Supporting information

to the paper

Structural and energetic factors controlling the enantioselectivity of dinucleotide formation under prebiotic conditions

by

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Calculation of HF/6-31G* dipoles for ImpA and ImpU

Explanation of the homochiral selectivity on the basis of dipole moment calculations has some apparent weaknesses. Namely, definition of molecular dipoles is unambiguous only for neutral systems, otherwise it becomes dependent on the choice of the reference coordinate system.[S1] Accordingly, only for neutral molecules we can unambiguously calculate the dipole moment. Quantum chemical softwares enable calculation of molecular dipoles also for charged systems, and these so-called field independent dipoles are often used in chemistry. The dipoles derived in this way can be used to provide qualitative information regarding the asymmetry of the charge distribution in molecules and molecular ions.

Joshi et al.[S2] used HF/6-31G* calculations to estimate the dipole moments of the anionic and zwitterionic forms of ImpA and ImpU. The dipoles derived from these calculations can be considered only as very approximate, since an accurate description of the electronic structure of highly polarizable anionic species would require at least inclusion of diffuse functions into the basis set. Notwithstanding, we have tried to reproduce their HF/6-31G* dipole moments computed on optimized geometries obtained at the same level. Unfortunately, our dipole moments shown on Figure S1 are entirely different from those reported by Joshi et al. Mainly, there is not much difference between the dipole moments when going from adenine to uracil, and the direction of the dipoles is mainly dictated by the total charge of the model (i.e. whether or not the imidazole ring is protonated). In addition, the dipole moment vectors of the corresponding zwitterionic and anionic species are not parallel, as was observed for ImpA by Joshi et al. We suspect that delicate conformational changes within the activated nucleotides might have a severe impact on the dipole moments, which could be also the reason for the difference between our computed results and those reported by Joshi et al. This, on the other hand, points at another weakness of the interpretation of the homochiral selectivity on the basis of dipole moments.

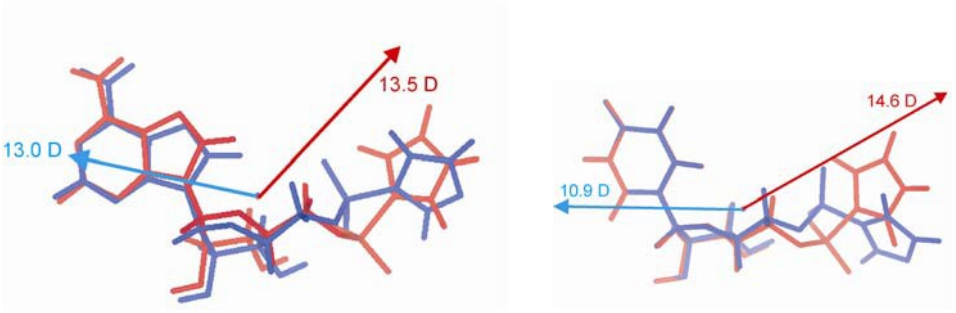


Figure S1. Computed HF/6-31G* dipole moments for the anionic (blue) and zwitterionic (red) forms of ImpA (left) and ImpU (right).

References:

S1. **C. J. Cramer, John Wiley & Sons, Chichester, 2nd edn., 2004, pp. 324-353.**
S2. **P. C. Joshi, M. F. Aldersley and J. P. Ferris, *Origins of Life and Evolution of Biospheres*, 2011, 41, 213-236.**

Figure S2. Optimized geometry of the *syn* D,D c-di-AMP model computed at TPSS/TZVP level oftheory.

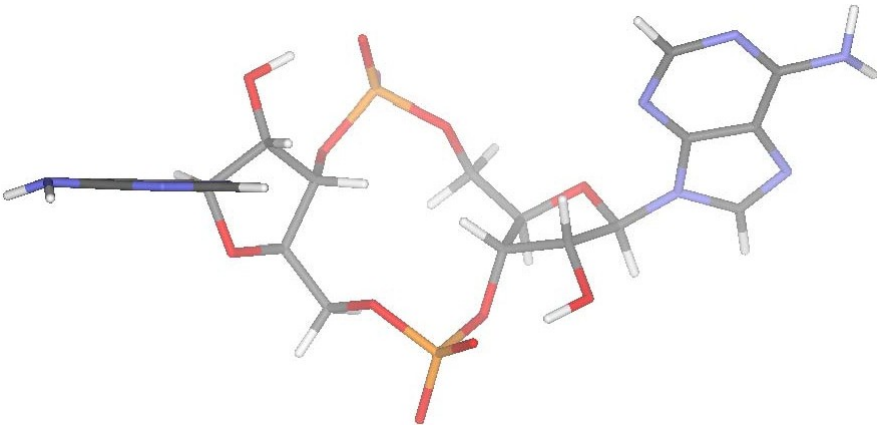
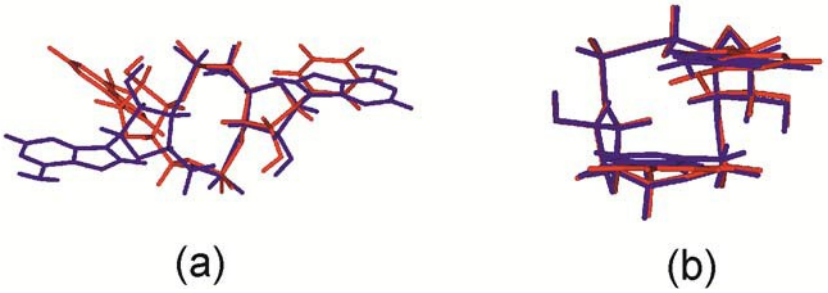


Figure S3. Overlay of (a) D,L c-di-AMP (blue) and D,L c-UMP-AMP (red) as well as (b) D,D c-di-AMP (blue) and D,D c-AMP-UMP (red) computed at TPSS-D3(BJ)/def2-TZVPPD level of theory. In (a) the minor deviation of the two structures is caused by a subtle C2'-endo /C3'-endo conformational change at the L AMP unit.



Optimized geometries of all structures reported in the paper:

D,D c-di-AMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, gas-phase

P	2.8756330	1.4370910	2.4543510
O	4.2432830	1.3134670	3.0286240
O	1.8194730	2.3759390	2.9748880
O	2.1398440	-0.0522300	2.4043040
C	2.9686100	-1.2245480	2.3117510
C	2.3195270	-2.2914780	1.4466890
O	1.0948860	-2.7875810	2.0622660
C	1.9016590	-1.8221310	0.0582890
O	3.0358740	-1.8389150	-0.7942010
C	0.7124480	-2.7379650	-0.3036210
O	1.1189800	-3.9777690	-0.8514650
C	0.0845480	-2.9640400	1.0806300
N	-1.0068770	-2.0033000	1.3642790
C	-0.8682540	-0.7005760	1.8206250
N	-2.0195980	-0.0597420	1.9304780
C	-2.9615580	-0.9868950	1.5254480
C	-4.3545140	-0.9151680	1.3943860
N	-5.0555380	0.2135110	1.7435740
N	-5.0291560	-1.9916580	0.9386130
C	-4.3173710	-3.1012180	0.6490010
H	-4.9041100	-3.9463500	0.2937730
N	-2.9971050	-3.3011880	0.7285490
C	-2.3564860	-2.2032360	1.1666420
H	0.1076860	-0.3036740	2.0798330
H	3.9387810	-0.9685410	1.8734000
H	3.1374280	-1.6119660	3.3234470
H	3.0218740	-3.1292210	1.3445440
H	1.5120500	-0.8055010	0.1444160
H	1.4574300	-3.6919910	-1.7455540
H	-0.3562990	-3.9608980	1.1526940
P	2.8630830	-1.5181250	-2.4117320
O	1.7883310	-2.4291940	-2.9433700
O	4.2396750	-1.4306970	-2.9711390
O	2.1664950	-0.0097930	-2.3696220
C	3.0256710	1.1398040	-2.2682650
C	2.3965030	2.2240700	-1.4100540
O	1.1930910	2.7536560	-2.0392370
C	1.9503770	1.7654630	-0.0268010
O	3.0745290	1.7531650	0.8389880
C	0.7805830	2.7110030	0.3216820
O	1.2118500	3.9393580	0.8763630
C	0.1758520	2.9558090	-1.0696650
N	-0.9383030	2.0267490	-1.3695750
C	-0.8310570	0.7198880	-1.8226290
N	-1.9991730	0.1144700	-1.9540340
C	-2.9198830	1.0704910	-1.5677040
C	-4.3168760	1.0426510	-1.4657030

N	-5.0460260	-0.0634850	-1.8292170
N	-4.9667510	2.1402160	-1.0244160
C	-4.2267920	3.2272840	-0.7206400
H	-4.7940160	4.0906100	-0.3776980
N	-2.8995760	3.3859560	-0.7734270
C	-2.2846540	2.2681440	-1.1979700
H	0.1367170	0.2933080	-2.0647730
H	3.9838610	0.8577170	-1.8197010
H	3.2155710	1.5222210	-3.2781130
H	3.1203360	3.0422310	-1.2994800
H	1.5363560	0.7588990	-0.1185850
H	0.0539870	2.2246970	0.9801780
H	1.5324330	3.6441990	1.7740910
H	-0.2365870	3.9645080	-1.1448770
H	0.0067640	-2.2344490	-0.9717920
H	-5.9547220	-0.1409620	-1.3906780
H	-4.5173730	-0.9282200	-1.8428640
H	-5.9512620	0.3211810	1.2851870
H	-4.4994600	1.0605500	1.7710200

