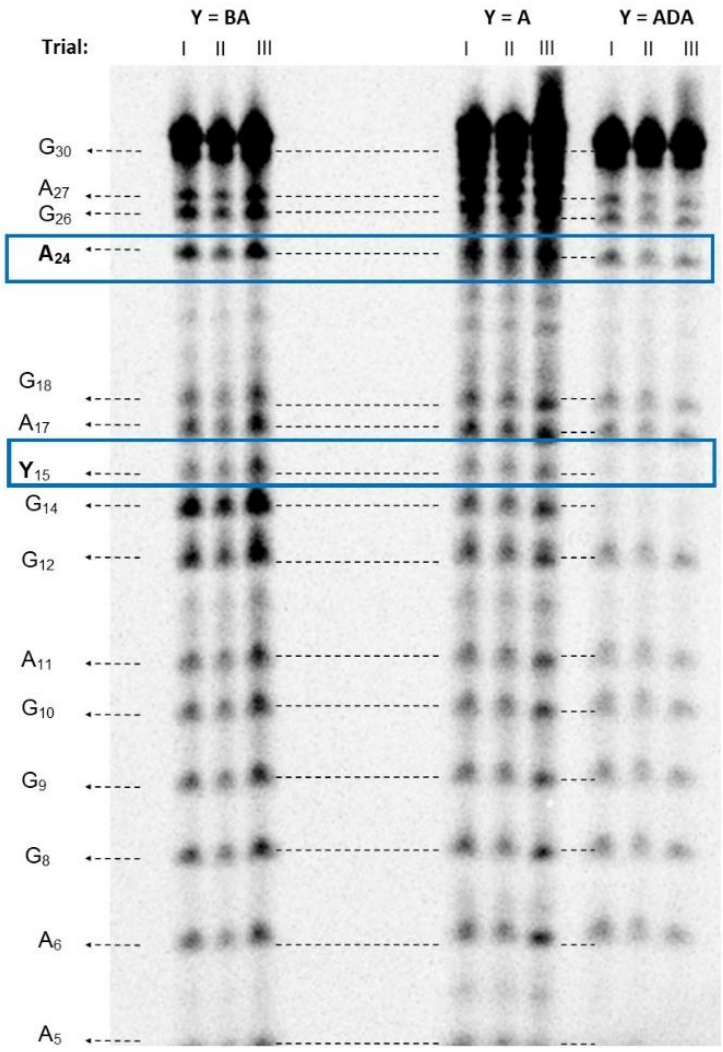


Figure S4 Representative gel showing bands formed by the depurination of A and G from a 30 nt ssDNA sequence after treatment with formic acid and piperidine. The relative intensities of the band corresponding to the analogue of interest (Y_{15}) with respect to a canonical adenine (A_{24}), as highlighted by the blue boxes, are used to determine the relative extent of acid catalyzed depurination of the nucleobase at position 15. Three trials for each analogue are averaged in quantitation.

Table S1 Quantitation of intensities of band corresponding to depurination of analogue at position 15

(Y_{15}) and canonical adenine at position 24 (A_{24}) to determine the relative extent of acid catalyzed depurination of the adenine analogues with respect to canonical adenine. S.D. represents standard deviation of the trials.

Analogue	Trial I			Trial II			Trial III			Average	S.D.
	Intensity of A_{24}	Intensity of Y_{15}	Y_{15}/A_{24}	Intensity of A_{24}	Intensity of Y_{15}	Y_{15}/A_{24}	Intensity of A_{24}	Intensity of Y_{15}	Y_{15}/A_{24}		
A	3206935	3693259	0.87	5122896	5043567	0.98	766436.2	0.984515	0.93	0.93	0.05
P	1110816	11207687	10.09	771259.1	7475590	9.69	3327828	48785493	14.66	11.48	2.25
2OA	861888	5945714	6.90	13661423	63366039	4.64	771070.2	4358296	5.65	5.73	0.92
6mA	2355452	2433459	1.03	1630671	1511099	0.93	2538994	2495640	0.98	0.98	0.04
Z3	10361867	2662677	0.26	10361867	2600025	0.25	10361867	2756320	0.28	0.26	0.01
2AP	6809224	16212884	2.38	2190856	4230497	1.93	1630897	2941600	1.80	2.04	0.25
I	755791.9	772906.7	1.02	399408	548707.1	1.37	831478.9	820489.9	0.99	1.13	0.17
BA	3693259	3206935	0.87	3095456	2904978	0.94	5290255	5326637	1.01	0.94	0.06
ADA	2320039	1275464	0.55	1989632	1070409	0.54	1778921	1004093	0.56	0.55	0.01

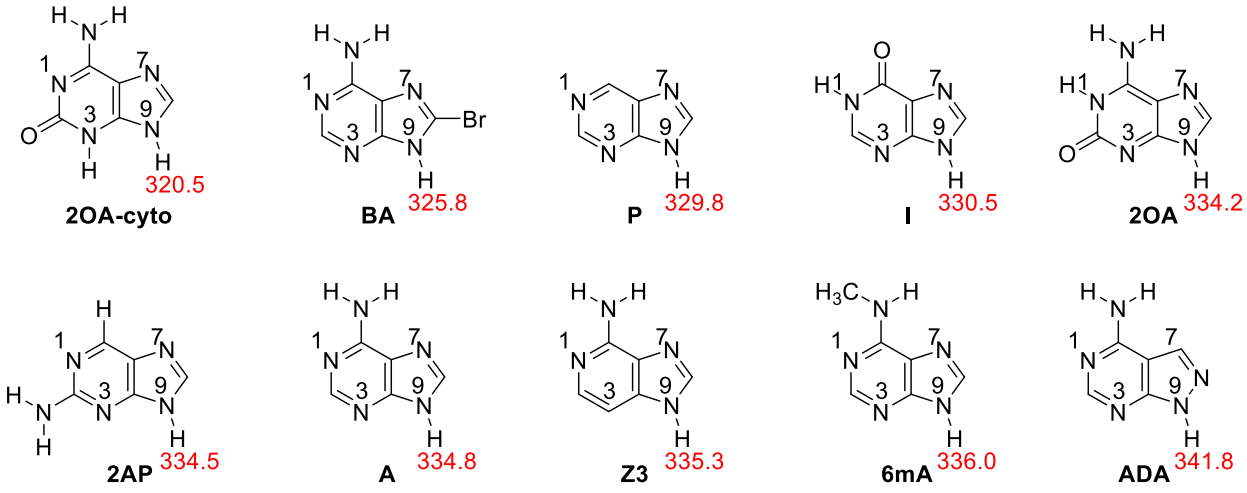


Figure S5 Calculated (B3LYP/6-31+G(d)) gas-phase acidities (ΔH, kcal mol^{-1}) of N9-H for neutral adenine analogues. Substrates are ordered in decreasing acidity (increasing ΔH_{acid} values).[1]

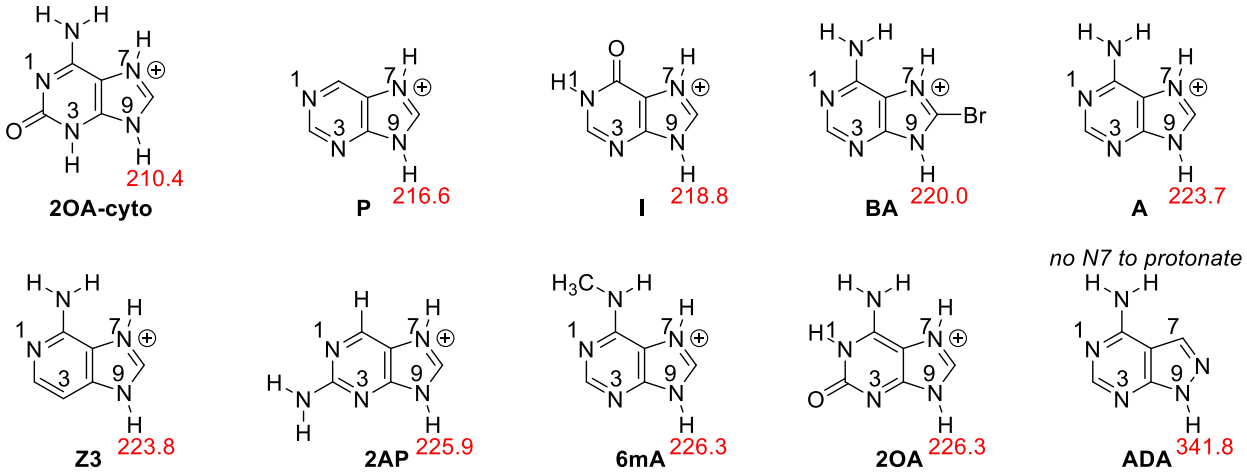


Figure S6 Calculated (B3LYP/6-31+G(d)) gas-phase acidities (ΔH, kcal mol^{-1}) of N9-H for N7-protonated nucleobase analogues. (ADA has no N7 to protonate; N9-H acidity of the neutral is shown for comparison.) Substrates are ordered in decreasing acidity (increasing ΔH_{acid} values).[1]

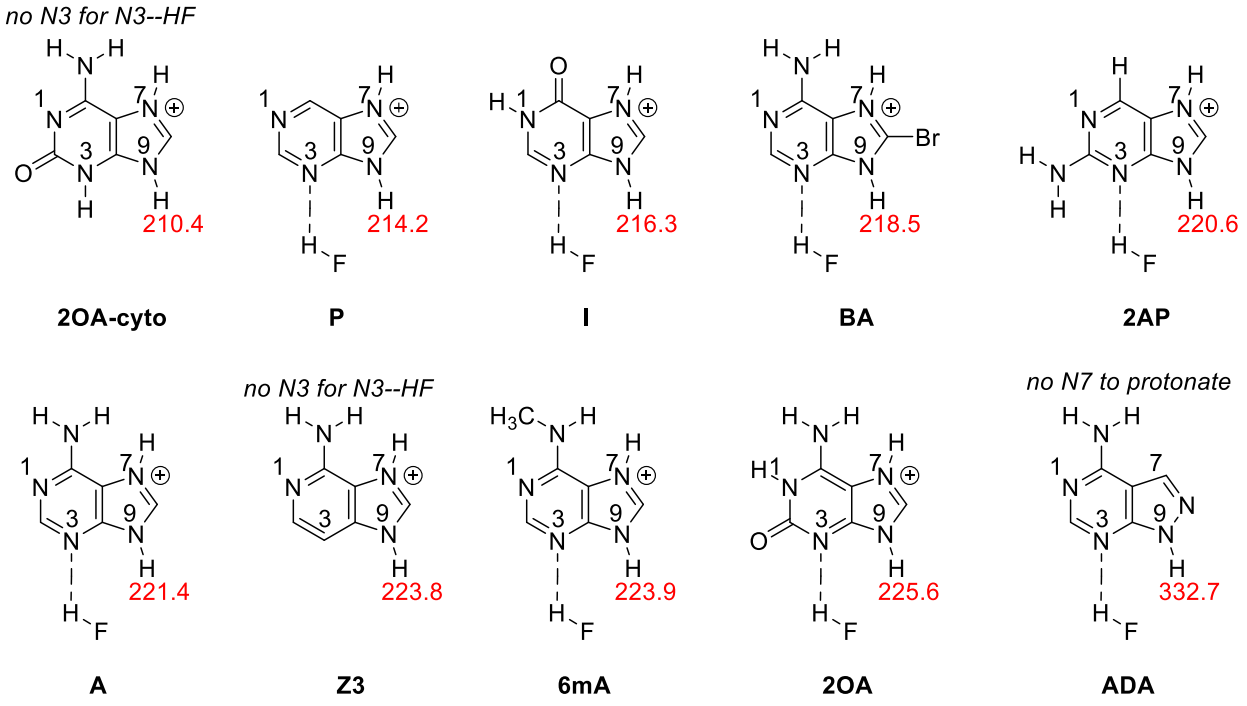


Figure S7 Calculated (B3LYP/6-31+G(d)) gas-phase acidities (ΔH, kcal mol^{-1}) of N9-H for N7-protonated, N3-hydrogen-bonded adenine analogues. Substrates are ordered in decreasing acidity (increasing ΔH_{acid} values). (Z3 has no N3-hydrogen-bonding site, so acidity of N9-H for N7-protonated site is shown for comparison; ADA has no N7 to protonate, so N9-H acidity of the neutral with N3-hydrogen-bonded is shown for comparison).[1]

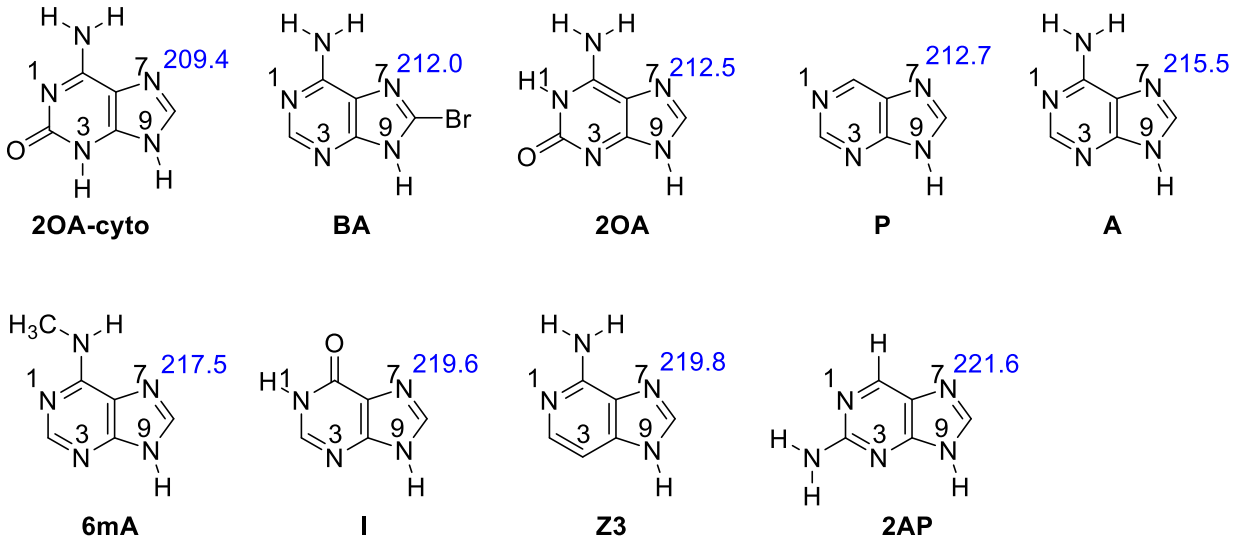


Figure S8 Calculated (B3LYP/6-31+G(d)) gas-phase proton affinities (PA; ΔH, kcal mol^{-1}) of N7 for adenine and analogues. Substrates are ordered in increasing PA. (ADA has no N7 and is therefore not included).[1]

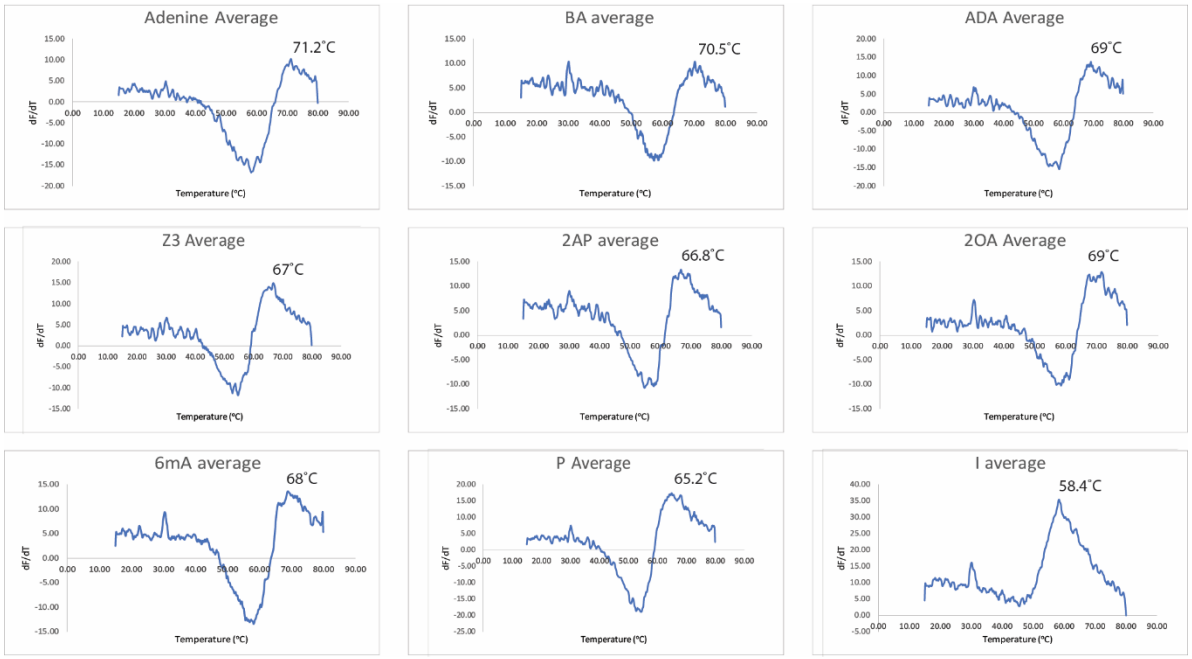


Figure S9: Duplex Melting Experiments with A analogues duplexes. First derivative of change of fluorescence vs temperature (-dF/dT) of EvaGreen dye during the high resolution melt analysis of 11 bp duplexes containing the OG:Y analogues. The melting temperature is the determined by the highest point in the curve, that represents the largest change in fluorescence.[2]

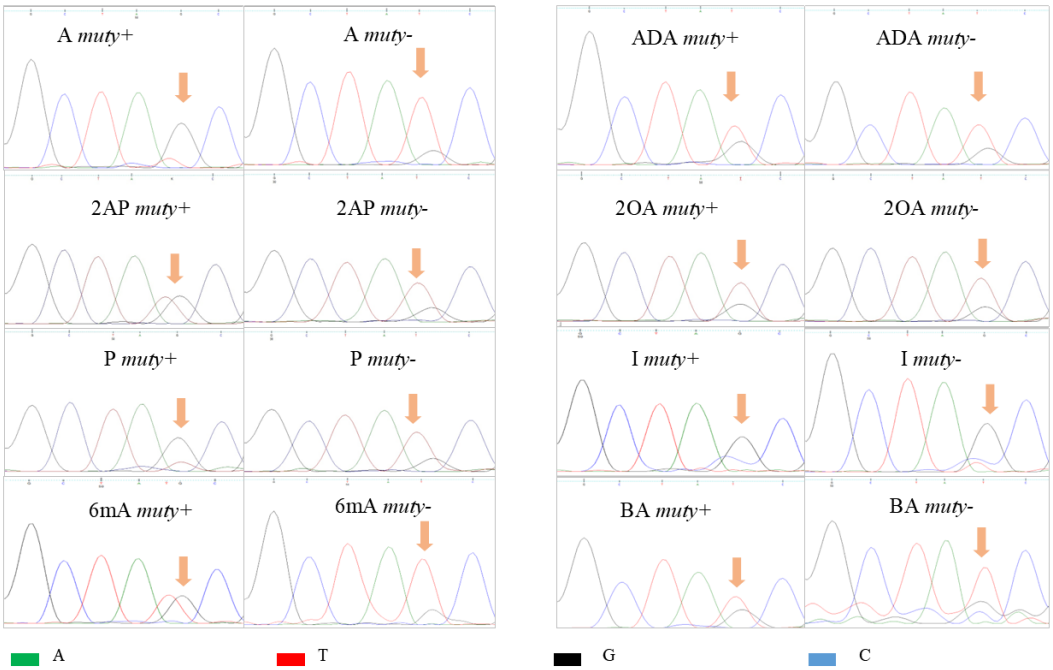


Figure S10: Cell Assay Sequencing. Representative sequencing traces of recovered plasmids from cell assay showing conversion of OG:Y to G:C or T:A at the *BmtI* restriction site (GCTAGC). The repaired site is indicated with the orange arrow.

MATERIALS AND METHODS

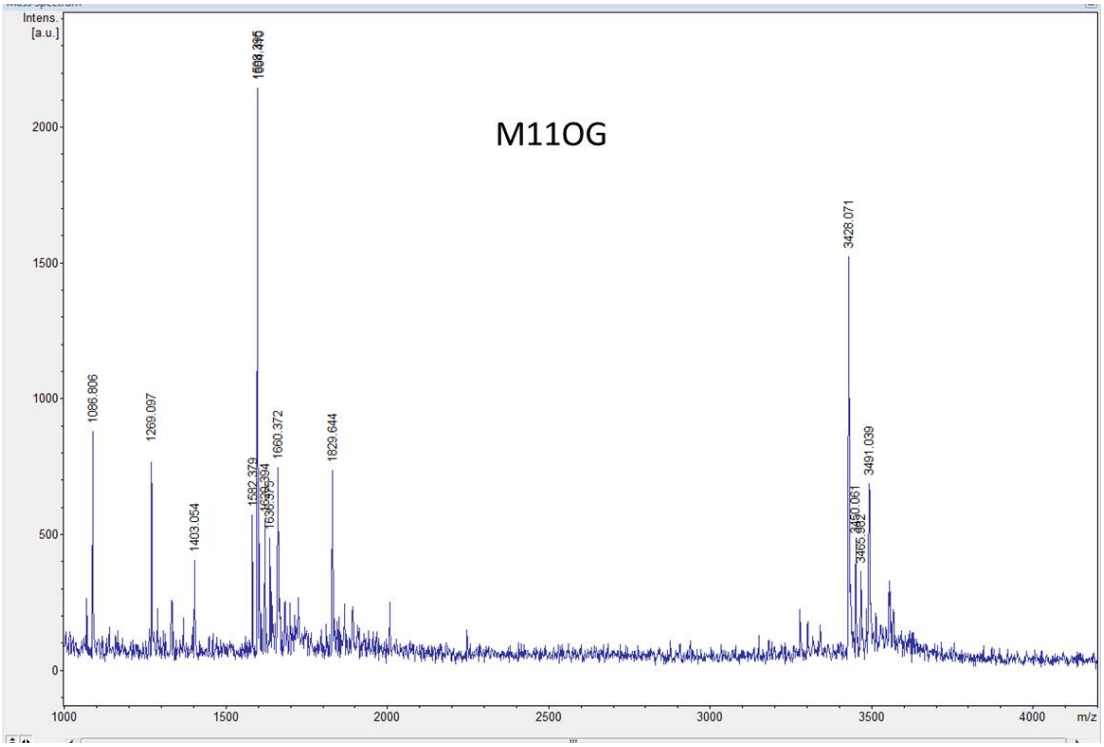
General materials and methods. [γ-^{32}P] – ATP used for DNA radiolabeling was purchased from PerkinElmer and storage phosphor autoradiographs were scanned on a GE Healthcare Typhoon Trio phosphorimager. Image quantitation and data analysis were performed using ImageQuant TL v8.2.0 (GE Healthcare Life Sciences), GraFit v5.0.2 (Erithacus Software) and Excel® for Office 365 (Microsoft). Electrostatic potential maps were generated using Gaussian 09 Revision B.01 (Gaussian, Inc)[3] and gas-phase acidities and tautomer free energies were calculated using Gaussian 16 Revision C.01 (Gaussian, Inc)[1]. Commercially available restriction enzymes were purchased from New England Biolabs and T4 ligase was purchased from Promega and used according to the manufacturer's protocol. Aqueous solutions were prepared using distilled, deionized water from a Milli-Q PR purification system. Other reagents and kits were purchased from Millipore-Sigma, Fisher Scientific, Qiagen or Promega.

DNA substrate preparation. A analogues and OG phosphoramidite monomers were purchased from Glen Research. Oligonucleotides were synthesized and deprotected at the University of Utah DNA and peptide synthesis core facility using standard procedures. DNA oligonucleotides containing only standard nucleobases were purchased from Integrated DNA Technologies or Millipore Sigma. All DNA oligonucleotides were HPLC purified using a Dionex 100 ion exchange column on a Beckman Gold Nouveau or Shimadzu Prominence instrument. Oligonucleotide lengths and sequences (30 nucleotides) were confirmed by Maxam-Gilbert sequencing and denaturing PAGE. Masses of the 11-nucleotide single-strands were confirmed by MALDI-MS.

Table S2 Oligonucleotide sequences used in this work. OG represents 8-oxo-7,8-dihydroguanine, Y represents A or an A analogue

Name	Sequence	Experiment
E30OG	5’ –CGA TCA TGG AGG CTA **OG**CG CTC CCG TTA CAG – 3’	*in vitro* assays
cE30Y	5’ - CTG TAA CGG GAG CG**Y** TAG CCT CCA TGA TCG – 3’	*in vitro* assays
E39OG	5’ - GAT CCG ATC ATG GAG GCT A**OG**C GCT CCC GTT ACA GCT GCA - 3’	Bacterial cell assay
cE31Y	5’ - GCT GTA ACG GGA GCG **Y**TA GCC TCC ATG ATC G -3’	Bacterial cell assay
M11OG	5’ – GAG CT**OG** GTG GC – 3’	Melting temperature
cM11Y	5’ - GCC AC**Y** AGC TC – 3'	Melting temperature

MALDI-TOF mass spectra of 11-nucleotide sequences used for determination of melting temperature: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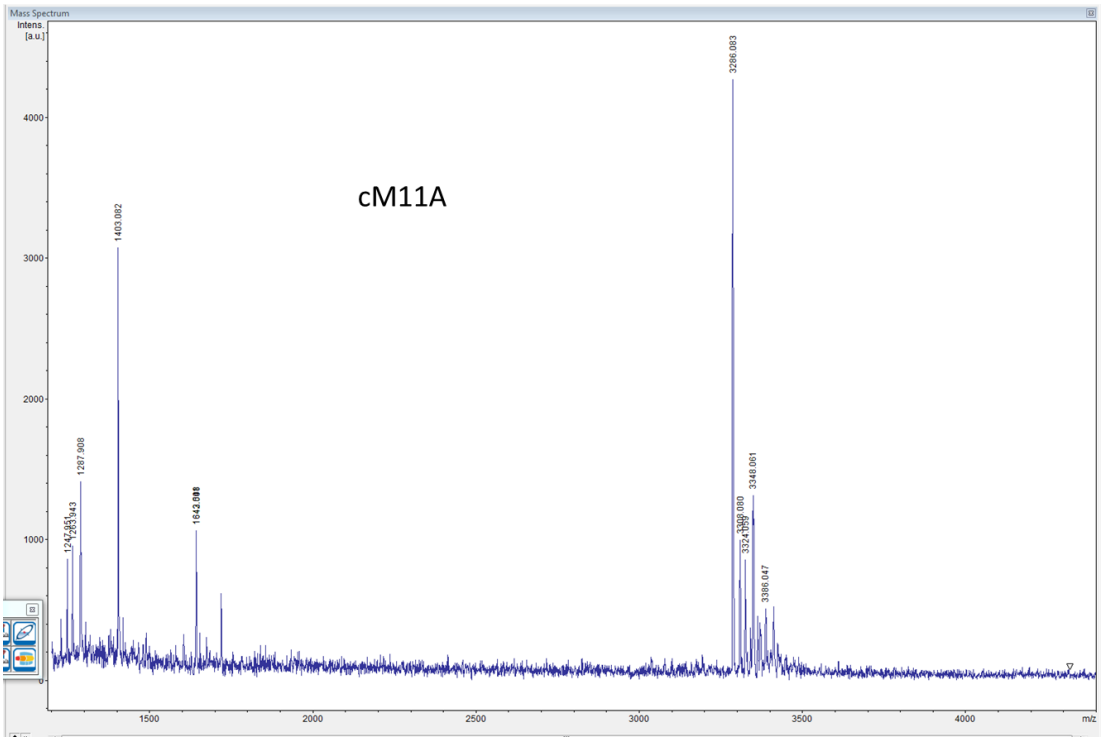
m/z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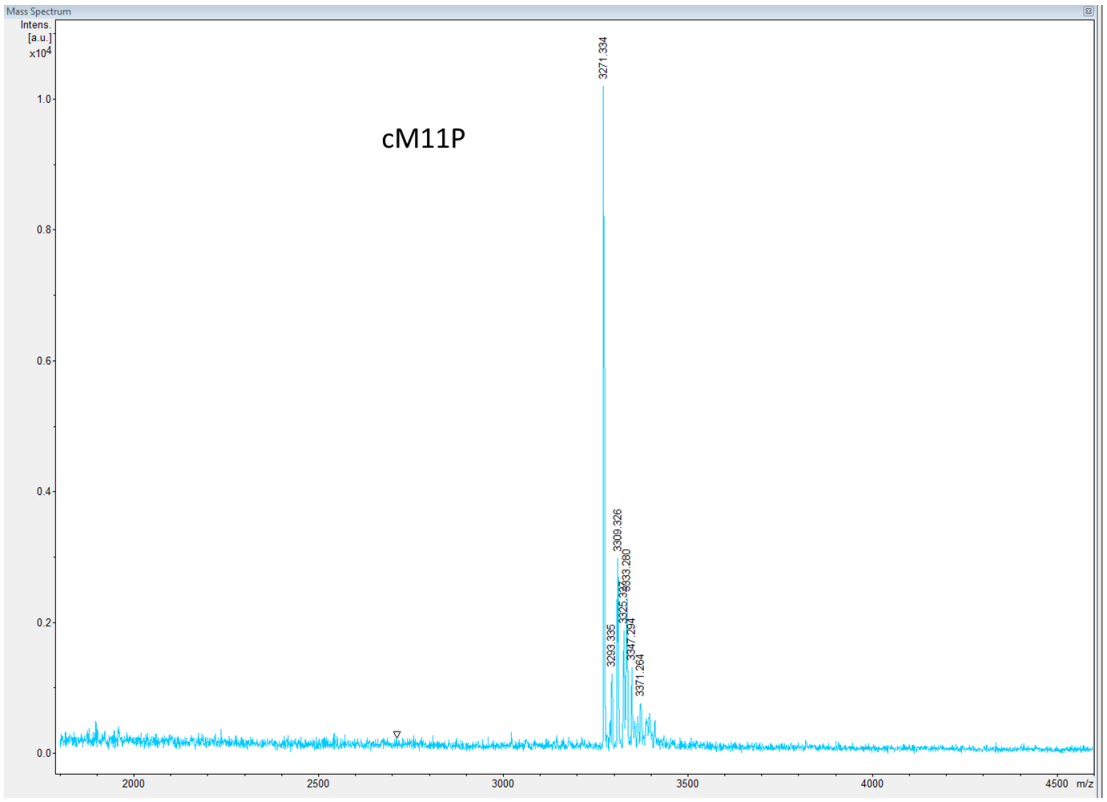
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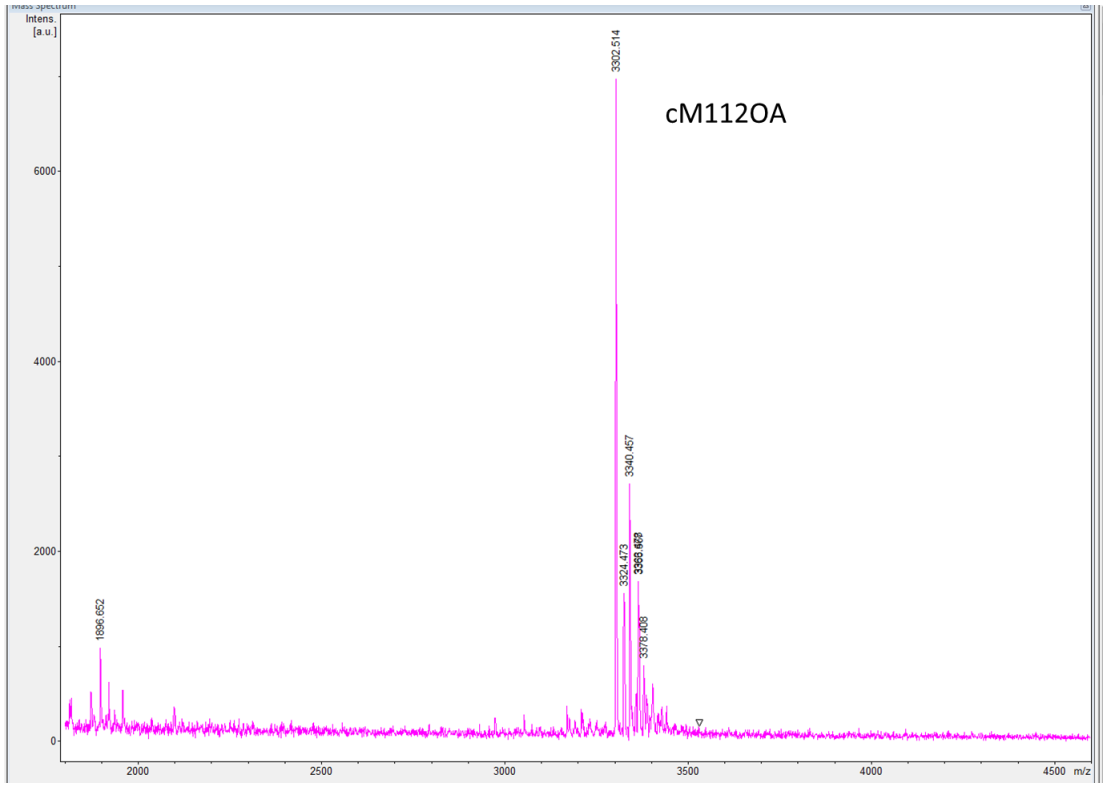
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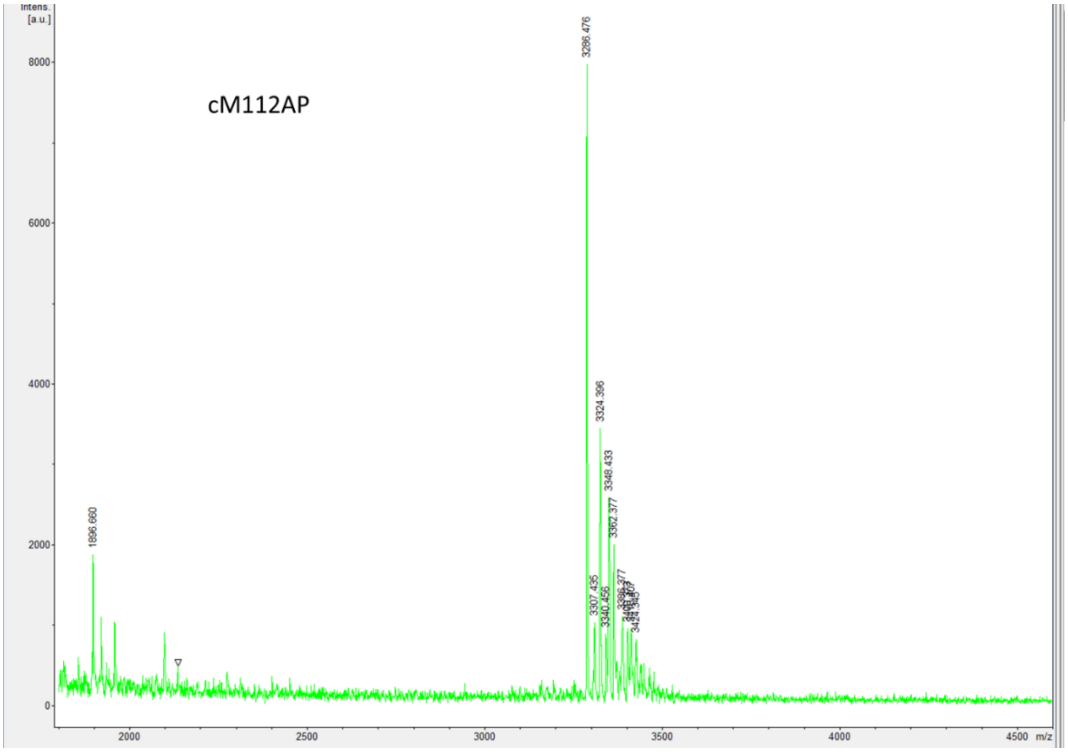
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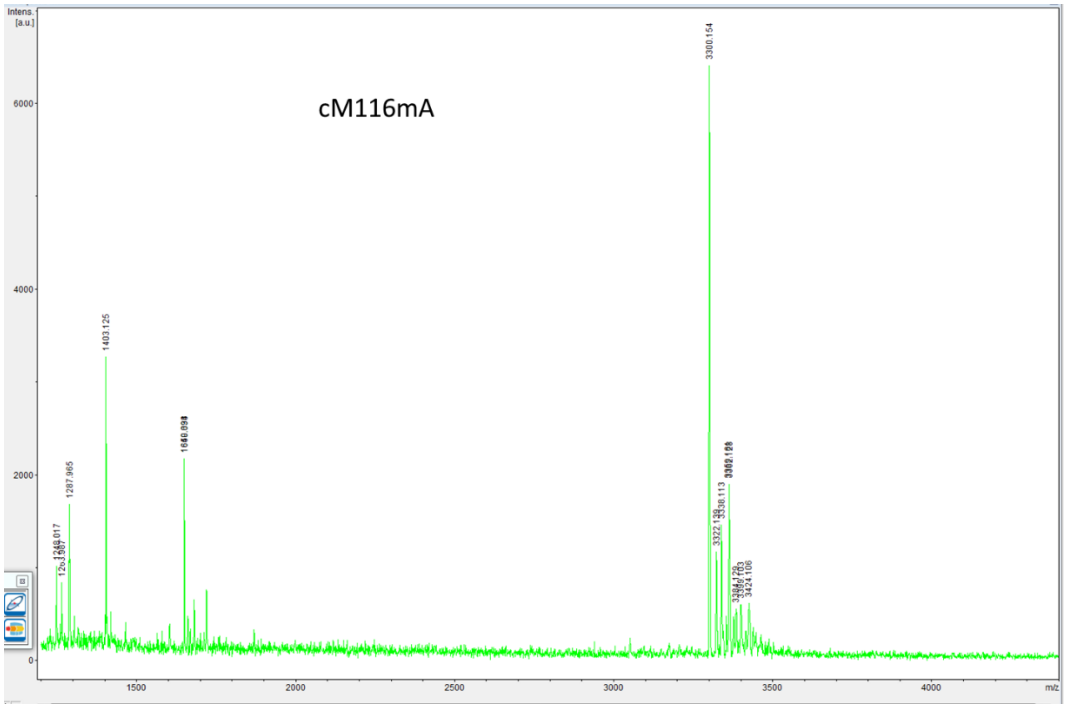
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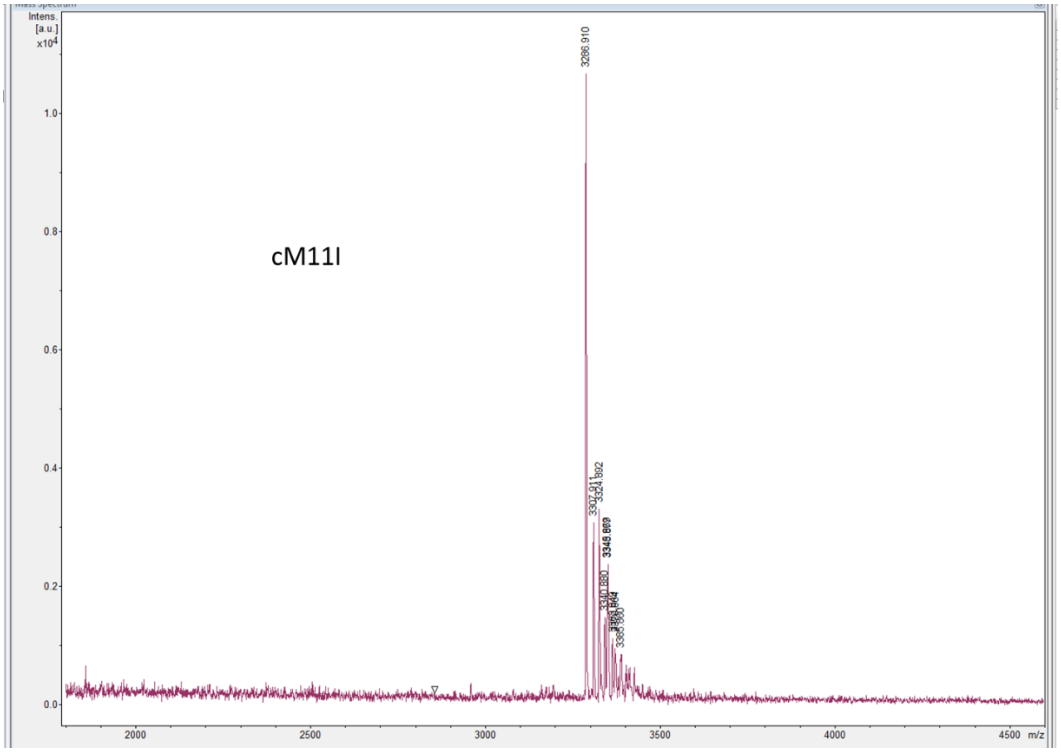
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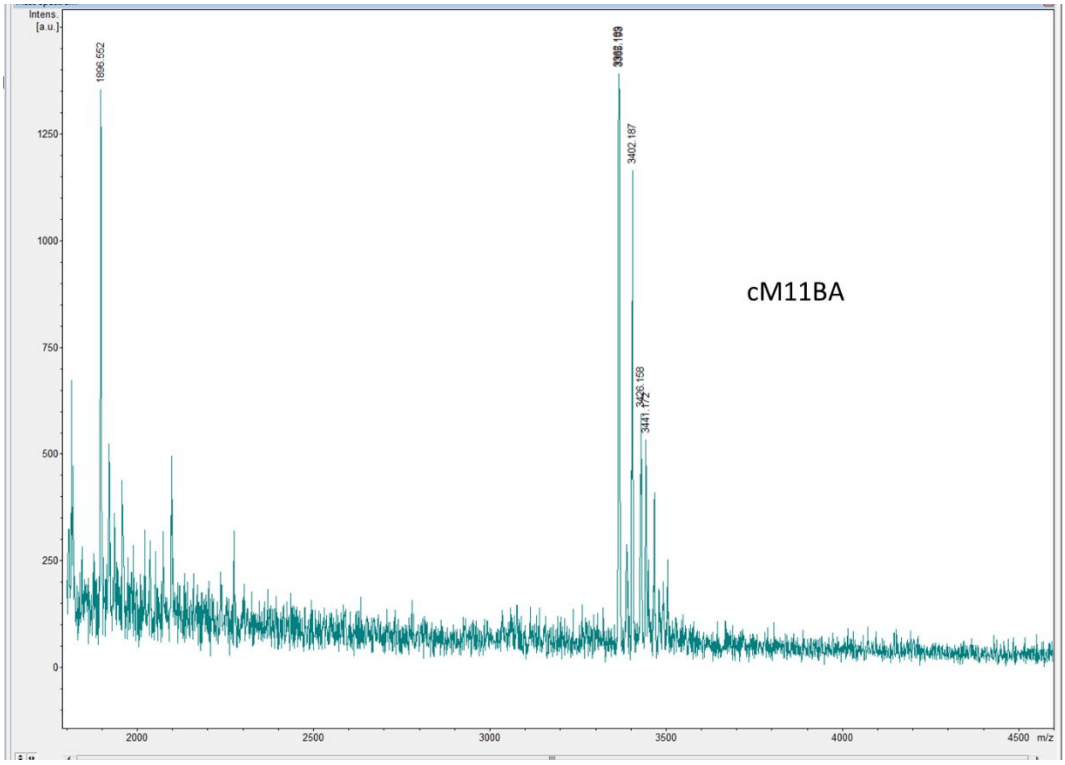
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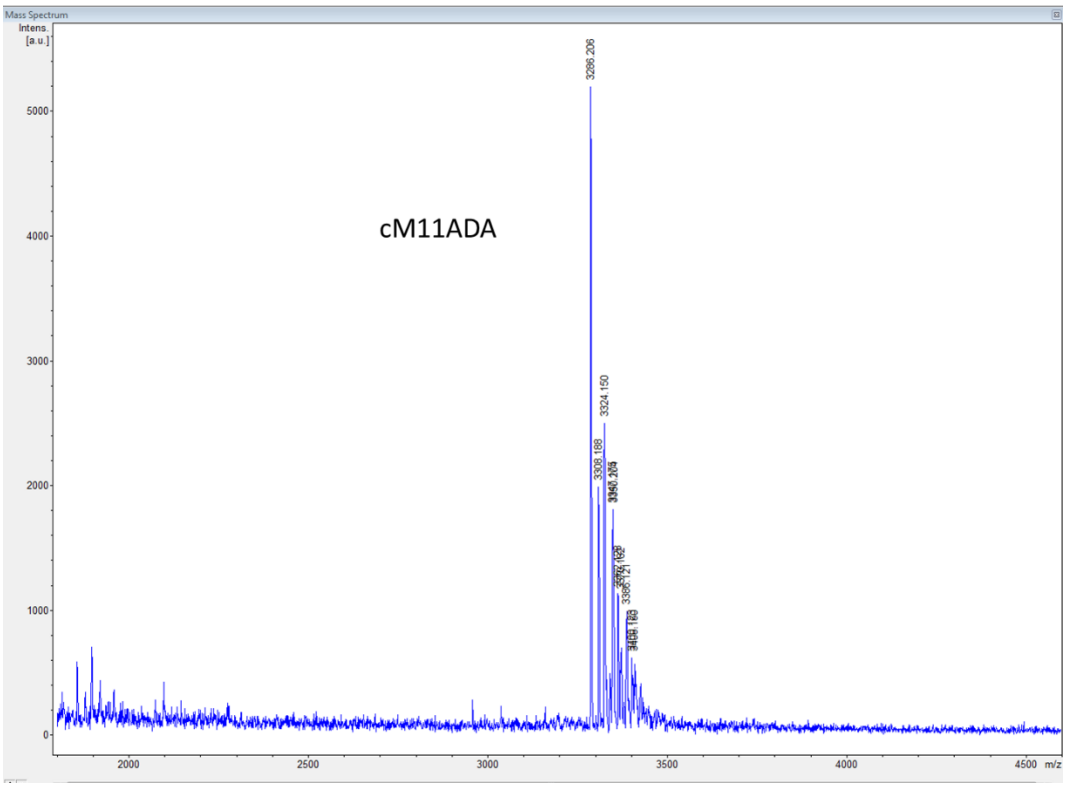
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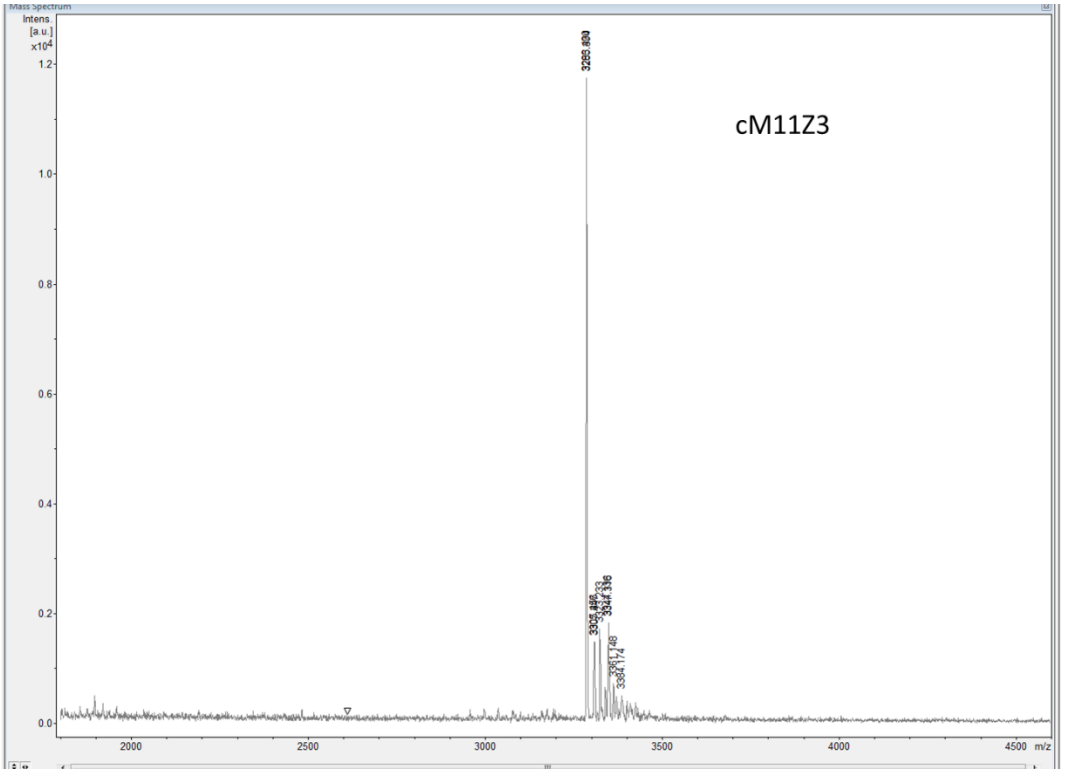
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2500
3000
3500
4000
4500 m/z
cM11Z3

Table S3 Expected and Observed masses of 11-mer oligonucleotide sequences from MALDI-TOF-MS

Oligonucleotide sequence	Expected Mass	Observed Mass
M11OG	3429.188	3428.071
cM11A	3286.207	3286.083
cM11P	3271.126	3271.334
cM112OA	3302.126	3302.514
cM112AP	3286.207	3286.476
cM116mA	3300.146	3300.154
cM11I	3287.116	3286.91
cM11BA	3364.046	3365.193
cM11ADA	3286.207	3286.206
cM11Z3	3285.136	3285.394

Radiolabeling DNA substrate for *in vitro* assays. For binding assays the 5' end labeled 30 bp long DNA duplex with a centrally placed OG:Y mispair is generated by incubating 5.0 pmol of the 30-mer Y (cE30Y, Table S2) containing ssDNA with 25 μCuries of [γ- ^{32}P] ATP (Perkin-Elmer) in the presence of 10 units of T4 polynucleotide kinase (NEB) and the provided buffer, at 37 °C for 30 min. The reaction is terminated by incubating at 90 °C for 5 min. The labeled product is purified using a G-50 microspin column (GE Healthcare), and then freeze dried. It is assumed that there is no loss of DNA during this purification step. The dry, labeled oligonucleotide is resuspended in 25 µL of 2x annealing buffer (40 mM Tris-HCl pH 7.6, 20 mM EDTA pH 8.0, 300 mM NaCl) and annealed to 20% excess (6.0 pmol) of complementary OG carrying strand to yield a solution of 100% labeled DNA. The final concentration of DNA duplex is brought to 100 nM with MilliQ H_2O and the solution is incubated for 5 min at 90 °C on a dry bath incubator, transferred to a Styrofoam box and allowed to cool slowly at 4°C for 12-16 h to ensure complete annealing.

Radiolabeling for glycosylase assays is carried out using an analogous procedure, wherein 2.5 pmol of the Y containing strand (cE30Y, Table S2) is incubated with 25 µCuries of [γ- ^{32}P] ATP and 10 units of T4 polynucleotide kinase in the provided buffer at 37 °C, quenched, purified through a G-50 microspin column and freeze dried as described above. The dried, labeled oligonucleotide is resuspended in 250 µL 2x annealing buffer, and combined with 47.5 pmol of unlabeled Y containing strand, followed by 20% excess

(60.0 pmol) of complementary OG containing strand, to yield a solution of 5% labeled DNA. The final duplex concentration is brought up to 100 nM by the addition of MilliQ H_2O and the solution is annealed as described above.

Note: (i) in the glycosylase assays, the final concentration (20 nM) of DNA used in the assays is known with greater accuracy due to the addition of 47.5 pmol unlabeled Y containing strand.

(ii) labeling for the Maxam-Gilbert sequencing reactions was carried out using a procedure identical to the one described for the glycosylase assay, with the exception that no OG containing oligonucleotide was added to the reaction mixture, and a solution of 100 nM ssDNA was created that was 5% end labeled with ^{32}P.

MutY purification. WT and Glu37Ser *Ec* MutY were overexpressed in JM101 *muty⁻ E coli* and purified using a GE Healthcare AKTA Pure FPLC system as previously described.[4] Active concentrations of WT *Ec* MutY was determined as described previously.[4] Active concentration of Glu37Ser *Ec* MutY was determined by electrophoretic mobility shift experiments under conditions of [DNA] >> K_D (in this case [DNA] = 20 nM) where MutY:DNA binding proceeded via a 1:1 complex formation. Under these conditions, approximately 40% of the sample contained active binding Glu37Ser MutY.[5]

Binding Assays to measure K_D. Briefly, binding affinities were measured by EMSA wherein a reaction mix with the composition 5 pM ^{32}P radiolabeled 30 bp DNA substrate, 20 mM Tris-HCl pH 7.5, 1 mM EDTA, 100 mM NaCl, 0.1 mg/mL BSA, 1 mM DTT and 10% glycerol was prepared and 20 µl of the reaction mix was aliquoted into each of 14 microcentrifuge tubes and allowed to equilibrate at 25 °C. Meanwhile, serial dilutions of the enzyme (based on active binding concentration) are carried out in MutY dilution buffer (20 mM Tris-HCl pH 7.5, 10 mM EDTA, 20% glycerol) to give 13 different concentrations. To initiate the experiment, 20 μl of the highest enzyme concentration is added to 20 μl of DNA solution, mixed gently and then incubated at 25 °C for 30 min. This is repeated for each of the enzyme concentrations as well as the negative control. The reaction mixtures are then loaded onto a 6% nondenaturing

polyacrylamide gel (29:1 acrylamide:bisacrylamide ratio) and electrophoresed for 2 h at 4 °C. The dried gel is exposed to a storage phosphor screen overnight, and the gel is quantitated using ImageQuant. Fitting of the percent DNA bound to a single binding isotherm allows for determination of the K_D:

$$K_D = \frac{[MutY][DNA]}{[MutY.DNA]}$$

For each of the analogues varying ranges of enzyme concentrations (from 100 nM to 20 pM) were used to determine the enzyme concentration at which 50% of the DNA substrate was bound. However, it was found that even at enzyme concentrations as low as 20 pM and DNA concentrations of 5 pM, the DNA substrate was more than 80% bound, prompting us estimate K_D < 5 pM (limit of detection of the storage phosphor screens).

