Supporting information

Gas phase studies of substrates for the DNA mismatch repair enzyme MutY

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Table of Contents:

1. Acid-catalyzed depurination

Acid-catalyzed depurination experiments were performed to determine the intrinsic lability of the Z1 and Z3 analogues compared to adenine (Figure S1). Adenine at position 11 of the 30 nt sequence was selected for comparison to all other purines in the sequence, except for G26 and A27 whose bands could not be well distinguished. In particular, the A, Z1, or Z3 at position 15 are depurinated at fractions of 0.9, 6.3, and 0.3 compared to A11, respectively. Plots of relative depurination show that Z1 is depurinated seven times *more than* adenine at the same position (Figure S2).

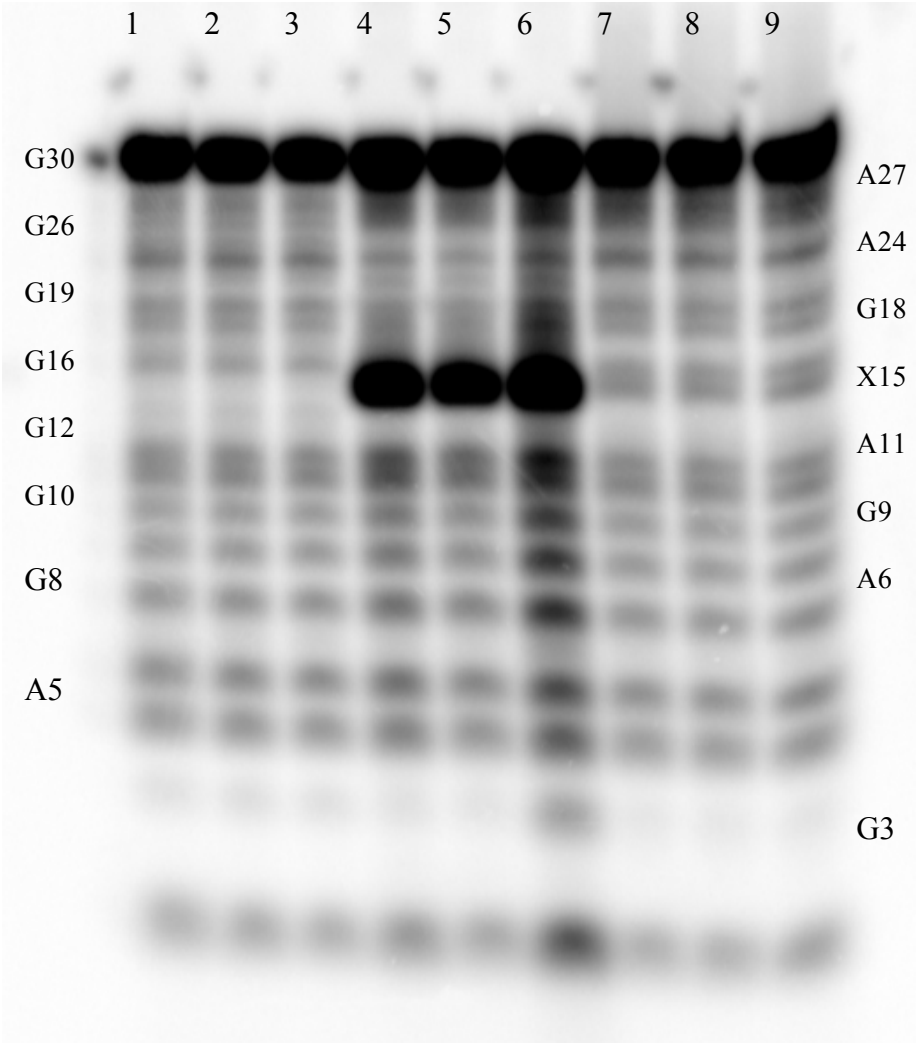


Figure S1: PAGE analysis of acid-catalyzed depurination reactions of X at position 15 in 30 nt sequence. Lanes 1 – 3, X = Z3, Lanes 4-6, X = Z1, Lanes 7-9, X = A. Purine position is indicated along both sides of the gel.

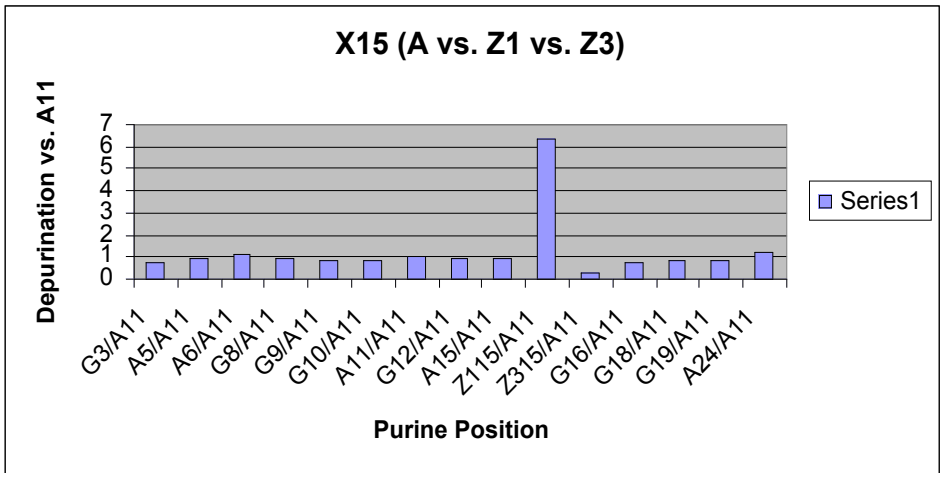


Figure S2: Comparison of acid-catalyzed depurination of purines of the B30 sequence. All positions are compared to depurination of A11 and are the result of nine experiments except position 15, which was either A, Z1, or Z3 and is the average of three experiments each.

2. General Synthetic Procedures.

Solvents were freshly distilled before use: THF and C_5H_5N from Na, benzophenone; CH_2Cl_2 and MeOH from CaH_2. Reactions were carried out in flame-dried round bottom flasks fitted with rubber septa under Ar at 23°. Air-, moisture- sensitive liquids and solutions were transferred via syringe or stainless steel canula. Organic solutions were concentrated by evaporation of the volatiles at 25°C / ca. 10 mm Hg. Products from reactions were dried in a vacuum dessicator (KOH) at 0.05 mm Hg prior to use in subsequent reactions. Thin-layer chromatography utilized *Merck* silica gel 60-F_{254} Al plates; detection by Mineralight multiband UV lamp at 254 and 365 nm and / or by heating with acidic *p*-anisaldehyde (prepared by adding 50 ml con. H_2SO_4 dropwise to an ice-cold solution of 15 mL AcOH, 3.5 mL *p*-anisaldehyde in 300 mL EtOH). Flash chromatography (FC) utilized silica gel *Merck* 60 (230-400 mesh. NMR Spectra: *Varian ASM*100 and *VXR*500. δ in ppm rel. to external TMS (^{1}H, ^{13}C) and to external 85% H_3PO_4 soln. (^{31}P); coupling constants *J* in Hz. High-resolution mass spectra: Finnigan Mat 95.

3. Experimental for synthetic intermediates

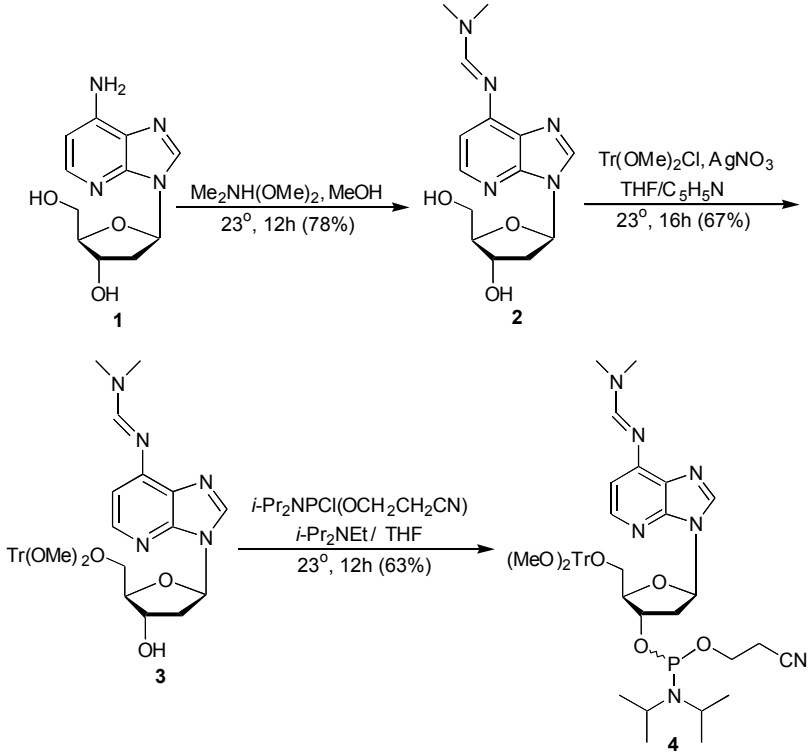
1-deazaadenine (Z1).

7-Nitro-1*H*-imidazo[4,5-*b*]pyridine 4-oxide (2.24 g, 12.4 mmol) was suspended in 22.5 mL water at 0 °C. The suspension was treated portionwise with 135 mL titanium(III) chloride in 20-30% HCl, mixing thoroughly after each addition. During this process, the reaction mixture became green and homogeneous, and gas evolution was evident. The reaction mixture was then stirred 2 d at rt until the solution was dark brownish-yellow. The solution was brought to pH 9 with saturated aq Na_2CO_3 then filtered. The blue-white precipitate was triturated with acetone (1 x 75 mL), and the filtrate was concentrated *in vacuo* to an amorphous yellow residue. This residue was triturated with acetone (3 x 75 mL). Acetone aliquots were combined and concentrated *in vacuo* to give 2.15 g of crude 1-deazaadenine.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.54 (s, 1H), 8.01 (s, 1H), 7.79 (d, *J* = 5.4, 1H), 6.31 (d, *J* = 5.4, 1H), 6.22 (s, 2H).

1-Deaza-2'-deoxyadenosine phosphoramidite (4).

The synthesis of the phosphoramidite monomer (4) was designed as shown in Scheme S1 starting with amine **1** (refs: Seela, F; Wenzel, T. *Helv. Chim. Acta*, **1994**, *77*, 1485; Seela, F; Wenzel, T. *Heterocycles*, **1993**, *36*, 237).



Scheme S1. Synthesis of 1-deaza-2'-deoxyadenosine phosphoramidite

1-Deaza-N^6-(N, N-Dimethylaminomethylene)-2'-deoxyadenosine (2)

A stirred mixture of 6-amino compound **1** (1.18 g, 4.7 mmol; R_f ($CHCl_3$ / MeOH / NEt_3 17:3:0.01)0.33) in MeOH (20 mL) was treated with N,N'-Dimethylformamide dimethyl acetal (2.1 mL, 14.1 mmol). After 12 h, the reaction solution was concentrated and coevaporated with toluene (2 x 25 mL). The residue was treated with MeOH (20 mL), stirred for 2 h and concentrated. FC ($CHCl_3$ / MeOH / NEt_3 9:1:0.01) gave the imine **2** (1.1 g, 78%). Colorless glass. R_f ($CHCl_3$ / MeOH / NEt_3 17:3:0.01) 0.46. ^{1}H-NMR (CD_3OD, 300 MHz): 2.32-2.42 (*m*, 1H), 2.84-2.93 (*m*, 1H), 3.11 (*s*, 3H), 3.17 (*s*, 3H),

3.75 (*dd*, *J* = 12.3, 3.0, 1H), 3.86 (*dd*, *J* = 12.3, 2.6, 1H), 4.08-4.11 (*m*, 1H), 4.57-4.61 (*m*, 1H), 4.91 (*s*, 2H, HOD), 6.50 (*dd*, *J* = 5.7, 8.24, 1H), 6.88 (*d*, *J* = 5.5, 1H), 8.08 (*d*, *J* = 5.5, 1H), 8.40 (*s*, 1H), 8.56 (*s*, 1H). ^{13}C-NMR (CD_3OD, 125 MHz): 37.22, 41.44 (2 x Me), 64.07, 73.59, 87.79, 90.17, 104.25, 113.37, 145.73. HRCI-MS: calcd. for $C_{14}H_{19}N_5O_3$ $(M+H)^+$ 306.1566, obsd. 306.1563.

1-Deaza-5'-O-(4.4'-dimethoxytrityl)-N^6-(N,N-dimethylaminomethylene)-2'-deoxyadenosine (3)

A stirred solution of the imine **2** (0.1 g, 0.33 mmol) in THF (3 mL), was treated with C_5H_5N (0.16 mL, 1.97 mmol) and trityl chloride (0.13 g, 0.36 mmol). After 3 min., $AgNO_3$ (0.06 g, 0.36 mmol) was added. The reaction solution acquired a pale orange color. Precipitation was observed after ten minutes. TLC (CH_2Cl_2 / MeOH / NEt_3 19:1:0.01) revealed complete disappearance of imine **2** after 16h. The suspension was passed through *Celite*, and the residue was washed with AcOEt (100 mL). The filtrate was washed with satd. aq. $NaHCO_3$ (20 mL), brine (20 mL), dried (anhyd. Na_2SO_4) and concentrated. FC (CH_2Cl_2 / MeOH / NEt_3 24:1:0.01) gave trityl derivative **3** (0.13 g, 67%). Pale yellow glass. R_f (CH_2Cl_2 / MeOH / NEt_3 19:1:0.01) 0.31. ^{1}H-NMR (CD_3OD, 300 MHz): 2.48-2.56 (*m*, 1H), 2.82-2.91 (*m*, 1H), 3.09 (*s*, 3H), 3.11 (*s*, 3H), 3.27-3.30 (*m*, 1H), 3.71 (*s*, 6H), 4.03-4.12 (*m*, 1H), 4.49-4.64 (*m*, 1H), 4.93 (*s*, 1H, HOD), 6.53 (*t*, *J* = 6.4, 1H), 6.71-6.75 (*m*, 4H), 6.84 (*d*, *J* = 5.5, 1H), 7.12-7.24 (*m*, 7H), 7.33-7.36 (*m*, 2H), 8.08 (*d*, *J* = 5.5, 1H), 8.28 (*s*, 1H), 8.47 (*s*, 1H). ^{13}C-NMR (CD_3OD, 75 MHz): 34.91, 41.20, 41.33, 55.82, 65.26, 72.87, 79.63, 85.70, 87.75, 87.94, 113.44, 114.18, 127.94, 128.89, 129.46, 130.28, 131.36, 131.46, 137.26, 141.87, 146.35, 146.43, 148.84, 152.43, 159.83, 160.21, 160.23. EI-MS: *m/z* (relative intensity) 608.3 ($[M+1]^+$, 13), 307.1 (15), 306.1 (100), 305.1 (34), 304.1 (16), 303 (44), 197.1 (34).

1-Deaza-5'-O-(4.4'-dimethoxytrityl)-N^6-(N,N-dimethylaminomethylene)-2'-deoxyadenosine-3'-O-[2-cyanoethyl)-N,N-diisopropylphosphoramidite] (4)

A stirred solution of compound **3** (82 mg, 0.135 mmol) and N,N'-diisopropyl ethyl amine (0.074 mL, 0.81 mmol) in THF (4 mL) was treated with 2-cyanoethyl diisopropylchlorophosphoramidite (0.071 mL, 0.27 mmol). Precipitation was observed in 20 minutes. After 12h, TLC (CH_2Cl_2 / MeOH / NEt_3 19:1:0.01) revealed disappearance of **3**, and formation of relatively non-polar spots. The suspension was diluted with AcOEt (50 mL), washed with satd. aq. $NaHCO_3$ (10 mL), brine (10 mL); the organic layer was separated, dried (anhyd. Na_2SO_4), filtered and concentrated. FC (AcOEt / MeOH / NEt_3 97:3:0.01) gave phosphoramidite diastereomers **4** (69 mg, 63%). Pale yellow oil. R_f (CH_2Cl_2 / MeOH / NEt_3 97:3:0.01) 0.28, 0.29; (CH_3CN / H_2O 9:1) 0.45). ^{1}H-NMR (CD_2Cl_2, 300 MHz): 1.01-1.18 (*m*), 1.35 (*d*, *J* = 6.6 Hz), 2.39 (m), 2.51-2.68 (*m*), 2.78-2.87 (*m*), 3.03 (*s*), 3.17-3.79 (*m*), 3.67 (*s*), 3.91-4.21 (*m*), 4.62-4.69 (*m*), 5.23-5.25 (*m*), 5.76 (*s*), 6.44 (*t*, 6.6 Hz), 6.65-6.73 (*m*), 7.10-7.23 (*m*), 7.30-7.35 (*m*), 7.89-7.98 (*m*). ^{31}P NMR (121 MHz, CD_2Cl_2): 149.10. HRFAB-MS: calcd. for $C_{44}H_{54}N_7O_6P$ $(M+H)^+$ 808.3951, obsd. 808.3911.

4. Oligonucleotide Synthesis

Oligonucleotides were synthesized at the University of Utah Medical School core facility. Oligonucleotides are purified via HPLC on a Beckman Gold Nouveau system using ion-exchange chromatography with a Waters AP1 DEAE 8HR column. The following duplex was used for MutY base excision assays:

5'-CGA TCA TGG AGC CAC ***(OG)***AG CTC CCG TTA CAG-3'

3'-GCT AGT ACC TCG GTG (***Y***)TC GAG GGC AAT GTC-5',

where Y = adenine analog, e.g. Z1 and OG = 8-oxoguanine.

5. MutY Cleavage Assays

MutY enzyme purification and glycosylase assays were performed as previously described (Francis, A. W.; Helquist, S. A.; Kool, E. T.; David, S. S. *J. Am. Chem. Soc.* **2003**, *125*, 16235-16242). Gels from cleavage assays were quantitated via storage phosphor autoradiography using ImageQuant software to generate plots of product formed as a function of time. The resulting data was fit to a single-exponential to determine k_{obs}. In these experiments, under single-turnover with base-quenching $k_{obs} = k_g$, as illustrated in the scheme below.

$$\text{Enzyme} + \text{(DNA)s} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \text{Enzyme}\cdot\text{(DNA)s} \xrightarrow{k_g} \text{Enzyme}\cdot\text{(AP-DNA)p}$$

Scheme S2. Kinetic scheme for glycosylase activities of MutY

6. Acid-Catalyzed Depurination reactions.

A modified Maxam-Gilbert G+A sequencing reaction was performed as previously described (Francis, A. W.; Helquist, S. A.; Kool, E. T.; David, S. S. *J. Am. Chem. Soc.* **2003**, *125*, 16235-16242). The X-containing DNA strand where X= **A, Z1, or Z3** at position 15 of the oligonucleotide sequence above was 5`-^{32}P labeled as described above. A solution of 25 µL final volume containing 32 nM DNA, 0.1 M piperidine, 13.2 % formic acid, and 1.2 mM calf thymus DNA was incubated at 37 ˚C for 30 min. The reaction was quenched with the addition of 225 µL of a stop solution (0.3 M sodium acetate, pH 7, 0.1mM EDTA, 76 mM calf thymus DNA). The DNA stands were ethanol precipitated (3X), dried in vacuo, followed by the addition of 1.0 M piperidine. The mixture was incubated at 90˚C for 45 min and dried in vacuo with several washes with ddH_2O. The samples were then electrophoresed on a 15% polyacrylamide gel for 4 h at 900 V. Bands were quantified using storage phosphor autoradiography.

7. Full References from Manuscript

Reference number refer to reference number in manuscript.

(44) Gaussian 03, *Revision E.01*, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

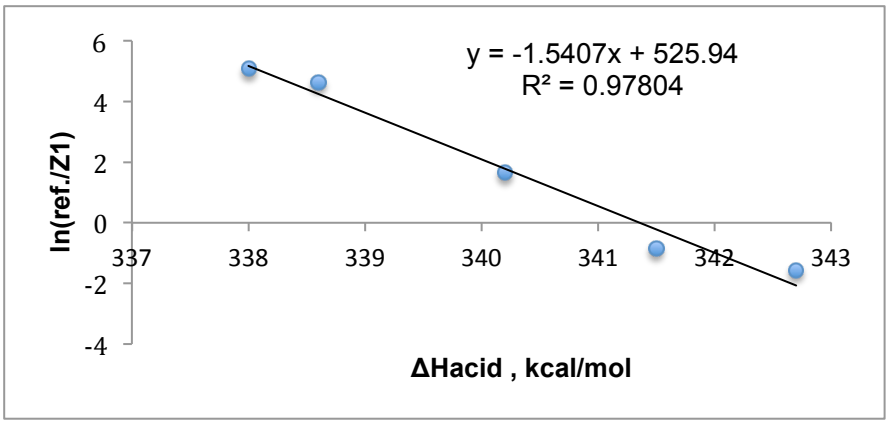
(45) Gaussian 09, *Revision A.02*, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

8. Cooks kinetic method

Figure S3. Plots for all Cooks kinetic method measurements

Z1 acidity

Trial 1



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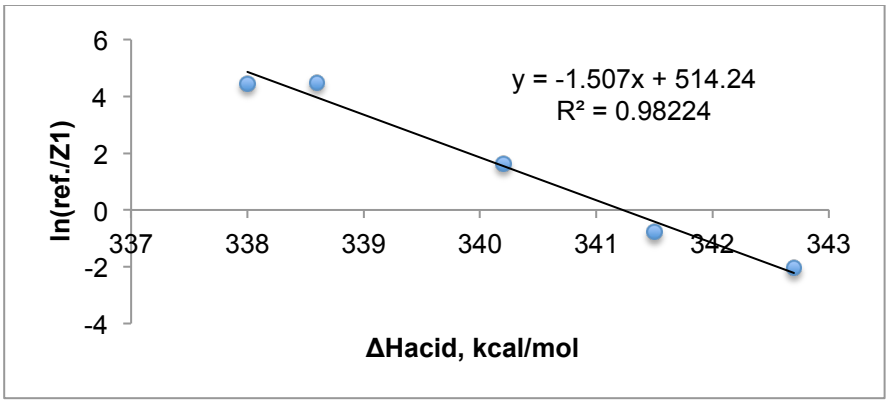

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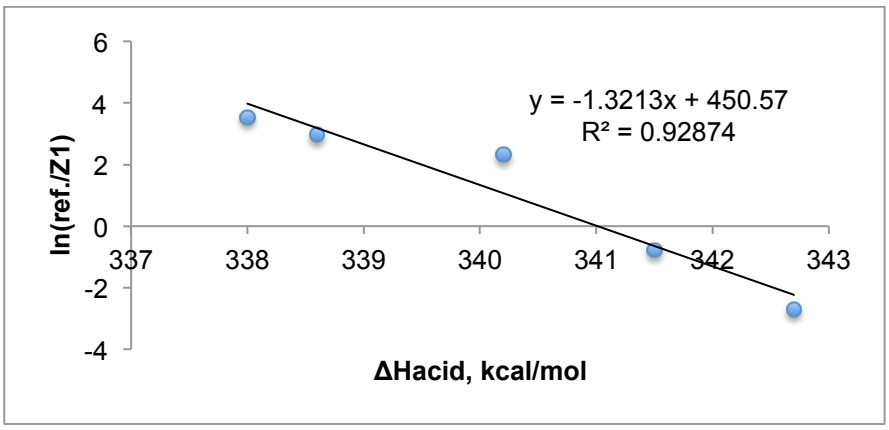
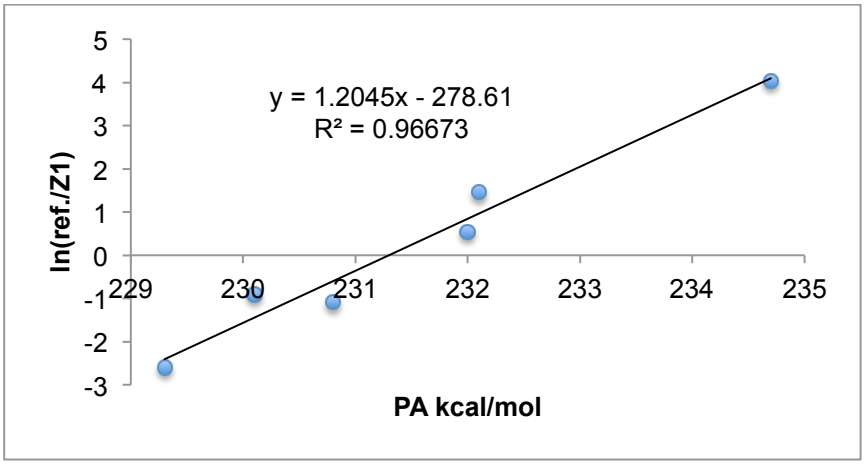


	slope	intercept	Teff, K	ΔHacid,kcal/mol
trial 1	-1.5407	525.94	327	341.4
trial 2	-1.507	514.24	334	341.2
trial 3	-1.3213	450.57	381	341.0
average			347	341.2

Z1 PA

Trial 1



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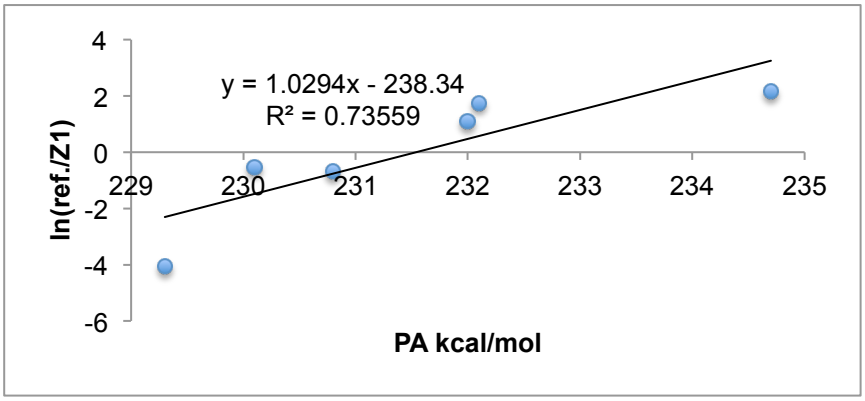

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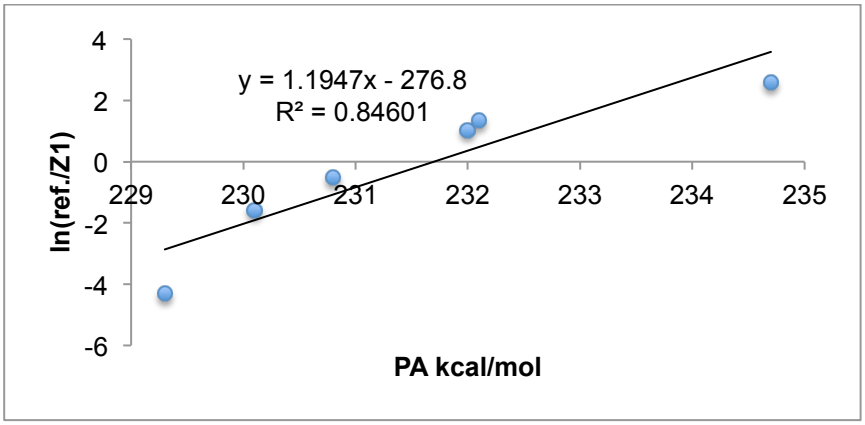
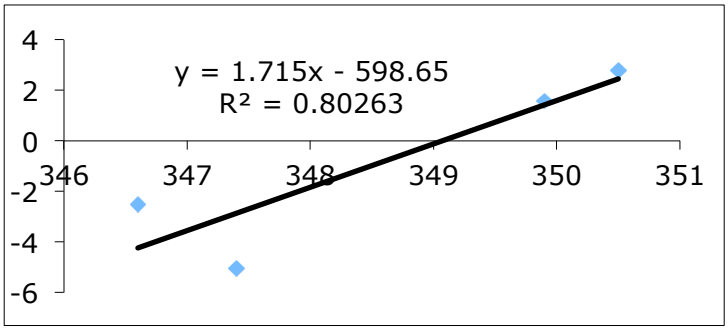


	slope	intercept	Teff, K	PA, kcal/mol
trial 1	1.2045	-278.61	418	231.3
trial 2	1.0294	-238.35	489	231.5
trial 3	1.1947	-276.8	421	231.7
average			443	231.5

M acidity

Trial 1



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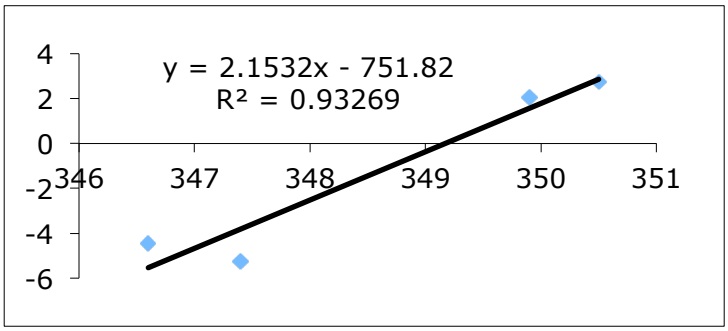

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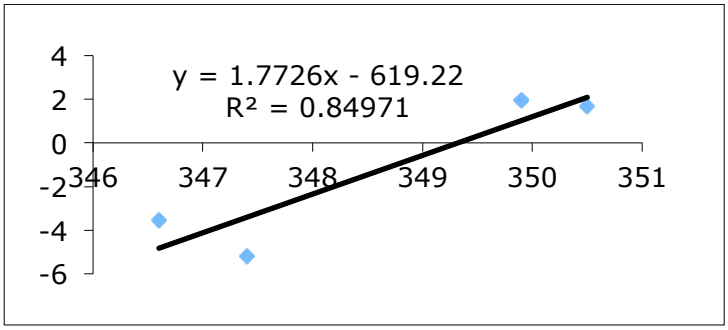
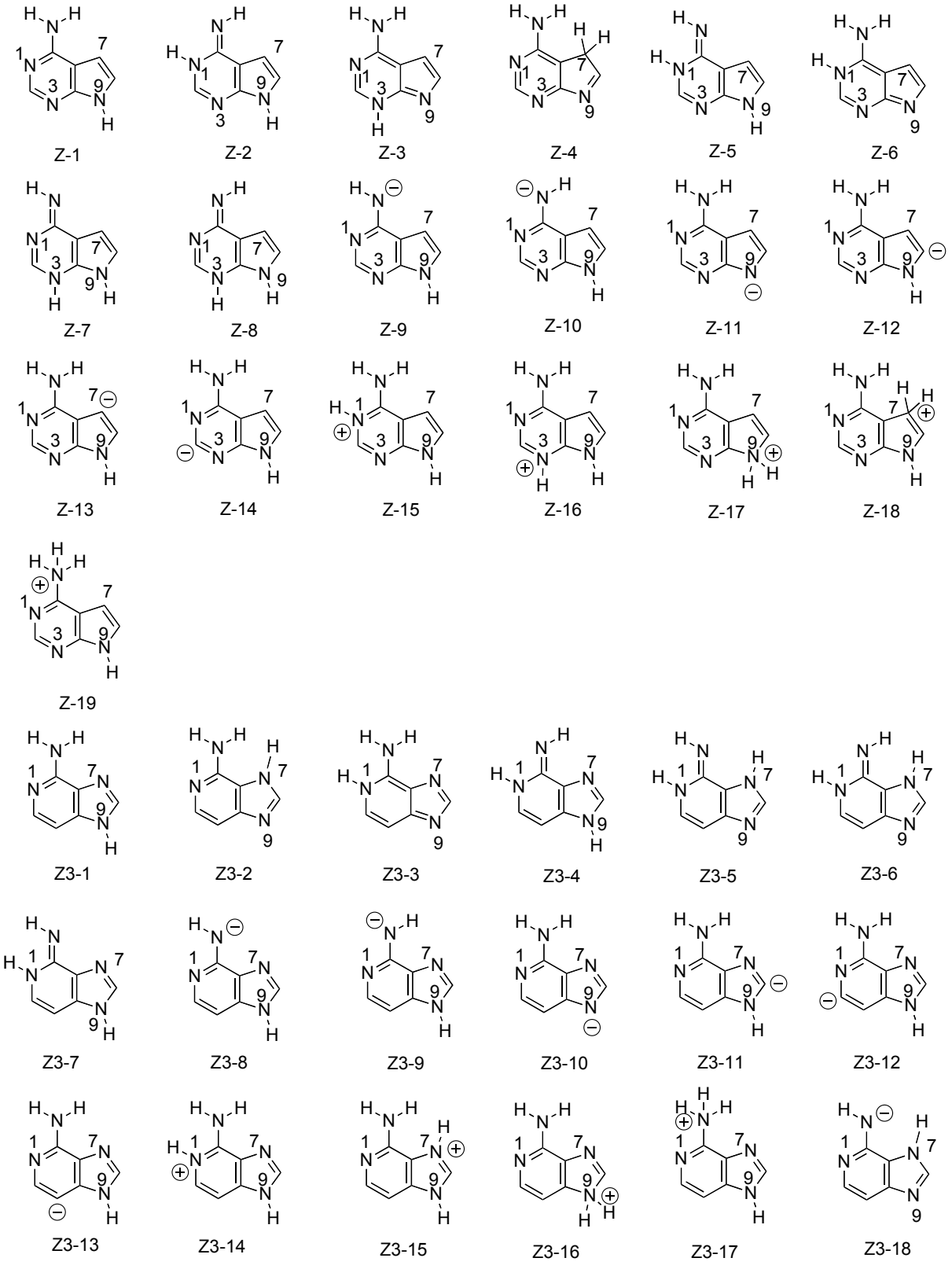
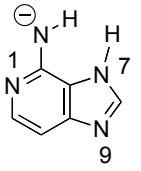