D,D c-di-AMP, TPSS-D3(BJ)/def2-TZVPPD level, constrained optimization, gas-phase

n	3.30212292364936	0.14934955688513	0.74647451217539
c	2.43822641671511	1.21994589310678	0.92269853136781
n	2.43932522075979	1.69366998817971	2.15767918495098
c	3.3481289465426	0.892669233123	2.82535708135249
c	3.78337591048268	0.8625756038991	4.15686200185068
n	3.34281308231959	1.77598239600819	5.08746091920482
n	4.6871374225692	-0.06081989065112	4.53752929761513
c	5.14324454721363	-0.9158796258888	3.59914214948556
h	5.87666812478243	-1.63915689729619	3.94987464427135
n	4.81250206286404	-1.00034322154721	2.30635569383699
c	3.89971055939891	-0.07385439376251	1.96741030005932
h	1.86592101253547	1.61686687530288	0.0913377096739
h	3.44152774849511	1.48835058187689	6.05215751136122
h	2.48241194570736	2.25423860131017	4.85012411854896
n	-3.28582201388697	-0.16729158479702	0.84341695817376
c	-2.41670618774558	-1.24053364075813	0.9713782284415
n	-2.36746049476997	-1.72854143309567	2.19980508274642
c	-3.24646388925292	-0.93423296824161	2.91377910851666
c	-3.62443064551084	-0.91765953832631	4.26290919604913
n	-3.1458171137768	-1.84107652465049	5.16437656332158
n	-4.50947285734108	0.00284503974087	4.69149637265198
c	-5.00348218863077	0.86861474235219	3.78258357571954
h	-5.72004936723262	1.58905051037483	4.17190488513746
n	-4.72752115572827	0.96684484058198	2.47796297994453
c	-3.83159857339160	.04280870804588	2.09066577471423
h	-1.87825954980622	-1.6265495743502	0.11260331542139
h	-3.20267850535532	-1.56290313196608	6.13522173955686
h	-2.2965534721876	-2.31701086115877	4.88576525988984
c	-3.53148575852646	0.64296886111024	-0.36667750289855

h	-4.46453660011191	1.18097018436648	-0.18091123112376
c	3.50387081635624	-0.64228451446897	-0.48375629648409
p	-0.10975274410486	-2.91624275177062	-2.54500705653875
o	-0.49271235179006	-3.5646611672498	-3.82918264019904
o	0.35594548655339	-3.66107730050243	-1.32175105602194
o	-1.33654464624487	-1.93405716491149	-2.01363565153347
c	-2.09587666972096	-1.25574627501763	-3.03073900595864
c	-2.67132512008311	0.03828155694685	-2.48607680314935
o	-3.66203974413977	-0.2455586788309	-1.46250392852363
c	-1.64245800012739	0.96848523921107	-1.84447135589836
o	-1.14805095856513	1.83442001005731	-2.85959299350891
c	-2.39923038802471	1.64423591404057	-0.66791119549157
o	-2.97021711113006	2.88986672308261	-1.01092521262683
h	-1.45293545943765	-1.0114818821651	-3.88416748937592
h	-2.89594761006623	-1.91766826117409	-3.37975133379993
h	-3.1616458712192	0.57691474777179	-3.3075074561203
h	-0.82491245512385	0.37433566631339	-1.42705832815268
h	-2.15974540138564	3.4532705326665	-1.15859436884794
p	0.02065921125534	2.95267397284099	-2.49023153222148
o	-0.41125824834561	3.67240292235376	-1.23990420132529
o	0.36495013262766	3.62629105641999	-3.77234251180582
o	1.26409449142618	1.9631526402611	-2.01418336225918
c	1.99186536683375	1.30504360183265	-3.06724769901351
c	2.58134866703174	-3.11636740431802E-4	-2.56616793969985
o	3.60348337499348	0.26358860155352	-1.56853399164804
c	1.57110772223767	-0.94202360975235	-1.91154849028642
o	1.0507059835437	-1.79335894364318	-2.92625690181428
c	2.35886825493417	-1.63487257848587	-0.76542999108549
o	2.9157858040759	-2.87782429700304	-1.13958629209986
h	1.32359376614644	1.07964563911005	-3.90624717098547
h	2.7827706552103	1.97294436053954	-3.4256463101394
h	3.04560662670259	-0.52312372107175	-3.41256308724483
h	0.76355936935539	-0.35576751882685	-1.46463939976438
h	1.72153138161478	-1.75087087992304	0.11869409883542
h	2.09983927457867	-3.43685131650184	-1.27563858812684
h	-1.73768333193721	1.75196168819291	0.19921294670116
h	4.43987557073773	-1.18708897380562	-0.33672253041766

D,D c-di-AMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, COSMO

N	2.4815	0.1129	0.8342
C	1.5867	1.1688	0.7819
N	1.1458	1.5340	1.9729
C	1.7806	0.6734	2.8560
C	1.7638	0.5614	4.2604
N	1.0648	1.4011	5.0575
N	2.5154	-0.4082	4.8355
C	3.2568	-1.2058	4.0469
H	3.8373	-1.9650	4.5650
N	3.3725	-1.1872	2.7102
C	2.6114	-0.2199	2.1686

H 1.3313 1.6328 -0.1604
H 0.9626 1.1687 6.0361
H 0.3643 2.0029 4.6479
N -2.4525 -0.1236 0.9227
C -1.5613 -1.1791 0.8240
N -1.0779 -1.5603 1.9932
C -1.6794 -0.7113 2.9101
C -1.6124 -0.6187 4.3145
N -0.8868 -1.4699 5.0745
N -2.3419 0.3434 4.9293
C -3.1100 1.1522 4.1787
H -3.6707 1.9047 4.7276
N -3.2737 1.1520 2.8469
C -2.5336 0.1917 2.2652
H -1.3406 -1.6302 -0.1332
H -0.7506 -1.2521 6.0523
H -0.2026 -2.0673 4.6321
C -3.2261 0.5310 -0.1493
H -4.1878 0.8060 0.2894
C 3.2155 -0.5279 -0.2733
P -0.1090 -2.8985 -2.6884
O -0.4528 -3.4962 -4.0200
O 0.1894 -3.7332 -1.4804
O -1.2710 -1.8603 -2.1903
C -2.0960 -1.1342 -3.1185
C -2.7014 0.0559 -2.4032
O -3.4271 -0.3854 -1.2198
C -1.7078 1.0851 -1.8661
O -1.2584 1.9184 -2.9282
C -2.5104 1.7581 -0.7479
O -3.4643 2.6348 -1.3436
H -1.5070 -0.7683 -3.9670
H -2.8809 -1.7969 -3.4935
H -3.3995 0.5518 -3.0880
H -0.8549 0.5714 -1.4086
H -3.8802 3.1510 -0.6358
P 0.0111 2.9344 -2.6498
O -0.2431 3.7520 -1.4204
O 0.3066 3.5504 -3.9846
O 1.1898 1.8892 -2.2092
C 1.9807 1.1770 -3.1770
C 2.6112 -0.0229 -2.5009
O 3.3791 0.4022 -1.3384
C 1.6366 -1.0589 -1.9424
O 1.1495 -1.8783 -2.9986
C 2.4778 -1.7467 -0.8622
O 3.4095 -2.6161 -1.5021
H 1.3613 0.8233 -4.0088
H 2.7515 1.8456 -3.5705
H 3.2839 -0.5095 -3.2170

H 0.8004 -0.5512 -1.4489
H 1.8762 -2.2748 -0.1209
H 3.8400 -3.1506 -0.8170
H -1.8832 2.2771 -0.0215

D,L c-di-AMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, gas-phase

C	3.7509860	1.1073710	0.9849130
N	4.7430300	0.1939090	0.3940790
C	4.5117400	-1.0820570	-0.0982290
N	5.5985270	-1.6620800	-0.5784750
C	6.5950000	-0.7206730	-0.3871890
C	7.9617430	-0.7150530	-0.6941900
N	8.5874590	-1.8068970	-1.2531510
N	8.7026950	0.3706570	-0.4010960
C	8.0824130	1.4086780	0.1973980
H	8.7205250	2.2605850	0.4233850
N	6.7972970	1.5344220	0.5429460
C	6.0872520	0.4402930	0.2204890
H	3.5258310	-1.5303230	-0.0434790
H	9.4586450	-1.6081900	-1.7269860
H	7.9740280	-2.4742600	-1.7039510
H	4.3225750	1.9648280	1.3515360
O	1.3669130	-1.6445500	0.8877940
C	1.0847430	-0.9039200	2.0829380
C	1.6666670	0.4932440	1.9505170
O	3.1139320	0.4153560	2.0421020
C	1.3153110	1.1965330	0.6329900
O	0.4404410	2.2837430	0.9254740
C	2.6824780	1.5922970	-0.0178180
O	2.8602220	2.9686250	-0.2381140
H	0.0041270	-0.8416340	2.2512710
H	1.5332640	-1.4139680	2.9439790
H	1.3067510	1.1133710	2.7801950
H	0.8202330	0.4892420	-0.0329980
H	2.0434090	3.2512650	-0.7507340
P	-0.4448380	2.9336250	-0.3165470
O	0.5166410	3.2382200	-1.4465550
O	-1.3622100	3.9258210	0.2954730
O	-1.3565720	1.6284120	-0.7847880
H	2.7869680	1.0266160	-0.9556790
C	-3.7140010	-1.1137430	-0.9449420
N	-4.7385260	-0.1974540	-0.4175910
C	-4.5402010	1.0879980	0.0643930
N	-5.6535070	1.6687330	0.4784840
C	-6.6334650	0.7177190	0.2524660
C	-8.0138500	0.7078920	0.4902770
N	-8.6734660	1.8046130	0.9987550
N	-8.7326510	-0.3874040	0.1784150
C	-8.0766320	-1.4309450	-0.3704000
H	-8.6974040	-2.2907860	-0.6139750