Glycosylase Assays to measure k_2 and k_3. Glycosylase assays were carried out either under conditions of single turnover (STO, 20 nM DNA, 40 nM active WT MutY) or multiple turnover (MTO, 20 nM DNA, 2 nM active WT MutY) to measure k_2 and k_3 respectively. Briefly, the reactions were carried out in 100 µl volumes in a mixture containing 20 nM radiolabeled 30 bp OG:Y carrying DNA substrate in 10 mM Tris-HCl pH 7.5, 10 mM EDTA, 20 mM NaCl and 0.1 mg/mL BSA equilibrated to 37 °C. The reaction was initiated by the addition of 40 nM WT MutY (for determination of k_2) or 2 nM WT MutY (for determination of k_3) . The contents of the tube were mixed by gentle pipetting, and, at each time point, 8 µl of the reaction mixture was quenched with 2 µl of 1.0 M NaOH, immediately incubated at 90 °C for 5 min, and then placed on ice. 10 µL of loading dye (80% formamide, 0.025% xylene cyanol, 0.025% bromophenol blue) is added to each sample prior to loading on a 15 % denaturing polyacrylamide gel (19:1 acrylamide:bisacrylamide) Resolution of the 14 nt product fragment hence formed from the 30 nt substrate by PAGE and visualization and quantitation of the bands by storage phosphor autoradiography enables determination of the rate constant k_2 by fitting the concentration of product to the following equation:

$$[P]_t = A_0\{1-\exp(-k_{obs}t)\},$$

where $k_{obs} = \frac{[E]_0 k_2}{K_D + [E]_0}$, where $[E]_0$ is initial enzyme concentration and k_{obs} is approximated to k_2 when $[E]_0 > K_D$

The rate of product release is determined by fitting the 14 nt product formation curves obtained under MTO conditions to the following equation:

$$[P]_t = A_0\{1\text{-}\exp(-k_{obs}t)\} + k_{ss}t$$

Where $k_{ss} = A_0 k_3$ and A_0 is the amplitude of the burst phase.

Experimental acid catalyzed depurination. Relative extents of acid catalyzed depurination were determined using a modified Maxam-Gilbert type sequencing reaction using a 30 mer ssDNA oligonucleotide carrying the adenine analogue (Y) at position 15 (cE30Y, Table S2). Briefly, the 5'-^{32}P labeled ssDNA strand (12 nM, 5% labeled) was incubated with calf thymus DNA (0.13 mg/mL), formic acid (11%) and piperidine (0.8 M) in a final volume of 32 µL for 30 min at 37°C. The reaction was quenched by the addition of 225 µL of cold stop solution (30 µg/mL calf thymus DNA, 1 mM EDTA pH 8.0, 0.3 M NaOAc pH 7.0) and further cooled on ice for 5 minutes. The DNA was ethanol precipitated and the pellet was completely dried. 100 µL of 1 M piperidine was added to the pellet and mixed, followed by incubation at 90°C for 30 min. The solution was then freeze-dried using a speed vac, and the pellet was resuspended in 20 µL of MilliQ water and mixed by vortexing. The resulting solution was freeze dried and resuspended in 20 µL of MilliQ water two more times prior to addition of 6 µL loading dye (80% formamide, 0.025% xylene cyanol, 0.025% bromophenol blue) loading the samples on a 20 % denaturing polyacrylamide gel (19:1 acrylamide:bisacrylamide ratio). Resolution of the fragments through PAGE, followed by visualization and quantitation of the bands through autoradiography revealed the relative extent of depurination of the analogues relative to an A (at position 24) on the same strand (Fig S4, Table S1).[6]

High resolution melt (HRM) analysis. The melting temperature (Tm) of an 11 bp duplex containing a centrally located OG:Y mispair was measured by incubating the duplex with EvaGreen DNA dye (Biotium Inc.) and monitoring its change in fluorescence while heating from 15°C to 80°C at a rate of 0.2°C s^{-1} using a qPCR (BioRad CFX Connect Real Time System).[2]

Overall cellular repair. MutY mediated cellular repair was measured using the bacterial cell assay previously described.[7,8] Briefly, substrate plasmids containing OG:Y mispairs (where Y is the A analogue) were created by ligating a duplex with the centrally located OG:Y pair and the appropriate sticky ends for ligation into double-digested pACYC177 (BamHI and PstI digested). The resultant reporter plasmids were transformed into XL1Blue *muty*$^+$ and JM101 *muty*$^-$ bacterial cell lines, amplified and then extracted by midiprep (Promega Wizard). Conversion to G:C was determined by BmtI digest and Sanger sequencing (Genewiz Inc). Overall repair defined as the normalized difference between percent G:C conversion in XL1Blue *muty*$^+$ and JM101 *muty*$^-$ was calculated using the following data and equations:

Column 1	**Column 2**	**Column 3**	**Column 4**	**Column 5**	**Column 6**	**Column 7**
Analogue	Mean difference in percent G:C in *muty*$^+$ and *muty*$^-$ cells (%)	Standard deviation	Maximum difference = mean + Standard deviation (%)	Minimum difference = mean – standard deviation (%)	Normalized value	Normalized standard deviation
OG:A	55	4	59	51	0.88	0.06
OG:P	47	12	59	35	0.75	0.19
OG:2OA	19	9	28	10	0.29	0.14
OG:6mA	12	9	21	3	0.18	0.14
OG:Z3	59	3	62	56	0.95	0.05
OG:2AP	21	13	34	8	0.32	0.21
OG:I	4	3	7	1	0.05	0.05
OG:ADA	24	6	30	18	0.37	0.09
OG:BA	31	3	34	28	0.49	0.04

Range = highest value from column 4 – lowest value from column 5

Range = 62 – 1 = 61

$$\text{Normalized values} = \frac{\text{mean difference from column 2 – lowest value from column 5}}{\text{Range}}$$

$$= \frac{\text{mean difference from column 2 – 1}}{61}$$

$$\text{Normalized standard deviation} = \frac{\text{Standard deviation from column 3}}{61}$$

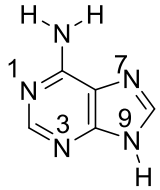
For example,

$$\text{Normalized value for OG:A} = \frac{55-1}{61} = 0.88$$

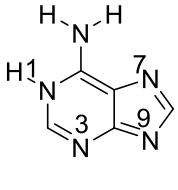
Normalized standard deviation for OG:A = $\frac{4}{61}$ = 0.06

Structures corresponding to neutral, deprotonated, and protonated species of adenine and adenine analogues studied in this paper

Adenine (A)



A-1



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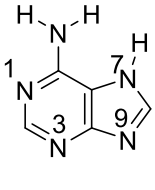

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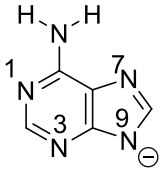

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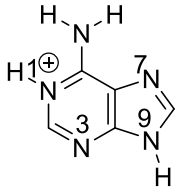

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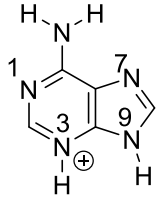

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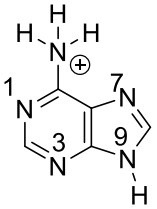

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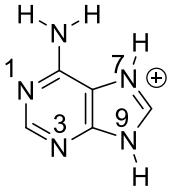

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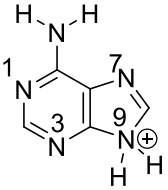

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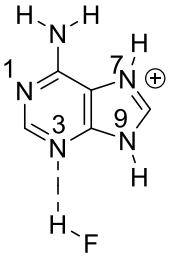

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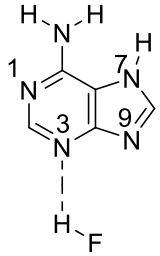

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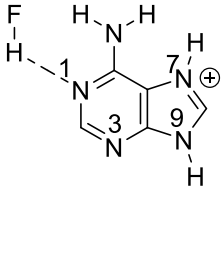

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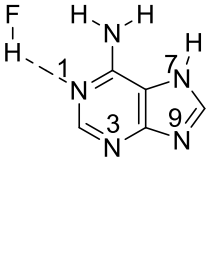

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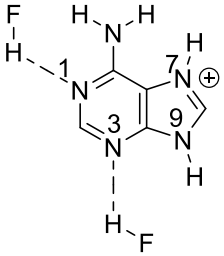

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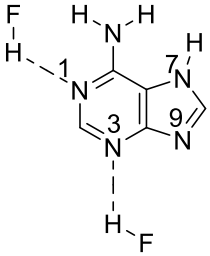
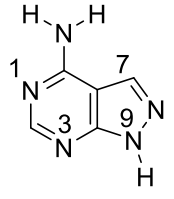
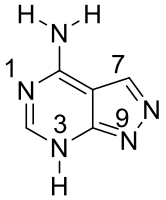


A-15

8-aza-7-deazaadenine (ADA)



ADA-1



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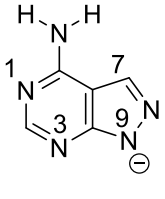

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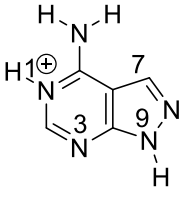

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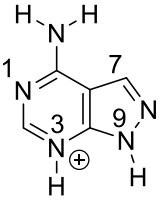

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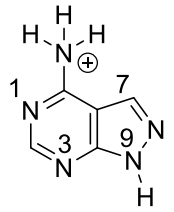

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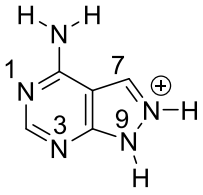

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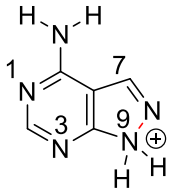
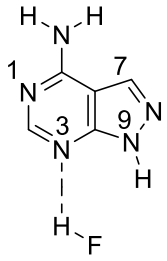


ADA-8

N^8-N^9 1.48655 Å



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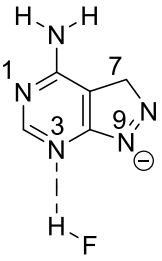

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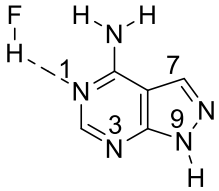

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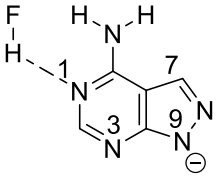

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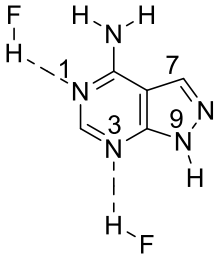

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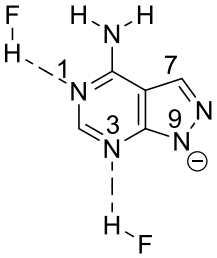
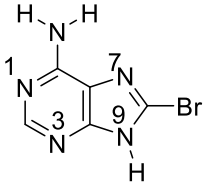


ADA-14

8-bromoadenine (BA)



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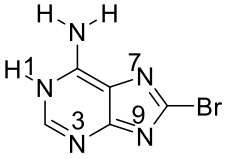

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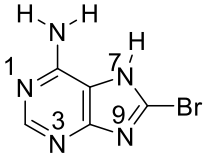

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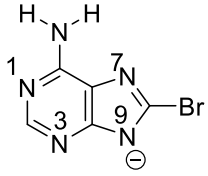

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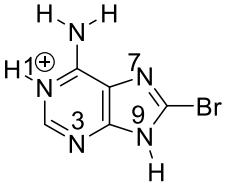

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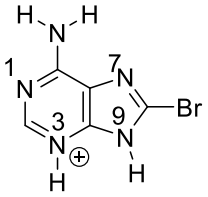

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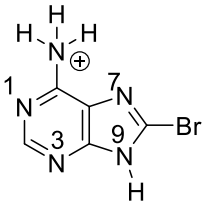

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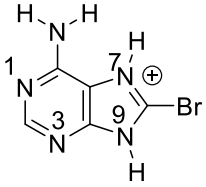

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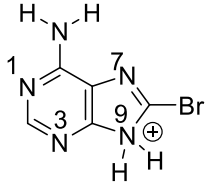

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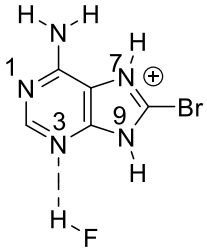

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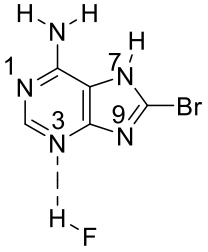

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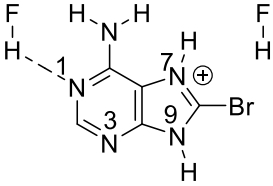

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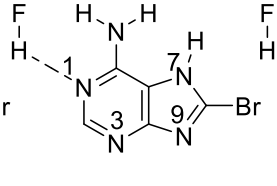

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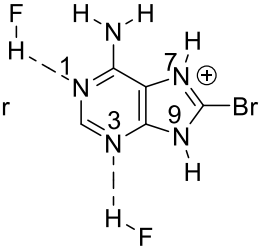

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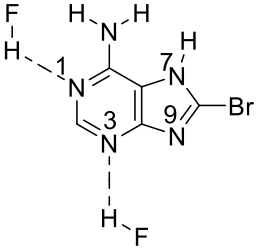
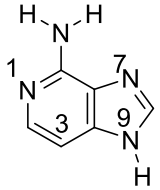
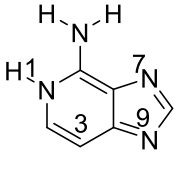


BA-15

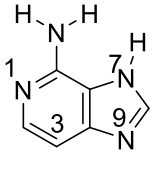
3-deazaadenine (Z3)



Z3-1



Z3-2



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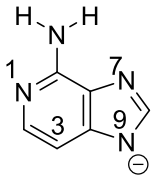

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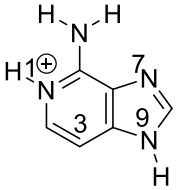

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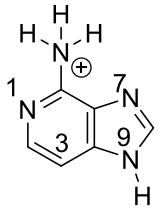
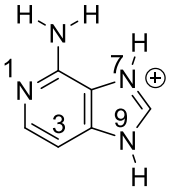
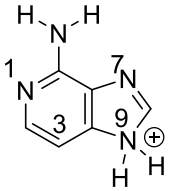


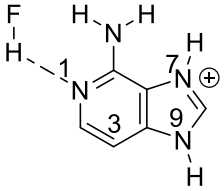
Z3-6



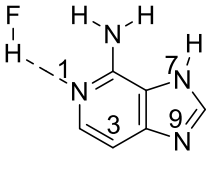
Z3-7



Z3-8

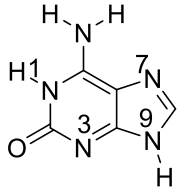


Z3-9

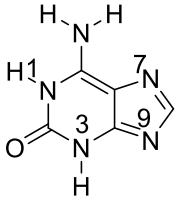


Z3-10

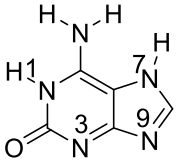
Isoguanine (2OA)



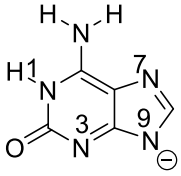
2OA-1



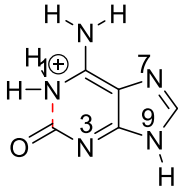
2OA-2



2OA-3

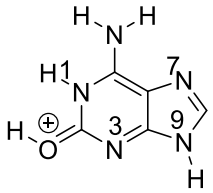


2OA-4

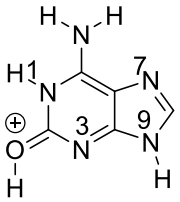


2OA-5

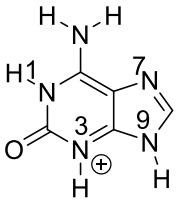
N^1-C^2 4.11706 Å



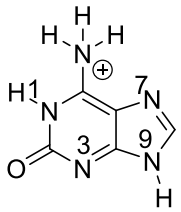
2OA-6



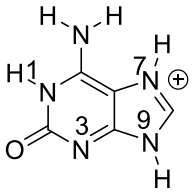
2OA-7



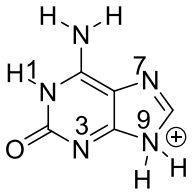
2OA-8



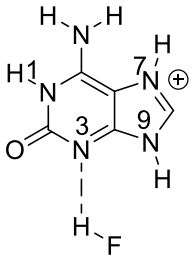
2OA-9



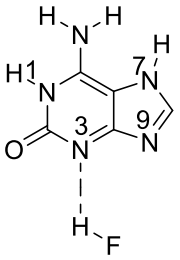
2OA-10



2OA-11

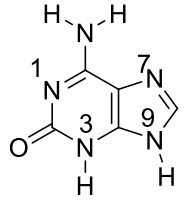


2OA-12

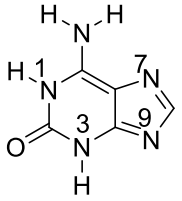


2OA-13

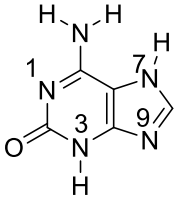
Isoguanine with cytosine-like face (2OA-cyto)



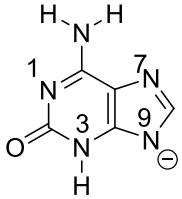
2OA-cyto-1



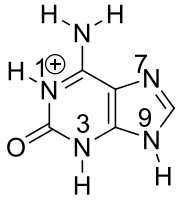
2OA-cyto-2



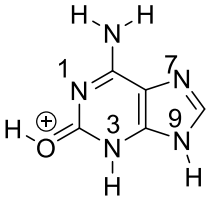
2OA-cyto-3



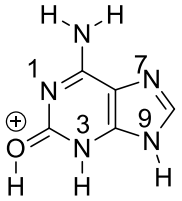
2OA-cyto-4



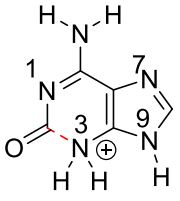
2OA-cyto-5



2OA-cyto-6

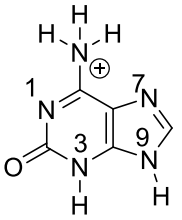


2OA-cyto-7

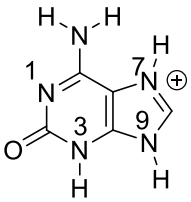


2OA-cyto-8

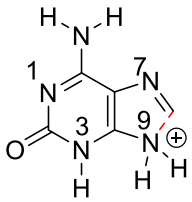
C^2-N^3 4.04895 Å



2OA-cyto-9

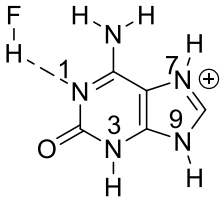


2OA-cyto-10

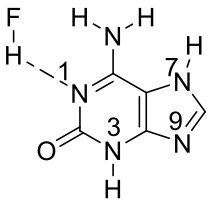


2OA-cyto-11

N^8-N^9 1.55980 Å

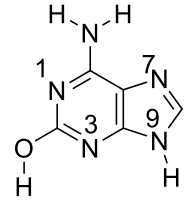


2OA-cyto-12

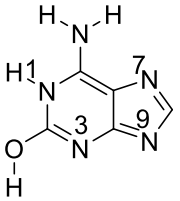


2OA-cyto-13

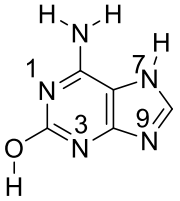
Isoguanine in enol form, with O2 hydrogen facing down (2OA-enol-d)



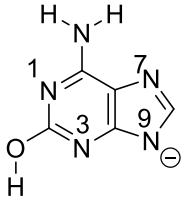
2OA-enol-d-1



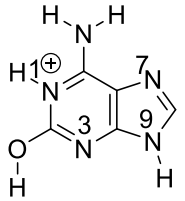
2OA-enol-d-2



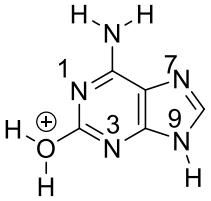
2OA-enol-d-3



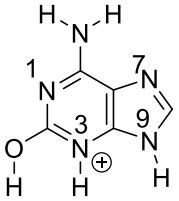
2OA-enol-d-4



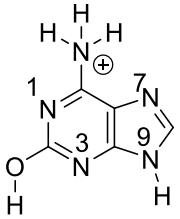
2OA-enol-d-5



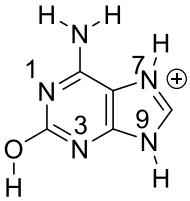
2OA-enol-d-6



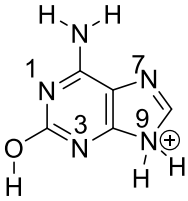
2OA-enol-d-7



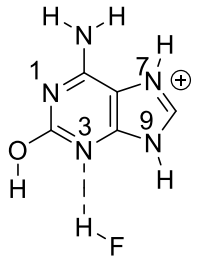
2OA-enol-d-8



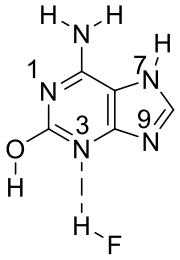
2OA-enol-d-9



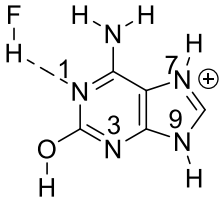
2OA-enol-d-10



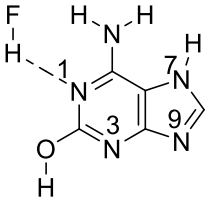
2OA-enol-d-11



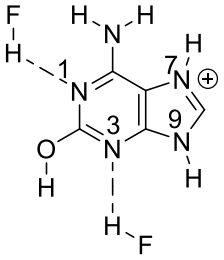
2OA-enol-d-12



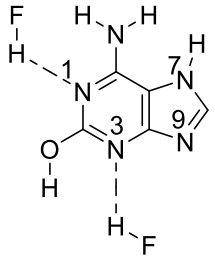
2OA-enol-d-13



2OA-enol-d-14

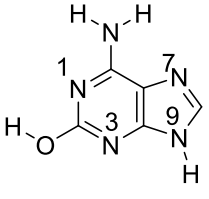


2OA-enol-d-15

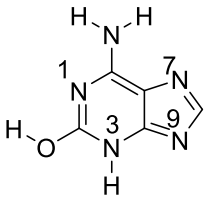


2OA-enol-d-16

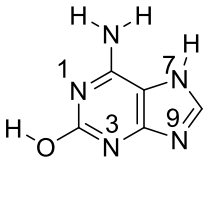
Isoguanine in enol form, with O2 hydrogen facing up (2OA-enol-u)



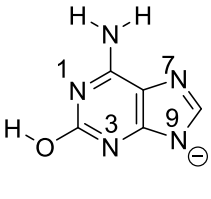
2OA-enol-u-1



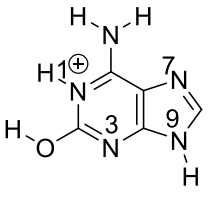
2OA-enol-u-2



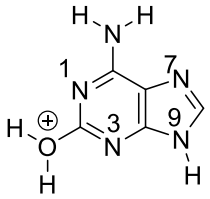
2OA-enol-u-3



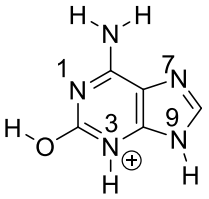
2OA-enol-u-4



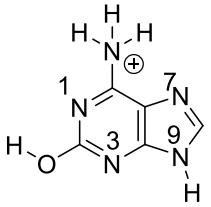
2OA-enol-u-5



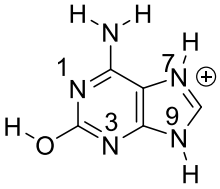
2OA-enol-u-6



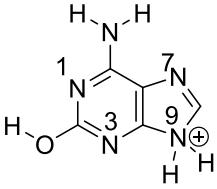
2OA-enol-u-7



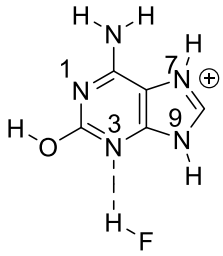
2OA-enol-u-8



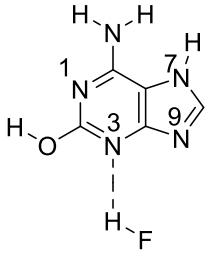
2OA-enol-u-9



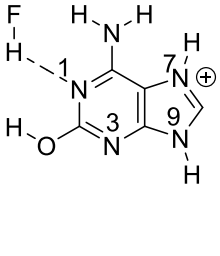
2OA-enol-u-10



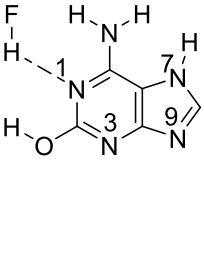
2OA-enol-u-11



2OA-enol-u-12



2OA-enol-u-13



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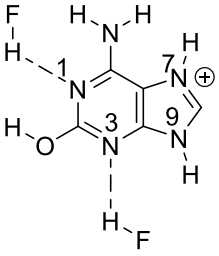
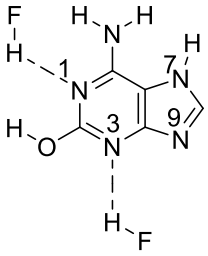
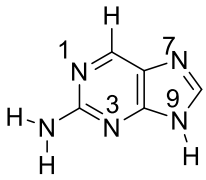


2OA-enol-u-15

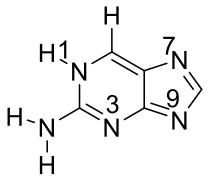


2OA-enol-u-16

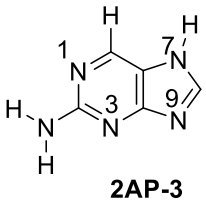
2-aminopurine (2AP)



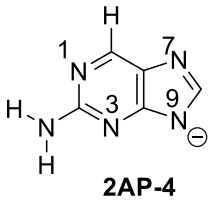
2AP-1



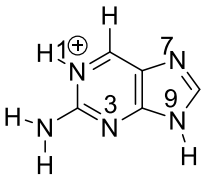
2AP-2



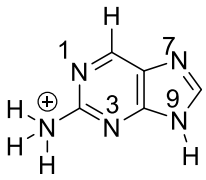
2AP-3



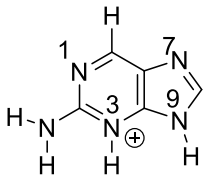
2AP-4



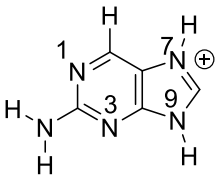
2AP-5



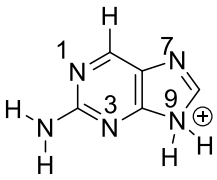
2AP-6



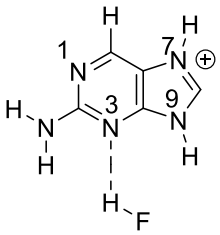
2AP-7



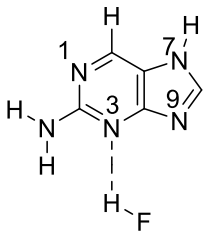
2AP-8



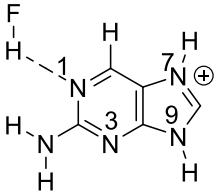
2AP-9



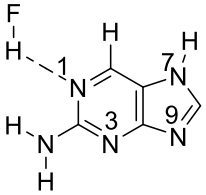
2AP-10



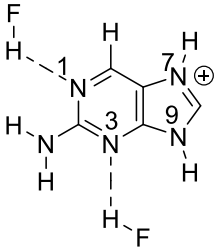
2AP-11



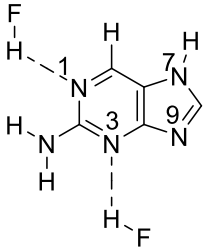
2AP-12



2AP-13

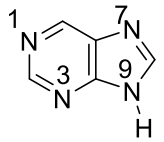


2AP-14

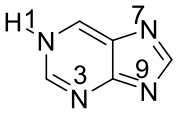


2AP-15

Purine (P)



P-1



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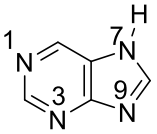
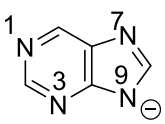
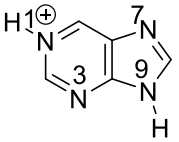


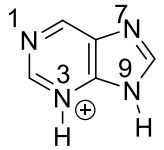
P-3



P-4



P-5



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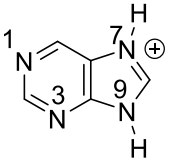
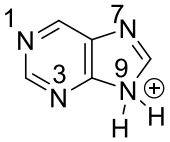
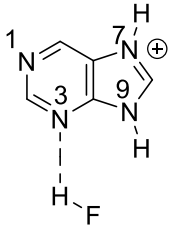


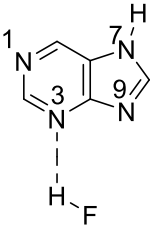
P-7



P-8



P-9



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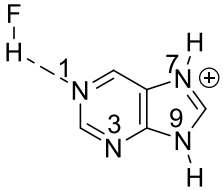
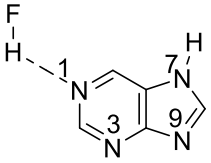


P-11



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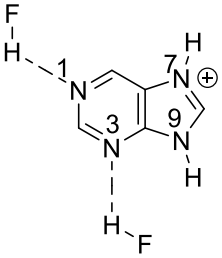

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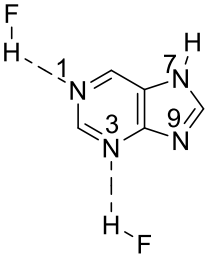
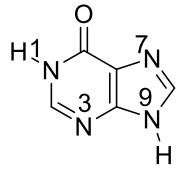
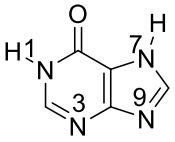


P-14

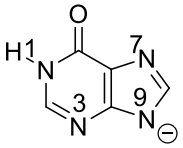
Hypoxanthine (I)



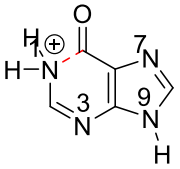
I-1



I-2

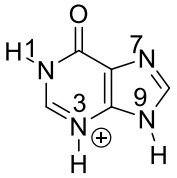


I-3

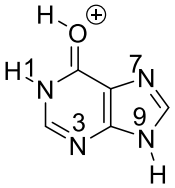


I-4

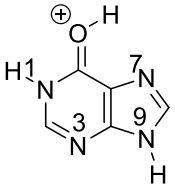
N^1-C^6 1.73025 Å



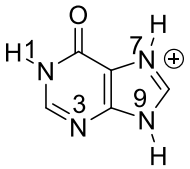
I-5



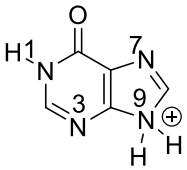
I-6



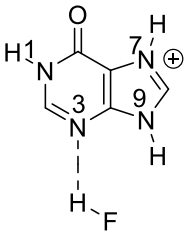
I-7



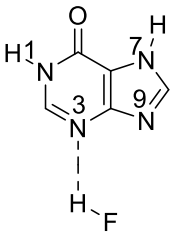
I-8



I-9

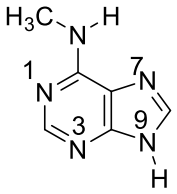


I-10

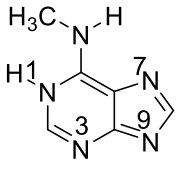


I-11

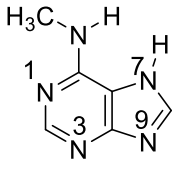
6-methyladenine, more stable (6mA)



6mA-1

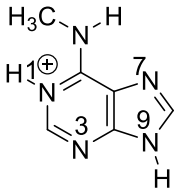


6mA-2

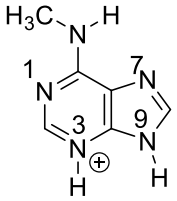


6mA-3

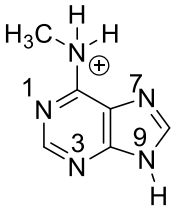
6mA-4



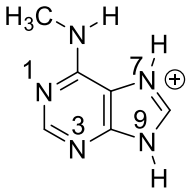
6mA-5



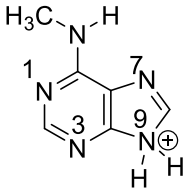
6mA-6



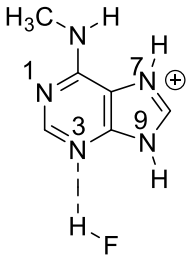
6mA-7



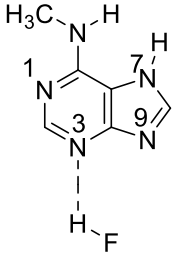
6mA-8



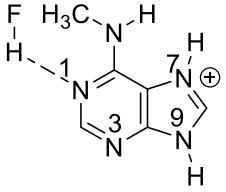
6mA-9



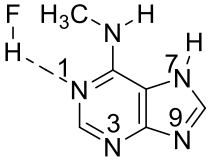
6mA-10



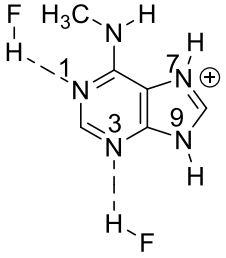
6mA-11



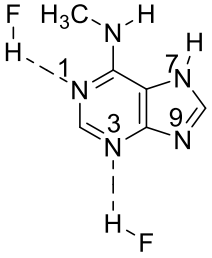
6mA-12



6mA-13

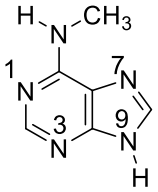


6mA-14

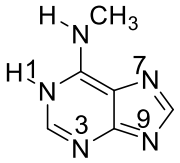


6mA-15

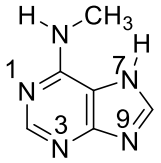
6-methyladenine, less stable (6mA_a)



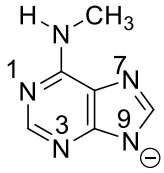
6mA_a-1



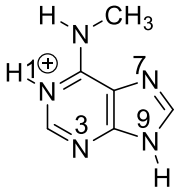
6mA_a-2



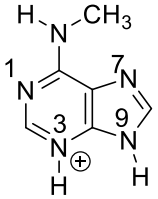
6mA_a-3



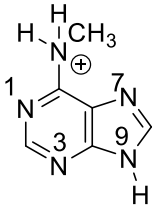
6mA_a-4



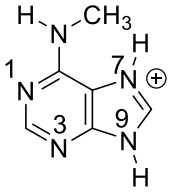
6mA_a-5



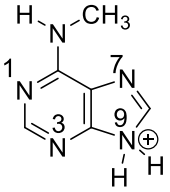
6mA_a-6



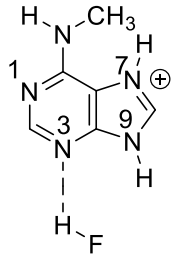
6mA_a-7



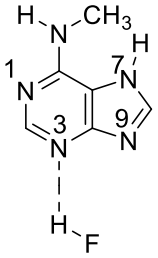
6mA_a-8



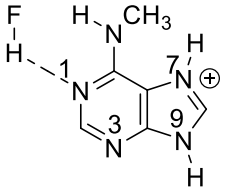
6mA_a-9



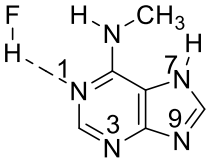
6mA_a-10



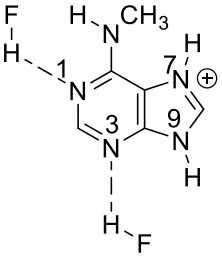
6mA_a-11



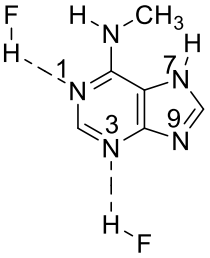
6mA_a-12



6mA_a-13



6mA_a-14



6mA_a-15

Cartesian coordinates and energies (in Hartree) for species of adenine (A)

N9H-amino A (A-1), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.339881191 A.U. after 1 cycles

Zero-point correction= 0.111957 (Hartree/Particle)
Thermal correction to Energy= 0.119331
Thermal correction to Enthalpy= 0.120275
Thermal correction to Gibbs Free Energy= 0.080084
Sum of electronic and zero-point Energies= -467.227924
Sum of electronic and thermal Energies= -467.220550
Sum of electronic and thermal Enthalpies= -467.219606
Sum of electronic and thermal Free Energies= -467.259797

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.881	28.910	84.588

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.711315	0.773997	-0.001931
2	6	0	-0.179627	-0.520661	-0.003380
3	6	0	1.229172	-0.609214	-0.002879
4	6	0	1.295074	1.702604	0.002598
5	6	0	-2.291834	-0.777562	0.002544
6	1	0	1.927526	2.586991	0.006698
7	1	0	-2.775138	1.317763	0.000977
8	1	0	-3.290892	-1.193726	0.005581
9	7	0	1.882703	-1.798044	-0.031675
10	7	0	-2.076904	0.586444	0.000429
11	7	0	1.948280	0.527537	0.003453
12	7	0	-0.023597	1.923342	-0.000397
13	7	0	-1.182303	-1.477617	0.000902
14	1	0	1.367862	-2.656923	0.098373
15	1	0	2.884563	-1.800724	0.097666

N1H-amino A (A-2), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.310080863 A.U. after 9 cycles

Zero-point correction= 0.111887 (Hartree/Particle)
Thermal correction to Energy= 0.119118
Thermal correction to Enthalpy= 0.120063
Thermal correction to Gibbs Free Energy= 0.080191
Sum of electronic and zero-point Energies= -467.198194
Sum of electronic and thermal Energies= -467.190962
Sum of electronic and thermal Enthalpies= -467.190018

```
Sum of electronic and thermal Free Energies=         -467.229890

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   74.748             28.726             83.918


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.811069   -0.802510    0.006760
     2          6           0       -0.254122    0.524937    0.011198
     3          6           0        1.117583    0.684292    0.003595
     4          6           0        1.234292   -1.736223   -0.004696
     5          6           0       -2.343511    0.645230   -0.007733
     6          1           0        1.927544   -2.572175   -0.011850
     7          1           0       -3.346790    1.056809   -0.015924
     8          7           0        1.773215    1.885542    0.065198
     9          7           0       -2.144635   -0.706675   -0.006558
    10          7           0        1.837971   -0.485323   -0.000199
    11          7           0       -0.046168   -1.937023   -0.003390
    12          7           0       -1.263968    1.443451   -0.001116
    13          1           0        1.157546    2.684820   -0.046351
    14          1           0        2.658862    1.981684   -0.417596
    15          1           0        2.848898   -0.445290    0.059431
---------------------------------------------------------------------
```

N1H-amino A (A-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

```
SCF Done:  E(RB3LYP) =  -467.358999118     A.U. after    1 cycles


Zero-point correction=                           0.111778 (Hartree/Particle)
Thermal correction to Energy=                    0.119222
Thermal correction to Enthalpy=                  0.120166
Thermal correction to Gibbs Free Energy=         0.079750
Sum of electronic and zero-point Energies=           -467.247221
Sum of electronic and thermal Energies=              -467.239777
Sum of electronic and thermal Enthalpies=            -467.238833
Sum of electronic and thermal Free Energies=         -467.279249

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   74.813             28.897             85.063


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.798954    0.785361   -0.000372
     2          6           0       -0.263261   -0.526640   -0.001337
     3          6           0        1.125634   -0.692030   -0.000759
     4          6           0        1.241666    1.723036    0.000701
```

5	6	0	-2.365912	-0.636554	0.001602
6	1	0	1.938096	2.553466	0.001416
7	1	0	-3.371192	-1.041292	0.003417
8	7	0	1.780846	-1.859911	-0.028198
9	7	0	-2.149522	0.707897	0.001532
10	7	0	1.832548	0.482219	0.002565
11	7	0	-0.045228	1.929936	-0.000847
12	7	0	-1.289550	-1.439200	-0.000326
13	1	0	1.257884	-2.720810	0.076263
14	1	0	2.786677	-1.902210	0.092707
15	1	0	2.849838	0.445205	0.004102

N1H-amino A (A-2), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water) RADII=UAKS

SCF Done: E(RB3LYP) = -467.382517390 A.U. after 1 cycles

Zero-point correction= 0.105688 (Hartree/Particle)
Thermal correction to Energy= 0.113092
Thermal correction to Enthalpy= 0.114036
Thermal correction to Gibbs Free Energy= 0.073715
Sum of electronic and zero-point Energies= -467.276829
Sum of electronic and thermal Energies= -467.269425
Sum of electronic and thermal Enthalpies= -467.268481
Sum of electronic and thermal Free Energies= -467.308803

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.966	28.880	84.864

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.799180	0.781796	-0.000015
2	6	0	-0.265565	-0.527159	-0.000051
3	6	0	1.128621	-0.692194	-0.000045
4	6	0	1.240922	1.718333	0.000048
5	6	0	-2.373269	-0.636013	0.000076
6	1	0	1.937821	2.556437	0.000128
7	1	0	-3.382951	-1.040959	0.000143
8	7	0	1.788415	-1.851980	0.000026
9	7	0	-2.153260	0.706515	-0.000111
10	7	0	1.832068	0.483805	-0.000030
11	7	0	-0.048469	1.928487	0.000042
12	7	0	-1.295716	-1.438550	0.000069
13	1	0	1.264531	-2.740612	-0.000663
14	1	0	2.821314	-1.880501	0.000651
15	1	0	2.908838	0.439121	-0.000302

N7H-amino A (A-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.326751813   A.U. after   9 cycles

Zero-point correction=   0.111947 (Hartree/Particle)
Thermal correction to Energy=   0.119170
Thermal correction to Enthalpy=   0.120114
Thermal correction to Gibbs Free Energy=   0.080274
Sum of electronic and zero-point Energies=   -467.214805
Sum of electronic and thermal Energies=   -467.207582
Sum of electronic and thermal Enthalpies=   -467.206637
Sum of electronic and thermal Free Energies=   -467.246477

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.780	28.715	83.850

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.739235	-0.811047	0.016319
2	6	0	0.183183	0.483407	-0.006579
3	6	0	-1.213761	0.615161	-0.003496
4	6	0	-1.313442	-1.692655	-0.011379
5	6	0	2.387228	0.544242	-0.007532
6	1	0	-1.965678	-2.562414	-0.024340
7	1	0	3.382259	0.971296	-0.021676
8	7	0	-1.871995	1.830170	-0.051364
9	7	0	2.121156	-0.738791	0.020696
10	7	0	-1.948596	-0.500864	-0.014528
11	7	0	-0.006347	-1.930280	0.015778
12	7	0	1.268813	1.346071	-0.013001
13	1	0	-1.445675	2.611794	0.430794
14	1	0	-2.869754	1.750580	0.114102
15	1	0	1.262971	2.349962	-0.125940

N9-deprotonated N9H-amino A (A-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -466.795425309   A.U. after   9 cycles

Zero-point correction=   0.099276 (Hartree/Particle)
Thermal correction to Energy=   0.106040
Thermal correction to Enthalpy=   0.106984
Thermal correction to Gibbs Free Energy=   0.067928
Sum of electronic and zero-point Energies=   -466.696149
Sum of electronic and thermal Energies=   -466.689385
Sum of electronic and thermal Enthalpies=   -466.688441
Sum of electronic and thermal Free Energies=   -466.727498

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

Total	66.541	26.769	82.201

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.785120	0.796719	-0.006708
2	6	0	-0.217924	-0.511297	-0.020848
3	6	0	1.177442	-0.608823	-0.018512
4	6	0	1.276654	1.690914	0.007395
5	6	0	-2.314835	-0.662918	0.010794
6	1	0	1.926498	2.566968	0.021384
7	1	0	-3.313301	-1.094683	0.025480
8	7	0	1.829308	-1.842488	-0.074095
9	7	0	-2.143267	0.682806	0.010313
10	7	0	1.930248	0.502767	0.002801
11	7	0	-0.030334	1.928187	0.001562
12	7	0	-1.221407	-1.452276	-0.006343
13	1	0	1.257019	-2.612462	0.254744
14	1	0	2.760649	-1.820362	0.326004

N1-protonated N9H-amino A (A-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.707533506 A.U. after 1 cycles

Zero-point correction=	0.125672 (Hartree/Particle)
Thermal correction to Energy=	0.132939
Thermal correction to Enthalpy=	0.133884
Thermal correction to Gibbs Free Energy=	0.094027
Sum of electronic and zero-point Energies=	-467.581861
Sum of electronic and thermal Energies=	-467.574594
Sum of electronic and thermal Enthalpies=	-467.573650
Sum of electronic and thermal Free Energies=	-467.613507

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.421	29.524	83.886

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.733770	0.779961	-0.000075
2	6	0	-0.221118	-0.525393	-0.000092
3	6	0	1.175479	-0.684937	0.000013
4	6	0	1.262536	1.743506	-0.000022
5	6	0	-2.325453	-0.746873	-0.000129
6	1	0	1.942187	2.589409	0.000109
7	1	0	-2.779629	1.356569	0.000488
8	1	0	-3.330261	-1.148617	-0.000160
9	7	0	1.793530	-1.865420	0.000232

10	7	0	-2.086675	0.615054	0.000180
11	7	0	1.870023	0.498415	-0.000046
12	7	0	-0.023559	1.929813	0.000069
13	7	0	-1.223655	-1.462277	-0.000135
14	1	0	1.227951	-2.708066	0.000217
15	1	0	2.799621	-1.975582	0.000094
16	1	0	2.886439	0.479604	-0.001015

N1-protonated N9H-amino A (A-5), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -467.816841343 A.U. after 1 cycles

Zero-point correction= 0.124905 (Hartree/Particle)
Thermal correction to Energy= 0.132466
Thermal correction to Enthalpy= 0.133410
Thermal correction to Gibbs Free Energy= 0.092886
Sum of electronic and zero-point Energies= -467.691936
Sum of electronic and thermal Energies= -467.684375
Sum of electronic and thermal Enthalpies= -467.683431
Sum of electronic and thermal Free Energies= -467.723956

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.124	30.043	85.291

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.739412	0.764497	-0.000073
2	6	0	0.221525	-0.534458	-0.000019
3	6	0	-1.179499	-0.681915	0.000060
4	6	0	-1.254698	1.735834	-0.000016
5	6	0	2.334639	-0.747920	-0.000327
6	1	0	-1.934882	2.578998	0.000028
7	1	0	2.793909	1.338101	0.000346
8	1	0	3.341846	-1.139985	-0.000380
9	7	0	-1.835719	-1.833815	0.000062
10	7	0	2.093182	0.602425	0.000168
11	7	0	-1.859993	0.507159	0.000048
12	7	0	0.038003	1.924996	-0.000047
13	7	0	1.233428	-1.472355	0.000003
14	1	0	-1.322314	-2.708383	0.000207
15	1	0	-2.849714	-1.873003	0.000240
16	1	0	-2.879420	0.489174	0.000176

N1-protonated N9H-amino A (A-5), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -467.850299859 A.U. after 8 cycles

```
Zero-point correction=                           0.114726 (Hartree/Particle)
Thermal correction to Energy=                    0.122079
Thermal correction to Enthalpy=                  0.123024
Thermal correction to Gibbs Free Energy=         0.083013
Sum of electronic and zero-point Energies=           -467.735574
Sum of electronic and thermal Energies=              -467.728220
Sum of electronic and thermal Enthalpies=            -467.727276
Sum of electronic and thermal Free Energies=         -467.767286

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   76.606             29.875             84.209


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.749359    0.755179   -0.000024
     2          6           0        0.219230   -0.539877   -0.000012
     3          6           0       -1.185929   -0.675469    0.000044
     4          6           0       -1.241794    1.737352    0.000059
     5          6           0        2.333846   -0.758362   -0.000099
     6          1           0       -1.917014    2.593466    0.000089
     7          1           0        2.843368    1.365903   -0.000103
     8          1           0        3.343940   -1.161339   -0.000142
     9          7           0       -1.860606   -1.815099    0.000065
    10          7           0        2.101826    0.589476   -0.000080
    11          7           0       -1.856153    0.519556    0.000076
    12          7           0        0.054803    1.921325    0.000010
    13          7           0        1.228004   -1.482343   -0.000059
    14          1           0       -1.351773   -2.715900    0.000041
    15          1           0       -2.896658   -1.824382    0.000106
    16          1           0       -2.945256    0.498903    0.000118
---------------------------------------------------------------------
```

N3-protonated N9H-amino A (A-6), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -467.705171440     A.U. after    1 cycles


Zero-point correction=                           0.125681 (Hartree/Particle)
Thermal correction to Energy=                    0.132912
Thermal correction to Enthalpy=                  0.133856
Thermal correction to Gibbs Free Energy=         0.094013
Sum of electronic and zero-point Energies=           -467.579491
Sum of electronic and thermal Energies=              -467.572260
Sum of electronic and thermal Enthalpies=            -467.571315
Sum of electronic and thermal Free Energies=         -467.611158

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   83.403             29.464             83.856
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.733773	0.747498	-0.000171
2	6	0	-0.204310	-0.539634	-0.000145
3	6	0	1.207473	-0.682026	-0.000198
4	6	0	1.423692	1.623102	0.000148
5	6	0	-2.318172	-0.774677	-0.000069
6	1	0	2.050386	2.509983	0.000286
7	1	0	-2.795508	1.323510	-0.000413
8	1	0	-3.324724	-1.171621	0.000001
9	7	0	1.816709	-1.859877	-0.000109
10	7	0	-2.085358	0.599936	0.000071
11	7	0	1.981460	0.446153	0.000123
12	7	0	0.072866	1.848496	0.000066
13	7	0	-1.215424	-1.474717	0.000355
14	1	0	1.283279	-2.721950	-0.000176
15	1	0	2.829670	-1.904961	0.000095
16	1	0	-0.284330	2.799521	-0.000725

N6-protonated N9H-amino A (A-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.673955192 A.U. after 1 cycles

Zero-point correction= 0.126410 (Hartree/Particle)
Thermal correction to Energy= 0.133893
Thermal correction to Enthalpy= 0.134837
Thermal correction to Gibbs Free Energy= 0.093920
Sum of electronic and zero-point Energies= -467.547545
Sum of electronic and thermal Energies= -467.540063
Sum of electronic and thermal Enthalpies= -467.539118
Sum of electronic and thermal Free Energies= -467.580036

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	84.019	28.548	86.117

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.813550	0.755947	-0.000055
2	6	0	0.176568	-0.513430	0.000060
3	6	0	-1.200747	-0.428220	0.000011
4	6	0	-1.135492	1.843363	0.000004
5	6	0	2.250085	-0.925224	-0.000083
6	1	0	-1.694949	2.772376	-0.000214
7	1	0	2.918261	1.114188	0.000457
8	1	0	3.211255	-1.423471	-0.000091

9	7	0	-2.024780	-1.675015	0.000085
10	7	0	2.151370	0.449915	0.000217
11	7	0	-1.865766	0.703434	-0.000050
12	7	0	0.199169	1.930717	-0.000074
13	7	0	1.086836	-1.542546	-0.000215
14	1	0	-1.415415	-2.506812	-0.000377
15	1	0	-2.635844	-1.708021	-0.827916
16	1	0	-2.634889	-1.708410	0.828776

N7-protonated N9H-amino A (A-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.694263079 A.U. after 1 cycles

Zero-point correction= 0.125068 (Hartree/Particle)
Thermal correction to Energy= 0.132627
Thermal correction to Enthalpy= 0.133572
Thermal correction to Gibbs Free Energy= 0.092968
Sum of electronic and zero-point Energies= -467.569195
Sum of electronic and thermal Energies= -467.561636
Sum of electronic and thermal Enthalpies= -467.560692
Sum of electronic and thermal Free Energies= -467.601295

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.225	29.925	85.458

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.675868	-0.784752	-0.000316
2	6	0	0.143876	0.507532	-0.000513
3	6	0	-1.273438	0.614224	-0.000030
4	6	0	-1.321149	-1.712961	0.000120
5	6	0	2.366777	0.669124	0.000278
6	1	0	-1.951072	-2.597344	0.000288
7	1	0	2.731140	-1.399423	0.000448
8	1	0	3.365216	1.083473	0.000565
9	7	0	-1.968653	1.766607	0.000044
10	7	0	2.063470	-0.632886	-0.000007
11	7	0	-1.961362	-0.538300	0.000204
12	7	0	0.004169	-1.924182	-0.000122
13	7	0	1.235987	1.381171	0.000205
14	1	0	-1.549056	2.684275	-0.000316
15	1	0	-2.980693	1.707975	0.000529
16	1	0	1.217598	2.395173	-0.001016

