Supporting Information (SI)

Impact of the substituents on the electronic structure of the four most stable tautomers of purine and their adenine analogues

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Supporting Information

Table S1. cSAR(X) and cSAR(NH_2) values for C8-X substitution of adenine.

C8-X	9H		7H		3H		1H	
	cSAR X	cSAR (NH_2)	cSAR X	cSAR (NH_2)	cSAR X	cSAR (NH_2)	cSAR X	cSAR (NH_2)
NO_2	-0.037	0.289	-0.005	0.229	-0.066	0.316	-0.051	0.301
CN	-0.002	0.277	0.019	0.216	-0.029	0.305	-0.018	0.289
CHO	0.008	0.274	0.039	0.219	-0.015	0.299	-0.002	0.291
Cl	0.099	0.246	0.113	0.191	0.057	0.276	0.066	0.250
F	0.122	0.241	0.132	0.187	0.091	0.269	0.099	0.241
H	**0.139**	**0.241**	**0.151**	**0.184**	**0.112**	**0.270**	**0.121**	**0.244**
Me	0.176	0.228	0.190	0.173	0.140	0.257	0.150	0.227
OMe	0.201	0.212	0.230	0.162	0.164	0.239	0.175	0.210
OH	0.193	0.217	0.210	0.168	0.163	0.244	0.171	0.215
NH_2	0.233	0.209	0.253	0.160	0.238	0.222	0.237	0.186
range	0.269	0.079	0.257	0.069	0.305	0.094	0.288	0.115
average	0.113	0.243	0.133	0.189	0.086	0.270	0.095	0.245
SD	0.094	0.028	0.091	0.025	0.098	0.030	0.095	0.038

Table S2. cSAR(X) and cSAR(NH_2) values for C2-X substitution of adenine.

C2-X	9H		7H		3H		1H	
	cSAR X	cSAR (NH_2)	cSAR X	cSAR (NH_2)	cSAR X	cSAR (NH_2)	cSAR X	cSAR (NH_2)
NO_2	-0.030	0.285	-0.008	0.231	0.014	0.303	-0.010	0.310
CN	0.000	0.275	0.004	0.220	0.034	0.294	0.011	0.288
CHO	0.024	0.267	0.029	0.210	0.060	0.279	0.030	0.300
Cl	0.061	0.268	0.062	0.210	0.119	0.287	0.104	0.263
F	0.096	0.266	0.097	0.210	0.138	0.290	0.124	0.258
H	**0.133**	**0.241**	**0.134**	**0.184**	**0.165**	**0.270**	**0.150**	**0.244**
Me	0.154	0.233	0.156	0.178	0.203	0.262	0.188	0.237
OMe	0.168	0.238	0.201	0.183	0.223	0.265	0.211	0.240
OH	0.167	0.243	0.167	0.189	0.214	0.271	0.199	0.244
NH_2	0.230	0.226	0.229	0.173	0.290	0.256	0.236	0.228
range	0.261	0.058	0.237	0.057	0.276	0.047	0.246	0.082
average	0.100	0.254	0.107	0.199	0.146	0.278	0.124	0.261
SD	0.085	0.020	0.083	0.020	0.090	0.015	0.089	0.029

Table S3. cSAR(X) and cSAR(C6H) values for C8 substitution of purine.

C8-X	9H		7H		3H		1H	
	cSAR X	cSAR (C6H)	cSAR X	cSAR (C6H)	cSAR X	cSAR (C6H)	cSAR X	cSAR (C6H)
NO_2	0.009	0.131	0.021	0.105	-0.015	0.142	-0.012	0.145
CN	0.032	0.126	0.040	0.099	0.019	0.135	0.021	0.139
CHO	0.052	0.122	0.064	0.098	0.039	0.131	0.043	0.134
Cl	0.122	0.110	0.129	0.086	0.100	0.116	0.098	0.119
F	0.140	0.108	0.145	0.084	0.125	0.113	0.123	0.115
H	**0.158**	**0.108**	**0.163**	**0.082**	**0.144**	**0.115**	**0.144**	**0.118**
Me	0.198	0.100	0.204	0.075	0.178	0.104	0.177	0.107
OMe	0.224	0.090	0.232	0.070	0.209	0.089	0.206	0.091
OH	0.213	0.094	0.220	0.074	0.202	0.094	0.198	0.099
NH_2	0.260	0.088	0.270	0.065	0.273	0.078	0.272	0.079
range	0.250	0.043	0.249	0.039	0.288	0.064	0.284	0.067
average	0.141	0.108	0.149	0.084	0.127	0.112	0.127	0.115
SD	0.086	0.015	0.085	0.013	0.092	0.021	0.090	0.021

Table S4. cSAR(X) and cSAR(C6H) values for C2 substitution of purine.

C2-X	9H		7H		3H		1H	
	cSAR X	cSAR (C6H)	cSAR X	cSAR (C6H)	cSAR X	cSAR (C6H)	cSAR X	cSAR (C6H)
NO_2	-0.011	0.143	-0.011	0.125	0.034	0.133	0.027	0.132
CN	0.018	0.138	0.017	0.121	0.045	0.128	0.035	0.126
CHO	0.042	0.129	0.044	0.117	0.074	0.121	0.065	0.128
Cl	0.082	0.131	0.077	0.114	0.130	0.120	0.119	0.112
F	0.112	0.130	0.108	0.113	0.145	0.120	0.135	0.110
H	**0.144**	**0.108**	**0.142**	**0.082**	**0.170**	**0.115**	**0.161**	**0.118**
Me	0.170	0.116	0.166	0.099	0.211	0.106	0.201	0.100
OMe	0.188	0.116	0.186	0.102	0.236	0.106	0.225	0.099
OH	0.184	0.119	0.181	0.106	0.224	0.110	0.212	0.101
NH_2	0.251	0.110	0.243	0.095	0.278	0.103	0.252	0.094
range	0.263	0.035	0.254	0.043	0.244	0.030	0.226	0.038
average	0.118	0.124	0.115	0.108	0.155	0.116	0.143	0.112
SD	0.084	0.012	0.082	0.013	0.084	0.010	0.081	0.013

Table S5. cSAR(X) and cSAR(NH_2) values for NX substitution of adenine.

N-X	9H		7H		3H		1H	
	cSAR X	cSAR (NH_2)	cSAR X	cSAR (NH_2)	cSAR X	cSAR (NH_2)	cSAR X	cSAR (NH_2)
NO_2	-0.058	0.267	-0.070	0.213	0.007	0.298	-0.003	0.272
CN	-0.088	0.270	-0.107	0.241	-0.051	0.307	-0.079	0.315
CHO	-0.037	0.262	-0.030	0.214	0.011	0.301	0.006	0.283
Cl	0.013	0.254	0.002	0.205	0.035	0.276	0.032	0.267
F	0.011	0.259	-0.030	0.225	0.027	0.275	0.016	0.278
H	**0.082**	**0.241**	**0.063**	**0.184**	**0.110**	**0.270**	**0.085**	**0.244**
Me	0.106	0.235	0.096	0.179	0.136	0.261	0.121	0.235
OMe	0.068	0.243	0.061	0.196	0.095	0.263	0.097	0.247
OH	0.068	0.254	0.060	0.191	0.093	0.265	0.092	0.243
NH_2	0.099	0.243	0.091	0.167	0.181	0.244	0.129	0.252
range	0.194	0.035	0.203	0.074	0.231	0.063	0.208	0.080
average	0.026	0.253	0.014	0.202	0.064	0.276	0.050	0.263
SD	0.069	0.012	0.071	0.023	0.070	0.020	0.066	0.024

Table S6. cSAR(X) and cSAR(C6H) values for NX substitution of purine.

N-X	9H		7H		3H		1H	
	cSAR X	cSAR (C6H)	cSAR X	cSAR (C6H)	cSAR X	cSAR (C6H)	cSAR X	cSAR (C6H)
NO_2	-0.044	0.123	-0.056	0.104	0.058	0.125	0.021	0.117
CN	-0.080	0.125	-0.088	0.111	-0.020	0.134	-0.048	0.143
CHO	-0.026	0.119	-0.033	0.109	0.050	0.128	0.018	0.128
Cl	0.020	0.115	0.012	0.095	0.050	0.120	0.051	0.127
F	0.015	0.118	-0.001	0.102	0.041	0.120	0.034	0.135
H	**0.086**	**0.108**	**0.077**	**0.082**	**0.129**	**0.115**	**0.108**	**0.118**
Me	0.113	0.104	0.111	0.077	0.162	0.109	0.148	0.108
OMe	0.077	0.109	0.103	0.092	0.120	0.111	0.116	0.116
OH	0.077	0.114	0.067	0.088	0.121	0.113	0.112	0.125
NH_2	0.108	0.105	0.105	0.085	0.154	0.109	0.137	0.118
range	0.193	0.021	0.199	0.033	0.183	0.025	0.196	0.035
average	0.035	0.114	0.030	0.094	0.087	0.118	0.070	0.123
SD	0.068	0.007	0.073	0.011	0.059	0.008	0.064	0.010

Table S7. CFI values for C8-X and C2-X substitution for adenine tautomers.

	9H		**7H**		**3H**		**1H**	
	C8-X	C2-X	C8-X	C2-X	C8-X	C2-X	C8-X	C2-X
NO_2	0.325	0.315	0.234	0.238	0.382	0.289	0.352	0.321
CN	0.279	0.275	0.197	0.216	0.216	0.260	0.307	0.276
CHO	0.266	0.243	0.180	0.180	0.180	0.218	0.292	0.271
Cl	0.148	0.207	0.078	0.148	0.148	0.168	0.184	0.159
F	0.120	0.170	0.055	0.113	0.113	0.152	0.143	0.134
H	**0.101**	**0.108**	**0.033**	**0.050**	**0.050**	**0.105**	**0.123**	**0.094**
Me	0.052	0.080	-0.016	0.022	0.022	0.059	0.077	0.049
OMe	0.011	0.069	-0.068	0.016	0.016	0.042	0.035	0.029
OH	0.024	0.077	-0.042	0.022	0.022	0.057	0.043	0.044
NH_2	-0.023	-0.004	-0.092	-0.056	-0.056	-0.034	-0.051	-0.008
range	0.348	0.319	0.326	0.294	0.438	0.323	0.403	0.328
average	0.130	0.154	0.056	0.095	0.109	0.131	0.151	0.137
SD	0.122	0.104	0.116	0.098	0.128	0.104	0.133	0.117

Table S8. CFI values for C8-X and C2-X substitution for purine tautomers.

	9H		**7H**		**3H**		**1H**	
	C8-X	C2-X	C8-X	C2-X	C8-X	C2-X	C8-X	C2-X
NO_2	0.122	0.154	0.083	0.136	0.156	0.099	0.157	0.105
CN	0.094	0.120	0.059	0.104	0.116	0.082	0.118	0.091
CHO	0.071	0.087	0.034	0.073	0.091	0.047	0.091	0.063
Cl	-0.012	0.049	-0.043	0.038	0.016	-0.010	0.021	-0.007
F	-0.032	0.018	-0.061	0.006	-0.012	-0.025	-0.008	-0.026
H	**-0.050**	**-0.036**	**-0.081**	**-0.059**	**-0.029**	**-0.055**	**-0.026**	**-0.043**
Me	-0.098	-0.054	-0.129	-0.067	-0.073	-0.105	-0.070	-0.101
OMe	-0.134	-0.072	-0.162	-0.084	-0.120	-0.129	-0.114	-0.126
OH	-0.119	-0.065	-0.146	-0.075	-0.108	-0.114	-0.099	-0.110
NH_2	-0.172	-0.141	-0.205	-0.149	-0.195	-0.175	-0.193	-0.158
range	0.293	0.295	0.288	0.285	0.352	0.274	0.351	0.264
average	-0.033	0.006	-0.065	-0.008	-0.016	-0.039	-0.012	-0.031
SD	0.101	0.095	0.099	0.093	0.113	0.094	0.111	0.094

Table S9. HOMA for imidazole (5) and pyrimidine (6) rings for C8-X of adenine.

	9H		7H		3H		1H	
C8-X	6	5	6	5	6	5	6	5
NO_2	0.890	0.820	0.894	0.789	0.843	0.871	0.731	0.790
CN	0.906	0.809	0.909	0.782	0.846	0.837	0.732	0.757
CHO	0.887	0.819	0.889	0.796	0.829	0.818	0.715	0.739
Cl	0.933	0.782	0.933	0.759	0.856	0.856	0.735	0.757
F	0.939	0.759	0.936	0.736	0.855	0.861	0.728	0.751
H	**0.929**	**0.802**	**0.927**	**0.776**	**0.850**	**0.840**	**0.720**	**0.736**
Me	0.935	0.790	0.933	0.770	0.848	0.818	0.714	0.711
OMe	0.943	0.770	0.938	0.752	0.847	0.831	0.721	0.716
OH	0.943	0.772	0.937	0.753	0.849	0.842	0.717	0.715
NH_2	0.943	0.772	0.942	0.734	0.842	0.809	0.699	0.678
range	0.057	0.061	0.053	0.062	0.027	0.062	0.036	0.112
average	0.925	0.789	0.924	0.765	0.846	0.838	0.721	0.735
SD	0.022	0.022	0.019	0.021	0.008	0.020	0.011	0.031

Table S10. HOMA for imidazole (5) and pyrimidine (6) rings for C2-X of adenine.

	9H		7H		3H		1H	
C2-X	6	5	6	5	6	5	6	5
NO_2	0.923	0.816	0.936	0.788	0.816	0.813	0.738	0.737
CN	0.920	0.814	0.918	0.780	0.833	0.829	0.717	0.744
CHO	0.914	0.814	0.917	0.776	0.830	0.813	0.747	0.739
Cl	0.935	0.808	0.932	0.789	0.836	0.835	0.708	0.743
F	0.934	0.805	0.930	0.790	0.826	0.830	0.687	0.724
H	**0.929**	**0.802**	**0.927**	**0.776**	**0.850**	**0.840**	**0.720**	**0.736**
Me	0.929	0.803	0.928	0.781	0.860	0.842	0.723	0.744
OMe	0.931	0.801	0.933	0.792	0.855	0.833	0.717	0.729
OH	0.933	0.796	0.934	0.788	0.855	0.838	0.712	0.719
NH_2	0.924	0.789	0.924	0.776	0.867	0.846	0.702	0.715
range	0.021	0.027	0.019	0.017	0.051	0.034	0.059	0.029
average	0.927	0.805	0.928	0.783	0.843	0.832	0.717	0.733
SD	0.007	0.008	0.007	0.007	0.017	0.011	0.017	0.011

Table S11. HOMA for imidazole (5) and pyrimidine (6) rings for N-X of adenine.

	9H		7H		3H		1H	
N-X	6	5	6	5	6	5	6	5
NO_2	0.935	0.677	0.911	0.612	0.772	0.797	0.632	0.802
CN	0.936	0.647	0.947	0.621	0.746	0.831	0.552	0.764
CHO	0.941	0.692	0.924	0.606	0.789	0.838	0.592	0.787
Cl	0.930	0.781	0.923	0.774	0.824	0.812	0.727	0.791
F	0.922	0.812	0.926	0.795	0.830	0.801	0.746	0.760
H	**0.929**	**0.802**	**0.927**	**0.776**	**0.850**	**0.840**	**0.720**	**0.736**
Me	0.930	0.806	0.914	0.770	0.856	0.843	0.736	0.769
OMe	0.927	0.801	0.927	0.797	0.847	0.828	0.732	0.751
OH	0.927	0.849	0.927	0.797	0.893	0.858	0.729	0.754
NH_2	0.933	0.798	0.922	0.763	0.857	0.842	0.723	0.783
range	0.019	0.201	0.037	0.191	0.147	0.062	0.194	0.066
average	0.931	0.766	0.925	0.731	0.826	0.829	0.689	0.770
SD	0.005	0.068	0.010	0.082	0.045	0.020	0.070	0.021

Table S12. HOMA for imidazole (5) and pyrimidine (6) rings for C8-X of purine.

	9H		7H		3H		1H	
C8-X	6	5	6	5	6	5	6	5
NO_2	0.904	0.769	0.897	0.761	0.782	0.730	0.626	0.600
CN	0.916	0.765	0.908	0.758	0.781	0.694	0.629	0.572
CHO	0.898	0.773	0.890	0.769	0.763	0.675	0.598	0.543
Cl	0.927	0.741	0.918	0.737	0.766	0.700	0.616	0.571
F	0.927	0.721	0.917	0.719	0.753	0.702	0.597	0.559
H	**0.926**	**0.757**	**0.915**	**0.752**	**0.761**	**0.680**	**0.602**	**0.548**
Me	0.928	0.747	0.918	0.745	0.750	0.652	0.591	0.522
OMe	0.921	0.731	0.911	0.729	0.730	0.664	0.576	0.521
OH	0.923	0.736	0.912	0.732	0.734	0.681	0.585	0.524
NH_2	0.922	0.733	0.910	0.726	0.716	0.640	0.569	0.494
range	0.029	0.052	0.028	0.049	0.066	0.089	0.060	0.107
average	0.919	0.747	0.909	0.743	0.754	0.682	0.599	0.545
SD	0.010	0.018	0.009	0.017	0.022	0.026	0.020	0.031

Table S13. HOMA for imidazole (5) and pyrimidine (6) rings for C2-X of purine.

	9H		7H		3H		1H	
C2-X	6	5	6	5	6	5	6	5
NO_2	0.921	0.762	0.909	0.747	0.704	0.621	0.600	0.530
CN	0.913	0.763	0.904	0.751	0.725	0.651	0.593	0.543
CHO	0.903	0.753	0.906	0.750	0.715	0.629	0.622	0.547
Cl	0.934	0.759	0.922	0.763	0.742	0.666	0.581	0.541
F	0.935	0.754	0.920	0.764	0.734	0.655	0.549	0.510
H	**0.926**	**0.757**	**0.915**	**0.753**	**0.761**	**0.680**	**0.602**	**0.548**
Me	0.927	0.763	0.917	0.762	0.776	0.694	0.606	0.562
OMe	0.936	0.760	0.927	0.776	0.773	0.678	0.588	0.536
OH	0.929	0.747	0.924	0.768	0.778	0.680	0.574	0.515
NH_2	0.919	0.745	0.909	0.757	0.801	0.708	0.575	0.527
range	0.033	0.018	0.023	0.029	0.098	0.087	0.074	0.051
average	0.924	0.756	0.915	0.759	0.751	0.666	0.589	0.536
SD	0.010	0.006	0.008	0.009	0.032	0.027	0.021	0.016

Table S14. HOMA for imidazole (5) and pyrimidine (6) ring for N-X of purine.

	9H		7H		3H		1H	
N-X	6	5	6	5	6	5	6	5
NO_2	0.937	0.647	0.931	0.656	0.646	0.558	0.569	0.536
CN	0.945	0.614	0.946	0.619	0.635	0.635	0.453	0.516
CHO	0.946	0.659	0.940	0.640	0.693	0.653	0.504	0.501
Cl	0.931	0.739	0.922	0.758	0.696	0.608	0.627	0.586
F	0.922	0.765	0.905	0.782	0.697	0.589	0.624	0.548
H	**0.926**	**0.757**	**0.915**	**0.753**	**0.761**	**0.680**	**0.602**	**0.548**
Me	0.924	0.761	0.911	0.756	0.778	0.702	0.635	0.591
OMe	0.924	0.755	0.909	0.782	0.755	0.668	0.619	0.557
OH	0.926	0.802	0.914	0.763	0.837	0.742	0.641	0.576
NH_2	0.927	0.728	0.923	0.750	0.703	0.636	0.619	0.579
range	0.024	0.187	0.040	0.163	0.201	0.184	0.188	0.090
average	0.931	0.723	0.922	0.726	0.720	0.647	0.589	0.554
SD	0.009	0.061	0.014	0.062	0.062	0.055	0.063	0.030

Table S15. pEDA values for C8-X substitution for adenine tautomers.

	9H		7H		3H		1H	
C8-X	6	5	6	5	6	5	6	5
NO_2	6.338	5.838	6.316	5.822	6.697	5.576	6.696	5.490
CN	6.360	5.886	6.327	5.860	6.708	5.603	6.702	5.506
CHO	6.340	5.811	6.316	5.791	6.701	5.537	6.701	5.449
Cl	6.360	5.886	6.327	5.860	6.708	5.603	6.702	5.506
F	6.422	5.965	6.382	5.936	6.753	5.657	6.731	5.539
H	**6.406**	**5.882**	**6.365**	**5.849**	**6.742**	**5.578**	**6.725**	**5.459**
Me	6.412	5.885	6.374	5.855	6.753	5.579	6.733	5.457
OMe	6.431	5.991	6.402	5.966	6.779	5.676	6.752	5.554
OH	6.429	5.988	6.399	5.963	6.772	5.673	6.747	5.553
NH_2	6.431	5.984	6.397	5.947	6.800	5.692	6.764	5.555
range	0.093	0.186	0.086	0.200	0.102	0.155	0.068	0.107
average	6.396	5.902	6.363	5.874	6.741	5.617	6.725	5.507
SD	0.038	0.070	0.035	0.069	0.036	0.053	0.024	0.042

Table S16. sEDA values for C8-X substitution for adenine tautomers.

	9H		7H		3H		1H	
C8-X	6	5	6	5	6	5	6	5
NO_2	19.414	16.091	19.421	16.088	19.098	16.373	19.079	16.428
CN	19.417	16.291	19.426	16.285	19.101	16.595	19.086	16.654
CHO	19.430	16.363	19.439	16.359	19.113	16.664	19.095	16.723
Cl	19.401	16.224	19.413	16.220	19.083	16.525	19.076	16.587
F	19.400	15.848	19.412	15.844	19.084	16.158	19.079	16.222
H	**19.429**	**16.462**	**19.440**	**16.458**	**19.111**	**16.780**	**19.104**	**16.845**
Me	19.420	16.278	19.431	16.274	19.096	16.603	19.092	16.669
OMe	19.404	15.922	19.414	15.918	19.077	16.235	19.079	16.302
OH	19.402	15.938	19.412	15.933	19.079	16.254	19.079	16.320
NH_2	19.408	16.062	19.420	16.073	19.072	16.371	19.079	16.446
range	0.066	1.219	0.070	1.221	0.077	1.238	0.069	1.241
average	19.418	16.232	19.428	16.229	19.097	16.541	19.090	16.605
SD	0.019	0.340	0.021	0.339	0.022	0.345	0.020	0.345

Table S17. The slopes of the linear dependences of cSAR(NH_2) on substituent constants σ_p, σ_m for C8-X, C2-X and N-X substituted derivatives of adenine.

	C8-X		**C2-X**		**N-X**	
	a	R^2	*a*	R^2	*a*	R^2
	cSAR(NH_2) vs σ_p					
9H	**0.060**	**0.948**	0.040	0.856	0.021	0.619
7H	**0.052**	**0.931**	0.039	0.850	0.039	0.644
3H	**0.065**	**0.980**	0.030	0.794	0.042	0.906
1H	**0.081**	**0.963**	0.058	0.867	0.039	0.549
average		0.955		0.842		
	cSAR(NH_2) vs σ_m					
9H	0.087	0.744	**0.070**	**0.957**	0.039	0.826
7H	0.077	0.757	**0.069**	**0.973**	0.070	0.756
3H	0.095	0.763	**0.053**	**0.935**	0.064	0.779
1H	0.118	0.746	**0.092**	**0.815***	0.066	0.584
average		0.752		0.920		

* without CHO *a* = 0.087, R^2 = 0.923

Table S18. Dependence HOMA vs cSAR(X) for all substituents and with separation on EA and ED substituents for all types substitution for 5- and 6-membered rings of adenine (a) and purine (b) tautomers.

a)		**HOMA vs cSAR(X)**											
AD	X	**C8-X**				**C2-X**				**N-X**			
		5		**6**		**5**		**6**		**5**		**6**	
		a	R^2	*a*	R^2	*a*	R^2	*a*	R^2	*a*	R^2	*a*	R^2
9H	all	-0.186	0.648	0.217	0.855	-0.097	0.946	0.039	0.226	0.870	0.773	-0.041	0.278
	EA	*-0.369*	*0.913*	*0.330*	*0.873*	*-0.091*	*0.944*	*0.122*	*0.452*	*1.547*	*0.931*	*-0.113*	*0.484*
	ED	*-0.363*	*0.791*	*0.168*	*0.830*	*-0.141*	*0.850*	*-0.059*	*0.403*	*-0.619*	*0.249**	*0.118*	*0.686*
7H	all	-0.180	0.589	0.189	0.791	-0.005	0.003	0.016	0.039	0.876	0.568	-0.051	0.139
	EA	*-0.370*	*0.811*	*0.322*	*0.793*	*-0.068*	*0.212*	*0.036*	*0.033*	*1.460*	*0.428*	*-0.158*	*0.255*
	ED	*-0.405*	*0.905*	*0.148*	*0.982*	*-0.037*	*0.031*	*-0.051*	*0.163*	*-0.752*	*0.697*	*-0.288*	*0.819*
3H	all	-0.104	0.253	0.022	0.079	0.111	0.705	0.178	0.837	0.169	0.270	0.638	0.778
	EA	*0.054*	*0.027*	*0.113*	*0.443*	*-0.070*	*0.450*	*0.067*	*0.217*	*-0.273*	*0.249*	*0.956*	*0.818*
	ED	*-0.200*	*0.449*	*-0.065*	*0.864*	*0.051*	*0.141*	*0.157*	*0.761*	*-0.040*	*0.004*	*-0.348*	*0.128*
1H	all	-0.297	0.804	-0.080	0.483	-0.073	0.365	-0.099	0.273	-0.090	0.083	0.844	0.636
	EA	*-0.156*	*0.268*	*0.014*	*0.013*	*0.129*	*0.272*	*-0.327*	*0.664*	*0.173*	*0.173*	*1.577*	*0.626*
	ED	*-0.470*	*0.902*	*-0.171*	*0.664*	*-0.257*	*0.453*	*-0.200*	*0.569*	*0.840*	*0.928*	*0.081*	*0.057*

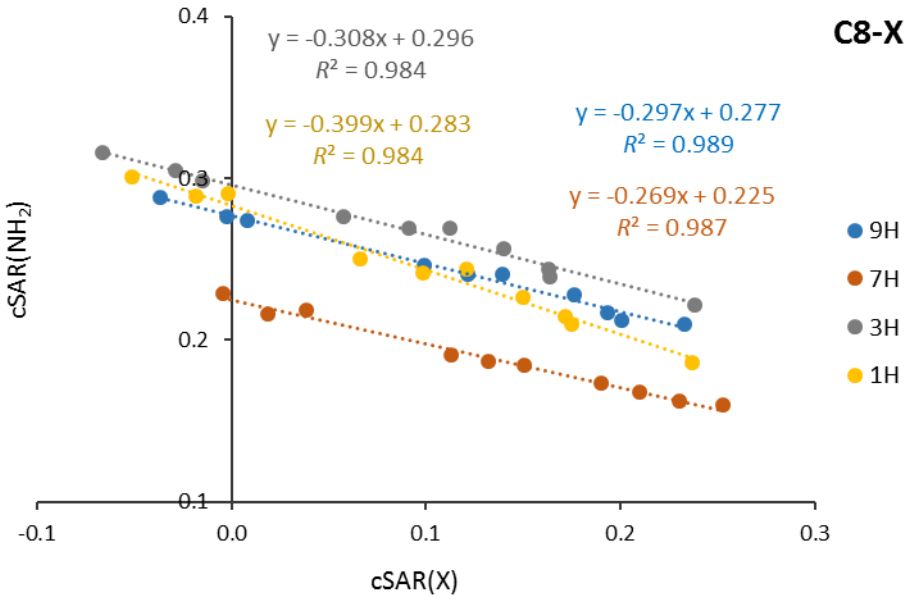
*****OH stands out

b)		**HOMA vs cSAR(X)**											
PU	X	**C8-X**				**C2-X**				**N-X**			
		5		**6**		**5**		**6**		**5**		**6**	
		a	R^2	*a*	R^2	*a*	R^2	*a*	R^2	*a*	R^2	*a*	R^2
9H	all	-0.159	0.591	0.080	0.451	-0.041	0.304	0.051	0.169	0.755	0.670	-0.106	0.673
	EA	*-0.357*	*0.844*	*0.181*	*0.624*	*-0.057*	*0.436*	*0.171*	*0.381*	*1.474*	*0.916*	*-0.188*	*0.621*
	ED	*-0.268*	*0.814*	*-0.056*	*0.516*	*-0.134*	*0.450*	*-0.075*	*0.233*	*-0.853*	*0.297*	*0.010*	*0.014*
7H	all	-0.146	0.570	0.064	0.345	0.072	0.412	0.049	0.254	0.688	0.651	-0.138	0.549
	EA	*-0.319*	*0.763*	*0.168*	*0.567*	*0.153*	*0.866*	*0.137*	*0.625*	*1.602*	*0.789*	*-0.309*	*0.624*
	ED	*-0.275*	*0.886*	*-0.059*	*0.527*	*0.024*	*0.009*	*-0.069*	*0.132*	*0.061*	*0.008*	*-0.017*	*0.003*
3H	all	-0.224	0.621	-0.223	0.907	0.298	0.836	0.364	0.938	0.536	0.333	0.786	0.551
	EA	*-0.095*	*0.077*	*-0.191*	*0.780*	*0.270*	*0.524*	*0.251*	*0.684*	*-0.508*	*0.189*	*0.556*	*0.347*
	ED	*-0.258*	*0.489*	*-0.352*	*0.937*	*0.217*	*0.422*	*0.351*	*0.876*	*-0.576*	*0.076*	*-1.027*	*0.163*
1H	all	-0.314	0.818	-0.201	0.829	-0.026	0.018	-0.088	0.118	0.359	0.577	0.794	0.647
	EA	*-0.198*	*0.275*	*-0.177*	*0.431*	*-0.147*	*0.238*	*-0.396*	*0.513*	*0.557*	*0.411*	*1.820*	*0.798*
	ED	*-0.397*	*0.931*	*-0.258*	*0.894*	*-0.280*	*0.268*	*-0.315*	*0.495*	*0.829*	*0.683*	*0.319*	*0.130*

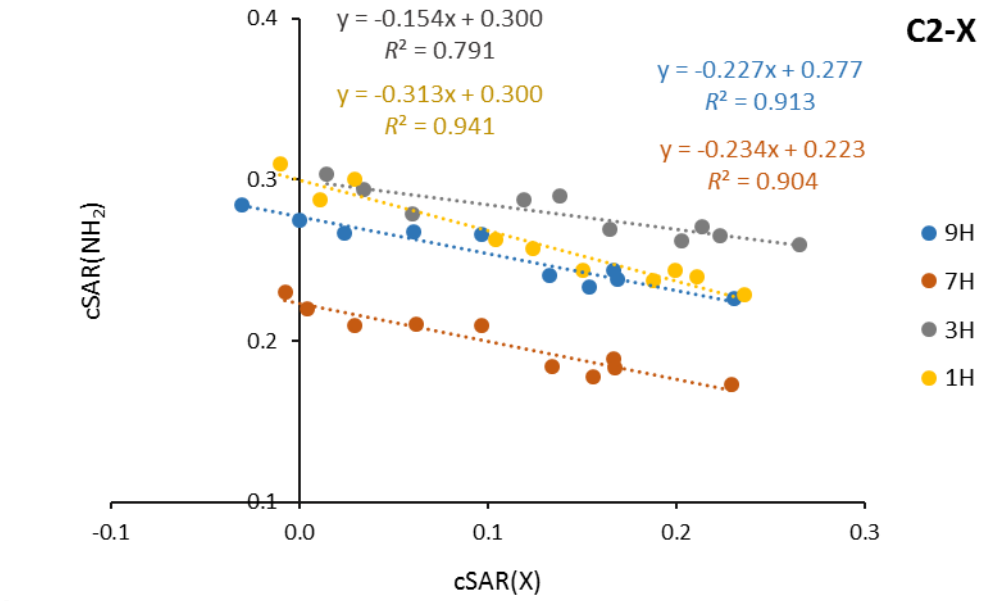
Table S19. The slopes of the obtained linear dependences of $HOMA(5)_{AD}$ vs $HOMA(5)_{PU}$ for C8-X, C2-X and N-X substitution.

	C8-X		C2-X		N-X	
	a	R^2	*a*	R^2	*a*	R^2
	$HOMA(5)_{AD}$ vs $HOMA(5)_{PU}$					
9H	1.211	0.989	0.890	0.445	1.105	0.982
7H	1.268	0.971	0.459/0.675*	0.410/0.748*	1.305	0.962
3H	0.716	0.869	0.400	0.942	0.335	0.846
1H	0.989	0.982	0.532	0.617	-0.051	0.004
	$HOMA(6)_{AD}$ vs $HOMA(6)_{PU}$					
9H	1.924	0.797	0.634	0.935	0.548	0.791
7H	1.813	0.756	0.596/0.755*	0.523/0.939*	0.373*	0.378*
3H	-0.013	0.004	0.513	0.945	0.646	0.807
1H	0.445	0.672	0.760	0.861	0.943	0.943

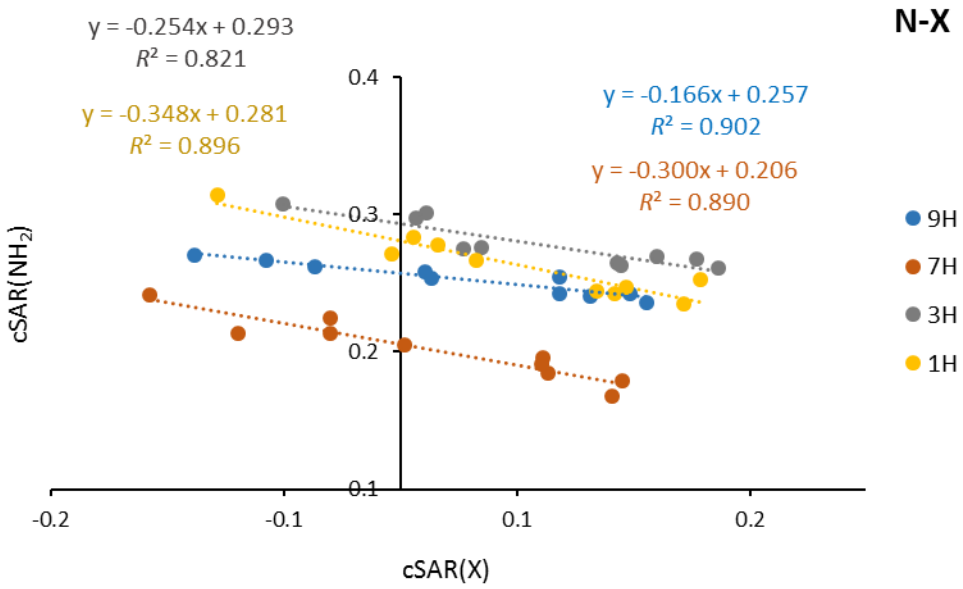
* without NO_2.



a)

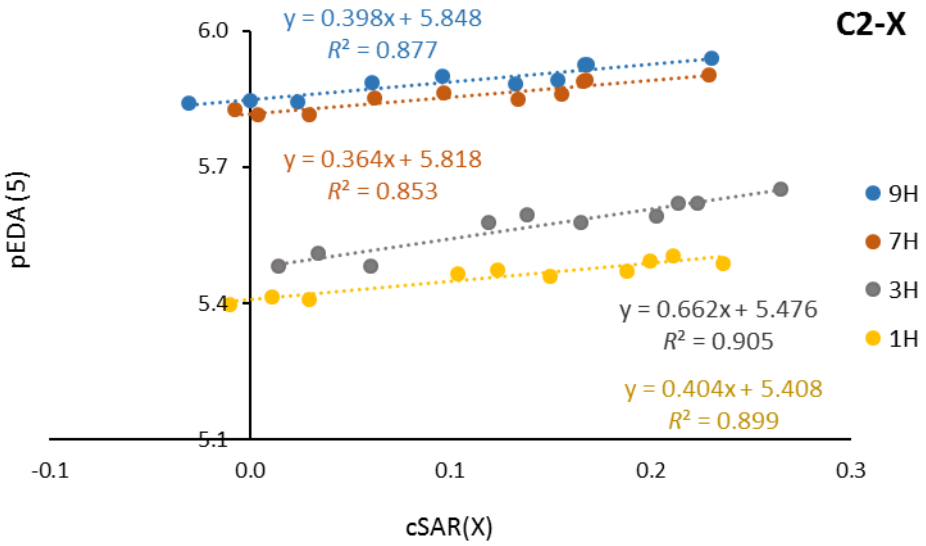


b)

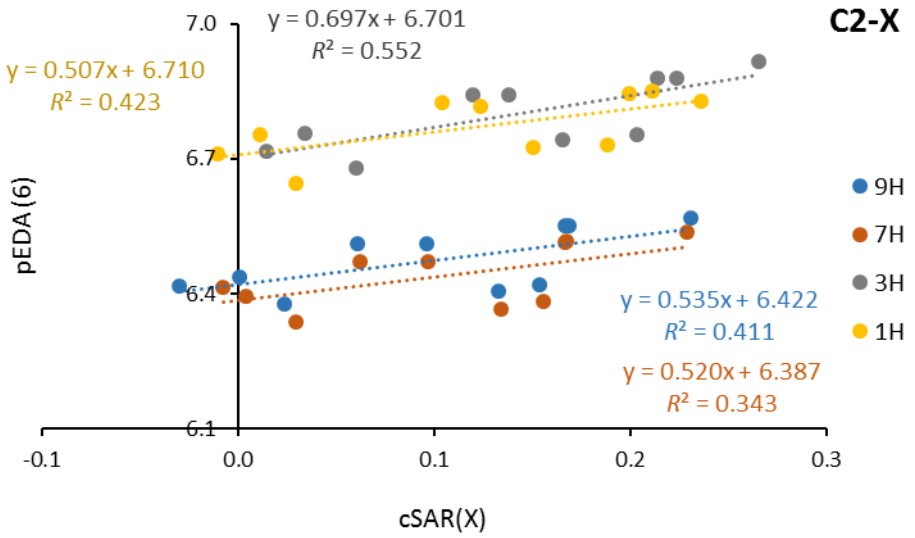


c)

Figure S1. Dependences of cSAR(NH_2) vs cSAR(X) for C8-X (a) C2-X (b) and N-X (c) substituted derivatives of adenine.

