

**Supporting Information for Theoretical Studies of the  
Quinolinic Acid to Nicotinic Acid Mononucleotide  
Transformation**

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## Table of Contents

**Structure numbers refer to structures on pages S5-S6, not structure numbers in manuscript.**

FULL REFERENCES FROM MANUSCRIPT ..... S7

### B3LYP/6-31+G\* CALCULATIONS

QUINOLINIC ACID NEUTRAL: PYRIDINE-2,3-DICARBOXYLIC ACID (1) ..... S8  
 QUINOLINIC ACID ANION: DEPROTONATED 3 CARBOXYL (2) ..... S8  
 QUINOLINIC ACID ANION: DEPROTONATED 2 CARBOXYL (3) ..... S9  
 QUINOLINIC ACID DIANION: DEPROTONATED 2&3 CARBOXYL (4) ..... S10

QUINOLINIC ACID CATION: PROTONATED N1 (1A) ..... S10  
 QUINOLINIC ACID ZWITTERION: DEPROTONATED 3 CARBOXYL & PROTONATED N1 (2A) ..... S11  
 QUINOLINIC ACID ZWITTERION: DEPROTONATED 2CARBOXYL & PROTONATED N1 (3A) ..... S12  
 QUINOLINIC ACID ZWITTERION: DEPROTONATED 2&3 CARBOXYL & PROTONATED N1 (4A) ... S12

QUINOLINIC ACID CATION: METHYLATED N1 (1B) ..... S13  
 QUINOLINIC ACID ZWITTERION: DEPROTONATED 3 CARBOXYL & METHYLATED N1 (2B) ..... S14  
 QUINOLINIC ACID ZWITTERION: DEPROTONATED 2CARBOXYL & METHYLATED N1 (3B) ..... S15  
 QUINOLINIC ACID ZWITTERION: DEPROTONATED 2&3 CARBOXYL & METHYLATED N1 (4B) ... S15

QUINOLINIC ACID CATION: THF ON N1 (1C) ..... S16  
 QUINOLINIC ACID ZWITTERION: DEPROTONATED 3 CARBOXYL & THF ON N1 (2C) ..... S17  
 QUINOLINIC ACID ZWITTERION: DEPROTONATED 2CARBOXYL & THF ON N1 (3C) ..... S18  
 QUINOLINIC ACID ZWITTERION: DEPROTONATED 2&3 CARBOXYL & THF ON N1 (4C) ..... S19

PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARXBOXYL (5) ..... S20  
 PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 (6) ..... S20  
 PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & 2 CARXBOXYL (7) ..... S21  
 PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 (8) ..... S21

PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED 3 CARXBOXYL (5A) ..... S22  
 PYRIDINE-3-CARBOXYLIC ACID (6A) ..... S23  
 PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED 2 CARXBOXYL (7A) ..... S23

PYRIDINE-3-CARBOXYLIC ACID: METHYLATED N1 (9A) ..... S24  
 PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARXBOXYL/METHYLATED N1 (10A) S25  
 PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED 3 CARBOXYL & METHYLATED N1 (11A) .... S25  
 PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & METHYLATED N1 (12A) ..... S26

PYRIDINE-2-CARBOXYLIC ACID: METHYLATED N1 (13A) ..... S27  
 PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & 2 CARXBOXYL/METHYLATED N1 (14A) S28  
 PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED 2 CARBOXYL & METHYLATED N1 (15A) .... S28  
 PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & METHYLATED N1 (16A) ..... S29

PYRIDINE-3-CARBOXYLIC ACID: THF ON N1 (9B) ..... S30  
 PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARXBOXYL & THF ON N1 (10B) .. S31  
 PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED 3 CARBOXYL & THF ON N1 (11B) ..... S31  
 PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & THF ON N1 (12B) ..... S32

PYRIDINE-2-CARBOXYLIC ACID: THF ON N1 (13B) ..... S33  
 PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & 2 CARXBOXYL & THF ON N1 (14B) .. S34

PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED 2 CARBOXYL & THF ON N1 (15B) .....	S35
PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & THF ON N1 (16B) .....	S36
METHYL CATION (17) .....	S36
THF CATION (18) .....	S37
CARBON DIOXIDE (19) .....	S38

### B3LYP/6-31+G\* TRANSITION STATE CALCULATIONS

QUINOLINIC ACID CATION: METHYLATED N1 (1B)	
NITROGEN-METHYL BOND FROZEN TO 1.5A° , 1.7A° , 1.9A° , 2.1A° , 2.3A° .....	S39-S41
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2CARBOXYL & METHYLATED N1 (3B)	
C2 CARBON-CARBOXYL BOND FROZEN TO 1.55 A° , 1.75 A° , 1.85 A° , 1.95 A° , 2.05 A° , 2.15 A° , 2.3 A° , 2.4 A° , 2.5 A° .....	S42-S46
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2CARBOXYL & METHYLATED N1 (3B)	
TRANSITION STATE CALCULATION .....	S47
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2&3 CARBOXYL & METHYLATED N1 (4B)	
C2 CARBON-CARBOXYL BOND FROZEN TO 1.55 A° , 1.75 A° , 1.8 A° , 1.85 A° , 1.9 A° , 1.95 A° , 2.05 A° , 2.1 A° , 2.15 A° , 2.2 A° , 2.3 A° , 2.4 A° , 2.5 A° , 2.6 A° , 2.7 A° , 2.8 A° .....	S48-S56
QUINOLINIC ACID ZWITTERION: DEPROTONATED CARBOXYL 2 OR 3 & THF ON N1 (2C OR 3C) C2 CARBON-CARBOXYL BOND FROZEN TO 1.55 A° , 1.75 A° , 1.85 A° , 1.95 A° , 2.05 A° , 2.15 A° , 2.3 A° , 2.4 A° , 2.5 A° , .....	S57-S64
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2 OR 3 CARBOXYL & THF ON N1 (2C OR 3C) TRANSITION STATE CALCULATION .....	S64

### B3LYP/6-31+G\* C-PCM CALCULATIONS IN WATER

QUINOLINIC ACID NEUTRAL: PYRIDINE-2,3-DICARBOXYLIC ACID (1) .....	S66
QUINOLINIC ACID ANION: DEPROTONATED 2 OR 3 CARBOXYL (2 OR 3) .....	S66
QUINOLINIC ACID DIANION: DEPROTONATED 2&3 CARBOXYL (4) .....	S66
QUINOLINIC ACID CATION: THF ON N1 (1C) .....	S67
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2OR3 CARBOXYL & THF ON N1 (2C OR 3C)	S68
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2&3 CARBOXYL & THF ON N1 (4C) .....	S69
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARXBOXYL (5) .....	S70
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 (6) .....	S70
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED 3 CARXBOXYL (5A) .....	S71
PYRIDINE-3-CARBOXYLIC ACID (6A) .....	S72
PYRIDINE-3-CARBOXYLIC ACID: THF ON N1 (9B) .....	S72
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARXBOXYL & THF ON N1 (10B) ..	S73
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED 3 CARBOXYL & THF ON N1 (11B) .....	S74
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & THF ON N1 (12B) .....	S75
PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & 2 CARXBOXYL (7) .....	S76
PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 (8) .....	S76
PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & 2 CARXBOXYL & THF ON N1 (14B) ..	S77
PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & THF ON N1 (16B) .....	S78

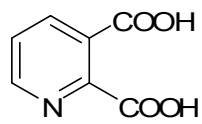
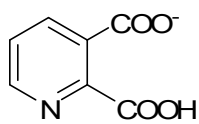
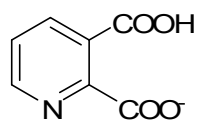
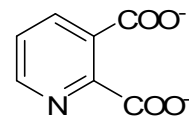
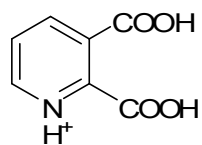
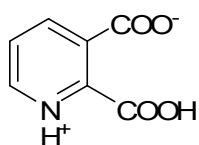
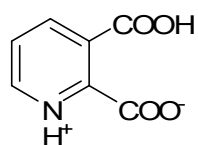
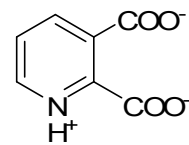
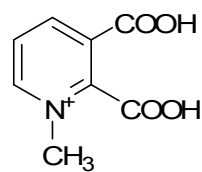
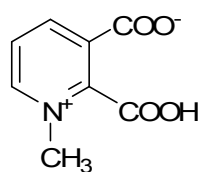
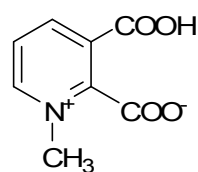
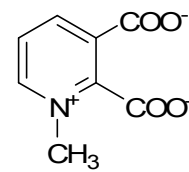
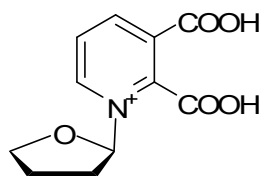
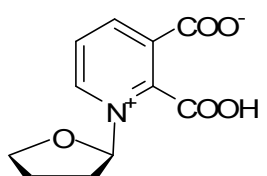
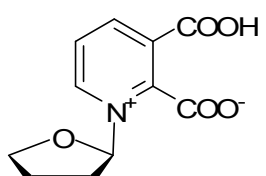
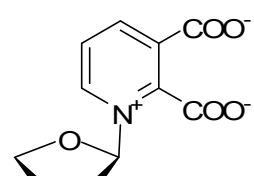
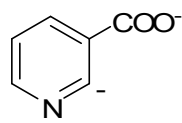
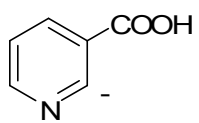
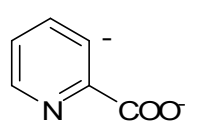
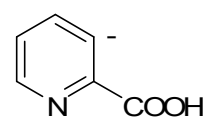
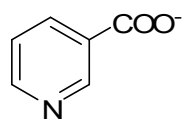
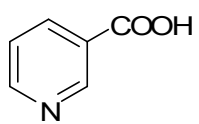
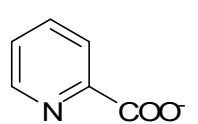
QUINOLINIC ACID ZWITTERION: DEPROTONATED CARBOXYL 2 OR 3 & THF ON N1 (2C OR 3C) TRANSITION STATE SINGLE POINT .....	S79
THF CATION (18) .....	S80
CARBON DIOXIDE (19) .....	S80

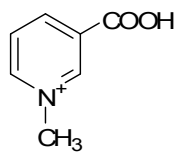
#### MP2/6-31+G\* SINGLE POINT CALCULATIONS

QUINOLINIC ACID NEUTRAL: PYRIDINE-2,3-DICARBOXYLIC ACID (1) .....	S82
QUINOLINIC ACID ANION: DEPROTONATED 2 OR 3 CARBOXYL (2 OR 3) .....	S82
QUINOLINIC ACID DIANION: DEPROTONATED 2&3 CARBOXYL (4) .....	S82
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED 3 CARBOXYL (5A) .....	S82
PYRIDINE-3-CARBOXYLIC ACID (6A) .....	S82
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARBOXYL (5) .....	S82
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 (6) .....	S82
PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & 2 CARBOXYL (7) .....	S82
PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 (8) .....	S83
QUINOLINIC ACID CATION: THF ON N1 (1C) .....	S83
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2 OR 3 CARBOXYL & THF ON N1 (2C/3C) ..	S83
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2&3 CARBOXYL & THF ON N1 (4C) .....	S83
PYRIDINE-3-CARBOXYLIC ACID: THF ON N1 (9B) .....	S83
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARBOXYL & THF ON N1 (10B) ..	S83
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED 3 CARBOXYL & THF ON N1 (11B) .....	S83
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & THF ON N1 (12B) .....	S83
PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & 2 CARBOXYL & THF ON N1 (14B) ..	S83
PYRIDINE-2-CARBOXYLIC ACID: DEPROTONATED C3 & THF ON N1 (16B) .....	S84
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2 OR 3 CARBOXYL & THF ON N1 (2C OR 3C) TRANSITION STATE CALCULATION .....	S84
THF CATION (18) .....	S84
CARBON DIOXIDE (19) .....	S84

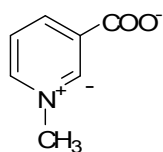
#### B3LYP/6-31+G\* CALCULATIONS FOR COMPLEXED STRUCTURES

QUINOLINIC ACID ANION: DEPROTONATED 2 CARBOXYL COMPLEXED WITH AMMONIUM (20) ..	S85
QUINOLINIC ACID ANION: DEPROTONATED 2&3 CARBOXYL COMPLEXED WITH AMMONIUM (21)	S86
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED 3 CARBOXYL COMPLEXED WITH AMMONIUM (22) .....	S86
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 COMPLEXED WITH AMMONIUM (20A) .....	S87
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARBOXYL COMPLEXED WITH AMMONIUM (21A) .....	S88
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2 CARBOXYL & THF ON N1 COMPLEXED WITH AMMONIUM (22) .....	S89
QUINOLINIC ACID ZWITTERION: DEPROTONATED 2&3 CARBOXYL & THF ON N1 COMPLEXED WITH AMMONIUM (23) .....	S90
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & THF ON N1 COMPLEXED WITH AMMONIUM (22A) .....	S91
PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARBOXYL & THF ON N1 COMPLEXED WITH AMMONIUM (23A) .....	S92

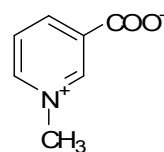
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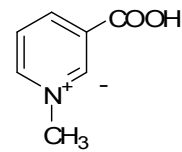
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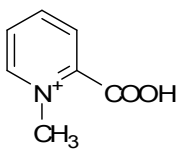
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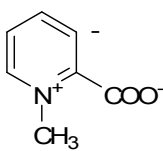
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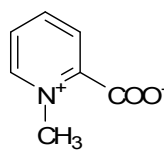
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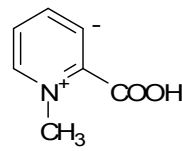
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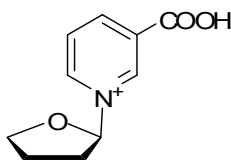
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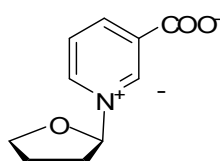
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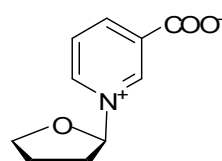
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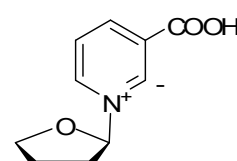
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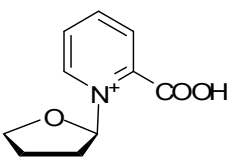
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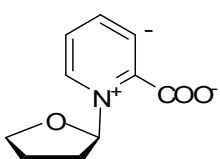
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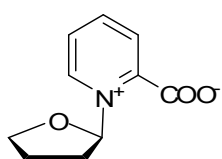
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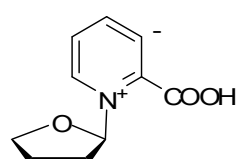
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14B



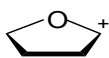
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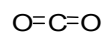
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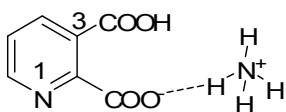
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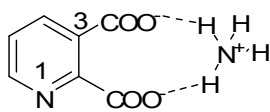
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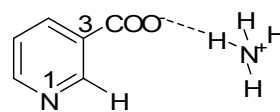
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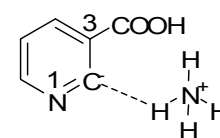
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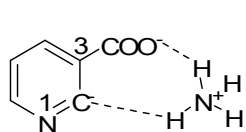
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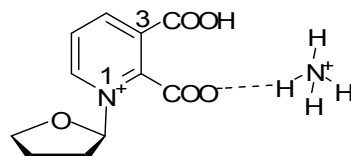
22



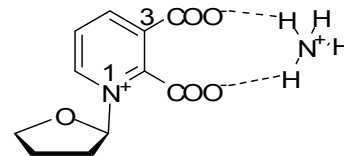
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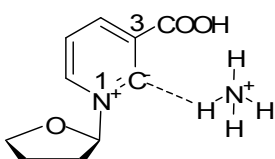
21A



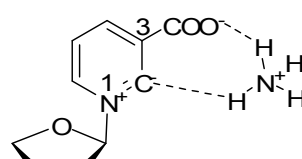
22



23



22A



23A

## Full References from Manuscript

Reference numbers refer to reference numbers in manuscript.

(17) Gerdes, S. Y.; Scholle, M. D.; D'Souza, M.; Bernal, A.; Baev, M. V.; Farrel, M.; Kurnasov, O. V.; Daugherty, M. D.; Mseeh, F.; Polanuyer, B. M.; Campbell, J. W.; Anantha, S.; Shatalin, K. Y.; Chowdhury, S. A.; Fonstein, M. Y.; Osterman, A. L. *J. Bacteriol.* **2002**, 184, 4555-4572.

(63) Schwarzenbacher, R.; Jaroszewski, L.; von Delft, F.; Abdubek, P.; Ambing, E.; Biorac, T.; Brinen, L. S.; Canaves, J. M.; Cambell, J.; Chiu, H.; Dai, X.; Deacon, A.; DiDonato, M.; Elsliger, M.; Eshagi, S.; Floyd, R.; Godzik, A.; Grittin, C.; Gzechnik, K.; Hampton, E.; Karlak, C.; Klock, H. E.; Koesema, E.; Kovarik, J. S.; Kreush, A.; Kuhn, P.. *Proteins: Struct. Funct. Bioinf.* **2004**, 55, 768-771.

(64) Frisch, M. J.; Trucks, G.W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; 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.; Peterson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nikai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; 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.; Salvador, P.; Dannenberg, J. J.; Zakrewski, V. G.; Dapprich, S.; Daniels, A.; Strain, M.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J.; Ortiz, J.; 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.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M.; Johnson, B.; Chen, W.; Wong, M.; Gonzalez, C.; Pople, J. A. GAUSSIAN03, Revision E.01; Gaussian, Inc., Wallingford CT, 2004.

**Quinolinic Acid Neutral: Pyridine-2,3-dicarboxylic acid (1)**

SCF Done: E(RB+HF-LYP) = -625.451309289

Zero-point correction= 0.118665 (Hartree/Particle)  
 Thermal correction to Energy= 0.127983  
 Thermal correction to Enthalpy= 0.128927  
 Thermal correction to Gibbs Free Energy= 0.082871  
 Sum of electronic and zero-point Energies= -625.332644  
 Sum of electronic and thermal Energies= -625.323327  
 Sum of electronic and thermal Enthalpies= -625.322382  
 Sum of electronic and thermal Free Energies= -625.368439

	E (E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	80.310	35.061	96.933

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.695099	0.011807	0.000045
2	6	0	-0.666224	0.395414	-0.000110
3	6	0	-0.913952	1.781290	-0.000169
4	6	0	0.124595	2.702163	-0.000047
5	6	0	1.433429	2.218274	0.000115
6	7	0	1.696724	0.914123	0.000160
7	1	0	-1.950735	2.099512	-0.000304
8	1	0	-0.071725	3.769853	-0.000082
9	1	0	2.291604	2.885661	0.000198
10	6	0	1.260254	-1.401906	0.000264
11	8	0	2.583982	-1.454574	0.000288
12	8	0	0.592717	-2.426056	0.000402
13	1	0	2.898298	-0.514608	0.000214
14	6	0	-1.956789	-0.445854	-0.000286
15	8	0	-1.895435	-1.766667	-0.000167
16	8	0	-3.024278	0.136031	-0.000536
17	1	0	-0.958865	-2.116271	0.000085

**Quinolinic Acid Anion: Deprotonated 3 Carboxyl (2)**

SCF Done: E(RB+HF-LYP) = -624.934277928

Zero-point correction= 0.103335 (Hartree/Particle)  
 Thermal correction to Energy= 0.112621  
 Thermal correction to Enthalpy= 0.113565  
 Thermal correction to Gibbs Free Energy= 0.067443  
 Sum of electronic and zero-point Energies= -624.830943  
 Sum of electronic and thermal Energies= -624.821657  
 Sum of electronic and thermal Enthalpies= -624.820713  
 Sum of electronic and thermal Free Energies= -624.866834

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.671	34.132	97.072



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.186756	-0.727492	-0.014935
2	6	0	-0.267082	0.690260	0.026123
3	6	0	-1.555521	1.250657	0.011866
4	6	0	-2.683779	0.448662	-0.098896
5	6	0	-2.488461	-0.931979	-0.175564
6	7	0	-1.287750	-1.500796	-0.113175
7	1	0	-1.624802	2.330997	0.090958
8	1	0	-3.684746	0.874453	-0.125891
9	1	0	-3.334506	-1.612348	-0.282789
10	6	0	0.881521	1.731490	0.055534
11	8	0	0.595469	2.853961	0.504412
12	8	0	2.006797	1.376189	-0.437510
13	6	0	1.092452	-1.582457	0.096619
14	8	0	1.024832	-2.712782	0.554751
15	8	0	2.218076	-1.061940	-0.347520
16	1	0	2.142670	-0.005802	-0.487587

### Quinolinic Acid Anion: Deprotonated 2 Carboxyl (3)

SCF Done: E(RB+HF-LYP) = -624.934277928

Zero-point correction= 0.103335 (Hartree/Particle)  
 Thermal correction to Energy= 0.112621  
 Thermal correction to Enthalpy= 0.113565  
 Thermal correction to Gibbs Free Energy= 0.067443  
 Sum of electronic and zero-point Energies= -624.830943  
 Sum of electronic and thermal Energies= -624.821657  
 Sum of electronic and thermal Enthalpies= -624.820713  
 Sum of electronic and thermal Free Energies= -624.866834

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.671	34.132	97.072

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.186756	-0.727492	-0.014935
2	6	0	-0.267082	0.690260	0.026123
3	6	0	-1.555521	1.250657	0.011866
4	6	0	-2.683779	0.448662	-0.098896
5	6	0	-2.488461	-0.931979	-0.175564
6	7	0	-1.287750	-1.500796	-0.113175
7	1	0	-1.624802	2.330997	0.090958
8	1	0	-3.684746	0.874453	-0.125891
9	1	0	-3.334506	-1.612348	-0.282789
10	6	0	0.881521	1.731490	0.055534
11	8	0	0.595469	2.853961	0.504412
12	8	0	2.006797	1.376189	-0.437510
13	6	0	1.092452	-1.582457	0.096619
14	8	0	1.024832	-2.712782	0.554751
15	8	0	2.218076	-1.061940	-0.347520

16            1            0            2.142670    -0.005802    -0.487587

### Quinolinic Acid Dianion: Deprotonated 2 & 3 Carboxyl (4)

SCF Done: E(RB+HF-LYP) = -624.248022638

Zero-point correction= 0.090716 (Hartree/Particle)  
 Thermal correction to Energy= 0.100494  
 Thermal correction to Enthalpy= 0.101438  
 Thermal correction to Gibbs Free Energy= 0.053850  
 Sum of electronic and zero-point Energies= -624.157307  
 Sum of electronic and thermal Energies= -624.147528  
 Sum of electronic and thermal Enthalpies= -624.146584  
 Sum of electronic and thermal Free Energies= -624.194173

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
-----					
1	6	0	0.068946	-0.742517	0.007025
2	6	0	-0.419190	0.597462	-0.036220
3	6	0	-1.806726	0.771285	-0.064414
4	6	0	-2.674456	-0.325799	-0.073576
5	6	0	-2.097337	-1.593236	-0.023012
6	7	0	-0.777409	-1.801593	0.023161
7	1	0	-2.188801	1.790124	-0.058649
8	1	0	-3.758495	-0.201963	-0.104999
9	1	0	-2.724405	-2.491162	-0.015427
10	6	0	0.422557	1.897736	-0.097919
11	8	0	1.344455	1.930212	-0.947652
12	8	0	0.019049	2.826416	0.665909
13	6	0	1.553108	-1.151737	0.132675
14	8	0	2.046708	-0.963445	1.277971
15	8	0	2.068808	-1.693809	-0.877530
-----					

### Quinolinic Acid Cation: Protonated N1 (1A)

SCF Done: E(RB+HF-LYP) = -625.763568319

Zero-point correction= 0.130862 (Hartree/Particle)  
 Thermal correction to Energy= 0.140960  
 Thermal correction to Enthalpy= 0.141905  
 Thermal correction to Gibbs Free Energy= 0.094483  
 Sum of electronic and zero-point Energies= -625.632707  
 Sum of electronic and thermal Energies= -625.622608  
 Sum of electronic and thermal Enthalpies= -625.621664  
 Sum of electronic and thermal Free Energies= -625.669086

Total	E (Thermal)		
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
	88.454	37.761	99.808