N9-protonated N9H-amino A (A-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.635757228 A.U. after 2 cycles

```
Zero-point correction=                           0.124307 (Hartree/Particle)
Thermal correction to Energy=                    0.131696
Thermal correction to Enthalpy=                  0.132640
Thermal correction to Gibbs Free Energy=         0.092459
Sum of electronic and zero-point Energies=           -467.511451
Sum of electronic and thermal Energies=              -467.504061
Sum of electronic and thermal Enthalpies=            -467.503117
Sum of electronic and thermal Free Energies=         -467.543299

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   82.640             29.759             84.569


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.639933    0.762568    0.000090
     2          6           0       -0.134577   -0.523297   -0.000140
     3          6           0        1.280850   -0.617518    0.000103
     4          6           0        1.337514    1.706548    0.000073
     5          6           0       -2.271786   -0.915625    0.000070
     6          1           0        1.946593    2.605218   -0.000183
     7          1           0       -2.559795    1.046820    0.827207
     8          1           0       -3.268297   -1.339510    0.000322
     9          7           0        1.959035   -1.767349   -0.000120
    10          7           0       -2.127334    0.608439   -0.000319
    11          7           0        1.977443    0.549216   -0.000271
    12          7           0       -0.014411    1.904243    0.000450
    13          7           0       -1.145944   -1.498467    0.000428
    14          1           0        1.493671   -2.665741   -0.000398
    15          1           0        2.972216   -1.740415    0.000327
    16          1           0       -2.558313    1.044994   -0.829625
---------------------------------------------------------------------
```

N7-protonated N9H-amino A with HF hydrogen-bonded to N3 (A-10), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -568.156135659     A.U. after    1 cycles


Zero-point correction=                           0.137725 (Hartree/Particle)
Thermal correction to Energy=                    0.147240
Thermal correction to Enthalpy=                  0.148184
Thermal correction to Gibbs Free Energy=         0.102819
Sum of electronic and zero-point Energies=           -568.018411
Sum of electronic and thermal Energies=              -568.008896
Sum of electronic and thermal Enthalpies=            -568.007952
Sum of electronic and thermal Free Energies=         -568.053317

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   92.394             36.455             95.479
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.553786	0.004839	0.000011
2	6	0	-0.702999	0.605515	-0.000017
3	6	0	-1.828776	-0.264436	-0.000014
4	6	0	-0.316630	-2.036102	0.000040
5	6	0	0.854810	2.200415	-0.000087
6	1	0	-0.192244	-3.114617	0.000073
7	1	0	2.502456	0.839952	0.000071
8	1	0	1.326681	3.173258	-0.000129
9	7	0	-3.113803	0.124841	-0.000049
10	7	0	1.491939	1.029022	0.000021
11	7	0	-1.571054	-1.584565	0.000017
12	7	0	0.809062	-1.302311	0.000042
13	7	0	-0.466982	1.984270	-0.000062
14	1	0	-3.415668	1.088096	-0.000073
15	1	0	-3.827684	-0.595451	-0.000046
16	1	0	-1.153667	2.730450	-0.000068
17	1	0	2.622787	-1.393217	0.000073
18	9	0	3.414672	-0.838740	0.000079

N7H-amino A with HF hydrogen-bonded to N3 (A-11), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -567.792258385 A.U. after 1 cycles

Zero-point correction= 0.124280 (Hartree/Particle)
Thermal correction to Energy= 0.133860
Thermal correction to Enthalpy= 0.134804
Thermal correction to Gibbs Free Energy= 0.088257
Sum of electronic and zero-point Energies= -567.667979
Sum of electronic and thermal Energies= -567.658398
Sum of electronic and thermal Enthalpies= -567.657454
Sum of electronic and thermal Free Energies= -567.704002

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.998	35.519	97.968

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.395421	0.594072	0.004940
2	6	0	-0.986013	0.326970	-0.004486
3	6	0	-1.416900	-1.009820	0.000079
4	6	0	0.811613	-1.618049	-0.024642
5	6	0	-0.566447	2.491927	-0.007025
6	1	0	1.527172	-2.435349	-0.041215

7	1	0	-0.764722	3.556225	-0.017052
8	7	0	-2.735765	-1.394619	-0.034063
9	7	0	0.629113	1.951419	0.007782
10	7	0	-0.484178	-1.971238	-0.018727
11	7	0	1.319824	-0.386452	-0.003244
12	7	0	-1.590367	1.574943	-0.005736
13	1	0	-3.429973	-0.792189	0.387832
14	1	0	-2.885513	-2.384646	0.125170
15	1	0	-2.574022	1.789649	-0.090219
16	1	0	2.998705	-0.229216	0.011477
17	9	0	3.970215	-0.292605	0.020970

N7-protonated N9H-amino A with HF hydrogen-bonded to N1 (A-12)

SCF Done: E(RB3LYP) = -568.151972920 A.U. after 8 cycles

Zero-point correction= 0.138074 (Hartree/Particle)
Thermal correction to Energy= 0.147489
Thermal correction to Enthalpy= 0.148434
Thermal correction to Gibbs Free Energy= 0.103075
Sum of electronic and zero-point Energies= -568.013899
Sum of electronic and thermal Energies= -568.004483
Sum of electronic and thermal Enthalpies= -568.003539
Sum of electronic and thermal Free Energies= -568.048898

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.551	36.131	95.465

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.262251	-0.751526	0.000000
2	6	0	0.648296	0.501415	0.000000
3	6	0	-0.774134	0.529657	-0.000000
4	6	0	-0.664900	-1.815723	-0.000000
5	6	0	2.853299	0.809045	0.000000
6	1	0	-1.238306	-2.737713	-0.000000
7	1	0	3.822529	1.288134	0.000000
8	7	0	-1.535489	1.629814	-0.000000
9	7	0	2.635555	-0.510532	0.000000
10	7	0	-1.380336	-0.680779	-0.000000
11	7	0	0.665969	-1.935329	-0.000000
12	7	0	1.678183	1.444925	0.000000
13	1	0	-1.159968	2.566798	0.000000
14	1	0	-2.552640	1.512582	-0.000000
15	1	0	1.592398	2.455909	-0.000000
16	1	0	-3.137493	-0.450453	0.000000
17	9	0	-3.897191	0.146989	0.000000
18	1	0	3.352149	-1.232062	0.000000

N7H-amino A with HF hydrogen-bonded to N1 (A-13)

SCF Done: E(RB3LYP) = -567.794770408 A.U. after 1 cycles

Zero-point correction= 0.124270 (Hartree/Particle)
Thermal correction to Energy= 0.133592
Thermal correction to Enthalpy= 0.134537
Thermal correction to Gibbs Free Energy= 0.089279
Sum of electronic and zero-point Energies= -567.670500
Sum of electronic and thermal Energies= -567.661178
Sum of electronic and thermal Enthalpies= -567.660234
Sum of electronic and thermal Free Energies= -567.705491

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.831	34.985	95.252

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.306252	-0.783478	0.015696
2	6	0	0.696111	0.485722	-0.010245
3	6	0	-0.705242	0.569870	-0.033558
4	6	0	-0.697425	-1.767594	-0.038070
5	6	0	2.893173	0.640459	0.025700
6	1	0	-1.318045	-2.659329	-0.056246
7	1	0	3.869311	1.108888	0.032157
8	7	0	-1.419195	1.733432	-0.089329
9	7	0	2.680022	-0.653627	0.041618
10	7	0	-1.377986	-0.596704	-0.052249
11	7	0	0.612312	-1.939489	0.002066
12	7	0	1.742779	1.392870	0.002232
13	1	0	-1.006628	2.584550	0.264499
14	1	0	-2.428093	1.648293	0.020427
15	1	0	1.697708	2.399081	-0.078231
16	1	0	-2.947585	-0.359468	0.012623
17	9	0	-3.832156	0.094748	0.079695

N7-protonated N9H-amino A with HF hydrogen-bonded to N1 and N3 (A-14)

SCF Done: E(RB3LYP) = -668.612927952 A.U. after 9 cycles

Zero-point correction= 0.150535 (Hartree/Particle)
Thermal correction to Energy= 0.162044
Thermal correction to Enthalpy= 0.162988
Thermal correction to Gibbs Free Energy= 0.112543
Sum of electronic and zero-point Energies= -668.462393
Sum of electronic and thermal Energies= -668.450884

```
Sum of electronic and thermal Enthalpies=           -668.449940
Sum of electronic and thermal Free Energies=        -668.500385

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  101.684             42.927           106.170


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.023137    0.074881   -0.000000
     2          6           0       -0.043200   -0.912526   -0.000001
     3          6           0        1.315262   -0.485544   -0.000001
     4          6           0        0.476258    1.708375   -0.000001
     5          6           0       -2.043782   -1.891209    0.000001
     6          1           0        0.725128    2.765084   -0.000001
     7          1           0       -3.138668   -0.055586    0.000001
     8          1           0       -2.815063   -2.649180    0.000001
     9          7           0        2.385576   -1.283685   -0.000001
    10          7           0       -2.249986   -0.573288    0.000001
    11          7           0        1.507703    0.857390   -0.000002
    12          7           0       -0.824409    1.394655   -0.000000
    13          7           0       -0.726263   -2.131170   -0.000000
    14          1           0        2.327458   -2.291856    0.000000
    15          1           0        3.313367   -0.849045   -0.000000
    16          1           0       -0.329164   -3.064707   -0.000000
    17          1           0        3.269503    1.198590    0.000001
    18          1           0       -2.531724    2.100400    0.000000
    19          9           0        4.169262    0.852104    0.000002
    20          9           0       -3.453438    1.818465    0.000001
---------------------------------------------------------------------
```

N7H-amino A with HF hydrogen-bonded to N1 and N3 (A-15), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -668.258262315     A.U. after    9 cycles


Zero-point correction=                           0.136542 (Hartree/Particle)
Thermal correction to Energy=                    0.148346
Thermal correction to Enthalpy=                  0.149291
Thermal correction to Gibbs Free Energy=         0.097005
Sum of electronic and zero-point Energies=           -668.121720
Sum of electronic and thermal Energies=              -668.109916
Sum of electronic and thermal Enthalpies=            -668.108972
Sum of electronic and thermal Free Energies=         -668.161258

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   93.089             42.035           110.045


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	-1.156066	-0.316065	0.006587
2	6	0	0.002476	-1.112874	-0.006964
3	6	0	1.263788	-0.492047	-0.024166
4	6	0	0.111934	1.541316	-0.035567
5	6	0	-1.832835	-2.331857	0.019860
6	1	0	0.199025	2.623738	-0.050770
7	1	0	-2.452551	-3.219430	0.026716
8	7	0	2.455876	-1.140274	-0.061179
9	7	0	-2.285142	-1.099173	0.025569
10	7	0	1.273018	0.858785	-0.042040
11	7	0	-1.112339	1.034322	-0.007592
12	7	0	-0.462280	-2.417827	0.005421
13	1	0	2.522796	-2.116304	0.184266
14	1	0	3.300105	-0.576728	0.022135
15	1	0	0.073322	-3.273286	-0.044614
16	1	0	2.788313	1.424437	0.008793
17	1	0	-2.420895	2.127886	0.005539
18	9	0	3.776799	1.423311	0.061386
19	9	0	-3.046780	2.868690	0.010634

Cartesian coordinates and energies (in Hartree) for species of 8-aza-7-deazaadenine (ADA)

N9H-amino ADA (ADA-1), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.315657706 A.U. after 9 cycles

Zero-point correction= 0.112036 (Hartree/Particle)
Thermal correction to Energy= 0.119329
Thermal correction to Enthalpy= 0.120273
Thermal correction to Gibbs Free Energy= 0.080276
Sum of electronic and zero-point Energies= -467.203622
Sum of electronic and thermal Energies= -467.196329
Sum of electronic and thermal Enthalpies= -467.195385
Sum of electronic and thermal Free Energies= -467.235382

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.880	28.849	84.182

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.722068	-0.743419	0.003305
2	6	0	0.162329	0.551658	-0.003919
3	6	0	-1.254618	0.592374	-0.003278
4	6	0	-1.269294	-1.716866	-0.001412
5	1	0	-1.884087	-2.613813	-0.001996
6	1	0	2.786205	-1.276892	0.007969

7	7	0	-1.963924	1.755311	-0.038013
8	7	0	2.069328	-0.565242	0.006531
9	7	0	-1.950096	-0.553776	-0.001695
10	7	0	0.048179	-1.906378	0.003915
11	1	0	-1.518674	2.632392	0.187897
12	1	0	-2.962042	1.687470	0.111929
13	7	0	2.421950	0.751282	-0.000891
14	6	0	1.286334	1.431141	-0.007336
15	1	0	1.319616	2.513129	-0.018881

N3H-amino ADA (ADA-2), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.288536803 A.U. after 1 cycles

Zero-point correction= 0.111045 (Hartree/Particle)
Thermal correction to Energy= 0.118601
Thermal correction to Enthalpy= 0.119545
Thermal correction to Gibbs Free Energy= 0.078808
Sum of electronic and zero-point Energies= -467.177492
Sum of electronic and thermal Energies= -467.169936
Sum of electronic and thermal Enthalpies= -467.168991
Sum of electronic and thermal Free Energies= -467.209729

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.423	29.287	85.739

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.809599	-0.712225	0.000009
2	6	0	0.213342	0.583814	0.000015
3	6	0	-1.185608	0.660333	0.000034
4	6	0	-1.348686	-1.644593	-0.000013
5	1	0	-1.956382	-2.544729	0.000026
6	7	0	-1.881386	1.818783	0.000031
7	7	0	2.127167	-0.680191	0.000121
8	7	0	-1.950429	-0.477845	0.000018
9	7	0	-0.010763	-1.822520	0.000000
10	1	0	-1.417145	2.714068	-0.000193
11	1	0	-2.891121	1.785612	-0.000149
12	7	0	2.467950	0.661236	-0.000178
13	6	0	1.369857	1.413571	0.000016
14	1	0	1.446546	2.494349	-0.000034
15	1	0	0.399292	-2.750942	0.000042

N3H-amino ADA (ADA-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -467.329272637 A.U. after 1 cycles

```
Zero-point correction=                           0.111523 (Hartree/Particle)
Thermal correction to Energy=                    0.118843
Thermal correction to Enthalpy=                  0.119788
Thermal correction to Gibbs Free Energy=         0.079673
Sum of electronic and zero-point Energies=           -467.217750
Sum of electronic and thermal Energies=              -467.210429
Sum of electronic and thermal Enthalpies=            -467.209485
Sum of electronic and thermal Free Energies=         -467.249599

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   74.575             28.875             84.428


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.799710    0.723387    0.000016
     2          6           0       -0.218100   -0.566503   -0.000004
     3          6           0        1.190135   -0.669106   -0.000009
     4          6           0        1.354931    1.639133    0.000027
     5          1           0        1.960446    2.538484    0.000042
     6          7           0        1.842819   -1.836343   -0.000007
     7          7           0       -2.127416    0.689083    0.000022
     8          7           0        1.958071    0.466995    0.000006
     9          7           0        0.023115    1.828724    0.000035
    10          1           0        1.340607   -2.715807   -0.000126
    11          1           0        2.855728   -1.854130   -0.000121
    12          7           0       -2.466739   -0.660150   -0.000032
    13          6           0       -1.359825   -1.405639   -0.000024
    14          1           0       -1.413709   -2.487085   -0.000048
    15          1           0       -0.356616    2.772745    0.000051
---------------------------------------------------------------------
```

N3H-amino ADA (ADA-2), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

```
SCF Done:  E(RB3LYP) =  -467.352330050     A.U. after    1 cycles


Zero-point correction=                           0.105430 (Hartree/Particle)
Thermal correction to Energy=                    0.112669
Thermal correction to Enthalpy=                  0.113613
Thermal correction to Gibbs Free Energy=         0.073697
Sum of electronic and zero-point Energies=           -467.246900
Sum of electronic and thermal Energies=              -467.239661
Sum of electronic and thermal Enthalpies=            -467.238717
Sum of electronic and thermal Free Energies=         -467.278633

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   70.701             28.882             84.010
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.798967	0.721014	0.000018
2	6	0	-0.215249	-0.566301	-0.000009
3	6	0	1.196891	-0.668147	-0.000019
4	6	0	1.342129	1.645603	0.000022
5	1	0	1.949447	2.551750	0.000046
6	7	0	1.849292	-1.831561	-0.000042
7	7	0	-2.129337	0.678802	0.000048
8	7	0	1.955961	0.475245	-0.000002
9	7	0	0.013115	1.832073	0.000037
10	1	0	1.336077	-2.726470	-0.000081
11	1	0	2.881186	-1.847678	-0.000076
12	7	0	-2.462583	-0.672494	-0.000004
13	6	0	-1.350759	-1.411914	-0.000035
14	1	0	-1.399961	-2.499985	-0.000074
15	1	0	-0.396158	2.826392	0.000068

N9-deprotonated N9H-amino ADA (ADA-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -466.759048830 A.U. after 10 cycles

Zero-point correction= 0.098210 (Hartree/Particle)
Thermal correction to Energy= 0.105095
Thermal correction to Enthalpy= 0.106039
Thermal correction to Gibbs Free Energy= 0.066749
Sum of electronic and zero-point Energies= -466.660839
Sum of electronic and thermal Energies= -466.653954
Sum of electronic and thermal Enthalpies= -466.653010
Sum of electronic and thermal Free Energies= -466.692300

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.948	27.310	82.694

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.795854	-0.764353	0.003998
2	6	0	0.199241	0.541541	-0.021212
3	6	0	-1.203476	0.592645	-0.017258
4	6	0	-1.250691	-1.706842	-0.001441
5	1	0	-1.885234	-2.594233	0.001308
6	7	0	-1.907698	1.803278	-0.065267
7	7	0	2.140108	-0.673238	0.019949
8	7	0	-1.934194	-0.526352	-0.005664
9	7	0	0.052518	-1.912152	0.008761
10	1	0	-1.428386	2.580644	0.374750

11	1	0	-2.865595	1.699174	0.253534
12	7	0	2.448325	0.660710	0.005692
13	6	0	1.326250	1.398061	-0.018529
14	1	0	1.382733	2.482371	-0.047235

N1-protonated N9H-amino ADA (ADA-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.677174599 A.U. after 1 cycles

Zero-point correction= 0.125408 (Hartree/Particle)
Thermal correction to Energy= 0.132758
Thermal correction to Enthalpy= 0.133702
Thermal correction to Gibbs Free Energy= 0.093659
Sum of electronic and zero-point Energies= -467.551767
Sum of electronic and thermal Energies= -467.544417
Sum of electronic and thermal Enthalpies= -467.543472
Sum of electronic and thermal Free Energies= -467.583516

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.307	29.759	84.278

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.744099	-0.744619	-0.000079
2	6	0	0.201831	0.563305	-0.000174
3	6	0	-1.201093	0.670113	-0.000020
4	6	0	-1.230332	-1.760279	0.000031
5	1	0	-1.890685	-2.621862	0.000153
6	1	0	2.789473	-1.314588	0.000125
7	7	0	-1.893475	1.812585	0.000157
8	7	0	2.078954	-0.590486	0.000064
9	7	0	-1.867855	-0.528346	-0.000036
10	7	0	0.055137	-1.912713	0.000077
11	1	0	-1.411807	2.702785	-0.000166
12	1	0	-2.905603	1.846899	0.000734
13	7	0	2.452785	0.716751	0.000088
14	6	0	1.340021	1.426391	-0.000108
15	1	0	1.396867	2.506913	-0.000226
16	1	0	-2.884224	-0.534147	-0.000974

N3-protonated N9H-amino ADA (ADA-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.677772097 A.U. after 1 cycles

Zero-point correction= 0.125590 (Hartree/Particle)
Thermal correction to Energy= 0.132868

```
Thermal correction to Enthalpy=                  0.133812
Thermal correction to Gibbs Free Energy=         0.093829
Sum of electronic and zero-point Energies=           -467.552182
Sum of electronic and thermal Energies=              -467.544904
Sum of electronic and thermal Enthalpies=            -467.543960
Sum of electronic and thermal Free Energies=         -467.583943

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   83.376             29.551             84.151


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.743064    0.714615   -0.000161
     2          6           0       -0.186624   -0.573036   -0.000085
     3          6           0        1.232244   -0.666042   -0.000020
     4          6           0        1.398315    1.641251   -0.000015
     5          1           0        2.004858    2.542272    0.000333
     6          1           0       -2.806514    1.280790    0.000353
     7          7           0        1.909645   -1.809490    0.000003
     8          7           0       -2.078474    0.576358    0.000296
     9          7           0        1.983497    0.478703    0.000197
    10          7           0        0.045315    1.831719   -0.000232
    11          1           0        1.455880   -2.713783   -0.000448
    12          1           0        2.923948   -1.780484   -0.000032
    13          7           0       -2.446599   -0.743032   -0.000218
    14          6           0       -1.327877   -1.437318    0.000154
    15          1           0       -1.372892   -2.518283    0.000273
    16          1           0       -0.336925    2.772863   -0.000024
---------------------------------------------------------------------
```

N3-protonated N9H-amino ADA (ADA-5), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

```
SCF Done:  E(RB3LYP) =  -467.787413088     A.U. after    1 cycles


Zero-point correction=                           0.125238 (Hartree/Particle)
Thermal correction to Energy=                    0.132595
Thermal correction to Enthalpy=                  0.133540
Thermal correction to Gibbs Free Energy=         0.093456
Sum of electronic and zero-point Energies=           -467.662175
Sum of electronic and thermal Energies=              -467.654818
Sum of electronic and thermal Enthalpies=            -467.653874
Sum of electronic and thermal Free Energies=         -467.693957

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   83.205             29.760             84.364


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	0.744971	0.707423	-0.000030
2	6	0	0.177439	-0.570826	0.000014
3	6	0	-1.241786	-0.656685	0.000022
4	6	0	-1.372082	1.654483	0.000007
5	1	0	-1.959447	2.565460	-0.000013
6	1	0	2.788779	1.289420	-0.000104
7	7	0	-1.902151	-1.806362	0.000065
8	7	0	2.076625	0.566381	-0.000096
9	7	0	-1.984989	0.495525	0.000031
10	7	0	-0.028990	1.827959	-0.000041
11	1	0	-1.412894	-2.694854	0.000139
12	1	0	-2.916632	-1.809969	0.000142
13	7	0	2.432898	-0.758937	-0.000029
14	6	0	1.301410	-1.444712	0.000041
15	1	0	1.317208	-2.525772	0.000087
16	1	0	0.369524	2.765657	-0.000079

N3-protonated N9H-amino ADA (ADA-5), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

[no coordinate information – structure never converged]

N6-protonated N9H-amino ADA (ADA-6), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.638506576 A.U. after 1 cycles

Zero-point correction= 0.126019 (Hartree/Particle)
Thermal correction to Energy= 0.133433
Thermal correction to Enthalpy= 0.134377
Thermal correction to Gibbs Free Energy= 0.093838
Sum of electronic and zero-point Energies= -467.512488
Sum of electronic and thermal Energies= -467.505074
Sum of electronic and thermal Enthalpies= -467.504129
Sum of electronic and thermal Free Energies= -467.544668

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.731	28.705	85.322

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.819626	0.711998	-0.000162
2	6	0	0.164344	-0.561000	-0.000118
3	6	0	-1.218059	-0.422333	0.000097
4	6	0	-1.102845	1.853058	0.000004
5	1	0	-1.649378	2.789957	0.000023

6	1	0	2.916726	1.094037	0.000190
7	7	0	-2.142910	-1.604355	-0.000014
8	7	0	2.144121	0.437352	0.000106
9	7	0	-1.857561	0.718702	0.000139
10	7	0	0.220597	1.904876	-0.000121
11	1	0	-2.025058	-2.197763	-0.833096
12	1	0	-3.104779	-1.229423	0.000595
13	7	0	2.395523	-0.893864	0.000130
14	6	0	1.230935	-1.515128	-0.000098
15	1	0	1.204381	-2.596876	-0.000186
16	1	0	-2.024297	-2.198480	0.832450

N8-protonated N9H-amino ADA (ADA-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.661241098 A.U. after 9 cycles

Zero-point correction= 0.124269 (Hartree/Particle)
Thermal correction to Energy= 0.132102
Thermal correction to Enthalpy= 0.133047
Thermal correction to Gibbs Free Energy= 0.091937
Sum of electronic and zero-point Energies= -467.536972
Sum of electronic and thermal Energies= -467.529139
Sum of electronic and thermal Enthalpies= -467.528194
Sum of electronic and thermal Free Energies= -467.569305

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.896	30.700	86.523

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.676298	-0.768860	-0.000000
2	6	0	0.135682	0.551186	-0.000000
3	6	0	-1.303954	0.612005	-0.000000
4	6	0	-1.323776	-1.704753	0.000000
5	1	0	-1.943410	-2.597113	0.000000
6	1	0	2.741338	-1.368978	0.000005
7	7	0	-1.999743	1.755391	0.000000
8	7	0	2.031581	-0.643772	-0.000001
9	7	0	-1.986430	-0.539240	-0.000000
10	7	0	0.001404	-1.909473	0.000000
11	1	0	-1.572713	2.670617	0.000001
12	1	0	-3.012561	1.699003	0.000001
13	7	0	2.341866	0.682520	0.000001
14	6	0	1.225867	1.424405	-0.000000
15	1	0	1.297419	2.504143	-0.000000
16	1	0	3.308480	0.990441	-0.000002

N9-protonated N9H-amino ADA (ADA-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.625337515 A.U. after 10 cycles

Zero-point correction=	0.125085 (Hartree/Particle)
Thermal correction to Energy=	0.132458
Thermal correction to Enthalpy=	0.133402
Thermal correction to Gibbs Free Energy=	0.093135
Sum of electronic and zero-point Energies=	-467.500252
Sum of electronic and thermal Energies=	-467.492879
Sum of electronic and thermal Enthalpies=	-467.491935
Sum of electronic and thermal Free Energies=	-467.532203

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.119	29.324	84.749

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.637240	0.738596	0.000000
2	6	0	-0.122655	-0.550199	-0.000000
3	6	0	1.302154	-0.608530	-0.000000
4	6	0	1.329133	1.712584	-0.000000
5	1	0	1.924245	2.620800	-0.000001
6	1	0	-2.559744	1.012702	-0.828541
7	7	0	2.025757	-1.731855	0.000000
8	7	0	-2.115457	0.590017	0.000000
9	7	0	1.984304	0.565933	-0.000000
10	7	0	-0.026490	1.886179	0.000000
11	1	0	1.618654	-2.656763	0.000002
12	1	0	3.037091	-1.653800	0.000001
13	7	0	-2.421821	-0.864622	-0.000000
14	6	0	-1.259932	-1.446261	-0.000001
15	1	0	-1.253317	-2.532344	-0.000001
16	1	0	-2.559743	1.012701	0.828543

N9H-amino ADA with HF hydrogen-bonded to N3 (ADA-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -567.782281743 A.U. after 8 cycles

Zero-point correction=	0.124105 (Hartree/Particle)
Thermal correction to Energy=	0.133948
Thermal correction to Enthalpy=	0.134893
Thermal correction to Gibbs Free Energy=	0.087266
Sum of electronic and zero-point Energies=	-567.658177
Sum of electronic and thermal Energies=	-567.648333
Sum of electronic and thermal Enthalpies=	-567.647389
Sum of electronic and thermal Free Energies=	-567.695015

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	84.054	35.376	100.238

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.545390	0.168866	-0.000001
2	6	0	-0.789745	0.613974	-0.000015
3	6	0	-1.767522	-0.413572	-0.000007
4	6	0	-0.071053	-1.982242	-0.000019
5	1	0	0.191817	-3.036642	-0.000025
6	1	0	2.335581	1.310331	0.000011
7	7	0	-3.098415	-0.170582	-0.000129
8	7	0	1.322351	1.277044	0.000009
9	7	0	-1.381005	-1.703444	-0.000008
10	7	0	0.946620	-1.119620	-0.000006
11	1	0	-3.474138	0.764919	0.000710
12	1	0	-3.734310	-0.956169	0.000455
13	7	0	0.582109	2.420531	-0.000007
14	6	0	-0.684883	2.038419	-0.000022
15	1	0	-1.463532	2.790126	-0.000055
16	1	0	2.587120	-1.147217	0.000013
17	9	0	3.506969	-0.800614	0.000029

N9-deprotonated N9H-amino ADA with HF hydrogen-bonded to N3 (ADA-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -567.239815687 A.U. after 10 cycles

Zero-point correction=	0.110250 (Hartree/Particle)
Thermal correction to Energy=	0.119298
Thermal correction to Enthalpy=	0.120242
Thermal correction to Gibbs Free Energy=	0.075039
Sum of electronic and zero-point Energies=	-567.129566
Sum of electronic and thermal Energies=	-567.120518
Sum of electronic and thermal Enthalpies=	-567.119573
Sum of electronic and thermal Free Energies=	-567.164777

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.861	33.540	95.138

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.364562	0.668491	-0.004466
2	6	0	-1.033363	0.346865	-0.017248
3	6	0	-1.374393	-1.012723	-0.012787

4	6	0	0.859868	-1.552097	-0.014412
5	1	0	1.607848	-2.342793	-0.016573
6	7	0	-2.694921	-1.453825	-0.051226
7	7	0	0.556583	1.995241	0.008892
8	7	0	-0.427930	-1.964353	-0.010852
9	7	0	1.322700	-0.310568	-0.007273
10	1	0	-3.372975	-0.822035	0.356857
11	1	0	-2.799855	-2.416287	0.250218
12	7	0	-0.688259	2.571965	0.005053
13	6	0	-1.638808	1.627557	-0.010089
14	1	0	-2.688276	1.904487	-0.027986
15	1	0	2.862843	-0.181949	0.007897
16	9	0	3.871778	-0.275467	0.019049

N9H-amino ADA with HF hydrogen-bonded to N1 (ADA-11), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -567.784033662 A.U. after 1 cycles

Zero-point correction= 0.124556 (Hartree/Particle)
Thermal correction to Energy= 0.133886
Thermal correction to Enthalpy= 0.134830
Thermal correction to Gibbs Free Energy= 0.089403
Sum of electronic and zero-point Energies= -567.659478
Sum of electronic and thermal Energies= -567.650148
Sum of electronic and thermal Enthalpies= -567.649204
Sum of electronic and thermal Free Energies= -567.694630

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	84.015	34.825	95.608

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.271672	-0.729759	0.000001
2	6	0	0.688976	0.554262	0.000054
3	6	0	-0.728198	0.581635	0.000030
4	6	0	-0.692057	-1.755771	-0.000012
5	1	0	-1.296582	-2.658820	0.000012
6	7	0	-1.463031	1.712281	-0.000187
7	7	0	2.612857	-0.527817	-0.000027
8	7	0	-1.388937	-0.597665	0.000025
9	7	0	0.622352	-1.910690	-0.000028
10	1	0	-1.027956	2.621566	0.000309
11	1	0	-2.477550	1.644650	-0.000031
12	7	0	2.942329	0.794347	0.000011
13	6	0	1.795469	1.454378	0.000045
14	1	0	1.808813	2.536685	0.000082
15	1	0	-2.960028	-0.382007	0.000061
16	9	0	-3.853701	0.060368	0.000041
17	1	0	3.342456	-1.227044	-0.000068

N9-deprotonated N9H-amino ADA with HF hydrogen-bonded to N1 (ADA-12), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -567.242536631 A.U. after 1 cycles

Zero-point correction= 0.108902 (Hartree/Particle)
Thermal correction to Energy= 0.117819
Thermal correction to Enthalpy= 0.118763
Thermal correction to Gibbs Free Energy= 0.074160
Sum of electronic and zero-point Energies= -567.133635
Sum of electronic and thermal Energies= -567.124718
Sum of electronic and thermal Enthalpies= -567.123774
Sum of electronic and thermal Free Energies= -567.168377

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.932	33.286	93.875

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.317817	-0.763457	0.009016
2	6	0	0.731478	0.548838	-0.021374
3	6	0	-0.665286	0.626954	-0.058846
4	6	0	-0.722493	-1.714552	-0.050647
5	1	0	-1.376009	-2.585189	-0.063835
6	7	0	-1.376972	1.807742	-0.127062
7	7	0	2.656692	-0.683105	0.053604
8	7	0	-1.382467	-0.515553	-0.071325
9	7	0	0.571632	-1.913844	-0.011021
10	1	0	-0.919329	2.625881	0.250295
11	1	0	-2.370913	1.726090	0.073210
12	7	0	2.977413	0.650127	0.054556
13	6	0	1.864742	1.395724	0.010044
14	1	0	1.929170	2.479254	-0.007426
15	1	0	-2.728722	-0.339011	0.016425
16	9	0	-3.757316	0.012707	0.123436

N9H-amino ADA with HF hydrogen-bonded to N1 and N3 (ADA-13), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -668.248632902 A.U. after 1 cycles

Zero-point correction= 0.137329 (Hartree/Particle)
Thermal correction to Energy= 0.148745
Thermal correction to Enthalpy= 0.149689
Thermal correction to Gibbs Free Energy= 0.098780
Sum of electronic and zero-point Energies= -668.111304
Sum of electronic and thermal Energies= -668.099888

```
Sum of electronic and thermal Enthalpies=           -668.098944
Sum of electronic and thermal Free Energies=        -668.149853

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   93.339             41.182           107.147


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.050041   -0.038632   -0.000024
     2          6           0       -0.044786   -1.023109    0.000055
     3          6           0        1.287748   -0.539475    0.000111
     4          6           0        0.431678    1.636010    0.000057
     5          1           0        0.664819    2.696766    0.000131
     6          1           0       -3.157383   -0.278659   -0.000040
     7          7           0        2.377548   -1.327434   -0.000129
     8          7           0       -2.231761   -0.693901   -0.000041
     9          7           0        1.486044    0.802739    0.000158
    10          7           0       -0.851435    1.299802   -0.000040
    11          1           0        2.298620   -2.332813    0.000899
    12          1           0        3.300976   -0.900319    0.000401
    13          7           0       -2.067166   -2.045546   -0.000084
    14          6           0       -0.761174   -2.257844   -0.000026
    15          1           0       -0.389558   -3.274144   -0.000041
    16          1           0        3.057556    1.159926   -0.000118
    17          1           0       -2.352453    2.030080   -0.000008
    18          9           0        4.040845    1.039393   -0.000158
    19          9           0       -3.329261    2.070367    0.000013
---------------------------------------------------------------------
```

N9-deprotonated N9H-amino ADA with HF hydrogen-bonded to N1 and N3 (ADA-14), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -667.719593679     A.U. after    9 cycles


Zero-point correction=                           0.121776 (Hartree/Particle)
Thermal correction to Energy=                    0.132944
Thermal correction to Enthalpy=                  0.133888
Thermal correction to Gibbs Free Energy=         0.083146
Sum of electronic and zero-point Energies=           -667.597818
Sum of electronic and thermal Energies=              -667.586649
Sum of electronic and thermal Enthalpies=            -667.585705
Sum of electronic and thermal Free Energies=         -667.636447

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   83.424             39.708           106.796


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	-1.194592	-0.317071	0.005683
2	6	0	-0.058824	-1.194603	-0.018011
3	6	0	1.211015	-0.609097	-0.053063
4	6	0	0.184079	1.488221	-0.051734
5	1	0	0.334123	2.564840	-0.065185
6	7	0	2.386549	-1.319215	-0.114710
7	7	0	-2.337875	-1.008319	0.046063
8	7	0	1.316531	0.740288	-0.067956
9	7	0	-1.056105	1.048914	-0.016128
10	1	0	2.364097	-2.273090	0.216042
11	1	0	3.237460	-0.796545	0.072373
12	7	0	-1.994951	-2.338089	0.050831
13	6	0	-0.664283	-2.474368	0.012968
14	1	0	-0.212417	-3.460859	0.000815
15	1	0	2.668303	1.229477	0.018083
16	1	0	-2.171877	2.172666	0.000887
17	9	0	3.703591	1.370886	0.114618
18	9	0	-2.735047	3.000220	0.007074

Cartesian coordinates and energies (in Hartree) for species of 8-bromoadenine (BA)

N9H-amino BA (BA-1), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3038.46426331 A.U. after 10 cycles

Zero-point correction= 0.101919 (Hartree/Particle)
Thermal correction to Energy= 0.110701
Thermal correction to Enthalpy= 0.111645
Thermal correction to Gibbs Free Energy= 0.066798
Sum of electronic and zero-point Energies= -3038.362344
Sum of electronic and thermal Energies= -3038.353562
Sum of electronic and thermal Enthalpies= -3038.352618
Sum of electronic and thermal Free Energies= -3038.397465

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.466	32.909	94.389

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.963439	-1.012961	-0.001692
2	6	0	-1.076872	0.381426	-0.002182
3	6	0	-2.390401	0.895726	-0.001857
4	6	0	-3.154884	-1.288080	0.003168
5	6	0	1.001496	-0.010078	-0.001541
6	1	0	-4.025116	-1.939634	0.006821
7	1	0	0.857671	-2.149809	-0.002188

8	7	0	-2.653685	2.224706	-0.023927
9	7	0	0.397695	-1.249371	-0.001673
10	7	0	-3.419886	0.028398	0.003678
11	7	0	-1.964009	-1.899147	0.000013
12	7	0	0.170827	0.992699	-0.001371
13	1	0	-1.904408	2.893986	0.075006
14	1	0	-3.610671	2.532941	0.072341
15	35	0	2.870586	0.119581	0.001017

N1H-amino BA (BA-2), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3038.43844939 A.U. after 8 cycles

Zero-point correction= 0.101790 (Hartree/Particle)
Thermal correction to Energy= 0.110345
Thermal correction to Enthalpy= 0.111289
Thermal correction to Gibbs Free Energy= 0.067073
Sum of electronic and zero-point Energies= -3038.336659
Sum of electronic and thermal Energies= -3038.328105
Sum of electronic and thermal Enthalpies= -3038.327160
Sum of electronic and thermal Free Energies= -3038.371377

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.242	32.771	93.061

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.855223	-1.045862	-0.007649
2	6	0	-1.017259	0.381447	-0.009098
3	6	0	-2.289158	0.921465	-0.001564
4	6	0	-3.077288	-1.370240	0.007977
5	6	0	1.005407	-0.088643	-0.003787
6	1	0	-3.975883	-1.979892	0.016749
7	7	0	-2.579169	2.256564	-0.064281
8	7	0	0.453035	-1.331201	-0.002437
9	7	0	-3.306886	-0.001754	0.003663
10	7	0	-1.903892	-1.921889	0.004358
11	7	0	0.209620	0.983203	-0.004314
12	1	0	-1.767664	2.856289	0.044315
13	1	0	-3.411616	2.601263	0.398714
14	35	0	2.877552	0.100577	0.003348
15	1	0	-4.266978	0.318689	-0.051154

N1H-amino BA (BA-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -3038.48903248 A.U. after 1 cycles

```
Zero-point correction=                           0.101152 (Hartree/Particle)
Thermal correction to Energy=                    0.109983
Thermal correction to Enthalpy=                  0.110927
Thermal correction to Gibbs Free Energy=         0.065902
Sum of electronic and zero-point Energies=          -3038.387881
Sum of electronic and thermal Energies=             -3038.379050
Sum of electronic and thermal Enthalpies=           -3038.378106
Sum of electronic and thermal Free Energies=        -3038.423131

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   69.015             33.079             94.763


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.859054   -1.023212   -0.000019
     2          6           0       -1.014879    0.381241   -0.000034
     3          6           0       -2.306559    0.922079    0.000009
     4          6           0       -3.074252   -1.370906    0.000002
     5          6           0        1.005671   -0.087531   -0.000019
     6          1           0       -3.969764   -1.980990    0.000037
     7          7           0       -2.618299    2.221193   -0.000221
     8          7           0        0.460925   -1.322909    0.000062
     9          7           0       -3.305128   -0.017389   -0.000041
    10          7           0       -1.892279   -1.920639    0.000029
    11          7           0        0.218777    0.984697   -0.000122
    12          1           0       -1.882877    2.916933    0.000897
    13          1           0       -3.581526    2.537464    0.000996
    14         35           0        2.890146    0.105334    0.000011
    15          1           0       -4.274475    0.295195    0.000095
---------------------------------------------------------------------
```

N1H-amino BA (BA-2), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

```
SCF Done:  E(RB3LYP) =  -3038.51317303     A.U. after    1 cycles


Zero-point correction=                           0.094973 (Hartree/Particle)
Thermal correction to Energy=                    0.103664
Thermal correction to Enthalpy=                  0.104609
Thermal correction to Gibbs Free Energy=         0.060110
Sum of electronic and zero-point Energies=          -3038.418200
Sum of electronic and thermal Energies=             -3038.409509
Sum of electronic and thermal Enthalpies=           -3038.408564
Sum of electronic and thermal Free Energies=        -3038.453063

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   65.050             33.100             93.655
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.859141	-1.020887	-0.000042
2	6	0	-1.016080	0.379765	0.000033
3	6	0	-2.312787	0.920384	0.000074
4	6	0	-3.073790	-1.368644	-0.000002
5	6	0	1.008932	-0.087545	-0.000089
6	1	0	-3.970859	-1.987885	-0.000019
7	7	0	-2.626678	2.214898	-0.000029
8	7	0	0.465243	-1.321026	-0.000162
9	7	0	-3.308407	-0.021166	0.000084
10	7	0	-1.889400	-1.921203	-0.000076
11	7	0	0.220283	0.983634	0.000064
12	1	0	-1.878230	2.925761	0.000686
13	1	0	-3.612873	2.525662	0.000686
14	35	0	2.893907	0.106777	-0.000013
15	1	0	-4.334851	0.314870	0.000097

N7H-amino BA (BA-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3038.45137178 A.U. after 9 cycles

Zero-point correction= 0.101977 (Hartree/Particle)
Thermal correction to Energy= 0.110520
Thermal correction to Enthalpy= 0.111465
Thermal correction to Gibbs Free Energy= 0.067288
Sum of electronic and zero-point Energies= -3038.349395
Sum of electronic and thermal Energies= -3038.340851
Sum of electronic and thermal Enthalpies= -3038.339907
Sum of electronic and thermal Free Energies= -3038.384084

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.353	32.698	92.977

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.914273	-1.029021	0.017347
2	6	0	-1.103620	0.366056	-0.004220
3	6	0	-2.413912	0.866653	-0.004462
4	6	0	-3.124512	-1.332520	-0.015678
5	6	0	1.025776	-0.171422	0.006492
6	1	0	-3.983873	-1.998129	-0.030746
7	7	0	-2.725941	2.210629	-0.052071
8	7	0	0.438377	-1.332796	0.029222
9	7	0	-3.418527	-0.016075	-0.018548
10	7	0	-1.926757	-1.910091	0.013150

11	7	0	0.176628	0.907651	-0.003421
12	1	0	-2.103844	2.857079	0.416787
13	1	0	-3.708782	2.402338	0.109628
14	35	0	2.877580	0.104371	-0.004627
15	1	0	0.457970	1.872034	-0.108927

N9-deprotonated N9H-amino BA (BA-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3037.93414896 A.U. after 8 cycles

Zero-point correction=	0.089278 (Hartree/Particle)
Thermal correction to Energy=	0.097395
Thermal correction to Enthalpy=	0.098339
Thermal correction to Gibbs Free Energy=	0.054869
Sum of electronic and zero-point Energies=	-3037.844871
Sum of electronic and thermal Energies=	-3037.836754
Sum of electronic and thermal Enthalpies=	-3037.835810
Sum of electronic and thermal Free Energies=	-3037.879280

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	61.116	30.890	91.491

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.906230	-1.042631	-0.008647
2	6	0	-1.063999	0.371061	-0.019977
3	6	0	-2.368090	0.877305	-0.014717
4	6	0	-3.133888	-1.295194	0.013304
5	6	0	0.957455	-0.100432	-0.007939
6	1	0	-4.010772	-1.942932	0.029887
7	7	0	-2.630040	2.243391	-0.072054
8	7	0	0.430165	-1.335449	-0.003126
9	7	0	-3.410187	0.031014	0.009389
10	7	0	-1.953267	-1.905312	0.003633
11	7	0	0.175148	0.979820	-0.016837
12	1	0	-1.862003	2.823073	0.246696
13	1	0	-3.533563	2.499556	0.308775
14	35	0	2.863203	0.104726	0.005585

N1-protonated N9H-amino BA (BA-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3038.82822954 A.U. after 8 cycles

Zero-point correction=	0.115577 (Hartree/Particle)
Thermal correction to Energy=	0.124162
Thermal correction to Enthalpy=	0.125107

```
Thermal correction to Gibbs Free Energy=         0.080918
Sum of electronic and zero-point Energies=          -3038.712652
Sum of electronic and thermal Energies=             -3038.704067
Sum of electronic and thermal Enthalpies=           -3038.703123
Sum of electronic and thermal Free Energies=        -3038.747311

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   77.913             33.509             93.003


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.921347   -1.016777    0.000000
     2          6           0       -1.030082    0.381026   -0.000000
     3          6           0       -2.318233    0.941477   -0.000000
     4          6           0       -3.111316   -1.354907    0.000000
     5          6           0        1.043321   -0.015666   -0.000000
     6          1           0       -4.007465   -1.966719   -0.000000
     7          1           0        0.879724   -2.160201    0.000000
     8          7           0       -2.565591    2.251410    0.000000
     9          7           0        0.421383   -1.254675    0.000000
    10          7           0       -3.328418    0.011578   -0.000000
    11          7           0       -1.934220   -1.908364    0.000000
    12          7           0        0.200900    0.988148   -0.000000
    13          1           0       -1.779669    2.893363    0.000000
    14          1           0       -3.495902    2.649885    0.000001
    15         35           0        2.890451    0.115119    0.000000
    16          1           0       -4.294921    0.326902   -0.000000
---------------------------------------------------------------------
```

N1-protonated N9H-amino BA (BA-5), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

```
SCF Done:  E(RB3LYP) =  -3038.93647230     A.U. after    1 cycles


Zero-point correction=                           0.115447 (Hartree/Particle)
Thermal correction to Energy=                    0.124082
Thermal correction to Enthalpy=                  0.125026
Thermal correction to Gibbs Free Energy=         0.080705
Sum of electronic and zero-point Energies=          -3038.821025
Sum of electronic and thermal Energies=             -3038.812391
Sum of electronic and thermal Enthalpies=           -3038.811446
Sum of electronic and thermal Free Energies=        -3038.855767

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   77.862             33.524             93.281


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
```

1	6	0	0.685403	-1.176565	0.000000
2	6	0	1.088256	0.160391	-0.000000
3	6	0	2.472375	0.431000	-0.000000
4	6	0	2.751787	-1.973246	0.000000
5	6	0	-1.022316	0.194340	-0.000000
6	1	0	3.500915	-2.756120	0.000000
7	1	0	-1.305879	-1.938452	0.000000
8	7	0	3.029290	1.633074	-0.000000
9	7	0	-0.681071	-1.136363	0.000000
10	7	0	3.249595	-0.699097	0.000000
11	7	0	1.478691	-2.272213	0.000000
12	7	0	-0.000000	1.010451	-0.000000
13	1	0	2.448423	2.464382	-0.000000
14	1	0	4.037907	1.752386	-0.000000
15	35	0	-2.809550	0.728691	-0.000000
16	1	0	4.264317	-0.592868	0.000000

N1-protonated N9H-amino (BA-5), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -3038.97277091 A.U. after 8 cycles

Zero-point correction= 0.104371 (Hartree/Particle)
Thermal correction to Energy= 0.113019
Thermal correction to Enthalpy= 0.113963
Thermal correction to Gibbs Free Energy= 0.069676
Sum of electronic and zero-point Energies= -3038.868400
Sum of electronic and thermal Energies= -3038.859752
Sum of electronic and thermal Enthalpies= -3038.858808
Sum of electronic and thermal Free Energies= -3038.903095

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.921	33.827	93.210

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.680420	-1.169759	-0.000000
2	6	0	1.089119	0.166584	0.000000
3	6	0	2.475249	0.433597	0.000000
4	6	0	2.751580	-1.963329	-0.000000
5	6	0	-1.021324	0.193038	0.000000
6	1	0	3.501168	-2.755266	-0.000000
7	1	0	-1.362441	-1.972080	-0.000000
8	7	0	3.037153	1.631541	0.000000
9	7	0	-0.683818	-1.131122	-0.000000
10	7	0	3.252008	-0.695472	-0.000000
11	7	0	1.476567	-2.266181	-0.000000
12	7	0	-0.000000	1.017003	0.000000

13	1	0	2.444984	2.480360	0.000000
14	1	0	4.068215	1.738396	0.000000
15	35	0	-2.811796	0.720943	0.000000
16	1	0	4.337292	-0.575593	-0.000000

N3-protonated N9H-amino BA (BA-6), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3038.82560656 A.U. after 8 cycles

Zero-point correction= 0.115619 (Hartree/Particle)
Thermal correction to Energy= 0.124165
Thermal correction to Enthalpy= 0.125109
Thermal correction to Gibbs Free Energy= 0.080950
Sum of electronic and zero-point Energies= -3038.709988
Sum of electronic and thermal Energies= -3038.701442
Sum of electronic and thermal Enthalpies= -3038.700498
Sum of electronic and thermal Free Energies= -3038.744657

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.914	33.444	92.940

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.918337	-0.985651	-0.000000
2	6	0	-1.040557	0.400125	0.000000
3	6	0	-2.345421	0.955699	0.000000
4	6	0	-3.237824	-1.181469	-0.000000
5	6	0	1.043523	0.001540	0.000000
6	1	0	-4.099285	-1.842583	-0.000000
7	1	0	0.892086	-2.142682	-0.000000
8	7	0	-2.577195	2.261955	0.000000
9	7	0	0.416458	-1.247251	0.000000
10	7	0	-3.418975	0.107848	-0.000000
11	7	0	-2.013703	-1.797494	0.000000
12	7	0	0.201818	0.996144	0.000000
13	1	0	-1.812336	2.927200	0.000000
14	1	0	-3.531067	2.605737	-0.000001
15	35	0	2.892475	0.110690	-0.000000
16	1	0	-1.953150	-2.811690	-0.000000

N6-protonated N9H-amino BA (BA-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3038.79532565 A.U. after 7 cycles

Zero-point correction= 0.116257 (Hartree/Particle)
Thermal correction to Energy= 0.125031

```
Thermal correction to Enthalpy=                  0.125975
Thermal correction to Gibbs Free Energy=         0.080798
Sum of electronic and zero-point Energies=          -3038.679068
Sum of electronic and thermal Energies=             -3038.670295
Sum of electronic and thermal Enthalpies=           -3038.669350
Sum of electronic and thermal Free Energies=        -3038.714527

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   78.458             32.520             95.083


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.906725   -1.066481   -0.000001
     2          6           0        1.034296    0.348989    0.000000
     3          6           0        2.349230    0.770199    0.000002
     4          6           0        3.116313   -1.373673    0.000001
     5          6           0       -1.042140   -0.025359   -0.000000
     6          1           0        3.974770   -2.036232    0.000002
     7          1           0       -0.929924   -2.167778   -0.000003
     8          7           0        2.695530    2.222047   -0.000002
     9          7           0       -0.450228   -1.273787   -0.000002
    10          7           0        3.379856   -0.047968    0.000003
    11          7           0        1.903052   -1.938233   -0.000002
    12          7           0       -0.188585    0.974346    0.000001
    13          1           0        2.323343    2.706778   -0.828865
    14          1           0        3.723557    2.300996    0.000128
    15         35           0       -2.885108    0.143215    0.000000
    16          1           0        2.323117    2.706837    0.828724
---------------------------------------------------------------------
```

N7-protonated N9H-amino BA (BA-8), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -3038.81286256     A.U. after    8 cycles


Zero-point correction=                           0.114955 (Hartree/Particle)
Thermal correction to Energy=                    0.123845
Thermal correction to Enthalpy=                  0.124789
Thermal correction to Gibbs Free Energy=         0.079818
Sum of electronic and zero-point Energies=          -3038.697908
Sum of electronic and thermal Energies=             -3038.689018
Sum of electronic and thermal Enthalpies=           -3038.688073
Sum of electronic and thermal Free Energies=        -3038.733045

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   77.714             33.907             94.651


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	-0.967958	-1.000124	0.000000
2	6	0	-1.118066	0.387757	0.000000
3	6	0	-2.446988	0.886070	0.000000
4	6	0	-3.144074	-1.334488	-0.000000
5	6	0	1.066643	-0.077207	0.000000
6	1	0	-3.995020	-2.008889	-0.000001
7	1	0	0.836686	-2.167025	0.000001
8	7	0	-2.793370	2.187126	-0.000000
9	7	0	0.407328	-1.245762	0.000000
10	7	0	-3.430631	-0.028838	-0.000000
11	7	0	-1.929238	-1.906997	0.000000
12	7	0	0.176119	0.925240	0.000000
13	1	0	-2.134007	2.950849	0.000003
14	1	0	-3.781428	2.413220	0.000001
15	35	0	2.893700	0.120615	-0.000000
16	1	0	0.445458	1.902851	-0.000001

N9-protonated N9H-amino BA (BA-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3038.75762777 A.U. after 1 cycles

Zero-point correction= 0.114638 (Hartree/Particle)
Thermal correction to Energy= 0.123312
Thermal correction to Enthalpy= 0.124257
Thermal correction to Gibbs Free Energy= 0.079767
Sum of electronic and zero-point Energies= -3038.642990
Sum of electronic and thermal Energies= -3038.634315
Sum of electronic and thermal Enthalpies= -3038.633371
Sum of electronic and thermal Free Energies= -3038.677861

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.380	33.522	93.636

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.043456	-1.001243	0.000104
2	6	0	1.094966	0.378537	0.000007
3	6	0	2.400311	0.932766	0.000017
4	6	0	3.220474	-1.243044	-0.000421
5	6	0	-1.050654	0.054112	0.000041
6	1	0	4.091815	-1.890529	0.000288
7	1	0	-0.686513	-1.894171	0.829034
8	7	0	2.660459	2.242832	0.000053
9	7	0	-0.412703	-1.345406	0.000219
10	7	0	3.442153	0.061206	-0.000043
11	7	0	2.009604	-1.873650	0.000046
12	7	0	-0.178340	0.973152	0.000044

13	1	0	1.923938	2.936178	0.000306
14	1	0	3.625378	2.552285	0.000004
15	35	0	-2.890499	0.144491	-0.000061
16	1	0	-0.686680	-1.894633	-0.828227

N7-protonated N9H-amino BA with HF hydrogen-bonded to N3 (BA-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3139.27507464 A.U. after 8 cycles

Zero-point correction=	0.127593 (Hartree/Particle)
Thermal correction to Energy=	0.138444
Thermal correction to Enthalpy=	0.139388
Thermal correction to Gibbs Free Energy=	0.089762
Sum of electronic and zero-point Energies=	-3139.147481
Sum of electronic and thermal Energies=	-3139.136631
Sum of electronic and thermal Enthalpies=	-3139.135686
Sum of electronic and thermal Free Energies=	-3139.185312

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.875	40.404	104.446

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.949175	0.634836	-0.000000
2	6	0	1.078727	-0.750620	0.000000
3	6	0	2.400731	-1.270622	0.000000
4	6	0	3.147429	0.935329	-0.000000
5	6	0	-1.094851	-0.231494	0.000000
6	1	0	4.008553	1.596467	-0.000000
7	1	0	-0.768641	1.882789	-0.000000
8	7	0	2.726301	-2.573883	0.000000
9	7	0	-0.411052	0.918973	-0.000000
10	7	0	3.403108	-0.372059	0.000000
11	7	0	1.938828	1.524652	-0.000000
12	7	0	-0.227267	-1.258710	0.000000
13	1	0	2.054119	-3.326889	0.000001
14	1	0	3.710713	-2.816998	0.000000
15	35	0	-2.924333	-0.385422	0.000000
16	1	0	-0.519921	-2.229445	0.000000
17	1	0	1.089707	3.120796	-0.000001
18	9	0	0.208937	3.520631	-0.000001

N7H-amino BA with HF hydrogen-bonded to N3 (BA-11), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3138.91608673 A.U. after 9 cycles