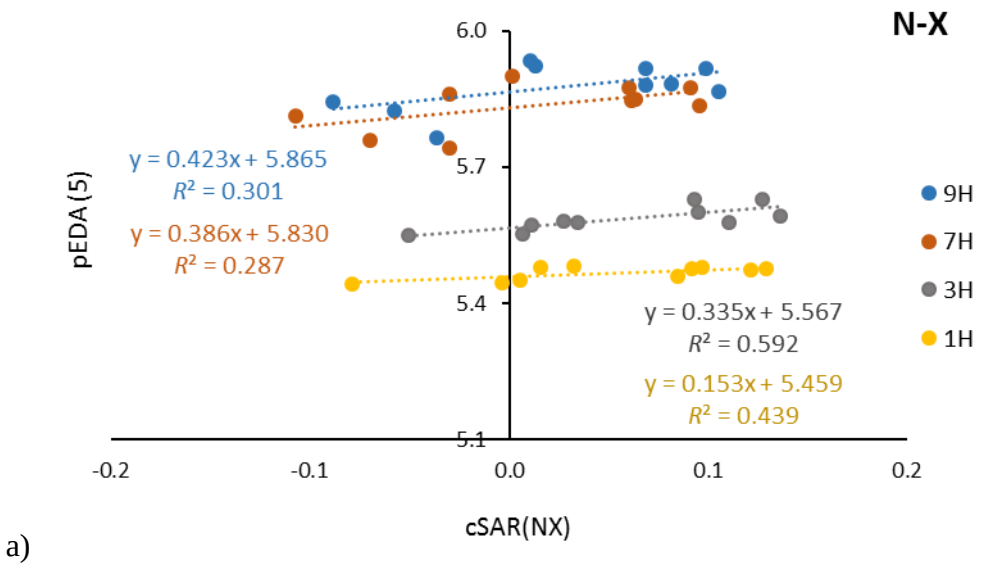


a)

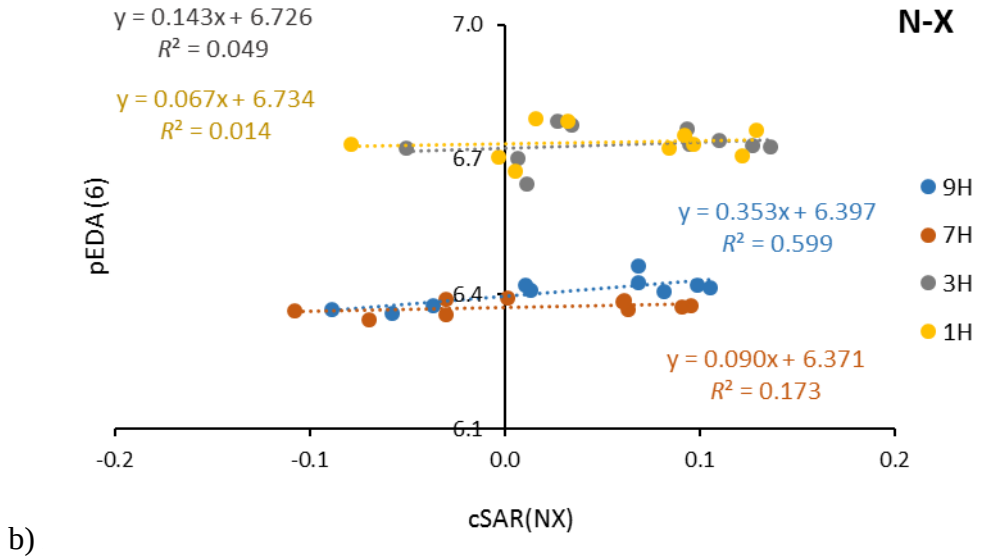


b)

Figure S2. Dependence of pEDA vs cSAR(X) for 5- (a) and 6-membered (b) rings of adenine tautomers for C2-X derivatives.



a)



b)

Figure S3. Dependence of pEDA vs cSAR(X) for 5- (a) and 6-membered (b) rings of adenine tautomers for N-X derivatives.

Table S20. Cartesian coordinates of equilibrium geometries of C8-X and C2-X substituted adenine (AD) 9H, 7H, 3H and 1H tautomers.

C8-NO_2-AD_9H E_{tot} = -671.528174 a.u.
Gibbs free energy E_G= -671.453526 a.u.

7	N	3.051385	-0.01772	0.000257
6	C	2.746118	-1.33337	0.00002
7	N	1.53543	-1.92744	-0.00014
6	C	0.550393	-1.01753	-0.00024
6	C	0.701554	0.39419	-0.0001
6	C	2.039737	0.87859	0.000164
7	N	-0.52075	1.035663	-0.00042
6	C	-1.38885	0.039864	-8.4E-05
7	N	-0.81619	-1.21783	-2E-06
7	N	2.329792	2.200113	-0.00034
1	H	3.297922	2.492331	0.00136
1	H	1.588182	2.886888	0.001235
1	H	3.606125	-2.01057	0.000368
1	H	-1.32741	-2.09385	0.000222
7	N	-2.83393	0.172764	0.000083
8	O	-3.46926	-0.89808	0.000245
8	O	-3.31558	1.302564	0.000032

C2-NO_2-AD_9H E_{tot} = -671.527920 a.u.
Gibbs free energy E_G= -671.452683 a.u.

7	N	3.046942	-0.01773	0.000271
6	C	2.721601	-1.30837	0.000153
7	N	1.536128	-1.91409	-5.5E-06
6	C	0.550419	-1.00068	-8.5E-05
6	C	0.699478	0.403469	-2.7E-05
6	C	2.036062	0.883051	0.000136
7	N	-0.53464	1.038806	-0.00028
6	C	-1.41325	0.046862	6.23E-05
7	N	-0.8178	-1.20576	-7.5E-05
7	N	2.341987	2.202056	-0.00032
1	H	3.312858	2.484092	0.001186
1	H	1.606485	2.894618	0.001048
1	H	-1.27995	-2.10767	-6.1E-05
7	N	3.919078	-2.26255	0.000517
8	O	3.670941	-3.46573	-3.5E-05
8	O	5.037433	-1.75457	0.001265
1	H	-2.49484	0.164399	0.000112

C8-CN-AD_9H E_{tot} = -559.285658 a.u.
Gibbs free energy E_G= -559.213562 a.u.

7	N	-2.69641	-0.02423	-0.00023
6	C	-2.38169	-1.33751	-1.6E-05
7	N	-1.16594	-1.91953	0.000096
6	C	-0.18879	-0.99872	0.000181
6	C	-0.34955	0.406884	0.00007
6	C	-1.69086	0.879203	-0.00015
7	N	0.868412	1.05841	0.000246
6	C	1.766702	0.072743	0.000038
7	N	1.178073	-1.19282	-6.1E-05
7	N	-1.99264	2.199695	0.000651
1	H	-2.96295	2.483723	-0.00187
1	H	-1.2568	2.892178	-0.00188
1	H	-3.23594	-2.022	-0.00031
1	H	1.659664	-2.08493	-0.00016
6	C	3.179585	0.236019	-7.3E-05
7	N	4.349025	0.332665	-0.00015

C2-CN-AD_9H E_{tot} = -559.285679 a.u.
Gibbs free energy E_G= -559.214063 a.u.

7	N	2.707322	-0.0276	0.000394
6	C	2.387419	-1.34143	0.000631
7	N	1.169701	-1.92426	0.0003
6	C	0.197908	-0.99881	0.000106
6	C	0.360527	0.403264	1.79E-05
6	C	1.699396	0.873706	5.63E-05
7	N	-0.86708	1.052321	5.02E-05
6	C	-1.75591	0.069837	-0.00012
7	N	-1.17327	-1.18903	-6.1E-05
7	N	2.007235	2.193509	-0.00063
1	H	2.977914	2.475431	0.001759
1	H	1.272208	2.886522	0.001618
1	H	-1.64609	-2.08525	-0.00011
1	H	-2.83649	0.198267	-0.00021
6	C	3.518081	-2.25069	0.000342
7	N	4.431238	-2.98403	0.000146

C8-CHO-AD_9H E_{tot} = -580.377851 a.u.
Gibbs free energy E_G= -580.295182 a.u.

7	N	-2.75516	-0.21694	-0.00021
6	C	-2.31075	-1.49311	-2.5E-05
7	N	-1.0445	-1.954	0.000129
6	C	-0.15797	-0.94504	0.000199
6	C	-0.45971	0.443685	0.000056
6	C	-1.84254	0.779489	-0.00015
7	N	0.686237	1.206	0.000255
6	C	1.681948	0.31035	0.000055
7	N	1.216827	-0.99926	-5.2E-05
7	N	-2.27373	2.063953	0.000543
1	H	-3.26751	2.250206	-0.00175
1	H	-1.6099	2.825688	-0.00176
1	H	-3.09419	-2.25783	-0.00019
1	H	1.805223	-1.82567	-0.00019
6	C	3.108805	0.633609	0.000004
8	O	3.988866	-0.22394	-0.00021
1	H	3.329063	1.726862	0.000115

C2-CHO-AD_9H E_{tot} = -580.368390 a.u.
Gibbs free energy E_G= -580.286234 a.u.

7	N	2.74373	-0.24696	-7.1E-06
6	C	2.293642	-1.52667	-0.00019
7	N	1.017433	-1.96458	-0.00016
6	C	0.154087	-0.94277	-0.00026
6	C	0.463469	0.436726	-0.00022
6	C	1.844206	0.760338	-7.1E-05
7	N	-0.68766	1.212792	-0.00072
6	C	-1.67625	0.329145	0.000106
7	N	-1.23217	-0.98339	0.000247
7	N	2.290952	2.04245	-0.00097
1	H	3.285719	2.219932	0.001386
1	H	1.633981	2.809665	0.001312
1	H	-1.79747	-1.8243	0.000641
6	C	3.396173	-2.55271	0.000419
8	O	3.228385	-3.75862	0.000795
1	H	4.41503	-2.08959	0.001152
1	H	-2.73684	0.573254	0.000341

C8-CHO-AD_9H E_{tot} = -580.369005 a.u.
Gibbs free energy E_G= -580.286774 a.u.

7	N	2.735495	-0.13251	0.000183
6	C	2.275491	-1.40377	0.000328
7	N	1.004037	-1.84911	8.79E-05
6	C	0.131231	-0.82676	8.1E-05
6	C	0.447833	0.556022	8.32E-05
6	C	1.835909	0.875336	2.46E-05
7	N	-0.68368	1.335977	0.000383
6	C	-1.69652	0.46487	4.76E-05
7	N	-1.24359	-0.86179	-9.9E-05
7	N	2.277168	2.155233	-0.00032
1	H	3.272029	2.335197	0.001323
1	H	1.617037	2.920739	0.001356
1	H	3.04972	-2.17784	-9.9E-06
1	H	-1.81356	-1.70036	-0.00027
6	C	-3.13722	0.762826	-1.6E-05
8	O	-3.62355	1.882712	0.000109
1	H	-3.7857	-0.15537	-0.00036

C2-CHO-AD_9H E_{tot} = --580.368769 a.u.
Gibbs free energy E_G= -580.287453 a.u.

7	N	0.980462	1.447537	0.000038
6	C	1.522341	0.211110	0.000264
7	N	0.886732	-0.985811	0.000332
6	C	-0.444536	-0.834088	0.000223
6	C	-1.155632	0.385198	-0.000023
6	C	-0.362706	1.564859	-0.000204
7	N	-2.526697	0.169261	0.000375
6	C	-2.650039	-1.151032	-0.000294
7	N	-1.430739	-1.809300	0.000387
7	N	-0.911612	2.805253	-0.000896
1	H	-0.302224	3.611883	0.001312
1	H	-1.915229	2.919038	0.001486
1	H	-1.273384	-2.810126	0.000608
6	C	3.022830	0.093499	0.000435
1	H	-3.592911	-1.694519	-0.000423
1	H	3.366962	-0.971638	0.000463
8	O	3.800990	1.029952	0.000561

C8-Cl-AD_9H E_{tot} = -926.728065 a.u.
Gibbs free energy E_G= -926.663 a.u.

7	N	-2.80562	-0.03014	0.006289
6	C	-2.49557	-1.34259	0.004669
7	N	-1.2781	-1.92359	-0.00085
6	C	-0.30372	-1.00156	-0.00329
6	C	-0.46172	0.399317	-0.00323
6	C	-1.79585	0.872003	-0.00096
7	N	0.773768	1.052237	-0.00043
6	C	1.643569	0.067604	-0.0005
7	N	1.072919	-1.19592	-0.00264
7	N	-2.1027	2.197444	-0.03228
1	H	-3.06853	2.469556	0.093513
1	H	-1.37022	2.882132	0.095229
1	H	-3.34983	-2.02713	0.009894
1	H	1.563556	-2.08186	-0.00282
17	Cl	3.357786	0.240379	0.002737

C8-F-AD_9H E_{tot} = -566.298514 a.u.
Gibbs free energy E_G= -566.230975 a.u.

7	N	-2.40905	-0.1512	0.005658
6	C	-2.01939	-1.44093	0.004872
7	N	-0.76661	-1.9437	-0.00078
6	C	0.14607	-0.96298	-0.00303
6	C	-0.09785	0.425072	-0.00321
6	C	-1.45683	0.812719	-0.00153
7	N	1.099946	1.156507	-9.5E-05
6	C	2.009867	0.222565	0.00071
7	N	1.537605	-1.07353	-0.0018
7	N	-1.8484	2.116848	-0.03467
1	H	-2.82904	2.324738	0.098849
1	H	-1.1623	2.846449	0.101304
1	H	-2.82869	-2.17797	0.008451
1	H	2.084715	-1.92593	-0.00173
9	F	3.327782	0.42881	0.003966

C8-H-AD_9H E_{tot} = -467.096786 a.u.
Gibbs free energy E_G= -467.019892 a.u.

7	N	1.962029	0.527275	0.004592
6	C	1.304445	1.706449	0.002924
7	N	-0.02351	1.934087	-0.00124
6	C	-0.71338	0.780032	-0.00262
6	C	-0.17923	-0.52523	-0.00271
6	C	1.234633	-0.6137	-0.00179
7	N	-1.18892	-1.48459	0.002006
6	C	-2.30842	-0.7791	0.002786
7	N	-2.08635	0.591594	-0.00028
7	N	1.889474	-1.80705	-0.03371
1	H	2.892382	-1.80781	0.096014
1	H	1.367686	-2.66248	0.09916
1	H	1.940976	2.597346	0.008033
1	H	-3.31484	-1.19342	0.006012
1	H	-2.78351	1.326384	-0.00041

C2-Cl-AD_9H E_{tot} = -926.732773 a.u.
Gibbs free energy E_G= -926.667577 a.u.

7	N	-2.80734	-0.0337	0.019792
6	C	-2.47941	-1.33143	0.005714
7	N	-1.27922	-1.91941	-0.00546
6	C	-0.3015	-0.99388	-0.00096
6	C	-0.46067	0.406281	0.013339
6	C	-1.79933	0.871222	0.023965
7	N	0.771099	1.053895	0.013972
6	C	1.656351	0.071058	0.000401
7	N	1.067699	-1.1887	-0.0091
7	N	-2.11524	2.189889	0.038241
1	H	-3.08736	2.466006	0.045147
1	H	-1.38355	2.886223	0.041454
1	H	1.537289	-2.08622	-0.01997
17	Cl	-3.85189	-2.43694	0.001266
1	H	2.737532	0.194593	-0.00335

C2-F-AD_9H E_{tot} = -566.310389 a.u.
Gibbs free energy E_G= -566.242457 a.u.

7	N	-2.41619	-0.15724	0.017325
6	C	-1.99565	-1.42294	0.004033
7	N	-0.77128	-1.94381	-0.00625
6	C	0.148608	-0.95875	-0.00144
6	C	-0.10093	0.428	0.011992
6	C	-1.4664	0.808703	0.021178
7	N	1.087373	1.153675	0.014247
6	C	2.033778	0.230743	0.002212
7	N	1.526292	-1.06537	-0.00773
7	N	-1.8615	2.105746	0.029822
1	H	-2.84784	2.32412	0.054519
1	H	-1.17204	2.843565	0.05246
1	H	2.052527	-1.93085	-0.01763
1	H	3.104888	0.422643	-4.1E-05
9	F	-2.99448	-2.33469	0.000832

C2-H-AD_9H E_{tot} = -467.096786 a.u.
Gibbs free energy E_G=-467.019892 a.u.

7	N	1.962029	0.527275	0.004592
6	C	1.304445	1.706449	0.002924
7	N	-0.02351	1.934087	-0.00124
6	C	-0.71338	0.780032	-0.00262
6	C	-0.17923	-0.52523	-0.00271
6	C	1.234633	-0.6137	-0.00179
7	N	-1.18892	-1.48459	0.002006
6	C	-2.30842	-0.7791	0.002786
7	N	-2.08635	0.591594	-0.00028
7	N	1.889474	-1.80705	-0.03371
1	H	2.892382	-1.80781	0.096014
1	H	1.367686	-2.66248	0.09916
1	H	1.940976	2.597346	0.008033
1	H	-3.31484	-1.19342	0.006012
1	H	-2.78351	1.326384	-0.00041

C8-Me-AD_9H E_{tot} = -506.398603 a.u.
Gibbs free energy E_G=-506.29734 a.u.

7	N	-2.45329	-0.10302	0.006983
6	C	-2.09174	-1.40278	0.005275
7	N	-0.8526	-1.9345	-0.00118
6	C	0.087738	-0.97488	-0.00427
6	C	-0.12524	0.41862	-0.00477
6	C	-1.47692	0.835079	-0.00242
7	N	1.083376	1.111687	-0.0004
6	C	2.017527	0.169197	0.000985
7	N	1.466576	-1.11222	-0.00276
7	N	-1.83636	2.151097	-0.04285
1	H	-2.8072	2.379831	0.126621
1	H	-1.12948	2.854179	0.126144
1	H	-2.9187	-2.12039	0.012297
1	H	1.970078	-1.991	-0.00227
6	C	3.491565	0.401851	0.004501
1	H	3.966429	-0.04837	0.893153
1	H	3.968099	-0.03556	-0.88967
1	H	3.677777	1.483323	0.012035

C2-Me-AD_9H E_{tot} = -506.396710 a.u.
Gibbs free energy E_G=-506.29638 a.u.

7	N	-2.44549	-0.10853	0.013165
6	C	-2.09655	-1.4204	0.007372
7	N	-0.84502	-1.93126	-0.00276
6	C	0.091644	-0.96828	-0.0053
6	C	-0.12178	0.423799	-0.00246
6	C	-1.4782	0.831503	0.003786
7	N	1.083738	1.122091	0.000967
6	C	2.00809	0.175341	-0.002
7	N	1.470793	-1.10612	-0.00647
7	N	-1.84127	2.145418	-0.03002
1	H	-2.81398	2.373773	0.12772
1	H	-1.13562	2.852904	0.124273
1	H	1.976208	-1.98378	-0.00885
1	H	3.083417	0.343029	-0.00082
6	C	-3.23822	-2.40422	0.014047
1	H	-3.8731	-2.24183	0.900442
1	H	-3.87628	-2.24936	-0.87152
1	H	-2.85449	-3.43236	0.017231

C8-OMe-AD_9H E_{tot} = -581.577754 a.u.
Gibbs free energy E_G= -581.472704 a.u.

7	N	-2.78495	0.270621	0.00619
6	C	-2.68422	-1.07221	0.005121
7	N	-1.56777	-1.83232	-0.0004
6	C	-0.46345	-1.07378	-0.00334
6	C	-0.40224	0.334835	-0.00473
6	C	-1.64433	1.002837	-0.00334
7	N	0.924131	0.787615	-0.00019
6	C	1.632019	-0.32703	0.001051
7	N	0.867814	-1.4836	-0.00093
7	N	-1.74707	2.368079	-0.05368
1	H	-2.65402	2.765224	0.158397
1	H	-0.92554	2.914755	0.17007
1	H	-3.63313	-1.61807	0.012029
1	H	1.212162	-2.43554	-0.00062
8	O	2.965689	-0.4561	0.003888
6	C	3.694486	0.798326	0.000613
1	H	4.752494	0.510708	-0.00232
1	H	3.438958	1.379873	-0.89786
1	H	3.444885	1.381156	0.900001

C2-OMe-AD_9H E_{tot} = -581.582143 a.u.
Gibbs free energy E_G= -581.477071 a.u.

7	N	1.172431	0.743748	-0.01034
6	C	1.271205	-0.60296	-0.00689
7	N	0.290019	-1.52498	-0.0008
6	C	-0.92248	-0.94173	0.000879
6	C	-1.19661	0.438243	0.000564
6	C	-0.05916	1.287303	-0.00255
7	N	-2.56853	0.681959	-0.00362
6	C	-3.11518	-0.52146	-0.00403
7	N	-2.16853	-1.54371	-0.00078
7	N	-0.17266	2.644035	0.029323
1	H	0.661257	3.199244	-0.10836
1	H	-1.08139	3.064806	-0.10774
1	H	-2.34393	-2.54101	-0.00067
8	O	2.557264	-1.0306	-0.01291
1	H	-4.18246	-0.73333	-0.00679
6	C	2.766683	-2.4562	-0.01125
1	H	3.85732	-2.57989	-0.01602
1	H	2.326762	-2.91418	0.888457
1	H	2.318457	-2.9176	-0.90512

C8-OMe-AD_9H E_{tot} = -581.569543 a.u.
Gibbs free energy E_G= -581.464982 a.u.

7	N	-2.78414	0.28138	0.008074
6	C	-2.70655	-1.06384	0.004425
7	N	-1.60305	-1.84225	-0.00209
6	C	-0.48762	-1.09937	-0.00241
6	C	-0.39955	0.305334	-0.00058
6	C	-1.63256	0.995011	0.000801
7	N	0.929066	0.736475	0.007161
6	C	1.625919	-0.38243	0.007135
7	N	0.837944	-1.53332	0.000768
7	N	-1.7078	2.359449	-0.04299
1	H	-2.60714	2.781977	0.148896
1	H	-0.8711	2.893517	0.152357
1	H	-3.66475	-1.59303	0.009449
1	H	1.134391	-2.50031	0.00049
8	O	2.97111	-0.39746	0.013974
6	C	3.61758	-1.68257	0.007826
1	H	3.35351	-2.26114	0.910553
1	H	3.359054	-2.24942	-0.90384
1	H	4.692797	-1.46844	0.012585

C2-OMe-AD_9H E_{tot} = -581.581759 a.u.
Gibbs free energy E_G= -581.476584 a.u.

7	N	1.174032	0.793835	-0.00302
6	C	1.298732	-0.55015	0.000068
7	N	0.333552	-1.48937	0.004074
6	C	-0.88268	-0.92642	0.004
6	C	-1.18606	0.452017	0.004112
6	C	-0.07064	1.320238	0.003429
7	N	-2.56347	0.668177	-0.00364
6	C	-3.08393	-0.54622	-0.00531
7	N	-2.11859	-1.5506	-0.00039
7	N	-0.20248	2.67699	0.041224
1	H	0.619943	3.2412	-0.12656
1	H	-1.11619	3.079552	-0.11916
1	H	-2.27349	-2.55137	-0.00152
8	O	2.550524	-1.07086	-0.0036
6	C	3.650528	-0.13995	-0.0022
1	H	4.549462	-0.77014	0.0003
1	H	3.625102	0.496978	-0.90012
1	H	3.620931	0.499075	0.894014
1	H	-4.14704	-0.77885	-0.01055

C8-OH-AD_9H E_{tot} = -542.301221 a.u.
Gibbs free energy E_G= -542.220982 a.u.

7	N	-2.41898	-0.12014	0.006536
6	C	-2.05175	-1.41558	0.005832
7	N	-0.80551	-1.93629	-9.1E-05
6	C	0.123263	-0.97187	-0.0032
6	C	-0.09789	0.420565	-0.0049
6	C	-1.4492	0.826579	-0.00324
7	N	1.11389	1.125945	7.95E-05
6	C	2.024621	0.173914	0.001081
7	N	1.511861	-1.10831	-0.00152
7	N	-1.82405	2.142048	-0.05131
1	H	-2.79394	2.35059	0.150426
1	H	-1.12976	2.846718	0.160293
1	H	-2.87192	-2.1405	0.01172
1	H	2.039039	-1.97271	-0.00136
8	O	3.362373	0.337007	0.004601
1	H	3.521142	1.296595	0.001374

C2-OH-AD_9H E_{tot} = -542.308123 a.u.
Gibbs free energy E_G= -542.228153 a.u.

7	N	-1.59565	0.732259	0.009828
6	C	-1.66958	-0.60926	0.003569
7	N	-0.67781	-1.52279	-0.00307
6	C	0.527595	-0.92613	-0.00176
6	C	0.779441	0.459732	0.002971
6	C	-0.36741	1.293121	0.006729
7	N	2.147765	0.724222	0.00758
6	C	2.712818	-0.46985	0.004374
7	N	1.782255	-1.50776	-0.002
7	N	-0.27569	2.648957	-0.01265
1	H	-1.1199	3.195832	0.088026
1	H	0.628313	3.088882	0.088176
1	H	1.973953	-2.50205	-0.00533
1	H	3.783234	-0.66528	0.006286
8	O	-2.93783	-1.09806	0.006018
1	H	-2.84534	-2.06625	0.002192

C8-OH-AD_9H E_{tot} = -542.292184 a.u.
Gibbs free energy E_G=-542.213349 a.u.

7	N	-2.42323	-0.11787	0.010082
6	C	-2.06755	-1.41671	0.005142
7	N	-0.82579	-1.94883	-0.00384
6	C	0.109685	-0.99026	-0.00603
6	C	-0.09648	0.402078	-0.0035
6	C	-1.44533	0.820569	0.00122
7	N	1.115572	1.100766	0.001627
6	C	2.025218	0.152989	-0.00011
7	N	1.498089	-1.13662	-0.00596
7	N	-1.80416	2.138255	-0.03962
1	H	-2.77254	2.364357	0.14763
1	H	-1.09749	2.837809	0.145993
1	H	-2.89424	-2.13417	0.012357
1	H	1.992386	-2.02091	-0.0042
8	O	3.353674	0.406679	0.005044
1	H	3.85417	-0.4228	-0.0066

C2-OH-AD_9H E_{tot} = -542.308312 a.u.
Gibbs free energy E_G= -542.227964 a.u.

7	N	-2.43487	-0.14946	0.014406
6	C	-2.04568	-1.44547	0.004444
7	N	-0.80976	-1.96237	-0.00556
6	C	0.113393	-0.98543	-0.00426
6	C	-0.11698	0.405257	0.002709
6	C	-1.47624	0.802052	0.009853
7	N	1.080742	1.117392	0.008368
6	C	2.0156	0.183208	0.002891
7	N	1.491193	-1.10712	-0.00516
7	N	-1.85105	2.110552	-0.01643
1	H	-2.82473	2.338512	0.132714
1	H	-1.14752	2.822712	0.125014
1	H	2.006242	-1.97917	-0.00954
1	H	3.089026	0.361871	0.004779
8	O	-3.05186	-2.35894	0.007065
1	H	-3.87436	-1.83998	0.011617

C8-NH_2-AD_9H E_{tot} = -522.439419 a.u
Gibbs free energy E_G= -522.347455 a.u

7	N	-2.43342	-0.11678	0.005091
6	C	-2.06818	-1.41293	0.005296
7	N	-0.82218	-1.93493	-0.00203
6	C	0.108298	-0.9712	-0.00281
6	C	-0.10979	0.420932	-0.00311
6	C	-1.46118	0.827325	-0.00474
7	N	1.098245	1.124344	-0.00715
6	C	2.025272	0.177659	0.000592
7	N	1.494623	-1.1088	-0.00459
7	N	-1.83257	2.145592	-0.05872
1	H	-2.79883	2.354933	0.160255
1	H	-1.13448	2.842291	0.168448
1	H	-2.8893	-2.13683	0.015086
1	H	2.001183	-1.98127	0.080494
7	N	3.391618	0.392401	0.0896
1	H	3.619174	1.372494	-0.05702
1	H	3.961502	-0.21507	-0.49406

C2-NH_2-AD_9H E_{tot} = -522.447764 a.u.
Gibbs free energy E_G= -522.355774 a.u

7	N	2.454677	-0.12805	-0.04902
6	C	2.08476	-1.43623	-0.06598
7	N	0.833293	-1.95446	-0.04613
6	C	-0.09416	-0.98555	-0.02743
6	C	0.128795	0.406344	-0.01512
6	C	1.487364	0.807918	-0.01969
7	N	-1.07291	1.112904	0.000541
6	C	-2.00412	0.175804	5.99E-05
7	N	-1.4728	-1.11331	-0.01461
7	N	1.850985	2.122375	0.043743
1	H	2.817561	2.354386	-0.14422
1	H	1.140814	2.824884	-0.11486
1	H	-1.98457	-1.98688	-0.02382
1	H	3.121273	-2.34304	-0.15612
7	N	-3.07829	0.34895	0.009487
1	H	4.034146	-1.9982	0.112351
1	H	2.897234	-3.29659	0.099345

C8-NO_2-AD_7H E_{tot} = -671.514633 a.u.
Gibbs free energy E_G= -671.440228 a.u.

7	N	-1.9551	-0.49365	0.001328
6	C	-1.32718	-1.69881	-0.00813
7	N	-0.01691	-1.9628	0.000457
6	C	0.743247	-0.8473	0.003918
6	C	0.1989	0.469894	0.000115
6	C	-1.20809	0.621382	0.009085
7	N	1.291625	1.318933	-0.00749
6	C	2.393614	0.495358	-0.00813
7	N	2.130259	-0.79467	0.002423
7	N	-1.84683	1.838198	-0.0314
1	H	-2.84661	1.801365	0.139275
1	H	-1.37044	2.655681	0.328739
1	H	-1.99665	-2.56469	-0.0176
1	H	1.347315	2.33058	-0.04855
7	N	3.722177	1.103841	-0.02084
8	O	3.73699	2.348694	-0.03759
8	O	4.698603	0.365949	-0.01452

C2-NO_2-AD_7H E_{tot} = -671.516624 a.u.
Gibbs free energy E_G= -671.4435 a.u.

7	N	-1.96367	-0.50606	0.037673
6	C	-1.30252	-1.66757	-0.01593
7	N	-0.01037	-1.94734	-0.04173
6	C	0.742849	-0.82309	-0.04754
6	C	0.181461	0.481418	0.004456
6	C	-1.22084	0.618285	0.06843
7	N	1.270973	1.340571	-0.02854
6	C	2.398151	0.539999	-0.1021
7	N	2.125827	-0.75373	-0.11019
7	N	-1.88304	1.824198	0.099021
1	H	-2.87722	1.754646	0.292676
1	H	-1.41755	2.618709	0.52037
1	H	1.259939	2.352361	-0.05921
1	H	3.396301	0.972684	-0.14591
7	N	-2.21211	-2.87548	-0.04973
8	O	-2.03281	-3.72798	0.815309
8	O	-3.05577	-2.90124	-0.94361

C8-CN-AD_7H E_{tot} = -559.272535 a.u.
Gibbs free energy E_G= -559.200373 a.u.

7	N	-1.94893	-0.49362	-0.00432
6	C	-1.31743	-1.69605	-0.00963
7	N	-0.00562	-1.95327	0.006606
6	C	0.750955	-0.8347	0.009112
6	C	0.202522	0.47697	-0.00122
6	C	-1.20334	0.62262	0.004976
7	N	1.290004	1.332338	-0.00979
6	C	2.419842	0.520159	-0.007
7	N	2.136124	-0.77856	0.010038
7	N	-1.84727	1.840887	-0.04088
1	H	-2.8465	1.789276	0.132767
1	H	-1.38499	2.644211	0.368294
1	H	-1.98278	-2.56512	-0.02029
1	H	1.297828	2.343152	-0.07565
6	C	3.724996	1.092976	-0.01994
7	N	4.775038	1.614725	-0.03159

C2-CN-AD_7H E_{tot} = -559.273660 a.u.
Gibbs free energy E_G= -559.201542 a.u.

7	N	-1.97013	-0.50756	-0.00283
6	C	-1.32569	-1.70242	-0.00818
7	N	-0.00852	-1.95518	0.006965
6	C	0.736926	-0.83186	0.010033
6	C	0.177302	0.474123	0.000512
6	C	-1.2263	0.611577	0.00518
7	N	1.266289	1.332777	-0.00865
6	C	2.396773	0.530303	-0.00808
7	N	2.124799	-0.76182	0.00883
7	N	-1.88386	1.822536	-0.04365
1	H	-2.88254	1.760483	0.130196
1	H	-1.43025	2.628715	0.36928
1	H	1.256791	2.343251	-0.06992
6	C	-2.19917	-2.86195	-0.02234
7	N	-2.91088	-3.79175	-0.03367
1	H	3.39563	0.96358	-0.0194

C8-CHO-AD_7H E_{tot} = -580.365063 a.u.
Gibbs free energy E_G= -580.282361 a.u.

7	N	-1.95033	-0.49711	-0.00057
6	C	-1.31556	-1.69992	-0.00777
7	N	-0.00501	-1.95661	0.003081
6	C	0.753473	-0.8365	0.006139
6	C	0.201704	0.478428	-0.00025
6	C	-1.20654	0.619514	0.006309
7	N	1.284544	1.332253	-0.00827
6	C	2.415237	0.533076	-0.00744
7	N	2.134453	-0.77159	0.004994
7	N	-1.85043	1.836299	-0.03904
1	H	-2.849	1.792514	0.138247
1	H	-1.37862	2.648827	0.338813
1	H	-1.98145	-2.56885	-0.01665
1	H	1.316818	2.345019	-0.0502
6	C	3.76111	1.123106	-0.02222
8	O	3.947976	2.336188	-0.03675
1	H	4.591993	0.381285	-0.01995

C2-CHO-AD_7H E_{tot} = -580.357663 a.u.
Gibbs free energy E_G= -580.275525 a.u.

7	N	-2.09234	-0.44428	-0.00546
6	C	-1.47836	-1.65277	-0.01005
7	N	-0.15878	-1.91802	0.006378
6	C	0.608989	-0.81194	0.009404
6	C	0.069998	0.502307	-0.00108
6	C	-1.33354	0.659957	0.003275
7	N	1.171178	1.343949	-0.01192
6	C	2.291027	0.525116	-0.01047
7	N	1.999933	-0.76231	0.008012
7	N	-1.9683	1.885566	-0.04714
1	H	-2.9681	1.8331	0.126406
1	H	-1.50671	2.676572	0.386845
1	H	1.175551	2.354382	-0.07424
6	C	-2.349	-2.88156	-0.02395
8	O	-3.56669	-2.87693	-0.0386
1	H	-1.75079	-3.82662	-0.0195
1	H	3.295874	0.944426	-0.02241

C8-CHO-AD_7H E_{tot} = -580.354559 a.u.
Gibbs free energy E_G= -580.272533 a.u.

7	N	-1.94976	-0.47843	-0.00692
6	C	-1.33544	-1.69234	-0.00912
7	N	-0.02981	-1.97146	0.01027
6	C	0.749427	-0.86579	0.013243
6	C	0.21869	0.457503	0.000448
6	C	-1.18619	0.623955	0.002457
7	N	1.316995	1.289869	-0.00934
6	C	2.443904	0.46405	-0.00373
7	N	2.129363	-0.82898	0.015307
7	N	-1.81001	1.853474	-0.04775
1	H	-2.81047	1.817852	0.123673
1	H	-1.33638	2.647913	0.365878
1	H	-2.01606	-2.54969	-0.02048
1	H	1.330035	2.301435	-0.07051
6	C	3.787685	1.077306	-0.01834
1	H	3.763855	2.202349	-0.03936
8	O	4.840326	0.465549	-0.00951

C2-CHO-AD_7H E_{tot} = -580.355458 a.u.
Gibbs free energy E_G= -580.273565 a.u.

7	N	-2.04106	-0.51287	-0.01246
6	C	-1.39158	-1.70959	-0.01466
7	N	-0.06985	-1.93659	0.005748
6	C	0.661116	-0.80854	0.009067
6	C	0.088	0.494212	-0.00371
6	C	-1.31566	0.616104	-0.00136
7	N	1.166346	1.364926	-0.01208
6	C	2.30721	0.574273	-0.00753
7	N	2.051107	-0.71963	0.011181
7	N	-1.98518	1.825501	-0.05281
1	H	-2.98168	1.746424	0.128563
1	H	-1.54523	2.623345	0.391781
1	H	1.144893	2.3748	-0.07907
1	H	3.300738	1.020144	-0.01778
6	C	-2.32768	-2.89202	-0.03374
8	O	-1.98191	-4.05803	-0.02232
1	H	-3.40499	-2.58736	-0.06031

C8-Cl-AD_7H E_{tot} = -926.716931 a.u.
Gibbs free energy E_G= -926.651791 a.u.

7	N	-1.95875	-0.50126	-0.00946
6	C	-1.31891	-1.695	-0.00885
7	N	-0.00139	-1.9409	0.011872
6	C	0.742744	-0.81749	0.01264
6	C	0.182794	0.486047	-0.00368
6	C	-1.2169	0.622053	-0.00155
7	N	1.276274	1.352138	-0.01102
6	C	2.39393	0.539297	-0.00469
7	N	2.136715	-0.74853	0.015895
7	N	-1.87474	1.839266	-0.05544
1	H	-2.87089	1.764327	0.130999
1	H	-1.42946	2.627346	0.401958
1	H	-1.97441	-2.57178	-0.0196
1	H	1.288121	2.360907	-0.09081
17	Cl	3.963231	1.248462	-0.02311

C2-Cl-AD_7H E_{tot} = -926.721057 a.u.
Gibbs free energy E_G= -926.656036 a.u.

7	N	-1.96296	-0.50317	-0.00367
6	C	-1.3148	-1.68161	-0.00791
7	N	-0.01408	-1.94355	0.007715
6	C	0.738561	-0.82027	0.010126
6	C	0.183463	0.485478	-0.0012
6	C	-1.21813	0.61867	0.002448
7	N	1.27774	1.342771	-0.00903
6	C	2.402496	0.5372	-0.00683
7	N	2.125372	-0.75604	0.010651
7	N	-1.88273	1.827707	-0.04844
1	H	-2.87933	1.756635	0.13462
1	H	-1.43303	2.630535	0.375864
1	H	1.271914	2.352642	-0.07563
17	Cl	-2.37746	-3.08891	-0.02569
1	H	3.40383	0.964717	-0.01749

C8-F-AD_7H E_{tot} = -566.287822 a.u.
Gibbs free energy E_G= -566.220271 a.u.

7	N	-1.95888	-0.50066	-0.01127
6	C	-1.32231	-1.69395	-0.01056
7	N	-0.00371	-1.94212	0.011935
6	C	0.741412	-0.82175	0.012946
6	C	0.183237	0.483026	-0.00353
6	C	-1.21361	0.622331	-0.00131
7	N	1.283625	1.350856	-0.00497
6	C	2.382742	0.523988	-0.00227
7	N	2.13917	-0.75681	0.019163
7	N	-1.87169	1.840279	-0.05439
1	H	-2.86781	1.762665	0.131443
1	H	-1.42918	2.625479	0.41074
1	H	-1.97824	-2.57042	-0.02191
1	H	1.301231	2.357335	-0.11065
9	F	3.594846	1.076551	-0.01678

C2-F-AD_7H E_{tot} = -566.298761 a.u.
Gibbs free energy E_G= -566.230971 a.u.

7	N	-1.96518	-0.50559	-0.00485
6	C	-1.3079	-1.67291	-0.0087
7	N	-0.01513	-1.94667	0.006793
6	C	0.738782	-0.82282	0.009409
6	C	0.18172	0.482473	-0.00121
6	C	-1.21984	0.616461	0.002052
7	N	1.276353	1.34131	-0.00757
6	C	2.400667	0.537202	-0.00628
7	N	2.124269	-0.75699	0.010387
7	N	-1.88343	1.825793	-0.04797
1	H	-2.8795	1.758043	0.138332
1	H	-1.43036	2.629197	0.371339
1	H	1.270184	2.350992	-0.0753
9	F	-2.12548	-2.75082	-0.02055
1	H	3.401919	0.964965	-0.0166

C8-H-AD_7H E_{tot} = -467.085338 a.u.
Gibbs free energy E_G= -467.00833 a.u.