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.306498	0.604146	-0.000663
2	6	0	0.081054	-0.771765	-0.033748
3	6	0	1.205554	-1.620543	-0.098617
4	6	0	2.498880	-1.108661	-0.188545
5	6	0	2.675603	0.266210	-0.166761
6	7	0	1.592362	1.063124	-0.054808
7	1	0	1.035021	-2.692894	-0.071092
8	1	0	3.361306	-1.761829	-0.266200
9	1	0	3.639253	0.759371	-0.232530
10	6	0	-0.767172	1.675939	-0.011192
11	8	0	-0.588487	2.736485	0.786871
12	8	0	-1.683458	1.607775	-0.791814
13	1	0	-0.069453	2.555181	1.592573
14	6	0	-1.265391	-1.495183	0.133120
15	8	0	-2.350156	-1.025379	-0.466026
16	8	0	-1.258569	-2.506783	0.789839
17	1	0	-2.217483	-0.172146	-0.931648
18	1	0	1.740033	2.072814	-0.059967

**Quinolinic Acid Zwitterion: Deprotonated 3 Carboxyl & Protonated N1 (2A)**

SCF Done: E(RB+HF-LYP) = -625.439414544

Zero-point correction= 0.117539 (Hartree/Particle)  
 Thermal correction to Energy= 0.126825  
 Thermal correction to Enthalpy= 0.127769  
 Thermal correction to Gibbs Free Energy= 0.082047  
 Sum of electronic and zero-point Energies= -625.321875  
 Sum of electronic and thermal Energies= -625.312590  
 Sum of electronic and thermal Enthalpies= -625.311646  
 Sum of electronic and thermal Free Energies= -625.357367

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.638921	-0.170635	0.000139
2	6	0	0.584234	0.517263	-0.000179
3	6	0	0.535919	1.923005	-0.000017
4	6	0	-0.671071	2.623210	0.000214
5	6	0	-1.851936	1.898677	0.000382
6	7	0	-1.777373	0.560593	0.000395
7	1	0	1.487496	2.445858	-0.000127
8	1	0	-0.695304	3.707232	0.000274
9	1	0	-2.842779	2.338822	0.000527
10	6	0	2.007062	-0.076088	-0.000079
11	8	0	2.155205	-1.375606	0.001291
12	8	0	2.940556	0.707728	-0.001266

13	6	0	-1.019355	-1.698491	-0.000226
14	8	0	-0.075651	-2.521223	0.000241
15	8	0	-2.251445	-1.876924	-0.001077
16	1	0	1.261339	-1.899827	0.001353
17	1	0	-2.594040	-0.089678	0.000289

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**Quinolinic Acid Zwitterion: Deprotonated 2 Carboxyl & Protonated N1 (3A)**

SCF Done: E(RB+HF-LYP) = -625.439414570

Zero-point correction= 0.117540 (Hartree/Particle)  
 Thermal correction to Energy= 0.126825  
 Thermal correction to Enthalpy= 0.127769  
 Thermal correction to Gibbs Free Energy= 0.082048  
 Sum of electronic and zero-point Energies= -625.321875  
 Sum of electronic and thermal Energies= -625.312589  
 Sum of electronic and thermal Enthalpies= -625.311645  
 Sum of electronic and thermal Free Energies= -625.357367

	E (Thermal)		CV	S		
	KCal/Mol		Cal/Mol-Kelvin	Cal/Mol-Kelvin		
Total	79.584		34.842	96.229		

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.638862	-0.170820	-0.000142
2	6	0	-0.584062	0.517447	0.000113
3	6	0	-0.535286	1.923180	0.000313
4	6	0	0.671956	2.622964	0.000218
5	6	0	1.852579	1.898010	-0.000084
6	7	0	1.777587	0.559968	-0.000191
7	1	0	-1.486698	2.446333	0.000544
8	1	0	0.696580	3.706977	0.000326
9	1	0	2.843549	2.337882	-0.000147
10	6	0	-2.007044	-0.075472	-0.000128
11	8	0	-2.155539	-1.374922	-0.000202
12	8	0	-2.940298	0.708662	-0.000265
13	6	0	1.018717	-1.698767	0.000035
14	8	0	0.074702	-2.521140	0.000654
15	8	0	2.250746	-1.877641	-0.000313
16	1	0	-1.261763	-1.899269	-0.000009
17	1	0	2.594003	-0.090633	-0.000331

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 Carboxyl & Protonated N1 (4A)**

SCF Done: E(RB+HF-LYP) = -624.895125380

Zero-point correction= 0.103862 (Hartree/Particle)  
 Thermal correction to Energy= 0.113715  
 Thermal correction to Enthalpy= 0.114659  
 Thermal correction to Gibbs Free Energy= 0.066985  
 Sum of electronic and zero-point Energies= -624.791264

Sum of electronic and thermal Energies= -624.781411  
 Sum of electronic and thermal Enthalpies= -624.780466  
 Sum of electronic and thermal Free Energies= -624.828141

		E (Thermal)	CV	S		
		KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin		
Total		71.357	35.187	100.339		

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.600108	-0.236563	-0.000106
2	6	0	0.595062	0.505902	-0.000183
3	6	0	0.460046	1.908136	-0.000167
4	6	0	-0.784135	2.544297	-0.000073
5	6	0	-1.930308	1.762819	-0.000013
6	7	0	-1.776690	0.429138	-0.000059
7	1	0	1.367248	2.507603	-0.000210
8	1	0	-0.864792	3.627356	0.000073
9	1	0	-2.943373	2.149564	-0.000068
10	6	0	2.036292	-0.041631	-0.000004
11	8	0	2.529047	-0.160833	-1.142879
12	8	0	2.528853	-0.159853	1.143092
13	6	0	-0.882925	-1.779493	0.000056
14	8	0	-2.137708	-2.011254	0.000143
15	8	0	0.086002	-2.539466	0.000080
16	1	0	-2.535354	-0.298051	0.000061

### Quinolinic Acid Cation: Methylated N1 (1B)

SCF Done: E(RB+HF-LYP) = -665.079283191

Zero-point correction= 0.158133 (Hartree/Particle)  
 Thermal correction to Energy= 0.170254  
 Thermal correction to Enthalpy= 0.171199  
 Thermal correction to Gibbs Free Energy= 0.118565  
 Sum of electronic and zero-point Energies= -664.921150  
 Sum of electronic and thermal Energies= -664.909029  
 Sum of electronic and thermal Enthalpies= -664.908085  
 Sum of electronic and thermal Free Energies= -664.960718

		E (Thermal)	CV	S		
		KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin		
Total		106.836	43.948	110.776		

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.401792	-0.164668	0.033650
2	6	0	0.627234	0.770791	-0.057928
3	6	0	0.302388	2.135656	-0.104915
4	6	0	-1.032978	2.527688	-0.112384
5	6	0	-2.020361	1.556634	-0.043063
6	7	0	-1.705861	0.242115	0.036432
7	1	0	1.104523	2.867526	-0.132324

8	1	0	-1.318232	3.572814	-0.165474
9	1	0	-3.076877	1.797850	-0.044247
10	6	0	-0.141056	-1.666599	0.007521
11	8	0	0.133329	-2.280394	1.158393
12	8	0	-0.189367	-2.244497	-1.049191
13	1	0	0.224995	-1.679762	1.921836
14	6	0	2.103463	0.400537	-0.006401
15	8	0	2.529662	-0.639831	-0.736286
16	8	0	2.841903	1.041162	0.695277
17	1	0	1.879855	-0.989764	-1.374025
18	6	0	-2.802951	-0.768831	0.073851
19	1	0	-2.807960	-1.322075	-0.867565
20	1	0	-2.643768	-1.452165	0.909950
21	1	0	-3.749408	-0.247998	0.209293

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**Quinolinic Acid Zwitterion: Deprotonated 3 Carboxyl & Methylated N1 (2B)**

SCF Done: E(RB+HF-LYP) = -664.735825073

Zero-point correction= 0.146329 (Hartree/Particle)  
 Thermal correction to Energy= 0.157356  
 Thermal correction to Enthalpy= 0.158300  
 Thermal correction to Gibbs Free Energy= 0.109028  
 Sum of electronic and zero-point Energies= -664.589496  
 Sum of electronic and thermal Energies= -664.578469  
 Sum of electronic and thermal Enthalpies= -664.577525  
 Sum of electronic and thermal Free Energies= -664.626797

	E (Thermal)		CV		S
	KCal/Mol		Cal/Mol-Kelvin		Cal/Mol-Kelvin
Total	98.742		40.984		103.701

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.425213	-0.176854	0.001007
2	6	0	-0.739896	0.616170	0.021227
3	6	0	-0.615940	2.006661	0.011499
4	6	0	0.640674	2.607954	-0.080299
5	6	0	1.752899	1.797746	-0.144197
6	7	0	1.639508	0.446460	-0.089738
7	1	0	-1.522860	2.599669	0.070488
8	1	0	0.757206	3.685492	-0.111187
9	1	0	2.758647	2.189266	-0.236521
10	6	0	-2.186692	0.104221	0.065985
11	8	0	-2.464833	-1.085514	-0.427243
12	8	0	-3.040498	0.850208	0.507442
13	6	0	0.440348	-1.723030	0.119304
14	8	0	-0.219916	-2.298172	-0.787867
15	8	0	1.098952	-2.163124	1.066507
16	1	0	-1.642544	-1.606297	-0.712386
17	6	0	2.889483	-0.359581	-0.130683
18	1	0	3.035929	-0.838070	0.837024
19	1	0	2.796416	-1.130895	-0.896171

20            1            0            3.714473    0.308706    -0.376857

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**Quinolinic Acid Zwitterion: Deprotonated 2 Carboxyl & Methylated N1 (3B)**

SCF Done: E(RB+HF-LYP) = -664.735825122

Zero-point correction= 0.146329 (Hartree/Particle)  
 Thermal correction to Energy= 0.157356  
 Thermal correction to Enthalpy= 0.158300  
 Thermal correction to Gibbs Free Energy= 0.109028  
 Sum of electronic and zero-point Energies= -664.589493  
 Sum of electronic and thermal Energies= -664.578468  
 Sum of electronic and thermal Enthalpies= -664.577525  
 Sum of electronic and thermal Free Energies= -664.626797

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	98.824	41.232	103.897

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.425213	-0.176854	0.001007
2	6	0	-0.739896	0.616170	0.021227
3	6	0	-0.615940	2.006661	0.011499
4	6	0	0.640674	2.607954	-0.080299
5	6	0	1.752899	1.797746	-0.144197
6	7	0	1.639508	0.446460	-0.089738
7	1	0	-1.522860	2.599669	0.070488
8	1	0	0.757206	3.685492	-0.111187
9	1	0	2.758647	2.189266	-0.236521
10	6	0	-2.186692	0.104221	0.065985
11	8	0	-2.464833	-1.085514	-0.427243
12	8	0	-3.040498	0.850208	0.507442
13	6	0	0.440348	-1.723030	0.119304
14	8	0	-0.219916	-2.298172	-0.787867
15	8	0	1.098952	-2.163124	1.066507
16	1	0	-1.642544	-1.606297	-0.712386
17	6	0	2.889483	-0.359581	-0.130683
18	1	0	3.035929	-0.838070	0.837024
19	1	0	2.796416	-1.130895	-0.896171
20	1	0	3.714473	0.308706	-0.376857

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 Carboxyl & Methylated N1 (4B)**

SCF Done: E(RB+HF-LYP) = -664.193634429

Zero-point correction= 0.132294 (Hartree/Particle)  
 Thermal correction to Energy= 0.143897  
 Thermal correction to Enthalpy= 0.144841  
 Thermal correction to Gibbs Free Energy= 0.093150  
 Sum of electronic and zero-point Energies= -664.061341

Sum of electronic and thermal Energies= -664.049737  
 Sum of electronic and thermal Enthalpies= -664.048793  
 Sum of electronic and thermal Free Energies= -664.100484

			E (Thermal)	CV	S
			KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total			90.297	41.171	108.794

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.383095	-0.145299	-0.006633
2	6	0	0.879161	0.495008	-0.030073
3	6	0	0.920030	1.884669	-0.060575
4	6	0	-0.256307	2.650210	-0.097930
5	6	0	-1.463773	1.996505	-0.049008
6	7	0	-1.509855	0.634924	0.008872
7	1	0	1.900315	2.351742	-0.030537
8	1	0	-0.235014	3.735304	-0.140859
9	1	0	-2.419190	2.508033	-0.044707
10	6	0	2.238098	-0.266222	-0.075417
11	8	0	2.222380	-1.317380	-0.745089
12	8	0	3.169495	0.333405	0.518583
13	6	0	-0.657242	-1.663308	0.098053
14	8	0	-0.496733	-2.096555	1.258223
15	8	0	-1.130098	-2.181706	-0.935200
16	6	0	-2.835711	-0.017861	0.072453
17	1	0	-2.974689	-0.626723	-0.822086
18	1	0	-2.867859	-0.672571	0.945933
19	1	0	-3.601901	0.755426	0.152792

### Quinolinic Acid Cation: THF on N1 (1C)

SCF Done: E(RB+HF-LYP) = -857.050483525

Zero-point correction= 0.228659 (Hartree/Particle)  
 Thermal correction to Energy= 0.243489  
 Thermal correction to Enthalpy= 0.244434  
 Thermal correction to Gibbs Free Energy= 0.185517  
 Sum of electronic and zero-point Energies= -856.821825  
 Sum of electronic and thermal Energies= -856.806994  
 Sum of electronic and thermal Enthalpies= -856.806050  
 Sum of electronic and thermal Free Energies= -856.864967

			E (Thermal)	CV	S
			KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total			152.792	56.136	124.001

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.796931	-0.783351	-0.820349
2	6	0	2.297745	-1.079554	-0.618052
3	8	0	2.935536	0.782298	0.708683
4	6	0	3.898345	0.674725	-0.387314



5	6	0	1.928791	-0.149102	0.562047
6	6	0	-0.519275	2.690794	-0.087187
7	6	0	0.625395	1.947087	0.167905
8	7	0	0.574261	0.606931	0.285998
9	6	0	-0.609526	-0.067288	0.154783
10	6	0	-1.790953	0.628689	-0.116535
11	6	0	-1.732601	2.031971	-0.215196
12	6	0	-3.212098	0.051821	-0.181801
13	8	0	-4.091586	0.682390	0.350450
14	8	0	-3.448643	-1.070283	-0.858593
15	6	0	-0.622156	-1.574782	0.301805
16	8	0	-0.182949	-1.986382	1.490936
17	8	0	-1.031574	-2.298658	-0.579945
18	1	0	4.114094	-0.942626	-1.854384
19	1	0	4.409723	-1.417195	-0.171724
20	1	0	2.102144	-2.130012	-0.391615
21	1	0	1.726145	-0.814072	-1.514296
22	1	0	3.616980	1.373187	-1.185836
23	1	0	4.863258	0.967829	0.027104
24	1	0	-0.447040	3.770171	-0.165544
25	1	0	1.606660	2.383802	0.302664
26	1	0	-2.656485	2.578456	-0.375718
27	1	0	-2.640440	-1.509905	-1.192747
28	1	0	1.749807	-0.648387	1.513718
29	1	0	-0.274525	-2.960755	1.553520

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**Quinolinic Acid Zwitterion: Deprotonated 3 Carboxyl & THF on N1 (2C)**

SCF Done: E(RB+HF-LYP) = -856.688711258

Zero-point correction= 0.215876 (Hartree/Particle)  
 Thermal correction to Energy= 0.230105  
 Thermal correction to Enthalpy= 0.231049  
 Thermal correction to Gibbs Free Energy= 0.173639  
 Sum of electronic and zero-point Energies= -856.472835  
 Sum of electronic and thermal Energies= -856.458607  
 Sum of electronic and thermal Enthalpies= -856.457662  
 Sum of electronic and thermal Free Energies= -856.515073

	E (Thermal)		CV		S
	KCal/Mol		Cal/Mol-Kelvin		Cal/Mol-Kelvin
Total	144.393		53.899		120.830

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.719469	-0.792044	-0.864715
2	6	0	2.240565	-1.107768	-0.576409
3	8	0	2.927081	0.811513	0.653466
4	6	0	3.810178	0.683171	-0.489090
5	6	0	1.892222	-0.127164	0.568200
6	6	0	-0.564937	2.678653	-0.029238
7	6	0	0.591837	1.956612	0.184844
8	7	0	0.558335	0.609523	0.302004
9	6	0	-0.607298	-0.101925	0.211331
10	6	0	-1.804099	0.595060	-0.046350

11	6	0	-1.770954	1.989853	-0.138851
12	6	0	-3.200380	-0.017827	-0.226484
13	8	0	-4.165946	0.691613	-0.013316
14	8	0	-3.313040	-1.256807	-0.663143
15	6	0	-0.531927	-1.631553	0.460493
16	8	0	-0.036984	-1.959836	1.544655
17	8	0	-0.978220	-2.322110	-0.495759
18	1	0	3.993348	-0.983314	-1.906616
19	1	0	4.377671	-1.386324	-0.221817
20	1	0	2.067120	-2.141897	-0.276605
21	1	0	1.618341	-0.910938	-1.455847
22	1	0	3.462743	1.337957	-1.301860
23	1	0	4.795785	1.016563	-0.158332
24	1	0	-0.516253	3.759265	-0.105725
25	1	0	1.570412	2.404778	0.288886
26	1	0	-2.709377	2.511595	-0.295488
27	1	0	1.743676	-0.604769	1.534727
28	1	0	-2.422990	-1.734968	-0.744953

**Quinolinic Acid Zwitterion: Deprotonated 2 Carboxyl & THF on N1 (3C)**

SCF Done: E(RB+HF-LYP) = -856.688711273

Zero-point correction=	0.215873 (Hartree/Particle)
Thermal correction to Energy=	0.230102
Thermal correction to Enthalpy=	0.231047
Thermal correction to Gibbs Free Energy=	0.173628
Sum of electronic and zero-point Energies=	-856.472838
Sum of electronic and thermal Energies=	-856.458609
Sum of electronic and thermal Enthalpies=	-856.457665
Sum of electronic and thermal Free Energies=	-856.515084

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	144.391	53.899	120.849

Atomic Number	Atomic Number	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.719469	-0.792044	-0.864715
2	6	0	2.240565	-1.107768	-0.576409
3	8	0	2.927081	0.811513	0.653466
4	6	0	3.810178	0.683171	-0.489090
5	6	0	1.892222	-0.127164	0.568200
6	6	0	-0.564937	2.678653	-0.029238
7	6	0	0.591837	1.956612	0.184844
8	7	0	0.558335	0.609523	0.302004
9	6	0	-0.607298	-0.101925	0.211331
10	6	0	-1.804099	0.595060	-0.046350
11	6	0	-1.770954	1.989853	-0.138851
12	6	0	-3.200380	-0.017827	-0.226484
13	8	0	-4.165946	0.691613	-0.013316
14	8	0	-3.313040	-1.256807	-0.663143
15	6	0	-0.531927	-1.631553	0.460493

16	8	0	-0.036984	-1.959836	1.544655
17	8	0	-0.978220	-2.322110	-0.495759
18	1	0	3.993348	-0.983314	-1.906616
19	1	0	4.377671	-1.386324	-0.221817
20	1	0	2.067120	-2.141897	-0.276605
21	1	0	1.618341	-0.910938	-1.455847
22	1	0	3.462743	1.337957	-1.301860
23	1	0	4.795785	1.016563	-0.158332
24	1	0	-0.516253	3.759265	-0.105725
25	1	0	1.570412	2.404778	0.288886
26	1	0	-2.709377	2.511595	-0.295488
27	1	0	1.743676	-0.604769	1.534727
28	1	0	-2.422990	-1.734968	-0.744953

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 Carboxyl & THF on N1 (4C)**

SCF Done: E(RB+HF-LYP) = -856.144212546

Zero-point correction= 0.202042 (Hartree/Particle)  
 Thermal correction to Energy= 0.216697  
 Thermal correction to Enthalpy= 0.217641  
 Thermal correction to Gibbs Free Energy= 0.158592  
 Sum of electronic and zero-point Energies= -855.942171  
 Sum of electronic and thermal Energies= -855.927516  
 Sum of electronic and thermal Enthalpies= -855.926572  
 Sum of electronic and thermal Free Energies= -855.985620

	E (Thermal)		CV		S
	KCal/Mol		Cal/Mol-Kelvin	Cal/Mol-Kelvin	
Total	135.979		53.941	124.278	

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.741876	-0.656769	0.851259
2	6	0	-2.234662	-0.951713	0.775656
3	8	0	-2.842711	0.682439	-0.852414
4	6	0	-3.822047	0.721918	0.200988
5	6	0	-1.793908	-0.207754	-0.506916
6	6	0	0.598457	2.648049	-0.063283
7	6	0	-0.551344	1.920288	-0.265297
8	7	0	-0.502539	0.559542	-0.301964
9	6	0	0.668425	-0.143584	-0.179944
10	6	0	1.867077	0.574217	0.037447
11	6	0	1.808284	1.962623	0.114160
12	6	0	3.268531	-0.091867	0.134484
13	8	0	4.020002	0.431362	0.993892
14	8	0	3.467736	-0.991878	-0.706533
15	6	0	0.542739	-1.688073	-0.184645
16	8	0	0.169418	-2.194372	-1.266501
17	8	0	0.709733	-2.179417	0.949944
18	1	0	-4.124743	-0.667112	1.877594
19	1	0	-4.314318	-1.384105	0.263016
20	1	0	-1.988944	-2.012474	0.719589
21	1	0	-1.706185	-0.545775	1.644342

22	1	0	-3.574217	1.520841	0.918544
23	1	0	-4.782730	0.954792	-0.267582
24	1	0	0.544516	3.732722	-0.036738
25	1	0	-1.526280	2.358516	-0.422323
26	1	0	2.732124	2.491022	0.331772
27	1	0	-1.592924	-0.874299	-1.345037

**Pyridine-3-carboxylic acid: Deprotonated C2 & 3 Carboxyl (5)**

SCF Done: E(RB+HF-LYP) = -435.551878861

Zero-point correction= 0.074340 (Hartree/Particle)  
 Thermal correction to Energy= 0.081573  
 Thermal correction to Enthalpy= 0.082517  
 Thermal correction to Gibbs Free Energy= 0.040655  
 Sum of electronic and zero-point Energies= -435.477539  
 Sum of electronic and thermal Energies= -435.470306  
 Sum of electronic and thermal Enthalpies= -435.469362  
 Sum of electronic and thermal Free Energies= -435.511224

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	51.188	25.575	88.106

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.481496	-1.353612	-0.008975
2	6	0	-0.250707	-0.098645	-0.000977
3	6	0	0.406282	1.134658	0.006270
4	6	0	1.811220	1.178996	0.007599
5	6	0	2.481263	-0.042398	0.000452
6	7	0	1.865409	-1.244292	-0.007979
7	1	0	-0.168980	2.066995	0.010787
8	1	0	2.360384	2.125764	0.013766
9	1	0	3.582094	-0.061462	0.001242
10	8	0	-2.355345	-0.017722	1.133669
11	8	0	-2.355214	0.014356	-1.133003
12	6	0	-1.787370	-0.051385	-0.000248

**Pyridine-3-carboxylic acid: Deprotonated C2 (6)**

SCF Done: E(RB+HF-LYP) = -436.241001825

Zero-point correction= 0.088178 (Hartree/Particle)  
 Thermal correction to Energy= 0.095443  
 Thermal correction to Enthalpy= 0.096388  
 Thermal correction to Gibbs Free Energy= 0.055711  
 Sum of electronic and zero-point Energies= -436.152824  
 Sum of electronic and thermal Energies= -436.145558  
 Sum of electronic and thermal Enthalpies= -436.144614  
 Sum of electronic and thermal Free Energies= -436.185291

Center	Atomic	Atomic	Coordinates (Angstroms)		
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Number	Number	Type	X	Y	Z
1	6	0	0.447177	-1.330261	-0.000152
2	6	0	-0.180735	-0.035327	-0.000134
3	6	0	0.526916	1.182083	-0.000216
4	6	0	1.914911	1.135549	0.000114
5	6	0	2.508180	-0.137543	0.000256
6	7	0	1.842811	-1.295687	-0.000140
7	1	0	-0.009103	2.130989	-0.000596
8	1	0	2.523767	2.039125	0.000141
9	1	0	3.602459	-0.212645	0.000471
10	6	0	-1.653941	0.087040	-0.000005
11	8	0	-2.351507	-1.084983	0.000101
12	8	0	-2.287054	1.147634	0.000077
13	1	0	-3.283359	-0.798105	0.000366

### Pyridine-2-carboxylic acid: Deprotonated C3 & 2 Carboxyl (7)

SCF Done: E(RB+HF-LYP) = -435.558302654

Zero-point correction= 0.074877 (Hartree/Particle)  
 Thermal correction to Energy= 0.081901  
 Thermal correction to Enthalpy= 0.082845  
 Thermal correction to Gibbs Free Energy= 0.042669  
 Sum of electronic and zero-point Energies= -435.483426  
 Sum of electronic and thermal Energies= -435.476402  
 Sum of electronic and thermal Enthalpies= -435.475457  
 Sum of electronic and thermal Free Energies= -435.515634

