

**非共价作用对气相中 B-DNA 双螺旋结构稳定性的贡献：  
基于 GEBF 方法的密度泛函理论计算**

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**Contribution of Non-Covalent Interactions to the Gas-Phase  
Stability of the Double-Helix of B-DNA: A Density Functional  
Theory Study with GEBF Approach**

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## Part 1 Cartesian coordinates optimized by different methods

1. 3'-GACTG-5'			C	5.657808	-4.399695	34.712250	
(optimized by GEBF-HF/6-31G**)			C	5.071672	-3.266159	33.866870	
C	-0.271296	-8.987913	29.564041	N	3.737403	-2.849918	34.218102
C	0.931768	-8.093529	29.790310	C	3.493923	-1.495520	34.350999
O	0.566597	-6.735250	29.434949	O	4.349841	-0.661957	34.235323
C	1.381377	-8.007431	31.258625	N	2.202362	-1.175125	34.649309
O	2.847946	-7.974575	31.256657	C	1.141446	-2.032456	34.794778
C	0.850558	-6.666970	31.734025	O	0.042218	-1.621090	35.055239
C	0.948222	-5.814843	30.469337	C	1.455277	-3.451290	34.605936
N	0.106971	-4.656455	30.425836	C	0.332363	-4.438418	34.749735
C	-1.269666	-4.575133	30.333075	C	2.708412	-3.770071	34.295717
N	-1.701487	-3.374705	30.354637	H	4.899374	-5.675047	30.792629
C	-0.569282	-2.590662	30.472382	H	6.213601	-6.716898	31.370501
C	-0.394371	-1.172554	30.561248	H	6.868525	-4.434744	31.741414
O	-1.222871	-0.295808	30.567076	H	6.733666	-6.155541	33.973529
N	0.961639	-0.842032	30.658336	H	4.891081	-5.099286	35.016340
C	1.996834	-1.722891	30.710233	H	6.152545	-4.020454	35.591504
N	3.220119	-1.214733	30.852544	H	5.689047	-2.388960	33.901767
N	1.837763	-3.016960	30.643588	H	2.011833	-0.187468	34.772272
C	0.551356	-3.375915	30.518237	H	0.700188	-5.455775	34.704748
H	-0.624249	-8.867764	28.550091	H	-0.171467	-4.296771	35.699777
H	-0.010745	-10.030114	29.717928	H	-0.414810	-4.297111	33.975759
H	1.767046	-8.396178	29.186892	H	2.997103	-4.782688	34.083409
H	1.074226	-8.849801	31.855597	P	9.089029	-4.574574	34.879728
H	-0.185273	-6.766749	32.033750	O	10.435292	-4.476736	34.338090
H	1.409915	-6.262942	32.560598	O	8.753785	-5.909207	35.663291
H	1.953281	-5.471814	30.307215	O	8.739320	-3.459382	35.950512
H	-1.869660	-5.454546	30.221659	C	8.969069	-2.037028	35.751757
H	1.158816	0.143963	30.730583	C	8.374834	-1.278331	36.905251
H	3.400722	-0.230186	30.840047	O	6.944572	-1.383034	36.859335
H	3.966433	-1.862497	30.965850	C	8.768120	-1.765085	38.318362
P	3.932548	-8.115954	32.370740	O	9.310298	-0.605484	39.024103
O	4.949953	-9.134098	32.152784	C	7.446574	-2.169465	38.963593
O	3.070708	-8.315198	33.686546	C	6.461818	-1.266341	38.220020
O	4.519764	-6.662947	32.569574	N	5.060803	-1.574200	38.283873
C	5.451198	-6.002261	31.657245	C	4.154198	-0.499962	38.366690
C	6.069579	-4.819422	32.356892	O	4.580644	0.628186	38.400279
O	5.071851	-3.798393	32.523943	N	2.833537	-0.781514	38.420123
C	6.616268	-5.106995	33.764158	C	2.391893	-2.014676	38.387914
O	7.942336	-4.498313	33.818878	N	1.088960	-2.222034	38.458891
				C	3.293279	-3.134941	38.265548

C	4.596594	-2.848590	38.208267	H	2.333637	3.134081	42.753072
H	8.497306	-1.728548	34.833600	P	10.024905	5.042347	44.440735
H	10.036211	-1.875149	35.689526	O	10.565861	6.391860	44.389952
H	8.663228	-0.240362	36.812176	O	10.966503	3.937359	45.067946
H	9.511445	-2.545713	38.309858	O	8.713594	4.900252	45.311042
H	7.265603	-3.211558	38.742334	C	7.512705	5.700711	45.128486
H	7.438611	-2.028606	40.031593	C	6.394378	5.125898	45.946871
H	6.563405	-0.246345	38.541204	O	6.040552	3.813905	45.490681
H	0.450089	-1.446554	38.521166	C	6.635497	4.949658	47.445534
H	0.720443	-3.141577	38.448355	O	6.244679	6.177155	48.063307
H	2.936002	-4.143967	38.213896	C	5.757555	3.741139	47.816052
H	5.334702	-3.617698	38.103951	C	5.136714	3.281818	46.481037
P	10.398499	-0.517640	40.149855	N	4.972982	1.873908	46.321449
O	11.769842	-0.789641	39.742880	C	5.932344	0.877280	46.336778
O	9.850183	-1.517490	41.252814	N	5.442719	-0.295283	46.224205
O	10.117459	0.880593	40.793255	C	4.076885	-0.102514	46.128101
C	10.109382	2.205565	40.190560	C	2.990885	-1.025303	46.012525
C	9.302257	3.119353	41.078197	O	3.007472	-2.235331	45.962532
O	7.919149	2.751618	40.977974	N	1.769203	-0.353117	45.964302
C	9.649009	3.041932	42.571558	C	1.594909	0.994959	46.013153
O	9.668069	4.422635	43.049106	N	0.335372	1.437546	45.965077
C	8.507498	2.253109	43.195446	N	2.581969	1.837918	46.133913
C	7.316894	2.519818	42.270260	C	3.778205	1.234499	46.179664
N	6.384378	1.438688	42.178148	H	7.245686	5.695170	44.084353
C	6.655118	0.119968	41.899491	H	7.725840	6.708943	45.447941
N	5.612938	-0.619959	41.837417	H	5.539815	5.786540	45.833558
C	4.564634	0.246629	42.086550	H	7.679629	4.750870	47.639187
C	3.179404	0.057352	42.181402	H	6.344577	2.941541	48.250040
N	2.602470	-1.137186	42.053378	H	4.990137	4.020857	48.526963
N	2.424488	1.129386	42.422006	H	4.160602	3.722221	46.333332
C	3.008071	2.317502	42.565421	H	6.972529	1.114684	46.423747
N	4.284224	2.605925	42.514096	H	0.956669	-0.935298	45.840591
C	5.023547	1.526345	42.278503	H	-0.415302	0.819696	45.725469
H	9.648495	2.144892	39.218352	H	0.219172	2.395193	45.719315
H	11.132432	2.536668	40.106723	C	-7.340523	-3.507563	46.016709
H	9.423744	4.134952	40.735439	C	-6.627383	-2.182199	45.839150
H	10.620404	2.619944	42.769667	O	-5.255708	-2.332991	46.292695
H	8.766474	1.206824	43.183623	C	-6.509181	-1.716712	44.376489
H	8.294593	2.546296	44.212411	O	-6.812534	-0.286573	44.332598
H	6.755994	3.390708	42.563751	C	-5.043089	-1.916932	44.023365
H	7.658214	-0.218176	41.751955	C	-4.344706	-1.717002	45.368517
H	1.606328	-1.214136	42.009747	N	-3.046000	-2.355637	45.499358
H	3.171705	-1.933604	41.897798	C	-1.895300	-1.558239	45.477055

O	-2.010680	-0.367800	45.315054	H	-2.684655	3.963355	43.544264
N	-0.698669	-2.162955	45.634860	H	0.436196	1.047411	42.600086
C	-0.601209	-3.465223	45.768651	H	-4.245627	-1.022836	40.798470
N	0.606135	-3.996497	45.895885	H	-2.749062	-1.189214	39.884798
C	-1.767103	-4.311904	45.785538	H	-2.975732	-2.118459	41.357001
C	-2.950760	-3.699940	45.662671	H	-4.256261	1.145264	41.942338
H	-8.396239	-3.404922	45.783812	P	-5.608944	7.090346	42.037556
H	-7.245787	-3.841796	47.038346	O	-6.066369	8.297841	42.704540
H	-7.094806	-1.405121	46.422468	O	-6.575209	6.510608	40.919444
H	-7.190233	-2.227328	43.714602	O	-4.260032	7.270673	41.234437
H	-4.887435	-2.925438	43.672867	C	-3.038538	7.846804	41.770546
H	-4.703057	-1.227416	43.268922	C	-1.941229	7.685570	40.748491
H	-4.218138	-0.675468	45.599159	O	-1.649101	6.288097	40.598636
H	1.422160	-3.412435	45.895447	C	-2.278915	8.186979	39.331882
H	0.714698	-4.974258	46.018038	O	-1.132614	8.984296	38.896828
H	-1.693171	-5.370061	45.916032	C	-2.367791	6.923545	38.489984
H	-3.880721	-4.227719	45.701614	C	-1.401539	5.979936	39.204167
P	-7.596488	0.560099	43.274164	N	-1.588332	4.588232	38.966018
O	-9.039381	0.614974	43.454207	C	-2.763360	3.876349	38.814868
O	-7.088702	-0.069180	41.912347	N	-2.582525	2.620523	38.691664
O	-6.870520	1.956171	43.272025	C	-1.210083	2.452957	38.761481
C	-6.687711	2.883294	44.374812	C	-0.394636	1.285743	38.660264
C	-5.470061	3.715979	44.077605	O	-0.733864	0.130698	38.528533
O	-4.334516	2.843725	44.077586	N	0.954553	1.611636	38.733228
C	-5.463036	4.416448	42.706411	C	1.465845	2.861770	38.895385
O	-5.395955	5.855392	42.967627	N	2.792263	2.964724	38.936995
C	-4.211301	3.913973	41.996314	N	0.720873	3.929947	39.011132
C	-3.365558	3.264396	43.098599	C	-0.587617	3.662315	38.928655
N	-2.586403	2.127968	42.676994	H	-2.768083	7.323242	42.673730
C	-1.231865	2.138282	42.917516	H	-3.219042	8.888392	41.989317
O	-0.667017	3.056236	43.448484	H	-1.061546	8.203015	41.101732
N	-0.568661	1.026701	42.491062	H	-3.158250	8.804552	39.288499
C	-1.109795	-0.104239	41.932882	H	-3.377538	6.544046	38.547401
O	-0.425116	-1.066594	41.700226	H	-2.116273	7.095291	37.457416
C	-2.544971	-0.035543	41.656151	H	-0.373258	6.207849	38.974949
C	-3.169384	-1.160616	40.883135	H	-3.714852	4.364549	38.804946
C	-3.196546	1.047756	42.067204	H	1.597125	0.835791	38.644118
H	-6.536002	2.323461	45.281091	H	3.400900	2.190758	38.771321
H	-7.577241	3.491471	44.451194	H	3.169360	3.881063	39.007415
H	-5.359267	4.465471	44.847372	P	-0.926204	10.046606	37.765096
H	-6.363813	4.242698	42.141636	O	-0.816416	11.433324	38.197384
H	-4.486445	3.187906	41.246571	O	-2.134396	9.765576	36.781828
H	-3.669031	4.706273	41.506089	O	0.316117	9.501742	36.965114



O	-1.294819	-0.351602	31.431533	H	5.779538	-2.379415	33.861697
N	0.931905	-0.862658	31.177062	H	2.105691	-0.209095	34.962671
C	1.987707	-1.732687	31.026425	H	0.805750	-5.538277	34.729588
N	3.228466	-1.208219	31.007486	H	-0.029346	-4.409004	35.815767
N	1.830747	-3.047041	30.909893	H	-0.344458	-4.333668	34.095707
C	0.540425	-3.419385	30.964027	H	3.118809	-4.845377	34.072373
H	-0.761394	-8.785050	28.683246	P	9.228851	-4.708921	34.803420
H	-0.059404	-10.054836	29.710066	O	10.613782	-4.611330	34.283563
H	1.696183	-8.367214	29.198609	O	8.812630	-6.075415	35.556630
H	1.153847	-9.039656	31.887457	O	8.837402	-3.611899	35.932951
H	-0.103487	-6.978424	32.306534	C	9.086901	-2.173747	35.678271
H	1.533076	-6.507213	32.794541	C	8.431873	-1.360523	36.768197
H	1.947010	-5.487494	30.575652	O	6.974771	-1.460063	36.639472
H	-1.912025	-5.542105	30.944743	C	8.759460	-1.781667	38.231017
H	1.129301	0.150028	31.263576	O	9.332459	-0.579740	38.892130
H	3.404094	-0.202805	31.059727	C	7.394479	-2.111128	38.846232
H	3.992334	-1.866700	31.020234	C	6.451866	-1.235196	38.010965
P	4.012857	-8.258550	32.389433	N	5.036560	-1.513872	38.065604
O	5.081200	-9.260875	32.141294	C	4.138821	-0.402546	38.185538
O	3.113897	-8.490822	33.715679	O	4.604886	0.740418	38.200164
O	4.547021	-6.749348	32.647253	N	2.813045	-0.666829	38.291117
C	5.458449	-6.100379	31.668676	C	2.337517	-1.915377	38.258895
C	6.122121	-4.900714	32.312317	N	1.019055	-2.090114	38.377816
O	5.134869	-3.829832	32.470750	C	3.218843	-3.044603	38.100694
C	6.726834	-5.159453	33.710529	C	4.546199	-2.787507	38.009262
O	8.094406	-4.576592	33.677579	H	8.663580	-1.901490	34.707420
C	5.812637	-4.413697	34.685321	H	10.168245	-2.009064	35.665570
C	5.181316	-3.289970	33.845486	H	8.737892	-0.313620	36.645059
N	3.843389	-2.897479	34.238932	H	9.479506	-2.598308	38.288806
C	3.602722	-1.522777	34.445629	H	7.187479	-3.172499	38.674338
O	4.480491	-0.677903	34.355328	H	7.343821	-1.909014	39.914900
N	2.303239	-1.225853	34.781484	H	6.558101	-0.179453	38.263952
C	1.243811	-2.109149	34.919573	H	0.377066	-1.282180	38.421620
O	0.117498	-1.708638	35.225176	H	0.623538	-3.012786	38.303969
C	1.560222	-3.518184	34.685338	H	2.841045	-4.057971	38.057382
C	0.444961	-4.512087	34.833668	H	5.277490	-3.575627	37.884647
C	2.825945	-3.832542	34.326702	P	10.353796	-0.576268	40.129548
H	4.863978	-5.779283	30.810496	O	11.789646	-0.820234	39.830143
H	6.209184	-6.833185	31.356588	O	9.666023	-1.635497	41.137990
H	6.919462	-4.554083	31.645092	O	9.989676	0.812823	40.852124
H	6.831646	-6.218316	33.946331	C	10.137151	2.150567	40.239148
H	5.044548	-5.106495	35.042113	C	9.386293	3.154099	41.095861
H	6.353537	-4.008007	35.541605	O	7.947680	2.958070	40.913558

C	9.656706	3.043044	42.609971	C	1.506614	1.050857	45.728895
O	9.770920	4.445781	43.099589	N	0.233824	1.506266	45.769006
C	8.429611	2.329626	43.175230	N	2.518314	1.897912	45.872172
C	7.286101	2.670657	42.200993	C	3.713925	1.284187	45.842063
N	6.327522	1.605263	42.023275	H	7.487793	5.657165	43.965083
C	6.579757	0.284888	41.689434	H	7.848649	6.732119	45.342402
N	5.496753	-0.445147	41.581852	H	5.577384	5.897273	45.563615
C	4.467501	0.436735	41.864463	H	7.540716	4.978856	47.627860
C	3.068450	0.260515	41.952585	H	6.469725	2.917425	47.879392
N	2.469743	-0.925909	41.764669	H	5.026135	3.827253	48.373790
N	2.318173	1.348435	42.249644	H	4.128368	3.777255	46.113845
C	2.925754	2.535105	42.450437	H	6.948625	1.125445	46.010167
N	4.227689	2.809712	42.414389	H	0.845328	-0.891505	45.413752
C	4.951579	1.718724	42.124196	H	-0.542901	0.888269	45.526762
H	9.703058	2.131929	39.236788	H	0.118233	2.481470	45.526282
H	11.203914	2.389602	40.188473	C	-7.324253	-3.700519	45.706175
H	9.647723	4.161366	40.755619	C	-6.625584	-2.350264	45.645163
H	10.593146	2.540386	42.851665	O	-5.203550	-2.553790	45.998566
H	8.623497	1.254438	43.161401	C	-6.622046	-1.679789	44.245462
H	8.185712	2.630684	44.194091	O	-7.112298	-0.291710	44.430632
H	6.714230	3.545455	42.514819	C	-5.154678	-1.687858	43.808123
H	7.588447	-0.070724	41.540536	C	-4.374422	-1.711283	45.132722
H	1.450927	-0.997249	41.735492	N	-3.041542	-2.305834	45.055567
H	3.047793	-1.735192	41.609273	C	-1.903434	-1.451294	45.113484
H	2.253466	3.358172	42.680263	O	-2.083170	-0.226789	45.158609
P	10.165047	4.934085	44.573313	N	-0.676718	-2.028426	45.108893
O	10.870047	6.239948	44.616058	C	-0.525721	-3.351469	44.972488
O	10.961090	3.664887	45.177195	N	0.716266	-3.844613	44.967403
O	8.787412	4.857009	45.418930	C	-1.664215	-4.225884	44.853155
C	7.630896	5.700041	45.048407	C	-2.892574	-3.658134	44.925369
C	6.401259	5.193706	45.760282	H	-8.392208	-3.586893	45.488226
O	6.043820	3.878061	45.235003	H	-7.219710	-4.134497	46.705341
C	6.495654	5.023395	47.305890	H	-7.063611	-1.646300	46.359414
O	5.793548	6.095219	48.000409	H	-7.282735	-2.179491	43.535443
C	5.764244	3.697370	47.579638	H	-4.946007	-2.604640	43.244245
C	5.112895	3.313682	46.233053	H	-4.888107	-0.834907	43.185830
N	4.935940	1.908364	45.998633	H	-4.249191	-0.711065	45.548482
C	5.894787	0.899595	45.929030	H	1.538856	-3.224161	45.081828
N	5.381603	-0.285649	45.738340	H	0.861810	-4.834563	44.856762
C	4.012488	-0.071535	45.689219	H	-1.548541	-5.297467	44.753686
C	2.917015	-0.978961	45.520402	H	-3.813166	-4.227788	44.916011
O	2.949656	-2.206688	45.343772	P	-7.836129	0.633572	43.324692
N	1.681606	-0.305075	45.574904	O	-9.276650	0.871265	43.579904

O	-7.488061	-0.058538	41.908364	N	-2.526903	2.658138	38.743860
O	-6.882348	1.941168	43.247127	C	-1.153282	2.473724	38.809434
C	-6.677456	2.819891	44.422124	C	-0.354651	1.295066	38.658074
C	-5.498102	3.725584	44.147766	O	-0.736572	0.130118	38.461688
O	-4.298723	2.894171	44.106299	N	1.015982	1.588103	38.751828
C	-5.546998	4.510459	42.813112	C	1.557251	2.834197	38.972759
O	-5.521601	5.951640	43.189339	N	2.898572	2.913315	39.038451
C	-4.296988	4.078001	42.037724	N	0.818899	3.929387	39.136391
C	-3.379038	3.412247	43.081750	C	-0.495839	3.682419	39.041105
N	-2.584674	2.304764	42.582613	H	-2.954428	7.458346	42.812358
C	-1.200153	2.322548	42.809096	H	-3.363875	9.013835	42.035104
O	-0.633518	3.257227	43.365649	H	-1.164981	8.247359	41.274562
N	-0.536390	1.210456	42.345257	H	-3.270612	8.710471	39.305899
C	-1.098788	0.073881	41.780080	H	-3.093100	6.577488	38.331659
O	-0.407724	-0.914908	41.513517	H	-1.617706	7.230065	37.606810
C	-2.535585	0.140038	41.528450	H	-0.226354	6.205403	39.367239
C	-3.164518	-0.973883	40.746375	H	-3.647895	4.447811	38.942046
C	-3.199746	1.229570	41.970107	H	1.660382	0.788213	38.603583
H	-6.466261	2.194507	45.292963	H	3.505680	2.143272	38.743024
H	-7.591128	3.398424	44.584650	H	3.284597	3.842025	39.101741
H	-5.421240	4.452784	44.965979	P	-0.968921	10.146133	37.895983
H	-6.468133	4.345999	42.254926	O	-0.633561	11.570306	38.142900
H	-4.583217	3.353365	41.270472	O	-2.261378	9.822256	36.983001
H	-3.792454	4.907563	41.540248	O	0.186636	9.327553	37.097578
H	-2.675599	4.116008	43.527799	C	1.589087	9.412935	37.573304
H	0.509689	1.246196	42.412535	C	2.479668	8.627718	36.637578
H	-4.252963	-0.867041	40.697860	O	2.156406	7.203912	36.773891
H	-2.767897	-0.959266	39.725455	C	2.336996	8.973562	35.135825
H	-2.923405	-1.949333	41.180566	O	3.721728	9.177523	34.635366
H	-4.273011	1.328847	41.865455	C	1.674058	7.743579	34.517223
P	-5.752891	7.202924	42.218766	C	2.100460	6.587518	35.436485
O	-6.132761	8.439947	42.938600	N	1.200995	5.466083	35.449448
O	-6.764530	6.590246	41.119607	C	-0.186090	5.455880	35.467485
O	-4.415910	7.347665	41.298701	N	-0.703005	4.253675	35.427791
C	-3.187588	7.948299	41.862853	C	0.397804	3.411727	35.392095
C	-2.053831	7.734095	40.887400	C	0.521765	2.002249	35.322558
O	-1.792459	6.298286	40.784656	N	-0.523313	1.164126	35.304610
C	-2.298061	8.238208	39.440012	N	1.778684	1.500476	35.255639
O	-1.271347	9.287404	39.206296	C	2.840542	2.326328	35.282226
C	-2.109879	7.002389	38.551464	N	2.837663	3.657356	35.366191
C	-1.303392	6.019242	39.416503	C	1.589080	4.137366	35.410910
N	-1.500174	4.631385	39.115235	H	1.642239	8.982676	38.576758
C	-2.694803	3.939470	38.925574	H	1.882584	10.466420	37.605747