7	N	-1.96277	-0.50017	-0.01
6	C	-1.32248	-1.69578	-0.00871
7	N	-0.0069	-1.94233	0.012901
6	C	0.742057	-0.8186	0.01347
6	C	0.182197	0.48572	-0.00383
6	C	-1.2189	0.620205	-0.00265
7	N	1.272567	1.348798	-0.01317
6	C	2.402066	0.548237	-0.00608
7	N	2.131882	-0.74505	0.016318
7	N	-1.87607	1.839342	-0.05822
1	H	-2.87193	1.76392	0.130168
1	H	-1.4308	2.624304	0.404726
1	H	-1.98003	-2.57131	-0.01873
1	H	3.400837	0.982174	-0.01724
1	H	1.261259	2.358063	-0.08695

C2-H-AD_7H E_{tot} = -467.085338 a.u.
Gibbs free energy E_G= -467.00833 a.u.

7	N	-1.96277	-0.50017	-0.01
6	C	-1.32248	-1.69578	-0.00871
7	N	-0.0069	-1.94233	0.012901
6	C	0.742057	-0.8186	0.01347
6	C	0.182197	0.48572	-0.00383
6	C	-1.2189	0.620205	-0.00265
7	N	1.272567	1.348798	-0.01317
6	C	2.402066	0.548237	-0.00608
7	N	2.131882	-0.74505	0.016318
7	N	-1.87607	1.839342	-0.05822
1	H	-2.87193	1.76392	0.130168
1	H	-1.4308	2.624304	0.404726
1	H	-1.98003	-2.57131	-0.01873
1	H	3.400837	0.982174	-0.01724
1	H	1.261259	2.358063	-0.08695

C8-Me-AD_7H E_{tot} = -506.387571 a.u.
Gibbs free energy E_G= -506.288694 a.u.

7	N	-1.96162	-0.49656	-0.01316
6	C	-1.32795	-1.6943	-0.00969
7	N	-0.01226	-1.94648	0.014821
6	C	0.741832	-0.82699	0.01535
6	C	0.188129	0.479216	-0.0047
6	C	-1.20994	0.620215	-0.00531
7	N	1.284606	1.335209	-0.01193
6	C	2.421692	0.535447	-0.00343
7	N	2.130636	-0.75835	0.021007
7	N	-1.86205	1.84491	-0.06291
1	H	-2.85782	1.768747	0.127214
1	H	-1.41791	2.619042	0.419812
1	H	-1.98864	-2.56749	-0.02022
1	H	1.275957	2.343873	-0.09482
6	C	3.797599	1.115011	-0.02216
1	H	3.967803	1.707928	-0.9371
1	H	3.964895	1.775544	0.845443
1	H	4.525217	0.294768	0.008704

C2-Me-AD_7H E_{tot} = -506.385299 a.u.
Gibbs free energy E_G= -506.284691 a.u.

7	N	-1.95518	-0.50342	-0.00291
6	C	-1.32927	-1.7151	-0.00614
7	N	-0.00544	-1.94077	0.012202
6	C	0.742092	-0.81759	0.011282
6	C	0.186536	0.486219	-0.00452
6	C	-1.21481	0.614578	0.00157
7	N	1.277982	1.348659	-0.0165
6	C	2.405867	0.546626	-0.01271
7	N	2.132852	-0.7467	0.010964
7	N	-1.87449	1.834449	-0.05197
1	H	-2.86875	1.754174	0.143853
1	H	-1.42992	2.614782	0.419939
1	H	1.267168	2.357594	-0.09408
6	C	-2.23899	-2.91685	-0.02423
1	H	-2.92176	-2.89108	0.840793
1	H	-2.86613	-2.90347	-0.93105
1	H	-1.64461	-3.83877	-0.00051
1	H	3.40551	0.978495	-0.0266

C8-OMe-AD_7H E_{tot} = -581.568845 a.u.
Gibbs free energy E_G= -581.464301 a.u.

7	N	2.784998	0.21089	0.018535
6	C	2.655038	-1.13404	0.017309
7	N	1.531583	-1.86992	-0.00846
6	C	0.410971	-1.12346	-0.01234
6	C	0.427089	0.29607	0.00486
6	C	1.661005	0.958412	0.005268
7	N	-0.9195	0.677888	-0.00099
6	C	-1.64098	-0.50156	-0.00205
7	N	-0.90075	-1.59584	-0.0223
7	N	1.798939	2.340628	0.058981
1	H	2.750201	2.643459	-0.13364
1	H	1.099481	2.882541	-0.43833
1	H	3.596911	-1.69242	0.031403
1	H	-1.31476	1.601192	0.12064
8	O	-2.97522	-0.41802	0.013844
6	C	-3.66417	-1.69904	0.016914
1	H	-3.4062	-2.26493	-0.89005
1	H	-3.37522	-2.27751	0.906485
1	H	-4.73029	-1.44398	0.036902

C2-OMe-AD_7H E_{tot} = -581.571698 a.u.
Gibbs free energy E_G= -581.466513 a.u.

7	N	-1.17118	0.746123	0.008924
6	C	-1.28018	-0.60615	0.01049
7	N	-0.31051	-1.52667	0.026179
6	C	0.92903	-0.99006	0.016863
6	C	1.168908	0.405401	-0.00477
6	C	0.059205	1.274876	0.003082
7	N	2.555867	0.535878	-0.02212
6	C	3.065965	-0.74763	-0.01648
7	N	2.131834	-1.68629	0.013889
7	N	0.168505	2.655337	-0.05679
1	H	-0.70628	3.133586	0.140391
1	H	0.974237	3.071066	0.397485
1	H	3.094685	1.387976	-0.10804
8	O	-2.57193	-1.01611	0.005856
1	H	4.139282	-0.93016	-0.03404
6	C	-2.79089	-2.44255	0.016496
1	H	-3.88242	-2.55775	0.010374
1	H	-2.34162	-2.91142	-0.87241
1	H	-2.35319	-2.89636	0.918924

C8-OMe-AD_7H E_{tot} = -581.559228 a.u.
Gibbs free energy E_G= -581.454953 a.u.

7	N	-1.93794	-0.48467	-0.01185
6	C	-1.29947	-1.67702	-0.00485
7	N	0.01921	-1.92543	0.022058
6	C	0.769375	-0.80549	0.015892
6	C	0.206014	0.496536	-0.00858
6	C	-1.18677	0.636002	-0.00448
7	N	1.300563	1.371007	-0.00618
6	C	2.42739	0.552541	-0.0137
7	N	2.157923	-0.73765	0.021206
7	N	-1.84316	1.862138	-0.06034
1	H	-2.83905	1.771906	0.125725
1	H	-1.41358	2.620301	0.461049
1	H	-1.95506	-2.55417	-0.01378
1	H	1.275874	2.363215	-0.20017
8	O	3.684105	1.023484	-0.03642
6	C	3.857207	2.451355	-0.05209
1	H	4.94098	2.61459	-0.03788
1	H	3.433773	2.88946	-0.97357
1	H	3.401189	2.912071	0.841445

C2-OMe-AD_7H E_{tot} = -581.569196 a.u.
Gibbs free energy E_G= -581.464275 a.u.

7	N	-1.98637	-0.49806	0.004537
6	C	-1.35407	-1.69608	0.005084
7	N	-0.04018	-1.95178	0.023541
6	C	0.709678	-0.83524	0.016674
6	C	0.163653	0.476894	-0.00448
6	C	-1.23284	0.616023	0.002763
7	N	1.265014	1.33076	-0.01772
6	C	2.383036	0.518224	-0.0111
7	N	2.100555	-0.77367	0.017439
7	N	-1.88963	1.836329	-0.05408
1	H	-2.88156	1.767046	0.154995
1	H	-1.43267	2.621635	0.396622
1	H	1.265111	2.33864	-0.10591
8	O	-2.12578	-2.81204	-0.00355
1	H	3.386853	0.940452	-0.02652
6	C	-3.5533	-2.62875	-0.02749
1	H	-3.86325	-2.07299	-0.92652
1	H	-3.96612	-3.64588	-0.04129
1	H	-3.89463	-2.08511	0.867737

C8-OH-AD_7H E_{tot} = -542.292302 a.u.
Gibbs free energy E_G= -542.212344 a.u.

7	N	-2.40804	-0.16261	4.04E-05
6	C	-2.01331	-1.45475	0.001022
7	N	-0.76579	-1.95258	0.008835
6	C	0.183065	-0.99803	-0.00719
6	C	-0.11523	0.390201	-0.02653
6	C	-1.45608	0.794447	-0.007
7	N	1.130381	1.032503	-0.0462
6	C	2.065343	0.021617	-0.05242
7	N	1.563621	-1.19714	-0.0184
7	N	-1.86834	2.119641	-0.06012
1	H	-2.85777	2.229344	0.14586
1	H	-1.28164	2.796904	0.416168
1	H	-2.8253	-2.18937	0.003725
1	H	1.332716	2.016766	-0.1644
8	O	3.369488	0.347685	-0.08872
1	H	3.860133	-0.49273	-0.09302

C2-OH-AD_7H E_{tot} = -542.297497 a.u.
Gibbs free energy E_G= -542.217166 a.u.

7	N	-1.59514	0.74378	-0.00116
6	C	-1.6849	-0.60279	-0.00055
7	N	-0.70887	-1.51907	0.017972
6	C	0.525843	-0.97335	0.014695
6	C	0.749811	0.426869	-0.00312
6	C	-0.36625	1.28527	0.000267
7	N	2.135743	0.57147	-0.01488
6	C	2.658961	-0.70631	-0.00933
7	N	1.735582	-1.65567	0.015305
7	N	-0.2745	2.665074	-0.05651
1	H	-1.15443	3.135653	0.135026
1	H	0.529681	3.094245	0.387199
1	H	2.666582	1.429099	-0.09512
1	H	3.73425	-0.87731	-0.02282
8	O	-2.96218	-1.06862	-0.01121
1	H	-2.88152	-2.03862	-0.00453

C8-OH-AD_7H E_{tot} = -542.281660 a.u.
Gibbs free energy E_G= -542.20272 a.u.

7	N	-1.94581	-0.49057	-0.01117
6	C	-1.30825	-1.68234	-0.00939
7	N	0.011649	-1.92983	0.015022
6	C	0.759117	-0.81042	0.007808
6	C	0.197895	0.49112	-0.01318
6	C	-1.19491	0.63087	0.000163
7	N	1.29475	1.368609	0.005172
6	C	2.417796	0.542178	-0.01405
7	N	2.152096	-0.74295	0.020448
7	N	-1.8504	1.856215	-0.04464
1	H	-2.84551	1.768767	0.145979
1	H	-1.41366	2.613977	0.47124
1	H	-1.96294	-2.55999	-0.01943
1	H	1.276488	2.332269	-0.3096
8	O	3.674739	1.03107	-0.0553
1	H	3.66824	1.98664	0.109126

C2-OH-AD_7H E_{tot} = -542.295711 a.u.
Gibbs free energy E_G= -542.215488 a.u.

7	N	-1.96797	-0.53171	-0.00775
6	C	-1.31543	-1.72309	-0.00974
7	N	-0.00646	-1.96778	0.01064
6	C	0.732121	-0.83892	0.011604
6	C	0.17049	0.464971	-0.00426
6	C	-1.22969	0.591476	-0.00246
7	N	1.26098	1.331752	-0.01108
6	C	2.388748	0.533511	-0.0051
7	N	2.119973	-0.76218	0.01605
7	N	-1.89603	1.804501	-0.05769
1	H	-2.88941	1.73074	0.141838
1	H	-1.44656	2.59537	0.390209
1	H	1.248972	2.340446	-0.08936
1	H	3.387584	0.967234	-0.01548
8	O	-2.11714	-2.82151	-0.02445
1	H	-3.0287	-2.48391	-0.03804

C8-NH_2-AD_7H E_{tot} = -522.430336 a.u.
Gibbs free energy E_G= -522.338657 a.u.

7	N	-1.93757	-0.49698	0.006836
6	C	-1.29406	-1.68474	0.014114
7	N	0.027849	-1.92563	0.025122
6	C	0.770638	-0.80228	-0.00306
6	C	0.202257	0.49697	-0.03242
6	C	-1.18999	0.628127	-0.00222
7	N	1.29198	1.380881	-0.0314
6	C	2.425938	0.573025	-0.04957
7	N	2.160672	-0.72372	0.001381
7	N	-1.85323	1.850544	-0.05147
1	H	-2.84386	1.75945	0.159506
1	H	-1.41094	2.615041	0.449673
1	H	-1.94411	-2.56606	0.021235
1	H	1.273429	2.338698	-0.36111
7	N	3.687295	1.119287	-0.17515
1	H	4.415744	0.4264	-0.02716
1	H	3.851412	1.974813	0.347514

C2-NH_2-AD_7H E_{tot} = -522.436103 a.u.
Gibbs free energy E_G= -522.344372 a.u.

7	N	-1.98356	-0.51386	0.031323
6	C	-1.34715	-1.72119	0.05001
7	N	-0.02282	-1.96304	0.055132
6	C	0.721525	-0.84163	0.035878
6	C	0.167422	0.464482	0.010102
6	C	-1.23312	0.596212	0.013945
7	N	1.263371	1.326265	-0.02274
6	C	2.386506	0.523074	-0.02124
7	N	2.111852	-0.77159	0.019953
7	N	-1.88801	1.818212	-0.06577
1	H	-2.87967	1.750105	0.146327
1	H	-1.43266	2.604602	0.385151
1	H	1.254956	2.333535	-0.11648
1	H	3.387307	0.951485	-0.04935
7	N	-2.17951	-2.82119	0.122191
1	H	-1.75211	-3.70611	-0.12208
1	H	-3.13507	-2.67619	-0.17829

C8-NO_2-AD_3H E_{tot} = -671.517325 a.u.
Gibbs free energy E_G= -671.444252 a.u.

7	N	1.942399	0.350453	0.000333
6	C	1.357998	1.532717	9E-05
7	N	0.01124	1.7428	-0.00024
6	C	-0.82023	0.644681	-0.00019
6	C	-0.24232	-0.65908	8.61E-05
6	C	1.164623	-0.78092	0.000252
7	N	-1.2569	-1.57917	0.000241
6	C	-2.33617	-0.77557	0.000129
7	N	-2.15781	0.585122	-0.00031
7	N	1.794987	-1.97211	-0.00012
1	H	2.805669	-2.00638	0.00221
1	H	1.251093	-2.82546	0.00182
1	H	1.981206	2.429908	0.00013
1	H	-0.37253	2.684577	-0.00045
7	N	-3.6986	-1.34202	0.000294
8	O	-4.6382	-0.54297	-2.6E-05
8	O	-3.79635	-2.57132	0.000745

C2-NO_2-AD_3H E_{tot} = -671.516501 a.u.
Gibbs free energy E_G= -671.442059 a.u.

7	N	1.962134	0.430105	0.000244
6	C	1.376937	1.59742	2.7E-05
7	N	0.043212	1.84366	-0.00027
6	C	-0.79382	0.75882	-0.00022
6	C	-0.22538	-0.55981	1.01E-05
6	C	1.179861	-0.69486	0.00014
7	N	-1.25009	-1.46273	0.000112
6	C	-2.34516	-0.65573	0.000265
7	N	-2.1341	0.705543	-0.00028
7	N	1.806112	-1.89151	-0.00046
1	H	2.816201	-1.93253	0.002552
1	H	1.256123	-2.74012	0.002085
1	H	-3.35672	-1.06315	0.000266
1	H	-0.27689	2.812888	-0.00044
7	N	2.219556	2.831299	0.000155
8	O	1.60186	3.909268	-0.00013
8	O	3.434895	2.694674	0.000616

C8-CN-AD_3H E_{tot} = -559.278473 a.u.
Gibbs free energy E_G= -559.205701 a.u.

7	N	1.937225	0.348865	0.000303
6	C	1.353518	1.53086	6.01E-05
7	N	0.005653	1.738676	-0.00027
6	C	-0.82641	0.641601	-0.00019
6	C	-0.24875	-0.6616	8.33E-05
6	C	1.157485	-0.78161	0.000214
7	N	-1.2614	-1.58384	0.000153
6	C	-2.36401	-0.78813	0.000429
7	N	-2.16356	0.585096	-0.00032
7	N	1.789495	-1.97373	-0.00031
1	H	2.800018	-2.00691	0.002384
1	H	1.24644	-2.82724	0.001993
1	H	1.975327	2.428951	8.99E-05
1	H	-0.37833	2.680183	-0.00051
6	C	-3.6864	-1.33644	0.00035
7	N	-4.76917	-1.78657	0.000273

C2-CN-AD_3H E_{tot} = -559.270093 a.u.
Gibbs free energy E_G= -559.198058 a.u.

7	N	1.969919	0.441826	9.36E-05
6	C	1.395761	1.635248	-7.4E-05
7	N	0.039807	1.852506	-0.00015
6	C	-0.79039	0.76321	-6.6E-05
6	C	-0.22026	-0.55013	9.46E-05
6	C	1.18343	-0.67957	0.000106
7	N	-1.24488	-1.45769	0.000654
6	C	-2.33981	-0.65502	-0.00056
7	N	-2.13095	0.708371	0.000241
7	N	1.810643	-1.87713	-0.00036
1	H	2.820565	-1.91771	0.002493
1	H	1.260862	-2.72582	0.002204
1	H	-3.35103	-1.06325	-0.00013
1	H	-0.33489	2.799067	-0.00017
6	C	2.221994	2.811869	3.37E-05
7	N	2.864326	3.792561	0.00012

C8-CHO-AD_3H E_{tot} = -580.361048 a.u.
Gibbs free energy E_G= -580.278319 a.u.

7	N	1.946593	0.439622	0.000281
6	C	1.376372	1.62904	2.83E-05
7	N	0.032432	1.854398	-0.00025
6	C	-0.81755	0.768605	-0.00016
6	C	-0.25331	-0.5452	0.000136
6	C	1.151785	-0.6804	0.000281
7	N	-1.27955	-1.44656	0.00039
6	C	-2.38045	-0.63826	0.0002
7	N	-2.15065	0.730415	-0.00035
7	N	1.771135	-1.87998	0.000139
1	H	2.781187	-1.9244	0.002086
1	H	1.218196	-2.72693	0.001823
1	H	2.0105	2.518611	-2.9E-05
1	H	-0.33959	2.800852	-0.00049
6	C	-3.72635	-1.2488	0.00021
8	O	-4.78329	-0.63389	0.000619
1	H	-3.69048	-2.36785	-0.00024

C2-CHO-AD_3H E_{tot} = -580.364512 a.u.
Gibbs free energy E_G= -580.281952 a.u.

7	N	1.967249	0.444632	0.000163
6	C	1.385433	1.639967	-9.6E-06
7	N	0.036415	1.848571	-0.00022
6	C	-0.79491	0.767183	-0.00014
6	C	-0.21934	-0.54858	2.03E-05
6	C	1.186738	-0.67672	8.34E-05
7	N	-1.237	-1.45941	7.85E-05
6	C	-2.33833	-0.6589	0.000505
7	N	-2.13752	0.702327	-0.00012
7	N	1.807966	-1.87954	-0.00057
1	H	2.817389	-1.9258	0.002422
1	H	1.253825	-2.72519	0.001997
1	H	-3.34678	-1.07442	0.000512
1	H	-0.2988	2.813487	-0.00032
6	C	2.232923	2.858215	4.28E-05
8	O	1.762611	3.989998	-0.00017
1	H	3.327529	2.652435	0.00045

C8-CHO-AD_3H E_{tot} = -580.360469 a.u.
Gibbs free energy E_G= -580.277681 a.u.

7	N	1.939583	0.360708	0.000362
6	C	1.340558	1.53633	0.000263
7	N	-0.00876	1.728975	-2.9E-05
6	C	-0.83155	0.622528	-0.0001
6	C	-0.23697	-0.67657	6.63E-06
6	C	1.172934	-0.77768	0.00014
7	N	-1.23144	-1.61016	6.01E-05
6	C	-2.35327	-0.83954	0.000144
7	N	-2.1642	0.541471	-0.00019
7	N	1.814384	-1.96414	-0.00044
1	H	2.825047	-1.99108	0.002133
1	H	1.274528	-2.82018	0.001521
1	H	1.952489	2.44128	0.00041
1	H	-0.40114	2.667024	-0.00013
6	C	-3.73452	-1.36951	0.000204
8	O	-4.03594	-2.55454	0.000184
1	H	-4.51003	-0.56183	0.000219

C2-CHO-AD_3H E_{tot} = -580.355066 a.u.
Gibbs free energy E_G= -580.272806 a.u.

7	N	2.082648	0.391685	0.000418
6	C	1.530983	1.595821	0.000176
7	N	0.173406	1.816548	-0.00021
6	C	-0.67187	0.745214	-0.00017
6	C	-0.11845	-0.57566	7.99E-05
6	C	1.288217	-0.71711	0.000283
7	N	-1.15031	-1.46995	-0.00012
6	C	-2.23988	-0.65238	0.000675
7	N	-2.01689	0.704355	-0.00035
7	N	1.896871	-1.92435	-0.00027
1	H	2.90654	-1.97574	0.002199
1	H	1.336622	-2.76601	0.001782
1	H	-3.25454	-1.05222	0.000468
1	H	-0.19423	2.767138	-0.00041
6	C	2.365103	2.831912	0.000283
8	O	3.580983	2.853228	0.000506
1	H	1.761939	3.781601	-0.00011

C8-Cl-AD_3H E_{tot} = -926.720746 a.u.
Gibbs free energy E_G= -926.655651 a.u.

7	N	1.944357	0.352402	0.000109
6	C	1.364181	1.534826	-2.3E-05
7	N	0.013865	1.740684	-0.0002
6	C	-0.81581	0.644167	-0.00016
6	C	-0.2391	-0.65832	-1.6E-05
6	C	1.162275	-0.77821	9.3E-06
7	N	-1.26291	-1.58123	0.000195
6	C	-2.34267	-0.77843	-7.2E-05
7	N	-2.15773	0.586168	-4E-05
7	N	1.798506	-1.97313	-0.0008
1	H	2.808502	-2.00421	0.002816
1	H	1.256972	-2.82682	0.002393
1	H	1.984988	2.4335	8.62E-05
1	H	-0.37152	2.681324	-0.00029
17	Cl	-3.94641	-1.42896	0.00033

C2-Cl-AD_3H E_{tot} = -926.717529 a.u.
Gibbs free energy E_G= -926.65264 a.u.

7	N	1.950454	0.455204	1.45E-05
6	C	1.370993	1.623858	-0.00016
7	N	0.02822	1.849829	-0.00023
6	C	-0.80512	0.748054	-0.00013
6	C	-0.23166	-0.55758	1.54E-05
6	C	1.168044	-0.67787	1.39E-05
7	N	-1.25976	-1.4732	0.000397
6	C	-2.35044	-0.67645	-0.00026
7	N	-2.14226	0.693789	0.000212
7	N	1.811083	-1.86767	-0.00073
1	H	2.821059	-1.89723	0.002857
1	H	1.269642	-2.72169	0.00231
1	H	-3.36249	-1.08289	3.69E-05
1	H	-0.34245	2.796156	-0.00027
17	Cl	2.354684	3.068155	6.73E-05

C8-F-AD_3H E_{tot} = -566.294574 a.u.
Gibbs free energy E_G= -566.227142 a.u.

7	N	1.942541	0.352287	7.07E-05
6	C	1.363983	1.534793	-2.7E-05
7	N	0.012879	1.739995	-0.00018
6	C	-0.81558	0.644249	-0.00016
6	C	-0.23934	-0.65966	-5E-05
6	C	1.160367	-0.77864	-4.3E-05
7	N	-1.26643	-1.58279	0.000145
6	C	-2.33029	-0.77191	-4.8E-05
7	N	-2.15928	0.585836	-3.7E-05
7	N	1.798454	-1.97405	-0.0009
1	H	2.808333	-2.00391	0.00292
1	H	1.258406	-2.82847	0.002473
1	H	1.984578	2.433568	8.89E-05
1	H	-0.37291	2.680417	-0.00026
9	F	-3.57022	-1.26913	0.000298

C2-F-AD_3H E_{tot} = -566.291563 a.u.
Gibbs free energy E_G= -566.224013 a.u.

7	N	1.957967	0.453321	6.76E-05
6	C	1.366241	1.607954	-6.8E-05
7	N	0.033841	1.853099	-0.00018
6	C	-0.80511	0.749031	-9.1E-05
6	C	-0.22844	-0.55425	4.79E-05
6	C	1.170204	-0.67906	5.39E-05
7	N	-1.2581	-1.47224	0.000544
6	C	-2.34801	-0.67897	-0.0003
7	N	-2.13973	0.694319	0.000104
7	N	1.809395	-1.87011	-0.00046
1	H	2.819202	-1.9043	0.002665
1	H	1.26418	-2.7218	0.002154
1	H	-3.36023	-1.08497	-4.6E-05
1	H	-0.32441	2.804612	-0.00022
9	F	2.119618	2.725312	1.69E-05

C8-H-AD_3H E_{tot} = -467.085495 a.u.
Gibbs free energy E_G= -467.008726 a.u.

7	N	1.956751	0.45435	0.000391
6	C	1.376085	1.637636	0.000118
7	N	0.027617	1.844188	-0.00022
6	C	-0.80757	0.749745	0.000092
6	C	-0.23136	-0.55468	0.000106
6	C	1.170301	-0.6737	-6.9E-05
7	N	-1.256	-1.47343	0.000079
6	C	-2.3504	-0.67884	0.000098
7	N	-2.14758	0.689367	-5.4E-05
7	N	1.805039	-1.86988	-0.00118
1	H	2.814875	-1.90314	0.00295
1	H	1.259925	-2.72134	0.002325
1	H	1.998167	2.535542	0.000062
1	H	-3.3607	-1.09023	0.000181
1	H	-0.35538	2.786045	-0.00071

C2-H-AD_3H E_{tot} = -467.085495 a.u.
Gibbs free energy E_G= -467.008726 a.u.

7	N	1.956751	0.45435	0.000391
6	C	1.376085	1.637636	0.000118
7	N	0.027617	1.844188	-0.00022
6	C	-0.80757	0.749745	0.000092
6	C	-0.23136	-0.55468	0.000106
6	C	1.170301	-0.6737	-6.9E-05
7	N	-1.256	-1.47343	0.000079
6	C	-2.3504	-0.67884	0.000098
7	N	-2.14758	0.689367	-5.4E-05
7	N	1.805039	-1.86988	-0.00118
1	H	2.814875	-1.90314	0.00295
1	H	1.259925	-2.72134	0.002325
1	H	1.998167	2.535542	0.000062
1	H	-3.3607	-1.09023	0.000181
1	H	-0.35538	2.786045	-0.00071

C8-Me-AD_3H E_{tot} = -506.386585 a.u.
Gibbs free energy E_G= -506.287823 a.u.

7	N	1.954797	0.453989	0.008523
6	C	1.375169	1.634386	-0.06502
7	N	0.024862	1.838206	-0.1008
6	C	-0.80932	0.744414	-0.05774
6	C	-0.23152	-0.55755	0.022239
6	C	1.167758	-0.6739	0.054013
7	N	-1.25768	-1.47401	0.052735
6	C	-2.36309	-0.69055	-0.00902
7	N	-2.14606	0.682377	-0.07864
7	N	1.805493	-1.86874	0.127953
1	H	2.814837	-1.89899	0.15448
1	H	1.261789	-2.71973	0.168963
1	H	1.995881	2.532558	-0.10139
1	H	-0.35857	2.777819	-0.15788
6	C	-3.74914	-1.24938	-0.00394
1	H	-4.29001	-0.94927	-0.91729
1	H	-3.71157	-2.34536	0.054097
1	H	-4.3209	-0.8564	0.853658

C2-Me-AD_3H E_{tot} = -506.386326 a.u.
Gibbs free energy E_G= -506.284818 a.u.

7	N	1.95918	0.443145	8.43E-05
6	C	1.399987	1.643224	-2.9E-05
7	N	0.044053	1.835623	-0.00016
6	C	-0.79668	0.744786	-0.00013
6	C	-0.2308	-0.56118	-3.2E-05
6	C	1.168214	-0.68058	-3E-05
7	N	-1.2631	-1.47542	0.00029
6	C	-2.3506	-0.67425	-0.0002
7	N	-2.13681	0.694627	0.000121
7	N	1.802556	-1.87821	-0.00089
1	H	2.812195	-1.91235	0.003031
1	H	1.256466	-2.7289	0.002404
1	H	-3.36432	-1.07729	3.44E-05
1	H	-0.34402	2.775182	-0.0002
6	C	2.26599	2.872665	0.000124
1	H	2.07211	3.4929	-0.89176
1	H	2.071441	3.493193	0.89166
1	H	3.318827	2.567453	0.000549

C8-OMe-AD_3H E_{tot} = -581.568580 a.u.
Gibbs free energy E_G= -581.463461 a.u.

7	N	1.963561	0.389726	-0.00019
6	C	1.35879	1.557638	-0.00017
7	N	0.000397	1.728438	-0.00018
6	C	-0.80373	0.614591	-0.0001
6	C	-0.19406	-0.67632	-0.00013
6	C	1.205376	-0.7593	-0.00027
7	N	-1.19917	-1.62098	0.000143
6	C	-2.30466	-0.84079	0.000325
7	N	-2.14046	0.531152	0.000152
7	N	1.877612	-1.94142	-0.00137
1	H	2.887446	-1.94351	0.003466
1	H	1.36116	-2.80944	0.003
1	H	1.956032	2.472018	-9.8E-05
1	H	-0.40913	2.658534	-0.00015
8	O	-3.55835	-1.32005	0.000564
6	C	-3.67081	-2.75833	0.000611
1	H	-4.74906	-2.96214	0.000787
1	H	-3.19248	-3.1814	-0.89676
1	H	-3.1922	-3.18137	0.897846

C2-OMe-AD_3H E_{tot} = -581.570115 a.u.
Gibbs free energy E_G= -581.466612 a.u.

7	N	1.972319	0.350517	9.59E-05
6	C	1.430021	1.549325	1.33E-05
7	N	0.090666	1.809088	-0.0002
6	C	-0.77874	0.733367	-0.00018
6	C	-0.24618	-0.58595	-0.00011
6	C	1.147034	-0.74958	-8.7E-05
7	N	-1.30516	-1.47431	4.05E-05
6	C	-2.36813	-0.6465	0.000204
7	N	-2.11641	0.719831	-0.00011
7	N	1.743392	-1.96645	-0.001
1	H	2.750674	-2.03878	0.003198
1	H	1.1662	-2.79647	0.002294
1	H	-3.39292	-1.02014	0.000323
1	H	-0.24321	2.768701	-0.0003
8	O	2.17722	2.672715	0.000137
6	C	3.612384	2.486442	0.000139
1	H	4.023796	3.502865	9.38E-05
1	H	3.925099	1.934533	0.89874
1	H	3.92509	1.934444	-0.89841

C8-OMe-AD_3H E_{tot} = -581.567454 a.u.
Gibbs free energy E_G= -581.462549 a.u.

7	N	1.911482	0.354717	4.32E-06
6	C	1.331842	1.536397	-3.9E-05
7	N	-0.02353	1.733605	-0.0002
6	C	-0.84858	0.636522	-0.0002
6	C	-0.26936	-0.66658	-0.00016
6	C	1.131282	-0.777	-0.00017
7	N	-1.28568	-1.5933	2.28E-07
6	C	-2.37806	-0.7983	3.93E-05
7	N	-2.19006	0.573896	-8.9E-05
7	N	1.772294	-1.97474	-0.0012
1	H	2.781738	-2.00424	0.003298
1	H	1.231138	-2.82816	0.002701
1	H	1.947266	2.438427	0.000106
1	H	-0.41277	2.672344	-0.00022
8	O	-3.60085	-1.35377	0.000148
6	C	-4.71392	-0.4369	4.29E-05
1	H	-5.60828	-1.07304	9.92E-05
1	H	-4.69055	0.200911	0.897632
1	H	-4.69053	0.200726	-0.89768

C2-OMe-AD_3H E_{tot} = -581.561330 a.u.
Gibbs free energy E_G= -581.456966 a.u.

7	N	1.9477	0.481835	0.000191
6	C	1.366897	1.662344	7.29E-05
7	N	0.014045	1.864121	-0.00019
6	C	-0.81	0.748831	-0.00018
6	C	-0.23038	-0.54511	-7.5E-05
6	C	1.172361	-0.64724	-1.5E-05
7	N	-1.25511	-1.47156	1.79E-05
6	C	-2.34964	-0.68392	0.000209
7	N	-2.14749	0.689696	-0.00017
7	N	1.819045	-1.83699	-0.00086
1	H	2.828967	-1.8623	0.002943
1	H	1.279739	-2.692	0.002245
1	H	-3.35979	-1.09528	0.000293
1	H	-0.4007	2.789942	-0.00037
8	O	2.201475	2.728761	0.000215
6	C	1.638062	4.050814	0.000236
1	H	1.034304	4.225987	0.908501
1	H	2.49843	4.730291	0.000473
1	H	1.034679	4.226169	-0.90824

C8-OH-AD_3H E_{tot} = -542.293445 a.u.
Gibbs free energy E_G= -542.213071 a.u.

7	N	1.934924	0.348774	-8.3E-05
6	C	1.355988	1.53011	-7.8E-05
7	N	0.001826	1.729642	-0.00014
6	C	-0.82508	0.633955	-0.0001
6	C	-0.24513	-0.67025	-0.00012
6	C	1.15324	-0.78329	-0.00021
7	N	-1.27473	-1.58889	6.76E-05
6	C	-2.35902	-0.78148	0.000226
7	N	-2.16657	0.580325	5.82E-05
7	N	1.798972	-1.97935	-0.0013
1	H	2.808652	-2.00346	0.003208
1	H	1.264406	-2.83639	0.00286
1	H	1.972889	2.431247	2.09E-05
1	H	-0.38786	2.668285	-0.00014
8	O	-3.61798	-1.26582	0.000321
1	H	-3.53189	-2.23418	0.000267

C2-OH-AD_3H E_{tot} = -542.294453 a.u.
Gibbs free energy E_G= -542.214882 a.u.

7	N	1.968854	0.453897	7.3E-05
6	C	1.385327	1.633357	-1.7E-05
7	N	0.045903	1.857692	-0.00017
6	C	-0.7914	0.753656	-0.00014
6	C	-0.21904	-0.54857	-6E-05
6	C	1.17952	-0.67293	-7.1E-05
7	N	-1.24993	-1.46756	0.000195
6	C	-2.33808	-0.67222	-1.9E-06
7	N	-2.12743	0.700435	1.67E-06
7	N	1.810886	-1.87047	-0.00092
1	H	2.819879	-1.91484	0.003085
1	H	1.257632	-2.71676	0.002307
1	H	-3.35077	-1.0771	0.000163
1	H	-0.31788	2.806515	-0.00026
8	O	2.131843	2.763371	0.000128
1	H	3.059969	2.470606	0.000138

C8-OH-AD_3H E_{tot} = -542.293128 a.u.
Gibbs free energy E_G= -542.212789 a.u.

7	N	1.922788	0.354763	4.54E-06
6	C	1.340122	1.534107	-2.4E-05
7	N	-0.01548	1.729401	-0.00017
6	C	-0.83797	0.630419	-0.00017
6	C	-0.25466	-0.67159	-0.00014
6	C	1.144958	-0.77974	-0.00017
7	N	-1.27096	-1.60349	3.63E-05
6	C	-2.35872	-0.81255	0.000115
7	N	-2.17942	0.55955	-6E-05
7	N	1.789539	-1.97505	-0.00119
1	H	2.799118	-2.00139	0.003203
1	H	1.251452	-2.83045	0.00263
1	H	1.953747	2.437498	0.000113
1	H	-0.40569	2.66766	-0.0002
8	O	-3.60183	-1.33767	0.000226
1	H	-4.21458	-0.58336	0.000178

C2-OH-AD_3H E_{tot} = -542.283675 a.u.
Gibbs free energy E_G= -542.204802 a.u.

7	N	1.964607	0.463798	0.00027
6	C	1.39449	1.644117	0.000111
7	N	0.04325	1.86271	-0.00025
6	C	-0.79402	0.756556	-0.00023
6	C	-0.22381	-0.54337	-5E-05
6	C	1.176196	-0.66004	4.97E-05
7	N	-1.25686	-1.46086	-5.6E-05
6	C	-2.34413	-0.66477	0.000391
7	N	-2.13049	0.708216	-0.00035
7	N	1.813559	-1.85371	-0.00075
1	H	2.823354	-1.88665	0.002853
1	H	1.267863	-2.70481	0.002127
1	H	-3.35773	-1.0674	0.000406
1	H	-0.36148	2.795377	-0.00056
8	O	2.22568	2.719664	0.000211
1	H	1.719766	3.546861	0.000327

C8-NH_2-AD_3H E_{tot} = -522.433418 a.u.
Gibbs free energy E_G= -522.342048 a.u.

7	N	1.93107	0.352474	-0.00023
6	C	1.353137	1.533539	-0.00011
7	N	-0.00483	1.729538	-0.00011
6	C	-0.83102	0.633961	-8.8E-05
6	C	-0.24918	-0.67086	-0.00021
6	C	1.149167	-0.77941	-0.0004
7	N	-1.26969	-1.59557	2.96E-06
6	C	-2.37073	-0.79957	0.000326
7	N	-2.17035	0.5758	0.000117
7	N	1.794946	-1.97929	-0.00172
1	H	2.804145	-2.00587	0.003595
1	H	1.256935	-2.83394	0.003155
1	H	1.96726	2.436377	1.59E-05
1	H	-0.39467	2.667754	-4E-05
7	N	-3.636	-1.30589	0.000474
1	H	-3.77374	-2.30456	7.16E-05
1	H	-4.42638	-0.68041	0.000128

C2-NH_2-AD_3H E_{tot} = -522.430863 a.u.
Gibbs free energy E_G= -522.340542 a.u.

7	N	1.966316	0.465645	0.000243
6	C	1.390457	1.661822	0.000166
7	N	0.033981	1.862307	-0.00028
6	C	-0.79571	0.75248	-0.00029
6	C	-0.22137	-0.54341	-0.00019
6	C	1.179641	-0.65437	-0.0001
7	N	-1.25092	-1.468	-0.0003
6	C	-2.34115	-0.67718	0.000657
7	N	-2.13319	0.697315	-0.0005
7	N	1.812928	-1.85314	-0.00106
1	H	2.822017	-1.89293	0.003175
1	H	1.261686	-2.70044	0.002213
1	H	-3.35319	-1.08401	0.000661
1	H	-0.37087	2.793687	-0.00058
7	N	2.196452	2.769199	0.000185
1	H	3.194702	2.622362	0.000326
1	H	1.833103	3.709533	0.000344

C8-NO_2-AD_1H E_{tot} = -671.500835 a.u.
Gibbs free energy E_G= -671.428109 a.u.