N	-6.7749580	-1.5536420	-0.6483830
C	-6.0885610	-0.4496620	-0.3088620
H	-3.5552210	1.5414720	0.0548860
H	-9.5660050	1.6074880	1.4317720
H	-8.0872770	2.4827660	1.4693040
H	-4.2610440	-1.9907500	-1.3024350
C	-1.0369880	0.8979330	-1.9766180
C	-1.6052210	-0.5065490	-1.8616240
O	-3.0498950	-0.4481840	-2.0026100
C	-1.2878080	-1.2028970	-0.5312930
O	-0.4436360	-2.3209190	-0.7974250
C	-2.6734540	-1.5477510	0.1085670
O	-2.8725110	-2.9058540	0.4089100
H	0.0479650	0.8498040	-2.1205220
H	-1.4721040	1.4061970	-2.8454720
H	-1.2115870	-1.1232110	-2.6781810
H	-0.7780500	-0.5036800	0.1318950
H	-2.0573340	-3.1798370	0.9291010
P	0.4344940	-2.9501680	0.4600120
O	-0.5258620	-3.2050280	1.6033540
O	1.3320150	-3.9757560	-0.1259850
H	-2.7918260	-0.9224630	1.0062200

D,L c-di-AMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, COSMO

C	3.6428	1.3375	1.6668
N	4.3270	0.3183	0.8512
C	3.8776	-0.9351	0.4793
N	4.7394	-1.5866	-0.2840
C	5.8093	-0.7132	-0.4238
C	7.0374	-0.8006	-1.1131
N	7.4203	-1.8959	-1.8039
N	7.8824	0.2575	-1.0512
C	7.5200	1.3370	-0.3368
H	8.2401	2.1514	-0.3244
N	6.3895	1.5410	0.3558
C	5.5718	0.4760	0.2746
H	2.9147	-1.3027	0.8065
H	8.2410	-1.8431	-2.3921
H	6.7519	-2.6298	-1.9916
H	4.4071	1.8081	2.2896
O	0.7518	-1.0187	1.1935
C	0.3735	-0.0409	2.1777
C	1.3280	1.1285	2.0894
O	2.6672	0.7083	2.4850
C	1.5257	1.7118	0.6908
O	0.4610	2.5946	0.3495
C	2.9007	2.3747	0.7986
O	2.7554	3.6047	1.5067
H	-0.6415	0.3214	1.9807
H	0.4011	-0.4776	3.1796

H 0.9841 1.9115 2.7754
H 1.5912 0.8914 -0.0301
H 3.6113 4.0612 1.4936
P -0.0984 2.5245 -1.1953
O 1.0459 2.5626 -2.1684
O -1.2136 3.5255 -1.2402
O -0.7501 1.0206 -1.1911
H 3.3830 2.5242 -0.1705
C -3.6406 -1.3364 -1.6638
N -4.3246 -0.3171 -0.8479
C -3.8764 0.9376 -0.4790
N -4.7379 1.5891 0.2845
C -5.8064 0.7147 0.4274
C -7.0336 0.8016 1.1184
N -7.4172 1.8977 1.8073
N -7.8771 -0.2581 1.0600
C -7.5141 -1.3384 0.3472
H -8.2331 -2.1538 0.3374
N -6.3845 -1.5419 -0.3469
C -5.5682 -0.4756 -0.2691
H -2.9144 1.3059 -0.8081
H -8.2361 1.8446 2.3980
H -6.7500 2.6337 1.9913
H -4.4051 -1.8068 -2.2866
C -0.3717 0.0424 -2.1749
C -1.3261 -1.1270 -2.0866
O -2.6652 -0.7071 -2.4822
C -1.5235 -1.7104 -0.6880
O -0.4586 -2.5931 -0.3470
C -2.8984 -2.3735 -0.7959
O -2.7527 -3.6034 -1.5043
H 0.6433 -0.3199 -1.9777
H -0.3990 0.4789 -3.1769
H -0.9819 -1.9099 -2.7725
H -1.5893 -0.8901 0.0331
H -3.6096 -4.0581 -1.4953
P 0.1010 -2.5230 1.1979
O -1.0430 -2.5620 2.1711
O 1.2168 -3.5235 1.2423
H -3.3809 -2.5234 0.1732

D,D c-di-UMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, gas-phase

P	2.8314510	1.4770230	2.4739640
O	4.1826240	1.3796430	3.0899100
O	1.7424930	2.4005560	2.9521690
O	2.1216580	-0.0241780	2.4142060
C	2.9712360	-1.1799950	2.3181640
C	2.3153690	-2.2597000	1.4770850
O	1.0796320	-2.7222380	2.0990850
C	1.9030800	-1.8258680	0.0757510

O	3.0422640	-1.8484050	-0.7695430
C	0.7360710	-2.7747910	-0.2703410
O	1.1768440	-4.0179850	-0.7810190
H	3.9262620	-0.9149710	1.8524340
H	3.1705280	-1.5531080	3.3295080
H	3.0059890	-3.1095120	1.3979240
H	1.4948560	-0.8137320	0.1320810
H	1.5023040	-3.7511600	-1.6825240
P	2.8670680	-1.5529430	-2.3920410
O	1.7666060	-2.4445860	-2.9030510
O	4.2421020	-1.5034660	-2.9589510
O	2.2050590	-0.0290350	-2.3674990
C	3.0879200	1.0981020	-2.2341720
C	2.4363230	2.1963720	-1.4138290
O	1.2350680	2.6913980	-2.0767460
C	1.9672940	1.7752060	-0.0261700
O	3.0745870	1.7777400	0.8607520
C	0.8083190	2.7484670	0.2788220
O	1.2560190	3.9803790	0.8103610
H	4.0159430	0.8001320	-1.7349370
H	3.3364920	1.4675180	-3.2359020
H	3.1474570	3.0267910	-1.3128510
H	1.5424390	0.7707930	-0.0953080
H	0.0685230	2.2913420	0.9415870
H	1.5457870	3.7047100	1.7214640
H	0.0310780	-2.3049450	-0.9613500
C	0.2229560	2.9622070	-1.1241570
H	-0.1647710	3.9742850	-1.2400260
N	-0.9361280	2.0453660	-1.3846480
C	-0.7524440	0.7895220	-1.9059770
H	0.2747590	0.5402870	-2.1622940
C	-1.7760800	-0.0821310	-2.1085270
H	-1.5852490	-1.0588870	-2.5319060
C	-3.1252630	0.2865130	-1.7628650
O	-4.1494720	-0.3904560	-1.8924060
N	-3.2133610	1.5846760	-1.2191870
H	-4.1214400	1.8581770	-0.8585620
C	-2.1986890	2.5028260	-1.0062060
O	-2.3998600	3.6185090	-0.5362890
C	0.0954630	-2.9688520	1.1114930
H	-0.3243070	-3.9693970	1.2157400
N	-1.0463680	-2.0188940	1.3282020
C	-0.8481340	-0.7718120	1.8647520
H	0.1748000	-0.5534720	2.1621060
C	-1.8535580	0.1282410	2.0309790
H	-1.6519010	1.0976470	2.4660040
C	-3.1977090	-0.1997500	1.6290900
O	-4.2064960	0.5056560	1.7219510
N	-3.3008500	-1.4919380	1.0736570
H	-4.1997690	-1.7352660	0.6709150