O	3.231497	-8.443392	33.602249	O	4.601396	0.684007	38.456590
O	4.484703	-6.567398	32.506535	N	2.758181	-0.683098	38.416096
C	5.384186	-5.886870	31.509622	C	2.254625	-1.927407	38.298570
C	6.071038	-4.708381	32.182162	N	0.922342	-2.061530	38.356261
O	5.084289	-3.620202	32.368675	C	3.117037	-3.071782	38.124795
C	6.668473	-5.010139	33.576516	C	4.460800	-2.844799	38.093892
O	8.033740	-4.375270	33.566925	H	8.521569	-1.761574	34.789764
C	5.731453	-4.320800	34.575718	H	10.065189	-1.925160	35.695013
C	5.112550	-3.149965	33.786710	H	8.662307	-0.275098	36.831649
N	3.756967	-2.783548	34.174119	H	9.470403	-2.635005	38.324067
C	3.489097	-1.400192	34.359451	H	7.157243	-3.309791	38.640327
O	4.364942	-0.540401	34.270237	H	7.329174	-2.169913	40.011171
N	2.172142	-1.122659	34.665663	H	6.516484	-0.279203	38.530118
C	1.121428	-2.030314	34.793935	H	0.302507	-1.220870	38.388136
O	-0.029076	-1.644570	35.078087	H	0.500119	-2.966370	38.196512
C	1.463434	-3.433753	34.567182	H	2.717888	-4.074534	38.013641
C	0.357224	-4.449342	34.675697	H	5.184397	-3.642468	37.957703
C	2.748436	-3.734356	34.232775	P	10.278589	-0.739640	40.297703
H	4.757724	-5.536131	30.684498	O	11.683722	-1.149064	39.977375
H	6.122423	-6.618460	31.159169	O	9.501942	-1.708252	41.357233
H	6.869620	-4.346240	31.521158	O	10.039322	0.700913	40.994043
H	6.811171	-6.075191	33.773279	C	10.140991	2.005142	40.270429
H	4.957598	-5.040129	34.871480	C	9.366615	3.040622	41.074655
H	6.256577	-3.968041	35.468117	O	7.921305	2.778441	40.917043
H	5.698206	-2.230026	33.853594	C	9.656802	3.035646	42.592151
H	1.947221	-0.096312	34.817089	O	9.724702	4.495121	42.969705
H	0.745627	-5.471401	34.601224	C	8.454396	2.330688	43.226951
H	-0.165722	-4.339310	35.634748	C	7.285950	2.593933	42.254651
H	-0.397558	-4.294226	33.893392	N	6.330011	1.506585	42.167212
H	3.061756	-4.742116	33.972791	C	6.583689	0.165516	41.901783
P	9.160026	-4.554806	34.710821	N	5.494851	-0.579984	41.853435
O	10.557863	-4.384625	34.213563	C	4.465919	0.320847	42.105580
O	8.746730	-5.984510	35.372197	C	3.062637	0.152060	42.205966
O	8.725269	-3.544190	35.925608	N	2.447603	-1.042980	42.086955
C	8.980852	-2.079338	35.732298	N	2.311805	1.261581	42.458009
C	8.356960	-1.330609	36.891390	C	2.926043	2.459832	42.595375
O	6.885055	-1.422554	36.776849	N	4.236214	2.739046	42.527327
C	8.707566	-1.852254	38.319351	C	4.950111	1.622474	42.286865
O	9.224881	-0.654616	39.071084	H	9.694423	1.893156	39.277771
C	7.356114	-2.267882	38.923749	H	11.203024	2.266084	40.195639
C	6.398474	-1.312606	38.193121	H	9.587340	4.036268	40.667674
N	4.976402	-1.582583	38.234686	H	10.616802	2.589738	42.862445
C	4.095356	-0.448311	38.372521	H	8.669868	1.256493	43.266770

H	8.226061	2.686267	44.236030	O	-6.762034	-0.149992	44.321738
H	6.709408	3.489827	42.504345	C	-5.029071	-1.822479	43.849170
H	7.592851	-0.194700	41.750146	C	-4.271327	-1.652241	45.179844
H	1.425510	-1.077688	41.953616	N	-2.947137	-2.281674	45.235122
H	3.017655	-1.840289	41.837496	C	-1.789549	-1.440036	45.325607
H	2.254877	3.294133	42.793042	O	-1.951621	-0.204828	45.301484
P	10.157671	5.070402	44.414474	N	-0.572609	-2.041307	45.424425
O	10.704780	6.460624	44.371268	C	-0.449644	-3.383332	45.409805
O	11.129967	3.888997	44.970692	N	0.792740	-3.888960	45.490192
O	8.857809	4.855474	45.382713	C	-1.602216	-4.245487	45.316243
C	7.636297	5.684314	45.125303	C	-2.825867	-3.645937	45.251075
C	6.501463	5.141051	45.963273	H	-8.337432	-3.427813	45.667542
O	6.123052	3.805118	45.464779	H	-7.111744	-3.931563	46.858813
C	6.766942	4.937661	47.479832	H	-7.026391	-1.423653	46.367948
O	6.354465	6.114171	48.255022	H	-7.215089	-2.099023	43.597557
C	5.861411	3.743161	47.856766	H	-4.882558	-2.842773	43.467209
C	5.202276	3.287075	46.525557	H	-4.716961	-1.108125	43.084975
N	5.033292	1.863636	46.364985	H	-4.130171	-0.600668	45.446567
C	5.987321	0.842199	46.406813	H	1.622355	-3.262063	45.623019
N	5.470057	-0.358926	46.269807	H	0.921446	-4.891388	45.531509
C	4.101700	-0.134709	46.141545	H	-1.509707	-5.327570	45.331400
C	3.003284	-1.045328	45.979162	H	-3.764829	-4.192673	45.240075
O	3.024432	-2.293624	45.891077	P	-7.761690	0.590688	43.265026
N	1.770150	-0.351568	45.919228	O	-9.215798	0.482044	43.586058
C	1.602447	1.018840	45.970750	O	-7.366141	-0.002778	41.801185
N	0.331582	1.488017	45.912815	O	-7.082659	2.066083	43.161440
N	2.620574	1.874574	46.114969	C	-6.803920	2.912439	44.362109
C	3.806714	1.237250	46.188248	C	-5.557362	3.731588	44.081233
H	7.392452	5.628663	44.058830	O	-4.418390	2.798005	44.033385
H	7.863229	6.721742	45.399242	C	-5.539774	4.518127	42.739744
H	5.641981	5.827934	45.867940	O	-5.538855	5.971686	43.140561
H	7.825134	4.712690	47.651266	C	-4.241870	4.097965	42.028674
H	6.439803	2.922973	48.292849	C	-3.404451	3.373756	43.108067
H	5.111910	4.068223	48.586201	N	-2.588467	2.271223	42.617059
H	4.210236	3.732258	46.381575	C	-1.205910	2.284289	42.906719
H	7.040935	1.068012	46.517311	O	-0.666190	3.213783	43.516152
H	0.928833	-0.943223	45.745344	N	-0.525756	1.178165	42.437617
H	-0.443021	0.857700	45.662816	C	-1.069784	0.058388	41.804667
H	0.233289	2.453456	45.616444	O	-0.362636	-0.930450	41.529117
C	-7.259349	-3.532912	45.848631	C	-2.494853	0.134386	41.493251
C	-6.563000	-2.177660	45.720801	C	-3.102199	-0.964400	40.663518
O	-5.141250	-2.352036	46.156288	C	-3.181482	1.219722	41.938232
C	-6.491281	-1.629355	44.270485	H	-6.636047	2.261637	45.225437

H	-7.674560	3.556687	44.522442	H	3.319311	3.819574	39.201254
H	-5.417923	4.455715	44.898466	P	-1.102259	10.395771	37.961096
H	-6.434261	4.358283	42.133602	O	-0.778452	11.819264	38.279422
H	-4.482445	3.401600	41.215722	O	-2.451892	10.099185	37.098348
H	-3.698814	4.943252	41.593374	O	0.007697	9.619812	37.035884
H	-2.726236	4.040928	43.647544	C	1.407945	9.532288	37.561879
H	0.528588	1.198955	42.550218	C	2.219994	8.659753	36.624879
H	-4.191980	-0.854059	40.591287	O	1.715138	7.269688	36.734236
H	-2.678877	-0.924474	39.650620	C	2.152985	9.033783	35.117310
H	-2.868326	-1.950310	41.085928	O	3.589166	9.051107	34.673139
H	-4.252857	1.327531	41.797689	C	1.373155	7.883403	34.472579
P	-5.762962	7.221979	42.148587	C	1.747943	6.684607	35.359643
O	-6.148078	8.477581	42.858712	N	0.861813	5.550225	35.297967
O	-6.782046	6.571045	41.059296	C	-0.529892	5.500233	35.268309
O	-4.417758	7.354666	41.215740	N	-1.014155	4.274762	35.201720
C	-3.199758	7.988142	41.809125	C	0.119054	3.466081	35.191881
C	-2.049873	7.780596	40.842165	C	0.291171	2.057239	35.108853
O	-1.808022	6.332153	40.727646	N	-0.724345	1.176212	35.061913
C	-2.265078	8.302512	39.394096	N	1.573309	1.594913	35.046579
O	-1.300206	9.450146	39.253213	C	2.609573	2.461292	35.098484
C	-1.931089	7.117750	38.469041	N	2.566397	3.798365	35.216942
C	-1.225141	6.083115	39.373130	C	1.292386	4.227025	35.251472
N	-1.456896	4.703271	39.029985	H	1.376968	9.081940	38.560126
C	-2.667604	4.036896	38.809871	H	1.819889	10.546820	37.617158
N	-2.523945	2.744914	38.612972	H	3.272790	8.692640	36.940324
C	-1.149685	2.532798	38.702664	H	1.734893	10.022535	34.916260
C	-0.367676	1.338103	38.567978	H	0.303092	8.101333	34.577149
O	-0.759605	0.167050	38.355132	H	1.612515	7.744143	33.415377
N	1.011828	1.610244	38.703010	H	2.754159	6.302301	35.149893
C	1.573316	2.847294	38.954251	H	-1.127079	6.402797	35.299735
N	2.916236	2.903040	39.059089	H	-0.525613	0.165892	35.117632
N	0.850212	3.965010	39.107862	H	-1.654403	1.505221	35.290125
C	-0.467309	3.730269	38.966899	H	3.594147	1.999963	35.034139
H	-2.979117	7.501557	42.765530	P	4.183420	9.264412	33.187784
H	-3.401967	9.053065	41.968993	O	5.386302	10.150446	33.121765
H	-1.156805	8.280625	41.247722	O	2.859894	9.722448	32.353949
H	-3.263720	8.708841	39.221425	O	4.410526	7.755530	32.593549
H	-2.860141	6.694342	38.073995	C	5.597947	6.985185	33.107906
H	-1.298559	7.415152	37.629503	C	5.862117	5.801988	32.195297
H	-0.138197	6.222095	39.409315	O	4.775566	4.821331	32.389748
H	-3.610297	4.569376	38.822520	C	5.935731	6.101814	30.661389
H	1.649407	0.787103	38.603119	O	7.115454	5.463352	30.056232
H	3.527605	2.102106	38.839827	C	4.713965	5.380977	30.076219

C	4.460110	4.222130	31.062454	N	0.324164	-4.653555	31.269090
N	3.084027	3.738768	31.122478	C	-1.053686	-4.591210	31.407785
C	2.824116	2.336950	30.937409	N	-1.477287	-3.401094	31.719414
O	3.780508	1.579382	30.691577	C	-0.333502	-2.631556	31.798615
N	1.531226	1.919105	31.027515	C	-0.141130	-1.244776	32.127846
C	0.535840	2.773269	31.340844	O	-0.977373	-0.397260	32.426096
N	-0.710347	2.278906	31.395872	N	1.220858	-0.908345	32.080745
C	0.791938	4.169013	31.603887	C	2.263412	-1.754694	31.788820
C	2.080750	4.595618	31.497077	N	3.494725	-1.233307	31.833936
H	5.356909	6.638443	34.118822	N	2.095649	-3.036953	31.493668
H	6.458424	7.667321	33.131928	C	0.797626	-3.389346	31.515274
H	6.813656	5.340952	32.507022	H	-0.761412	-8.477907	28.963974
H	5.928185	7.180381	30.454085	H	-0.138765	-9.830166	29.933716
H	3.851935	6.059769	30.064845	H	1.740833	-8.292829	29.383830
H	4.918432	5.033055	29.059580	H	1.285266	-9.024475	32.037187
H	5.090692	3.349900	30.873514	H	0.030500	-6.948267	32.526088
H	-0.889313	1.261120	31.229228	H	1.667862	-6.545909	33.077214
H	-1.464874	2.867160	31.725085	H	2.171409	-5.447478	30.930041
H	-0.002358	4.844491	31.905278	H	-1.670339	-5.460923	31.226419
H	2.399302	5.609979	31.720514	H	1.421332	0.086027	32.275303
H	-6.849107	-4.254690	45.129116	H	3.649178	-0.232016	31.945794
H	7.098232	6.760863	48.289487	H	4.264727	-1.887181	31.778386
H	-6.754089	0.521180	41.237389	P	4.103246	-7.830460	32.539648
H	-7.040992	7.115289	40.282198	O	5.382161	-8.539143	32.354979
H	-2.752728	10.812801	36.492221	O	3.301786	-8.151131	33.890877
H	3.007637	10.251885	31.538375	O	4.250243	-6.232155	32.648851
H	11.806893	4.138198	45.638230	C	5.082219	-5.515129	31.658732
H	10.063059	-2.227631	41.975569	C	5.978972	-4.530149	32.374609
H	9.466248	-6.505594	35.792182	O	5.217056	-3.352503	32.739801
H	3.688737	-8.925145	34.327646	C	6.580194	-5.065569	33.679862
H	-1.056285	-8.911819	30.436929	O	7.944266	-4.529141	33.741046
H	7.931198	5.950089	30.327488	C	5.698807	-4.477691	34.783178

4. 3'-GACTG-5'

(optimized by GEBF-M062X/6-31G\*\*)

C	-0.314927	-8.750971	29.921941	N	3.789701	-2.849983	34.569986
C	0.982488	-7.985385	30.107320	C	3.523372	-1.515705	34.916963
O	0.704646	-6.558077	29.911278	O	4.394551	-0.671425	35.006585
C	1.558483	-8.098349	31.529569	N	2.207193	-1.248769	35.169399
O	3.028664	-8.079211	31.399325	C	1.154227	-2.137878	35.183642
C	1.072775	-6.829590	32.210742	O	0.025778	-1.772455	35.495914
C	1.149429	-5.808541	31.074552	C	1.491170	-3.512948	34.810223
				C	0.367673	-4.503250	34.797930
				C	2.770161	-3.780175	34.472578
				H	4.404964	-4.975569	30.993611

H	5.684582	-6.244830	31.108890	O	9.395585	-1.530267	41.064359
H	6.784869	-4.224828	31.702009	O	9.825128	0.883537	40.712430
H	6.643375	-6.155778	33.706319	C	9.987162	2.166674	40.020167
H	4.894158	-5.183239	35.005773	C	9.311153	3.222134	40.865634
H	6.268657	-4.277127	35.693168	O	7.874640	3.114383	40.705782
H	5.752585	-2.306562	34.474333	C	9.595392	3.062305	42.364347
H	1.998516	-0.246775	35.432037	O	9.775818	4.424094	42.889200
H	0.739087	-5.525039	34.704106	C	8.347561	2.388844	42.927699
H	-0.201435	-4.422954	35.729827	C	7.214819	2.781437	41.963536
H	-0.341701	-4.292457	33.989077	N	6.264533	1.724064	41.720874
H	3.076235	-4.754787	34.096027	C	6.532107	0.463962	41.234032
P	9.000123	-4.759648	34.912450	N	5.464954	-0.267682	41.058121
O	10.405774	-4.777110	34.481347	C	4.428662	0.559100	41.445230
O	8.433021	-6.070577	35.630341	C	3.037555	0.348969	41.567968
O	8.635999	-3.627116	35.996341	N	2.453674	-0.829576	41.310962
C	8.934414	-2.229221	35.662935	N	2.286961	1.393914	41.963800
C	8.292435	-1.354028	36.701679	C	2.874507	2.568711	42.256041
O	6.851662	-1.449420	36.565306	N	4.166948	2.856416	42.250317
C	8.605831	-1.738999	38.169710	C	4.895258	1.807982	41.842267
O	9.137433	-0.528584	38.815211	H	9.500118	2.108110	39.044023
C	7.240714	-2.069960	38.768319	H	11.056818	2.365528	39.909793
C	6.320162	-1.196135	37.913094	H	9.627423	4.214302	40.534198
N	4.914670	-1.480617	37.955987	H	10.507109	2.501121	42.572732
C	4.013931	-0.391895	38.107639	H	8.493745	1.305251	42.908425
O	4.458863	0.751543	38.133264	H	8.122168	2.712087	43.945951
N	2.697417	-0.682156	38.243320	H	6.641679	3.637462	42.325497
C	2.253498	-1.932143	38.174404	H	7.547804	0.156325	41.024731
N	0.961130	-2.156654	38.397117	H	1.452526	-0.946652	41.470265
C	3.134509	-3.034556	37.875898	H	3.048509	-1.641229	41.256558
C	4.451328	-2.748202	37.790516	H	2.185866	3.355140	42.558833
H	8.521499	-2.000724	34.675468	P	10.194048	4.807355	44.377154
H	10.019831	-2.097926	35.651241	O	10.967608	6.055192	44.493649
H	8.611634	-0.316322	36.548135	O	10.899766	3.476479	44.914149
H	9.338413	-2.545000	38.248098	O	8.810626	4.771690	45.189719
H	7.030577	-3.129285	38.588455	C	7.735589	5.689396	44.809425
H	7.168918	-1.860271	39.835241	C	6.452732	5.170198	45.391485
H	6.429132	-0.138827	38.162258	O	6.118282	3.923359	44.731500
H	0.310362	-1.370502	38.532457	C	6.466406	4.856606	46.911665
H	0.576382	-3.069422	38.215488	O	5.680745	5.820427	47.645154
H	2.762321	-4.040226	37.732487	C	5.777124	3.490736	47.007728
H	5.203590	-3.502823	37.589492	C	5.155658	3.278691	45.617666
P	10.136481	-0.535139	40.054902	N	4.967706	1.915214	45.225670
O	11.552965	-0.847285	39.780394	C	5.910023	0.928861	44.986233

N	5.380397	-0.217966	44.672737	H	0.749101	-4.687673	44.216408
C	4.018163	0.007230	44.716627	H	-1.647529	-5.105570	44.410831
C	2.902603	-0.865795	44.500139	H	-3.869205	-3.970855	44.716203
O	2.913081	-2.060989	44.193053	P	-7.698369	0.785240	43.162289
N	1.689030	-0.192548	44.679549	O	-9.086823	1.218630	43.373274
C	1.541795	1.132588	45.007162	O	-7.370319	0.060738	41.777113
N	0.282598	1.587914	45.148942	O	-6.588791	1.950045	43.151041
N	2.560401	1.944416	45.219324	C	-6.372339	2.757772	44.359980
C	3.741894	1.326763	45.053326	C	-5.277011	3.743683	44.050582
H	7.666656	5.731669	43.717952	O	-4.046891	3.001539	43.904258
H	7.971687	6.684010	45.199193	C	-5.502065	4.506959	42.732101
H	5.651036	5.901406	45.216505	O	-5.475642	5.936680	43.073693
H	7.491448	4.817157	47.291311	C	-4.342944	4.097044	41.822076
H	6.506516	2.698343	47.197114	C	-3.285589	3.503627	42.764965
H	5.032505	3.495160	47.804169	N	-2.518259	2.400979	42.233896
H	4.181291	3.770413	45.526759	C	-1.135672	2.414263	42.437624
H	6.967158	1.137417	45.069464	O	-0.546898	3.377328	42.899530
H	0.833959	-0.755463	44.528236	N	-0.497624	1.254214	42.083940
H	-0.509392	1.012269	44.859783	C	-1.084921	0.074263	41.677129
H	0.176967	2.585925	45.055263	O	-0.420155	-0.946265	41.526175
C	-6.957920	-3.735656	45.363759	C	-2.525607	0.139437	41.427828
C	-6.532778	-2.279096	45.390659	C	-3.165555	-1.055125	40.797820
O	-5.115200	-2.221655	45.759564	C	-3.162712	1.276540	41.755949
C	-6.639448	-1.579531	44.025234	H	-6.067599	2.092272	45.170825
O	-7.158703	-0.233236	44.273662	H	-7.306400	3.267227	44.612097
C	-5.204531	-1.518917	43.512788	H	-5.190440	4.469533	44.866124
C	-4.360674	-1.453315	44.789464	H	-6.475359	4.297894	42.288306
N	-3.047106	-2.071566	44.645973	H	-4.688305	3.349400	41.103412
C	-1.908207	-1.243877	44.549074	H	-3.926371	4.942401	41.269733
O	-2.062194	-0.022958	44.545283	H	-2.564388	4.255451	43.087028
N	-0.697579	-1.846873	44.465208	H	0.553798	1.279565	42.142218
C	-0.585678	-3.167667	44.383451	H	-4.240593	-0.904126	40.660922
N	0.634586	-3.689854	44.265724	H	-2.706954	-1.221877	39.819232
C	-1.739670	-4.028626	44.443224	H	-3.002787	-1.953516	41.403470
C	-2.938731	-3.427938	44.596090	H	-4.238319	1.388421	41.659615
H	-8.033707	-3.820918	45.200351	P	-5.784035	7.128420	42.068530
H	-6.710651	-4.208028	46.314405	O	-6.242848	8.358779	42.724790
H	-7.101563	-1.707637	46.127195	O	-6.718713	6.419551	40.983968
H	-7.319871	-2.090557	43.341444	O	-4.439497	7.307565	41.188350
H	-4.968894	-2.436724	42.962043	C	-3.244361	7.864107	41.828907
H	-5.015909	-0.667436	42.858891	C	-2.097405	7.659890	40.878170
H	-4.196945	-0.430691	45.130585	O	-1.813392	6.235004	40.818780
H	1.466895	-3.080655	44.220035	C	-2.404432	8.101294	39.429376