	Slope	Intercept	Teff	ΔHacid, kcal/mol
Trial 1	1.715	-598.65	293.5	349.1
Trial 2	2.1532	-751.82	233.7	349.2
Trial 3	1.7726	-619.22	283.9	349.3
Average			270	349.2

9. Cartesian coordinates and energies (in Hartree) for species calculated

Figure S2. Structures for species calculated





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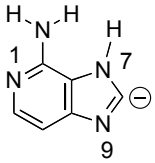

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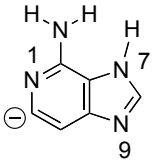

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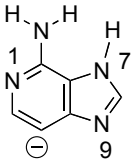

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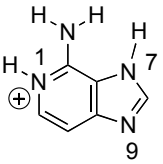

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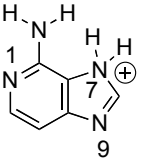

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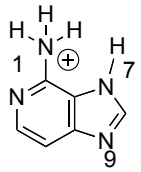

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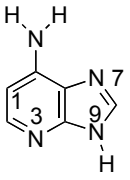
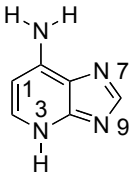


Z1-1



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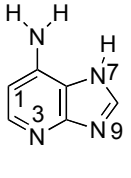

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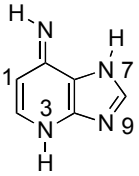

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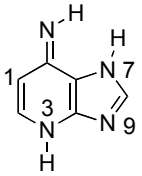

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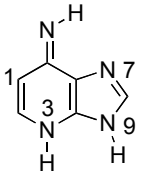

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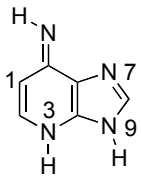

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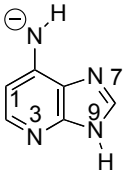

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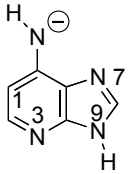

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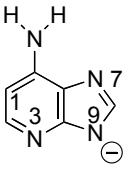

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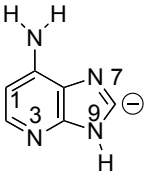

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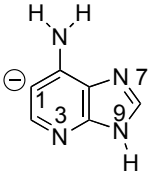

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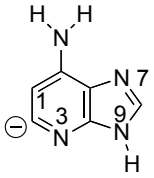

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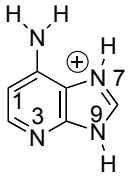

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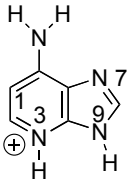

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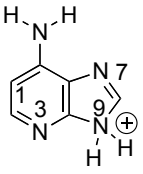

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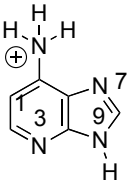

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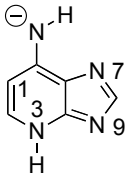

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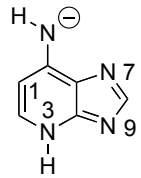

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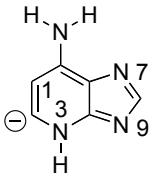

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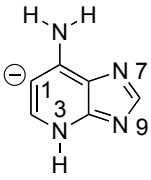

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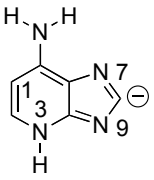

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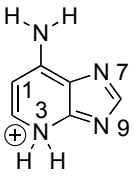

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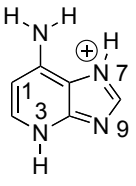

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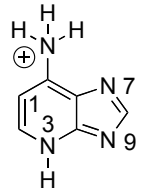

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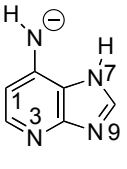

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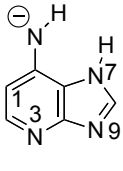

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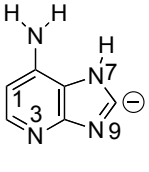

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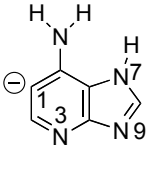

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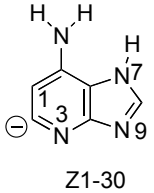

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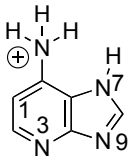

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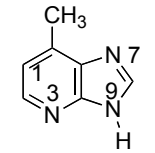

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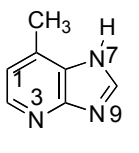

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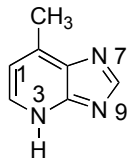

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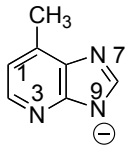

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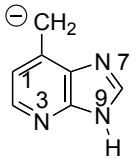

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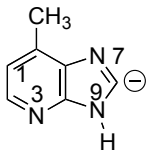

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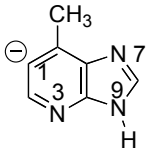

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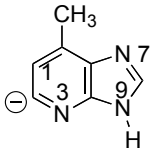

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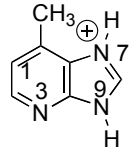

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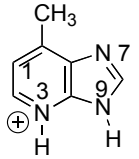

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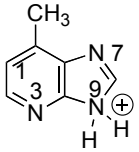

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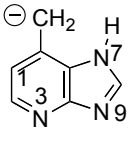

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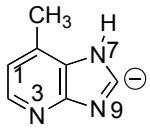

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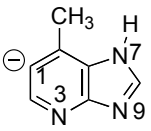

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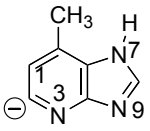

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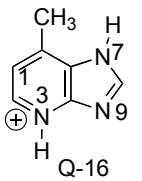

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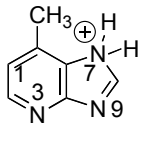

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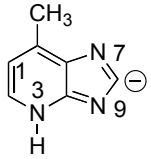

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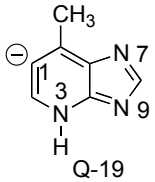

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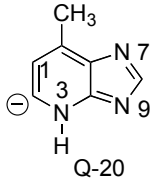

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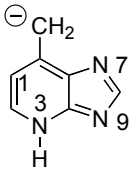

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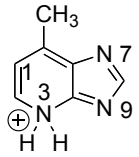

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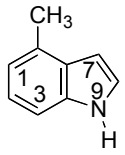

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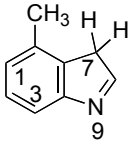

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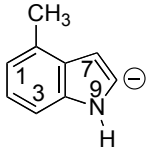

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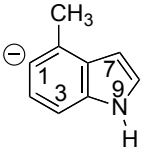

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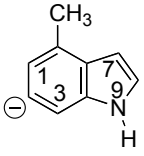

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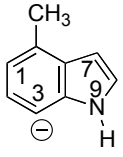

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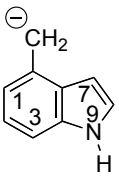

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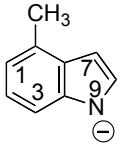

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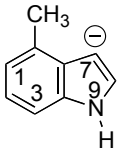

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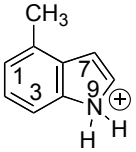

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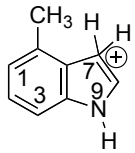

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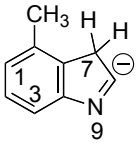

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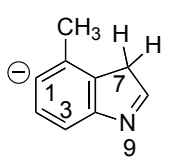

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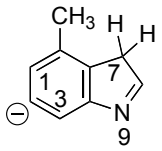

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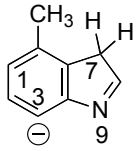

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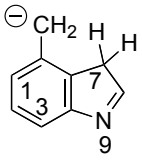

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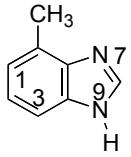

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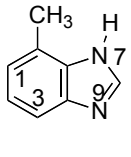
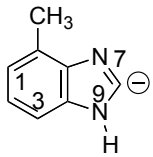


B-2



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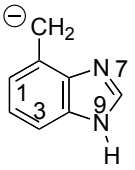

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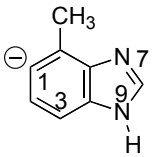

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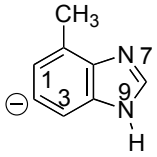
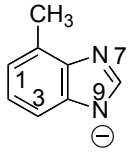
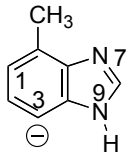


B-6



B-7



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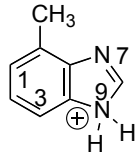

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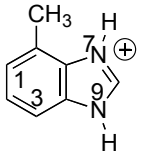
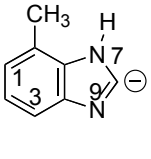


B-10



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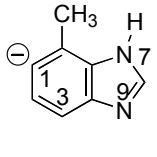

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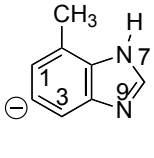

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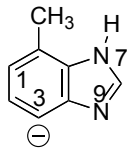
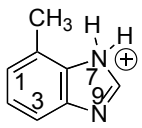


B-14

B-15



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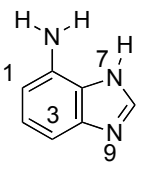
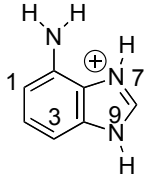
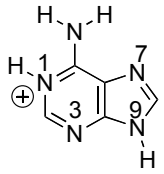


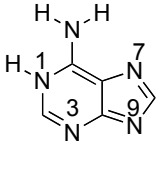
Z13-1



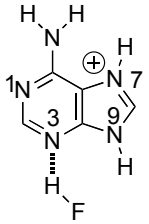
Z13-2



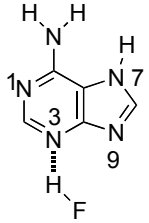
A-1



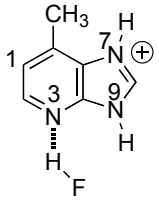
A-2



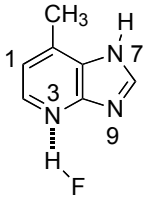
A-N3HF-1



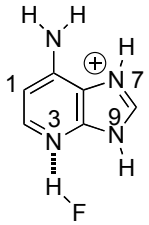
A-N3HF-2



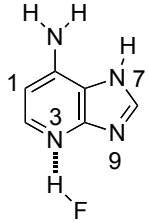
Q-N3HF-1



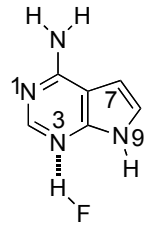
Q-N3HF-2



Z1-N3HF-1



Z1-N3HF-2



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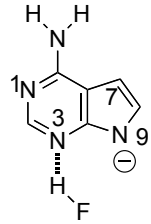

Z-N3HF-2

Note: *Structure numbers in the section below correlate to structures shown on pages S19-S22 of SI, not to structures in the paper.*

Z (7-deazaadenine): neutral, protonated and deprotonated species

Amino N9H Z (Z-1) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.290219726     A.U.

Zero-point correction=                           0.123731
(Hartree/Particle)
 Thermal correction to Energy=                   0.131087
 Thermal correction to Enthalpy=                 0.132031
 Thermal correction to Gibbs Free Energy=        0.092037
 Sum of electronic and zero-point Energies=          -451.166489
 Sum of electronic and thermal Energies=             -451.159133
 Sum of electronic and thermal Enthalpies=           -451.158189
 Sum of electronic and thermal Free Energies=        -451.198183

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  82.258             29.915            84.175
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        0.162259    0.548532   -0.006252
    2          6             0        0.699802   -0.758058    0.004302
    3          6             0       -1.310938   -1.702866   -0.002393
    4          6             0       -1.250566    0.603028   -0.005181
    5          6             0        1.268115    1.466120   -0.010426
    6          6             0        2.409467    0.702070   -0.000596
    7          1             0       -1.937185   -2.591843   -0.003426
    8          1             0        1.238549    2.547409   -0.029543
    9          1             0        3.447643    1.003173   -0.002830
   10          7             0       -1.969353   -0.529419   -0.002996
   11          7             0        0.005674   -1.905886    0.005102
   12          7             0       -1.944807    1.785442   -0.049547
   13          1             0       -2.934760    1.718991    0.151123
   14          1             0       -1.486259    2.630870    0.259575
   15          7             0        2.065722   -0.641053    0.009709
   16          1             0        2.702533   -1.425146    0.012500
 -------------------------------------------------------------------
```

N1H-N9H-imino_N7side Z (Z-2) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.273176261     A.U.
Zero-point correction=                           0.124050
(Hartree/Particle)
 Thermal correction to Energy=                   0.131188
 Thermal correction to Enthalpy=                 0.132133
 Thermal correction to Gibbs Free Energy=        0.092384
 Sum of electronic and zero-point Energies=          -451.149126
 Sum of electronic and thermal Energies=             -451.141988
 Sum of electronic and thermal Enthalpies=           -451.141044
```

```
 Sum of electronic and thermal Free Energies=         -451.180793

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  82.322             29.081             83.658
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.214357    0.575425   -0.000185
    2          6             0        0.640139   -0.758074   -0.000055
    3          6             0       -1.407678   -1.622155   -0.000141
    4          6             0       -1.209360    0.843587   -0.000027
    5          6             0        1.384282    1.394643   -0.000264
    6          6             0        2.468012    0.543536    0.000049
    7          1             0       -2.125067   -2.438531    0.000510
    8          1             0        1.432329    2.475369   -0.000143
    9          1             0        3.527289    0.756407    0.000350
   10          7             0       -1.943661   -0.367076   -0.000099
   11          7             0       -0.133362   -1.887585    0.000046
   12          7             0       -1.890488    1.936697    0.000235
   13          7             0        2.007149   -0.761182    0.000153
   14          1             0        2.572383   -1.598720    0.000295
   15          1             0       -1.271495    2.747603    0.000363
   16          1             0       -2.951419   -0.249877    0.000021
 ---------------------------------------------------------------------
```

Amino N3H Z (Z-3) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.271763751     A.U.

Zero-point correction=                           0.123374
(Hartree/Particle)
 Thermal correction to Energy=                   0.130825
 Thermal correction to Enthalpy=                 0.131769
 Thermal correction to Gibbs Free Energy=        0.091543
 Sum of electronic and zero-point Energies=          -451.148390
 Sum of electronic and thermal Energies=             -451.140939
 Sum of electronic and thermal Enthalpies=           -451.139994
 Sum of electronic and thermal Free Energies=        -451.180221

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  82.094             30.034             84.663
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.211947   -0.581834   -0.004782
    2          6             0       -0.794053    0.730173    0.001939
    3          6             0        1.382511    1.635521   -0.000746
    4          6             0        1.185709   -0.665808   -0.004330
    5          6             0       -1.344047   -1.450913   -0.004697
    6          6             0       -2.444585   -0.600602    0.001331
    7          1             0        1.998369    2.529664    0.002090
    8          1             0       -1.358662   -2.533465   -0.016381
```

9	1	0	-3.489629	-0.889348	0.001342
10	7	0	1.964548	0.458909	-0.001328
11	7	0	0.043374	1.822692	0.002293
12	7	0	1.867988	-1.844497	-0.037403
13	1	0	2.864745	-1.814185	0.128078
14	1	0	1.385949	-2.708434	0.162152
15	7	0	-2.116503	0.743146	0.005578
16	1	0	-0.358150	2.754794	0.006443

Amino C7H Z (Z-4) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.267779609 A.U.

Zero-point correction= 0.122450
(Hartree/Particle)
Thermal correction to Energy= 0.129846
Thermal correction to Enthalpy= 0.130790
Thermal correction to Gibbs Free Energy= 0.090595
Sum of electronic and zero-point Energies= -451.145330
Sum of electronic and thermal Energies= -451.137933
Sum of electronic and thermal Enthalpies= -451.136989
Sum of electronic and thermal Free Energies= -451.177185

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	81.480	29.480	84.599

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.176703	0.494695	-0.002446
2	6	0	0.683198	-0.808934	-0.005987
3	6	0	-1.374408	-1.667075	0.001049
4	6	0	-1.216000	0.626324	0.002510
5	6	0	1.348887	1.429497	0.007847
6	6	0	2.476191	0.411433	0.002370
7	7	0	-1.988938	-0.480798	0.002206
8	7	0	-0.057519	-1.917299	-0.004441
9	7	0	-1.866784	1.834618	0.054756
10	7	0	2.107533	-0.822249	-0.005983
11	1	0	3.529829	0.682792	0.004407
12	1	0	1.413395	2.091864	-0.869066
13	1	0	-2.028601	-2.536073	0.001709
14	1	0	-1.382504	2.665757	-0.253991
15	1	0	-2.860228	1.804966	-0.138458
16	1	0	1.400641	2.075151	0.897568

N1H-N9H-imino_N1side Z (Z-5) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.267779676 A.U.

Zero-point correction= 0.123644
(Hartree/Particle)
Thermal correction to Energy= 0.130843

```
 Thermal correction to Enthalpy=                  0.131787
 Thermal correction to Gibbs Free Energy=         0.091957
 Sum of electronic and zero-point Energies=           -451.144135
 Sum of electronic and thermal Energies=              -451.136937
 Sum of electronic and thermal Enthalpies=            -451.135993
 Sum of electronic and thermal Free Energies=         -451.175822

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  82.105             29.341             83.828
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
-------------------------------------------------------------------
    1          6             0        0.212203    0.575591   -0.000060
    2          6             0        0.655128   -0.750414   -0.000021
    3          6             0       -1.380487   -1.643472    0.000011
    4          6             0       -1.209082    0.839521   -0.000019
    5          6             0        1.365416    1.412914   -0.000067
    6          6             0        2.462019    0.578046    0.000025
    7          1             0       -2.089405   -2.467655    0.000108
    8          1             0        1.376611    2.493390   -0.000036
    9          1             0        3.518350    0.805693    0.000085
   10          7             0       -1.937057   -0.387028   -0.000015
   11          7             0       -0.106399   -1.889863   -0.000031
   12          7             0       -1.739666    2.012048    0.000062
   13          7             0        2.022223   -0.735173    0.000041
   14          1             0        2.600221   -1.563605    0.000157
   15          1             0       -2.948212   -0.320657   -0.000026
   16          1             0       -2.762453    1.979829    0.000100
-------------------------------------------------------------------
```

Amino N1H Z (Z-6) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.253289134     A.U.

Zero-point correction=                           0.122834
(Hartree/Particle)
 Thermal correction to Energy=                   0.130352
 Thermal correction to Enthalpy=                 0.131296
 Thermal correction to Gibbs Free Energy=        0.090932
 Sum of electronic and zero-point Energies=           -451.130455
 Sum of electronic and thermal Energies=              -451.122937
 Sum of electronic and thermal Enthalpies=            -451.121993
 Sum of electronic and thermal Free Energies=         -451.162357

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  81.797             30.249             84.954
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
-------------------------------------------------------------------
    1          6             0        0.234758    0.557444   -0.013796
    2          6             0        0.803282   -0.791736   -0.004720
    3          6             0       -1.248029   -1.739006    0.003050
```

4	6	0	-1.139300	0.678971	-0.005310
5	6	0	1.358183	1.430749	-0.002198
6	6	0	2.454160	0.574317	0.006832
7	1	0	-1.934334	-2.580752	0.007345
8	1	0	1.375817	2.513899	-0.012379
9	1	0	3.498532	0.868227	0.011641
10	7	0	-1.857349	-0.490572	-0.002694
11	7	0	0.032738	-1.922136	0.006605
12	7	0	-1.854924	1.860117	-0.065225
13	1	0	-2.723726	1.900616	0.457124
14	1	0	-1.292158	2.691137	0.071095
15	7	0	2.131543	-0.762599	0.010428
16	1	0	-2.866511	-0.451224	-0.081783

Amino N1H Z (Z-6) B3LYP/6-31+G(d) cpcm in water, RADII=UAKS

Total free energy in solution:		
with all non electrostatic terms	(a.u.) =	-451.297065
(Polarized solute)-Solvent	(kcal/mol) =	-38.87
Cavitation energy	(kcal/mol) =	16.77
Dispersion energy	(kcal/mol) =	-20.87
Repulsion energy	(kcal/mol) =	4.86
Total non electrostatic	(kcal/mol) =	0.76

N3H-N9H-imino_N1side Z (Z-7) B3LYP/6-31+G(d)

Zero-point correction=	0.122520
(Hartree/Particle)	
Thermal correction to Energy=	0.130346
Thermal correction to Enthalpy=	0.131291
Thermal correction to Gibbs Free Energy=	0.090092
Sum of electronic and zero-point Energies=	-451.126130
Sum of electronic and thermal Energies=	-451.118304
Sum of electronic and thermal Enthalpies=	-451.117360
Sum of electronic and thermal Free Energies=	-451.158558

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	81.794	30.530	86.709

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.200085	0.580385	0.000366
2	6	0	0.652107	-0.726882	0.000303
3	6	0	-1.563623	-1.498074	-0.000018
4	6	0	-1.235504	0.842082	0.000074
5	6	0	1.364781	1.412297	0.000165
6	6	0	2.460771	0.585455	-0.000133
7	1	0	-2.220540	-2.366736	0.000592
8	1	0	1.370114	2.492703	0.000174
9	1	0	3.518818	0.802903	-0.000384
10	7	0	-2.069784	-0.314752	0.000007

11	7	0	-0.215741	-1.802109	-0.000253
12	7	0	-1.718356	2.033673	-0.000230
13	1	0	-2.740725	1.977696	-0.000436
14	7	0	2.017027	-0.739789	-0.000158
15	1	0	2.613339	-1.553849	-0.000090
16	1	0	0.095266	-2.763453	0.000049

N3H-N9H-imino_N7side Z (Z-8) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.242019836 A.U.

Zero-point correction= 0.122271
(Hartree/Particle)
Thermal correction to Energy= 0.130133
Thermal correction to Enthalpy= 0.131077
Thermal correction to Gibbs Free Energy= 0.089686
Sum of electronic and zero-point Energies= -451.119749
Sum of electronic and thermal Energies= -451.111887
Sum of electronic and thermal Enthalpies= -451.110943
Sum of electronic and thermal Free Energies= -451.152334

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	81.660	30.581	87.115

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.195555	0.571955	-0.000095
2	6	0	0.629111	-0.743314	0.000011
3	6	0	-1.598628	-1.473992	0.000015
4	6	0	-1.244214	0.856300	-0.000016
5	6	0	1.379652	1.381438	-0.000088
6	6	0	2.461545	0.536244	0.000004
7	1	0	-2.268023	-2.333112	0.000168
8	1	0	1.426906	2.462092	-0.000207
9	1	0	3.522724	0.736946	0.000113
10	7	0	-2.085951	-0.286908	-0.000056
11	7	0	-0.251505	-1.803595	-0.000195
12	7	0	-1.817548	2.009682	0.000121
13	7	0	1.993498	-0.778315	0.000176
14	1	0	2.575414	-1.603108	-0.000345
15	1	0	0.044708	-2.769604	0.000797
16	1	0	-1.109308	2.748949	0.000168

N10-deprotonated N9H-amino(N10H_N1side) Z (Z-9) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.717281219 A.U.

Zero-point correction= 0.109693
(Hartree/Particle)
Thermal correction to Energy= 0.116844
Thermal correction to Enthalpy= 0.117789
Thermal correction to Gibbs Free Energy= 0.077964

```
 Sum of electronic and zero-point Energies=           -450.607589
 Sum of electronic and thermal Energies=              -450.600437
 Sum of electronic and thermal Enthalpies=            -450.599493
 Sum of electronic and thermal Free Energies=         -450.639317

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.321             28.445             83.817
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        0.168005    0.563154    0.000068
    2          6             0        0.632034   -0.758279   -0.000077
    3          6             0       -1.426638   -1.585280   -0.000209
    4          6             0       -1.270017    0.770541    0.000068
    5          6             0        1.315973    1.418260    0.000187
    6          6             0        2.433550    0.609886    0.000112
    7          7             0       -2.035604   -0.404002   -0.000082
    8          7             0       -0.113923   -1.890089   -0.000222
    9          7             0       -1.802804    1.967964    0.000200
   10          7             0        2.010571   -0.718706   -0.000049
   11          1             0        2.595461   -1.540306   -0.000136
   12          1             0        3.487624    0.854626    0.000158
   13          1             0        1.306923    2.500454    0.000311
   14          1             0       -2.094408   -2.451822   -0.000321
   15          1             0       -2.820726    1.841194    0.000168
 -------------------------------------------------------------------
```

N10-deprotonated N9H-amino (N10H_N7side) Z (Z-10) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -450.710594177     A.U.

Zero-point correction=                           0.109373
(Hartree/Particle)
 Thermal correction to Energy=                   0.116553
 Thermal correction to Enthalpy=                 0.117497
 Thermal correction to Gibbs Free Energy=        0.077592
 Sum of electronic and zero-point Energies=           -450.601221
 Sum of electronic and thermal Energies=              -450.594041
 Sum of electronic and thermal Enthalpies=            -450.593097
 Sum of electronic and thermal Free Energies=         -450.633002

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.138             28.580             83.988


-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.160119    0.551738   -0.000231
    2          6             0       -0.606125   -0.777558   -0.000251
    3          6             0        1.465997   -1.563863    0.000138
    4          6             0        1.282197    0.782424   -0.000007
```

5	6	0	-1.326627	1.386155	-0.000022
6	6	0	-2.431338	0.559803	0.000413
7	7	0	2.057277	-0.378258	0.000059
8	7	0	0.154908	-1.894271	0.000032
9	7	0	1.881641	1.951787	0.000073
10	7	0	-1.986113	-0.759191	-0.000211
11	1	0	-2.557350	-1.590773	0.000779
12	1	0	-3.488641	0.789244	-0.000316
13	1	0	-1.357083	2.469768	-0.000084
14	1	0	2.145447	-2.421078	-0.000124
15	1	0	1.159724	2.680168	-0.000159

N9-deprotonated N9H-amino Z (Z-11) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.731170139 A.U.

Zero-point correction= 0.110010
(Hartree/Particle)
Thermal correction to Energy= 0.117025
Thermal correction to Enthalpy= 0.117969
Thermal correction to Gibbs Free Energy= 0.078514
Sum of electronic and zero-point Energies= -450.621160
Sum of electronic and thermal Energies= -450.614146
Sum of electronic and thermal Enthalpies= -450.613201
Sum of electronic and thermal Free Energies= -450.652656

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.434	28.260	83.038

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.198704	0.537330	-0.023828
2	6	0	0.777831	-0.786546	0.003853
3	6	0	-1.292453	-1.692385	-0.001948
4	6	0	-1.200505	0.602651	-0.019546
5	6	0	1.306494	1.434933	-0.021147
6	6	0	2.425512	0.593709	0.006514
7	1	0	-1.936824	-2.572945	0.001696
8	1	0	1.301898	2.519860	-0.061263
9	1	0	3.466642	0.912062	0.011784
10	7	0	-1.952908	-0.505416	-0.007163
11	7	0	0.013094	-1.913708	0.009278
12	7	0	-1.889920	1.830004	-0.065656
13	1	0	-2.843040	1.730091	0.270702
14	1	0	-1.398009	2.584152	0.402466
15	7	0	2.131996	-0.741076	0.022287

C8-deprotonated N9H-amino Z (Z-12) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -450.676087841
Zero-point correction= 0.110114
(Hartree/Particle)

```
 Thermal correction to Energy=                    0.117285
 Thermal correction to Enthalpy=                  0.118230
 Thermal correction to Gibbs Free Energy=         0.078533
 Sum of electronic and zero-point Energies=           -450.565974
 Sum of electronic and thermal Energies=              -450.558802
 Sum of electronic and thermal Enthalpies=            -450.557858
 Sum of electronic and thermal Free Energies=         -450.597555

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.598             28.960             83.548

-------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 -------------------------------------------------------------------
      1          6           0       -0.188929   -0.569326   -0.025349
      2          6           0       -0.768222    0.732476   -0.002014
      3          6           0        1.235275    1.732055    0.000596
      4          6           0        1.214480   -0.569223   -0.019064
      5          6           0       -1.284973   -1.497414   -0.017162
      6          6           0       -2.518107   -0.817414    0.009903
      7          1           0        1.837478    2.640187    0.007338
      8          1           0       -1.194571   -2.580155   -0.048052
      9          7           0        1.924320    0.573867   -0.003660
     10          7           0       -0.090884    1.895093    0.005469
     11          7           0        1.950448   -1.762618   -0.065567
     12          1           0        2.893882   -1.643905    0.288808
     13          1           0        1.471309   -2.551778    0.354693
     14          7           0       -2.122182    0.544532    0.018174
     15          1           0       -2.777158    1.312608    0.034853
 -------------------------------------------------------------------
```

C7-deprotonated N9H-amino Z (Z-13)

```
SCF Done:  E(RB3LYP) =  -450.665067114

Zero-point correction=                           0.109555
(Hartree/Particle)
 Thermal correction to Energy=                    0.116885
 Thermal correction to Enthalpy=                  0.117829
 Thermal correction to Gibbs Free Energy=         0.077866
 Sum of electronic and zero-point Energies=           -450.555512
 Sum of electronic and thermal Energies=              -450.548182
 Sum of electronic and thermal Enthalpies=            -450.547238
 Sum of electronic and thermal Free Energies=         -450.587202

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.346             29.393             84.110

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

1	6	0	-0.188718	-0.568973	-0.019937
2	6	0	-0.730148	0.745726	-0.017768
3	6	0	1.288504	1.695848	0.015191
4	6	0	1.216833	-0.603222	-0.017916
5	6	0	-1.218523	-1.598415	0.010673
6	6	0	-2.354660	-0.812977	0.018684
7	7	0	1.957637	0.524970	0.012534
8	7	0	-0.030349	1.902442	-0.005765
9	7	0	1.880327	-1.817629	-0.078116
10	1	0	2.800591	-1.824742	0.343652
11	1	0	1.275940	-2.600290	0.158258
12	7	0	-2.082150	0.593852	-0.006015
13	1	0	-2.742450	1.359017	0.025185
14	1	0	-3.404849	-1.097137	0.042784
15	1	0	1.912784	2.589783	0.038096

C2-deprotonated N9H-amino Z (Z-14) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -450.636115223
Zero-point correction=                           0.107756
(Hartree/Particle)
 Thermal correction to Energy=                    0.115399
 Thermal correction to Enthalpy=                  0.116343
 Thermal correction to Gibbs Free Energy=         0.075728
 Sum of electronic and zero-point Energies=           -450.528359
 Sum of electronic and thermal Energies=              -450.520716
 Sum of electronic and thermal Enthalpies=            -450.519772
 Sum of electronic and thermal Free Energies=         -450.560387

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.414             30.416             85.481
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.120849	-0.535323	-0.020679
2	6	0	-0.691534	0.756977	0.009298
3	6	0	1.328630	1.907194	-0.009346
4	6	0	1.290377	-0.504993	-0.018306
5	6	0	-1.196279	-1.494150	-0.029719
6	6	0	-2.369967	-0.774091	-0.002309
7	1	0	-1.126458	-2.575188	-0.069801
8	7	0	1.957006	0.640405	-0.013956
9	7	0	-0.055627	1.928865	0.015567
10	7	0	2.043609	-1.700439	-0.060554
11	1	0	3.008359	-1.497306	0.191067
12	1	0	1.658777	-2.448027	0.510519
13	7	0	-2.068263	0.581353	0.025696
14	1	0	-2.722398	1.349965	0.032163
15	1	0	-3.397612	-1.114423	-0.004844

N1-protonated N9H-amino Z (Z-15) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.665297307     A.U.