7	N	1.834676	-0.48512	0.014291
6	C	1.226675	-1.74285	0.03459
7	N	-0.06008	-1.94874	0.036463
6	C	-0.82134	-0.80815	0.014241
6	C	-0.2636	0.524884	-0.00218
6	C	1.121792	0.69155	-0.00311
7	N	-1.26678	1.45127	0.005142
6	C	-2.34183	0.637259	0.014035
7	N	-2.16766	-0.71415	0.019853
7	N	1.760681	1.890938	-0.06918
1	H	2.716643	1.987454	0.250711
1	H	1.162226	2.703177	0.043519
1	H	1.928838	-2.57969	0.050451
1	H	2.849173	-0.4517	-0.01114
7	N	-3.70469	1.215275	0.014327
8	O	-4.6306	0.466033	-0.29823
8	O	-3.80801	2.404486	0.325092

C2-NO_2-AD_1H E_{tot} = -671.504987 a.u.
Gibbs free energy E_G= -671.430871 a.u.

7	N	1.821619	-0.51578	0.020951
6	C	1.181953	-1.74067	0.006213
7	N	-0.10129	-1.9492	-0.00893
6	C	-0.84489	-0.80942	-0.01002
6	C	-0.26955	0.522251	0.00551
6	C	1.123324	0.664806	0.021758
7	N	-1.26139	1.450247	0.012589
6	C	-2.37767	0.656213	-0.00137
7	N	-2.19569	-0.69466	-0.01409
7	N	1.779484	1.851849	-0.00352
1	H	2.75937	1.920913	0.238398
1	H	1.205111	2.67876	0.114596
1	H	-3.37713	1.093473	-0.00084
1	H	2.841691	-0.57048	0.020559
7	N	2.133114	-2.87444	0.011338
8	O	3.345284	-2.56463	0.026709
8	O	1.686322	-4.01182	-2.7E-05

C8-CN-AD_1H E_{tot} = -559.262127 a.u.
Gibbs free energy E_G= -559.1899 a.u.

7	N	1.829419	-0.48385	0.011031
6	C	1.22123	-1.74045	0.003563
7	N	-0.06624	-1.94398	-0.00705
6	C	-0.82771	-0.80274	-0.01096
6	C	-0.26925	0.530265	-0.00238
6	C	1.11567	0.692885	0.01007
7	N	-1.26982	1.458168	0.008929
6	C	-2.37015	0.652475	0.004175
7	N	-2.17242	-0.71135	-0.00558
7	N	1.760668	1.893482	-0.03735
1	H	2.701108	1.981222	0.329511
1	H	1.158086	2.7005	0.092031
1	H	1.921902	-2.57869	0.008805
1	H	2.843818	-0.44913	-0.01383
6	C	-3.69164	1.208938	0.012448
7	N	-4.76872	1.671109	0.020038

C2-CN-AD_1H E_{tot} = -559.256303 a.u.
Gibbs free energy E_G= -559.184415 a.u.

7	N	1.849765	-0.49622	0.011055
6	C	1.235683	-1.75808	0.005503
7	N	-0.06336	-1.95463	-0.00473
6	C	-0.81373	-0.81841	-0.0104
6	C	-0.25205	0.517852	-0.00153
6	C	1.133536	0.6764	0.010278
7	N	-1.25526	1.439388	0.008855
6	C	-2.35904	0.636588	0.002411
7	N	-2.16343	-0.7166	-0.00702
7	N	1.781229	1.875701	-0.037
1	H	2.724546	1.960257	0.323168
1	H	1.179766	2.682331	0.098183
1	H	-3.36388	1.061586	0.006653
1	H	2.865026	-0.46861	-0.01392
6	C	2.154187	-2.85981	0.015832
7	N	2.956517	-3.71584	0.024327

C8-CHO-AD_1H E_{tot} = -580.344124 a.u.
Gibbs free energy E_G=-580.262066 a.u.

7	N	1.824815	-0.39242	0.012742
6	C	1.198066	-1.64202	0.005143
7	N	-0.09178	-1.828	-0.00606
6	C	-0.83975	-0.67609	-0.01016
6	C	-0.26146	0.650834	-0.00121
6	C	1.127695	0.793115	0.011211
7	N	-1.2425	1.593035	0.010535
6	C	-2.36301	0.815045	0.00478
7	N	-2.17964	-0.55633	-0.00601
7	N	1.783482	1.986351	-0.03396
1	H	2.729685	2.06718	0.318577
1	H	1.186897	2.798929	0.090445
1	H	1.888241	-2.48906	0.01087
1	H	2.839621	-0.37267	-0.01034
6	C	-3.74391	1.356184	0.013206
8	O	-4.03306	2.543727	0.028817
1	H	-4.52521	0.555447	0.004283

C2-CHO-AD_1H E_{tot} = -580.355145 a.u.
Gibbs free energy E_G= -580.272473 a.u.

7	N	1.846864	-0.48795	0.020428
6	C	1.246716	-1.74433	0.007174
7	N	-0.05792	-1.95168	-0.00805
6	C	-0.81064	-0.82289	-0.00948
6	C	-0.25383	0.515971	0.00455
6	C	1.138827	0.679091	0.019773
7	N	-1.25539	1.432922	0.0118
6	C	-2.3637	0.625782	-0.00021
7	N	-2.16668	-0.72087	-0.01218
7	N	1.770431	1.88125	-0.00925
1	H	2.745377	1.968311	0.246787
1	H	1.178082	2.694477	0.115466
1	H	-3.36767	1.05299	0.000999
1	H	2.868505	-0.51373	0.01939
6	C	2.196654	-2.86874	0.012616
8	O	3.416484	-2.69823	0.028107
1	H	1.721036	-3.87412	0.001342

C8-CHO-AD_1H E_{tot} = -580.343273 a.u.
Gibbs free energy E_G= -580.261129 a.u.

7	N	1.835315	-0.47635	0.009655
6	C	1.240486	-1.74087	0.003623
7	N	-0.04334	-1.96048	-0.00553
6	C	-0.82271	-0.82845	-0.00965
6	C	-0.27592	0.513957	-0.00282
6	C	1.106961	0.691347	0.008456
7	N	-1.28957	1.4235	0.009079
6	C	-2.38884	0.607748	0.005607
7	N	-2.16397	-0.7525	-0.00364
7	N	1.741318	1.89888	-0.04027
1	H	2.678072	1.995117	0.334269
1	H	1.129326	2.69823	0.092136
1	H	1.952152	-2.57013	0.008581
1	H	2.849093	-0.42994	-0.01768
6	C	-3.73298	1.233221	0.013937
8	O	-4.79521	0.630856	0.014141
1	H	-3.68517	2.352495	0.020193

C2-CHO-AD_1H E_{tot} = -580.339473 a.u.
Gibbs free energy E_G= -580.257639 a.u.

7	N	1.786291	-0.60532	0.009309
6	C	1.173971	-1.86923	0.00744
7	N	-0.13168	-2.04462	-0.00064
6	C	-0.869	-0.90781	-0.0081
6	C	-0.29868	0.428191	-0.00336
6	C	1.090425	0.572917	0.007434
7	N	-1.2907	1.35622	0.006638
6	C	-2.40527	0.559427	0.003585
7	N	-2.22238	-0.79066	-0.00291
7	N	1.74711	1.769864	-0.04379
1	H	2.683871	1.847603	0.33529
1	H	1.148865	2.578428	0.095434
1	H	-3.40546	0.99566	0.008416
1	H	2.803263	-0.58343	-0.01487
6	C	2.135773	-3.00104	0.017516
8	O	1.838329	-4.1804	0.014989
1	H	3.216316	-2.67472	0.02734

C8-Cl-AD_1H E_{tot} = -926.705777 a.u.
Gibbs free energy E_G= -926.640506 a.u.

7	N	1.837789	-0.4892	0.000646
6	C	1.232278	-1.74099	0.00534
7	N	-0.05883	-1.9433	0.001961
6	C	-0.81674	-0.80341	-0.00794
6	C	-0.25652	0.531318	-0.00855
6	C	1.122496	0.690442	-0.00155
7	N	-1.26753	1.459108	0.003135
6	C	-2.3463	0.647837	0.006855
7	N	-2.16447	-0.70921	0.0036
7	N	1.787438	1.891284	-0.06952
1	H	2.67337	1.975032	0.41947
1	H	1.171782	2.690103	0.058749
1	H	1.929619	-2.58196	0.013618
1	H	2.851252	-0.4507	-0.0433
17	Cl	-3.94584	1.308399	0.019091

C2-Cl-AD_1H E_{tot} = -926.702403 a.u.
Gibbs free energy E_G= -926.637384 a.u.

7	N	1.839498	-0.50067	0.003836
6	C	1.214501	-1.73975	0.00555
7	N	-0.06	-1.9451	0.001651
6	C	-0.8258	-0.80317	-0.00911
6	C	-0.26069	0.529465	-0.00784
6	C	1.117217	0.680296	0.000973
7	N	-1.2735	1.45576	0.004548
6	C	-2.36612	0.656237	0.006024
7	N	-2.16716	-0.70805	0.001465
7	N	1.790564	1.872721	-0.06103
1	H	2.693949	1.945781	0.395416
1	H	1.185714	2.678605	0.071615
1	H	-3.37473	1.072794	0.013251
1	H	2.852985	-0.47948	-0.04213
17	Cl	2.34794	-3.07591	0.019723

C8-F-AD_1H E_{tot} = -566.280394 a.u.
Gibbs free energy E_G= -566.212364 a.u

7	N	1.836326	-0.48973	-0.002
6	C	1.232704	-1.73978	0.005166
7	N	-0.05975	-1.94192	0.004103
6	C	-0.81691	-0.80403	-0.00625
6	C	-0.25667	0.533276	-0.0084
6	C	1.120624	0.690954	-0.00312
7	N	-1.27105	1.460369	0.003607
6	C	-2.33347	0.640819	0.008733
7	N	-2.16573	-0.70979	0.00666
7	N	1.791527	1.891161	-0.07474
1	H	2.664229	1.974009	0.438479
1	H	1.174778	2.689995	0.049438
1	H	1.928802	-2.58173	0.013133
1	H	2.849503	-0.44964	-0.05048
9	F	-3.56853	1.148494	0.018907

C2-F-AD_1H E_{tot} = -566.275710 a.u.
Gibbs free energy E_G= -566.208069 a.u

7	N	1.843815	-0.50091	0.004092
6	C	1.207702	-1.72522	0.005575
7	N	-0.05601	-1.9514	0.002792
6	C	-0.82559	-0.80647	-0.00858
6	C	-0.25775	0.52692	-0.00788
6	C	1.117268	0.682431	0.000439
7	N	-1.27365	1.45435	0.004599
6	C	-2.36311	0.65644	0.007624
7	N	-2.16333	-0.71148	0.003321
7	N	1.793902	1.874269	-0.06641
1	H	2.681683	1.951429	0.420228
1	H	1.184008	2.678536	0.055461
1	H	-3.37261	1.070858	0.015243
1	H	2.857219	-0.48724	-0.05111
9	F	2.09651	-2.74372	0.015823

C8-H-AD_1H E_{tot} = -467.069792 a.u.
Gibbs free energy E_G= -466.99272 a.u.

7	N	1.843838	-0.48974	-0.00037
6	C	1.238324	-1.74401	0.005322
7	N	-0.0518	-1.94645	0.002588
6	C	-0.8139	-0.80699	-0.00787
6	C	-0.25316	0.529442	-0.00976
6	C	1.1257	0.687191	-0.00332
7	N	-1.26468	1.454384	0.003038
6	C	-2.35845	0.651982	0.008009
7	N	-2.15946	-0.7083	0.0051
7	N	1.789146	1.88985	-0.07085
1	H	2.673125	1.975185	0.421389
1	H	1.168191	2.684323	0.060485
1	H	1.937806	-2.58348	0.014141
1	H	-3.36668	1.070055	0.017315
1	H	2.857129	-0.45	-0.04418

C2-H-AD_1H E_{tot} = -467.069792 a.u.
Gibbs free energy E_G= -466.99272 a.u.

7	N	1.843838	-0.48974	-0.00037
6	C	1.238324	-1.74401	0.005322
7	N	-0.0518	-1.94645	0.002588
6	C	-0.8139	-0.80699	-0.00787
6	C	-0.25316	0.529442	-0.00976
6	C	1.1257	0.687191	-0.00332
7	N	-1.26468	1.454384	0.003038
6	C	-2.35845	0.651982	0.008009
7	N	-2.15946	-0.7083	0.0051
7	N	1.789146	1.88985	-0.07085
1	H	2.673125	1.975185	0.421389
1	H	1.168191	2.684323	0.060485
1	H	1.937806	-2.58348	0.014141
1	H	-3.36668	1.070055	0.017315
1	H	2.857129	-0.45	-0.04418

C8-Me-AD_1H E_{tot} = -506.371454 a.u.
Gibbs free energy E_G=-506.270763 a.u.

7	N	1.843535	-0.48706	-0.01734
6	C	1.237493	-1.73316	-0.13095
7	N	-0.05357	-1.93059	-0.18135
6	C	-0.81431	-0.79191	-0.11493
6	C	-0.25087	0.539179	0.009985
6	C	1.125494	0.689609	0.062473
7	N	-1.26358	1.459842	0.075298
6	C	-2.36879	0.671633	-0.01406
7	N	-2.15562	-0.69071	-0.12643
7	N	1.801366	1.891636	0.108384
1	H	2.644818	1.92835	0.674259
1	H	1.173207	2.672783	0.282048
1	H	1.934043	-2.57391	-0.1763
1	H	2.857259	-0.44432	-0.04181
6	C	-3.7523	1.235966	0.00874
1	H	-3.71507	2.328406	0.114507
1	H	-4.2866	0.973632	-0.91974
1	H	-4.32803	0.802781	0.843526

C2-Me-AD_1H E_{tot} = -506.370739 a.u.
Gibbs free energy E_G=-506.269624 a.u.

7	N	1.824737	-0.51139	-0.00187
6	C	1.223773	-1.77437	0.005661
7	N	-0.07544	-1.94579	0.004994
6	C	-0.82817	-0.80073	-0.00605
6	C	-0.26165	0.530891	-0.01079
6	C	1.116069	0.67202	-0.0061
7	N	-1.26968	1.463531	0.002705
6	C	-2.36589	0.667497	0.010598
7	N	-2.17315	-0.69559	0.009362
7	N	1.796838	1.866368	-0.07663
1	H	2.675315	1.940506	0.427642
1	H	1.18493	2.668176	0.05293
1	H	-3.3725	1.089643	0.0204
1	H	2.837556	-0.47029	-0.05306
6	C	2.167402	-2.94443	0.017053
1	H	2.823631	-2.94107	-0.87095
1	H	2.810303	-2.9338	0.914613
1	H	1.574576	-3.86642	0.015819

C8-OMe-AD_1H E_{tot} = -581.554600 a.u.
Gibbs free energy E_G= -581.44955 a.u

7	N	1.805936	-0.49501	-0.00723
6	C	1.200013	-1.7403	0.00435
7	N	-0.09658	-1.93558	0.004287
6	C	-0.8491	-0.79565	-0.01086
6	C	-0.28477	0.542683	-0.01496
6	C	1.093523	0.688977	-0.00816
7	N	-1.28876	1.472047	-0.00634
6	C	-2.3805	0.66851	-0.00033
7	N	-2.19397	-0.69607	0.00185
7	N	1.780262	1.888841	-0.08445
1	H	2.600206	1.977537	0.511351
1	H	1.14969	2.681686	0.015694
1	H	1.890976	-2.58629	0.015144
1	H	2.818569	-0.45538	-0.06411
8	O	-3.59844	1.227965	0.00746
6	C	-4.71593	0.310136	0.00971
1	H	-5.60779	0.949931	0.017016
1	H	-4.69561	-0.32326	-0.89025
1	H	-4.68581	-0.3309	0.903948

C2-OMe-AD_1H E_{tot} = -581.555696 a.u.
Gibbs free energy E_G= -581.450664 a.u

7	N	1.827005	-0.54669	0.006125
6	C	1.194045	-1.78279	0.014064
7	N	-0.0935	-1.97076	0.011439
6	C	-0.84244	-0.81663	-0.00369
6	C	-0.26029	0.508381	-0.01021
6	C	1.115771	0.640904	-0.00377
7	N	-1.26624	1.45175	0.000163
6	C	-2.36402	0.667733	0.007319
7	N	-2.18145	-0.7034	0.008653
7	N	1.809574	1.826449	-0.07662
1	H	2.688583	1.8912	0.428086
1	H	1.206457	2.635328	0.049037
1	H	-3.36865	1.094528	0.014367
1	H	2.84021	-0.5412	-0.05129
8	O	2.099784	-2.78712	0.025872
6	C	1.535234	-4.12448	0.023657
1	H	0.923589	-4.27431	-0.87761
1	H	2.404964	-4.792	0.030459
1	H	0.911183	-4.272	0.916699

C8-OMe-AD_1H E_{tot} = -581.554279 a.u.
Gibbs free energy E_G= -581.449095 a.u

7	N	1.856561	-0.52292	-0.013
6	C	1.224597	-1.75528	0.000212
7	N	-0.07334	-1.92728	0.008899
6	C	-0.80785	-0.77195	0.000444
6	C	-0.2127	0.554824	-0.00486
6	C	1.164726	0.67564	-0.00758
7	N	-1.20621	1.501581	0.010464
6	C	-2.31043	0.713514	0.020164
7	N	-2.14689	-0.65241	0.019746
7	N	1.881458	1.860193	-0.08775
1	H	2.697438	1.928038	0.516883
1	H	1.269641	2.666714	0.016954
1	H	1.899327	-2.61486	0.004259
1	H	2.868715	-0.50243	-0.08403
8	O	-3.56009	1.196844	0.032855
6	C	-3.67351	2.635815	0.032144
1	H	-4.75207	2.837895	0.039169
1	H	-3.19019	3.059828	0.926354
1	H	-3.20184	3.057961	-0.86902

C2-OMe-AD_1H E_{tot} = -581.542138 a.u.
Gibbs free energy E_G= -581.437865 a.u

7	N	1.848803	-0.41708	-0.00839
6	C	1.266695	-1.68131	-0.00435
7	N	-0.01535	-1.90644	0.000716
6	C	-0.80504	-0.78786	-0.00762
6	C	-0.27749	0.564845	-0.00651
6	C	1.08821	0.745701	-0.00598
7	N	-1.31978	1.465913	0.013787
6	C	-2.38437	0.635366	0.018763
7	N	-2.14851	-0.72594	0.010994
7	N	1.753768	1.954318	-0.08345
1	H	2.575874	2.059894	0.506518
1	H	1.109904	2.737114	0.009669
1	H	-3.40536	1.02172	0.031537
8	H	2.852576	-0.32365	-0.1112
6	O	2.089585	-2.76382	0.000253
6	C	3.510152	-2.57507	0.017092
1	H	3.859701	-2.05711	-0.89569
1	H	3.833337	-2.02977	0.922623
1	H	3.936343	-3.58511	0.035804

C8-OH-AD_1H E_{tot} = -542.280433 a.u.
Gibbs free energy E_G= -542.199927 a.u.

7	N	1.816125	-0.49437	-0.00733
6	C	1.205483	-1.73724	0.005059
7	N	-0.09085	-1.92938	0.007204
6	C	-0.84026	-0.78664	-0.006
6	C	-0.27037	0.549593	-0.01115
6	C	1.106954	0.692628	-0.00782
7	N	-1.27387	1.485218	-0.00044
6	C	-2.36075	0.687344	0.007085
7	N	-2.18427	-0.67845	0.008173
7	N	1.79695	1.889311	-0.08721
1	H	2.623856	1.974622	0.499115
1	H	1.171787	2.685993	0.014996
1	H	1.893698	-2.58564	0.014322
1	H	2.82875	-0.45839	-0.06641
8	O	-3.59948	1.215709	0.016929
1	H	-4.2109	0.459445	0.020811

C2-OH-AD_1H E_{tot} = -542.279325 a.u.
Gibbs free energy E_G= -542.199126 a.u.

7	N	1.852626	-0.516	0.004206
6	C	1.234392	-1.75244	0.009176
7	N	-0.04849	-1.96464	0.006771
6	C	-0.81667	-0.82282	-0.00635
6	C	-0.24992	0.510874	-0.0092
6	C	1.123218	0.663892	-0.00231
7	N	-1.26818	1.440162	0.002996
6	C	-2.35567	0.642239	0.00777
7	N	-2.15581	-0.72682	0.006375
7	N	1.802484	1.857459	-0.07343
1	H	2.677461	1.934771	0.436679
1	H	1.188289	2.658763	0.047988
1	H	-3.36572	1.055864	0.015606
1	H	2.865393	-0.4947	-0.05611
8	O	2.13575	-2.76893	0.018711
1	H	1.607303	-3.58637	0.015014

C8-OH-AD_1H E_{tot} = -542.279278 a.u.
Gibbs free energy E_G= -542.198816 a.u.

7	N	1.829347	-0.4886	-0.01015
6	C	1.223827	-1.73397	0.004035
7	N	-0.071	-1.9315	0.009978
6	C	-0.82725	-0.79302	-0.00182
6	C	-0.26123	0.54651	-0.00896
6	C	1.114659	0.695331	-0.00852
7	N	-1.27751	1.468365	0.003324
6	C	-2.3616	0.653896	0.013518
7	N	-2.17225	-0.70186	0.015884
7	N	1.805345	1.893637	-0.08878
1	H	2.629087	1.977325	0.502687
1	H	1.181121	2.690102	0.017306
1	H	1.915824	-2.57942	0.011197
1	H	2.841529	-0.44787	-0.07351
8	O	-3.61487	1.146275	0.02405
1	H	-3.52419	2.114505	0.019462

C2-OH-AD_1H E_{tot} = -542.264826 a.u.
Gibbs free energy E_G= -542.186423 a.u.

7	N	1.860778	-0.48852	-0.04538
6	C	1.248802	-1.74352	-0.05383
7	N	-0.03095	-1.94791	-0.0424
6	C	-0.8003	-0.80913	-0.03557
6	C	-0.24588	0.530132	0.007002
6	C	1.124393	0.689312	-0.0067
7	N	-1.26999	1.450289	0.056571
6	C	-2.3513	0.642924	0.034208
7	N	-2.14062	-0.72276	-0.01502
7	N	1.804215	1.886081	-0.06911
1	H	2.661728	1.961674	0.471265
1	H	1.183499	2.682383	0.055877
1	H	-3.36449	1.048281	0.057408
1	H	2.847942	-0.42781	-0.27423
8	O	2.098016	-2.81278	-0.12277
1	H	2.899823	-2.64419	0.396937

C8-NH_2-AD_1H E_{tot} = -522.421093 a.u.
Gibbs free energy E_G= -522.329075 a.u.

7	N	1.821857	-0.49234	-0.02741
6	C	1.21548	-1.73462	-0.00935
7	N	-0.08137	-1.9297	0.017763
6	C	-0.83563	-0.78924	0.024631
6	C	-0.26752	0.551266	0.014924
6	C	1.10838	0.694076	-0.00595
7	N	-1.2755	1.478128	0.042265
6	C	-2.37496	0.67575	0.068735
7	N	-2.17676	-0.69266	0.062461
7	N	1.807606	1.892835	-0.09238
1	H	2.598649	1.982696	0.543099
1	H	1.173336	2.683854	0.002073
1	H	1.90458	-2.58243	-0.01845
1	H	2.83225	-0.45043	-0.11261
7	N	-3.64262	1.187497	0.150532
1	H	-3.75299	2.157641	-0.11676
1	H	-4.39191	0.556552	-0.10547

C2-NH_2-AD_1H E_{tot} = -522.414063 a.u.
Gibbs free energy E_G= -522.322177 a.u.

7	N	1.867562	-0.50066	-0.05628
6	C	1.268699	-1.7602	-0.05508
7	N	-0.0244	-1.96193	-0.03304
6	C	-0.79338	-0.82558	-0.02672
6	C	-0.23962	0.513722	0.007689
6	C	1.130796	0.672629	-0.01391
7	N	-1.26452	1.434731	0.062252
6	C	-2.34543	0.627138	0.050375
7	N	-2.1353	-0.73858	0.003588
7	N	1.807358	1.872476	-0.07883
1	H	2.66835	1.946645	0.456202
1	H	1.185269	2.665748	0.057663
1	H	-3.35857	1.032572	0.080142
1	H	2.857444	-0.44475	-0.2724
7	N	2.164839	-2.82777	-0.15604
1	H	2.936185	-2.80332	0.508435
1	H	1.660408	-3.70925	-0.09495

Table S21. Cartesian coordinates of equilibrium geometries of NX substituted adenine (AD) 9H, 7H, 3H and 1H tautomers.

N9-NO_2-AD_9H E_{tot} = -671.492041 a.u.
Gibbs free energy E_G= -671.419679 a.u.

7	N	3.075438	-0.009967	0.000172
6	C	2.785791	-1.324234	0.000101
7	N	1.576966	-1.929022	0.000073
6	C	0.587013	-1.031651	0.000010
6	C	0.720821	0.369295	-0.000006
6	C	2.045854	0.870583	0.000057
7	N	-0.516285	1.020554	-0.000059
6	C	-1.411119	0.061619	0.000068
7	N	-0.814654	-1.212695	0.000005
7	N	2.320976	2.198131	-0.000386
1	H	3.285411	2.500587	0.001177
1	H	1.571673	2.875653	0.001082
1	H	3.648551	-1.997558	0.000365
1	H	-2.491476	0.165958	0.000098
7	N	-1.562733	-2.447789	0.000013
8	O	-2.779166	-2.307408	0.000331
8	O	-0.910202	-3.470692	0.000254

N9-CN-AD_9H E_{tot} = -559.263292 a.u.
Gibbs free energy E_G= -559.192009 a.u.

7	N	2.701585	-0.026905	0.000157
6	C	2.400440	-1.339361	0.000688
7	N	1.182962	-1.926024	0.000356
6	C	0.212950	-1.010358	0.000267
6	C	0.352256	0.386750	0.000077
6	C	1.685776	0.869443	-0.000176
7	N	-0.886302	1.031726	0.000551
6	C	-1.776775	0.071917	0.000063
7	N	-1.185026	-1.218516	0.000036
7	N	1.982513	2.192212	-0.000805
1	H	2.951901	2.478624	0.001488
1	H	1.245428	2.882884	0.001609
1	H	3.256400	-2.020992	-0.000068
1	H	-2.859268	0.176949	-0.000017
6	C	-1.838178	-2.395507	-0.000152
7	N	-2.440106	-3.401936	-0.000275

N7-NO_2-AD_7H E_{tot} = -671.4901144 a.u.
Gibbs free energy E_G= -671.41608 a.u.

7	N	-3.06426	-0.0483	0.048716
6	C	-2.74386	-1.35259	0.087473
7	N	-1.52304	-1.91601	0.051302
6	C	-0.53534	-1.01093	0.008296
6	C	-0.73839	0.392584	0.013428
6	C	-2.07208	0.873166	-0.02083
7	N	0.569442	0.91627	-0.09651
6	C	1.455828	-0.18047	-0.1253
7	N	0.833249	-1.32502	-0.07293
7	N	-2.44421	2.17163	-0.17177
1	H	-3.43052	2.366275	-0.05002
1	H	-1.76584	2.900924	0.009197
1	H	-3.592	-2.0425	0.146075
1	H	2.528461	-0.01473	-0.17337
7	N	1.031958	2.246792	0.109752
8	O	0.193977	3.075621	0.457497
8	O	2.22501	2.432731	-0.07979

N7-CN-AD_7H E_{tot} = -559.256945 a.u.
Gibbs free energy E_G= -559.186408 a.u.

7	N	-2.69055	-0.03091	0.035411
6	C	-2.37146	-1.34331	0.023268
7	N	-1.15698	-1.91725	-0.00054
6	C	-0.15779	-1.01634	-0.01179
6	C	-0.37287	0.376347	-0.001
6	C	-1.69058	0.877746	0.021718
7	N	0.917929	0.950648	-0.01759
6	C	1.821281	-0.14327	-0.03742
7	N	1.216158	-1.29945	-0.035
7	N	-2.01811	2.199233	0.017204
1	H	-2.99787	2.441892	0.080521
1	H	-1.32089	2.928828	0.067306
1	H	-3.22616	-2.02723	0.034941
1	H	2.893943	0.039487	-0.05223
6	C	1.219311	2.257667	-0.0069
7	N	1.451731	3.409719	0.004696

N9-CHO-AD_9H E_{tot} = -580.374927 a.u.
Gibbs free energy E_G= -580.293037 a.u.

7	N	2.744507	-0.235900	0.000188
6	C	2.301101	-1.506963	-0.000104
7	N	1.026912	-1.957136	-0.000144
6	C	0.156390	-0.939526	-0.000190
6	C	0.455421	0.431478	-0.000065
6	C	1.831625	0.766475	0.000142
7	N	-0.710496	1.206354	-0.000355
6	C	-1.696693	0.337886	0.000088
7	N	-1.250211	-0.998650	0.000031
7	N	2.271668	2.049652	-0.000506
1	H	3.266142	2.229982	0.001736
1	H	1.612548	2.815148	0.001639
1	H	3.078234	-2.277574	0.000388
1	H	-2.759786	0.563381	0.000238
6	C	-2.040600	-2.165596	0.000212
8	O	-3.255316	-2.143632	0.000225
1	H	-1.414883	-3.081083	0.000244

N9-CHO-AD_9H E_{tot} = -580.367327 a.u.
Gibbs free energy E_G= -580.285083 a.u.

7	N	2.829687	-0.290032	0.000066
6	C	2.414950	-1.572474	0.000336
7	N	1.155530	-2.057890	0.000194
6	C	0.252752	-1.069693	0.000140
6	C	0.523524	0.311043	-0.000008
6	C	1.890042	0.684220	-0.000166
7	N	-0.650901	1.071436	0.000364
6	C	-1.617521	0.185400	0.000039
7	N	-1.158114	-1.148565	0.000076
7	N	2.291016	1.981124	-0.000799
1	H	3.279680	2.190620	0.001609
1	H	1.609197	2.726222	0.001652
1	H	3.211422	-2.323298	0.000032
1	H	-2.683730	0.405767	0.000020
6	C	-2.014575	-2.271879	0.000005
8	O	-1.654413	-3.425705	-0.000028
1	H	-3.082074	-1.949620	0.000080

N7-CHO-AD_7H E_{tot} = -580.371250 a.u.
Gibbs free energy E_G= -580.287887 a.u.

7	N	-2.82581	0.188357	0.030636
6	C	-2.60311	-1.13892	0.012089
7	N	-1.43124	-1.79929	-0.01165
6	C	-0.37481	-0.96968	-0.01645
6	C	-0.47225	0.439213	0.001274
6	C	-1.76072	1.028716	0.025865
7	N	0.863568	0.902896	-0.01164
6	C	1.662068	-0.26481	-0.03616
7	N	0.974726	-1.37286	-0.03962
7	N	-1.99969	2.360637	0.04468
1	H	-2.96243	2.668359	0.061535
1	H	-1.2224	3.015703	0.041572
1	H	-3.50418	-1.76146	0.017204
1	H	2.748618	-0.18635	-0.05013
6	C	1.394297	2.188458	-0.00404
8	O	0.74628	3.224504	0.016704
1	H	2.504262	2.170943	-0.01925

N7-CHO-AD_7H E_{tot} = -580.362767 a.u.
Gibbs free energy E_G= -580.27991 a.u.

7	N	-2.72643	0.156198	-0.03273
6	C	-2.53719	-1.1793	-0.04222
7	N	-1.37889	-1.85769	0.002623
6	C	-0.30371	-1.05362	0.022024
6	C	-0.37285	0.360776	-0.00431
6	C	-1.64565	0.964271	0.000403
7	N	0.969323	0.795639	0.001528
6	C	1.745875	-0.38133	0.043379
7	N	1.033892	-1.47855	0.057239
7	N	-1.88156	2.326517	-0.02012
1	H	-2.85771	2.557447	0.143859
1	H	-1.23031	2.923931	0.476716
1	H	-3.45082	-1.78117	-0.07764
1	H	2.83096	-0.31192	0.049127
6	C	1.495604	2.092409	-0.11808
8	O	2.686155	2.336609	-0.10238
1	H	0.709247	2.86498	-0.24622

N9-Cl-AD_9H E_{tot} = -926.679501 a.u.
Gibbs free energy E_G= -926.61612 a.u.

7	N	-2.813263	-0.031582	0.010803
6	C	-2.501077	-1.344464	0.004543
7	N	-1.283828	-1.923309	-0.00297
6	C	-0.312389	-1.001406	-0.00256
6	C	-0.465135	0.399257	0.002792
6	C	-1.803147	0.868714	0.007798
7	N	0.765089	1.055549	0.005446
6	C	1.664284	0.088161	0.000623
7	N	1.068107	-1.170600	-0.00488
7	N	-2.106724	2.192875	-0.00685
1	H	-3.074814	2.471794	0.075864
1	H	-1.371716	2.881319	0.073814
1	H	-3.354046	-2.030472	0.006672
1	H	2.745850	0.197955	0.000728
17	Cl	1.894575	-2.681357	-0.01067

N9-F-AD_9H E_{tot} = -566.212576 a.u.
Gibbs free energy E_G= -566.149434 a.u

7	N	-2.420863	-0.153021	0.018612
6	C	-2.029488	-1.444873	0.003636
7	N	-0.781008	-1.952904	-0.006947
6	C	0.130221	-0.969674	-0.000767
6	C	-0.103011	0.422643	0.014515
6	C	-1.468545	0.807711	0.024368
7	N	1.080350	1.157816	0.016989
6	C	2.046185	0.252334	0.003543
7	N	1.513205	-1.023904	-0.007128
7	N	-1.851221	2.109529	0.039282
1	H	-2.836826	2.332922	0.046444
1	H	-1.159120	2.845250	0.044523
1	H	-2.840201	-2.180417	-0.000426
1	H	3.119039	0.424615	0.000723
9	F	2.261545	-2.177326	-0.022663

N9-H-AD_9H E_{tot} = -467.096786 a.u.
Gibbs free energy E_G= -467.019892 a.u.

7	N	1.962029	0.527275	0.004592
6	C	1.304445	1.706449	0.002924
7	N	-0.02351	1.934087	-0.00124
6	C	-0.71338	0.780032	-0.00262
6	C	-0.17923	-0.52523	-0.00271
6	C	1.234633	-0.6137	-0.00179
7	N	-1.18892	-1.48459	0.002006
6	C	-2.30842	-0.7791	0.002786
7	N	-2.08635	0.591594	-0.00028
7	N	1.889474	-1.80705	-0.03371
1	H	2.892382	-1.80781	0.096014
1	H	1.367686	-2.66248	0.09916
1	H	1.940976	2.597346	0.008033
1	H	-3.31484	-1.19342	0.006012
1	H	-2.78351	1.326384	-0.00041

N7-Cl-AD_7H E_{tot} = -926.670997 a.u.
Gibbs free energy E_G= -926.60822 a.u.

7	N	-2.80994	-0.06949	0.017768
6	C	-2.47553	-1.38183	0.008677
7	N	-1.25707	-1.93534	-0.00542
6	C	-0.26094	-1.02558	-0.00659
6	C	-0.4934	0.373434	0.000519
6	C	-1.82357	0.847701	0.007338
7	N	0.788468	0.920042	-0.01854
6	C	1.701343	-0.11971	-0.01863
7	N	1.104268	-1.29765	-0.02061
7	N	-2.17925	2.171512	-0.04328
1	H	-3.15529	2.369302	0.144027
1	H	-1.50309	2.88129	0.204152
1	H	-3.32272	-2.07531	0.015881
1	H	2.772026	0.07174	-0.0225
17	Cl	1.200857	2.610378	0.058586

N7-F-AD_7H E_{tot} = -566.205716 a.u.
Gibbs free energy E_G= -566.141068 a.u

7	N	-2.41746	-0.18549	0.027054
6	C	-2.00367	-1.47591	0.019985
7	N	-0.75362	-1.95657	-0.00561
6	C	0.1879	-0.99223	-0.00537
6	C	-0.13359	0.389182	0.001511
6	C	-1.48697	0.786921	0.003553
7	N	1.107094	0.994942	-0.10065
6	C	2.094015	0.033891	-0.03796
7	N	1.569943	-1.18118	-0.04036
7	N	-1.90212	2.091333	-0.05353
1	H	-2.88617	2.252387	0.126297
1	H	-1.25617	2.831819	0.185109
1	H	-2.80726	-2.2191	0.035566
1	H	3.148841	0.297721	-0.03675
9	F	1.333613	2.347926	0.200396

N7-H-AD_7H E_{tot} = -467.085338 a.u.
Gibbs free energy E_G= -467.00833 a.u.

7	N	-1.96277	-0.50017	-0.01
6	C	-1.32248	-1.69578	-0.00871
7	N	-0.0069	-1.94233	0.012901
6	C	0.742057	-0.8186	0.01347
6	C	0.182197	0.48572	-0.00383
6	C	-1.2189	0.620205	-0.00265
7	N	1.272567	1.348798	-0.01317
6	C	2.402066	0.548237	-0.00608
7	N	2.131882	-0.74505	0.016318
7	N	-1.87607	1.839342	-0.05822
1	H	-2.87193	1.76392	0.130168
1	H	-1.4308	2.624304	0.404726
1	H	-1.98003	-2.57131	-0.01873
1	H	3.400837	0.982174	-0.01724

N9-Me-AD_9H E_{tot} = -506.385688 a.u.
Gibbs free energy E_G= -506.283306 a.u.

7	N	-2.450516	-0.103569	0.009877
6	C	-2.083262	-1.403057	0.006481
7	N	-0.843296	-1.930292	-0.000717
6	C	0.094587	-0.965434	-0.002740
6	C	-0.124525	0.427846	-0.001128
6	C	-1.479411	0.839344	0.002305
7	N	1.080340	1.123197	0.002965
6	C	2.000718	0.169386	0.001831
7	N	1.472158	-1.114897	-0.002203
7	N	-1.842904	2.152234	-0.030960
1	H	-2.816749	2.381943	0.116650
1	H	-1.137460	2.861610	0.114693
1	H	-2.908600	-2.122618	0.011991
1	H	3.077584	0.332237	0.004023
6	C	2.191342	-2.381488	-0.003453
1	H	1.926846	-2.966437	0.890166
1	H	1.927557	-2.964163	-0.898744
1	H	3.269596	-2.173625	-0.002827

N9-OMe-AD_9H E_{tot} = -581.508846 a.u.
Gibbs free energy E_G= -581.405627 a.u.

7	N	-2.510247	0.037766	-0.391422
6	C	-2.198395	-1.274229	-0.329004
7	N	-1.020709	-1.850729	-0.017466
6	C	-0.089209	-0.921640	0.258895
6	C	-0.248257	0.480013	0.231682
6	C	-1.541527	0.942143	-0.117268
7	N	0.928927	1.141277	0.572816
6	C	1.801912	0.169407	0.794762
7	N	1.242028	-1.086467	0.615578
7	N	-1.837083	2.267341	-0.214445
1	H	-2.804804	2.534803	-0.336688
1	H	-1.169525	2.948552	0.120960
1	H	-3.017382	-1.962058	-0.563158
1	H	2.840565	0.281035	1.097021
8	O	1.890796	-2.276989	0.870633
6	C	2.145052	-2.986402	-0.374840
1	H	2.678234	-3.895158	-0.065137
1	H	1.192975	-3.243140	-0.862516
1	H	2.777799	-2.371971	-1.036586
1	H	1.261259	2.358063	-0.08695

N7-Me-AD_7H E_{tot} = -506.37318104 a.u.
Gibbs free energy E_G= -506.270869 a.u.