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	51.394	25.188	84.558

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.236541	0.086605	-0.000194
2	6	0	0.457698	1.348819	-0.000198
3	6	0	1.855014	1.183987	-0.000086
4	6	0	2.496931	-0.075426	0.000093
5	6	0	1.684142	-1.205908	0.000074
6	7	0	0.340401	-1.144614	-0.000063
7	1	0	2.511002	2.071475	-0.000051
8	1	0	3.591114	-0.176275	0.000081
9	1	0	2.121547	-2.212632	0.000012
10	6	0	-1.777628	0.034034	-0.000017
11	8	0	-2.343002	0.005928	-1.134049
12	8	0	-2.342519	0.006206	1.134344

### Pyridine-2-carboxylic acid: Deprotonated C3 (8)

SCF Done: E(RB+HF-LYP) = -436.275417413

Zero-point correction= 0.087929 (Hartree/Particle)

Thermal correction to Energy= 0.094717  
 Thermal correction to Enthalpy= 0.095661  
 Thermal correction to Gibbs Free Energy= 0.056306  
 Sum of electronic and zero-point Energies= -436.187488  
 Sum of electronic and thermal Energies= -436.180701  
 Sum of electronic and thermal Enthalpies= -436.179757  
 Sum of electronic and thermal Free Energies= -436.219111

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	59.436	25.114	82.828

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.195354	-0.085623	-0.000714
2	6	0	0.346402	1.222977	-0.000359
3	6	0	1.753931	1.233027	0.000098
4	6	0	2.490809	0.040765	0.000251
5	6	0	1.798909	-1.177032	0.000210
6	7	0	0.463809	-1.261267	-0.000196
7	1	0	2.302342	2.180544	-0.000030
8	1	0	3.582433	0.041646	0.000383
9	1	0	2.342507	-2.124307	0.000352
10	6	0	-1.718121	-0.111245	-0.000075
11	8	0	-2.197159	1.140754	0.000344
12	8	0	-2.432980	-1.103069	0.000161
13	1	0	-1.292286	1.692283	0.000157

### Pyridine-3-carboxylic acid: Deprotonated 3 Carboxyl (5A)

SCF Done: E(RB+HF-LYP) = -436.338580453

Zero-point correction= 0.090314 (Hartree/Particle)  
 Thermal correction to Energy= 0.097179  
 Thermal correction to Enthalpy= 0.098123  
 Thermal correction to Gibbs Free Energy= 0.058216  
 Sum of electronic and zero-point Energies= -436.248267  
 Sum of electronic and thermal Energies= -436.241402  
 Sum of electronic and thermal Enthalpies= -436.240458  
 Sum of electronic and thermal Free Energies= -436.280365

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	60.980	25.117	83.991

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.473602	-1.182333	-0.000020
2	6	0	0.267102	0.009157	0.000002
3	6	0	-0.456301	1.205512	0.000065
4	6	0	-1.853063	1.164612	0.000011
5	6	0	-2.483494	-0.082073	-0.000034

6	7	0	-1.817787	-1.247427	-0.000007
7	1	0	0.101153	2.138502	0.000158
8	1	0	-2.447462	2.077230	0.000075
9	1	0	-3.572292	-0.152719	0.000008
10	6	0	1.818189	0.004438	-0.000107
11	8	0	2.354349	1.143759	-0.000057
12	8	0	2.353728	-1.133881	0.000111
13	1	0	0.065505	-2.125924	-0.000132

### Pyridine-3-carboxylic acid(6A)

SCF Done: E(RB+HF-LYP) = -436.876694881

Zero-point correction= 0.103780 (Hartree/Particle)  
 Thermal correction to Energy= 0.110810  
 Thermal correction to Enthalpy= 0.111755  
 Thermal correction to Gibbs Free Energy= 0.071721  
 Sum of electronic and zero-point Energies= -436.772915  
 Sum of electronic and thermal Energies= -436.765884  
 Sum of electronic and thermal Enthalpies= -436.764940  
 Sum of electronic and thermal Free Energies= -436.804973

	E (Thermal)		CV	S		
	KCal/Mol		Cal/Mol-Kelvin	Cal/Mol-Kelvin		
Total	69.535		26.331	84.257		

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.546814	-1.201354	0.000156
2	6	0	-0.208171	-0.017557	-0.000187
3	6	0	0.472666	1.206750	-0.000185
4	6	0	1.865353	1.191124	0.000040
5	6	0	2.519564	-0.044383	-0.000012
6	7	0	1.882821	-1.224828	0.000064
7	1	0	-0.079856	2.140467	-0.000261
8	1	0	2.436977	2.114581	0.000083
9	1	0	3.606947	-0.091802	-0.000033
10	6	0	-1.690112	-0.117117	0.000015
11	8	0	-2.299500	1.098349	0.000205
12	8	0	-2.320212	-1.156373	-0.000189
13	1	0	0.037590	-2.161402	0.000346
14	1	0	-3.260397	0.931364	0.000320

### Pyridine-2-carboxylic acid: Deprotonated 2 Carboxyl (7A)

SCF Done: E(RB+HF-LYP) = -436.326286352

Zero-point correction= 0.089691 (Hartree/Particle)  
 Thermal correction to Energy= 0.096713  
 Thermal correction to Enthalpy= 0.097657  
 Sum of electronic and zero-point Energies= -436.236596  
 Sum of electronic and thermal Energies= -436.229573

Sum of electronic and thermal Enthalpies= -436.228629  
 Sum of electronic and thermal Free Energies= -436.269909

		E (Thermal)	CV	S		
		KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin		
Total		60.688	25.334	86.880		

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.258132	-0.042749	-0.012083
2	6	0	0.437307	1.171170	0.163941
3	6	0	1.827976	1.174695	0.195926
4	6	0	2.507108	-0.035263	0.008990
5	6	0	1.737653	-1.183540	-0.188686
6	7	0	0.398292	-1.206310	-0.183282
7	1	0	2.378670	2.101943	0.352625
8	1	0	3.594178	-0.089298	0.012251
9	1	0	2.227473	-2.145528	-0.354619
10	6	0	-1.811811	-0.022680	-0.004759
11	8	0	-2.302796	1.056196	-0.442922
12	8	0	-2.382415	-1.040320	0.447070
13	1	0	-0.147280	2.080252	0.259568

### Pyridine-3-carboxylic acid: Methylated N1 (9A)

SCF Done: E(RB+HF-LYP) = -476.552412749

Zero-point correction= 0.145026 (Hartree/Particle)  
 Thermal correction to Energy= 0.153108  
 Thermal correction to Enthalpy= 0.154052  
 Thermal correction to Gibbs Free Energy= 0.111611  
 Sum of electronic and zero-point Energies= -476.407386  
 Sum of electronic and thermal Energies= -476.399304  
 Sum of electronic and thermal Enthalpies= -476.398360  
 Sum of electronic and thermal Free Energies= -476.440802

		E (Thermal)	CV	S		
		KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin		
Total		96.077	30.910	89.326		

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.432224	-0.784903	-0.000494
2	6	0	-0.604827	0.138652	-0.000008
3	6	0	-0.301453	1.505696	0.000268
4	6	0	1.037674	1.903005	0.000109
5	6	0	2.034125	0.940327	-0.000388
6	7	0	1.721461	-0.380311	-0.000754
7	1	0	-1.100752	2.239439	0.000444
8	1	0	1.315634	2.951397	0.000206
9	1	0	3.089109	1.187652	-0.000544
10	6	0	-2.004533	-0.414694	0.000014



11	8	0	-2.922572	0.561187	0.000232
12	8	0	-2.235530	-1.601552	-0.000122
13	6	0	2.794915	-1.410368	0.000777
14	1	0	-3.814524	0.160284	0.000258
15	1	0	3.764163	-0.913725	-0.016836
16	1	0	2.686678	-2.038489	-0.885693
17	1	0	2.706704	-2.015194	0.905620
18	1	0	0.238836	-1.852554	-0.000726

**Pyridine-3-carboxylic acid: Deprotonated C2 & 3 Carboxyl/Methylated N1 (10A)**

SCF Done: E(RB+HF-LYP) = -475.558538677

Zero-point correction= 0.116593 (Hartree/Particle)  
 Thermal correction to Energy= 0.125624  
 Thermal correction to Enthalpy= 0.126569  
 Thermal correction to Gibbs Free Energy= 0.080559  
 Sum of electronic and zero-point Energies= -475.441946  
 Sum of electronic and thermal Energies= -475.432914  
 Sum of electronic and thermal Enthalpies= -475.431970  
 Sum of electronic and thermal Free Energies= -475.477979

Total Center Number	Atomic Number	E (Thermal) KCal/Mol Atomic Type	CV		S
			Cal/Mol-Kelvin	Cal/Mol-Kelvin	Cal/Mol-Kelvin
			Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.361388	-0.956179	0.049206
2	6	0	0.641623	0.078223	0.004506
3	6	0	0.308188	1.427446	-0.042426
4	6	0	-1.041957	1.828994	-0.084090
5	6	0	-2.014497	0.861005	-0.051736
6	7	0	-1.640817	-0.462393	0.023746
7	1	0	1.094045	2.181592	-0.048462
8	1	0	-1.324720	2.877668	-0.139045
9	1	0	-3.078894	1.078930	-0.081554
10	6	0	2.123985	-0.309552	0.005714
11	8	0	2.586659	-0.632060	-1.118271
12	8	0	2.702824	-0.218467	1.119661
13	6	0	-2.740453	-1.437865	0.084360
14	1	0	-3.374267	-1.357988	-0.808388
15	1	0	-3.356429	-1.266408	0.976691
16	1	0	-2.282884	-2.425264	0.130225

**Pyridine-3-carboxylic acid: Deprotonated 3 Carboxyl & Methylated N1 (11A)**

SCF Done: E(RB+HF-LYP) = -476.145296655

Zero-point correction= 0.131219 (Hartree/Particle)  
 Thermal correction to Energy= 0.140149  
 Thermal correction to Enthalpy= 0.141093  
 Thermal correction to Gibbs Free Energy= 0.095864

Sum of electronic and zero-point Energies= -476.014078  
 Sum of electronic and thermal Energies= -476.005148  
 Sum of electronic and thermal Enthalpies= -476.004204  
 Sum of electronic and thermal Free Energies= -476.049433

			E (Thermal)	CV	S
			KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total			87.945	32.040	95.193

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.363727	-0.775478	-0.009674
2	6	0	0.667188	0.154050	-0.001462
3	6	0	0.333541	1.509069	0.002530
4	6	0	-1.013676	1.895867	-0.003695
5	6	0	-1.999115	0.926182	-0.010822
6	7	0	-1.663748	-0.392175	-0.013847
7	1	0	1.147431	2.229243	0.008561
8	1	0	-1.306274	2.941192	-0.005317
9	1	0	-3.059041	1.152689	-0.014859
10	6	0	2.144033	-0.357927	0.001050
11	8	0	2.989994	0.556711	0.020550
12	8	0	2.230149	-1.606782	-0.016506
13	6	0	-2.733042	-1.410848	0.022483
14	1	0	-3.539134	-1.116106	-0.652142
15	1	0	-3.117009	-1.504882	1.042026
16	1	0	-2.320697	-2.366208	-0.301676
17	1	0	-0.131392	-1.835623	-0.014483

**Pyridine-3-carboxylic acid: Deprotonated C2 & Methylated N1  
(12A)**

SCF Done: E(RB+HF-LYP) = -476.126706344

Zero-point correction= 0.131278 (Hartree/Particle)  
 Thermal correction to Energy= 0.139132  
 Thermal correction to Enthalpy= 0.140076  
 Thermal correction to Gibbs Free Energy= 0.098250  
 Sum of electronic and zero-point Energies= -475.995428  
 Sum of electronic and thermal Energies= -475.987574  
 Sum of electronic and thermal Enthalpies= -475.986630  
 Sum of electronic and thermal Free Energies= -476.028457

			E (Thermal)	CV	S
			KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total			87.307	29.924	88.032

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.344879	-0.855894	-0.000962
2	6	0	-0.606198	0.191770	-0.000116
3	6	0	-0.274495	1.541271	0.000124
4	6	0	1.082637	1.894696	0.000024

5	6	0	2.024127	0.886878	-0.000400
6	7	0	1.641280	-0.423400	-0.001073
7	1	0	-1.057035	2.295529	0.000407
8	1	0	1.405354	2.930366	-0.000044
9	1	0	3.089964	1.088509	-0.000296
10	6	0	-2.055501	-0.227805	0.000201
11	8	0	-2.225008	-1.558275	-0.000519
12	8	0	-2.983157	0.556499	0.000825
13	6	0	2.689474	-1.465742	0.001124
14	1	0	3.679755	-1.004702	-0.021295
15	1	0	2.554496	-2.102565	-0.874785
16	1	0	2.581671	-2.073409	0.901531
17	1	0	-1.307376	-1.946762	-0.000414

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**Pyridine-2-carboxylic acid: Methylated N1 (13A)**

SCF Done: E(RB+HF-LYP) = -476.528542630

Zero-point correction= 0.144701 (Hartree/Particle)  
 Thermal correction to Energy= 0.153555  
 Thermal correction to Enthalpy= 0.154499  
 Thermal correction to Gibbs Free Energy= 0.110605  
 Sum of electronic and zero-point Energies= -476.383841  
 Sum of electronic and thermal Energies= -476.374987  
 Sum of electronic and thermal Enthalpies= -476.374043  
 Sum of electronic and thermal Free Energies= -476.417937

	E (Thermal)		CV	S		
	KCal/Mol		Cal/Mol-Kelvin	Cal/Mol-Kelvin		
Total	96.357		33.241	92.383		

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.186739	-0.289219	-0.007806
2	6	0	-0.529840	-1.472956	0.130977
3	6	0	-1.926918	-1.450786	0.166099
4	6	0	-2.583760	-0.227790	0.047250
5	6	0	-1.830789	0.928601	-0.098263
6	7	0	-0.477547	0.899814	-0.118024
7	1	0	-2.486806	-2.373287	0.286496
8	1	0	-3.665768	-0.154717	0.065004
9	1	0	-2.288621	1.904986	-0.203784
10	6	0	1.702979	-0.273416	0.110361
11	8	0	2.373616	-1.177597	-0.615565
12	8	0	2.251909	0.481432	0.869200
13	6	0	0.257598	2.193455	-0.256227
14	1	0	-0.461387	2.958027	-0.546106
15	1	0	1.022395	2.098527	-1.027461
16	1	0	0.726337	2.441098	0.696200
17	1	0	0.010427	-2.407848	0.244533
18	1	0	1.825986	-1.643497	-1.272135

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**Pyridine-2-carboxylic acid: Deprotonated C3 & 2 Carboxyl/Methylated N1 (14A)**

SCF Done: E(RB+HF-LYP) = -475.547508577

Zero-point correction= 0.116691 (Hartree/Particle)  
 Thermal correction to Energy= 0.125698  
 Thermal correction to Enthalpy= 0.126642  
 Thermal correction to Gibbs Free Energy= 0.081350  
 Sum of electronic and zero-point Energies= -475.430818  
 Sum of electronic and thermal Energies= -475.421811  
 Sum of electronic and thermal Enthalpies= -475.420867  
 Sum of electronic and thermal Free Energies= -475.466159

Total	E (Thermal)		CV	S	
	KCal/Mol		Cal/Mol-Kelvin	Cal/Mol-Kelvin	
	78.876		31.817		95.325

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.164660	-0.447534	-0.001234
2	6	0	0.645296	-1.617837	-0.003638
3	6	0	2.018527	-1.329678	-0.002192
4	6	0	2.565163	-0.023975	0.001595
5	6	0	1.704253	1.047398	0.001935
6	7	0	0.356746	0.828240	-0.000154
7	1	0	2.739299	-2.155377	-0.004473
8	1	0	3.640123	0.160398	0.003293
9	1	0	2.025615	2.083911	0.003466
10	6	0	-1.700518	-0.486645	0.000360
11	8	0	-2.228171	-0.471998	1.140486
12	8	0	-2.232356	-0.464732	-1.137792
13	6	0	-0.549604	1.991677	-0.000445
14	1	0	-1.186938	1.947875	-0.886715
15	1	0	-1.186017	1.949195	0.886658
16	1	0	0.044174	2.909721	-0.001001

**Pyridine-2-carboxylic acid: Deprotonated 2 Carboxyl & Methylated N1 (15A)**

SCF Done: E(RB+HF-LYP) = -476.154825807

Zero-point correction= 0.131492 (Hartree/Particle)  
 Thermal correction to Energy= 0.140305  
 Thermal correction to Enthalpy= 0.141249  
 Thermal correction to Gibbs Free Energy= 0.096862  
 Sum of electronic and zero-point Energies= -476.023334  
 Sum of electronic and thermal Energies= -476.014521  
 Sum of electronic and thermal Enthalpies= -476.013576  
 Sum of electronic and thermal Free Energies= -476.057964

Total	E (Thermal)		CV	S	
	KCal/Mol		Cal/Mol-Kelvin	Cal/Mol-Kelvin	
	88.043		31.963		93.422

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.217147	-0.322460	0.034658
2	6	0	0.587415	-1.466716	0.151478
3	6	0	1.967096	-1.363767	0.162324
4	6	0	2.563414	-0.097257	0.021005
5	6	0	1.750491	1.005012	-0.111145
6	7	0	0.392507	0.888421	-0.087896
7	1	0	2.586019	-2.250766	0.264048
8	1	0	3.640267	0.029242	0.006613
9	1	0	2.140054	2.008018	-0.238430
10	6	0	-1.759603	-0.422952	0.034060
11	8	0	-2.313889	0.204864	0.958423
12	8	0	-2.181951	-1.131156	-0.898330
13	6	0	-0.440713	2.109883	-0.197650
14	1	0	0.218653	2.974199	-0.279805
15	1	0	-1.081573	2.171227	0.682698
16	1	0	-1.072297	2.033083	-1.085372
17	1	0	0.082320	-2.424072	0.216396

**Pyridine-2-carboxylic acid: Deprotonated C3 & Methylated N1  
(16A)**

SCF Done: E(RB+HF-LYP) = -476.106345483

Zero-point correction= 0.130543 (Hartree/Particle)  
 Thermal correction to Energy= 0.138997  
 Thermal correction to Enthalpy= 0.139941  
 Thermal correction to Gibbs Free Energy= 0.096836  
 Sum of electronic and zero-point Energies= -475.975803  
 Sum of electronic and thermal Energies= -475.967348  
 Sum of electronic and thermal Enthalpies= -475.966404  
 Sum of electronic and thermal Free Energies= -476.009509

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	87.222	31.584	90.722

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.193339	-0.266571	0.000042
2	6	0	-0.406803	-1.529827	0.000163
3	6	0	-1.814617	-1.513097	0.000127
4	6	0	-2.536368	-0.314459	-0.000134
5	6	0	-1.849130	0.889450	-0.000162
6	7	0	-0.495208	0.922543	-0.000043
7	1	0	-2.372024	-2.449985	0.000407
8	1	0	-3.623169	-0.290821	-0.000260
9	1	0	-2.352146	1.849010	-0.000253
10	6	0	1.718923	-0.284049	0.000004
11	8	0	2.157781	-1.530856	-0.000150
12	8	0	2.432578	0.705457	-0.000033

13	6	0	0.166723	2.252328	0.000144
14	1	0	0.797115	2.350655	0.882869
15	1	0	0.798017	2.350490	-0.881923
16	1	0	-0.613987	3.014831	-0.000262
17	1	0	1.277372	-2.081440	0.000081

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**Pyridine-3-carboxylic acid: THF on N1 (9B)**

SCF Done: E(RB+HF-LYP) = -668.510774097

Zero-point correction=	0.214717 (Hartree/Particle)
Thermal correction to Energy=	0.226650
Thermal correction to Enthalpy=	0.227594
Thermal correction to Gibbs Free Energy=	0.175354
Sum of electronic and zero-point Energies=	-668.296057
Sum of electronic and thermal Energies=	-668.284124
Sum of electronic and thermal Enthalpies=	-668.283180
Sum of electronic and thermal Free Energies=	-668.335420

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	142.225	45.793	109.949

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.672266	-0.451625	-0.328259
2	6	0	-1.876410	0.161491	-0.008361
3	6	0	-1.888052	1.536320	0.264020
4	6	0	-0.689947	2.248856	0.200506
5	6	0	0.484834	1.584614	-0.125249
6	7	0	0.474767	0.255349	-0.369881
7	1	0	-2.820438	2.032270	0.512610
8	1	0	-0.658414	3.315666	0.393642
9	1	0	1.448627	2.069179	-0.218404
10	6	0	-3.098669	-0.712661	0.017493
11	8	0	-4.204206	-0.015426	0.317550
12	8	0	-3.059025	-1.900740	-0.208587
13	1	0	-4.970226	-0.622915	0.321447
14	6	0	1.787926	-0.481775	-0.775078
15	8	0	2.809008	0.440835	-0.845489
16	6	0	2.182146	-1.541439	0.264568
17	1	0	1.556775	-0.874629	-1.769201
18	6	0	3.814223	0.193377	0.196578
19	6	0	3.141401	-0.761814	1.180330
20	1	0	2.709549	-2.344258	-0.262286
21	1	0	1.333815	-1.989614	0.787944
22	1	0	4.685381	-0.248169	-0.296333
23	1	0	4.091358	1.162552	0.616054
24	1	0	3.858984	-1.414619	1.683717
25	1	0	2.590344	-0.211391	1.951602
26	1	0	-0.626456	-1.510933	-0.558709

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**Pyridine-3-carboxylic acid: Deprotonated C2 & 3 Carboxyl & THF on N1 (10B)**

SCF Done: E(RB+HF-LYP) = -667.510517442

Zero-point correction= 0.186689 (Hartree/Particle)  
 Thermal correction to Energy= 0.198726  
 Thermal correction to Enthalpy= 0.199670  
 Thermal correction to Gibbs Free Energy= 0.145481  
 Sum of electronic and zero-point Energies= -667.323828  
 Sum of electronic and thermal Energies= -667.311792  
 Sum of electronic and thermal Enthalpies= -667.310848  
 Sum of electronic and thermal Free Energies= -667.365036

Center Number	Atomic Number	Atomic Type	E (Thermal)		
			KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total			124.702	44.390	114.049

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.424052	-1.319381	-0.479728
2	6	0	2.037485	-1.538584	0.164442
3	8	0	2.804602	0.685532	0.551274
4	6	0	3.477655	0.201840	-0.619922
5	6	0	1.709082	-0.181077	0.831885
6	6	0	-0.845196	2.246553	-0.395435
7	6	0	0.364744	1.706628	-0.026902
8	7	0	0.404369	0.385470	0.345277
9	6	0	-0.644598	-0.491327	0.400948
10	6	0	-1.893841	0.089039	0.000946
11	6	0	-1.990478	1.428601	-0.367065
12	6	0	-3.158214	-0.777959	-0.042264
13	8	0	-3.202241	-1.595163	-0.997502
14	8	0	-4.011145	-0.539042	0.852961
15	1	0	3.528808	-1.837748	-1.439525
16	1	0	4.230584	-1.659844	0.181877
17	1	0	2.034236	-2.349144	0.897102
18	1	0	1.259485	-1.773949	-0.564398
19	1	0	2.953242	0.541979	-1.526786
20	1	0	4.484813	0.629912	-0.611649
21	1	0	-0.897625	3.290917	-0.694213
22	1	0	1.297220	2.256427	-0.004209
23	1	0	-2.960913	1.847889	-0.629091
24	1	0	1.625692	-0.241337	1.918654

**Pyridine-3-carboxylic acid: Deprotonated 3 Carboxyl & THF on N1 (11B)**

SCF Done: E(RB+HF-LYP) = -668.098136835

Zero-point correction= 0.201158 (Hartree/Particle)  
 Thermal correction to Energy= 0.213000  
 Thermal correction to Enthalpy= 0.213944  
 Thermal correction to Gibbs Free Energy= 0.161576  
 Sum of electronic and zero-point Energies= -667.896979  
 Sum of electronic and thermal Energies= -667.885137

Sum of electronic and thermal Enthalpies= -667.884193  
 Sum of electronic and thermal Free Energies= -667.936561

		E (Thermal)	CV	S		
		KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin		
Total		133.659	44.699	110.218		

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.716366	-0.438850	-0.350438
2	6	0	-1.917679	0.163253	-0.012729
3	6	0	-1.909621	1.533819	0.264304
4	6	0	-0.710783	2.251155	0.190868
5	6	0	0.462589	1.593540	-0.145331
6	7	0	0.442371	0.262766	-0.398722
7	1	0	-2.854882	2.001419	0.526583
8	1	0	-0.673313	3.317845	0.388919
9	1	0	1.424519	2.078236	-0.240707
10	6	0	-3.208392	-0.713141	0.050968
11	8	0	-4.232568	-0.077447	0.368491
12	8	0	-3.000042	-1.917760	-0.222944
13	6	0	1.714270	-0.485842	-0.783613
14	8	0	2.783824	0.403807	-0.864823
15	6	0	2.087875	-1.540481	0.268431
16	1	0	1.506208	-0.897048	-1.774723
17	6	0	3.719940	0.194971	0.233380
18	6	0	3.011356	-0.747636	1.207460
19	1	0	2.638707	-2.343285	-0.234612
20	1	0	1.223228	-1.984887	0.765972
21	1	0	4.628798	-0.246283	-0.190501
22	1	0	3.963641	1.174783	0.653108
23	1	0	3.710464	-1.388997	1.751133
24	1	0	2.426548	-0.185450	1.944226
25	1	0	-0.699369	-1.499224	-0.583946