```
Zero-point correction=                           0.114296 (Hartree/Particle)
Thermal correction to Energy=                    0.125214
Thermal correction to Enthalpy=                  0.126158
Thermal correction to Gibbs Free Energy=         0.075255
Sum of electronic and zero-point Energies=          -3138.801791
Sum of electronic and thermal Energies=             -3138.790872
Sum of electronic and thermal Enthalpies=           -3138.789928
Sum of electronic and thermal Free Energies=        -3138.840832

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   78.573             39.522           107.136


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.855988    0.453121    0.005006
     2          6           0        0.734135   -0.947794   -0.003262
     3          6           0        1.900928   -1.728677   -0.000585
     4          6           0        3.094962    0.249920   -0.027379
     5          6           0       -1.222228    0.053455    0.003066
     6          1           0        4.076167    0.715852   -0.044961
     7          7           0        1.912075   -3.100706   -0.034076
     8          7           0       -0.385588    1.053893    0.013362
     9          7           0        3.080440   -1.091635   -0.021119
    10          7           0        2.048187    1.076188   -0.005503
    11          7           0       -0.634760   -1.186797    0.001352
    12          1           0        1.139010   -3.609025    0.373958
    13          1           0        2.822933   -3.517744    0.120982
    14         35           0       -3.084362    0.204349   -0.003207
    15          1           0       -1.126730   -2.065594   -0.077992
    16          1           0        2.367543    2.738486    0.010679
    17          9           0        2.705395    3.649895    0.021156
---------------------------------------------------------------------
```

N7-protonated N9H-amino BA with HF hydrogen-bonded to N1 (BA-12), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -3139.27078146     A.U. after    2 cycles


Zero-point correction=                           0.127968 (Hartree/Particle)
Thermal correction to Energy=                    0.138717
Thermal correction to Enthalpy=                  0.139661
Thermal correction to Gibbs Free Energy=         0.090018
Sum of electronic and zero-point Energies=          -3139.142813
Sum of electronic and thermal Energies=             -3139.132064
Sum of electronic and thermal Enthalpies=           -3139.131120
Sum of electronic and thermal Free Energies=        -3139.180764

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   87.046             40.088           104.484
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.375488	1.175792	0.000038
2	6	0	0.665701	-0.187387	0.000265
3	6	0	2.036204	-0.561366	0.000357
4	6	0	2.503091	1.739378	0.000197
5	6	0	-1.553547	0.050444	0.000075
6	1	0	3.282930	2.494808	0.000228
7	7	0	2.507416	-1.814268	0.000461
8	7	0	-1.015624	1.280691	-0.000189
9	7	0	2.920136	0.465330	0.000395
10	7	0	1.240380	2.178840	-0.000044
11	7	0	-0.564338	-0.855195	0.000255
12	1	0	1.914664	-2.631248	-0.000077
13	1	0	3.522199	-1.948441	0.000043
14	35	0	-3.349916	-0.331610	-0.000126
15	1	0	-0.731089	-1.855827	0.000475
16	1	0	4.565495	-0.184312	-0.000388
17	9	0	5.161341	-0.945705	-0.000812
18	1	0	-1.536640	2.153775	-0.000296

N7H-amino BA with HF hydrogen-bonded to N1 (BA-13), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3138.91881028 A.U. after 9 cycles

Zero-point correction= 0.114295 (Hartree/Particle)
Thermal correction to Energy= 0.124969
Thermal correction to Enthalpy= 0.125913
Thermal correction to Gibbs Free Energy= 0.076310
Sum of electronic and zero-point Energies= -3138.804516
Sum of electronic and thermal Energies= -3138.793841
Sum of electronic and thermal Enthalpies= -3138.792897
Sum of electronic and thermal Free Energies= -3138.842501

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.419	38.987	104.400

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.330365	1.176761	0.006359
2	6	0	0.643834	-0.194999	-0.021229
3	6	0	1.991409	-0.587662	-0.036082
4	6	0	2.499347	1.694507	-0.029494
5	6	0	-1.524064	0.148577	0.005792
6	1	0	3.300252	2.428665	-0.039013
7	7	0	2.432170	-1.877613	-0.090723

8	7	0	-1.039853	1.358452	0.026490
9	7	0	2.904537	0.404008	-0.044763
10	7	0	1.258332	2.151518	0.002329
11	7	0	-0.581204	-0.848545	-0.016203
12	1	0	1.835784	-2.624283	0.235128
13	1	0	3.434207	-2.020194	0.021399
14	35	0	-3.341711	-0.288870	0.010038
15	1	0	-0.777589	-1.836361	-0.096007
16	1	0	4.390522	-0.178776	0.023805
17	9	0	5.145945	-0.821830	0.090153

N7-protonated N9H-amino BA with HF hydrogen-bonded to N1 and N3 (BA-14), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3239.73206716 A.U. after 9 cycles

Zero-point correction= 0.140413 (Hartree/Particle)
Thermal correction to Energy= 0.153261
Thermal correction to Enthalpy= 0.154205
Thermal correction to Gibbs Free Energy= 0.099547
Sum of electronic and zero-point Energies= -3239.591654
Sum of electronic and thermal Energies= -3239.578806
Sum of electronic and thermal Enthalpies= -3239.577862
Sum of electronic and thermal Free Energies= -3239.632520

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	96.173	46.850	115.038

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.382819	0.866517	-0.000000
2	6	0	0.735950	-0.477521	-0.000000
3	6	0	2.123169	-0.789096	-0.000000
4	6	0	2.498771	1.529212	0.000000
5	6	0	-1.491694	-0.322240	-0.000000
6	1	0	3.242778	2.319766	0.000001
7	1	0	-1.514395	1.817741	-0.000000
8	7	0	2.649987	-2.016710	0.000000
9	7	0	-1.003878	0.925042	-0.000000
10	7	0	2.964173	0.276796	0.000000
11	7	0	1.214945	1.908799	0.000000
12	7	0	-0.466926	-1.193092	-0.000000
13	1	0	2.093904	-2.859557	-0.000000
14	1	0	3.670319	-2.105913	0.000000
15	35	0	-3.270721	-0.771877	0.000000
16	1	0	-0.595600	-2.199158	-0.000000
17	1	0	4.655323	-0.308854	-0.000000
18	1	0	0.097154	3.368577	0.000000
19	9	0	5.265613	-1.055718	-0.000000

20	9	0	-0.840773	3.593055	-0.000000

N7H-amino BA with HF hydrogen-bonded to N1 and N3 (BA-15), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -3239.38166472 A.U. after 8 cycles

Zero-point correction= 0.126538 (Hartree/Particle)
Thermal correction to Energy= 0.139720
Thermal correction to Enthalpy= 0.140664
Thermal correction to Gibbs Free Energy= 0.083973
Sum of electronic and zero-point Energies= -3239.255127
Sum of electronic and thermal Energies= -3239.241945
Sum of electronic and thermal Enthalpies= -3239.241000
Sum of electronic and thermal Free Energies= -3239.297691

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.676	46.041	119.316

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.299058	0.773571	-0.002199
2	6	0	0.506971	-0.616191	-0.014814
3	6	0	1.821032	-1.114722	-0.023573
4	6	0	2.519480	1.115952	-0.027995
5	6	0	-1.628203	-0.099573	0.002278
6	1	0	3.368740	1.792791	-0.036412
7	7	0	2.162811	-2.426246	-0.055601
8	7	0	-1.044693	1.068522	0.010408
9	7	0	2.813832	-0.196765	-0.033472
10	7	0	1.311755	1.664652	-0.008888
11	7	0	-0.767224	-1.167365	-0.008735
12	1	0	1.490636	-3.148023	0.154701
13	1	0	3.150704	-2.660843	0.022746
14	35	0	-3.472357	-0.383598	0.007788
15	1	0	-1.043387	-2.138259	-0.054211
16	1	0	4.267699	-0.921520	0.016086
17	1	0	1.228715	3.373829	0.005613
18	9	0	4.935978	-1.648040	0.064001
19	9	0	1.355578	4.334059	0.012745

Cartesian coordinates and energies (in Hartree) for species of 3-deazaadenine (Z3)

N9H-amino Z3 (Z3-1), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.289799967 A.U. after 1 cycles

```
Zero-point correction=                           0.123556 (Hartree/Particle)
Thermal correction to Energy=                    0.130915
Thermal correction to Enthalpy=                  0.131859
Thermal correction to Gibbs Free Energy=         0.091896
Sum of electronic and zero-point Energies=           -451.166244
Sum of electronic and thermal Energies=              -451.158885
Sum of electronic and thermal Enthalpies=            -451.157941
Sum of electronic and thermal Free Energies=         -451.197904

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   82.150             29.955             84.109


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.731932    0.811492   -0.005151
     2          6           0       -0.203292   -0.488366   -0.006161
     3          6           0        1.202886   -0.649774   -0.006105
     4          6           0        1.461181    1.654459    0.006740
     5          6           0       -2.320102   -0.744520    0.005860
     6          1           0        2.180345    2.470938    0.016040
     7          1           0       -2.811176    1.337666    0.000901
     8          7           0        1.767312   -1.898677   -0.060840
     9          7           0       -2.100432    0.619763    0.000209
    10          7           0        2.006995    0.417731    0.007936
    11          7           0       -1.212514   -1.441628    0.002947
    12          1           0        1.184721   -2.688077    0.183606
    13          1           0        2.747212   -1.958816    0.181660
    14          1           0       -3.321236   -1.156160    0.012784
    15          6           0        0.100830    1.941929   -0.002569
    16          1           0       -0.266821    2.962812   -0.002438
---------------------------------------------------------------------
```

N1H-amino Z3 (Z3-2), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -451.271638825     A.U. after   10 cycles


Zero-point correction=                           0.123827 (Hartree/Particle)
Thermal correction to Energy=                    0.131188
Thermal correction to Enthalpy=                  0.132132
Thermal correction to Gibbs Free Energy=         0.092099
Sum of electronic and zero-point Energies=           -451.147811
Sum of electronic and thermal Energies=              -451.140451
Sum of electronic and thermal Enthalpies=            -451.139507
Sum of electronic and thermal Free Energies=         -451.179540

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   82.322             29.685             84.258
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.819720	0.828856	0.009510
2	6	0	0.278782	-0.500933	0.011763
3	6	0	-1.090678	-0.716838	0.004906
4	6	0	-1.401441	1.692570	-0.006819
5	6	0	2.374158	-0.607285	-0.008775
6	1	0	-2.162246	2.463003	-0.016722
7	7	0	-1.673093	-1.964484	0.070620
8	7	0	2.163054	0.740883	-0.005276
9	7	0	-1.887699	0.392284	0.002450
10	7	0	1.299462	-1.410607	-0.003429
11	1	0	-0.988468	-2.709316	-0.022672
12	1	0	-2.502078	-2.123962	-0.491649
13	1	0	3.380578	-1.011765	-0.017842
14	6	0	-0.057453	1.945148	-0.004122
15	1	0	0.310411	2.965510	-0.016868
16	1	0	-2.888788	0.260904	0.076414

N1H-amino Z3 (Z3-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -451.310392845 A.U. after 1 cycles

Zero-point correction= 0.124029 (Hartree/Particle)
Thermal correction to Energy= 0.131323
Thermal correction to Enthalpy= 0.132267
Thermal correction to Gibbs Free Energy= 0.092397
Sum of electronic and zero-point Energies= -451.186364
Sum of electronic and thermal Energies= -451.179070
Sum of electronic and thermal Enthalpies= -451.178126
Sum of electronic and thermal Free Energies= -451.217995

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.406	29.611	83.912

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.815180	0.813326	0.001175
2	6	0	-0.283443	-0.504003	-0.002647
3	6	0	1.101903	-0.717607	-0.002445
4	6	0	1.391656	1.691665	0.001323
5	6	0	-2.391364	-0.613579	0.001306
6	1	0	2.152882	2.461340	0.004401
7	7	0	1.693196	-1.939390	-0.059677
8	7	0	-2.175331	0.728695	0.003915
9	7	0	1.879822	0.399180	-0.000151

10	7	0	-1.314878	-1.415532	-0.002632
11	1	0	1.114764	-2.734301	0.186588
12	1	0	2.669094	-2.019401	0.207811
13	1	0	-3.397095	-1.018530	0.002271
14	6	0	0.048434	1.940544	0.001688
15	1	0	-0.320749	2.960588	0.004194
16	1	0	2.889409	0.277558	0.002153

N1H-amino Z3 (Z3-2), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -451.332187760 A.U. after 1 cycles

Zero-point correction= 0.117874 (Hartree/Particle)
Thermal correction to Energy= 0.125222
Thermal correction to Enthalpy= 0.126166
Thermal correction to Gibbs Free Energy= 0.086197
Sum of electronic and zero-point Energies= -451.214314
Sum of electronic and thermal Energies= -451.206966
Sum of electronic and thermal Enthalpies= -451.206021
Sum of electronic and thermal Free Energies= -451.245991

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.578	29.821	84.123

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.815624	0.811107	0.001106
2	6	0	-0.284537	-0.502893	-0.001704
3	6	0	1.105001	-0.716176	-0.002429
4	6	0	1.389493	1.688276	0.001465
5	6	0	-2.396615	-0.615083	0.001326
6	1	0	2.150220	2.464366	0.003678
7	7	0	1.697286	-1.933244	-0.061208
8	7	0	-2.179527	0.725958	0.003312
9	7	0	1.881388	0.399917	0.003144
10	7	0	-1.318042	-1.415162	-0.001567
11	1	0	1.116902	-2.747293	0.190793
12	1	0	2.696557	-2.001084	0.192060
13	1	0	-3.405646	-1.022592	0.002764
14	6	0	0.045493	1.940057	0.000126
15	1	0	-0.327618	2.965698	-0.000404
16	1	0	2.942594	0.266903	0.006007

N7H-amino Z3 (Z3-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.283481511 A.U. after 9 cycles

```
Zero-point correction=                           0.123638 (Hartree/Particle)
Thermal correction to Energy=                    0.130989
Thermal correction to Enthalpy=                  0.131933
Thermal correction to Gibbs Free Energy=         0.091917
Sum of electronic and zero-point Energies=           -451.159843
Sum of electronic and thermal Energies=              -451.152493
Sum of electronic and thermal Enthalpies=            -451.151549
Sum of electronic and thermal Free Energies=         -451.191564

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   82.197             29.653             84.220


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.756830    0.833846    0.025396
     2          6           0       -0.202557   -0.459433   -0.000333
     3          6           0        1.190821   -0.648810   -0.001258
     4          6           0        1.463928    1.656468   -0.017680
     5          6           0       -2.411863   -0.521079   -0.015324
     6          1           0        2.192748    2.463194   -0.038347
     7          7           0        1.765719   -1.922869   -0.056497
     8          7           0       -2.142977    0.761894    0.021690
     9          7           0        1.996426    0.409480   -0.017505
    10          7           0       -1.293132   -1.319298   -0.017283
    11          1           0        1.359656   -2.609664    0.571134
    12          1           0        2.774422   -1.875425    0.054886
    13          1           0       -3.407571   -0.946425   -0.037264
    14          6           0        0.107160    1.942860    0.018722
    15          1           0       -0.266096    2.961163    0.031121
    16          1           0       -1.279364   -2.320405   -0.151508
---------------------------------------------------------------------
```

N9-deprotonated N9H-amino Z3 (Z3-4), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -450.744450348     A.U. after    1 cycles


Zero-point correction=                           0.110581 (Hartree/Particle)
Thermal correction to Energy=                    0.117526
Thermal correction to Enthalpy=                  0.118471
Thermal correction to Gibbs Free Energy=         0.079152
Sum of electronic and zero-point Energies=           -450.633870
Sum of electronic and thermal Energies=              -450.626924
Sum of electronic and thermal Enthalpies=            -450.625980
Sum of electronic and thermal Free Energies=         -450.665298

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   73.749             27.948             82.753
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.797517	0.823390	-0.009344
2	6	0	-0.242548	-0.486987	-0.021099
3	6	0	1.156191	-0.647505	-0.019960
4	6	0	1.440333	1.647963	0.009578
5	6	0	-2.347635	-0.623468	0.011502
6	1	0	2.166664	2.461577	0.026968
7	7	0	1.721568	-1.932999	-0.080689
8	7	0	-2.163681	0.720169	0.009325
9	7	0	1.985511	0.398707	0.003922
10	7	0	-1.258797	-1.417140	-0.003426
11	1	0	1.088584	-2.648888	0.261784
12	1	0	2.639235	-1.971789	0.350251
13	1	0	-3.349748	-1.047280	0.028024
14	6	0	0.081610	1.931183	-0.000616
15	1	0	-0.279556	2.957770	0.008686

N1-protonated N9H-amino Z3 (Z3-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.673002103 A.U. after 1 cycles

Zero-point correction= 0.137380 (Hartree/Particle)
Thermal correction to Energy= 0.144915
Thermal correction to Enthalpy= 0.145859
Thermal correction to Gibbs Free Energy= 0.105573
Sum of electronic and zero-point Energies= -451.535622
Sum of electronic and thermal Energies= -451.528087
Sum of electronic and thermal Enthalpies= -451.527143
Sum of electronic and thermal Free Energies= -451.567429

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.935	30.845	84.789

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.749940	0.818849	0.000014
2	6	0	-0.246091	-0.491676	0.000114
3	6	0	1.143847	-0.722165	0.000003
4	6	0	1.436158	1.691457	-0.000016
5	6	0	-2.353194	-0.712156	0.000032
6	1	0	2.194218	2.464354	0.000094
7	1	0	-2.811551	1.377640	-0.000299
8	7	0	1.672565	-1.951682	-0.000003
9	7	0	-2.107578	0.648507	-0.000107
10	7	0	1.923963	0.395549	0.000226

11	7	0	-1.254268	-1.425897	0.000040
12	1	0	1.042346	-2.746107	-0.000034
13	1	0	2.666517	-2.137708	-0.000709
14	1	0	-3.360037	-1.108810	0.000004
15	6	0	0.095796	1.953671	-0.000020
16	1	0	-0.266598	2.974754	-0.000051
17	1	0	2.932869	0.282651	-0.000866

N1-protonated N9H-amino Z3 (Z3-5), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -451.773279676 A.U. after 1 cycles

Zero-point correction=	0.136468 (Hartree/Particle)
Thermal correction to Energy=	0.144457
Thermal correction to Enthalpy=	0.145401
Thermal correction to Gibbs Free Energy=	0.103372
Sum of electronic and zero-point Energies=	-451.636812
Sum of electronic and thermal Energies=	-451.628823
Sum of electronic and thermal Enthalpies=	-451.627879
Sum of electronic and thermal Free Energies=	-451.669908

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.648	31.277	88.457

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.760442	0.793573	-0.000026
2	6	0	0.241855	-0.509794	-0.000035
3	6	0	-1.155559	-0.709377	0.000031
4	6	0	-1.403814	1.705977	0.000086
5	6	0	2.358510	-0.729511	0.000019
6	1	0	-2.153196	2.487021	0.000125
7	1	0	2.822129	1.350388	-0.000123
8	7	0	-1.744955	-1.909475	-0.000067
9	7	0	2.117301	0.619870	-0.000100
10	7	0	-1.909349	0.424027	0.000083
11	7	0	1.256574	-1.450083	-0.000123
12	1	0	-1.180759	-2.750105	0.000228
13	1	0	-2.754379	-2.005371	0.000416
14	1	0	3.365725	-1.122061	0.000016
15	6	0	-0.059343	1.944921	0.000029
16	1	0	0.333213	2.954260	0.000018
17	1	0	-2.922277	0.320761	0.000142

N1-protonated N9H-amino Z3 (Z3-5), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -451.803178661   A.U. after   1 cycles

Zero-point correction=   0.126836 (Hartree/Particle)
Thermal correction to Energy=   0.134636
Thermal correction to Enthalpy=   0.135580
Thermal correction to Gibbs Free Energy=   0.094631
Sum of electronic and zero-point Energies=   -451.676343
Sum of electronic and thermal Energies=   -451.668543
Sum of electronic and thermal Enthalpies=   -451.667599
Sum of electronic and thermal Free Energies=   -451.708547

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	84.485	31.373	86.183

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.768859	0.785690	-0.000022
2	6	0	0.239045	-0.513057	-0.000003
3	6	0	-1.162558	-0.702415	0.000034
4	6	0	-1.392547	1.709234	0.000035
5	6	0	2.356401	-0.738970	-0.000157
6	1	0	-2.136494	2.502056	0.000065
7	1	0	2.871438	1.374988	-0.000006
8	7	0	-1.760794	-1.895361	-0.000017
9	7	0	2.125273	0.608132	-0.000021
10	7	0	-1.909776	0.434856	0.000063
11	7	0	1.249287	-1.458376	0.000002
12	1	0	-1.193099	-2.756731	0.000284
13	1	0	-2.791279	-1.974741	0.000294
14	1	0	3.365660	-1.144065	-0.000211
15	6	0	-0.045488	1.941975	-0.000005
16	1	0	0.354784	2.953049	-0.000012
17	1	0	-2.981214	0.325940	0.000102

N6-protonated N9H-amino Z3 (Z3-6), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.641985586   A.U. after   1 cycles

Zero-point correction=   0.138352 (Hartree/Particle)
Thermal correction to Energy=   0.145962
Thermal correction to Enthalpy=   0.146906
Thermal correction to Gibbs Free Energy=   0.105937
Sum of electronic and zero-point Energies=   -451.503633
Sum of electronic and thermal Energies=   -451.496023
Sum of electronic and thermal Enthalpies=   -451.495079
Sum of electronic and thermal Free Energies=   -451.536048

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	91.593	29.595	86.227

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.829124	0.796111	-0.000019
2	6	0	0.202375	-0.473145	-0.000044
3	6	0	-1.183036	-0.472557	-0.000030
4	6	0	-1.320016	1.799422	-0.000000
5	6	0	2.279826	-0.885798	0.000007
6	1	0	-1.977066	2.662801	0.000005
7	1	0	2.947227	1.140025	-0.000374
8	7	0	-1.891526	-1.788458	0.000019
9	7	0	2.172103	0.487733	0.000072
10	7	0	-1.939277	0.594719	-0.000013
11	7	0	1.118732	-1.501109	-0.000013
12	1	0	-1.200217	-2.554173	0.000203
13	1	0	-2.494370	-1.882470	-0.828301
14	1	0	3.243780	-1.378489	0.000064
15	6	0	0.067082	1.966644	0.000029
16	1	0	0.502849	2.960307	0.000067
17	1	0	-2.494563	-1.882247	0.828227

N7-protonated N9H-amino Z3 (Z3-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.651318697 A.U. after 1 cycles

Zero-point correction=	0.136968 (Hartree/Particle)
Thermal correction to Energy=	0.144501
Thermal correction to Enthalpy=	0.145445
Thermal correction to Gibbs Free Energy=	0.105083
Sum of electronic and zero-point Energies=	-451.514351
Sum of electronic and thermal Energies=	-451.506818
Sum of electronic and thermal Enthalpies=	-451.505874
Sum of electronic and thermal Free Energies=	-451.546236

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.675	30.808	84.949

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.701960	0.821776	0.024048
2	6	0	-0.161709	-0.471801	0.008824
3	6	0	1.245277	-0.648850	0.007593
4	6	0	1.474369	1.672449	-0.018491
5	6	0	-2.384503	-0.653594	-0.017727

6	1	0	2.192013	2.487912	-0.042463
7	1	0	-2.779120	1.394565	0.024704
8	7	0	1.850115	-1.873507	-0.038683
9	7	0	-2.088336	0.651423	0.015603
10	7	0	2.014024	0.440127	-0.016404
11	7	0	-1.249346	-1.352062	-0.021547
12	1	0	1.415574	-2.681567	0.386990
13	1	0	2.861891	-1.850725	0.037168
14	1	0	-3.380910	-1.071982	-0.041030
15	6	0	0.109999	1.955622	0.015644
16	1	0	-0.270807	2.969971	0.025202
17	1	0	-1.212668	-2.363657	-0.082703

N9-protonated N9H-amino Z3 (Z3-8) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.592211825 A.U. after 1 cycles

Zero-point correction= 0.135630 (Hartree/Particle)
Thermal correction to Energy= 0.143303
Thermal correction to Enthalpy= 0.144247
Thermal correction to Gibbs Free Energy= 0.103610
Sum of electronic and zero-point Energies= -451.456582
Sum of electronic and thermal Energies= -451.448909
Sum of electronic and thermal Enthalpies= -451.447965
Sum of electronic and thermal Free Energies= -451.488602

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.924	31.193	85.527

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.673840	0.798552	-0.000039
2	6	0	-0.152935	-0.494033	-0.000009
3	6	0	1.253552	-0.653970	0.000015
4	6	0	1.484716	1.663810	0.000022
5	6	0	-2.289783	-0.906847	0.000080
6	1	0	2.185546	2.495345	0.000139
7	1	0	-2.598122	1.044904	0.828596
8	7	0	1.858728	-1.852566	-0.000137
9	7	0	-2.149003	0.628750	-0.000062
10	7	0	2.031715	0.455056	0.000071
11	7	0	-1.157682	-1.471536	0.000060
12	1	0	1.335978	-2.717481	0.000195
13	1	0	2.870337	-1.889239	0.000009
14	1	0	-3.286522	-1.329000	0.000133
15	6	0	0.093754	1.939073	-0.000008
16	1	0	-0.288326	2.953410	-0.000024
17	1	0	-2.597977	1.044620	-0.828947

N7-protonated N9H-amino Z3 with HF hydrogen-bonded to N1 (Z3-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -552.109898733 A.U. after 8 cycles

Zero-point correction= 0.149092 (Hartree/Particle)
Thermal correction to Energy= 0.159101
Thermal correction to Enthalpy= 0.160045
Thermal correction to Gibbs Free Energy= 0.111946
Sum of electronic and zero-point Energies= -551.960807
Sum of electronic and thermal Energies= -551.950798
Sum of electronic and thermal Enthalpies= -551.949853
Sum of electronic and thermal Free Energies= -551.997953

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	99.837	37.570	101.233

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.316029	0.764181	0.001881
2	6	0	-0.651903	-0.468978	0.000194
3	6	0	0.768901	-0.515971	-0.001408
4	6	0	0.756923	1.838879	-0.002914
5	6	0	-2.844905	-0.869551	0.000503
6	1	0	1.390873	2.720667	-0.004909
7	1	0	-3.437852	1.131327	0.004007
8	7	0	1.497987	-1.649690	-0.006133
9	7	0	-2.677723	0.458760	0.002639
10	7	0	1.416284	0.664265	-0.003470
11	7	0	-1.646568	-1.452275	-0.000953
12	1	0	1.095289	-2.573588	0.023015
13	1	0	2.516474	-1.567150	0.000273
14	1	0	-3.795174	-1.384969	-0.000203
15	6	0	-0.626004	1.977978	0.000605
16	1	0	-1.109059	2.947396	0.001689
17	1	0	3.114748	0.384374	0.000490
18	9	0	3.898752	-0.189638	0.004824
19	1	0	-1.515822	-2.457951	-0.005525

N7H-amino Z3 with HF hydrogen-bonded to N1 (Z3-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -551.760300879 A.U. after 9 cycles

Zero-point correction= 0.135638 (Hartree/Particle)
Thermal correction to Energy= 0.145288
Thermal correction to Enthalpy= 0.146233
Thermal correction to Gibbs Free Energy= 0.099851

```
Sum of electronic and zero-point Energies=          -551.624663
Sum of electronic and thermal Energies=             -551.615013
Sum of electronic and thermal Enthalpies=           -551.614068
Sum of electronic and thermal Free Energies=        -551.660450

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   91.170             36.196             97.618


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.322883    0.767296   -0.000000
     2          6           0       -0.707223   -0.491915    0.000002
     3          6           0        0.707153   -0.566228    0.000009
     4          6           0        0.797309    1.778972    0.000007
     5          6           0       -2.798070   -0.895058   -0.000008
     6          1           0        1.464220    2.636642    0.000008
     7          1           0       -3.431309    1.148610   -0.000010
     8          7           0        1.360521   -1.751281    0.000020
     9          7           0       -2.672444    0.481255   -0.000006
    10          7           0        1.420811    0.575063    0.000009
    11          7           0       -1.643918   -1.512411   -0.000002
    12          1           0        0.836435   -2.613317   -0.000015
    13          1           0        2.374259   -1.767735   -0.000005
    14          1           0       -3.767801   -1.375554   -0.000013
    15          6           0       -0.574970    1.959834    0.000002
    16          1           0       -1.017173    2.949897    0.000000
    17          1           0        2.949395    0.300132   -0.000005
    18          9           0        3.858809   -0.127165   -0.000019
---------------------------------------------------------------------
```

Cartesian coordinates and energies (in Hartree) for species of isoguanine (2OA)

N9H-amino 2OA (2OA-1), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -542.569482088     A.U. after    1 cycles


Zero-point correction=                           0.116149 (Hartree/Particle)
Thermal correction to Energy=                    0.124582
Thermal correction to Enthalpy=                  0.125526
Thermal correction to Gibbs Free Energy=         0.082958
Sum of electronic and zero-point Energies=          -542.453333
Sum of electronic and thermal Energies=             -542.444901
Sum of electronic and thermal Enthalpies=           -542.443956
Sum of electronic and thermal Free Energies=        -542.486524

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   78.176             33.319             89.592
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.490993	-0.931462	-0.004038
2	6	0	0.758142	0.459278	-0.005752
3	6	0	-0.342610	1.305613	-0.003595
4	6	0	-1.770351	-0.767310	0.002175
5	6	0	2.673542	-0.458058	0.005078
6	1	0	1.941200	-2.487866	0.004705
7	7	0	-0.262407	2.661535	-0.051586
8	7	0	1.750027	-1.494796	0.001038
9	7	0	-1.545536	0.675934	0.005693
10	7	0	2.122250	0.725707	0.002462
11	1	0	0.656268	3.063397	0.088818
12	1	0	-1.046404	3.228845	0.240521
13	1	0	3.738571	-0.650001	0.010976
14	1	0	-2.409513	1.206189	-0.026689
15	8	0	-2.940599	-1.125893	0.001160
16	7	0	-0.666280	-1.568635	0.000847

N9H-amino 2OA (2OA-1), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -542.618627289 A.U. after 1 cycles

Zero-point correction= 0.115978 (Hartree/Particle)
Thermal correction to Energy= 0.124489
Thermal correction to Enthalpy= 0.125433
Thermal correction to Gibbs Free Energy= 0.082532
Sum of electronic and zero-point Energies= -542.502649
Sum of electronic and thermal Energies= -542.494139
Sum of electronic and thermal Enthalpies= -542.493195
Sum of electronic and thermal Free Energies= -542.536095

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.118	33.035	90.292

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.530107	-0.909236	-0.000001
2	6	0	0.755820	0.476161	0.000017
3	6	0	-0.374005	1.302460	0.000001
4	6	0	-1.727708	-0.774669	0.000011
5	6	0	2.689687	-0.413405	0.000006
6	1	0	2.015718	-2.444238	0.000007
7	7	0	-0.361421	2.637158	-0.000197
8	7	0	1.787555	-1.455496	0.000004
9	7	0	-1.563453	0.632731	0.000062

10	7	0	2.115764	0.767096	-0.000002
11	1	0	0.520749	3.134456	0.000405
12	1	0	-1.219203	3.177510	0.000451
13	1	0	3.755581	-0.593797	0.000035
14	1	0	-2.428276	1.168958	0.000211
15	8	0	-2.909644	-1.202204	-0.000031
16	7	0	-0.637133	-1.569078	-0.000018

N3H-amino 2OA (2OA-2), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.571202997 A.U. after 11 cycles

Zero-point correction=	0.116731 (Hartree/Particle)
Thermal correction to Energy=	0.125123
Thermal correction to Enthalpy=	0.126067
Thermal correction to Gibbs Free Energy=	0.083506
Sum of electronic and zero-point Energies=	-542.454472
Sum of electronic and thermal Energies=	-542.446080
Sum of electronic and thermal Enthalpies=	-542.445136
Sum of electronic and thermal Free Energies=	-542.487697

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.516	32.988	89.578

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.574204	-0.976112	0.006338
2	6	0	-0.829725	0.420592	0.010257
3	6	0	0.223200	1.310555	0.003384
4	6	0	1.812880	-0.611444	-0.002990
5	6	0	-2.646033	-0.636317	-0.006549
6	7	0	0.088611	2.660228	0.051773
7	7	0	-1.706577	-1.657513	-0.004916
8	7	0	1.489345	0.763214	-0.007573
9	7	0	-2.197815	0.612424	-0.001099
10	1	0	-0.856742	3.007553	-0.063219
11	1	0	0.826500	3.264002	-0.285342
12	1	0	-3.704367	-0.869260	-0.014058
13	1	0	2.308273	1.357839	0.044472
14	8	0	2.977959	-0.980544	0.000237
15	7	0	0.722536	-1.451472	-0.001443
16	1	0	0.913239	-2.447591	-0.003585

N3H-amino 2OA (2OA-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -542.614693486 A.U. after 1 cycles

```
Zero-point correction=                           0.116089 (Hartree/Particle)
Thermal correction to Energy=                    0.124523
Thermal correction to Enthalpy=                  0.125467
Thermal correction to Gibbs Free Energy=         0.082843
Sum of electronic and zero-point Energies=           -542.498605
Sum of electronic and thermal Energies=              -542.490170
Sum of electronic and thermal Enthalpies=            -542.489226
Sum of electronic and thermal Free Energies=         -542.531851

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   78.140             33.040             89.711


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.596404   -0.947026   -0.000203
     2          6           0        0.826390    0.438611   -0.000119
     3          6           0       -0.260778    1.316034   -0.000133
     4          6           0       -1.777229   -0.641038    0.000000
     5          6           0        2.668993   -0.591831    0.000185
     6          7           0       -0.186999    2.646280    0.000361
     7          7           0        1.752149   -1.618763    0.000012
     8          7           0       -1.505063    0.725278   -0.000754
     9          7           0        2.194090    0.652412    0.000171
    10          1           0        0.718749    3.100143   -0.000233
    11          1           0       -1.016691    3.229700    0.000218
    12          1           0        3.731596   -0.801316    0.000386
    13          1           0       -2.332176    1.319208    0.000116
    14          8           0       -2.945303   -1.056124    0.000608
    15          7           0       -0.684023   -1.460125   -0.000414
    16          1           0       -0.852819   -2.462818    0.000630
---------------------------------------------------------------------
```

N3H-amino 2OA (2OA-2), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

```
SCF Done:  E(RB3LYP) =  -542.645842167     A.U. after    1 cycles


Zero-point correction=                           0.107437 (Hartree/Particle)
Thermal correction to Energy=                    0.115801
Thermal correction to Enthalpy=                  0.116745
Thermal correction to Gibbs Free Energy=         0.074311
Sum of electronic and zero-point Energies=           -542.538406
Sum of electronic and thermal Energies=              -542.530041
Sum of electronic and thermal Enthalpies=            -542.529097
Sum of electronic and thermal Free Energies=         -542.571531

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   72.666             33.091             89.310
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.597952	-0.941302	0.000028
2	6	0	0.824877	0.441882	-0.000008
3	6	0	-0.270973	1.315924	-0.000029
4	6	0	-1.769749	-0.647054	-0.000052
5	6	0	2.675721	-0.581836	-0.000046
6	7	0	-0.204373	2.644417	0.000006
7	7	0	1.763355	-1.609045	0.000062
8	7	0	-1.509021	0.719500	0.000000
9	7	0	2.193468	0.661571	0.000061
10	1	0	0.715201	3.113431	-0.000140
11	1	0	-1.061246	3.223237	-0.000248
12	1	0	3.743755	-0.786080	-0.000023
13	1	0	-2.379110	1.346440	-0.000104
14	8	0	-2.937809	-1.071761	-0.000001
15	7	0	-0.674834	-1.463620	0.000020
16	1	0	-0.843261	-2.518387	0.000119

N7H-amino 2OA (2OA-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.547002275 A.U. after 10 cycles

Zero-point correction=	0.115394 (Hartree/Particle)
Thermal correction to Energy=	0.124065
Thermal correction to Enthalpy=	0.125009
Thermal correction to Gibbs Free Energy=	0.081871
Sum of electronic and zero-point Energies=	-542.431609
Sum of electronic and thermal Energies=	-542.422937
Sum of electronic and thermal Enthalpies=	-542.421993
Sum of electronic and thermal Free Energies=	-542.465131

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.852	33.757	90.791

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.505147	-0.974073	-0.008853
2	6	0	-0.740328	0.435506	0.044960
3	6	0	0.336837	1.292687	0.007411
4	6	0	1.774137	-0.768381	0.003641
5	6	0	-2.634276	-0.684476	0.000034
6	7	0	0.282584	2.670033	0.028738
7	7	0	-1.734115	-1.630831	-0.040574
8	7	0	1.544786	0.671266	0.009242
9	7	0	-2.129447	0.595500	0.006263

10	1	0	-0.567038	3.089008	-0.328807
11	1	0	1.112751	3.164110	-0.277685
12	1	0	-3.704353	-0.855122	0.015684
13	1	0	2.404489	1.208855	0.034330
14	8	0	2.945942	-1.121944	0.026361
15	7	0	0.672559	-1.569925	-0.036997
16	1	0	-2.655289	1.408818	0.295729

N9-deprotonated N9H-amino 2OA (2OA-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.025953809 A.U. after 1 cycles

Zero-point correction= 0.103142 (Hartree/Particle)
Thermal correction to Energy= 0.111208
Thermal correction to Enthalpy= 0.112153
Thermal correction to Gibbs Free Energy= 0.070125
Sum of electronic and zero-point Energies= -541.922812
Sum of electronic and thermal Energies= -541.914745
Sum of electronic and thermal Enthalpies= -541.913801
Sum of electronic and thermal Free Energies= -541.955829

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.784	31.397	88.454

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.524560	-1.004113	-0.006432
2	6	0	0.804015	0.414284	-0.023521
3	6	0	-0.255901	1.278411	-0.016060
4	6	0	-1.760672	-0.717929	0.004340
5	6	0	2.621094	-0.628356	0.010623
6	7	0	-0.157804	2.673565	-0.075369
7	7	0	1.718826	-1.652176	0.014282
8	7	0	-1.496121	0.706364	0.007507
9	7	0	2.173466	0.632018	-0.006889
10	1	0	0.811402	2.957293	0.044451
11	1	0	-0.757572	3.156897	0.588907
12	1	0	3.688379	-0.839533	0.023583
13	1	0	-2.327477	1.275558	-0.091990
14	8	0	-2.968256	-1.027887	-0.003128
15	7	0	-0.705118	-1.557042	0.009951

N1-protonated N9H-amino 2OA (2OA-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.934567897 A.U. after 1 cycles

```
Zero-point correction=                           0.127682 (Hartree/Particle)
Thermal correction to Energy=                    0.137490
Thermal correction to Enthalpy=                  0.138434
Thermal correction to Gibbs Free Energy=         0.091986
Sum of electronic and zero-point Energies=           -542.806886
Sum of electronic and thermal Energies=              -542.797078
Sum of electronic and thermal Enthalpies=            -542.796134
Sum of electronic and thermal Free Energies=         -542.842582

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   86.276             36.722             97.758


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.513416   -0.402731    0.000157
     2          6           0        0.870479   -0.261196   -0.000039
     3          6           0        1.684081    0.934249   -0.000038
     4          6           0       -2.695590    0.621439   -0.000147
     5          6           0        0.505124   -2.373572    0.000025
     6          1           0       -1.628519   -2.224935   -0.000657
     7          7           0        3.001199    0.767153   -0.000391
     8          7           0       -0.728463   -1.757328    0.000411
     9          7           0        1.128810    2.145941    0.000412
    10          7           0        1.476918   -1.501280   -0.000145
    11          1           0        3.360049   -0.183924   -0.000709
    12          1           0        3.659712    1.535865   -0.000604
    13          1           0        0.612132   -3.449878    0.000127
    14          1           0        1.680493    2.995044    0.000148
    15          8           0       -3.846003    0.795625   -0.000485
    16          7           0       -1.469871    0.575571    0.000451
    17          1           0        0.119937    2.243285    0.000659
---------------------------------------------------------------------
```

O2-protonated (N1 side) N9H-amino 2OA (2OA-6), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -542.928771024     A.U. after    9 cycles


Zero-point correction=                           0.128733 (Hartree/Particle)
Thermal correction to Energy=                    0.137603
Thermal correction to Enthalpy=                  0.138547
Thermal correction to Gibbs Free Energy=         0.095127
Sum of electronic and zero-point Energies=           -542.800038
Sum of electronic and thermal Energies=              -542.791168
Sum of electronic and thermal Enthalpies=            -542.790224
Sum of electronic and thermal Free Energies=         -542.833644

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   86.347             34.793             91.386
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.520103	-0.932727	0.000000
2	6	0	0.819520	0.438747	-0.000000
3	6	0	-0.251856	1.334759	0.000000
4	6	0	-1.678837	-0.644810	0.000000
5	6	0	2.694744	-0.542422	-0.000000
6	1	0	1.897672	-2.547336	0.000001
7	7	0	-0.126475	2.662370	-0.000000
8	7	0	1.734818	-1.545801	0.000000
9	7	0	-1.498099	0.738406	-0.000000
10	7	0	2.178932	0.661151	-0.000000
11	1	0	0.808624	3.056869	0.000001
12	1	0	-0.906078	3.307244	0.000002
13	1	0	3.752518	-0.770414	-0.000000
14	1	0	-2.316119	1.340281	-0.000003
15	8	0	-2.919592	-1.121475	-0.000001
16	7	0	-0.700031	-1.499272	0.000001
17	1	0	-3.625943	-0.454105	0.000004

O2-protonated (N3 side) N9H-amino 2OA (2OA-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.945031921 A.U. after 1 cycles

Zero-point correction= 0.129935 (Hartree/Particle)
Thermal correction to Energy= 0.138255
Thermal correction to Enthalpy= 0.139199
Thermal correction to Gibbs Free Energy= 0.097013
Sum of electronic and zero-point Energies= -542.815097
Sum of electronic and thermal Energies= -542.806777
Sum of electronic and thermal Enthalpies= -542.805833
Sum of electronic and thermal Free Energies= -542.848019

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.756	33.797	88.788

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.513132	-0.937222	-0.000080
2	6	0	0.815489	0.432610	-0.000254
3	6	0	-0.251778	1.340720	-0.000126
4	6	0	-1.678352	-0.617133	-0.000043
5	6	0	2.689143	-0.554511	-0.000200
6	1	0	1.887303	-2.556369	0.000585
7	7	0	-0.114127	2.665435	0.000439
8	7	0	1.725300	-1.554987	0.000302

9	7	0	-1.495476	0.754357	-0.000208
10	7	0	2.175533	0.649478	-0.000081
11	1	0	0.823453	3.053759	-0.000295
12	1	0	-0.891755	3.313240	0.000206
13	1	0	3.746026	-0.786367	-0.000170
14	1	0	-2.339400	1.322284	-0.000555
15	8	0	-2.963966	-0.943865	0.000169
16	7	0	-0.717383	-1.495205	0.000141
17	1	0	-3.056633	-1.915960	-0.001059

N3-protonated N9H-amino 2OA (2OA-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.948929838 A.U. after 9 cycles

Zero-point correction= 0.130030 (Hartree/Particle)
Thermal correction to Energy= 0.138453
Thermal correction to Enthalpy= 0.139398
Thermal correction to Gibbs Free Energy= 0.096864
Sum of electronic and zero-point Energies= -542.818900
Sum of electronic and thermal Energies= -542.810476
Sum of electronic and thermal Enthalpies= -542.809532
Sum of electronic and thermal Free Energies= -542.852066

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.881	33.927	89.520

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.542165	-0.927080	-0.000000
2	6	0	0.778847	0.443480	-0.000000
3	6	0	-0.315070	1.332682	0.000000
4	6	0	-1.838705	-0.643782	0.000000
5	6	0	2.699921	-0.462123	-0.000000
6	1	0	1.984222	-2.498096	0.000001
7	7	0	-0.171323	2.651876	-0.000000
8	7	0	1.767423	-1.507334	0.000000
9	7	0	-1.548808	0.747486	0.000001
10	7	0	2.132899	0.710260	-0.000000
11	1	0	0.767057	3.040102	-0.000001
12	1	0	-0.949702	3.299942	-0.000000
13	1	0	3.763431	-0.659452	-0.000000
14	1	0	-2.392955	1.314632	0.000002
15	8	0	-2.971856	-1.054247	-0.000001
16	7	0	-0.709230	-1.467496	0.000001
17	1	0	-0.896870	-2.465760	-0.000004

N3-protonated N9H-amino 2OA (2OA-8), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -543.066157837   A.U. after   1 cycles

Zero-point correction=   0.129414 (Hartree/Particle)
Thermal correction to Energy=   0.137873
Thermal correction to Enthalpy=   0.138817
Thermal correction to Gibbs Free Energy=   0.096256
Sum of electronic and zero-point Energies=   -542.936744
Sum of electronic and thermal Energies=   -542.928285
Sum of electronic and thermal Enthalpies=   -542.927341
Sum of electronic and thermal Free Energies=   -542.969901

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.517	34.005	89.577

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.568830	-0.894175	0.000000
2	6	0	0.780906	0.478051	0.000000
3	6	0	-0.343250	1.330528	0.000000
4	6	0	-1.793492	-0.678822	0.000000
5	6	0	2.708733	-0.426610	0.000000
6	1	0	2.008964	-2.459388	0.000000
7	7	0	-0.293100	2.650566	0.000000
8	7	0	1.793851	-1.465713	0.000000
9	7	0	-1.558561	0.697325	0.000000
10	7	0	2.139110	0.753640	0.000000
11	1	0	0.605125	3.122735	0.000000
12	1	0	-1.134984	3.219057	0.000001
13	1	0	3.771558	-0.621063	0.000000
14	1	0	-2.407259	1.262393	0.000000
15	8	0	-2.935493	-1.132952	0.000000
16	7	0	-0.665878	-1.469395	0.000000
17	1	0	-0.797765	-2.478918	-0.000001

N3-protonated N9H-amino 2OA (2OA-8), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -543.109724999   A.U. after   1 cycles

Zero-point correction=   0.115527 (Hartree/Particle)
Thermal correction to Energy=   0.124026
Thermal correction to Enthalpy=   0.124970
Thermal correction to Gibbs Free Energy=   0.082371
Sum of electronic and zero-point Energies=   -542.994198
Sum of electronic and thermal Energies=   -542.985699
Sum of electronic and thermal Enthalpies=   -542.984755
Sum of electronic and thermal Free Energies=   -543.027354

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.827	34.391	89.656

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.575208	-0.886817	-0.000000
2	6	0	0.778351	0.486884	0.000000
3	6	0	-0.354698	1.330494	0.000000
4	6	0	-1.782335	-0.686787	-0.000000
5	6	0	2.709041	-0.414993	-0.000000
6	1	0	2.029117	-2.507890	-0.000000
7	7	0	-0.313059	2.650708	0.000000
8	7	0	1.802707	-1.455453	-0.000000
9	7	0	-1.565010	0.689833	0.000000
10	7	0	2.136646	0.768285	0.000000
11	1	0	0.599485	3.139872	0.000000
12	1	0	-1.183834	3.213878	0.000000
13	1	0	3.780171	-0.600358	-0.000000
14	1	0	-2.464409	1.289374	0.000000
15	8	0	-2.924363	-1.154736	-0.000000
16	7	0	-0.652762	-1.471418	-0.000000
17	1	0	-0.778690	-2.543354	-0.000000

N6-protonated N9H-amino 2OA (2OA-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.875745081 A.U. after 9 cycles

Zero-point correction= 0.129665 (Hartree/Particle)
Thermal correction to Energy= 0.138392
Thermal correction to Enthalpy= 0.139336
Thermal correction to Gibbs Free Energy= 0.095934
Sum of electronic and zero-point Energies= -542.746080
Sum of electronic and thermal Energies= -542.737353
Sum of electronic and thermal Enthalpies= -542.736409
Sum of electronic and thermal Free Energies= -542.779811

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.842	33.654	91.347

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.454589	-1.012795	0.000000
2	6	0	-0.762093	0.400617	0.000001
3	6	0	0.309680	1.223850	0.000001

4	6	0	1.822150	-0.755180	-0.000000
5	6	0	-2.641868	-0.565351	0.000000
6	1	0	-1.898245	-2.583907	-0.000001
7	7	0	0.093509	2.686386	-0.000001
8	7	0	-1.707804	-1.587581	-0.000001
9	7	0	1.556741	0.700591	-0.000001
10	7	0	-2.124564	0.637908	0.000001
11	1	0	-0.931358	2.840524	-0.000002
12	1	0	0.483176	3.151770	-0.834361
13	1	0	-3.704331	-0.775455	-0.000000
14	1	0	2.405750	1.258749	0.000003
15	8	0	2.977750	-1.096799	0.000001
16	7	0	0.710711	-1.582435	-0.000002
17	1	0	0.483176	3.151774	0.834356

N7-protonated N9H-amino 2OA (2OA-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.918809389 A.U. after 8 cycles

Zero-point correction=	0.128794 (Hartree/Particle)
Thermal correction to Energy=	0.137678
Thermal correction to Enthalpy=	0.138622
Thermal correction to Gibbs Free Energy=	0.095069
Sum of electronic and zero-point Energies=	-542.790016
Sum of electronic and thermal Energies=	-542.781131
Sum of electronic and thermal Enthalpies=	-542.780187
Sum of electronic and thermal Free Energies=	-542.823740

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.394	34.878	91.666

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.477276	-0.911148	0.000000
2	6	0	0.701559	0.486289	0.000000
3	6	0	-0.427423	1.322300	0.000000
4	6	0	-1.781843	-0.824207	0.000000
5	6	0	2.690185	-0.511085	-0.000000
6	1	0	1.945290	-2.477875	-0.000000
7	7	0	-0.422562	2.667158	-0.000000
8	7	0	1.764214	-1.477858	0.000000
9	7	0	-1.592564	0.638227	0.000000
10	7	0	2.088970	0.677227	-0.000000
11	1	0	0.431490	3.206154	0.000000
12	1	0	-1.284397	3.198635	0.000000
13	1	0	3.760328	-0.664283	-0.000000
14	1	0	-2.479181	1.136434	0.000000
15	8	0	-2.920257	-1.221895	-0.000000
16	7	0	-0.633488	-1.583384	0.000000

17	1	0	2.598009	1.553611	-0.000000

N9-protonated N9H-amino 2OA (2OA-11), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.872000472 A.U. after 9 cycles

Zero-point correction=	0.128506 (Hartree/Particle)
Thermal correction to Energy=	0.137140
Thermal correction to Enthalpy=	0.138084
Thermal correction to Gibbs Free Energy=	0.095059
Sum of electronic and zero-point Energies=	-542.743495
Sum of electronic and thermal Energies=	-542.734861
Sum of electronic and thermal Enthalpies=	-542.733916
Sum of electronic and thermal Free Energies=	-542.776941