7	N	2.446743	-0.14999	0.009402
6	C	2.057048	-1.44874	-0.00936
7	N	0.816832	-1.94935	-0.03205
6	C	-0.13973	-0.99552	-0.01999
6	C	0.147375	0.397285	0.010573
6	C	1.49752	0.803244	0.018128
7	N	-1.09358	1.031363	0.039096
6	C	-2.03139	0.015335	0.017295
7	N	-1.51288	-1.20176	-0.01895
7	N	1.922128	2.121822	0.1011
1	H	2.914047	2.228108	-0.09156
1	H	1.339939	2.82766	-0.33339
1	H	2.875441	-2.17637	-0.01296
1	H	-3.0969	0.244056	0.033242
6	C	-1.37121	2.459976	0.087823
1	H	-0.84714	2.923233	0.937307
1	H	-1.06715	2.953372	-0.8506
1	H	-2.45227	2.601812	0.219406

N7-OMe-AD_7H E_{tot} = -581.501347 a.u.
Gibbs free energy E_G= -581.397678 a.u.

7	N	-2.53626	-0.35058	0.323233
6	C	-1.94163	-1.50205	0.729734
7	N	-0.64819	-1.84254	0.680655
6	C	0.139075	-0.87098	0.168613
6	C	-0.3744	0.378346	-0.26526
6	C	-1.75965	0.617505	-0.19282
7	N	0.74333	1.068171	-0.71135
6	C	1.842231	0.253733	-0.53159
7	N	1.517218	-0.92331	-0.01428
7	N	-2.34603	1.81091	-0.57093
1	H	-3.35613	1.760662	-0.66067
1	H	-1.87391	2.337653	-1.29776
1	H	-2.62441	-2.25098	1.144179
1	H	2.839577	0.584679	-0.81426
8	O	0.763669	2.365429	-1.20413
6	C	0.847447	3.314218	-0.10088
1	H	-0.03796	3.22091	0.547772
1	H	1.77189	3.144644	0.473627
1	H	0.869213	4.299656	-0.58569

N9-OH-AD_9H E_{tot} = -542.229559 a.u.
Gibbs free energy E_G= -542.152512 a.u.

7	N	-2.305009	-0.204970	-0.042086
6	C	-1.853037	-1.475369	-0.093507
7	N	-0.576833	-1.912508	-0.080414
6	C	0.273483	-0.875755	-0.005510
6	C	-0.023402	0.499803	0.055895
6	C	-1.407512	0.808426	0.034837
7	N	1.136007	1.262268	0.122557
6	C	2.127457	0.373339	0.103196
7	N	1.647577	-0.918968	0.027065
7	N	-1.870580	2.083049	0.099941
1	H	-2.865064	2.248886	0.029327
1	H	-1.222714	2.858162	0.102415
1	H	-2.624935	-2.248814	-0.154308
1	H	3.192765	0.584911	0.140208
8	O	2.417125	-2.073211	-0.011583
1	H	1.740027	-2.779454	-0.064406

N7-OH-AD_7H E_{tot} = -542.219894 a.u.
Gibbs free energy E_G= -542.14133 a.u.

7	N	-2.38376	-0.12831	0.13653
6	C	-2.00841	-1.43297	0.114493
7	N	-0.77869	-1.95154	0.015696
6	C	0.190107	-1.0126	-0.0563
6	C	-0.08837	0.377706	-0.02098
6	C	-1.42567	0.811945	0.066478
7	N	1.162893	0.972569	-0.08982
6	C	2.105878	-0.02905	-0.19567
7	N	1.559197	-1.23555	-0.16685
7	N	-1.7939	2.140213	0.134858
1	H	-2.7849	2.303951	-0.01177
1	H	-1.17014	2.814024	-0.29445
1	H	-2.83295	-2.15038	0.179653
1	H	3.164979	0.203483	-0.28749
8	O	1.415166	2.342025	-0.1898
1	H	1.535616	2.640703	0.730742

N9-NH_2-AD_9H E_{tot} = -522.395376 a.u.
Gibbs free energy E_G= -522.297862 a.u.

7	N	2.380696	-0.164701	0.078897
6	C	1.979598	-1.452799	0.093225
7	N	0.724962	-1.946608	0.046701
6	C	-0.178350	-0.954815	-0.023435
6	C	0.072554	0.430527	-0.047080
6	C	1.437249	0.805318	0.011817
7	N	-1.112897	1.158866	-0.130738
6	C	-2.062925	0.236648	-0.155738
7	N	-1.562133	-1.056921	-0.093003
7	N	1.836036	2.106226	0.027819
1	H	2.823544	2.309695	-0.048243
1	H	1.158404	2.835760	-0.145995
1	H	2.783363	-2.194158	0.148709
1	H	-3.134771	0.411760	-0.217875
7	N	-2.348879	-2.220731	-0.104496
1	H	-2.029775	-2.795552	-0.890194
1	H	-2.120496	-2.750431	0.742201

N7-NH_2-AD_7H E_{tot} = -522.384077 a.u.
Gibbs free energy E_G= -522.292721 a.u.

7	N	-2.12393	0.625906	-0.07454
6	C	-2.34242	-0.71339	-0.09109
7	N	-1.45503	-1.71394	-0.02447
6	C	-0.17887	-1.27892	0.08035
6	C	0.166873	0.092241	0.110552
6	C	-0.85333	1.061854	0.019326
7	N	1.552105	0.117297	0.226936
6	C	1.966397	-1.2065	0.262553
7	N	0.966373	-2.06777	0.176647
7	N	-0.6077	2.409811	-0.02213
1	H	-1.40515	3.021511	0.100249
1	H	0.310055	2.73795	0.252611
1	H	-3.39487	-1.00595	-0.17013
1	H	3.022307	-1.46061	0.355977
7	N	2.320652	1.293652	0.335376
1	H	2.871907	1.245883	1.195308
1	H	2.96801	1.337992	-0.45529

N3-NO_2-AD_3H E_{tot} = -671.477355 a.u.
Gibbs free energy E_G= -671.403201 a.u.

7	N	-2.7773	0.027249	0.0004
6	C	-2.52707	-1.25953	7.52E-05
7	N	-1.26534	-1.81187	-0.00025
6	C	-0.15275	-0.97858	-0.0002
6	C	-0.40536	0.435891	0.000162
6	C	-1.72224	0.914953	0.000426
7	N	0.804574	1.085182	0.000267
6	C	1.681111	0.061891	-8.4E-05
7	N	1.164392	-1.22254	-0.00032
7	N	-2.03047	2.229246	0.000536
1	H	-2.99894	2.51909	0.00163
1	H	-1.28541	2.913659	0.001334
1	H	-3.3461	-1.97689	5.04E-05
1	H	2.7599	0.220202	-9.3E-05
7	N	-1.16273	-3.33664	-0.00068
8	O	-0.03913	-3.7683	-0.0012
8	O	-2.23121	-3.9196	-0.00024

N1-NO_2-AD_1H E_{tot} = -671.46525243 a.u.
Gibbs free energy E_G= -671.392863a.u.

7	N	2.656686	0.24338	0.011821
6	C	2.502994	-1.17429	0.011646
7	N	1.360796	-1.78633	0.012885
6	C	0.249064	-0.97894	0.006173
6	C	0.327018	0.454863	0.017978
6	C	1.551423	1.118154	0.015819
7	N	-0.9407	0.985578	0.009605
6	C	-1.69917	-0.13504	-0.00432
7	N	-1.04413	-1.34975	-0.00626
7	N	1.647155	2.462755	-0.06229
1	H	2.507471	2.944408	0.155964
1	H	0.755688	2.946426	-0.02149
1	H	3.447904	-1.71175	0.024863
1	H	-2.78896	-0.08555	-0.01111
7	N	4.040067	0.738297	0.035553
8	O	4.901758	-0.07913	-0.21965
8	O	4.198566	1.918163	0.323123

N3-CN-AD_3H E_{tot} = -559.245777 a.u.
Gibbs free energy E_G= -559.173896 a.u.

7	N	-2.77514	0.005039	0.000294
6	C	-2.54144	-1.27687	2.19E-05
7	N	-1.26724	-1.85239	-0.00027
6	C	-0.16932	-0.98391	-0.00021
6	C	-0.40507	0.422687	9.14E-05
6	C	-1.72256	0.901019	0.000283
7	N	0.819897	1.050807	0.00031
6	C	1.677521	0.009539	-0.00026
7	N	1.131584	-1.2668	-0.0003
7	N	-2.04057	2.212037	0.000129
1	H	-3.01088	2.495988	0.002036
1	H	-1.30106	2.902502	0.001626
1	H	-3.365	-1.99348	4E-05
1	H	2.758718	0.148425	-0.00021
6	C	-1.129	-3.20313	-0.00055
7	N	-1.06102	-4.37267	-0.00078

N1-CN-AD_1H E_{tot} = -559.234917 a.u.
Gibbs free energy E_G= -559.165285 a.u.

7	N	2.663727	0.240794	0.024688
6	C	2.51102	-1.18871	-0.0039
7	N	1.371089	-1.79331	-0.02279
6	C	0.257725	-0.9846	-0.01417
6	C	0.322554	0.457298	0.014199
6	C	1.54886	1.10367	0.034375
7	N	-0.9501	0.973484	0.016141
6	C	-1.6971	-0.15437	-0.01042
7	N	-1.03171	-1.36268	-0.0296
7	N	1.743437	2.438327	0.061228
1	H	2.662832	2.860819	0.07593
1	H	0.917644	3.023942	0.067534
1	H	3.464585	-1.71948	-0.00812
1	H	-2.78729	-0.11543	-0.0165
6	C	3.907769	0.766064	0.042725
7	N	4.977422	1.24908	0.058885

N3-CHO-AD_3H E_{tot} = -580.360120 a.u.
Gibbs free energy E_G= -580.27727 a.u.

7	N	-2.81742	0.167658	0.000128
6	C	-2.71025	-1.13648	-3.7E-05
7	N	-1.51578	-1.83841	-9.6E-05
6	C	-0.33895	-1.09138	-2.5E-05
6	C	-0.41172	0.331053	0.00014
6	C	-1.67226	0.944424	0.000204
7	N	0.874989	0.824711	0.00069
6	C	1.613536	-0.30296	-0.00068
7	N	0.931896	-1.51144	0.000157
7	N	-1.85054	2.281935	0.000175
1	H	-2.78689	2.663566	0.001551
1	H	-1.04344	2.891916	0.001408
1	H	-3.604	-1.76174	-3.6E-05
1	H	2.703656	-0.28212	-0.00035
6	C	-1.49166	-3.27221	-0.00018
8	O	-2.49661	-3.94893	-0.00017
1	H	-0.45082	-3.64914	-6.2E-05

N1-CHO-AD_1H E_{tot} = -580.339335 a.u.
Gibbs free energy E_G= -580.256612 a.u.

7	N	2.682397	0.133981	0.023441
6	C	2.507068	-1.27607	0.067464
7	N	1.363567	-1.89071	0.050699
6	C	0.2572	-1.07735	-0.01431
6	C	0.341987	0.365783	-0.04657
6	C	1.571717	0.991625	0.007244
7	N	-0.9278	0.899153	-0.04941
6	C	-1.68627	-0.21665	-0.03309
7	N	-1.0352	-1.43815	-0.0003
7	N	1.738374	2.357876	-0.00684
1	H	2.431454	2.763706	0.614171
1	H	0.839273	2.83367	0.040359
1	H	3.450507	-1.82023	0.099519
1	H	-2.77627	-0.16678	-0.03925
6	C	4.009798	0.637719	-0.12443
8	O	5.00343	-0.04652	-0.01227
1	H	4.02893	1.713806	-0.38612

N3-CHO-AD_3H E_{tot} = -580.351426 a.u.
Gibbs free energy E_G= -580.269146 a.u.

7	N	-2.70587	0.178098	0.000313
6	C	-2.55931	-1.11987	0.000141
7	N	-1.35554	-1.81146	-9.2E-05
6	C	-0.18793	-1.04419	-8.7E-05
6	C	-0.30803	0.382933	9.2E-05
6	C	-1.57654	0.975815	0.000251
7	N	0.956436	0.921791	0.000143
6	C	1.733898	-0.18154	-7.7E-06
7	N	1.09886	-1.41164	-0.00014
7	N	-1.77495	2.310673	9.2E-05
1	H	-2.71574	2.680627	0.001536
1	H	-0.9749	2.930064	0.001114
1	H	-3.4516	-1.75128	0.00019
1	H	2.822858	-0.12243	-1E-05
6	C	-1.41108	-3.24592	-0.0003
8	O	-0.45212	-3.97389	-0.00052
1	H	-2.46932	-3.59287	-0.00019

N1-CHO-AD_1H E_{tot} = -580.347637 a.u.
Gibbs free energy E_G= -580.264507 a.u.

7	N	2.674345	0.288923	0.005122
6	C	2.517332	-1.13291	-0.01834
7	N	1.393466	-1.77108	-0.02806
6	C	0.267558	-0.97659	-0.01397
6	C	0.321466	0.461053	0.009918
6	C	1.540615	1.129849	0.02001
7	N	-0.95657	0.966886	0.019343
6	C	-1.69464	-0.16599	0.001081
7	N	-1.01813	-1.36963	-0.01951
7	N	1.673777	2.469452	0.042029
1	H	2.590322	2.902331	0.048634
1	H	0.815109	3.006575	0.052018
1	H	3.467892	-1.67118	-0.02798
6	H	-2.7853	-0.13707	0.002477
1	C	3.996225	0.776626	0.012002
1	O	4.316658	1.952708	0.031242
8	H	4.735718	-0.04976	-0.00243

N3-Cl-AD_3H E_{tot} = -926.669178 a.u.
Gibbs free energy E_G= -926.605777 a.u.

7	N	-2.78318	0.029191	0.000415
6	C	-2.54584	-1.26662	0.000168
7	N	-1.28957	-1.80613	-0.00035
6	C	-0.18704	-0.98552	-0.00042
6	C	-0.41517	0.430865	-0.00014
6	C	-1.73654	0.913298	0.000174
7	N	0.808648	1.051031	-0.00057
6	C	1.665108	0.006326	0.000617
7	N	1.120357	-1.26408	-0.00078
7	N	-2.03281	2.234643	-0.00049
1	H	-2.99709	2.535912	0.002599
1	H	-1.2813	2.9109	0.001832
1	H	-3.36908	-1.98193	0.000289
1	H	2.746258	0.145058	0.000346
17	Cl	-1.10206	-3.55386	-0.00074

N1-Cl-AD_1H E_{tot} = -926.654125 a.u.
Gibbs free energy E_G= -926.590587 a.u.

7	N	2.633253	0.220162	0.003839
6	C	2.507219	-1.17674	0.004585
7	N	1.356754	-1.78511	-0.00784
6	C	0.244851	-0.98511	-0.01426
6	C	0.31428	0.453804	-0.01017
6	C	1.557079	1.092119	-0.00311
7	N	-0.94717	0.980988	-0.0032
6	C	-1.70473	-0.14925	-0.00551
7	N	-1.05305	-1.357	-0.01156
7	N	1.729864	2.438417	-0.05745
1	H	2.601808	2.853112	0.246752
1	H	0.879231	2.974822	0.078561
1	H	3.456401	-1.71383	0.01611
1	H	-2.79488	-0.09768	-0.00126
17	Cl	4.258061	0.884796	0.039076

N3-F-AD_3H E_{tot} = -566.205357 a.u.
Gibbs free energy E_G= -566.140402 a.u.

7	N	-2.79193	0.033398	0.000232
6	C	-2.5517	-1.26487	8.72E-05
7	N	-1.29448	-1.77683	-0.00032
6	C	-0.17656	-0.98886	-0.00039
6	C	-0.41728	0.42757	-0.00022
6	C	-1.7406	0.911017	1.46E-05
7	N	0.804483	1.049975	-0.00027
6	C	1.666947	0.009941	0.000238
7	N	1.131881	-1.26556	-0.00063
7	N	-2.02974	2.234132	-0.00057
1	H	-2.99237	2.540495	0.002776
1	H	-1.27483	2.906609	0.002011
1	H	-3.36158	-1.99544	0.000197
1	H	2.747514	0.154001	0.000279
9	F	-1.16951	-3.16962	-0.00044

N1-F-AD_1H E_{tot} = -566.192113 a.u.
Gibbs free energy E_G= -566.126786 a.u.

7	N	2.586115	0.209885	0.000213
6	C	2.503965	-1.17488	0.006816
7	N	1.352731	-1.79269	-0.00444
6	C	0.24316	-0.9892	-0.01311
6	C	0.298387	0.456345	-0.01196
6	C	1.537952	1.100457	-0.0037
7	N	-0.96585	0.971803	-0.00836
6	C	-1.7141	-0.16626	-0.00882
7	N	-1.05388	-1.36682	-0.01167
7	N	1.75796	2.439718	-0.05575
1	H	2.652107	2.81653	0.230666
1	H	0.933034	3.00913	0.098098
1	H	3.465811	-1.68906	0.020065
1	H	-2.80445	-0.12243	-0.00582
9	F	3.868404	0.771293	0.04035

N3-H-AD_3H E_{tot} = -467.085495 a.u.
Gibbs free energy E_G= -467.008726 a.u.

7	N	1.956751	0.45435	0.000391
6	C	1.376085	1.637636	0.000118
7	N	0.027617	1.844188	-0.00022
6	C	-0.80757	0.749745	0.000092
6	C	-0.23136	-0.55468	0.000106
6	C	1.170301	-0.6737	-6.9E-05
7	N	-1.256	-1.47343	0.000079
6	C	-2.3504	-0.67884	0.000098
7	N	-2.14758	0.689367	-5.4E-05
7	N	1.805039	-1.86988	-0.00118
1	H	2.814875	-1.90314	0.00295
1	H	1.259925	-2.72134	0.002325
1	H	1.998167	2.535542	0.000062
1	H	-3.3607	-1.09023	0.000181
1	H	-0.35538	2.786045	-0.00071

N1-H-AD_1H E_{tot} = -467.069792 a.u.
Gibbs free energy E_G= -466.99272 a.u.

7	N	1.843838	-0.48974	-0.00037
6	C	1.238324	-1.74401	0.005322
7	N	-0.0518	-1.94645	0.002588
6	C	-0.8139	-0.80699	-0.00787
6	C	-0.25316	0.529442	-0.00976
6	C	1.1257	0.687191	-0.00332
7	N	-1.26468	1.454384	0.003038
6	C	-2.35845	0.651982	0.008009
7	N	-2.15946	-0.7083	0.0051
7	N	1.789146	1.88985	-0.07085
1	H	2.673125	1.975185	0.421389
1	H	1.168191	2.684323	0.060485
1	H	1.937806	-2.58348	0.014141
1	H	-3.36668	1.070055	0.017315
1	H	2.857129	-0.45	-0.04418

N3-Me-AD_3H E_{tot} = -506.375091 a.u.
Gibbs free energy E_G= -506.274446 a.u.

7	N	2.433879	-0.03502	-0.00038
6	C	2.132468	-1.32064	-0.00034
7	N	0.872358	-1.84534	-4.1E-05
6	C	-0.17634	-0.95029	0.000148
6	C	0.083123	0.451046	0.000169
6	C	1.419235	0.887757	4.86E-05
7	N	-1.12589	1.109401	-0.0001
6	C	-2.00879	0.086039	0.00031
7	N	-1.49708	-1.19853	-1.5E-05
7	N	1.766694	2.197921	0.001489
1	H	2.742485	2.459345	-0.00503
1	H	1.042711	2.903242	-0.00384
1	H	2.946441	-2.05004	-0.0007
1	H	-3.08674	0.254249	0.000125
6	C	0.612774	-3.28982	5.17E-05
1	H	0.029884	-3.55391	0.89405
1	H	0.027508	-3.55348	-0.8925
1	H	1.572452	-3.82277	-0.00133

N1-Me-AD_1H E_{tot} = -506.356916 a.u.
Gibbs free energy E_G= -506.254292 a.u.

7	N	2.662128	0.234278	0.010102
6	C	2.494049	-1.15377	0.033182
7	N	1.352484	-1.78851	0.026004
6	C	0.244131	-0.98728	-0.00241
6	C	0.321675	0.454198	-0.018
6	C	1.564767	1.074732	-0.00841
7	N	-0.94187	0.985295	-0.02402
6	C	-1.7024	-0.1405	-0.01487
7	N	-1.05674	-1.35255	0.000867
7	N	1.739022	2.437828	-0.09845
1	H	2.513371	2.862052	0.400795
1	H	0.859505	2.937655	0.008365
1	H	3.432492	-1.71321	0.059074
1	H	-2.79254	-0.08601	-0.01769
6	C	4.014637	0.79914	-0.00635
1	H	4.126665	1.480111	-0.86342
1	H	4.224933	1.343454	0.929327
1	H	4.735788	-0.02087	-0.10197

N3-OMe-AD_3H E_{tot} = -581.500654 a.u.
Gibbs free energy E_G= -581.397613 a.u.

7	N	-2.67211	-0.08031	-0.10663
6	C	-2.3482	-1.35395	0.029047
7	N	-1.07675	-1.81068	0.198799
6	C	-0.03107	-0.91541	0.237496
6	C	-0.33896	0.471363	0.079519
6	C	-1.68055	0.864214	-0.08684
7	N	0.840908	1.174803	0.14876
6	C	1.752992	0.195308	0.331347
7	N	1.288963	-1.1062	0.393596
7	N	-2.04721	2.160154	-0.24557
1	H	-3.02795	2.400177	-0.28496
1	H	-1.34528	2.883596	-0.16623
1	H	-3.11731	-2.12793	0.024922
1	H	2.818209	0.408162	0.428407
8	O	-0.90237	-3.17445	0.43292
6	C	-0.15726	-3.78749	-0.6587
1	H	-0.70431	-3.65551	-1.60699
1	H	0.852475	-3.35657	-0.71303
1	H	-0.11537	-4.84953	-0.38314

N1-OMe-AD_1H E_{tot} = -581.487770 a.u.
Gibbs free energy E_G= -581.383897 a.u.

7	N	2.560577	0.518413	-0.11374
6	C	2.560108	-0.85331	0.117397
7	N	1.474944	-1.56455	0.274565
6	C	0.301352	-0.86291	0.190088
6	C	0.236649	0.559261	-0.07123
6	C	1.416246	1.279827	-0.23667
7	N	-1.0708	0.960587	-0.12982
6	C	-1.71878	-0.21225	0.100211
7	N	-0.95917	-1.3377	0.296345
7	N	1.521052	2.628317	-0.43966
1	H	2.339315	2.957343	-0.94083
1	H	0.638822	3.063554	-0.69096
1	H	3.557973	-1.29519	0.143636
1	H	-2.80897	-0.25864	0.12635
8	O	3.791816	1.156387	-0.28211
6	C	4.291493	1.615728	1.008648
1	H	5.238727	2.117999	0.770762
1	H	3.579737	2.32123	1.464316
1	H	4.466672	0.75491	1.672768

N3-OH-AD_3H E_{tot} = -542.223954 a.u.
Gibbs free energy E_G= -542.14811 a.u.

7	N	-2.78957	0.024269	-0.00676
6	C	-2.55563	-1.28091	-0.02666
7	N	-1.30844	-1.80994	-0.03826
6	C	-0.2217	-0.98303	-0.03004
6	C	-0.41823	0.422508	-0.00888
6	C	-1.74437	0.906212	0.0025
7	N	0.827934	1.008972	-0.00451
6	C	1.658971	-0.05701	-0.02236
7	N	1.077726	-1.31427	-0.03847
7	N	-2.03989	2.229665	0.021921
1	H	-3.0046	2.529321	0.030061
1	H	-1.29045	2.907524	0.029646
1	H	-3.37879	-1.99658	-0.03407
1	H	2.743342	0.054696	-0.02401
8	O	-1.13206	-3.19383	-0.05954
1	H	-0.15251	-3.27441	-0.06358

N1-OH-AD_1H E_{tot} = -542.206189 a.u.
Gibbs free energy E_G= -542.127644 a.u.

7	N	2.612927	0.298102	0.013935
6	C	2.521286	-1.091	-0.03545
7	N	1.389184	-1.74226	-0.02538
6	C	0.264625	-0.96106	0.020835
6	C	0.296903	0.485398	0.044968
6	C	1.522705	1.145406	0.03073
7	N	-0.98006	0.977437	0.061838
6	C	-1.70688	-0.17146	0.051098
7	N	-1.02516	-1.36192	0.024963
7	N	1.715699	2.496032	0.107975
1	H	2.559693	2.872702	-0.30974
1	H	0.865603	3.031146	-0.04153
1	H	3.48861	-1.59406	-0.08922
1	H	-2.79801	-0.14879	0.061289
8	O	3.887732	0.875445	-0.07129
1	H	4.168377	1.001706	0.854884

N3-NH_2-AD_3H E_{tot} = -522.386047 a.u.
Gibbs free energy E_G= -522.295526 a.u.

7	N	-0.89433	-1.49178	0.83506
6	C	0.42147	-1.59342	0.843451
7	N	1.264938	-0.86687	0.054485
6	C	0.712729	0.044616	-0.8203
6	C	-0.70256	0.194426	-0.86983
6	C	-1.4932	-0.5988	-0.01816
7	N	-0.99301	1.155839	-1.81292
6	C	0.234357	1.507922	-2.25321
7	N	1.324093	0.866354	-1.68758
7	N	-2.84562	-0.52798	0.005911
1	H	-3.36827	-1.11708	0.638874
1	H	-3.32073	0.120818	-0.60664
1	H	0.918109	-2.29691	1.513911
1	H	0.376109	2.266587	-3.02385
7	N	2.664732	-1.07788	0.166769
1	H	3.074207	-0.15884	0.366481
1	H	2.992493	-1.30954	-0.7772

N1-NH_2-AD_1H E_{tot} = -522.369277 a.u.
Gibbs free energy E_G= -522.278009 a.u.

7	N	2.64099	0.32375	-0.01331
6	C	2.52917	-1.07	-0.11784
7	N	1.407725	-1.73309	-0.15395
6	C	0.275914	-0.96077	-0.08247
6	C	0.302855	0.476917	0.020337
6	C	1.526447	1.145218	0.052974
7	N	-0.97754	0.960641	0.077905
6	C	-1.69995	-0.18856	0.007666
7	N	-1.0119	-1.37165	-0.09045
7	N	1.686737	2.489665	0.10423
1	H	2.603647	2.86803	0.304212
1	H	0.854602	3.033472	0.295713
1	H	3.494024	-1.58337	-0.16497
1	H	-2.79108	-0.17257	0.029008
7	N	3.90802	0.953791	0.049412
1	H	4.442643	0.527946	0.809108
1	H	4.403617	0.778963	-0.82769

Table S22. Cartesian coordinates of equilibrium geometries of C8-X and C2-X substituted purine (PU) 9H, 7H, 3H and 1H tautomers.

C8-NO_2-PU_9H E_{tot} = -616.168587 a.u.
Gibbs free energy E_G=-616.108778 a.u.

7	N	-3.21234	0.665164	0.000032
6	C	-3.09987	-0.68752	0.000431
7	N	-1.97707	-1.43298	0.000239
6	C	-0.87638	-0.6769	0.000192
6	C	-0.83899	0.751088	0.000089
6	C	-2.0872	1.396861	-8.9E-05
7	N	0.472261	1.210068	0.00031
6	C	1.180865	0.102093	-0.00005
7	N	0.447624	-1.06877	0.000045
1	H	-4.04243	-1.24295	-0.00019
1	H	0.836168	-2.00608	0.000203
1	H	-2.18138	2.487997	-9.3E-05
7	N	2.64252	0.027359	-0.00025
8	O	3.11465	-1.12157	-0.00031
8	O	3.273602	1.07674	-0.00044

C2-NO_2-PU_9H E_{tot} = -616.169698 a.u.
Gibbs free energy E_G=-616.108863 a.u

7	N	-0.77871	1.400018	-0.00011
6	C	-1.05727	0.095056	-9.3E-05
7	N	-0.2431	-0.96291	-8E-06
6	C	1.035035	-0.58335	0.000125
6	C	1.511644	0.762079	0.000166
6	C	0.520509	1.754883	-6E-06
7	N	2.901634	0.785829	0.000547
6	C	3.251993	-0.48944	0.000097
7	N	2.173086	-1.36453	0.00023
1	H	2.200888	-2.37792	0.000512
1	H	0.754512	2.824021	0.000135
1	H	4.27696	-0.85636	0.00012
7	N	-2.54562	-0.2517	-0.00031
8	O	-2.83395	-1.44614	0.000405
8	O	-3.33541	0.687129	-0.00103

C8-CN-PU_9H E_{tot} = -503.927175 a.u.
Gibbs free energy E_G= -503.86959 a.u.

7	N	-2.84737	0.654904	-1E-06
6	C	-2.73288	-0.69601	0.000342
7	N	-1.60678	-1.43792	0.000208
6	C	-0.50826	-0.67817	0.000136
6	C	-0.47233	0.74656	0.000039
6	C	-1.72215	1.388475	-0.00011
7	N	0.835442	1.208886	0.000313
6	C	1.572081	0.101683	-0.00029
7	N	0.813518	-1.07079	0.000063
1	H	-3.6734	-1.25492	-0.00013
1	H	1.165045	-2.02216	0.000484
1	H	-1.81927	2.479371	-0.0001
6	C	2.996748	0.054507	-0.0004
7	N	4.16638	-0.02716	-0.00038

C2-CN-PU_9H E_{tot} = -503.928272 a.u.
Gibbs free energy E_G= -503.870719 a.u.

7	N	-1.15942	1.351228	-0.00021
6	C	-1.44397	0.025322	-0.00045
7	N	-0.58349	-1.01995	-0.00022
6	C	0.684989	-0.6142	-3E-06
6	C	1.138827	0.737907	0.000105
6	C	0.134012	1.716294	0.000025
7	N	2.528666	0.786696	0.000238
6	C	2.901728	-0.48179	0.000431
7	N	1.83765	-1.37532	0.000115
1	H	1.883573	-2.38794	0.000307
1	H	0.35734	2.788048	0.000063
1	H	3.932967	-0.83126	0.000586
6	C	-2.85155	-0.3164	-0.00019
7	N	-3.98885	-0.59574	0.000008

C8-CHO-PU_9H E_{tot} = -525.019300 a.u.
Gibbs free energy E_G= -524.951194 a.u.

7	N	-2.95537	0.495729	0.000129
6	C	-2.72403	-0.84238	0.000165
7	N	-1.54149	-1.48716	0.000132
6	C	-0.50713	-0.63933	0.000047
6	C	-0.59515	0.78785	-5E-06
6	C	-1.89633	1.320591	0.000029
7	N	0.667682	1.353881	-8.9E-05
6	C	1.498639	0.310168	-0.00012
7	N	0.839811	-0.9138	0.000004
1	H	-3.6149	-1.47778	0.000271
1	H	1.292682	-1.82196	0.000126
1	H	-2.08569	2.399624	-3E-06
6	C	2.966847	0.401155	-0.00019
8	O	3.689421	-0.58903	-0.00011
1	H	3.361121	1.443433	-0.0003

C2-CHO-PU_9H E_{tot} = -525.012356 a.u.
Gibbs free energy E_G= -524.944891 a.u.

7	N	0.996012	1.511681	0.000007
6	C	1.394739	0.212853	0.00008
7	N	0.611533	-0.89063	0.000007
6	C	-0.68106	-0.58563	0.00001
6	C	-1.24452	0.727092	-1E-06
6	C	-0.32019	1.781704	-5.3E-05
7	N	-2.63364	0.663992	0.000234
6	C	-2.9028	-0.63159	-0.0003
7	N	-1.77275	-1.43639	0.000118
1	H	-1.7371	-2.44936	-0.00001
1	H	-0.62874	2.832534	0.000076
1	H	-3.90352	-1.06143	-0.00037
6	C	2.887993	0.024921	-0.00017
8	O	3.451561	-1.0542	0.000094
1	H	3.443726	0.995177	-0.00039

C8-CHO-PU_9H E_{tot} = -525.009688 a.u.
Gibbs free energy E_G= -524.94224 a.u

7	N	2.852408	0.823963	-4.5E-05
6	C	2.858304	-0.53441	0.000139
7	N	1.805447	-1.37398	0.000027
6	C	0.640616	-0.71582	0.000021
6	C	0.476799	0.702668	-0.00002
6	C	1.667294	1.453256	-0.00013
7	N	-0.86196	1.044001	0.000164
6	C	-1.50792	-0.11952	-0.00019
7	N	-0.63815	-1.21911	0.000095
7	H	3.846157	-1.00501	-0.00018
1	H	-0.89217	-2.20108	-5.2E-05
1	H	1.666127	2.548675	-4.4E-05
6	C	-2.97199	-0.33404	-0.00024
8	O	-3.8042	0.554751	0.00017
1	H	-3.26945	-1.41754	-0.00026

C2-CHO-PU_9H E_{tot} = -525.011257 a.u.
Gibbs free energy E_G= -524.94385 a.u

7	N	-1.17705	1.189913	0.000049
6	C	-1.36426	-0.15223	0.000121
7	N	-0.41313	-1.12061	0.000085
6	C	0.819633	-0.61971	0.000033
6	C	1.163147	0.763449	-6E-06
6	C	0.079273	1.657916	0.000012
7	N	2.543981	0.925254	-0.00008
6	C	3.019611	-0.30958	0.000051
7	N	2.032898	-1.28556	-0.00011
1	H	2.162148	-2.29073	0.000023
1	H	0.219943	2.744411	-5.4E-05
1	H	4.076177	-0.57302	0.000031
6	C	-2.77296	-0.68318	0.000093
8	O	-3.77783	0.002306	-0.00013
1	H	-2.80915	-1.80211	-0.00034

C8-Cl-PU_9H E_{tot} = -871.372525 a.u.
Gibbs free energy E_G= -871.321934 a.u

7	N	-2.9564	0.662746	0.000026
6	C	-2.85072	-0.68453	-0.00016
7	N	-1.7248	-1.43232	-0.00003
6	C	-0.62593	-0.6783	-4.3E-05
6	C	-0.58024	0.744395	-0.00004
6	C	-1.82229	1.390895	0.000039
7	N	0.742719	1.197608	-0.00026
6	C	1.450794	0.092886	0.000107
7	N	0.702847	-1.07678	-8.3E-05
1	H	-3.79307	-1.24052	0.000355
1	H	1.059307	-2.02521	0.000484
1	H	-1.91439	2.482211	-5.9E-05
17	Cl	3.1687	0.0078	0.000131

C2-Cl-PU_9H E_{tot} = -871.375960 a.u.
Gibbs free energy E_G= -871.325514 a.u

7	N	-1.06265	1.345126	0.000155
6	C	-1.32641	0.0283	0.000745
7	N	-0.4776	-1.00924	0.00041
6	C	0.794294	-0.59892	0.000268
6	C	1.242963	0.752134	0.000145
6	C	0.231568	1.720825	-5.3E-05
7	N	2.636168	0.80477	0.000237
6	C	3.01219	-0.46034	0.000057
7	N	1.946758	-1.35772	0.000168
1	H	1.994174	-2.36995	0.00043
1	H	0.441966	2.795162	-0.00019
1	H	4.043406	-0.80945	-1.3E-05
17	Cl	-3.02976	-0.39696	-0.00082

C8-F-PU_9H E_{tot} = -510.943647 a.u.
Gibbs free energy E_G= -510.890557 a.u

7	N	-2.54161	0.661651	0.000001
6	C	-2.43692	-0.68408	-0.00017
7	N	-1.30939	-1.43157	-2.5E-05
6	C	-0.21272	-0.67821	-2.2E-05
6	C	-0.16538	0.744952	-1.4E-05
6	C	-1.40627	1.390228	0.000042
7	N	1.161569	1.198929	-0.00019
6	C	1.850667	0.093303	0.000113
7	N	1.120378	-1.07982	-4.7E-05
1	H	-3.37872	-1.24089	0.000281
1	H	1.47934	-2.0274	0.000564
1	H	-1.49882	2.481461	-4.9E-05
9	F	3.178369	0.016139	0.000142

C2-F-PU_9H E_{tot} = -510.953511 a.u.
Gibbs free energy E_G= -510.900289 a.u

7	N	-1.57944	1.142159	-0.00014
6	C	-1.70193	-0.18896	-8.7E-05
7	N	-0.77368	-1.14668	0.000026
6	C	0.455979	-0.61875	0.000054
6	C	0.772276	0.769349	-1.2E-05
6	C	-0.32563	1.638699	-0.00012
7	N	2.155262	0.954766	0.000149
6	C	2.650683	-0.2673	-2.3E-05
7	N	1.67439	-1.26324	0.000101
1	H	1.818377	-2.26625	0.000405
1	H	-0.21602	2.72778	-0.00013
1	H	3.710467	-0.51716	-0.00004
9	F	-2.97298	-0.63907	-7E-06

C8-H-PU_9H E_{tot} = -411.741198 a.u.
Gibbs free energy E_G= -411.678769 a.u

7	N	2.133176	0.656495	0.000257
6	C	2.020379	-0.69113	0.000211
7	N	0.89314	-1.43447	0.000044
6	C	-0.20576	-0.67547	-4.3E-05
6	C	-0.24493	0.747737	0.000004
6	C	1.001414	1.387556	0.000157
7	N	-1.56412	1.203032	-9.8E-05
6	C	-2.29031	0.100127	-0.0002
7	N	-1.53258	-1.06594	-0.00028
1	H	1.099483	2.478907	0.000216
1	H	-3.37889	0.065738	-0.00032
1	H	2.960683	-1.25118	0.000252
1	H	-1.87332	-2.02021	-0.00041

C2-H-PU_9H E_{tot} = -411.741198 a.u.
Gibbs free energy E_G= -411.678769 a.u

7	N	2.133176	0.656495	0.000257
6	C	2.020379	-0.69113	0.000211
7	N	0.89314	-1.43447	0.000044
6	C	-0.20576	-0.67547	-4.3E-05
6	C	-0.24493	0.747737	0.000004
6	C	1.001414	1.387556	0.000157
7	N	-1.56412	1.203032	-9.8E-05
6	C	-2.29031	0.100127	-0.0002
7	N	-1.53258	-1.06594	-0.00028
1	H	1.099483	2.478907	0.000216
1	H	-3.37889	0.065738	-0.00032
1	H	2.960683	-1.25118	0.000252
1	H	-1.87332	-2.02021	-0.00041

C8-Me-PU_9H E_{tot} = -451.043994 a.u.
Gibbs free energy E_G= -450.957287 a.u

7	N	2.586578	0.669494	-0.00031
6	C	2.48465	-0.67772	0.000005
7	N	1.360823	-1.42888	-5.6E-05
6	C	0.257082	-0.67899	0.000052
6	C	0.206609	0.743328	0.000009
6	C	1.44716	1.391772	-0.00024
7	N	-1.11641	1.18448	0.000493
6	C	-1.84841	0.079977	-1.6E-05
7	N	-1.06677	-1.07812	0.00014
1	H	3.428843	-1.23112	-0.00077
1	H	-1.3966	-2.03604	-0.00036
1	H	1.536806	2.483653	-0.00014
6	C	-3.33922	0.026244	0.000051
1	H	-3.71821	-0.50229	-0.89159
1	H	-3.7181	-0.50265	0.891521
1	H	-3.72954	1.051921	0.000275