Zero-point correction=                           0.137046
(Hartree/Particle)
 Thermal correction to Energy=                   0.144645
 Thermal correction to Enthalpy=                 0.145589
 Thermal correction to Gibbs Free Energy=        0.105170
 Sum of electronic and zero-point Energies=          -451.528252
 Sum of electronic and thermal Energies=             -451.520653
 Sum of electronic and thermal Enthalpies=           -451.519708
 Sum of electronic and thermal Free Energies=        -451.560127

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.766             31.085            85.068
 ------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ------------------------------------------------------------------------
    1          6             0       -0.203543    0.561704   -0.000282
    2          6             0       -0.723140   -0.759554   -0.000050
    3          6             0        1.271299   -1.747034   -0.000078
    4          6             0        1.197208    0.678150   -0.000682
    5          6             0       -1.317826    1.459615   -0.000300
    6          6             0       -2.442495    0.671323    0.000180
    7          1             0        1.941750   -2.600010    0.000656
    8          1             0       -1.311225    2.540683   -0.000709
    9          1             0       -3.485860    0.953098   -0.000083
   10          7             0        1.885449   -0.507205   -0.000191
   11          7             0       -0.015053   -1.910580    0.000036
   12          7             0        1.875590    1.834615    0.000637
   13          1             0        2.886216    1.884506    0.000554
   14          7             0       -2.073956   -0.663782    0.000334
   15          1             0       -2.704376   -1.457621    0.000455
   16          1             0        1.378977    2.715504    0.000404
   17          1             0        2.901290   -0.492722    0.000278
 ------------------------------------------------------------------------
```

N1-protonated N9H-amino Z (Z-15) B3LYP/6-31+G(d) cpcm, water, RADII=UAKS

```
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -451.770294
 ------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -70.49
 ------------------------------------------------------------------
 Cavitation energy                         (kcal/mol) =      16.98
 Dispersion energy                         (kcal/mol) =     -21.38
 Repulsion energy                          (kcal/mol) =       5.16
 Total non electrostatic                   (kcal/mol) =       0.76
```

N3-protonated N9H-amino Z (Z-16) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.663618885 A.U.

Zero-point correction= (Hartree/Particle)	0.137233
Thermal correction to Energy=	0.144725
Thermal correction to Enthalpy=	0.145670
Thermal correction to Gibbs Free Energy=	0.105396
Sum of electronic and zero-point Energies=	-451.526386
Sum of electronic and thermal Energies=	-451.518893
Sum of electronic and thermal Enthalpies=	-451.517949
Sum of electronic and thermal Free Energies=	-451.558223

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.817	30.883	84.762

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.188044	-0.571328	0.000035
2	6	0	0.720642	0.727831	-0.000112
3	6	0	-1.435265	1.626790	0.000162
4	6	0	-1.229233	-0.675437	-0.000035
5	6	0	1.307521	-1.470036	0.000135
6	6	0	2.435467	-0.695540	0.000076
7	1	0	-2.054116	2.518961	0.000243
8	1	0	1.289718	-2.550730	0.000287
9	1	0	3.479603	-0.973047	0.000130
10	7	0	-2.000368	0.452769	0.000066
11	7	0	-0.087104	1.830723	0.000094
12	7	0	-1.887612	-1.835100	-0.000358
13	1	0	-2.901355	-1.826347	0.000597
14	1	0	-1.414761	-2.728539	0.000495
15	7	0	2.071081	0.652088	-0.000190
16	1	0	2.723806	1.425880	0.000286
17	1	0	0.282077	2.776766	-0.000893

N9-protonated N9H-amino Z (Z-17) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.605986624 A.U.

Zero-point correction= (Hartree/Particle)	0.136660
Thermal correction to Energy=	0.144261
Thermal correction to Enthalpy=	0.145205
Thermal correction to Gibbs Free Energy=	0.104625
Sum of electronic and zero-point Energies=	-451.469326
Sum of electronic and thermal Energies=	-451.461726
Sum of electronic and thermal Enthalpies=	-451.460782
Sum of electronic and thermal Free Energies=	-451.501362

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

Total	90.525	30.639	85.409

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.118124	0.553511	-0.000003
2	6	0	0.617671	-0.737477	-0.000048
3	6	0	-1.352141	-1.706413	0.000024
4	6	0	-1.304423	0.612641	-0.000047
5	6	0	1.238698	1.489421	-0.000114
6	6	0	2.401092	0.816156	-0.000062
7	1	0	-1.954540	-2.609602	0.000013
8	1	0	1.175387	2.571168	-0.000102
9	1	0	3.433404	1.134524	-0.000233
10	7	0	-1.998497	-0.551959	0.000006
11	7	0	-0.003289	-1.883790	-0.000133
12	7	0	-2.018183	1.748508	0.000090
13	1	0	-3.029435	1.683147	-0.000120
14	1	0	-1.598583	2.666856	0.000251
15	7	0	2.113869	-0.648834	0.000156
16	1	0	2.501391	-1.130591	-0.824816
17	1	0	2.500941	-1.130003	0.825677

C7-protonated N9H-amino Z (Z-18) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.626685996 A.U. after
Zero-point correction= 0.135424
(Hartree/Particle)
Thermal correction to Energy= 0.143056
Thermal correction to Enthalpy= 0.144000
Thermal correction to Gibbs Free Energy= 0.103352
Sum of electronic and zero-point Energies= -451.491262
Sum of electronic and thermal Energies= -451.483630
Sum of electronic and thermal Enthalpies= -451.482686
Sum of electronic and thermal Free Energies= -451.523334

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.769	30.535	85.550

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.137519	0.526202	0.000464
2	6	0	-0.616116	-0.773738	0.000258
3	6	0	1.377964	-1.694962	-0.000082
4	6	0	1.276233	0.623890	0.000056
5	6	0	-1.307226	1.470719	0.000119
6	6	0	-2.468830	0.528701	-0.000312
7	1	0	2.008739	-2.578812	-0.000270
8	1	0	-1.372633	2.133258	0.879145
9	1	0	-3.524439	0.780703	-0.000521
10	7	0	1.999055	-0.520790	-0.000284

11	7	0	0.043406	-1.910587	0.000257
12	7	0	1.961121	1.781659	-0.000030
13	1	0	2.973474	1.742470	-0.000674
14	1	0	1.518337	2.688631	0.000172
15	7	0	-2.051770	-0.700237	-0.000125
16	1	0	-2.641123	-1.534630	-0.000579
17	1	0	-1.372067	2.133192	-0.879018

N10-protonated N9H-amino Z (Z-19) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.628824677 A.U.

Zero-point correction= 0.137918
(Hartree/Particle)
Thermal correction to Energy= 0.145482
Thermal correction to Enthalpy= 0.146426
Thermal correction to Gibbs Free Energy= 0.105672
Sum of electronic and zero-point Energies= -451.490906
Sum of electronic and thermal Energies= -451.483343
Sum of electronic and thermal Enthalpies= -451.482398
Sum of electronic and thermal Free Energies= -451.523152

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.291	29.780	85.774

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.166901	-0.560248	-0.000221
2	6	0	-0.797393	0.733207	-0.000119
3	6	0	1.153424	1.835831	0.000051
4	6	0	1.214807	-0.437231	-0.000441
5	6	0	-1.208275	-1.542161	-0.000229
6	6	0	-2.390665	-0.839247	0.000175
7	1	0	1.710488	2.766201	0.000417
8	1	0	-1.123335	-2.620177	-0.000394
9	1	0	-3.406203	-1.210721	0.000229
10	7	0	1.881287	0.695141	-0.000046
11	7	0	-0.175787	1.906313	-0.000050
12	7	0	2.118656	-1.635122	0.000292
13	1	0	3.085513	-1.274884	-0.000715
14	1	0	1.990882	-2.225510	0.833352
15	7	0	-2.143671	0.518937	0.000173
16	1	0	-2.840453	1.254654	0.000527
17	1	0	1.989735	-2.227353	-0.831287

Z3 (3-deazaadenine): neutral, protonated and deprotonated species

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

SCF Done: E(RB+HF-LYP) = -451.289796555 A.U.

Zero-point correction= 0.123581
(Hartree/Particle)
Thermal correction to Energy= 0.130930
Thermal correction to Enthalpy= 0.131874
Thermal correction to Gibbs Free Energy= 0.091929
Sum of electronic and zero-point Energies= -451.166215
Sum of electronic and thermal Energies= -451.158866
Sum of electronic and thermal Enthalpies= -451.157922
Sum of electronic and thermal Free Energies= -451.197868

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.160	29.932	84.073

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.203219	-0.488326	-0.006298
2	6	0	-0.732119	0.811630	-0.005261
3	6	0	1.460988	1.654532	0.007115
4	6	0	1.202881	-0.649684	-0.006143
5	6	0	-2.319963	-0.744834	0.006128
6	1	0	2.180091	2.471110	0.015376
7	7	0	1.767717	-1.898592	-0.061705
8	1	0	2.747068	-1.958219	0.183693
9	1	0	1.185229	-2.687752	0.184048
10	7	0	2.006894	0.417842	0.008404
11	7	0	-1.212273	-1.441761	0.003241
12	7	0	-2.100603	0.619508	-0.000189
13	6	0	0.100599	1.942066	-0.002692
14	1	0	-2.811611	1.337168	0.001628
15	1	0	-3.321070	-1.156596	0.013341
16	1	0	-0.266859	2.963014	-0.003421

Amino N7H Z3 (Z3-2) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.283481399 A.U.

Zero-point correction= 0.123643
(Hartree/Particle)
Thermal correction to Energy= 0.130995
Thermal correction to Enthalpy= 0.131939
Thermal correction to Gibbs Free Energy= 0.091921
Sum of electronic and zero-point Energies= -451.159839
Sum of electronic and thermal Energies= -451.152487
Sum of electronic and thermal Enthalpies= -451.151542
Sum of electronic and thermal Free Energies= -451.191561

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.201	29.658	84.226

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.202522	-0.459476	-0.000304
2	6	0	-0.756897	0.833905	0.025304
3	6	0	1.463869	1.656458	-0.017563
4	6	0	1.190788	-0.648863	-0.001436
5	6	0	-2.411888	-0.521179	-0.015209
6	1	0	2.192580	2.463303	-0.037453
7	7	0	1.766102	-1.922663	-0.056489
8	1	0	2.774695	-1.875061	0.055316
9	1	0	1.359657	-2.609992	0.570214
10	7	0	1.996431	0.409593	-0.017591
11	7	0	-1.293107	-1.319314	-0.017530
12	7	0	-2.143126	0.761732	0.021517
13	6	0	0.107009	1.942921	0.018685
14	1	0	-3.407519	-0.946724	-0.037215
15	1	0	-0.266198	2.961210	0.031615
16	1	0	-1.279471	-2.320769	-0.148687

Amino N1H Z3 (Z3-3) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.271638149 A.U.

Zero-point correction= 0.123841
(Hartree/Particle)
Thermal correction to Energy= 0.131203
Thermal correction to Enthalpy= 0.132147
Thermal correction to Gibbs Free Energy= 0.092109
Sum of electronic and zero-point Energies= -451.147797
Sum of electronic and thermal Energies= -451.140435
Sum of electronic and thermal Enthalpies= -451.139491
Sum of electronic and thermal Free Energies= -451.179529

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.331	29.683	84.268

1	6	0	-0.278751	-0.500829	-0.011945
2	6	0	-0.819817	0.829014	-0.009452
3	6	0	1.401578	1.692405	0.006788
4	6	0	1.090598	-0.716917	-0.005059
5	6	0	-2.374110	-0.607273	0.008794
6	1	0	2.162399	2.462833	0.016584
7	7	0	1.672909	-1.964554	-0.070381
8	1	0	2.501896	-2.123810	0.491893
9	1	0	0.988278	-2.709354	0.022938
10	7	0	1.887724	0.392169	-0.002648
11	7	0	-1.299420	-1.410516	0.003246
12	7	0	-2.163121	0.740902	0.005491
13	6	0	0.057568	1.945198	0.004171
14	1	0	-3.380534	-1.011765	0.017657
15	1	0	-0.309938	2.965697	0.016990
16	1	0	2.888856	0.260807	-0.075814

Amino N1H Z3 (Z3-3) B3LYP/6-31+G(d) cpcm, water, RADII=UAKS

```
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -451.309521
 ------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -31.98
 ------------------------------------------------------------------
 Cavitation energy                         (kcal/mol) =      16.89
 Dispersion energy                         (kcal/mol) =     -20.65
 Repulsion energy                          (kcal/mol) =       4.66
 Total non electrostatic                   (kcal/mol) =       0.91
```

Imino (H taward N7) N1H N9H Z3 (Z3-4) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.270111768     A.U.

Zero-point correction=                           0.123866
(Hartree/Particle)
 Thermal correction to Energy=                   0.131059
 Thermal correction to Enthalpy=                 0.132003
 Thermal correction to Gibbs Free Energy=        0.092164
 Sum of electronic and zero-point Energies=          -451.146246
 Sum of electronic and thermal Energies=             -451.139053
 Sum of electronic and thermal Enthalpies=           -451.138108
 Sum of electronic and thermal Free Energies=        -451.177948

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  82.241             29.240            83.850
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.260721   -0.520491   -0.000092
    2          6             0       -0.667512    0.811241    0.000156
    3          6             0        1.563291    1.560987   -0.000208
    4          6             0        1.144578   -0.888625   -0.000030
    5          6             0       -2.392640   -0.583280   -0.000165
    6          1             0        2.360203    2.296350   -0.000141
    7          7             0        1.709464   -2.045261    0.000321
    8          7             0        1.973672    0.253117   -0.000357
    9          7             0       -1.344136   -1.372065   -0.000068
   10          7             0       -2.043708    0.751903   -0.000049
   11          6             0        0.243578    1.911305    0.000428
   12          1             0       -3.425713   -0.904301   -0.000096
   13          1             0       -0.064701    2.949633    0.000775
   14          1             0        2.964153    0.038530   -0.000507
   15          1             0       -2.681733    1.535842   -0.000126
   16          1             0        0.997309   -2.776730    0.000628
 -------------------------------------------------------------------
```

Imino (H taward N1) N1H N7H Z3 (Z3-5) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.269314720     A.U.
```

Zero-point correction= 0.123714
(Hartree/Particle)
Thermal correction to Energy= 0.130901
Thermal correction to Enthalpy= 0.131845
Thermal correction to Gibbs Free Energy= 0.092060
Sum of electronic and zero-point Energies= -451.145601
Sum of electronic and thermal Energies= -451.138414
Sum of electronic and thermal Enthalpies= -451.137470
Sum of electronic and thermal Free Energies= -451.177254

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.141	29.295	83.734

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.255658	-0.464352	0.000001
2	6	0	0.692913	0.855435	-0.000171
3	6	0	-1.574117	1.557638	0.000059
4	6	0	-1.116637	-0.890654	-0.000083
5	6	0	2.449088	-0.364977	0.000034
6	1	0	-2.388356	2.273418	0.000178
7	7	0	-1.456907	-2.140400	-0.000013
8	7	0	-1.971619	0.226006	0.000155
9	7	0	1.392509	-1.233652	-0.000105
10	7	0	2.071845	0.900317	0.000252
11	6	0	-0.264402	1.922631	-0.000223
12	1	0	3.474959	-0.708917	0.000297
13	1	0	0.034287	2.963702	-0.000328
14	1	0	-2.964700	0.031499	0.000299
15	1	0	1.408416	-2.245366	-0.000228
16	1	0	-2.470429	-2.274574	0.000059

Imino (H taward N7) N1H N7H Z3 (Z3-6) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.267897381 A.U.

Zero-point correction= 0.123597
(Hartree/Particle)
Thermal correction to Energy= 0.130839
Thermal correction to Enthalpy= 0.131784
Thermal correction to Gibbs Free Energy= 0.091851
Sum of electronic and zero-point Energies= -451.144301
Sum of electronic and thermal Energies= -451.137058
Sum of electronic and thermal Enthalpies= -451.136114
Sum of electronic and thermal Free Energies= -451.176047

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.103	29.414	84.046

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

1	6	0	0.256933	0.476083	0.000131
2	6	0	0.680847	-0.852232	0.000008
3	6	0	-1.585397	-1.544128	-0.000058
4	6	0	-1.123295	0.895967	0.000003
5	6	0	2.458389	0.336705	-0.000037
6	1	0	-2.402915	-2.256154	0.000302
7	7	0	-1.670706	2.071487	-0.000043
8	7	0	-1.969469	-0.220138	-0.000027
9	7	0	1.417052	1.225801	-0.000052
10	7	0	2.059431	-0.918308	0.000022
11	6	0	-0.275795	-1.916784	-0.000019
12	1	0	3.489425	0.665542	0.000030
13	1	0	0.023591	-2.957243	-0.000087
14	1	0	-2.955195	0.015082	0.000089
15	1	0	-0.971151	2.813538	0.000141
16	1	0	1.491995	2.233683	0.000061

Imino (H taward N1) N1H N9H Z3 (Z3-7) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.258846801 A.U.

Zero-point correction= 0.123177
(Hartree/Particle)
Thermal correction to Energy= 0.130466
Thermal correction to Enthalpy= 0.131410
Thermal correction to Gibbs Free Energy= 0.091388
Sum of electronic and zero-point Energies= -451.135670
Sum of electronic and thermal Energies= -451.128381
Sum of electronic and thermal Enthalpies= -451.127437
Sum of electronic and thermal Free Energies= -451.167459

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	81.868	29.615	84.234

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.257852	-0.540614	-0.000014
2	6	0	-0.692005	0.784417	0.000011
3	6	0	1.511453	1.605494	0.000004
4	6	0	1.158112	-0.875139	-0.000022
5	6	0	-2.388604	-0.638067	0.000022
6	1	0	2.288950	2.361526	-0.000010
7	7	0	1.621801	-2.075433	0.000029
8	1	0	2.645701	-2.091210	0.000053
9	7	0	1.957740	0.301716	0.000001
10	7	0	-1.328252	-1.408222	-0.000018
11	7	0	-2.065971	0.703711	-0.000109
12	6	0	0.185204	1.911927	-0.000010
13	1	0	-3.415768	-0.978169	0.000048
14	1	0	-0.156567	2.939995	0.000006
15	1	0	2.958353	0.149625	0.000020
16	1	0	-2.715742	1.477725	0.000603

N10-deprotonated N9H-amino (N10H_N1side) Z3 (Z3-8) B3LYP/6-31+G(d)

```
 SCF Done:  E(RB+HF-LYP) =  -450.698872237     A.U.

Zero-point correction=                           0.108641
(Hartree/Particle)
 Thermal correction to Energy=                   0.115905
 Thermal correction to Enthalpy=                 0.116849
 Thermal correction to Gibbs Free Energy=        0.076814
 Sum of electronic and zero-point Energies=          -450.590231
 Sum of electronic and thermal Energies=             -450.582968
 Sum of electronic and thermal Enthalpies=           -450.582023
 Sum of electronic and thermal Free Energies=        -450.622058

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.731             28.929             84.261
-------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------------
    1          6             0       -0.212522   -0.533803   -0.000144
    2          6             0       -0.672534    0.790202   -0.000212
    3          6             0        1.549030    1.545693    0.000181
    4          6             0        1.222418   -0.811713    0.000086
    5          6             0       -2.359395   -0.665926    0.000245
    6          7             0        1.694792   -2.035149   -0.000125
    7          7             0        2.058437    0.312640    0.000178
    8          7             0       -1.286716   -1.416988   -0.000044
    9          7             0       -2.053889    0.687688   -0.000134
   10          6             0        0.194755    1.905886   -0.000182
   11          1             0       -2.709500    1.454739    0.000923
   12          1             0       -3.384130   -1.018388    0.000167
   13          1             0       -0.136199    2.941087   -0.000031
   14          1             0        2.293708    2.349166   -0.000181
   15          1             0        2.717236   -1.945974    0.000147
 -------------------------------------------------------------------------
```

N10-deprotonated N9H-amino (N10H_N7side) Z3 (Z3-9) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -450.698027344     A.U.

Zero-point correction=                           0.108634
(Hartree/Particle)
 Thermal correction to Energy=                   0.115899
 Thermal correction to Enthalpy=                 0.116843
 Thermal correction to Gibbs Free Energy=        0.076828
 Sum of electronic and zero-point Energies=          -450.589393
 Sum of electronic and thermal Energies=             -450.582128
 Sum of electronic and thermal Enthalpies=           -450.581184
 Sum of electronic and thermal Free Energies=        -450.621200

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.728             28.980             84.220
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.207444	-0.503375	-0.000360
2	6	0	0.632422	0.830193	0.000156
3	6	0	-1.618854	1.491367	-0.000174
4	6	0	-1.217209	-0.841256	-0.000007
5	6	0	2.357910	-0.585981	-0.000091
6	7	0	-1.697512	-2.063922	0.000585
7	1	0	-0.899664	-2.706911	0.000858
8	7	0	-2.090071	0.246142	-0.000411
9	7	0	1.300950	-1.362106	-0.000449
10	7	0	2.017655	0.758764	0.000292
11	6	0	-0.276081	1.909221	0.000175
12	1	0	2.657030	1.539654	0.000440
13	1	0	3.390590	-0.913587	-0.000224
14	1	0	0.010689	2.957420	0.001017
15	1	0	-2.389599	2.270266	-0.000396

N9-deprotonated N9H-amino Z3 (Z3-10) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.744457816 A.U.

Zero-point correction= 0.110612
(Hartree/Particle)
Thermal correction to Energy= 0.117550
Thermal correction to Enthalpy= 0.118494
Thermal correction to Gibbs Free Energy= 0.079191
Sum of electronic and zero-point Energies= -450.633846
Sum of electronic and thermal Energies= -450.626908
Sum of electronic and thermal Enthalpies= -450.625964
Sum of electronic and thermal Free Energies= -450.665267

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.764	27.930	82.721

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.242461	-0.486750	-0.021211
2	6	0	-0.797609	0.823668	-0.009386
3	6	0	1.440585	1.647739	0.009640
4	6	0	1.156093	-0.647674	-0.020112
5	6	0	-2.347682	-0.623182	0.012418
6	1	0	2.166947	2.461337	0.027092
7	7	0	1.721171	-1.933274	-0.080646
8	1	0	2.638177	-1.972527	0.351563
9	1	0	1.087357	-2.649067	0.260436
10	7	0	1.985762	0.398424	0.003961
11	7	0	-1.258929	-1.416967	-0.003722
12	7	0	-2.163603	0.720289	0.008655
13	6	0	0.081962	1.931232	-0.000441
14	1	0	-3.349748	-1.047223	0.028803

15	1	0	-0.278862	2.957981	0.008927

C8-deprotonated N9H-amino Z3 (Z3-11) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.680097381 A.U.

Zero-point correction= (Hartree/Particle)	0.109455
Thermal correction to Energy=	0.116707
Thermal correction to Enthalpy=	0.117651
Thermal correction to Gibbs Free Energy=	0.077858
Sum of electronic and zero-point Energies=	-450.570642
Sum of electronic and thermal Energies=	-450.563391
Sum of electronic and thermal Enthalpies=	-450.562446
Sum of electronic and thermal Free Energies=	-450.602239

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.235	29.353	83.751

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.235726	-0.502701	-0.022164
2	6	0	-0.797761	0.789212	-0.014972
3	6	0	1.401534	1.681510	0.013270
4	6	0	1.167100	-0.617213	-0.020071
5	6	0	-2.427643	-0.868616	0.021449
6	1	0	2.100797	2.518237	0.034006
7	7	0	1.755683	-1.885300	-0.081943
8	1	0	2.665192	-1.926774	0.363736
9	1	0	1.117867	-2.618988	0.211688
10	7	0	1.973520	0.453531	0.007897
11	7	0	-1.219098	-1.478046	0.002651
12	7	0	-2.148937	0.537068	0.004012
13	6	0	0.029249	1.927143	-0.004111
14	1	0	-0.354736	2.945809	0.002134
15	1	0	-2.877818	1.234949	0.019709

C2-deprotonated N9H-amino Z3 (Z3-12) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.636603127 A.U.

Zero-point correction= (Hartree/Particle)	0.108214
Thermal correction to Energy=	0.115779
Thermal correction to Enthalpy=	0.116723
Thermal correction to Gibbs Free Energy=	0.076292
Sum of electronic and zero-point Energies=	-450.528389
Sum of electronic and thermal Energies=	-450.520824
Sum of electronic and thermal Enthalpies=	-450.519880
Sum of electronic and thermal Free Energies=	-450.560311

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.653	30.102	85.096

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.157393	-0.482406	-0.021369
2	6	0	-0.735484	0.801170	-0.009159
3	6	0	1.467604	1.859387	0.014492
4	6	0	1.251208	-0.541557	-0.018701
5	6	0	-2.270868	-0.835451	0.010335
6	7	0	1.910035	-1.786791	-0.085419
7	1	0	2.861438	-1.698115	0.260972
8	1	0	1.397531	-2.542740	0.357877
9	7	0	1.996114	0.559725	0.012907
10	7	0	-1.133316	-1.485192	-0.005962
11	7	0	-2.109470	0.538448	0.007238
12	6	0	0.047866	1.961358	-0.002727
13	1	0	-2.846666	1.227036	0.017557
14	1	0	-3.253720	-1.292819	0.025170
15	1	0	-0.419722	2.948309	-0.000151

C3-deprotonated N9H-amino Z3 (Z3-13) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.662815357 A.U.

Zero-point correction= 0.109864
(Hartree/Particle)
Thermal correction to Energy= 0.117121
Thermal correction to Enthalpy= 0.118065
Thermal correction to Gibbs Free Energy= 0.078211
Sum of electronic and zero-point Energies= -450.552951
Sum of electronic and thermal Energies= -450.545695
Sum of electronic and thermal Enthalpies= -450.544751
Sum of electronic and thermal Free Energies= -450.584605

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.494	29.051	83.880

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.188064	-0.470983	-0.020986
2	6	0	-0.712964	0.841185	-0.007130
3	6	0	1.366354	1.737350	0.008424
4	6	0	1.215290	-0.591040	-0.019856
5	6	0	-2.307323	-0.737646	0.009221
6	1	0	2.108883	2.540703	0.026208
7	7	0	1.842861	-1.859090	-0.084726
8	1	0	2.774965	-1.818017	0.317027
9	1	0	1.280380	-2.590159	0.340722

10	7	0	1.973692	0.495569	0.003648
11	7	0	-1.193556	-1.441019	-0.006611
12	7	0	-2.095110	0.615737	0.006914
13	6	0	-0.001565	2.054013	0.003339
14	1	0	-2.784933	1.354958	0.019521
15	1	0	-3.304882	-1.163142	0.023882

N1-protonated N9H-amino Z3 (Z3-14) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.672997623 A.U.

Zero-point correction=	0.137397
(Hartree/Particle)	
Thermal correction to Energy=	0.144930
Thermal correction to Enthalpy=	0.145874
Thermal correction to Gibbs Free Energy=	0.105592
Sum of electronic and zero-point Energies=	-451.535600
Sum of electronic and thermal Energies=	-451.528068
Sum of electronic and thermal Enthalpies=	-451.527123
Sum of electronic and thermal Free Energies=	-451.567405

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.945	30.836	84.781

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.246123	-0.491503	-0.000101
2	6	0	-0.749831	0.819017	-0.000169
3	6	0	1.436440	1.691201	0.000138
4	6	0	1.143776	-0.722301	-0.000097
5	6	0	-2.353272	-0.711929	0.000195
6	7	0	1.671979	-1.951941	-0.000124
7	7	0	1.924166	0.395243	0.000185
8	7	0	-1.254397	-1.425687	-0.000003
9	7	0	-2.107487	0.648737	0.000040
10	6	0	0.096138	1.953755	-0.000130
11	1	0	-2.811444	1.377872	-0.000031
12	1	0	-3.360169	-1.108466	0.000262
13	1	0	-0.266096	2.974907	-0.000350
14	1	0	2.194708	2.463925	0.000123
15	1	0	1.041520	-2.746182	-0.000350
16	1	0	2.665874	-2.138233	0.000584
17	1	0	2.933021	0.282275	0.000051

N1-protonated N9H-amino Z3 (Z3-14) B3LYP/6-31+G(d) (cpcm, water, RADII=UAKS)

Total free energy in solution:

with all non electrostatic terms (a.u.) =	-451.776854
(Polarized solute)-Solvent (kcal/mol) =	-69.40

```
 Cavitation energy                        (kcal/mol) =      16.97
 Dispersion energy                        (kcal/mol) =     -21.39
 Repulsion energy                         (kcal/mol) =       5.16
 Total non electrostatic                  (kcal/mol) =       0.74
```

N7-protonated N9H-amino Z3 (Z3-15) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.651316608     A.U.

Zero-point correction=                           0.136987
(Hartree/Particle)
 Thermal correction to Energy=                   0.144517
 Thermal correction to Enthalpy=                 0.145461
 Thermal correction to Gibbs Free Energy=        0.105103
 Sum of electronic and zero-point Energies=          -451.514330
 Sum of electronic and thermal Energies=             -451.506799
 Sum of electronic and thermal Enthalpies=           -451.505855
 Sum of electronic and thermal Free Energies=        -451.546214

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.686             30.796            84.942
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0        0.161701   -0.471809    0.008878
    2          6             0        0.702068    0.821776    0.023879
    3          6             0       -1.474272    1.672396   -0.018348
    4          6             0       -1.245258   -0.648845    0.007438
    5          6             0        2.384513   -0.653716   -0.017733
    6          7             0       -1.850450   -1.873316   -0.038918
    7          7             0       -2.013989    0.440223   -0.016370
    8          7             0        1.249320   -1.352067   -0.021326
    9          7             0        2.088424    0.651304    0.015469
   10          6             0       -0.109889    1.955601    0.015625
   11          1             0        2.779331    1.394333    0.023840
   12          1             0        3.380916   -1.072126   -0.040975
   13          1             0        0.270737    2.970018    0.025443
   14          1             0       -2.191872    2.487927   -0.041604
   15          1             0       -1.416000   -2.681763    0.386012
   16          1             0       -2.862139   -1.850072    0.037636
   17          1             0        1.212722   -2.363744   -0.080764
 -------------------------------------------------------------------
```

N9-protonated N9H-amino Z3 (Z3-16) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.592204494     A.U.