**Pyridine-3-carboxylic acid: Deprotonated C2 & THF on N1 (12B)**

SCF Done: E(RB+HF-LYP) = -668.079423474

Zero-point correction= 0.201246 (Hartree/Particle)  
 Thermal correction to Energy= 0.212938  
 Thermal correction to Enthalpy= 0.213882  
 Thermal correction to Gibbs Free Energy= 0.161894  
 Sum of electronic and zero-point Energies= -667.878177  
 Sum of electronic and thermal Energies= -667.866486  
 Sum of electronic and thermal Enthalpies= -667.865542  
 Sum of electronic and thermal Free Energies= -667.917529

		E (Thermal)	CV	S		
		KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin		
Total		133.620	44.599	109.417		

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



1	6	0	-3.602949	-1.156501	0.588572
2	6	0	-2.081472	-1.356350	0.499577
3	8	0	-2.721677	0.552692	-0.767888
4	6	0	-3.740112	0.322614	0.231770
5	6	0	-1.671816	-0.378610	-0.621709
6	6	0	0.827368	2.291866	0.229384
7	6	0	-0.359509	1.652734	-0.071942
8	7	0	-0.369907	0.313304	-0.312988
9	6	0	0.726114	-0.499579	-0.305360
10	6	0	1.929789	0.171618	0.007266
11	6	0	2.005791	1.534993	0.274857
12	6	0	3.178104	-0.673411	0.036210
13	8	0	2.955025	-1.964656	-0.256199
14	8	0	4.282038	-0.238836	0.297681
15	1	0	-4.005408	-1.393971	1.578359
16	1	0	-4.124939	-1.774780	-0.150897
17	1	0	-1.778819	-2.380174	0.272444
18	1	0	-1.592336	-1.066278	1.435977
19	1	0	-3.557441	0.969949	1.102258
20	1	0	-4.696384	0.597855	-0.219389
21	1	0	0.827066	3.360375	0.417136
22	1	0	-1.312203	2.161489	-0.147199
23	1	0	2.964586	1.991679	0.506305
24	1	0	-1.501511	-0.874527	-1.579890
25	1	0	1.975785	-2.034587	-0.424695

**Pyridine-2-carboxylic acid: THF on N1 (13B)**

SCF Done: E(RB+HF-LYP) = -668.500990110

Zero-point correction= 0.214705 (Hartree/Particle)  
 Thermal correction to Energy= 0.226583  
 Thermal correction to Enthalpy= 0.227528  
 Thermal correction to Gibbs Free Energy= 0.175532  
 Sum of electronic and zero-point Energies= -668.286285  
 Sum of electronic and thermal Energies= -668.274407  
 Sum of electronic and thermal Enthalpies= -668.273463  
 Sum of electronic and thermal Free Energies= -668.325458

Center Number	Atomic Number	Atomic Type	E (Thermal)	CV	S
			KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total			142.183	45.868	109.433

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.145901	-0.762620	0.770753
2	6	0	-1.644604	-1.097117	0.676257
3	8	0	-2.181752	0.632198	-0.859431
4	6	0	-3.204569	0.642759	0.183802
5	6	0	-1.192391	-0.284700	-0.558577
6	6	0	1.158340	2.656127	0.056189
7	6	0	0.060417	1.851505	-0.231963
8	7	0	0.146248	0.507489	-0.261253

9	6	0	1.348679	-0.105967	-0.027426
10	6	0	2.468820	0.661107	0.278542
11	6	0	2.381968	2.055595	0.325843
12	6	0	1.485089	-1.601776	-0.185753
13	8	0	2.610127	-2.039066	0.396625
14	8	0	0.706132	-2.303950	-0.788293
15	1	0	-3.519181	-0.808528	1.797407
16	1	0	-3.734914	-1.454603	0.160657
17	1	0	-1.449176	-2.161401	0.543407
18	1	0	-1.113671	-0.761216	1.574811
19	1	0	-2.961785	1.417896	0.922909
20	1	0	-4.141462	0.898777	-0.312015
21	1	0	1.033840	3.733663	0.063063
22	1	0	-0.918856	2.251777	-0.459724
23	1	0	3.259020	2.650930	0.560456
24	1	0	-0.948499	-0.875372	-1.438276
25	1	0	3.406304	0.152397	0.466058
26	1	0	2.693509	-2.999680	0.232817

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**Pyridine-2-carboxylic acid: Deprotonated C3 & 2 Carboxyl & THF on N1 (14B)**

SCF Done: E(RB+HF-LYP) = -667.497242703

Zero-point correction=	0.186436 (Hartree/Particle)
Thermal correction to Energy=	0.198404
Thermal correction to Enthalpy=	0.199348
Thermal correction to Gibbs Free Energy=	0.146733
Sum of electronic and zero-point Energies=	-667.310807
Sum of electronic and thermal Energies=	-667.298839
Sum of electronic and thermal Enthalpies=	-667.297895
Sum of electronic and thermal Free Energies=	-667.350510

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	124.500	44.623	110.737

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.119133	0.371101	-0.617202
2	6	0	-1.643492	0.785535	-0.720990
3	8	0	-1.907539	-0.920241	0.926845
4	6	0	-3.001802	-1.019432	0.005316
5	6	0	-0.998240	0.097418	0.503741
6	6	0	1.695786	-2.377091	-0.260594
7	6	0	0.458799	-1.830675	-0.009376
8	7	0	0.346361	-0.485398	0.190214
9	6	0	1.443902	0.350140	0.077422
10	6	0	2.765651	-0.140231	-0.072177
11	6	0	2.829550	-1.532347	-0.224316
12	6	0	1.126930	1.854848	0.111889
13	8	0	0.832285	2.329848	1.241675
14	8	0	1.144410	2.414355	-1.010093
15	1	0	-3.630922	0.363188	-1.586580
16	1	0	-3.669021	1.040576	0.056218

17	1	0	-1.473289	1.862738	-0.704932
18	1	0	-1.188912	0.400283	-1.640301
19	1	0	-2.785419	-1.782284	-0.761534
20	1	0	-3.878371	-1.339351	0.578372
21	1	0	1.771985	-3.452715	-0.424655
22	1	0	-0.451153	-2.405596	0.093071
23	1	0	3.806981	-2.021580	-0.302940
24	1	0	-0.827349	0.785247	1.332091

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**Pyridine-2-carboxylic acid: Deprotonated 2 Carboxyl & THF on N1 (15B)**

SCF Done: E(RB+HF-LYP) = -668.108723303

Zero-point correction= 0.201303 (Hartree/Particle)  
 Thermal correction to Energy= 0.213099  
 Thermal correction to Enthalpy= 0.214044  
 Thermal correction to Gibbs Free Energy= 0.162417  
 Sum of electronic and zero-point Energies= -667.907420  
 Sum of electronic and thermal Energies= -667.895624  
 Sum of electronic and thermal Enthalpies= -667.894680  
 Sum of electronic and thermal Free Energies= -667.946307

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	133.722	44.740	108.658

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.326032	-0.195618	-0.053364
2	6	0	-2.477916	0.542532	0.252258
3	6	0	-2.439677	1.926612	0.299190
4	6	0	-1.223173	2.585957	0.060604
5	6	0	-0.102454	1.833776	-0.221007
6	7	0	-0.163816	0.477207	-0.276199
7	1	0	-3.337388	2.495686	0.524560
8	1	0	-1.144421	3.667253	0.089955
9	1	0	0.867765	2.261587	-0.432930
10	6	0	-1.384985	-1.741933	-0.136307
11	8	0	-1.011131	-2.213839	-1.229584
12	8	0	-1.805734	-2.257819	0.916139
13	6	0	1.100184	-0.320725	-0.646401
14	8	0	2.127535	0.574277	-0.963107
15	6	0	1.596079	-1.172823	0.530019
16	1	0	0.799781	-0.899778	-1.518632
17	6	0	3.175616	0.542894	0.045265
18	6	0	2.589367	-0.229949	1.227022
19	1	0	2.107019	-2.047206	0.112600
20	1	0	0.794633	-1.538264	1.174729
21	1	0	4.042113	0.035368	-0.394452
22	1	0	3.451382	1.577166	0.273156
23	1	0	3.353979	-0.766660	1.796037
24	1	0	2.068795	0.444518	1.917603
25	1	0	-3.384367	-0.015411	0.459511

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**Pyridine-2-carboxylic acid: Deprotonated C3 & THF on N1 (16B)**

SCF Done: E(RB+HF-LYP) = -668.057169394

Zero-point correction= 0.199607 (Hartree/Particle)  
 Thermal correction to Energy= 0.211242  
 Thermal correction to Enthalpy= 0.212187  
 Thermal correction to Gibbs Free Energy= 0.160839  
 Sum of electronic and zero-point Energies= -667.857563  
 Sum of electronic and thermal Energies= -667.845927  
 Sum of electronic and thermal Enthalpies= -667.844983  
 Sum of electronic and thermal Free Energies= -667.896331

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	132.557	44.510	108.071

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.183101	-0.725968	0.720715
2	6	0	-1.666121	-0.949229	0.829365
3	8	0	-2.136158	0.550142	-0.957296
4	6	0	-3.250160	0.598269	-0.035997
5	6	0	-1.133406	-0.312297	-0.471351
6	6	0	1.182396	2.602357	0.102812
7	6	0	0.064128	1.828687	-0.175959
8	7	0	0.147779	0.480603	-0.228654
9	6	0	1.370187	-0.116571	-0.031585
10	6	0	2.546839	0.578048	0.263233
11	6	0	2.409604	1.976518	0.339722
12	6	0	1.563024	-1.628334	-0.153101
13	8	0	0.685362	-2.433727	-0.426771
14	8	0	2.824943	-1.934592	0.071413
15	1	0	-3.676556	-0.683249	1.696749
16	1	0	-3.652343	-1.523326	0.133474
17	1	0	-1.371752	-1.996436	0.898510
18	1	0	-1.257517	-0.419544	1.698256
19	1	0	-3.136360	1.460238	0.638626
20	1	0	-4.151163	0.736984	-0.637985
21	1	0	1.068653	3.683185	0.130118
22	1	0	-0.910776	2.246043	-0.383299
23	1	0	3.271978	2.598958	0.578885
24	1	0	-0.880251	-1.044238	-1.234375
25	1	0	3.248118	-0.986293	0.255717

**Methyl Cation (17)**

SCF Done: E(RB+HF-LYP) = -39.4322712601

Zero-point correction= 0.032128 (Hartree/Particle)  
 Thermal correction to Energy= 0.034995  
 Thermal correction to Enthalpy= 0.035939  
 Thermal correction to Gibbs Free Energy= 0.014130  
 Sum of electronic and zero-point Energies= -39.400143

Sum of electronic and thermal Energies= -39.397276  
 Sum of electronic and thermal Enthalpies= -39.479332  
 Sum of electronic and thermal Free Energies= -39.418141

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	21.960	6.416	45.901

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.118889
2	1	0	0.000000	1.008806	-0.237778
3	1	0	-0.873651	-0.504403	-0.237778
4	1	0	0.873651	-0.504403	-0.237778

### THF Cation (18)

SCF Done: E(RB+HF-LYP) = -231.546733464

Zero-point correction= 0.104606 (Hartree/Particle)  
 Thermal correction to Energy= 0.109079  
 Thermal correction to Enthalpy= 0.110023  
 Thermal correction to Gibbs Free Energy= 0.077402  
 Sum of electronic and zero-point Energies= -231.442128  
 Sum of electronic and thermal Energies= -231.437654  
 Sum of electronic and thermal Enthalpies= -231.406710  
 Sum of electronic and thermal Free Energies= -231.469332

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.448	16.347	68.658

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.122878	0.439371	0.174190
2	8	0	-0.826300	-0.939504	-0.124196
3	6	0	0.525819	-1.131206	0.054329
4	6	0	1.262930	0.180045	0.129717
5	6	0	0.149773	1.204195	-0.207135
6	1	0	-2.010128	0.713145	-0.401613
7	1	0	-1.346617	0.528173	1.246743
8	1	0	0.894783	-2.053011	-0.381499
9	1	0	1.671668	0.363814	1.135525
10	1	0	2.109652	0.236312	-0.567386
11	1	0	0.250365	2.149088	0.336086
12	1	0	0.146810	1.424084	-1.280888

**Carbon Dioxide (19)**

SCF Done: E(RB+HF-LYP) = -188.590392614

Zero-point correction=	0.011565 (Hartree/Particle)
Thermal correction to Energy=	0.014202
Thermal correction to Enthalpy=	0.015147
Thermal correction to Gibbs Free Energy=	-0.009803
Sum of electronic and zero-point Energies=	-188.578827
Sum of electronic and thermal Energies=	-188.576190
Sum of electronic and thermal Enthalpies=	-188.575246
Sum of electronic and thermal Free Energies=	-188.600196

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	8.912	6.942	52.512

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	-0.000021
2	8	0	0.000000	0.000000	-1.169331
3	8	0	0.000000	0.000000	1.169347

**B3LYP/6-31+G\* TRANSITION STATE CALCULATIONS**

**Quinolinic Acid Cation: Methylated N1 (1B)**  
**Nitrogen-Methyl bond frozen to 1.5A°**

SCF Done: E(RB+HF-LYP) = -665.079257271

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.401641	-0.163244	0.033467
2	6	0	0.629925	0.769569	-0.057885
3	6	0	0.308486	2.135252	-0.104804
4	6	0	-1.025852	2.530881	-0.112371
5	6	0	-2.015808	1.562307	-0.043259
6	7	0	-1.704060	0.247431	0.036134
7	1	0	1.112513	2.865050	-0.132149
8	1	0	-1.308247	3.576785	-0.165437
9	1	0	-3.071722	1.806154	-0.044572
10	6	0	-0.145403	-1.665922	0.007676
11	8	0	0.128543	-2.279849	1.158623
12	8	0	-0.197023	-2.244407	-1.048550
13	1	0	0.222855	-1.679004	1.921570
14	6	0	2.105095	0.395353	-0.006369
15	8	0	2.528348	-0.646199	-0.736382
16	8	0	2.845391	1.033736	0.695389
17	1	0	1.877691	-0.993862	-1.374476
18	6	0	-2.809658	-0.765616	0.073433
19	1	0	-2.814161	-1.316947	-0.868854
20	1	0	-2.650266	-1.448186	0.909883
21	1	0	-3.753172	-0.239733	0.209132

**Quinolinic Acid Cation: Methylated N1 (1B)**  
**Nitrogen-Methyl bond frozen to 1.7A°**

SCF Done: E(RB+HF-LYP) = -665.069283191

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.401792	-0.164668	0.033650
2	6	0	0.627234	0.770791	-0.057928
3	6	0	0.302388	2.135656	-0.104915
4	6	0	-1.032978	2.527688	-0.112384
5	6	0	-2.020361	1.556634	-0.043063
6	7	0	-1.705861	0.242115	0.036432
7	1	0	1.104523	2.867526	-0.132324
8	1	0	-1.318232	3.572814	-0.165474
9	1	0	-3.076877	1.797850	-0.044247
10	6	0	-0.141056	-1.666599	0.007521
11	8	0	0.133329	-2.280394	1.158393

12	8	0	-0.189367	-2.244497	-1.049191
13	1	0	0.224995	-1.679762	1.921836
14	6	0	2.103463	0.400537	-0.006401
15	8	0	2.529662	-0.639831	-0.736286
16	8	0	2.841903	1.041162	0.695277
17	1	0	1.879855	-0.989764	-1.374025
18	6	0	-2.802951	-0.768831	0.073851
19	1	0	-2.807960	-1.322075	-0.867565
20	1	0	-2.643768	-1.452165	0.909950
21	1	0	-3.749408	-0.247998	0.209293

**Quinolinic Acid Cation: Methylated N1 (1B)**  
**Nitrogen-Methyl bond frozen to 1.9A°**

SCF Done: E(RB+HF-LYP) = -665.053994293

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.401715	-0.112861	-0.002334
2	6	0	-0.816710	0.593564	0.018494
3	6	0	-0.795782	1.995614	-0.034171
4	6	0	0.414594	2.676340	-0.124929
5	6	0	1.587019	1.932893	-0.153735
6	7	0	1.551210	0.593105	-0.079188
7	1	0	-1.728585	2.553768	-0.037995
8	1	0	0.457527	3.758624	-0.182433
9	1	0	2.563030	2.397446	-0.234237
10	6	0	0.580235	-1.630145	0.189719
11	8	0	-0.122897	-2.452487	-0.563653
12	8	0	1.407447	-1.997155	0.990793
13	1	0	-0.897353	-2.018751	-1.002762
14	6	0	-2.150012	-0.121296	-0.043367
15	8	0	-3.140366	0.334954	0.723528
16	8	0	-2.337579	-1.034808	-0.819213
17	1	0	-2.851508	0.963311	1.408804
18	6	0	3.248631	-0.259410	-0.123683
19	1	0	3.367189	-0.586241	0.902900
20	1	0	3.101822	-1.048452	-0.853973
21	1	0	3.858434	0.576331	-0.453582

**Quinolinic Acid Cation: Methylated N1 (1B)**  
**Nitrogen-Methyl bond frozen to 2.1A°**

SCF Done: E(RB+HF-LYP) = -665.034052229

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.390707	-0.094499	-0.005636
2	6	0	-0.858394	0.561586	0.011709



3	6	0	-0.890672	1.963642	-0.054565
4	6	0	0.290624	2.691521	-0.152172
5	6	0	1.492253	1.991890	-0.164819
6	7	0	1.506001	0.656483	-0.077523
7	1	0	-1.844530	2.484875	-0.064101
8	1	0	0.289637	3.774057	-0.221815
9	1	0	2.449381	2.495824	-0.241735
10	6	0	0.647242	-1.605692	0.158675
11	8	0	-0.094685	-2.456742	-0.518829
12	8	0	1.566670	-1.946464	0.867768
13	1	0	-0.903323	-2.049598	-0.923593
14	6	0	-2.170985	-0.191399	-0.024803
15	8	0	-3.165629	0.255855	0.742573
16	8	0	-2.347226	-1.127194	-0.777153
17	1	0	-2.886264	0.909366	1.407808
18	6	0	3.426574	-0.192662	-0.058764
19	1	0	3.474392	-0.497595	0.979470
20	1	0	3.300828	-0.974517	-0.799200
21	1	0	3.940738	0.712237	-0.366795

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**Quinolinic Acid Cation: Methylated N1 (1B)**  
**Nitrogen-Methyl bond frozen to 2.3A°**

SCF Done: E(RB+HF-LYP) = -665.017475256

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.379886	-0.073903	-0.017372
2	6	0	-0.898550	0.528759	0.002548
3	6	0	-0.984489	1.928637	-0.078520
4	6	0	0.165542	2.702590	-0.186133
5	6	0	1.394508	2.048587	-0.184295
6	7	0	1.460410	0.718593	-0.087540
7	1	0	-1.957986	2.412047	-0.092093
8	1	0	0.119985	3.783358	-0.268830
9	1	0	2.331378	2.590965	-0.258787
10	6	0	0.714677	-1.575982	0.111890
11	8	0	-0.065025	-2.461985	-0.465531
12	8	0	1.726185	-1.883152	0.705414
13	1	0	-0.910363	-2.085701	-0.828104
14	6	0	-2.189190	-0.261219	0.001128
15	8	0	-3.188384	0.186411	0.762949
16	8	0	-2.353473	-1.228824	-0.713942
17	1	0	-2.920175	0.872470	1.399157
18	6	0	3.593423	-0.130824	0.049375
19	1	0	3.583410	-0.398378	1.098919
20	1	0	3.516315	-0.928603	-0.679926
21	1	0	4.005314	0.824232	-0.260405

Quinolinic Acid Zwitterion: Deprotonated 2carboxyl & Methylated  
N1 (3b) C2 Carbon-Carboxyl bond frozen to 1.55 Å°

SCF Done: E(RB+HF-LYP) = -664.735824878

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.425176	-0.177073	0.001072
2	6	0	-0.739853	0.616097	0.021254
3	6	0	-0.615764	2.006567	0.011571
4	6	0	0.640903	2.607748	-0.080246
5	6	0	1.753043	1.797433	-0.144213
6	7	0	1.639541	0.446156	-0.089728
7	1	0	-1.522627	2.599660	0.070568
8	1	0	0.757535	3.685275	-0.111124
9	1	0	2.758821	2.188859	-0.236589
10	6	0	-2.186693	0.104272	0.065897
11	8	0	-2.464802	-1.085494	-0.427298
12	8	0	-3.040493	0.850318	0.507263
13	6	0	0.440075	-1.722475	0.119437
14	8	0	-0.219891	-2.297758	-0.787902
15	8	0	1.098567	-2.162680	1.066715
16	1	0	-1.642400	-1.606164	-0.712424
17	6	0	2.889466	-0.359961	-0.130795
18	1	0	3.035933	-0.838519	0.836873
19	1	0	2.796306	-1.131224	-0.896331
20	1	0	3.714483	0.308290	-0.376978

Quinolinic Acid Zwitterion: Deprotonated 2carboxyl & Methylated  
N1 (3b) C2 Carbon-Carboxyl bond frozen to 1.75 Å°

SCF Done: E(RB+HF-LYP) = -664.726818

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.423689	-0.121764	-0.018834
2	6	0	-0.768018	0.624016	0.018768
3	6	0	-0.703479	2.020692	0.027392
4	6	0	0.527700	2.672281	-0.051788
5	6	0	1.671511	1.907559	-0.126996
6	7	0	1.607744	0.550796	-0.098489
7	1	0	-1.633955	2.575454	0.094270
8	1	0	0.601782	3.754059	-0.063559
9	1	0	2.661036	2.340794	-0.210221
10	6	0	-2.191662	0.054467	0.060278
11	8	0	-2.417330	-1.164385	-0.389619
12	8	0	-3.085327	0.775502	0.463180
13	6	0	0.531283	-1.862763	0.122045
14	8	0	-0.185202	-2.432376	-0.719673
15	8	0	1.292957	-2.211283	1.010514
16	1	0	-1.584723	-1.675718	-0.647549
17	6	0	2.890229	-0.201311	-0.168517
18	1	0	3.051232	-0.722085	0.774267

19	1	0	2.831290	-0.935790	-0.972470
20	1	0	3.690823	0.508986	-0.374602

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**Quinolinic Acid Zwitterion: Deprotonated 2carboxyl & Methylated  
N1 (3b) C2 Carbon-Carboxyl bond frozen to 1.85 Å°**

SCF Done: E(RB+HF-LYP) = -664.723058451

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.420814	-0.093682	-0.032721
2	6	0	-0.789846	0.620880	0.016859
3	6	0	-0.769800	2.019051	0.039576
4	6	0	0.441182	2.708226	-0.032103
5	6	0	1.606643	1.978289	-0.117064
6	7	0	1.581055	0.619113	-0.106462
7	1	0	-1.716676	2.544766	0.112112
8	1	0	0.483140	3.791831	-0.030970
9	1	0	2.582928	2.441788	-0.195176
10	6	0	-2.192994	0.007366	0.054456
11	8	0	-2.376227	-1.229117	-0.372508
12	8	0	-3.117467	0.701166	0.434549
13	6	0	0.603603	-1.927735	0.126458
14	8	0	-0.125284	-2.504250	-0.685402
15	8	0	1.407403	-2.208475	0.991973
16	1	0	-1.534217	-1.721926	-0.616740
17	6	0	2.885596	-0.091355	-0.191891
18	1	0	3.072442	-0.613318	0.745427
19	1	0	2.842731	-0.821237	-1.000795
20	1	0	3.663674	0.643464	-0.398955

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**Quinolinic Acid Zwitterion: Deprotonated 2carboxyl & Methylated  
N1 (3b) C2 Carbon-Carboxyl bond frozen to 1.95 Å°**

SCF Done: E(RB+HF-LYP) = -664.718214981

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.415877	-0.062566	-0.051172
2	6	0	-0.820922	0.606815	0.015339
3	6	0	-0.863088	2.003935	0.059138
4	6	0	0.317337	2.745266	-0.003894
5	6	0	1.511409	2.065940	-0.105900
6	7	0	1.540945	0.706051	-0.119733
7	1	0	-1.831497	2.487629	0.140772
8	1	0	0.313663	3.829535	0.015599
9	1	0	2.467197	2.571367	-0.179511
10	6	0	-2.192774	-0.068389	0.044492
11	8	0	-2.313025	-1.323140	-0.359909
12	8	0	-3.158242	0.581695	0.398244
13	6	0	0.708371	-1.981301	0.136978
14	8	0	-0.018715	-2.577937	-0.647013

15	8	0	1.546406	-2.171310	0.984960
16	1	0	-1.454255	-1.781655	-0.588417
17	6	0	2.873631	0.054942	-0.226291
18	1	0	3.103034	-0.453359	0.709215
19	1	0	2.848393	-0.679207	-1.031763
20	1	0	3.616406	0.821007	-0.450172