C2-Me- PU _9H E_{tot} = -451.041421 a.u.
Gibbs free energy E_G= -450.95599 a.u

7	N	1.501101	1.193626	0.000014
6	C	1.709726	-0.1518	0.000021
7	N	0.755725	-1.11289	0.00002
6	C	-0.4826	-0.6139	0.000006
6	C	-0.838	0.761681	0.000002
6	C	0.240404	1.656825	0.000009
7	N	-2.2255	0.912782	-1.6E-05
6	C	-2.68894	-0.32362	-9E-06
7	N	-1.68882	-1.29108	-1.1E-05
1	H	-1.80631	-2.29733	0.000084
1	H	0.097707	2.743341	-7E-06
1	H	-3.74231	-0.59971	-2.3E-05
6	C	3.145628	-0.6045	-2.3E-05
1	H	3.66708	-0.20529	0.885218
1	H	3.202129	-1.70046	0.000281
1	H	3.666852	-0.20583	-0.88564

C8-OMe- PU _9H E_{tot} = -526.215871 a.u.
Gibbs free energy E_G= -526.126105 a.u

7	N	3.041032	0.41492	-0.00032
6	C	2.767354	-0.90512	-0.0003
7	N	1.551127	-1.50177	-0.00017
6	C	0.561001	-0.61391	-0.00006
6	C	0.690752	0.803172	-9.3E-05
6	C	2.005484	1.282605	-0.00023
7	N	-0.56164	1.417619	0.000011
6	C	-1.41414	0.41293	0.000099
7	N	-0.81005	-0.84747	0.000187
1	H	3.629598	-1.57872	-0.0004
1	H	-1.24985	-1.75859	-0.00035
1	H	2.237825	2.352865	-0.00024
8	O	-2.74274	0.595497	0.000239
6	C	-3.57752	-0.57874	0.000491
1	H	-4.60733	-0.20347	0.000716
1	H	-3.40481	-1.18244	-0.90731
1	H	-3.40436	-1.18237	0.908252

C2-OMe- PU _9H E_{tot} = -526.226856 a.u.
Gibbs free energy E_G= -526.136473 a.u

7	N	1.168668	1.068913	-6.5E-05
6	C	1.275745	-0.2798	-0.00012
7	N	0.284448	-1.19685	-3.6E-05
6	C	-0.91758	-0.62342	0.000004
6	C	-1.19279	0.774687	-6E-06
6	C	-0.06747	1.603708	-2.4E-05
7	N	-2.57101	1.00516	0.000061
6	C	-3.10471	-0.20005	-2.1E-05
7	N	-2.16023	-1.22712	0.000087
1	H	-2.33601	-2.22472	-0.00017
1	H	-0.14269	2.696396	0.000012
1	H	-4.17195	-0.4161	0
8	O	2.511448	-0.82765	-0.00001
6	C	3.632839	0.082009	0.000094
1	H	4.517229	-0.56786	0.000195
1	H	3.616295	0.719944	-0.89652
1	H	3.616113	0.719975	0.896681

C8-OMe- PU _9H E_{tot} = -526.224915 a.u.
Gibbs free energy E_G= -526.134812 a.u

7	N	-2.86968	0.912592	0.000064
6	C	-2.94804	-0.4322	0.000287
7	N	-1.92971	-1.32642	0.000154
6	C	-0.74071	-0.73074	0.000052
6	C	-0.50013	0.67421	-2.9E-05
6	C	-1.6418	1.479295	-6.9E-05
7	N	0.873437	0.940904	-4E-06
6	C	1.427273	-0.25722	-0.00012
7	N	0.521473	-1.31044	-0.00013
1	H	-3.95592	-0.85846	0.000077
1	H	0.74228	-2.29874	0.000327
1	H	-1.58693	2.57328	-0.00012
8	O	2.728439	-0.55702	-0.00014
6	C	3.618428	0.59254	-6.2E-05
1	H	4.627738	0.165268	-5.8E-05
6	H	3.44324	1.201568	-0.89887
1	H	3.443196	1.201483	0.898792

C2-OMe- PU _9H E_{tot} = -526.226415 a.u.
Gibbs free energy E_G= -526.135919 a.u

7	N	0.872466	1.628833	0.000001
6	C	1.333519	0.353883	0.000077
7	N	0.623972	-0.79271	0.000094
6	C	-0.69405	-0.56333	-8.3E-05
6	C	-1.32554	0.707604	-0.00024
6	C	-0.45574	1.809613	-0.00017
7	N	-2.71492	0.567124	-0.00038
6	C	-2.91401	-0.7363	-0.00043
7	N	-1.73013	-1.47584	-0.00012
1	H	-1.63686	-2.48443	-0.00029
1	H	-0.82233	2.842041	-0.00024
1	H	-3.88586	-1.22703	-0.00053
8	O	2.683112	0.280653	0.000385
6	C	3.264953	-1.03855	0.000634
1	H	4.34868	-0.86755	0.000862
1	H	2.958295	-1.59875	0.897695
1	H	2.958697	-1.5989	-0.89647

C8-OH- PU _9H E_{tot} = -486.938320 a.u.
Gibbs free energy E_G= -486.874055 a.u

7	N	2.556834	0.652548	0.000001
6	C	2.448037	-0.69047	-0.00034
7	N	1.314215	-1.43286	-0.00013
6	C	0.222506	-0.67438	-4.2E-05
6	C	0.177412	0.747923	0.00003
6	C	1.421781	1.385941	0.000135
7	N	-1.14321	1.204335	-0.00012
6	C	-1.86154	0.105471	0.000092
7	N	-1.1112	-1.07242	0.000188
1	H	3.386456	-1.25309	0.000137
1	H	-1.43955	-2.03111	-0.00044
1	H	1.520011	2.476661	0.000157
8	O	-3.20981	0.1117	0.00009
1	H	-3.55413	-0.79418	0.000582

C8-OH- PU _9H E_{tot} = -486.948145 a.u.
Gibbs free energy E_G= -486.88269 a.u

7	N	-2.54592	0.681927	0.000005
6	C	-2.4566	-0.66242	0.000187
7	N	-1.33427	-1.42171	0.000108
6	C	-0.22992	-0.68212	0.000033
6	C	-0.16568	0.741396	-4.5E-05
6	C	-1.39951	1.397867	-0.0001
7	N	1.165611	1.17337	-3.8E-05
6	C	1.858696	0.053357	-6.1E-05
7	N	1.097047	-1.10153	-7.2E-05
1	H	-3.40334	-1.21098	0.000062
1	H	1.438809	-2.05497	0.000415
1	H	-1.482	2.489994	-0.00016
8	O	3.197102	-0.06042	-5.2E-05
1	H	3.550537	0.846452	-1.3E-05

C8-NH_2- PU _9H E_{tot} = -467.086682 a.u.
Gibbs free energy E_G= -467.009632 a.u

7	N	-2.5647	0.671329	0.003387
6	C	-2.4689	-0.67129	0.000119
7	N	-1.34113	-1.42528	0.000245
6	C	-0.24124	-0.67898	-0.00105
6	C	-0.18249	0.744548	-0.00091
6	C	-1.42076	1.393514	0.003496
7	N	1.141784	1.183367	0.007028
6	C	1.858892	0.069586	0.000442
7	N	1.08603	-1.09103	0.0028
1	H	-3.41215	-1.22594	-0.00337
1	H	1.409753	-2.04766	-0.07306
1	H	-1.50978	2.485132	0.00697
7	N	3.233981	0.013406	-0.07985
1	H	3.664291	0.91868	0.085432
1	H	3.683126	-0.73705	0.436153

C2-OH- PU _9H E_{tot} = -486.953186 a.u.
Gibbs free energy E_G= -486.887437 a.u

7	N	1.5719	1.124812	0.000317
6	C	1.708047	-0.2241	0.000646
7	N	0.749558	-1.1652	0.000287
6	C	-0.4697	-0.62033	0.000015
6	C	-0.77877	0.769144	-5.5E-05
6	C	0.325084	1.629853	0.000072
7	N	-2.16144	0.965362	-0.00026
6	C	-2.66581	-0.25257	-0.00044
7	N	-1.69488	-1.25505	-0.00024
1	H	-1.8448	-2.25699	-0.00053
1	H	0.222217	2.719926	0
1	H	-3.72708	-0.49541	-0.00063
8	O	2.978844	-0.69523	-8.6E-05
1	H	3.549791	0.092881	-0.00039

C2-OH- PU _9H E_{tot} = -486.951744 a.u.
Gibbs free energy E_G= -486.88609 a.u

7	N	1.557025	1.185213	0.000152
6	C	1.723573	-0.15349	0.000351
7	N	0.783402	-1.12223	0.000195
6	C	-0.45352	-0.61545	0.000019
6	C	-0.79016	0.765769	-0.00008
6	C	0.296236	1.650934	-1.7E-05
7	N	-2.17706	0.93219	-0.00024
6	C	-2.65639	-0.29529	-0.00025
7	N	-1.66361	-1.27771	-8.4E-05
1	H	-1.79427	-2.28217	-0.00036
1	H	0.163626	2.738145	-0.0001
1	H	-3.71213	-0.56114	-0.00033
8	O	3.01653	-0.56217	0.000062
1	H	2.993732	-1.53456	-3.7E-05

C2-NH_2- PU _9H E_{tot} = -467.093074 a.u.
Gibbs free energy E_G= -467.016016 a.u

7	N	1.54184	1.176136	0.00488
6	C	1.717681	-0.17729	-0.00287
7	N	0.759091	-1.13752	0.004223
6	C	-0.4694	-0.6174	-0.00073
6	C	-0.80438	0.764518	-0.00411
6	C	0.285626	1.645634	0.003742
7	N	-2.19101	0.936357	-0.0026
6	C	-2.67479	-0.28956	0.000545
7	N	-1.68436	-1.27473	0.003782
1	H	-1.81706	-2.27877	0.002638
1	H	0.155556	2.733523	0.013831
1	H	-3.73146	-0.55191	0.001158
7	N	3.022212	-0.60817	-0.0601
1	H	3.732152	0.07314	0.174947
1	H	3.198	-1.5759	0.176695

C8-NO_2-PU_7H E_{tot} = -616.162730 a.u.
Gibbs free energy E_G= -616.103174 a.u.

7	N	3.216658	0.647833	0.000053
6	C	3.097687	-0.70874	-0.00017
7	N	1.979247	-1.44724	0.000043
6	C	0.85242	-0.71574	0.000089
6	C	0.861159	0.715935	0.00009
6	C	2.094873	1.379461	0.000087
7	N	-0.472	1.082893	0.000098
6	C	-1.17701	-0.09881	-8E-06
7	N	-0.45102	-1.19536	0.000195
1	H	4.042441	-1.26069	0.000378
1	H	-0.89882	2.003292	0.000202
1	H	2.193231	2.470913	0.000108
7	N	-2.64341	-0.0421	-0.00013
8	O	-3.12865	1.101536	-0.00022
8	O	-3.2611	-1.09759	-0.00016

C8-CN-PU_7H E_{tot} = -503.921405 a.u.
Gibbs free energy E_G= -503.864055 a.u.

7	N	2.848838	0.655869	0.000043
6	C	2.733274	-0.69931	-0.00021
7	N	1.615239	-1.4401	0.000021
6	C	0.4859	-0.71206	0.00006
6	C	0.491673	0.716993	0.000069
6	C	1.723033	1.383299	0.00008
7	N	-0.83964	1.083723	0.000116
6	C	-1.56935	-0.10173	-0.00022
7	N	-0.81321	-1.19538	0.000269
1	H	3.678579	-1.25044	0.0004
1	H	-1.23008	2.01924	0.000329
1	H	1.818583	2.475154	0.000137
6	C	-2.99562	-0.07756	-0.00024
7	N	-4.16559	-0.00436	-0.00018

C8-CHO-PU_7H E_{tot} = -525.013652 a.u.
Gibbs free energy E_G= -524.945777 a.u.

7	N	2.844098	0.815538	-0.00002
6	C	2.845361	-0.54703	0.000019
7	N	1.797586	-1.38134	0.000093
6	C	0.606663	-0.75388	0.000023
6	C	0.488809	0.674017	-7.3E-05
6	C	1.660753	1.442802	-8.4E-05
7	N	-0.86599	0.922584	-0.00014
6	C	-1.49474	-0.31131	-0.00014
7	N	-0.64561	-1.34004	0.000095
1	H	3.835943	-1.01228	0.000217
1	H	-1.35651	1.810795	-0.00021
1	H	1.661576	2.539006	-0.00016
6	C	-2.96458	-0.42086	-0.00023
8	O	-3.69438	0.563568	0.00049
1	H	-3.35028	-1.46565	-0.00102

C2-NO_2-AD_7H E_{tot} = -616.164390 a.u.
Gibbs free energy E_G= -616.103789 a.u

7	N	-0.778286	1.394437	0.00003
6	C	-1.05578	0.085755	-0.000039
7	N	-0.253008	-0.97154	-0.00004
6	C	1.046685	-0.636799	0.000055
6	C	1.483745	0.727106	0.000138
6	C	0.520629	1.739294	0.000137
7	N	2.863665	0.651672	0.000196
6	C	3.185962	-0.697903	0.000395
7	N	2.134251	-1.497187	-0.000083
1	H	3.519211	1.42408	0.000131
1	H	0.758995	2.808366	0.000226
1	H	4.223454	-1.028278	0.000485
7	N	-2.55264	-0.245193	-0.00024
8	O	-2.855151	-1.434027	0.000455
8	O	-3.330722	0.70475	-0.000955

C2-CN-PU_7H E_{tot} = -503.922890 a.u.
Gibbs free energy E_G= -503.865575 a.u.

7	N	-1.160143	1.346391	-0.000178
6	C	-1.444089	0.016587	-0.000381
7	N	-0.594212	-1.028503	-0.000187
6	C	0.696014	-0.666001	0.000006
6	C	1.109813	0.703521	0.000097
6	C	0.132959	1.702128	0.000025
7	N	2.491962	0.65321	0.000302
6	C	2.837914	-0.689868	0.000239
7	N	1.800191	-1.50749	0.000192
1	H	3.133293	1.437443	0.000332
1	H	0.360448	2.773896	0.00011
1	H	3.881128	-1.002523	0.00037
6	C	-2.857071	-0.310695	-0.000199
7	N	-3.998955	-0.569728	-0.000062

C2-CHO-PU_7H E_{tot} = -525.005733 a.u.
Gibbs free energy E_G= -524.938678 a.u.

7	N	0.995362	1.507603	-0.000148
6	C	1.394479	0.205626	-0.000486
7	N	0.621999	-0.897894	-0.000252
6	C	-0.689202	-0.639235	-0.000099
6	C	-1.214014	0.694329	0.000061
6	C	-0.320136	1.767499	0.000069
7	N	-2.586981	0.534154	0.000245
6	C	-2.824898	-0.834041	-0.000229
7	N	-1.727345	-1.566231	0.000215
1	H	-3.288825	1.264642	0.000585
1	H	-0.633932	2.817808	0.000191
1	H	-3.840713	-1.227231	-0.000195
6	C	2.892859	0.034436	-0.000026
8	O	3.471382	-1.035354	0.000324
1	H	3.436639	1.0125	0.000662

C8-CHO-PU_7H E_{tot} = -525.003418 a.u.
Gibbs free energy E_G= -524.936268 a.u.

7	N	2.970464	0.487118	-3.9E-05
6	C	2.733412	-0.85547	-7.9E-05
7	N	1.557347	-1.49514	0.000024
6	C	0.49196	-0.67113	0.000035
6	C	0.62689	0.754518	0.000004
6	C	1.913817	1.309395	-1.5E-05
7	N	-0.66428	1.233197	-5.6E-05
6	C	-1.50578	0.118192	0.000083
7	N	-0.83993	-1.03338	0.000126
1	H	3.628102	-1.48576	0.000108
1	H	-0.95993	2.203261	-7.7E-05
1	H	2.105104	2.389038	-6.9E-05
6	C	-2.97445	0.313981	0.000114
8	O	-3.79627	-0.58263	-0.00022
1	H	-3.2834	1.395086	0.000574

C2-CHO-PU_7H E_{tot} = -525.006594 a.u.
Gibbs free energy E_G= -524.939398 a.u.

7	N	-1.17644	1.188475	0.000053
6	C	-1.364897	-0.157068	0.00009
7	N	-0.426089	-1.127526	0.000068
6	C	0.832802	-0.671024	0.000015
6	C	1.137149	0.725565	-0.000004
6	C	0.081318	1.644597	0.000023
7	N	2.518348	0.785624	0.000006
6	C	2.971463	-0.526164	-0.000146
7	N	2.002426	-1.423244	0.000059
1	H	3.094647	1.618805	-0.000051
1	H	0.228816	2.731216	0.000015
1	H	4.036571	-0.753492	-0.00019
6	C	-2.780711	-0.674207	0.000101
8	O	-3.778009	0.022746	-0.000162
1	H	-2.826422	-1.791997	-0.000252

C8-Cl-PU_7H E_{tot} = -871.367421 a.u.
Gibbs free energy E_G= -871.31708 a.u.

7	N	2.968099	0.639871	0.000137
6	C	2.839325	-0.70945	0.000338
7	N	1.71181	-1.44255	0.000045
6	C	0.591451	-0.70601	-1.1E-05
6	C	0.611177	0.721789	0.000021
6	C	1.842561	1.376751	0.000053
7	N	-0.72887	1.094856	-9.4E-05
6	C	-1.44846	-0.08588	0.000033
7	N	-0.71949	-1.17912	-0.00023
1	H	3.778351	-1.2718	-0.00018
1	H	-1.12337	2.027582	0.000034
1	H	1.946895	2.467893	0.000031
17	Cl	-3.16701	-0.03519	-8.6E-05

C2-Cl-PU_7H E_{tot} = -871.370729 a.u.
Gibbs free energy E_G= -871.320551 a.u.

7	N	-1.061812	1.342753	-0.00007
6	C	-1.326318	0.021505	-0.00012
7	N	-0.488964	-1.015364	-0.00004
6	C	0.805032	-0.650891	0.00003
6	C	1.215678	0.717073	0.000034
6	C	0.232771	1.706831	0.000009
7	N	2.601478	0.668536	0.000088
6	C	2.947112	-0.671574	0.000181
7	N	1.908524	-1.49136	0.000054
1	H	3.242133	1.452793	-0.00000
1	H	0.448982	2.780886	0.000011
1	H	3.990266	-0.984774	0.000248
17	Cl	-3.037742	-0.383443	-0.00008

C8-F-PU_7H E_{tot} = -510.938689 a.u.
Gibbs free energy E_G= -510.885856 a.u.

7	N	2.550567	0.650149	0.000117
6	C	2.428655	-0.69817	0.000303
7	N	1.30401	-1.43792	0.000031
6	C	0.180803	-0.70903	-0.00002
6	C	0.193978	0.719616	0.000009
6	C	1.41938	1.380996	0.000027
7	N	-1.15332	1.086933	-8.5E-05
6	C	-1.84741	-0.10128	0.000005
7	N	-1.1299	-1.19143	-0.00021
1	H	3.3701	-1.25653	-0.00017
1	H	-1.5566	2.015961	0.00007
1	H	1.517268	2.472754	0.00001
9	F	-3.17586	-0.0599	-9.4E-05

C2-F-PU_7H E_{tot} = -510.948485 a.u.
Gibbs free energy E_G= -510.895513 a.u.

7	N	-1.574291	1.148209	-0.000048
6	C	-1.703512	-0.186637	-0.000063
7	N	-0.790435	-1.149075	-0.000019
6	C	0.466944	-0.669475	0.000018
6	C	0.750479	0.731072	0.000006
6	C	-0.317041	1.628546	-0.000006
7	N	2.136255	0.80843	0.000022
6	C	2.601586	-0.49328	0.000164
7	N	1.64132	-1.404863	0.000005
1	H	2.703188	1.647398	-0.000111
1	H	-0.197769	2.717459	-0.000019
1	H	3.668793	-0.710914	0.000218
9	F	-2.983876	-0.614911	-0.000057

C8-H-AD_7H E_{tot} = -411.735954 a.u.
Gibbs free energy E_G= -411.673762 a.u.

7	N	-2.12563	0.684039	-0.00026
6	C	-2.0303	-0.66959	-9.7E-05
7	N	-0.92259	-1.42993	0.000027
6	C	0.219001	-0.72192	0.000092
6	C	0.234645	0.706284	-5.1E-05
6	C	-0.98209	1.390693	-0.00022
7	N	1.579429	1.045547	0.000083
6	C	2.285114	-0.14627	0.000431
7	N	1.516735	-1.22169	0.000003
1	H	-1.0606	2.484487	-0.0003
1	H	3.374333	-0.15507	0.000616
1	H	-2.98376	-1.20761	-0.00027
1	H	1.97617	1.977259	0.000072

C2-H-AD_7H E_{tot} = -411.735954 a.u.
Gibbs free energy E_G= -411.673762 a.u.

7	N	-2.12563	0.684039	-0.00026
6	C	-2.0303	-0.66959	-9.7E-05
7	N	-0.92259	-1.42993	0.000027
6	C	0.219001	-0.72192	0.000092
6	C	0.234645	0.706284	-5.1E-05
6	C	-0.98209	1.390693	-0.00022
7	N	1.579429	1.045547	0.000083
6	C	2.285114	-0.14627	0.000431
7	N	1.516735	-1.22169	0.000003
1	N	-1.0606	2.484487	-0.0003
1	H	3.374333	-0.15507	0.000616
1	H	-2.98376	-1.20761	-0.00027
1	H	1.97617	1.977259	0.000072

C8-Me-PU_7H E_{tot} = -451.038815 a.u.
Gibbs free energy E_G= -450.952769 a.u.

7	N	-2.60006	0.641637	-0.00019
6	C	-2.47222	-0.70748	-0.00048
7	N	-1.3452	-1.44164	-9.1E-05
6	C	-0.22117	-0.70756	0.000014
6	C	-0.23995	0.720219	0.000001
6	C	-1.4709	1.375028	-6.3E-05
7	N	1.097406	1.088611	0.000175
6	C	1.845648	-0.08439	-1.3E-05
7	N	1.087752	-1.17354	0.000384
1	H	-3.41207	-1.269	0.000219
1	H	1.470007	2.030214	0.000098
1	H	-1.57472	2.466668	-6E-06
6	C	3.337952	-0.06806	0.000099
1	H	3.729059	0.451038	-0.89175
1	H	3.728928	0.451445	0.891764
1	H	3.703342	-1.10245	0.000358

C2-Me-PU_7H E_{tot} = -451.035984 a.u.
Gibbs free energy E_G= -450.95092 a.u.

7	N	1.496747	1.199555	-0.000042
6	C	1.712007	-0.148928	-0.000046
7	N	0.772433	-1.115108	-0.000032
6	C	-0.492567	-0.665247	0.000012
6	C	-0.814002	0.723426	0.000034
6	C	0.233029	1.646748	-0.00002
7	N	-2.201237	0.768519	-0.000057
6	C	-2.635626	-0.545832	0.000002
7	N	-1.653773	-1.431727	-0.000004
1	H	-2.787769	1.593873	0.000521
1	H	0.079495	2.732811	-0.00002
1	H	-3.697526	-0.788367	-0.000019
6	C	3.154414	-0.584359	0.000041
1	H	3.671682	-0.181647	0.886251
1	H	3.219264	-1.679614	-0.000518
1	H	3.672135	-0.180589	-0.885407

C8-OMe- PU _7H E_{tot} = -526.220894 a.u.
Gibbs free energy E_G= -526.131069 a.u.

7	N	-3.05633	0.368489	-0.00012
6	C	-2.74174	-0.94521	0.000067
7	N	-1.52014	-1.51663	-0.00001
6	C	-0.5119	-0.63535	-5E-06
6	C	-0.73081	0.778008	-4.6E-05
6	C	-2.03673	1.25438	-0.00012
7	N	0.546612	1.33624	0.000037
6	C	1.427135	0.268626	0.000099
7	N	0.84993	-0.92142	-6E-06
1	H	-3.59202	-1.63497	-0.00031
1	H	0.80651	2.314456	-0.00015
1	H	-2.29063	2.320772	-0.00017
8	O	2.733313	0.537797	0.000105
6	C	3.599356	-0.63222	0.000065
1	H	4.617222	-0.22576	0.000075
1	H	3.410018	-1.23656	0.898774
1	H	3.410015	-1.23651	-0.89868

C2-OMe- PU _7H E_{tot} = -526.222037 a.u.
Gibbs free energy E_G= -526.131784 a.u.

7	N	-0.87114	1.628906	-0.000144
6	C	-1.33506	0.350464	0.000054
7	N	-0.636292	-0.794465	0.000141
6	C	0.696294	-0.614405	0.00011
6	C	1.293736	0.678106	-0.000038
6	C	0.456547	1.797655	-0.000174
7	N	2.663003	0.436389	0.00004
6	C	2.817884	-0.935884	0.000154
7	N	1.671908	-1.601882	0.000246
1	H	3.406517	1.123348	-0.00012
1	H	0.829316	2.828901	-0.000284
1	H	3.80622	-1.393335	0.000213
8	O	-2.686472	0.289639	-0.000136
6	C	-3.272229	-1.029651	-0.000148
1	H	-2.965251	-1.590829	0.895763
1	H	-4.355436	-0.854595	-0.000326
1	H	-2.964977	-1.590945	-0.895892

C8-OMe- PU _7H E_{tot} = -526.211236 a.u.
Gibbs free energy E_G= -526.121766 a.u.

7	N	-2.89475	0.872809	-0.00019
6	C	-2.9321	-0.47915	-0.00019
7	N	-1.904	-1.3496	-0.00011
6	C	-0.69806	-0.76271	-3.9E-05
6	C	-0.54512	0.65798	-3.8E-05
6	C	-1.67955	1.460684	-9.7E-05
7	N	0.83491	0.86638	0.000074
6	C	1.410196	-0.40146	0.000069
7	N	0.538137	-1.39254	0.000032
1	H	-3.9334	-0.92228	-0.00026
1	H	1.311685	1.758058	-0.00011
1	H	-1.64534	2.556757	-9.9E-05
8	O	2.732727	-0.61341	0.000146
6	C	3.594418	0.540888	0.00026
1	H	4.615129	0.141887	0.000367
1	H	3.43577	1.148069	-0.90791
1	H	3.435561	1.148045	0.90841

C2-OMe- PU _7H E_{tot} = -526.220388 a.u.
Gibbs free energy E_G= -526.130338 a.u.

7	N	1.167766	1.068588	0.00002
6	C	1.277406	-0.283115	-0.000011
7	N	0.297709	-1.203454	-0.00002
6	C	-0.931554	-0.674188	-0.000037
6	C	-1.169425	0.736103	-0.000042
6	C	-0.071579	1.591281	-0.000008
7	N	-2.554096	0.863382	-0.00013
6	C	-3.063692	-0.421545	-0.000075
7	N	-2.137747	-1.36676	-0.000118
1	H	-3.091364	1.72123	-0.000037
1	H	-0.15354	2.684388	-0.00002
1	H	-4.138155	-0.600946	-0.000105
8	O	2.520977	-0.818682	0.000121
6	C	3.633499	0.098462	0.000212
1	H	3.613997	0.736985	0.89693
1	H	4.52378	-0.543523	0.000252
1	H	3.614106	0.737031	-0.896473

C8-OH- PU _7H E_{tot} = -486.944078 a.u.
Gibbs free energy E_G= -486.878838 a.u.

7	N	2.570194	0.625693	0.000088
6	C	2.431312	-0.71819	-6.8E-05
7	N	1.295864	-1.44548	0
6	C	0.18069	-0.70452	0.000005
6	C	0.212035	0.725244	0.000039
6	C	1.443486	1.369789	0.000104
7	N	-1.12971	1.111524	-3.8E-05
6	C	-1.85621	-0.05941	-8.1E-05
7	N	-1.13378	-1.16397	-1.1E-05
1	H	3.365036	-1.28985	0.000226
1	H	-1.51562	2.047378	0.000135
1	H	1.554787	2.460305	0.000134
8	O	-3.19603	0.014181	-8.7E-05
1	H	-3.52175	-0.90311	-0.00006

C2-OH- PU _7H E_{tot} = -486.947466 a.u.
Gibbs free energy E_G= -486.882007 a.u.

7	N	1.551645	1.192762	0.00015
6	C	1.72563	-0.149076	0.000406
7	N	0.800436	-1.122605	0.000187
6	C	-0.462768	-0.665405	0.000026
6	C	-0.767733	0.728254	-0.000038
6	C	0.287061	1.641855	-0.000012
7	N	-2.157194	0.785092	-0.000183
6	C	-2.602445	-0.521756	-0.000157
7	N	-1.627323	-1.419278	-0.000114
1	H	-2.736305	1.615409	-0.000154
1	H	0.144246	2.728696	-0.000106
1	H	-3.665982	-0.756241	-0.000253
8	O	3.024932	-0.541097	-0.000106
1	H	3.00717	-1.51412	-0.000276

C8-OH- PU _7H E_{tot} = -486.933447 a.u.
Gibbs free energy E_G= -486.869533 a.u.

7	N	2.562673	0.655807	0.00007
6	C	2.44341	-0.69066	-0.00027
7	N	1.319565	-1.43452	-1.1E-05
6	C	0.191991	-0.7114	0.000017
6	C	0.204105	0.71731	0.000036
6	C	1.424821	1.381994	0.00011
7	N	-1.14377	1.081613	-2.6E-05
6	C	-1.85849	-0.11182	-0.0001
7	N	-1.11173	-1.19469	0.000109
1	H	3.385766	-1.24799	0.000478
1	H	-1.5175	2.022975	0.000235
1	H	1.5195	2.474305	0.000177
8	O	-3.20418	-0.15716	-0.00006
1	H	-3.57656	0.737926	-0.00016

C2-OH- PU _7H E_{tot} = -486.946823 a.u.
Gibbs free energy E_G= -486.881414 a.u.

7	N	1.56693	1.131727	0.000219
6	C	1.710908	-0.21991	0.000453
7	N	0.767112	-1.167274	0.000181
6	C	-0.480168	-0.671373	-0.000002
6	C	-0.75696	0.730464	-0.000022
6	C	0.315504	1.620254	0.000057
7	N	-2.144126	0.818747	-0.000198
6	C	-2.617661	-0.479074	-0.000225
7	N	-1.663705	-1.397412	-0.000184
1	H	-2.705071	1.661452	-0.000153
1	H	0.202387	2.710188	-0.000009
1	H	-3.686341	-0.689296	-0.000351
8	O	2.990436	-0.67323	-0.000106
1	H	3.552325	0.120813	-0.000326

C8-NH_2- PU _7H E_{tot} = -467.082512 a.u.
Gibbs free energy E_G= -467.00578 a.u.

7	N	2.583791	0.634514	0.000082
6	C	2.449926	-0.7089	0.002612
7	N	1.317595	-1.44232	0.002619
6	C	0.196764	-0.70749	-0.00184
6	C	0.223813	0.722397	-0.00168
6	C	1.450884	1.372637	0.001094
7	N	-1.11831	1.103081	0.009631
6	C	-1.85648	-0.07435	0.000707
7	N	-1.11077	-1.1724	0.006696
1	H	3.385954	-1.27717	0.004728
1	H	-1.48478	2.039684	-0.1053
1	H	1.557448	2.463839	0.000997
7	N	-3.22982	-0.06102	-0.0774
1	H	-3.63843	-0.97517	0.091965
1	H	-3.707	0.690016	0.410844

C2-NH_2- PU _7H E_{tot} = -467.087348 a.u.
Gibbs free energy E_G= -467.010526 a.u.

7	N	-1.536799	1.183797	0.007392
6	C	-1.720715	-0.171669	-0.00314
7	N	-0.776714	-1.137809	0.005359
6	C	0.478449	-0.667724	-0.000251
6	C	0.781574	0.72661	-0.006434
6	C	-0.276049	1.636627	0.005818
7	N	2.172069	0.789526	-0.0053
6	C	2.621476	-0.515675	0.001604
7	N	1.650057	-1.416743	0.006692
1	H	2.748209	1.621665	-0.011058
1	H	-0.13514	2.724111	0.018397
1	H	3.686113	-0.745971	0.002199
7	N	-3.032326	-0.588226	-0.065868
1	H	-3.207453	-1.555795	0.174187
1	H	-3.734149	0.093154	0.192774

C8-NO_2-PU_3H E_{tot} = -616.154310 a.u.
Gibbs free energy E_G= -616.093342 a.u.

7	N	0.726731	1.436678	0.000046
6	C	1.062845	0.173891	0.000039
7	N	0.214242	-0.892265	0.00002
6	C	-1.121382	-0.640365	0.000036
6	C	-1.565853	0.754405	0.000053
6	C	-0.59918	1.75636	0.000041
7	N	-2.93381	0.741005	0.000143
6	C	-3.215506	-0.581887	0.000137
7	N	-2.156081	-1.478015	-0.000061
1	H	0.618149	-1.832519	-0.000032
1	H	-0.846591	2.821367	0.000111
1	H	-4.243444	-0.947949	0.000092
7	N	2.507275	-0.210606	-0.000011
8	O	2.736153	-1.431982	-0.000208
8	O	3.338578	0.682869	-0.000161

C2-NO_2-PU_3H E_{tot} = -616.156681 a.u.
Gibbs free energy E_G= -616.097011 a.u.

7	N	0.726731	1.436678	0.000046
6	C	1.062845	0.173891	0.000039
7	N	0.214242	-0.892265	0.00002
6	C	-1.121382	-0.640365	0.000036
6	C	-1.565853	0.754405	0.000053
6	C	-0.59918	1.75636	0.000041
7	N	-2.93381	0.741005	0.000143
6	C	-3.215506	-0.581887	0.000137
7	N	-2.156081	-1.478015	-0.000061
1	H	0.618149	-1.832519	-0.000032
1	H	-0.846591	2.821367	0.000111
1	H	-4.243444	-0.947949	0.000092
7	N	2.507275	-0.210606	-0.000011
8	O	2.736153	-1.431982	-0.000208
8	O	3.338578	0.682869	-0.000161

C8-CN- PU _3H E_{tot} = -503.916727 a.u.
Gibbs free energy E_G= -503.859019 a.u.

7	N	-2.804898	0.707231	0.000209
6	C	-2.75132	-0.612758	0.000277
7	N	-1.590048	-1.337483	0.000183
6	C	-0.394882	-0.677618	0.000077
6	C	-0.409123	0.772658	0.000008
6	C	-1.641325	1.420477	0.000054
7	N	0.896551	1.197873	-0.000144
6	C	1.576328	0.028116	0.000266
7	N	0.845061	-1.16029	-0.000134
1	H	-3.676213	-1.193519	0.000341
1	H	-1.611493	-2.356472	0.000179
1	H	-1.732907	2.510755	0.000026
6	C	3.009032	-0.010064	-0.000205
7	N	4.180242	-0.048135	-0.000601

C2-CN- PU _3H E_{tot} = -503.910832 a.u.
Gibbs free energy E_G= -503.853456 a.u.

7	N	1.091952	1.391241	-0.000006
6	C	1.444886	0.112897	-0.000129
7	N	0.550448	-0.938958	-0.000083
6	C	-0.781173	-0.667978	0.000007
6	C	-1.208977	0.727107	0.000121
6	C	-0.230529	1.715746	0.00015
7	N	-2.579522	0.729353	0.000051
6	C	-2.875693	-0.588009	-0.00018
7	N	-1.824078	-1.496002	0.000302
1	H	0.885397	-1.902649	-0.000066
1	H	-0.469156	2.783189	0.000081
1	H	-3.906866	-0.944474	0.000106
6	C	2.835666	-0.24546	-0.000127
7	N	3.959136	-0.580189	-0.000146

C8-CHO- PU _3H E_{tot} = -524.999636 a.u.
Gibbs free energy E_G= -524.931972 a.u.

7	N	-2.92171	0.565815	-0.000067
6	C	-2.766844	-0.747008	0.000077
7	N	-1.556038	-1.382807	0.0001
6	C	-0.409931	-0.636037	0.000046
6	C	-0.536583	0.811698	-0.000077
6	C	-1.814064	1.363939	-0.000176
7	N	0.734403	1.326915	0.00011
6	C	1.507642	0.211836	0.000209
7	N	0.859286	-1.022901	-0.000175
1	H	-3.646091	-1.395066	0.000046
1	H	-1.501361	-2.40062	0.0001
1	H	-1.988597	2.444301	-0.000092
6	C	2.987071	0.353462	0.000253
8	O	3.775093	-0.578255	-0.000226
1	H	3.319957	1.420939	-0.000013

C2-CHO- PU _3H E_{tot} = -525.006500 a.u.
Gibbs free energy E_G= -524.938374 a.u.

7	N	0.932823	1.567859	-0.000141
6	C	1.390479	0.318788	0.000021
7	N	0.59096	-0.795487	0.00008
6	C	-0.754252	-0.647247	0.000046
6	C	-1.301552	0.710099	-0.000116
6	C	-0.409589	1.781838	-0.000255
7	N	-2.664416	0.597899	0.000249
6	C	-2.848111	-0.74426	0.000145
7	N	-1.72886	-1.559211	-0.000227
1	H	1.050694	-1.710337	0.000072
1	H	-0.744038	2.823608	-0.000087
1	H	-3.847392	-1.182923	0.000097
6	C	2.852291	0.067271	-0.000001
8	O	3.32206	-1.064563	0.000183
1	H	3.475107	0.989812	-0.000313

C8-CHO- PU _3H E_{tot} = -524.998002 a.u.
Gibbs free energy E_G= -524.930509 a.u.

7	N	2.813552	0.85776	-0.000017
6	C	2.867003	-0.463683	-0.000008
7	N	1.769576	-1.279969	0.00005
6	C	0.522381	-0.720493	0.000035
6	C	0.418375	0.728845	-0.000006
6	C	1.596642	1.473429	-0.000011
7	N	-0.913541	1.047149	0.000018
6	C	-1.507494	-0.168125	-0.000452
7	N	-0.675509	-1.294427	0.000261
1	H	3.836598	-0.966505	0.000075
1	H	1.875841	-2.293644	0.000148
1	H	1.599396	2.567744	-0.000068
6	C	-2.980195	-0.384058	-0.000366
8	O	-3.813393	0.506215	0.000381
1	H	-3.263502	-1.466399	-0.000535

C2-CHO- PU _3H E_{tot} = -524.995120 a.u.
Gibbs free energy E_G= -524.927741 a.u.

7	N	-1.124141	1.212194	0.000152
6	C	-1.367109	-0.092932	0.000176
7	N	-0.370475	-1.048664	0.000002
6	C	0.928662	-0.664147	-0.000056
6	C	1.228767	0.762538	-0.000065
6	C	0.157659	1.656701	-0.000033
7	N	2.590729	0.890569	0.000153
6	C	3.007086	-0.398416	0.00025
7	N	2.046375	-1.395414	-0.0006
1	H	-0.610754	-2.041488	-0.000153
1	H	0.300977	2.741761	0.00025
1	H	4.06731	-0.656208	-0.000215
6	C	-2.757556	-0.634418	0.000147
8	O	-3.767024	0.041047	-0.000113
1	H	-2.803808	-1.759194	0.000558

C8-Cl- PU _3H E_{tot} = -871.362744 a.u.
Gibbs free energy E_G= -871.31204 a.u.