O	-1.325743	9.019270	39.050296	C	2.829005	2.178817	35.663945
C	-2.374419	6.805461	38.626287	N	2.883784	3.504005	35.704386
C	-1.449415	5.898227	39.440679	C	1.668848	4.029591	35.885485
N	-1.627622	4.497726	39.225996	H	1.611024	8.790507	38.662899
C	-2.799409	3.796445	38.990588	H	1.691323	10.299309	37.691712
N	-2.620010	2.516722	38.863875	H	3.596203	8.922731	37.058814
C	-1.255492	2.347793	39.011710	H	1.755844	9.710217	35.095257
C	-0.442523	1.177269	38.893986	H	0.645438	7.635815	34.894079
O	-0.816259	0.016506	38.704493	H	1.944902	7.356588	33.723356
N	0.915926	1.483441	38.994836	H	3.194971	5.993067	35.335478
C	1.437753	2.746911	39.141097	H	-0.527220	6.378470	36.175381
N	2.774698	2.850244	39.123567	H	-0.440287	0.142550	35.889324
N	0.693649	3.831994	39.303265	H	-1.443817	1.530228	36.231259
C	-0.617276	3.563754	39.220344	H	3.763167	1.636559	35.539910
H	-3.053842	7.326968	42.763037	P	4.049133	9.258394	33.161089
H	-3.415887	8.923762	42.034426	O	5.061854	10.288565	32.878751
H	-1.215754	8.204215	41.229576	O	2.613231	9.455454	32.485576
H	-3.346493	8.641130	39.337695	O	4.440129	7.776074	32.671816
H	-3.384270	6.388648	38.627313	C	5.706325	7.217815	33.179544
H	-2.056635	6.947528	37.596151	C	5.966504	5.915922	32.473203
H	-0.388987	6.122224	39.275051	O	4.973144	4.958244	32.922802
H	-3.753944	4.297425	38.922943	C	5.850383	5.978798	30.928188
H	1.572444	0.701990	38.797637	O	6.859407	5.155515	30.305617
H	3.367876	2.088554	38.788636	C	4.521362	5.293033	30.642587
H	3.138627	3.790953	39.098700	C	4.446561	4.248206	31.760029
P	-1.020603	9.732815	37.673366	N	3.118189	3.780560	32.083134
O	-0.799708	11.188565	37.728175	C	2.857097	2.391397	32.081548
O	-2.215684	9.204293	36.748882	O	3.763750	1.617922	31.785537
O	0.239187	8.917551	37.085651	N	1.601396	1.988444	32.390236
C	1.564575	9.213503	37.657164	C	0.654503	2.861051	32.723442
C	2.601613	8.567338	36.777652	N	-0.567308	2.390150	32.965891
O	2.541602	7.128846	36.965052	C	0.925108	4.276485	32.815424
C	2.368289	8.827635	35.283989	C	2.174516	4.673259	32.493359
O	3.690635	9.059068	34.697525	H	5.602291	7.050912	34.255671
C	1.726752	7.541995	34.775213	H	6.505463	7.940512	32.986914
C	2.271378	6.448429	35.707232	H	6.965074	5.554963	32.747855
N	1.345635	5.366917	35.921832	H	5.885778	7.008198	30.557618
C	-0.022307	5.424837	36.082968	H	3.701998	6.011398	30.737830
N	-0.596277	4.252038	36.124640	H	4.516105	4.846144	29.648777
C	0.454766	3.360060	36.005217	H	5.056094	3.373279	31.543026
C	0.514712	1.947648	35.909457	H	-0.744411	1.381986	32.877921
N	-0.561269	1.155425	35.917216	H	-1.269888	2.991245	33.367829
N	1.736135	1.402456	35.754007	H	0.167227	4.977177	33.145125

H	2.515756	5.703720	32.543286
H	-6.439810	-4.275950	44.566073
H	6.172168	6.647001	47.795194
H	-6.717434	0.401822	41.141026
H	-6.684852	6.644124	40.035345
H	-2.384446	9.598090	35.868514
H	2.511208	10.030911	31.707660
H	11.708370	3.538308	45.450426
H	9.874467	-1.986189	41.774979
H	9.037508	-6.714029	36.033471
H	3.729612	-8.681750	34.586433
H	-1.028971	-8.500068	30.711586
H	7.745158	5.559298	30.350645

5. 3'-GACTGGATGT-5'  
(optimized by GEBF-HF/6-31G\*\*)

C	-4.230351	7.442939	-6.949051
H	-5.122143	7.576904	-7.540878
O	-3.624100	6.177295	-7.299026
C	-3.912893	5.194459	-6.278560
H	-4.890252	4.782376	-6.444665
N	-2.985952	4.100719	-6.374651
C	-1.655975	4.245329	-6.036983
H	-1.374816	5.229563	-5.723273
C	-0.762307	3.261872	-6.083294
C	0.670711	3.406672	-5.659132
H	0.884517	4.428234	-5.364087
H	0.882149	2.757359	-4.816022
H	1.346198	3.129278	-6.460776
C	-1.215544	1.957456	-6.567686
O	-0.495403	0.996529	-6.685364
N	-2.535081	1.898969	-6.933876
H	-2.892565	1.007166	-7.245114
C	-3.465630	2.895013	-6.852269
O	-4.605234	2.724794	-7.178739
C	-3.888272	6.042729	-5.007358
H	-2.876636	6.316524	-4.738660
H	-4.334601	5.566104	-4.155246
C	-4.622884	7.293937	-5.466425
H	-4.409827	8.166546	-4.872302
O	-6.076485	7.063685	-5.419887
P	-7.021274	7.178533	-4.168502

O	-8.048347	8.328498	-4.543487
H	-8.094692	9.150962	-4.069736
O	-6.320764	7.384007	-2.907521
O	-7.909303	5.894696	-4.213117
C	-8.867304	5.403703	-5.190581
H	-8.364106	5.282200	-6.135876
H	-9.659276	6.132973	-5.274020
C	-9.386867	4.069298	-4.711465
H	-10.218917	3.777295	-5.333750
O	-8.349228	3.089907	-4.841425
C	-8.007605	2.462364	-3.585413
H	-8.425807	1.471212	-3.569559
N	-6.587112	2.321074	-3.482677
C	-5.649369	3.321499	-3.330371
H	-5.946377	4.332996	-3.156675
N	-4.446349	2.902400	-3.394734
C	-4.558326	1.542351	-3.618214
C	-3.566893	0.527469	-3.781994
O	-2.361110	0.629782	-3.770505
N	-4.156463	-0.719027	-3.979808
H	-3.517589	-1.491338	-4.089399
C	-5.492637	-0.966597	-4.030499
N	-5.861851	-2.227643	-4.258158
H	-5.203373	-2.981512	-4.246063
H	-6.824706	-2.427807	-4.125450
N	-6.401164	-0.041100	-3.881432
C	-5.877394	1.176296	-3.686817
C	-8.628384	3.379418	-2.524930
H	-8.927728	2.835949	-1.644352
C	-9.803022	4.032136	-3.236732
H	-10.071074	4.990765	-2.828382
O	-10.991691	3.171514	-3.168961
P	-11.830291	2.840409	-1.873186
O	-13.294362	2.620672	-2.428863
H	-13.970597	3.288042	-2.403954
O	-11.691498	3.826516	-0.812730
O	-11.416315	1.382761	-1.474208
C	-11.567145	0.153923	-2.233987
H	-11.130057	0.289839	-3.210547
H	-12.622406	-0.052520	-2.326213
C	-10.856610	-0.951067	-1.501748
H	-11.109241	-1.893320	-1.967290
O	-9.440667	-0.734861	-1.599082

C	-8.809807	-1.149460	-0.362507	N	-2.265660	-2.711913	2.776071
H	-8.700626	-2.218772	-0.368244	C	-2.719967	-3.963572	2.786347
N	-7.488085	-0.603465	-0.264442	H	-1.958897	-4.722334	2.754356
C	-7.268135	0.733318	0.019344	N	-3.962186	-4.377246	2.834918
H	-8.152779	1.317284	0.164804	C	-4.819395	-3.361617	2.879552
C	-6.063371	1.280757	0.128624	C	-7.945904	-4.646890	4.264362
C	-5.809760	2.716572	0.490401	H	-8.347308	-3.664926	4.471555
H	-6.742846	3.267845	0.570421	H	-7.461826	-5.012953	5.153713
H	-5.292879	2.782816	1.444314	C	-9.075951	-5.555349	3.783998
H	-5.180719	3.192600	-0.254011	H	-10.041166	-5.245646	4.141066
C	-4.905411	0.412497	-0.094407	O	-8.874281	-6.944258	4.209853
O	-3.765228	0.775870	0.037442	P	-8.980575	-7.519919	5.675042
N	-5.196568	-0.870698	-0.481906	O	-9.532332	-8.985852	5.448378
H	-4.418163	-1.497410	-0.629868	H	-10.426185	-9.233353	5.658675
C	-6.431956	-1.442948	-0.579101	O	-9.753691	-6.703632	6.597058
O	-6.580506	-2.587371	-0.894325	O	-7.493736	-7.774086	6.096026
C	-9.833727	-0.711460	0.684013	C	-6.418721	-8.360568	5.321874
H	-9.709236	-1.206951	1.632895	H	-6.520311	-8.063144	4.290867
C	-11.157337	-1.049678	0.007145	H	-6.499536	-9.434079	5.403565
H	-11.971020	-0.428177	0.334253	C	-5.107987	-7.874108	5.870807
O	-11.529638	-2.445454	0.259431	H	-4.310596	-8.412579	5.378804
P	-11.946122	-3.064673	1.652210	O	-4.970994	-6.470514	5.606315
O	-13.009795	-4.169297	1.262033	C	-4.219013	-5.883316	6.704465
H	-13.948474	-4.029602	1.315282	H	-3.183789	-6.161129	6.595070
O	-12.387183	-2.075438	2.623009	N	-4.249434	-4.464572	6.669997
O	-10.724159	-3.934933	2.095365	C	-5.288587	-3.570481	6.871828
C	-10.182286	-5.138791	1.486636	H	-6.282183	-3.908064	7.081910
H	-9.924592	-4.926420	0.461353	N	-4.923241	-2.352769	6.782945
H	-10.943747	-5.901974	1.528656	C	-3.566267	-2.400423	6.518199
C	-8.954286	-5.557348	2.247186	C	-2.581998	-1.373592	6.366876
H	-8.680947	-6.554288	1.929022	O	-2.707634	-0.170551	6.394290
O	-7.885838	-4.651859	1.944404	N	-1.314909	-1.924476	6.159271
C	-6.986746	-4.585495	3.072231	H	-0.565447	-1.263729	6.045875
H	-6.312094	-5.426049	3.056253	C	-1.016336	-3.250149	6.110980
N	-6.183429	-3.408196	2.984789	N	0.260132	-3.578912	5.923593
C	-6.601795	-2.097873	2.983751	H	0.995400	-2.903807	5.888934
H	-7.641061	-1.851525	3.043985	H	0.484386	-4.544969	5.976239
N	-5.648422	-1.251178	2.899515	N	-1.914572	-4.186566	6.237493
C	-4.505824	-2.026506	2.845931	C	-3.144204	-3.700000	6.446646
C	-3.140006	-1.702759	2.799431	C	-4.849156	-6.586416	7.902765
N	-2.694325	-0.449505	2.805952	H	-5.852398	-6.217593	8.068492
H	-1.729805	-0.263920	2.629155	H	-4.288877	-6.489401	8.817598
H	-3.345578	0.290081	2.690459	C	-4.928573	-8.020524	7.396674

H	-5.682252	-8.619027	7.876369	H	6.068660	-7.094120	9.382972
O	-3.629174	-8.692355	7.564357	C	5.921748	-5.213370	10.411094
P	-2.894158	-9.190072	8.857942	H	6.693950	-4.800055	9.778629
O	-2.757349	-10.757988	8.650855	O	4.902958	-4.226914	10.623309
H	-3.157382	-11.383849	9.244084	C	4.960561	-3.696185	11.970102
O	-3.514890	-8.808532	10.118034	H	5.604354	-2.837743	11.983630
O	-1.427681	-8.680181	8.675753	N	3.660274	-3.242525	12.373618
C	-0.487496	-8.787078	7.576122	C	2.614810	-4.134971	12.543181
H	-0.925239	-8.338661	6.699870	H	2.870157	-5.161330	12.372648
H	-0.290713	-9.835228	7.405509	C	1.385451	-3.774004	12.895197
C	0.772777	-8.049480	7.960447	C	0.247892	-4.722920	13.143851
H	1.553356	-8.299877	7.258412	H	0.575518	-5.753226	13.069131
O	0.533917	-6.633125	7.903596	H	-0.160824	-4.567948	14.136262
C	0.835098	-5.986384	9.167299	H	-0.561350	-4.553057	12.444745
H	1.828199	-5.575384	9.111363	C	1.109816	-2.339013	13.021411
N	-0.045584	-4.891334	9.402907	O	0.025522	-1.893471	13.279275
C	-1.406261	-4.897002	9.654973	N	2.187299	-1.511476	12.815570
H	-1.957589	-5.812625	9.696994	H	2.024017	-0.516704	12.921122
N	-1.887344	-3.729101	9.828411	C	3.457790	-1.873792	12.479129
C	-0.812101	-2.871784	9.677332	O	4.330128	-1.073787	12.308137
C	-0.705692	-1.445986	9.768947	C	5.552455	-4.852759	12.778418
O	-1.559671	-0.622433	9.988446	H	4.798532	-5.572525	13.058161
N	0.613713	-1.032053	9.558625	H	6.046120	-4.502716	13.670231
H	0.764720	-0.037940	9.611189	C	6.513233	-5.513027	11.798461
C	1.675335	-1.841600	9.301708	H	6.667523	-6.560113	11.990309
N	2.862222	-1.255728	9.145883	O	7.822505	-4.854717	11.843174
H	3.010060	-0.277246	9.295257	P	8.879524	-5.004031	13.010060
H	3.642341	-1.857085	9.026043	O	10.251474	-4.682337	12.295652
N	1.577816	-3.139493	9.214332	H	10.847500	-5.350186	11.969962
C	0.326811	-3.581023	9.406241	O	8.801872	-6.276865	13.710509
C	0.744065	-7.126947	10.179830	O	8.676169	-3.742446	13.914334
H	-0.281398	-7.306865	10.462785	C	8.837779	-2.337134	13.579502
H	1.316552	-6.943375	11.072725	H	8.320902	-2.132033	12.655666
C	1.247678	-8.323200	9.392887	H	9.893204	-2.146048	13.463150
H	0.934195	-9.272182	9.789892	C	8.256772	-1.507509	14.689741
O	2.717903	-8.318630	9.339029	H	8.543109	-0.476048	14.537695
P	3.723456	-8.476335	10.543608	O	6.824367	-1.610581	14.664865
O	4.869892	-9.400296	9.963598	C	6.357926	-1.335987	16.008075
H	4.950978	-10.324459	10.170712	H	6.460409	-0.285204	16.210683
O	3.103920	-8.943638	11.775175	N	4.954954	-1.634575	16.128074
O	4.448060	-7.094700	10.661606	C	4.491832	-2.913385	16.127307
C	5.310212	-6.401863	9.715545	H	5.226893	-3.680852	16.001326
H	4.708626	-6.074858	8.883380	C	3.195734	-3.209527	16.271328

H	2.848323	-4.223208	16.268378	H	7.915569	2.307199	22.180657
C	2.285194	-2.102573	16.409133	C	9.372943	2.757855	20.618838
N	0.985329	-2.308896	16.554258	H	10.301293	2.253538	20.824264
H	0.344359	-1.534743	16.592447	O	9.463606	4.113039	21.171371
H	0.607917	-3.223783	16.595409	P	9.880929	4.464473	22.740896
N	2.733813	-0.856422	16.375212	O	10.475414	6.013237	22.598925
C	4.048188	-0.566318	16.239813	H	11.409093	6.186486	22.676654
O	4.468677	0.598555	16.225113	O	10.848303	3.433587	23.410541
C	7.336148	-2.169799	16.836703	O	8.439593	4.715691	23.490184
H	7.111458	-3.223933	16.758611	C	7.338689	5.536478	23.008323
H	7.352818	-1.912789	17.880001	H	7.254663	5.426020	21.939043
C	8.661856	-1.917706	16.121350	H	7.557725	6.563296	23.257238
H	9.325274	-2.763630	16.154031	C	6.080887	5.082388	23.688378
O	9.361551	-0.758535	16.685459	H	5.282995	5.756899	23.401586
P	10.188061	-0.751236	18.119751	O	5.743625	3.751303	23.270610
O	11.766909	-0.520763	17.632215	C	4.820092	3.235767	24.251878
H	12.467279	-1.060994	17.989191	H	3.853892	3.691464	24.106150
O	9.963889	-1.999266	19.032599	N	4.642981	1.829131	24.088782
O	9.777708	0.692346	18.785719	C	5.611820	0.826651	24.030784
C	9.862503	2.028524	18.213271	H	6.650126	1.040618	24.115825
H	9.419871	2.019388	17.231028	N	5.091275	-0.340460	23.855079
H	10.905121	2.302506	18.161041	C	3.715499	-0.137897	23.790674
C	9.082327	2.942931	19.123712	C	2.631385	-1.038206	23.615391
H	9.275669	3.968100	18.845730	O	2.655377	-2.268780	23.462611
O	7.687624	2.663049	18.956010	N	1.401965	-0.379889	23.624432
C	7.020374	2.387296	20.204174	H	0.594805	-0.967359	23.463203
H	6.471831	3.257477	20.515732	C	1.221063	0.968101	23.762191
N	6.066158	1.337885	20.021852	N	-0.028038	1.426645	23.727453
C	6.329895	0.013711	19.717509	H	-0.819419	0.832155	23.570244
H	7.323205	-0.344066	19.595113	H	-0.155699	2.408211	23.682217
N	5.255847	-0.699518	19.617917	N	2.233021	1.800389	23.932438
C	4.210244	0.180380	19.874260	C	3.440334	1.204810	23.928474
C	2.826587	-0.008453	19.971125	C	5.462270	3.684447	25.570081
N	2.241870	-1.200574	19.841288	H	6.219530	2.969756	25.863607
H	1.247361	-1.282150	19.832999	H	4.737338	3.767569	26.367447
H	2.799667	-2.016081	19.768544	C	6.107585	5.035095	25.226323
N	2.077422	1.079048	20.233071	H	7.114872	5.103821	25.607267
C	2.661496	2.279272	20.393022	O	5.337965	6.164816	25.662514
H	2.002600	3.098001	20.582017	H	5.369677	6.314192	26.600902
N	3.958303	2.531605	20.354841	C	-7.445445	-3.747138	23.803266
C	4.701696	1.448074	20.099469	H	-7.163695	-4.193663	24.746999
C	8.157467	2.026678	21.168538	C	-6.789821	-2.386397	23.667633
H	8.353396	0.965608	21.146889	H	-7.208564	-1.677249	24.363765

O	-5.377243	-2.536213	23.956198	O	-0.765070	-1.192202	19.615810
C	-4.581090	-1.797839	23.015102	N	-0.875015	0.967713	20.221155
H	-4.437027	-0.785948	23.343252	H	0.134075	0.992737	20.343533
N	-3.269610	-2.413414	22.947925	C	-1.536173	2.103037	20.581493
C	-3.146392	-3.768529	22.811514	O	-0.973017	3.043945	21.069815
H	-4.060547	-4.315990	22.748447	C	-4.721655	3.760312	19.827924
C	-1.948050	-4.368444	22.779988	H	-5.153719	2.984167	19.216539
H	-1.856643	-5.426906	22.664775	H	-4.294654	4.505904	19.178188
C	-0.786724	-3.532650	22.944692	C	-5.799124	4.333348	20.739863
N	0.431500	-4.050632	22.951488	H	-6.790500	4.248177	20.329206
H	1.236859	-3.459356	23.089537	O	-5.547441	5.755436	21.008521
H	0.576631	-5.021398	22.819089	P	-5.874077	6.966895	19.920061
N	-0.922653	-2.223868	23.114633	O	-6.010930	8.299542	20.908144
C	-2.128950	-1.617413	23.095782	H	-6.863796	8.658174	21.136089
O	-2.258024	-0.386660	23.196052	O	-7.091953	6.682876	18.981106
C	-6.844173	-1.794022	22.246944	O	-4.438784	7.265050	19.172494
H	-7.551021	-2.293267	21.605870	C	-3.189466	7.697419	19.781366
C	-5.412052	-1.874554	21.735036	H	-2.985915	7.091571	20.649772
H	-5.259944	-2.828625	21.244198	H	-3.299218	8.732661	20.064920
H	-5.175875	-1.097288	21.030846	C	-2.104082	7.513804	18.755141
O	-7.261829	-0.393843	22.364378	H	-1.207197	8.005754	19.103371
P	-7.830497	0.506661	21.201288	O	-1.851883	6.110281	18.598936
O	-9.287444	0.892522	21.694455	C	-1.561476	5.821177	17.208057
H	-10.066256	0.725492	21.175965	H	-0.528604	6.059218	17.010652
O	-7.787310	-0.118803	19.886144	N	-1.729594	4.431634	16.947735
O	-7.035785	1.842871	21.320679	C	-2.896011	3.713083	16.755840
C	-6.760123	2.695323	22.464113	H	-3.850306	4.193843	16.715206
H	-6.474823	2.077370	23.299737	N	-2.701166	2.460498	16.624562
H	-7.659848	3.247025	22.691922	C	-1.331352	2.302915	16.729127
C	-5.624337	3.608209	22.084896	C	-0.508186	1.140355	16.634987
H	-5.482442	4.343533	22.863760	O	-0.847823	-0.016369	16.511149
O	-4.446581	2.808821	21.949250	N	0.840523	1.468844	16.710348
C	-3.670502	3.209647	20.796581	H	1.491065	0.700269	16.598848
H	-2.972391	3.970522	21.089090	C	1.338197	2.722334	16.888836
N	-2.896106	2.092752	20.331495	N	2.665854	2.837247	16.937790
C	-3.502536	0.988351	19.761265	H	3.277313	2.087618	16.669271
H	-4.552688	1.087062	19.579100	H	3.020172	3.764210	16.948109
C	-2.854033	-0.121039	19.424407	N	0.586350	3.783984	17.025667
C	-3.475565	-1.265158	18.675969	C	-0.720381	3.513038	16.921918
H	-4.542365	-1.114005	18.553326	C	-2.514864	6.772222	16.486759
H	-3.025757	-1.337952	17.692240	H	-3.526374	6.395894	16.527681
H	-3.308068	-2.206963	19.188374	H	-2.257973	6.951067	15.456805
C	-1.429386	-0.193208	19.746103	C	-2.443511	8.029543	17.343064