C	-2.3046950	-2.4370710	0.8944340
O	-2.5174760	-3.5431420	0.4071930

D,D c-di-UMP, TPSS-D3(BJ)/def2-TZVPPD level, constrained optimization, gas-phase

P	1.1887	-2.9830	-1.5255
O	1.7127	-3.7074	-2.7146
O	0.6823	-3.6460	-0.2712
O	-0.0298	-1.9524	-1.9753
C	0.0807	-1.3011	-3.2516
C	-0.7151	-0.0076	-3.2330
O	-2.1285	-0.2967	-3.0760
C	-0.3416	0.9400	-2.0940
O	0.6786	1.8121	-2.5671
C	-1.6801	1.6040	-1.6666
O	-1.9008	2.8614	-2.2701
C	-2.7435	0.6103	-2.1749
C	-3.1530	-1.9630	0.5250
C	-4.5047	-1.7632	0.9834
O	-5.1092	-2.3813	1.8632
N	-5.1658	-0.7262	0.2884
C	-4.6920	0.0778	-0.7380
O	-5.3920	0.9328	-1.2736
N	-3.3708	-0.1914	-1.0874
C	-2.6531	-1.1930	-0.4750
H	1.1281	-1.0599	-3.4677
H	-0.2889	-1.9757	-4.0311
H	-0.5659	0.5153	-4.1866
H	0.0305	0.3581	-1.2467
H	-1.1804	3.4174	-1.8634
H	-3.5650	1.1462	-2.6504
P	1.3576	2.9076	-1.5229
O	0.2364	3.6163	-0.8092
O	2.4430	3.5872	-2.2798
O	2.0046	1.8925	-0.3827
C	3.2228	1.2043	-0.7107
C	3.3233	-0.0693	0.1107
O	3.4376	0.2566	1.5203
C	2.1131	-0.9932	-0.0194
O	2.3670	-1.9017	-1.0847
C	1.9256	-1.6133	1.3930
O	2.5316	-2.8809	1.5342
C	2.6436	-0.6091	2.3161
C	0.1305	2.0527	3.1420
C	-0.0789	1.8953	4.5591
O	-0.8165	2.5530	5.2974
N	0.6967	0.8506	5.1093
C	1.5975	0.0056	4.4778
O	2.2276	-0.8521	5.0903
N	1.7087	0.2378	3.1089
C	1.0021	1.2425	2.4888

H 3.2336 0.9326 -1.7727
H 4.0726 1.8659 -0.5118
H 4.2206 -0.6214 -0.1977
H 1.2256 -0.3957 -0.2444
H 0.8589 -1.6700 1.6407
H 1.9855 -3.4427 0.9180
H 3.2494 -1.1383 3.0517
H -1.7245 1.6915 -0.5745
H -2.5485 -2.7456 0.9629
H -1.6575 -1.3599 -0.8803
H -0.3894 2.8356 2.6068
H 1.2237 1.3772 1.4324
H -6.1240 -0.5437 0.5642
H 0.5947 0.6954 6.1058

D,D c-di-UMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, COSMO
p -0.96882817 -2.754665305 -2.113942619
o -1.466509977 -3.258919635 -3.410145864
o -0.933107261 -3.603103481 -0.903374591
o -1.781394079 -1.407684461 -1.668482025
c -2.319360311 -0.477034838 -2.606444165
c -2.515819731 0.859317988 -1.934883564
o -3.356796895 0.700201849 -0.773580859
c -1.255984045 1.528777325 -1.403582616
o -0.535156561 2.141015126 -2.44463182
c -1.828513187 2.467785048 -0.350638305
o -2.451459399 3.591929453 -0.959338755
c -2.913820416 1.560349174 0.243535468
c -1.540038745 -1.315345652 2.224928266
c -1.523932348 -0.776427497 3.53360348
o -1.189800467 -1.365655709 4.549950104
n -1.942269007 0.563054125 3.598114331
c -2.366736984 1.368704271 2.582651005
o -2.695536906 2.545758153 2.733443766
n -2.394309683 0.741316232 1.364299154
c -1.981417356 -0.556251222 1.20885035
h -1.634670394 -0.338107396 -3.434342172
h -3.271386951 -0.861315104 -2.975811862
h -3.014282654 1.538457223 -2.623274689
h -0.627171374 0.780737117 -0.914005805
h -2.16274154 4.388887745 -0.501284408
h -3.748909219 2.138289087 0.630169442
p 0.959764073 2.756234835 -2.123122423
o 0.907414571 3.614046071 -0.91891564
o 1.465714361 3.255767663 -3.417843988
o 1.775463657 1.415551956 -1.663541092
c 2.301390199 0.477032389 -2.601237926
c 2.508287209 -0.856412949 -1.92739074
o 3.353168242 -0.689170821 -0.770679924
c 1.257465562 -1.540625154 -1.38974847

o 0.533564184 -2.152163567 -2.428864587
c 1.847308422 -2.475089833 -0.345271601
o 2.472371652 -3.578176506 -0.984750473
c 2.921443345 -1.551560026 0.248015655
c 1.527650973 1.310581499 2.235406455
c 1.511865096 0.766524656 3.542216721
o 1.17411869 1.350707469 4.560077337
n 1.935439038 -0.571631467 3.602587843
c 2.366153167 -1.370735856 2.58486292
o 2.702084626 -2.546554054 2.730992739
n 2.392346129 -0.738684319 1.369003815
c 1.973843402 0.557471855 1.217011522
h 1.606408225 0.333530452 -3.420164394
h 3.248640242 0.858708415 -2.984693261
h 3.009098209 -1.53169161 -2.617567757
h 0.626027946 -0.802251882 -0.88931777
h 1.110881362 -2.806977957 0.371584794
h 2.553240203 -4.298450477 -0.353669679
h 3.765459399 -2.116196116 0.635976239
h -1.084707853 2.780567165 0.365091033
h -1.229794834 -2.338383713 2.064130158
h -2.041978774 -0.934748166 0.21356182
h 1.214121985 2.333307859 2.078926051
h 2.034249683 0.939340371 0.222878213
h -1.91390367 1.005912539 4.494995079
h 1.90816153 -1.017750139 4.497951687

D,L c-di-UMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, gas-phase

C	5.3434980	-1.6210180	-0.5141300
C	6.7343260	-1.2515690	-0.5916230
O	7.6722630	-1.9120260	-1.0481490
N	6.9881280	0.0288310	-0.0543790
C	6.0997310	0.9284240	0.5207550
O	6.4723020	1.9991750	0.9899870
N	4.7796210	0.4850330	0.5027380
C	4.4415110	-0.7602940	0.0225050
H	5.0250000	-2.5922200	-0.8673420
H	3.3928160	-1.0260750	0.1376960
H	7.9550730	0.3327120	-0.0607680
C	3.7149860	1.3465770	1.0724550
H	4.2279130	2.2205160	1.4762630
O	1.4582000	-1.4823880	0.8519410
C	1.0916720	-0.7874740	2.0512220
C	1.6272360	0.6321650	1.9631580
O	3.0729990	0.5951130	2.0886400
C	1.2892660	1.3415480	0.6449430
O	0.3754640	2.4002340	0.9223480
C	2.6609330	1.7804820	0.0334680
O	2.7943400	3.1584240	-0.2051440
H	0.0028900	-0.7703830	2.1714130

H	1.5227670	-1.3004610	2.9188530
H	1.2253430	1.2272260	2.7918710
H	0.8299960	0.6290010	-0.0407340
H	1.9777510	3.4097020	-0.7320080
P	-0.5119340	3.0030670	-0.3403680
O	0.4532960	3.3599950	-1.4495480
O	-1.5043770	3.9360460	0.2483300
O	-1.3321890	1.6429080	-0.8253300
H	2.8126790	1.2043510	-0.8926630
C	-0.9867720	0.9436580	-2.0284140
C	-1.5296140	-0.4726150	-1.9315360
O	-2.9769820	-0.4269780	-2.0305590
C	-1.1733310	-1.1842710	-0.6198630
O	-0.2433730	-2.2250510	-0.9098760
C	-2.5338800	-1.6496500	-0.0026510
O	-2.6555810	-3.0362090	0.1894650
H	0.1002000	0.9191300	-2.1627540
H	-1.4259610	1.4581530	-2.8910850
H	-1.1452810	-1.0694980	-2.7673570
H	-0.7224680	-0.4673860	0.0670540
H	-1.8394880	-3.2925210	0.7142020
P	0.6468650	-2.8394000	0.3453310
O	-0.3184870	-3.2202760	1.4463890
O	1.6478260	-3.7556850	-0.2550710
H	-2.6757730	-1.1082050	0.9454450
C	-3.6047080	-1.1876450	-1.0124630
C	-5.1755770	1.7761880	0.6398340
C	-6.5653890	1.4121280	0.7530610
O	-7.4874200	2.0728850	1.2404640
N	-6.8396030	0.1370410	0.2132000
C	-5.9712170	-0.7622680	-0.3920050
O	-6.3612050	-1.8281910	-0.8582160
N	-4.6491790	-0.3245910	-0.4075860
C	-4.2924860	0.9155360	0.0725150
H	-4.8432220	2.7436690	0.9905170
H	-3.2462070	1.1778500	-0.0692950
H	-7.8073100	-0.1629090	0.2440400
H	-4.1345780	-2.0502140	-1.4187840

D,L c-di-UMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, COSMO

C	4.5708	-1.6487	-0.4842
C	5.8136	-1.2840	-1.1095
O	6.4906	-1.9797	-1.8805
N	6.2560	0.0054	-0.7725
C	5.6348	0.9203	0.0496
O	6.0867	2.0459	0.2702
N	4.4466	0.4715	0.6141
C	3.9433	-0.7749	0.3436
H	4.1437	-2.6234	-0.6765
H	3.0049	-1.0066	0.8333