**Quinolinic Acid Zwitterion: Deprotonated 2carboxyl & Methylated  
N1 (3b) C2 Carbon-Carboxyl bond frozen to 2.05 Å°**

SCF Done: E(RB+HF-LYP) = -664.714450844

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.407522	-0.027501	-0.079363
2	6	0	-0.862324	0.577334	0.013945
3	6	0	-0.987721	1.967574	0.092130
4	6	0	0.147948	2.777171	0.040472
5	6	0	1.376817	2.169284	-0.091805
6	7	0	1.481630	0.813224	-0.142818
7	1	0	-1.981952	2.392631	0.189611
8	1	0	0.082897	3.858623	0.088978
9	1	0	2.301604	2.730194	-0.161813
10	6	0	-2.187324	-0.179968	0.027118
11	8	0	-2.218397	-1.449223	-0.359315
12	8	0	-3.203539	0.404117	0.351532
13	6	0	0.852772	-2.014209	0.159895
14	8	0	0.145569	-2.650375	-0.595963
15	8	0	1.710879	-2.081512	0.997085
16	1	0	-1.334172	-1.853468	-0.566712
17	6	0	2.846999	0.244106	-0.283636
18	1	0	3.134083	-0.244501	0.646740
19	1	0	2.843289	-0.493284	-1.086326
20	1	0	3.538612	1.050449	-0.530001

**Quinolinic Acid Zwitterion: Deprotonated 2carboxyl & Methylated  
N1 (3b) C2 Carbon-Carboxyl bond frozen to 2.15 Å°**

SCF Done: E(RB+HF-LYP) = -664.711921317

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.392884	0.015261	-0.113073
2	6	0	-0.919955	0.519101	0.012162
3	6	0	-1.165110	1.889600	0.129965
4	6	0	-0.101766	2.793638	0.090936
5	6	0	1.170658	2.294072	-0.076391
6	7	0	1.386293	0.952834	-0.170397
7	1	0	-2.190851	2.226332	0.245622
8	1	0	-0.255950	3.864045	0.172329
9	1	0	2.044248	2.932596	-0.142614
10	6	0	-2.167731	-0.353641	0.007568

11	8	0	-2.068835	-1.626068	-0.369047
12	8	0	-3.243954	0.126079	0.307296
13	6	0	1.063139	-2.004925	0.190418
14	8	0	0.404094	-2.700135	-0.541870
15	8	0	1.918996	-1.914280	1.018649
16	1	0	-1.149975	-1.938959	-0.556874
17	6	0	2.791583	0.508270	-0.349837
18	1	0	3.163609	0.086325	0.583664
19	1	0	2.823782	-0.256531	-1.125181
20	1	0	3.396465	1.363331	-0.654880

**Quinolinic Acid Zwitterion: Deprotonated 2carboxyl & Methylated  
N1 (3b) C2 Carbon-Carboxyl bond frozen to 2.3 Å°**

SCF Done: E(RB+HF-LYP) = -664.710368126

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.354405	0.094579	-0.174048
2	6	0	-1.024026	0.358562	0.006211
3	6	0	-1.518975	1.650613	0.189373
4	6	0	-0.640167	2.736753	0.166290
5	6	0	0.695235	2.485532	-0.056947
6	7	0	1.147888	1.210237	-0.217548
7	1	0	-2.585664	1.788761	0.339540
8	1	0	-0.984116	3.756678	0.299443
9	1	0	1.434601	3.276488	-0.117329
10	6	0	-2.070619	-0.739444	-0.022382
11	8	0	-1.696875	-1.963265	-0.407021
12	8	0	-3.228421	-0.505911	0.262918
13	6	0	1.498542	-1.855454	0.248235
14	8	0	0.995007	-2.654535	-0.480591
15	8	0	2.254223	-1.484048	1.083401
16	1	0	-0.734059	-2.049257	-0.581544
17	6	0	2.602685	1.040762	-0.449294
18	1	0	3.087681	0.728948	0.476567
19	1	0	2.748848	0.272671	-1.207934
20	1	0	3.023533	1.984705	-0.800195

**Quinolinic Acid Zwitterion: Deprotonated 2carboxyl & Methylated  
N1 (3b) C2 Carbon-Carboxyl bond frozen to 2.4 Å°**

SCF Done: E(RB+HF-LYP) = -664.710708010

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.317698	0.124071	-0.248970
2	6	0	-1.070776	0.269023	-0.006094
3	6	0	-1.671585	1.499885	0.253373
4	6	0	-0.888833	2.658909	0.249185
5	6	0	0.452524	2.533563	-0.036157
6	7	0	1.004683	1.309877	-0.273914

7	1	0	-2.739963	1.538427	0.445671
8	1	0	-1.311920	3.638782	0.442023
9	1	0	1.119145	3.387746	-0.088071
10	6	0	-1.997656	-0.926030	-0.058572
11	8	0	-1.479762	-2.089088	-0.475190
12	8	0	-3.173042	-0.836413	0.233989
13	6	0	1.714809	-1.740786	0.325823
14	8	0	1.333511	-2.592810	-0.403572
15	8	0	2.333778	-1.194619	1.170608
16	1	0	-0.517701	-2.024436	-0.650680
17	6	0	2.456936	1.279804	-0.564843
18	1	0	3.012794	1.084248	0.354174
19	1	0	2.649087	0.482148	-1.280946
20	1	0	2.761190	2.236762	-0.993928

Quinolinic Acid Zwitterion: Deprotonated 2carboxyl & Methylated  
N1 (3b) C2 Carbon-Carboxyl bond frozen to 2.5 Å°

SCF Done: E(RB+HF-LYP) = -664.711890686

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.281910	0.137703	-0.330761
2	6	0	-1.100195	0.218257	-0.023296
3	6	0	-1.744302	1.405709	0.313909
4	6	0	-1.009367	2.597107	0.328917
5	6	0	0.322909	2.541370	-0.015286
6	7	0	0.914294	1.353669	-0.331576
7	1	0	-2.804648	1.390789	0.550126
8	1	0	-1.463139	3.549220	0.581860
9	1	0	0.951563	3.424859	-0.054633
10	6	0	-1.951153	-1.027579	-0.095066
11	8	0	-1.347309	-2.130891	-0.562684
12	8	0	-3.122109	-1.036864	0.225880
13	6	0	1.840833	-1.669522	0.413348
14	8	0	1.568164	-2.543417	-0.327806
15	8	0	2.308081	-1.003257	1.264365
16	1	0	-0.403733	-1.944191	-0.755856
17	6	0	2.353082	1.398303	-0.676171
18	1	0	2.953428	1.295214	0.230881
19	1	0	2.567169	0.571222	-1.351165
20	1	0	2.582382	2.344552	-1.171789

QUINOLINIC ACID ZWITTERION: DEPROTONATED 2CARBOXYL & METHYLATED  
N1 (3B) TRANSITION STATE CALCULATION

Negative frequency -199.3823

Zero-point correction= 0.144132 (Hartree/Particle)  
 Thermal correction to Energy= 0.155675  
 Thermal correction to Enthalpy= 0.156620  
 Thermal correction to Gibbs Free Energy= 0.105231  
 Sum of electronic and zero-point Energies= -664.566226  
 Sum of electronic and thermal Energies= -664.554682  
 Sum of electronic and thermal Enthalpies= -664.553738  
 Sum of electronic and thermal Free Energies= -664.605126

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	97.688	41.606	108.156

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.348493	0.097051	-0.190065
2	6	0	-1.030615	0.349425	0.004363
3	6	0	-1.535657	1.634561	0.205162
4	6	0	-0.665822	2.728308	0.186573
5	6	0	0.669359	2.490563	-0.052023
6	7	0	1.131016	1.220723	-0.230560
7	1	0	-2.602299	1.762307	0.364871
8	1	0	-1.016898	3.743856	0.333880
9	1	0	1.401615	3.288303	-0.111313
10	6	0	-2.064602	-0.759262	-0.030961
11	8	0	-1.672791	-1.976893	-0.419490
12	8	0	-3.226181	-0.542427	0.251755
13	6	0	1.525672	-1.846069	0.264512
14	8	0	1.035243	-2.657082	-0.457483
15	8	0	2.265187	-1.441711	1.097574
16	1	0	-0.708320	-2.044902	-0.589535
17	6	0	2.584945	1.067458	-0.477092
18	1	0	3.087398	0.787770	0.450015
19	1	0	2.732373	0.282184	-1.217368
20	1	0	2.986716	2.008118	-0.858294

**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 1.55 A°**

SCF Done: E(RB+HF-LYP) = -664.193629764 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.383025	-0.143788	-0.006708
2	6	0	0.880122	0.494488	-0.030019
3	6	0	0.923022	1.884138	-0.060293
4	6	0	-0.252250	2.651328	-0.097692
5	6	0	-1.460679	1.999347	-0.048942
6	7	0	-1.508586	0.637802	0.008866
7	1	0	1.903959	2.349852	-0.030182
8	1	0	-0.229393	3.736390	-0.140559
9	1	0	-2.415365	2.512259	-0.044714
10	6	0	2.237857	-0.268823	-0.075701
11	8	0	2.220335	-1.319921	-0.745444
12	8	0	3.170318	0.329311	0.518134
13	6	0	-0.660497	-1.665126	0.098360
14	8	0	-0.500682	-2.097917	1.258506
15	8	0	-1.133875	-2.181867	-0.935223
16	6	0	-2.835251	-0.013351	0.072476
17	1	0	-2.974332	-0.623257	-0.821341
18	1	0	-2.868696	-0.666867	0.946799
19	1	0	-3.600651	0.760885	0.151278

**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 1.75 A°**

SCF Done: E(RB+HF-LYP) = -664.1840199

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.380829	-0.073168	-0.011031
2	6	0	0.924379	0.465509	-0.027991
3	6	0	1.077064	1.849798	-0.044566
4	6	0	-0.036714	2.702919	-0.082366
5	6	0	-1.292809	2.144920	-0.044248
6	7	0	-1.438343	0.788235	0.006927
7	1	0	2.090071	2.241002	-0.008502
8	1	0	0.068627	3.783496	-0.119970
9	1	0	-2.206001	2.729089	-0.044119
10	6	0	2.215514	-0.402784	-0.083863
11	8	0	2.114896	-1.439657	-0.769707
12	8	0	3.193820	0.106811	0.519703
13	6	0	-0.833524	-1.759633	0.104739
14	8	0	-0.660526	-2.181590	1.249544
15	8	0	-1.356374	-2.177599	-0.933507
16	6	0	-2.809308	0.235623	0.074320
17	1	0	-2.962406	-0.432017	-0.774591



18	1	0	-2.914681	-0.342649	0.995141
19	1	0	-3.524365	1.060606	0.065327

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 1.8 A°**

SCF Done: E(RB+HF-LYP) = -664.182639037

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.380362	-0.055894	-0.011032
2	6	0	0.935622	0.455797	-0.027437
3	6	0	1.119469	1.836658	-0.040453
4	6	0	0.024396	2.713682	-0.078132
5	6	0	-1.243690	2.183038	-0.042548
6	7	0	-1.417183	0.828986	0.007222
7	1	0	2.140526	2.206426	-0.003202
8	1	0	0.153187	3.791809	-0.114564
9	1	0	-2.144068	2.786966	-0.043643
10	6	0	2.206070	-0.441121	-0.087455
11	8	0	2.083128	-1.469938	-0.782430
12	8	0	3.195338	0.039530	0.522212
13	6	0	-0.882300	-1.780455	0.107063
14	8	0	-0.696884	-2.201950	1.245479
15	8	0	-1.422322	-2.168727	-0.929751
16	6	0	-2.799435	0.305634	0.075844
17	1	0	-2.960243	-0.375362	-0.760858
18	1	0	-2.923086	-0.251741	1.007365
19	1	0	-3.498730	1.143645	0.045156

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 1.85 A°**

SCF Done: E(RB+HF-LYP) = -664.179702113

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.378835	-0.035954	-0.008584
2	6	0	0.951591	0.437308	-0.026196
3	6	0	1.178542	1.811976	-0.038119
4	6	0	0.110791	2.722162	-0.076394
5	6	0	-1.172961	2.230527	-0.041150
6	7	0	-1.386230	0.881702	0.009955
7	1	0	2.210472	2.150493	-0.001260
8	1	0	0.272569	3.795855	-0.113688
9	1	0	-2.054542	2.861800	-0.043654
10	6	0	2.193105	-0.498933	-0.087577
11	8	0	2.035169	-1.528474	-0.774834
12	8	0	3.200769	-0.046700	0.514312
13	6	0	-0.950569	-1.791694	0.105425
14	8	0	-0.768615	-2.216360	1.238744
15	8	0	-1.500860	-2.141128	-0.935440
16	6	0	-2.783261	0.400015	0.079708

17	1	0	-2.965306	-0.276180	-0.756514
18	1	0	-2.923084	-0.152634	1.011741
19	1	0	-3.458617	1.257596	0.048759

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 1.9 A°**

SCF Done: E(RB+HF-LYP) = -664.176904346

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.378761	-0.017942	-0.009251
2	6	0	0.963158	0.423637	-0.025472
3	6	0	1.226385	1.791944	-0.032372
4	6	0	0.182381	2.729481	-0.070491
5	6	0	-1.113644	2.271007	-0.039804
6	7	0	-1.360194	0.927050	0.008398
7	1	0	2.266472	2.104494	0.006588
8	1	0	0.371980	3.798743	-0.105682
9	1	0	-1.978862	2.924705	-0.044391
10	6	0	2.178575	-0.544697	-0.092275
11	8	0	1.993554	-1.564990	-0.787421
12	8	0	3.198541	-0.125751	0.513253
13	6	0	-1.006231	-1.807434	0.109067
14	8	0	-0.809507	-2.230027	1.236153
15	8	0	-1.572949	-2.126423	-0.928517
16	6	0	-2.768643	0.481057	0.079391
17	1	0	-2.957239	-0.220596	-0.733917
18	1	0	-2.932753	-0.032897	1.029728
19	1	0	-3.424670	1.351398	0.008392

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 1.95 A°**

SCF Done: E(RB+HF-LYP) = -664.174294587

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.377517	0.003144	-0.008958
2	6	0	0.978784	0.401056	-0.024590
3	6	0	1.290241	1.759121	-0.027376
4	6	0	0.279347	2.732574	-0.065463
5	6	0	-1.031800	2.319293	-0.038574
6	7	0	-1.323550	0.983735	0.007842
7	1	0	2.340573	2.035332	0.013145
8	1	0	0.506257	3.794663	-0.098981
9	1	0	-1.873943	3.002625	-0.045313
10	6	0	2.158409	-0.609966	-0.094796
11	8	0	1.933135	-1.626958	-0.783482
12	8	0	3.197407	-0.226348	0.502402
13	6	0	-1.080397	-1.811844	0.110534
14	8	0	-0.882929	-2.232870	1.233783

15	8	0	-1.656647	-2.094535	-0.927917
16	6	0	-2.746116	0.586303	0.078620
17	1	0	-2.954759	-0.121323	-0.724442
18	1	0	-2.932751	0.094340	1.036567
19	1	0	-3.373967	1.475819	-0.010518

**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.0 A°**

SCF Done: E(RB+HF-LYP) = -664.171885690

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.375680	0.026421	-0.007451
2	6	0	0.995778	0.372412	-0.023048
3	6	0	1.362978	1.716339	-0.021738
4	6	0	0.392281	2.730293	-0.060405
5	6	0	-0.934507	2.370388	-0.037738
6	7	0	-1.278874	1.046864	0.007865
7	1	0	2.423721	1.949336	0.020499
8	1	0	0.662354	3.782348	-0.092608
9	1	0	-1.748444	3.087203	-0.047649
10	6	0	2.131766	-0.686814	-0.097208
11	8	0	1.858427	-1.698974	-0.776314
12	8	0	3.192243	-0.344620	0.487947
13	6	0	-1.165252	-1.807266	0.111567
14	8	0	-0.969156	-2.228861	1.230625
15	8	0	-1.750158	-2.048606	-0.928177
16	6	0	-2.715890	0.706645	0.078083
17	1	0	-2.949900	-0.001813	-0.717132
18	1	0	-2.925655	0.234762	1.041498
19	1	0	-3.309662	1.618086	-0.024680

**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.05 A°**

SCF Done: E(RB+HF-LYP) = -664.169716093 ]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.372196	0.052500	-0.003907
2	6	0	1.015130	0.333190	-0.021674
3	6	0	1.450517	1.656549	-0.019700
4	6	0	0.531896	2.718339	-0.058495
5	6	0	-0.811176	2.425133	-0.036469
6	7	0	-1.220206	1.119837	0.010336
7	1	0	2.521711	1.835789	0.021503
8	1	0	0.854323	3.755586	-0.091686
9	1	0	-1.588196	3.181942	-0.048116
10	6	0	2.095222	-0.782658	-0.097966
11	8	0	1.765691	-1.785249	-0.766997
12	8	0	3.177404	-0.492604	0.476269

13	6	0	-1.269585	-1.787143	0.109715
14	8	0	-1.077690	-2.215442	1.222820
15	8	0	-1.863644	-1.976312	-0.931519
16	6	0	-2.671936	0.851772	0.082837
17	1	0	-2.938202	0.140111	-0.699156
18	1	0	-2.907452	0.410539	1.055042
19	1	0	-3.222051	1.787939	-0.040563

Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl &  
Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.1 A°

SCF Done: E(RB+HF-LYP) = -664.167824237

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.366112	0.083782	0.005048
2	6	0	1.036478	0.280249	-0.019327
3	6	0	1.555206	1.573125	-0.021921
4	6	0	0.705104	2.690837	-0.062366
5	6	0	-0.653591	2.482565	-0.036125
6	7	0	-1.142643	1.204913	0.017923
7	1	0	2.635772	1.684723	0.015426
8	1	0	1.092046	3.705641	-0.100702
9	1	0	-1.381555	3.286874	-0.050743
10	6	0	2.042284	-0.902826	-0.094561
11	8	0	1.640181	-1.893750	-0.741672
12	8	0	3.149868	-0.675383	0.459983
13	6	0	-1.395031	-1.744313	0.101976
14	8	0	-1.223246	-2.184943	1.209507
15	8	0	-1.986912	-1.869408	-0.946097
16	6	0	-2.607466	1.027448	0.094561
17	1	0	-2.921799	0.342018	-0.693115
18	1	0	-2.866127	0.592327	1.063560
19	1	0	-3.100197	1.996703	-0.017366

Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl &  
Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.15 A°

SCF Done: E(RB+HF-LYP) = -664.166184204

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.357365	0.119947	0.010723
2	6	0	1.057013	0.211834	-0.018098
3	6	0	1.673982	1.460564	-0.023742
4	6	0	0.911814	2.640458	-0.064274
5	6	0	-0.458656	2.536957	-0.035620
6	7	0	-1.043033	1.299713	0.021802
7	1	0	2.760077	1.488913	0.009978
8	1	0	1.375571	3.622473	-0.105856
9	1	0	-1.122951	3.394749	-0.051774

10	6	0	1.967717	-1.046181	-0.091429
11	8	0	1.480105	-2.015018	-0.713436
12	8	0	3.099682	-0.897306	0.441038
13	6	0	-1.540249	-1.673410	0.095319
14	8	0	-1.394540	-2.120739	1.200071
15	8	0	-2.124574	-1.734029	-0.958746
16	6	0	-2.516268	1.233530	0.103773
17	1	0	-2.882669	0.558792	-0.670504
18	1	0	-2.804389	0.837835	1.081465
19	1	0	-2.937723	2.233794	-0.027246

Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.2 A°

SCF Done: E(RB+HF-LYP) = -664.164784275

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.343398	0.158488	0.019047
2	6	0	1.074780	0.127790	-0.016209
3	6	0	1.801480	1.315819	-0.026600
4	6	0	1.147694	2.559267	-0.068883
5	6	0	-0.226405	2.578123	-0.036038
6	7	0	-0.917609	1.397118	0.028296
7	1	0	2.885960	1.247759	0.003821
8	1	0	1.697185	3.495827	-0.115566
9	1	0	-0.811723	3.491718	-0.054437
10	6	0	1.867938	-1.206632	-0.090130
11	8	0	1.295279	-2.127846	-0.713009
12	8	0	3.008786	-1.162992	0.442927
13	6	0	-1.703515	-1.569215	0.090621
14	8	0	-1.582596	-2.029105	1.189534
15	8	0	-2.279737	-1.553814	-0.965677
16	6	0	-2.390332	1.462907	0.114639
17	1	0	-2.818849	0.830126	-0.663270
18	1	0	-2.710743	1.087798	1.090400
19	1	0	-2.721874	2.497720	-0.007902

Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.3 A°

SCF Done: E(RB+HF-LYP) = -664.162567373

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.270586	0.271407	0.046567
2	6	0	1.074384	-0.184902	-0.004635
3	6	0	2.129508	0.722546	-0.039075
4	6	0	1.886817	2.107177	-0.084679
5	6	0	0.584747	2.544523	-0.037983
6	7	0	-0.431478	1.629592	0.045783
7	1	0	3.140042	0.322003	-0.027126

8	1	0	2.695741	2.830662	-0.145476
9	1	0	0.306723	3.593568	-0.061241
10	6	0	1.419355	-1.703044	-0.050706
11	8	0	0.510937	-2.449502	-0.478023
12	8	0	2.594261	-1.979101	0.316607
13	6	0	-2.158863	-1.041749	0.040548
14	8	0	-2.257325	-1.420527	1.166269
15	8	0	-2.567262	-0.905135	-1.075051
16	6	0	-1.814541	2.136886	0.131460
17	1	0	-2.393349	1.743258	-0.706007
18	1	0	-2.264694	1.789650	1.064377
19	1	0	-1.813931	3.230780	0.107599

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.4 A°**

SCF Done: E(RB+HF-LYP) = -664.161224508

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.141846	0.380302	0.032473
2	6	0	0.941335	-0.542628	0.002180
3	6	0	2.259836	-0.098790	-0.018567
4	6	0	2.556027	1.276793	-0.042201
5	6	0	1.511753	2.169715	-0.019342
6	7	0	0.225448	1.700168	0.025551
7	1	0	3.043353	-0.852450	-0.016559
8	1	0	3.578580	1.644147	-0.075447
9	1	0	1.648341	3.246804	-0.034755
10	6	0	0.689647	-2.082510	-0.022462
11	8	0	-0.495644	-2.441995	-0.203645
12	8	0	1.730661	-2.780998	0.127967
13	6	0	-2.458655	-0.245812	0.012970
14	8	0	-2.682456	-0.409350	1.166931
15	8	0	-2.718864	-0.113297	-1.139556
16	6	0	-0.870872	2.685733	0.069758
17	1	0	-1.550752	2.498522	-0.763623
18	1	0	-1.422026	2.568413	1.006049
19	1	0	-0.468561	3.701695	0.003055

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.5 A°**

SCF Done: E(RB+HF-LYP) = -664.160622650

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.054878	-0.451572	-0.052621
2	6	0	0.646535	0.845084	-0.011453
3	6	0	2.027194	1.009041	0.029418
4	6	0	2.883046	-0.108409	0.058592
5	6	0	2.320376	-1.361698	0.024435

6	7	0	0.956992	-1.484761	-0.038071
7	1	0	2.413800	2.025120	0.038907
8	1	0	3.964153	-0.003689	0.104053
9	1	0	2.904607	-2.277069	0.043521
10	6	0	-0.240246	2.128596	-0.003916
11	8	0	-1.475615	1.946057	0.100785
12	8	0	0.405101	3.210083	-0.093391
13	6	0	-2.432483	-0.692026	0.019576
14	8	0	-2.681785	-0.691527	-1.135952
15	8	0	-2.565833	-0.837734	1.186388
16	6	0	0.384429	-2.842610	-0.081481
17	1	0	-0.242390	-2.995713	0.800305
18	1	0	-0.239045	-2.936588	-0.973169
19	1	0	1.182625	-3.592214	-0.105058

Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl &  
Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.6 A°

SCF Done: E(RB+HF-LYP) = -664.160594838

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.152375	-0.473474	-0.094740
2	6	0	0.526565	0.902960	-0.024769
3	6	0	1.859413	1.292161	0.053866
4	6	0	2.886693	0.330405	0.102434
5	6	0	2.538899	-0.997536	0.042490
6	7	0	1.216191	-1.341223	-0.064342
7	1	0	2.075084	2.357529	0.077771
8	1	0	3.934015	0.611177	0.181076
9	1	0	3.265380	-1.804486	0.074321
10	6	0	-0.557306	2.023083	-0.027795
11	8	0	-1.748553	1.643175	0.075753
12	8	0	-0.101117	3.196252	-0.121066
13	6	0	-2.394263	-0.975540	0.055414
14	8	0	-2.650624	-1.021772	-1.093974
15	8	0	-2.435975	-1.112698	1.226636
16	6	0	0.878769	-2.774437	-0.130422
17	1	0	0.333861	-3.059914	0.773514
18	1	0	0.232736	-2.943306	-0.993771
19	1	0	1.788858	-3.377829	-0.220191

Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl &  
Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.7 A°