H	-3.336095	8.626255	17.298268	C	5.454752	5.751954	10.077064
O	-1.311090	8.873115	16.932268	H	6.331080	5.189346	10.364325
P	-1.184147	9.741632	15.625008	O	4.273972	5.010420	10.426160
O	-0.799994	11.187018	16.150325	C	3.802253	4.308088	9.252840
H	-1.395952	11.926042	16.106830	H	4.401846	3.431140	9.100825
O	-2.352493	9.697213	14.758105	N	2.456267	3.844392	9.438563
O	0.145135	9.257328	14.961703	C	1.422526	4.710777	9.628722
C	1.502637	9.215334	15.475612	H	1.678413	5.751328	9.634186
H	1.499818	8.719293	16.432513	C	0.169094	4.285009	9.798884
H	1.848627	10.232478	15.580704	H	-0.641654	4.966873	9.957979
C	2.346764	8.441808	14.496171	C	-0.036401	2.852776	9.795366
H	3.389010	8.572528	14.746693	N	-1.251818	2.356608	9.926779
O	2.003590	7.049380	14.597296	H	-1.390809	1.359561	9.953431
C	1.826040	6.468319	13.285135	H	-2.020712	2.948955	10.130873
H	2.776737	6.104100	12.932197	N	0.968357	2.021608	9.647022
N	0.952383	5.341591	13.339787	C	2.233659	2.456634	9.507857
C	-0.423547	5.308194	13.392131	O	3.178304	1.709487	9.410784
H	-1.003045	6.206921	13.426587	C	4.044940	5.342860	8.155667
N	-0.911216	4.126885	13.383092	H	3.337173	6.157230	8.223838
C	0.194365	3.296704	13.337212	H	4.013466	4.944258	7.155338
C	0.336435	1.897204	13.283364	C	5.421913	5.869012	8.538692
N	-0.696389	1.066121	13.288682	H	5.633676	6.854545	8.164673
H	-0.548764	0.077800	13.323895	O	6.467628	4.959182	8.050875
H	-1.608283	1.420907	13.455162	P	6.861469	4.616552	6.562658
N	1.579640	1.412599	13.212859	O	8.436062	4.766470	6.534539
C	2.611316	2.249957	13.206784	H	8.883992	5.477400	6.089539
H	3.577362	1.782045	13.151379	O	6.145672	5.394254	5.562285
N	2.592702	3.561770	13.259267	O	6.665361	3.068365	6.451616
C	1.352493	4.031683	13.318323	C	7.252771	1.980571	7.220047
C	1.321784	7.652293	12.460511	H	6.923496	2.067791	8.242235
H	0.277491	7.839504	12.658356	H	8.327126	2.071135	7.161086
H	1.453318	7.526303	11.398956	C	6.780684	0.673248	6.635700
C	2.121128	8.817416	13.021496	H	7.332264	-0.130211	7.101038
H	1.647128	9.771514	12.878561	O	5.383189	0.514798	6.919349
O	3.450038	8.875529	12.400141	C	4.649653	0.110996	5.739107
P	3.780846	9.207815	10.892034	H	4.601511	-0.959848	5.691432
O	5.056811	10.136882	10.978792	N	3.291223	0.585969	5.829365
H	5.027980	11.079358	10.857190	C	3.035996	1.911179	5.995198
O	2.656587	9.750678	10.144119	H	3.897514	2.545836	6.052388
O	4.371693	7.878181	10.316569	C	1.788675	2.381071	6.079300
C	5.451556	7.053517	10.829428	H	1.586300	3.427142	6.196261
H	5.285074	6.872217	11.878972	C	0.726743	1.403331	6.054121
H	6.377611	7.590156	10.688513	N	-0.532264	1.794016	6.161892

H	-1.280271	1.118386	6.205525	O	5.620524	-6.484715	1.949594
H	-0.750441	2.752536	6.287520	P	5.572051	-7.299595	0.597120
N	0.978537	0.122054	5.931983	O	6.012495	-8.757657	1.023853
C	2.237374	-0.343413	5.810814	H	6.905303	-9.077651	0.953952
O	2.491833	-1.516632	5.666957	O	6.346847	-6.687384	-0.472185
C	5.482439	0.702899	4.600930	O	4.055120	-7.505599	0.275450
H	5.266142	1.753137	4.465906	C	3.060741	-8.362541	0.909393
H	5.325937	0.203384	3.661486	H	2.854724	-7.978833	1.895222
C	6.907887	0.561553	5.107771	H	3.473799	-9.357173	0.971434
H	7.592069	1.268459	4.672308	C	1.803986	-8.344431	0.078333
O	7.411082	-0.790952	4.836972	H	1.163557	-9.150782	0.405091
P	7.850510	-1.375178	3.436667	O	1.130904	-7.093368	0.282627
O	9.326527	-1.891948	3.682577	C	0.579191	-6.602532	-0.956806
H	10.083603	-1.538075	3.230026	H	-0.401135	-7.022248	-1.113687
O	7.703600	-0.436650	2.333327	N	0.417400	-5.184063	-0.889526
O	7.032284	-2.694672	3.285230	C	1.397694	-4.228580	-0.777679
C	6.902435	-3.852507	4.154085	H	2.432445	-4.498985	-0.770939
H	6.621216	-3.514631	5.138356	N	0.950722	-3.033924	-0.684908
H	7.857864	-4.354360	4.187074	C	-0.425706	-3.179402	-0.718539
C	5.823382	-4.740365	3.590114	C	-1.485343	-2.255009	-0.661908
H	5.800404	-5.662267	4.152631	N	-1.297999	-0.943230	-0.559824
O	4.568593	-4.061998	3.727200	H	-2.080704	-0.338174	-0.418407
C	3.809115	-4.127194	2.494840	H	-0.394083	-0.594943	-0.349931
H	3.210734	-5.018413	2.502831	N	-2.727410	-2.737282	-0.736030
N	2.899427	-3.022765	2.414265	C	-2.909917	-4.048761	-0.848698
C	3.346609	-1.733703	2.204992	H	-3.936442	-4.362864	-0.902842
H	4.407543	-1.632395	2.099822	N	-2.001676	-4.996241	-0.902319
C	2.541137	-0.681319	2.111622	C	-0.771268	-4.502344	-0.832989
C	2.996760	0.716156	1.801132	C	1.591542	-7.103073	-1.990159
H	4.065102	0.746327	1.620334	H	2.456581	-6.455915	-2.015674
H	2.492499	1.089605	0.917260	H	1.179648	-7.167152	-2.983229
H	2.757204	1.397291	2.610982	C	2.018773	-8.458685	-1.441805
C	1.107073	-0.907278	2.302260	H	3.019287	-8.732075	-1.723688
O	0.287346	-0.027474	2.212496	O	1.117277	-9.516446	-1.910608
N	0.740932	-2.194017	2.588653	P	1.057284	-10.109586	-3.373763
H	-0.246543	-2.386527	2.705358	O	0.744400	-11.642220	-3.141766
C	1.555060	-3.286250	2.634447	H	1.404667	-12.324173	-3.196730
O	1.139747	-4.391877	2.824706	O	2.235849	-9.819433	-4.175600
C	4.899304	-4.198593	1.424939	O	-0.290145	-9.581737	-3.966498
H	5.329666	-3.230690	1.222854	C	-1.644457	-9.731857	-3.461735
H	4.548453	-4.612236	0.493968	H	-1.660136	-9.473274	-2.415145
C	5.958474	-5.062640	2.092120	H	-1.934865	-10.762786	-3.594228
H	6.947423	-4.918405	1.694567	C	-2.540747	-8.804318	-4.234814

H -3.569269 -9.030419 -3.992830  
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 C -2.407936 -6.603895 -5.020251  
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 H -1.761114 -9.663503 -6.113658  
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 O -4.561375 -10.848595 -7.756279  
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 O -3.102845 -9.046612 -8.817044  
 O -5.448971 -8.532152 -8.019070  
 C -6.613236 -8.319038 -7.173567  
 H -6.282879 -8.182777 -6.156898  
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 C -7.321615 -7.080720 -7.656309  
 H -8.255731 -6.980839 -7.124027  
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 C -6.308084 -5.099736 -8.513079  
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 C -3.794271 -5.182170 -8.477280  
 H -3.744495 -6.236872 -8.651334  
 N -2.783877 -4.423093 -8.275372  
 C -3.329677 -3.162119 -8.116691  
 C -2.759797 -1.905680 -7.864198  
 N -1.443298 -1.718518 -7.749877  
 H -1.086391 -0.838215 -7.435875

H -0.845850 -2.509833 -7.769363  
 N -3.583487 -0.864179 -7.751134  
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 H -5.492767 -0.166870 -7.787953  
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 C -4.698129 -3.205203 -8.225862  
 C -6.559730 -6.038785 -9.697572  
 H -5.658390 -6.578369 -9.948432  
 H -6.891253 -5.504063 -10.578020  
 C -7.607073 -7.013406 -9.165262  
 H -7.553033 -7.980938 -9.642282  
 O -8.938662 -6.485931 -9.282478  
 H -7.129733 -4.413886 23.008066  
 H -8.524564 -3.660294 23.770452  
 H -9.155037 -6.169256 -10.149437  
 C -3.222820 8.545338 -7.213039  
 H -2.838776 8.450727 -8.219244  
 H -3.681392 9.522240 -7.107163  
 H -2.384689 8.479867 -6.528590  
 H -9.805533 0.354057 0.850533  
 H -7.936979 4.151272 -2.226947

6. 3'-GACTGGATGT-5'  
 (optimized by GEBF-B3LYP/6-31G\*\*)

C -4.220056 7.353818 -6.984306  
 H -5.131287 7.517737 -7.568969  
 O -3.613997 6.073120 -7.399985  
 C -3.930314 5.058935 -6.370960  
 H -4.915669 4.631662 -6.560150  
 N -2.991247 3.962379 -6.473687  
 C -1.652134 4.131824 -6.183556  
 H -1.366796 5.142850 -5.919756  
 C -0.742662 3.132061 -6.225771  
 C 0.703041 3.305930 -5.863222  
 H 0.928325 4.348167 -5.620360  
 H 0.957216 2.688017 -4.994846  
 H 1.356807 2.986584 -6.681341  
 C -1.200655 1.809568 -6.640537  
 O -0.454122 0.825411 -6.731454  
 N -2.542170 1.721125 -6.973467  
 H -2.909465 0.783897 -7.249982  
 C -3.492931 2.715729 -6.897515

O	-4.668450	2.532116	-7.176026	O	-11.800949	3.965295	-0.720648
C	-3.910191	5.878527	-5.074532	O	-11.489305	1.452677	-1.276624
H	-2.881140	6.118187	-4.784896	C	-11.648764	0.231649	-2.093071
H	-4.374546	5.368830	-4.234106	H	-11.268015	0.423667	-3.099621
C	-4.610534	7.168981	-5.496015	H	-12.714101	-0.008685	-2.139588
H	-4.358292	8.025240	-4.868631	C	-10.867847	-0.890707	-1.450864
O	-6.099076	7.001091	-5.459420	H	-11.122864	-1.825508	-1.968819
P	-6.964242	7.152527	-4.107859	O	-9.441551	-0.613586	-1.608303
O	-8.065885	8.284453	-4.474617	C	-8.746461	-1.245031	-0.463970
H	-7.986725	9.158422	-4.049755	H	-8.603054	-2.308386	-0.663550
O	-6.176449	7.390904	-2.871646	N	-7.427798	-0.677960	-0.329174
O	-7.867174	5.833694	-4.059880	C	-7.255591	0.656202	0.000458
C	-8.852930	5.397168	-5.071968	H	-8.173268	1.218136	0.123300
H	-8.337746	5.264187	-6.026003	C	-6.045473	1.232860	0.161273
H	-9.617401	6.175348	-5.157007	C	-5.840055	2.669537	0.542847
C	-9.453296	4.073061	-4.628759	H	-6.793516	3.197690	0.629966
H	-10.309879	3.855946	-5.275949	H	-5.317407	2.742745	1.502460
O	-8.473322	3.003922	-4.801450	H	-5.217199	3.180106	-0.198132
C	-8.092720	2.410808	-3.501059	C	-4.864756	0.397514	-0.040327
H	-8.471478	1.387597	-3.473106	O	-3.709851	0.799184	0.143240
N	-6.655531	2.318946	-3.404361	N	-5.105874	-0.899363	-0.468516
C	-5.731601	3.344080	-3.227821	H	-4.277152	-1.518405	-0.621556
H	-6.048506	4.355607	-3.022063	C	-6.329617	-1.507516	-0.633098
N	-4.490964	2.943170	-3.321340	O	-6.455381	-2.669602	-0.989793
C	-4.579231	1.584356	-3.584918	C	-9.713286	-1.008485	0.707128
C	-3.563736	0.592345	-3.784556	H	-9.561868	-1.733483	1.508981
O	-2.331218	0.734077	-3.778383	C	-11.104818	-1.113554	0.066771
N	-4.128762	-0.677158	-4.009404	H	-11.822560	-0.418048	0.501166
H	-3.453356	-1.451406	-4.132697	O	-11.672445	-2.486736	0.194551
C	-5.473579	-0.962564	-4.049150	P	-12.152389	-3.062350	1.633291
N	-5.823626	-2.238294	-4.308267	O	-13.109983	-4.283093	1.185828
H	-5.138767	-2.997670	-4.291978	H	-14.050806	-4.104218	1.006125
H	-6.795546	-2.455555	-4.159087	O	-12.709001	-2.048067	2.560671
N	-6.418051	-0.046629	-3.868252	O	-10.891129	-3.863464	2.213430
C	-5.913764	1.178926	-3.650135	C	-10.256209	-5.018390	1.545411
C	-8.738443	3.317619	-2.435721	H	-10.058564	-4.764799	0.500680
H	-9.069136	2.746138	-1.567936	H	-10.951389	-5.860458	1.596301
C	-9.892804	4.017457	-3.154850	C	-8.965143	-5.352683	2.253261
H	-10.133443	4.990726	-2.725553	H	-8.620388	-6.328395	1.881598
O	-11.139896	3.195188	-3.132070	O	-7.962510	-4.335324	1.948375
P	-11.946744	2.913052	-1.755574	C	-6.945881	-4.435046	3.017093
O	-13.429607	2.590088	-2.306312	H	-6.280637	-5.283509	2.827156
H	-14.043538	3.323739	-2.490133	N	-6.123936	-3.256044	2.994053

C	-6.524290	-1.928668	3.027989	H	1.056618	-2.967447	5.903554
H	-7.568859	-1.663614	3.105670	H	0.505043	-4.625250	6.059049
N	-5.531461	-1.079839	2.947002	N	-1.915168	-4.227436	6.258731
C	-4.404820	-1.880843	2.868518	C	-3.139975	-3.716560	6.454389
C	-3.025046	-1.577433	2.786124	C	-4.887157	-6.621304	7.888741
N	-2.546443	-0.321257	2.768682	H	-5.899718	-6.242802	8.060953
H	-1.567931	-0.175035	2.519384	H	-4.321452	-6.539166	8.817270
H	-3.195538	0.416345	2.537634	C	-4.983428	-8.054790	7.366181
N	-2.159094	-2.620162	2.752096	H	-5.743040	-8.657889	7.862794
C	-2.635033	-3.880811	2.769223	O	-3.671187	-8.767378	7.478371
H	-1.873861	-4.656252	2.734319	P	-2.938461	-9.195322	8.844973
N	-3.905555	-4.278582	2.824574	O	-2.635181	-10.773597	8.629629
C	-4.742817	-3.234009	2.882803	H	-3.137346	-11.413329	9.167329
C	-7.793022	-4.651728	4.286886	O	-3.631318	-8.835172	10.106578
H	-8.111659	-3.684886	4.686824	O	-1.473592	-8.566285	8.698618
H	-7.224545	-5.177138	5.055900	C	-0.544190	-8.742849	7.564047
C	-9.023599	-5.439248	3.800726	H	-0.985242	-8.284601	6.676321
H	-9.955299	-5.055555	4.215303	H	-0.397579	-9.815863	7.405033
O	-8.958599	-6.892715	4.117994	C	0.770948	-8.059633	7.901843
P	-9.109337	-7.476068	5.620885	H	1.519351	-8.368593	7.164520
O	-9.556878	-9.001000	5.326841	O	0.613187	-6.603403	7.818959
H	-10.509027	-9.208530	5.292471	C	0.904321	-5.982440	9.139176
O	-9.959360	-6.684424	6.541722	H	1.908626	-5.554674	9.098746
O	-7.603363	-7.691100	6.127241	N	0.016100	-4.886721	9.387376
C	-6.548423	-8.332458	5.319224	C	-1.356693	-4.878433	9.637642
H	-6.664947	-8.035409	4.274387	H	-1.924630	-5.797330	9.667541
H	-6.665694	-9.416504	5.409124	N	-1.835837	-3.676858	9.811615
C	-5.201262	-7.889300	5.838077	C	-0.744390	-2.832206	9.661119
H	-4.427916	-8.469056	5.319150	C	-0.621113	-1.404548	9.744248
O	-5.020662	-6.464365	5.552736	O	-1.499038	-0.560318	9.963163
C	-4.249798	-5.898200	6.697726	N	0.714905	-0.995026	9.534250
H	-3.198816	-6.179045	6.580913	H	0.874158	0.023804	9.590625
N	-4.274330	-4.473159	6.680163	C	1.786173	-1.822307	9.289718
C	-5.311333	-3.556781	6.872482	N	2.996314	-1.249545	9.131531
H	-6.321297	-3.882829	7.078189	H	3.160608	-0.254833	9.291245
N	-4.918627	-2.316326	6.778204	H	3.778614	-1.883665	9.079121
C	-3.556631	-2.389239	6.521036	N	1.671505	-3.141309	9.201475
C	-2.553975	-1.374980	6.367012	C	0.410943	-3.563131	9.390101
O	-2.680612	-0.142357	6.401531	C	0.806133	-7.146558	10.133334
N	-1.279746	-1.944410	6.155162	H	-0.234221	-7.319593	10.417349
H	-0.503225	-1.272868	6.051894	H	1.388043	-6.983508	11.040677
C	-0.988164	-3.287976	6.122583	C	1.285428	-8.347418	9.325137
N	0.296141	-3.646041	5.935198	H	0.960328	-9.305763	9.730713

O	2.777099	-8.380986	9.217253	H	8.473459	-0.503059	14.570798
P	3.753932	-8.456878	10.504501	O	6.729631	-1.673404	14.655278
O	5.035441	-9.242498	9.912243	C	6.253907	-1.353015	16.024271
H	5.058510	-10.216010	9.956745	H	6.347202	-0.279013	16.196168
O	3.125992	-8.998043	11.735729	N	4.844430	-1.648834	16.143945
O	4.365478	-6.986301	10.680749	C	4.369987	-2.931007	16.140318
C	5.224217	-6.287685	9.693627	H	5.109993	-3.711578	16.019388
H	4.594845	-5.956763	8.864604	C	3.049660	-3.208628	16.275738
H	5.980277	-6.993693	9.339993	H	2.691839	-4.230213	16.269256
C	5.872405	-5.092646	10.364284	C	2.143981	-2.096543	16.415512
H	6.658502	-4.713442	9.700142	N	0.826738	-2.282043	16.559527
O	4.866205	-4.049481	10.560709	H	0.182634	-1.474741	16.599246
C	4.939888	-3.530210	11.947126	H	0.433600	-3.208999	16.581321
H	5.556395	-2.631885	11.965487	N	2.606390	-0.827454	16.394908
N	3.620791	-3.114758	12.368082	C	3.932949	-0.548901	16.257135
C	2.589993	-4.032471	12.496696	O	4.385148	0.627708	16.244339
H	2.863936	-5.056495	12.271097	C	7.230035	-2.161890	16.889335
C	1.333129	-3.692596	12.859263	H	6.994823	-3.229558	16.842613
C	0.208342	-4.668737	13.046032	H	7.228603	-1.867097	17.937055
H	0.549871	-5.700569	12.929194	C	8.573529	-1.937415	16.181445
H	-0.229744	-4.560629	14.044219	H	9.232322	-2.803992	16.235431
H	-0.602257	-4.476100	12.336571	O	9.300430	-0.744606	16.710079
C	1.035369	-2.271485	13.043090	P	10.112625	-0.881977	18.210171
O	-0.086050	-1.845239	13.324764	O	11.739623	-0.641615	17.696890
N	2.108194	-1.405938	12.876014	H	12.401003	-1.090862	18.264973
H	1.916255	-0.380881	13.010595	O	9.835720	-2.168825	19.083928
C	3.399851	-1.729985	12.536720	O	9.691992	0.579387	18.984745
O	4.288423	-0.900777	12.410061	C	9.832388	1.894219	18.312957
C	5.566103	-4.682144	12.748898	H	9.385690	1.842349	17.317781
H	4.803281	-5.394834	13.072742	H	10.898356	2.131442	18.241587
H	6.096720	-4.308396	13.626241	C	9.089771	2.915784	19.156875
C	6.491270	-5.382539	11.750682	H	9.358731	3.916864	18.800643
H	6.617921	-6.445321	11.959087	O	7.652785	2.729263	18.977443
O	7.847836	-4.761253	11.737045	C	6.985173	2.461915	20.264148
P	8.891821	-5.021411	12.951924	H	6.399042	3.335289	20.552998
O	10.288328	-4.588824	12.271874	N	6.043212	1.380215	20.098921
H	10.792600	-5.240737	11.753365	C	6.324250	0.043642	19.807920
O	8.804242	-6.366014	13.571628	H	7.334731	-0.310992	19.703235
O	8.665926	-3.812257	13.977595	N	5.232631	-0.697446	19.692233
C	8.814147	-2.382290	13.632794	C	4.177585	0.189920	19.929285
H	8.316680	-2.186619	12.679613	C	2.780752	-0.007104	19.999273
H	9.882110	-2.167544	13.544575	N	2.194966	-1.208974	19.855058
C	8.187727	-1.552059	14.726122	H	1.176711	-1.286415	19.811115