H 7.1262 0.3173 -1.1952
C 3.7535 1.4359 1.5248
H 4.5338 1.8947 2.1329
O 0.8952 -0.9646 1.0872
C 0.5434 -0.0430 2.1331
C 1.4696 1.1491 2.0497
O 2.8388 0.7380 2.3476
C 1.5811 1.8013 0.6729
O 0.4809 2.6720 0.4295
C 2.9475 2.4883 0.7363
O 2.8215 3.6881 1.4974
H -0.4864 0.3066 2.0004
H 0.6277 -0.5243 3.1109
H 1.1545 1.8908 2.7925
H 1.6245 1.0159 -0.0880
H 3.6618 4.1690 1.4356
P -0.1705 2.6421 -1.0800
O 0.9104 2.7452 -2.1187
O -1.3149 3.6079 -1.0224
O -0.7720 1.1153 -1.0878
H 3.3737 2.6838 -0.2500
C -0.4635 0.1963 -2.1496
C -1.3904 -0.9927 -2.0386
O -2.7675 -0.5764 -2.2947
C -1.4656 -1.6464 -0.6603
O -0.3583 -2.5143 -0.4431
C -2.8327 -2.3337 -0.6903
O -2.7278 -3.5267 -1.4651
H 0.5697 -0.1560 -2.0569
H -0.5830 0.6806 -3.1224
H -1.1013 -1.7342 -2.7920
H -1.4916 -0.8604 0.1008
H -3.5634 -4.0119 -1.3790
P 0.3116 -2.4974 1.0595
O -0.7565 -2.6325 2.1078
O 1.4697 -3.4440 0.9721
H -3.2303 -2.5378 0.3060
C -3.6590 -1.2739 -1.4464
C -4.3816 1.7969 0.6201
C -5.5998 1.4317 1.2919
O -6.2400 2.1219 2.0985
N -6.0636 0.1490 0.9583
C -5.4817 -0.7601 0.1018
O -5.9490 -1.8805 -0.1127
N -4.3139 -0.3119 -0.5048
C -3.7934 0.9288 -0.2421
H -3.9419 2.7673 0.8058
H -2.8743 1.1609 -0.7671
H -6.9182 -0.1625 1.4118
H -4.4621 -1.7232 -2.0311

D,D c-AMP-UMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, gas-phase

P	2.9253900	1.4678490	2.4851100
O	4.2918630	1.3867810	3.0697930
O	1.8428720	2.3876560	2.9845300
O	2.2281390	-0.0380410	2.4428970
C	3.1038870	-1.1745290	2.3413930
C	2.4605800	-2.2879760	1.5365600
O	1.2729390	-2.7890070	2.2162910
C	1.9810300	-1.8912270	0.1441280
O	3.0781380	-1.9170340	-0.7563190
C	0.8201000	-2.8712040	-0.1349250
O	1.2589400	-4.1095820	-0.6591260
C	0.2477430	-3.0647210	1.2769310
N	-0.8834130	-2.1417240	1.5171120
C	-0.8179420	-0.7880090	1.8129540
N	-1.9942500	-0.1855470	1.7619520
C	-2.8770980	-1.1928050	1.4086940
C	-4.2512540	-1.1966690	1.1287560
N	-5.0199180	-0.0580370	1.2139130
N	-4.8494990	-2.3533550	0.7859130
C	-4.0858120	-3.4584290	0.7033980
H	-4.6139170	-4.3673860	0.4222470
N	-2.7685470	-3.5885940	0.9050200
C	-2.2087360	-2.4182060	1.2535550
H	0.1251220	-0.3251410	2.0829240
H	4.0407870	-0.8910570	1.8501310
H	3.3379940	-1.5271940	3.3525850
H	3.1831280	-3.1096350	1.4414560
H	1.5589710	-0.8840550	0.1939730
H	1.5306890	-3.8426140	-1.5779340
H	-0.1442830	-4.0752090	1.4119970
P	2.8055740	-1.6258130	-2.3670200
O	1.6788440	-2.5212460	-2.8103560
O	4.1435320	-1.5781650	-3.0168800
O	2.1464010	-0.1014160	-2.3034730
C	3.0561750	1.0108170	-2.2197050
C	2.4557840	2.1368130	-1.3995850
O	1.2650200	2.6632180	-2.0509740
C	2.0025950	1.7443240	0.0022700
O	3.1289410	1.7648390	0.8650390
C	0.8507970	2.7297220	0.3131980
O	1.3065580	3.9477530	0.8690370
C	0.2786910	2.9952810	-1.0889040
C	-0.8323990	0.8664130	-1.7696460
H	0.1869080	0.5053620	-1.8897110
H	3.9932130	0.7019910	-1.7445630
H	3.2809380	1.3567690	-3.2351250
H	3.1971350	2.9427030	-1.3174340
H	1.5765820	0.7379270	-0.0336470

H	0.0982320	2.2679310	0.9608210
H	1.6041600	3.6516560	1.7741820
H	-0.0363380	4.0340780	-1.1872130
H	0.0727620	-2.4220730	-0.7957390
H	-5.8235830	-0.0673770	0.5968580
H	-4.4836840	0.8020030	1.1888160
N	-0.9418510	2.1795010	-1.3784270
C	-1.9069950	0.0783610	-2.0364900
H	-1.7688790	-0.9475270	-2.3490140
C	-3.2400670	0.6130650	-1.9347930
O	-4.3116230	0.0474140	-2.1690040
N	-3.2517810	1.9635140	-1.5226200
H	-4.1620530	2.4047870	-1.4600040
C	-2.1800960	2.7995800	-1.2457270
O	-2.3361350	3.9758000	-0.9286690

D,D c-AMP-UMP, TPSS-D3(BJ)/def2-TZVPPD level, constrained optimization, gas-phase

P	2.3833	-0.4408	2.8317
O	3.4283	-1.2486	3.5180
O	1.5453	0.6155	3.5016
O	1.2975	-1.4386	2.0712
C	1.8283	-2.6569	1.5190
C	0.9763	-3.1229	0.3529
O	-0.3395	-3.5186	0.8225
C	0.7497	-2.0665	-0.7280
O	1.7857	-2.2023	-1.6950
C	-0.6991	-2.3144	-1.2315
O	-0.7624	-3.1369	-2.3779
C	-1.3556	-3.0533	-0.0488
N	-2.2684	-2.2001	0.7362
C	-1.9207	-1.2036	1.6362
N	-2.9654	-0.5705	2.1426
C	-4.0532	-1.1821	1.5450
C	-5.4340	-0.9616	1.6404
N	-5.9641	-0.0140	2.4856
N	-6.2769	-1.7204	0.9138
C	-5.7415	-2.6742	0.1251
H	-6.4601	-3.2655	-0.4388
N	-4.4545	-2.9845	-0.0638
C	-3.6446	-2.2005	0.6678
H	-0.8828	-1.0239	1.8941
H	2.8494	-2.4948	1.1545
H	1.8591	-3.4209	2.3033
H	1.4595	-3.9944	-0.1080
H	0.7865	-1.0715	-0.2760
H	-0.3390	-2.5586	-3.0708
H	-1.9667	-3.8800	-0.4201
P	1.8521	-1.1518	-2.9758
O	0.4686	-1.0556	-3.5645
O	3.0743	-1.5112	-3.7446

O 2.0773 0.2906 -2.1895
C 3.3925 0.5674 -1.6789
C 3.2951 1.5150 -0.4972
O 2.7833 2.8026 -0.9321
C 2.3626 1.0392 0.6154
O 3.1301 0.2616 1.5255
C 1.7214 2.3379 1.1779
O 2.4050 2.8595 2.2984
C 1.8564 3.3275 0.0041
C 0.0619 2.5911 -1.5433
H 0.6879 1.7087 -1.6570
H 3.8727 -0.3578 -1.3401
H 4.0018 1.0025 -2.4785
H 4.2979 1.6592 -0.0746
H 1.5645 0.4293 0.1832
H 0.6663 2.1651 1.4203
H 2.2322 2.1596 2.9883
H 2.1701 4.3062 0.3670
H -1.2052 -1.3601 -1.4173
H -6.8974 0.2963 2.2489
H -5.3188 0.7067 2.7847
N 0.5726 3.5650 -0.7166
C -1.1091 2.7254 -2.2174
H -1.4592 1.9315 -2.8630
C -1.8762 3.9392 -2.0983
O -2.9452 4.2222 -2.6458
N -1.2661 4.8846 -1.2444
H -1.7562 5.7642 -1.1286
C -0.0733 4.7860 -0.5425
O 0.3513 5.7046 0.1535

D,D c-AMP-UMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, COSMO
P 2.6465 1.4212 2.5746
O 3.9701 1.4479 3.2781
O 1.4264 2.1007 3.1169
O 2.1640 -0.1144 2.2833
C 3.1011 -1.1924 2.1133
C 2.4007 -2.3393 1.4149
O 1.2032 -2.7199 2.1525
C 1.8871 -2.0511 0.0049
O 2.9641 -2.0976 -0.9230
C 0.7862 -3.1047 -0.1560
O 1.4033 -4.3725 -0.3649
C 0.1535 -3.0472 1.2484
N -0.9202 -2.0405 1.3475
C -0.8237 -0.7106 1.7215
N -1.9885 -0.0862 1.7204
C -2.9003 -1.0553 1.3265
C -4.2999 -1.0380 1.1547
N -5.0531 0.0565 1.3893