Zero-point correction=                           0.135617
(Hartree/Particle)
 Thermal correction to Energy=                   0.143293
 Thermal correction to Enthalpy=                 0.144237
 Thermal correction to Gibbs Free Energy=        0.103594
 Sum of electronic and zero-point Energies=          -451.456588
 Sum of electronic and thermal Energies=             -451.448911
```

```
 Sum of electronic and thermal Enthalpies=           -451.447967
 Sum of electronic and thermal Free Energies=        -451.488610

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.918             31.201             85.541
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.152888   -0.493965    0.000067
    2          6             0        0.673865    0.798682    0.000096
    3          6             0       -1.484753    1.663774   -0.000037
    4          6             0       -1.253550   -0.654005    0.000066
    5          6             0        2.289727   -0.906931   -0.000312
    6          7             0       -1.858535   -1.852692   -0.000027
    7          7             0       -2.031825    0.455048   -0.000006
    8          7             0        1.157529   -1.471449    0.000013
    9          7             0        2.149100    0.628763    0.000150
   10          6             0       -0.093796    1.939160   -0.000028
   11          1             0        2.598281    1.045024   -0.828350
   12          1             0        3.286515   -1.328931   -0.000532
   13          1             0        0.288279    2.953473   -0.000292
   14          1             0       -2.185616    2.495283   -0.000348
   15          1             0       -1.335557   -2.717471    0.000615
   16          1             0       -2.870104   -1.889498   -0.000345
   17          1             0        2.598041    1.044150    0.829231
 ---------------------------------------------------------------------
```

N10-protonated N9H-amino Z3 (Z3-17) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.641986137     A.U.

Zero-point correction=                           0.138353
(Hartree/Particle)
 Thermal correction to Energy=                   0.145967
 Thermal correction to Enthalpy=                 0.146911
 Thermal correction to Gibbs Free Energy=        0.105916
 Sum of electronic and zero-point Energies=          -451.503633
 Sum of electronic and thermal Energies=             -451.496019
 Sum of electronic and thermal Enthalpies=           -451.495075
 Sum of electronic and thermal Free Energies=        -451.536070

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.596             29.595             86.281
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.202404   -0.473402   -0.000241
    2          6             0        0.829202    0.795872    0.000051
    3          6             0       -1.319677    1.799553   -0.000035
    4          6             0       -1.182983   -0.472514   -0.000288
    5          6             0        2.279933   -0.885934   -0.000026
    6          7             0       -1.892229   -1.787971    0.000458
```

7	7	0	-1.939069	0.594899	-0.000492
8	7	0	1.118816	-1.501318	-0.000299
9	7	0	2.172122	0.487553	0.000214
10	6	0	0.067339	1.966519	0.000138
11	1	0	2.947115	1.139984	0.000019
12	1	0	3.243874	-1.378655	0.000169
13	1	0	0.503213	2.960146	0.000764
14	1	0	-1.976712	2.662957	0.000636
15	1	0	-1.201857	-2.554477	0.000395
16	1	0	-2.495004	-1.881094	0.828931
17	1	0	-2.495416	-1.881561	-0.827685

N10-deprotonated N7H-amino (N10H_N1side) Z3 (Z3-18) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -450.713074310

Zero-point correction=                           0.109660
(Hartree/Particle)
 Thermal correction to Energy=                    0.116644
 Thermal correction to Enthalpy=                  0.117588
 Thermal correction to Gibbs Free Energy=         0.078149
 Sum of electronic and zero-point Energies=           -450.603415
 Sum of electronic and thermal Energies=              -450.596431
 Sum of electronic and thermal Enthalpies=            -450.595486
 Sum of electronic and thermal Free Energies=         -450.634925

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.195             28.193             83.006
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.209285	-0.442088	0.000071
2	6	0	0.672879	0.872137	-0.000003
3	6	0	-1.615879	1.490404	-0.000092
4	6	0	-1.177798	-0.830584	0.000008
5	6	0	2.414941	-0.391130	-0.000113
6	1	0	-2.404236	2.248908	0.000021
7	1	0	3.435046	-0.757030	-0.000038
8	7	0	1.339773	-1.235224	-0.000099
9	7	0	2.067527	0.885241	0.000111
10	7	0	-1.490196	-2.117446	-0.000015
11	6	0	-0.289504	1.919552	0.000050
12	1	0	-0.018741	2.971210	0.000041
13	7	0	-2.074098	0.218821	-0.000042
14	1	0	1.315836	-2.245381	0.000378
15	1	0	-2.512494	-2.187209	0.000381

N10-deprotonated N7H-amino (N10H_N7side) Z3 (Z3-19) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -450.699727143

Zero-point correction= 0.108542
(Hartree/Particle)
 Thermal correction to Energy= 0.115779
 Thermal correction to Enthalpy= 0.116724
 Thermal correction to Gibbs Free Energy= 0.076766
 Sum of electronic and zero-point Energies= -450.591186
 Sum of electronic and thermal Energies= -450.583948
 Sum of electronic and thermal Enthalpies= -450.583004
 Sum of electronic and thermal Free Energies= -450.622961

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.653	28.936	84.097

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.202302	0.445874	0.000045
2	6	0	0.642471	-0.881420	0.000199
3	6	0	-1.648372	-1.463894	0.000246
4	6	0	-1.189468	0.853496	0.000226
5	6	0	2.419204	0.329959	0.000014
6	1	0	-2.447448	-2.211652	-0.000613
7	1	0	3.448175	0.670918	-0.000373
8	7	0	1.367861	1.206203	0.000332
9	7	0	2.037299	-0.931919	-0.000488
10	7	0	-1.624133	2.109503	-0.000537
11	6	0	-0.327007	-1.914837	0.000032
12	1	0	-0.066703	-2.968942	-0.000238
13	7	0	-2.085850	-0.192739	0.000057
14	1	0	1.420859	2.214234	0.001011
15	1	0	-0.815902	2.743034	0.000088

C8-deprotonated N7H-amino Z3 (Z3-20) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -450.676049169

Zero-point correction= 0.109267
(Hartree/Particle)
 Thermal correction to Energy= 0.116634
 Thermal correction to Enthalpy= 0.117579
 Thermal correction to Gibbs Free Energy= 0.077529
 Sum of electronic and zero-point Energies= -450.566782
 Sum of electronic and thermal Energies= -450.559415
 Sum of electronic and thermal Enthalpies= -450.558471
 Sum of electronic and thermal Free Energies= -450.598520

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.189	29.422	84.292

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.225743	-0.484579	-0.021386
2	6	0	0.842898	0.790504	0.014560
3	6	0	-1.373602	1.694837	-0.009411
4	6	0	-1.164830	-0.605997	-0.016208
5	6	0	2.531440	-0.661895	-0.005858
6	1	0	-2.067408	2.536143	-0.014664
7	7	0	1.298189	-1.361412	-0.018638
8	7	0	2.211583	0.662033	0.026925
9	7	0	-1.803205	-1.873968	-0.061558
10	1	0	-2.787602	-1.765605	0.169586
11	1	0	-1.370665	-2.551998	0.560905
12	6	0	-0.001962	1.921203	0.015101
13	1	0	0.402546	2.930589	0.031934
14	7	0	-1.961104	0.471704	-0.014311
15	1	0	1.246775	-2.362067	-0.135477

C2-deprotonated N7H-amino Z3 (Z3-21) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -450.629468796 A.U. after

Zero-point correction= 0.108160
(Hartree/Particle)
Thermal correction to Energy= 0.115772
Thermal correction to Enthalpy= 0.116716
Thermal correction to Gibbs Free Energy= 0.076153
Sum of electronic and zero-point Energies= -450.521308
Sum of electronic and thermal Energies= -450.513697
Sum of electronic and thermal Enthalpies= -450.512753
Sum of electronic and thermal Free Energies= -450.553316

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.648	29.935	85.371

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.159717	-0.443208	-0.000417
2	6	0	0.761216	0.829457	0.029148
3	6	0	-1.483653	1.853671	-0.026610
4	6	0	-1.231764	-0.545795	-0.010476
5	6	0	2.369383	-0.612305	-0.024418
6	7	0	1.215254	-1.365486	-0.000475
7	7	0	2.163932	0.680324	0.020552
8	7	0	-1.873261	-1.828848	-0.049704
9	1	0	-2.877601	-1.641800	-0.049532
10	1	0	-1.657462	-2.378581	0.782725

11	6	0	-0.066211	1.963847	0.031020
12	1	0	0.392961	2.952568	0.067590
13	7	0	-1.991305	0.545432	-0.039377
14	1	0	1.142350	-2.340154	-0.254451
15	1	0	3.345287	-1.085997	-0.052783

C3-deprotonated N7H-amino Z3 (Z3-22) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -450.643129177
Zero-point correction= 0.108882
(Hartree/Particle)
Thermal correction to Energy= 0.116381
Thermal correction to Enthalpy= 0.117326
Thermal correction to Gibbs Free Energy= 0.076950
Sum of electronic and zero-point Energies= -450.534247
Sum of electronic and thermal Energies= -450.526748
Sum of electronic and thermal Enthalpies= -450.525804
Sum of electronic and thermal Free Energies= -450.566180

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.030	29.456	84.978

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.194535	-0.412848	-0.008323
2	6	0	0.742569	0.894623	0.029848
3	6	0	-1.409311	1.712731	-0.019146
4	6	0	-1.187656	-0.600303	-0.010442
5	6	0	2.401601	-0.510830	-0.021062
6	7	0	1.266159	-1.305243	-0.004678
7	7	0	2.157023	0.768590	0.029671
8	7	0	-1.765553	-1.916758	-0.049948
9	6	0	-0.046306	2.069773	0.028781
10	7	0	-1.983557	0.460681	-0.023141
11	1	0	3.389836	-0.959642	-0.047149
12	1	0	-2.172189	2.496716	-0.049881
13	1	0	-1.555368	-2.434095	0.805247
14	1	0	-2.777374	-1.795208	-0.090704
15	1	0	1.224005	-2.277537	-0.278778

N1-protonated N7H-amino Z3 (Z3-23) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.659243466
Zero-point correction= 0.136110
(Hartree/Particle)
Thermal correction to Energy= 0.144317
Thermal correction to Enthalpy= 0.145261
Thermal correction to Gibbs Free Energy= 0.103141
Sum of electronic and zero-point Energies= -451.523133

```
 Sum of electronic and thermal Energies=             -451.514927
 Sum of electronic and thermal Enthalpies=           -451.513982
 Sum of electronic and thermal Free Energies=        -451.556103

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.560             31.891             88.650
-------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 -------------------------------------------------------------------
      1          6           0        0.000000    0.541395    0.000000
      2          6           0       -1.065944   -0.388651    0.000000
      3          6           0        0.503020   -2.160075    0.000000
      4          6           0        1.339416    0.129940    0.000000
      5          6           0       -1.961403    1.543562    0.000000
      6          7           0       -0.611525    1.781825    0.000000
      7          7           0       -2.267355    0.264359    0.000000
      8          7           0        2.419806    0.942344    0.000000
      9          6           0       -0.806763   -1.780349    0.000000
     10          1           0       -1.608259   -2.509170    0.000000
     11          7           0        1.519536   -1.221179    0.000000
     12          1           0       -2.678621    2.354823    0.000000
     13          1           0        0.835472   -3.190490    0.000000
     14          1           0        2.470684   -1.575636    0.000000
     15          1           0        3.367233    0.587116    0.000000
     16          1           0        2.324211    1.947318    0.000000
     17          1           0       -0.183915    2.699660    0.000000
 -------------------------------------------------------------------
```

N7-protonated N7H-amino Z3 (Z3-24) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -451.584683200

Zero-point correction=                           0.135560
(Hartree/Particle)
 Thermal correction to Energy=                    0.143288
 Thermal correction to Enthalpy=                  0.144232
 Thermal correction to Gibbs Free Energy=         0.103408
 Sum of electronic and zero-point Energies=           -451.449124
 Sum of electronic and thermal Energies=              -451.441395
 Sum of electronic and thermal Enthalpies=            -451.440451
 Sum of electronic and thermal Free Energies=         -451.481275

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.915             31.091             85.921

-------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 -------------------------------------------------------------------
      1          6           0        0.166547   -0.435558   -0.033718
      2          6           0        0.689651    0.861425   -0.028495
```

3	6	0	-1.523193	1.642250	0.014344
4	6	0	-1.212171	-0.670434	-0.012478
5	6	0	2.495153	-0.359286	0.023615
6	1	0	-2.260480	2.440614	0.039842
7	1	0	3.499907	-0.765426	0.049094
8	7	0	1.318938	-1.358201	0.014203
9	7	0	2.108955	0.838338	-0.005657
10	7	0	-1.804366	-1.899600	0.051951
11	1	0	-2.817044	-1.891132	-0.015505
12	1	0	-1.360919	-2.719948	-0.338791
13	6	0	-0.150348	1.958204	-0.013078
14	1	0	0.215027	2.978147	-0.009004
15	7	0	-2.023704	0.407632	0.012742
16	1	0	1.396553	-1.987894	-0.799056
17	1	0	1.334353	-1.951151	0.859613

N10-protonated N7H-amino Z3 (Z3-25) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -451.622462063

Zero-point correction=                           0.137605
(Hartree/Particle)
 Thermal correction to Energy=                    0.145226
 Thermal correction to Enthalpy=                  0.146170
 Thermal correction to Gibbs Free Energy=         0.105455
 Sum of electronic and zero-point Energies=           -451.484857
 Sum of electronic and thermal Energies=              -451.477236
 Sum of electronic and thermal Enthalpies=            -451.476292
 Sum of electronic and thermal Free Energies=         -451.517007

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.131             30.059             85.692
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.213782	-0.491183	0.000119
2	6	0	0.862192	0.780096	0.000022
3	6	0	-1.287590	1.811669	-0.000026
4	6	0	-1.174596	-0.481185	0.000051
5	6	0	2.417812	-0.680159	0.000050
6	1	0	-1.942355	2.676529	-0.000043
7	1	0	3.381589	-1.174234	-0.000018
8	7	0	1.241818	-1.412961	-0.000158
9	7	0	2.230964	0.611377	-0.000016
10	7	0	-2.023509	-1.718259	-0.000053
11	1	0	-2.997461	-1.373559	-0.000871
12	1	0	-1.894378	-2.306612	-0.834263
13	6	0	0.098518	1.950534	-0.000044
14	1	0	0.570107	2.927368	-0.000079
15	7	0	-1.905767	0.611431	0.000072

16	1	0	1.192835	-2.423340	0.000472
17	1	0	-1.895574	-2.305892	0.834855

Z1 (1-deazaadenine): neutral, protonated and deprotonated species

Amino N9H Z1 (Z1-1) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.290354912 A.U.

Zero-point correction= (Hartree/Particle)	0.123743
Thermal correction to Energy=	0.131065
Thermal correction to Enthalpy=	0.132010
Thermal correction to Gibbs Free Energy=	0.092129
Sum of electronic and zero-point Energies=	-451.166612
Sum of electronic and thermal Energies=	-451.159289
Sum of electronic and thermal Enthalpies=	-451.158345
Sum of electronic and thermal Free Energies=	-451.198226

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.245	29.829	83.936

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.171392	-0.512525	-0.006323
2	6	0	0.712005	0.786384	-0.003781
3	6	0	-1.273202	1.788883	0.004786
4	6	0	-1.946509	0.556810	0.002590
5	6	0	-1.229839	-0.654211	-0.006081
6	6	0	2.287502	-0.776451	0.004875
7	1	0	-1.857568	2.706743	0.009872
8	1	0	-3.033507	0.547591	-0.000919
9	1	0	3.283856	-1.199611	0.011026
10	7	0	0.059651	1.950080	0.000947
11	7	0	1.173759	-1.470994	0.001007
12	7	0	2.081291	0.584674	0.001692
13	1	0	2.782988	1.312244	0.004460
14	7	0	-1.815401	-1.895901	-0.058916
15	1	0	-1.221164	-2.687855	0.150964
16	1	0	-2.777793	-1.987466	0.235093

Amino N3H Z1 (Z1-2) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.279813940 A.U.

Zero-point correction= (Hartree/Particle)	0.123770
Thermal correction to Energy=	0.131230
Thermal correction to Enthalpy=	0.132174
Thermal correction to Gibbs Free Energy=	0.091951

```
 Sum of electronic and zero-point Energies=           -451.156043
 Sum of electronic and thermal Energies=              -451.148584
 Sum of electronic and thermal Enthalpies=            -451.147640
 Sum of electronic and thermal Free Energies=         -451.187863

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  82.348             29.928             84.656
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.225969   -0.546283   -0.006396
    2          6             0        0.799095    0.755169   -0.003742
    3          6             0       -1.353740    1.721016    0.003453
    4          6             0       -1.947093    0.476009    0.002578
    5          6             0       -1.162975   -0.717159   -0.004024
    6          6             0        2.331662   -0.667630    0.004817
    7          7             0       -0.001124    1.866261   -0.001041
    8          7             0        1.249401   -1.457379    0.000686
    9          7             0        2.132741    0.687977    0.003121
   10          7             0       -1.718147   -1.959884   -0.039960
   11          1             0        3.335796   -1.076464    0.009396
   12          1             0       -3.030984    0.417850    0.000305
   13          1             0       -1.934032    2.636015    0.007169
   14          1             0       -2.695339   -2.096449    0.172299
   15          1             0       -1.100584   -2.751331    0.088327
   16          1             0        0.427538    2.784825    0.002742
 ---------------------------------------------------------------------
```

Amino N3H Z1 (Z1-2) B3LYP/6-31+G(d) cpcm, water, RADII=UAKS

```
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -451.312371
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -26.16
 ---------------------------------------------------------------------
 Cavitation energy                         (kcal/mol) =      16.89
 Dispersion energy                         (kcal/mol) =     -20.51
 Repulsion energy                          (kcal/mol) =       4.57
 Total non electrostatic                   (kcal/mol) =       0.94
```

Amino N7H Z1 (Z1-3) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.276749462     A.U.

Zero-point correction=                           0.123384
(Hartree/Particle)
 Thermal correction to Energy=                   0.130810
 Thermal correction to Enthalpy=                 0.131754
 Thermal correction to Gibbs Free Energy=        0.091617
 Sum of electronic and zero-point Energies=           -451.153366
 Sum of electronic and thermal Energies=              -451.145939
 Sum of electronic and thermal Enthalpies=            -451.144995
 Sum of electronic and thermal Free Energies=         -451.185133
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.085	29.882	84.477

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.176335	-0.473864	-0.008404
2	6	0	0.741951	0.823326	0.016409
3	6	0	-1.292502	1.779185	-0.009493
4	6	0	-1.947308	0.532535	-0.018150
5	6	0	-1.211804	-0.658885	-0.004325
6	6	0	2.385381	-0.546091	-0.009597
7	7	0	0.029070	1.958882	0.018185
8	7	0	1.258048	-1.341365	-0.008878
9	7	0	2.127734	0.735140	0.020787
10	7	0	-1.795994	-1.928035	-0.055537
11	1	0	3.376653	-0.981947	-0.026294
12	1	0	-3.034169	0.500356	-0.025712
13	1	0	-1.895831	2.685340	-0.015213
14	1	0	-2.796457	-1.933431	0.110010
15	1	0	-1.338098	-2.640681	0.502654
16	1	0	1.243573	-2.339230	-0.165988

Imino (H toward C1) N7H N3H Z1 (Z1-4) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.265854166 A.U.

Zero-point correction= 0.123872
(Hartree/Particle)
Thermal correction to Energy= 0.131133
Thermal correction to Enthalpy= 0.132077
Thermal correction to Gibbs Free Energy= 0.092147
Sum of electronic and zero-point Energies= -451.141983
Sum of electronic and thermal Energies= -451.134721
Sum of electronic and thermal Enthalpies= -451.133777
Sum of electronic and thermal Free Energies= -451.173707

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.287	29.361	84.040

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.213174	0.507754	-0.000068
2	6	0	0.670088	-0.797478	-0.000017
3	6	0	-1.560143	-1.556999	-0.000001
4	6	0	-2.041334	-0.278273	0.000054
5	6	0	-1.174882	0.905947	-0.000035
6	6	0	2.417389	0.399831	0.000033
7	7	0	-0.217275	-1.849763	-0.000084
8	7	0	1.364767	1.266139	-0.000026
9	7	0	2.033632	-0.870035	0.000056
10	7	0	-1.501232	2.164663	-0.000012

11	1	0	3.445874	0.733815	0.000063
12	1	0	-3.117808	-0.133673	0.000203
13	1	0	-2.221981	-2.416446	0.000148
14	1	0	-2.518304	2.277539	0.000069
15	1	0	1.383589	2.277804	0.000137
16	1	0	0.123640	-2.800762	0.000051

Imino (H toward N7) N7H N3H Z1 (Z1-5) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.259557676 A.U.

Zero-point correction= 0.123342
(Hartree/Particle)
Thermal correction to Energy= 0.130727
Thermal correction to Enthalpy= 0.131672
Thermal correction to Gibbs Free Energy= 0.091483
Sum of electronic and zero-point Energies= -451.136216
Sum of electronic and thermal Energies= -451.128830
Sum of electronic and thermal Enthalpies= -451.127886
Sum of electronic and thermal Free Energies= -451.168075

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.033	29.747	84.584

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.214781	0.516170	-0.000313
2	6	0	0.653501	-0.799353	-0.000078
3	6	0	-1.582004	-1.542025	-0.000032
4	6	0	-2.047656	-0.262199	-0.000067
5	6	0	-1.180519	0.917808	-0.000115
6	6	0	2.426615	0.359675	0.000049
7	7	0	-0.236832	-1.843259	-0.000028
8	7	0	1.392539	1.250078	-0.000293
9	7	0	2.016237	-0.897967	0.000294
10	7	0	-1.689090	2.115729	0.000355
11	1	0	3.461309	0.674532	0.000252
12	1	0	-3.117733	-0.085993	-0.000155
13	1	0	-2.248948	-2.396973	0.000021
14	1	0	1.473606	2.257473	-0.000059
15	1	0	0.101328	-2.795050	0.000576
16	1	0	-0.957854	2.833486	0.000399

Imino (H toward N7) N9H N3H Z1 (Z1-6) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.247981427 A.U.

Zero-point correction= 0.122721
(Hartree/Particle)
Thermal correction to Energy= 0.130435
Thermal correction to Enthalpy= 0.131379
Thermal correction to Gibbs Free Energy= 0.090504

```
 Sum of electronic and zero-point Energies=           -451.125260
 Sum of electronic and thermal Energies=              -451.117547
 Sum of electronic and thermal Enthalpies=            -451.116602
 Sum of electronic and thermal Free Energies=         -451.157478

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  81.849             30.323            86.030
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.219564    0.557015    0.002603
    2          6             0        0.636908   -0.761512    0.001881
    3          6             0       -1.573973   -1.555729    0.003185
    4          6             0       -2.054252   -0.288369    0.002073
    5          6             0       -1.199674    0.908375    0.000527
    6          6             0        2.365060    0.606260    0.001545
    7          7             0       -0.209613   -1.841881   -0.032362
    8          7             0        1.322020    1.394117    0.002776
    9          7             0        2.009780   -0.736282   -0.000809
   10          7             0       -1.721575    2.091448   -0.001281
   11          1             0        3.401664    0.915114    0.006884
   12          1             0       -3.127305   -0.128781    0.003883
   13          1             0       -2.219508   -2.426855    0.010273
   14          1             0        0.113740   -2.780453    0.150611
   15          1             0       -0.977887    2.796528    0.000273
   16          1             0        2.643214   -1.523604   -0.021069
 ---------------------------------------------------------------------
```

Imino (H toward C1) N9H N3H Z1 (Z1-7) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -451.241719280     A.U.

Zero-point correction=                           0.122351
(Hartree/Particle)
 Thermal correction to Energy=                    0.130161
 Thermal correction to Enthalpy=                  0.131105
 Thermal correction to Gibbs Free Energy=         0.089942
 Sum of electronic and zero-point Energies=           -451.119369
 Sum of electronic and thermal Energies=              -451.111558
 Sum of electronic and thermal Enthalpies=            -451.110614
 Sum of electronic and thermal Free Energies=         -451.151777

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  81.677             30.479            86.634
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.215669   -0.579767    0.002206
    2          6             0       -0.667219    0.729730    0.000851
    3          6             0        1.510592    1.603352    0.003301
    4          6             0        2.028753    0.349512    0.001752
    5          6             0        1.215017   -0.883142    0.000341
```

6	6	0	-2.359981	-0.675372	0.001533
7	7	0	0.143937	1.839574	-0.026214
8	7	0	-1.301360	-1.439149	0.003196
9	7	0	-2.038043	0.676370	-0.000919
10	7	0	1.665758	-2.095267	-0.001429
11	1	0	-3.389247	-1.008439	0.006212
12	1	0	3.110207	0.243883	0.003516
13	1	0	2.130042	2.493611	0.010898
14	1	0	-0.215278	2.771387	0.119444
15	1	0	-2.687453	1.450353	-0.019753
16	1	0	2.690730	-2.087374	-0.002658

N10-deprotonated (N10H toward N7) amino N9H Z1 (Z1-8) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.712342526 A.U.

Zero-point correction= 0.109547
(Hartree/Particle)
Thermal correction to Energy= 0.116600
Thermal correction to Enthalpy= 0.117544
Thermal correction to Gibbs Free Energy= 0.077989
Sum of electronic and zero-point Energies= -450.602795
Sum of electronic and thermal Energies= -450.595743
Sum of electronic and thermal Enthalpies= -450.594799
Sum of electronic and thermal Free Energies= -450.634354

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.167	28.355	83.250

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.180524	0.538473	0.000032
2	6	0	0.618931	-0.796269	-0.000014
3	6	0	-1.429833	-1.651204	0.000044
4	6	0	-2.012619	-0.393449	-0.000008
5	6	0	-1.241359	0.838425	-0.000053
6	6	0	2.329184	0.636687	0.000191
7	7	0	-0.096038	-1.932906	0.000118
8	7	0	1.266594	1.408121	0.000084
9	7	0	2.006338	-0.706924	-0.000516
10	7	0	-1.808228	2.028764	0.000042
11	1	0	-1.066719	2.736505	-0.000547
12	1	0	2.636625	-1.495601	0.001155
13	1	0	3.357763	0.978082	0.000205
14	1	0	-3.097445	-0.305220	0.000117
15	1	0	-2.079860	-2.529129	-0.000182

N10-deprotonated (N10H toward C1) amino N9H Z1 (Z1-9) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.706788616 A.U.

Zero-point correction= 0.109202

(Hartree/Particle)
 Thermal correction to Energy= 0.116271
 Thermal correction to Enthalpy= 0.117216
 Thermal correction to Gibbs Free Energy= 0.077615
 Sum of electronic and zero-point Energies= -450.597587
 Sum of electronic and thermal Energies= -450.590517
 Sum of electronic and thermal Enthalpies= -450.589573
 Sum of electronic and thermal Free Energies= -450.629174

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.961	28.422	83.348

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.181231	-0.562957	-0.000005
2	6	0	0.652024	0.763113	0.000029
3	6	0	-1.363516	1.691137	0.000040
4	6	0	-1.980388	0.448725	0.000007
5	6	0	-1.250155	-0.815185	-0.000010
6	6	0	2.327601	-0.703845	-0.000014
7	7	0	-0.026197	1.925788	0.000059
8	7	0	1.251704	-1.452827	-0.000070
9	7	0	2.035063	0.646955	0.000023
10	7	0	-1.771253	-2.026389	-0.000058
11	1	0	2.678540	1.424572	0.000091
12	1	0	3.348992	-1.067051	-0.000046
13	1	0	-3.070701	0.404995	0.000015
14	1	0	-1.988022	2.588004	0.000045
15	1	0	-2.794816	-1.931141	-0.000071

N9-deprotonated amino N9H Z1 (Z1-10) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.736318593 A.U.

Zero-point correction= 0.110358
(Hartree/Particle)
 Thermal correction to Energy= 0.117348
 Thermal correction to Enthalpy= 0.118293
 Thermal correction to Gibbs Free Energy= 0.078897
 Sum of electronic and zero-point Energies= -450.625961
 Sum of electronic and thermal Energies= -450.618970
 Sum of electronic and thermal Enthalpies= -450.618026
 Sum of electronic and thermal Free Energies= -450.657422

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.637	28.036	82.915

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.212535	-0.504428	-0.021042

2	6	0	0.781028	0.811622	-0.006385
3	6	0	-1.265355	1.774130	0.007599
4	6	0	-1.927907	0.526816	-0.005584
5	6	0	-1.178656	-0.658618	-0.019152
6	6	0	2.314324	-0.652192	0.010828
7	1	0	-1.871525	2.683152	0.018643
8	1	0	-3.017354	0.495375	-0.018189
9	1	0	3.311837	-1.087410	0.024171
10	7	0	0.058146	1.957227	0.006322
11	7	0	1.217366	-1.441859	-0.006414
12	7	0	2.145039	0.688187	0.011672
13	7	0	-1.757481	-1.943437	-0.077826
14	1	0	-1.077090	-2.658322	0.166034
15	1	0	-2.603174	-2.037594	0.475482

C8-deprotonated amino N9H Z1 (Z1-11) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.676544116 A.U.
Zero-point correction= 0.109474
(Hartree/Particle)
Thermal correction to Energy= 0.116741
Thermal correction to Enthalpy= 0.117685
Thermal correction to Gibbs Free Energy= 0.077858
Sum of electronic and zero-point Energies= -450.567071
Sum of electronic and thermal Energies= -450.559803
Sum of electronic and thermal Enthalpies= -450.558859
Sum of electronic and thermal Free Energies= -450.598686

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.256	29.297	83.824

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.199236	-0.532087	-0.021883
2	6	0	0.780902	0.759680	-0.010671
3	6	0	-1.199131	1.820440	0.009031
4	6	0	-1.900751	0.603522	-0.003317
5	6	0	-1.197326	-0.616619	-0.018348
6	6	0	2.387602	-0.912720	0.017615
7	1	0	-1.758675	2.756830	0.021500
8	1	0	-2.990376	0.612461	-0.013547
9	7	0	0.142399	1.939409	0.003757
10	7	0	1.167725	-1.516114	-0.003119
11	7	0	2.127391	0.489632	0.007393
12	7	0	-1.823861	-1.874003	-0.078181
13	1	0	-1.159690	-2.615001	0.133836
14	1	0	-2.663188	-1.950792	0.486436
15	1	0	2.853160	1.190743	0.028259

C1-deprotonated amino N9H Z1 (Z1-12) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -450.656404107 A.U.

```
Zero-point correction=                           0.109386
(Hartree/Particle)
 Thermal correction to Energy=                   0.116750
 Thermal correction to Enthalpy=                 0.117694
 Thermal correction to Gibbs Free Energy=        0.077621
 Sum of electronic and zero-point Energies=          -450.547018
 Sum of electronic and thermal Energies=             -450.539654
 Sum of electronic and thermal Enthalpies=           -450.538710
 Sum of electronic and thermal Free Energies=        -450.578784

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.262             29.427            84.343
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.122228   -0.509412   -0.019125
    2          6             0        0.696761    0.777992   -0.007332
    3          6             0       -1.295359    1.786752    0.008994
    4          6             0       -2.056659    0.600077    0.005416
    5          6             0       -1.288401   -0.583104   -0.018293
    6          6             0        2.251875   -0.820020    0.007883
    7          1             0       -1.815095    2.749685    0.026654
    8          7             0        0.069487    1.946561    0.003028
    9          7             0        1.124249   -1.492148   -0.005673
   10          7             0        2.073816    0.546684    0.004714
   11          7             0       -1.914293   -1.842334   -0.077200
   12          1             0       -1.392246   -2.600058    0.352882
   13          1             0       -2.876394   -1.774584    0.243522
   14          1             0        2.785986    1.261646    0.017548
   15          1             0        3.242255   -1.261740    0.020045
 ---------------------------------------------------------------------
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C2-deprotonated amino N9H Z1 (Z1-13) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -450.638928031     A.U.

Zero-point correction=                           0.108560
(Hartree/Particle)
 Thermal correction to Energy=                   0.116039
 Thermal correction to Enthalpy=                 0.116983
 Thermal correction to Gibbs Free Energy=        0.076747
 Sum of electronic and zero-point Energies=          -450.530368
 Sum of electronic and thermal Energies=             -450.522889
 Sum of electronic and thermal Enthalpies=           -450.521945
 Sum of electronic and thermal Free Energies=        -450.562181

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.816             29.878            84.685
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
```

1	6	0	0.125151	-0.502669	-0.019254
2	6	0	0.716232	0.775775	-0.006922
3	6	0	-1.249608	1.997085	0.011821
4	6	0	-1.907828	0.709632	-0.000209
5	6	0	-1.281441	-0.540178	-0.018881
6	6	0	2.234949	-0.869667	0.008747
7	7	0	0.138806	1.975119	0.004235
8	7	0	1.087069	-1.513138	-0.005363
9	7	0	2.086969	0.499101	0.006797
10	7	0	-1.964491	-1.775760	-0.081349
11	1	0	-1.408725	-2.549489	0.271954
12	1	0	-2.875923	-1.745614	0.363660
13	1	0	2.812577	1.201564	0.018983
14	1	0	3.211421	-1.340537	0.021311
15	1	0	-3.002549	0.716957	0.002047

N7-protonated amino N9H Z1 (Z1-14) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.654634307 A.U.

Zero-point correction= 0.136881
(Hartree/Particle)
Thermal correction to Energy= 0.144528
Thermal correction to Enthalpy= 0.145472
Thermal correction to Gibbs Free Energy= 0.104933
Sum of electronic and zero-point Energies= -451.517754
Sum of electronic and thermal Energies= -451.510106
Sum of electronic and thermal Enthalpies= -451.509162
Sum of electronic and thermal Free Energies= -451.549701

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.693	31.072	85.321

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.133844	-0.494925	0.003564
2	6	0	0.682271	0.796984	0.011197
3	6	0	-1.291014	1.802382	-0.006512
4	6	0	-1.963322	0.572971	-0.009224
5	6	0	-1.270389	-0.653602	0.003660
6	6	0	2.359747	-0.677706	-0.008535
7	7	0	0.044260	1.951835	0.009010
8	7	0	1.218971	-1.377324	-0.010756
9	7	0	2.070940	0.624302	0.009116
10	7	0	-1.897054	-1.864283	-0.035329
11	1	0	2.745943	1.383719	0.013729
12	1	0	3.352578	-1.104437	-0.022611
13	1	0	-3.049192	0.569321	-0.016415
14	1	0	-1.868806	2.722139	-0.010831
15	1	0	-2.904722	-1.889448	0.056399
16	1	0	-1.431901	-2.709983	0.263280
17	1	0	1.189460	-2.389651	-0.052744

N3-protonated amino N9H Z1 (Z1-15) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.668329052 A.U.