H	2.773551	-2.029631	19.776839	C	6.124316	5.035148	25.276334
N	2.007592	1.094623	20.245120	H	7.126440	5.185932	25.689290
C	2.592588	2.310951	20.416609	O	5.229256	6.105997	25.702223
H	1.913018	3.132919	20.599423	H	5.253731	6.204158	26.674714
N	3.908691	2.581661	20.401193	C	-7.525745	-3.796100	23.685365
C	4.658376	1.483676	20.160015	H	-7.391362	-4.234645	24.679498
C	8.122249	2.148075	21.256819	C	-6.810406	-2.455570	23.601728
H	8.302984	1.071183	21.300232	H	-7.237317	-1.735729	24.307724
H	7.868384	2.497430	22.259416	O	-5.391397	-2.670652	23.953989
C	9.361670	2.826238	20.671607	C	-4.557519	-1.828014	23.090767
H	10.288749	2.307399	20.920784	H	-4.423262	-0.830476	23.511074
O	9.491535	4.245819	21.121432	N	-3.227533	-2.434396	23.022617
P	9.972631	4.543525	22.749144	C	-3.081060	-3.795516	22.888117
O	10.444183	6.188974	22.625430	H	-4.000606	-4.362290	22.848246
H	11.409870	6.329641	22.532108	C	-1.851148	-4.373171	22.851065
O	11.024414	3.531057	23.358620	H	-1.742150	-5.444047	22.745460
O	8.512964	4.696341	23.610993	C	-0.699131	-3.517762	22.997570
C	7.416980	5.546758	23.079709	N	0.543720	-4.016034	23.016534
H	7.365280	5.436964	21.994097	H	1.366025	-3.394864	23.145260
H	7.638945	6.585761	23.337342	H	0.698490	-5.005729	22.908060
C	6.128832	5.102909	23.725647	N	-0.850800	-2.181711	23.138816
H	5.340175	5.812693	23.437990	C	-2.079859	-1.592589	23.127536
O	5.776306	3.763846	23.249630	O	-2.247365	-0.342474	23.197985
C	4.883234	3.203035	24.285159	C	-6.803026	-1.806957	22.193578
H	3.890550	3.654740	24.194427	H	-7.445053	-2.324133	21.478445
N	4.714458	1.793082	24.086234	C	-5.332631	-1.798283	21.764088
C	5.684913	0.774246	24.053123	H	-5.118111	-2.708926	21.192870
H	6.734943	0.982992	24.167518	H	-5.070630	-0.942773	21.142813
N	5.155898	-0.418372	23.855890	O	-7.338251	-0.426161	22.356385
C	3.775252	-0.197395	23.756171	P	-7.864270	0.447883	21.101497
C	2.685694	-1.098170	23.563056	O	-9.303401	0.985376	21.613247
O	2.724398	-2.353969	23.405655	H	-10.104130	0.677279	21.150708
N	1.441362	-0.432406	23.554786	O	-7.856203	-0.254642	19.793274
H	0.609738	-1.031418	23.386715	O	-6.973040	1.773091	21.156934
C	1.260380	0.934165	23.682741	C	-6.787979	2.615532	22.360002
N	0.000535	1.404097	23.619465	H	-6.540401	1.970104	23.205600
H	-0.808160	0.795073	23.467000	H	-7.725230	3.146540	22.549705
H	-0.117161	2.397872	23.499419	C	-5.648749	3.575708	22.090765
N	2.287037	1.781097	23.867636	H	-5.599650	4.299004	22.914666
C	3.491010	1.168337	23.888108	O	-4.414086	2.803788	22.035895
C	5.586178	3.624627	25.588093	C	-3.590355	3.245785	20.891256
H	6.415740	2.939711	25.789041	H	-2.863044	3.983049	21.230367
H	4.908553	3.617294	26.446016	N	-2.822383	2.114337	20.413519

C	-3.445592	1.024664	19.831607	H	3.300839	2.041309	16.647274
H	-4.513039	1.129589	19.681131	H	3.029477	3.753807	16.896135
C	-2.788344	-0.093284	19.452169	N	0.579701	3.782521	16.990717
C	-3.426812	-1.218756	18.692707	C	-0.731405	3.509265	16.911447
H	-4.509321	-1.084020	18.613069	C	-2.490047	6.799564	16.442903
H	-3.004204	-1.246600	17.682465	H	-3.509758	6.405831	16.418217
H	-3.215961	-2.184962	19.163004	H	-2.169570	6.981877	15.417401
C	-1.359514	-0.175198	19.742016	C	-2.493591	8.062765	17.307320
O	-0.683445	-1.193171	19.545403	H	-3.420044	8.628635	17.220640
N	-0.783670	0.975742	20.258989	O	-1.364520	8.982621	16.974088
H	0.272568	0.998824	20.342759	P	-1.268596	9.784437	15.573976
C	-1.435247	2.120576	20.650060	O	-0.725651	11.239581	16.026648
O	-0.860222	3.076360	21.160365	H	-1.372451	11.952086	16.186744
C	-4.600097	3.841464	19.893131	O	-2.496168	9.751492	14.741831
H	-4.979080	3.075642	19.212452	O	0.033126	9.191357	14.856090
H	-4.137839	4.629744	19.296421	C	1.396378	9.202465	15.431952
C	-5.752259	4.355044	20.759238	H	1.372599	8.702702	16.403196
H	-6.726031	4.255018	20.276631	H	1.704633	10.244943	15.551395
O	-5.569258	5.795297	21.127462	C	2.319336	8.457976	14.489323
P	-6.000807	6.980685	19.955347	H	3.356000	8.650335	14.788898
O	-6.035002	8.384917	20.941089	O	2.042943	7.022261	14.604086
H	-6.914153	8.624210	21.286734	C	1.881382	6.440889	13.254226
O	-7.279856	6.654924	19.084492	H	2.843592	6.046862	12.915173
O	-4.580944	7.283057	19.062518	N	0.981384	5.321409	13.306051
C	-3.338750	7.739218	19.730968	C	-0.405213	5.307216	13.370828
H	-3.159594	7.138655	20.626183	H	-0.978500	6.223034	13.401746
H	-3.463637	8.790247	20.004025	N	-0.916771	4.102129	13.382454
C	-2.207411	7.552541	18.743711	C	0.185486	3.262366	13.338266
H	-1.320423	8.072388	19.126918	C	0.311415	1.850262	13.301550
O	-1.927172	6.121063	18.625169	N	-0.731021	1.012522	13.328612
C	-1.574530	5.836754	17.210069	H	-0.580343	0.001688	13.360862
H	-0.513936	6.056966	17.056261	H	-1.651296	1.382320	13.505453
N	-1.754017	4.442085	16.945538	N	1.568857	1.348983	13.218163
C	-2.936339	3.718170	16.791930	C	2.625686	2.179361	13.186297
H	-3.899625	4.207001	16.771728	H	3.592081	1.686650	13.114865
N	-2.741902	2.434177	16.668528	N	2.621528	3.513062	13.227375
C	-1.365131	2.279484	16.741723	C	1.373136	3.991353	13.298138
C	-0.545400	1.108708	16.655568	C	1.399930	7.626721	12.406256
O	-0.913542	-0.071169	16.535630	H	0.331685	7.796568	12.561026
N	0.821464	1.426688	16.725234	H	1.578759	7.495855	11.338709
H	1.480326	0.624637	16.617640	C	2.145908	8.822065	12.997555
C	1.336920	2.694094	16.874271	H	1.629592	9.767226	12.832302
N	2.678930	2.809508	16.924831	O	3.523768	8.952446	12.441036

P	3.797232	9.297654	10.880967	H	4.552677	-1.105539	5.674361
O	5.170032	10.143384	10.951124	N	3.267231	0.472022	5.837313
H	5.131188	11.111051	11.065760	C	3.019516	1.803427	6.022623
O	2.648217	9.902726	10.164005	H	3.894878	2.438828	6.087558
O	4.323146	7.927174	10.241349	C	1.754267	2.275851	6.131094
C	5.451825	7.139062	10.782072	H	1.560014	3.332418	6.266771
H	5.292804	6.980135	11.851380	C	0.683432	1.309840	6.106600
H	6.371395	7.709313	10.623628	N	-0.589291	1.693537	6.239705
C	5.503408	5.811576	10.063050	H	-1.360202	0.995208	6.275085
H	6.419049	5.290376	10.367653	H	-0.803289	2.665818	6.387679
O	4.333999	5.019242	10.459415	N	0.931251	0.004953	5.957302
C	3.880241	4.279419	9.260965	C	2.192619	-0.472035	5.817598
H	4.493170	3.387594	9.127737	O	2.455457	-1.667839	5.656996
N	2.532674	3.798492	9.450750	C	5.465571	0.587376	4.603239
C	1.480880	4.654102	9.636728	H	5.219755	1.644804	4.467903
H	1.727126	5.709333	9.646960	H	5.316951	0.081988	3.650115
C	0.218446	4.194333	9.808409	C	6.902624	0.492468	5.108469
H	-0.608719	4.873675	9.969563	H	7.562773	1.235923	4.661155
C	0.029146	2.761533	9.804793	O	7.487508	-0.857145	4.855276
N	-1.184578	2.227840	9.941527	P	7.887865	-1.371867	3.373073
H	-1.306697	1.196453	9.957270	O	9.349032	-2.027649	3.598251
H	-1.977298	2.819416	10.133245	H	10.134643	-1.540518	3.287878
N	1.064705	1.927697	9.651945	O	7.774983	-0.347390	2.304853
C	2.331526	2.379579	9.508128	O	6.987996	-2.672838	3.143875
O	3.313962	1.640965	9.396281	C	6.919264	-3.836623	4.056552
C	4.109702	5.300645	8.140026	H	6.679565	-3.477354	5.059995
H	3.370353	6.105955	8.194300	H	7.896393	-4.328215	4.054179
H	4.084461	4.877083	7.135384	C	5.827096	-4.766815	3.569914
C	5.474891	5.881128	8.512732	H	5.867281	-5.685651	4.167684
H	5.649140	6.878004	8.108848	O	4.541475	-4.103549	3.777418
O	6.594104	4.999895	8.062998	C	3.715027	-4.230910	2.556469
P	6.869452	4.599276	6.519005	H	3.071081	-5.106304	2.643943
O	8.482779	4.559349	6.449019	N	2.831619	-3.092914	2.453138
H	8.964415	5.360972	6.171254	C	3.329743	-1.825043	2.226273
O	6.162903	5.436924	5.518860	H	4.410512	-1.759516	2.179297
O	6.527343	3.036986	6.424518	C	2.541706	-0.739924	2.060993
C	7.178538	1.961688	7.213436	C	3.055755	0.633745	1.739759
H	6.840494	2.043786	8.248571	H	4.140954	0.633093	1.605456
H	8.261369	2.103253	7.153681	H	2.595599	1.007374	0.819333
C	6.774569	0.615838	6.642349	H	2.795597	1.351065	2.526245
H	7.395178	-0.152932	7.117273	C	1.097620	-0.923115	2.181999
O	5.369786	0.358147	6.964594	O	0.288915	-0.001678	2.000346
C	4.629922	-0.020571	5.740084	N	0.670590	-2.194731	2.515371

H	-0.362592	-2.354254	2.618121	O	0.636970	-11.728442	-3.076968
C	1.448445	-3.325433	2.622261	H	1.296795	-12.416012	-2.875389
O	0.991441	-4.439516	2.819294	O	2.383953	-10.020185	-4.111044
C	4.746227	-4.374835	1.425626	O	-0.169024	-9.589250	-4.037470
H	5.120537	-3.398376	1.108827	C	-1.538004	-9.687091	-3.486592
H	4.332438	-4.884063	0.554007	H	-1.513350	-9.449781	-2.420205
C	5.895640	-5.147030	2.072413	H	-1.886386	-10.713337	-3.631176
H	6.861834	-4.946437	1.608667	C	-2.418309	-8.703292	-4.220906
O	5.660769	-6.620630	2.009566	H	-3.464835	-8.910781	-3.965347
P	5.705579	-7.410289	0.592860	O	-2.069560	-7.344323	-3.796022
O	6.022329	-8.920235	1.067333	C	-2.303451	-6.478049	-4.983472
H	6.946169	-9.191711	1.208191	H	-3.377310	-6.331202	-5.107478
O	6.598313	-6.798134	-0.421863	N	-1.753032	-5.164906	-4.758661
O	4.182700	-7.557352	0.120779	C	-0.407087	-4.927042	-4.735162
C	3.146172	-8.357096	0.812586	H	0.233815	-5.784128	-4.902405
H	3.015919	-7.966931	1.825038	C	0.091193	-3.686016	-4.515986
H	3.491338	-9.393136	0.852215	H	1.158890	-3.507928	-4.492718
C	1.846640	-8.248237	0.045821	C	-0.858639	-2.619301	-4.305280
H	1.163039	-9.021806	0.420151	N	-0.450524	-1.365963	-4.103151
O	1.270719	-6.926984	0.288459	H	-1.135014	-0.601612	-3.977111
C	0.508472	-6.533872	-0.909723	H	0.530883	-1.143129	-4.115510
H	-0.500492	-6.956688	-0.881155	N	-2.174870	-2.855734	-4.304548
N	0.356505	-5.102820	-0.905912	C	-2.676765	-4.099152	-4.494674
C	1.353877	-4.145588	-0.825919	O	-3.882862	-4.358219	-4.470158
H	2.397120	-4.427223	-0.823354	C	-1.720411	-7.334497	-6.112276
N	0.901045	-2.919229	-0.743712	H	-0.629135	-7.383373	-6.041599
C	-0.478380	-3.064408	-0.762580	H	-1.990564	-6.993592	-7.110257
C	-1.539632	-2.127730	-0.690782	C	-2.279028	-8.717969	-5.768336
N	-1.353957	-0.802527	-0.579548	H	-1.670077	-9.541217	-6.140280
H	-2.161949	-0.208148	-0.382536	O	-3.668122	-8.870802	-6.301493
H	-0.454255	-0.469760	-0.267141	P	-3.988217	-9.235543	-7.832289
N	-2.801775	-2.616179	-0.764613	O	-4.307485	-10.826456	-7.740285
C	-3.000171	-3.942132	-0.870878	H	-4.058596	-11.373598	-8.509680
H	-4.042484	-4.246240	-0.925490	O	-2.971065	-8.866460	-8.852595
N	-2.082442	-4.910384	-0.914512	O	-5.396963	-8.527120	-8.083469
C	-0.842865	-4.407954	-0.856646	C	-6.532523	-8.364590	-7.150576
C	1.346068	-7.113633	-2.064865	H	-6.143786	-8.233742	-6.138974
H	2.156156	-6.422201	-2.315371	H	-7.146977	-9.268210	-7.210335
H	0.740944	-7.289288	-2.955775	C	-7.311382	-7.133032	-7.568388
C	1.950593	-8.405048	-1.493281	H	-8.239750	-7.087671	-6.987964
H	2.967593	-8.581413	-1.842278	O	-6.498439	-5.953595	-7.259709
O	1.141630	-9.608178	-1.838604	C	-6.330869	-5.117721	-8.458959
P	1.131373	-10.215725	-3.342032	H	-7.025980	-4.276582	-8.407743

N	-4.999411	-4.556433	-8.454230	H	0.669763	4.374407	-5.081503
C	-3.791014	-5.235603	-8.500751	H	0.580763	2.818407	-4.221503
H	-3.744253	-6.295610	-8.710322	H	1.120763	2.868407	-5.916503
N	-2.749631	-4.465508	-8.295888	C	-1.409236	1.806407	-5.976503
C	-3.292067	-3.205649	-8.095307	O	-0.711236	0.791407	-5.919503
C	-2.705663	-1.947411	-7.825894	N	-2.724236	1.730407	-6.386503
N	-1.377597	-1.757310	-7.726703	H	-3.077236	0.806407	-6.634503
H	-1.010632	-0.859610	-7.396366	C	-3.610236	2.784407	-6.493503
H	-0.777259	-2.564567	-7.772984	O	-4.759236	2.618407	-6.867503
N	-3.538272	-0.891308	-7.677354	C	-4.084236	6.059407	-5.011503
C	-4.867584	-1.069679	-7.793987	H	-3.096236	6.330407	-4.638503
H	-5.460998	-0.167393	-7.664800	H	-4.734236	5.559407	-4.293503
N	-5.525615	-2.201821	-8.046511	C	-4.783236	7.304407	-5.556503
C	-4.684679	-3.235640	-8.178671	H	-4.484236	8.203407	-5.018503
C	-6.630395	-6.062355	-9.636654	O	-6.198236	7.147407	-5.552503
H	-5.728934	-6.611219	-9.920719	P	-6.996236	7.304407	-4.175503
H	-6.997604	-5.521400	-10.514072	O	-7.996236	8.386407	-4.300503
C	-7.668022	-7.039579	-9.067155	H	-7.939236	9.151407	-3.658503
H	-7.634985	-8.015772	-9.564862	O	-6.034236	7.433407	-3.057503
O	-9.020834	-6.491572	-9.102959	O	-7.741236	5.892407	-4.078503
H	-7.129173	-4.498950	22.943692	C	-8.777236	5.559407	-5.052503
H	-8.600303	-3.667454	23.505870	H	-8.324236	5.536407	-6.044503
H	-9.292624	-6.315584	-10.026407	H	-9.556236	6.320407	-5.023503
C	-3.201140	8.458790	-7.232658	C	-9.377236	4.203407	-4.741503
H	-2.861674	8.420774	-8.271527	H	-10.157236	3.975407	-5.467503
H	-3.642011	9.444957	-7.046169	O	-8.373236	3.145407	-4.912503
H	-2.325212	8.336350	-6.585921	C	-8.084236	2.563407	-3.650503
H	-9.588308	-0.003621	1.118850	H	-8.570236	1.587407	-3.646503
H	-8.034953	4.080139	-2.096307	N	-6.616236	2.387407	-3.469503

### 7. 3'-GACTGGATGT-5'

(optimized by GEBF-TPSS/6-31G\*\*)

C	-4.263236	7.377407	-6.991503	H	-5.897236	4.370407	-2.948503
H	-5.074590	7.552841	-7.666652	N	-4.447236	2.839407	-3.052503
O	-3.640236	6.078407	-7.280503	C	-4.606236	1.488407	-3.358503
C	-4.032236	5.179407	-6.255503	C	-3.643236	0.449407	-3.433503
H	-5.033236	4.826407	-6.506503	O	-2.432236	0.506407	-3.241503
N	-3.107236	4.016407	-6.152503	N	-4.237236	-0.773592	-3.776503
C	-1.813236	4.183407	-5.735503	H	-3.626236	-1.586592	-3.855503
H	-1.459236	5.181407	-5.475503	C	-5.583236	-0.966592	-4.016503
C	-0.971236	3.140407	-5.639503	N	-5.951236	-2.210592	-4.331503
C	0.446763	3.312407	-5.183503	H	-5.251236	-2.951592	-4.382503
				H	-6.931236	-2.420592	-4.520503
				N	-6.485236	0.010407	-3.946503
				C	-5.926236	1.203407	-3.614503

C	-8.728236	3.455407	-2.594503	H	-10.043236	-4.904592	0.363496
H	-9.040287	2.877299	-1.749923	H	-11.095236	-5.718592	1.549496
C	-9.936236	4.035407	-3.328503	C	-9.029236	-5.613592	2.110496
H	-10.227236	5.008407	-2.933503	H	-8.810236	-6.598592	1.698496
O	-11.035236	3.130407	-3.331503	O	-7.850236	-4.804592	1.797496
P	-11.839236	2.878407	-1.971503	C	-7.043236	-4.701592	2.960496
O	-13.277236	2.701407	-2.270503	H	-6.384236	-5.569592	2.961496
H	-13.925236	3.325407	-1.833503	N	-6.225236	-3.456592	2.945496
O	-11.503236	3.937407	-0.993503	C	-6.638236	-2.144592	3.010496
O	-11.216236	1.485407	-1.488503	H	-7.687236	-1.858592	3.084496
C	-11.465236	0.283407	-2.276503	N	-5.669236	-1.284592	2.974496
H	-11.100236	0.446407	-3.290503	C	-4.528236	-2.068592	2.878496
H	-12.537236	0.092407	-2.298503	C	-3.163236	-1.748592	2.802496
C	-10.747236	-0.903592	-1.666503	N	-2.695236	-0.491592	2.809496
H	-10.986236	-1.803592	-2.233503	H	-1.692236	-0.319592	2.751496
O	-9.292236	-0.742592	-1.804503	H	-3.344236	0.292407	2.873496
C	-8.693236	-1.209592	-0.606503	N	-2.291236	-2.770592	2.716496
H	-8.617236	-2.293592	-0.692503	C	-2.762236	-4.017592	2.710496
N	-7.335236	-0.630592	-0.408503	H	-2.008236	-4.800592	2.639496
C	-7.171236	0.707407	-0.166503	N	-4.006236	-4.435592	2.776496
H	-8.047236	1.354407	-0.119503	C	-4.859236	-3.392592	2.860496
C	-5.950236	1.238407	0.012496	C	-8.017236	-4.791592	4.130496
C	-5.758236	2.702407	0.277496	H	-8.456236	-3.825592	4.379496
H	-6.675236	3.238407	0.033496	H	-7.479236	-5.283592	4.939496
H	-5.519236	2.852407	1.330496	C	-9.124236	-5.720592	3.633496
H	-4.942236	3.079407	-0.338503	H	-10.108236	-5.376592	3.952496
C	-4.769236	0.409407	-0.044503	O	-8.889236	-7.063592	4.041496
O	-3.611236	0.805407	0.107496	P	-8.990236	-7.433592	5.595496
N	-5.027236	-0.923592	-0.292503	O	-9.572236	-8.785592	5.746496
H	-4.221236	-1.546592	-0.340503	H	-10.409236	-8.875592	6.286496
C	-6.270236	-1.495592	-0.480503	O	-9.680236	-6.342592	6.320496
O	-6.398236	-2.688592	-0.694503	O	-7.447236	-7.462592	6.014496
C	-9.696236	-0.844592	0.482496	C	-6.535236	-8.350592	5.302496
H	-9.554461	-1.455257	1.349611	H	-6.682236	-8.211592	4.231496
C	-11.035236	-1.153592	-0.185503	H	-6.760236	-9.382592	5.571496
H	-11.818236	-0.470592	0.146496	C	-5.097236	-8.033592	5.658496
O	-11.413236	-2.510592	0.016496	H	-4.428236	-8.648592	5.056496
P	-11.900236	-2.974592	1.468496	O	-4.771236	-6.638592	5.291496
O	-13.024236	-3.926592	1.334496	C	-3.986236	-6.106592	6.347496
H	-13.889236	-3.693592	1.779496	H	-2.970236	-6.477592	6.212496
O	-12.152236	-1.783592	2.311496	N	-3.975236	-4.616592	6.341496
O	-10.605236	-3.745592	2.004496	C	-5.027236	-3.737592	6.468496
C	-10.252236	-5.039592	1.424496	H	-6.060236	-4.061592	6.597496