N -4.9118 -2.1825 0.7674
C -4.1627 -3.2781 0.5602
H -4.7088 -4.1640 0.2456
N -2.8348 -3.4236 0.6919
C -2.2571 -2.2753 1.0866
H 0.1280 -0.2840 2.0068
H 3.9553 -0.8805 1.5019
H 3.4662 -1.5062 3.0951
H 3.0875 -3.1932 1.3801
H 1.4143 -1.0622 -0.0209
H 0.7078 -5.0136 -0.5791
H -0.2927 -4.0040 1.5278
P 2.6984 -1.5441 -2.4543
O 1.4749 -2.1893 -3.0293
O 4.0392 -1.6032 -3.1223
O 2.2501 0.0053 -2.1762
C 3.2007 1.0648 -1.9737
C 2.4923 2.2220 -1.3003
O 1.3239 2.6171 -2.0788
C 1.9226 1.9414 0.0887
O 2.9681 1.9688 1.0516
C 0.8323 3.0118 0.2150
O 1.4584 4.2667 0.4711
C 0.2626 2.9920 -1.2167
C -0.7000 0.7650 -1.8699
H 0.3278 0.5016 -2.0940
H 4.0256 0.7388 -1.3304
H 3.6071 1.3717 -2.9413
H 3.1860 3.0686 -1.2429
H 1.4342 0.9593 0.0937
H 0.0833 2.7737 0.9712
H 0.7608 4.9166 0.6496
H -0.1294 3.9670 -1.5068
H 0.0762 -2.8661 -0.9493
H -6.0299 0.0557 1.1302
H -4.6104 0.9421 1.5864
N -0.8753 2.0311 -1.3712
C -1.7347 -0.0857 -2.0853
H -1.5579 -1.0739 -2.4871
C -3.0852 0.3441 -1.8360
O -4.1217 -0.2915 -2.0612
N -3.1674 1.6363 -1.2879
H -4.0989 1.9874 -1.0850
C -2.1341 2.5114 -1.0284
O -2.3055 3.6314 -0.5436

D,L c-UMP-AMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, gas-phase

C	3.1887530	1.3159670	1.1018430
H	3.4670600	2.3278860	1.3986280
O	1.3051840	-1.5853960	0.4823060

C	0.5306990	-0.8513450	1.4384980
C	0.9424820	0.6123470	1.4064490
O	2.2643600	0.7321100	2.0089770
C	1.0201850	1.2358750	0.0034730
O	0.3611980	2.5065140	0.0340670
C	2.5419820	1.3071280	-0.2929680
O	2.9910980	2.4047920	-1.0414330
H	-0.5407770	-0.9555440	1.2368380
H	0.7268670	-1.2616940	2.4365340
H	0.2482920	1.2032990	2.0144150
H	0.5526250	0.5888860	-0.7394120
H	2.2465820	2.6636290	-1.6677480
P	-0.2460230	3.0854420	-1.3926680
O	0.8271620	2.9416160	-2.4515290
O	-0.9355800	4.3602060	-1.0759720
O	-1.3960040	1.9251010	-1.7171330
H	2.7930650	0.3553030	-0.7871510
C	-3.8051390	-1.0116310	-1.4728330
N	-4.4592850	-0.1651220	-0.4518690
C	-4.0359490	1.0701270	0.0148510
N	-4.8148690	1.5636600	0.9638010
C	-5.7987200	0.6047070	1.1259330
C	-6.9060670	0.5180170	1.9807800
N	-7.2346020	1.5298790	2.8526890
N	-7.7003150	-0.5685060	1.9272450
C	-7.3935270	-1.5269750	1.0292870
H	-8.0662480	-2.3820530	1.0172100
N	-6.3765470	-1.5719210	0.1621780
C	-5.5992160	-0.4794510	0.2548810
H	-3.1623500	1.5553790	-0.4080260
H	-7.8268420	1.2593870	3.6265440
H	-6.4911330	2.1841970	3.0619870
H	-4.5761920	-1.6968790	-1.8335400
C	-1.3058730	1.1173940	-2.8975040
C	-1.8954890	-0.2575790	-2.6400990
O	-3.3435430	-0.1674860	-2.5111540
C	-1.4142370	-0.9212590	-1.3518180
O	-0.1787910	-1.5678160	-1.6340480
C	-2.6081750	-1.8028320	-0.9145890
O	-2.5980300	-3.0901470	-1.4950680
H	-0.2581920	1.0138890	-3.1969290
H	-1.8559590	1.6055340	-3.7126010
H	-1.6602340	-0.9132500	-3.4877430
H	-1.2784350	-0.1369070	-0.5990710
H	-1.8244230	-3.5125280	-1.0278800
P	0.5843020	-2.6132340	-0.5950990
O	-0.4948850	-3.3889760	0.1245200
O	1.6993210	-3.2317150	-1.3531150
H	-2.6665940	-1.8747290	0.1776980
C	5.4770950	-1.6290800	0.8811940

C	6.7507980	-1.1124780	1.3115000
O	7.8224390	-1.7196960	1.4096620
N	6.6934740	0.2528290	1.6569190
C	5.6021810	1.1140030	1.6451160
O	5.6925110	2.2759570	2.0253420
N	4.4351810	0.5191860	1.1684580
C	4.3916840	-0.8141000	0.8331990
H	5.3935150	-2.6698760	0.6007970
H	3.4091440	-1.1791600	0.5425980
H	7.5561070	0.6679190	1.9897810

D,L c-UMP-AMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, COSMO

C	3.8168	1.4933	1.3570
H	4.6645	1.9720	1.8479
O	0.8284	-0.8029	1.3652
C	0.6231	0.2096	2.3644
C	1.5762	1.3508	2.0891
O	2.9535	0.9212	2.3205
C	1.5984	1.8522	0.6472
O	0.4963	2.7135	0.3855
C	2.9817	2.4958	0.5351
O	2.9496	3.7665	1.1822
H	-0.4040	0.5860	2.3128
H	0.7990	-0.1941	3.3657
H	1.3462	2.1745	2.7743
H	1.5715	0.9851	-0.0198
H	3.8021	4.2023	1.0255
P	-0.1871	2.6005	-1.1091
O	0.8729	2.6823	-2.1701
O	-1.3502	3.5450	-1.0621
O	-0.7770	1.0728	-1.0543
H	3.3299	2.5808	-0.4964
C	-3.5503	-1.4207	-1.5088
N	-4.3232	-0.3830	-0.8060
C	-3.9311	0.8955	-0.4550
N	-4.8728	1.5653	0.1884
C	-5.9382	0.6789	0.2665
C	-7.2312	0.7780	0.8226
N	-7.6967	1.8987	1.4137
N	-8.0515	-0.2974	0.7297
C	-7.6041	-1.4034	0.1106
H	-8.3082	-2.2307	0.0673
N	-6.4070	-1.6199	-0.4546
C	-5.6159	-0.5376	-0.3455
H	-2.9488	1.2688	-0.7111
H	-8.5756	1.8640	1.9122
H	-7.0640	2.6581	1.6218
H	-4.2597	-1.9669	-2.1351
C	-0.3157	0.0546	-1.9603
C	-1.2274	-1.1462	-1.8432

O -2.5608 -0.8004 -2.3178
C -1.4606 -1.6586 -0.4214
O -0.3884 -2.4989 -0.0022
C -2.8115 -2.3690 -0.5411
O -2.5991 -3.6386 -1.1572
H 0.7016 -0.2575 -1.6983
H -0.3122 0.4338 -2.9852
H -0.8240 -1.9521 -2.4676
H -1.5699 -0.8064 0.2560
H -3.4423 -4.1181 -1.1540
P 0.1777 -2.3003 1.5257
O -0.9565 -2.2370 2.5095
O 1.2841 -3.3036 1.6587
H -3.3310 -2.4697 0.4152
C 4.3387 -1.8101 -0.3861
C 5.5234 -1.5610 -1.1628
O 6.0970 -2.3574 -1.9200
N 6.0375 -0.2640 -1.0043
C 5.5314 0.7527 -0.2237
O 6.0408 1.8734 -0.1607
N 4.3881 0.4137 0.4906
C 3.8237 -0.8326 0.4025
H 3.8662 -2.7816 -0.4342
H 2.9313 -0.9746 1.0003
H 6.8727 -0.0332 -1.5355

Sugar-phosphate ring model, Figure 4a, TPSS-D3(BJ)/def2-TZVPPD level, gas-phase
o -1.789306687 -1.743957762 -0.266298297
p -0.681026771 -2.269248169 -1.11664263
o -0.31529905 -1.186209533 -2.294320907
o -0.747946109 -3.598282579 -1.785316536
o 0.749605743 -2.113258665 -0.300471165
c 0.446967418 -1.028129103 4.095979024
h 0.21974104 -1.797442302 4.830376711
c 0.750021566 -2.371842029 1.075915062
c 1.089352145 -1.111298119 1.863114455
o 1.409005518 -1.567210221 3.199011851
c -0.083763932 -0.146909988 1.993632619
o 0.324253919 1.203063133 2.2907373
c -0.768839949 -0.616445848 3.268001549
o -1.557311892 0.404385005 3.862467703
h 1.518472012 -3.126763771 1.282119778
h -0.224038032 -2.763155685 1.387822492
h 1.959887456 -0.60305714 1.44859402
h -0.745655701 -0.175979748 1.141641794
h -1.121893089 1.225381998 3.551360805
h -1.421611403 -1.469054431 3.064717616
h 0.847557432 -0.135823888 4.590583931
o 1.798042618 1.761427159 0.262690159
p 0.689591548 2.286287244 1.113077464

o	0.756131096	3.615289361	1.781853982
o	-0.740989144	2.129904536	0.296904144
c	-0.437211173	1.045253693	-4.099488166
h	-0.209642043	1.814706869	-4.833647168
c	-0.741403819	2.38862768	-1.079474584
c	-1.080361045	1.128100628	-1.866833102
o	-1.399575789	1.584171513	-3.20274863
c	0.092780609	0.163722044	-1.997024562
c	0.778276337	0.63329321	-3.271167396
o	1.56686316	-0.387511857	-3.865532205
h	-1.51000003	3.143410177	-1.285653221
h	0.232583198	2.780179109	-1.391298601
h	-1.951020269	0.619766968	-1.45266653
h	0.754442251	0.192698271	-1.144870402
h	1.131413203	-1.208524101	-3.55450628
h	1.431090634	1.485776114	-3.067526333
h	-0.837691858	0.153094741	-4.59443183