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.057	34.341	90.553

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.467677	-0.866751	-0.000000
2	6	0	0.696244	0.511883	-0.000000
3	6	0	-0.453153	1.324049	-0.000000
4	6	0	-1.782027	-0.816254	-0.000000
5	6	0	2.737181	-0.224867	0.000000
6	1	0	1.997535	-2.067441	0.827624
7	7	0	-0.430796	2.658159	-0.000000
8	7	0	1.851216	-1.470613	0.000000
9	7	0	-1.621023	0.627354	0.000000
10	7	0	2.045380	0.842312	0.000000
11	1	0	0.456466	3.147513	0.000000
12	1	0	-1.272961	3.219932	0.000000
13	1	0	3.811853	-0.349954	0.000000
14	1	0	-2.512536	1.116734	0.000001
15	8	0	-2.896958	-1.269821	0.000000
16	7	0	-0.601600	-1.572802	-0.000000
17	1	0	1.997535	-2.067441	-0.827624

N7-protonated N9H-amino 2OA with HF hydrogen-bonded to N3 (2OA-12), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -643.382760981 A.U. after 1 cycles

Zero-point correction=	0.141501 (Hartree/Particle)
Thermal correction to Energy=	0.152318
Thermal correction to Enthalpy=	0.153262
Thermal correction to Gibbs Free Energy=	0.105005

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Sum of electronic and zero-point Energies=          -643.241260
Sum of electronic and thermal Energies=             -643.230443
Sum of electronic and thermal Enthalpies=           -643.229499
Sum of electronic and thermal Free Energies=        -643.277756

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   95.581             41.236           101.567


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.000000    0.638220   -0.000000
     2          6           0       -1.096734   -0.243867   -0.000000
     3          6           0       -0.821606   -1.623952    0.000000
     4          6           0        1.626012   -0.958985    0.000000
     5          6           0       -1.881908    1.837917   -0.000000
     6          1           0        0.052090    2.757204   -0.000000
     7          7           0       -1.728234   -2.613657    0.000000
     8          7           0       -0.549387    1.921746   -0.000000
     9          7           0        0.501786   -1.903427    0.000000
    10          7           0       -2.248616    0.554523   -0.000000
    11          1           0       -2.722873   -2.436396    0.000000
    12          1           0       -1.450284   -3.587704    0.000000
    13          1           0       -2.564228    2.676767   -0.000000
    14          1           0        0.819992   -2.869587    0.000000
    15          8           0        2.738225   -1.423263    0.000000
    16          7           0        1.283815    0.375613    0.000000
    17          1           0       -3.216591    0.254500   -0.000000
    18          1           0        2.109710    1.979633   -0.000000
    19          9           0        1.921807    2.930234   -0.000000
---------------------------------------------------------------------
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N7H-amino 2OA with HF hydrogen-bonded to N3 (2OA-13), B3LYP/6-31+G(d)

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SCF Done:  E(RB3LYP) =  -643.012101076     A.U. after    9 cycles


Zero-point correction=                           0.127642 (Hartree/Particle)
Thermal correction to Energy=                    0.138739
Thermal correction to Enthalpy=                  0.139684
Thermal correction to Gibbs Free Energy=         0.089617
Sum of electronic and zero-point Energies=          -642.884460
Sum of electronic and thermal Energies=             -642.873362
Sum of electronic and thermal Enthalpies=           -642.872418
Sum of electronic and thermal Free Energies=        -642.922484

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   87.060             40.752           105.373


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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.199665	-0.769505	-0.022129
2	6	0	1.174639	-0.392605	-0.034706
3	6	0	1.507355	0.946405	0.011951
4	6	0	-0.961666	1.407418	-0.035678
5	6	0	0.943373	-2.580501	-0.017641
6	7	0	2.776899	1.466471	0.019899
7	7	0	-0.293602	-2.150289	-0.007721
8	7	0	0.441356	1.786908	-0.010376
9	7	0	1.893040	-1.590290	0.002537
10	1	0	3.520014	0.867743	0.355891
11	1	0	2.888461	2.433335	0.300510
12	1	0	1.229507	-3.625269	-0.031619
13	1	0	0.573929	2.792610	-0.022007
14	8	0	-1.771358	2.319735	-0.063799
15	7	0	-1.230758	0.067681	-0.016046
16	1	0	2.872108	-1.728586	-0.205549
17	1	0	-2.868170	-0.488953	0.040074
18	9	0	-3.770861	-0.837711	0.082696

Cartesian coordinates and energies (in Hartree) for species of isoguanine with cytosine-like face (2OA-cyto)

N9H-amino 2OA-cyto (2OA-cyto-1), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.568914877 A.U. after 8 cycles

Zero-point correction= 0.115547 (Hartree/Particle)
Thermal correction to Energy= 0.124325
Thermal correction to Enthalpy= 0.125269
Thermal correction to Gibbs Free Energy= 0.081811
Sum of electronic and zero-point Energies= -542.453368
Sum of electronic and thermal Energies= -542.444590
Sum of electronic and thermal Enthalpies= -542.443646
Sum of electronic and thermal Free Energies= -542.487104

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.015	33.894	91.466

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.529342	-0.908859	0.000000
2	6	0	0.754972	0.454028	-0.000000
3	6	0	-0.400030	1.302981	-0.000000
4	6	0	-1.861878	-0.550766	0.000000
5	6	0	2.690741	-0.446222	-0.000000

6	7	0	-0.241202	2.644495	0.000000
7	7	0	1.766515	-1.493143	0.000000
8	7	0	-1.625882	0.801403	0.000000
9	7	0	2.113634	0.725613	-0.000000
10	1	0	0.681351	3.054570	-0.000000
11	1	0	-1.060343	3.235880	0.000000
12	1	0	3.755181	-0.636063	-0.000000
13	8	0	-2.968340	-1.073687	-0.000000
14	7	0	-0.721693	-1.431005	0.000000
15	1	0	-0.928022	-2.422217	0.000000
16	1	0	1.980054	-2.481181	0.000000

N9H-amino 2OA-cyto (2OA-cyto-1), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -542.616207858 A.U. after 1 cycles

Zero-point correction= 0.115773 (Hartree/Particle)
Thermal correction to Energy= 0.124305
Thermal correction to Enthalpy= 0.125249
Thermal correction to Gibbs Free Energy= 0.082381
Sum of electronic and zero-point Energies= -542.500435
Sum of electronic and thermal Energies= -542.491903
Sum of electronic and thermal Enthalpies= -542.490959
Sum of electronic and thermal Free Energies= -542.533827

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.003	33.275	90.223

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.535006	-0.892718	0.000087
2	6	0	0.753395	0.472389	0.000165
3	6	0	-0.396698	1.312429	0.000036
4	6	0	-1.818880	-0.571817	0.000007
5	6	0	2.681874	-0.449279	-0.000097
6	7	0	-0.280627	2.648977	0.000123
7	7	0	1.760667	-1.480779	-0.000045
8	7	0	-1.629178	0.774613	0.000011
9	7	0	2.118490	0.736765	-0.000044
10	1	0	0.628275	3.093554	-0.000414
11	1	0	-1.108973	3.231676	-0.000623
12	1	0	3.743683	-0.649894	-0.000161
13	8	0	-2.960823	-1.093362	-0.000125
14	7	0	-0.711901	-1.429282	0.000095
15	1	0	-0.875474	-2.432057	0.000028
16	1	0	1.968743	-2.474458	-0.000006

N1H-amino 2OA-cyto (2OA-cyto-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -542.614693608 A.U. after 1 cycles

Zero-point correction= 0.116088 (Hartree/Particle)
Thermal correction to Energy= 0.124523
Thermal correction to Enthalpy= 0.125467
Thermal correction to Gibbs Free Energy= 0.082841
Sum of electronic and zero-point Energies= -542.498606
Sum of electronic and thermal Energies= -542.490171
Sum of electronic and thermal Enthalpies= -542.489226
Sum of electronic and thermal Free Energies= -542.531853

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.139	33.041	89.714

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.596345	-0.947069	-0.000024
2	6	0	0.826411	0.438593	0.000104
3	6	0	-0.260639	1.316116	0.000082
4	6	0	-1.777254	-0.640903	0.000120
5	6	0	2.668895	-0.591975	-0.000064
6	7	0	-0.186821	2.646263	0.000028
7	7	0	1.752061	-1.618836	0.000056
8	7	0	-1.505070	0.725311	-0.000011
9	7	0	2.194112	0.652336	-0.000015
10	1	0	0.719029	3.099904	-0.000287
11	1	0	-1.016330	3.229878	-0.000276
12	1	0	3.731512	-0.801459	-0.000182
13	8	0	-2.945365	-1.056018	-0.000069
14	7	0	-0.684085	-1.460103	-0.000033
15	1	0	-0.853024	-2.462765	-0.000103
16	1	0	-2.332189	1.319212	-0.000088

N7H-amino 2OA-cyto (2OA-cyto-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.567730709 A.U. after 8 cycles

Zero-point correction= 0.116275 (Hartree/Particle)
Thermal correction to Energy= 0.124712
Thermal correction to Enthalpy= 0.125656
Thermal correction to Gibbs Free Energy= 0.082907
Sum of electronic and zero-point Energies= -542.451456
Sum of electronic and thermal Energies= -542.443019
Sum of electronic and thermal Enthalpies= -542.442075
Sum of electronic and thermal Free Energies= -542.484824

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.258	33.177	89.973

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.541841	-0.935494	0.024465
2	6	0	0.742747	0.436246	-0.001066
3	6	0	-0.394016	1.296748	0.002295
4	6	0	-1.852941	-0.570615	-0.007756
5	6	0	2.646511	-0.683372	-0.017840
6	7	0	-0.260196	2.665792	-0.045069
7	7	0	1.718857	-1.627858	0.019369
8	7	0	-1.610335	0.794464	-0.003621
9	7	0	2.129533	0.578353	-0.024648
10	1	0	0.548627	3.088489	0.391646
11	1	0	-1.128985	3.167212	0.105860
12	1	0	3.712484	-0.866731	-0.039466
13	8	0	-2.971983	-1.064126	-0.031183
14	7	0	-0.723713	-1.430799	0.035797
15	1	0	-0.900477	-2.428610	0.042597
16	1	0	2.660332	1.431909	-0.124562

N9-deprotonated N9H-amino 2OA-cyto (2OA-cyto-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.047892792 A.U. after 1 cycles

Zero-point correction=	0.103695 (Hartree/Particle)
Thermal correction to Energy=	0.111643
Thermal correction to Enthalpy=	0.112587
Thermal correction to Gibbs Free Energy=	0.070774
Sum of electronic and zero-point Energies=	-541.944197
Sum of electronic and thermal Energies=	-541.936250
Sum of electronic and thermal Enthalpies=	-541.935306
Sum of electronic and thermal Free Energies=	-541.977118

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.057	31.243	88.003

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.559809	-0.956708	-0.012262
2	6	0	0.803477	0.422832	-0.021860
3	6	0	-0.312277	1.283100	-0.018669
4	6	0	-1.832251	-0.518265	0.001582

5	6	0	2.634935	-0.625959	0.016727
6	7	0	-0.133252	2.654924	-0.065002
7	7	0	1.712591	-1.648016	0.008995
8	7	0	-1.568398	0.831702	-0.000692
9	7	0	2.174768	0.628135	0.001307
10	1	0	0.777760	2.978281	0.236843
11	1	0	-0.925994	3.191251	0.265367
12	1	0	3.698651	-0.845660	0.035171
13	8	0	-2.980023	-0.997186	0.019944
14	7	0	-0.739417	-1.406903	-0.014719
15	1	0	-0.956431	-2.395283	0.000723

N1-protonated N9H-amino 2OA-cyto (2OA-cyto-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.948929838 A.U. after 8 cycles

Zero-point correction= 0.130030 (Hartree/Particle)
Thermal correction to Energy= 0.138453
Thermal correction to Enthalpy= 0.139398
Thermal correction to Gibbs Free Energy= 0.096864
Sum of electronic and zero-point Energies= -542.818900
Sum of electronic and thermal Energies= -542.810476
Sum of electronic and thermal Enthalpies= -542.809532
Sum of electronic and thermal Free Energies= -542.852066

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.881	33.927	89.520

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.542165	-0.927080	0.000000
2	6	0	0.778848	0.443480	-0.000000
3	6	0	-0.315070	1.332682	0.000000
4	6	0	-1.838706	-0.643782	-0.000000
5	6	0	2.699921	-0.462123	-0.000000
6	7	0	-0.171323	2.651877	0.000000
7	7	0	1.767423	-1.507334	0.000000
8	7	0	-1.548808	0.747487	0.000000
9	7	0	2.132899	0.710260	-0.000000
10	1	0	0.767058	3.040102	-0.000000
11	1	0	-0.949702	3.299942	-0.000000
12	1	0	3.763431	-0.659452	-0.000000
13	8	0	-2.971857	-1.054247	-0.000000
14	7	0	-0.709230	-1.467496	0.000000
15	1	0	-0.896870	-2.465760	-0.000000
16	1	0	1.984222	-2.498097	0.000000
17	1	0	-2.392956	1.314632	-0.000000

N1-protonated N9H-amino 2OA-cyto (2OA-cyto-5), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

```
 SCF Done:  E(RB3LYP) =  -543.066157783     A.U. after    1 cycles


 Zero-point correction=                           0.129421 (Hartree/Particle)
 Thermal correction to Energy=                    0.137877
 Thermal correction to Enthalpy=                  0.138821
 Thermal correction to Gibbs Free Energy=         0.096266
 Sum of electronic and zero-point Energies=           -542.936736
 Sum of electronic and thermal Energies=              -542.928280
 Sum of electronic and thermal Enthalpies=            -542.927336
 Sum of electronic and thermal Free Energies=         -542.969892

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.519             33.996             89.565


 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        0.568864   -0.894110    0.000077
      2          6           0        0.780994    0.478035   -0.000047
      3          6           0       -0.343199    1.330404    0.000312
      4          6           0       -1.793400   -0.678767    0.000269
      5          6           0        2.708841   -0.426608   -0.000156
      6          7           0       -0.293422    2.650584   -0.000082
      7          7           0        1.793882   -1.465513    0.000264
      8          7           0       -1.558477    0.697090    0.000159
      9          7           0        2.139219    0.753604   -0.000632
     10          1           0        0.604578    3.123346    0.000749
     11          1           0       -1.135722    3.218595    0.000902
     12          1           0        3.771680   -0.621025   -0.000174
     13          8           0       -2.935497   -1.133104   -0.000655
     14          7           0       -0.665936   -1.469235    0.000436
     15          1           0       -0.797865   -2.478775   -0.000053
     16          1           0        2.008815   -2.459268    0.000393
     17          1           0       -2.406966    1.262523   -0.000331
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```

O2-protonated (N1 side) N9H-amino (2OA-cyto-6), B3LYP/6-31+G(d)

```
 SCF Done:  E(RB3LYP) =  -542.944335253     A.U. after    1 cycles


 Zero-point correction=                           0.129983 (Hartree/Particle)
 Thermal correction to Energy=                    0.138267
 Thermal correction to Enthalpy=                  0.139211
 Thermal correction to Gibbs Free Energy=         0.097034
 Sum of electronic and zero-point Energies=           -542.814353
 Sum of electronic and thermal Energies=              -542.806068
 Sum of electronic and thermal Enthalpies=            -542.805124
```

Sum of electronic and thermal Free Energies= -542.847301

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.764	33.724	88.770

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.556725	-0.911912	-0.000199
2	6	0	0.803956	0.453264	-0.000133
3	6	0	-0.311048	1.335230	-0.000054
4	6	0	-1.728854	-0.490831	0.000030
5	6	0	2.712511	-0.486265	0.000106
6	7	0	-0.176924	2.655130	-0.000071
7	7	0	1.771491	-1.518160	0.000121
8	7	0	-1.565192	0.806439	0.000184
9	7	0	2.160849	0.696580	-0.000030
10	1	0	0.743703	3.079563	0.000696
11	1	0	-0.995202	3.252876	-0.000505
12	1	0	3.773628	-0.696619	0.000296
13	8	0	-2.931263	-1.045086	0.000216
14	7	0	-0.717134	-1.413013	-0.000094
15	1	0	1.976297	-2.511042	0.000093
16	1	0	-0.945775	-2.403342	-0.001015
17	1	0	-3.613909	-0.346492	-0.000549

O2-protonated (N3 side) N9H-amino 2OA-cyto (2OA-cyto-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.928928406 A.U. after 1 cycles

Zero-point correction= 0.129081 (Hartree/Particle)
Thermal correction to Energy= 0.137725
Thermal correction to Enthalpy= 0.138669
Thermal correction to Gibbs Free Energy= 0.095772
Sum of electronic and zero-point Energies= -542.799847
Sum of electronic and thermal Energies= -542.791203
Sum of electronic and thermal Enthalpies= -542.790259
Sum of electronic and thermal Free Energies= -542.833156

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.424	34.508	90.285

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.542622	-0.911290	-0.000051
2	6	0	0.816838	0.446256	-0.000167

3	6	0	-0.286703	1.344486	-0.000103
4	6	0	-1.750478	-0.448115	-0.000022
5	6	0	2.706642	-0.530293	-0.000003
6	7	0	-0.135987	2.661986	0.000263
7	7	0	1.745788	-1.543266	0.000173
8	7	0	-1.545638	0.838843	-0.000115
9	7	0	2.177835	0.663085	-0.000190
10	1	0	0.788273	3.078179	0.000370
11	1	0	-0.950995	3.265085	-0.000082
12	1	0	3.763439	-0.761464	0.000112
13	8	0	-3.014287	-0.854261	0.000061
14	7	0	-0.743770	-1.393123	0.000002
15	1	0	1.933432	-2.539369	0.000102
16	1	0	-0.943027	-2.388488	0.000638
17	1	0	-3.137956	-1.818790	-0.000485

N3-protonated N9H-amino 2OA-cyto (2OA-cyto-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.924550423 A.U. after 9 cycles

Zero-point correction= 0.126563 (Hartree/Particle)
Thermal correction to Energy= 0.136755
Thermal correction to Enthalpy= 0.137700
Thermal correction to Gibbs Free Energy= 0.090633
Sum of electronic and zero-point Energies= -542.797988
Sum of electronic and thermal Energies= -542.787795
Sum of electronic and thermal Enthalpies= -542.786851
Sum of electronic and thermal Free Energies= -542.833918

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.815	37.689	99.060

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.322604	-0.915599	-0.000014
2	6	0	0.696213	0.362388	-0.000026
3	6	0	-0.664935	0.695546	-0.000053
4	6	0	-2.819487	-0.367063	0.000018
5	6	0	2.806640	0.754731	0.000059
6	7	0	-1.035445	1.976679	-0.000036
7	7	0	2.656035	-0.634029	0.000039
8	7	0	-1.589502	-0.320100	-0.000105
9	7	0	1.666881	1.364876	0.000020
10	1	0	-0.304781	2.683948	-0.000006
11	1	0	-2.001428	2.277262	-0.000087
12	1	0	3.784919	1.216768	0.000100
13	8	0	-3.965222	-0.550854	0.000117
14	7	0	0.813294	-2.155061	0.000009
15	1	0	-0.188924	-2.286016	-0.000228

16	1	0	3.411115	-1.310130	0.000079
17	1	0	1.395827	-2.981578	-0.000184

N6-protonated N9H-amino 2OA-cyto (2OA-cyto-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.898977065 A.U. after 1 cycles

Zero-point correction= 0.130232 (Hartree/Particle)
Thermal correction to Energy= 0.138980
Thermal correction to Enthalpy= 0.139924
Thermal correction to Gibbs Free Energy= 0.096050
Sum of electronic and zero-point Energies= -542.768745
Sum of electronic and thermal Energies= -542.759997
Sum of electronic and thermal Enthalpies= -542.759053
Sum of electronic and thermal Free Energies= -542.802927

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.211	33.291	92.342

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.536725	-0.969401	-0.000175
2	6	0	-0.760140	0.412241	-0.000068
3	6	0	0.398208	1.187735	0.000019
4	6	0	1.871935	-0.616497	0.000008
5	6	0	-2.691689	-0.464806	0.000049
6	7	0	0.236874	2.682673	0.000020
7	7	0	-1.776218	-1.526593	0.000071
8	7	0	1.614475	0.765940	0.000016
9	7	0	-2.110550	0.703165	0.000011
10	1	0	-0.761250	2.942315	-0.000219
11	1	0	0.694667	3.088249	-0.828049
12	1	0	-3.758015	-0.646618	0.000326
13	8	0	2.974388	-1.103939	0.000188
14	7	0	0.712733	-1.475512	-0.000281
15	1	0	0.917319	-2.471499	-0.000120
16	1	0	0.694518	3.088309	0.828116
17	1	0	-2.013071	-2.512588	0.000601

N7-protonated N9H-amino 2OA-cyto (2OA-cyto-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.913483357 A.U. after 8 cycles

Zero-point correction= 0.128490 (Hartree/Particle)
Thermal correction to Energy= 0.137521
Thermal correction to Enthalpy= 0.138465

```
Thermal correction to Gibbs Free Energy=         0.094180
Sum of electronic and zero-point Energies=           -542.784994
Sum of electronic and thermal Energies=              -542.775963
Sum of electronic and thermal Enthalpies=            -542.775018
Sum of electronic and thermal Free Energies=         -542.819304

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   86.296             34.981             93.206


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.517971   -0.898865    0.013435
     2          6           0        0.699788    0.473415    0.006326
     3          6           0       -0.481801    1.316242    0.005598
     4          6           0       -1.883615   -0.603624   -0.003947
     5          6           0        2.709184   -0.497209   -0.012176
     6          7           0       -0.396039    2.662516   -0.013573
     7          7           0        1.774786   -1.474953    0.005053
     8          7           0       -1.666135    0.755823   -0.000164
     9          7           0        2.078499    0.674286   -0.012501
    10          1           0        0.460396    3.178673    0.122497
    11          1           0       -1.265994    3.183365    0.019193
    12          1           0        3.778433   -0.649217   -0.024095
    13          8           0       -2.959427   -1.149994   -0.017685
    14          7           0       -0.697629   -1.459185    0.017873
    15          1           0       -0.869145   -2.459822    0.019209
    16          1           0        1.986044   -2.468020    0.007738
    17          1           0        2.562138    1.565820   -0.035286
---------------------------------------------------------------------
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N9-protonated N9H-amino 2OA-cyto (2OA-cyto-11), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -542.844911009     A.U. after    1 cycles


Zero-point correction=                           0.127057 (Hartree/Particle)
Thermal correction to Energy=                    0.135979
Thermal correction to Enthalpy=                  0.136923
Thermal correction to Gibbs Free Energy=         0.093249
Sum of electronic and zero-point Energies=           -542.717854
Sum of electronic and thermal Energies=              -542.708932
Sum of electronic and thermal Enthalpies=            -542.707988
Sum of electronic and thermal Free Energies=         -542.751662

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   85.328             35.298             91.919


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	0.506725	-0.860806	0.000139
2	6	0	0.693813	0.490663	0.000380
3	6	0	-0.499154	1.318585	0.000120
4	6	0	-1.905994	-0.585931	-0.000132
5	6	0	2.757872	-0.213540	-0.000068
6	7	0	-0.385715	2.651600	-0.000119
7	7	0	1.849351	-1.481436	-0.000059
8	7	0	-1.693784	0.758799	-0.000477
9	7	0	2.051654	0.833785	0.000232
10	1	0	0.512341	3.116659	0.000062
11	1	0	-1.229866	3.213145	0.000099
12	1	0	3.829907	-0.361620	-0.000451
13	8	0	-2.955231	-1.176939	0.000405
14	7	0	-0.677942	-1.456820	-0.000281
15	1	0	2.025812	-2.064341	-0.832878
16	1	0	-0.846789	-2.458942	-0.000253
17	1	0	2.025924	-2.064707	0.832476

N7-protonated N9H-amino 2OA-cyto with HF hydrogen-bonded to N1 (2OA-cyto-12), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -643.373594853 A.U. after 1 cycles

Zero-point correction= 0.141490 (Hartree/Particle)
Thermal correction to Energy= 0.152359
Thermal correction to Enthalpy= 0.153303
Thermal correction to Gibbs Free Energy= 0.104576
Sum of electronic and zero-point Energies= -643.232105
Sum of electronic and thermal Energies= -643.221236
Sum of electronic and thermal Enthalpies= -643.220292
Sum of electronic and thermal Free Energies= -643.269019

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.607	41.231	102.555

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.339670	-0.664683	-0.000062
2	6	0	0.854353	0.630696	0.000079
3	6	0	-0.581192	0.831401	0.000001
4	6	0	-0.908127	-1.544385	0.000019
5	6	0	3.082050	0.721729	0.000070
6	7	0	-1.142341	2.046547	-0.000039
7	7	0	2.719145	-0.580988	-0.000103
8	7	0	-1.358481	-0.240261	-0.000086
9	7	0	1.974775	1.458274	0.000172
10	1	0	-0.618794	2.909290	-0.000130

11	1	0	-2.166826	2.094057	-0.000106
12	1	0	4.097067	1.091658	0.000150
13	8	0	-1.609129	-2.526327	0.000327
14	7	0	0.533062	-1.734633	-0.000362
15	1	0	0.855086	-2.697586	0.000184
16	1	0	-3.093246	0.248968	-0.000056
17	9	0	-3.706645	0.995238	-0.000054
18	1	0	1.981812	2.473192	0.000352
19	1	0	3.374091	-1.357228	-0.000243

N7H-amino 2OA-cyto with HF hydrogen-bonded to N1 (2OA-cyto-13), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -643.037611100 A.U. after 8 cycles

Zero-point correction= 0.128514 (Hartree/Particle)
Thermal correction to Energy= 0.139096
Thermal correction to Enthalpy= 0.140040
Thermal correction to Gibbs Free Energy= 0.091878
Sum of electronic and zero-point Energies= -642.909097
Sum of electronic and thermal Energies= -642.898515
Sum of electronic and thermal Enthalpies= -642.897571
Sum of electronic and thermal Free Energies= -642.945733

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.284	39.468	101.367

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.363759	-0.692571	-0.019128
2	6	0	0.908231	0.617616	0.005924
3	6	0	-0.492680	0.868019	0.025973
4	6	0	-0.917661	-1.493474	0.020406
5	6	0	3.112441	0.504402	-0.014517
6	7	0	-1.020347	2.116374	0.072334
7	7	0	2.725582	-0.762080	-0.034548
8	7	0	-1.330156	-0.167615	0.034329
9	7	0	2.072276	1.384193	0.006572
10	1	0	-0.466136	2.925260	-0.163695
11	1	0	-2.034600	2.193523	-0.005464
12	1	0	4.142706	0.834379	-0.015119
13	8	0	-1.689593	-2.439283	0.031159
14	7	0	0.476697	-1.723100	-0.016491
15	1	0	0.787556	-2.687574	-0.031338
16	1	0	-2.864308	0.320241	-0.020590
17	9	0	-3.612797	0.975634	-0.069531
18	1	0	2.153807	2.389372	0.065401

Cartesian coordinates and energies (in Hartree) for species of isoguanine in enol form, with O2 facing down (2OA-enol-d)

N9H-amino 2OA-enol-d (2OA-enol-d-1), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.575871843 A.U. after 8 cycles

Zero-point correction= 0.116208 (Hartree/Particle)
Thermal correction to Energy= 0.124798
Thermal correction to Enthalpy= 0.125742
Thermal correction to Gibbs Free Energy= 0.082429
Sum of electronic and zero-point Energies= -542.459664
Sum of electronic and thermal Energies= -542.451074
Sum of electronic and thermal Enthalpies= -542.450130
Sum of electronic and thermal Free Energies= -542.493442

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.312	33.184	91.159

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.484371	-0.917673	-0.001473
2	6	0	0.789602	0.446102	-0.001713
3	6	0	-0.318595	1.323117	-0.001675
4	6	0	-1.690989	-0.519960	0.000092
5	6	0	2.670242	-0.550945	0.001768
6	1	0	1.860847	-2.546798	0.000566
7	7	0	-0.173993	2.668156	-0.013651
8	7	0	1.707252	-1.547575	0.000297
9	7	0	-1.559601	0.811098	0.000830
10	7	0	2.160674	0.655711	0.000812
11	1	0	0.744355	3.082849	0.044042
12	1	0	-0.995284	3.252927	0.042939
13	1	0	3.726605	-0.785324	0.003699
14	8	0	-2.970702	-0.954695	0.002018
15	7	0	-0.740497	-1.462076	-0.001315
16	1	0	-2.935541	-1.927131	0.001811

N9H-amino 2OA-enol-d (2OA-enol-d-1), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -542.609804671 A.U. after 8 cycles

Zero-point correction= 0.115632 (Hartree/Particle)
Thermal correction to Energy= 0.124090
Thermal correction to Enthalpy= 0.125034
Thermal correction to Gibbs Free Energy= 0.082493
Sum of electronic and zero-point Energies= -542.494173

```
Sum of electronic and thermal Energies=             -542.485715
Sum of electronic and thermal Enthalpies=           -542.484771
Sum of electronic and thermal Free Energies=        -542.527311

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   77.868             33.371             89.534


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.495194   -0.912133   -0.000314
     2          6           0        0.788348    0.452901   -0.002461
     3          6           0       -0.319088    1.329125   -0.002395
     4          6           0       -1.681392   -0.532181    0.000070
     5          6           0        2.670596   -0.552010    0.001277
     6          1           0        1.885043   -2.540043    0.004361
     7          7           0       -0.190686    2.672443   -0.034516
     8          7           0        1.713678   -1.539981    0.002292
     9          7           0       -1.562504    0.800547    0.000186
    10          7           0        2.163081    0.662165   -0.001531
    11          1           0        0.715517    3.095780    0.119135
    12          1           0       -1.009810    3.249306    0.113921
    13          1           0        3.724755   -0.791835    0.002949
    14          8           0       -2.975419   -0.961443    0.001645
    15          7           0       -0.731835   -1.466460    0.000173
    16          1           0       -2.976236   -1.936869    0.003184
---------------------------------------------------------------------
```

N1H-amino 2OA-enol-d (2OA-enol-d-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

```
SCF Done:  E(RB3LYP) =  -542.595461534     A.U. after    8 cycles


Zero-point correction=                           0.115218 (Hartree/Particle)
Thermal correction to Energy=                    0.124010
Thermal correction to Enthalpy=                  0.124954
Thermal correction to Gibbs Free Energy=         0.081457
Sum of electronic and zero-point Energies=           -542.480244
Sum of electronic and thermal Energies=              -542.471451
Sum of electronic and thermal Enthalpies=            -542.470507
Sum of electronic and thermal Free Energies=         -542.514005

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   77.818             33.655             91.548


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.563333   -0.976537    0.000008
```

2	6	0	0.858475	0.408072	0.000004
3	6	0	-0.195775	1.321775	0.000004
4	6	0	-1.646573	-0.604778	0.000005
5	6	0	2.659869	-0.683561	-0.000010
6	7	0	-0.091513	2.654142	0.000097
7	7	0	1.718092	-1.674443	-0.000003
8	7	0	-1.448941	0.753721	-0.000016
9	7	0	2.226612	0.582367	-0.000005
10	1	0	0.824547	3.085198	-0.000266
11	1	0	-0.906585	3.256834	-0.000314
12	1	0	3.717337	-0.920618	-0.000022
13	8	0	-2.955120	-0.922757	0.000017
14	7	0	-0.706058	-1.499803	0.000018
15	1	0	-3.045483	-1.895165	-0.000213
16	1	0	-2.272183	1.354089	-0.000020

N7H-amino 2OA-enol-d (2OA-enol-d-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.563498620 A.U. after 1 cycles

Zero-point correction= 0.116439 (Hartree/Particle)
Thermal correction to Energy= 0.124689
Thermal correction to Enthalpy= 0.125633
Thermal correction to Gibbs Free Energy= 0.083482
Sum of electronic and zero-point Energies= -542.447059
Sum of electronic and thermal Energies= -542.438809
Sum of electronic and thermal Enthalpies= -542.437865
Sum of electronic and thermal Free Energies= -542.480016

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.244	32.897	88.715

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.497713	-0.962515	0.017505
2	6	0	0.770053	0.417915	-0.008148
3	6	0	-0.313218	1.311143	-0.002322
4	6	0	-1.692131	-0.524220	-0.002929
5	6	0	2.622658	-0.776659	-0.009428
6	7	0	-0.176850	2.682946	-0.050144
7	7	0	1.674465	-1.685177	0.021469
8	7	0	-1.550871	0.811874	-0.007071
9	7	0	2.156642	0.514279	-0.015385
10	1	0	0.630334	3.093007	0.401953
11	1	0	-1.042060	3.183320	0.122479
12	1	0	3.684005	-0.990652	-0.025083
13	8	0	-2.977587	-0.942721	-0.015752
14	7	0	-0.750953	-1.461895	0.022465
15	1	0	2.720386	1.343806	-0.134773

16	1	0	-2.949459	-1.915901	-0.005964

N9-deprotonated N9H-amino 2OA-enol-d (2OA-enol-d-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.032728799 A.U. after 9 cycles

Zero-point correction= 0.103808 (Hartree/Particle)
Thermal correction to Energy= 0.111598
Thermal correction to Enthalpy= 0.112543
Thermal correction to Gibbs Free Energy= 0.071195
Sum of electronic and zero-point Energies= -541.928921
Sum of electronic and thermal Energies= -541.921130
Sum of electronic and thermal Enthalpies= -541.920186
Sum of electronic and thermal Free Energies= -541.961534

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.029	31.004	87.024

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.510831	-0.990704	-0.009449
2	6	0	0.830675	0.396345	-0.021005
3	6	0	-0.232983	1.300596	-0.019468
4	6	0	-1.672647	-0.470228	-0.000916
5	6	0	2.607848	-0.727832	0.013951
6	7	0	-0.031567	2.676934	-0.070321
7	7	0	1.661990	-1.709273	0.009837
8	7	0	-1.505168	0.860685	-0.002742
9	7	0	2.202426	0.552874	-0.002319
10	1	0	0.886006	2.964071	0.250924
11	1	0	-0.799093	3.214048	0.316509
12	1	0	3.665654	-0.980653	0.030952
13	8	0	-2.992323	-0.871077	0.012852
14	7	0	-0.775846	-1.443406	-0.005367
15	1	0	-2.939171	-1.842612	0.016501

N1-protonated N9H-amino 2OA-enol-d (2OA-enol-d-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.945032460 A.U. after 9 cycles

Zero-point correction= 0.129940 (Hartree/Particle)
Thermal correction to Energy= 0.138262
Thermal correction to Enthalpy= 0.139206
Thermal correction to Gibbs Free Energy= 0.097015
Sum of electronic and zero-point Energies= -542.815092
Sum of electronic and thermal Energies= -542.806770

```
Sum of electronic and thermal Enthalpies=           -542.805826
Sum of electronic and thermal Free Energies=        -542.848017

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   86.761             33.799             88.799


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.512919   -0.937250    0.000000
     2          6           0        0.815721    0.432652   -0.000000
     3          6           0       -0.251318    1.340794    0.000000
     4          6           0       -1.678457   -0.616716    0.000000
     5          6           0        2.688889   -0.554965    0.000000
     6          1           0        1.886624   -2.556619    0.000000
     7          7           0       -0.113825    2.665351   -0.000000
     8          7           0        1.724805   -1.555190    0.000000
     9          7           0       -1.495405    0.754420    0.000000
    10          7           0        2.175702    0.649250   -0.000000
    11          1           0        0.823607    3.053956    0.000000
    12          1           0       -0.891394    3.313156    0.000002
    13          1           0        3.745730   -0.786915   -0.000000
    14          8           0       -2.963785   -0.943782   -0.000000
    15          7           0       -0.717797   -1.494912    0.000000
    16          1           0       -3.056361   -1.915887    0.000000
    17          1           0       -2.338815    1.323036   -0.000002
---------------------------------------------------------------------
```

N1-protonated N9H-amino 2OA-enol-d (2OA-enol-d-5), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

```
SCF Done:  E(RB3LYP) =  -543.054457809     A.U. after    1 cycles


Zero-point correction=                           0.128480 (Hartree/Particle)
Thermal correction to Energy=                    0.137210
Thermal correction to Enthalpy=                  0.138154
Thermal correction to Gibbs Free Energy=         0.095125
Sum of electronic and zero-point Energies=           -542.925978
Sum of electronic and thermal Energies=              -542.917248
Sum of electronic and thermal Enthalpies=            -542.916304
Sum of electronic and thermal Free Energies=         -542.959333

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   86.101             34.612             90.562


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
```

1	6	0	0.537812	-0.914380	-0.000105
2	6	0	0.816424	0.456526	0.000062
3	6	0	-0.276491	1.340362	-0.000042
4	6	0	-1.659306	-0.641342	-0.000199
5	6	0	2.703171	-0.521799	0.000255
6	1	0	1.938206	-2.520675	-0.000233
7	7	0	-0.211301	2.664242	0.000262
8	7	0	1.756600	-1.521030	-0.000106
9	7	0	-1.501323	0.720729	-0.000186
10	7	0	2.181253	0.685029	-0.000011
11	1	0	0.691944	3.125174	-0.000595
12	1	0	-1.045998	3.242084	-0.000491
13	1	0	3.759692	-0.749559	0.000376
14	8	0	-2.941299	-1.003446	0.000169
15	7	0	-0.680057	-1.505672	-0.000192
16	1	0	-3.010714	-1.978584	0.001449
17	1	0	-2.348597	1.289859	-0.000050

O2-protonated N9H-amino 2OA-enol-d (2OA-enol-d-6), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -542.877339647     A.U. after    1 cycles


Zero-point correction=                           0.128181 (Hartree/Particle)
Thermal correction to Energy=                    0.136874
Thermal correction to Enthalpy=                  0.137818
Thermal correction to Gibbs Free Energy=         0.094916
Sum of electronic and zero-point Energies=           -542.749159
Sum of electronic and thermal Energies=              -542.740466
Sum of electronic and thermal Enthalpies=            -542.739522
Sum of electronic and thermal Free Energies=         -542.782423

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   85.890             34.822             90.294
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.521912	-0.939206	0.002353
2	6	0	0.841575	0.425893	0.001570
3	6	0	-0.229022	1.356066	0.001481
4	6	0	-1.564708	-0.449595	0.015819
5	6	0	2.698640	-0.604099	-0.006437
6	7	0	-0.054552	2.677813	-0.006787
7	7	0	1.721519	-1.587064	-0.003320
8	7	0	-1.498397	0.848218	0.007350
9	7	0	2.205149	0.610587	-0.004757
10	1	0	0.880707	3.066588	-0.004455
11	1	0	-0.847531	3.306026	0.008570
12	1	0	3.751412	-0.853929	-0.009572
13	8	0	-2.998001	-0.914764	0.069284

14	7	0	-0.740092	-1.446553	0.008553
15	1	0	-3.106148	-1.813800	-0.318605
16	1	0	1.868846	-2.589781	0.002493
17	1	0	-3.609047	-0.252353	-0.328688

N3-protonated N9H-amino 2OA-enol-d (2OA-enol-d-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.928928425 A.U. after 9 cycles

Zero-point correction= 0.129082 (Hartree/Particle)
Thermal correction to Energy= 0.137726
Thermal correction to Enthalpy= 0.138670
Thermal correction to Gibbs Free Energy= 0.095773
Sum of electronic and zero-point Energies= -542.799846
Sum of electronic and thermal Energies= -542.791202
Sum of electronic and thermal Enthalpies= -542.790258
Sum of electronic and thermal Free Energies= -542.833156

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.425	34.508	90.286

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.542611	-0.911266	-0.000000
2	6	0	0.816842	0.446268	0.000000
3	6	0	-0.286711	1.344492	-0.000000
4	6	0	-1.750478	-0.448098	0.000000
5	6	0	2.706650	-0.530290	0.000000
6	1	0	1.933423	-2.539353	0.000000
7	7	0	-0.136002	2.661949	-0.000000
8	7	0	1.745773	-1.543251	-0.000000
9	7	0	-1.545637	0.838853	0.000000
10	7	0	2.177838	0.663069	0.000000
11	1	0	0.788257	3.078140	-0.000001
12	1	0	-0.951002	3.265055	-0.000000
13	1	0	3.763437	-0.761500	0.000000
14	8	0	-3.014270	-0.854291	-0.000000
15	7	0	-0.743764	-1.393100	0.000000
16	1	0	-3.137868	-1.818828	0.000002
17	1	0	-0.943040	-2.388462	-0.000004

N6-protoanted N9H-amino 2OA-enol-d (2OA-enol-d-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.910104582 A.U. after 1 cycles

Zero-point correction= 0.130897 (Hartree/Particle)

```
Thermal correction to Energy=                    0.139351
Thermal correction to Enthalpy=                  0.140295
Thermal correction to Gibbs Free Energy=         0.097298
Sum of electronic and zero-point Energies=           -542.779208
Sum of electronic and thermal Energies=              -542.770753
Sum of electronic and thermal Enthalpies=            -542.769809
Sum of electronic and thermal Free Energies=         -542.812806

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   87.444             32.675             90.495


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.492265   -0.974404   -0.000081
     2          6           0       -0.800119    0.411960   -0.000083
     3          6           0        0.321621    1.211079    0.000034
     4          6           0        1.706403   -0.579424    0.000062
     5          6           0       -2.671006   -0.574650    0.000130
     6          7           0        0.177313    2.697226    0.000004
     7          7           0       -1.719340   -1.582074    0.000053
     8          7           0        1.554500    0.765333    0.000084
     9          7           0       -2.160540    0.634141   -0.000140
    10          1           0       -0.819674    2.960144   -0.000606
    11          1           0        0.633283    3.105952   -0.827912
    12          1           0       -3.729728   -0.800065    0.000228
    13          8           0        2.969058   -0.990914   -0.000027
    14          7           0        0.726365   -1.495371   -0.000029
    15          1           0        2.990710   -1.965980   -0.000071
    16          1           0       -1.895155   -2.580842   -0.000112
    17          1           0        0.632205    3.105947    0.828515
---------------------------------------------------------------------
```

N7-protonated N9H-amino 2OA-enol-d (2OA-enol-d-9), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -542.932268256     A.U. after    1 cycles


Zero-point correction=                           0.129568 (Hartree/Particle)
Thermal correction to Energy=                    0.138139
Thermal correction to Enthalpy=                  0.139083
Thermal correction to Gibbs Free Energy=         0.096166
Sum of electronic and zero-point Energies=           -542.802700
Sum of electronic and thermal Energies=              -542.794129
Sum of electronic and thermal Enthalpies=            -542.793185
Sum of electronic and thermal Free Energies=         -542.836102

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   86.683             34.034             90.326
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.475134	-0.896262	-0.000239
2	6	0	0.735240	0.476107	-0.000306
3	6	0	-0.402505	1.336216	-0.000039
4	6	0	-1.707545	-0.578601	-0.000003
5	6	0	2.687633	-0.597253	0.000181
6	1	0	1.863347	-2.530760	0.000499
7	7	0	-0.349357	2.680929	-0.000003
8	7	0	1.719253	-1.525110	-0.000048
9	7	0	-1.603163	0.756472	0.000115
10	7	0	2.125607	0.612988	0.000238
11	1	0	0.506917	3.214465	-0.000042
12	1	0	-1.226050	3.189926	0.000348
13	1	0	3.749982	-0.795170	0.000528
14	8	0	-2.953512	-1.034949	0.000137
15	7	0	-0.708752	-1.483051	-0.000185
16	1	0	2.660945	1.474155	-0.000934
17	1	0	-2.939897	-2.009857	0.000123

N9-protonated N9H-amino 2OA-enol-d (2OA-enol-d-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.873311152 A.U. after 9 cycles

Zero-point correction= 0.128801 (Hartree/Particle)
Thermal correction to Energy= 0.137198
Thermal correction to Enthalpy= 0.138142
Thermal correction to Gibbs Free Energy= 0.095683
Sum of electronic and zero-point Energies= -542.744510
Sum of electronic and thermal Energies= -542.736113
Sum of electronic and thermal Enthalpies= -542.735169
Sum of electronic and thermal Free Energies= -542.777628

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.093	33.875	89.362

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.462704	-0.851045	0.000000
2	6	0	0.732031	0.501732	0.000000
3	6	0	-0.418574	1.342774	0.000000
4	6	0	-1.714845	-0.573257	-0.000000
5	6	0	2.744317	-0.319944	-0.000000
6	1	0	1.922048	-2.126501	0.828706
7	7	0	-0.356566	2.676137	-0.000000
8	7	0	1.794198	-1.526557	0.000000
9	7	0	-1.627586	0.749179	-0.000000

10	7	0	2.105924	0.775614	-0.000000
11	1	0	0.525792	3.170689	0.000001
12	1	0	-1.218363	3.209368	0.000000
13	1	0	3.810867	-0.504611	-0.000001
14	8	0	-2.941879	-1.071565	-0.000000
15	7	0	-0.681176	-1.475197	0.000000
16	1	0	-2.904726	-2.045716	0.000000
17	1	0	1.922047	-2.126501	-0.828706

N7-protonated N9H-amino 2OA-enol-d with HF hydrogen-bonded to N3 (2OA-enol-d-11), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -643.391593622 A.U. after 9 cycles

Zero-point correction=	0.142114 (Hartree/Particle)
Thermal correction to Energy=	0.152711
Thermal correction to Enthalpy=	0.153655
Thermal correction to Gibbs Free Energy=	0.105836
Sum of electronic and zero-point Energies=	-643.249479
Sum of electronic and thermal Energies=	-643.238883
Sum of electronic and thermal Enthalpies=	-643.237938
Sum of electronic and thermal Free Energies=	-643.285758

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.828	40.702	100.644

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.579724	-0.280188	-0.000003
2	6	0	0.638382	-0.952282	-0.000001
3	6	0	1.813040	-0.140727	0.000001
4	6	0	0.412182	1.709828	-0.000001
5	6	0	-1.003481	-2.458560	-0.000001
6	7	0	3.070866	-0.610696	0.000004
7	7	0	-1.573321	-1.248738	-0.000002
8	7	0	1.639244	1.182744	0.000000
9	7	0	0.325773	-2.314645	0.000000
10	1	0	3.309092	-1.591450	-0.000002
11	1	0	3.829853	0.061875	0.000005
12	1	0	-1.530789	-3.402113	0.000000
13	8	0	0.381609	3.035063	-0.000001
14	7	0	-0.760789	1.040325	-0.000003
15	1	0	0.971061	-3.096723	0.000000
16	1	0	-2.559109	1.212673	0.000003
17	9	0	-3.395335	0.730922	0.000005
18	1	0	-0.537790	3.357043	-0.000003
19	1	0	-2.571993	-1.011459	-0.000001

N7H-amino 2OA-enol-d with HF hydrogen-bonded to N3 (2OA-enol-d-12), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -643.031990350 A.U. after 9 cycles

Zero-point correction=	0.128985 (Hartree/Particle)
Thermal correction to Energy=	0.139190
Thermal correction to Enthalpy=	0.140134
Thermal correction to Gibbs Free Energy=	0.093033
Sum of electronic and zero-point Energies=	-642.903006
Sum of electronic and thermal Energies=	-642.892801
Sum of electronic and thermal Enthalpies=	-642.891857
Sum of electronic and thermal Free Energies=	-642.938958

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.343	38.796	99.132

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.208536	-0.907765	0.011077
2	6	0	1.295439	-0.020997	-0.005685
3	6	0	1.032171	1.361289	0.000866
4	6	0	-1.214704	0.851933	-0.008947
5	6	0	1.953217	-2.125319	-0.009853
6	7	0	2.008412	2.325042	-0.038117
7	7	0	0.640612	-2.213082	0.012693
8	7	0	-0.237843	1.771504	-0.007954
9	7	0	2.420911	-0.837293	-0.011696
10	1	0	2.914665	2.120357	0.360561
11	1	0	1.675046	3.268643	0.123754
12	1	0	2.628591	-2.971241	-0.023350
13	8	0	-2.455039	1.350107	-0.022780
14	7	0	-1.070140	-0.481009	0.012254
15	1	0	3.388156	-0.562033	-0.106814
16	1	0	-2.486845	-1.209876	0.018552
17	9	0	-3.484433	-1.218355	0.014516
18	1	0	-3.101016	0.607511	-0.016118

N7-protonated N9H-amino 2OA-enol-d with HF hydrogen-bonded to N1 (2OA-enol-d-13), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -643.390821781 A.U. after 8 cycles

Zero-point correction=	0.142463 (Hartree/Particle)
Thermal correction to Energy=	0.152937
Thermal correction to Enthalpy=	0.153881
Thermal correction to Gibbs Free Energy=	0.106169
Sum of electronic and zero-point Energies=	-643.248359

Sum of electronic and thermal Energies= -643.237885
Sum of electronic and thermal Enthalpies= -643.236941
Sum of electronic and thermal Free Energies= -643.284653

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.969	40.396	100.419

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.295429	-0.690498	0.000000
2	6	0	0.884815	0.642903	0.000000
3	6	0	-0.520723	0.886158	0.000000
4	6	0	-0.778499	-1.436844	0.000000
5	6	0	3.110460	0.607612	-0.000000
6	1	0	3.285794	-1.487362	-0.000000
7	7	0	-1.098751	2.092306	-0.000000
8	7	0	2.687962	-0.665573	-0.000000
9	7	0	-1.309757	-0.203704	0.000000
10	7	0	2.048181	1.414518	0.000000
11	1	0	-0.579409	2.957670	-0.000000
12	1	0	-2.121822	2.135116	0.000000
13	1	0	4.142310	0.929181	-0.000000
14	8	0	-1.674671	-2.413295	-0.000000
15	7	0	0.522837	-1.765180	0.000000
16	1	0	2.118075	2.426525	0.000000
17	1	0	-3.051747	0.284567	-0.000001
18	9	0	-3.675330	1.019363	0.000000
19	1	0	-1.220064	-3.276163	-0.000000

N7H-amino 2OA-enol-d with HF hydrogen-bonded to N1 (2OA-enol-d-14), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -643.031291133 A.U. after 8 cycles

Zero-point correction= 0.128773 (Hartree/Particle)
Thermal correction to Energy= 0.139164
Thermal correction to Enthalpy= 0.140108
Thermal correction to Gibbs Free Energy= 0.092521
Sum of electronic and zero-point Energies= -642.902518
Sum of electronic and thermal Energies= -642.892127
Sum of electronic and thermal Enthalpies= -642.891183
Sum of electronic and thermal Free Energies= -642.938770

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.327	39.294	100.156

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.336336	-0.743053	0.022379
2	6	0	0.940530	0.606635	-0.013510
3	6	0	-0.430139	0.911008	-0.037412
4	6	0	-0.801709	-1.381760	-0.023405
5	6	0	3.133406	0.403783	0.025353
6	7	0	-0.949044	2.169907	-0.098050
7	7	0	2.710457	-0.840492	0.049623
8	7	0	-1.290051	-0.125252	-0.046181
9	7	0	2.124918	1.332106	-0.004333
10	1	0	-0.396328	2.953380	0.217293
11	1	0	-1.958387	2.252189	0.011601
12	1	0	4.173708	0.703729	0.030106
13	8	0	-1.756224	-2.332349	-0.038415
14	7	0	0.462105	-1.768689	0.017811
15	1	0	2.245778	2.330962	-0.094407
16	1	0	-2.839922	0.374042	0.028026
17	9	0	-3.595117	1.009241	0.094990
18	1	0	-1.298246	-3.191410	-0.012721

N7-protonated N9H-amino 2OA-enol-d with HF hydrogen-bonded to N1 and N3 (2OA-enol-d-15), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -743.849279790 A.U. after 8 cycles

Zero-point correction= 0.154810 (Hartree/Particle)
Thermal correction to Energy= 0.167447
Thermal correction to Enthalpy= 0.168391
Thermal correction to Gibbs Free Energy= 0.115440
Sum of electronic and zero-point Energies= -743.694469
Sum of electronic and thermal Energies= -743.681833
Sum of electronic and thermal Enthalpies= -743.680889
Sum of electronic and thermal Free Energies= -743.733840

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	105.074	47.327	111.445

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.096565	-0.089707	-0.000000
2	6	0	-0.197276	-1.149636	0.000000
3	6	0	1.192426	-0.822091	0.000000
4	6	0	0.530435	1.422478	-0.000000
5	6	0	-2.264317	-1.976079	-0.000000
6	1	0	-3.218309	-0.066559	-0.000000
7	7	0	2.195334	-1.703049	0.000000
8	7	0	-2.368163	-0.642484	-0.000000
9	7	0	1.492537	0.491102	0.000000

10	7	0	-0.970646	-2.312514	0.000000
11	1	0	2.056266	-2.703062	0.000000
12	1	0	3.154123	-1.341781	0.000000
13	1	0	-3.091958	-2.671546	-0.000000
14	8	0	0.982864	2.667352	-0.000000
15	7	0	-0.798257	1.211622	-0.000000
16	1	0	0.246417	3.305411	-0.000000
17	1	0	-0.643545	-3.272636	0.000000
18	1	0	-2.444323	2.020836	0.000000
19	1	0	3.311685	0.726091	-0.000000
20	9	0	4.159550	0.272558	0.000000
21	9	0	-3.390342	1.843208	0.000000

N7H-amino 2OA-enol-d with HF hydrogen-bonded to N1 and N3 (2OA-enol-d-16), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -743.498580109 A.U. after 8 cycles

Zero-point correction= 0.141306 (Hartree/Particle)
Thermal correction to Energy= 0.153732
Thermal correction to Enthalpy= 0.154676
Thermal correction to Gibbs Free Energy= 0.101959
Sum of electronic and zero-point Energies= -743.357274
Sum of electronic and thermal Energies= -743.344848
Sum of electronic and thermal Enthalpies= -743.343904
Sum of electronic and thermal Free Energies= -743.396621