N	-4.677236	-2.475592	6.420496	H	3.877763	-1.824592	9.116496
C	-3.294236	-2.521592	6.249496	N	1.703763	-3.132592	9.133496
C	-2.352236	-1.466592	6.128496	C	0.404763	-3.526592	9.195496
O	-2.547236	-0.254592	6.148496	C	0.856763	-7.002592	9.980496
N	-1.050236	-1.960592	5.969496	H	-0.131236	-7.197592	10.397496
H	-0.298236	-1.278592	5.873496	H	1.600763	-6.639592	10.688496
C	-0.703236	-3.296592	5.930496	C	1.377763	-8.264592	9.294496
N	0.595763	-3.560592	5.770496	H	1.054763	-9.170592	9.807496
H	1.264763	-2.796592	5.684496	O	2.793763	-8.233592	9.144496
H	0.918763	-4.527592	5.733496	P	3.718763	-8.468592	10.428496
N	-1.588236	-4.285592	6.043496	O	4.801763	-9.417592	10.093496
C	-2.856236	-3.823592	6.199496	H	4.872763	-10.254592	10.635496
C	-4.619236	-6.733592	7.585496	O	2.872763	-8.828592	11.589496
H	-5.610236	-6.339592	7.807496	O	4.332763	-7.007592	10.646496
H	-3.891236	-6.654592	8.392496	C	5.249763	-6.455592	9.649496
C	-4.733236	-8.189592	7.135496	H	4.678763	-6.166592	8.767496
H	-5.536236	-8.714592	7.653496	H	5.979763	-7.219592	9.379496
O	-3.494236	-8.878592	7.271496	C	5.965763	-5.242592	10.207496
P	-3.003236	-9.316592	8.729496	H	6.720763	-4.906592	9.496496
O	-2.878236	-10.788592	8.789496	O	5.031763	-4.114592	10.329496
H	-3.412236	-11.274592	9.481496	C	5.032763	-3.657592	11.673496
O	-3.872236	-8.693592	9.753496	H	5.706763	-2.801592	11.704496
O	-1.549236	-8.651592	8.785496	N	3.668763	-3.231592	12.092496
C	-0.557236	-9.019592	7.774496	C	2.655763	-4.144592	12.221496
H	-0.986236	-8.851592	6.786496	H	2.853763	-5.196592	12.013496
H	-0.307236	-10.073592	7.892496	C	1.421763	-3.769592	12.598496
C	0.693763	-8.177592	7.930496	C	0.305763	-4.760592	12.742496
H	1.409763	-8.443592	7.153496	H	0.705763	-5.771592	12.659496
O	0.384763	-6.755592	7.694496	H	-0.167236	-4.635592	13.716496
C	0.829763	-6.013592	8.819496	H	-0.430236	-4.595592	11.955496
H	1.843763	-5.684592	8.593496	C	1.126763	-2.384592	12.881496
N	-0.036236	-4.825592	9.058496	O	0.028763	-1.946592	13.232496
C	-1.405236	-4.757592	9.190496	N	2.203763	-1.535592	12.726496
H	-2.052236	-5.632592	9.129496	H	2.039763	-0.546592	12.915496
N	-1.862236	-3.546592	9.396496	C	3.479763	-1.893592	12.340496
C	-0.714236	-2.755592	9.401496	O	4.369763	-1.067592	12.230496
C	-0.570236	-1.354592	9.578496	C	5.607763	-4.788592	12.520496
O	-1.440236	-0.509592	9.771496	H	4.857763	-5.525592	12.804496
N	0.774763	-0.966592	9.511496	H	6.139763	-4.318592	13.348496
H	0.983763	0.024407	9.627496	C	6.617763	-5.437592	11.575496
C	1.840763	-1.819592	9.299496	H	6.727763	-6.504592	11.772496
N	3.048763	-1.251592	9.268496	O	7.874763	-4.771592	11.621496
H	3.141763	-0.243592	9.397496	P	8.842763	-5.019592	12.871496

O	10.251763	-4.868592	12.446496	N	6.125763	1.398407	19.929496
H	10.866763	-5.645592	12.583496	C	6.371763	0.063407	19.698496
O	8.492763	-6.302592	13.522496	H	7.377763	-0.352592	19.645496
O	8.437763	-3.804592	13.830496	N	5.299763	-0.651592	19.550496
C	8.834763	-2.448592	13.470496	C	4.265763	0.262407	19.690496
H	8.410763	-2.211592	12.494496	C	2.868763	0.126407	19.638496
H	9.922763	-2.394592	13.421496	N	2.245763	-1.039592	19.419496
C	8.321763	-1.459592	14.497496	H	1.226763	-1.077592	19.392496
H	8.686763	-0.461592	14.255496	H	2.790763	-1.890592	19.280496
O	6.853763	-1.359592	14.427496	N	2.131763	1.238407	19.819496
C	6.380763	-1.286592	15.762496	C	2.755763	2.395407	20.036496
H	6.538763	-0.264592	16.105496	H	2.105763	3.258407	20.175496
N	4.932763	-1.624592	15.862496	N	4.044763	2.642407	20.106496
C	4.498763	-2.903592	15.702496	C	4.760763	1.513407	19.921496
H	5.220763	-3.694592	15.499496	C	8.206763	2.158407	21.130496
C	3.179763	-3.211592	15.793496	H	8.425763	1.091407	21.147496
H	2.823763	-4.233592	15.667496	H	7.915763	2.592407	22.087496
C	2.278763	-2.130592	16.063496	C	9.426763	2.905407	20.594496
N	0.978763	-2.358592	16.164496	H	10.350763	2.357407	20.783496
H	0.338763	-1.587592	16.356496	O	9.495763	4.228407	21.116496
H	0.616763	-3.305592	16.050496	P	9.894763	4.440407	22.651496
N	2.717763	-0.875592	16.218496	O	10.562763	5.749407	22.814496
C	4.041763	-0.587592	16.123496	H	11.485763	5.757407	23.198496
O	4.483763	0.559407	16.261496	O	10.645763	3.260407	23.136496
C	7.310763	-2.241592	16.502496	O	8.454763	4.481407	23.348496
H	7.145763	-3.288592	16.248496	C	7.492763	5.501407	22.942496
H	7.242763	-2.000592	17.563496	H	7.455763	5.535407	21.853496
C	8.659763	-1.781592	15.953496	H	7.816763	6.468407	23.328496
H	9.403763	-2.578592	15.983496	C	6.117763	5.169407	23.485496
O	9.125763	-0.614592	16.622496	H	5.405763	5.929407	23.161496
P	9.923763	-0.773592	18.000496	O	5.628763	3.917407	22.898496
O	11.377763	-0.706592	17.742496	C	4.772763	3.319407	23.859496
H	11.937763	-1.485592	18.024496	H	3.817763	3.840407	23.799496
O	9.443763	-1.977592	18.715496	N	4.565763	1.870407	23.586496
O	9.456763	0.538407	18.788496	C	5.497763	0.860407	23.489496
C	9.831763	1.853407	18.279496	H	6.567763	1.026407	23.613496
H	9.514763	1.927407	17.239496	N	4.982763	-0.318592	23.236496
H	10.914763	1.963407	18.341496	C	3.612763	-0.071592	23.159496
C	9.161763	2.944407	19.090496	C	2.537763	-0.962592	22.908496
H	9.452763	3.919407	18.699496	O	2.571763	-2.171592	22.698496
O	7.706763	2.884407	18.920496	N	1.305763	-0.291592	22.918496
C	7.095763	2.508407	20.144496	H	0.467763	-0.847592	22.746496
H	6.564763	3.391407	20.500496	C	1.136763	1.059407	23.141496

N	-0.121236	1.506407	23.110496	H	-6.591236	2.059407	23.204496
H	-0.888236	0.858407	22.928496	H	-7.765236	3.143407	22.414496
H	-0.316236	2.495407	23.267496	C	-5.710236	3.652407	22.077496
N	2.146763	1.894407	23.377496	H	-5.672236	4.339407	22.922496
C	3.348763	1.260407	23.371496	O	-4.414236	2.992407	22.079496
C	5.444763	3.617407	25.196496	C	-3.727236	3.328407	20.883496
H	6.254763	2.922407	25.420496	H	-3.055236	4.147407	21.138496
H	4.648763	3.663407	25.938496	N	-2.933236	2.170407	20.385496
C	6.030763	5.015407	25.003496	C	-3.553236	1.041407	19.919496
H	7.032763	5.089407	25.425496	H	-4.641236	0.992407	19.914496
O	5.169763	6.008407	25.541496	C	-2.844236	-0.007592	19.468496
H	5.061763	5.978407	26.494496	C	-3.512236	-1.247592	18.956496
C	-7.323236	-3.822592	23.606496	H	-4.587236	-1.081592	18.892496
H	-6.540531	-4.434894	24.003181	H	-3.123236	-1.488592	17.966496
C	-6.867236	-2.377592	23.574496	H	-3.312236	-2.075592	19.636496
H	-7.391236	-1.813592	24.346496	C	-1.400236	0.026407	19.462496
O	-5.454236	-2.288592	23.939496	O	-0.668236	-0.884592	19.068496
C	-4.730236	-1.674592	22.885496	N	-0.861236	1.199407	19.948496
H	-4.587236	-0.633592	23.175496	H	0.156763	1.267407	19.962496
N	-3.403236	-2.324592	22.697496	C	-1.564236	2.291407	20.417496
C	-3.292236	-3.675592	22.591496	O	-0.997236	3.289407	20.828496
H	-4.188236	-4.293592	22.645496	C	-4.773236	3.822407	19.888496
C	-2.082236	-4.266592	22.421496	H	-5.228236	3.011407	19.321496
H	-1.985236	-5.349592	22.335496	H	-4.292236	4.598407	19.293496
C	-0.941236	-3.402592	22.358496	C	-5.832236	4.461407	20.785496
N	0.269763	-3.912592	22.193496	H	-6.835236	4.337407	20.377496
H	1.080763	-3.296592	22.149496	O	-5.542236	5.832407	21.035496
H	0.390763	-4.921592	22.110496	P	-5.863236	6.915407	19.902496
N	-1.062236	-2.074592	22.463496	O	-6.174236	8.216407	20.532496
C	-2.281236	-1.501592	22.634496	H	-7.062236	8.630407	20.334496
O	-2.432236	-0.277592	22.735496	O	-6.888236	6.377407	18.979496
C	-7.039236	-1.666592	22.232496	O	-4.457236	7.007407	19.145496
H	-7.758236	-2.213592	21.622496	C	-3.310236	7.576407	19.840496
C	-5.627236	-1.741592	21.653496	H	-3.104236	6.976407	20.726496
H	-5.517236	-2.678592	21.107496	H	-3.545236	8.598407	20.136496
H	-5.429236	-0.837592	21.077496	C	-2.095236	7.573407	18.935496
O	-7.451236	-0.319592	22.433496	H	-1.287236	8.130407	19.409496
P	-7.957236	0.536407	21.180496	O	-1.578236	6.209407	18.782496
O	-9.304236	1.078407	21.459496	C	-1.420236	5.940407	17.398496
H	-10.043236	0.838407	20.829496	H	-0.406236	6.241407	17.136496
O	-7.822236	-0.268592	19.944496	N	-1.599236	4.490407	17.105496
O	-6.891236	1.729407	21.161496	C	-2.762236	3.777407	16.916496
C	-6.809236	2.632407	22.303496	H	-3.752236	4.232407	16.964496

N	-2.574236	2.503407	16.672496	N	2.670763	3.534407	13.331496
C	-1.187236	2.362407	16.702496	C	1.398763	3.973407	13.438496
C	-0.382236	1.210407	16.509496	C	1.354763	7.622407	12.640496
O	-0.731236	0.058407	16.267496	H	0.299763	7.839407	12.805496
N	0.981763	1.514407	16.626496	H	1.630763	7.391407	11.611496
H	1.645763	0.749407	16.503496	C	2.198763	8.792407	13.143496
C	1.498763	2.766407	16.894496	H	1.710763	9.753407	12.977496
N	2.829763	2.848407	16.966496	O	3.509763	8.777407	12.589496
H	3.399763	2.014407	16.825496	P	3.711763	9.185407	11.055496
H	3.275763	3.744407	17.161496	O	4.825763	10.151407	10.940496
N	0.741763	3.846407	17.076496	H	4.631763	11.040407	10.526496
C	-0.583236	3.569407	16.965496	O	2.415763	9.614407	10.481496
C	-2.424236	6.844407	16.692496	O	4.145763	7.786407	10.410496
H	-3.444236	6.463407	16.733496	C	5.411763	7.184407	10.810496
H	-2.034236	7.032407	15.691496	H	5.446763	7.137407	11.898496
C	-2.324236	8.121407	17.526496	H	6.230763	7.802407	10.443496
H	-3.252236	8.691407	17.507496	C	5.532763	5.785407	10.240496
O	-1.218236	8.921407	17.122496	H	6.435763	5.312407	10.626496
P	-1.316236	9.756407	15.761496	O	4.425763	4.941407	10.715496
O	-1.085236	11.190407	16.041496	C	3.931763	4.215407	9.601496
H	-1.804236	11.837407	15.787496	H	4.571763	3.340407	9.484496
O	-2.581236	9.425407	15.067496	N	2.523763	3.776407	9.809496
O	-0.081236	9.163407	14.936496	C	1.537763	4.678407	10.064496
C	1.263763	9.273407	15.491496	H	1.781763	5.739407	10.116496
H	1.262763	8.873407	16.505496	C	0.254763	4.277407	10.254496
H	1.554763	10.323407	15.511496	H	-0.540236	4.994407	10.458496
C	2.242763	8.489407	14.641496	C	-0.004236	2.870407	10.172496
H	3.255763	8.652407	15.008496	N	-1.233236	2.410407	10.347496
O	2.008763	7.037407	14.801496	H	-1.415236	1.408407	10.289496
C	1.870763	6.476407	13.504496	H	-1.997236	3.057407	10.540496
H	2.869763	6.188407	13.179496	N	0.973763	1.992407	9.921496
N	0.986763	5.277407	13.518496	C	2.251763	2.412407	9.734496
C	-0.385236	5.211407	13.612496	O	3.180763	1.630407	9.500496
H	-1.016236	6.096407	13.691496	C	4.127763	5.165407	8.424496
N	-0.857236	4.003407	13.597496	H	3.417763	5.992407	8.418496
C	0.271763	3.204407	13.486496	H	4.144763	4.555407	7.520496
C	0.443763	1.812407	13.419496	C	5.530763	5.693407	8.714496
N	-0.572236	0.938407	13.455496	H	5.685763	6.687407	8.292496
H	-0.386236	-0.063592	13.402496	O	6.532763	4.783407	8.272496
H	-1.531236	1.275407	13.536496	P	6.859763	4.683407	6.709496
N	1.702763	1.348407	13.312496	O	8.290763	4.977407	6.480496
C	2.708763	2.221407	13.277496	H	8.519763	5.733407	5.866496
H	3.703763	1.785407	13.190496	O	5.895763	5.510407	5.947496

O	6.576763	3.134407	6.426496	C	2.469763	-0.802592	2.421496
C	7.405763	2.123407	7.081496	C	2.993763	0.595407	2.288496
H	7.335763	2.252407	8.161496	H	4.070763	0.566407	2.122496
H	8.439763	2.256407	6.762496	H	2.509763	1.086407	1.444496
C	6.931763	0.733407	6.707496	H	2.781763	1.151407	3.202496
H	7.520763	-0.008592	7.246496	C	1.036763	-0.982592	2.440496
O	5.560763	0.529407	7.166496	O	0.204763	-0.076592	2.356496
C	4.774763	0.096407	6.067496	N	0.634763	-2.296592	2.565496
H	4.767763	-0.993592	6.105496	H	-0.370236	-2.469592	2.583496
N	3.378763	0.605407	6.174496	C	1.459763	-3.399592	2.668496
C	3.127763	1.898407	6.514496	O	1.008763	-4.526592	2.775496
H	3.960763	2.572407	6.711496	C	4.788763	-4.346592	1.652496
C	1.855763	2.362407	6.611496	H	5.211763	-3.368592	1.425496
H	1.646763	3.396407	6.883496	H	4.344763	-4.873592	0.808496
C	0.802763	1.428407	6.339496	C	5.859763	-5.226592	2.295496
N	-0.461236	1.813407	6.416496	H	6.853763	-5.011592	1.901496
H	-1.209236	1.147407	6.222496	O	5.543763	-6.609592	2.173496
H	-0.687236	2.775407	6.668496	P	5.644763	-7.307592	0.736496
N	1.061763	0.158407	6.006496	O	6.164763	-8.683592	0.888496
C	2.341763	-0.286592	5.914496	H	7.001763	-8.923592	0.396496
O	2.618763	-1.452592	5.608496	O	6.392763	-6.427592	-0.190503
C	5.502763	0.558407	4.809496	O	4.106763	-7.358592	0.301496
H	5.299763	1.599407	4.561496	C	3.187763	-8.241592	1.020496
H	5.268763	-0.163592	4.027496	H	3.003763	-7.827592	2.011496
C	6.968763	0.410407	5.213496	H	3.645763	-9.225592	1.112496
H	7.603763	1.135407	4.703496	C	1.875763	-8.357592	0.271496
O	7.433763	-0.918592	5.007496	H	1.285763	-9.171592	0.694496
P	7.790763	-1.398592	3.523496	O	1.061763	-7.151592	0.483496
O	9.168763	-1.933592	3.491496	C	0.603763	-6.671592	-0.771503
H	9.820763	-1.506592	2.864496	H	-0.370236	-7.130592	-0.943503
O	7.493763	-0.308592	2.565496	N	0.459763	-5.188592	-0.765503
O	6.745763	-2.591592	3.317496	C	1.435763	-4.221592	-0.858503
C	6.816763	-3.762592	4.184496	H	2.495763	-4.458592	-0.953503
H	6.616763	-3.452592	5.210496	N	0.980763	-3.008592	-0.822503
H	7.814763	-4.194592	4.120496	C	-0.392236	-3.169592	-0.697503
C	5.787763	-4.791592	3.758496	C	-1.448236	-2.249592	-0.605503
H	5.865763	-5.670592	4.398496	N	-1.277236	-0.919592	-0.627503
O	4.432763	-4.277592	3.982496	H	-2.084236	-0.299592	-0.556503
C	3.729763	-4.297592	2.749496	H	-0.339236	-0.528592	-0.713503
H	3.151763	-5.221592	2.740496	N	-2.694236	-2.746592	-0.490503
N	2.807763	-3.133592	2.641496	C	-2.859236	-4.068592	-0.469503
C	3.294763	-1.858592	2.520496	H	-3.890236	-4.409592	-0.374503
H	4.372763	-1.697592	2.503496	N	-1.954236	-5.018592	-0.546503



O	-3.711614	5.794383	-7.090863	N	-4.076821	-0.692486	-3.339287
C	-3.991101	4.961828	-5.918287	H	-3.432043	-1.497023	-3.412612
H	-4.991826	4.530989	-5.988939	C	-5.421138	-0.942450	-3.428639
N	-3.068382	3.856357	-5.902948	N	-5.798871	-2.222246	-3.537012
C	-1.723472	4.065214	-5.689775	H	-5.144289	-2.984168	-3.719715
H	-1.426840	5.106991	-5.633735	H	-6.788059	-2.378137	-3.640706
C	-0.822894	3.072693	-5.579958	N	-6.340259	0.006431	-3.392902
C	0.635291	3.276171	-5.316563	C	-5.798747	1.228552	-3.295194
H	0.872301	4.336979	-5.209071	C	-8.572097	3.479986	-2.351665
H	0.923664	2.755321	-4.399310	H	-8.875253	3.015975	-1.411478
H	1.239251	2.856770	-6.126219	C	-9.748283	4.070127	-3.122331
C	-1.299894	1.702259	-5.743326	H	-10.032606	5.065193	-2.776426
O	-0.560806	0.721801	-5.684710	O	-10.935157	3.197300	-3.045443
N	-2.642157	1.573498	-6.025955	P	-11.576478	2.777745	-1.635392
H	-3.009690	0.602294	-6.155455	O	-13.081545	2.425281	-2.044974
C	-3.585244	2.569818	-6.090503	H	-13.761915	3.115008	-2.113397
O	-4.763509	2.350491	-6.298139	O	-11.364358	3.754256	-0.554475
C	-3.881781	5.955589	-4.759440	O	-11.006601	1.320758	-1.338189
H	-2.833694	6.190424	-4.549783	C	-11.247270	0.179169	-2.231009
H	-4.326469	5.609583	-3.829066	H	-10.756368	0.370650	-3.188587
C	-4.549686	7.191283	-5.347315	H	-12.326659	0.078411	-2.371018
H	-4.293867	8.119119	-4.832617	C	-10.667382	-1.048683	-1.577612
O	-6.021790	7.047529	-5.334826	H	-11.033390	-1.941505	-2.095450
P	-6.887766	7.079700	-3.991533	O	-9.221426	-0.983504	-1.673481
O	-8.037120	8.156915	-4.288708	C	-8.636309	-1.374117	-0.385538
H	-7.973234	9.063956	-3.946671	H	-8.493529	-2.456686	-0.348590
O	-6.103762	7.273750	-2.758251	N	-7.333975	-0.780543	-0.266647
O	-7.723136	5.734121	-4.025012	C	-7.199855	0.594209	-0.187861
C	-8.658477	5.304605	-5.064171	H	-8.133246	1.145546	-0.247162
H	-8.101512	5.123816	-5.986077	C	-6.014944	1.213211	-0.048524
H	-9.400019	6.095600	-5.207306	C	-5.826349	2.687910	0.114264
C	-9.297504	4.019452	-4.585608	H	-6.772864	3.223190	0.006246
H	-10.145185	3.774524	-5.230855	H	-5.417496	2.907631	1.105397
O	-8.339469	2.936580	-4.662351	H	-5.107301	3.061874	-0.619540
C	-7.947075	2.475484	-3.331008	C	-4.813945	0.380427	-0.070664
H	-8.320563	1.455985	-3.193957	O	-3.679625	0.828365	0.086582
N	-6.516321	2.395364	-3.236096	N	-5.017647	-0.958619	-0.315078
C	-5.586417	3.416713	-3.170797	H	-4.167476	-1.565976	-0.353136
H	-5.904992	4.447860	-3.098730	C	-6.217264	-1.622120	-0.341858
N	-4.356159	2.988897	-3.143058	O	-6.301174	-2.833831	-0.411807
C	-4.465927	1.610036	-3.211586	C	-9.680528	-0.897963	0.629286
C	-3.478932	0.567158	-3.213997	H	-9.600962	-1.407844	1.590734
O	-2.253316	0.662391	-3.129406	C	-11.003675	-1.169194	-0.078820