Zero-point correction= (Hartree/Particle)	0.137522
Thermal correction to Energy=	0.144951
Thermal correction to Enthalpy=	0.145895
Thermal correction to Gibbs Free Energy=	0.105822
Sum of electronic and zero-point Energies=	-451.530807
Sum of electronic and thermal Energies=	-451.523378
Sum of electronic and thermal Enthalpies=	-451.522434
Sum of electronic and thermal Free Energies=	-451.562507

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.958	30.737	84.342

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.197966	-0.530344	-0.000037
2	6	0	-0.728584	0.760145	0.000066
3	6	0	1.409245	1.706821	0.000108
4	6	0	1.993143	0.464554	0.000008
5	6	0	1.205371	-0.728037	-0.000070
6	6	0	-2.315991	-0.764051	-0.000027
7	7	0	0.050491	1.874412	0.000139
8	7	0	-1.213283	-1.463335	-0.000093
9	7	0	-2.084156	0.607701	0.000073
10	7	0	1.726522	-1.957066	-0.000167
11	1	0	-2.794631	1.330229	0.000135
12	1	0	-3.321985	-1.162431	-0.000043
13	1	0	3.076060	0.403493	-0.000011
14	1	0	1.994035	2.618711	0.000168
15	1	0	2.724938	-2.119240	-0.000193
16	1	0	1.116105	-2.766577	-0.000220
17	1	0	-0.342848	2.809308	0.000214

N3-protonated amino N9H Z1 (Z1-15) B3LYP/6-31+G(d), cpcm, water, RADII=UAKS

Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-451.772659
(Polarized solute)-Solvent	(kcal/mol) =	-70.23
Cavitation energy	(kcal/mol) =	16.90
Dispersion energy	(kcal/mol) =	-21.49
Repulsion energy	(kcal/mol) =	5.24
Total non electrostatic	(kcal/mol) =	0.65

N9-protonated amino N9H Z1 (Z1-16) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.599657906 A.U.

Zero-point correction= 0.136095
(Hartree/Particle)
Thermal correction to Energy= 0.143696
Thermal correction to Enthalpy= 0.144641
Thermal correction to Gibbs Free Energy= 0.104184
Sum of electronic and zero-point Energies= -451.463563
Sum of electronic and thermal Energies= -451.455962
Sum of electronic and thermal Enthalpies= -451.455017
Sum of electronic and thermal Free Energies= -451.495474

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.171	30.983	85.149

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.126100	-0.513692	-0.000172
2	6	0	-0.643467	0.775121	-0.000176
3	6	0	1.311947	1.793729	0.000062
4	6	0	1.981890	0.579312	0.000083
5	6	0	1.279021	-0.660933	-0.000118
6	6	0	-2.265826	-0.914215	0.000151
7	7	0	-0.047406	1.927897	-0.000139
8	7	0	-1.135830	-1.489906	-0.000114
9	7	0	-2.132819	0.605327	0.000128
10	7	0	1.885645	-1.861199	0.000074
11	1	0	-2.568488	1.038286	-0.827741
12	1	0	-3.258096	-1.347703	0.000234
13	1	0	3.067799	0.577712	0.000172
14	1	0	1.871679	2.723521	0.000481
15	1	0	2.893227	-1.941758	0.000006
16	1	0	1.350250	-2.719363	0.000268
17	1	0	-2.568283	1.038543	0.827962

N10-protonated amino N9H Z1 (Z1-17) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -451.631395754 A.U.

Zero-point correction= 0.138288
(Hartree/Particle)
Thermal correction to Energy= 0.145799
Thermal correction to Enthalpy= 0.146743
Thermal correction to Gibbs Free Energy= 0.106157
Sum of electronic and zero-point Energies= -451.493108
Sum of electronic and thermal Energies= -451.485597
Sum of electronic and thermal Enthalpies= -451.484652
Sum of electronic and thermal Free Energies= -451.525238

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

Total	91.490	29.529	85.421

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.167737	-0.483784	-0.000004
2	6	0	-0.798420	0.782399	-0.000043
3	6	0	1.139857	1.913556	0.000035
4	6	0	1.903214	0.721872	0.000080
5	6	0	1.217588	-0.483497	0.000059
6	6	0	-2.246125	-0.894111	-0.000095
7	7	0	-0.198786	1.963580	-0.000026
8	7	0	-1.078301	-1.510943	-0.000036
9	7	0	-2.144240	0.473918	-0.000102
10	7	0	1.870956	-1.819432	0.000101
11	1	0	-2.909123	1.139546	-0.000142
12	1	0	-3.206026	-1.394253	-0.000134
13	1	0	2.987786	0.779368	0.000129
14	1	0	1.653499	2.870352	0.000051
15	1	0	2.456709	-1.974369	0.831434
16	1	0	2.456793	-1.974381	-0.831170
17	1	0	1.122691	-2.534740	0.000069

N10-deprotonated (N10H toward N7) amino N3H Z1 (Z1-18) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -450.716729976
Zero-point correction= 0.109821
(Hartree/Particle)
Thermal correction to Energy= 0.117075
Thermal correction to Enthalpy= 0.118019
Thermal correction to Gibbs Free Energy= 0.077937
Sum of electronic and zero-point Energies= -450.606909
Sum of electronic and thermal Energies= -450.599655
Sum of electronic and thermal Enthalpies= -450.598711
Sum of electronic and thermal Free Energies= -450.638793

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.466	28.480	84.360

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.253266	0.562784	-0.000094
2	6	0	0.701223	-0.767333	0.000122
3	6	0	-1.528750	-1.561609	0.000269
4	6	0	-1.155355	0.908290	-0.000141
5	6	0	2.377906	0.490601	-0.000100
6	1	0	-2.184127	-2.428678	0.000416
7	1	0	3.417827	0.806366	-0.000161
8	7	0	1.368692	1.373875	-0.000238
9	7	0	2.050071	-0.836752	0.000123
10	7	0	-1.693427	2.104303	-0.000334
11	1	0	-0.932002	2.790699	-0.000452

12	7	0	-0.182662	-1.835551	0.000305
13	6	0	-2.012525	-0.283433	0.000061
14	1	0	-3.087540	-0.125024	0.000042
15	1	0	0.172533	-2.780290	0.000457

N10-deprotonated (N10H toward C1) amino N3H Z1 (Z1-19) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -450.706896413

Zero-point correction= 0.109295
(Hartree/Particle)
Thermal correction to Energy= 0.116554
Thermal correction to Enthalpy= 0.117498
Thermal correction to Gibbs Free Energy= 0.077420
Sum of electronic and zero-point Energies= -450.597601
Sum of electronic and thermal Energies= -450.590342
Sum of electronic and thermal Enthalpies= -450.589398
Sum of electronic and thermal Free Energies= -450.629477

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.139	28.647	84.353

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.247317	-0.595942	-0.000080
2	6	0	-0.741621	0.723681	0.000042
3	6	0	1.443906	1.623492	0.000263
4	6	0	1.176742	-0.876772	-0.000033
5	6	0	-2.374650	-0.584121	-0.000199
6	1	0	2.063616	2.516706	0.000397
7	1	0	-3.404504	-0.932059	-0.000297
8	7	0	-1.341455	-1.435285	-0.000237
9	7	0	-2.089721	0.754070	-0.000030
10	7	0	1.692525	-2.084127	-0.000140
11	7	0	0.092072	1.832162	0.000214
12	6	0	1.976284	0.363534	0.000149
13	1	0	3.061126	0.267568	0.000197
14	1	0	-0.310961	2.757747	0.000293
15	1	0	2.716707	-2.000930	-0.000075

C2-deprotonated amino N3H Z1 (Z1-20) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -450.680328252

Zero-point correction= 0.110632
(Hartree/Particle)
Thermal correction to Energy= 0.117721
Thermal correction to Enthalpy= 0.118666
Thermal correction to Gibbs Free Energy= 0.079109

```
 Sum of electronic and zero-point Energies=           -450.569696
 Sum of electronic and thermal Energies=              -450.562607
 Sum of electronic and thermal Enthalpies=            -450.561663
 Sum of electronic and thermal Free Energies=         -450.601219

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.871             28.526             83.254
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.183596	-0.526935	-0.022351
2	6	0	-0.801333	0.738516	-0.008571
3	6	0	1.341594	1.914767	0.010866
4	6	0	1.219302	-0.598942	-0.018112
5	6	0	-2.285263	-0.752408	0.011510
6	1	0	-3.271531	-1.209502	0.026245
7	7	0	-1.168397	-1.497412	-0.006249
8	7	0	-2.149293	0.606744	0.011593
9	7	0	1.851401	-1.846293	-0.072926
10	1	0	2.763353	-1.878861	0.367910
11	1	0	1.248155	-2.611140	0.212382
12	7	0	-0.036445	1.879221	0.001213
13	6	0	1.925552	0.620944	0.001064
14	1	0	-0.535424	2.761403	0.010553
15	1	0	3.017063	0.566620	0.001064

C1-deprotonated amino N3H Z1 (Z1-21) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -450.668639394

Zero-point correction=                           0.109924
(Hartree/Particle)
 Thermal correction to Energy=                    0.117157
 Thermal correction to Enthalpy=                  0.118101
 Thermal correction to Gibbs Free Energy=         0.078231
 Sum of electronic and zero-point Energies=           -450.558716
 Sum of electronic and thermal Energies=              -450.551482
 Sum of electronic and thermal Enthalpies=            -450.550538
 Sum of electronic and thermal Free Energies=         -450.590409

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.517             29.058             83.915
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.186965	-0.533866	-0.017585
2	6	0	-0.773326	0.752690	-0.008551
3	6	0	1.410337	1.693067	0.009930

4	6	0	1.216882	-0.658966	-0.015594
5	6	0	-2.303772	-0.682295	0.010353
6	1	0	1.928103	2.655069	0.027551
7	1	0	-3.306760	-1.101959	0.024252
8	7	0	-1.216780	-1.464564	-0.002053
9	7	0	-2.123830	0.673763	0.006237
10	7	0	1.776741	-1.925500	-0.062931
11	1	0	2.746060	-1.953767	0.231586
12	1	0	1.186600	-2.694800	0.232001
13	7	0	0.023604	1.856300	-0.004464
14	6	0	2.075375	0.485853	0.007432
15	1	0	-0.403340	2.776560	0.011180

C8-deprotonated amino N3H Z1 (Z1-22) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -450.624790942
Zero-point correction=                           0.108155
(Hartree/Particle)
 Thermal correction to Energy=                    0.115726
 Thermal correction to Enthalpy=                  0.116670
 Thermal correction to Gibbs Free Energy=         0.076259
 Sum of electronic and zero-point Energies=           -450.516636
 Sum of electronic and thermal Energies=              -450.509065
 Sum of electronic and thermal Enthalpies=            -450.508121
 Sum of electronic and thermal Free Energies=         -450.548532
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.619	30.309	85.053

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.237348	-0.580481	-0.029087
2	6	0	-0.892308	0.709357	-0.013819
3	6	0	1.247430	1.783710	0.010513
4	6	0	1.146488	-0.659024	-0.017088
5	6	0	-2.428654	-0.861865	0.024811
6	7	0	-1.214130	-1.529595	-0.006891
7	7	0	-2.198111	0.578536	0.015664
8	7	0	1.793529	-1.911210	-0.077194
9	1	0	2.578137	-1.999335	0.562442
10	1	0	1.113565	-2.652711	0.082400
11	7	0	-0.123242	1.849651	-0.001255
12	6	0	1.888962	0.562369	-0.005635
13	1	0	-0.599646	2.743481	0.025643
14	1	0	2.976620	0.542227	-0.021174
15	1	0	1.777587	2.730267	0.020242

N3-protonated amino N3H Z1 (Z1-23) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -451.669848030
```

```
Zero-point correction=                           0.137258
(Hartree/Particle)
 Thermal correction to Energy=                    0.144888
 Thermal correction to Enthalpy=                  0.145832
 Thermal correction to Gibbs Free Energy=         0.105345
 Sum of electronic and zero-point Energies=           -451.532590
 Sum of electronic and thermal Energies=              -451.524961
 Sum of electronic and thermal Enthalpies=            -451.524016
 Sum of electronic and thermal Free Energies=         -451.564503

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.918             31.065             85.211
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.194203	-0.522149	-0.000033
2	6	0	0.758208	0.762960	-0.000057
3	6	0	-1.380223	1.724563	0.000059
4	6	0	-1.203334	-0.720508	-0.000015
5	6	0	2.407039	-0.550407	0.000067
6	1	0	-1.963539	2.637485	0.000059
7	1	0	3.411044	-0.954617	0.000110
8	7	0	1.302645	-1.356617	-0.000049
9	7	0	2.113038	0.736637	-0.000007
10	7	0	-1.794618	-1.930937	-0.000092
11	1	0	-2.802738	-2.016552	0.000071
12	1	0	-1.275409	-2.796996	-0.000191
13	7	0	-0.031196	1.870139	-0.000061
14	6	0	-1.971335	0.480873	0.000115
15	1	0	-3.054487	0.423965	0.000190
16	1	0	1.324388	-2.368467	0.000612
17	1	0	0.404319	2.788635	-0.000210

N7-protonated amino N3H Z1 (Z1-24) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -451.581556085

Zero-point correction=                           0.135212
(Hartree/Particle)
 Thermal correction to Energy=                    0.143163
 Thermal correction to Enthalpy=                  0.144107
 Thermal correction to Gibbs Free Energy=         0.102830
 Sum of electronic and zero-point Energies=           -451.446344
 Sum of electronic and thermal Energies=              -451.438393
 Sum of electronic and thermal Enthalpies=            -451.437449
 Sum of electronic and thermal Free Energies=         -451.478726

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

Total	89.836	31.569	86.875

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.147183	0.445509	-0.015585
2	6	0	-0.672347	-0.854275	-0.011156
3	6	0	1.366579	-1.764192	0.003455
4	6	0	1.231350	0.681687	-0.005530
5	6	0	-2.479903	0.371785	0.010930
6	7	0	-1.287457	1.373487	0.004205
7	7	0	-2.098598	-0.823155	-0.000937
8	7	0	1.820218	1.908667	0.035067
9	1	0	2.827523	1.975009	-0.035580
10	1	0	1.322742	2.760315	-0.181419
11	7	0	0.028312	-1.962143	-0.005194
12	6	0	1.988310	-0.520794	0.004634
13	1	0	3.072992	-0.465187	0.013726
14	1	0	1.974211	-2.664547	0.008225
15	1	0	-3.477976	0.794057	0.021914
16	1	0	-1.354160	1.988606	-0.820796
17	1	0	-1.323482	1.975444	0.841462

N10-protonated amino N3H Z1 (Z1-25) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.613047976

Zero-point correction= (Hartree/Particle)	0.138373
Thermal correction to Energy=	0.145840
Thermal correction to Enthalpy=	0.146784
Thermal correction to Gibbs Free Energy=	0.106317
Sum of electronic and zero-point Energies=	-451.474675
Sum of electronic and thermal Energies=	-451.467208
Sum of electronic and thermal Enthalpies=	-451.466264
Sum of electronic and thermal Free Energies=	-451.506731

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.516	29.387	85.170

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.199926	-0.522451	-0.000295
2	6	0	-0.895759	0.743749	-0.000134
3	6	0	1.191731	1.869377	0.000042
4	6	0	1.170979	-0.528232	-0.000173
5	6	0	-2.275159	-0.829684	0.000055
6	7	0	-1.115685	-1.519488	-0.000178
7	7	0	-2.204419	0.539455	0.000219

8	7	0	1.794374	-1.876701	0.000197
9	1	0	2.373358	-2.051687	0.832768
10	1	0	1.015012	-2.562457	0.000063
11	7	0	-0.170823	1.890670	0.000005
12	6	0	1.898649	0.674306	-0.000049
13	1	0	2.982899	0.704382	-0.000079
14	1	0	1.686619	2.832281	0.000081
15	1	0	-3.234750	-1.332565	0.000237
16	1	0	-0.664427	2.782085	0.000353
17	1	0	2.374074	-2.051975	-0.831799

N10-deprotonated (N10H toward C1) amino N7H Z1 (Z1-26) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -450.713850691
Zero-point correction=                           0.109637
(Hartree/Particle)
 Thermal correction to Energy=                    0.116593
 Thermal correction to Enthalpy=                  0.117537
 Thermal correction to Gibbs Free Energy=         0.078184
 Sum of electronic and zero-point Energies=           -450.604214
 Sum of electronic and thermal Energies=              -450.597258
 Sum of electronic and thermal Enthalpies=            -450.596313
 Sum of electronic and thermal Free Energies=         -450.635667

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.163             28.134             82.826
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.184155	0.499545	-0.019836
2	6	0	-0.672366	-0.828840	-0.003537
3	6	0	1.415186	-1.662557	0.014977
4	6	0	1.190445	0.765612	-0.049918
5	6	0	-2.393385	0.441857	0.013569
6	1	0	2.071038	-2.531261	0.033986
7	1	0	-3.408339	0.819061	0.034631
8	7	0	-1.315090	1.301739	-0.024376
9	7	0	-2.060873	-0.822358	0.011215
10	7	0	1.699188	2.067774	-0.039454
11	7	0	0.106285	-1.920227	0.012098
12	6	0	1.995206	-0.379792	-0.017661
13	1	0	3.078264	-0.283638	-0.027688
14	1	0	-1.357463	2.302444	0.107595
15	1	0	2.504356	2.289948	0.509534

N10-deprotonated (N10H toward N7) amino N7H Z1 (Z1-27) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -450.707429554
```

```
Zero-point correction=                           0.108863
(Hartree/Particle)
 Thermal correction to Energy=                    0.116063
 Thermal correction to Enthalpy=                  0.117008
 Thermal correction to Gibbs Free Energy=         0.077174
 Sum of electronic and zero-point Energies=           -450.598567
 Sum of electronic and thermal Energies=              -450.591366
 Sum of electronic and thermal Enthalpies=            -450.590422
 Sum of electronic and thermal Free Energies=         -450.630255

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.831             28.747             83.836

---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -0.178319    0.470440    0.000815
      2          6           0       -0.634501   -0.860490    0.000118
      3          6           0        1.473092   -1.616743   -0.000014
      4          6           0        1.207808    0.856848   -0.000119
      5          6           0       -2.394324    0.380197   -0.000365
      6          1           0        2.162270   -2.465388    0.000170
      7          1           0       -3.418447    0.736311   -0.000248
      8          7           0       -1.332306    1.247755    0.000742
      9          7           0       -2.032236   -0.883346   -0.000509
     10          7           0        1.715103    2.088450   -0.000468
     11          1           0        0.953327    2.777487   -0.000592
     12          7           0        0.165324   -1.950599   -0.000045
     13          6           0        2.020425   -0.332378    0.000137
     14          1           0        3.101600   -0.207693   -0.000227
     15          1           0       -1.375042    2.256211   -0.000580
 ---------------------------------------------------------------------
```

C8-deprotonated amino N7H Z1 (Z1-28) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -450.665088043
Zero-point correction=                           0.108722
(Hartree/Particle)
 Thermal correction to Energy=                    0.116216
 Thermal correction to Enthalpy=                  0.117161
 Thermal correction to Gibbs Free Energy=         0.076870
 Sum of electronic and zero-point Energies=           -450.556366
 Sum of electronic and thermal Energies=              -450.548872
 Sum of electronic and thermal Enthalpies=            -450.547928
 Sum of electronic and thermal Free Energies=         -450.588218

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  72.927             29.781             84.798

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

Number	Number	Type	X	Y	Z
1	6	0	-0.195949	-0.502793	-0.031790
2	6	0	-0.829565	0.778206	0.007940
3	6	0	1.191500	1.816150	-0.004218
4	6	0	1.188618	-0.613770	-0.018617
5	6	0	-2.500847	-0.694014	-0.000781
6	7	0	-1.253479	-1.389867	-0.011402
7	7	0	-2.194686	0.625569	0.030132
8	7	0	1.847062	-1.872499	-0.059769
9	1	0	2.796901	-1.819607	0.297640
10	1	0	1.338882	-2.589806	0.451074
11	7	0	-0.140924	1.940815	0.018441
12	6	0	1.898183	0.601586	-0.019784
13	1	0	-1.199130	-2.387029	-0.155521
14	1	0	2.988018	0.606030	-0.028436
15	1	0	1.757881	2.750097	-0.003080

C1-deprotonated amino N7H Z1 (Z1-29) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -450.651539092
Zero-point correction= 0.109268
(Hartree/Particle)
Thermal correction to Energy= 0.116665
Thermal correction to Enthalpy= 0.117610
Thermal correction to Gibbs Free Energy= 0.077459
Sum of electronic and zero-point Energies= -450.542272
Sum of electronic and thermal Energies= -450.534874
Sum of electronic and thermal Enthalpies= -450.533930
Sum of electronic and thermal Free Energies= -450.574080

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.209	29.265	84.505

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.126613	-0.455686	-0.011224
2	6	0	-0.728957	0.820897	0.026073
3	6	0	1.314584	1.776930	-0.016938
4	6	0	1.268733	-0.588500	-0.015457
5	6	0	-2.346643	-0.595630	-0.019310
6	1	0	1.864200	2.723484	-0.024374
7	1	0	-3.327900	-1.057226	-0.040291
8	7	0	-1.195293	-1.358369	-0.010711
9	7	0	-2.124422	0.694553	0.028258
10	7	0	1.850953	-1.902810	-0.050580
11	1	0	2.861685	-1.763501	0.006703
12	1	0	1.561510	-2.466133	0.751199
13	7	0	-0.027825	1.962257	0.032423
14	6	0	2.060229	0.564339	-0.038275

15	1	0	-1.131391	-2.340127	-0.238171

C2-deprotonated amino N7H Z1 (Z1-30) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -450.623088858

Zero-point correction= 0.107964
(Hartree/Particle)
Thermal correction to Energy= 0.115588
Thermal correction to Enthalpy= 0.116533
Thermal correction to Gibbs Free Energy= 0.075942
Sum of electronic and zero-point Energies= -450.515125
Sum of electronic and thermal Energies= -450.507500
Sum of electronic and thermal Enthalpies= -450.506556
Sum of electronic and thermal Free Energies= -450.547147

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.533	29.998	85.431

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.110314	-0.446137	-0.008476
2	6	0	-0.786344	0.797081	0.016283
3	6	0	1.157473	1.925887	-0.009608
4	6	0	1.288660	-0.509987	-0.004309
5	6	0	-2.304771	-0.709761	-0.009786
6	1	0	-3.254451	-1.230035	-0.026522
7	7	0	-1.112607	-1.404239	-0.008985
8	7	0	-2.159255	0.588974	0.020597
9	7	0	1.980729	-1.723652	-0.055427
10	1	0	2.977949	-1.642286	0.109726
11	1	0	1.586475	-2.473342	0.502804
12	7	0	-0.174714	1.990217	0.018045
13	6	0	1.917991	0.740766	-0.018129
14	1	0	-1.011603	-2.397074	-0.166145
15	1	0	2.986398	0.796537	-0.035319

N7-protonated amino N7H Z1 (Z1-31) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.581556085
Zero-point correction= 0.135212
(Hartree/Particle)
Thermal correction to Energy= 0.143163
Thermal correction to Enthalpy= 0.144107
Thermal correction to Gibbs Free Energy= 0.102830
Sum of electronic and zero-point Energies= -451.446344
Sum of electronic and thermal Energies= -451.438393
Sum of electronic and thermal Enthalpies= -451.437449
Sum of electronic and thermal Free Energies= -451.478726

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.836	31.569	86.875

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.147183	0.445509	-0.015585
2	6	0	-0.672347	-0.854275	-0.011156
3	6	0	1.366579	-1.764192	0.003455
4	6	0	1.231350	0.681687	-0.005530
5	6	0	-2.479903	0.371785	0.010930
6	7	0	-1.287457	1.373487	0.004205
7	7	0	-2.098598	-0.823155	-0.000937
8	7	0	1.820218	1.908667	0.035067
9	1	0	2.827523	1.975009	-0.035580
10	1	0	1.322742	2.760315	-0.181419
11	7	0	0.028312	-1.962143	-0.005194
12	6	0	1.988310	-0.520794	0.004634
13	1	0	3.072992	-0.465187	0.013726
14	1	0	1.974211	-2.664547	0.008225
15	1	0	-3.477976	0.794057	0.021914
16	1	0	-1.354160	1.988606	-0.820796
17	1	0	-1.323482	1.975444	0.841462

N10-protonated amino N7H Z1 (Z1-32) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -451.602410280

Zero-point correction= 0.137149
(Hartree/Particle)
Thermal correction to Energy= 0.144923
Thermal correction to Enthalpy= 0.145867
Thermal correction to Gibbs Free Energy= 0.104749
Sum of electronic and zero-point Energies= -451.465262
Sum of electronic and thermal Energies= -451.457488
Sum of electronic and thermal Enthalpies= -451.456544
Sum of electronic and thermal Free Energies= -451.497662

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.940	30.357	86.540

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.184893	-0.494637	-0.000079
2	6	0	0.843973	0.779504	0.000000
3	6	0	-1.116056	1.917963	-0.000084
4	6	0	-1.204141	-0.487051	-0.000044
5	6	0	2.388878	-0.691323	0.000028

6	7	0	1.203250	-1.420652	-0.000016
7	7	0	2.211061	0.597444	0.000064
8	7	0	-2.000404	-1.752100	0.000068
9	1	0	-3.006291	-1.534590	-0.000080
10	1	0	-1.820403	-2.331808	-0.832067
11	7	0	0.214785	1.952468	0.000031
12	6	0	-1.875039	0.729614	-0.000001
13	1	0	-2.960777	0.783999	0.000032
14	1	0	-1.628712	2.875871	0.000083
15	1	0	3.347324	-1.195303	0.000051
16	1	0	1.153540	-2.431202	-0.000421
17	1	0	-1.820573	-2.331500	0.832456

Q ("6-methylated" 1-deazaadenine): neutral, protonated and deprotonated species

Amino N9H Q (Q-1) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -435.246411281 A.U.

Zero-point correction= 0.134517
(Hartree/Particle)
Thermal correction to Energy= 0.142177
Thermal correction to Enthalpy= 0.143121
Thermal correction to Gibbs Free Energy= 0.102006
Sum of electronic and zero-point Energies= -435.111894
Sum of electronic and thermal Energies= -435.104235
Sum of electronic and thermal Enthalpies= -435.103290
Sum of electronic and thermal Free Energies= -435.144406

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.217	29.842	86.534

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.138158	-0.514047	0.000172
2	6	0	-0.784291	0.743760	0.000209
3	6	0	1.119115	1.901546	-0.000047
4	6	0	1.877261	0.714161	-0.000435
5	6	0	1.265692	-0.544776	0.000035
6	6	0	-2.234625	-0.927264	-0.000312
7	1	0	1.626447	2.863859	-0.000524
8	1	0	2.961876	0.787570	-0.000477
9	1	0	-3.197081	-1.423472	-0.000319
10	6	0	2.033402	-1.837595	0.000155
11	1	0	1.779408	-2.441434	0.879513
12	1	0	1.778664	-2.441962	-0.878661
13	1	0	3.112985	-1.658208	-0.000436
14	7	0	-0.220236	1.948928	0.000363
15	7	0	-2.134424	0.445250	-0.000014
16	1	0	-2.889106	1.117834	-0.000309
17	7	0	-1.074420	-1.539735	0.000015

Amino N9H-Q (Q1) B3LYP/6-31+G(d) cpcm in water; RADII=UAKS

```
SCF Done:  E(RB+HF-LYP) =  -435.266619084
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -435.264828
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -15.17
 ---------------------------------------------------------------------
 Cavitation energy                         (kcal/mol) =      17.50
 Dispersion energy                         (kcal/mol) =     -20.92
 Repulsion energy                          (kcal/mol) =       4.54
 Total non electrostatic                   (kcal/mol) =       1.12
 ---------------------------------------------------------------------
```

Amino N7H Q (Q-2) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -435.238739643     A.U.

Zero-point correction=                           0.134231
(Hartree/Particle)
 Thermal correction to Energy=                   0.141913
 Thermal correction to Enthalpy=                 0.142857
 Thermal correction to Gibbs Free Energy=        0.101905
 Sum of electronic and zero-point Energies=          -435.104508
 Sum of electronic and thermal Energies=             -435.096827
 Sum of electronic and thermal Enthalpies=           -435.095883
 Sum of electronic and thermal Free Energies=        -435.136834

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.052             30.046            86.190
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.147415   -0.466283   -0.000056
    2          6             0        0.807896    0.789594    0.000049
    3          6             0       -1.161394    1.882173   -0.000006
    4          6             0       -1.893948    0.676291   -0.000067
    5          6             0       -1.247631   -0.562290    0.000010
    6          6             0        2.350051   -0.687638    0.000015
    7          6             0       -1.978150   -1.880082    0.000094
    8          1             0       -1.725579   -2.479408   -0.885004
    9          1             0       -1.725430   -2.479366    0.885194
   10          1             0       -3.061763   -1.728658    0.000195
   11          7             0        0.169920    1.966514    0.000025
   12          7             0        2.183760    0.609442    0.000072
   13          7             0        1.168830   -1.400450   -0.000182
   14          1             0        3.308359   -1.192128    0.000247
   15          1             0       -2.980286    0.718051   -0.000059
   16          1             0       -1.698409    2.828972   -0.000141
   17          1             0        1.080096   -2.406598   -0.000071
 ---------------------------------------------------------------------
```

Amino N7H-Q (Q2) B3LYP/6-31+G(d) cpcm in water; RADII=UAKS

```
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -435.264473
 ------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -23.33
 ------------------------------------------------------------------
 Cavitation energy                         (kcal/mol) =      17.45
 Dispersion energy                         (kcal/mol) =     -20.68
 Repulsion energy                          (kcal/mol) =       4.35
 Total non electrostatic                   (kcal/mol) =       1.12
 ------------------------------------------------------------------
```

Amino N3H Q (Q-3) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -435.232274269     A.U.

Zero-point correction=                           0.134649
(Hartree/Particle)
 Thermal correction to Energy=                    0.142370
 Thermal correction to Enthalpy=                  0.143314
 Thermal correction to Gibbs Free Energy=         0.101472
 Sum of electronic and zero-point Energies=           -435.097625
 Sum of electronic and thermal Energies=              -435.089905
 Sum of electronic and thermal Enthalpies=            -435.088960
 Sum of electronic and thermal Free Energies=         -435.130802

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.338             29.709            88.063
 ------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ------------------------------------------------------------------
    1          6             0       -0.174912   -0.561445   -0.001701
    2          6             0       -0.887518    0.692651    0.001020
    3          6             0        1.162541    1.864790   -0.000208
    4          6             0        1.866205    0.676473   -0.003437
    5          6             0        1.214029   -0.587006   -0.003371
    6          6             0       -2.265845   -0.873255   -0.000749
    7          1             0        1.642232    2.836109   -0.000530
    8          1             0        2.950942    0.724147   -0.006738
    9          1             0       -3.227754   -1.374169   -0.001274
   10          6             0        1.990391   -1.874659    0.002871
   11          1             0        2.538990   -1.991111    0.946819
   12          1             0        1.318434   -2.728098   -0.111563
   13          1             0        2.730111   -1.891813   -0.807068
   14          7             0       -0.200474    1.866120    0.002368
   15          7             0       -2.203143    0.500482    0.001932
   16          7             0       -1.119448   -1.557744   -0.002940
   17          1             0       -0.720843    2.737638    0.004281
 ------------------------------------------------------------------
```

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

SCF Done: E(RB+HF-LYP) = -434.695464953 A.U.