Sugar-phosphate ring model, Figure 4b, TPSS-D3(BJ)/def2-TZVPPD level, gas-phase

c	4.046869403	-1.211913834	0.208794929
h	4.390963223	-0.522906151	0.979499751
o	-0.480321868	-2.445632817	0.433844306
c	0.853161024	-2.590934777	-0.065254305
c	1.760222288	-1.570396356	0.609586838
o	3.098710383	-2.159750674	0.708735926
c	1.923541565	-0.227479007	-0.107597183
o	1.984063677	0.794851252	0.885191848
c	3.265129262	-0.440919039	-0.838514103
o	3.933666011	0.663901332	-1.378749832
h	1.214863199	-3.595211215	0.18280634
h	0.858485022	-2.486208449	-1.134996326
h	1.382321653	-1.381929731	1.600533585
h	1.093762955	-0.021670671	-0.776822836
h	3.595987562	1.519661402	-0.961604596
p	1.799754165	2.400502929	0.537614117
o	2.95240761	2.826975853	-0.32381579
o	1.474427462	3.083327825	1.799100113
o	0.496587735	2.372412317	-0.451167527
h	3.044595041	-1.150595725	-1.637866007
c	-4.027560824	1.136959262	-0.197265629
h	-4.87542969	1.694226189	0.206726692
c	-0.834972907	2.52237391	0.051518977
c	-1.745866954	1.502317063	-0.618454492
o	-3.086616409	2.088737209	-0.703335721
c	-1.898525274	0.156980525	0.09628149
o	-1.964687296	-0.862341804	-0.898935298
c	-3.233582839	0.364669997	0.840301488
o	-3.893455936	-0.743204832	1.384705624
h	-1.195037548	3.527068626	-0.197349398
h	-0.837561177	2.41978923	1.121455617

h -1.377075905 1.317865509 -1.613436561
h -1.06201994 -0.048094897 0.757528578
h -3.56560122 -1.596310711 0.955048844
p -1.78059857 -2.469572013 -0.558633017
o -2.935694648 -2.900835841 0.297335848
o -1.451670885 -3.146257719 -1.822424688
h -3.007038225 1.072425372 1.639558117
h -4.377555781 0.449638922 -0.966873895
h 4.897332843 -1.772520893 -0.185412779

Sugar-phosphate ring model, Figure 4c, TPSS-D3(BJ)/def2-TZVPPD level, gas-phase
c 4.070176352 -0.36938245 0.1723256
h 4.457874313 0.61674923 0.476909222
o 0.734278044 -2.465118653 0.639712518
c 0.969741618 -1.443206445 1.593603337
c 1.984568849 -0.386380328 1.181326446
o 3.31875586 -0.992013459 1.189936792
c 1.772354619 0.194937081 -0.202729452
o 1.700930454 1.636640005 -0.257543086
c 3.068736133 -0.180961617 -0.951224703
o 3.455856303 0.81009339 -1.882754645
h 0.040870804 -0.941993188 1.870596641
h 1.364436515 -1.955364229 2.464123646
h 1.947984025 0.429847404 1.897340345
h 0.91057906 -0.257900609 -0.684015363
h 2.979937614 1.609685552 -1.572519945
p 0.486233522 2.53435731 0.445626995
o 0.96967159 3.945954518 0.431195244
o 0.074582225 1.827721879 1.6834393
o -0.748331687 2.448648123 -0.63182463
h 2.904684488 -1.125542277 -1.466669203
c -4.083879256 0.352138382 -0.168624597
h -4.924026645 1.010935579 0.071999554
c -0.983049243 1.428095143 -1.587226288
c -1.9974019 0.370309816 -1.176097219
o -3.332098147 0.975091081 -1.185800855
c -1.786020464 -0.210490674 0.208274026
o -1.713941532 -1.652109434 0.263843466
c -3.083176952 0.164847316 0.955713911
o -3.470244695 -0.826125006 1.887335741
h -0.053803701 0.927887431 -1.864747312
h -1.377987916 1.941070969 -2.457174149
h -1.959756917 -0.445929762 -1.891992557
h -0.924862978 0.243004023 0.690086061
h -2.993707335 -1.625540457 1.577542494
p -0.499129649 -2.55010926 -0.438867477
o -0.982863823 -3.961613057 -0.424898626
o -0.086749344 -1.843450912 -1.676448435
h -2.920185464 1.109734705 1.470945108
h -4.470547002 -0.634380492 -0.473233043

h 4.909614558 -1.028772731 -0.069079022

Sugar-phosphate ring model, Figure 4d, TPSS-D3(BJ)/def2-TZVPPD level, gas-phase
c 3.906315099 -1.489024571 -0.316278484
h 4.561352778 -1.108609441 0.470160217
o -0.024803975 -2.218290474 -0.488505031
c 0.566841304 -2.267912197 0.790673423
c 1.902574076 -1.546454267 0.800318075
o 2.911474852 -2.380312082 0.185192634
c 1.940685119 -0.175644167 0.102004741
o 2.154257452 0.836795986 1.07762404
c 3.113191247 -0.325203443 -0.899829097
o 3.926328314 0.806678479 -1.101552197
h -0.100658501 -1.81069387 1.514972301
h 0.721980268 -3.314763621 1.07814039
h 2.191196299 -1.371182209 1.828569179
h 1.002576872 0.008803649 -0.412495809
h 3.34813518 1.620027725 -0.965778704
p 1.658826196 2.378165195 0.738964618
o 2.221209355 2.75197807 -0.595211545
o 1.89708117 3.181457787 1.944268752
o 0.030253689 2.165411373 0.55555236
h 2.658435908 -0.667350805 -1.826449018
c -3.894587543 1.434537645 0.37069982
h -4.494252632 1.996132943 1.080009058
c -0.553873363 2.213009877 -0.727093419
c -1.887989464 1.488405273 -0.743874664
o -2.904058246 2.324284439 -0.141835712
c -1.928137525 0.12209499 -0.037286453
o -2.152383738 -0.895533057 -1.005741046
c -3.094492669 0.283042466 0.96836144
o -3.901375676 -0.848726812 1.193858473
h 0.119201756 1.757201332 -1.4472469
h -0.709829276 3.25937731 -1.015819372
h -2.167715223 1.306337337 -1.773203616
h -0.988072421 -0.06397873 0.473104827
h -3.325532486 -1.663007715 1.054114842
p -1.654145149 -2.434753719 -0.662599086
o -2.208747121 -2.802702161 0.676202896
o -1.898339928 -3.244352735 -1.862746091
h -2.635155898 0.642997082 1.88623815
h -4.548042342 1.040857594 -0.410645196
h 4.503624687 -2.044540088 -1.032067374

syn D,D c-di-AMP, TPSS/TZVP level
C 4.174745 -0.745910 0.809868
N 5.328916 0.104860 0.517778
C 6.626714 -0.235890 0.839446
N 7.542938 0.628144 0.449497

C	6.794447	1.610660	-0.182609
C	7.164254	2.793870	-0.842490
N	8.475868	3.220677	-0.899156
N	6.217462	3.562678	-1.406348
C	4.932413	3.154583	-1.294809
H	4.196803	3.805946	-1.761365
N	4.447547	2.061805	-0.699753
C	5.419348	1.311719	-0.161005
H	6.826956	-1.152719	1.379164
H	8.670388	3.883641	-1.640047
H	9.173576	2.501118	-0.751733
H	4.532906	-1.472931	1.557688
C	-4.183910	-0.826725	-0.731215
N	-5.331930	0.056924	-0.524714
C	-6.633765	-0.309665	-0.798237
N	-7.543463	0.593910	-0.491580
C	-6.785971	1.632998	0.029776
C	-7.145674	2.879043	0.568353
N	-8.455450	3.314663	0.594047
N	-6.190912	3.698052	1.040716
C	-4.908193	3.275572	0.959453
H	-4.166102	3.968699	1.349202
N	-4.432709	2.125031	0.476124
C	-5.412197	1.327532	0.027090
H	-6.842018	-1.276456	-1.238646
H	-8.640054	4.050380	1.265593
H	-9.156529	2.586254	0.529000
P	-0.160844	-1.637930	-2.950167
O	0.180666	-2.855716	-3.777506
O	-0.590331	-0.279943	-3.508346
O	1.090124	-1.282737	-1.880063
C	1.722826	-2.420281	-1.276540
C	2.504186	-2.034848	-0.032116
O	3.765967	-1.392866	-0.388273
C	1.809182	-1.103779	0.991343
O	1.363608	-1.930613	2.075155
C	2.923899	-0.061623	1.376675
O	3.105041	0.196690	2.748558
H	0.967031	-3.158613	-0.974314
H	2.395109	-2.902346	-1.998098
H	2.741488	-2.966737	0.507249
H	0.961823	-0.581880	0.541934
H	2.178817	0.253295	3.149948
P	0.153976	-1.312268	3.096488
O	0.576756	0.100244	3.503740
O	-0.185205	-2.433747	4.051238
O	-1.095283	-1.080070	1.991431
C	-1.725438	-2.276110	1.511954
C	-2.512116	-2.022448	0.237476
O	-3.770479	-1.342121	0.527540