SCF Done: E(RB+HF-LYP) = -664.1608133

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.210018	-0.493831	-0.108135
2	6	0	0.487917	0.906443	-0.028221

3	6	0	1.788551	1.390271	0.064333
4	6	0	2.881907	0.504962	0.121454
5	6	0	2.630257	-0.843997	0.052366
6	7	0	1.336755	-1.280270	-0.071755
7	1	0	1.926838	2.468291	0.092138
8	1	0	3.905437	0.859806	0.213106
9	1	0	3.412448	-1.596915	0.089920
10	6	0	-0.668834	1.950813	-0.035819
11	8	0	-1.833833	1.496235	0.076678
12	8	0	-0.294607	3.151539	-0.139714
13	6	0	-2.425195	-1.055182	0.066619
14	8	0	-2.666971	-1.108648	-1.083423
15	8	0	-2.426982	-1.194807	1.236132
16	6	0	1.105849	-2.733903	-0.149780
17	1	0	0.570993	-3.063780	0.744976
18	1	0	0.484756	-2.944157	-1.022334
19	1	0	2.058562	-3.269363	-0.229807

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 carboxyl & Methylated N1 (4B) C2 Carbon-Carboxyl Bond frozen to 2.8 Å**

SCF Done: E(RB+HF-LYP) = -664.1610158

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.242536	-0.503527	-0.157469
2	6	0	0.492888	0.900479	-0.041843
3	6	0	1.781269	1.406505	0.093946
4	6	0	2.888444	0.540437	0.174742
5	6	0	2.664337	-0.811430	0.076078
6	7	0	1.383812	-1.268377	-0.100465
7	1	0	1.900060	2.486392	0.136884
8	1	0	3.901541	0.912523	0.305663
9	1	0	3.458498	-1.550848	0.129684
10	6	0	-0.680535	1.924646	-0.055798
11	8	0	-1.836578	1.455320	0.089303
12	8	0	-0.329061	3.128978	-0.191195
13	6	0	-2.489846	-1.058677	0.099232
14	8	0	-2.764498	-1.100156	-1.042159
15	8	0	-2.422216	-1.204513	1.264546
16	6	0	1.184315	-2.724251	-0.209729
17	1	0	0.672199	-3.089354	0.685273
18	1	0	0.552496	-2.925025	-1.076251
19	1	0	2.146899	-3.237166	-0.316922

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**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) C2 Carbon-Carboxyl Bond frozen to 1.55 Å**

SCF Done: E(RB+HF-LYP) = -856.688710462

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.720467	-0.792617	-0.863251
2	6	0	2.240779	-1.106893	-0.577677
3	8	0	2.926765	0.811691	0.653552
4	6	0	3.811733	0.682536	-0.487481
5	6	0	1.892060	-0.127163	0.567511
6	6	0	-0.565318	2.678383	-0.029858
7	6	0	0.591555	1.956447	0.184026
8	7	0	0.558171	0.609408	0.301610
9	6	0	-0.607475	-0.102203	0.211344
10	6	0	-1.804394	0.594732	-0.046142
11	6	0	-1.771341	1.989492	-0.138875
12	6	0	-3.200686	-0.018277	-0.225768
13	8	0	-4.166230	0.690943	-0.011781
14	8	0	-3.313345	-1.257084	-0.662911
15	6	0	-0.532055	-1.630289	0.459868
16	8	0	-0.037476	-1.959278	1.544101
17	8	0	-0.977845	-2.320898	-0.496763
18	1	0	3.996108	-0.984179	-1.904634
19	1	0	4.376922	-1.387472	-0.219091
20	1	0	2.065441	-2.141189	-0.279557
21	1	0	1.620244	-0.907929	-1.457848
22	1	0	3.466248	1.337603	-1.300850
23	1	0	4.797058	1.015090	-0.155036
24	1	0	-0.516708	3.758976	-0.106642
25	1	0	1.570153	2.404662	0.287631
26	1	0	-2.709846	2.511150	-0.295294
27	1	0	-2.423160	-1.734916	-0.745359
28	1	0	1.743434	-0.605532	1.533657

**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) C2 Carbon-Carboxyl Bond frozen to 1.75 Å**

SCF Done: E(RB+HF-LYP) = -856.681248283

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.696723	-0.747035	-0.932245
2	6	0	2.215949	-1.060684	-0.651385
3	8	0	2.929533	0.787825	0.667856
4	6	0	3.805311	0.706653	-0.483653
5	6	0	1.882695	-0.134483	0.541758
6	6	0	-0.546442	2.709313	0.044873
7	6	0	0.604323	1.973449	0.245304
8	7	0	0.556674	0.621916	0.316191

9	6	0	-0.608540	-0.078117	0.199844
10	6	0	-1.795761	0.633945	-0.042845
11	6	0	-1.755160	2.032429	-0.098858
12	6	0	-3.191823	0.035179	-0.253472
13	8	0	-4.157700	0.757242	-0.089226
14	8	0	-3.311559	-1.214448	-0.661349
15	6	0	-0.529184	-1.802365	0.488242
16	8	0	0.032072	-2.075830	1.539600
17	8	0	-1.050871	-2.451920	-0.435483
18	1	0	3.963603	-0.889304	-1.983809
19	1	0	4.351247	-1.379730	-0.323142
20	1	0	2.036296	-2.107347	-0.402882
21	1	0	1.590719	-0.812858	-1.515886
22	1	0	3.461962	1.404627	-1.261620
23	1	0	4.796521	1.011980	-0.142568
24	1	0	-0.490556	3.791609	0.003596
25	1	0	1.585002	2.411627	0.370820
26	1	0	-2.688762	2.564472	-0.250851
27	1	0	-2.440427	-1.722238	-0.707505
28	1	0	1.737340	-0.658911	1.483948

**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) C2 Carbon-Carboxyl Bond frozen to 1.85 Å°**

SCF Done: E(RB+HF-LYP) = -856.675568097

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.675910	-0.725064	-0.976500
2	6	0	2.198029	-1.042158	-0.683419
3	8	0	2.933346	0.775407	0.666500
4	6	0	3.793304	0.718317	-0.497511
5	6	0	1.877768	-0.136364	0.529038
6	6	0	-0.537703	2.725719	0.098712
7	6	0	0.610010	1.982540	0.288394
8	7	0	0.556535	0.628980	0.325636
9	6	0	-0.606909	-0.069671	0.191409
10	6	0	-1.788626	0.654935	-0.041949
11	6	0	-1.746478	2.054552	-0.070068
12	6	0	-3.181061	0.062587	-0.278205
13	8	0	-4.149999	0.787293	-0.148578
14	8	0	-3.300719	-1.194358	-0.670632
15	6	0	-0.527666	-1.889858	0.512564
16	8	0	0.055135	-2.121284	1.554293
17	8	0	-1.076345	-2.521823	-0.394808
18	1	0	3.929129	-0.844872	-2.034252
19	1	0	4.336936	-1.371966	-0.389758
20	1	0	2.022653	-2.093375	-0.451135
21	1	0	1.562040	-0.779888	-1.535586
22	1	0	3.441395	1.433608	-1.255756
23	1	0	4.789743	1.014225	-0.163330
24	1	0	-0.479453	3.808604	0.083007

25	1	0	1.591227	2.415250	0.428617
26	1	0	-2.677671	2.591656	-0.219772
27	1	0	-2.440845	-1.713395	-0.692865
28	1	0	1.738280	-0.677785	1.462369

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**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) C2 Carbon-Carboxyl Bond frozen to 1.95 Å<sup>o</sup>**

SCF Done: E(RB+HF-LYP) = -856.670476640

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.650203	-0.705486	-1.025137
2	6	0	2.176140	-1.025140	-0.715133
3	8	0	2.938057	0.763794	0.658091
4	6	0	3.778205	0.728284	-0.520291
5	6	0	1.872508	-0.136914	0.514691
6	6	0	-0.530910	2.741490	0.164305
7	6	0	0.614364	1.991205	0.338917
8	7	0	0.556444	0.636441	0.335662
9	6	0	-0.604291	-0.062888	0.180230
10	6	0	-1.780259	0.676488	-0.041341
11	6	0	-1.738855	2.076374	-0.033883
12	6	0	-3.165713	0.089261	-0.311346
13	8	0	-4.139482	0.812983	-0.220866
14	8	0	-3.280409	-1.175024	-0.691351
15	6	0	-0.527122	-1.976546	0.546917
16	8	0	0.066362	-2.154725	1.585092
17	8	0	-1.092385	-2.593809	-0.347297
18	1	0	3.886784	-0.805567	-2.088807
19	1	0	4.319025	-1.364560	-0.461183
20	1	0	2.004798	-2.080179	-0.496820
21	1	0	1.527223	-0.750375	-1.553290
22	1	0	3.415421	1.458480	-1.259019
23	1	0	4.780780	1.015961	-0.197340
24	1	0	-0.471347	3.824344	0.179846
25	1	0	1.595820	2.418250	0.494851
26	1	0	-2.667877	2.618421	-0.180045
27	1	0	-2.430521	-1.699944	-0.685790
28	1	0	1.742014	-0.692429	1.441030

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**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) C2 Carbon-Carboxyl Bond frozen to 2.05 Å<sup>o</sup>**

SCF Done: E(RB+HF-LYP) = -856.666497432

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

1	6	0	3.622282	-0.686373	-1.075374
2	6	0	2.153728	-1.011436	-0.744134
3	8	0	2.942868	0.752278	0.646372
4	6	0	3.760179	0.738320	-0.547532
5	6	0	1.867147	-0.137424	0.500147
6	6	0	-0.525038	2.755042	0.236603
7	6	0	0.618029	1.997711	0.392866
8	7	0	0.556480	0.643139	0.344393
9	6	0	-0.601085	-0.057487	0.164844
10	6	0	-1.771078	0.698495	-0.041782
11	6	0	-1.731902	2.097225	0.006993
12	6	0	-3.147111	0.115971	-0.349245
13	8	0	-4.126231	0.835662	-0.297271
14	8	0	-3.253052	-1.155069	-0.721199
15	6	0	-0.528838	-2.062136	0.587532
16	8	0	0.064537	-2.178489	1.626735
17	8	0	-1.100307	-2.665038	-0.299659
18	1	0	3.839365	-0.767665	-2.144820
19	1	0	4.301424	-1.355058	-0.535529
20	1	0	1.989428	-2.069858	-0.535911
21	1	0	1.489232	-0.729534	-1.567268
22	1	0	3.383857	1.481383	-1.266443
23	1	0	4.768942	1.020171	-0.238890
24	1	0	-0.464532	3.836809	0.287137
25	1	0	1.599570	2.418475	0.565300
26	1	0	-2.658820	2.644569	-0.133581
27	1	0	-2.410305	-1.679369	-0.687214
28	1	0	1.746090	-0.704086	1.421126

**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) C2 Carbon-Carboxyl Bond frozen to 2.15 Å°**

SCF Done: E(RB+HF-LYP) = -856.663780334

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.598512	0.668645	-1.118754
2	6	0	-2.134043	0.997593	-0.772454
3	8	0	-2.945691	-0.742606	0.634738
4	6	0	-3.745087	-0.747607	-0.570464
5	6	0	-1.860875	0.137017	0.484355
6	6	0	0.521685	-2.765786	0.307307
7	6	0	-0.619587	-2.002160	0.443507
8	7	0	-0.555419	-0.649397	0.348890
9	6	0	0.598755	0.052757	0.144214
10	6	0	1.763039	-0.720112	-0.044308
11	6	0	1.727487	-2.116107	0.047702
12	6	0	3.128315	-0.141157	-0.386933
13	8	0	4.113694	-0.853157	-0.365994
14	8	0	3.221163	1.135365	-0.756710
15	6	0	0.532395	2.145986	0.630514
16	8	0	-0.051314	2.193771	1.673124
17	8	0	1.099258	2.733814	-0.257370

18	1	0	-3.800758	0.733315	-2.192276
19	1	0	-4.284788	1.345912	-0.598915
20	1	0	-1.973957	2.058951	-0.574945
21	1	0	-1.458021	0.708044	-1.583112
22	1	0	-3.358953	-1.501971	-1.272218
23	1	0	-4.758645	-1.023959	-0.272569
24	1	0	0.460571	-3.845288	0.393566
25	1	0	-1.601033	-2.416426	0.632205
26	1	0	2.652693	-2.668609	-0.084768
27	1	0	2.379968	1.649890	-0.699737
28	1	0	-1.747455	0.714010	1.400127

**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) C2 Carbon-Carboxyl Bond frozen to 2.3 Å°**

SCF Done: E(RB+HF-LYP) = -856.662310575

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.578145	0.656446	-1.155772
2	6	0	-2.115023	0.982924	-0.801639
3	8	0	-2.946541	-0.737523	0.618313
4	6	0	-3.733709	-0.753729	-0.593966
5	6	0	-1.853737	0.133927	0.465581
6	6	0	0.524335	-2.772892	0.381895
7	6	0	-0.616552	-2.004924	0.495077
8	7	0	-0.552732	-0.656092	0.349472
9	6	0	0.597117	0.047995	0.115981
10	6	0	1.756558	-0.740484	-0.050803
11	6	0	1.728008	-2.131641	0.090235
12	6	0	3.107595	-0.161672	-0.430914
13	8	0	4.102615	-0.859653	-0.435008
14	8	0	3.176457	1.118336	-0.807370
15	6	0	0.537882	2.224020	0.685110
16	8	0	-0.020074	2.186738	1.735241
17	8	0	1.082600	2.803785	-0.210004
18	1	0	-3.771951	0.710922	-2.231460
19	1	0	-4.266317	1.341075	-0.648049
20	1	0	-1.951783	2.046146	-0.616029
21	1	0	-1.433304	0.681890	-1.603002
22	1	0	-3.342612	-1.516146	-1.284164
23	1	0	-4.751053	-1.024404	-0.303623
24	1	0	0.464298	-3.848550	0.507986
25	1	0	-1.597114	-2.413179	0.701407
26	1	0	2.652544	-2.688084	-0.031366
27	1	0	2.328579	1.609928	-0.729281
28	1	0	-1.748593	0.719769	1.377174

**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) C2 Carbon-Carboxyl Bond frozen to 2.4 Å°**

SCF Done: E(RB+HF-LYP) = -856.662017739

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.559184	0.648136	-1.189168
2	6	0	-2.098949	0.975773	-0.823615
3	8	0	-2.946471	-0.734100	0.599818
4	6	0	-3.720507	-0.758663	-0.620287
5	6	0	-1.847330	0.131103	0.448265
6	6	0	0.530352	-2.774734	0.458891
7	6	0	-0.610791	-2.003994	0.548552
8	7	0	-0.549814	-0.661578	0.345919
9	6	0	0.594316	0.041665	0.077063
10	6	0	1.750044	-0.760327	-0.064846
11	6	0	1.731182	-2.143678	0.131217
12	6	0	3.083489	-0.177846	-0.483730
13	8	0	4.093001	-0.853518	-0.501889
14	8	0	3.113992	1.102181	-0.877596
15	6	0	0.549592	2.291814	0.753324
16	8	0	0.043754	2.150045	1.814561
17	8	0	1.045961	2.873705	-0.157245
18	1	0	-3.742879	0.696197	-2.266975
19	1	0	-4.252242	1.335791	-0.692120
20	1	0	-1.936892	2.040079	-0.642001
21	1	0	-1.409272	0.672388	-1.616831
22	1	0	-3.321838	-1.525203	-1.301443
23	1	0	-4.740922	-1.027785	-0.339255
24	1	0	0.472602	-3.844430	0.629259
25	1	0	-1.589149	-2.405929	0.777118
26	1	0	2.655462	-2.703637	0.022731
27	1	0	2.247587	1.551255	-0.786196
28	1	0	-1.748930	0.720324	1.359112

**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) C2 Carbon-Carboxyl Bond frozen to 2.5 Å°**

SCF Done: E(RB+HF-LYP) = -856.662767085

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.555346	0.651059	-1.217044
2	6	0	-2.087224	0.963018	-0.870905
3	8	0	-2.946453	-0.710643	0.588721
4	6	0	-3.728893	-0.745055	-0.625597
5	6	0	-1.839232	0.141641	0.416351
6	6	0	0.534621	-2.762970	0.551359
7	6	0	-0.606716	-1.989103	0.610178
8	7	0	-0.549392	-0.659395	0.331300

9	6	0	0.588363	0.033222	0.012445
10	6	0	1.740295	-0.781437	-0.095543
11	6	0	1.732557	-2.150272	0.176073
12	6	0	3.049666	-0.193048	-0.564902
13	8	0	4.080542	-0.834386	-0.585765
14	8	0	3.017864	1.077961	-0.997442
15	6	0	0.597228	2.330843	0.862951
16	8	0	0.197965	2.039348	1.933805
17	8	0	0.993428	2.948586	-0.062529
18	1	0	-3.749199	0.685664	-2.293637
19	1	0	-4.234674	1.354962	-0.723483
20	1	0	-1.902551	2.028004	-0.716337
21	1	0	-1.409111	0.628672	-1.661421
22	1	0	-3.343169	-1.526184	-1.297411
23	1	0	-4.750448	-0.998313	-0.333962
24	1	0	0.479265	-3.821596	0.781429
25	1	0	-1.582083	-2.379641	0.869824
26	1	0	2.656084	-2.715522	0.087750
27	1	0	2.120331	1.457120	-0.894767
28	1	0	-1.737401	0.748271	1.316392

**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) Transition State Calculation**

Negative Frequency -203.3494

SCF Done: E(RB+HF-LYP) = -856.661987165

Zero-point correction= 0.213824 (Hartree/Particle)  
 Thermal correction to Energy= 0.228534  
 Thermal correction to Enthalpy= 0.229478  
 Thermal correction to Gibbs Free Energy= 0.169961  
 Sum of electronic and zero-point Energies= -856.448163  
 Sum of electronic and thermal Energies= -856.433453  
 Sum of electronic and thermal Enthalpies= -856.432509  
 Sum of electronic and thermal Free Energies= -856.492026

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	143.407	54.410	125.265

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.562331	0.649500	-1.182445
2	6	0	-2.102310	0.978198	-0.816962
3	8	0	-2.946706	-0.735653	0.603472
4	6	0	-3.722054	-0.758417	-0.615955
5	6	0	-1.849102	0.131296	0.453168
6	6	0	0.528845	-2.774865	0.440777
7	6	0	-0.612240	-2.004786	0.536156

8	7	0	-0.550517	-0.660531	0.347549
9	6	0	0.594942	0.043313	0.087623
10	6	0	1.751548	-0.755564	-0.060632
11	6	0	1.730331	-2.141060	0.121833
12	6	0	3.089334	-0.174203	-0.470456
13	8	0	4.094990	-0.855880	-0.486495
14	8	0	3.130198	1.106278	-0.859099
15	6	0	0.545259	2.276842	0.735661
16	8	0	0.023853	2.161841	1.794003
17	8	0	1.056331	2.856972	-0.170416
18	1	0	-3.746568	0.699210	-2.260074
19	1	0	-4.255753	1.335670	-0.683911
20	1	0	-1.941838	2.042255	-0.632732
21	1	0	-1.412864	0.677472	-1.611468
22	1	0	-3.323608	-1.523481	-1.298915
23	1	0	-4.741959	-1.028747	-0.334282
24	1	0	0.470591	-3.846203	0.600266
25	1	0	-1.591168	-2.408401	0.759125
26	1	0	2.654656	-2.700169	0.009927
27	1	0	2.269226	1.567311	-0.769950
28	1	0	-1.749765	0.718797	1.364840

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**B3LYP/6-31+G\* C-PCM CALCULATIONS IN WATER**

**Quinolinic Acid Neutral: Pyridine-2,3-dicarboxylic acid (1)**

SCF Done: E(RB+HF-LYP) = -625.473572579

Zero-point correction=	0.116948 (Hartree/Particle)
Thermal correction to Energy=	0.126289
Thermal correction to Enthalpy=	0.127233
Thermal correction to Gibbs Free Energy=	0.081329
Sum of electronic and zero-point Energies=	-625.356625
Sum of electronic and thermal Energies=	-625.347284
Sum of electronic and thermal Enthalpies=	-625.346340
Sum of electronic and thermal Free Energies=	-625.392243

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.247	35.325	96.612

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.691534	0.019207	0.000038
2	6	0	-0.672508	0.402091	-0.002480
3	6	0	-0.923344	1.786788	-0.006954
4	6	0	0.113965	2.709715	-0.008228
5	6	0	1.423446	2.227198	-0.002618
6	7	0	1.687732	0.921213	0.001571
7	1	0	-1.956145	2.119137	-0.008578
8	1	0	-0.084390	3.779724	-0.012273
9	1	0	2.281406	2.898739	-0.001429
10	6	0	1.259548	-1.385891	0.001230
11	8	0	2.576763	-1.462047	0.015644
12	8	0	0.593938	-2.420844	-0.010968
13	1	0	2.948159	-0.536095	0.019625
14	6	0	-1.938413	-0.449598	0.003543
15	8	0	-1.864353	-1.771056	-0.016978
16	8	0	-3.033112	0.096454	0.025730
17	1	0	-0.914406	-2.107119	-0.022949

**Quinolinic Acid Anion: Deprotonated 3 Carboxyl or 2 Carboxyl (2&3)**

SCF Done: E(RB+HF-LYP) = -625.027604715

Zero-point correction=	0.103561 (Hartree/Particle)
Thermal correction to Energy=	0.113361
Thermal correction to Enthalpy=	0.114305
Thermal correction to Gibbs Free Energy=	0.067112
Sum of electronic and zero-point Energies=	-624.924044

Sum of electronic and thermal Energies= -624.914244  
 Sum of electronic and thermal Enthalpies= -624.913300  
 Sum of electronic and thermal Free Energies= -624.960493

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	71.135	35.457	99.326

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.242264	-0.693819	-0.025996
2	6	0	-0.310031	0.708588	0.040121
3	6	0	-1.588776	1.281892	0.047402
4	6	0	-2.715660	0.464489	0.007956
5	6	0	-2.531906	-0.919871	-0.047207
6	7	0	-1.321737	-1.493316	-0.063303
7	1	0	-1.689104	2.364072	0.092392
8	1	0	-3.719379	0.885569	0.023590
9	1	0	-3.385917	-1.596161	-0.081618
10	6	0	0.921173	1.598712	0.172277
11	8	0	1.738053	1.293889	1.086558
12	8	0	0.996607	2.584893	-0.612928
13	6	0	1.070026	-1.433636	-0.073159
14	8	0	1.891743	-0.954487	-1.017181
15	8	0	1.334274	-2.396031	0.627783
16	1	0	2.745771	-1.464509	-0.993467

#### Quinolinic Acid Dianion: Deprotonated 2 & 3 Carboxyl (4)

SCF Done: E(RB+HF-LYP) = -624.576577479

Zero-point correction= 0.091990 (Hartree/Particle)  
 Thermal correction to Energy= 0.101510  
 Thermal correction to Enthalpy= 0.102455  
 Thermal correction to Gibbs Free Energy= 0.055921  
 Sum of electronic and zero-point Energies= -624.484587  
 Sum of electronic and thermal Energies= -624.475067  
 Sum of electronic and thermal Enthalpies= -624.474123  
 Sum of electronic and thermal Free Energies= -624.520657

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	63.699	33.938	97.939

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.186046	-0.707570	0.021041
2	6	0	-0.281579	0.697965	-0.054581
3	6	0	-1.563125	1.259458	-0.083324

4	6	0	-2.687865	0.435028	-0.052176
5	6	0	-2.487865	-0.942987	0.022519
6	7	0	-1.269905	-1.506887	0.060390
7	1	0	-1.669823	2.340775	-0.133571
8	1	0	-3.694889	0.847192	-0.082529
9	1	0	-3.335516	-1.628288	0.054969
10	6	0	0.936996	1.605874	-0.135850
11	8	0	1.864543	1.261496	-0.923747
12	8	0	0.913992	2.656996	0.571521
13	6	0	1.147301	-1.442909	0.146015
14	8	0	1.799148	-1.241304	1.210937
15	8	0	1.462649	-2.232266	-0.789144

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**Quinolinic Acid Cation: THF on N1 (1C)**

SCF Done: E(RB+HF-LYP) = -857.158056715

Zero-point correction=	0.224252 (Hartree/Particle)
Thermal correction to Energy=	0.239289
Thermal correction to Enthalpy=	0.240234
Thermal correction to Gibbs Free Energy=	0.180205
and zero-point Energies=	-856.933805
Sum of electronic and thermal Energies=	-856.918767
Sum of electronic and thermal Enthalpies=	-856.917823
Sum of electronic and thermal Free Energies=	-856.977852