Zero-point correction= 0.120772
(Hartree/Particle)
Thermal correction to Energy= 0.128156
Thermal correction to Enthalpy= 0.129101
Thermal correction to Gibbs Free Energy= 0.088480
Sum of electronic and zero-point Energies= -434.574693
Sum of electronic and thermal Energies= -434.567309
Sum of electronic and thermal Enthalpies= -434.566364
Sum of electronic and thermal Free Energies= -434.606985

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	80.419	28.470	85.493

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.178864	-0.516217	-0.000012
2	6	0	-0.861769	0.755265	-0.000015
3	6	0	1.095673	1.891726	0.000000
4	6	0	1.853824	0.701627	0.000033
5	6	0	1.222294	-0.550005	0.000004
6	6	0	-2.268142	-0.823892	0.000022
7	1	0	1.617181	2.851608	0.000056
8	1	0	2.942316	0.766010	0.000026
9	1	0	-3.227093	-1.339257	-0.000030
10	6	0	1.984616	-1.851158	-0.000026
11	1	0	1.728538	-2.458360	0.878583
12	1	0	1.727990	-2.458629	-0.878292
13	1	0	3.069093	-1.679461	-0.000383
14	7	0	-0.240854	1.952834	-0.000016
15	7	0	-2.211379	0.524701	-0.000018
16	7	0	-1.111169	-1.524104	0.000034

CH3-deprotonated amino N9H Q (Q-5) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -434.647666329

Zero-point correction= 0.119549
(Hartree/Particle)
Thermal correction to Energy= 0.126971
Thermal correction to Enthalpy= 0.127916
Thermal correction to Gibbs Free Energy= 0.087787
Sum of electronic and zero-point Energies= -434.528117
Sum of electronic and thermal Energies= -434.520695
Sum of electronic and thermal Enthalpies= -434.519751
Sum of electronic and thermal Free Energies= -434.559879

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

Total	79.676	30.274	84.458

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.160351	-0.541130	-0.000157
2	6	0	-0.682183	0.762963	-0.000199
3	6	0	1.305118	1.753186	0.000134
4	6	0	1.966071	0.536963	-0.000030
5	6	0	1.277767	-0.747968	-0.000083
6	6	0	-2.301680	-0.771220	0.000266
7	1	0	1.899560	2.670095	0.000212
8	1	0	3.056171	0.538166	-0.000012
9	1	0	-3.306805	-1.176064	-0.000061
10	6	0	1.901561	-1.973849	0.000084
11	1	0	2.987807	-2.046523	-0.000111
12	7	0	-0.045084	1.949488	0.000093
13	7	0	-2.059864	0.589562	-0.000562
14	1	0	-2.734155	1.340709	0.002145
15	7	0	-1.190737	-1.473847	0.000119
16	1	0	1.329401	-2.896469	0.000181

C8-deprotonated amino N9H Q (Q-6) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -434.634764086 A.U.

Zero-point correction= 0.119812
(Hartree/Particle)
Thermal correction to Energy= 0.127517
Thermal correction to Enthalpy= 0.128461
Thermal correction to Gibbs Free Energy= 0.087251
Sum of electronic and zero-point Energies= -434.514953
Sum of electronic and thermal Energies= -434.507247
Sum of electronic and thermal Enthalpies= -434.506303
Sum of electronic and thermal Free Energies= -434.547513

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	80.018	29.795	86.734

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.161026	-0.546735	0.000133
2	6	0	-0.863028	0.697145	0.000088
3	6	0	1.011985	1.938036	-0.000002
4	6	0	1.813136	0.785903	-0.000083
5	6	0	1.239325	-0.499735	-0.000010
6	6	0	-2.316057	-1.103441	-0.000107
7	1	0	1.478131	2.924005	-0.000080
8	1	0	2.897589	0.896903	-0.000197
9	6	0	2.064449	-1.760730	-0.000014
10	1	0	1.835322	-2.378991	0.877859
11	1	0	1.833815	-2.379923	-0.876817

12	1	0	3.139233	-1.537000	-0.000995
13	7	0	-0.336849	1.924236	0.000065
14	7	0	-2.179850	0.314900	-0.000060
15	7	0	-1.048123	-1.601886	0.000042
16	1	0	-2.963040	0.951597	-0.000133

C1-deprotonated amino N9H Q (Q-7) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -434.608064455 A.U.
Zero-point correction= 0.119434
(Hartree/Particle)
Thermal correction to Energy= 0.127325
Thermal correction to Enthalpy= 0.128269
Thermal correction to Gibbs Free Energy= 0.086634
Sum of electronic and zero-point Energies= -434.488631
Sum of electronic and thermal Energies= -434.480740
Sum of electronic and thermal Enthalpies= -434.479796
Sum of electronic and thermal Free Energies= -434.521431

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.897	30.085	87.628

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.084345	-0.496711	-0.000018
2	6	0	-0.764255	0.738115	0.000006
3	6	0	1.136631	1.906125	0.000027
4	6	0	1.999470	0.773759	0.000014
5	6	0	1.329647	-0.471241	-0.000119
6	6	0	-2.189230	-0.967269	0.000063
7	1	0	1.579441	2.907108	0.000106
8	6	0	2.089632	-1.781990	0.000023
9	1	0	1.845382	-2.395148	0.881541
10	1	0	1.843865	-2.396254	-0.880301
11	1	0	3.163491	-1.568399	-0.000952
12	7	0	-0.225839	1.952955	-0.000014
13	7	0	-2.119317	0.407930	-0.000029
14	7	0	-1.013443	-1.551502	-0.000019
15	1	0	-2.884388	1.066417	0.000073
16	1	0	-3.142895	-1.484127	-0.000005

C2-deprotonated amino N9H Q (Q-8) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -434.598944701 A.U.

Zero-point correction= 0.119096
(Hartree/Particle)
Thermal correction to Energy= 0.126931
Thermal correction to Enthalpy= 0.127875
Thermal correction to Gibbs Free Energy= 0.086613
Sum of electronic and zero-point Energies= -434.479849
Sum of electronic and thermal Energies= -434.472014

```
 Sum of electronic and thermal Enthalpies=           -434.471070
 Sum of electronic and thermal Free Energies=        -434.512331

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  79.650             30.271            86.842

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.101234   -0.500362    0.000012
    2          6             0        0.779853    0.734710   -0.000093
    3          6             0       -1.095645    2.095837    0.000004
    4          6             0       -1.835821    0.846477    0.000114
    5          6             0       -1.306958   -0.446261    0.000124
    6          6             0        2.188323   -0.997902   -0.000137
    7          6             0       -2.148162   -1.699830    0.000242
    8          1             0       -1.940256   -2.324755   -0.880008
    9          1             0       -1.940122   -2.324680    0.880514
   10          1             0       -3.216251   -1.448816    0.000313
   11          7             0        0.281965    1.972077   -0.000102
   12          7             0        2.129405    0.376809   -0.000188
   13          7             0        1.002261   -1.567862   -0.000018
   14          1             0        2.897597    1.032856   -0.000276
   15          1             0        3.133186   -1.529831   -0.000192
   16          1             0       -2.926512    0.932055    0.000198
 ---------------------------------------------------------------------
```

N7-protonated amino N9H Q (Q-9) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -435.613036687     A.U.

Zero-point correction=                           0.148154
(Hartree/Particle)
 Thermal correction to Energy=                   0.155887
 Thermal correction to Enthalpy=                 0.156831
 Thermal correction to Gibbs Free Energy=        0.115710
 Sum of electronic and zero-point Energies=          -435.464882
 Sum of electronic and thermal Energies=             -435.457150
 Sum of electronic and thermal Enthalpies=           -435.456206
 Sum of electronic and thermal Free Energies=        -435.497327

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  97.821             30.650            86.548
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.104041   -0.474909   -0.000018
    2          6             0        0.745304    0.772367    0.000004
    3          6             0       -1.164210    1.905666    0.000002
    4          6             0       -1.910579    0.705161   -0.000019
    5          6             0       -1.298845   -0.550312   -0.000035
    6          6             0        2.312015   -0.811557    0.000001
```

7	6	0	-2.053448	-1.850604	0.000027
8	1	0	-1.813923	-2.451233	-0.886780
9	1	0	-1.814372	-2.450859	0.887213
10	1	0	-3.131674	-1.675091	-0.000279
11	7	0	0.171835	1.963578	0.000012
12	7	0	2.118117	0.508630	0.000003
13	7	0	1.124245	-1.429415	-0.000019
14	1	0	2.847580	1.216270	0.000049
15	1	0	3.273056	-1.306378	0.000021
16	1	0	-2.994509	0.769179	-0.000025
17	1	0	-1.681024	2.861126	0.000038
18	1	0	1.009816	-2.437446	0.000021

N7-protonated amino N9H Q (Q-9) B3LYP/6-31+G(d) cpcm in water, RADII=UAKS

Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-419.672183
(Polarized solute)-Solvent	(kcal/mol) =	-64.44
Cavitation energy	(kcal/mol) =	18.16
Dispersion energy	(kcal/mol) =	-21.40
Repulsion energy	(kcal/mol) =	4.62
Total non electrostatic	(kcal/mol) =	1.38

N3-protonated amino N9H Q (Q-10) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -435.610389303 A.U.

Zero-point correction= (Hartree/Particle)	0.147625
Thermal correction to Energy=	0.155598
Thermal correction to Enthalpy=	0.156542
Thermal correction to Gibbs Free Energy=	0.114077
Sum of electronic and zero-point Energies=	-435.462764
Sum of electronic and thermal Energies=	-435.454792
Sum of electronic and thermal Enthalpies=	-435.453847
Sum of electronic and thermal Free Energies=	-435.496312

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	97.639	31.057	89.374

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.149522	-0.535027	-0.000010
2	6	0	0.808475	0.713570	0.000000
3	6	0	-1.234351	1.850259	0.000008
4	6	0	-1.918787	0.648430	-0.000005
5	6	0	-1.252083	-0.598125	-0.000034
6	6	0	2.245293	-0.946106	0.000000
7	6	0	-1.978490	-1.904929	-0.000002
8	1	0	-1.692664	-2.498416	-0.876825

9	1	0	-1.694311	-2.497356	0.878097
10	1	0	-3.061586	-1.765636	-0.001036
11	7	0	0.129150	1.881103	0.000004
12	7	0	2.141686	0.445560	0.000010
13	7	0	1.089968	-1.548052	-0.000007
14	1	0	2.915712	1.100217	0.000024
15	1	0	3.213596	-1.430224	-0.000018
16	1	0	-3.003019	0.680892	-0.000031
17	1	0	-1.729057	2.814010	0.000022
18	1	0	0.608231	2.777810	-0.000030

N9-protonated amino N9H Q (Q-11) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -435.549286102 A.U.

Zero-point correction= 0.146696
(Hartree/Particle)
Thermal correction to Energy= 0.154714
Thermal correction to Enthalpy= 0.155658
Thermal correction to Gibbs Free Energy= 0.113430
Sum of electronic and zero-point Energies= -435.402590
Sum of electronic and thermal Energies= -435.394572
Sum of electronic and thermal Enthalpies= -435.393628
Sum of electronic and thermal Free Energies= -435.435856

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	97.084	31.064	88.876

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.093277	-0.503188	-0.001504
2	6	0	-0.711741	0.744004	0.001798
3	6	0	1.170957	1.901990	-0.000431
4	6	0	1.916370	0.719394	-0.004327
5	6	0	1.304964	-0.552808	-0.004082
6	6	0	-2.205787	-1.047717	-0.001745
7	6	0	2.085670	-1.834402	0.003492
8	1	0	2.602958	-1.955265	0.963554
9	1	0	1.440172	-2.701966	-0.148107
10	1	0	2.852796	-1.822557	-0.778281
11	7	0	-0.185390	1.932342	0.002805
12	7	0	-2.182553	0.481030	0.002514
13	7	0	-1.045492	-1.550068	-0.004166
14	1	0	-2.650843	0.882095	-0.824139
15	1	0	-3.168558	-1.545037	-0.002939
16	1	0	3.000452	0.788952	-0.008703
17	1	0	1.663342	2.869264	-0.000853
18	1	0	-2.649208	0.877754	0.832178

CH3-deprotonated amino N7H Q (Q-12) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -434.645238353

```
 Zero-point correction=                           0.119106
(Hartree/Particle)
 Thermal correction to Energy=                    0.126703
 Thermal correction to Enthalpy=                  0.127647
 Thermal correction to Gibbs Free Energy=         0.087211
 Sum of electronic and zero-point Energies=           -434.526132
 Sum of electronic and thermal Energies=              -434.518536
 Sum of electronic and thermal Enthalpies=            -434.517592
 Sum of electronic and thermal Free Energies=         -434.558027

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  79.507             30.688             85.103
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.160510	0.464195	-0.000344
2	6	0	-0.696751	-0.833779	0.000057
3	6	0	1.360866	-1.718309	-0.000065
4	6	0	1.984774	-0.470430	-0.000300
5	6	0	1.243589	0.770434	-0.000097
6	6	0	-2.377115	0.514107	0.000063
7	6	0	1.773228	2.052420	0.000401
8	7	0	0.035411	-1.975829	0.000212
9	7	0	-2.092078	-0.770251	0.000359
10	7	0	-1.260729	1.311078	-0.000413
11	1	0	1.141062	2.938525	0.000849
12	1	0	2.847981	2.216752	0.000963
13	1	0	3.073798	-0.429552	-0.000508
14	1	0	2.000338	-2.605639	-0.000078
15	1	0	-3.376897	0.933413	-0.000072
16	1	0	-1.232996	2.319678	-0.000555

C8-deprotonated amino N7H Q (Q-13) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -434.628281387
Zero-point correction=                           0.119370
(Hartree/Particle)
 Thermal correction to Energy=                    0.127133
 Thermal correction to Enthalpy=                  0.128077
 Thermal correction to Gibbs Free Energy=         0.086950
 Sum of electronic and zero-point Energies=           -434.508912
 Sum of electronic and thermal Energies=              -434.501148
 Sum of electronic and thermal Enthalpies=            -434.500204
 Sum of electronic and thermal Free Energies=         -434.541332

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  79.777             30.100             86.560
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.160596	-0.499978	-0.000193
2	6	0	0.902824	0.728776	-0.000016
3	6	0	-1.034676	1.922076	0.000043
4	6	0	-1.830677	0.765273	-0.000011
5	6	0	-1.230292	-0.508774	0.000009
6	6	0	2.446188	-0.873041	0.000024
7	6	0	-2.035049	-1.786923	0.000010
8	7	0	0.306846	1.936555	-0.000043
9	7	0	2.251146	0.468476	-0.000001
10	7	0	1.142839	-1.461741	0.000246
11	1	0	-1.814908	-2.404084	0.883550
12	1	0	-1.814040	-2.404625	-0.882917
13	1	0	-3.112001	-1.577556	-0.000584
14	1	0	0.998529	-2.460268	-0.000888
15	1	0	-2.916369	0.858930	0.000172
16	1	0	-1.520512	2.900118	0.000073

C1-deprotonated amino N7H Q (Q-14) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -434.606067732
Zero-point correction=                           0.119255
(Hartree/Particle)
 Thermal correction to Energy=                    0.127123
 Thermal correction to Enthalpy=                  0.128067
 Thermal correction to Gibbs Free Energy=         0.086711
 Sum of electronic and zero-point Energies=           -434.486813
 Sum of electronic and thermal Energies=              -434.478945
 Sum of electronic and thermal Enthalpies=            -434.478001
 Sum of electronic and thermal Free Energies=         -434.519357
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.771	30.158	87.042

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.094496	-0.440510	-0.000038
2	6	0	-0.789269	0.788963	0.000007
3	6	0	1.182765	1.884133	-0.000008
4	6	0	2.020557	0.722159	-0.000018
5	6	0	1.311055	-0.493297	-0.000011
6	6	0	-2.306926	-0.730214	0.000066
7	1	0	1.666085	2.866510	-0.000090
8	1	0	-3.253805	-1.258947	0.000052
9	6	0	2.015183	-1.837384	0.000049
10	7	0	-0.164759	1.975978	0.000045
11	7	0	-2.171509	0.573403	0.000068
12	7	0	-1.104552	-1.407576	-0.000337

13	1	0	1.761059	-2.444927	-0.886404
14	1	0	1.761930	-2.444322	0.887156
15	1	0	3.096774	-1.665473	-0.000504
16	1	0	-0.979512	-2.408577	0.001078

C2-deprotonated amino N7H Q (Q-15) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -434.585634271

Zero-point correction= 0.118125
(Hartree/Particle)
Thermal correction to Energy= 0.126274
Thermal correction to Enthalpy= 0.127218
Thermal correction to Gibbs Free Energy= 0.085327
Sum of electronic and zero-point Energies= -434.467510
Sum of electronic and thermal Energies= -434.459360
Sum of electronic and thermal Enthalpies= -434.458416
Sum of electronic and thermal Free Energies= -434.500308

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.238	30.879	88.168

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.111203	-0.443068	-0.000150
2	6	0	-0.806719	0.786648	0.000015
3	6	0	1.150985	2.074998	-0.000087
4	6	0	1.859934	0.809652	-0.000330
5	6	0	1.288497	-0.465569	-0.000060
6	6	0	-2.306490	-0.767324	-0.000205
7	1	0	-3.243167	-1.314886	-0.000269
8	6	0	2.081269	-1.753206	0.000246
9	7	0	-0.224425	1.997725	0.000273
10	7	0	-2.191263	0.536006	-0.000036
11	7	0	-1.095520	-1.430621	0.000843
12	1	0	1.867890	-2.373792	-0.885229
13	1	0	1.867151	-2.373706	0.885581
14	1	0	3.156958	-1.539670	0.000615
15	1	0	-0.961286	-2.430953	-0.004241
16	1	0	2.953263	0.858448	-0.000590

N3-protonated amino N7H Q (Q-16) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -435.621210671
Zero-point correction= 0.148363
(Hartree/Particle)
Thermal correction to Energy= 0.156123
Thermal correction to Enthalpy= 0.157067
Thermal correction to Gibbs Free Energy= 0.115764

```
 Sum of electronic and zero-point Energies=           -435.472848
 Sum of electronic and thermal Energies=              -435.465088
 Sum of electronic and thermal Enthalpies=            -435.464143
 Sum of electronic and thermal Free Energies=         -435.505446

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  97.969             30.581             86.930
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.149709	-0.510276	0.000017
2	6	0	0.830422	0.728249	-0.000023
3	6	0	-1.230040	1.852008	-0.000036
4	6	0	-1.912499	0.642567	-0.000001
5	6	0	-1.245089	-0.600506	0.000025
6	6	0	2.353235	-0.721423	0.000101
7	6	0	-1.978679	-1.909874	0.000038
8	1	0	-1.718598	-2.503973	-0.885306
9	1	0	-1.718553	-2.503986	0.885360
10	1	0	-3.060618	-1.760817	0.000066
11	7	0	0.123212	1.882796	-0.000051
12	7	0	2.176308	0.588708	-0.000043
13	7	0	1.182686	-1.430316	-0.000020
14	1	0	3.319071	-1.210375	0.000123
15	1	0	-2.996786	0.668707	-0.000005
16	1	0	-1.734698	2.810712	-0.000063
17	1	0	1.103465	-2.440263	-0.000012
18	1	0	0.628912	2.767212	-0.000085

N7-protonated amino N7H Q (Q-17) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -435.539104459
Zero-point correction=                           0.146402
(Hartree/Particle)
 Thermal correction to Energy=                    0.154511
 Thermal correction to Enthalpy=                  0.155456
 Thermal correction to Gibbs Free Energy=         0.112422
 Sum of electronic and zero-point Energies=           -435.392703
 Sum of electronic and thermal Energies=              -435.384593
 Sum of electronic and thermal Enthalpies=            -435.383649
 Sum of electronic and thermal Free Energies=         -435.426683

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  96.957             31.168             90.573
```

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

1	6	0	-0.118964	-0.422942	-0.001575
2	6	0	-0.733004	0.833088	0.001105
3	6	0	1.253306	1.866359	0.000139
4	6	0	1.944347	0.646285	-0.003365
5	6	0	1.260560	-0.585022	-0.003573
6	6	0	-2.455122	-0.503977	0.000108
7	6	0	1.959823	-1.917985	0.003555
8	7	0	-0.087028	1.979863	0.002164
9	7	0	-2.152989	0.715597	0.001822
10	7	0	-1.204705	-1.422047	-0.002379
11	1	0	1.600792	-2.571532	-0.801285
12	1	0	1.806504	-2.442018	0.956094
13	1	0	3.036705	-1.792918	-0.130580
14	1	0	-1.202857	-2.036781	0.825295
15	1	0	3.030242	0.652443	-0.006863
16	1	0	1.806274	2.801522	0.000182
17	1	0	-3.426067	-0.985657	-0.000103
18	1	0	-1.204211	-2.033783	-0.832360

C8-deprotonated amino N3H Q (Q-18) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -434.583520511
Zero-point correction=                           0.118365
(Hartree/Particle)
 Thermal correction to Energy=                    0.126451
 Thermal correction to Enthalpy=                  0.127395
 Thermal correction to Gibbs Free Energy=         0.085201
 Sum of electronic and zero-point Energies=           -434.465156
 Sum of electronic and thermal Energies=              -434.457070
 Sum of electronic and thermal Enthalpies=            -434.456125
 Sum of electronic and thermal Free Energies=         -434.498320

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  79.349             30.935             88.805
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.180541	-0.603818	-0.000002
2	6	0	-0.985663	0.619462	0.000005
3	6	0	1.022126	1.927070	-0.000004
4	6	0	1.789426	0.783247	-0.000019
5	6	0	1.204368	-0.523417	-0.000012
6	6	0	-2.335541	-1.113373	-0.000017
7	6	0	2.064742	-1.762452	0.000016
8	7	0	-0.350726	1.834235	0.000020
9	7	0	-2.264687	0.353010	0.000001
10	7	0	-1.058947	-1.643229	0.000000
11	1	0	1.426458	-2.650650	-0.000137
12	1	0	2.718590	-1.803059	-0.884663
13	1	0	-0.927054	2.667964	0.000045

14	1	0	2.718326	-1.803196	0.884885
15	1	0	2.872678	0.891360	-0.000051
16	1	0	1.438025	2.929149	-0.000020

C1-deprotonated amino N3H Q (Q-19) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -434.615508714

Zero-point correction= 0.120081
(Hartree/Particle)

Thermal correction to Energy= 0.127833
Thermal correction to Enthalpy= 0.128778
Thermal correction to Gibbs Free Energy= 0.086915
Sum of electronic and zero-point Energies= -434.495427
Sum of electronic and thermal Energies= -434.487675
Sum of electronic and thermal Enthalpies= -434.486731
Sum of electronic and thermal Free Energies= -434.528593

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	80.217	29.417	88.107

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.132268	-0.538352	-0.000362
2	6	0	0.859260	0.689954	0.000004
3	6	0	-1.211284	1.850860	-0.000053
4	6	0	-1.999535	0.711656	-0.000224
5	6	0	-1.271483	-0.521673	-0.000256
6	6	0	2.231293	-0.888906	0.000047
7	6	0	-2.023512	-1.834604	0.000365
8	7	0	0.179483	1.861096	0.000063
9	7	0	2.192556	0.480186	0.000244
10	7	0	1.075709	-1.560338	-0.000302
11	1	0	-1.346550	-2.696179	-0.001366
12	1	0	-2.678818	-1.887802	0.880542
13	1	0	-1.620926	2.864075	-0.000170
14	1	0	3.188040	-1.406055	0.000095
15	1	0	0.704196	2.732450	0.001048
16	1	0	-2.682216	-1.886711	-0.877316

C2-deprotonated amino N3H Q (Q-20) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -434.636680123

Zero-point correction= 0.121171
(Hartree/Particle)

Thermal correction to Energy= 0.128654
Thermal correction to Enthalpy= 0.129598
Thermal correction to Gibbs Free Energy= 0.088833
Sum of electronic and zero-point Energies= -434.515509

```
 Sum of electronic and thermal Energies=             -434.508026
 Sum of electronic and thermal Enthalpies=           -434.507082
 Sum of electronic and thermal Free Energies=        -434.547847

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  80.732             28.833             85.798
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.147222	-0.533600	-0.000142
2	6	0	0.873348	0.681729	-0.000026
3	6	0	-1.158469	2.040470	0.000040
4	6	0	-1.845366	0.789813	0.000004
5	6	0	-1.256594	-0.487088	-0.000138
6	6	0	2.230652	-0.917990	0.000048
7	6	0	-2.073808	-1.755262	0.000040
8	7	0	0.206818	1.878534	0.000049
9	7	0	2.205651	0.448188	0.000034
10	7	0	1.059692	-1.573418	-0.000007
11	1	0	-1.842803	-2.371089	0.879531
12	1	0	-3.148325	-1.534088	-0.000996
13	1	0	3.178172	-1.451407	0.000099
14	1	0	0.783465	2.713647	-0.000178
15	1	0	-1.841180	-2.372398	-0.878045
16	1	0	-2.936360	0.833771	0.000095

CH3-deprotonated amino N3H Q (Q-21) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -434.652557581
Zero-point correction=                           0.119750
(Hartree/Particle)
 Thermal correction to Energy=                    0.127476
 Thermal correction to Enthalpy=                  0.128421
 Thermal correction to Gibbs Free Energy=         0.087316
 Sum of electronic and zero-point Energies=           -434.532807
 Sum of electronic and thermal Energies=              -434.525081
 Sum of electronic and thermal Enthalpies=            -434.524137
 Sum of electronic and thermal Free Energies=         -434.565242

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  79.993             30.381             86.513
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.227076	-0.570854	-0.004268
2	6	0	-0.769131	0.721981	-0.006436
3	6	0	1.395107	1.682414	0.007720

4	6	0	1.968775	0.442888	0.007085
5	6	0	1.205881	-0.811196	-0.001629
6	6	0	-2.354304	-0.648580	0.006699
7	6	0	1.812592	-2.038577	-0.003317
8	7	0	0.031999	1.859667	-0.023588
9	7	0	-2.120226	0.697611	0.000098
10	7	0	-1.282761	-1.457401	0.003461
11	1	0	1.224250	-2.950359	-0.007556
12	1	0	2.897832	-2.128936	0.001174
13	1	0	3.055683	0.386474	0.014181
14	1	0	1.989352	2.592574	0.017134
15	1	0	-3.368954	-1.038339	0.014661
16	1	0	-0.392309	2.770997	0.065494

N3-protonated amino N3H Q (Q-22) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -435.512799314
 Zero-point correction=                           0.146496
(Hartree/Particle)
 Thermal correction to Energy=                    0.154632
 Thermal correction to Enthalpy=                  0.155576
 Thermal correction to Gibbs Free Energy=         0.113506
 Sum of electronic and zero-point Energies=           -435.366303
 Sum of electronic and thermal Energies=              -435.358168
 Sum of electronic and thermal Enthalpies=            -435.357224
 Sum of electronic and thermal Free Energies=         -435.399293

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  97.033             31.273             88.542
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.192307	-0.602496	-0.001102
2	6	0	-0.886659	0.662424	-0.000445
3	6	0	1.314697	1.807190	-0.000300
4	6	0	1.889344	0.595949	-0.000883
5	6	0	1.171422	-0.690263	-0.000467
6	6	0	-2.294915	-0.885068	-0.000044
7	6	0	1.931802	-1.970182	0.001159
8	7	0	-0.169431	1.944939	0.001040
9	7	0	-2.165680	0.537862	0.000357
10	7	0	-1.183186	-1.572521	-0.000447
11	1	0	1.259377	-2.829239	0.001822
12	1	0	2.588019	-2.024258	-0.878848
13	1	0	-0.468186	2.500487	-0.817891
14	1	0	2.587131	-2.022234	0.881902
15	1	0	2.976264	0.572440	-0.002100
16	1	0	1.834497	2.757245	-0.001072
17	1	0	-3.282319	-1.329482	-0.000243
18	1	0	-0.467010	2.497744	0.822265

M ("6-methylated" 1,3,7-deazaadenine): neutral, protonated and deprotonated species

Amino N9H M (M-1) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -403.150879504 A.U.

Zero-point correction= 0.157439
(Hartree/Particle)
Thermal correction to Energy= 0.165461
Thermal correction to Enthalpy= 0.166405
Thermal correction to Gibbs Free Energy= 0.125013
Sum of electronic and zero-point Energies= -402.993440
Sum of electronic and thermal Energies= -402.985419
Sum of electronic and thermal Enthalpies= -402.984474
Sum of electronic and thermal Free Energies= -403.025866

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	103.828	32.396	87.116

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.152635	-0.507383	-0.000022
2	6	0	-0.781740	0.768239	-0.000069
3	6	0	-0.055449	1.966292	0.000021
4	6	0	1.330668	1.863290	0.000159
5	6	0	1.973195	0.605001	0.000207
6	6	0	1.259569	-0.591644	0.000119
7	6	0	-1.203276	-1.490891	-0.000142
8	6	0	-2.395295	-0.809919	-0.000253
9	1	0	-0.550434	2.934401	-0.000016
10	1	0	1.934729	2.766998	0.000232
11	1	0	3.060611	0.571294	0.000314
12	1	0	-1.092967	-2.566852	-0.000146
13	1	0	-3.411191	-1.181185	-0.000361
14	6	0	1.950143	-1.932893	0.000172
15	1	0	1.674322	-2.525755	0.882710
16	1	0	1.674497	-2.525735	-0.882433
17	1	0	3.039174	-1.818463	0.000282
18	7	0	-2.146708	0.550543	-0.000209
19	1	0	-2.852863	1.270936	-0.000270

Amino C7H M (M-2) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -403.137864824 A.U.

Zero-point correction= 0.156435
(Hartree/Particle)
Thermal correction to Energy= 0.164455
Thermal correction to Enthalpy= 0.165399
Thermal correction to Gibbs Free Energy= 0.123688

```
 Sum of electronic and zero-point Energies=           -402.981430
 Sum of electronic and thermal Energies=              -402.973410
 Sum of electronic and thermal Enthalpies=            -402.972466
 Sum of electronic and thermal Free Energies=         -403.014177

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 103.197             31.722            87.788
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.167792   -0.462259    0.000051
    2          6             0       -0.755159    0.816321   -0.000020
    3          6             0        0.015487    1.976409   -0.000168
    4          6             0        1.405782    1.822857   -0.000243
    5          6             0        1.992274    0.550198   -0.000172
    6          6             0        1.218414   -0.624857   -0.000024
    7          6             0       -1.303989   -1.452483    0.000205
    8          6             0       -2.485539   -0.503846    0.000200
    9          6             0        1.856704   -1.993845    0.000048
   10          1             0        1.559500   -2.575976    0.882536
   11          1             0        1.559395   -2.576117   -0.882311
   12          1             0        2.949305   -1.923717   -0.000023
   13          7             0       -2.176404    0.747377    0.000075
   14          1             0       -3.524737   -0.826442    0.000292
   15          1             0       -1.316996   -2.112057   -0.880497
   16          1             0        3.076955    0.465759   -0.000233
   17          1             0        2.045008    2.702206   -0.000358
   18          1             0       -0.453804    2.955641   -0.000222
   19          1             0       -1.316886   -2.111912    0.881017
 ---------------------------------------------------------------------
```

C8-deprotonated amino N9H M (M-3) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -402.526292465     A.U.

Zero-point correction=                           0.143010
(Hartree/Particle)
 Thermal correction to Energy=                   0.150927
 Thermal correction to Enthalpy=                 0.151871
 Thermal correction to Gibbs Free Energy=        0.110708
 Sum of electronic and zero-point Energies=          -402.383282
 Sum of electronic and thermal Energies=             -402.375366
 Sum of electronic and thermal Enthalpies=           -402.374422
 Sum of electronic and thermal Free Energies=        -402.415585

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  94.708             31.903            86.635
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.179967   -0.539729    0.000211
    2          6             0       -0.853947    0.725779    0.000263
```

3	6	0	-0.163685	1.940492	0.000287
4	6	0	1.236933	1.904200	-0.000250
5	6	0	1.918881	0.668526	-0.000354
6	6	0	1.235515	-0.553683	0.000020
7	6	0	-1.212825	-1.535097	-0.000156
8	6	0	-2.496473	-0.949874	-0.000321
9	1	0	-0.695624	2.892648	0.000519
10	1	0	1.805041	2.833731	-0.000309
11	1	0	3.010109	0.665299	-0.000521
12	1	0	-1.039649	-2.608073	-0.000416
13	6	0	1.977416	-1.869181	0.000229
14	1	0	1.719887	-2.476053	0.881327
15	1	0	1.718627	-2.476984	-0.879842
16	1	0	3.065194	-1.717832	-0.000609
17	7	0	-2.204101	0.429195	0.000004
18	1	0	-2.925964	1.134291	0.000244

C1-deprotonated amino N9H M (M-4) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -402.495523772 A.U.