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	96.468	45.324	110.953

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.356813	-0.084396	0.011338
2	6	0	-0.584001	-1.254737	-0.008700
3	6	0	0.819011	-1.144286	-0.025385
4	6	0	0.525445	1.167593	-0.023892
5	6	0	-2.741975	-1.698277	0.017860
6	7	0	1.680699	-2.189941	-0.064851
7	7	0	-2.696381	-0.382673	0.029935
8	7	0	1.341714	0.097665	-0.035824
9	7	0	-1.508464	-2.292012	-0.000106
10	1	0	1.373922	-3.125146	0.154335
11	1	0	2.675377	-1.984587	0.015304
12	1	0	-3.651528	-2.285121	0.022500
13	8	0	1.155187	2.342044	-0.037056
14	7	0	-0.809013	1.150024	0.004227
15	1	0	0.488918	3.068336	-0.022345
16	1	0	-1.334191	-3.285558	-0.055881
17	1	0	-1.389313	2.657402	0.017507

18	1	0	2.992311	0.061351	0.020453
19	9	0	3.882433	-0.357719	0.071342
20	9	0	-1.263199	3.642181	0.015723

Cartesian coordinates and energies (in Hartree) for species of isoguanine in enol form, with O2 facing up (2OA-enol-u)

N9H-amino 2OA-enol-u (2OA-enol-u-1), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.576175216 A.U. after 9 cycles

Zero-point correction= 0.116421 (Hartree/Particle)
Thermal correction to Energy= 0.124824
Thermal correction to Enthalpy= 0.125768
Thermal correction to Gibbs Free Energy= 0.083262
Sum of electronic and zero-point Energies= -542.459754
Sum of electronic and thermal Energies= -542.451352
Sum of electronic and thermal Enthalpies= -542.450407
Sum of electronic and thermal Free Energies= -542.492913

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.328	33.100	89.461

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.519719	-0.914004	-0.002670
2	6	0	0.778101	0.461140	-0.003855
3	6	0	-0.357833	1.297723	-0.003494
4	6	0	-1.658134	-0.613557	0.000453
5	6	0	2.691570	-0.469113	0.003461
6	1	0	1.951601	-2.492308	0.002065
7	7	0	-0.263972	2.649766	-0.029585
8	7	0	1.765164	-1.498478	0.001043
9	7	0	-1.576200	0.731306	0.002148
10	7	0	2.140676	0.719728	0.001063
11	1	0	0.637163	3.088907	0.092297
12	1	0	-1.100481	3.200993	0.097586
13	1	0	3.755689	-0.665486	0.007407
14	8	0	-2.910060	-1.121866	0.003402
15	7	0	-0.677832	-1.511952	-0.002055
16	1	0	-3.518883	-0.362909	0.001749

N9H-amino 2OA-enol-u (2OA-enol-u-1), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -542.609937450 A.U. after 1 cycles

```
Zero-point correction=                           0.115597 (Hartree/Particle)
Thermal correction to Energy=                    0.124054
Thermal correction to Enthalpy=                  0.124998
Thermal correction to Gibbs Free Energy=         0.082457
Sum of electronic and zero-point Energies=           -542.494341
Sum of electronic and thermal Energies=              -542.485884
Sum of electronic and thermal Enthalpies=            -542.484939
Sum of electronic and thermal Free Energies=         -542.527480

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   77.845             33.376             89.535


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.529319   -0.908374   -0.000030
     2          6           0        0.777915    0.466353   -0.002874
     3          6           0       -0.356611    1.305577   -0.002438
     4          6           0       -1.654649   -0.607309    0.000145
     5          6           0        2.692272   -0.475143    0.000940
     6          1           0        1.973722   -2.487999    0.005629
     7          7           0       -0.276495    2.652519   -0.034516
     8          7           0        1.768846   -1.494272    0.002937
     9          7           0       -1.580143    0.730553    0.000045
    10          7           0        2.144854    0.721515   -0.002482
    11          1           0        0.614287    3.106634    0.121526
    12          1           0       -1.115071    3.199892    0.117078
    13          1           0        3.753845   -0.679852    0.002510
    14          8           0       -2.908972   -1.141437    0.001559
    15          7           0       -0.675569   -1.507918    0.000823
    16          1           0       -3.554928   -0.410588   -0.001316
---------------------------------------------------------------------
```

N3H-amino 2OA-enol-u (2OA-enol-u-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

```
SCF Done:  E(RB3LYP) =  -542.599130086     A.U. after    8 cycles


Zero-point correction=                           0.115311 (Hartree/Particle)
Thermal correction to Energy=                    0.123841
Thermal correction to Enthalpy=                  0.124785
Thermal correction to Gibbs Free Energy=         0.082038
Sum of electronic and zero-point Energies=           -542.483819
Sum of electronic and thermal Energies=              -542.475289
Sum of electronic and thermal Enthalpies=            -542.474345
Sum of electronic and thermal Free Energies=         -542.517092

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   77.711             33.441             89.970
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.591787	-0.947541	-0.000001
2	6	0	0.847497	0.431051	-0.000005
3	6	0	-0.241927	1.322151	-0.000002
4	6	0	-1.693056	-0.480232	-0.000001
5	6	0	2.665249	-0.650579	0.000002
6	7	0	-0.107427	2.655214	0.000002
7	7	0	1.729961	-1.654206	0.000002
8	7	0	-1.515003	0.821615	-0.000006
9	7	0	2.218492	0.608880	-0.000002
10	1	0	0.809622	3.083086	0.000020
11	1	0	-0.924657	3.253311	0.000017
12	1	0	3.723402	-0.882613	0.000004
13	8	0	-2.929008	-1.003329	0.000001
14	7	0	-0.708077	-1.403566	0.000002
15	1	0	-3.582031	-0.276383	0.000014
16	1	0	-0.937185	-2.395422	0.000007

N7H-amino 2OA-enol-u (2OA-enol-u-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.561396313 A.U. after 8 cycles

Zero-point correction= 0.116297 (Hartree/Particle)
Thermal correction to Energy= 0.124586
Thermal correction to Enthalpy= 0.125530
Thermal correction to Gibbs Free Energy= 0.083319
Sum of electronic and zero-point Energies= -542.445099
Sum of electronic and thermal Energies= -542.436811
Sum of electronic and thermal Enthalpies= -542.435867
Sum of electronic and thermal Free Energies= -542.478078

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.179	33.025	88.841

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.534281	-0.959724	0.017293
2	6	0	0.759726	0.431418	-0.010394
3	6	0	-0.351006	1.285605	-0.002187
4	6	0	-1.660682	-0.616186	-0.001693
5	6	0	2.652693	-0.696471	-0.009462
6	7	0	-0.266504	2.662740	-0.049821
7	7	0	1.738751	-1.637769	0.022651
8	7	0	-1.567785	0.732806	-0.005261
9	7	0	2.141690	0.578276	-0.015931

10	1	0	0.527383	3.098301	0.402301
11	1	0	-1.145917	3.133119	0.133407
12	1	0	3.721183	-0.871984	-0.025247
13	8	0	-2.920197	-1.108766	-0.015026
14	7	0	-0.689573	-1.512857	0.023435
15	1	0	-3.522766	-0.345570	-0.032931
16	1	0	2.675569	1.426049	-0.144169

N9-deprotonated N9H-amino 2OA-enol-u (2OA-enol-u-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.030716566 A.U. after 9 cycles

Zero-point correction=	0.103686 (Hartree/Particle)
Thermal correction to Energy=	0.111515
Thermal correction to Enthalpy=	0.112459
Thermal correction to Gibbs Free Energy=	0.071048
Sum of electronic and zero-point Energies=	-541.927031
Sum of electronic and thermal Energies=	-541.919202
Sum of electronic and thermal Enthalpies=	-541.918258
Sum of electronic and thermal Free Energies=	-541.959669

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.977	31.115	87.157

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.558831	-0.986254	-0.008288
2	6	0	0.817837	0.415454	-0.022468
3	6	0	-0.282348	1.271611	-0.019777
4	6	0	-1.635822	-0.585857	0.000186
5	6	0	2.643176	-0.625581	0.013632
6	7	0	-0.146354	2.657621	-0.071477
7	7	0	1.743877	-1.648437	0.011789
8	7	0	-1.528575	0.762980	-0.001980
9	7	0	2.180096	0.636001	-0.004633
10	1	0	0.763238	2.979494	0.240668
11	1	0	-0.925148	3.158150	0.341465
12	1	0	3.711571	-0.829364	0.030507
13	8	0	-2.939912	-1.038401	0.011406
14	7	0	-0.701053	-1.509485	-0.002983
15	1	0	-3.476350	-0.228062	0.001391

N1-protonated N9H-amino 2OA-enol-u (2OA-enol-u-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.928771024 A.U. after 9 cycles

```
Zero-point correction=                           0.128733 (Hartree/Particle)
Thermal correction to Energy=                    0.137603
Thermal correction to Enthalpy=                  0.138547
Thermal correction to Gibbs Free Energy=         0.095127
Sum of electronic and zero-point Energies=           -542.800038
Sum of electronic and thermal Energies=              -542.791168
Sum of electronic and thermal Enthalpies=            -542.790224
Sum of electronic and thermal Free Energies=         -542.833644

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   86.347             34.792             91.385


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.520107   -0.932727   -0.000000
     2          6           0        0.819520    0.438748    0.000001
     3          6           0       -0.251861    1.334758    0.000000
     4          6           0       -1.678833   -0.644819    0.000001
     5          6           0        2.694747   -0.542414    0.000000
     6          1           0        1.897683   -2.547330   -0.000001
     7          7           0       -0.126485    2.662369   -0.000000
     8          7           0        1.734824   -1.545796   -0.000001
     9          7           0       -1.498100    0.738398   -0.000001
    10          7           0        2.178930    0.661157    0.000001
    11          1           0        0.808612    3.056873   -0.000001
    12          1           0       -0.906092    3.307238    0.000002
    13          1           0        3.752521   -0.770402    0.000000
    14          8           0       -2.919594   -1.121475   -0.000003
    15          7           0       -0.700025   -1.499277    0.000001
    16          1           0       -3.625932   -0.454090    0.000026
    17          1           0       -2.316127    1.340265   -0.000010
---------------------------------------------------------------------
```

O2-protonated N9H-amino 2OA-enol-u (2OA-enol-u-6), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -542.877339647     A.U. after    1 cycles


Zero-point correction=                           0.128181 (Hartree/Particle)
Thermal correction to Energy=                    0.136874
Thermal correction to Enthalpy=                  0.137818
Thermal correction to Gibbs Free Energy=         0.094916
Sum of electronic and zero-point Energies=           -542.749159
Sum of electronic and thermal Energies=              -542.740466
Sum of electronic and thermal Enthalpies=            -542.739522
Sum of electronic and thermal Free Energies=         -542.782423

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   85.890             34.822             90.294
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.521912	-0.939206	0.002353
2	6	0	0.841575	0.425893	0.001570
3	6	0	-0.229022	1.356066	0.001481
4	6	0	-1.564708	-0.449595	0.015819
5	6	0	2.698640	-0.604099	-0.006437
6	7	0	-0.054552	2.677813	-0.006787
7	7	0	1.721519	-1.587064	-0.003320
8	7	0	-1.498397	0.848218	0.007350
9	7	0	2.205149	0.610587	-0.004757
10	1	0	0.880707	3.066588	-0.004455
11	1	0	-0.847531	3.306026	0.008570
12	1	0	3.751412	-0.853929	-0.009572
13	8	0	-2.998001	-0.914764	0.069284
14	7	0	-0.740092	-1.446553	0.008553
15	1	0	-3.106148	-1.813800	-0.318605
16	1	0	1.868846	-2.589781	0.002493
17	1	0	-3.609047	-0.252353	-0.328688

N3-protonated N9H-amino 2OA-enol-u (2OA-enol-u-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.944335327 A.U. after 9 cycles

Zero-point correction= 0.129982 (Hartree/Particle)
Thermal correction to Energy= 0.138267
Thermal correction to Enthalpy= 0.139211
Thermal correction to Gibbs Free Energy= 0.097033
Sum of electronic and zero-point Energies= -542.814353
Sum of electronic and thermal Energies= -542.806069
Sum of electronic and thermal Enthalpies= -542.805124
Sum of electronic and thermal Free Energies= -542.847302

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.764	33.725	88.771

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.556744	-0.911918	-0.000000
2	6	0	0.803952	0.453295	-0.000000
3	6	0	-0.311073	1.335231	0.000000
4	6	0	-1.728842	-0.490870	0.000000
5	6	0	2.712502	-0.486228	0.000000
6	1	0	1.976337	-2.511043	0.000000
7	7	0	-0.176977	2.655092	-0.000000
8	7	0	1.771523	-1.518168	0.000000

9	7	0	-1.565198	0.806408	0.000000
10	7	0	2.160838	0.696662	0.000000
11	1	0	0.743662	3.079475	0.000000
12	1	0	-0.995269	3.252798	0.000000
13	1	0	3.773623	-0.696553	0.000000
14	8	0	-2.931243	-1.045070	0.000000
15	7	0	-0.717114	-1.413042	0.000000
16	1	0	-3.613886	-0.346478	0.000000
17	1	0	-0.945728	-2.403367	-0.000002

N3-protonated N9H-amino 2OA-enol-u (2OA-enol-u-7), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -543.051793299 A.U. after 1 cycles

Zero-point correction= 0.128651 (Hartree/Particle)
Thermal correction to Energy= 0.137242
Thermal correction to Enthalpy= 0.138187
Thermal correction to Gibbs Free Energy= 0.095428
Sum of electronic and zero-point Energies= -542.923142
Sum of electronic and thermal Energies= -542.914551
Sum of electronic and thermal Enthalpies= -542.913607
Sum of electronic and thermal Free Energies= -542.956365

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.121	34.466	89.992

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.563198	-0.894097	0.000004
2	6	0	0.804683	0.471025	0.000041
3	6	0	-0.319103	1.337568	-0.000119
4	6	0	-1.715800	-0.509474	-0.000135
5	6	0	2.709354	-0.490670	-0.000216
6	1	0	1.960065	-2.503709	-0.000058
7	7	0	-0.212655	2.661876	0.000082
8	7	0	1.771105	-1.505089	0.000033
9	7	0	-1.569586	0.794636	-0.000192
10	7	0	2.170699	0.706775	0.000311
11	1	0	0.695299	3.111915	-0.000603
12	1	0	-1.043867	3.242934	0.000461
13	1	0	3.767117	-0.711527	-0.000278
14	8	0	-2.920870	-1.073075	0.000153
15	7	0	-0.697549	-1.408783	0.000022
16	1	0	-3.608696	-0.377403	-0.000121
17	1	0	-0.891043	-2.409629	0.000130

N6-protonated N9H-amino 2OA-enol-u (2OA-enol-u-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.907401351 A.U. after 1 cycles

Zero-point correction= 0.130826 (Hartree/Particle)
Thermal correction to Energy= 0.139282
Thermal correction to Enthalpy= 0.140226
Thermal correction to Gibbs Free Energy= 0.097298
Sum of electronic and zero-point Energies= -542.776575
Sum of electronic and thermal Energies= -542.768119
Sum of electronic and thermal Enthalpies= -542.767175
Sum of electronic and thermal Free Energies= -542.810104

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.401	32.747	90.351

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.516655	-0.971898	-0.000000
2	6	0	-0.791164	0.423934	-0.000011
3	6	0	0.346722	1.194487	-0.000014
4	6	0	1.683757	-0.644497	0.000002
5	6	0	-2.684954	-0.516330	-0.000011
6	7	0	0.231749	2.681760	0.000017
7	7	0	-1.760463	-1.546892	0.000035
8	7	0	1.570307	0.708974	-0.000020
9	7	0	-2.145394	0.680635	-0.000023
10	1	0	-0.762682	2.956084	0.000004
11	1	0	0.688954	3.086662	-0.828937
12	1	0	-3.749253	-0.714172	-0.000003
13	8	0	2.907401	-1.162503	-0.000020
14	7	0	0.680483	-1.529895	0.000023
15	1	0	3.571283	-0.449809	0.000079
16	1	0	-1.959392	-2.541576	-0.000057
17	1	0	0.688864	3.086595	0.829058

N7-protonated N9H-amino 2OA-enol-u (2OA-enol-u-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -542.932839897 A.U. after 8 cycles

Zero-point correction= 0.129531 (Hartree/Particle)
Thermal correction to Energy= 0.138123
Thermal correction to Enthalpy= 0.139067
Thermal correction to Gibbs Free Energy= 0.096100
Sum of electronic and zero-point Energies= -542.803309
Sum of electronic and thermal Energies= -542.794717
Sum of electronic and thermal Enthalpies= -542.793773

```
Sum of electronic and thermal Free Energies=         -542.836739

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   86.673             34.073             90.431


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.501024   -0.893173    0.000000
     2          6           0        0.725953    0.486962   -0.000000
     3          6           0       -0.431619    1.314905    0.000000
     4          6           0       -1.680138   -0.650455    0.000000
     5          6           0        2.705091   -0.535480   -0.000000
     6          1           0        1.930374   -2.490569    0.000000
     7          7           0       -0.417603    2.661145   -0.000000
     8          7           0        1.762883   -1.488187    0.000000
     9          7           0       -1.615478    0.694225   -0.000000
    10          7           0        2.112695    0.660715   -0.000000
    11          1           0        0.424715    3.216436    0.000004
    12          1           0       -1.305045    3.149884    0.000001
    13          1           0        3.772441   -0.704859   -0.000000
    14          8           0       -2.887060   -1.200815   -0.000000
    15          7           0       -0.658772   -1.519270    0.000000
    16          1           0       -3.560770   -0.495924   -0.000001
    17          1           0        2.626817    1.534596   -0.000001
---------------------------------------------------------------------
```

N9-protonated N9H-amino 2OA-enol-u (2OA-enol-u-10), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -542.875881271     A.U. after    1 cycles


Zero-point correction=                           0.128907 (Hartree/Particle)
Thermal correction to Energy=                    0.137283
Thermal correction to Enthalpy=                  0.138227
Thermal correction to Gibbs Free Energy=         0.095811
Sum of electronic and zero-point Energies=           -542.746974
Sum of electronic and thermal Energies=              -542.738599
Sum of electronic and thermal Enthalpies=            -542.737655
Sum of electronic and thermal Free Energies=         -542.780070

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   86.146             33.792             89.271


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.486094   -0.848851   -0.000047
     2          6           0        0.722882    0.512045   -0.000085
```

3	6	0	-0.445877	1.322196	-0.000045
4	6	0	-1.687368	-0.641535	0.000320
5	6	0	2.753613	-0.260589	0.000299
6	1	0	1.975682	-2.088505	0.827509
7	7	0	-0.420870	2.657451	-0.000312
8	7	0	1.836077	-1.489791	-0.000258
9	7	0	-1.638931	0.689070	0.000133
10	7	0	2.088681	0.819944	0.000138
11	1	0	0.449489	3.173010	-0.000283
12	1	0	-1.293294	3.172002	0.000922
13	1	0	3.824720	-0.416517	0.000827
14	8	0	-2.869958	-1.234615	-0.000020
15	7	0	-0.633208	-1.508188	0.000077
16	1	0	-3.570783	-0.555290	-0.000585
17	1	0	1.975538	-2.086777	-0.829327

N7-protonated N9H-amino 2OA-enol-u with HF hydrogen-bonded to N3 (2OA-enol-u-11), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -643.395238457 A.U. after 1 cycles

Zero-point correction= 0.142135 (Hartree/Particle)
Thermal correction to Energy= 0.152720
Thermal correction to Enthalpy= 0.153664
Thermal correction to Gibbs Free Energy= 0.105906
Sum of electronic and zero-point Energies= -643.253103
Sum of electronic and thermal Energies= -643.242519
Sum of electronic and thermal Enthalpies= -643.241574
Sum of electronic and thermal Free Energies= -643.289333

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.833	40.682	100.516

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.604008	-0.237110	-0.000082
2	6	0	0.565332	-0.994003	0.000241
3	6	0	1.791182	-0.267518	0.000091
4	6	0	0.506241	1.675571	-0.000040
5	6	0	-1.180090	-2.379304	-0.000150
6	7	0	3.014941	-0.822034	0.000021
7	7	0	-1.663339	-1.133513	-0.000314
8	7	0	1.702840	1.068432	0.000081
9	7	0	0.156864	-2.331499	0.000086
10	1	0	3.182385	-1.817308	-0.000178
11	1	0	3.821418	-0.208256	-0.000149
12	1	0	-1.772029	-3.283779	-0.000169
13	8	0	0.482184	3.000043	-0.000084
14	7	0	-0.701079	1.087445	-0.000229

15	1	0	0.743317	-3.158457	0.000711
16	1	0	-2.500891	1.424618	0.000201
17	9	0	-3.347752	0.961280	0.000304
18	1	0	-2.641254	-0.817904	-0.000358
19	1	0	1.395810	3.341584	0.000015

N7H-amino 2OA-enol-u with HF hydrogen-bonded to N3 (2OA-enol-u-12), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -643.025588770 A.U. after 8 cycles

Zero-point correction= 0.128524 (Hartree/Particle)
Thermal correction to Energy= 0.139234
Thermal correction to Enthalpy= 0.140178
Thermal correction to Gibbs Free Energy= 0.091109
Sum of electronic and zero-point Energies= -642.897065
Sum of electronic and thermal Energies= -642.886355
Sum of electronic and thermal Enthalpies= -642.885411
Sum of electronic and thermal Free Energies= -642.934480

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.370	40.038	103.275

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.059982	-0.830326	0.001087
2	6	0	1.231495	-0.272416	-0.007376
3	6	0	1.358271	1.124808	0.007057
4	6	0	-0.949782	1.223957	-0.016276
5	6	0	1.291608	-2.475104	-0.016051
6	7	0	2.558471	1.791404	-0.021698
7	7	0	0.006136	-2.204312	-0.000092
8	7	0	0.238432	1.857467	-0.005184
9	7	0	2.093610	-1.362122	-0.009590
10	1	0	3.371524	1.343659	0.379384
11	1	0	2.496057	2.787293	0.155170
12	1	0	1.712602	-3.472477	-0.030059
13	8	0	-2.041153	2.009551	-0.035179
14	7	0	-1.182148	-0.083165	-0.001537
15	1	0	3.099198	-1.360291	-0.105367
16	1	0	-1.735609	2.933083	-0.043666
17	1	0	-2.780107	-0.760385	0.021277
18	9	0	-3.673956	-1.129746	0.040083

N7-protonated N9H-amino 2OA-enol-u with HF hydrogen-bonded to N1 (2OA-enol-u-13), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -643.388035847 A.U. after 1 cycles

```
Zero-point correction=                           0.142212 (Hartree/Particle)
Thermal correction to Energy=                    0.152786
Thermal correction to Enthalpy=                  0.153730
Thermal correction to Gibbs Free Energy=         0.105865
Sum of electronic and zero-point Energies=           -643.245824
Sum of electronic and thermal Energies=              -643.235250
Sum of electronic and thermal Enthalpies=            -643.234306
Sum of electronic and thermal Free Energies=         -643.282171

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   95.875             40.420           100.741


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        1.114416   -0.845976   -0.000146
     2          6           0        1.106258    0.552089   -0.000167
     3          6           0       -0.168793    1.177707   -0.000179
     4          6           0       -1.083613   -0.992997   -0.000139
     5          6           0        3.226972   -0.123788    0.000297
     6          1           0        2.791111   -2.181551    0.000073
     7          7           0       -0.371311    2.507365   -0.000012
     8          7           0        2.458171   -1.220930    0.000055
     9          7           0       -1.232756    0.361481   -0.000286
    10          7           0        2.443869    0.956909    0.000140
    11          1           0        0.376846    3.184784   -0.000486
    12          1           0       -1.318062    2.867718   -0.000057
    13          1           0        4.307846   -0.111821    0.000462
    14          8           0       -2.164868   -1.738970    0.000019
    15          7           0        0.079361   -1.659187   -0.000156
    16          1           0       -2.987658   -1.191980    0.000276
    17          1           0        2.806292    1.904072    0.000328
    18          1           0       -2.921112    0.704326   -0.000595
    19          9           0       -3.838789    0.390504    0.000408
---------------------------------------------------------------------
```

N7H-amino 2OA-enol-u with HF hydrogen-bonded to N1 (2OA-enol-u-14), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -643.026617954     A.U. after    1 cycles


Zero-point correction=                           0.128427 (Hartree/Particle)
Thermal correction to Energy=                    0.138832
Thermal correction to Enthalpy=                  0.139776
Thermal correction to Gibbs Free Energy=         0.092124
Sum of electronic and zero-point Energies=           -642.898191
Sum of electronic and thermal Energies=              -642.887786
Sum of electronic and thermal Enthalpies=            -642.886841
Sum of electronic and thermal Free Energies=         -642.934494
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.119	39.187	100.293

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.196355	-0.882156	0.013464
2	6	0	1.108449	0.526225	-0.009007
3	6	0	-0.158486	1.116482	-0.000000
4	6	0	-1.024497	-1.059903	-0.000762
5	6	0	3.202350	-0.153781	-0.008542
6	7	0	-0.388716	2.469289	-0.043258
7	7	0	2.519625	-1.274399	0.017970
8	7	0	-1.217228	0.290942	-0.003651
9	7	0	2.422752	0.976154	-0.012103
10	1	0	0.312836	3.087332	0.341371
11	1	0	-1.341931	2.765725	0.131142
12	1	0	4.283137	-0.088261	-0.022775
13	8	0	-2.128812	-1.819041	-0.009663
14	7	0	0.130666	-1.698048	0.018839
15	1	0	2.758688	1.921760	-0.128188
16	1	0	-2.729815	0.640013	-0.008892
17	9	0	-3.726375	0.539036	-0.003838
18	1	0	-2.929756	-1.254336	-0.016309

N7-protonated N9H-amino 2OA-enol-u with HF hydrogen-bonded to N1 and N3 (2OA-enol-u-15), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -743.849987035 A.U. after 9 cycles

Zero-point correction=	0.154670 (Hartree/Particle)
Thermal correction to Energy=	0.167319
Thermal correction to Enthalpy=	0.168264
Thermal correction to Gibbs Free Energy=	0.115402
Sum of electronic and zero-point Energies=	-743.695317
Sum of electronic and thermal Energies=	-743.682668
Sum of electronic and thermal Enthalpies=	-743.681724
Sum of electronic and thermal Free Energies=	-743.734585

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	104.994	47.213	111.256

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.058519	0.138914	-0.000001
2	6	0	-0.619714	-1.182983	-0.000001

3	6	0	0.787632	-1.386384	-0.000002
4	6	0	1.003327	0.959647	-0.000003
5	6	0	-2.846301	-1.174309	0.000003
6	7	0	1.386793	-2.587960	-0.000001
7	7	0	-2.445649	0.100224	0.000001
8	7	0	1.553089	-0.282919	-0.000005
9	7	0	-1.773426	-1.973171	0.000002
10	1	0	0.881081	-3.461806	0.000001
11	1	0	2.398551	-2.642563	-0.000001
12	1	0	-3.873737	-1.510912	0.000004
13	8	0	1.797022	2.004362	-0.000003
14	7	0	-0.310430	1.234128	-0.000002
15	1	0	-1.834029	-2.985353	0.000002
16	1	0	-1.524717	2.644175	0.000000
17	1	0	3.286142	-0.081644	-0.000017
18	9	0	4.042358	0.522194	0.000009
19	9	0	-2.477926	2.782399	0.000001
20	1	0	2.750914	1.741561	-0.000001
21	1	0	-3.011454	0.958878	0.000002

N7H-amino 2OA-enol-u with HF hydrogen-bonded to N1 and N3 (2OA-enol-u-16), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -743.488908283 A.U. after 9 cycles

Zero-point correction= 0.140682 (Hartree/Particle)
Thermal correction to Energy= 0.153559
Thermal correction to Enthalpy= 0.154503
Thermal correction to Gibbs Free Energy= 0.099898
Sum of electronic and zero-point Energies= -743.348226
Sum of electronic and thermal Energies= -743.335349
Sum of electronic and thermal Enthalpies= -743.334405
Sum of electronic and thermal Free Energies= -743.389010

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	96.360	46.387	114.926

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.224600	0.249051	-0.000670
2	6	0	-0.917106	-1.125318	-0.006338
3	6	0	0.427573	-1.513697	0.008693
4	6	0	0.959138	0.767698	-0.012052
5	6	0	-3.090674	-0.774911	-0.015452
6	7	0	0.863559	-2.808547	-0.015980
7	7	0	-2.585379	0.437929	-0.002821
8	7	0	1.348632	-0.534979	-0.001968
9	7	0	-2.147366	-1.770135	-0.007718
10	1	0	0.253748	-3.543193	0.314011

11	1	0	1.850614	-2.965851	0.147507
12	1	0	-4.148996	-1.002777	-0.028468
13	8	0	1.920256	1.691255	-0.025527
14	7	0	-0.287588	1.217193	-0.002119
15	1	0	-2.335378	-2.759215	-0.091828
16	1	0	-0.684162	2.930028	0.017756
17	1	0	2.923939	-0.631148	-0.008275
18	9	0	3.874691	-0.337960	-0.006795
19	9	0	-0.907665	3.867527	0.034456
20	1	0	2.805958	1.268850	-0.026283

Cartesian coordinates and energies (in Hartree) for species of 2-aminopurine (2AP)

N9H-amino 2AP (2AP-1), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.336418261 A.U. after 1 cycles

Zero-point correction= 0.111860 (Hartree/Particle)
Thermal correction to Energy= 0.119022
Thermal correction to Enthalpy= 0.119967
Thermal correction to Gibbs Free Energy= 0.080293
Sum of electronic and zero-point Energies= -467.224558
Sum of electronic and thermal Energies= -467.217396
Sum of electronic and thermal Enthalpies= -467.216452
Sum of electronic and thermal Free Energies= -467.256125

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.688	28.827	83.500

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.468630	-0.612802	-0.000702
2	6	0	0.803655	0.758105	-0.003316
3	6	0	-0.280476	1.636433	0.003457
4	6	0	-1.711654	-0.175917	-0.004320
5	1	0	1.809808	-2.272084	0.000371
6	7	0	1.676079	-1.269937	0.003315
7	7	0	-1.529753	1.169942	0.003158
8	7	0	-0.757227	-1.126089	0.001717
9	1	0	3.709932	-0.548472	0.002419
10	7	0	2.183936	0.928423	-0.001202
11	6	0	2.659054	-0.288916	0.001514
12	1	0	-0.152432	2.717140	0.012345
13	7	0	-3.013993	-0.603296	-0.058888
14	1	0	-3.722506	0.075465	0.181857
15	1	0	-3.193344	-1.566771	0.186502

N1H-amino 2AP (2AP-2), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.308713439 A.U. after 8 cycles

Zero-point correction= 0.111849 (Hartree/Particle)
Thermal correction to Energy= 0.119042
Thermal correction to Enthalpy= 0.119986
Thermal correction to Gibbs Free Energy= 0.080202
Sum of electronic and zero-point Energies= -467.196865
Sum of electronic and thermal Energies= -467.189672
Sum of electronic and thermal Enthalpies= -467.188728
Sum of electronic and thermal Free Energies= -467.228512

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.700	28.676	83.733

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.553002	-0.690541	-0.006351
2	6	0	-0.888081	0.735603	0.009733
3	6	0	0.133269	1.634030	-0.002833
4	6	0	1.663438	-0.239028	-0.000331
5	7	0	-1.677689	-1.396505	-0.009774
6	7	0	1.413019	1.116336	-0.015370
7	7	0	0.724088	-1.150642	0.006831
8	1	0	-3.692466	-0.679611	0.002957
9	7	0	-2.255373	0.864189	0.018321
10	6	0	-2.641269	-0.410795	0.003796
11	1	0	0.038060	2.713908	-0.009138
12	7	0	3.000185	-0.609590	-0.065123
13	1	0	3.638893	-0.111149	0.546113
14	1	0	3.105163	-1.615388	0.019272
15	1	0	2.194611	1.750108	-0.127485

N1H-amino 2AP (2AP-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -467.356269019 A.U. after 1 cycles

Zero-point correction= 0.112066 (Hartree/Particle)
Thermal correction to Energy= 0.119178
Thermal correction to Enthalpy= 0.120122
Thermal correction to Gibbs Free Energy= 0.080540
Sum of electronic and zero-point Energies= -467.244203
Sum of electronic and thermal Energies= -467.237091
Sum of electronic and thermal Enthalpies= -467.236147
Sum of electronic and thermal Free Energies= -467.275729

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.785	28.574	83.308

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.553001	-0.672944	-0.002137
2	6	0	-0.877100	0.732642	-0.001062
3	6	0	0.155859	1.623917	0.000664
4	6	0	1.672447	-0.249120	-0.001957
5	7	0	-1.694752	-1.384356	0.001100
6	7	0	1.419259	1.101619	-0.001953
7	7	0	0.707654	-1.157499	-0.000136
8	1	0	-3.704033	-0.661873	0.006237
9	7	0	-2.253883	0.871579	0.002802
10	6	0	-2.651900	-0.400882	0.003596
11	1	0	0.077904	2.704814	0.005339
12	7	0	2.978860	-0.632773	-0.064495
13	1	0	3.684704	0.020539	0.259328
14	1	0	3.156648	-1.600811	0.179570
15	1	0	2.206981	1.745672	-0.006321

N1H-amino 2AP (2AP-2), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -467.379672021 A.U. after 7 cycles

Zero-point correction= 0.105843 (Hartree/Particle)
Thermal correction to Energy= 0.112976
Thermal correction to Enthalpy= 0.113921
Thermal correction to Gibbs Free Energy= 0.074305
Sum of electronic and zero-point Energies= -467.273829
Sum of electronic and thermal Energies= -467.266696
Sum of electronic and thermal Enthalpies= -467.265751
Sum of electronic and thermal Free Energies= -467.305367

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.894	28.697	83.378

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.555578	-0.670301	-0.000367
2	6	0	-0.873973	0.732233	-0.001941
3	6	0	0.165282	1.619801	0.001497
4	6	0	1.673398	-0.252981	-0.002129
5	7	0	-1.703785	-1.379490	0.002948
6	7	0	1.423752	1.096956	0.002054

7	7	0	0.700792	-1.161356	0.000887
8	1	0	-3.715244	-0.652030	0.003713
9	7	0	-2.252211	0.876320	-0.000287
10	6	0	-2.657487	-0.394958	0.002257
11	1	0	0.087112	2.710077	0.006201
12	7	0	2.974241	-0.639870	-0.066717
13	1	0	3.692321	0.041536	0.227066
14	1	0	3.163719	-1.620101	0.192139
15	1	0	2.262714	1.769824	0.002782

N7H-amino 2AP (2AP-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.329320468 A.U. after 11 cycles

Zero-point correction= 0.111629 (Hartree/Particle)
Thermal correction to Energy= 0.118857
Thermal correction to Enthalpy= 0.119801
Thermal correction to Gibbs Free Energy= 0.080001
Sum of electronic and zero-point Energies= -467.217692
Sum of electronic and thermal Energies= -467.210463
Sum of electronic and thermal Enthalpies= -467.209519
Sum of electronic and thermal Free Energies= -467.249320

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.584	28.976	83.767

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.477214	-0.660491	-0.000578
2	6	0	0.782527	0.722755	-0.005323
3	6	0	-0.272048	1.627917	0.004935
4	6	0	-1.715748	-0.170183	-0.004571
5	7	0	1.639695	-1.409931	0.005400
6	7	0	-1.525427	1.177114	0.004989
7	7	0	-0.774336	-1.124669	0.002217
8	1	0	3.661640	-0.755788	0.003613
9	7	0	2.169354	0.782731	-0.002820
10	6	0	2.604882	-0.518618	0.002485
11	1	0	-0.135508	2.708514	0.015911
12	7	0	-3.025052	-0.584508	-0.063973
13	1	0	-3.725416	0.093079	0.202670
14	1	0	-3.202115	-1.548064	0.184499
15	1	0	2.750796	1.608822	-0.009079

N9-deprotonated N9H-amino 2AP (2AP-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -466.792511587 A.U. after 9 cycles

```
Zero-point correction=                           0.098991 (Hartree/Particle)
Thermal correction to Energy=                    0.105761
Thermal correction to Enthalpy=                  0.106706
Thermal correction to Gibbs Free Energy=         0.067650
Sum of electronic and zero-point Energies=           -466.693520
Sum of electronic and thermal Energies=              -466.686750
Sum of electronic and thermal Enthalpies=            -466.685806
Sum of electronic and thermal Free Energies=         -466.724861

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   66.366             26.853             82.199


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.526913   -0.669916   -0.007307
     2          6           0        0.848034    0.733097   -0.005630
     3          6           0       -0.217581    1.619533    0.002457
     4          6           0       -1.669348   -0.163047   -0.016075
     5          7           0        1.678284   -1.387786    0.003805
     6          7           0       -1.491213    1.177194   -0.003471
     7          7           0       -0.746822   -1.125187   -0.009905
     8          1           0        3.678998   -0.656118    0.017152
     9          7           0        2.221642    0.878696    0.005512
    10          6           0        2.620797   -0.402237    0.009563
    11          1           0       -0.077000    2.701502    0.018473
    12          7           0       -3.016149   -0.587980   -0.078854
    13          1           0       -3.644604    0.086199    0.344010
    14          1           0       -3.130472   -1.520734    0.302710
---------------------------------------------------------------------
```

N1-protonated N9H-amino 2AP (2AP-5), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -467.703036190     A.U. after    1 cycles


Zero-point correction=                           0.124861 (Hartree/Particle)
Thermal correction to Energy=                    0.132377
Thermal correction to Enthalpy=                  0.133321
Thermal correction to Gibbs Free Energy=         0.092969
Sum of electronic and zero-point Energies=           -467.578175
Sum of electronic and thermal Energies=              -467.570660
Sum of electronic and thermal Enthalpies=            -467.569715
Sum of electronic and thermal Free Energies=         -467.610068

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   83.068             30.168             84.928
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.493584	-0.632781	0.000051
2	6	0	0.843685	0.759420	0.000103
3	6	0	-0.194911	1.646697	-0.000030
4	6	0	-1.712320	-0.241621	-0.000012
5	1	0	1.821123	-2.286713	0.000201
6	7	0	1.684496	-1.281387	-0.000088
7	7	0	-1.459421	1.116913	0.000093
8	7	0	-0.729662	-1.141542	-0.000042
9	1	0	3.728760	-0.568501	-0.000132
10	7	0	2.218740	0.918861	0.000063
11	6	0	2.680106	-0.298470	-0.000058
12	1	0	-0.104394	2.726994	-0.000123
13	7	0	-2.987867	-0.660529	-0.000026
14	1	0	-3.786969	-0.041852	-0.000198
15	1	0	-3.160088	-1.658445	0.000479
16	1	0	-2.243302	1.762838	-0.000550

N1-protonated N9H-amino 2AP (2AP-5), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -467.813251472 A.U. after 1 cycles

Zero-point correction= 0.124546 (Hartree/Particle)
Thermal correction to Energy= 0.132287
Thermal correction to Enthalpy= 0.133231
Thermal correction to Gibbs Free Energy= 0.091976
Sum of electronic and zero-point Energies= -467.688706
Sum of electronic and thermal Energies= -467.680964
Sum of electronic and thermal Enthalpies= -467.680020
Sum of electronic and thermal Free Energies= -467.721276

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.012	30.212	86.830

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.501235	-0.625634	0.000039
2	6	0	0.833192	0.761292	-0.000039
3	6	0	-0.215894	1.638841	-0.000098
4	6	0	-1.709672	-0.254207	0.000024
5	1	0	1.854087	-2.272068	0.000196
6	7	0	1.698621	-1.267921	0.000032
7	7	0	-1.464778	1.101222	-0.000048
8	7	0	-0.717276	-1.152728	0.000059
9	1	0	3.726767	-0.563130	0.000095
10	7	0	2.214421	0.931352	-0.000096

11	6	0	2.680028	-0.291808	0.000079
12	1	0	-0.146033	2.719935	-0.000191
13	7	0	-2.983265	-0.660109	0.000020
14	1	0	-3.755213	-0.003797	0.000055
15	1	0	-3.186027	-1.652302	0.000193
16	1	0	-2.260977	1.737751	-0.000142

N1-protonated N9H-amino 2AP (2AP-5), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -467.846612324 A.U. after 1 cycles

Zero-point correction= 0.113864 (Hartree/Particle)
Thermal correction to Energy= 0.121585
Thermal correction to Enthalpy= 0.122529
Thermal correction to Gibbs Free Energy= 0.081554
Sum of electronic and zero-point Energies= -467.732748
Sum of electronic and thermal Energies= -467.725028
Sum of electronic and thermal Enthalpies= -467.724084
Sum of electronic and thermal Free Energies= -467.765058

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.295	30.509	86.238

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.508726	-0.624274	0.000052
2	6	0	0.829642	0.763944	-0.000049
3	6	0	-0.226770	1.636147	-0.000122
4	6	0	-1.707902	-0.259710	-0.000004
5	1	0	1.874199	-2.323764	0.000219
6	7	0	1.708386	-1.262659	0.000138
7	7	0	-1.470464	1.096630	-0.000097
8	7	0	-0.709376	-1.156797	0.000084
9	1	0	3.736040	-0.546905	-0.000014
10	7	0	2.210497	0.941593	-0.000005
11	6	0	2.680054	-0.284072	-0.000033
12	1	0	-0.158239	2.727913	-0.000184
13	7	0	-2.979500	-0.667938	0.000002
14	1	0	-3.758965	0.009787	0.000038
15	1	0	-3.185886	-1.678872	0.000155
16	1	0	-2.326450	1.763826	-0.000130

N2-protonated N9H-amino 2AP (2AP-6), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.677561773 A.U. after 1 cycles

```
Zero-point correction=                           0.126164 (Hartree/Particle)
Thermal correction to Energy=                    0.133674
Thermal correction to Enthalpy=                  0.134618
Thermal correction to Gibbs Free Energy=         0.093394
Sum of electronic and zero-point Energies=           -467.551398
Sum of electronic and thermal Energies=              -467.543888
Sum of electronic and thermal Enthalpies=            -467.542944
Sum of electronic and thermal Free Energies=         -467.584168

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   83.881             28.694             86.762


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.517770   -0.628367   -0.000004
     2          6           0       -0.859073    0.754476    0.000011
     3          6           0        0.197514    1.662369   -0.000003
     4          6           0        1.602450   -0.115131   -0.000028
     5          1           0       -1.847301   -2.294753   -0.000014
     6          7           0       -1.708279   -1.290519   -0.000006
     7          7           0        1.463050    1.195309   -0.000021
     8          7           0        0.731746   -1.106094   -0.000022
     9          1           0       -3.744796   -0.579038    0.000014
    10          7           0       -2.228026    0.908911    0.000018
    11          6           0       -2.695061   -0.313544    0.000009
    12          1           0        0.058138    2.739170   -0.000008
    13          7           0        3.032413   -0.566299    0.000025
    14          1           0        3.529500   -0.208881   -0.826925
    15          1           0        3.070738   -1.594124   -0.000830
    16          1           0        3.529026   -0.210355    0.827898
---------------------------------------------------------------------
```

N3-protonated N9H-amino 2AP (2AP-7), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -467.688744211     A.U. after    1 cycles


Zero-point correction=                           0.124360 (Hartree/Particle)
Thermal correction to Energy=                    0.131933
Thermal correction to Enthalpy=                  0.132877
Thermal correction to Gibbs Free Energy=         0.092413
Sum of electronic and zero-point Energies=           -467.564384
Sum of electronic and thermal Energies=              -467.556812
Sum of electronic and thermal Enthalpies=            -467.555867
Sum of electronic and thermal Free Energies=         -467.596332

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   82.789             30.406             85.164
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.534696	-0.613462	-0.000009
2	6	0	0.824426	0.757588	-0.000077
3	6	0	-0.261855	1.641543	0.000059
4	6	0	-1.761441	-0.122133	-0.000032
5	1	0	1.898448	-2.258563	0.000410
6	7	0	1.721824	-1.259989	-0.000020
7	7	0	-1.515783	1.192282	0.000109
8	7	0	-0.751510	-1.064464	0.000141
9	1	0	3.753196	-0.500622	-0.000059
10	7	0	2.194296	0.947319	-0.000098
11	6	0	2.700504	-0.249766	-0.000002
12	1	0	-0.123543	2.720029	0.000212
13	7	0	-3.034829	-0.536908	-0.000171
14	1	0	-3.757206	0.174085	0.000056
15	1	0	-3.319900	-1.506964	0.000042
16	1	0	-0.966954	-2.058266	-0.000027

N7-protonated N9H-amino 2AP (2AP-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.700738401 A.U. after 9 cycles

Zero-point correction= 0.125324 (Hartree/Particle)
Thermal correction to Energy= 0.132602
Thermal correction to Enthalpy= 0.133546
Thermal correction to Gibbs Free Energy= 0.093622
Sum of electronic and zero-point Energies= -467.575414
Sum of electronic and thermal Energies= -467.568137
Sum of electronic and thermal Enthalpies= -467.567193
Sum of electronic and thermal Free Energies= -467.607117

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.209	29.634	84.027

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.423093	-0.612419	0.000001
2	6	0	0.744832	0.751242	0.000000
3	6	0	-0.336060	1.650502	0.000001
4	6	0	-1.757286	-0.186310	0.000000
5	1	0	1.748167	-2.305247	-0.000001
6	7	0	1.640657	-1.295061	0.000000
7	7	0	-1.563432	1.172475	-0.000000
8	7	0	-0.785046	-1.130829	0.000001
9	1	0	3.698701	-0.646649	-0.000001

10	7	0	2.137394	0.829477	-0.000001
11	6	0	2.645690	-0.403318	-0.000001
12	1	0	-0.214813	2.731843	0.000001
13	7	0	-3.032316	-0.597896	-0.000001
14	1	0	-3.779537	0.083116	-0.000000
15	1	0	-3.252645	-1.584438	0.000002
16	1	0	2.697708	1.676031	0.000001

N9-protonated N9H-amino 2AP (2AP-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -467.635910744 A.U. after 1 cycles

Zero-point correction=	0.123955 (Hartree/Particle)
Thermal correction to Energy=	0.131377
Thermal correction to Enthalpy=	0.132321
Thermal correction to Gibbs Free Energy=	0.092076
Sum of electronic and zero-point Energies=	-467.511956
Sum of electronic and thermal Energies=	-467.504534
Sum of electronic and thermal Enthalpies=	-467.503589
Sum of electronic and thermal Free Energies=	-467.543835

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.440	29.974	84.703

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.412351	-0.561843	-0.000148
2	6	0	0.744955	0.785472	-0.000094
3	6	0	-0.354596	1.659352	0.000512
4	6	0	-1.763703	-0.180208	0.000001
5	1	0	1.808753	-1.909724	-0.828960
6	7	0	1.707399	-1.305526	0.000016
7	7	0	-1.584975	1.167091	-0.000090
8	7	0	-0.758189	-1.118949	0.000230
9	1	0	3.769629	-0.375871	0.000179
10	7	0	2.133551	0.988062	-0.000333
11	6	0	2.713553	-0.137265	0.000152
12	1	0	-0.240848	2.740854	-0.000182
13	7	0	-3.020596	-0.635417	-0.000235
14	1	0	-3.789246	0.022884	0.000056
15	1	0	-3.212302	-1.628249	0.000241
16	1	0	1.808324	-1.909779	0.829004

N7-protonated N9H-amino 2AP with HF hydrogen-bonded to N3 (2AP-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -568.160073693 A.U. after 1 cycles

```
Zero-point correction=                           0.137831 (Hartree/Particle)
Thermal correction to Energy=                    0.147205
Thermal correction to Enthalpy=                  0.148149
Thermal correction to Gibbs Free Energy=         0.103046
Sum of electronic and zero-point Energies=           -568.022242
Sum of electronic and thermal Energies=              -568.012869
Sum of electronic and thermal Enthalpies=            -568.011925
Sum of electronic and thermal Free Energies=         -568.057028

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   92.372             36.326             94.927


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.430292    0.141028    0.000000
     2          6           0       -0.639711   -1.239018   -0.000001
     3          6           0        0.510449   -2.050169   -0.000001
     4          6           0        1.794274   -0.111421    0.000001
     5          1           0       -1.815560    1.754305   -0.000001
     6          7           0       -1.684530    0.737007   -0.000001
     7          7           0        1.696880   -1.478249    0.000000
     8          7           0        0.746253    0.751505    0.000000
     9          1           0       -3.686974   -0.057155   -0.000001
    10          7           0       -2.023412   -1.419712   -0.000000
    11          6           0       -2.618836   -0.223704   -0.000001
    12          1           0        0.476257   -3.137622   -0.000001
    13          7           0        3.035332    0.389569    0.000001
    14          1           0        3.825182   -0.242442    0.000000
    15          1           0        3.199234    1.387059    0.000001
    16          1           0       -2.520569   -2.304749    0.000000
    17          1           0        0.305536    2.502120    0.000001
    18          9           0       -0.430230    3.126372    0.000001
---------------------------------------------------------------------
```

N7H-amino 2AP with HF hydrogen-bonded to N3 (2AP-11), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -567.797039363     A.U. after    8 cycles


Zero-point correction=                           0.123824 (Hartree/Particle)
Thermal correction to Energy=                    0.133398
Thermal correction to Enthalpy=                  0.134342
Thermal correction to Gibbs Free Energy=         0.088133
Sum of electronic and zero-point Energies=           -567.673215
Sum of electronic and thermal Energies=              -567.663642
Sum of electronic and thermal Enthalpies=            -567.662698
Sum of electronic and thermal Free Energies=         -567.708906

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
```

Total	83.708	35.521	97.254

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.575780	0.515928	0.015337
2	6	0	-1.391136	-0.637418	-0.006501
3	6	0	-0.772878	-1.884082	-0.024614
4	6	0	1.270200	-0.808556	0.014989
5	7	0	-1.343134	1.657998	0.022149
6	7	0	0.554182	-1.966341	-0.013335
7	7	0	0.761082	0.441672	0.024639
8	1	0	-3.460949	1.851146	0.006433
9	7	0	-2.691038	-0.148572	-0.012453
10	6	0	-2.583585	1.216659	0.005773
11	1	0	-1.323465	-2.823418	-0.049190
12	7	0	2.620395	-0.933501	0.049929
13	1	0	3.024844	-1.851165	-0.053535
14	1	0	3.202686	-0.106211	-0.012437
15	1	0	-3.549409	-0.681452	-0.025231
16	1	0	1.908952	1.605281	-0.007398
17	9	0	2.800668	2.025760	-0.042783

N7-protonated N9H-amino 2AP with HF hydrogen-bonded to N1 (2AP-12), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -568.156292891 A.U. after 7 cycles

Zero-point correction=	0.138123 (Hartree/Particle)
Thermal correction to Energy=	0.147462
Thermal correction to Enthalpy=	0.148406
Thermal correction to Gibbs Free Energy=	0.103123
Sum of electronic and zero-point Energies=	-568.018170
Sum of electronic and thermal Energies=	-568.008831
Sum of electronic and thermal Enthalpies=	-568.007887
Sum of electronic and thermal Free Energies=	-568.053170

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.534	36.103	95.307

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.090395	0.623594	0.000000
2	6	0	-1.082292	-0.779724	-0.000000
3	6	0	0.174274	-1.398645	0.000000
4	6	0	1.133880	0.738226	0.000000
5	7	0	-2.435368	0.998066	0.000000
6	7	0	1.254320	-0.638151	0.000000

7	7	0	-0.043026	1.413459	0.000000
8	1	0	-4.281143	-0.118725	-0.000000
9	7	0	-2.417395	-1.185121	-0.000000
10	6	0	-3.200112	-0.106544	-0.000000
11	1	0	0.315363	-2.476978	0.000000
12	7	0	2.268845	1.437847	-0.000000
13	1	0	3.167722	0.958298	-0.000000
14	1	0	2.233940	2.448632	-0.000000
15	1	0	-2.763591	-2.139790	-0.000000
16	1	0	2.962716	-1.108836	0.000000
17	9	0	3.904517	-0.906786	-0.000000
18	1	0	-2.779425	1.954336	0.000000

N7H-amino 2AP with HF hydrogen-bonded to N1 (2AP-13), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -567.796621532 A.U. after 1 cycles

Zero-point correction= 0.123638 (Hartree/Particle)
Thermal correction to Energy= 0.133246
Thermal correction to Enthalpy= 0.134190
Thermal correction to Gibbs Free Energy= 0.087910
Sum of electronic and zero-point Energies= -567.672983
Sum of electronic and thermal Energies= -567.663376
Sum of electronic and thermal Enthalpies= -567.662431
Sum of electronic and thermal Free Energies= -567.708711

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.613	35.554	97.404

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.160207	0.657920	-0.007756
2	6	0	-1.078216	-0.760838	0.016856
3	6	0	0.175129	-1.345626	0.033506
4	6	0	1.085538	0.800937	0.019630
5	7	0	-2.481439	1.059314	-0.032808
6	7	0	1.254021	-0.556346	0.034815
7	7	0	-0.088333	1.449147	-0.007666
8	1	0	-4.248201	-0.120568	-0.035572
9	7	0	-2.396146	-1.195641	0.006272
10	6	0	-3.166821	-0.061873	-0.022823
11	1	0	0.350005	-2.419130	0.043332
12	7	0	2.222648	1.544325	0.053390
13	1	0	3.125005	1.094570	-0.038298
14	1	0	2.145100	2.542186	-0.072816
15	1	0	-2.732136	-2.148489	0.018703
16	1	0	2.774952	-1.022164	-0.007830
17	9	0	3.764165	-1.086124	-0.058001

N7-protonated N9H-amino 2AP with HF hydrogen-bonded to N1 and N3 (2AP-14), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -668.614848000 A.U. after 1 cycles

Zero-point correction= 0.150498 (Hartree/Particle)
Thermal correction to Energy= 0.161991
Thermal correction to Enthalpy= 0.162936
Thermal correction to Gibbs Free Energy= 0.112412
Sum of electronic and zero-point Energies= -668.464350
Sum of electronic and thermal Energies= -668.452857
Sum of electronic and thermal Enthalpies= -668.451912
Sum of electronic and thermal Free Energies= -668.502436

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.651	43.006	106.336

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.961006	0.034944	-0.000356
2	6	0	-0.664486	-1.331505	-0.000130
3	6	0	0.693610	-1.680373	0.000080
4	6	0	1.208951	0.606883	-0.000333
5	1	0	-2.831452	1.045743	-0.000105
6	7	0	-2.345421	0.141650	-0.000236
7	7	0	1.597395	-0.717570	-0.000042
8	7	0	-0.083807	1.025102	-0.000527
9	1	0	-3.931363	-1.315659	0.000216
10	7	0	-1.892385	-1.995275	0.000135
11	6	0	-2.873825	-1.090039	0.000091
12	1	0	1.051752	-2.707223	0.000265
13	7	0	2.183157	1.515277	-0.000416
14	1	0	3.157870	1.214637	-0.000335
15	1	0	1.964193	2.502597	-0.000803
16	1	0	-1.143579	2.528011	0.000388
17	1	0	3.389828	-0.838198	0.000553
18	1	0	-2.041964	-2.999608	0.000265
19	9	0	4.256563	-0.422621	0.000533
20	9	0	-2.061821	2.816615	0.000694

N7H-amino 2AP with HF hydrogen-bonded to N1 and N3 (2AP-15), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -668.262287314 A.U. after 1 cycles

Zero-point correction= 0.136648 (Hartree/Particle)
Thermal correction to Energy= 0.148193