C	-1.817922	-1.205721	-0.879673
O	-1.365677	-2.145115	-1.863994
C	-2.934384	-0.215205	-1.379279
O	-3.122154	-0.121857	-2.771547
H	-0.967981	-3.038730	1.282531
H	-2.392494	-2.683998	2.282469
H	-2.753591	-3.005290	-0.200047
H	-0.974165	-0.634875	-0.486405
H	-2.740832	0.763005	-0.919326
H	-2.197116	-0.102546	-3.178814
H	2.733415	0.854910	0.802273
H	-4.551208	-1.628188	-1.393581

ImpA$^-$, HF/6-31G* level

P	-2.987609	-0.294677	-0.478242
O	-2.721317	0.627869	0.838420
O	-2.071346	-1.444058	-0.434248
O	-3.114286	0.613756	-1.634740
N	-4.580681	-0.862368	-0.135802
C	-4.929687	-1.955664	0.623089
C	-6.276936	-1.973854	0.653478
N	-6.787555	-0.918882	-0.068104
C	-5.750277	-0.292769	-0.513107
H	-4.188123	-2.602878	1.036732
H	-5.761382	0.582931	-1.126411
H	-6.919556	-2.680683	1.138710
C	-0.501937	1.597980	1.019725
C	1.187866	2.145815	-0.541704
C	-0.260892	1.667690	-0.495940
C	1.797926	1.421663	0.665465
O	0.764914	1.225278	1.567990
C	-1.504428	0.565902	1.530018
H	-1.714985	0.762892	2.574372
H	-1.076028	-0.421083	1.451863
H	-0.763125	2.590681	1.364346
H	1.683122	1.885217	-1.470441
H	2.579159	2.015092	1.116165
O	1.225760	3.527858	-0.321807
O	-1.111684	2.504204	-1.185298
H	-0.286377	0.662517	-0.908265
H	2.114496	3.834061	-0.437161
H	-1.890241	2.000173	-1.440071
N	2.427146	0.145972	0.332499
C	1.851168	-1.088258	0.129206
N	2.697590	-2.018458	-0.131044
C	3.919909	-1.381626	-0.107677
C	5.228556	-1.825680	-0.298776
N	5.514292	-3.108892	-0.617926

N	6.225670	-0.956293	-0.187656
C	5.926675	0.308302	0.087715
H	6.770643	0.971313	0.161809
N	4.748441	0.851198	0.280249
C	3.766216	-0.043290	0.178737
H	0.791133	-1.230770	0.181958
H	6.458574	-3.401601	-0.512416
H	4.801234	-3.790180	-0.486999

HImpA HF/6-31G* level

P	3.716950	-0.721826	-0.423972
O	2.901533	-0.781579	0.939637
O	2.821029	-0.439485	-1.549139
O	4.848476	-1.630736	-0.365228
N	4.559489	0.895419	-0.198899
C	4.134525	2.151302	-0.573964
C	5.104413	3.022967	-0.260376
N	6.123114	2.274867	0.300361
C	5.757150	1.004198	0.308136
H	3.191121	2.294216	-1.050920
H	6.340259	0.178927	0.655329
H	5.178065	4.080047	-0.386774
C	0.510092	-1.244426	0.914505
C	-1.414979	-1.969367	-0.238057
C	-0.008081	-1.450036	-0.513201
C	-1.813738	-1.131344	0.987343
O	-0.629248	-0.731115	1.599084
C	1.617016	-0.225166	1.140087
H	1.584411	0.087831	2.173662
H	1.467463	0.643558	0.510509
H	0.804222	-2.194791	1.341446
H	-2.083012	-1.816691	-1.074618
H	-2.407178	-1.717513	1.674157
O	-1.345714	-3.316167	0.118836
O	0.722675	-2.304245	-1.309644
H	-0.107630	-0.469862	-0.977533
H	6.999457	2.620315	0.623171
H	-2.215346	-3.691596	0.091038
H	1.458818	-1.816634	-1.671172
N	-2.581938	0.059087	0.642888
C	-2.238301	1.380752	0.775246
N	-3.166078	2.199147	0.435478
C	-4.213322	1.382244	0.059088
C	-5.508874	1.634337	-0.406331
N	-5.992951	2.880512	-0.555212
N	-6.294742	0.603240	-0.691230
C	-5.822498	-0.624296	-0.513932
H	-6.505958	-1.417380	-0.758259
N	-4.637043	-0.992747	-0.084814
C	-3.865809	0.057191	0.187690

H	-1.274980	1.659822	1.141633
H	-6.857518	2.992911	-1.032834
H	-5.370969	3.654046	-0.505030

ImpU$^-$, HF/6-31G* level

P	-2.844398	-0.734643	-0.482298
O	-2.242525	-0.019654	0.857866
O	-2.569827	-2.173146	-0.421445
O	-2.503482	0.118344	-1.641911
N	-4.519774	-0.481181	-0.167434
C	-5.352840	-1.281169	0.580278
C	-6.553136	-0.668817	0.584373
N	-6.498855	0.498681	-0.143210
C	-5.281434	0.566329	-0.565284
H	-5.004757	-2.195451	1.007569
H	-4.872553	1.343320	-1.175460
H	-7.460237	-0.990774	1.054984
C	-0.012955	0.867147	1.001702
C	1.668330	1.865221	-0.339377
C	0.295053	1.205820	-0.460404
C	2.297639	1.092214	0.831740
O	1.266059	0.502547	1.537365
C	-0.938431	-0.307601	1.274440
H	-0.957862	-0.494496	2.342012
H	-0.564262	-1.201721	0.790227
H	-0.376550	1.754418	1.504686
H	2.246709	1.769434	-1.249230
H	2.855989	1.759177	1.469015
O	1.526282	3.207646	0.018229
O	-0.615950	2.013882	-1.094635
H	0.433100	0.267570	-0.999945
H	2.382127	3.614223	-0.015251
H	-1.360241	1.466419	-1.370388
O	4.763806	1.651542	-0.076768
O	6.028579	-2.612658	-0.720971
C	5.152594	-1.871727	-0.377734
C	3.825002	-2.246093	0.077239
C	2.958590	-1.296729	0.437082
N	3.249399	0.043146	0.395279
C	4.476147	0.485186	-0.025519
N	5.357422	-0.496517	-0.385593
H	6.250044	-0.177471	-0.696704
H	3.569250	-3.284752	0.114988
H	1.976992	-1.525870	0.791603

HImpU, HF/6-31G* level

P	3.289585	-0.797711	-0.289081
O	2.378063	-0.687570	1.010688
O	2.495004	-0.541257	-1.493868
O	4.337826	-1.780459	-0.078280

N	4.241151	0.763439	-0.122340
C	3.943651	2.015135	-0.615738
C	4.959290	2.832223	-0.300288
N	5.876751	2.054683	0.381917
C	5.409716	0.819986	0.456603
H	3.047354	2.191756	-1.166470
H	5.901290	-0.017826	0.901679
H	5.126518	3.867446	-0.498277
C	-0.021246	-1.055561	0.843033
C	-1.888061	-1.841380	-0.373275
C	-0.451521	-1.374704	-0.591889
C	-2.337257	-0.948281	0.799554
O	-1.184529	-0.434102	1.382984
C	1.111603	-0.063017	1.058035
H	1.017262	0.349484	2.052335
H	1.049784	0.745193	0.339446
H	0.196397	-1.971397	1.378482
H	-2.498412	-1.696643	-1.253955
H	-2.890739	-1.529474	1.519412
O	-1.890966	-3.174806	0.026771
O	0.306981	-2.304280	-1.266919
H	-0.495953	-0.432151	-1.137849
H	-2.787380	-3.485427	0.036736
H	1.079913	-1.865638	-1.614179
O	-4.853256	-1.320669	0.007415
O	-5.805367	3.026612	-0.653078
C	-4.987362	2.219430	-0.327172
C	-3.619443	2.495290	0.088876
C	-2.815638	1.487109	0.424564
N	-3.205519	0.170814	0.388237
C	-4.484102	-0.178186	0.026391
N	-5.298458	0.863674	-0.314858
H	-6.226269	0.612961	-0.585525
H	-3.294113	3.514499	0.124346
H	-1.811225	1.642107	0.753680
H	6.756480	2.356498	0.737797