Zero-point correction= 0.141317
(Hartree/Particle)
Thermal correction to Energy= 0.149816
Thermal correction to Enthalpy= 0.150760
Thermal correction to Gibbs Free Energy= 0.108119
Sum of electronic and zero-point Energies= -402.354207
Sum of electronic and thermal Energies= -402.345708
Sum of electronic and thermal Enthalpies= -402.344764
Sum of electronic and thermal Free Energies= -402.387405

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	94.011	32.959	89.745

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.101534	-0.488633	-0.000022
2	6	0	-0.757503	0.769122	0.000051
3	6	0	-0.034105	1.968278	0.000029
4	6	0	1.363908	1.857949	-0.000049
5	6	0	2.108956	0.635999	-0.000034
6	6	0	1.324047	-0.532941	-0.000008
7	6	0	-1.146395	-1.490669	-0.000093
8	6	0	-2.358311	-0.837535	-0.000042
9	1	0	-0.540296	2.938656	0.000011
10	1	0	1.916275	2.805354	-0.000094
11	6	0	1.982568	-1.903089	0.000040
12	1	0	1.703288	-2.502445	0.884588
13	1	0	1.702764	-2.502748	-0.884118
14	1	0	3.069861	-1.772451	-0.000263
15	7	0	-2.130510	0.530339	0.000210
16	1	0	-2.843571	1.242507	-0.000724
17	1	0	-3.369755	-1.226048	-0.000045

18	1	0	-1.014786	-2.566083	-0.000064

C2-deprotonated amino N9H M (M-5) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -402.497547408 A.U.

Zero-point correction= 0.141761
(Hartree/Particle)
Thermal correction to Energy= 0.150062
Thermal correction to Enthalpy= 0.151006
Thermal correction to Gibbs Free Energy= 0.109051
Sum of electronic and zero-point Energies= -402.355787
Sum of electronic and thermal Energies= -402.347486
Sum of electronic and thermal Enthalpies= -402.346542
Sum of electronic and thermal Free Energies= -402.388497

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	94.165	32.707	88.302

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.110553	-0.495251	0.000049
2	6	0	-0.781375	0.755226	-0.000045
3	6	0	-0.097687	1.987584	-0.000181
4	6	0	1.308158	2.052569	-0.000230
5	6	0	1.940366	0.760407	-0.000131
6	6	0	1.306186	-0.487249	0.000003
7	6	0	-1.122031	-1.523896	0.000176
8	6	0	-2.349303	-0.897174	0.000159
9	1	0	-0.700812	2.906335	-0.000248
10	6	0	2.078375	-1.787876	0.000096
11	1	0	1.850073	-2.406588	0.883165
12	1	0	1.850019	-2.406746	-0.882848
13	1	0	3.159283	-1.595243	0.000046
14	7	0	-2.148171	0.474917	0.000025
15	1	0	-2.875060	1.173267	-0.000012
16	1	0	-3.349916	-1.312219	0.000230
17	1	0	-0.967350	-2.596824	0.000270
18	1	0	3.038152	0.727563	-0.000161

C3-deprotonated amino N9H M (M-6) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -402.512883933 A.U.

Zero-point correction= 0.142611
(Hartree/Particle)
Thermal correction to Energy= 0.150592
Thermal correction to Enthalpy= 0.151536
Thermal correction to Gibbs Free Energy= 0.110239
Sum of electronic and zero-point Energies= -402.370273
Sum of electronic and thermal Energies= -402.362292
Sum of electronic and thermal Enthalpies= -402.361348

```
 Sum of electronic and thermal Free Energies=         -402.402645

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  94.498             32.033             86.917
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
-------------------------------------------------------------------
    1          6             0       -0.148896   -0.486689   -0.000168
    2          6             0       -0.759083    0.806643   -0.000012
    3          6             0       -0.138933    2.073659    0.000064
    4          6             0        1.259362    1.913511    0.000170
    5          6             0        1.941070    0.660332   -0.000184
    6          6             0        1.266522   -0.558641   -0.000244
    7          6             0       -1.202059   -1.468744   -0.000048
    8          6             0       -2.399683   -0.776028    0.000038
    9          6             0        1.983272   -1.888075    0.000182
   10          1             0        1.728396   -2.497216    0.882736
   11          1             0        1.728008   -2.497886   -0.881784
   12          1             0        3.072549   -1.747520   -0.000099
   13          7             0       -2.135961    0.571807   -0.000023
   14          1             0       -2.803664    1.330389    0.000347
   15          1             0       -3.417308   -1.148791    0.000158
   16          1             0       -1.104285   -2.549603   -0.000009
   17          1             0        3.036118    0.650018    0.000045
   18          1             0        1.902477    2.802156   -0.000028
-------------------------------------------------------------------
```

CH3-deprotonated amino N9H M (M-7) B3LYP/6-31+G(d)

```
Zero-point correction=                           0.140804
(Hartree/Particle)
 Thermal correction to Energy=                    0.149129
 Thermal correction to Enthalpy=                  0.150073
 Thermal correction to Gibbs Free Energy=         0.108234
 Sum of electronic and zero-point Energies=           -402.388583
 Sum of electronic and thermal Energies=              -402.380259
 Sum of electronic and thermal Enthalpies=            -402.379315
 Sum of electronic and thermal Free Energies=         -402.421153

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  93.580             33.989             88.056
```

N9-deprotonated amino N9H M (M-8) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -402.584141757     A.U.

Zero-point correction=                           0.142986
(Hartree/Particle)
 Thermal correction to Energy=                    0.150691
 Thermal correction to Enthalpy=                  0.151635
 Thermal correction to Gibbs Free Energy=         0.110822
 Sum of electronic and zero-point Energies=           -402.441156
```

```
 Sum of electronic and thermal Energies=             -402.433451
 Sum of electronic and thermal Enthalpies=           -402.432506
 Sum of electronic and thermal Free Energies=        -402.473319

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  94.560             31.114             85.898
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.191037   -0.517302    0.000104
    2          6             0       -0.852253    0.772820    0.000116
    3          6             0       -0.085702    1.954525    0.000163
    4          6             0        1.304702    1.860752   -0.000114
    5          6             0        1.948981    0.597208   -0.000180
    6          6             0        1.222509   -0.595108    0.000125
    7          6             0       -1.250771   -1.469443   -0.000040
    8          6             0       -2.427038   -0.699250   -0.000109
    9          1             0       -0.584967    2.923192    0.000301
   10          1             0        1.911363    2.766570   -0.000130
   11          1             0        3.039548    0.555873   -0.000406
   12          1             0       -1.178702   -2.552859   -0.000020
   13          1             0       -3.446619   -1.084433   -0.000287
   14          6             0        1.914015   -1.938893    0.000055
   15          1             0        1.635762   -2.536698    0.881744
   16          1             0        1.634655   -2.537163   -0.880959
   17          1             0        3.007027   -1.829056   -0.000652
   18          7             0       -2.216929    0.643246   -0.000045
 ---------------------------------------------------------------------
```

C7-deprotonated amino N9H M (M-9) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -402.507828035     A.U.

Zero-point correction=                           0.141605
(Hartree/Particle)
 Thermal correction to Energy=                    0.150124
 Thermal correction to Enthalpy=                  0.151068
 Thermal correction to Gibbs Free Energy=         0.108082
 Sum of electronic and zero-point Energies=          -402.366224
 Sum of electronic and thermal Energies=             -402.357704
 Sum of electronic and thermal Enthalpies=           -402.356760
 Sum of electronic and thermal Free Energies=        -402.399746

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  94.204             32.781             90.471
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.182224   -0.556381    0.000319
    2          6             0       -0.818575    0.734429    0.005070
    3          6             0       -0.107761    1.942712    0.001610
    4          6             0        1.287284    1.868485   -0.004661
```

5	6	0	1.944112	0.617792	-0.003258
6	6	0	1.233842	-0.589284	0.001083
7	6	0	-1.166437	-1.638665	-0.006355
8	6	0	-2.347131	-0.928801	-0.007759
9	1	0	-0.613352	2.909773	0.006108
10	1	0	1.876695	2.785262	-0.008846
11	1	0	3.034873	0.594122	-0.005862
12	6	0	1.952501	-1.917504	0.002416
13	1	0	1.688492	-2.505066	0.891235
14	1	0	1.646831	-2.527579	-0.856933
15	1	0	3.043214	-1.783310	-0.023767
16	7	0	-2.169326	0.488271	0.023366
17	1	0	-2.886823	1.192780	-0.088287
18	1	0	-3.378308	-1.280581	-0.008000

N9-protonated amino N9H M (M-10) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -403.480744448 A.U.

Zero-point correction= 0.171033
(Hartree/Particle)
Thermal correction to Energy= 0.179260
Thermal correction to Enthalpy= 0.180205
Thermal correction to Gibbs Free Energy= 0.138039
Sum of electronic and zero-point Energies= -403.309712
Sum of electronic and thermal Energies= -403.301484
Sum of electronic and thermal Enthalpies= -403.300540
Sum of electronic and thermal Free Energies= -403.342706

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	112.488	32.804	88.746

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.101336	-0.496008	-0.000005
2	6	0	-0.709166	0.763577	0.000054
3	6	0	-0.035767	1.967911	0.000070
4	6	0	1.363951	1.867335	-0.000030
5	6	0	2.003550	0.622265	-0.000119
6	6	0	1.299886	-0.594478	-0.000092
7	6	0	-1.156700	-1.511090	0.000050
8	6	0	-2.363938	-0.931278	-0.000135
9	6	0	2.006984	-1.925619	0.000101
10	1	0	1.744942	-2.518403	0.885014
11	1	0	1.744815	-2.518677	-0.884604
12	1	0	3.091720	-1.792451	0.000006
13	7	0	-2.186647	0.555790	0.000047
14	1	0	-2.630488	0.981245	-0.825872
15	1	0	-3.373014	-1.317946	-0.000195
16	1	0	-1.000104	-2.583054	-0.000086
17	1	0	3.089579	0.594969	-0.000144
18	1	0	1.959838	2.774672	0.000007
19	1	0	-0.535007	2.932355	0.000132

20	1	0	-2.630538	0.981078	0.826054

C7-protonated amino N9H M (M-11) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -403.504822556

Zero-point correction=                           0.169918
(Hartree/Particle)
 Thermal correction to Energy=                    0.178113
 Thermal correction to Enthalpy=                  0.179058
 Thermal correction to Gibbs Free Energy=         0.136906
 Sum of electronic and zero-point Energies=           -403.334904
 Sum of electronic and thermal Energies=              -403.326709
 Sum of electronic and thermal Enthalpies=            -403.325765
 Sum of electronic and thermal Free Energies=         -403.367917

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 111.768             32.598             88.717
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.124949	-0.473390	0.000000
2	6	0	-0.700652	0.805047	0.000000
3	6	0	0.020855	1.992638	0.000001
4	6	0	1.409769	1.846464	0.000000
5	6	0	2.008125	0.577631	-0.000001
6	6	0	1.264440	-0.617398	-0.000001
7	6	0	-1.242551	-1.488421	0.000000
8	6	0	-2.460406	-0.629249	-0.000001
9	1	0	-0.452303	2.969703	0.000001
10	1	0	2.038755	2.731137	0.000000
11	1	0	3.092758	0.513783	-0.000002
12	1	0	-1.249019	-2.156273	-0.876448
13	1	0	-3.500451	-0.936397	-0.000001
14	6	0	1.924795	-1.972197	0.000000
15	1	0	1.639710	-2.556275	0.884247
16	1	0	1.639665	-2.556299	-0.884216
17	1	0	3.013912	-1.881532	-0.000029
18	7	0	-2.113230	0.626091	0.000000
19	1	0	-2.777969	1.399031	-0.000001
20	1	0	-1.249020	-2.156270	0.876451

C8-deprotonated amino C7H M (M-12) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -402.507105783
Zero-point correction=                           0.141058
(Hartree/Particle)
 Thermal correction to Energy=                    0.149238
 Thermal correction to Enthalpy=                  0.150182
```

```
 Thermal correction to Gibbs Free Energy=         0.108154
 Sum of electronic and zero-point Energies=           -402.366048
 Sum of electronic and thermal Energies=              -402.357868
 Sum of electronic and thermal Enthalpies=            -402.356924
 Sum of electronic and thermal Free Energies=         -402.398951

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  93.648             32.030             88.455
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.188357	-0.487414	0.000054
2	6	0	-0.844367	0.764846	-0.000015
3	6	0	-0.096274	1.950487	-0.000163
4	6	0	1.301537	1.862574	-0.000239
5	6	0	1.947799	0.618096	-0.000170
6	6	0	1.203158	-0.580909	-0.000022
7	6	0	-1.306118	-1.498266	0.000208
8	6	0	-2.618421	-0.635527	0.000213
9	6	0	1.900132	-1.925595	0.000051
10	1	0	1.623299	-2.522534	0.880505
11	1	0	1.623202	-2.522679	-0.880274
12	1	0	2.992301	-1.812249	-0.000019
13	7	0	-2.252993	0.644463	0.000081
14	1	0	-1.299128	-2.162531	-0.879422
15	1	0	-1.299023	-2.162381	0.879950
16	1	0	3.037441	0.574482	-0.000231
17	1	0	1.901585	2.773185	-0.000355
18	1	0	-0.603253	2.913714	-0.000217

C1-deprotonated amino C7H M (M-13) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -402.494533394

Zero-point correction=                           0.141099
(Hartree/Particle)
 Thermal correction to Energy=                    0.149190
 Thermal correction to Enthalpy=                  0.150135
 Thermal correction to Gibbs Free Energy=         0.108252
 Sum of electronic and zero-point Energies=           -402.353434
 Sum of electronic and thermal Energies=              -402.345343
 Sum of electronic and thermal Enthalpies=            -402.344399
 Sum of electronic and thermal Free Energies=         -402.386282

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  93.618             31.672             88.150
```

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.121652	-0.442899	0.000046
2	6	0	-0.726649	0.828633	-0.000022
3	6	0	0.059421	1.980555	-0.000170
4	6	0	1.456323	1.805222	-0.000245
5	6	0	2.134953	0.554690	-0.000183
6	6	0	1.272207	-0.581806	-0.000032
7	6	0	-1.258276	-1.446409	0.000201
8	6	0	-2.453842	-0.512258	0.000199
9	6	0	1.861737	-1.984150	0.000047
10	1	0	1.551758	-2.568809	0.883856
11	1	0	1.551654	-2.568952	-0.883630
12	1	0	2.954468	-1.911323	-0.000023
13	7	0	-2.147938	0.743769	0.000075
14	1	0	-3.494337	-0.839006	0.000292
15	1	0	-1.261869	-2.109455	-0.880626
16	1	0	2.056350	2.722915	-0.000362
17	1	0	-0.406027	2.968092	-0.000224
18	1	0	-1.261759	-2.109310	0.881138

C2-deprotonated amino C7H M (M-14) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -402.491088014
Zero-point correction= 0.141259
(Hartree/Particle)
Thermal correction to Energy= 0.149324
Thermal correction to Enthalpy= 0.150268
Thermal correction to Gibbs Free Energy= 0.108588
Sum of electronic and zero-point Energies= -402.349829
Sum of electronic and thermal Energies= -402.341764
Sum of electronic and thermal Enthalpies= -402.340820
Sum of electronic and thermal Free Energies= -402.382500

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.702	31.614	87.724

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.129335	-0.449198	0.000048
2	6	0	-0.758799	0.810660	-0.000025
3	6	0	-0.023420	2.000882	-0.000173
4	6	0	1.399195	2.011920	-0.000258
5	6	0	1.966225	0.707933	-0.000177
6	6	0	1.262861	-0.522627	-0.000029
7	6	0	-1.219049	-1.493207	0.000203
8	6	0	-2.444827	-0.595410	0.000196
9	6	0	1.980428	-1.856026	0.000043
10	1	0	1.727182	-2.464586	0.882993
11	1	0	1.727085	-2.464732	-0.882779

12	1	0	3.068571	-1.710765	-0.000030
13	7	0	-2.185828	0.667858	0.000072
14	1	0	-3.471746	-0.964259	0.000288
15	1	0	-1.211292	-2.156596	-0.881356
16	1	0	-0.588806	2.938621	-0.000224
17	1	0	-1.211190	-2.156443	0.881875
18	1	0	3.061316	0.614189	-0.000233

C3-deprotonated amino C7H M (M-15) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -402.493139686
Zero-point correction= 0.141147
(Hartree/Particle)
Thermal correction to Energy= 0.149202
Thermal correction to Enthalpy= 0.150146
Thermal correction to Gibbs Free Energy= 0.108428
Sum of electronic and zero-point Energies= -402.351993
Sum of electronic and thermal Energies= -402.343938
Sum of electronic and thermal Enthalpies= -402.342993
Sum of electronic and thermal Free Energies= -402.384712

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.626	31.597	87.805

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.172483	0.413181	0.000047
2	6	0	0.728805	-0.893442	-0.000027
3	6	0	0.014325	-2.106878	-0.000174
4	6	0	-1.385235	-1.846257	-0.000243
5	6	0	-1.983361	-0.571959	-0.000175
6	6	0	-1.208316	0.603696	-0.000027
7	6	0	1.302354	1.410816	0.000201
8	6	0	2.486090	0.458714	0.000197
9	6	0	-1.831009	1.982095	0.000047
10	1	0	-1.535619	2.572480	0.882120
11	1	0	-1.535510	2.572624	-0.881892
12	1	0	-2.927253	1.918716	-0.000026
13	7	0	2.174229	-0.789004	0.000074
14	1	0	3.526892	0.788102	0.000290
15	1	0	1.315317	2.073676	-0.882083
16	1	0	1.315206	2.073531	0.882595
17	1	0	-3.074758	-0.480441	-0.000237
18	1	0	-2.080693	-2.695467	-0.000359

CH3-deprotonated amino C7H M (M-16) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -402.525540047
Zero-point correction= 0.140673
(Hartree/Particle)

```
 Thermal correction to Energy=                    0.148489
 Thermal correction to Enthalpy=                  0.149433
 Thermal correction to Gibbs Free Energy=         0.108646
 Sum of electronic and zero-point Energies=           -402.384867
 Sum of electronic and thermal Energies=              -402.377051
 Sum of electronic and thermal Enthalpies=            -402.376107
 Sum of electronic and thermal Free Energies=         -402.416894

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  93.178             32.387             85.843
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.183648	0.474917	0.000050
2	6	0	0.658212	-0.837823	-0.000016
3	6	0	-0.182834	-1.959163	-0.000167
4	6	0	-1.566218	-1.665353	-0.000248
5	6	0	-2.060045	-0.366596	-0.000178
6	6	0	-1.213908	0.813990	-0.000026
7	6	0	1.380091	1.375820	0.000208
8	6	0	2.492816	0.350441	0.000211
9	6	0	-1.701530	2.119510	0.000039
10	7	0	2.091864	-0.876346	0.000082
11	1	0	1.439416	2.043893	-0.880045
12	1	0	1.439289	2.043757	0.880573
13	1	0	-3.140268	-0.213998	-0.000238
14	1	0	-2.281353	-2.490305	-0.000362
15	1	0	0.206682	-2.972833	-0.000218
16	1	0	3.557076	0.591963	0.000307
17	1	0	-2.771209	2.319591	0.000145
18	1	0	-1.034066	2.977901	0.000022

B ("6-methylated" 1,3-deazaadenine): neutral, protonated and deprotonated species

Amino N9H B (B-1) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -419.201787472     A.U.

Zero-point correction=                           0.145967
(Hartree/Particle)
 Thermal correction to Energy=                   0.153823
 Thermal correction to Enthalpy=                 0.154767
 Thermal correction to Gibbs Free Energy=        0.113455
 Sum of electronic and zero-point Energies=          -419.055820
 Sum of electronic and thermal Energies=             -419.047964
 Sum of electronic and thermal Enthalpies=           -419.047020
 Sum of electronic and thermal Free Energies=        -419.088332

                    E (Thermal)             CV                S
```

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	96.525	31.108	86.948

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.799341	0.777053	-0.000024
2	6	0	-0.167620	-0.488821	0.000024
3	6	0	1.237593	-0.594275	0.000008
4	6	0	1.945955	0.608413	0.000102
5	6	0	1.304031	1.866226	0.000006
6	6	0	-0.083769	1.978661	-0.000024
7	6	0	-2.272370	-0.884675	0.000010
8	1	0	3.033244	0.577100	-0.000007
9	1	0	1.910781	2.768046	-0.000033
10	1	0	-0.575302	2.947851	-0.000084
11	1	0	-3.241478	-1.368107	0.000041
12	7	0	-1.119495	-1.504297	0.000061
13	7	0	-2.155152	0.487366	-0.000055
14	1	0	-2.915929	1.151665	0.000072
15	6	0	1.913026	-1.940431	-0.000073
16	1	0	1.622395	-2.528032	0.879304
17	1	0	1.620988	-2.528663	-0.878552
18	1	0	3.002807	-1.834258	-0.000956

Amino N7H B (B-2) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -419.200960900 A.U.

Zero-point correction= 0.145916
(Hartree/Particle)
Thermal correction to Energy= 0.153761
Thermal correction to Enthalpy= 0.154705
Thermal correction to Gibbs Free Energy= 0.113522
Sum of electronic and zero-point Energies= -419.055045
Sum of electronic and thermal Energies= -419.047200
Sum of electronic and thermal Enthalpies= -419.046256
Sum of electronic and thermal Free Energies= -419.087439

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	96.486	31.136	86.676

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.815903	0.810682	0.000172
2	6	0	-0.172185	-0.449473	0.000173
3	6	0	1.221935	-0.608674	0.000149
4	6	0	1.952611	0.581407	-0.000475
5	6	0	1.333913	1.851295	-0.000252
6	6	0	-0.050397	1.985714	0.000333
7	6	0	-2.384113	-0.645988	-0.000385
8	7	0	-1.211663	-1.369277	-0.000162
9	7	0	-2.197561	0.649119	0.000152

10	6	0	1.871309	-1.970223	0.000298
11	1	0	1.587709	-2.556734	0.885504
12	1	0	1.587662	-2.556875	-0.884804
13	1	0	2.962477	-1.883721	0.000226
14	1	0	-3.349337	-1.137147	-0.000057
15	1	0	3.039034	0.525356	-0.000740
16	1	0	1.960455	2.739372	-0.000196
17	1	0	-0.533243	2.958296	0.000663
18	1	0	-1.133201	-2.375885	-0.000604

Amino N7H B (B-2) B3LYP/6-31+G(d) cpcm, water, RADII=UAKS

Total free energy in solution:

with all non electrostatic terms	(a.u.) =	-419.217997
(Polarized solute)-Solvent	(kcal/mol) =	-15.36
Cavitation energy	(kcal/mol) =	17.98
Dispersion energy	(kcal/mol) =	-20.63
Repulsion energy	(kcal/mol) =	4.13
Total non electrostatic	(kcal/mol) =	1.47

C8-deprotonated amino N9H B (B-3) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -418.585089690 A.U.

Zero-point correction= (Hartree/Particle)	0.131011
Thermal correction to Energy=	0.138916
Thermal correction to Enthalpy=	0.139860
Thermal correction to Gibbs Free Energy=	0.098476
Sum of electronic and zero-point Energies=	-418.454079
Sum of electronic and thermal Energies=	-418.446174
Sum of electronic and thermal Enthalpies=	-418.445230
Sum of electronic and thermal Free Energies=	-418.486614

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.171	31.121	87.100

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.874605	0.732540	0.000027
2	6	0	-0.196694	-0.519909	0.000042
3	6	0	1.212477	-0.552301	-0.000061
4	6	0	1.892085	0.674724	-0.000175
5	6	0	1.208956	1.908028	-0.000188
6	6	0	-0.192107	1.952058	-0.000087
7	6	0	-2.363407	-1.048981	0.000230
8	1	0	2.982978	0.674361	-0.000254
9	1	0	1.778577	2.836795	-0.000279
10	1	0	-0.719361	2.906323	-0.000098
11	7	0	-1.106880	-1.561427	0.000163
12	7	0	-2.204621	0.365441	0.000145

13	6	0	1.940428	-1.873673	-0.000048
14	1	0	1.667391	-2.475969	0.876819
15	1	0	1.667262	-2.476058	-0.876813
16	1	0	3.029325	-1.729474	-0.000135
17	1	0	-2.988463	1.001011	0.000171

CH3-deprotonated amino N9H B (B-4) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -418.583367925
Zero-point correction=                           0.129731
(Hartree/Particle)
 Thermal correction to Energy=                    0.137634
 Thermal correction to Enthalpy=                  0.138578
 Thermal correction to Gibbs Free Energy=         0.097654
 Sum of electronic and zero-point Energies=           -418.453637
 Sum of electronic and thermal Energies=              -418.445734
 Sum of electronic and thermal Enthalpies=            -418.444790
 Sum of electronic and thermal Free Energies=         -418.485714

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.366             32.442            86.132
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.191011	-0.518380	-0.000200
2	6	0	-1.238495	-0.794023	-0.000130
3	6	0	-2.029450	0.425232	-0.000242
4	6	0	-1.484123	1.703982	-0.000012
5	6	0	-0.093867	1.962289	-0.000209
6	6	0	0.699374	0.797111	-0.000010
7	1	0	-3.114547	0.317645	-0.000458
8	1	0	-2.169117	2.554449	0.000116
9	1	0	0.318999	2.967823	0.001872
10	6	0	2.338105	-0.727265	0.000049
11	6	0	-1.775977	-2.067978	0.000396
12	1	0	-1.140528	-2.947803	0.000618
13	1	0	-2.854693	-2.215759	0.000939
14	7	0	2.080339	0.633962	-0.000044
15	1	0	2.764410	1.375362	0.001619
16	1	0	3.348627	-1.118723	0.000119
17	7	0	1.235001	-1.436647	-0.000340

C1-deprotonated amino N9H B (B-5) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -418.550879505     A.U.

Zero-point correction=                           0.130142
(Hartree/Particle)
 Thermal correction to Energy=                    0.138327
```

```
 Thermal correction to Enthalpy=                  0.139271
 Thermal correction to Gibbs Free Energy=         0.097217
 Sum of electronic and zero-point Energies=           -418.420738
 Sum of electronic and thermal Energies=              -418.412552
 Sum of electronic and thermal Enthalpies=            -418.411608
 Sum of electronic and thermal Free Energies=         -418.453663

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.802             31.583             88.511
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.775933    0.774442    0.000003
    2          6             0        0.115354   -0.475063   -0.000027
    3          6             0       -1.301497   -0.534898   -0.000031
    4          6             0       -2.077293    0.645210   -0.000023
    5          6             0       -1.331330    1.864797   -0.000010
    6          6             0        0.068776    1.979639    0.000020
    7          6             0        2.233149   -0.911607   -0.000008
    8          1             0       -1.883819    2.812112   -0.000012
    9          1             0        0.576658    2.948693    0.000085
   10          7             0        1.069213   -1.512043   -0.000017
   11          7             0        2.137108    0.463873    0.000033
   12          6             0       -1.958331   -1.903314    0.000035
   13          1             0       -1.671116   -2.500090   -0.880703
   14          1             0       -1.671346   -2.499886    0.880976
   15          1             0       -3.045255   -1.769775   -0.000121
   16          1             0        2.904153    1.119121   -0.000085
   17          1             0        3.197911   -1.408216   -0.000004
 ---------------------------------------------------------------------
```

C2-deprotonated amino N9H B (B-6) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -418.554131873     A.U.

Zero-point correction=                           0.130634
(Hartree/Particle)
 Thermal correction to Energy=                    0.138660
 Thermal correction to Enthalpy=                  0.139604
 Thermal correction to Gibbs Free Energy=         0.098069
 Sum of electronic and zero-point Energies=           -418.423498
 Sum of electronic and thermal Energies=              -418.415472
 Sum of electronic and thermal Enthalpies=            -418.414528
 Sum of electronic and thermal Free Energies=         -418.456063

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  87.011             31.293             87.418
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.802264    0.760984   -0.000039
    2          6             0        0.125919   -0.478878   -0.000018
```

3	6	0	-1.285026	-0.486414	0.000078
4	6	0	-1.909262	0.769262	0.000144
5	6	0	-1.273809	2.059330	0.000127
6	6	0	0.134568	1.998882	0.000032
7	6	0	2.219549	-0.973225	-0.000171
8	1	0	0.737003	2.916713	0.000010
9	7	0	1.037080	-1.542366	-0.000102
10	7	0	2.155729	0.403808	-0.000139
11	6	0	-2.051833	-1.787819	0.000105
12	1	0	-1.814009	-2.403538	-0.879912
13	1	0	-1.813902	-2.403565	0.880075
14	1	0	-3.132748	-1.595258	0.000174
15	1	0	2.938703	1.040172	-0.000178
16	1	0	3.167811	-1.499813	-0.000248
17	1	0	-3.006739	0.742459	0.000216

N9-deprotonated amino N9H B (B-7) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -418.649247360 A.U.

Zero-point correction= 0.132202
(Hartree/Particle)
Thermal correction to Energy= 0.139739
Thermal correction to Enthalpy= 0.140683
Thermal correction to Gibbs Free Energy= 0.099950
Sum of electronic and zero-point Energies= -418.517045
Sum of electronic and thermal Energies= -418.509508
Sum of electronic and thermal Enthalpies= -418.508564
Sum of electronic and thermal Free Energies= -418.549297

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.688	29.638	85.731

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.868436	0.776752	-0.000042
2	6	0	-0.209251	-0.499554	-0.000024
3	6	0	1.198549	-0.596095	-0.000036
4	6	0	1.918992	0.602799	0.000006
5	6	0	1.275063	1.864742	0.000134
6	6	0	-0.116692	1.965271	-0.000040
7	6	0	-2.310457	-0.776463	0.000001
8	1	0	3.009428	0.564854	0.000040
9	1	0	1.883596	2.769166	0.000059
10	1	0	-0.612735	2.935346	-0.000296
11	1	0	-3.277963	-1.276079	0.000140
12	7	0	-1.163504	-1.490961	0.000074
13	7	0	-2.228847	0.570648	-0.000017
14	6	0	1.878414	-1.943821	-0.000024
15	1	0	1.587717	-2.537045	0.878109
16	1	0	1.587382	-2.537147	-0.877994
17	1	0	2.971940	-1.838690	-0.000310

C3-deprotonated amino N9H B (B-8) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -418.570675103 A.U.

Zero-point correction= 0.131506
(Hartree/Particle)
Thermal correction to Energy= 0.139298
Thermal correction to Enthalpy= 0.140242
Thermal correction to Gibbs Free Energy= 0.099108
Sum of electronic and zero-point Energies= -418.439169
Sum of electronic and thermal Energies= -418.431378
Sum of electronic and thermal Enthalpies= -418.430433
Sum of electronic and thermal Free Energies= -418.471567

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	87.411	30.643	86.573

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.774969	0.814275	0.000020
2	6	0	0.165087	-0.468934	-0.000122
3	6	0	-1.243240	-0.559867	-0.000217
4	6	0	-1.911081	0.666156	-0.000207
5	6	0	-1.228722	1.918071	0.000071
6	6	0	0.171853	2.085314	0.000109
7	6	0	2.276472	-0.850615	-0.000002
8	7	0	1.121437	-1.488696	-0.000065
9	7	0	2.143757	0.507740	0.000027
10	6	0	-1.952189	-1.891851	0.000175
11	1	0	-1.686711	-2.497587	-0.878849
12	1	0	-1.687282	-2.496827	0.879920
13	1	0	-3.041688	-1.753094	-0.000193
14	1	0	2.872229	1.208896	0.000214
15	1	0	3.247351	-1.335023	0.000058
16	1	0	-3.005894	0.659633	0.000127
17	1	0	-1.873264	2.805392	0.000027

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

SCF Done: E(RB+HF-LYP) = -419.512049720 A.U.

Zero-point correction= 0.158484
(Hartree/Particle)
Thermal correction to Energy= 0.166700
Thermal correction to Enthalpy= 0.167644
Thermal correction to Gibbs Free Energy= 0.124731
Sum of electronic and zero-point Energies= -419.353566
Sum of electronic and thermal Energies= -419.345350
Sum of electronic and thermal Enthalpies= -419.344406
Sum of electronic and thermal Free Energies= -419.387318

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	104.606	32.135	90.317

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.741882	0.774348	-0.000004
2	6	0	0.114921	-0.479651	-0.000001
3	6	0	-1.276605	-0.595217	0.000005
4	6	0	-1.975776	0.630253	-0.000004
5	6	0	-1.333706	1.870644	-0.000002
6	6	0	0.070422	1.976526	-0.000002
7	6	0	2.229550	-1.032221	-0.000010
8	7	0	1.069598	-1.525130	0.000004
9	7	0	2.200341	0.506999	0.000005
10	6	0	-1.985166	-1.922190	0.000002
11	1	0	-2.629159	-2.013345	-0.882410
12	1	0	-1.280899	-2.756477	-0.000079
13	1	0	-2.629042	-2.013415	0.882492
14	1	0	2.682277	0.884580	0.828652
15	1	0	3.196244	-1.521129	-0.000018
16	1	0	-3.062228	0.605597	-0.000008
17	1	0	-1.928023	2.779069	0.000007
18	1	0	0.565816	2.942470	0.000009
19	1	0	2.682305	0.884619	-0.828605

N7-protonated amino N9H B (B-10) B3LYP/6-31+G(d)

SCF Done: E(RB+HF-LYP) = -419.577177433 A.U.

Zero-point correction= 0.159986
(Hartree/Particle)
Thermal correction to Energy= 0.167896
Thermal correction to Enthalpy= 0.168840
Thermal correction to Gibbs Free Energy= 0.127431
Sum of electronic and zero-point Energies= -419.417191
Sum of electronic and thermal Energies= -419.409282
Sum of electronic and thermal Enthalpies= -419.408337
Sum of electronic and thermal Free Energies= -419.449746

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	105.356	31.738	87.152

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.762482	0.808002	0.000000
2	6	0	-0.128350	-0.447442	-0.000006
3	6	0	1.267290	-0.600132	-0.000014
4	6	0	1.974468	0.602500	-0.000008
5	6	0	1.344162	1.866891	0.000005
6	6	0	-0.039224	2.002524	0.000005
7	6	0	-2.341278	-0.775673	0.000000
8	7	0	-1.158418	-1.395381	-0.000005

9	7	0	-2.135569	0.544200	0.000005
10	6	0	1.928433	-1.953725	0.000011
11	1	0	1.654753	-2.538419	0.888002
12	1	0	1.653768	-2.538958	-0.887319
13	1	0	3.016483	-1.852425	-0.000622
14	1	0	-2.876252	1.237289	0.000002
15	1	0	-3.306601	-1.261594	0.000004
16	1	0	3.060041	0.564350	-0.000016
17	1	0	1.962654	2.758964	0.000004
18	1	0	-0.521881	2.974207	0.000002
19	1	0	-1.043177	-2.402808	-0.000006

N7-protonated amino N9H B (B-10) B3LYP/6-31+G(d) cpcm, water, RADII=UAKS