```
Thermal correction to Enthalpy=                  0.149138
Thermal correction to Gibbs Free Energy=         0.097793
Sum of electronic and zero-point Energies=           -668.125640
Sum of electronic and thermal Energies=              -668.114094
Sum of electronic and thermal Enthalpies=            -668.113150
Sum of electronic and thermal Free Energies=         -668.164494

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   92.993             41.669            108.064


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.193734    0.353362    0.000310
     2          6           0       -1.257822   -1.062408    0.000103
     3          6           0       -0.071482   -1.777147   -0.000607
     4          6           0        1.078414    0.254157   -0.000146
     5          7           0       -2.455844    0.896728    0.000448
     6          7           0        1.086571   -1.113901   -0.000701
     7          7           0       -0.034293    1.017909    0.000329
     8          1           0       -4.341575   -0.085517    0.000242
     9          7           0       -2.615410   -1.353084   -0.000106
    10          6           0       -3.260468   -0.145906    0.000176
    11          1           0       -0.015055   -2.863378   -0.001138
    12          7           0        2.277117    0.871867   -0.000149
    13          1           0        3.128718    0.324100    0.000115
    14          1           0        2.313872    1.885147    0.000137
    15          1           0        0.304526    2.647118   -0.000057
    16          1           0        2.573511   -1.747302    0.000034
    17          1           0       -3.051030   -2.265053   -0.000482
    18          9           0        3.548374   -1.896292    0.000683
    19          9           0        0.841692    3.466950   -0.000307
---------------------------------------------------------------------
```

Cartesian coordinates and energies (in Hartree) for species of purine (P)

N9H-amino P (P-1), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -411.963191873     A.U. after    1 cycles


Zero-point correction=                           0.095205 (Hartree/Particle)
Thermal correction to Energy=                    0.100939
Thermal correction to Enthalpy=                  0.101884
Thermal correction to Gibbs Free Energy=         0.065187
Sum of electronic and zero-point Energies=           -411.867987
Sum of electronic and thermal Energies=              -411.862252
Sum of electronic and thermal Enthalpies=            -411.861308
Sum of electronic and thermal Free Energies=         -411.898005

                    E (Thermal)             CV                S
```

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	63.340	22.775	77.235

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.205096	-0.671264	0.000014
2	6	0	-0.245473	0.741536	0.000071
3	6	0	0.994079	1.380193	-0.000076
4	6	0	2.012648	-0.687433	-0.000288
5	6	0	-2.275524	0.099434	0.000274
6	1	0	-1.865883	-2.014237	0.000080
7	7	0	-1.525041	-1.061949	0.000131
8	7	0	2.119942	0.654213	-0.000251
9	7	0	-1.558036	1.194864	0.000296
10	1	0	-3.357965	0.067765	0.000384
11	7	0	0.891764	-1.422936	-0.000172
12	1	0	2.947589	-1.241486	-0.000445
13	1	0	1.092060	2.463813	-0.000031

N1H-amino P (P-2), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -411.942269262 A.U. after 1 cycles

Zero-point correction=	0.095184 (Hartree/Particle)
Thermal correction to Energy=	0.100906
Thermal correction to Enthalpy=	0.101850
Thermal correction to Gibbs Free Energy=	0.065163
Sum of electronic and zero-point Energies=	-411.847086
Sum of electronic and thermal Energies=	-411.841363
Sum of electronic and thermal Enthalpies=	-411.840419
Sum of electronic and thermal Free Energies=	-411.877106

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	63.320	22.798	77.215

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.315316	-0.729692	-0.000003
2	6	0	0.330356	0.735064	-0.000078
3	6	0	-0.867176	1.395837	0.000038
4	6	0	-1.936338	-0.763796	0.000281
5	6	0	2.290258	-0.003781	-0.000287
6	7	0	1.570268	-1.171534	-0.000138
7	7	0	-1.990803	0.609262	0.000219
8	7	0	1.627997	1.159273	-0.000262
9	1	0	3.374702	-0.030558	-0.000422

10	7	0	-0.831090	-1.457891	0.000178
11	1	0	-2.898022	-1.268369	0.000427
12	1	0	-1.003653	2.471544	0.000001
13	1	0	-2.902129	1.051813	0.000311

N1H-amino P (P-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -411.982149049 A.U. after 1 cycles

Zero-point correction= 0.096063 (Hartree/Particle)
Thermal correction to Energy= 0.101661
Thermal correction to Enthalpy= 0.102605
Thermal correction to Gibbs Free Energy= 0.066132
Sum of electronic and zero-point Energies= -411.886086
Sum of electronic and thermal Energies= -411.880488
Sum of electronic and thermal Enthalpies= -411.879544
Sum of electronic and thermal Free Energies= -411.916017

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	63.793	22.287	76.763

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.311538	-0.714368	-0.000003
2	6	0	0.323934	0.727744	-0.000078
3	6	0	-0.879581	1.386833	0.000039
4	6	0	-1.939546	-0.761636	0.000282
5	6	0	2.298399	-0.001580	-0.000283
6	7	0	1.578361	-1.164262	-0.000142
7	7	0	-1.989387	0.600132	0.000221
8	7	0	1.629729	1.157797	-0.000263
9	1	0	3.381889	-0.025787	-0.000423
10	7	0	-0.823703	-1.455623	0.000175
11	1	0	-2.899112	-1.264257	0.000427
12	1	0	-1.029373	2.460107	0.000002
13	1	0	-2.906867	1.041667	0.000310

N1H-amino P (P-2), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -411.997503352 A.U. after 1 cycles

Zero-point correction= 0.091250 (Hartree/Particle)
Thermal correction to Energy= 0.096875
Thermal correction to Enthalpy= 0.097819
Thermal correction to Gibbs Free Energy= 0.061301
Sum of electronic and zero-point Energies= -411.906253

Sum of electronic and thermal Energies= -411.900629
Sum of electronic and thermal Enthalpies= -411.899684
Sum of electronic and thermal Free Energies= -411.936203

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	60.790	22.440	76.859

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.315110	-0.712996	-0.000005
2	6	0	0.321371	0.726113	-0.000081
3	6	0	-0.887156	1.380072	0.000037
4	6	0	-1.936423	-0.764943	0.000282
5	6	0	2.302762	0.004656	-0.000291
6	7	0	1.587027	-1.158501	-0.000136
7	7	0	-1.994385	0.593586	0.000216
8	7	0	1.626248	1.161163	-0.000256
9	1	0	3.391158	-0.013564	-0.000418
10	7	0	-0.816090	-1.457471	0.000176
11	1	0	-2.897544	-1.279024	0.000431
12	1	0	-1.037929	2.463307	0.000006
13	1	0	-2.969262	1.060420	0.000323

N7H-amino P (P-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -411.956816796 A.U. after 1 cycles

Zero-point correction= 0.094982 (Hartree/Particle)
Thermal correction to Energy= 0.100771
Thermal correction to Enthalpy= 0.101716
Thermal correction to Gibbs Free Energy= 0.064921
Sum of electronic and zero-point Energies= -411.861835
Sum of electronic and thermal Energies= -411.856045
Sum of electronic and thermal Enthalpies= -411.855101
Sum of electronic and thermal Free Energies= -411.891896

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	63.235	22.929	77.441

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.217839	-0.715676	-0.000011
2	6	0	-0.235783	0.702139	0.000069
3	6	0	0.976738	1.383201	-0.000051
4	6	0	2.023487	-0.666712	-0.000298

5	6	0	-2.270514	-0.149971	0.000284
6	7	0	-1.507464	-1.215629	0.000126
7	7	0	2.113255	0.680954	-0.000235
8	7	0	-1.576864	1.039312	0.000262
9	1	0	-3.353413	-0.165501	0.000423
10	7	0	0.920768	-1.417324	-0.000197
11	1	0	2.970781	-1.199558	-0.000450
12	1	0	1.056831	2.469226	0.000000
13	1	0	-1.978598	1.966753	0.000370

N9-deprotonated N9H-amino P (P-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -411.426500545 A.U. after 1 cycles

Zero-point correction= 0.081979 (Hartree/Particle)
Thermal correction to Energy= 0.087424
Thermal correction to Enthalpy= 0.088368
Thermal correction to Gibbs Free Energy= 0.052140
Sum of electronic and zero-point Energies= -411.344521
Sum of electronic and thermal Energies= -411.339077
Sum of electronic and thermal Enthalpies= -411.338133
Sum of electronic and thermal Free Energies= -411.374361

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	54.859	21.280	76.249

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.268201	-0.715461	0.000002
2	6	0	0.290238	0.725631	-0.000072
3	6	0	-0.937871	1.376922	0.000051
4	6	0	-1.983561	-0.670511	0.000285
5	6	0	2.259161	-0.019823	-0.000281
6	7	0	1.548334	-1.176363	-0.000156
7	7	0	-2.089068	0.676869	0.000233
8	7	0	1.597524	1.153090	-0.000248
9	1	0	3.347112	-0.042682	-0.000419
10	7	0	-0.881506	-1.424021	0.000179
11	1	0	-2.931465	-1.210179	0.000425
12	1	0	-1.019642	2.465287	0.000016

N1-protonated N9H-amino P (P-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -412.323833697 A.U. after 9 cycles

Zero-point correction= 0.108853 (Hartree/Particle)

```
Thermal correction to Energy=                    0.114642
Thermal correction to Enthalpy=                  0.115586
Thermal correction to Gibbs Free Energy=         0.078797
Sum of electronic and zero-point Energies=           -412.214980
Sum of electronic and thermal Energies=              -412.209192
Sum of electronic and thermal Enthalpies=            -412.208247
Sum of electronic and thermal Free Energies=         -412.245036

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   71.939             23.478             77.428


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.256730   -0.684938    0.000005
     2          6           0        0.285189    0.745843   -0.000075
     3          6           0       -0.932812    1.389805    0.000041
     4          6           0       -1.965559   -0.782147    0.000286
     5          6           0        2.307538    0.120049   -0.000293
     6          1           0        1.917809   -2.004944   -0.000131
     7          7           0        1.561037   -1.053895   -0.000137
     8          7           0       -2.029962    0.584997    0.000220
     9          7           0        1.580416    1.207842   -0.000261
    10          1           0        3.390291    0.096241   -0.000426
    11          7           0       -0.835877   -1.452070    0.000181
    12          1           0       -2.912403   -1.311872    0.000431
    13          1           0       -1.079297    2.464380    0.000002
    14          1           0       -2.952224    1.016395    0.000312
---------------------------------------------------------------------
```

N1-protonated N9H-amino P (P-5), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

```
SCF Done:  E(RB3LYP) =  -412.433610995     A.U. after    1 cycles


Zero-point correction=                           0.109411 (Hartree/Particle)
Thermal correction to Energy=                    0.115153
Thermal correction to Enthalpy=                  0.116097
Thermal correction to Gibbs Free Energy=         0.079398
Sum of electronic and zero-point Energies=           -412.324200
Sum of electronic and thermal Energies=              -412.318458
Sum of electronic and thermal Enthalpies=            -412.317514
Sum of electronic and thermal Free Energies=         -412.354213

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   72.259             23.279             77.240


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
```

1	6	0	0.260675	-0.677469	0.000006
2	6	0	0.277354	0.745477	-0.000073
3	6	0	-0.942794	1.383009	0.000040
4	6	0	-1.961440	-0.782507	0.000285
5	6	0	2.305745	0.118795	-0.000289
6	1	0	1.938062	-1.990307	-0.000142
7	7	0	1.566693	-1.043476	-0.000141
8	7	0	-2.029599	0.575274	0.000220
9	7	0	1.578442	1.213498	-0.000259
10	1	0	3.386661	0.087813	-0.000428
11	7	0	-0.828257	-1.455437	0.000182
12	1	0	-2.909013	-1.305986	0.000431
13	1	0	-1.107184	2.453767	-0.000001
14	1	0	-2.956708	1.001874	0.000307

N1-protonated N9H-amino P (P-5), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -412.458986649 A.U. after 1 cycles

Zero-point correction= 0.099079 (Hartree/Particle)
Thermal correction to Energy= 0.104911
Thermal correction to Enthalpy= 0.105855
Thermal correction to Gibbs Free Energy= 0.069013
Sum of electronic and zero-point Energies= -412.359908
Sum of electronic and thermal Energies= -412.354075
Sum of electronic and thermal Enthalpies= -412.353131
Sum of electronic and thermal Free Energies= -412.389973

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.833	23.804	77.541

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.271254	-0.676011	-0.000014
2	6	0	0.272247	0.747430	-0.000071
3	6	0	-0.954784	1.374718	0.000050
4	6	0	-1.954019	-0.791147	0.000281
5	6	0	2.303856	0.130850	-0.000323
6	1	0	1.977186	-2.039400	-0.000083
7	7	0	1.578471	-1.034583	-0.000115
8	7	0	-2.037316	0.563819	0.000225
9	7	0	1.569112	1.225284	-0.000243
10	1	0	3.392276	0.113375	-0.000447
11	7	0	-0.815205	-1.459111	0.000163
12	1	0	-2.901907	-1.329697	0.000427
13	1	0	-1.124486	2.455805	0.000022
14	1	0	-3.039827	1.016994	0.000328

N3-protonated N9H-amino P (P-6), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -412.306124973 A.U. after 9 cycles

Zero-point correction=	0.108043 (Hartree/Particle)
Thermal correction to Energy=	0.113999
Thermal correction to Enthalpy=	0.114943
Thermal correction to Gibbs Free Energy=	0.077859
Sum of electronic and zero-point Energies=	-412.198082
Sum of electronic and thermal Energies=	-412.192126
Sum of electronic and thermal Enthalpies=	-412.191182
Sum of electronic and thermal Free Energies=	-412.228266

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	71.535	24.000	78.051

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.252774	0.663603	0.000000
2	6	0	-0.280843	-0.753401	-0.000071
3	6	0	0.938216	-1.423490	0.000048
4	6	0	2.077307	0.578894	0.000285
5	6	0	-2.307760	-0.105296	-0.000291
6	1	0	-1.904243	2.019118	-0.000139
7	7	0	-1.540695	1.071578	-0.000140
8	7	0	2.098322	-0.731993	0.000225
9	7	0	-1.590387	-1.189991	-0.000254
10	1	0	-3.389574	-0.057706	-0.000423
11	7	0	0.925922	1.322487	0.000178
12	1	0	3.006516	1.140257	0.000427
13	1	0	1.004560	-2.508230	0.000005
14	1	0	0.985738	2.340130	0.000234

N7-protonated N9H-amino P (P-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -412.313155701 A.U. after 1 cycles

Zero-point correction=	0.108538 (Hartree/Particle)
Thermal correction to Energy=	0.114392
Thermal correction to Enthalpy=	0.115336
Thermal correction to Gibbs Free Energy=	0.078422
Sum of electronic and zero-point Energies=	-412.204617
Sum of electronic and thermal Energies=	-412.198764
Sum of electronic and thermal Enthalpies=	-412.197819
Sum of electronic and thermal Free Energies=	-412.234734

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	71.782	23.634	77.693

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.159894	-0.674893	-0.000021
2	6	0	-0.195586	0.725081	0.000070
3	6	0	1.036075	1.391764	-0.000046
4	6	0	2.052716	-0.687709	-0.000303
5	6	0	-2.287802	-0.030853	0.000293
6	1	0	-1.795826	-2.072440	0.000111
7	7	0	-1.488530	-1.102722	0.000129
8	7	0	2.144967	0.659441	-0.000235
9	7	0	-1.545367	1.080570	0.000254
10	1	0	-3.369210	-0.056901	0.000430
11	7	0	0.930554	-1.419221	-0.000205
12	1	0	2.990342	-1.234254	-0.000459
13	1	0	1.137402	2.474686	0.000001
14	1	0	-1.927137	2.022093	0.000360

N9-protonated N9H-amino P (P-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -412.245705100 A.U. after 1 cycles

Zero-point correction=	0.107007 (Hartree/Particle)
Thermal correction to Energy=	0.113071
Thermal correction to Enthalpy=	0.114015
Thermal correction to Gibbs Free Energy=	0.076665
Sum of electronic and zero-point Energies=	-412.138698
Sum of electronic and thermal Energies=	-412.132634
Sum of electronic and thermal Enthalpies=	-412.131690
Sum of electronic and thermal Free Energies=	-412.169040

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.953	24.157	78.611

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.145137	-0.635364	-0.000012
2	6	0	-0.184450	0.751977	0.000071
3	6	0	1.059670	1.383806	-0.000022
4	6	0	2.055152	-0.702774	-0.000340
5	6	0	-2.300504	0.258332	0.000304
6	1	0	-1.793877	-1.662950	-0.829075

7	7	0	-1.566118	-1.092215	0.000142
8	7	0	2.167161	0.627715	-0.000236
9	7	0	-1.509054	1.243734	0.000227
10	1	0	-3.384492	0.246779	0.000439
11	7	0	0.895865	-1.413485	-0.000182
12	1	0	2.973107	-1.281510	-0.000393
13	1	0	1.175557	2.464611	-0.000002
14	1	0	-1.793667	-1.663029	0.829362

N7-protonated N9H-amino P with HF hydrogen-bonded to N3 (P-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -512.772621819 A.U. after 7 cycles

Zero-point correction= 0.120805 (Hartree/Particle)
Thermal correction to Energy= 0.128841
Thermal correction to Enthalpy= 0.129785
Thermal correction to Gibbs Free Energy= 0.087499
Sum of electronic and zero-point Energies= -512.651816
Sum of electronic and thermal Energies= -512.643781
Sum of electronic and thermal Enthalpies= -512.642837
Sum of electronic and thermal Free Energies= -512.685122

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	80.849	30.726	88.998

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.201360	0.010687	-0.000000
2	6	0	-0.970189	-0.752667	0.000100
3	6	0	-2.184713	-0.054727	-0.000006
4	6	0	-0.959462	1.909959	-0.000276
5	6	0	0.783581	-2.122504	0.000305
6	1	0	2.247102	-0.566990	0.000095
7	7	0	1.267889	-0.879471	0.000132
8	7	0	-2.147419	1.274769	-0.000194
9	7	0	-0.555454	-2.084976	0.000291
10	1	0	1.379830	-3.025309	0.000436
11	7	0	0.253088	1.337339	-0.000187
12	1	0	-0.988133	2.994827	-0.000429
13	1	0	-3.159417	-0.537218	0.000056
14	1	0	-1.150624	-2.908273	0.000403
15	1	0	2.136522	1.708241	-0.000228
16	9	0	2.953837	1.206290	-0.000152

N7H-amino P with HF hydrogen-bonded to N3 (P-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -512.420340983 A.U. after 1 cycles

```
Zero-point correction=                           0.107408 (Hartree/Particle)
Thermal correction to Energy=                    0.115533
Thermal correction to Enthalpy=                  0.116477
Thermal correction to Gibbs Free Energy=         0.072946
Sum of electronic and zero-point Energies=           -512.312933
Sum of electronic and thermal Energies=              -512.304808
Sum of electronic and thermal Enthalpies=            -512.303864
Sum of electronic and thermal Free Energies=         -512.347395

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   72.498             29.712             91.618


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.109325   -0.430088    0.000053
     2          6           0       -1.257516    0.400157    0.000119
     3          6           0       -1.085024    1.779756   -0.000031
     4          6           0        1.187698    1.418093   -0.000277
     5          6           0       -1.777593   -1.743243    0.000219
     6          7           0       -0.465224   -1.759983    0.000258
     7          7           0        0.154534    2.280208   -0.000223
     8          7           0       -2.322930   -0.480431    0.000394
     9          1           0       -2.405151   -2.625640    0.000341
    10          7           0        1.128364    0.082448   -0.000147
    11          1           0        2.181667    1.855690   -0.000424
    12          1           0       -1.910904    2.488845    0.000038
    13          1           0       -3.308251   -0.254053    0.000567
    14          1           0        2.607474   -0.776744   -0.000233
    15          9           0        3.513614   -1.121314   -0.000306
---------------------------------------------------------------------
```

N7-protonated N9H-amino P with HF hydrogen-bonded to N1 (P-11), B3LYP/6-31+G(d)

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SCF Done:  E(RB3LYP) =  -512.764770930     A.U. after    1 cycles


Zero-point correction=                           0.120631 (Hartree/Particle)
Thermal correction to Energy=                    0.129011
Thermal correction to Enthalpy=                  0.129955
Thermal correction to Gibbs Free Energy=         0.085944
Sum of electronic and zero-point Energies=           -512.644140
Sum of electronic and thermal Energies=              -512.635760
Sum of electronic and thermal Enthalpies=            -512.634816
Sum of electronic and thermal Free Energies=         -512.678827

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   80.956             31.213             92.629
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.056976	0.662976	0.000026
2	6	0	0.473083	-0.610242	0.000108
3	6	0	-0.922761	-0.672661	-0.000010
4	6	0	-0.922378	1.653979	-0.000257
5	6	0	2.682037	-0.853102	0.000402
6	7	0	2.437172	0.462096	0.000170
7	7	0	-1.592314	0.480132	-0.000197
8	7	0	1.526720	-1.524008	0.000259
9	1	0	3.664707	-1.305985	0.000576
10	7	0	0.404955	1.811680	-0.000155
11	1	0	-1.525734	2.556010	-0.000413
12	1	0	-1.503019	-1.592779	0.000019
13	1	0	1.453404	-2.537962	0.000319
14	1	0	-3.384100	-0.107553	-0.000306
15	9	0	-3.942638	-0.878197	-0.000277
16	1	0	3.141008	1.197048	0.000152

N7H-amino P with HF hydrogen-bonded to N1 (P-12), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -512.421707345 A.U. after 1 cycles

Zero-point correction=	0.107398 (Hartree/Particle)
Thermal correction to Energy=	0.115484
Thermal correction to Enthalpy=	0.116428
Thermal correction to Gibbs Free Energy=	0.072902
Sum of electronic and zero-point Energies=	-512.314309
Sum of electronic and thermal Energies=	-512.306223
Sum of electronic and thermal Enthalpies=	-512.305279
Sum of electronic and thermal Free Energies=	-512.348806

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.467	29.501	91.609

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.070345	0.705050	0.000059
2	6	0	0.655436	-0.653563	0.000130
3	6	0	-0.702249	-0.936418	-0.000007
4	6	0	-1.075596	1.353371	-0.000241
5	6	0	2.850158	-0.460317	0.000232
6	7	0	2.447549	0.787939	0.000295
7	7	0	-1.560939	0.090925	-0.000193
8	7	0	1.828270	-1.382189	0.000378
9	1	0	3.886451	-0.774649	0.000360

10	7	0	0.201646	1.722513	-0.000118
11	1	0	-1.820791	2.143471	-0.000381
12	1	0	-1.121755	-1.939823	0.000043
13	1	0	1.928972	-2.388309	0.000533
14	1	0	-3.174226	-0.281268	-0.000342
15	9	0	-4.100321	-0.593609	-0.000420

N7-protonated N9H-amino P with HF hydrogen-bonded to N1 and N3 (P-13), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -613.223443172 A.U. after 1 cycles

Zero-point correction= 0.132641 (Hartree/Particle)
Thermal correction to Energy= 0.143336
Thermal correction to Enthalpy= 0.144280
Thermal correction to Gibbs Free Energy= 0.094653
Sum of electronic and zero-point Energies= -613.090802
Sum of electronic and thermal Energies= -613.080107
Sum of electronic and thermal Enthalpies= -613.079163
Sum of electronic and thermal Free Energies= -613.128790

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.945	38.673	104.450

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.787159	-0.034382	0.000042
2	6	0	0.179071	0.977480	0.000115
3	6	0	1.519527	0.583290	-0.000011
4	6	0	0.773899	-1.620828	-0.000247
5	6	0	-1.838751	1.910352	0.000348
6	1	0	-2.910468	0.062133	0.000175
7	7	0	-2.027487	0.589057	0.000192
8	7	0	1.781764	-0.725286	-0.000192
9	7	0	-0.527205	2.179786	0.000308
10	1	0	-2.625520	2.653383	0.000487
11	7	0	-0.534385	-1.338045	-0.000137
12	1	0	1.052306	-2.669666	-0.000395
13	1	0	2.367801	1.264248	0.000026
14	1	0	3.702623	-0.720762	-0.000307
15	1	0	-2.331533	-2.150074	-0.000138
16	1	0	-0.133976	3.117085	0.000404
17	9	0	4.441617	-0.123610	-0.000278
18	9	0	-3.224901	-1.808656	-0.000045

N7H-amino P with HF hydrogen-bonded to N1 and N3 (P-14), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -612.882686068 A.U. after 8 cycles

```
Zero-point correction=                           0.119757 (Hartree/Particle)
Thermal correction to Energy=                    0.130272
Thermal correction to Enthalpy=                  0.131216
Thermal correction to Gibbs Free Energy=         0.080649
Sum of electronic and zero-point Energies=           -612.762930
Sum of electronic and thermal Energies=              -612.752414
Sum of electronic and thermal Enthalpies=            -612.751470
Sum of electronic and thermal Free Energies=         -612.802037

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   81.747             36.563            106.426
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.020501	-0.065621	0.000100
2	6	0	0.272136	-1.271912	0.000161
3	6	0	-1.112438	-1.201203	0.000026
4	6	0	-0.907291	1.108761	-0.000203
5	6	0	2.444528	-1.638177	0.000400
6	7	0	2.368848	-0.326927	0.000252
7	7	0	-1.686735	0.009633	-0.000157
8	7	0	1.224327	-2.271437	0.000355
9	1	0	3.369279	-2.201404	0.000545
10	7	0	0.425150	1.134915	-0.000083
11	1	0	-1.419756	2.065780	-0.000352
12	1	0	-1.772246	-2.065535	0.000058
13	1	0	-3.369416	0.007664	-0.000309
14	1	0	1.200596	2.690658	-0.000178
15	1	0	1.068058	-3.270746	0.000448
16	9	0	-4.331386	-0.131137	-0.000381
17	9	0	1.475579	3.615493	-0.000251

Cartesian coordinates and energies (in Hartree) for species of hypoxanthine (I)

N9H-amino I (I-1), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -487.207701754     A.U. after    1 cycles

Zero-point correction=                           0.100177 (Hartree/Particle)
Thermal correction to Energy=                    0.106939
Thermal correction to Enthalpy=                  0.107883
Thermal correction to Gibbs Free Energy=         0.068732
Sum of electronic and zero-point Energies=           -487.107525
Sum of electronic and thermal Energies=              -487.100763
Sum of electronic and thermal Enthalpies=            -487.099819
Sum of electronic and thermal Free Energies=         -487.138970
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.105	26.772	82.400

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.633857	-0.767028	-0.000020
2	6	0	-0.245424	0.574776	0.000070
3	6	0	1.164056	0.896281	-0.000015
4	6	0	1.420790	-1.590513	-0.000274
5	6	0	-2.374414	0.589366	0.000286
6	1	0	-2.611078	-1.550350	0.000086
7	7	0	-2.004926	-0.740413	0.000106
8	7	0	1.923173	-0.320590	-0.000196
9	7	0	-1.346261	1.403948	0.000229
10	1	0	-3.413265	0.891729	0.000421
11	7	0	0.149676	-1.881303	-0.000188
12	1	0	2.152921	-2.393696	-0.000410
13	1	0	2.929221	-0.183478	-0.000270
14	8	0	1.737957	1.973376	0.000030

N7H-amino I (I-2), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -487.209050022 A.U. after 2 cycles

Zero-point correction= 0.100286 (Hartree/Particle)
Thermal correction to Energy= 0.107045
Thermal correction to Enthalpy= 0.107989
Thermal correction to Gibbs Free Energy= 0.068843
Sum of electronic and zero-point Energies= -487.108764
Sum of electronic and thermal Energies= -487.102005
Sum of electronic and thermal Enthalpies= -487.101061
Sum of electronic and thermal Free Energies= -487.140207

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.172	26.698	82.391

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.644551	-0.839245	0.000010
2	6	0	0.244876	0.499831	-0.000064
3	6	0	-1.126739	0.908475	0.000031
4	6	0	-1.479450	-1.546347	0.000269
5	6	0	2.430995	0.322158	-0.000258
6	7	0	2.014256	-0.929328	-0.000114

7	7	0	-1.940536	-0.248835	0.000204
8	7	0	1.408907	1.231849	-0.000235
9	1	0	3.468222	0.630640	-0.000382
10	7	0	-0.229628	-1.896208	0.000181
11	1	0	-2.252170	-2.311040	0.000406
12	1	0	-2.940377	-0.073051	0.000283
13	8	0	-1.601234	2.042578	-0.000021
14	1	0	1.477804	2.241249	-0.000324

N7H-amino I (I-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -487.244399076 A.U. after 1 cycles

Zero-point correction= 0.100492 (Hartree/Particle)
Thermal correction to Energy= 0.107191
Thermal correction to Enthalpy= 0.108136
Thermal correction to Gibbs Free Energy= 0.069111
Sum of electronic and zero-point Energies= -487.143907
Sum of electronic and thermal Energies= -487.137208
Sum of electronic and thermal Enthalpies= -487.136263
Sum of electronic and thermal Free Energies= -487.175289

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.264	26.486	82.135

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.635686	-0.840391	-0.000003
2	6	0	-0.250225	0.502012	0.000069
3	6	0	1.116558	0.897461	-0.000028
4	6	0	1.496070	-1.530593	-0.000270
5	6	0	-2.431611	0.314267	0.000252
6	7	0	-2.004610	-0.943959	0.000112
7	7	0	1.937380	-0.236033	-0.000206
8	7	0	-1.423110	1.221471	0.000236
9	1	0	-3.468615	0.619179	0.000371
10	7	0	0.240848	-1.891938	-0.000176
11	1	0	2.278942	-2.281275	-0.000409
12	1	0	2.942201	-0.070857	-0.000293
13	8	0	1.593339	2.049761	0.000014
14	1	0	-1.523428	2.231540	0.000334

N7H-amino I (I-2), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -487.265237451 A.U. after 1 cycles

```
Zero-point correction=                           0.093475 (Hartree/Particle)
Thermal correction to Energy=                    0.100191
Thermal correction to Enthalpy=                  0.101135
Thermal correction to Gibbs Free Energy=         0.062087
Sum of electronic and zero-point Energies=           -487.171763
Sum of electronic and thermal Energies=              -487.165047
Sum of electronic and thermal Enthalpies=            -487.164103
Sum of electronic and thermal Free Energies=         -487.203150

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   62.871             26.657             82.182


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.634901   -0.844781    0.000001
     2          6           0       -0.254566    0.499117    0.000074
     3          6           0        1.113716    0.897068   -0.000021
     4          6           0        1.500993   -1.523334   -0.000272
     5          6           0       -2.430090    0.310201    0.000247
     6          7           0       -2.003303   -0.951937    0.000109
     7          7           0        1.939473   -0.231633   -0.000207
     8          7           0       -1.426412    1.217867    0.000239
     9          1           0       -3.474725    0.611795    0.000362
    10          7           0        0.245512   -1.893378   -0.000172
    11          1           0        2.288358   -2.278279   -0.000419
    12          1           0        2.996803   -0.053347   -0.000305
    13          8           0        1.582683    2.052765    0.000009
    14          1           0       -1.529697    2.281650    0.000333
---------------------------------------------------------------------
```

N9-deprotonated N9H-amino I (I-3), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -486.669580597     A.U. after    2 cycles


Zero-point correction=                           0.086528 (Hartree/Particle)
Thermal correction to Energy=                    0.093096
Thermal correction to Enthalpy=                  0.094041
Thermal correction to Gibbs Free Energy=         0.055192
Sum of electronic and zero-point Energies=           -486.583052
Sum of electronic and thermal Energies=              -486.576484
Sum of electronic and thermal Enthalpies=            -486.575540
Sum of electronic and thermal Free Energies=         -486.614389

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   58.419             25.616             81.764


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	0.710479	-0.793388	0.000006
2	6	0	0.281001	0.568545	-0.000079
3	6	0	-1.112309	0.895617	0.000014
4	6	0	-1.389445	-1.588683	0.000272
5	6	0	2.387421	0.485683	-0.000270
6	7	0	2.063194	-0.834204	-0.000107
7	7	0	-1.886887	-0.303803	0.000200
8	7	0	1.384896	1.380386	-0.000247
9	1	0	3.426832	0.804669	-0.000392
10	7	0	-0.128573	-1.891092	0.000183
11	1	0	-2.140853	-2.378000	0.000416
12	1	0	-2.888849	-0.151849	0.000281
13	8	0	-1.711053	1.982440	-0.000021

N1-protonated N9H-amino I (I-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -487.496429081 A.U. after 9 cycles

Zero-point correction= 0.111026 (Hartree/Particle)
Thermal correction to Energy= 0.118649
Thermal correction to Enthalpy= 0.119593
Thermal correction to Gibbs Free Energy= 0.078395
Sum of electronic and zero-point Energies= -487.385404
Sum of electronic and thermal Energies= -487.377780
Sum of electronic and thermal Enthalpies= -487.376836
Sum of electronic and thermal Free Energies= -487.418034

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.454	29.194	86.710

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.620942	0.768095	0.000011
2	6	0	-0.328856	-0.602591	-0.000085
3	6	0	1.002780	-1.096583	-0.000005
4	6	0	1.455215	1.667281	0.000286
5	6	0	-2.447538	-0.466819	-0.000271
6	1	0	-2.528842	1.683835	-0.000086
7	7	0	-1.976896	0.830522	-0.000111
8	7	0	2.030633	0.295285	0.000217
9	7	0	-1.477094	-1.351134	-0.000260
10	1	0	-3.505096	-0.695379	-0.000391
11	7	0	0.203946	1.868217	0.000187
12	1	0	2.178348	2.479445	0.000427
13	1	0	2.642902	0.166313	0.818808
14	8	0	1.592693	-2.114651	-0.000041
15	1	0	2.643055	0.166460	-0.818282

N3-protonated N9H-amino I (I-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -487.544097041 A.U. after 1 cycles

Zero-point correction= 0.112776 (Hartree/Particle)
Thermal correction to Energy= 0.119894
Thermal correction to Enthalpy= 0.120838
Thermal correction to Gibbs Free Energy= 0.081030
Sum of electronic and zero-point Energies= -487.431321
Sum of electronic and thermal Energies= -487.424203
Sum of electronic and thermal Enthalpies= -487.423259
Sum of electronic and thermal Free Energies= -487.463067

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.235	28.390	83.785

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.654987	0.743040	0.000012
2	6	0	-0.278262	-0.594870	-0.000059
3	6	0	1.119195	-0.977716	0.000105
4	6	0	1.549749	1.506027	0.000287
5	6	0	-2.405964	-0.571555	-0.000234
6	1	0	-2.635863	1.563605	-0.000131
7	7	0	-2.015284	0.761227	-0.000137
8	7	0	1.959610	0.249656	0.000221
9	7	0	-1.388459	-1.394858	-0.000355
10	1	0	-3.451078	-0.851635	-0.000358
11	7	0	0.246527	1.794557	0.000198
12	1	0	2.266626	2.320399	0.000404
13	1	0	2.961614	0.059222	0.000268
14	8	0	1.663822	-2.045313	-0.000073
15	1	0	-0.047026	2.767272	0.000244

6O-protonated (N1 side) N9H-amino I (I-6), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -487.546613217 A.U. after 1 cycles

Zero-point correction= 0.112584 (Hartree/Particle)
Thermal correction to Energy= 0.119609
Thermal correction to Enthalpy= 0.120553
Thermal correction to Gibbs Free Energy= 0.081047
Sum of electronic and zero-point Energies= -487.434029
Sum of electronic and thermal Energies= -487.427004
Sum of electronic and thermal Enthalpies= -487.426060

Sum of electronic and thermal Free Energies= -487.465566

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.056	28.217	83.148

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.717310	0.779801	0.000021
2	6	0	-0.233913	-0.551796	-0.000075
3	6	0	1.150751	-0.715961	0.000023
4	6	0	1.300511	1.703518	0.000283
5	6	0	-2.342895	-0.708173	-0.000260
6	1	0	-2.741665	1.412033	-0.000086
7	7	0	-2.068927	0.651500	-0.000106
8	7	0	1.876047	0.444525	0.000203
9	7	0	-1.266881	-1.455653	-0.000264
10	1	0	-3.359356	-1.080656	-0.000382
11	7	0	0.015695	1.908211	0.000198
12	1	0	1.995259	2.536897	0.000426
13	1	0	2.892936	0.401260	0.000289
14	8	0	1.711559	-1.904972	-0.000050
15	1	0	2.685948	-1.914167	-0.000013

6O-protonated (5C side) N9H-amino I (I-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -487.559374957 A.U. after 8 cycles

Zero-point correction= 0.113279 (Hartree/Particle)
Thermal correction to Energy= 0.120115
Thermal correction to Enthalpy= 0.121059
Thermal correction to Gibbs Free Energy= 0.081872
Sum of electronic and zero-point Energies= -487.446096
Sum of electronic and thermal Energies= -487.439260
Sum of electronic and thermal Enthalpies= -487.438316
Sum of electronic and thermal Free Energies= -487.477503

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.373	27.612	82.475

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.697904	0.800205	0.000010
2	6	0	-0.238744	-0.535183	-0.000069
3	6	0	1.138893	-0.727405	0.000036
4	6	0	1.344343	1.673984	0.000269

5	6	0	-2.347808	-0.666982	-0.000268
6	1	0	-2.718534	1.455017	-0.000111
7	7	0	-2.053799	0.687225	-0.000121
8	7	0	1.890586	0.407913	0.000204
9	7	0	-1.280037	-1.429590	-0.000241
10	1	0	-3.369232	-1.025332	-0.000391
11	7	0	0.060821	1.910625	0.000176
12	1	0	2.055314	2.493440	0.000405
13	1	0	2.904777	0.303769	0.000285
14	8	0	1.802012	-1.862163	-0.000007
15	1	0	1.195895	-2.630524	-0.000129

N7-protonated N9H-amino I (I-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -487.569076581 A.U. after 1 cycles

Zero-point correction= 0.113936 (Hartree/Particle)
Thermal correction to Energy= 0.120767
Thermal correction to Enthalpy= 0.121712
Thermal correction to Gibbs Free Energy= 0.082425
Sum of electronic and zero-point Energies= -487.455141
Sum of electronic and thermal Energies= -487.448309
Sum of electronic and thermal Enthalpies= -487.447365
Sum of electronic and thermal Free Energies= -487.486651

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.783	27.341	82.685

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.580723	-0.813728	-0.000014
2	6	0	-0.208537	0.516898	0.000066
3	6	0	1.185643	0.906038	-0.000021
4	6	0	1.501051	-1.558587	-0.000274
5	6	0	-2.418908	0.443174	0.000259
6	1	0	-2.550764	-1.657443	0.000096
7	7	0	-1.969354	-0.823051	0.000113
8	7	0	1.975166	-0.279138	-0.000208
9	7	0	-1.369031	1.267440	0.000234
10	1	0	-3.457217	0.743395	0.000378
11	7	0	0.232881	-1.888382	-0.000181
12	1	0	2.249908	-2.345358	-0.000417
13	1	0	2.981959	-0.123961	-0.000294
14	8	0	1.653904	2.024826	0.000015
15	1	0	-1.413901	2.283900	0.000321

N7-protonated N9H-amino I (I-8), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -487.685309026   A.U. after   1 cycles

Zero-point correction=   0.113785 (Hartree/Particle)
Thermal correction to Energy=   0.120607
Thermal correction to Enthalpy=   0.121551
Thermal correction to Gibbs Free Energy=   0.082318
Sum of electronic and zero-point Energies=   -487.571524
Sum of electronic and thermal Energies=   -487.564702
Sum of electronic and thermal Enthalpies=   -487.563758
Sum of electronic and thermal Free Energies=   -487.602991

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.682	27.376	82.571

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.588677	-0.812332	-0.000003
2	6	0	-0.207213	0.518590	0.000075
3	6	0	1.177727	0.884852	-0.000033
4	6	0	1.498286	-1.554480	-0.000273
5	6	0	-2.410018	0.447503	0.000253
6	1	0	-2.568946	-1.642095	0.000088
7	7	0	-1.969231	-0.818850	0.000112
8	7	0	1.966328	-0.275566	-0.000216
9	7	0	-1.365382	1.271267	0.000231
10	1	0	-3.447067	0.748616	0.000364
11	7	0	0.230307	-1.888951	-0.000172
12	1	0	2.258624	-2.327428	-0.000413
13	1	0	2.976237	-0.134925	-0.000308
14	8	0	1.669459	2.018543	0.000016
15	1	0	-1.429302	2.287394	0.000336

N7-protonated N9H-amino I (I-8), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -487.720081158   A.U. after   1 cycles

Zero-point correction=   0.100000 (Hartree/Particle)
Thermal correction to Energy=   0.106915
Thermal correction to Enthalpy=   0.107860
Thermal correction to Gibbs Free Energy=   0.068503
Sum of electronic and zero-point Energies=   -487.620081
Sum of electronic and thermal Energies=   -487.613166
Sum of electronic and thermal Enthalpies=   -487.612222
Sum of electronic and thermal Free Energies=   -487.651578

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	67.090	28.016	82.833

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.597198	-0.811622	-0.000018
2	6	0	-0.207367	0.519624	0.000052
3	6	0	1.180129	0.876931	-0.000037
4	6	0	1.492571	-1.555668	-0.000263
5	6	0	-2.402300	0.454989	0.000275
6	1	0	-2.618984	-1.696928	0.000082
7	7	0	-1.973860	-0.816377	0.000101
8	7	0	1.966278	-0.282244	-0.000195
9	7	0	-1.357946	1.279978	0.000250
10	1	0	-3.446622	0.762901	0.000407
11	7	0	0.222503	-1.891016	-0.000181
12	1	0	2.253264	-2.337752	-0.000393
13	1	0	3.038428	-0.134890	-0.000275
14	8	0	1.674510	2.012221	-0.000005
15	1	0	-1.415996	2.370982	0.000347

N9-protonated N9H-amino I (I-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -487.491560884 A.U. after 1 cycles

Zero-point correction=	0.112042 (Hartree/Particle)
Thermal correction to Energy=	0.119139
Thermal correction to Enthalpy=	0.120083
Thermal correction to Gibbs Free Energy=	0.080241
Sum of electronic and zero-point Energies=	-487.379519
Sum of electronic and thermal Energies=	-487.372422
Sum of electronic and thermal Enthalpies=	-487.371478
Sum of electronic and thermal Free Energies=	-487.411320

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.761	28.079	83.853

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.555483	0.755559	-0.000075
2	6	0	0.203397	-0.564082	-0.000012
3	6	0	-1.214480	-0.904551	-0.000323
4	6	0	-1.479731	1.580449	-0.000232
5	6	0	2.366598	-0.716643	0.000356
6	1	0	2.421456	1.267568	0.829321
7	7	0	2.043745	0.782741	0.000113

8	7	0	-1.976468	0.327367	-0.000186
9	7	0	1.316640	-1.422155	0.000341
10	1	0	3.406893	-1.019269	0.000545
11	7	0	-0.185876	1.860086	-0.000264
12	1	0	-2.194105	2.398706	-0.000260
13	1	0	-2.987230	0.192614	-0.000120
14	8	0	-1.755323	-1.980956	0.000164
15	1	0	2.421680	1.267364	-0.829113

N7-protonated N9H-amino I with HF hydrogen-bonded to N3 (I-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -588.027971841 A.U. after 1 cycles

Zero-point correction= 0.126236 (Hartree/Particle)
Thermal correction to Energy= 0.135268
Thermal correction to Enthalpy= 0.136212
Thermal correction to Gibbs Free Energy= 0.091557
Sum of electronic and zero-point Energies= -587.901736
Sum of electronic and thermal Energies= -587.892704
Sum of electronic and thermal Enthalpies= -587.891760
Sum of electronic and thermal Free Energies= -587.936415

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	84.882	34.427	93.984

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.519813	0.015205	-0.000006
2	6	0	0.709060	0.640780	0.000087
3	6	0	1.939905	-0.121167	0.000005
4	6	0	0.349214	-2.034814	-0.000255
5	6	0	-0.857145	2.204211	0.000285
6	1	0	-2.483040	0.816004	0.000103
7	7	0	-1.475294	1.015299	0.000125
8	7	0	1.603557	-1.510749	-0.000173
9	7	0	0.465087	2.001536	0.000233
10	1	0	-1.346743	3.168021	0.000413
11	7	0	-0.752300	-1.321708	-0.000179
12	1	0	0.277174	-3.118355	-0.000390
13	1	0	2.402815	-2.142627	-0.000243
14	8	0	3.080821	0.284685	0.000067
15	1	0	1.175680	2.729513	0.000311
16	1	0	-2.643662	-1.449675	-0.000213
17	9	0	-3.404831	-0.866254	-0.000140

N7H-amino I with HF hydrogen-bonded to N3 (I-11), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -587.672157867   A.U. after   1 cycles

Zero-point correction= 0.112696 (Hartree/Particle)
Thermal correction to Energy= 0.121818
Thermal correction to Enthalpy= 0.122762
Thermal correction to Gibbs Free Energy= 0.076802
Sum of electronic and zero-point Energies= -587.559462
Sum of electronic and thermal Energies= -587.550340
Sum of electronic and thermal Enthalpies= -587.549395
Sum of electronic and thermal Free Energies= -587.595356

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.442	33.502	96.732

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.270325	0.658617	0.000047
2	6	0	1.059926	0.236532	0.000104
3	6	0	1.447624	-1.141912	-0.000027
4	6	0	-1.010367	-1.472107	-0.000241
5	6	0	0.911218	2.425213	0.000211
6	7	0	-0.346849	2.024261	0.000221
7	7	0	0.274220	-1.942581	-0.000189
8	7	0	1.805976	1.390900	0.000358
9	1	0	1.231655	3.458557	0.000304
10	7	0	-1.333660	-0.210841	-0.000134
11	1	0	-1.796281	-2.221973	-0.000371
12	1	0	0.436909	-2.944950	-0.000267
13	8	0	2.569596	-1.635913	0.000052
14	1	0	2.816519	1.447096	0.000507
15	1	0	-3.017470	0.091413	-0.000221
16	9	0	-3.983817	0.020769	-0.000302

Cartesian coordinates and energies (in Hartree) for species of 6-methyladenine (6mA) (more stable)

N9H-amino 6mA, more stable (6mA-1), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -506.649142879   A.U. after   1 cycles

Zero-point correction= 0.140513 (Hartree/Particle)
Thermal correction to Energy= 0.149440
Thermal correction to Enthalpy= 0.150384
Thermal correction to Gibbs Free Energy= 0.105890
Sum of electronic and zero-point Energies= -506.508630
Sum of electronic and thermal Energies= -506.499703
Sum of electronic and thermal Enthalpies= -506.498759
Sum of electronic and thermal Free Energies= -506.543253

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.775	33.470	93.646

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.336854	0.556543	-0.000015
2	6	0	-0.399996	-0.479830	0.000012
3	6	0	0.960811	-0.088168	0.000017
4	6	0	0.235980	2.110326	0.000013
5	6	0	-2.300600	-1.437669	0.000005
6	1	0	-3.463640	0.370164	0.000028
7	7	0	1.964377	-0.995299	0.000025
8	7	0	-2.559248	-0.081969	-0.000044
9	7	0	1.251429	1.227077	0.000032
10	7	0	-1.018259	-1.719410	0.000024
11	1	0	-3.099417	-2.167796	0.000002
12	7	0	-1.078698	1.873056	-0.000014
13	1	0	0.531168	3.157053	0.000033
14	6	0	3.373635	-0.637730	-0.000042
15	1	0	3.630833	-0.047776	-0.886642
16	1	0	3.631017	-0.048006	0.886664
17	1	0	3.960116	-1.559559	-0.000226
18	1	0	1.694854	-1.969098	0.000050

N1H-amino 6mA (6mA-2), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -506.619712340 A.U. after 1 cycles

Zero-point correction=	0.139912 (Hartree/Particle)
Thermal correction to Energy=	0.148932
Thermal correction to Enthalpy=	0.149876
Thermal correction to Gibbs Free Energy=	0.104967
Sum of electronic and zero-point Energies=	-506.479801
Sum of electronic and thermal Energies=	-506.470780
Sum of electronic and thermal Enthalpies=	-506.469836
Sum of electronic and thermal Free Energies=	-506.514745

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.456	33.777	94.519

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.457434	0.501291	-0.000019
2	6	0	0.441106	-0.507906	0.000005

3	6	0	-0.896526	-0.134251	0.000009
4	6	0	-0.073556	2.148373	-0.000033
5	6	0	2.325578	-1.419850	0.000004
6	7	0	-1.932000	-1.005291	0.000031
7	7	0	2.656818	-0.098056	-0.000019
8	7	0	-1.114861	1.222885	-0.000010
9	7	0	1.018797	-1.742671	0.000020
10	1	0	3.093307	-2.185702	0.000010
11	7	0	1.184452	1.844227	-0.000038
12	1	0	-0.396135	3.185464	-0.000047
13	6	0	-3.339365	-0.655192	0.000036
14	1	0	-3.619083	-0.082733	0.895777
15	1	0	-3.619097	-0.082761	-0.895719
16	1	0	-3.923193	-1.577213	0.000055
17	1	0	-1.653956	-1.978680	0.000044
18	1	0	-2.062311	1.579178	-0.000009

N1H-amino 6mA (6mA-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -506.667188294 A.U. after 1 cycles

Zero-point correction= 0.141106 (Hartree/Particle)
Thermal correction to Energy= 0.149798
Thermal correction to Enthalpy= 0.150742
Thermal correction to Gibbs Free Energy= 0.107204
Sum of electronic and zero-point Energies= -506.526082
Sum of electronic and thermal Energies= -506.517391
Sum of electronic and thermal Enthalpies= -506.516446
Sum of electronic and thermal Free Energies= -506.559984

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.999	33.184	91.633

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.430401	0.514399	-0.000021
2	6	0	0.457720	-0.511738	0.000007
3	6	0	-0.903916	-0.164593	0.000012
4	6	0	-0.128895	2.129982	-0.000033
5	6	0	2.378846	-1.377626	0.000005
6	7	0	-1.924668	-1.027238	0.000032
7	7	0	2.663162	-0.047172	-0.000023
8	7	0	-1.133302	1.188829	-0.000007
9	7	0	1.082858	-1.733847	0.000020
10	1	0	3.168542	-2.119953	0.000010
11	7	0	1.144061	1.856298	-0.000041
12	1	0	-0.476982	3.156207	-0.000047
13	6	0	-3.338972	-0.666342	0.000035
14	1	0	-3.600968	-0.088641	0.893564

15	1	0	-3.600979	-0.088665	-0.893508
16	1	0	-3.918358	-1.589383	0.000051
17	1	0	-1.678703	-2.009851	0.000044
18	1	0	-2.088439	1.537695	-0.000006

N1H-amino 6mA (6mA-2), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -506.690851349 A.U. after 1 cycles

Zero-point correction= 0.134039 (Hartree/Particle)
Thermal correction to Energy= 0.142739
Thermal correction to Enthalpy= 0.143683
Thermal correction to Gibbs Free Energy= 0.100061
Sum of electronic and zero-point Energies= -506.556812
Sum of electronic and thermal Energies= -506.548112
Sum of electronic and thermal Enthalpies= -506.547168
Sum of electronic and thermal Free Energies= -506.590790

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.570	33.242	91.811

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.429787	0.512264	-0.000018
2	6	0	0.456396	-0.508492	0.000002
3	6	0	-0.909013	-0.157393	0.000008
4	6	0	-0.125525	2.130008	-0.000031
5	6	0	2.379615	-1.380905	0.000009
6	7	0	-1.923141	-1.022947	0.000029
7	7	0	2.664788	-0.052108	-0.000021
8	7	0	-1.131991	1.197586	-0.000010
9	7	0	1.081365	-1.732667	0.000015
10	1	0	3.170451	-2.127792	0.000013
11	7	0	1.149924	1.855353	-0.000036
12	1	0	-0.468663	3.164535	-0.000045
13	6	0	-3.341128	-0.675690	0.000037
14	1	0	-3.611021	-0.096798	0.896167
15	1	0	-3.611039	-0.096829	-0.896108
16	1	0	-3.912481	-1.609399	0.000059
17	1	0	-1.656959	-2.045453	0.000042
18	1	0	-2.137701	1.576467	-0.000011

N7H-amino 6mA (6mA-3), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -506.634717681 A.U. after 10 cycles