7	N	-2.915236	0.70673	0.000108
6	C	-2.863898	-0.60994	0.000224
7	N	-1.698123	-1.335566	0.000192
6	C	-0.505379	-0.675812	0.000093
6	C	-0.518404	0.775801	-0.00002
6	C	-1.748147	1.421744	-0.00006
7	N	0.794006	1.196575	0.000104
6	C	1.454764	0.029645	0.000052
7	N	0.737642	-1.158016	-0.00011
1	H	-3.787265	-1.193159	0.000269
1	H	-1.718424	-2.354106	0.000212
1	H	-1.840943	2.511697	0.000019
17	Cl	3.176764	-0.028301	-0.00025

C2-Cl- PU _3H E_{tot} = -871.358895 a.u.
Gibbs free energy E_G= -871.308459 a.u.

7	N	1.002408	1.373047	0.000046
6	C	1.329778	0.109361	0.000051
7	N	0.445577	-0.9361	-0.00004
6	C	-0.894277	-0.652501	-0.00003
6	C	-1.308786	0.740672	-0.00000
6	C	-0.324809	1.716556	-0.00001
7	N	-2.68764	0.751995	-0.00004
6	C	-2.990031	-0.556666	0.000553
7	N	-1.937577	-1.474538	-0.00029
1	H	0.779104	-1.898543	-0.00015
1	H	-0.546329	2.787428	0.000044
1	H	-4.022173	-0.910962	0.000181
17	Cl	3.009339	-0.360194	-0.00007

C8-F- PU_3H E_{tot} = -510.937515 a.u.
Gibbs free energy E_G= -510.884072 a.u.

7	N	-2.493728	0.717531	0.000044
6	C	-2.451702	-0.598259	0.00016
7	N	-1.289058	-1.331503	0.000151
6	C	-0.094022	-0.679703	0.000072
6	C	-0.096707	0.774028	-0.000048
6	C	-1.321632	1.426146	-0.000104
7	N	1.22044	1.184906	0.000107
6	C	1.855805	0.012509	0.000046
7	N	1.147853	-1.169438	-0.000106
1	H	-3.378184	-1.176495	0.000194
1	H	-1.31561	-2.34987	0.000173
1	H	-1.408584	2.516525	-0.000032
9	F	3.183709	-0.04544	-0.000274

C2-F- PU_3H E_{tot} = -510.932605 a.u.
Gibbs free energy E_G= -510.879613 a.u.

7	N	1.513638	1.192017	-0.000008
6	C	1.708033	-0.091007	-0.000295
7	N	0.754806	-1.062751	-0.000195
6	C	-0.559902	-0.662358	-0.000012
6	C	-0.846009	0.762427	0.000189
6	C	0.217555	1.649344	0.000322
7	N	-2.221346	0.896034	-0.000227
6	C	-2.638611	-0.37783	-0.000156
7	N	-1.669377	-1.387572	0.000544
1	H	1.013546	-2.048277	-0.000159
1	H	0.088874	2.73506	0.000102
1	H	-3.697652	-0.640365	0.000142
9	F	2.962754	-0.57711	-0.00013

C8-H- PU_3H E_{tot} = -411.727345 a.u.
Gibbs free energy E_G= -411.664858 a.u.

7	N	2.072937	0.745955	0.000539
6	C	2.048809	-0.57306	0.000429
7	N	0.901102	-1.3226	-9E-06
6	C	-0.30896	-0.69164	-0.00031
6	C	-0.327	0.761381	-0.00014
6	C	0.888871	1.432181	0.000271
7	N	-1.6492	1.149621	-0.00059
6	C	-2.29914	-0.0285	0.000644
7	N	-1.54133	-1.19673	-0.00084
1	H	0.958232	2.524362	0.000366
1	H	-3.38904	-0.08448	0.000104
1	H	2.985325	-1.13528	0.000592
1	H	0.945502	-2.34051	-0.00015

C2-H- PU_3H E_{tot} = -411.727345 a.u.
Gibbs free energy E_G= -411.664858 a.u.

7	N	2.072937	0.745955	0.000539
6	C	2.048809	-0.57306	0.000429
7	N	0.901102	-1.3226	-9E-06
6	C	-0.30896	-0.69164	-0.00031
6	C	-0.327	0.761381	-0.00014
6	C	0.888871	1.432181	0.000271
7	N	-1.6492	1.149621	-0.00059
6	C	-2.29914	-0.0285	0.000644
7	N	-1.54133	-1.19673	-0.00084
1	H	0.958232	2.524362	0.000366
1	H	-3.38904	-0.08448	0.000104
1	H	2.985325	-1.13528	0.000592
1	H	0.945502	-2.34051	-0.00015

C8-Me- PU_3H E_{tot} = -451.030158 a.u.
Gibbs free energy E_G= -450.943926 a.u.

7	N	2.544541	0.715094	-0.000173
6	C	2.498045	-0.601375	-0.000283
7	N	1.335088	-1.331912	-0.000198
6	C	0.136032	-0.680142	-0.000061
6	C	0.144076	0.773607	0.000057
6	C	1.370568	1.422782	0.000042
7	N	-1.16971	1.183228	-0.000011
6	C	-1.856055	0.020096	-0.000037
7	N	-1.102111	-1.161698	0.000227
1	H	3.423758	-1.181168	-0.000356
1	H	1.361675	-2.350128	-0.000205
1	H	1.459328	2.513366	-0.000044
6	C	-3.34656	-0.037763	0.000352
1	H	-3.70622	-0.587411	-0.88567
1	H	-3.705807	-0.588034	0.886152
1	H	-3.764033	0.977166	0.00078

C2-Me- PU_3H E_{tot} = -451.028624 a.u.
Gibbs free energy E_G= -450.9412 a.u.

7	N	-1.440553	1.236491	0.000004
6	C	-1.713073	-0.060779	0.000129
7	N	-0.728303	-1.02184	0.000104
6	C	0.587614	-0.657864	0.000011
6	C	0.911099	0.755026	-0.000103
6	C	-0.139829	1.659643	-0.000141
7	N	2.287952	0.857846	0.000006
6	C	2.67409	-0.429581	0.000033
7	N	1.685086	-1.412484	-0.00019
1	H	-0.974528	-2.010433	0.000117
1	H	0.01686	2.742897	-0.000081
1	H	3.727425	-0.71521	-0.000086
6	C	-3.13648	-0.541864	0.000116
1	H	-3.348309	-1.156344	-0.891645
1	H	-3.348239	-1.156601	0.891712
1	H	-3.802995	0.32812	0.000258

C8-OMe- PU_3H E_{tot} = -526.215092 a.u.
Gibbs free energy E_G= -526.124594 a.u.

7	N	-2.821288	0.951938	0.000203
6	C	-2.949884	-0.355737	0.000228
7	N	-1.888695	-1.234815	0.000153
6	C	-0.617191	-0.745403	0.000017
6	C	-0.43304	0.698701	-0.000017
6	C	-1.563314	1.502571	0.000086
7	N	0.922491	0.933876	-0.00005
6	C	1.425797	-0.318308	-0.000343
7	N	0.543017	-1.393967	-0.000122
1	H	-3.942504	-0.811383	0.000314
1	H	-2.046443	-2.240681	0.000174
1	H	-1.509232	2.595047	0.000129
8	O	2.729463	-0.597194	-0.000217
6	C	3.614824	0.549188	-0.000015
1	H	4.626593	0.125817	0.000063
1	H	3.442125	1.161803	-0.897479
1	H	3.441928	1.161655	0.897514

C2-OMe- PU_3H E_{tot} = -526.212989 a.u.
Gibbs free energy E_G= -526.122762 a.u.

7	N	1.118481	1.102136	-0.00004
6	C	1.281589	-0.204989	-0.000049
7	N	0.260839	-1.118824	0.000039
6	C	-1.032124	-0.661023	0.00004
6	C	-1.258648	0.769998	0.000049
6	C	-0.155669	1.606773	0.000002
7	N	-2.630141	0.964523	0.000552
6	C	-3.100176	-0.289906	-0.000798
7	N	-2.173874	-1.339366	0.000159
1	H	0.470527	-2.1152	0.00009
1	H	-0.241765	2.697486	0.000204
1	H	-4.169404	-0.507903	-0.000367
8	O	2.495857	-0.786784	-0.00002
6	C	3.633431	0.114394	-0.000023
1	H	3.614178	0.747891	-0.898216
1	H	3.61414	0.747947	0.898131
1	H	4.507906	-0.546705	0.000016

C8-OMe- PU_3H E_{tot} = -526.212890 a.u.
Gibbs free energy E_G= -526.122596 a.u.

7	N	3.005447	0.443715	-0.00002
6	C	2.778203	-0.851569	0.000002
7	N	1.517731	-1.409748	0.000008
6	C	0.428395	-0.594716	0.000014
6	C	0.636425	0.84537	-0.000007
6	C	1.945878	1.312893	-0.000035
7	N	-0.599462	1.440543	0.000018
6	C	-1.425721	0.375481	0.000082
7	N	-0.867677	-0.902776	0.000012
1	H	3.610464	-1.55847	0
1	H	1.398591	-2.421013	0.000012
1	H	2.188315	2.37937	-0.000037
8	O	-2.746998	0.564693	0.000007
6	C	-3.572786	-0.623291	-0.00005
1	H	-4.604345	-0.250163	-0.000091
1	H	-3.3758	-1.227197	-0.898632
1	H	-3.375878	-1.227223	0.898532

C2-OMe- PU_3H E_{tot} = -526.203064 a.u.
Gibbs free energy E_G= -526.113033 a.u.

7	N	-0.814486	1.625303	-0.000015
6	C	-1.320984	0.407918	-0.000067
7	N	-0.567049	-0.739351	-0.000016
6	C	0.804403	-0.627295	-0.000034
6	C	1.394806	0.688695	-0.000039
6	C	0.54009	1.782637	0.000042
7	N	2.768578	0.51836	-0.000299
6	C	2.89515	-0.816599	-0.00031
7	N	1.726256	-1.584818	0.000237
1	H	-0.984218	-1.666606	0.000084
1	H	0.904251	2.814709	-0.000133
1	H	3.870027	-1.306773	-0.000198
8	O	-2.669586	0.320424	0.000083
6	C	-3.285208	-0.97912	0.000281
1	H	-3.016096	-1.54641	-0.908374
1	H	-3.015849	-1.546262	0.908955
1	H	-4.364063	-0.785932	0.000412

C8-OH- PU_3H E_{tot} = -486.939490 a.u.
Gibbs free energy E_G= -486.873581 a.u.

7	N	-2.49731	0.737968	0.000016
6	C	-2.471129	-0.576255	0.000013
7	N	-1.31293	-1.322676	-0.00002
6	C	-0.110056	-0.685983	0.00003
6	C	-0.096398	0.769508	0.000032
6	C	-1.315031	1.433885	0.000004
7	N	1.223518	1.15778	-0.000162
6	C	1.865763	-0.027816	0.000517
7	N	1.121323	-1.194955	0.000069
1	H	-3.402719	-1.146111	0.000016
1	H	-1.349511	-2.340341	-0.000033
1	H	-1.391206	2.524994	-0.000106
8	O	3.203109	-0.119946	-0.00026
1	H	3.537458	0.79416	-0.000691

C2-OH- PU_3H E_{tot} = -486.937002 a.u.
Gibbs free energy E_G= -486.871473 a.u.

7	N	1.510664	1.174249	-0.00005
6	C	1.712858	-0.127247	-0.000105
7	N	0.732913	-1.075942	-0.000045
6	C	-0.576998	-0.660725	0.000022
6	C	-0.851454	0.761647	0.000065
6	C	0.221313	1.637891	0.000039
7	N	-2.22819	0.908762	0.000233
6	C	-2.655746	-0.360825	-0.000162
7	N	-1.693552	-1.377796	0.000127
1	H	0.975337	-2.065019	-0.000048
1	H	0.099181	2.724844	0.000097
1	H	-3.716712	-0.615233	0.000004
8	O	2.965555	-0.635651	-0.000119
1	H	3.565076	0.131258	-0.000107

C8-OH- PU_3H E_{tot} = -486.938355 a.u.
Gibbs free energy E_G= -486.872502 a.u.

7	N	2.513791	0.692686	-0.000238
6	C	2.456961	-0.620366	-0.00027
7	N	1.280703	-1.33917	-0.000176
6	C	0.094165	-0.673264	-0.000019
6	C	0.113729	0.78236	0.000021
6	C	1.348941	1.416709	-0.000091
7	N	-1.192808	1.213473	0.000004
6	C	-1.867619	0.054506	0.000398
7	N	-1.152923	-1.142482	0.000168
1	H	3.374563	-1.212456	-0.000364
1	H	1.295319	-2.357277	-0.000194
1	H	1.449816	2.505708	-0.000178
8	O	-3.208656	0.029981	0.000241
1	H	-3.468851	-0.907035	0.000271

C2-OH- PU_3H E_{tot} = -486.924866 a.u.
Gibbs free energy E_G= -486.860497 a.u.

7	N	1.491343	1.210464	-0.000038
6	C	1.727887	-0.081328	-0.000216
7	N	0.751592	-1.048302	-0.000122
6	C	-0.566696	-0.654299	0.000014
6	C	-0.866235	0.759516	0.000147
6	C	0.196548	1.649262	0.000197
7	N	-2.245461	0.881019	0.000036
6	C	-2.649684	-0.396359	-0.000159
7	N	-1.668162	-1.394947	0.000376
1	H	0.967922	-2.044062	-0.000099
1	H	0.058004	2.734591	0.000109
1	H	-3.705609	-0.67077	0.000098
8	O	3.027393	-0.472388	-0.000196
1	H	3.10444	-1.439052	-0.000198

C8-NH_2- PU_3H E_{tot} = -467.081976 a.u.
Gibbs free energy E_G= -467.0048 a.u.

7	N	-2.522604	0.712205	0.003991
6	C	-2.480656	-0.59974	0.003232
7	N	-1.308658	-1.331697	0.000187
6	C	-0.114222	-0.679297	-0.002707
6	C	-0.118907	0.777832	-0.002659
6	C	-1.34854	1.424788	0.001171
7	N	1.190386	1.189357	-0.001494
6	C	1.86654	0.015951	-0.003468
7	N	1.122831	-1.168451	-0.00252
1	H	-3.403274	-1.183931	0.004794
1	H	-1.332856	-2.349237	-0.000948
1	H	-1.439289	2.514629	0.002132
7	N	3.225037	-0.043906	-0.04324
1	H	3.736081	0.807076	0.150315
1	H	3.665107	-0.9283	0.171835

C2-NH_2- PU_3H E_{tot} = -467.073558 a.u.
Gibbs free energy E_G= -466.996686 a.u.

7	N	1.481805	1.203572	0.005288
6	C	1.720895	-0.102657	-0.001532
7	N	0.731229	-1.055968	-0.015315
6	C	-0.58305	-0.65583	0.000584
6	C	-0.876934	0.757634	0.006785
6	C	0.18999	1.643677	-0.005605
7	N	-2.256546	0.887137	0.010205
6	C	-2.666898	-0.388395	0.005034
7	N	-1.690227	-1.390995	-0.002568
1	H	0.952521	-2.047507	-0.07979
1	H	0.051944	2.729408	-0.016503
1	H	-3.724373	-0.65769	0.005794
7	N	3.029011	-0.548417	-0.064036
1	H	3.69756	0.195973	0.106743
1	H	3.251424	-1.414061	0.417151

C8-NO_2-PU_1H E_{tot} = -616.150185 a.u.
Gibbs free energy E_G= -616.089244 a.u.

7	N	3.092628	0.602164	0.000434
6	C	3.03158	-0.778356	0.000301
7	N	1.91666	-1.471762	0.000091
6	C	0.776908	-0.728514	0.000023
6	C	0.770026	0.742416	0.00014
6	C	1.980075	1.403689	0.00036
7	N	-0.525469	1.182826	0
6	C	-1.180454	0.010505	-0.0001
7	N	-0.492306	-1.170186	-0.000275
1	H	3.998514	-1.286864	0.000368
1	H	4.010101	1.037249	0.000589
1	H	2.127003	2.484645	0.000476
7	N	-2.672119	-0.002616	-0.000319
8	O	-3.217633	-1.105046	-0.000147
8	O	-3.237392	1.09049	-0.000514

C2-NO_2-PU_1H E_{tot} = -616.154259 a.u.
Gibbs free energy E_G= -616.094487 a.u.

7	N	0.698681	1.293746	0.000192
6	C	1.021605	-0.035864	0.000056
7	N	0.188416	-1.041301	-0.000133
6	C	-1.117484	-0.678739	-0.000174
6	C	-1.564016	0.729424	-0.000056
6	C	-0.601642	1.720796	0.000142
7	N	-2.92584	0.756571	-0.000264
6	C	-3.230954	-0.569236	-0.000056
7	N	-2.199678	-1.476696	-0.00052
1	H	1.492281	1.936195	0.000307
1	H	-0.778341	2.796835	0.000227
1	H	-4.269206	-0.906068	-0.000463
7	N	2.49265	-0.281374	0.000123
8	O	2.883438	-1.436684	0.000125
8	O	3.207888	0.73895	0.000458

C8-CN-PU_1H E_{tot} = -503.912548 a.u.
Gibbs free energy E_G= -503.85486 a.u.

7	N	2.720685	0.598393	0.000405
6	C	2.657642	-0.780934	0.000284
7	N	1.54095	-1.472108	0.000077
6	C	0.401006	-0.727777	-0.000093
6	C	0.395393	0.742703	0.000046
6	C	1.607463	1.400961	0.000307
7	N	-0.89645	1.187806	0.000031
6	C	-1.580145	0.013376	-0.000865
7	N	-0.865572	-1.170904	-0.000091
1	H	3.623351	-1.291813	0.000439
1	H	3.638247	1.032891	0.000616
1	H	1.756556	2.481582	0.00047
6	C	-3.015617	-0.002694	-0.000401
7	N	-4.187129	-0.014112	-0.000021

C2-CN-PU_1H E_{tot} = -503.907115 a.u.
Gibbs free energy E_G= -503.849669 a.u.

7	N	1.066651	1.245509	0.000184
6	C	1.400964	-0.102479	0.000063
7	N	0.519849	-1.088984	-0.000085
6	C	-0.776893	-0.700136	-0.000169
6	C	-1.20392	0.712239	-0.000015
6	C	-0.229541	1.688131	0.000147
7	N	-2.567012	0.760913	0.000086
6	C	-2.890492	-0.558017	-0.000806
7	N	-1.871159	-1.481636	-0.000019
1	H	1.825658	1.920939	0.000342
1	H	-0.393229	2.766627	0.000301
1	H	-3.93305	-0.881117	-0.000393
6	C	2.810598	-0.379269	0.000194
7	N	3.971147	-0.545698	0.000301

C8-CHO- PU_1H E_{tot} = -524.993922 a.u.
Gibbs free energy E_G= -524.926397 a.u.

7	N	2.83078	0.466544	0.000403
6	C	2.663968	-0.906207	0.000155
7	N	1.501332	-1.513442	-0.000072
6	C	0.415131	-0.687357	-0.000068
6	C	0.522387	0.782468	0.000202
6	C	1.779541	1.348799	0.000427
7	N	-0.734564	1.315339	0.000264
6	C	-1.511436	0.196026	-0.000327
7	N	-0.877477	-1.03285	-0.000182
1	H	3.59052	-1.485591	0.000185
1	H	3.778249	0.830775	0.000591
1	H	2.009247	2.415508	0.000659
6	C	-2.991893	0.362401	-0.00036
8	O	-3.797378	-0.552876	-0.000463
1	H	-3.305672	1.436396	-0.000801

C2-CHO- PU_1H E_{tot} = -524.990732 a.u.
Gibbs free energy E_G= -524.923335 a.u.

7	N	0.889993	1.424246	0.000217
6	C	1.360015	0.117938	0.000136
7	N	0.565688	-0.942494	-0.000024
6	C	-0.75611	-0.677019	-0.000108
6	C	-1.318523	0.689635	-0.000011
6	C	-0.435763	1.752987	0.000157
7	N	-2.676624	0.61061	-0.000141
6	C	-2.874634	-0.738591	-0.00027
7	N	-1.778184	-1.558926	-0.000235
1	H	1.582062	2.16995	0.000333
1	H	-0.699973	2.811649	0.000232
1	H	-3.883926	-1.154786	-0.000372
6	C	2.845661	-0.003263	0.000243
8	O	3.461428	-1.050041	-0.000047
1	H	3.38043	0.989347	0.000572

C8-CHO- PU_1H E_{tot} = -524.993886 a.u.
Gibbs free energy E_G= -524.926391 a.u.

7	N	2.739122	0.735461	0.000036
6	C	2.784877	-0.64599	0.00007
7	N	1.726112	-1.422501	0.000048
6	C	0.530095	-0.769813	-0.000021
6	C	0.408484	0.698364	-0.000053
6	C	1.567715	1.448565	-0.00003
7	N	-0.911075	1.041066	-0.000076
6	C	-1.511524	-0.177301	-0.000236
7	N	-0.699452	-1.302012	0.000057
1	H	3.788437	-1.077954	0.000135
1	H	3.620144	1.23994	0.000067
1	H	1.632362	2.537708	-0.000047
6	C	-2.990489	-0.369754	-0.000213
8	O	-3.808507	0.53483	0.000302
1	H	-3.290781	-1.446852	-0.000125

C2-CHO- PU_1H E_{tot} = -525.004460 a.u.
Gibbs free energy E_G= -524.936198 a.u.

7	N	1.102854	1.055043	0.000251
6	C	1.308136	-0.308051	0.000114
7	N	0.334962	-1.211442	-0.000095
6	C	-0.915487	-0.701357	-0.000163
6	C	-1.203278	0.745818	-0.000029
6	C	-0.134363	1.625336	0.000187
7	N	-2.552453	0.92774	-0.000186
6	C	-3.006776	-0.356981	-0.000269
7	N	-2.086908	-1.372331	-0.00038
1	H	1.955298	1.617671	0.000405
1	H	-0.197114	2.714664	0.000294
1	H	-4.077014	-0.57215	-0.00047
6	C	2.726908	-0.730285	0.000212
8	O	3.649965	0.079043	0.000254
1	H	2.879084	-1.83248	0.000296

C8-Cl- PU_1H E_{tot} = -871.359156 a.u.
Gibbs free energy E_G= -871.308481 a.u.

7	N	2.832796	0.593994	0.000373
6	C	2.767002	-0.78089	0.000256
7	N	1.647131	-1.471771	0.000073
6	C	0.51038	-0.725927	-0.00000
6	C	0.505878	0.746548	0.000113
6	C	1.717171	1.401544	0.000308
7	N	-0.791165	1.188252	0.000005
6	C	-1.458137	0.017383	-0.00019
7	N	-0.759301	-1.166705	-0.00019
1	H	3.73087	-1.295471	0.000328
1	H	3.750546	1.026949	0.000516
1	H	1.870345	2.481235	0.000414
17	Cl	-3.183044	-0.010062	-0.00035

C2-Cl- PU_1H E_{tot} = -871.354833 a.u.
Gibbs free energy E_G= -871.304418 a.u.

7	N	-0.965273	1.256414	-0.00021
6	C	-1.284298	-0.082421	-0.00009
7	N	-0.429934	-1.061912	0.000072
6	C	0.882333	-0.686582	0.000139
6	C	1.31235	0.722882	0.000031
6	C	0.343523	1.695915	-0.00015
7	N	2.684446	0.762615	0.000108
6	C	2.995573	-0.55026	0.000359
7	N	1.963467	-1.473783	0.000318
1	H	-1.725571	1.928136	-0.00035
1	H	0.502879	2.774841	-0.00026
1	H	4.034638	-0.885408	0.000448
17	Cl	-3.004575	-0.399889	-0.00021

C8-F- PU_1H E_{tot} = -510.934568 a.u.
Gibbs free energy E_G= -510.881123 a.u.

7	N	2.413951	0.596893	0.000321
6	C	2.351342	-0.776312	0.000205
7	N	1.231985	-1.470084	0.000025
6	C	0.095163	-0.72815	-0.000047
6	C	0.086609	0.747072	0.000065
6	C	1.296019	1.403254	0.000258
7	N	-1.213289	1.18379	-0.000041
6	C	-1.860307	0.010439	-0.000235
7	N	-1.174973	-1.171309	-0.000239
1	H	3.315795	-1.289753	0.000275
1	H	3.330643	1.031951	0.000462
1	H	1.448059	2.482993	0.000364
9	F	-3.19013	-0.015337	-0.000338

C2-F- PU_1H E_{tot} = -510.928373 a.u.
Gibbs free energy E_G= -510.875401 a.u.

7	N	1.469456	1.068095	0.000236
6	C	1.644023	-0.28909	0.000117
7	N	0.722793	-1.195048	-0.000048
6	C	-0.552911	-0.698638	-0.000112
6	C	-0.848478	0.747548	-0.000005
6	C	0.202292	1.628832	0.000176
7	N	-2.213861	0.913196	-0.000078
6	C	-2.644048	-0.362346	-0.000332
7	N	-1.699803	-1.379937	-0.000289
1	H	2.294665	1.658616	0.000374
1	H	0.143167	2.717421	0.000288
1	H	-3.709324	-0.60139	-0.000417
9	F	2.946237	-0.641847	0.000216

C8-H- PU_1H E_{tot} = -411.722874 a.u.
Gibbs free energy E_G= -411.660423 a.u.

7	N	1.998293	0.60907	0.000281
6	C	1.944534	-0.76881	0.000166
7	N	0.831723	-1.46826	-2.5E-05
6	C	-0.31401	-0.73292	-9.3E-05
6	C	-0.33035	0.740831	0.00001
6	C	0.875838	1.404443	0.000212
7	N	-1.63187	1.170039	-0.00012
6	C	-2.30446	-0.00402	-0.00017
7	N	-1.58092	-1.1785	-0.00034
1	H	1.020069	2.486083	0.000314
1	H	-3.39633	-0.02647	-0.00036
1	H	2.913982	-1.27315	0.000243
1	H	2.912345	1.049889	0.000424

C2-H- PU_1H E_{tot} = -411.722874 a.u.
Gibbs free energy E_G= -411.660423 a.u.

7	N	1.998293	0.60907	0.000281
6	C	1.944534	-0.76881	0.000166
7	N	0.831723	-1.46826	-2.5E-05
6	C	-0.31401	-0.73292	-9.3E-05
6	C	-0.33035	0.740831	0.00001
6	C	0.875838	1.404443	0.000212
7	N	-1.63187	1.170039	-0.00012
6	C	-2.30446	-0.00402	-0.00017
7	N	-1.58092	-1.1785	-0.00034
1	H	1.020069	2.486083	0.000314
1	H	-3.39633	-0.02647	-0.00036
1	H	2.913982	-1.27315	0.000243
1	H	2.912345	1.049889	0.000424

C8-Me- PU_1H E_{tot} = -451.025819 a.u.
Gibbs free energy E_G= -450.939693 a.u.

7	N	-2.463188	0.595764	0.000055
6	C	-2.397897	-0.779803	0.000061
7	N	-1.279177	-1.471421	0
6	C	-0.137902	-0.727484	0.000003
6	C	-0.133516	0.747381	-0.000043
6	C	-1.343978	1.401181	-0.000013
7	N	1.163733	1.182722	-0.000196
6	C	1.860814	0.017928	0.000342
7	N	1.128063	-1.162006	-0.000251
1	H	-3.362826	-1.292929	0.000072
1	H	-3.380023	1.029767	0.000093
1	H	-1.498113	2.481111	-0.000028
6	C	3.352727	-0.013089	0.00001
1	H	3.719219	-0.555915	0.887249
1	H	3.718936	-0.562167	-0.883422
1	H	3.755306	1.00804	-0.003381

C2-Me- PU_1H E_{tot} = -451.023980 a.u.
Gibbs free energy E_G= -450.93801 a.u.

7	N	-1.382972	1.124998	-0.000232
6	C	-1.659978	-0.231989	-0.000302
7	N	-0.713267	-1.151004	-0.000166
6	C	0.567893	-0.692025	-0.000004
6	C	0.918058	0.737319	0.000138
6	C	-0.109275	1.649002	-0.000012
7	N	2.28575	0.859988	0.000553
6	C	2.673493	-0.433919	-0.000269
7	N	1.699733	-1.414138	0.000484
1	H	-2.168557	1.766887	-0.000302
1	H	-0.012475	2.735827	0.000055
1	H	3.731228	-0.705791	0.000427
6	C	-3.112288	-0.6212	-0.000233
1	H	-3.631451	-0.232771	0.89304
1	H	-3.63214	-0.230849	-0.892258
1	H	-3.178726	-1.715341	-0.001339

C8-OMe- PU_1H E_{tot} = -526.211017 a.u.
Gibbs free energy E_G= -526.120493 a.u.

7	N	-2.755709	0.822855	-0.000366
6	C	-2.871348	-0.54508	-0.000267
7	N	-1.853396	-1.380571	-0.000094
6	C	-0.624842	-0.794983	-0.000037
6	C	-0.424089	0.668337	-0.000136
6	C	-1.536935	1.476835	-0.000298
7	N	0.91863	0.928563	-0.000019
6	C	1.43126	-0.326608	0.000018
7	N	0.567358	-1.403165	0.000159
1	H	-3.894916	-0.928298	-0.000326
1	H	-3.607028	1.373901	-0.000488
1	H	-1.548161	2.567056	-0.00038
8	O	2.74064	-0.581533	0.000374
6	C	3.609291	0.575768	0.000517
1	H	3.429621	1.186872	0.897913
1	H	4.627067	0.166623	0.00082
1	H	3.430093	1.186723	-0.897075

C2-OMe- PU_1H E_{tot} = -526.196289 a.u.
Gibbs free energy E_G= -526.10652 a.u.

7	N	1.0487	1.02521	0.000126
6	C	1.228286	-0.343589	-0.000003
7	N	0.251568	-1.216914	-0.000103
6	C	-1.003828	-0.695667	-0.000205
6	C	-1.279598	0.75405	-0.000034
6	C	-0.210942	1.60862	0.000124
7	N	-2.642966	0.945017	0.000152
6	C	-3.092593	-0.325282	-0.001059
7	N	-2.168774	-1.357371	0.000101
1	H	1.855722	1.636426	0.000283
1	H	-0.246226	2.698548	0.000303
1	H	-4.162514	-0.545146	-0.000418
8	O	2.490855	-0.840866	0.000157
6	C	3.605849	0.062269	0.000392
1	H	3.613579	0.69036	0.910052
1	H	4.496014	-0.577749	0.000476
1	H	3.613846	0.690495	-0.909172

C8-OMe- PU_1H E_{tot} = -526.210636 a.u.
Gibbs free energy E_G= -526.120166 a.u.

7	N	-2.909529	0.344349	-0.000431
6	C	-2.657801	-1.004138	-0.000288
7	N	-1.450268	-1.535705	-0.000087
6	C	-0.428174	-0.642347	-0.000043
6	C	-0.620633	0.821759	-0.000184
6	C	-1.913403	1.301119	-0.000378
7	N	0.597942	1.433791	-0.00008
6	C	1.430532	0.364859	0.000032
7	N	0.887246	-0.90597	0.000182
1	H	-3.540922	-1.647374	-0.000341
1	H	-3.87748	0.647643	-0.000576
1	H	-2.216805	2.348161	-0.000499
8	O	2.748906	0.572044	0.000358
6	C	3.584864	-0.610915	0.000709
1	H	3.390528	-1.216698	-0.896773
1	H	4.613329	-0.228845	0.000938
1	H	3.39006	-1.216509	0.898217

C2-OMe- PU_1H E_{tot} = -526.208965 a.u.
Gibbs free energy E_G= -526.118637 a.u.

7	N	0.775122	1.532804	0.000254
6	C	1.297382	0.257452	0.000142
7	N	0.587924	-0.843633	-0.00006
6	C	-0.765409	-0.662273	-0.000128
6	C	-1.398884	0.667188	-0.000022
6	C	-0.586596	1.771239	0.000174
7	N	-2.767575	0.502528	-0.000212
6	C	-2.879369	-0.838106	-0.000129
7	N	-1.719192	-1.599945	-0.000405
1	H	1.431391	2.306268	0.000389
1	H	-0.906501	2.813796	0.000258
1	H	-3.856893	-1.325021	-0.000415
8	O	2.646844	0.267645	0.000219
6	C	3.281461	-1.037825	0.000093
1	H	2.987773	-1.601084	-0.897446
1	H	4.356339	-0.822125	0.000183
1	H	2.987668	-1.601308	0.897457

C8-OH- PU_1H E_{tot} = -486.935811 a.u.
Gibbs free energy E_G= -486.869894a.u.

7	N	2.419491	0.615631	0.000308
6	C	2.370953	-0.75581	0.000187
7	N	1.258402	-1.462186	-0.000001
6	C	0.111256	-0.734372	-0.000021
6	C	0.086337	0.742835	0.000097
6	C	1.289567	1.411362	0.000251
7	N	-1.216784	1.156925	-0.000013
6	C	-1.871617	-0.029512	0.000075
7	N	-1.148458	-1.1971	-0.000266
1	H	3.340593	-1.259774	0.000225
1	H	3.330978	1.060566	0.000432
1	H	1.432218	2.492189	0.000343
8	O	-3.210916	-0.090512	-0.000515
1	H	-3.523998	0.831198	-0.000602

C2-OH- PU_1H E_{tot} = -486.918429 a.u.
Gibbs free energy E_G= -486.854697 a.u.

7	N	1.45011	1.080308	0.000235
6	C	1.66376	-0.285815	0.000118
7	N	0.715805	-1.18359	-0.000046
6	C	-0.555457	-0.694228	-0.000117
6	C	-0.868456	0.747481	-0.000007
6	C	0.175291	1.63176	0.000174
7	N	-2.237186	0.902129	-0.000074
6	C	-2.653076	-0.378159	-0.000377
7	N	-1.70004	-1.386114	-0.000262
1	H	2.241095	1.714915	0.000377
1	H	0.110854	2.720361	0.000289
1	H	-3.716263	-0.627414	-0.000417
8	O	2.951163	-0.728762	0.000211
1	H	3.581813	0.006875	0.000343

C8-OH- PU_1H E_{tot} = -486.936245 a.u.
Gibbs free energy E_G= -486.870299 a.u.

7	N	2.433062	0.571228	0.000292
6	C	2.35179	-0.79824	0.000195
7	N	1.221384	-1.477302	0.000026
6	C	0.094466	-0.719562	0.000003
6	C	0.103221	0.757321	0.000086
6	C	1.32388	1.394963	0.000223
7	N	-1.185832	1.214283	-0.000002
6	C	-1.872151	0.054445	0.000089
7	N	-1.179306	-1.141177	-0.000261
1	H	3.308545	-1.325991	0.000236
1	H	3.355284	0.993577	0.000407
1	H	1.492209	2.472	0.000301
8	O	-3.213202	0.054743	-0.000512
1	H	-3.482805	-0.880324	-0.000809

C2-OH- PU_1H E_{tot} = -486.932603 a.u.
Gibbs free energy E_G= -486.867106 a.u.

7	N	1.445227	1.107741	0.000181
6	C	1.665817	-0.246305	0.000055
7	N	0.735701	-1.167545	-0.000047
6	C	-0.545258	-0.695288	-0.000129
6	C	-0.867215	0.744072	0.000017
6	C	0.167411	1.641913	0.000172
7	N	-2.238354	0.885681	0.000182
6	C	-2.644424	-0.396369	-0.000874
7	N	-1.681975	-1.397515	0.000039
1	H	2.255104	1.718536	0.000329
1	H	0.086747	2.72923	0.000342
1	H	-3.705263	-0.65503	-0.000406
8	O	2.982771	-0.567393	0.000206
1	H	3.019074	-1.540268	0.000161

C8-NH_2- PU_1H E_{tot} = -467.078817 a.u.
Gibbs free energy E_G= -467.001666 a.u.

7	N	-2.44375	0.589642	0.00269
6	C	-2.376093	-0.778511	0.003045
7	N	-1.25264	-1.47066	0.000977
6	C	-0.115094	-0.725487	-0.002372
6	C	-0.108136	0.753059	-0.002081
6	C	-1.323059	1.403812	0.000475
7	N	1.184199	1.189835	-0.000814
6	C	1.87207	0.015061	-0.003665
7	N	1.148643	-1.168223	-0.003138
1	H	-3.33813	-1.297005	0.005342
1	H	-3.361071	1.021617	0.004038
1	H	-1.483021	2.48196	0.00082
7	N	3.230244	-0.019373	-0.039668
1	H	3.731798	0.838697	0.145314
1	H	3.685413	-0.901424	0.151735

C2-NH_2- PU_1H E_{tot} = -467.067709 a.u.
Gibbs free energy E_G= -466.990713 a.u.

7	N	-1.420004	1.118265	-0.016349
6	C	-1.670248	-0.241475	-0.000483
7	N	-0.725396	-1.160614	0.007226
6	C	0.552851	-0.692938	-0.006119
6	C	0.889767	0.74198	0.008474
6	C	-0.139592	1.644722	-0.002758
7	N	2.261762	0.874018	0.017874
6	C	2.656802	-0.412734	0.004088
7	N	1.687803	-1.404535	-0.009559
1	H	-2.206264	1.751352	-0.110466
1	H	-0.051636	2.731866	-0.007669
1	H	3.716008	-0.679296	0.00392
7	N	-3.010703	-0.614643	-0.069347
1	H	-3.1069	-1.621003	0.040545
1	H	-3.642923	-0.107697	0.54553

Table S23. Cartesian coordinates of equilibrium geometries of NX substituted purine (PU) 9H, 7H, 3H and 1H tautomers.

N9-NO_2- PU_9H E_{tot} = -616.134907 a.u
Gibbs free energy E_G= -616.076861 a.u.

7	N	-3.03509	-0.44948	-0.0002
6	C	-2.17337	-1.48916	-0.00037
7	N	-0.82136	-1.4556	-0.00024
6	C	-0.3507	-0.21251	0.000043
6	C	-1.13088	0.974354	0.000235
6	C	-2.51907	0.794221	0.000208
7	N	-0.32518	2.121217	0.000251
6	C	0.906596	1.675697	-8E-06
7	N	0.971735	0.269562	0.000088
1	H	-2.62143	-2.48709	-0.00075
1	H	1.816901	2.268613	-7.8E-05
1	H	-3.2146	1.64029	0.00022
7	N	2.21308	-0.48359	0.000015
8	O	2.102086	-1.69077	0.000965
8	O	3.223075	0.204243	-0.0009

N7-NO_2- PU_7H E_{tot} = -616.137609 a.u.
Gibbs free energy E_G= -616.078701 a.u.

7	N	-2.28333	-1.52189	-0.00007
6	C	-2.96115	-0.35174	-0.0002
7	N	-2.46228	0.89968	-0.00027
6	C	-1.12684	0.945111	0.000016
6	C	-0.31652	-0.22572	0.000422
6	C	-0.93815	-1.4765	0.00033
7	N	0.987502	0.280011	0.000696
6	C	0.900854	1.68316	0.000156
7	N	-0.33804	2.1064	-0.0002
1	H	-4.05232	-0.43439	-0.00044
1	H	1.801955	2.290814	0.000187
1	H	-0.38821	-2.41952	0.000324
7	N	2.209212	-0.47021	-5.4E-05
8	O	2.076692	-1.68407	-0.00032
8	O	3.235541	0.191485	-0.00032

N9-CN- PU_9H E_{tot} = -503.905930 a.u.
Gibbs free energy E_G= -503.848773 a.u.