H	-11.801502	-0.500032	0.245014	C	-5.208917	-7.976535	5.586502
O	-11.450980	-2.558258	0.132882	H	-4.480534	-8.635135	5.101683
P	-11.832193	-3.059649	1.613559	O	-4.991865	-6.603785	5.159520
O	-12.871631	-4.238876	1.317761	C	-4.167351	-5.969258	6.196648
H	-13.822453	-4.058739	1.231771	H	-3.127703	-6.297222	6.085457
O	-12.253596	-1.980800	2.521206	N	-4.152979	-4.554505	6.060023
O	-10.568986	-3.893251	2.097402	C	-5.181373	-3.625527	6.150031
C	-10.113996	-5.118903	1.438071	H	-6.208539	-3.934647	6.280610
H	-9.899714	-4.900798	0.388711	N	-4.762612	-2.397905	6.078406
H	-10.909513	-5.863732	1.514796	C	-3.390832	-2.502221	5.950073
C	-8.866487	-5.586855	2.138207	C	-2.357907	-1.508084	5.985758
H	-8.633392	-6.608396	1.810633	O	-2.468149	-0.287338	6.096472
O	-7.786124	-4.693384	1.795151	N	-1.087153	-2.095264	5.907424
C	-6.812544	-4.723296	2.882979	H	-0.298836	-1.435828	6.003804
H	-6.113146	-5.558119	2.767262	C	-0.815470	-3.439722	5.895386
N	-6.042771	-3.516893	2.824366	N	0.475913	-3.801233	5.917104
C	-6.531158	-2.229175	2.761725	H	1.233173	-3.121817	5.875663
H	-7.597535	-2.046724	2.756773	H	0.668934	-4.788730	6.011990
N	-5.599830	-1.320584	2.683831	N	-1.759940	-4.366569	5.890740
C	-4.426927	-2.047377	2.698475	C	-2.990791	-3.830113	5.937793
C	-3.069863	-1.656899	2.691314	C	-4.793406	-6.528876	7.473951
N	-2.681373	-0.381750	2.671577	H	-5.787093	-6.091867	7.614167
H	-1.692449	-0.148732	2.619677	H	-4.205669	-6.360100	8.376970
H	-3.373628	0.337747	2.536480	C	-4.951828	-7.999994	7.111529
N	-2.143135	-2.637654	2.724418	H	-5.724738	-8.515147	7.681965
C	-2.530678	-3.926343	2.758569	O	-3.680818	-8.739323	7.267522
H	-1.713165	-4.644784	2.773736	P	-2.864234	-8.878924	8.635281
N	-3.767312	-4.402543	2.791607	O	-2.394666	-10.413078	8.631223
C	-4.671126	-3.412976	2.767573	H	-2.926492	-11.092461	9.078994
C	-7.682257	-4.869924	4.145391	O	-3.564684	-8.402480	9.839301
H	-7.940052	-3.878487	4.527163	O	-1.479052	-8.156885	8.347563
H	-7.145482	-5.420066	4.921747	C	-0.523342	-8.506660	7.295843
C	-8.952348	-5.589968	3.677659	H	-0.861835	-8.057103	6.360438
H	-9.858592	-5.110766	4.048994	H	-0.480349	-9.596555	7.210804
O	-9.001183	-7.005321	4.082206	C	0.828200	-7.942251	7.681311
P	-9.061435	-7.429391	5.629169	H	1.592307	-8.349548	7.014020
O	-9.558213	-8.946035	5.528115	O	0.819415	-6.494895	7.540084
H	-10.504119	-9.165122	5.565855	C	0.960852	-5.852957	8.852461
O	-9.813184	-6.520255	6.507776	H	1.976844	-5.458635	8.937686
O	-7.533722	-7.638639	6.031906	N	0.090617	-4.730292	8.964960
C	-6.599634	-8.384790	5.190427	C	-1.294669	-4.671540	9.016119
H	-6.781405	-8.138363	4.140824	H	-1.888998	-5.567929	8.892784
H	-6.765012	-9.452240	5.357344	N	-1.740032	-3.464124	9.204599

C	-0.603232	-2.676790	9.278142	O	4.101114	-0.817210	12.757956
C	-0.420786	-1.279216	9.549070	C	5.328087	-4.586996	12.577973
O	-1.271300	-0.417712	9.759726	H	4.518004	-5.277152	12.827684
N	0.945578	-0.947147	9.582741	H	5.874127	-4.327598	13.488222
H	1.140612	0.039880	9.808900	C	6.239127	-5.238576	11.538959
C	1.996358	-1.802986	9.366363	H	6.303097	-6.324068	11.644727
N	3.237145	-1.287808	9.403895	O	7.603229	-4.686765	11.619340
H	3.410888	-0.312521	9.639774	P	8.549316	-5.042227	12.873280
H	3.989288	-1.965405	9.429525	O	10.001814	-4.733746	12.287805
N	1.836594	-3.091956	9.126160	H	10.522751	-5.406542	11.818230
C	0.540332	-3.443939	9.115092	O	8.299145	-6.368596	13.460092
C	0.697658	-6.965940	9.867540	O	8.370703	-3.819915	13.876481
H	-0.372524	-7.069244	10.056169	C	8.659860	-2.437984	13.481971
H	1.201774	-6.793533	10.818521	H	8.202556	-2.239393	12.508571
C	1.207219	-8.202996	9.144893	H	9.744142	-2.321584	13.416836
H	0.829945	-9.145546	9.544169	C	8.072853	-1.528664	14.524079
O	2.687440	-8.243842	9.168440	H	8.430592	-0.505371	14.359612
P	3.546420	-8.016258	10.505611	O	6.628068	-1.571453	14.410660
O	4.942613	-8.695226	10.124344	C	6.116148	-1.293601	15.758524
H	5.086244	-9.651412	10.218958	H	6.224542	-0.232130	15.991873
O	2.885873	-8.449160	11.749184	N	4.707610	-1.582397	15.796308
O	3.965956	-6.477873	10.504307	C	4.247482	-2.842893	15.573224
C	4.831286	-5.840754	9.498553	H	5.006769	-3.591060	15.380434
H	4.190276	-5.369877	8.750427	C	2.928669	-3.137810	15.598151
H	5.465463	-6.609492	9.049054	H	2.568725	-4.142464	15.420286
C	5.672898	-4.787631	10.186023	C	2.021415	-2.055011	15.881565
H	6.495453	-4.499554	9.524751	N	0.712932	-2.272930	16.000864
O	4.863226	-3.616048	10.454402	H	0.062738	-1.494513	16.196809
C	4.795158	-3.321012	11.890400	H	0.327295	-3.191248	15.854377
H	5.409699	-2.446571	12.109715	N	2.474414	-0.799663	16.025283
N	3.441100	-2.959361	12.233101	C	3.802664	-0.507406	15.974530
C	2.407032	-3.875110	12.128012	O	4.248039	0.656524	16.100444
H	2.706524	-4.857719	11.770108	C	7.028996	-2.165583	16.624076
C	1.128940	-3.579662	12.438947	H	6.780334	-3.223327	16.494576
C	-0.017982	-4.541153	12.402296	H	6.977977	-1.931893	17.687601
H	0.327520	-5.569578	12.290224	C	8.395646	-1.916737	15.987088
H	-0.589873	-4.467604	13.332042	H	9.070432	-2.770886	16.066986
H	-0.715369	-4.295335	11.593717	O	9.046754	-0.721230	16.559728
C	0.815454	-2.197999	12.808137	P	9.803317	-0.861748	18.058909
O	-0.315064	-1.810818	13.077775	O	11.432574	-0.707407	17.625136
N	1.891695	-1.335765	12.852219	H	12.073072	-1.208858	18.166128
H	1.696758	-0.334312	13.138068	O	9.435618	-2.120127	18.918234
C	3.205309	-1.631839	12.618997	O	9.435605	0.620701	18.756568

C	9.689825	1.885868	18.052707	H	6.677578	1.021030	23.086018
H	9.224167	1.849161	17.065489	N	5.082950	-0.304511	22.605893
H	10.771611	2.020643	17.968005	C	3.707336	-0.065359	22.586133
C	9.051836	2.972417	18.890296	C	2.602124	-0.935205	22.359103
H	9.425323	3.948480	18.568061	O	2.631566	-2.162516	22.080972
O	7.617320	2.944217	18.704918	N	1.373647	-0.275766	22.489128
C	6.915665	2.581487	19.933275	H	0.529364	-0.868424	22.339433
H	6.323941	3.430279	20.281813	C	1.212536	1.058892	22.800220
N	5.979832	1.524373	19.650772	N	-0.038637	1.531591	22.879272
C	6.267106	0.236786	19.218167	H	-0.859485	0.951498	22.689738
H	7.282604	-0.099556	19.102780	H	-0.145510	2.531396	22.936249
N	5.184214	-0.483524	19.000483	N	2.246200	1.873471	23.033734
C	4.128265	0.369271	19.315520	C	3.443264	1.263848	22.909578
C	2.736466	0.158138	19.389225	C	5.585040	3.421834	24.868297
N	2.160385	-1.032146	19.177326	H	6.471680	2.781086	24.895325
H	1.146273	-1.145522	19.256202	H	4.958704	3.212062	25.737766
H	2.750783	-1.842498	19.076339	C	6.002838	4.891640	24.774101
N	1.973057	1.225314	19.741290	H	6.949484	5.090736	25.284612
C	2.541697	2.422752	20.029089	O	4.964181	5.787527	25.233288
H	1.849659	3.215514	20.283707	H	4.842700	5.725168	26.198075
N	3.851834	2.688585	20.053226	C	-7.079894	-3.808850	23.467293
C	4.601620	1.623073	19.698970	H	-6.742984	-4.207158	24.425658
C	8.013911	2.174808	20.931913	C	-6.661967	-2.354627	23.345327
H	8.119502	1.087546	20.962018	H	-7.185839	-1.723997	24.067523
H	7.765985	2.541211	21.931347	O	-5.224746	-2.264887	23.613773
C	9.300049	2.792319	20.391314	C	-4.540322	-1.597536	22.517560
H	10.183998	2.193115	20.618791	H	-4.366093	-0.543069	22.737969
O	9.510061	4.153197	20.919286	N	-3.230791	-2.214561	22.368262
P	9.896968	4.307547	22.564059	C	-3.118483	-3.580579	22.316709
O	10.487581	5.888263	22.595988	H	-4.047220	-4.129033	22.408995
H	11.450243	6.011543	22.510314	C	-1.914103	-4.184750	22.193118
O	10.810936	3.171587	23.144532	H	-1.825853	-5.260654	22.149498
O	8.411364	4.530478	23.312638	C	-0.745618	-3.337787	22.161963
C	7.475577	5.524478	22.764572	N	0.480153	-3.851850	22.057896
H	7.516962	5.500771	21.671881	H	1.307219	-3.224416	22.036749
H	7.770536	6.509969	23.131662	H	0.615644	-4.847514	21.996388
C	6.107587	5.142380	23.251090	N	-0.868115	-2.005967	22.265890
H	5.390928	5.933477	23.000809	C	-2.081016	-1.395090	22.336548
O	5.720037	3.901032	22.598927	O	-2.218264	-0.149053	22.378178
C	4.849548	3.204483	23.542292	C	-6.857287	-1.777362	21.934570
H	3.858041	3.668913	23.546311	H	-7.600104	-2.320084	21.346764
N	4.670347	1.844594	23.145824	C	-5.464179	-1.806903	21.317106
C	5.625761	0.843201	22.947711	H	-5.283303	-2.791029	20.869882

H	-5.320771	-1.059475	20.537226	C	-2.220675	7.414377	18.775862
O	-7.329856	-0.394184	22.102147	H	-1.311440	7.907802	19.133822
P	-7.612507	0.553131	20.834003	O	-1.997254	5.984366	18.657582
O	-8.971249	1.298257	21.229590	C	-1.723952	5.688220	17.244666
H	-9.828793	1.007655	20.878151	H	-0.673998	5.913872	17.025367
O	-7.582415	-0.147541	19.537997	N	-1.912611	4.297165	17.004346
O	-6.559747	1.728385	20.995056	C	-3.081764	3.585682	16.777151
C	-6.408915	2.498719	22.236749	H	-4.041231	4.080244	16.715212
H	-6.067529	1.825509	23.025479	N	-2.884173	2.309161	16.634437
H	-7.379790	2.932033	22.493763	C	-1.515645	2.155859	16.768451
C	-5.380987	3.566684	21.965592	C	-0.686003	0.996674	16.646213
H	-5.349003	4.267796	22.805906	O	-1.055366	-0.169153	16.470817
O	-4.096317	2.930333	21.804418	N	0.669421	1.319181	16.717375
C	-3.453784	3.347292	20.554127	H	1.342064	0.541543	16.518551
H	-2.707659	4.113950	20.763516	C	1.173918	2.587891	16.885194
N	-2.737949	2.215449	20.018297	N	2.508263	2.714523	16.873761
C	-3.415753	1.091780	19.580574	H	3.138586	1.959493	16.578381
H	-4.493919	1.200124	19.505348	H	2.853615	3.661142	16.892046
C	-2.794584	-0.051612	19.240553	N	0.415964	3.661375	17.059706
C	-3.461274	-1.233813	18.611823	C	-0.891133	3.376255	16.978670
H	-4.529682	-1.056168	18.462044	C	-2.684974	6.638081	16.532698
H	-2.994717	-1.410769	17.638259	H	-3.711896	6.281438	16.652828
H	-3.318838	-2.138183	19.215805	H	-2.483943	6.778802	15.471278
C	-1.349980	-0.130219	19.444226	C	-2.543464	7.917672	17.351673
O	-0.709023	-1.169808	19.285110	H	-3.428302	8.551901	17.306271
N	-0.730335	1.039915	19.820291	O	-1.372341	8.711819	16.933408
H	0.341634	1.079398	19.840057	P	-1.248499	9.396507	15.491853
C	-1.342831	2.222770	20.136370	O	-0.793122	10.897883	15.815836
O	-0.722685	3.209068	20.500418	H	-1.440931	11.612542	15.930563
C	-4.595004	3.886508	19.680423	O	-2.426678	9.223812	14.624816
H	-5.009394	3.105919	19.038577	O	0.103995	8.809527	14.905311
H	-4.230379	4.702363	19.049555	C	1.426683	9.000118	15.508470
C	-5.659567	4.347459	20.672455	H	1.448440	8.494038	16.476011
H	-6.676667	4.210917	20.297374	H	1.596333	10.073074	15.629806
O	-5.488461	5.769303	21.032464	C	2.432034	8.376795	14.570451
P	-5.974893	6.927206	19.898127	H	3.442368	8.690527	14.845797
O	-6.047811	8.307513	20.867565	O	2.339765	6.932545	14.681466
H	-6.905954	8.527444	21.275887	C	1.968765	6.334420	13.403584
O	-7.241131	6.553619	19.050753	H	2.859476	5.883352	12.951222
O	-4.574939	7.262473	19.035858	N	1.033480	5.264421	13.617105
C	-3.346231	7.630020	19.752272	C	-0.333348	5.320441	13.810956
H	-3.219675	6.984521	20.625886	H	-0.849810	6.268689	13.891673
H	-3.429642	8.674671	20.059857	N	-0.898991	4.145911	13.875766

C	0.152267	3.257233	13.742535	H	4.089965	4.757340	7.443716
C	0.212229	1.845679	13.646615	C	5.554960	5.849436	8.665754
N	-0.864822	1.058580	13.664620	H	5.639893	6.842952	8.224799
H	-0.753055	0.046283	13.608711	O	6.648582	5.008902	8.143341
H	-1.749814	1.443600	13.960696	P	6.708395	4.502392	6.619115
N	1.434718	1.299662	13.492446	O	8.279390	4.444423	6.329692
C	2.524046	2.076915	13.378320	H	8.765937	5.223572	6.013549
H	3.459088	1.537689	13.240122	O	5.866469	5.273342	5.689914
N	2.574394	3.403501	13.397254	O	6.371751	2.948468	6.693914
C	1.360605	3.927751	13.592525	C	7.188154	1.960920	7.415513
C	1.404010	7.496386	12.576997	H	6.924131	2.006769	8.473997
H	0.345503	7.646098	12.794900	H	8.242353	2.209229	7.266779
H	1.515287	7.363895	11.499875	C	6.870722	0.593377	6.859959
C	2.158774	8.713398	13.098110	H	7.596760	-0.126677	7.249337
H	1.605559	9.643049	12.957954	O	5.539939	0.207693	7.291946
O	3.475845	8.854840	12.455156	C	4.713978	-0.150627	6.141577
P	3.620930	9.074457	10.869757	H	4.675949	-1.233811	6.020122
O	4.897851	10.027609	10.758184	N	3.358191	0.288642	6.381904
H	4.822831	10.994549	10.812785	C	3.123263	1.563229	6.804556
O	2.379347	9.498908	10.202236	H	4.012537	2.169396	6.958048
O	4.234427	7.706172	10.339846	C	1.864376	2.000721	7.019151
C	5.492039	7.159113	10.865009	H	1.661946	3.011678	7.351389
H	5.393422	7.028011	11.945660	C	0.801433	1.043359	6.838020
H	6.293997	7.866162	10.639384	N	-0.458484	1.375240	7.100912
C	5.719963	5.829474	10.199963	H	-1.223929	0.732244	6.835767
H	6.720742	5.462067	10.446342	H	-0.680654	2.309890	7.400452
O	4.719442	4.902866	10.703794	N	1.044613	-0.195934	6.417001
C	4.149154	4.173430	9.575473	C	2.300273	-0.624697	6.158064
H	4.748515	3.287521	9.359428	O	2.564880	-1.747319	5.730803
N	2.834749	3.703538	9.921381	C	5.386844	0.557214	4.963583
C	1.851637	4.586543	10.265227	H	5.055311	1.599066	4.913382
H	2.162999	5.625538	10.315693	H	5.164309	0.082170	4.008558
C	0.596606	4.167533	10.527867	C	6.864402	0.532862	5.323190
H	-0.188662	4.854452	10.819069	H	7.437403	1.332862	4.851079
C	0.349670	2.746996	10.401366	O	7.486387	-0.756612	4.968086
N	-0.884585	2.264226	10.487895	P	7.493307	-1.308879	3.457895
H	-1.048350	1.256537	10.318178	O	8.885063	-2.090092	3.375505
H	-1.645651	2.860662	10.769521	H	9.703804	-1.648621	3.096143
N	1.339410	1.888143	10.170316	O	7.214838	-0.283875	2.437036
C	2.613902	2.305794	9.997240	O	6.474182	-2.524478	3.455324
O	3.568280	1.548810	9.848133	C	6.562409	-3.697263	4.333129
C	4.198163	5.194104	8.438243	H	6.242183	-3.401094	5.333731
H	3.424174	5.955556	8.570123	H	7.599084	-4.045221	4.345456

C	5.633141	-4.752530	3.781660	C	-1.459099	-2.126052	-0.291883
H	5.784438	-5.686310	4.331864	N	-1.252859	-0.816419	-0.139922
O	4.266871	-4.310684	3.955089	H	-2.057528	-0.188077	-0.092080
C	3.579713	-4.215306	2.661206	H	-0.353658	-0.487059	0.175895
H	2.930416	-5.084140	2.538523	N	-2.715740	-2.582608	-0.459427
N	2.720150	-3.061719	2.659034	C	-2.940672	-3.894670	-0.633207
C	3.246441	-1.785685	2.628533	H	-3.988683	-4.165750	-0.750148
H	4.331521	-1.733098	2.635844	N	-2.045933	-4.874741	-0.681256
C	2.481477	-0.681039	2.575331	C	-0.806026	-4.403245	-0.513706
C	3.006136	0.716305	2.452587	C	1.486537	-7.006465	-1.748783
H	4.075201	0.722016	2.224854	H	2.344755	-6.329953	-1.785999
H	2.475086	1.239021	1.653073	H	1.034105	-7.063576	-2.739373
H	2.827666	1.289149	3.370870	C	1.959568	-8.367091	-1.245020
C	1.030370	-0.857565	2.608424	H	2.976862	-8.599570	-1.561650
O	0.244432	0.081622	2.479956	O	1.075560	-9.450407	-1.708195
N	0.579643	-2.143686	2.786833	P	1.074495	-9.887344	-3.256481
H	-0.470456	-2.310524	2.786239	O	0.677779	-11.433651	-3.179105
C	1.336586	-3.284693	2.749527	H	1.348742	-12.126802	-3.062449
O	0.856014	-4.401878	2.764927	O	2.302675	-9.524042	-3.982355
C	4.711744	-4.187332	1.625846	O	-0.263391	-9.270802	-3.851988
H	5.083692	-3.174033	1.468172	C	-1.594473	-9.592223	-3.323230
H	4.409621	-4.589004	0.657583	H	-1.616030	-9.361302	-2.255341
C	5.816153	-5.007741	2.279594	H	-1.776811	-10.657130	-3.486123
H	6.812468	-4.763738	1.905917	C	-2.591832	-8.736113	-4.058590
O	5.593282	-6.453659	2.088705	H	-3.605763	-9.094154	-3.854034
P	5.523281	-7.085394	0.612883	O	-2.441541	-7.371175	-3.594898
O	5.958674	-8.601688	0.870011	C	-2.480923	-6.486025	-4.766564
H	6.893026	-8.865368	0.903016	H	-3.517491	-6.291160	-5.047712
O	6.262193	-6.314895	-0.401322	N	-1.911073	-5.217848	-4.395342
O	3.974522	-7.275054	0.306390	C	-0.579139	-5.082574	-4.147557
C	3.106294	-8.217828	1.025829	H	0.024195	-5.965699	-4.322816
H	2.946603	-7.844723	2.039820	C	-0.050248	-3.911634	-3.731680
H	3.603672	-9.190232	1.048189	H	1.009530	-3.802086	-3.540285
C	1.795409	-8.287085	0.284095	C	-0.966247	-2.805248	-3.574846
H	1.223202	-9.154249	0.629242	N	-0.509833	-1.587619	-3.301223
O	1.057093	-7.070826	0.560163	H	-1.147062	-0.779175	-3.232884
C	0.494450	-6.539765	-0.675757	H	0.470411	-1.445640	-3.121367
H	-0.514674	-6.931010	-0.840588	N	-2.277910	-2.969275	-3.720556
N	0.373031	-5.117165	-0.549838	C	-2.806869	-4.159303	-4.092806
C	1.382990	-4.201037	-0.362680	O	-4.013021	-4.358422	-4.206049
H	2.415657	-4.520696	-0.307741	C	-1.760004	-7.314458	-5.830920
N	0.959932	-2.972020	-0.239288	H	-0.688008	-7.379820	-5.626892
C	-0.416826	-3.083769	-0.322157	H	-1.909585	-6.950765	-6.846665

C	-2.367296	-8.692300	-5.583993	H	-1.070186	-1.008296	-6.201523
H	-1.761357	-9.519995	-5.957094	H	-0.824820	-2.678709	-6.721897
O	-3.712785	-8.759897	-6.190125	N	-3.592870	-1.048064	-6.455863
P	-3.945322	-9.025299	-7.743344	C	-4.916158	-1.209370	-6.630198
O	-4.147728	-10.618496	-7.787121	H	-5.515605	-0.327873	-6.405545
H	-3.867664	-11.112282	-8.577241	N	-5.555924	-2.294715	-7.045452
O	-2.921839	-8.508280	-8.673054	C	-4.704314	-3.299468	-7.276354
O	-5.377578	-8.396288	-7.986084	C	-6.479232	-5.899938	-9.238654
C	-6.542154	-8.427242	-7.099421	H	-5.553627	-6.428970	-9.475751
H	-6.201786	-8.411986	-6.062048	H	-6.749317	-5.261911	-10.083636
H	-7.104489	-9.339922	-7.310751	C	-7.571966	-6.909162	-8.888243
C	-7.348397	-7.184533	-7.392916	H	-7.509760	-7.822394	-9.489761
H	-8.320387	-7.239538	-6.894706	O	-8.888885	-6.317993	-8.967973
O	-6.607843	-6.046719	-6.876185	H	-6.631364	-4.408858	22.668671
C	-6.317154	-5.097074	-7.941329	H	-8.166842	-3.907330	23.407561
H	-7.013517	-4.257927	-7.874266	H	-9.085293	-6.008861	-9.871712
N	-4.996769	-4.561947	-7.742370	C	-2.957431	8.089313	-7.126579
C	-3.796136	-5.236600	-7.809305	H	-2.589871	7.893325	-8.135310
H	-3.735935	-6.257112	-8.168900	H	-3.256789	9.139148	-7.056809
N	-2.770362	-4.509879	-7.453918	H	-2.137051	7.907478	-6.424459
C	-3.323207	-3.287251	-7.127492	H	-9.596825	0.177349	0.801644
C	-2.752155	-2.068544	-6.704348	H	-7.869294	4.283031	-2.123697
N	-1.431888	-1.888561	-6.575551				