```
Zero-point correction=                           0.139998 (Hartree/Particle)
Thermal correction to Energy=                    0.148945
Thermal correction to Enthalpy=                  0.149889
Thermal correction to Gibbs Free Energy=         0.105920
Sum of electronic and zero-point Energies=           -506.494719
Sum of electronic and thermal Energies=              -506.485773
Sum of electronic and thermal Enthalpies=            -506.484829
Sum of electronic and thermal Free Energies=         -506.528798

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   93.464             33.862             92.541


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.371339    0.583716    0.020083
     2          6           0       -0.414701   -0.446423   -0.016302
     3          6           0        0.951716   -0.102073   -0.030577
     4          6           0        0.262626    2.105501   -0.016244
     5          6           0       -2.471259   -1.245255    0.006532
     6          7           0        1.962727   -1.031419   -0.077399
     7          7           0       -2.649384    0.052571    0.038181
     8          7           0        1.264676    1.198423   -0.036112
     9          7           0       -1.148116   -1.623955   -0.016825
    10          1           0       -3.264918   -1.981921    0.001871
    11          7           0       -1.046462    1.891304    0.022118
    12          1           0        0.584350    3.144330   -0.025784
    13          6           0        3.360844   -0.634274    0.059062
    14          1           0        3.608537    0.101074   -0.708992
    15          1           0        3.575347   -0.188963    1.039528
    16          1           0        3.982124   -1.522486   -0.082820
    17          1           0        1.732993   -1.957962    0.254697
    18          1           0       -0.809843   -2.569689   -0.123566
---------------------------------------------------------------------
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N9-deprotonated N9H-amino 6mA (6mA-4), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -506.102381022     A.U. after    9 cycles


Zero-point correction=                           0.127259 (Hartree/Particle)
Thermal correction to Energy=                    0.135678
Thermal correction to Enthalpy=                  0.136622
Thermal correction to Gibbs Free Energy=         0.093396
Sum of electronic and zero-point Energies=           -505.975122
Sum of electronic and thermal Energies=              -505.966703
Sum of electronic and thermal Enthalpies=            -505.965759
Sum of electronic and thermal Free Energies=         -506.008985

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   85.139             31.618             90.978
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.425638	0.520473	0.019878
2	6	0	-0.417105	-0.480480	-0.050098
3	6	0	0.918600	-0.055676	-0.103090
4	6	0	0.157129	2.115528	-0.010500
5	6	0	-2.304537	-1.402779	0.042315
6	7	0	1.951028	-0.979928	-0.213602
7	7	0	-2.643832	-0.090549	0.077143
8	7	0	1.206239	1.255879	-0.072134
9	7	0	-0.996327	-1.727146	-0.033201
10	1	0	-3.069336	-2.175728	0.075535
11	7	0	-1.143017	1.852264	0.035568
12	1	0	0.436633	3.170008	0.006948
13	6	0	3.301666	-0.634269	0.186130
14	1	0	3.626313	0.255815	-0.358898
15	1	0	3.396848	-0.414952	1.264428
16	1	0	3.968715	-1.467417	-0.065066
17	1	0	1.641495	-1.918153	0.012819

N1-protonated N9H-amino 6mA (6mA-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -507.022642620 A.U. after 10 cycles

Zero-point correction= 0.154314 (Hartree/Particle)
Thermal correction to Energy= 0.163113
Thermal correction to Enthalpy= 0.164057
Thermal correction to Gibbs Free Energy= 0.120395
Sum of electronic and zero-point Energies= -506.868328
Sum of electronic and thermal Energies= -506.859529
Sum of electronic and thermal Enthalpies= -506.858585
Sum of electronic and thermal Free Energies= -506.902247

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.355	34.149	91.895

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.368504	0.531010	0.000019
2	6	0	-0.418207	-0.496230	-0.000005
3	6	0	0.946073	-0.138305	-0.000009
4	6	0	0.139057	2.156699	0.000033
5	6	0	-2.298090	-1.468902	-0.000005
6	1	0	-3.485328	0.323966	0.000032
7	7	0	1.949613	-1.010257	-0.000031

8	7	0	-2.570539	-0.114974	0.000018
9	7	0	1.160575	1.219359	0.000010
10	7	0	-1.010111	-1.733404	-0.000020
11	1	0	-3.087087	-2.209339	-0.000011
12	7	0	-1.125804	1.862491	0.000038
13	1	0	0.463473	3.192215	0.000047
14	6	0	3.376091	-0.683332	-0.000037
15	1	0	3.652019	-0.120661	-0.899488
16	1	0	3.652033	-0.120689	0.899428
17	1	0	3.937129	-1.617903	-0.000056
18	1	0	1.669756	-1.986333	-0.000044
19	1	0	2.113342	1.570594	0.000008

N1-protonated N9H-amino 6mA (6mA-5), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -507.126174558 A.U. after 1 cycles

Zero-point correction= 0.154686 (Hartree/Particle)
Thermal correction to Energy= 0.163423
Thermal correction to Enthalpy= 0.164367
Thermal correction to Gibbs Free Energy= 0.120926
Sum of electronic and zero-point Energies= -506.971488
Sum of electronic and thermal Energies= -506.962751
Sum of electronic and thermal Enthalpies= -506.961807
Sum of electronic and thermal Free Energies= -507.005248

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.550	34.077	91.429

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.356917	0.536669	-0.000021
2	6	0	0.425325	-0.503302	0.000008
3	6	0	-0.947244	-0.162270	0.000014
4	6	0	-0.179666	2.135860	-0.000033
5	6	0	2.337762	-1.430141	0.000006
6	1	0	3.485217	0.370187	-0.000041
7	7	0	-1.950753	-1.027921	0.000033
8	7	0	2.574296	-0.080196	-0.000023
9	7	0	-1.174512	1.191738	-0.000004
10	7	0	1.053411	-1.731213	0.000022
11	1	0	3.148665	-2.144973	0.000011
12	7	0	1.097998	1.869304	-0.000043
13	1	0	-0.528133	3.161375	-0.000048
14	6	0	-3.372179	-0.683025	0.000033
15	1	0	-3.633969	-0.108439	0.894569
16	1	0	-3.633974	-0.108464	-0.894518
17	1	0	-3.937342	-1.614188	0.000048
18	1	0	-1.697532	-2.010310	0.000045

19	1	0	-2.131506	1.540081	-0.000002

N1-protonated N9H-amino 6mA (6mA-5), B3LYP/6-31+G(d), scrf=(read,smd,solvent=water), RADII=UAKS

SCF Done: E(RB3LYP) = -507.159347864 A.U. after 9 cycles

Zero-point correction= 0.142696 (Hartree/Particle)
Thermal correction to Energy= 0.151589
Thermal correction to Enthalpy= 0.152533
Thermal correction to Gibbs Free Energy= 0.108681
Sum of electronic and zero-point Energies= -507.016652
Sum of electronic and thermal Energies= -507.007759
Sum of electronic and thermal Enthalpies= -507.006815
Sum of electronic and thermal Free Energies= -507.050667

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.123	34.566	92.294

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.360731	0.530285	-0.000018
2	6	0	0.421301	-0.502874	0.000003
3	6	0	-0.952723	-0.154829	0.000007
4	6	0	-0.172895	2.134512	-0.000031
5	6	0	2.334671	-1.432024	0.000005
6	1	0	3.537798	0.389151	-0.000029
7	7	0	-1.952967	-1.021835	0.000029
8	7	0	2.576870	-0.087175	-0.000016
9	7	0	-1.171899	1.200951	-0.000011
10	7	0	1.046425	-1.732854	0.000017
11	1	0	3.145147	-2.156974	0.000011
12	7	0	1.106756	1.865607	-0.000035
13	1	0	-0.515472	3.169665	-0.000044
14	6	0	-3.375971	-0.686085	0.000038
15	1	0	-3.645210	-0.109286	0.897222
16	1	0	-3.645230	-0.109323	-0.897164
17	1	0	-3.937408	-1.625595	0.000064
18	1	0	-1.678283	-2.047682	0.000043
19	1	0	-2.188323	1.583283	-0.000013

N3-protonated N9H-amino 6mA (6mA-6), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -507.019224913 A.U. after 1 cycles

Zero-point correction= 0.153939 (Hartree/Particle)

```
Thermal correction to Energy=                    0.162992
Thermal correction to Enthalpy=                  0.163937
Thermal correction to Gibbs Free Energy=         0.119058
Sum of electronic and zero-point Energies=           -506.865286
Sum of electronic and thermal Energies=              -506.856233
Sum of electronic and thermal Enthalpies=            -506.855288
Sum of electronic and thermal Free Energies=         -506.900167

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  102.279             34.485             94.455


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.360847    0.491149    0.000012
     2          6           0       -0.392778   -0.504264    0.000005
     3          6           0        0.977605   -0.114832   -0.000008
     4          6           0        0.316635    2.106705   -0.000007
     5          6           0       -2.268160   -1.509302    0.000009
     6          1           0       -3.490481    0.259144    0.000047
     7          7           0        1.967760   -0.993433   -0.000017
     8          7           0       -2.562550   -0.148677    0.000020
     9          7           0        1.273765    1.223523   -0.000012
    10          7           0       -0.982543   -1.747983    0.000011
    11          1           0       -3.053754   -2.253115    0.000011
    12          7           0       -1.021221    1.815711    0.000006
    13          1           0        0.567063    3.163629   -0.000010
    14          6           0        3.394595   -0.650614   -0.000020
    15          1           0        3.646066   -0.068695   -0.890314
    16          1           0        3.646140   -0.068957    0.890428
    17          1           0        3.961318   -1.581783   -0.000180
    18          1           0        1.700837   -1.972933   -0.000001
    19          1           0       -1.705965    2.565676    0.000011
---------------------------------------------------------------------
```

N6-protonated N9H-amino 6mA (6mA-7), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -506.993709928     A.U. after    9 cycles


Zero-point correction=                           0.155235 (Hartree/Particle)
Thermal correction to Energy=                    0.163950
Thermal correction to Enthalpy=                  0.164894
Thermal correction to Gibbs Free Energy=         0.120530
Sum of electronic and zero-point Energies=           -506.838475
Sum of electronic and thermal Energies=              -506.829760
Sum of electronic and thermal Enthalpies=            -506.828816
Sum of electronic and thermal Free Energies=         -506.873180

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  102.880             33.119             93.372
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.378366	0.471309	-0.087314
2	6	0	-0.320006	-0.447326	0.136326
3	6	0	0.913693	0.159331	0.279123
4	6	0	-0.002664	2.225031	-0.007940
5	6	0	-2.068087	-1.628250	-0.023826
6	1	0	-3.441863	-0.011203	-0.346831
7	7	0	2.132301	-0.657575	0.511617
8	7	0	-2.490927	-0.326356	-0.187526
9	7	0	1.092079	1.461464	0.212936
10	7	0	-0.771604	-1.745939	0.172702
11	1	0	-2.763406	-2.457352	-0.058125
12	7	0	-1.257358	1.789619	-0.166005
13	1	0	0.160499	3.296154	-0.057531
14	6	0	3.016394	-0.806957	-0.713134
15	1	0	2.439805	-1.320192	-1.482816
16	1	0	3.299484	0.193699	-1.038667
17	1	0	3.893596	-1.391361	-0.430800
18	1	0	2.673258	-0.210330	1.263341
19	1	0	1.841411	-1.586735	0.845953

N7-protonated N9H-amino 6mA (6mA-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -507.006707596 A.U. after 3 cycles

Zero-point correction= 0.153674 (Hartree/Particle)
Thermal correction to Energy= 0.162768
Thermal correction to Enthalpy= 0.163712
Thermal correction to Gibbs Free Energy= 0.119281
Sum of electronic and zero-point Energies= -506.853033
Sum of electronic and thermal Energies= -506.843940
Sum of electronic and thermal Enthalpies= -506.842996
Sum of electronic and thermal Free Energies= -506.887427

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.138	34.689	93.514

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.287879	0.607835	0.000014
2	6	0	-0.387585	-0.458680	0.000003
3	6	0	1.000953	-0.129008	-0.000008
4	6	0	0.328283	2.102697	-0.000002
5	6	0	-2.456153	-1.291691	0.000018

6	1	0	-3.431652	0.568533	0.000041
7	7	0	2.003377	-1.023846	-0.000022
8	7	0	-2.562866	0.041087	0.000023
9	7	0	1.299802	1.181750	-0.000010
10	7	0	-1.160825	-1.623222	0.000004
11	1	0	-3.280042	-1.991158	0.000021
12	7	0	-0.997146	1.900536	0.000013
13	1	0	0.657125	3.137732	-0.000004
14	6	0	3.419168	-0.634613	-0.000028
15	1	0	3.652644	-0.043282	-0.889087
16	1	0	3.652718	-0.043483	0.889148
17	1	0	4.016185	-1.547426	-0.000157
18	1	0	1.790546	-2.011017	0.000009
19	1	0	-0.834647	-2.583284	-0.000008

N9-protonated N9H-amino 6mA (6mA-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -506.948762462 A.U. after 1 cycles

Zero-point correction= 0.152697 (Hartree/Particle)
Thermal correction to Energy= 0.161804
Thermal correction to Enthalpy= 0.162748
Thermal correction to Gibbs Free Energy= 0.118132
Sum of electronic and zero-point Energies= -506.796065
Sum of electronic and thermal Energies= -506.786958
Sum of electronic and thermal Enthalpies= -506.786014
Sum of electronic and thermal Free Energies= -506.830630

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.534	34.646	93.902

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.248397	0.598262	-0.000003
2	6	0	0.372650	-0.467022	0.000000
3	6	0	-1.008975	-0.121505	0.000004
4	6	0	-0.338731	2.107684	-0.000008
5	6	0	2.285065	-1.500752	-0.000002
6	1	0	3.161490	0.275016	-0.828367
7	7	0	-1.997589	-1.014846	0.000013
8	7	0	2.616806	-0.008495	-0.000004
9	7	0	-1.307492	1.207149	-0.000001
10	7	0	1.033071	-1.706048	0.000001
11	1	0	3.101021	-2.212482	-0.000002
12	7	0	1.007992	1.879568	-0.000005
13	1	0	-0.638850	3.151246	0.000000
14	6	0	-3.421153	-0.659764	0.000005
15	1	0	-3.669355	-0.074890	0.889449
16	1	0	-3.669407	-0.075103	-0.889566

17	1	0	-3.996080	-1.586265	0.000133
18	1	0	-1.743348	-1.995250	-0.000002
19	1	0	3.161492	0.275017	0.828357

N7-protonated N9H-amino 6mA with HF hydrogen-bonded to N3 (6mA-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -607.469089459 A.U. after 1 cycles

Zero-point correction= 0.166260 (Hartree/Particle)
Thermal correction to Energy= 0.177373
Thermal correction to Enthalpy= 0.178317
Thermal correction to Gibbs Free Energy= 0.128943
Sum of electronic and zero-point Energies= -607.302830
Sum of electronic and thermal Energies= -607.291717
Sum of electronic and thermal Enthalpies= -607.290772
Sum of electronic and thermal Free Energies= -607.340147

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.303	41.204	103.917

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.952998	-0.013115	0.000012
2	6	0	-0.231749	0.715549	-0.000007
3	6	0	-1.449663	-0.030975	-0.000023
4	6	0	-0.126457	-1.951723	0.000008
5	6	0	1.486860	2.137826	0.000015
6	1	0	2.979174	0.608919	0.000011
7	7	0	-2.678544	0.504499	-0.000035
8	7	0	1.994938	0.904868	0.000010
9	7	0	-1.327893	-1.373076	-0.000013
10	7	0	0.148996	2.060946	0.000000
11	1	0	2.058658	3.055223	0.000020
12	7	0	1.070131	-1.342227	0.000019
13	1	0	-0.114820	-3.037544	0.000006
14	6	0	-3.905321	-0.304234	-0.000038
15	1	0	-3.943478	-0.938046	-0.889487
16	1	0	-3.943536	-0.937975	0.889462
17	1	0	-4.754945	0.379420	-0.000093
18	1	0	-2.782677	1.509388	-0.000014
19	1	0	-0.454180	2.875867	-0.000008
20	1	0	2.844254	-1.620583	0.000039
21	9	0	3.699794	-1.166634	0.000044

N7H-amino 6mA with HF hydrogen-bonded to N3 (6mA-11), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -607.100925440 A.U. after 1 cycles

```
Zero-point correction=                           0.152293 (Hartree/Particle)
Thermal correction to Energy=                    0.163673
Thermal correction to Enthalpy=                  0.164618
Thermal correction to Gibbs Free Energy=         0.113724
Sum of electronic and zero-point Energies=           -606.948633
Sum of electronic and thermal Energies=              -606.937252
Sum of electronic and thermal Enthalpies=            -606.936308
Sum of electronic and thermal Free Energies=         -606.987202

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  102.707             40.670           107.115
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.973162	0.516683	0.004202
2	6	0	-0.397501	0.821059	-0.012329
3	6	0	-1.331252	-0.236695	-0.023451
4	6	0	0.477595	-1.678249	-0.032129
5	6	0	0.850107	2.641229	0.006299
6	7	0	-2.683596	-0.051980	-0.049619
7	7	0	1.729642	1.668097	0.018746
8	7	0	-0.853151	-1.490043	-0.037869
9	7	0	-0.454388	2.207016	-0.005786
10	1	0	1.091836	3.696498	0.007029
11	7	0	1.433464	-0.752672	-0.004041
12	1	0	0.809456	-2.712929	-0.046173
13	6	0	-3.620718	-1.166626	0.055266
14	1	0	-3.412387	-1.899070	-0.727372
15	1	0	-3.551339	-1.672215	1.026397
16	1	0	-4.631338	-0.774101	-0.080661
17	1	0	-3.032507	0.862373	0.198667
18	1	0	-1.269396	2.800119	-0.071942
19	1	0	3.027513	-1.274155	0.016215
20	9	0	3.895110	-1.719317	0.026741

N7-protonated N9H-amino 6mA with HF hydrogen-bonded to N1 (6mA-12), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -607.459136692     A.U. after   10 cycles

Zero-point correction=                           0.166155 (Hartree/Particle)
Thermal correction to Energy=                    0.177537
Thermal correction to Enthalpy=                  0.178481
Thermal correction to Gibbs Free Energy=         0.127653
Sum of electronic and zero-point Energies=           -607.292981
Sum of electronic and thermal Energies=              -607.281600
Sum of electronic and thermal Enthalpies=            -607.280656
Sum of electronic and thermal Free Energies=         -607.331483
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.406	41.717	106.976

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.516060	0.821155	0.000004
2	6	0	-0.965948	-0.459321	-0.000000
3	6	0	0.458387	-0.559782	0.000007
4	6	0	0.460249	1.787741	0.000019
5	6	0	-3.185538	-0.654427	-0.000015
6	7	0	1.136334	-1.715151	0.000006
7	7	0	-2.899574	0.651621	-0.000006
8	7	0	1.122068	0.616069	0.000015
9	7	0	-2.042742	-1.348743	-0.000012
10	1	0	-4.177553	-1.083976	-0.000023
11	7	0	-0.860649	1.975006	0.000014
12	1	0	1.082143	2.678380	0.000026
13	6	0	2.604199	-1.818871	0.000016
14	1	0	3.025413	-1.345602	-0.890227
15	1	0	3.025400	-1.345593	0.890259
16	1	0	2.858783	-2.879082	0.000024
17	1	0	0.617417	-2.582015	-0.000003
18	1	0	-2.011448	-2.362624	-0.000017
19	1	0	2.851665	0.926754	-0.000013
20	9	0	3.776170	1.181476	-0.000036
21	1	0	-3.577143	1.409897	-0.000006

N7H-amino 6mA with HF hydrogen-bonded to N1 (6mA-13), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -607.099551803 A.U. after 8 cycles

Zero-point correction=	0.152301 (Hartree/Particle)
Thermal correction to Energy=	0.163606
Thermal correction to Enthalpy=	0.164550
Thermal correction to Gibbs Free Energy=	0.114174
Sum of electronic and zero-point Energies=	-606.947251
Sum of electronic and thermal Energies=	-606.935946
Sum of electronic and thermal Enthalpies=	-606.935002
Sum of electronic and thermal Free Energies=	-606.985378

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.664	40.596	106.025

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.588284	0.831510	0.015584
2	6	0	-0.982158	-0.436039	-0.011653
3	6	0	0.424930	-0.528229	-0.013884
4	6	0	0.418517	1.806522	0.005661
5	6	0	-3.181874	-0.584774	-0.007489
6	7	0	1.095244	-1.713934	-0.045482
7	7	0	-2.963491	0.707498	0.020541
8	7	0	1.104049	0.632860	-0.009279
9	7	0	-2.032409	-1.340577	-0.020915
10	1	0	-4.159147	-1.050722	-0.017803
11	7	0	-0.888979	1.985745	0.025357
12	1	0	1.044060	2.695318	0.005820
13	6	0	2.548951	-1.829816	0.051729
14	1	0	3.032367	-1.292404	-0.767000
15	1	0	2.930883	-1.430686	0.998231
16	1	0	2.805030	-2.888953	-0.023378
17	1	0	0.559410	-2.544890	0.156450
18	1	0	-1.994403	-2.347040	-0.099270
19	1	0	2.719688	0.913749	-0.017732
20	9	0	3.668969	1.165493	-0.029618

N7-protonated N9H-amino 6mA with HF hydrogen-bonded to N1 and N3 (6mA-14), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -707.920449029 A.U. after 9 cycles

Zero-point correction= 0.178599 (Hartree/Particle)
Thermal correction to Energy= 0.192090
Thermal correction to Enthalpy= 0.193034
Thermal correction to Gibbs Free Energy= 0.137051
Sum of electronic and zero-point Energies= -707.741850
Sum of electronic and thermal Energies= -707.728359
Sum of electronic and thermal Enthalpies= -707.727415
Sum of electronic and thermal Free Energies= -707.783398

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	120.538	48.493	117.826

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.299942	0.086105	0.000002
2	6	0	-0.389015	-0.963125	-0.000009
3	6	0	0.999986	-0.627220	-0.000007
4	6	0	0.303378	1.615914	0.000015
5	6	0	-2.452938	-1.804737	-0.000015
6	1	0	-3.418615	0.102091	0.000004
7	7	0	1.995284	-1.519696	-0.000017
8	7	0	-2.568075	-0.476327	-0.000002

9	7	0	1.279617	0.696600	0.000005
10	7	0	-1.153346	-2.132453	-0.000020
11	1	0	-3.273275	-2.509108	-0.000021
12	7	0	-1.013370	1.391233	0.000014
13	1	0	0.626117	2.653060	0.000025
14	6	0	3.426662	-1.174791	-0.000015
15	1	0	3.684166	-0.596769	-0.890771
16	1	0	3.684168	-0.596787	0.890752
17	1	0	3.989469	-2.108518	-0.000025
18	1	0	1.763322	-2.503421	-0.000026
19	1	0	-0.823205	-3.091441	-0.000029
20	1	0	-2.665508	2.208843	0.000024
21	1	0	2.841736	1.520532	0.000013
22	9	0	3.636374	2.054608	0.000018
23	9	0	-3.605034	1.991297	0.000023

N7H-amino 6mA with HF hydrogen-bonded to N1 and N3 (6mA-15), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -707.563298286 A.U. after 1 cycles

Zero-point correction= 0.164481 (Hartree/Particle)
Thermal correction to Energy= 0.178393
Thermal correction to Enthalpy= 0.179338
Thermal correction to Gibbs Free Energy= 0.121057
Sum of electronic and zero-point Energies= -707.398817
Sum of electronic and thermal Energies= -707.384905
Sum of electronic and thermal Enthalpies= -707.383961
Sum of electronic and thermal Free Energies= -707.442241

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.944	47.636	122.661

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.445633	0.288486	0.000006
2	6	0	0.342588	1.155634	-0.000008
3	6	0	-0.962789	0.617711	-0.000011
4	6	0	0.059471	-1.480939	0.000003
5	6	0	2.254384	2.254956	-0.000018
6	7	0	-2.085347	1.376208	-0.000025
7	7	0	2.624443	0.996005	0.000018
8	7	0	-1.062627	-0.727614	-0.000007
9	7	0	0.890934	2.428533	-0.000010
10	1	0	2.929541	3.101094	-0.000027
11	7	0	1.313538	-1.057554	0.000013
12	1	0	-0.099935	-2.555588	0.000008
13	6	0	-3.447545	0.845006	-0.000002
14	1	0	-3.633889	0.233241	-0.887271
15	1	0	-3.633887	0.233293	0.887304

16	1	0	-4.135371	1.692836	-0.000028
17	1	0	-1.975746	2.378566	0.000026
18	1	0	0.414960	3.319701	-0.000035
19	1	0	2.564607	-2.214411	0.000034
20	1	0	-2.416266	-1.696382	-0.000012
21	9	0	-3.162527	-2.326323	-0.000017
22	9	0	3.170188	-2.972180	0.000045

Cartesian coordinates and energies (in Hartree) for species of 6-methyladenine (6mA_a) (less stable)

N9H-amino 6mA_a (6mA_a-1), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -506.646582408 A.U. after 8 cycles

Zero-point correction=	0.140540 (Hartree/Particle)
Thermal correction to Energy=	0.149399
Thermal correction to Enthalpy=	0.150343
Thermal correction to Gibbs Free Energy=	0.105879
Sum of electronic and zero-point Energies=	-506.506042
Sum of electronic and thermal Energies=	-506.497183
Sum of electronic and thermal Enthalpies=	-506.496239
Sum of electronic and thermal Free Energies=	-506.540703

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.749	33.319	93.582

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.381339	0.189898	0.011461
2	6	0	-0.094011	-0.372734	-0.017743
3	6	0	0.976773	0.556100	-0.032349
4	6	0	-0.606086	2.256880	0.017540
5	6	0	-1.450573	-2.022920	-0.015379
6	1	0	-3.246147	-0.839421	0.030385
7	7	0	2.293714	0.238905	-0.089663
8	7	0	-2.236451	-0.889272	0.013462
9	7	0	0.676846	1.875417	-0.008856
10	7	0	-0.166820	-1.762011	-0.034517
11	1	0	2.904105	1.042873	-0.008057
12	1	0	-1.883938	-3.014650	-0.019344
13	7	0	-1.701705	1.488829	0.029564
14	1	0	-0.774816	3.331178	0.033161
15	6	0	2.867295	-1.088604	0.078090
16	1	0	2.862425	-1.412267	1.128283
17	1	0	2.306640	-1.820273	-0.505168
18	1	0	3.900295	-1.062237	-0.278915

N1H-amino 6mA_a (6mA_a-2), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -506.616921577 A.U. after 1 cycles

Zero-point correction= 0.139944 (Hartree/Particle)
Thermal correction to Energy= 0.148949
Thermal correction to Enthalpy= 0.149893
Thermal correction to Gibbs Free Energy= 0.105443
Sum of electronic and zero-point Energies= -506.476978
Sum of electronic and thermal Energies= -506.467972
Sum of electronic and thermal Enthalpies= -506.467028
Sum of electronic and thermal Free Energies= -506.511479

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.467	33.848	93.555

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.469799	0.024976	0.014867
2	6	0	-0.099340	-0.423136	-0.015613
3	6	0	0.919346	0.525482	-0.031043
4	6	0	-0.866958	2.186032	0.018648
5	6	0	-1.393503	-2.080569	-0.016612
6	7	0	2.260622	0.319632	-0.102491
7	7	0	-2.275806	-1.041860	0.015693
8	7	0	0.474644	1.833252	-0.008851
9	7	0	-0.084098	-1.793528	-0.036552
10	1	0	2.855913	1.124766	0.048494
11	1	0	-1.742874	-3.107268	-0.025731
12	7	0	-1.846375	1.341915	0.033641
13	1	0	-1.051935	3.256461	0.029911
14	6	0	2.896337	-0.987053	0.081524
15	1	0	3.111588	-1.182826	1.139957
16	1	0	2.225203	-1.763993	-0.284111
17	1	0	3.829358	-1.002356	-0.488567
18	1	0	1.153326	2.584952	-0.040663

N1H-amino 6mA_a (6mA_a-2), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -506.663880980 A.U. after 1 cycles

Zero-point correction= 0.140776 (Hartree/Particle)
Thermal correction to Energy= 0.149716
Thermal correction to Enthalpy= 0.150660
Thermal correction to Gibbs Free Energy= 0.106188
Sum of electronic and zero-point Energies= -506.523105

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Sum of electronic and thermal Energies=             -506.514165
Sum of electronic and thermal Enthalpies=           -506.513221
Sum of electronic and thermal Free Energies=        -506.557693

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   93.948             33.432             93.599


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.454265    0.060471   -0.000008
     2          6           0       -0.117713   -0.426310   -0.000023
     3          6           0        0.936808    0.503187    0.000009
     4          6           0       -0.798010    2.204533   -0.000007
     5          6           0       -1.463762   -2.055004    0.000009
     6          7           0        2.255532    0.274426    0.000093
     7          7           0       -2.307933   -0.986466    0.000013
     8          7           0        0.516227    1.816069   -0.000039
     9          7           0       -0.147671   -1.804518    0.000004
    10          1           0        2.868667    1.082743    0.000045
    11          1           0       -1.844900   -3.069736    0.000024
    12          7           0       -1.810027    1.385012   -0.000001
    13          1           0       -0.950702    3.277670   -0.000006
    14          6           0        2.890570   -1.042088   -0.000044
    15          1           0        2.617762   -1.612735    0.891078
    16          1           0        2.617928   -1.612478   -0.891386
    17          1           0        3.968918   -0.879280    0.000081
    18          1           0        1.217663    2.553414    0.000056
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N7H-amino 6mA_a (6mA_a-3), B3LPY/6-31+G(d)

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SCF Done:  E(RB3LYP) =  -506.633809619     A.U. after    9 cycles


Zero-point correction=                           0.140104 (Hartree/Particle)
Thermal correction to Energy=                    0.148970
Thermal correction to Enthalpy=                  0.149915
Thermal correction to Gibbs Free Energy=         0.105839
Sum of electronic and zero-point Energies=           -506.493706
Sum of electronic and thermal Energies=              -506.484839
Sum of electronic and thermal Enthalpies=            -506.483895
Sum of electronic and thermal Free Energies=         -506.527971

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   93.480             33.618             92.765


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Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
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1	6	0	1.428850	0.169356	-0.024741
2	6	0	0.112054	-0.339287	0.031170
3	6	0	-0.957710	0.576689	0.055932
4	6	0	0.636174	2.256008	-0.024514
5	6	0	1.618302	-1.955620	0.018132
6	7	0	-2.287875	0.256308	0.135706
7	7	0	2.345378	-0.865804	-0.033956
8	7	0	-0.657029	1.884984	0.023978
9	7	0	0.267052	-1.720998	0.061781
10	1	0	-2.890053	1.063780	0.035472
11	1	0	2.012306	-2.964363	0.027983
12	7	0	1.716790	1.482589	-0.054364
13	1	0	0.806923	3.329906	-0.045191
14	6	0	-2.852314	-1.052407	-0.133453
15	1	0	-2.557637	-1.449318	-1.116293
16	1	0	-2.578691	-1.775230	0.646704
17	1	0	-3.941179	-0.967294	-0.118480
18	1	0	-0.454007	-2.425465	0.102644

N9-deprotonated N9H-amino 6mA_a (6mA_a-4), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -506.100548951 A.U. after 1 cycles

Zero-point correction= 0.127452 (Hartree/Particle)
Thermal correction to Energy= 0.135708
Thermal correction to Enthalpy= 0.136653
Thermal correction to Gibbs Free Energy= 0.093947
Sum of electronic and zero-point Energies= -505.973097
Sum of electronic and thermal Energies= -505.964841
Sum of electronic and thermal Enthalpies= -505.963896
Sum of electronic and thermal Free Energies= -506.006602

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.158	31.419	89.882

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.448328	0.128021	0.045909
2	6	0	-0.120657	-0.396799	-0.065004
3	6	0	0.930563	0.533928	-0.111325
4	6	0	-0.642456	2.222224	0.053672
5	6	0	-1.513508	-1.982239	-0.044786
6	7	0	2.276745	0.210688	-0.275576
7	7	0	-2.332289	-0.907376	0.059214
8	7	0	0.654174	1.852407	-0.043142
9	7	0	-0.186011	-1.774570	-0.125273
10	1	0	2.847112	1.034974	-0.114180
11	1	0	-1.920102	-2.991275	-0.062833

12	7	0	-1.726052	1.456956	0.106625
13	1	0	-0.807444	3.299832	0.099291
14	6	0	2.823472	-1.028571	0.261815
15	1	0	2.904089	-1.022179	1.364085
16	1	0	2.172268	-1.857842	-0.021066
17	1	0	3.823601	-1.189630	-0.159910

N1-protonated N9H-amino 6mA_a (6mA_a-5), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -507.018938498 A.U. after 1 cycles

Zero-point correction= 0.154052 (Hartree/Particle)
Thermal correction to Energy= 0.163039
Thermal correction to Enthalpy= 0.163983
Thermal correction to Gibbs Free Energy= 0.119630
Sum of electronic and zero-point Energies= -506.864887
Sum of electronic and thermal Energies= -506.855900
Sum of electronic and thermal Enthalpies= -506.854956
Sum of electronic and thermal Free Energies= -506.899308

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.308	34.461	93.348

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.396120	0.117787	0.000019
2	6	0	-0.085921	-0.394171	-0.000022
3	6	0	0.978205	0.535889	-0.000047
4	6	0	-0.771591	2.240640	0.000036
5	6	0	-1.370298	-2.086195	0.000025
6	1	0	-3.213827	-0.975881	-0.000028
7	7	0	2.280849	0.263557	-0.000202
8	7	0	-2.199125	-0.981410	-0.000024
9	7	0	0.552902	1.850602	0.000004
10	7	0	-0.096555	-1.771449	-0.000031
11	1	0	2.932469	1.039675	-0.000197
12	1	0	-1.763272	-3.094327	0.000041
13	7	0	-1.774696	1.415829	0.000009
14	1	0	-0.939222	3.312943	0.000030
15	6	0	2.866809	-1.090367	0.000127
16	1	0	2.557851	-1.640957	0.890684
17	1	0	2.556865	-1.641759	-0.889580
18	1	0	3.950551	-0.972607	-0.000543
19	1	0	1.248457	2.591511	0.000469

N1-protonated N9H-amino 6mA_a (6mA_a-5), B3LYP/6-31+G(d), scrf=(smd,solvent=water)

SCF Done: E(RB3LYP) = -507.122837033   A.U. after   1 cycles

Zero-point correction=   0.154153 (Hartree/Particle)
Thermal correction to Energy=   0.163057
Thermal correction to Enthalpy=   0.164001
Thermal correction to Gibbs Free Energy=   0.120191
Sum of electronic and zero-point Energies=   -506.968684
Sum of electronic and thermal Energies=   -506.959780
Sum of electronic and thermal Enthalpies=   -506.958836
Sum of electronic and thermal Free Energies=   -507.002646

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.320	34.475	92.205

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.389611	0.161301	-0.000029
2	6	0	-0.104928	-0.403318	0.000121
3	6	0	0.995201	0.486998	0.000130
4	6	0	-0.671462	2.255894	-0.000068
5	6	0	-1.476827	-2.034219	0.000053
6	1	0	-3.259864	-0.854550	-0.000279
7	7	0	2.289366	0.194997	0.000130
8	7	0	-2.244961	-0.898241	-0.000056
9	7	0	0.619561	1.813681	0.000169
10	7	0	-0.184234	-1.785259	0.000149
11	1	0	2.943055	0.972628	-0.000142
12	1	0	-1.923955	-3.018331	0.000051
13	7	0	-1.719619	1.476310	-0.000163
14	1	0	-0.785971	3.333141	-0.000154
15	6	0	2.862552	-1.153215	-0.000235
16	1	0	2.560504	-1.704948	0.892595
17	1	0	2.559494	-1.704908	-0.892756
18	1	0	3.946398	-1.038750	-0.000834
19	1	0	1.349989	2.524667	0.000085

N3-protonated N9H-amino 6mA_a, (6mA_a-6), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -507.017297222   A.U. after   1 cycles

Zero-point correction=   0.153880 (Hartree/Particle)
Thermal correction to Energy=   0.162873
Thermal correction to Enthalpy=   0.163817
Thermal correction to Gibbs Free Energy=   0.119409
Sum of electronic and zero-point Energies=   -506.863417
Sum of electronic and thermal Energies=   -506.854424
Sum of electronic and thermal Enthalpies=   -506.853480
Sum of electronic and thermal Free Energies=   -506.897888

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.204	34.538	93.465

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.378135	0.066205	0.000029
2	6	0	-0.061725	-0.395406	-0.000016
3	6	0	0.980928	0.577131	-0.000020
4	6	0	-0.620315	2.266021	-0.000047
5	6	0	-1.307164	-2.128720	-0.000024
6	1	0	-3.184237	-1.077629	-0.000151
7	7	0	2.280029	0.319478	0.000071
8	7	0	-2.171409	-1.036361	0.000069
9	7	0	0.627071	1.907731	-0.000076
10	7	0	-0.050384	-1.777438	-0.000083
11	1	0	2.871476	1.145426	0.000003
12	1	0	-1.684674	-3.142551	-0.000023
13	7	0	-1.680715	1.397294	0.000099
14	1	0	-0.873952	3.322081	-0.000057
15	6	0	2.920311	-1.000962	0.000023
16	1	0	2.634192	-1.568131	0.888937
17	1	0	2.635094	-1.567654	-0.889496
18	1	0	3.998935	-0.843192	0.000622
19	1	0	-2.632379	1.751113	-0.000066

N6-protonted N9H-amino 6mA_a (6mA_a-7), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -506.993709925 A.U. after 1 cycles

Zero-point correction=	0.155235 (Hartree/Particle)
Thermal correction to Energy=	0.163950
Thermal correction to Enthalpy=	0.164894
Thermal correction to Gibbs Free Energy=	0.120531
Sum of electronic and zero-point Energies=	-506.838474
Sum of electronic and thermal Energies=	-506.829760
Sum of electronic and thermal Enthalpies=	-506.828816
Sum of electronic and thermal Free Energies=	-506.873179

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.880	33.119	93.371

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.378367	0.471382	0.087288

2	6	0	-0.320082	-0.447337	-0.136288
3	6	0	0.913681	0.159200	-0.279090
4	6	0	-0.002519	2.224992	0.007873
5	6	0	-2.068240	-1.628137	0.023900
6	7	0	2.132161	-0.657898	-0.511529
7	7	0	-2.490983	-0.326199	0.187542
8	7	0	1.092183	1.461313	-0.212949
9	7	0	-0.771764	-1.745923	-0.172617
10	1	0	2.672935	-0.211099	-1.263648
11	1	0	-2.763623	-2.457184	0.058231
12	7	0	-1.257236	1.789691	0.165938
13	1	0	0.160731	3.296107	0.057377
14	6	0	3.016609	-0.806727	0.713011
15	1	0	3.299864	0.194073	1.037957
16	1	0	2.440246	-1.319553	1.483131
17	1	0	3.893697	-1.391310	0.430693
18	1	0	-3.441913	-0.010967	0.346727
19	1	0	1.841055	-1.587195	-0.845325

N7-protonated N9H-amino 6mA_a (6mA_a-8), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -507.006623074 A.U. after 8 cycles

Zero-point correction= 0.154022 (Hartree/Particle)
Thermal correction to Energy= 0.162815
Thermal correction to Enthalpy= 0.163759
Thermal correction to Gibbs Free Energy= 0.120092
Sum of electronic and zero-point Energies= -506.852601
Sum of electronic and thermal Energies= -506.843808
Sum of electronic and thermal Enthalpies= -506.842864
Sum of electronic and thermal Free Energies= -506.886531

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.168	34.170	91.906

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.359189	0.261043	-0.000000
2	6	0	-0.088449	-0.326614	0.000000
3	6	0	1.024051	0.562570	0.000001
4	6	0	-0.529524	2.300995	0.000000
5	6	0	-1.613343	-1.955553	0.000000
6	1	0	-3.284647	-0.681214	-0.000001
7	7	0	2.320472	0.209114	0.000001
8	7	0	-2.274507	-0.792398	-0.000001
9	7	0	0.736215	1.879426	0.000001
10	7	0	-0.301535	-1.710333	0.000001
11	1	0	2.962729	0.994368	0.000001
12	1	0	-2.065422	-2.937295	0.000001

13	7	0	-1.645397	1.551456	-0.000001
14	1	0	-0.672981	3.377407	0.000000
15	6	0	2.856496	-1.143630	-0.000001
16	1	0	2.560900	-1.695008	0.902262
17	1	0	2.560898	-1.695006	-0.902265
18	1	0	3.945368	-1.081170	-0.000002
19	1	0	0.406159	-2.435800	0.000002

N9-protonated N9H-amino 6mA_a (6mA_a-9), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -506.947374136 A.U. after 8 cycles

Zero-point correction= 0.152744 (Hartree/Particle)
Thermal correction to Energy= 0.161754
Thermal correction to Enthalpy= 0.162698
Thermal correction to Gibbs Free Energy= 0.118479
Sum of electronic and zero-point Energies= -506.794630
Sum of electronic and thermal Energies= -506.785620
Sum of electronic and thermal Enthalpies= -506.784676
Sum of electronic and thermal Free Energies= -506.828895

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.502	34.553	93.067

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.306363	0.307853	0.000000
2	6	0	-0.081235	-0.341049	-0.000000
3	6	0	1.052716	0.521240	-0.000000
4	6	0	-0.435995	2.317961	-0.000000
5	6	0	-1.463573	-2.026144	-0.000000
6	1	0	-2.950608	-0.717434	-0.828050
7	7	0	2.330622	0.144992	0.000000
8	7	0	-2.338864	-0.774284	0.000000
9	7	0	0.800523	1.864834	-0.000000
10	7	0	-0.227946	-1.739829	-0.000000
11	1	0	2.991383	0.915532	-0.000000
12	1	0	-1.946302	-2.995140	0.000000
13	7	0	-1.587593	1.576785	0.000000
14	1	0	-0.568029	3.395649	0.000000
15	6	0	2.840718	-1.226000	0.000000
16	1	0	2.509757	-1.767740	0.891091
17	1	0	2.509764	-1.767738	-0.891095
18	1	0	3.929841	-1.176339	0.000004
19	1	0	-2.950608	-0.717435	0.828050

N7H-amino 6mA_a with HF hydrogen-bonded to N3 (6mA_a-10), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -607.100243197   A.U. after   8 cycles

Zero-point correction=   0.152393 (Hartree/Particle)
Thermal correction to Energy=   0.163696
Thermal correction to Enthalpy=   0.164640
Thermal correction to Gibbs Free Energy=   0.113216
Sum of electronic and zero-point Energies=   -606.947850
Sum of electronic and thermal Energies=   -606.936547
Sum of electronic and thermal Enthalpies=   -606.935603
Sum of electronic and thermal Free Energies=   -606.987027

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.721	40.381	108.232

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.805447	0.584105	-0.000002
2	6	0	-0.595096	0.421720	-0.000013
3	6	0	-1.121410	-0.886688	-0.000021
4	6	0	1.065879	-1.650502	-0.000007
5	6	0	-0.006046	2.551168	-0.000008
6	7	0	-2.441305	-1.218377	-0.000042
7	7	0	1.143909	1.917962	0.000002
8	7	0	-0.247286	-1.911212	-0.000017
9	7	0	-1.095500	1.719541	-0.000018
10	1	0	-2.614111	-2.215182	-0.000001
11	1	0	-0.119903	3.627901	-0.000009
12	7	0	1.660973	-0.457613	0.000002
13	1	0	1.722432	-2.516452	-0.000005
14	6	0	-3.563936	-0.302418	0.000060
15	1	0	-3.577065	0.331321	0.897606
16	1	0	-3.577135	0.331419	-0.897415
17	1	0	-4.485521	-0.887902	0.000059
18	1	0	-2.061369	2.011666	-0.000026
19	1	0	3.335515	-0.417006	0.000017
20	9	0	4.302511	-0.546909	0.000026

N7-protonated N9H-amino 6mA_a with HF hydrogen-bonded to N3 (6mA_a-11), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -607.468927509   A.U. after   1 cycles

Zero-point correction=   0.166573 (Hartree/Particle)
Thermal correction to Energy=   0.177422
Thermal correction to Enthalpy=   0.178367
Thermal correction to Gibbs Free Energy=   0.129691

```
Sum of electronic and zero-point Energies=           -607.302354
Sum of electronic and thermal Energies=              -607.291505
Sum of electronic and thermal Enthalpies=            -607.290561
Sum of electronic and thermal Free Energies=         -607.339236

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  111.334             40.730           102.446


---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.897503    0.040358    0.000000
     2          6           0        0.455389    0.381067   -0.000001
     3          6           0        1.386612   -0.698633   -0.000002
     4          6           0       -0.452981   -2.134059    0.000001
     5          6           0       -0.760334    2.253000    0.000002
     6          1           0       -2.643205    1.241275   -0.000004
     7          7           0        2.722638   -0.591098   -0.000001
     8          7           0       -1.615549    1.228600   -0.000002
     9          7           0        0.862823   -1.943926   -0.000000
    10          7           0        0.491172    1.781109    0.000001
    11          1           0        3.209506   -1.481584   -0.000001
    12          1           0       -1.032097    3.299354    0.000002
    13          7           0       -1.410400   -1.188122    0.000001
    14          1           0       -0.792669   -3.165339    0.000001
    15          6           0        3.501451    0.639849   -0.000001
    16          1           0        3.311961    1.234913   -0.902434
    17          1           0        3.311960    1.234913    0.902432
    18          1           0        4.559421    0.375277   -0.000000
    19          1           0        1.315349    2.370612    0.000001
    20          1           0       -3.187224   -0.921161    0.000002
    21          9           0       -3.867066   -0.231521    0.000001
---------------------------------------------------------------------
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N7-protonated N9H-amino 6mA_a with HF hydrogen-bonded to N1 (6mA_a-12), B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -607.465037641     A.U. after    8 cycles


Zero-point correction=                           0.166813 (Hartree/Particle)
Thermal correction to Energy=                    0.177624
Thermal correction to Enthalpy=                  0.178568
Thermal correction to Gibbs Free Energy=         0.129887
Sum of electronic and zero-point Energies=           -607.298225
Sum of electronic and thermal Energies=              -607.287413
Sum of electronic and thermal Enthalpies=            -607.286469
Sum of electronic and thermal Free Energies=         -607.335150

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  111.461             40.555           102.458
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.478684	-0.843068	0.000000
2	6	0	0.706903	0.322320	0.000000
3	6	0	-0.710375	0.163411	0.000000
4	6	0	-0.290954	-2.152036	0.000001
5	6	0	2.857620	0.908841	-0.000001
6	7	0	-1.619059	1.142823	0.000000
7	7	0	2.809187	-0.428781	-0.000000
8	7	0	-1.147915	-1.124207	0.000001
9	7	0	1.612264	1.387982	-0.000001
10	1	0	3.757786	1.507331	-0.000001
11	7	0	1.045547	-2.095251	0.000000
12	1	0	-0.736868	-3.142139	0.000001
13	1	0	1.389046	2.376932	-0.000001
14	1	0	-2.892684	-1.154512	-0.000001
15	9	0	-3.745224	-0.692714	-0.000001
16	6	0	-1.345786	2.573312	0.000001
17	1	0	-0.802141	2.879976	0.903021
18	1	0	-0.802142	2.879977	-0.903020
19	1	0	-2.300589	3.100217	0.000002
20	1	0	-2.592734	0.826241	-0.000000
21	1	0	3.610623	-1.054237	-0.000000

N7H-amino 6mA_a (less stable) with HF hydrogen-bonded to N1 (6mA_a-13), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -607.103213575 A.U. after 1 cycles

Zero-point correction= 0.152631 (Hartree/Particle)
Thermal correction to Energy= 0.163479
Thermal correction to Enthalpy= 0.164423
Thermal correction to Gibbs Free Energy= 0.115258
Sum of electronic and zero-point Energies= -606.950583
Sum of electronic and thermal Energies= -606.939735
Sum of electronic and thermal Enthalpies= -606.938791
Sum of electronic and thermal Free Energies= -606.987955

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.584	39.552	103.475

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.512404	-0.882221	-0.000225
2	6	0	0.746587	0.303650	-0.000164
3	6	0	-0.659839	0.206197	0.000040

4	6	0	-0.344981	-2.118243	-0.000313
5	6	0	2.912703	0.725540	0.000413
6	7	0	-1.544197	1.234939	0.000388
7	7	0	2.858789	-0.585751	0.000107
8	7	0	-1.169707	-1.048096	-0.000137
9	7	0	1.682485	1.330206	0.000529
10	1	0	3.824806	1.309099	0.000717
11	7	0	0.976284	-2.120149	-0.000358
12	1	0	-0.845929	-3.082827	-0.000440
13	1	0	1.512287	2.324936	-0.000637
14	1	0	-2.734397	-1.040507	0.000223
15	9	0	-3.686523	-0.723362	0.000499
16	6	0	-1.208658	2.644626	-0.000684
17	1	0	-0.644994	2.934401	0.896955
18	1	0	-0.644605	2.932877	-0.898576
19	1	0	-2.139083	3.215620	-0.001398
20	1	0	-2.524255	0.961325	0.000558

N7-protonated N9H-amino 6mA_a (less stable) with HF hydrogen-bonded to N1 and N3 (6mA_a-14), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -707.926382193 A.U. after 1 cycles

Zero-point correction= 0.179244 (Hartree/Particle)
Thermal correction to Energy= 0.192186
Thermal correction to Enthalpy= 0.193131
Thermal correction to Gibbs Free Energy= 0.139304
Sum of electronic and zero-point Energies= -707.747139
Sum of electronic and thermal Energies= -707.734196
Sum of electronic and thermal Enthalpies= -707.733252
Sum of electronic and thermal Free Energies= -707.787078

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	120.599	47.358	113.288

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.251522	-0.070914	0.000084
2	6	0	0.105223	0.721045	-0.000048
3	6	0	-1.153667	0.047744	-0.000211
4	6	0	0.083065	-1.955705	-0.000151
5	6	0	1.896838	2.048917	0.000377
6	1	0	3.306690	0.441496	0.000330
7	7	0	-2.358069	0.619024	-0.000256
8	7	0	2.339156	0.789340	0.000311
9	7	0	-1.085912	-1.313668	-0.000288
10	7	0	0.559505	2.043978	0.000228
11	1	0	-3.145783	-0.036037	-0.000135
12	1	0	2.517449	2.934247	0.000580

13	7	0	1.303778	-1.404306	0.000054
14	1	0	0.036757	-3.040446	-0.000216
15	6	0	-2.636437	2.049954	-0.000403
16	1	0	-2.245157	2.535021	0.902764
17	1	0	-2.244804	2.534855	-0.903507
18	1	0	-3.718709	2.183293	-0.000657
19	1	0	-2.716048	-1.992392	0.000317
20	1	0	3.091697	-1.779796	-0.000287
21	1	0	-0.007953	2.883893	-0.000036
22	9	0	3.955538	-1.348788	-0.000305
23	9	0	-3.673606	-1.856875	0.000595

N7H-amino 6mA_a (less stable) with HF hydrogen-bonded to N1 and N3 (6mA_a-15), B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -707.567419818 A.U. after 8 cycles

Zero-point correction= 0.165231 (Hartree/Particle)
Thermal correction to Energy= 0.178403
Thermal correction to Enthalpy= 0.179347
Thermal correction to Gibbs Free Energy= 0.123661
Sum of electronic and zero-point Energies= -707.402189
Sum of electronic and thermal Energies= -707.389017
Sum of electronic and thermal Enthalpies= -707.388073
Sum of electronic and thermal Free Energies= -707.443759

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	111.950	46.337	117.201

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.260606	0.558300	0.000000
2	6	0	-0.100684	0.922792	-0.000000
3	6	0	-1.082001	-0.090888	-0.000000
4	6	0	0.696998	-1.618012	0.000001
5	6	0	1.229135	2.684247	-0.000001
6	7	0	-2.422959	0.082405	-0.000001
7	7	0	2.065090	1.670529	-0.000000
8	7	0	-0.623359	-1.368597	-0.000000
9	7	0	-0.088771	2.311720	-0.000002
10	1	0	-2.969945	-0.776575	-0.000001
11	1	0	1.520194	3.726978	-0.000002
12	7	0	1.678319	-0.727164	0.000001
13	1	0	0.980730	-2.666548	0.000001
14	6	0	-3.117720	1.355933	0.000003
15	1	0	-2.891026	1.945745	0.898334
16	1	0	-2.891028	1.945750	-0.898325
17	1	0	-4.190795	1.156830	0.000004
18	1	0	-1.823167	-2.421946	-0.000001

19	1	0	3.273729	-1.308638	0.000001
20	1	0	-0.880174	2.938286	-0.000002
21	9	0	4.115845	-1.792286	0.000001
22	9	0	-2.749707	-2.785088	-0.000002

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