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	150.156	56.350	126.341

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.663604	-0.792313	1.024491
2	6	0	-2.207353	-1.137973	0.654597
3	8	0	-2.998010	0.637279	-0.713178
4	6	0	-3.801219	0.633777	0.507343
5	6	0	-1.937585	-0.244909	-0.580704
6	6	0	0.430154	2.709339	-0.197369
7	6	0	-0.691512	1.917559	-0.402301
8	7	0	-0.611068	0.571511	-0.398323
9	6	0	0.585451	-0.052502	-0.213103
10	6	0	1.731553	0.701154	0.032113
11	6	0	1.656357	2.100535	0.037117
12	6	0	3.081396	0.031448	0.171560
13	8	0	3.639483	-0.466636	-0.785397
14	8	0	3.667661	0.075610	1.365495
15	6	0	0.709520	-1.562688	-0.243519
16	8	0	0.150350	-2.102180	-1.315940
17	8	0	1.315494	-2.152400	0.628058
18	1	0	-3.844730	-0.868195	2.101155
19	1	0	-4.363916	-1.455062	0.504299
20	1	0	-2.074497	-2.196115	0.415528
21	1	0	-1.530410	-0.880936	1.477687

22	1	0	-3.397569	1.375885	1.209247
23	1	0	-4.811016	0.922947	0.209415
24	1	0	0.325271	3.793361	-0.214894
25	1	0	-1.677629	2.335370	-0.574834
26	1	0	2.551420	2.699910	0.214228
27	1	0	3.064048	0.399360	2.097018
28	1	0	-1.792804	-0.776047	-1.523534
29	1	0	0.270536	-3.105006	-1.300712

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**Quinolinic Acid Zwitterion: Deprotonated 3 Carboxyl (or 2 Carboxyl) & THF on N1 (2C or 3C)**

SCF Done: E(RB+HF-LYP) = -856.729192721

Zero-point correction= 0.214095 (Hartree/Particle)  
 Thermal correction to Energy= 0.228391  
 Thermal correction to Enthalpy= 0.229335  
 Thermal correction to Gibbs Free Energy= 0.171495 Sum of electronic  
 and zero-point Energies= -856.515098  
 Sum of electronic and thermal Energies= -856.500802  
 Sum of electronic and thermal Enthalpies= -856.499858  
 Sum of electronic and thermal Free Energies= -856.557697

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	143.317	54.106	121.734

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.718582	-0.787621	-0.893302
2	6	0	2.237880	-1.104255	-0.611989
3	8	0	2.940552	0.752366	0.697444
4	6	0	3.821468	0.669829	-0.461606
5	6	0	1.899222	-0.165933	0.570894
6	6	0	-0.520308	2.681078	-0.034599
7	6	0	0.622335	1.937994	0.199067
8	7	0	0.568394	0.593695	0.318682
9	6	0	-0.607217	-0.094174	0.211981
10	6	0	-1.788250	0.619156	-0.054835
11	6	0	-1.733699	2.016740	-0.158317
12	6	0	-3.173560	0.018366	-0.232518
13	8	0	-4.160103	0.687822	0.037086
14	8	0	-3.300283	-1.199884	-0.735708
15	6	0	-0.579674	-1.616941	0.466143
16	8	0	-0.154436	-1.985462	1.572724
17	8	0	-1.015688	-2.325809	-0.490018
18	1	0	3.981575	-0.935118	-1.945575
19	1	0	4.375095	-1.413259	-0.278037
20	1	0	2.068037	-2.151573	-0.352250
21	1	0	1.617780	-0.862362	-1.482671
22	1	0	3.467818	1.361209	-1.238890
23	1	0	4.810703	0.981625	-0.119548
24	1	0	-0.448241	3.764001	-0.118517
25	1	0	1.602446	2.387193	0.310327
26	1	0	-2.651476	2.571594	-0.343567

27	1	0	1.745516	-0.667036	1.526385
28	1	0	-2.409034	-1.669835	-0.846166

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**Quinolinic Acid Zwitterion: Deprotonated 2&3 Carboxyl & THF on N1 (4C)**

SCF Done: E(RB+HF-LYP) = -856.281426025

Zero-point correction=	0.201469 (Hartree/Particle)
Thermal correction to Energy=	0.215208
Thermal correction to Enthalpy=	0.216152
Thermal correction to Gibbs Free Energy=	0.159749
Sum of electronic and zero-point Energies=	-856.079957
Sum of electronic and thermal Energies=	-856.066218
Sum of electronic and thermal Enthalpies=	-856.065274
Sum of electronic and thermal Free Energies=	-856.121677

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	135.045	51.744	118.709

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.751228	-0.730024	0.897019
2	6	0	-2.235101	-0.983063	0.826083
3	8	0	-2.883082	0.561966	-0.864397
4	6	0	-3.879396	0.617444	0.196527
5	6	0	-1.828257	-0.280199	-0.489740
6	6	0	0.483574	2.673933	-0.087623
7	6	0	-0.638902	1.892302	-0.280444
8	7	0	-0.544641	0.540782	-0.312293
9	6	0	0.652626	-0.100723	-0.179483
10	6	0	1.815084	0.655773	0.028674
11	6	0	1.718297	2.048015	0.085982
12	6	0	3.191318	-0.002299	0.169273
13	8	0	3.868729	0.354175	1.171178
14	8	0	3.528024	-0.797174	-0.746934
15	6	0	0.692258	-1.640535	-0.225119
16	8	0	0.392858	-2.170189	-1.323592
17	8	0	1.011260	-2.188091	0.856616
18	1	0	-4.122366	-0.706703	1.926639
19	1	0	-4.302373	-1.499972	0.344692
20	1	0	-1.974458	-2.043707	0.811961
21	1	0	-1.722002	-0.518096	1.675741
22	1	0	-3.651029	1.456741	0.868123
23	1	0	-4.841450	0.793773	-0.290088
24	1	0	0.381958	3.757447	-0.067626
25	1	0	-1.628910	2.306627	-0.424920
26	1	0	2.615325	2.640302	0.263461
27	1	0	-1.606161	-0.961125	-1.311797

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**Pyridine-3-carboxylic acid: Deprotonated C2 & 3 Carboxyl (5)**

SCF Done: E(RB+HF-LYP) = -435.886045020

Zero-point correction= 0.076166 (Hartree/Particle)  
 Thermal correction to Energy= 0.083041  
 Thermal correction to Enthalpy= 0.083985  
 Thermal correction to Gibbs Free Energy= 0.044285  
 Sum of electronic and zero-point Energies= -435.809879  
 Sum of electronic and thermal Energies= -435.803004  
 Sum of electronic and thermal Enthalpies= -435.802060  
 Sum of electronic and thermal Free Energies= -435.841760

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	52.109	24.868	83.556

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.417868	-1.309352	0.084726
2	6	0	-0.243686	-0.040700	-0.000057
3	6	0	0.453717	1.168289	-0.073152
4	6	0	1.854062	1.143106	-0.076221
5	6	0	2.474181	-0.099290	0.003885
6	7	0	1.800823	-1.273313	0.085018
7	1	0	-0.074725	2.122085	-0.129037
8	1	0	2.442186	2.057862	-0.137250
9	1	0	3.564854	-0.168784	0.005296
10	8	0	-2.352494	0.158032	1.123182
11	8	0	-2.361903	-0.178502	-1.119334
12	6	0	-1.759960	-0.017755	0.000000

**Pyridine-3-carboxylic acid: Deprotonated C2 (6)**

SCF Done: E(RB+HF-LYP) = -436.349061582

Zero-point correction= 0.088157 (Hartree/Particle)  
 Thermal correction to Energy= 0.095260  
 Thermal correction to Enthalpy= 0.096204  
 Thermal correction to Gibbs Free Energy= 0.055682  
 Sum of electronic and zero-point Energies= -436.260905  
 Sum of electronic and thermal Energies= -436.253802  
 Sum of electronic and thermal Enthalpies= -436.252858  
 Sum of electronic and thermal Free Energies= -436.293379

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	59.776	26.121	85.285

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.450780	-1.314578	-0.038584
2	6	0	0.188546	-0.033864	-0.004076
3	6	0	-0.528790	1.175249	0.030073
4	6	0	-1.919178	1.127217	0.035447
5	6	0	-2.517734	-0.134847	0.000091
6	7	0	-1.834526	-1.295921	-0.036018
7	1	0	-0.008548	2.132594	0.056744
8	1	0	-2.523452	2.033359	0.066805
9	1	0	-3.607888	-0.221415	0.001381
10	6	0	1.674237	0.083129	-0.013019
11	8	0	2.336866	-1.080703	0.071915
12	8	0	2.287146	1.152911	-0.071307
13	1	0	3.311672	-0.864594	0.062738

### Pyridine-3-carboxylic acid: Deprotonated 3 Carboxyl (5A)

SCF Done: E(RB+HF-LYP) = -436.445401261

Zero-point correction=	0.090510 (Hartree/Particle)
Thermal correction to Energy=	0.097322
Thermal correction to Enthalpy=	0.098266
Thermal correction to Gibbs Free Energy=	0.058497
Sum of electronic and zero-point Energies=	-436.354891
Sum of electronic and thermal Energies=	-436.348080
Sum of electronic and thermal Enthalpies=	-436.347136
Sum of electronic and thermal Free Energies=	-436.386904

KCal/Mol	E (Thermal)		CV	S
	Cal/Mol-Kelvin	Cal/Mol-Kelvin		
Total	61.070	24.959		83.701

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.465059	-1.184896	-0.006473
2	6	0	-0.263629	0.013100	0.000390
3	6	0	0.465310	1.208564	0.007010
4	6	0	1.859677	1.160969	0.007087
5	6	0	2.484090	-0.088230	-0.000792
6	7	0	1.806746	-1.249815	-0.007722
7	1	0	-0.063872	2.157638	0.012100
8	1	0	2.456258	2.071561	0.012826
9	1	0	3.571793	-0.164585	-0.001359
10	6	0	-1.788574	0.008139	0.000095
11	8	0	-2.368803	1.133406	-0.016330
12	8	0	-2.365925	-1.119251	0.016146
13	1	0	-0.065180	-2.135023	-0.011949