```
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -419.672183
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -64.44
 ---------------------------------------------------------------------
 Cavitation energy                         (kcal/mol) =      18.16
 Dispersion energy                         (kcal/mol) =     -21.40
 Repulsion energy                          (kcal/mol) =       4.62
 Total non electrostatic                   (kcal/mol) =       1.38
```

C8-deprotonated amino N7H B (B-11) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -418.584242278

Zero-point correction=                           0.130935
(Hartree/Particle)
 Thermal correction to Energy=                    0.138822
 Thermal correction to Enthalpy=                  0.139766
 Thermal correction to Gibbs Free Energy=         0.098570
 Sum of electronic and zero-point Energies=           -418.453307
 Sum of electronic and thermal Energies=              -418.445420
 Sum of electronic and thermal Enthalpies=            -418.444476
 Sum of electronic and thermal Free Energies=         -418.485672

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  87.112             31.197             86.705
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.907476	0.749706	0.000037
2	6	0	0.190643	-0.481900	0.000044
3	6	0	-1.208079	-0.555295	-0.000086
4	6	0	-1.899172	0.668013	-0.000073
5	6	0	-1.214531	1.900518	0.000037
6	6	0	0.183632	1.953017	0.000037
7	6	0	2.487558	-0.823776	-0.000108
8	7	0	1.195536	-1.428040	0.000002

9	7	0	2.270177	0.513282	0.000003
10	6	0	-1.929544	-1.883308	0.000036
11	1	0	1.065250	-2.428391	0.000324
12	1	0	-3.018098	-1.742954	0.000115
13	1	0	-1.673485	-2.488649	-0.883004
14	1	0	-1.673383	-2.488571	0.883091
15	1	0	-2.989699	0.659657	-0.000202
16	1	0	-1.790844	2.825576	0.000048
17	1	0	0.712381	2.904796	0.000045

C1-deprotonated amino N7H B (B-12) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -418.556348350
Zero-point correction=                           0.130428
(Hartree/Particle)
 Thermal correction to Energy=                    0.138467
 Thermal correction to Enthalpy=                  0.139412
 Thermal correction to Gibbs Free Energy=         0.097815
 Sum of electronic and zero-point Energies=           -418.425920
 Sum of electronic and thermal Energies=              -418.417881
 Sum of electronic and thermal Enthalpies=            -418.416937
 Sum of electronic and thermal Free Energies=         -418.458533
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.890	31.353	87.547

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.792055	0.818255	0.000059
2	6	0	0.121697	-0.425332	0.000046
3	6	0	-1.281728	-0.557443	-0.000026
4	6	0	-2.090398	0.596500	-0.000035
5	6	0	-1.373767	1.840450	-0.000003
6	6	0	0.017097	1.990977	0.000132
7	6	0	2.347700	-0.666676	-0.000194
8	7	0	1.160647	-1.367000	0.000075
9	7	0	2.179285	0.634636	-0.000058
10	6	0	-1.886099	-1.951319	-0.000094
11	1	0	3.307397	-1.172018	-0.000307
12	1	0	-1.957612	2.767829	-0.000236
13	1	0	0.499208	2.970422	0.000052
14	1	0	1.055414	-2.370022	0.001219
15	1	0	-2.977391	-1.856799	-0.000984
16	1	0	-1.592141	-2.543059	-0.886564
17	1	0	-1.593739	-2.542282	0.887381

C2-deprotonated amino N7H B (B-13) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -418.549096259
```

```
Zero-point correction=                           0.130269
(Hartree/Particle)
 Thermal correction to Energy=                    0.138438
 Thermal correction to Enthalpy=                  0.139382
 Thermal correction to Gibbs Free Energy=         0.097590
 Sum of electronic and zero-point Energies=           -418.418827
 Sum of electronic and thermal Energies=              -418.410659
 Sum of electronic and thermal Enthalpies=            -418.409714
 Sum of electronic and thermal Free Energies=         -418.451507

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.871             31.534            87.959

-------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 -------------------------------------------------------------------
      1          6           0        0.822320    0.801092    0.000022
      2          6           0        0.131592   -0.430939    0.000061
      3          6           0       -1.267080   -0.504420    0.000014
      4          6           0       -1.923627    0.740835    0.000108
      5          6           0       -1.318875    2.039681    0.000026
      6          6           0        0.092166    2.010260   -0.000059
      7          6           0        2.338191   -0.739204    0.000076
      8          7           0        1.131869   -1.408444   -0.000362
      9          7           0        2.209349    0.564177    0.000019
     10          6           0       -1.995483   -1.829046   -0.000070
     11          1           0        3.280025   -1.278096    0.000077
     12          1           0        0.672151    2.938989   -0.000188
     13          1           0        1.002543   -2.408565    0.001661
     14          1           0       -3.080789   -1.665427   -0.000727
     15          1           0       -1.757896   -2.443578   -0.885059
     16          1           0       -1.758940   -2.443163    0.885490
     17          1           0       -3.020847    0.680161    0.000084
 -------------------------------------------------------------------
```

C3-deprotonated amino N7H B (B-14) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -418.552250401
Zero-point correction=                           0.129938
(Hartree/Particle)
 Thermal correction to Energy=                    0.138154
 Thermal correction to Enthalpy=                  0.139098
 Thermal correction to Gibbs Free Energy=         0.097125
 Sum of electronic and zero-point Energies=           -418.422312
 Sum of electronic and thermal Energies=              -418.414097
 Sum of electronic and thermal Enthalpies=            -418.413153
 Sum of electronic and thermal Free Energies=         -418.455126

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.693             31.606            88.340
-------------------------------------------------------------------
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.790562	0.882995	0.000118
2	6	0	-0.175830	-0.402429	-0.000092
3	6	0	1.213644	-0.589990	0.000004
4	6	0	1.943284	0.604367	-0.000270
5	6	0	1.313545	1.875074	-0.000158
6	6	0	-0.082378	2.112167	0.000070
7	6	0	-2.390482	-0.593055	-0.000392
8	7	0	-1.216031	-1.328872	0.000958
9	7	0	-2.196089	0.695438	0.000239
10	6	0	1.847526	-1.959878	0.000254
11	1	0	-3.356785	-1.087848	-0.000577
12	1	0	-1.141059	-2.336065	-0.005390
13	1	0	2.942208	-1.879125	-0.000064
14	1	0	1.567327	-2.556831	0.884967
15	1	0	1.567026	-2.557547	-0.883910
16	1	0	3.037114	0.541975	-0.000355
17	1	0	1.996521	2.733963	-0.000255

CH3-deprotonated amino N7H B (B-15) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -418.588396752
Zero-point correction=                           0.129786
(Hartree/Particle)
 Thermal correction to Energy=                    0.137759
 Thermal correction to Enthalpy=                  0.138703
 Thermal correction to Gibbs Free Energy=         0.097653
 Sum of electronic and zero-point Energies=           -418.458610
 Sum of electronic and thermal Energies=              -418.450638
 Sum of electronic and thermal Enthalpies=            -418.449694
 Sum of electronic and thermal Free Energies=         -418.490744
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.445	32.499	86.397

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.705511	-0.859948	-0.000045
2	6	0	-0.185937	0.446725	-0.000055
3	6	0	1.204288	0.815587	0.000122
4	6	0	2.038309	-0.359646	0.000323
5	6	0	1.532810	-1.667990	0.000336
6	6	0	0.164432	-1.977429	0.000157
7	6	0	-2.408625	0.463202	-0.000384
8	7	0	-1.304001	1.272947	-0.000276
9	7	0	-2.103758	-0.817713	-0.000254
10	6	0	1.648197	2.140061	0.000097
11	1	0	-3.414879	0.866937	-0.000560
12	1	0	3.118652	-0.213494	0.000469

13	1	0	2.253409	-2.488358	0.000496
14	1	0	-0.211437	-2.996290	0.000171
15	1	0	-1.287567	2.281545	-0.000338
16	1	0	2.709368	2.376978	0.000230
17	1	0	0.958989	2.982666	-0.000069

N7-protonated amino N7H B (B-16) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -419.511158580
Zero-point correction=                           0.158377
(Hartree/Particle)
 Thermal correction to Energy=                    0.166582
 Thermal correction to Enthalpy=                  0.167526
 Thermal correction to Gibbs Free Energy=         0.125024
 Sum of electronic and zero-point Energies=           -419.352781
 Sum of electronic and thermal Energies=              -419.344576
 Sum of electronic and thermal Enthalpies=            -419.343632
 Sum of electronic and thermal Free Energies=         -419.386135

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                104.532             32.151             89.454
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.743037	0.856862	-0.000024
2	6	0	-0.138506	-0.405584	-0.000058
3	6	0	1.228678	-0.634043	-0.000037
4	6	0	1.997110	0.550140	0.000006
5	6	0	1.421279	1.826266	0.000009
6	6	0	0.031810	2.008343	-0.000030
7	6	0	-2.477595	-0.465462	0.000045
8	7	0	-1.247980	-1.389888	-0.000042
9	7	0	-2.154884	0.753122	0.000061
10	6	0	1.846875	-2.009436	0.000041
11	1	0	-1.249103	-2.004279	0.827594
12	1	0	2.937509	-1.944122	-0.001436
13	1	0	1.557619	-2.586538	0.888231
14	1	0	1.555276	-2.587775	-0.886568
15	1	0	3.079640	0.459540	0.000032
16	1	0	2.071297	2.695793	0.000053
17	1	0	-0.424441	2.992349	0.000000
18	1	0	-3.458241	-0.926050	0.000084
19	1	0	-1.249203	-2.004076	-0.827834

Z13 (1,3-deazaadenine): neutral and protonated species

Amino N7H Z13 (Z13-1) B3LYP/6-31+G(d)

```
SCF Done:  E(RB+HF-LYP) =  -435.614774893
Zero-point correction=                           0.148954
(Hartree/Particle)
 Thermal correction to Energy=                    0.156626
 Thermal correction to Enthalpy=                  0.157570
 Thermal correction to Gibbs Free Energy=         0.117000
 Sum of electronic and zero-point Energies=           -435.465821
 Sum of electronic and thermal Energies=              -435.458149
 Sum of electronic and thermal Enthalpies=            -435.457205
 Sum of electronic and thermal Free Energies=         -435.497774

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  98.284             31.655             85.386
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 -------------------------------------------------------------------
    1          6             0       -0.154221   -0.458880    0.010484
    2          6             0       -0.703478    0.835341    0.030591
    3          6             0        1.460477    1.759782   -0.020240
    4          6             0        1.235164   -0.691088    0.010187
    5          6             0       -2.378807   -0.651033   -0.025211
    6          1             0        2.132957    2.611832   -0.036523
    7          1             0       -3.371883   -1.075901   -0.057736
    8          7             0       -1.237069   -1.342791   -0.027922
    9          7             0       -2.090851    0.653072    0.018414
   10          7             0        1.745786   -1.983455   -0.045470
   11          1             0        2.758388   -2.041352   -0.068306
   12          1             0        1.367714   -2.654268    0.615953
   13          6             0        2.019829    0.468080   -0.021030
   14          1             0        3.101315    0.364467   -0.034486
   15          6             0        0.086384    1.985041    0.019165
   16          1             0       -0.334654    2.984128    0.032455
   17          1             0       -2.786601    1.390965    0.031609
   18          1             0       -1.184390   -2.351107   -0.121797
 -------------------------------------------------------------------
```

Amino N7H Z13 (Z13-1) B3LYP/6-31+G(d) cpcm, water, RADII=UAKS

```
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -435.261959
 ------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -21.21
 ------------------------------------------------------------------
 Cavitation energy                         (kcal/mol) =      17.30
 Dispersion energy                         (kcal/mol) =     -20.85
 Repulsion energy                          (kcal/mol) =       4.70
 Total non electrostatic                   (kcal/mol) =       1.14
```

N7-protonated amino N9H Z13 (Z13-2) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -435.614774709
```

Zero-point correction= 0.148952
(Hartree/Particle)
Thermal correction to Energy= 0.156623
Thermal correction to Enthalpy= 0.157568
Thermal correction to Gibbs Free Energy= 0.116999
Sum of electronic and zero-point Energies= -435.465823
Sum of electronic and thermal Energies= -435.458151
Sum of electronic and thermal Enthalpies= -435.457207
Sum of electronic and thermal Free Energies= -435.497776

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	98.283	31.656	85.384

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.154225	-0.458617	0.010321
2	6	0	-0.703377	0.835600	0.030361
3	6	0	1.460832	1.759627	-0.020160
4	6	0	1.235040	-0.691176	0.010092
5	6	0	-2.378740	-0.650834	-0.025083
6	1	0	2.133445	2.611567	-0.036269
7	1	0	-3.371947	-1.075412	-0.057401
8	7	0	-1.237121	-1.342602	-0.027979
9	7	0	-2.090750	0.653325	0.018506
10	7	0	1.745010	-1.983964	-0.045204
11	1	0	2.757558	-2.042660	-0.068300
12	1	0	1.366314	-2.654566	0.616084
13	6	0	2.019984	0.467783	-0.020997
14	1	0	3.101447	0.364041	-0.034517
15	6	0	0.086795	1.985135	0.019035
16	1	0	-0.333983	2.984330	0.032339
17	1	0	-2.786609	1.391091	0.032535
18	1	0	-1.184068	-2.350807	-0.123147

N7-protonated amino N9H Z13 (Z13-2) B3LYP/6-31+G(d) cpcm, water, RADII=UAKS

Total free energy in solution:
with all non electrostatic terms (a.u.) = -435.717875
(Polarized solute)-Solvent (kcal/mol) = -69.38
Cavitation energy (kcal/mol) = 17.46
Dispersion energy (kcal/mol) = -21.66
Repulsion energy (kcal/mol) = 5.21
Total non electrostatic (kcal/mol) = 1.00

Adenine hydrogen-bonded to HF at N3: N7-protonated and N7-protonated-N9-deprotonated species

N7-protonated N9H-adenine HF hydrogen-bound to N3 (A-N3HF-1) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -568.156155523
Zero-point correction= 0.137790
(Hartree/Particle)
Thermal correction to Energy= 0.147286
Thermal correction to Enthalpy= 0.148230
Thermal correction to Gibbs Free Energy= 0.102911
Sum of electronic and zero-point Energies= -568.018366
Sum of electronic and thermal Energies= -568.008870
Sum of electronic and thermal Enthalpies= -568.007926
Sum of electronic and thermal Free Energies= -568.053244

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.423	36.407	95.381

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.702735	0.605684	0.000040
2	6	0	-0.553986	0.004886	-0.000007
3	6	0	0.316441	-2.036011	-0.000096
4	6	0	1.828572	-0.264261	0.000012
5	6	0	-0.855143	2.200468	0.000098
6	1	0	0.192194	-3.114544	-0.000151
7	1	0	-1.327059	3.173294	0.000141
8	7	0	1.570818	-1.584413	-0.000057
9	7	0	-0.809274	-1.302298	-0.000076
10	7	0	0.466675	1.984383	0.000105
11	7	0	-1.492229	1.029061	0.000031
12	7	0	3.113645	0.124844	0.000047
13	1	0	3.827321	-0.595649	0.000023
14	1	0	3.415978	1.087965	0.000101
15	1	0	1.153324	2.730570	0.000151
16	1	0	-2.502803	0.840200	0.000009
17	9	0	-3.413116	-0.839430	-0.000089
18	1	0	-2.620085	-1.392602	-0.000105

N9-deprotoanted N7-protonated N9H-adenine HF hydrogen-bound to N3 (A-N3HF-2) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -567.792267091
Zero-point correction= 0.124293
(Hartree/Particle)
Thermal correction to Energy= 0.133874
Thermal correction to Enthalpy= 0.134818
Thermal correction to Gibbs Free Energy= 0.088268
Sum of electronic and zero-point Energies= -567.667974
Sum of electronic and thermal Energies= -567.658393

```
 Sum of electronic and thermal Enthalpies=            -567.657449
 Sum of electronic and thermal Free Energies=         -567.703999

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  84.007             35.518             97.973

-------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 -------------------------------------------------------------------
      1          6           0       -0.986257    0.326712   -0.004977
      2          6           0        0.395047    0.594361    0.004226
      3          6           0        0.812527   -1.617432   -0.025390
      4          6           0       -1.416343   -1.010368    0.000048
      5          6           0       -0.567550    2.491817   -0.006920
      6          1           0        1.528450   -2.434410   -0.042072
      7          1           0       -0.766376    3.556020   -0.016527
      8          7           0       -0.483118   -1.971281   -0.019106
      9          7           0        1.320045   -0.385572   -0.004129
     10          7           0       -1.591147    1.574397   -0.005139
     11          7           0        0.628207    1.951880    0.007326
     12          7           0       -2.734903   -1.395929   -0.032937
     13          1           0       -2.884417   -2.385952    0.126288
     14          1           0       -3.429603   -0.793231    0.387667
     15          1           0       -2.574806    1.788692   -0.090557
     16          9           0        3.970013   -0.292018    0.022164
     17          1           0        2.998502   -0.227955    0.011694
 -------------------------------------------------------------------
```

Q hydrogen-bound to HF at N3: N7-protonated and N7-protonated-N9-deprotonated species

N7-protonated N9H-Q HF hydrogen-bound to N3 (Q-N3HF-1) B3LYP/6-31+G(d)

```
SCF Done:  E(RB3LYP) =  -536.074166096

Zero-point correction=                           0.160584
(Hartree/Particle)
 Thermal correction to Energy=                    0.170445
 Thermal correction to Enthalpy=                  0.171389
 Thermal correction to Gibbs Free Energy=         0.124932
 Sum of electronic and zero-point Energies=           -535.913582
 Sum of electronic and thermal Energies=              -535.903721
 Sum of electronic and thermal Enthalpies=            -535.902777
 Sum of electronic and thermal Free Energies=         -535.949234

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 106.956             37.335             97.779

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

Number	Number	Type	X	Y	Z
1	6	0	-0.710127	0.539677	0.000044
2	6	0	0.584048	0.007605	0.000029
3	6	0	-0.144632	-2.106723	-0.000082
4	6	0	-1.828299	-0.312071	0.000015
5	6	0	0.768258	2.214623	-0.000167
6	1	0	0.080284	-3.168908	-0.000244
7	1	0	1.186823	3.211521	0.000047
8	7	0	0.909200	-1.281486	-0.000042
9	7	0	-0.542059	1.926699	-0.000020
10	7	0	1.468235	1.082380	-0.000022
11	1	0	-1.276855	2.626108	-0.000067
12	9	0	3.493242	-0.687244	0.000136
13	1	0	2.724540	-1.272752	0.000069
14	6	0	-1.485534	-1.667443	-0.000070
15	1	0	-2.272404	-2.415288	-0.000208
16	1	0	2.487245	0.953909	-0.000109
17	6	0	-3.244589	0.189693	0.000114
18	1	0	-3.449178	0.801509	0.887990
19	1	0	-3.448324	0.804926	-0.885580
20	1	0	-3.953686	-0.641137	-0.001833

N9-deprotoanted N7-protonated N9H-Q HF hydrogen-bound to N3 (Q-N3HF-2) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -535.705164777
Zero-point correction= 0.146666
(Hartree/Particle)
Thermal correction to Energy= 0.156693
Thermal correction to Enthalpy= 0.157637
Thermal correction to Gibbs Free Energy= 0.109931
Sum of electronic and zero-point Energies= -535.558499
Sum of electronic and thermal Energies= -535.548472
Sum of electronic and thermal Enthalpies= -535.547528
Sum of electronic and thermal Free Energies= -535.595234

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	98.326	36.668	100.406

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.953945	0.334740	0.000000
2	6	0	-0.441835	0.580527	-0.000006
3	6	0	-0.872837	-1.647072	-0.000007
4	6	0	1.474820	-0.962732	0.000000
5	6	0	0.483441	2.497579	0.000000
6	1	0	-1.614941	-2.441296	-0.000010
7	1	0	0.664439	3.565083	0.000002
8	7	0	-1.355179	-0.400935	-0.000009

9	7	0	1.525023	1.595273	0.000004
10	7	0	-0.699840	1.937372	-0.000006
11	1	0	2.509521	1.821957	0.000010
12	9	0	-3.994145	-0.352391	0.000013
13	1	0	-3.022948	-0.255086	0.000001
14	6	0	0.498279	-1.963376	-0.000003
15	1	0	0.795747	-3.008241	-0.000005
16	6	0	2.953224	-1.249777	0.000007
17	1	0	3.442979	-0.822763	-0.885179
18	1	0	3.442944	-0.822890	0.885274
19	1	0	3.145318	-2.326551	-0.000067

Z1 hydrogen-bound to HF at N3: N7-protonated and N7-protonated-N9-deprotonated species

N7-protonated N9H-Z1 HF hydrogen-bound to N3 (Z1-N3HF-1) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -552.117429292

Zero-point correction= 0.149075
(Hartree/Particle)
Thermal correction to Energy= 0.159071
Thermal correction to Enthalpy= 0.160015
Thermal correction to Gibbs Free Energy= 0.113253
Sum of electronic and zero-point Energies= -551.968355
Sum of electronic and thermal Energies= -551.958358
Sum of electronic and thermal Enthalpies= -551.957414
Sum of electronic and thermal Free Energies= -552.004176

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	99.819	37.789	98.419

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.711951	0.577963	0.000095
2	6	0	0.563975	0.004634	0.000125
3	6	0	-0.208639	-2.089378	0.000077
4	6	0	-1.852390	-0.261174	0.000007
5	6	0	0.814087	2.210150	0.000034
6	1	0	-0.007554	-3.156152	0.000091
7	1	0	1.261327	3.194260	0.000030
8	7	0	0.871795	-1.286968	0.000135
9	7	0	-0.503649	1.961942	-0.000061
10	7	0	1.476673	1.056622	0.000080
11	7	0	-3.129236	0.189730	-0.000306
12	1	0	-3.901623	-0.462975	0.000291
13	1	0	-3.376435	1.167752	0.000408
14	1	0	-1.205137	2.693208	0.000115
15	1	0	2.491134	0.892041	-0.000059

16	9	0	3.441419	-0.769494	-0.000179
17	1	0	2.636794	-1.314214	-0.000169
18	6	0	-1.529870	-1.637004	0.000005
19	1	0	-2.331642	-2.368896	-0.000098

N9-deprotoanted N7-protonated N9H-Z1 HF hydrogen-bound to N3 (Z1-N3HF-2) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -551.744199222
Zero-point correction= 0.135835
(Hartree/Particle)
Thermal correction to Energy= 0.145555
Thermal correction to Enthalpy= 0.146499
Thermal correction to Gibbs Free Energy= 0.099842
Sum of electronic and zero-point Energies= -551.608365
Sum of electronic and thermal Energies= -551.598644
Sum of electronic and thermal Enthalpies= -551.597700
Sum of electronic and thermal Free Energies= -551.644357

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.337	36.521	98.198

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.976411	0.319843	-0.008034
2	6	0	0.411758	0.583534	0.001440
3	6	0	0.885595	-1.631378	-0.029780
4	6	0	-1.468433	-0.992587	0.000532
5	6	0	-0.547189	2.488304	-0.009390
6	1	0	1.640106	-2.413848	-0.041926
7	1	0	-0.745299	3.552675	-0.021149
8	7	0	1.349726	-0.377773	-0.006969
9	7	0	-1.574949	1.570635	-0.001120
10	7	0	0.643662	1.945883	0.005315
11	7	0	-2.827781	-1.281819	-0.033840
12	1	0	-3.067548	-2.249844	0.146256
13	1	0	-3.437226	-0.649291	0.471460
14	1	0	-2.553674	1.785338	-0.130375
15	9	0	3.975976	-0.278924	0.030379
16	1	0	3.000390	-0.203508	0.015560
17	6	0	-0.472767	-1.980782	-0.025556
18	1	0	-0.750454	-3.031288	-0.032210

Z hydrogen-bonded to HF at N3: neutral and N7-protonated-N9-deprotonated species

N9H-Z HF hydrogen-bound to N3 (Z-N3HF-1) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -551.759481990
Zero-point correction=   0.136180
(Hartree/Particle)
 Thermal correction to Energy=   0.145703
 Thermal correction to Enthalpy=   0.146647
 Thermal correction to Gibbs Free Energy=   0.100964
 Sum of electronic and zero-point Energies=   -551.623302
 Sum of electronic and thermal Energies=   -551.613779
 Sum of electronic and thermal Enthalpies=   -551.612835
 Sum of electronic and thermal Free Energies=   -551.658518

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.430	36.176	96.147

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.787945	0.615727	-0.004652
2	6	0	0.545203	0.158174	-0.000198
3	6	0	-0.086397	-1.994782	-0.005268
4	6	0	-1.763873	-0.408584	-0.002466
5	6	0	0.596545	2.392771	-0.001494
6	1	0	0.172252	-3.050065	-0.007112
7	1	0	1.063420	3.367494	-0.003052
8	7	0	-1.391789	-1.702728	-0.002698
9	7	0	0.932554	-1.132250	-0.001519
10	7	0	1.370939	1.244053	0.002935
11	7	0	-3.102454	-0.153005	-0.034072
12	9	0	3.476974	-0.842276	0.007680
13	1	0	2.544122	-1.175708	0.003425
14	1	0	2.383201	1.175457	0.004153
15	6	0	-0.734873	2.051784	-0.006174
16	1	0	-1.560753	2.750059	-0.017989
17	1	0	-3.722812	-0.936163	0.123753
18	1	0	-3.448911	0.766371	0.196688

N9-deprotonated N9H-Z HF hydrogen-bound to N3 (Z-N3HF-2) B3LYP/6-31+G(d)

SCF Done: E(RB3LYP) = -551.214184424
Zero-point correction=   0.122028
(Hartree/Particle)
 Thermal correction to Energy=   0.131167
 Thermal correction to Enthalpy=   0.132111
 Thermal correction to Gibbs Free Energy=   0.086870
 Sum of electronic and zero-point Energies=   -551.092156
 Sum of electronic and thermal Energies=   -551.083018
 Sum of electronic and thermal Enthalpies=   -551.082073
 Sum of electronic and thermal Free Energies=   -551.127314

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

Total	82.308	34.368	95.218

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.030413	0.342795	-0.020060
2	6	0	-0.379007	0.655238	-0.005941
3	6	0	-0.853556	-1.577611	-0.016997
4	6	0	1.372517	-1.013828	-0.014887
5	6	0	0.644299	2.536572	0.005600
6	1	0	-1.599765	-2.369863	-0.019720
7	1	0	0.746996	3.619409	0.011631
8	7	0	0.433426	-1.975963	-0.013265
9	7	0	-1.320809	-0.332674	-0.008968
10	7	0	-0.607995	1.982221	0.009556
11	7	0	2.703361	-1.448519	-0.050843
12	1	0	2.800933	-2.406575	0.269114
13	1	0	3.358571	-0.816367	0.394904
14	9	0	-3.855557	-0.280256	0.022561
15	1	0	-2.836536	-0.201524	0.009071
16	6	0	1.688809	1.607652	-0.011723
17	1	0	2.753065	1.816851	-0.039369

N1 protonated adenine (cpcm calculations in water)

N1-protonated N9H-adenine (A-1) B3LYP/6-31+G(d) (cpcm, water, RADII=UAKS)

```
B3LYP/6-31+G* scrf=(read,cpcm,solvent=water) RADII=UAKS

SCF Done:  E(RB+HF-LYP) =  -467.819505843     A.U.
Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -467.818917
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent                (kcal/mol) =     -74.62
 ---------------------------------------------------------------------
 Cavitation energy                         (kcal/mol) =      16.47
 Dispersion energy                         (kcal/mol) =     -21.46
 Repulsion energy                          (kcal/mol) =       5.36
 Total non electrostatic                   (kcal/mol) =       0.37
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.734051    0.780031    0.000000
    2          6             0       -0.220977   -0.525437    0.000000
    3          6             0        1.175335   -0.685161    0.000000
    4          6             0        1.262181    1.743391    0.000000
    5          6             0       -2.325241   -0.747580    0.000000
    6          1             0        1.941759    2.589352    0.000000
    7          1             0       -3.330153   -1.148743    0.000000
```

8	7	0	1.869922	0.498898	0.000000
9	7	0	-0.024130	1.930110	0.000000
10	7	0	-1.223488	-1.462505	0.000000
11	7	0	-2.086594	0.614838	0.000000
12	7	0	1.794125	-1.864990	0.000000
13	1	0	2.800194	-1.974456	0.000004
14	1	0	1.229318	-2.708138	0.000000
15	1	0	-2.779608	1.356180	0.000000
16	1	0	2.886164	0.479884	-0.000002

N9-deprotonated N1-protonated N9H-adenine (neutral) (A-2) B3LYP/6-31+G(d) (cpcm, water, RADII=UAKS)

SCF Done: E(RB+HF-LYP) = -467.356678961 A.U.

Total free energy in solution:
with all non electrostatic terms (a.u.) = -467.355590

(Polarized solute)-Solvent	(kcal/mol) =	-39.11
Cavitation energy	(kcal/mol) =	16.41
Dispersion energy	(kcal/mol) =	-20.33
Repulsion energy	(kcal/mol) =	4.61
Total non electrostatic	(kcal/mol) =	0.68

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.810944	0.802569	-0.006850
2	6	0	-0.254140	-0.524888	-0.012005
3	6	0	1.117571	-0.684413	-0.003859
4	6	0	1.234375	1.736197	0.004785
5	6	0	-2.343517	-0.645029	0.008056
6	1	0	1.927849	2.571964	0.011843
7	1	0	-3.346808	-1.056551	0.017012
8	7	0	1.838060	0.485162	0.000107
9	7	0	-0.046017	1.937064	0.003309
10	7	0	-1.264005	-1.443344	0.000544
11	7	0	-2.144568	0.706753	0.006973
12	7	0	1.772720	-1.885747	-0.064669
13	1	0	2.659361	-1.981556	0.416231
14	1	0	1.157114	-2.684862	0.048118
15	1	0	2.849084	0.445169	-0.057818