7	N	2.711185	-0.49264	-0.0002
6	C	1.854541	-1.53745	0.000417
7	N	0.502193	-1.50214	0.00008
6	C	0.04102	-0.25871	0.000068
6	C	0.807555	0.931992	-2.7E-05
6	C	2.19741	0.752092	-0.00033
7	N	-0.01706	2.062649	0.000579
6	C	-1.23928	1.600189	-0.00044
7	N	-1.29892	0.179944	0.000133
1	H	2.306094	-2.53354	-0.00079
1	H	-2.15992	2.180734	-0.00057
1	H	2.895665	1.595636	-0.00022
6	C	-2.41303	-0.57653	0.00004
7	N	-3.40185	-1.20673	-0.00013

N7-CN- PU_7H E_{tot} = -503.902987 a.u.
Gibbs free energy E_G= -503.845936 a.u.

7	N	-1.97322	-1.57119	0.000239
6	C	-2.64684	-0.39544	0.000678
7	N	-2.14725	0.854702	-0.00012
6	C	-0.80921	0.897519	-0.00014
6	C	-0.01222	-0.27661	0.000049
6	C	-0.62875	-1.52577	0.000182
7	N	1.31614	0.189068	-0.00018
6	C	1.226464	1.604986	0.000286
7	N	-0.00426	2.042777	-0.00078
1	H	-3.73802	-0.47686	-0.00092
1	H	2.135154	2.204474	0.000302
1	H	-0.07737	-2.47197	0.000191
6	C	2.438779	-0.55155	-0.00019
7	N	3.418715	-1.19742	0.000151

N9-CHO- PU_9H E_{tot} = -525.017987 a.u.
Gibbs free energy E_G= -524.949910 a.u.

7	N	-2.84998	-0.27953	0.00008
6	C	-2.09967	-1.40133	-0.00025
7	N	-0.74964	-1.49937	-5.6E-05
6	C	-0.16303	-0.30511	-2E-06
6	C	-0.81661	0.951705	-1.4E-05
6	C	-2.21566	0.910699	0.000034
7	N	0.120609	1.995267	0.000416
6	C	1.290848	1.402654	-0.00056
7	N	1.20841	-0.00571	-8.2E-05
1	H	-2.64675	-2.34858	0.000292
1	H	2.262306	1.891491	-0.00076
1	H	-2.82981	1.817351	0.000354
6	C	2.27873	-0.92579	0.000101
8	O	3.442969	-0.58227	0.00016
1	H	1.917104	-1.97375	0.000477

N7-CHO- PU_7H E_{tot} = -525.012837 a.u.
Gibbs free energy E_G= -524.945000 a.u.

7	N	-2.2512	-1.40624	-0.00012
6	C	-2.78737	-0.1637	0.00008
7	N	-2.1474	1.021497	0.000005
6	C	-0.81407	0.909777	-0.00013
6	C	-0.14466	-0.34442	-0.00001
6	C	-0.90865	-1.51048	-0.00013
7	N	1.224542	-0.02706	0.0001
6	C	1.287745	1.380942	-0.00047
7	N	0.11308	1.961633	0.000434
1	H	-3.88091	-0.12029	-6.4E-05
1	H	2.254284	1.879809	-0.00051
1	H	-0.48213	-2.51954	-0.00016
6	C	2.320547	-0.90851	0.000509
8	O	3.476236	-0.53713	-0.00026
1	H	2.004444	-1.97347	0.000747

N9-CHO- PU_9H E_{tot} = -525.011084 a.u.
Gibbs free energy E_G= -524.943514 a.u.

7	N	2.700881	-0.5777	-0.00015
6	C	1.783474	-1.57017	0.000297
7	N	0.43605	-1.46335	0.000196
6	C	0.031895	-0.19575	0.000109
6	C	0.87661	0.944755	-6.7E-05
6	C	2.253697	0.692441	-0.00027
7	N	0.126027	2.129069	0.000128
6	C	-1.1207	1.729613	0.000014
7	N	-1.27719	0.326655	0.000171
1	H	2.179069	-2.59018	-0.00027
1	H	-1.99378	2.381346	0.000046
1	H	2.995233	1.498522	-0.00034
6	C	-2.53034	-0.33035	-4.6E-05
8	O	-2.68583	-1.5284	-0.00025
1	H	-3.36208	0.411496	-6.6E-05

N7-CHO- PU_7H E_{tot} = -525.014519 a.u.
Gibbs free energy E_G= -524.946347 a.u.

7	N	-1.88575	-1.6093	-3.6E-05
6	C	-2.62641	-0.47678	0.000327
7	N	-2.20093	0.801851	-0.00001
6	C	-0.86826	0.918443	-6E-06
6	C	0.003922	-0.20306	-1.5E-05
6	C	-0.54437	-1.4866	-0.00009
7	N	1.297238	0.342124	-2.4E-05
6	C	1.117992	1.740918	0.000238
7	N	-0.13539	2.116945	-0.00025
1	H	-3.71146	-0.62086	-0.00058
1	H	1.979837	2.407647	0.000273
1	H	0.061619	-2.39564	-0.00014
6	C	2.528699	-0.32948	-1E-06
8	O	2.636016	-1.53901	0.000015
1	H	3.386315	0.378942	-0.00012

N9-Cl- PU_9H E_{tot} = -871.323437 a.u.
Gibbs free energy E_G= -871.274114 a.u.

7	N	2.809599	-0.45155	0.000055
6	C	1.958755	-1.50413	-0.00022
7	N	0.609271	-1.48213	0.000049
6	C	0.130818	-0.2401	0.000031
6	C	0.892761	0.960346	-1.1E-05
6	C	2.283875	0.787158	0.000142
7	N	0.063297	2.084755	-0.00049
6	C	-1.16247	1.600452	0.000399
7	N	-1.18279	0.205676	0.000188
1	H	2.420456	-2.49597	0.000452
1	H	-2.08944	2.170092	0.000536
1	H	2.974554	1.637788	-4.3E-05
17	Cl	-2.58963	-0.79009	-9.3E-05

N7-Cl- PU_7H E_{tot} = -871.320300 a.u.
Gibbs free energy E_G= -871.271340 a.u.

7	N	2.088335	-1.53647	0.000143
6	C	2.750518	-0.35108	0.000638
7	N	2.237895	0.890598	0.000189
6	C	0.896957	0.927437	0.0001
6	C	0.108943	-0.26158	0.000053
6	C	0.745511	-1.50349	0.000014
7	N	-1.19361	0.208775	0.000015
6	C	-1.15119	1.595261	0.00041
7	N	0.086123	2.058283	-0.00041
1	H	3.842578	-0.42197	-0.00046
1	H	-2.06664	2.18334	0.000416
1	H	0.203538	-2.45517	-0.00007
17	Cl	-2.62442	-0.77022	-0.0004

N9-F- PU_9H E_{tot} = -510.856023 a.u.
Gibbs free energy E_G= -510.804949 a.u.

7	N	2.537585	0.088479	0.000031
6	C	1.990566	-1.1506	0.000089
7	N	0.683792	-1.48618	-8.8E-05
6	C	-0.09942	-0.40807	-6.3E-05
6	C	0.318931	0.953534	0.000103
6	C	1.707849	1.147092	0.000131
7	N	-0.76982	1.828008	0.000535
6	C	-1.83541	1.047527	-0.00048
7	N	-1.47495	-0.29019	-0.0002
7	H	2.696313	-1.98659	-0.00044
1	H	-2.87927	1.352446	-0.00061
1	H	2.152681	2.14852	0.000315
9	F	-2.36679	-1.3369	0.000009

N7-F- PU_7H E_{tot} = -510.854103 a.u.
Gibbs free energy E_G= -510.803556 a.u.

7	N	-2.10207	-1.17526	-6.8E-05
6	C	-2.45093	0.137951	-0.00032
7	N	-1.64747	1.213053	-5.9E-05
6	C	-0.33826	0.921031	-1.9E-05
6	C	0.129391	-0.43109	0.000002
6	C	-0.79554	-1.47883	0.000059
7	N	1.494405	-0.26652	0.000026
6	C	1.81355	1.072087	-0.00032
7	N	0.720356	1.821715	0.000304
7	H	-3.52654	0.338936	0.000201
1	H	2.84591	1.41391	-0.00036
1	H	-0.50644	-2.5346	0.000079
9	F	2.420137	-1.29956	0.000247

N9-H-PU_9H E_{tot} = -411.741198 a.u.
Gibbs free energy E_G= -411.678769 a.u

7	N	2.133176	0.656495	0.000257
6	C	2.020379	-0.69113	0.000211
7	N	0.89314	-1.43447	0.000044
6	C	-0.20576	-0.67547	-4.3E-05
6	C	-0.24493	0.747737	0.000004
6	C	1.001414	1.387556	0.000157
7	N	-1.56412	1.203032	-9.8E-05
6	C	-2.29031	0.100127	-0.0002
7	N	-1.53258	-1.06594	-0.00028
1	H	1.099483	2.478907	0.000216
1	H	-3.37889	0.065738	-0.00032
1	H	2.960683	-1.25118	0.000252
1	H	-1.87332	-2.02021	-0.00041

N7-H-AD_7H E_{tot} = -411.735954 a.u.
Gibbs free energy E_G= -411.673762 a.u.

7	N	-2.12563	0.684039	-0.00026
6	C	-2.0303	-0.66959	-9.7E-05
7	N	-0.92259	-1.42993	0.000027
6	C	0.219001	-0.72192	0.000092
6	C	0.234645	0.706284	-5.1E-05
6	C	-0.98209	1.390693	-0.00022
7	N	1.579429	1.045547	0.000083
6	C	2.285114	-0.14627	0.000431
7	N	1.516735	-1.22169	0.000003
1	H	-1.0606	2.484487	-0.0003
1	H	3.374333	-0.15507	0.000616
1	H	-2.98376	-1.20761	-0.00027
1	H	1.97617	1.977259	0.000072

N9-Me- PU_9H E_{tot} = -451.030304 a.u.
Gibbs free energy E_G= -450.943859 a.u.

7	N	-2.55503	-0.05808	0.000154
6	C	-1.91621	-1.25073	-0.00017
7	N	-0.58657	-1.48419	-0.00017
6	C	0.120613	-0.34977	-0.00015
6	C	-0.40918	0.972117	0.000028
6	C	-1.80717	1.063223	0.000231
7	N	0.623242	1.908045	-0.00024
6	C	1.723629	1.173729	0.000124
7	N	1.494738	-0.1977	-0.00023
1	H	-2.55774	-2.13743	0.000242
1	H	2.739912	1.567163	0.000115
1	H	-2.33134	2.025359	0.000236
6	C	2.477373	-1.27458	0.00023
1	H	2.349174	-1.90076	0.895872
1	H	2.348364	-1.90221	-0.89427
1	H	3.482629	-0.83262	-0.00059

N7-Me- PU_7H E_{tot} = -451.024895 a.u.
Gibbs free energy E_G= -450.937923 a.u.

7	N	-2.04051	-1.27589	0.000107
6	C	-2.4762	0.00967	0.000192
7	N	-1.75065	1.141135	-0.00014
6	C	-0.42377	0.93226	-0.00011
6	C	0.143416	-0.37949	0.000028
6	C	-0.71133	-1.48289	0.000108
7	N	1.516125	-0.18712	-2.7E-05
6	C	1.702906	1.185054	0.000078
7	N	0.581882	1.890138	-0.00043
1	H	-3.56371	0.135731	-0.00039
1	H	2.70767	1.607782	0.000058
1	H	-0.35798	-2.52104	0.000187
6	C	2.53953	-1.22273	0.000179
1	H	2.445574	-1.85388	0.898459
1	H	2.445482	-1.85436	-0.89775
1	H	3.527763	-0.74332	-5E-06

N9-OMe-PU_9H E_{tot} = -526.152929 a.u.
Gibbs free energy E_G= -526.06453 a.u.

7	N	2.754488	-0.58466	0.113884
6	C	1.851843	-1.57062	-0.09667
7	N	0.513534	-1.46141	-0.23577
6	C	0.107819	-0.19193	-0.14963
6	C	0.932269	0.947993	0.072354
6	C	2.301804	0.680981	0.201876
7	N	0.173181	2.118408	0.110824
6	C	-1.0717	1.712044	-0.07136
7	N	-1.17018	0.335562	-0.22691
7	H	2.256713	-2.58526	-0.16048
1	H	-1.95964	2.33958	-0.11584
1	H	3.03621	1.475431	0.375536
1	O	-2.33329	-0.33761	-0.53752
8	C	-2.76995	-1.14119	0.596549
6	H	-3.70707	-1.60103	0.256049
1	H	-2.01924	-1.91299	0.821701
1	H	-2.95027	-0.4938	1.470306

N7-OMe- PU_7H E_{tot} = -526.143533 a.u.
Gibbs free energy E_G= -526.053804 a.u.

7	N	2.320222	-1.41318	0.000512
6	C	2.861286	-0.16541	0.001195
7	N	2.23157	1.01935	0.001021
6	C	0.890334	0.923883	0.000029
6	C	0.223638	-0.34033	-0.00073
6	C	0.981755	-1.51435	-0.0005
7	N	-1.11538	-0.01189	-0.00151
6	C	-1.21537	1.368164	-0.00137
7	N	-0.02471	1.9624	-0.00034
1	H	3.955406	-0.12994	0.001972
1	H	-2.1708	1.884154	-0.00191
1	H	0.537729	-2.51504	-0.00105
8	O	-2.10065	-1.00391	-0.00353
6	C	-3.42659	-0.45084	0.00383
1	H	-3.60894	0.15342	-0.90182
1	H	-4.07936	-1.33249	0.003685
1	H	-3.6011	0.147633	0.91485

N9-OH- PU_9H E_{tot} = -486.872939 a.u.
Gibbs free energy E_G= -486.809613 a.u.

7	N	2.523059	0.043752	0
6	C	1.945214	-1.17992	-8E-06
7	N	0.626196	-1.47137	-3.6E-05
6	C	-0.11607	-0.36252	-5.8E-05
6	C	0.33466	0.986924	0.000007
6	C	1.72923	1.133963	0.000049
7	N	-0.74643	1.863983	0.000003
6	C	-1.8189	1.080363	0.000005
7	N	-1.4847	-0.26158	-1.2E-05
1	H	2.626979	-2.03537	-4.6E-05
1	H	-2.85748	1.40303	0.000004
1	H	2.214938	2.115979	0.000035
8	O	-2.38248	-1.3195	-0.00007
1	H	-1.79636	-2.10405	0.000912

N7-OMe- PU_7H E_{tot} = -526.141230 a.u.
Gibbs free energy E_G= -526.051497 a.u.

7	N	1.860871	-1.67661	0.000442
6	C	2.660919	-0.5801	0.000523
7	N	2.295189	0.708238	0.000191
6	C	0.967221	0.908559	0.000017
6	C	0.023807	-0.18039	0.000033
6	C	0.533469	-1.48837	0.000222
7	N	-1.20341	0.473071	0.00006
6	C	-0.96739	1.827938	-0.00044
7	N	0.324313	2.131129	0.000117
1	H	3.736877	-0.78066	0.000296
1	H	-1.79688	2.531867	-0.00055
1	H	-0.08894	-2.38659	0.000437
8	O	-2.52773	0.011744	0.000376
6	C	-2.63253	-1.42164	-0.0011
1	H	-2.18269	-1.85348	0.907794
1	H	-3.71548	-1.60033	-0.00121
1	H	-2.18281	-1.85157	-0.91095

N7-OH- PU_7H E_{tot} = -486.868409 a.u.
Gibbs free energy E_G= -486.805107 a.u.

7	N	2.082536	-1.20873	-0.00765
6	C	2.459118	0.095706	0.003501
7	N	1.680988	1.190874	0.008534
6	C	0.36549	0.923323	0.004628
6	C	-0.13507	-0.41465	0.003122
6	C	0.766407	-1.48023	-0.0078
7	N	-1.50874	-0.25005	0.021732
6	C	-1.77707	1.105881	-0.0063
7	N	-0.6777	1.843183	-0.00247
1	H	3.539284	0.272475	0.006439
1	H	-2.80238	1.471079	-0.02563
1	H	0.455916	-2.53049	-0.02358
8	O	-2.45825	-1.25793	-0.11019
1	H	-2.63964	-1.55678	0.800296

N7-OH- PU_7H E_{tot} = -486.863033 a.u.
Gibbs free energy E_G= -486.800056 a.u.

7	N	-2.08042	-1.20465	-4.8E-05
6	C	-2.45583	0.101332	-0.00057
7	N	-1.6771	1.194777	-0.00023
6	C	-0.36038	0.932037	-9.8E-05
6	C	0.139726	-0.41202	0.00003
6	C	-0.76552	-1.47607	0.000124
7	N	1.508596	-0.2453	0.000047
6	C	1.781922	1.101793	-0.00035
7	N	0.679622	1.845055	0.000409
1	H	-3.5359	0.277748	0.000316
1	H	2.80745	1.464916	-0.00033
1	H	-0.46853	-2.53252	0.000289
8	O	2.513027	-1.21923	0.000494
1	H	2.038374	-2.06798	-0.00033

N9-NH_2- PU_9H E_{tot} = -467.033124 a.u.
Gibbs free energy E_G= -466.956984 a.u.

7	N	-2.55977	0.000158	-7.8E-05
6	C	-1.95688	-1.21238	0.000259
7	N	-0.63701	-1.49099	0.000017
6	C	0.108928	-0.38424	0.000024
6	C	-0.37945	0.95263	-5E-06
6	C	-1.77335	1.093033	-0.00018
7	N	0.673936	1.86926	0.000386
6	C	1.758014	1.118234	-0.0003
7	N	1.492011	-0.25282	-0.00014
1	H	-2.62661	-2.07814	-0.00043
1	H	2.78583	1.481794	-0.00041
1	H	-2.26034	2.074629	-7.6E-05
7	N	2.398944	-1.32127	0.000175
1	H	2.989935	-1.25682	-0.83082
1	H	2.990838	-1.25558	0.830421

N7-NH_2- PU_7H E_{tot} = -467.031592 a.u.
Gibbs free energy E_G= -466.955304 a.u.

7	N	-2.06876	-1.23992	-4.4E-05
6	C	-2.47113	0.05698	-0.00047
7	N	-1.71559	1.168069	-0.00011
6	C	-0.39498	0.921898	-4.6E-05
6	C	0.13426	-0.40174	-2E-06
6	C	-0.74659	-1.48454	0.000049
7	N	1.510939	-0.23413	0.000033
6	C	1.740464	1.136477	-0.00033
7	N	0.634201	1.860052	0.000354
1	H	-3.55485	0.211959	0.000457
1	H	2.757392	1.529885	-0.00036
1	H	-0.41048	-2.52655	0.000131
7	N	2.43607	-1.29153	0.000337
1	H	3.028833	-1.21395	-0.82897
1	H	3.028888	-1.21352	0.829568

N3-NO_2- PU_3H E_{tot} = -616.117010 a.u.
Gibbs free energy E_G= - 616.058258 a.u.

7	N	-0.34809	2.373466	0.000179
6	C	0.739387	1.629408	0.000201
7	N	0.726203	0.255127	0.000199
6	C	-0.46055	-0.43268	0.000151
6	C	-1.68192	0.383958	0.000124
6	C	-1.57247	1.762835	0.00013
7	N	-2.74773	-0.48447	-9.1E-05
6	C	-2.154	-1.68542	0.000575
7	N	-0.75972	-1.72892	0.000119
1	H	1.726339	2.089856	0.000215
1	H	-2.72429	-2.61544	0.000339
1	H	-2.4466	2.420171	-1.4E-05
7	N	2.135671	-0.4869	0.000067
8	O	2.06469	-1.68256	-0.00095
8	O	3.0825	0.264903	-0.00042

N1-NO_2- PU_1H E_{tot} = -616.120089 a.u.
Gibbs free energy E_G= -616.061928 a.u.

7	N	1.04705	0.057802	-0.00015
6	C	0.635688	1.388564	-2.5E-05
7	N	-0.62326	1.748897	0.000165
6	C	-1.53656	0.733598	0.000236
6	C	-1.15379	-0.68824	0.000112
6	C	0.178547	-1.01567	-8.3E-05
7	N	-2.29706	-1.45316	0.000244
6	C	-3.25569	-0.50881	0.000375
7	N	-2.86802	0.827176	0.000432
1	H	1.439147	2.122864	-9.6E-05
1	H	-4.31462	-0.7742	0.000536
1	H	0.612911	-2.01337	-0.00019
7	N	2.528665	-0.23668	-0.00036
8	O	2.818419	-1.41379	-0.00041
8	O	3.249297	0.738768	-0.00038

N3-CN- PU_3H E_{tot} = -503.884158 a.u.
Gibbs free energy E_G= -503.827426 a.u.

7	N	0.109033	2.292427	-8.4E-05
6	C	1.149605	1.506368	0.000095
7	N	1.072742	0.102319	0.000106
6	C	-0.18667	-0.47977	0.000037
6	C	-1.35057	0.394688	-0.00013
6	C	-1.16005	1.763501	-0.00033
7	N	-2.46128	-0.42412	0.000774
6	C	-1.92293	-1.65128	0.000362
7	N	-0.52557	-1.75579	-0.00062
1	H	2.166129	1.904287	-2.4E-05
1	H	-2.53485	-2.55422	0.000153
1	H	-1.98663	2.47918	0.000188
6	C	2.211316	-0.64484	-5.2E-05
7	N	3.220951	-1.23788	-0.00021

N1-CN- PU_1H E_{tot} = -503.882294 a.u.
Gibbs free energy E_G= -503.825574 a.u.

7	N	1.432611	-0.0258	-0.00019
6	C	1.021369	1.328048	-6.3E-05
7	N	-0.22205	1.711225	0.000128
6	C	-1.15823	0.716843	0.000204
6	C	-0.80873	-0.71613	0.000064
6	C	0.50977	-1.07972	-0.00013
7	N	-1.97133	-1.45084	0.000223
6	C	-2.90626	-0.48327	0.000322
7	N	-2.48572	0.841911	0.000352
1	H	1.846041	2.043521	-0.00013
1	H	-3.97127	-0.72255	0.000468
1	H	0.918791	-2.09005	-0.00023
6	C	2.762795	-0.29786	-0.00038
7	N	3.915358	-0.51056	-0.00054

N3-CHO- PU_3H E_{tot} = -524.989977 a.u.
Gibbs free energy E_G= -524.922834 a.u

7	N	-0.23901	2.364611	-8.8E-05
6	C	0.895032	1.712687	-0.00017
7	N	1.03607	0.326184	-7.6E-05
6	C	-0.12367	-0.43283	0.00005
6	C	-1.40403	0.272238	0.000122
6	C	-1.41654	1.652586	0.000051
7	N	-2.39775	-0.68434	0.00058
6	C	-1.69966	-1.82759	-0.00045
7	N	-0.30297	-1.74651	0.000246
1	H	1.83612	2.268766	-0.00025
1	H	-2.18564	-2.80449	0.000085
1	H	-2.3407	2.237334	0.000224
6	C	2.37697	-0.2152	-0.00011
8	O	2.640104	-1.38752	-0.00018
1	H	3.126358	0.60757	-0.00025

N1-CHO- PU_1H E_{tot} = -524.996050 a.u.
Gibbs free energy E_G= -524.928256 a.u

7	N	-1.38263	0.198685	0.000154
6	C	-0.84681	1.492327	0.000044
7	N	0.426391	1.779464	-0.00013
6	C	1.266774	0.700302	-0.0002
6	C	0.781797	-0.69349	-8.8E-05
6	C	-0.56664	-0.92737	0.00009
7	N	1.872832	-1.53447	-0.00021
6	C	2.893448	-0.66057	-0.00037
7	N	2.599691	0.700903	-0.00033
1	H	-1.59114	2.293146	0.000114
1	H	3.931874	-0.99772	-0.00046
1	H	-1.07531	-1.89128	0.00018
6	C	-2.80558	0.048058	0.000332
8	O	-3.36167	-1.02515	0.000557
1	H	-3.32406	1.029396	0.00048

N3-CHO- PU_3H E_{tot} = -524.998093 a.u.
Gibbs free energy E_G= -524.930545 a.u

7	N	0.343274	2.208838	0.000014
6	C	1.255045	1.266158	-0.00019
7	N	0.979738	-0.09619	-0.00014
6	C	-0.34619	-0.48588	0.000016
6	C	-1.37791	0.538466	0.000233
6	C	-0.98888	1.865134	0.000311
7	N	-2.59599	-0.11238	0.000065
6	C	-2.23859	-1.40317	-0.00032
7	N	-0.87171	-1.70492	0.000464
1	H	2.317097	1.514099	-0.00023
1	H	-2.97363	-2.20929	0.000098
1	H	-1.70433	2.692572	0.000193
6	C	2.041186	-1.078	-0.00014
8	O	3.209387	-0.77191	-0.00029
1	H	1.630592	-2.1058	-3.6E-05

N1-CHO- PU_1H E_{tot} = -524.995159 a.u.
Gibbs free energy E_G= -524.927547

7	N	-1.34593	-0.21817	0.000198
6	C	-1.05368	1.152846	0.000066
7	N	0.153484	1.653318	-0.00012
6	C	1.173393	0.743744	-0.0002
6	C	0.9497	-0.71264	-6.5E-05
6	C	-0.33682	-1.17572	0.000134
7	N	2.173361	-1.34551	-0.0002
6	C	3.020458	-0.3014	-0.00038
7	N	2.486198	0.983196	-0.00035
1	N	-1.93497	1.794801	0.000137
1	H	4.102495	-0.44658	-0.00049
1	H	-0.64623	-2.22319	0.000239
6	C	-2.7113	-0.65173	0.000403
8	O	-3.65724	0.099456	0.000404
1	H	-2.78362	-1.76111	0.000417

N3-Cl- PU_3H E_{tot} = -871.312447 a.u.
Gibbs free energy E_G= -871.263308 a.u.

7	N	0.008437	2.317039	-0.00015
6	C	1.059333	1.520998	-0.00011
7	N	0.953657	0.151991	-4E-06
6	C	-0.26434	-0.45374	0.000052
6	C	-1.44244	0.416952	0.000022
6	C	-1.2476	1.791919	-0.0001
7	N	-2.54202	-0.4037	0.000567
6	C	-1.99838	-1.63403	-0.00017
7	N	-0.61273	-1.73586	-8E-06
7	H	2.074639	1.918997	-0.00018
1	H	-2.612	-2.53606	0.000015
1	H	-2.07918	2.502376	0.000143
17	Cl	2.430921	-0.82613	-5.8E-05

N1-Cl- PU_1H E_{tot} = -871.305480 a.u.
Gibbs free energy E_G= -871.256569 a.u.

7	N	1.292863	0.008534	-0.00015
6	C	0.910976	1.33877	-3.6E-05
7	N	-0.34706	1.712556	0.000132
6	C	-1.27926	0.723028	0.000203
6	C	-0.92517	-0.7034	0.000085
6	C	0.411337	-1.04747	-9.6E-05
7	N	-2.07292	-1.44736	0.000145
6	C	-3.0212	-0.47997	0.000462
7	N	-2.61594	0.839141	0.000322
1	H	1.727823	2.061672	-0.00011
1	H	-4.08312	-0.73372	0.000488
1	H	0.825882	-2.05454	-0.00021
17	Cl	3.008866	-0.35584	-0.00041

N3-F- PU_3H E_{tot} = -510.848903 a.u.
Gibbs free energy E_G= -510.797916 a.u.

7	N	1.455888	1.68292	0.00006
6	C	1.915763	0.443999	-0.00039
7	N	1.079207	-0.63247	-0.00028
6	C	-0.27044	-0.52851	-1E-06
6	C	-0.78924	0.843868	0.000296
6	C	0.112002	1.902545	0.000496
7	N	-2.1568	0.740379	-0.00043
6	C	-2.36235	-0.58893	-0.00025
7	N	-1.25175	-1.42518	0.000801
7	H	2.982679	0.217973	-0.0004
1	H	-3.36544	-1.01777	-8.4E-05
1	H	-0.21407	2.94625	0.00001
9	F	1.675178	-1.90486	-0.00017

N1-F- PU_1H E_{tot} = -510.844843 a.u.
Gibbs free energy E_G= -510.794099

7	N	1.647114	-0.16703	-0.0002
6	C	1.406374	1.18318	-0.00011
7	N	0.178172	1.658354	0.000048
6	C	-0.82341	0.740237	0.000104
6	C	-0.58881	-0.71588	0.00003
6	C	0.718256	-1.16671	-0.00014
7	N	-1.79094	-1.36139	0.000056
6	C	-2.65843	-0.31749	0.000346
7	N	-2.14825	0.960978	0.000388
7	H	2.2903	1.822088	-0.00018
1	H	-3.73723	-0.48539	0.000447
1	H	1.081232	-2.19406	-0.00026
9	F	2.982129	-0.56878	-0.00039

N3-H- PU_3H E_{tot} = -411.727345 a.u.
Gibbs free energy E_G= -411.664858 a.u.

7	N	2.072937	0.745955	0.000539
6	C	2.048809	-0.57306	0.000429
7	N	0.901102	-1.3226	-9E-06
6	C	-0.30896	-0.69164	-0.00031
6	C	-0.327	0.761381	-0.00014
6	C	0.888871	1.432181	0.000271
7	N	-1.6492	1.149621	-0.00059
6	C	-2.29914	-0.0285	0.000644
7	N	-1.54133	-1.19673	-0.00084
1	H	0.958232	2.524362	0.000366
1	H	-3.38904	-0.08448	0.000104
1	H	2.985325	-1.13528	0.000592
1	H	0.945502	-2.34051	-0.00015

N1-H- PU_1H E_{tot} = -411.722874 a.u.
Gibbs free energy E_G= -411.660423 a.u.

7	N	1.998293	0.60907	0.000281
6	C	1.944534	-0.76881	0.000166
7	N	0.831723	-1.46826	-2.5E-05
6	C	-0.31401	-0.73292	-9.3E-05
6	C	-0.33035	0.740831	0.00001
6	C	0.875838	1.404443	0.000212
7	N	-1.63187	1.170039	-0.00012
6	C	-2.30446	-0.00402	-0.00017
7	N	-1.58092	-1.1785	-0.00034
1	H	1.020069	2.486083	0.000314
1	H	-3.39633	-0.02647	-0.00036
1	H	2.913982	-1.27315	0.000243
1	H	2.912345	1.049889	0.000424

N3-Me- PU_3H E_{tot} = -451.017870 a.u.
Gibbs free energy E_G= -450.930743 a.u.

7	N	-1.2689	1.849171	-0.00003
6	C	-1.83101	0.653586	0.000013
7	N	-1.15325	-0.53917	0.000074
6	C	0.212758	-0.4884	0.000019
6	C	0.879626	0.79907	-3.6E-05
6	C	0.093052	1.943477	-3.2E-05
7	N	2.236326	0.555153	-0.00005
6	C	2.291318	-0.78928	-0.00049
7	N	1.092142	-1.49379	0.000229
1	H	-2.92084	0.573639	0.000093
1	H	3.241552	-1.32608	-0.00023
1	H	0.515801	2.952788	-0.00011
6	C	-1.8413	-1.83915	0.000196
1	H	-1.54158	-2.40459	-0.89296
1	H	-1.54118	-2.40462	0.893191
1	H	-2.92461	-1.66651	0.000439

N1-Me- PU_1H E_{tot} = -451.009572 a.u.
Gibbs free energy E_G= -450.921889 a.u.

7	N	-1.67365	-0.15413	0.000273
6	C	-1.33739	1.186998	0.000155
7	N	-0.1123	1.666916	-8.5E-05
6	C	0.877218	0.735878	-0.00013
6	C	0.610062	-0.70855	-5.5E-05
6	C	-0.70185	-1.12835	0.000164
7	N	1.804247	-1.38067	-0.00045
6	C	2.691779	-0.35745	0.000371
7	N	2.207619	0.932797	-0.00078
1	H	-2.18812	1.873412	0.000182
1	H	3.767459	-0.54587	-0.00043
1	H	-1.03376	-2.16796	0.000202
6	C	-3.09976	-0.52155	0.000454
1	H	-3.59108	-0.12065	0.899258
1	H	-3.59131	-0.12067	-0.89823
1	H	-3.18494	-1.61449	0.000476

N3-OMe- PU_3H E_{tot} = -526.143912 a.u.
Gibbs free energy E_G= -526.055290 a.u.

7	N	0.28004	2.359251	0.082993
6	C	-0.85311	1.704759	-0.10474
7	N	-0.93567	0.343441	-0.21916
6	C	0.191026	-0.42262	-0.13789
6	C	1.451892	0.270605	0.082277
6	C	1.444349	1.657402	0.179287
7	N	2.434974	-0.69237	0.128362
6	C	1.744287	-1.83195	-0.0514
7	N	0.366854	-1.74311	-0.22084
1	H	-1.80574	2.229141	-0.19344
1	H	2.234105	-2.80681	-0.06756
1	H	2.357609	2.239503	0.333299
8	O	-2.18746	-0.19998	-0.51313
6	C	-2.64337	-1.06648	0.568536
1	H	-2.71046	-0.48986	1.505437
1	H	-3.64102	-1.38539	0.240188
1	H	-1.96868	-1.92756	0.671092

N1-OMe- PU_1H E_{tot} = -526.138516 a.u.
Gibbs free energy E_G= -526.050245 a.u.

7	N	1.271897	0.041568	0.309704
6	C	0.883339	1.354782	0.164942
7	N	-0.36663	1.725412	-0.01668
6	C	-1.27826	0.717799	-0.05699
6	C	-0.92005	-0.70249	0.101558
6	C	0.407924	-1.02258	0.294505
7	N	-2.05785	-1.45871	0.026568
6	C	-3.00377	-0.50758	-0.16736
7	N	-2.60863	0.810498	-0.22607
1	H	1.696905	2.079829	0.225093
1	H	-4.05665	-0.7765	-0.27512
1	H	0.83924	-2.01225	0.445815
8	O	2.626801	-0.21363	0.53682
6	C	3.305796	-0.47308	-0.72212
1	H	3.234306	0.404596	-1.38484
1	H	4.349719	-0.65529	-0.43493
1	H	2.880604	-1.3639	-1.21243

N3-OH- PU_3H E_{tot} = -486.868000 a.u.
Gibbs free energy E_G= -486.803932 a.u.

7	N	-1.50236	1.658162	0.000008
6	C	-1.93276	0.403854	-0.00002
7	N	-1.08333	-0.66166	-4.4E-05
6	C	0.256884	-0.46648	-2.4E-05
6	C	0.764006	0.884424	-1.5E-05
6	C	-0.16745	1.922564	-1.6E-05
7	N	2.138815	0.782915	0.000103
6	C	2.346393	-0.54751	0.000028
7	N	1.230386	-1.37872	-0.00015
1	H	-2.99678	0.164056	0.000017
1	H	3.349741	-0.97516	0.000044
1	H	0.122383	2.977179	-4.5E-05
8	O	-1.59751	-1.95575	0.000071
1	H	-0.78227	-2.50603	0.000285

N1-OH- PU_1H E_{tot} = -486.853390 a.u.
Gibbs free energy E_G= -486.790443 a.u.

7	N	-1.66575	-0.16515	-0.00524
6	C	-1.38176	1.18371	-0.01293
7	N	-0.15675	1.663722	-0.00367
6	C	0.839374	0.738844	0.005915
6	C	0.59257	-0.71388	-0.00402
6	C	-0.71472	-1.15384	-0.01977
7	N	1.793645	-1.3685	-0.00262
6	C	2.667431	-0.33258	0.009225
7	N	2.166081	0.950599	0.013905
1	H	-2.25781	1.834384	-0.03159
1	H	3.745328	-0.50714	0.014326
1	H	-1.0722	-2.18329	-0.04665
8	O	-3.01194	-0.54829	-0.08329
1	H	-3.29774	-0.65588	0.843046

N3-OH- PU_3H E_{tot} = -486.867999 a.u.
Gibbs free energy E_G= -486.803936 a.u.

7	N	1.50276	1.65784	-6.9E-05
6	C	1.933052	0.403605	-0.00018
7	N	1.083279	-0.66174	-0.00011
6	C	-0.25686	-0.46632	0.000006
6	C	-0.76378	0.884742	0.000122
6	C	0.16792	1.922632	0.000092
7	N	-2.1387	0.783327	0.000362
6	C	-2.34636	-0.54703	-0.00024
7	N	-1.23048	-1.37857	0.000179
1	H	2.997031	0.163654	-0.00025
1	H	-3.34977	-0.97458	0.000018
1	H	-0.12167	2.97736	0.000205
8	O	1.596477	-1.95655	-0.00015
1	H	0.780628	-2.50587	-5.7E-05

N1-OH- PU_1H E_{tot} = -486.852982 a.u.
Gibbs free energy E_G= -486.790022 a.u

7	N	-1.66871	-0.15297	0.000172
6	C	-1.38033	1.190513	0.000058
7	N	-0.14946	1.663061	-7.1E-05
6	C	0.842382	0.739622	-0.00016
6	C	0.590238	-0.71132	-1.5E-05
6	C	-0.72234	-1.14216	0.000148
7	N	1.783558	-1.3732	0.000075
6	C	2.665641	-0.33901	-0.00079
7	N	2.173577	0.943419	-3.5E-05
1	H	-2.25189	1.846281	0.00015
1	H	3.742073	-0.52207	-0.00044
1	H	-1.06387	-2.17989	0.0003
8	O	-3.03649	-0.46222	0.000385
1	H	-3.08068	-1.4346	0.000459

N3-NH_2-PU_3H E_{tot} = -467.018518 a.u.
Gibbs free energy E_G= -466.942304 a.u.

7	N	-1.29864	1.809859	-2.1E-05
6	C	-1.83895	0.608173	0.000186
7	N	-1.1355	-0.57734	0.000159
6	C	0.233649	-0.52499	0.000019
6	C	0.866383	0.791167	-0.00018
6	C	0.063545	1.921733	-0.00027
7	N	2.227055	0.587595	0.000081
6	C	2.319641	-0.75522	0.000088
7	N	1.144184	-1.49685	-0.00034
1	H	-2.92658	0.494676	0.000232
1	H	3.285112	-1.26445	-0.00011
1	H	0.473514	2.935965	-0.00014
7	N	-1.78478	-1.84242	0.000159
1	H	-2.3817	-1.88873	0.828918
1	H	-2.3822	-1.88847	-0.82825

N1-NH_2-PU_1H E_{tot} = -467.018746 a.u.
Gibbs free energy E_G= -466.942667 a.u.

7	N	-1.67314	-0.18019	0.000204
6	C	-1.36445	1.171215	0.000085
7	N	-0.14541	1.660718	-7.9E-05
6	C	0.853993	0.737588	-0.00015
6	C	0.605099	-0.71144	-2.7E-05
6	C	-0.70056	-1.1523	0.000151
7	N	1.808761	-1.36678	-5.5E-05
6	C	2.682141	-0.33274	-0.00048
7	N	2.180139	0.951859	-0.00024
1	H	-2.23215	1.836769	0.000161
1	H	3.760255	-0.50627	-0.00045
1	H	-1.05087	-2.18415	0.000276
7	N	-3.02248	-0.62845	0.000408
1	H	-3.48471	-0.24015	0.826298
1	H	-3.48492	-0.24025	-0.82541