**Pyridine-3-carboxylic acid(6A)**

SCF Done: E(RB+HF-LYP) = -436.896238268

```

Zero-point correction=          0.102228 (Hartree/Particle)
Thermal correction to Energy=    0.109289
Thermal correction to Enthalpy=  0.110233
Thermal correction to Gibbs Free Energy= 0.070094
Sum of electronic and zero-point Energies= -436.794010
Sum of electronic and thermal Energies= -436.786949
Sum of electronic and thermal Enthalpies= -436.786005
Sum of electronic and thermal Free Energies= -436.826144

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	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	68.580	26.442	84.481

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.540928	-1.201866	-0.000049
2	6	0	0.210364	-0.017013	-0.000030
3	6	0	-0.475406	1.205499	0.000018
4	6	0	-1.868600	1.188864	0.000087
5	6	0	-2.522965	-0.045610	0.000112
6	7	0	-1.879448	-1.226870	0.000025
7	1	0	0.070132	2.144781	0.000023
8	1	0	-2.442119	2.113683	0.000124
9	1	0	-3.612154	-0.092585	0.000141
10	6	0	1.695631	-0.107221	-0.000114
11	8	0	2.294162	1.095818	0.000019
12	8	0	2.319042	-1.159724	-0.000114
13	1	0	-0.033249	-2.165067	-0.000067
14	1	0	3.279317	0.962610	0.000218

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**Pyridine-3-carboxylic acid: THF on N1 (9B)**

SCF DONE: E(RB+HF-LYP) = -668.603830603

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Zero-point correction=          0.210141 (Hartree/Particle)
Thermal correction to Energy=    0.221310
Thermal correction to Enthalpy=  0.222254
Thermal correction to Gibbs Free Energy= 0.172135
Sum of electronic and zero-point Energies= -668.393689
Sum of electronic and thermal Energies= -668.382521
Sum of electronic and thermal Enthalpies= -668.381576
Sum of electronic and thermal Free Energies= -668.431696

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	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	138.874	44.049	105.485

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.662173	-1.130157	0.618389
2	6	0	-2.152599	-1.385948	0.465854
3	8	0	-2.773524	0.546328	-0.775429
4	6	0	-3.765098	0.353430	0.280228
5	6	0	-1.760061	-0.402756	-0.657818
6	6	0	0.802277	2.258847	0.226140
7	6	0	-0.400019	1.633594	-0.073480
8	7	0	-0.436620	0.306416	-0.318377
9	6	0	0.684577	-0.440686	-0.292167
10	6	0	1.914410	0.133048	-0.000535
11	6	0	1.976174	1.508253	0.265466
12	6	0	3.115596	-0.763458	0.004821
13	8	0	4.239744	-0.101133	0.283403
14	8	0	3.053724	-1.957256	-0.230473
15	1	0	-4.022053	-1.356973	1.627508
16	1	0	-4.235630	-1.726376	-0.101342
17	1	0	-1.909273	-2.419324	0.201108
18	1	0	-1.627140	-1.133017	1.395601
19	1	0	-3.512126	0.995086	1.135619
20	1	0	-4.725722	0.663672	-0.138181
21	1	0	0.808974	3.327768	0.420717
22	1	0	-1.348238	2.155367	-0.134327
23	1	0	2.926922	1.981782	0.493358
24	1	0	-1.566352	-0.886447	-1.667178
25	1	0	0.581078	-1.498841	-0.517658
26	1	0	5.007843	-0.736130	0.272022

**Pyridine-3-carboxylic acid: Deprotonated C2 & 3 Carboxyl & THF on N1 (10B)**

SCF Done: E(RB+HF-LYP) = -667.637450368

Zero-point correction= 0.186448 (Hartree/Particle)  
 Thermal correction to Energy= 0.197416  
 Thermal correction to Enthalpy= 0.198360  
 Thermal correction to Gibbs Free Energy= 0.148349  
 Sum of electronic and zero-point Energies= -667.451003  
 Sum of electronic and thermal Energies= -667.440034  
 Sum of electronic and thermal Enthalpies= -667.439090  
 Sum of electronic and thermal Free Energies= -667.489102

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	123.881	42.142	105.259

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.691549	-1.071410	-0.537608
2	6	0	2.173531	-1.292916	-0.624533
3	8	0	2.646281	0.420505	0.957321
4	6	0	3.761929	0.342774	0.033475

5	6	0	1.636546	-0.508242	0.590380
6	6	0	-0.759198	2.156578	-0.478463
7	6	0	0.399420	1.500283	-0.124567
8	7	0	0.345545	0.197549	0.274586
9	6	0	-0.784465	-0.572009	0.366451
10	6	0	-1.969538	0.119884	-0.011024
11	6	0	-1.971217	1.451061	-0.423294
12	6	0	-3.279581	-0.648943	0.050007
13	8	0	-3.635427	-1.265502	-0.998245
14	8	0	-3.921086	-0.620105	1.142045
15	1	0	4.190769	-1.157939	-1.509124
16	1	0	4.153288	-1.785736	0.155634
17	1	0	1.878682	-2.345452	-0.583693
18	1	0	1.772957	-0.863238	-1.551584
19	1	0	3.642795	1.104463	-0.751766
20	1	0	4.668600	0.559106	0.606184
21	1	0	-0.717098	3.197196	-0.788218
22	1	0	1.372535	1.975902	-0.125376
23	1	0	-2.899353	1.952319	-0.698525
24	1	0	1.406017	-1.161013	1.470444

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**Pyridine-3-carboxylic acid: Deprotonated 3 Carboxyl & THF on N1 (11B)**

SCF Done: E(RB+HF-LYP) = -668.157647073

Zero-point correction=	0.198707 (Hartree/Particle)
Thermal correction to Energy=	0.210498
Thermal correction to Enthalpy=	0.211443
Thermal correction to Gibbs Free Energy=	0.158769
Sum of electronic and zero-point Energies=	-667.958940
Sum of electronic and thermal Energies=	-667.947149
Sum of electronic and thermal Enthalpies=	-667.946204
Sum of electronic and thermal Free Energies=	-667.998878

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	132.090	44.567	110.862

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.629832	-1.068233	0.664744
2	6	0	-2.119285	-1.342388	0.558749
3	8	0	-2.714474	0.477670	-0.855610
4	6	0	-3.718439	0.380994	0.198212
5	6	0	-1.696079	-0.453075	-0.632653
6	6	0	0.820591	2.241750	0.233336
7	6	0	-0.374070	1.605612	-0.071773
8	7	0	-0.389009	0.279238	-0.322279
9	6	0	0.747665	-0.452540	-0.294226
10	6	0	1.973186	0.126080	0.004236
11	6	0	2.001743	1.500051	0.274851
12	6	0	3.242845	-0.740831	0.020228
13	8	0	4.311798	-0.146580	0.317921
14	8	0	3.084345	-1.957732	-0.266790

15	1	0	-4.007936	-1.206287	1.683298
16	1	0	-4.194842	-1.721739	-0.010650
17	1	0	-1.879501	-2.394611	0.378178
18	1	0	-1.604100	-1.023821	1.473653
19	1	0	-3.473447	1.090102	1.001723
20	1	0	-4.672629	0.661411	-0.254891
21	1	0	0.813596	3.310194	0.431088
22	1	0	-1.325904	2.118373	-0.138955
23	1	0	2.951925	1.972180	0.508583
24	1	0	-1.486656	-1.021858	-1.590411
25	1	0	0.659245	-1.509995	-0.524052

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**Pyridine-3-carboxylic acid: Deprotonated C2 & THF on N1 (12B)**

SCF Done: E(RB+HF-LYP) = -668.106745392

Zero-point correction= 0.197932 (Hartree/Particle)  
 Thermal correction to Energy= 0.209638  
 Thermal correction to Enthalpy= 0.210582  
 Thermal correction to Gibbs Free Energy= 0.158634  
 Sum of electronic and zero-point Energies= -667.908813  
 Sum of electronic and thermal Energies= -667.897107  
 Sum of electronic and thermal Enthalpies= -667.896163  
 Sum of electronic and thermal Free Energies= -667.948111

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	131.550	44.777	109.334

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.635983	-1.067098	0.645724
2	6	0	-2.117242	-1.305189	0.615482
3	8	0	-2.691700	0.453142	-0.882499
4	6	0	-3.734173	0.364257	0.126194
5	6	0	-1.659327	-0.466540	-0.597438
6	6	0	0.785383	2.272609	0.242262
7	6	0	-0.383203	1.594047	-0.056449
8	7	0	-0.362805	0.258863	-0.306683
9	6	0	0.759726	-0.515258	-0.296559
10	6	0	1.943485	0.188611	0.013008
11	6	0	1.985734	1.556571	0.280656
12	6	0	3.189785	-0.641024	0.027822
13	8	0	2.978292	-1.932930	-0.259330
14	8	0	4.312229	-0.218329	0.273318
15	1	0	-4.061315	-1.181531	1.648848
16	1	0	-4.155058	-1.754649	-0.033569
17	1	0	-1.839968	-2.357064	0.504071
18	1	0	-1.647810	-0.924734	1.531415
19	1	0	-3.541363	1.101797	0.919276
20	1	0	-4.677458	0.608263	-0.370362
21	1	0	0.749366	3.340839	0.435430
22	1	0	-1.347286	2.084988	-0.118835

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23	1	0	2.925722	2.055448	0.508014
24	1	0	-1.446095	-1.078888	-1.516140
25	1	0	1.985224	-2.007477	-0.417475

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**Pyridine-2-carboxylic acid: Deprotonated C3 & 2 carxboxyl (7)**

SCF Done: E(RB+HF-LYP) = -435.888999821

Zero-point correction=	0.076584 (Hartree/Particle)
Thermal correction to Energy=	0.083469
Thermal correction to Enthalpy=	0.084413
Thermal correction to Gibbs Free Energy=	0.044454
Sum of electronic and zero-point Energies=	-435.812415
Sum of electronic and thermal Energies=	-435.805531
Sum of electronic and thermal Enthalpies=	-435.804586
Sum of electronic and thermal Free Energies=	-435.844546

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	52.378	24.606	84.101

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.227248	0.074056	-0.005692
2	6	0	0.428801	1.333659	-0.006959
3	6	0	1.835353	1.193918	-0.005950
4	6	0	2.484059	-0.054454	0.000828
5	6	0	1.695776	-1.202424	0.006940
6	7	0	0.348688	-1.156228	0.003020
7	1	0	2.474597	2.084630	-0.007680
8	1	0	3.572698	-0.139272	0.002565
9	1	0	2.146405	-2.197738	0.011830
10	6	0	-1.751528	0.026883	0.000799
11	8	0	-2.342098	-0.004812	-1.124687
12	8	0	-2.336126	0.019332	1.128730

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**Pyridine-2-carboxylic acid: Deprotonated C3 (8)**

SCF Done: E(RB+HF-LYP) = -436.357040855

Zero-point correction=	0.088907 (Hartree/Particle)
Thermal correction to Energy=	0.095769
Thermal correction to Enthalpy=	0.096713
Thermal correction to Gibbs Free Energy=	0.057184
Sum of electronic and zero-point Energies=	-436.268134
Sum of electronic and thermal Energies=	-436.261272
Sum of electronic and thermal Enthalpies=	-436.260328
Sum of electronic and thermal Free Energies=	-436.299857

E (Thermal)	CV	S
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Total	KCal/Mol 60.096	Cal/Mol-Kelvin 25.647	Cal/Mol-Kelvin 83.196
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.186542	-0.176918	-0.000248
2	6	0	-0.523800	-1.396007	0.001527
3	6	0	-1.928964	-1.171542	0.001715
4	6	0	-2.503720	0.102092	-0.000110
5	6	0	-1.655216	1.218047	-0.001744
6	7	0	-0.328243	1.087955	-0.001660
7	1	0	-2.611529	-2.027166	0.003379
8	1	0	-3.585315	0.246532	-0.000170
9	1	0	-2.051851	2.234577	-0.003173
10	6	0	1.693525	-0.151475	-0.000163
11	8	0	2.245270	1.083221	0.003416
12	8	0	2.435054	-1.126839	-0.003134
13	1	0	1.493599	1.734134	0.003465

Pyridine-2-carboxylic acid: Deprotonated C3 & 2 carboxyl & THF on N1 (14B)

SCF Done: E(RB+HF-LYP) = -667.623995309

Zero-point correction=	0.185611 (Hartree/Particle)
Thermal correction to Energy=	0.196566
Thermal correction to Enthalpy=	0.197510
Thermal correction to Gibbs Free Energy=	0.147971
Sum of electronic and zero-point Energies=	-667.438385
Sum of electronic and thermal Energies=	-667.427429
Sum of electronic and thermal Enthalpies=	-667.426485
Sum of electronic and thermal Free Energies=	-667.476024

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	123.347	42.283	104.264

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.158864	-0.562773	-0.659666
2	6	0	1.657871	-0.824484	-0.863128
3	8	0	1.985778	0.552943	1.049502
4	6	0	3.140806	0.708753	0.182312
5	6	0	1.031423	-0.299204	0.447431
6	6	0	-1.329693	2.549190	-0.174815
7	6	0	-0.191982	1.820575	0.105223
8	7	0	-0.253416	0.466530	0.192739
9	6	0	-1.448336	-0.186865	0.005095
10	6	0	-2.665168	0.463759	-0.284206
11	6	0	-2.542998	1.865512	-0.366601
12	6	0	-1.468692	-1.710483	0.120694
13	8	0	-1.314316	-2.364944	-0.946657

14	8	0	-1.696047	-2.187236	1.269951
15	1	0	3.695548	-0.434141	-1.606056
16	1	0	3.627260	-1.382997	-0.101660
17	1	0	1.415198	-1.876151	-1.030697
18	1	0	1.275566	-0.248259	-1.714900
19	1	0	3.016093	1.608855	-0.437810
20	1	0	4.009725	0.838943	0.833435
21	1	0	-1.256637	3.634513	-0.234701
22	1	0	0.775227	2.269448	0.285647
23	1	0	-3.425076	2.473461	-0.585990
24	1	0	0.785117	-1.099356	1.187158

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Pyridine-2-carboxylic acid: Deprotonated C3 & THF on N1 (16B)

SCF Done: E(RB+HF-LYP) = -668.067272180

Zero-point correction=	0.197028 (Hartree/Particle)
Thermal correction to Energy=	0.209144
Thermal correction to Enthalpy=	0.210088
Thermal correction to Gibbs Free Energy=	0.156925
Sum of electronic and zero-point Energies=	-667.870244
Sum of electronic and thermal Energies=	-667.858128
Sum of electronic and thermal Enthalpies=	-667.857184
Sum of electronic and thermal Free Energies=	-667.910348

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	131.240	45.800	111.893

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.155584	-0.631697	-0.590581
2	6	0	1.658330	-0.978582	-0.651943
3	8	0	2.037703	0.719572	0.967231
4	6	0	3.126429	0.769994	0.003306
5	6	0	1.069592	-0.215291	0.559360
6	6	0	-1.369246	2.568557	-0.190235
7	6	0	-0.206302	1.872968	0.108637
8	7	0	-0.220725	0.526120	0.195525
9	6	0	-1.404530	-0.144174	-0.017838
10	6	0	-2.635841	0.446575	-0.304302
11	6	0	-2.559272	1.859986	-0.380639
12	6	0	-1.395573	-1.656376	-0.018029
13	8	0	-1.178781	-2.313908	-1.020023
14	8	0	-1.721007	-2.274176	1.130109
15	1	0	3.631247	-0.664735	-1.576823
16	1	0	3.690083	-1.316705	0.078691
17	1	0	1.465312	-2.051499	-0.590286
18	1	0	1.212397	-0.606571	-1.581637
19	1	0	2.910813	1.536504	-0.755198
20	1	0	4.022774	1.053268	0.561209
21	1	0	-1.323906	3.655189	-0.251649
22	1	0	0.743007	2.353596	0.302989

23	1	0	-3.460584	2.439387	-0.594999
24	1	0	0.805568	-0.858630	1.450357
25	1	0	-1.889984	-1.626308	1.863734

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**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) Transition State Single Point**

SCF Done: E(RB+HF-LYP) = -856.686856260

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.562331	0.649500	-1.182445
2	6	0	-2.102310	0.978198	-0.816962
3	8	0	-2.946706	-0.735653	0.603472
4	6	0	-3.722054	-0.758417	-0.615955
5	6	0	-1.849102	0.131296	0.453168
6	6	0	0.528845	-2.774865	0.440777
7	6	0	-0.612240	-2.004786	0.536156
8	7	0	-0.550517	-0.660531	0.347549
9	6	0	0.594942	0.043313	0.087623
10	6	0	1.751548	-0.755564	-0.060632
11	6	0	1.730331	-2.141060	0.121833
12	6	0	3.089334	-0.174203	-0.470456
13	8	0	4.094990	-0.855880	-0.486495
14	8	0	3.130198	1.106278	-0.859099
15	6	0	0.545259	2.276842	0.735661
16	8	0	0.023853	2.161841	1.794003
17	8	0	1.056331	2.856972	-0.170416
18	1	0	-3.746568	0.699210	-2.260074
19	1	0	-4.255753	1.335670	-0.683911
20	1	0	-1.941838	2.042255	-0.632732
21	1	0	-1.412864	0.677472	-1.611468
22	1	0	-3.323608	-1.523481	-1.298915
23	1	0	-4.741959	-1.028747	-0.334282
24	1	0	0.470591	-3.846203	0.600266
25	1	0	-1.591168	-2.408401	0.759125
26	1	0	2.654656	-2.700169	0.009927
27	1	0	2.269226	1.567311	-0.769950
28	1	0	-1.749765	0.718797	1.364840

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**THF Cation (18)**

SCF Done: E(RB+HF-LYP) = -231.670436486

Zero-point correction= 0.104204 (Hartree/Particle)  
 Thermal correction to Energy= 0.108961  
 Thermal correction to Enthalpy= 0.109905  
 Thermal correction to Gibbs Free Energy= 0.076236  
 Sum of electronic and zero-point Energies= -231.566233  
 Sum of electronic and thermal Energies= -231.561476  
 Sum of electronic and thermal Enthalpies= -231.560532  
 Sum of electronic and thermal Free Energies= -231.594200

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	68.374	16.505	70.862

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.168760	-0.447521	0.092478
2	8	0	0.120287	-1.230667	-0.052399
3	6	0	1.113958	-0.455973	-0.039144
4	6	0	0.793531	0.972336	0.083877
5	6	0	-0.740511	1.007388	-0.113409
6	1	0	-1.834372	-0.866756	-0.662741
7	1	0	-1.512904	-0.695681	1.099652
8	1	0	2.106496	-0.922214	-0.102015
9	1	0	1.126002	1.291318	1.089822
10	1	0	1.378180	1.568798	-0.630315
11	1	0	-1.229936	1.667819	0.606747
12	1	0	-0.985069	1.344664	-1.124772

**Carbon Dioxide (19)**

SCF Done: E(RB+HF-LYP) = -188.593474840

Zero-point correction= 0.011458 (Hartree/Particle)  
 Thermal correction to Energy= 0.014100  
 Thermal correction to Enthalpy= 0.015044  
 Thermal correction to Gibbs Free Energy= -0.009912  
 Sum of electronic and zero-point Energies= -188.582017  
 Sum of electronic and thermal Energies= -188.579375  
 Sum of electronic and thermal Enthalpies= -188.578431  
 Sum of electronic and thermal Free Energies= -188.603387

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	8.848	6.960	52.525

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



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1	6	0	0.000000	0.000000	-0.000005
2	8	0	0.000000	0.000000	-1.169109
3	8	0	0.000000	0.000000	1.169113

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**MP2/6-31+G\* SINGLE POINT CALCULATIONS****Quinolinic Acid Neutral: Pyridine-2,3-dicarboxylic acid (1)**

SCF Done: E(RHF) = -621.928476419

**Quinolinic Acid Anion: Deprotonated 2 or 3 Carboxyl (2 or 3)**

SCF Done: E(RHF) = -621.401504435

**Quinolinic Acid Dianion: Deprotonated 2 & 3 Carboxyl (4)**

SCF Done: E(RHF) = -620.711528629

**Pyridine-3-carboxylic acid: Deprotonated 3 Carboxyl (5A)**

SCF Done: E(RHF) = -433.775167722

**Pyridine-3-carboxylic acid(6A)**

SCF Done: E(RHF) = -434.324776043

**Pyridine-3-carboxylic acid: Deprotonated C2 & 3 Carboxyl (5)**

SCF Done: E(RHF) = -432.975615320

**Pyridine-3-carboxylic acid: Deprotonated C2 (6)**

SCF Done: E(RHF) = -433.680606554

**Pyridine-2-carboxylic acid: Deprotonated C3 & 2 Carboxyl (7)**

SCF Done: E(RHF) = -432.982391246

**Pyridine-2-carboxylic acid: Deprotonated C3 (8)**

SCF Done: E(RHF) = -433.702847607

**Quinolinic Acid Cation: THF on N1 (1C)**

SCF Done: E(RHF) = -852.096024458

**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF on N1 (2C or 3C)**

SCF Done: E(RHF) = -851.721919652

**Quinolinic Acid Zwitterion: Deprotonated 2 and 3 Carboxyl & THF on N1 (4C)**

SCF Done: E(RHF) = -851.168447659

**Pyridine-3-carboxylic acid: THF on N1 (9B)**

SCF Done: E(RHF) = -664.651975678

**Pyridine-3-carboxylic acid: Deprotonated C2 & 3 Carboxyl & THF on N1 (10B)**

SCF Done: E(RHF) = -663.489805036

**Pyridine-3-carboxylic acid: Deprotonated 3 Carboxyl & THF on N1 (11B)**

SCF Done: E(RHF) = -663.977327954

**Pyridine-3-carboxylic acid: Deprotonated C2 & THF on N1 (12B)**

SCF Done: E(RHF) = -664.086710115

**Pyridine-2-carboxylic acid: Deprotonated C3 & 2 Carboxyl & THF on N1 (14B)**

SCF Done: E(RHF) = -663.483856882

**Pyridine-2-carboxylic acid: Deprotonated C3 & THF on N1 (16B)**

SCF Done: E(RHF) = -664.049202568

**Quinolinic Acid Zwitterion: Deprotonated 2 or 3 Carboxyl & THF  
on N1 (2C or 3C) Transition State Calculation**

SCF Done: E(RHF) = -851.722092345

**THF Cation (18)**

SCF Done: E(RHF) = -230.109802703

**Carbon Dioxide (19)**

SCF Done: E(RHF) = -187.635647609

**B3LYP/6-31+G\* CALCULATIONS FOR COMPLEXED STRUCTURES**

**QUINOLINIC ACID ANION: DEPROTONATED 2 CARBOXYL COMPLEXED WITH AMMONIUM (20)**

SCF Done: E(RB+HF-LYP) = -682.023391968

Zero-point correction=	0.155677 (Hartree/Particle)
Thermal correction to Energy=	0.168641
Thermal correction to Enthalpy=	0.169585
Thermal correction to Gibbs Free Energy=	0.114301
Sum of electronic and zero-point Energies=	-681.867715
Sum of electronic and thermal Energies=	-681.854751
Sum of electronic and thermal Enthalpies=	-681.853807
Sum of electronic and thermal Free Energies=	-681.909091

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	105.824	45.521	116.356

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.160027	-0.620188	-0.057331
2	6	0	1.270427	0.259594	-0.000965
3	6	0	2.541673	-0.340080	0.017665
4	6	0	2.677222	-1.719234	-0.059209
5	6	0	1.513956	-2.488900	-0.123208
6	7	0	0.293732	-1.956100	-0.103285
7	1	0	3.406868	0.308732	0.099611
8	1	0	3.656609	-2.188730	-0.060801
9	1	0	1.559699	-3.574560	-0.183913
10	6	0	1.320194	1.784806	0.108410
11	8	0	2.308124	2.312199	0.582189
12	8	0	0.312455	2.515815	-0.359258
13	6	0	-1.287048	-0.180338	-0.087947
14	8	0	-1.658442	0.868512	-0.630448
15	8	0	-2.117796	-1.019933	0.478780
16	1	0	-3.078726	-0.669784	0.389725
17	7	0	-4.614267	-0.026633	0.197270
18	1	0	-5.253724	-0.590423	-0.360902
19	1	0	-5.093505	0.220222	1.062001
20	1	0	-4.429390	0.836234	-0.314497
21	1	0	-0.457515	1.950732	-0.643705

**QUINOLINIC ACID ANION: DEPROTONATED 2&3 CARBOXYL COMPLEXED WITH AMMONIUM (21)**

SCF DONE: E(RB+HF-LYP) = -681.483557362  
 Zero-point correction= 0.141979 (Hartree/Particle)  
 Thermal correction to Energy= 0.154097  
 Thermal correction to Enthalpy= 0.155041  
 Thermal correction to Gibbs Free Energy= 0.102788  
 Sum of electronic and zero-point Energies= -681.341578  
 Sum of electronic and thermal Energies= -681.329460  
 Sum of electronic and thermal Enthalpies= -681.328516  
 Sum of electronic and thermal Free Energies= -681.380770

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	96.697	43.766	109.977

CENTER NUMBER	ATOMIC NUMBER	ATOMIC TYPE	COORDINATES (ANGSTROMS)		
			X	Y	Z
1	6	0	0.531863	-0.757462	0.028334
2	6	0	0.786938	0.635545	-0.040442
3	6	0	2.127429	1.032145	-0.085378
4	6	0	3.147914	0.080827	-0.087722
5	6	0	2.783128	-1.262936	-0.020897
6	7	0	1.513527	-1.679099	0.041406
7	1	0	2.341967	2.096816	-0.107679
8	1	0	4.195900	0.371567	-0.131922
9	1	0	3.541934	-2.047159	-0.013580
10	6	0	-0.270731	1.755147	-0.065253
11	8	0	0.072142	2.848181	0.423734
12	8	0	-1.387502	1.504986	-0.642672
13	6	0	-0.878594	-1.322462	0.132654
14	8	0	-1.387631	-1.841611	-0.884821
15	8	0	-1.452099	-1.164515	1.267223
16	1	0	-2.848396	-0.600113	0.706528
17	7	0	-3.371562	-0.032092	-0.046712
18	1	0	-3.504302	-0.673241	-0.830000
19	1	0	-4.241661	0.392876	0.265581
20	1	0	-2.606165	0.696441	-0.327276

**PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED 3 CARXBOXYL COMPLEXED WITH AMMONIUM(22)**

SCF Done: E(RB+HF-LYP) = -493.454731102

Zero-point correction= 0.141375 (Hartree/Particle)  
 Thermal correction to Energy= 0.151742  
 Thermal correction to Enthalpy= 0.152686  
 Thermal correction to Gibbs Free Energy= 0.104421  
 Sum of electronic and zero-point Energies= -493.313356  
 Sum of electronic and thermal Energies= -493.302989

Sum of electronic and thermal Enthalpies= -493.302045  
 Sum of electronic and thermal Free Energies= -493.350310

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.219	36.209	101.583

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.665689	1.062679	0.000076
2	6	0	3.190961	-0.233495	0.000136
3	7	0	2.437228	-1.341889	0.000049
4	6	0	1.107954	-1.182092	-0.000074
5	6	0	0.477744	0.071696	-0.000054
6	6	0	1.282245	1.217182	-0.000005
7	6	0	-1.008160	0.219572	-0.000134
8	8	0	-1.566129	1.311032	-0.000129
9	8	0	-1.660884	-0.945420	-0.000148
10	1	0	3.328599	1.923291	0.000110
11	1	0	4.268066	-0.391620	0.000163
12	1	0	0.812970	2.196364	-0.000026
13	7	0	-4.289467	-0.194474	0.000245
14	1	0	0.511309	-2.089537	-0.000042
15	1	0	-4.063410	0.801120	-0.000643
16	1	0	-2.659691	-0.764298	-0.000275
17	1	0	-4.857034	-0.388828	0.823527
18	1	0	-4.857631	-0.390087	-0.822324

**PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 COMPLEXED WITH AMMONIUM(20A)**

SCF Done: E(RB+HF-LYP) = -493.335080180

Zero-point correction=	0.138852 (Hartree/Particle)
Thermal correction to Energy=	0.148682
Thermal correction to Enthalpy=	0.149627
Thermal correction to Gibbs Free Energy=	0.103291
Sum of electronic and zero-point Energies=	-493.196228
Sum of electronic and thermal Energies=	-493.186398
Sum of electronic and thermal Enthalpies=	-493.185453
Sum of electronic and thermal Free Energies=	-493.231789

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.300	35.603	97.521

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.175268	-1.003725	-0.000460
2	6	0	0.312849	0.414896	-0.000078

3	6	0	1.576559	1.040170	0.000201
4	6	0	2.706899	0.237328	0.000260
5	6	0	2.515410	-1.151517	-0.000010
6	7	0	1.319501	-1.753179	-0.000393
7	1	0	1.650856	2.124962	0.000311
8	1	0	3.707752	0.661458	0.000492
9	1	0	3.382110	-1.815337	0.000033
10	6	0	-0.842741	1.326301	-0.000035
11	8	0	-0.811006	2.543915	0.000373
12	8	0	-2.116783	0.733241	-0.000641
13	1	0	-3.224137	-2.354438	0.845026
14	7	0	-2.788817	-1.975289	0.000489
15	1	0	-3.229529	-2.353867	-0.841515
16	1	0	-2.801000	-0.933837	0.001157
17	1	0	-1.726097	-2.130184	-0.002194
18	1	0	-2.717887	1.502551	-0.001104

**PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARXBOXYL  
COMPLEXED WITH AMMONIUM(21A)**

SCF Done: E(RB+HF-LYP) = -492.776304766

Zero-point correction=	0.127749 (Hartree/Particle)
Thermal correction to Energy=	0.134781
Thermal correction to Enthalpy=	0.135726
Thermal correction to Gibbs Free Energy=	0.095507
Sum of electronic and zero-point Energies=	-492.648556
Sum of electronic and thermal Energies=	-492.641523
Sum of electronic and thermal Enthalpies=	-492.640579
Sum of electronic and thermal Free Energies=	-492.680797

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	84.577	26.804	84.646

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.275437	-1.033636	-0.134036
2	6	0	0.105238	0.381640	-0.073066
3	6	0	1.262518	1.160406	0.029358
4	6	0	2.529429	0.570878	0.092817
5	6	0	2.588026	-0.819508	0.019230
6	7	0	1.507486	-1.598366	-0.097246
7	1	0	1.144838	2.242130	0.037721
8	1	0	3.438480	1.168443	0.182297
9	1	0	3.551608	-1.339129	0.051590
10	6	0	-1.233614	1.162971	-0.065683
11	8	0	-2.283669	0.478367	-0.106912
12	8	0	-1.113582	2.417788	0.074766
13	1	0	-2.470739	-1.498313	-0.667661
14	7	0	-2.242867	-2.053511	0.132232
15	1	0	-2.145280	-3.010000	-0.142734
16	1	0	-2.972519	-1.974729	0.811498



17            1            0            -1.382929    -1.731002    0.527827

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**QUINOLINIC ACID ZWITTERION: DEPROTONATED 2 CARBOXYL & THF ON N1  
COMPLEXED WITH AMMONIUM(22)**

SCF Done: E(RB+HF-LYP) = -913.656547992

Zero-point correction= 0.264934 (Hartree/Particle)  
 Thermal correction to Energy= 0.282373  
 Thermal correction to Enthalpy= 0.283318  
 Thermal correction to Gibbs Free Energy= 0.217362  
 Sum of electronic and zero-point Energies= -913.391614  
 Sum of electronic and thermal Energies= -913.374175  
 Sum of electronic and thermal Enthalpies= -913.373230  
 Sum of electronic and thermal Free Energies= -913.439186

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.192	63.765	138.816

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.960804	0.704892	0.888283
2	6	0	2.457644	0.537464	1.165539
3	8	0	2.936184	-0.228729	-1.028366
4	6	0	4.182562	-0.269039	-0.266186
5	6	0	1.902520	0.277598	-0.249138
6	6	0	0.094328	-3.033980	-0.376571
7	6	0	1.066131	-2.052100	-0.414527
8	7	0	0.748814	-0.748972	-0.237205
9	6	0	-0.535676	-0.341831	-0.041056
10	6	0	-1.552338	-1.304763	0.015232
11	6	0	-1.226513	-2.656015	-0.153192
12	6	0	-3.010963	-1.007240	0.253782
13	8	0	-3.852903	-1.875258	0.236145
14	8	0	-3.265503	0.287969	0.496988
15	6	0	-0.757581	1.161656	0.146557
16	8	0	-1.119841	1.744908	-0.962513
17	8	0	-0.544303	1.663156	1.234455
18	1	0	4.575581	0.471239	1.761899
19	1	0	4.187923	1.729832	0.575663
20	1	0	1.985079	1.399633	1.637882
21	1	0	2.274472	-0.335318	1.803638
22	1	0	4.353477	-1.296300	0.080788
23	1	0	4.977840	0.011482	-0.958166
24	1	0	0.372405	-4.071405	-0.525147
25	1	0	2.110671	-2.252200	-0.612536
26	1	0	-2.027585	-3.387678	-0.113218
27	1	0	1.472159	1.156453	-0.733619
28	1	0	-2.651992	4.425580	-0.673907

29	7	0	-1.643447	4.272031	-0.683873
30	1	0	-1.258236	4.838563	-1.440009
31	1	0	-1.273925	4.633890	0.195896
32	1	0	-1.323817	2.793038	-0.826159
33	1	0	-4.226195	0.385552	0.648540

**QUINOLINIC ACID ZWITTERION: DEPROTONATED 2&3 CARBOXYL & THF ON N1 COMPLEXED WITH AMMONIUM (23)**

SCF Done: E(RB+HF-LYP) = -913.257602423

Zero-point correction=	0.254352 (Hartree/Particle)
Thermal correction to Energy=	0.271597
Thermal correction to Enthalpy=	0.272541
Thermal correction to Gibbs Free Energy=	0.208410
Sum of electronic and zero-point Energies=	-913.003250
Sum of electronic and thermal Energies=	-912.986006
Sum of electronic and thermal Enthalpies=	-912.985062
Sum of electronic and thermal Free Energies=	-913.049192

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	170.429	63.616	134.974

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.816899	-1.215165	0.883386
2	6	0	-2.280290	-1.145705	0.856201
3	8	0	-3.191829	0.170908	-0.907305
4	6	0	-4.202356	0.049518	0.121825
5	6	0	-1.992781	-0.420485	-0.480237
6	6	0	-0.320330	2.947890	-0.245326
7	6	0	-1.268473	1.958898	-0.405244
8	7	0	-0.916229	0.650950	-0.321351
9	6	0	0.373739	0.261880	-0.115226
10	6	0	1.373397	1.236843	0.045630
11	6	0	1.006125	2.580779	0.001997
12	6	0	2.863354	0.893211	0.264268
13	8	0	3.472533	1.638064	1.038162
14	8	0	3.304677	-0.074825	-0.439131
15	6	0	0.680877	-1.237491	-0.010895
16	8	0	0.602226	-1.897363	-1.085320
17	8	0	1.002067	-1.627522	1.127787
18	1	0	-4.218246	-1.238239	1.901199
19	1	0	-4.178272	-2.102159	0.351059
20	1	0	-1.795725	-2.122220	0.895417
21	1	0	-1.896409	-0.556351	1.695485
22	1	0	-4.182436	0.938814	0.769098
23	1	0	-5.165888	0.003377	-0.390240
24	1	0	-0.620817	3.988362	-0.310996
25	1	0	-2.311450	2.148091	-0.616158
26	1	0	1.777202	3.326559	0.170187
27	1	0	-1.611682	-1.075060	-1.264388

28	1	0	3.334952	-1.575746	-0.348205
29	7	0	3.156334	-2.650159	-0.395374
30	1	0	3.881503	-3.137239	-0.921038
31	1	0	3.077012	-3.010888	0.556513
32	1	0	2.213957	-2.727975	-0.842663

**PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & THF ON N1  
COMPLEXED WITH AMMONIUM(22A)**

SCF Done: E(RB+HF-LYP) = -725.037563866

Zero-point correction=	0.252240 (Hartree/Particle)
Thermal correction to Energy=	0.266774
Thermal correction to Enthalpy=	0.267718
Thermal correction to Gibbs Free Energy=	0.209227
Sum of electronic and zero-point Energies=	-724.785323
Sum of electronic and thermal Energies=	-724.770790
Sum of electronic and thermal Enthalpies=	-724.769846
Sum of electronic and thermal Free Energies=	-724.828337

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	167.403	54.107	123.106

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.900318	0.886181	0.792736
2	6	0	2.388911	0.831036	1.062878
3	8	0	2.840691	-0.239512	-1.000109
4	6	0	4.073315	-0.237588	-0.230092
5	6	0	1.826114	0.449933	-0.319706
6	6	0	-0.339122	-2.587555	-0.052715
7	6	0	0.750209	-1.754668	-0.201749
8	7	0	0.586090	-0.404962	-0.224109
9	6	0	-0.606722	0.257304	-0.132604
10	6	0	-1.719215	-0.611295	0.027247
11	6	0	-1.602841	-2.007156	0.071839
12	6	0	-3.074588	-0.005722	0.137595
13	8	0	-4.044696	-0.901675	0.352168
14	8	0	-3.355244	1.192386	0.048978
15	1	0	4.498979	0.732278	1.695046
16	1	0	4.184932	1.850014	0.355620
17	1	0	1.968622	1.767723	1.438062
18	1	0	2.152277	0.043148	1.788220
19	1	0	4.196036	-1.217237	0.250813
20	1	0	4.891952	-0.085326	-0.936153
21	1	0	-0.202010	-3.662972	-0.042128
22	1	0	1.762151	-2.118023	-0.330520
23	1	0	-2.479899	-2.635162	0.189664
24	1	0	1.502911	1.315519	-0.904441
25	7	0	-1.707887	3.243955	-0.409095
26	1	0	-2.425595	2.474270	-0.232195
27	1	0	-1.745877	3.962693	0.318187

28	1	0	-0.813389	2.726682	-0.376658
29	1	0	-1.844793	3.670680	-1.329085
30	1	0	-4.898002	-0.429645	0.407132

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**PYRIDINE-3-CARBOXYLIC ACID: DEPROTONATED C2 & 3 CARXBOXYL & THE  
ON N1 COMPLEXED WITH AMMONIUM (23A)**

SCF Done: E(RB+HF-LYP) = -724.617126003

Zero-point correction=	0.238110 (Hartree/Particle)
Thermal correction to Energy=	0.252385
Thermal correction to Enthalpy=	0.253329
Thermal correction to Gibbs Free Energy=	0.194877
Sum of electronic and zero-point Energies=	-724.379016
Sum of electronic and thermal Energies=	-724.364741
Sum of electronic and thermal Enthalpies=	-724.363797
Sum of electronic and thermal Free Energies=	-724.422249

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	158.374	52.592	123.022

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.654632	0.257942	-0.154226
2	6	0	-1.783689	-0.583582	0.022919
3	6	0	-1.646092	-1.970161	0.074606
4	6	0	-0.383621	-2.564797	-0.067894
5	6	0	0.713226	-1.748945	-0.224606
6	7	0	0.545313	-0.395405	-0.250855
7	1	0	-2.543803	-2.564465	0.220845
8	1	0	-0.254243	-3.642719	-0.058672
9	1	0	1.722509	-2.116427	-0.359517
10	6	0	-3.219122	-0.003366	0.168254
11	8	0	-3.345112	1.242793	-0.051317
12	8	0	-4.100305	-0.824366	0.479800
13	1	0	-2.324821	2.982384	0.384031
14	7	0	-1.655320	3.051022	-0.392521
15	1	0	-1.096655	3.906649	-0.393004
16	1	0	-2.235700	2.957527	-1.229406
17	1	0	-1.086218	2.118198	-0.320786
18	6	0	1.763344	0.464391	-0.314345
19	6	0	2.324954	0.801789	1.081905
20	1	0	1.444128	1.352247	-0.864949
21	6	0	3.839363	0.850057	0.833996
22	1	0	2.069930	-0.001910	1.782611
23	1	0	1.906591	1.731567	1.476150
24	6	0	4.006858	-0.238465	-0.228109
25	1	0	4.140049	1.824792	0.431420
26	1	0	4.428479	0.657100	1.736120
27	1	0	4.853534	-0.084935	-0.902190
28	1	0	4.094937	-1.236512	0.226214
29	8	0	2.806391	-0.176175	-1.026013

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