**Part 2. Cartesian coordinates of primitive subsystems of one step during the optimization with GEBF-B3LYP/6-31G\*\***

(3'-GACTGGATGT-5')				O	-0.585986	0.952552	-6.506050
1. Subsystem I				N	-2.612024	1.870456	-6.808325
C	-4.240235	7.441701	-6.935356	C	-3.531313	2.879778	-6.769440
O	-3.653810	6.162374	-7.268770	O	-4.666841	2.715573	-7.112502
C	-3.961995	5.194924	-6.239775	N	-6.606488	2.364175	-3.479311
C	-3.934428	6.055077	-4.976290	C	-5.666573	3.353547	-3.276767
C	-4.633114	7.320522	-5.450136	N	-4.464527	2.925986	-3.308200
C	-3.216606	8.523292	-7.220612	C	-4.580729	1.569685	-3.551574
N	-3.045100	4.090561	-6.311705	C	-3.592211	0.547247	-3.679274
C	-1.720782	4.225052	-5.947404	O	-2.386199	0.640228	-3.622456
C	-0.840366	3.228994	-5.949089	N	-4.183059	-0.692944	-3.907439
C	0.581028	3.360753	-5.484272	C	-5.518349	-0.927849	-4.018360
C	-1.298613	1.921913	-6.418841	N	-5.886462	-2.183567	-4.260491



C	-6.020862	1.263528	0.114639	O	7.704917	2.713223	18.917969
C	-5.771205	2.701878	0.468231	C	7.028078	2.417799	20.158882
C	-4.861587	0.389951	-0.076460	C	8.154824	2.030178	21.124901
O	-3.721923	0.752052	0.063130	C	9.387216	2.740464	20.586265
N	-5.149131	-0.898045	-0.452252	N	6.065184	1.380378	19.952049
C	-6.382250	-1.472572	-0.556118	C	6.319436	0.057000	19.634293
O	-6.524898	-2.626075	-0.841506	N	5.239997	-0.644209	19.513430
H	-5.141689	7.256463	-5.432489	C	4.200752	0.242180	19.770521
H	-8.091377	9.209066	-4.004562	C	2.815718	0.060674	19.858270
H	-8.388839	5.367196	-6.116903	N	2.228753	-1.128033	19.719164
H	-9.675462	6.207886	-5.233325	N	2.071390	1.151064	20.124360
H	-10.230852	3.847893	-5.325736	C	2.663580	2.345615	20.298799
H	-8.449773	1.527348	-3.589593	N	3.962193	2.589016	20.275371
H	-5.960860	4.364778	-3.096942	C	4.700543	1.502245	20.015798
H	-3.546485	-1.468962	-4.005045	O	9.504638	4.088268	21.151413
H	-5.236218	-2.944512	-4.272525	P	9.894514	4.417982	22.731949
H	-6.861694	-2.367702	-4.260982	O	10.503309	5.963229	22.616068
H	-8.943960	2.871512	-1.644719	O	10.839362	3.373631	23.412579
H	-10.087470	5.037392	-2.807895	O	8.439558	4.670926	23.455783
H	-13.990010	3.271961	-2.380694	C	7.364800	5.522593	22.968048
H	-11.110086	0.325527	-3.219820	C	6.082884	5.078594	23.609539
H	-12.593599	-0.028438	-2.326223	O	5.732984	3.761807	23.155050
H	-11.064625	-1.857411	-1.986482	C	4.812020	3.220500	24.125199
H	-8.661013	-2.227275	-0.450045	C	5.471555	3.621962	25.447888
H	-8.112122	1.305768	0.091271	C	6.072368	5.001199	25.148198
H	-6.699899	3.262209	0.488754	O	5.239035	6.086645	25.582290
H	-5.308895	2.778052	1.447165	N	4.623385	1.821191	23.919498
H	-5.098692	3.160245	-0.246452	C	5.584780	0.814386	23.825652
H	-4.370234	-1.529627	-0.572162	N	5.055940	-0.343048	23.615016
H	-9.650232	-1.302185	1.590886	C	3.681741	-0.128847	23.562495
H	-11.902848	-0.389999	0.336727	C	2.592362	-1.015637	23.360529
H	-11.418801	-2.044609	0.161015	O	2.611202	-2.239920	23.160933
H	-9.718707	0.300398	0.894735	N	1.366706	-0.353229	23.403257
H	-7.953006	4.191628	-2.216077	C	1.194022	0.989777	23.589979

### 3. Subsystem 3

O	9.331557	-0.789377	16.655073	N	-0.053354	1.453878	23.585963
P	10.118465	-0.789276	18.111291	N	2.211799	1.811463	23.778116
O	11.715656	-0.619708	17.661879	C	3.415643	1.210299	23.745720
O	9.825545	-2.013827	19.036607	H	8.888155	-1.547556	16.267570
O	9.727976	0.672040	18.746116	H	12.393647	-1.148742	18.074218
C	9.865812	2.006738	18.182404	H	9.435350	2.018180	17.194507
C	9.108982	2.942989	19.091664	H	10.918037	2.245874	18.143154
				H	9.336167	3.962381	18.818150
				H	6.485423	3.286855	20.482715

H	7.309720	-0.309023	19.516349	O	-4.463958	2.849097	21.948865
H	1.234532	-1.208348	19.705470	C	-3.693646	3.243807	20.790618
H	2.785361	-1.945103	19.653230	C	-4.750483	3.777672	19.817287
H	2.008992	3.167669	20.488668	C	-5.841634	4.336825	20.721367
H	8.329511	0.965720	21.101915	N	-2.915181	2.126471	20.332247
H	7.913696	2.313012	22.136445	C	-3.521936	1.012259	19.783385
H	10.304128	2.215493	20.791778	C	-2.865315	-0.084523	19.422457
H	11.434275	6.131538	22.735174	C	-3.485545	-1.241850	18.694717
H	7.303205	5.436890	21.894851	C	-1.429378	-0.132769	19.694917
H	7.597901	6.539604	23.243355	O	-0.752890	-1.116292	19.521479
H	5.304127	5.772449	23.317357	N	-0.880857	1.029605	20.172394
H	3.848414	3.688451	24.003126	C	-1.548751	2.158282	20.543051
H	6.624468	1.017641	23.915888	O	-0.986805	3.110605	21.010089
H	0.553708	-0.930377	23.231916	H	-7.160373	-4.231511	24.680766
H	-0.850271	0.866846	23.427512	H	-7.257358	-1.722249	24.334090
H	-0.177632	2.436809	23.570035	H	-4.500263	-0.753929	23.271274
H	6.256535	2.916257	25.685805	H	-4.105861	-4.271495	22.629358
H	4.766518	3.645865	26.266963	H	-1.896909	-5.359277	22.439488
H	7.063782	5.106931	25.561544	H	1.195298	-3.375677	22.784964
H	5.209068	6.196101	26.526517	H	0.534829	-4.932562	22.491009

#### 4. Subsystem 4

C	-7.444415	-3.787841	23.741633
C	-6.828981	-2.407175	23.619877
O	-5.408231	-2.520540	23.886906
C	-4.641151	-1.763823	22.935306
C	-6.921818	-1.796537	22.209784
C	-5.498214	-1.840192	21.671813
N	-3.324974	-2.364156	22.828672
C	-3.194579	-3.716362	22.665089
C	-1.993351	-4.303797	22.576103
C	-0.832646	-3.460449	22.712249
N	0.387992	-3.967359	22.658294
N	-0.974319	-2.156613	22.917474
C	-2.185984	-1.560850	22.953064
O	-2.320485	-0.332702	23.080506
O	-7.370548	-0.408119	22.355492
P	-7.893994	0.525559	21.196051
O	-9.323147	0.995689	21.695615
O	-7.887525	-0.101652	19.881378
O	-7.031050	1.819685	21.313968
C	-6.778761	2.689806	22.450631
C	-5.659965	3.623145	22.071042

O	-4.463958	2.849097	21.948865
C	-3.693646	3.243807	20.790618
C	-4.750483	3.777672	19.817287
C	-5.841634	4.336825	20.721367
N	-2.915181	2.126471	20.332247
C	-3.521936	1.012259	19.783385
C	-2.865315	-0.084523	19.422457
C	-3.485545	-1.241850	18.694717
C	-1.429378	-0.132769	19.694917
O	-0.752890	-1.116292	19.521479
N	-0.880857	1.029605	20.172394
C	-1.548751	2.158282	20.543051
O	-0.986805	3.110605	21.010089
H	-7.160373	-4.231511	24.680766
H	-7.257358	-1.722249	24.334090
H	-4.500263	-0.753929	23.271274
H	-4.105861	-4.271495	22.629358
H	-1.896909	-5.359277	22.439488
H	1.195298	-3.375677	22.784964
H	0.534829	-4.932562	22.491009
H	-7.630193	-2.300191	21.573948
H	-5.337253	-2.784064	21.164862
H	-5.290190	-1.051282	20.972175
H	-10.122249	0.814036	21.214305
H	-6.484705	2.083698	23.291972
H	-7.690768	3.224043	22.670490
H	-5.539050	4.366121	22.846042
H	-2.998654	4.011253	21.073081
H	-4.580057	1.094438	19.641714
H	-4.552547	-1.095305	18.569413
H	-3.035164	-1.330030	17.712926
H	-3.315314	-2.175259	19.221353
H	0.131903	1.068038	20.262938
H	-5.166086	2.994655	19.203273
H	-4.331412	4.528814	19.169001
H	-6.829756	4.233051	20.307011
H	-5.677365	5.376616	20.913066
H	-7.102971	-4.438840	22.949411
H	-8.522022	-3.735443	23.699040

#### 5. Subsystem 5

N	4.623385	1.821191	23.919498
C	5.584780	0.814386	23.825652

N	5.055940	-0.343048	23.615016	N	-3.045100	4.090561	-6.311705
C	3.681741	-0.128847	23.562495	C	-1.720782	4.225052	-5.947404
C	2.592362	-1.015637	23.360529	C	-0.840366	3.228994	-5.949089
O	2.611202	-2.239920	23.160933	C	0.581028	3.360753	-5.484272
N	1.366706	-0.353229	23.403257	C	-1.298613	1.921913	-6.418841
C	1.194022	0.989777	23.589979	O	-0.585986	0.952552	-6.506050
N	-0.053354	1.453878	23.585963	N	-2.612024	1.870456	-6.808325
N	2.211799	1.811463	23.778116	C	-3.531313	2.879778	-6.769440
C	3.415643	1.210299	23.745720	O	-4.666841	2.715573	-7.112502
C	-7.444415	-3.787841	23.741633	C	-1.611787	-9.728397	-3.366923
C	-6.828981	-2.407175	23.619877	C	-2.522942	-8.808633	-4.132557
O	-5.408231	-2.520540	23.886906	O	-2.250593	-7.454114	-3.741913
C	-4.641151	-1.763823	22.935306	C	-2.432768	-6.597917	-4.898637
C	-6.921818	-1.796537	22.209784	C	-1.817759	-7.448409	-6.008571
C	-5.498214	-1.840192	21.671813	C	-2.349808	-8.833911	-5.666160
N	-3.324974	-2.364156	22.828672	N	-1.864554	-5.301671	-4.656395
C	-3.194579	-3.716362	22.665089	C	-0.520993	-5.118350	-4.563969
C	-1.993351	-4.303797	22.576103	C	0.016808	-3.918397	-4.333563
C	-0.832646	-3.460449	22.712249	C	-0.904880	-2.818320	-4.174594
N	0.387992	-3.967359	22.658294	N	-0.444311	-1.596498	-3.977001
N	-0.974319	-2.156613	22.917474	N	-2.202592	-3.001697	-4.228630
C	-2.185984	-1.560850	22.953064	C	-2.737501	-4.220954	-4.437914
O	-2.320485	-0.332702	23.080506	O	-3.929955	-4.415910	-4.460752
H	4.755587	2.801874	24.063660	O	-3.695837	-9.014903	-6.228498
H	6.624468	1.017641	23.915888	P	-4.097205	-9.319435	-7.717369
H	0.553708	-0.930377	23.231916	O	-4.584947	-10.830206	-7.677057
H	-0.850271	0.866846	23.427512	O	-3.057758	-9.063972	-8.706757
H	-0.177632	2.436809	23.570035	O	-5.400167	-8.492631	-7.936687
H	-7.160373	-4.231511	24.680766	C	-6.616451	-8.354748	-7.150021
H	-7.257358	-1.722249	24.334090	C	-7.355033	-7.134097	-7.633220
H	-4.500263	-0.753929	23.271274	O	-6.576239	-5.973294	-7.298227
H	-4.105861	-4.271495	22.629358	C	-6.348519	-5.124657	-8.437883
H	-1.896909	-5.359277	22.439488	C	-6.552603	-6.056053	-9.638296
H	1.195298	-3.375677	22.784964	C	-7.603155	-7.046751	-9.146876
H	0.534829	-4.932562	22.491009	O	-8.935593	-6.525003	-9.284638
H	-7.630193	-2.300191	21.573948	N	-5.040900	-4.542855	-8.352357
H	-5.337253	-2.784064	21.164862	C	-3.834676	-5.203448	-8.343575
H	-5.290190	-1.051282	20.972175	N	-2.830054	-4.441948	-8.122954
H	-7.249249	-0.783431	22.316105	C	-3.383055	-3.184685	-7.962735
H	-7.102971	-4.438840	22.949411	C	-2.820435	-1.927939	-7.697816
H	-8.522022	-3.735443	23.699040	N	-1.505658	-1.737354	-7.571838
				N	-3.649991	-0.890453	-7.588228
				C	-4.957373	-1.084524	-7.741094

6. Subsystem 6

N	-5.588238	-2.205851	-7.997811	C	1.407415	-3.766759	12.783058
C	-4.749554	-3.232120	-8.089603	C	0.267828	-4.718513	13.011315
H	-3.683082	4.858984	-6.261655	C	1.136061	-2.335400	12.943572
H	-1.432426	5.212396	-5.651140	O	0.054842	-1.893297	13.219819
H	0.810658	4.390192	-5.231044	N	2.214561	-1.505159	12.752537
H	0.746181	2.748173	-4.603441	C	3.484535	-1.862279	12.409611
H	1.275048	3.027464	-6.247923	O	4.360481	-1.060146	12.266048
H	-2.972391	0.976560	-7.111026	O	7.838558	-4.872042	11.761074
H	-0.615913	-9.600315	-3.736691	P	8.881064	-5.021886	12.940740
H	-1.631029	-9.479004	-2.318043	O	10.262126	-4.706762	12.241756
H	-1.886617	-10.762578	-3.507828	O	8.792573	-6.293336	13.642934
H	-3.547331	-9.054426	-3.891939	O	8.669145	-3.758775	13.841074
H	-3.483075	-6.443873	-5.060310	C	8.856764	-2.353513	13.519342
H	0.084465	-5.992230	-4.689218	C	8.274806	-1.522498	14.628525
H	1.076724	-3.779503	-4.260004	O	6.841245	-1.602967	14.583700
H	-1.077301	-0.824195	-3.860467	C	6.359438	-1.348040	15.925676
H	0.528992	-1.431618	-3.887519	C	7.316485	-2.209478	16.750763
H	-0.740357	-7.475770	-5.929184	C	8.654391	-1.947272	16.063277
H	-2.076843	-7.124855	-7.000632	N	4.952411	-1.634109	16.023899
H	-1.725359	-9.635174	-6.018942	C	4.479648	-2.909061	16.000472
H	-4.270914	-11.478374	-8.297516	C	3.181195	-3.197829	16.134637
H	-6.344035	-8.233296	-6.113961	C	2.279393	-2.086777	16.292405
H	-7.200259	-9.253543	-7.285021	N	0.978974	-2.287290	16.438150
H	-8.305809	-7.079033	-7.124156	N	2.736992	-0.843837	16.278251
H	-7.056712	-4.313885	-8.420810	C	4.053402	-0.561346	16.147278
H	-3.779009	-6.256211	-8.524913	O	4.481770	0.600855	16.148702
H	-1.156257	-0.861555	-7.236661	N	6.065184	1.380378	19.952049
H	-0.910056	-2.530420	-7.573176	C	6.319436	0.057000	19.634293
H	-5.561727	-0.200658	-7.639350	N	5.239997	-0.644209	19.513430
H	-5.638824	-6.584212	-9.866367	C	4.200752	0.242180	19.770521
H	-6.861638	-5.516511	-10.524476	C	2.815718	0.060674	19.858270
H	-7.533045	-8.006746	-9.637439	N	2.228753	-1.128033	19.719164
H	-9.133552	-6.180182	-10.156916	N	2.071390	1.151064	20.124360

#### 7. Subsystem 7

C	5.310777	-6.397709	9.630488	C	4.700543	1.502245	20.015798
C	5.939441	-5.214952	10.321294	H	4.667677	-6.894286	10.326717
O	4.937410	-4.209025	10.523809	H	4.715859	-6.065269	8.795719
C	4.984846	-3.679812	11.870430	H	6.059258	-7.103330	9.303087
C	5.566244	-4.837209	12.685695	H	6.719887	-4.818547	9.688079
C	6.521466	-5.514583	11.712456	H	5.628610	-2.821476	11.889873
N	3.681310	-3.227302	12.266202	H	2.888178	-5.143124	12.218606
C	2.634703	-4.121559	12.417659	H	0.600759	-5.747583	12.946053

H	-0.159818	-4.562085	13.995461	O	-11.006124	3.221030	-3.167927
H	-0.529090	-4.553851	12.296678	P	-11.836047	2.867176	-1.872528
H	2.056029	-0.513289	12.886015	O	-13.296044	2.623558	-2.429048
H	4.804406	-5.546144	12.971402	O	-11.716303	3.849749	-0.806437
H	6.063037	-4.484565	13.574759	O	-11.392567	1.415617	-1.482105
H	6.662093	-6.562614	11.910317	C	-11.539427	0.185702	-2.240278
H	10.869174	-5.378174	11.949470	C	-10.817292	-0.916255	-1.515289
H	8.353859	-2.133510	12.591111	O	-9.403670	-0.690061	-1.614943
H	9.916290	-2.178085	13.416153	C	-8.765170	-1.158527	-0.401891
H	8.579671	-0.494891	14.487049	C	-9.775156	-0.753901	0.671542
H	6.471493	-0.302697	16.149554	C	-11.112678	-1.033056	-0.006164
H	5.209438	-3.679507	15.865417	N	-7.441751	-0.621371	-0.291189
H	2.826434	-4.208615	16.114641	C	-7.224277	0.718522	-0.019117
H	0.343385	-1.510866	16.495711	C	-6.020862	1.263528	0.114639
H	0.595870	-3.200277	16.455356	C	-5.771205	2.701878	0.468231
H	7.086050	-3.259659	16.640529	C	-4.861587	0.389951	-0.076460
H	7.317519	-1.979556	17.801248	O	-3.721923	0.752052	0.063130
H	9.322053	-2.789947	16.100029	N	-5.149131	-0.898045	-0.452252
H	9.148600	-1.102218	16.495181	C	-6.382250	-1.472572	-0.556118
H	6.738324	2.105619	20.096642	O	-6.524898	-2.626075	-0.841506
H	7.309720	-0.309023	19.516349	H	-8.171960	5.827118	-4.448107
H	1.234532	-1.208348	19.705470	H	-8.388839	5.367196	-6.116903
H	2.785361	-1.945103	19.653230	H	-9.675462	6.207886	-5.233325
H	2.008992	3.167669	20.488668	H	-10.230852	3.847893	-5.325736

#### 8. Subsystem 8

C	-8.883898	5.476600	-5.165868	H	-8.449773	1.527348	-3.589593
C	-9.400030	4.136418	-4.700136	H	-5.960860	4.364778	-3.096942
O	-8.357287	3.163269	-4.838635	H	-3.546485	-1.468962	-4.005045
C	-8.024974	2.515769	-3.590231	H	-5.236218	-2.944512	-4.272525
C	-8.644765	3.422771	-2.520471	H	-6.861694	-2.367702	-4.260982
C	-9.818258	4.083310	-3.226209	H	-8.943960	2.871512	-1.644719
N	-6.606488	2.364175	-3.479311	H	-10.087470	5.037392	-2.807895
C	-5.666573	3.353547	-3.276767	H	-13.990010	3.271961	-2.380694
N	-4.464527	2.925986	-3.308200	H	-11.110086	0.325527	-3.219820
C	-4.580729	1.569685	-3.551574	H	-12.593599	-0.028438	-2.326223
C	-3.592211	0.547247	-3.679274	H	-11.064625	-1.857411	-1.986482
O	-2.386199	0.640228	-3.622456	H	-8.661013	-2.227275	-0.450045
N	-4.183059	-0.692944	-3.907439	H	-8.112122	1.305768	0.091271
C	-5.518349	-0.927849	-4.018360	H	-6.699899	3.262209	0.488754
N	-5.886462	-2.183567	-4.260491	H	-5.308895	2.778052	1.447165
N	-6.425380	0.005352	-3.903643	H	-5.098692	3.160245	-0.246452
C	-5.900011	1.215801	-3.674135	H	-4.370234	-1.529627	-0.572162
				H	-9.650232	-1.302185	1.590886
				H	-11.902848	-0.389999	0.336727

H	-11.418801	-2.044609	0.161015
H	-9.718707	0.300398	0.894735
H	-7.953006	4.191628	-2.216077

H	-9.675462	6.207886	-5.233325
H	-10.230852	3.847893	-5.325736
H	-8.449773	1.527348	-3.589593

9. Subsystem 9

C	-8.883898	5.476600	-5.165868
C	-9.400030	4.136418	-4.700136
O	-8.357287	3.163269	-4.838635
C	-8.024974	2.515769	-3.590231
C	-8.644765	3.422771	-2.520471
C	-9.818258	4.083310	-3.226209
O	-11.006124	3.221030	-3.167927
P	-11.836047	2.867176	-1.872528
O	-13.296044	2.623558	-2.429048
O	-11.716303	3.849749	-0.806437
O	-11.392567	1.415617	-1.482105
C	-11.539427	0.185702	-2.240278
C	-10.817292	-0.916255	-1.515289
O	-9.403670	-0.690061	-1.614943
C	-8.765170	-1.158527	-0.401891
C	-9.775156	-0.753901	0.671542
C	-11.112678	-1.033056	-0.006164
N	-7.441751	-0.621371	-0.291189
C	-7.224277	0.718522	-0.019117
C	-6.020862	1.263528	0.114639
C	-5.771205	2.701878	0.468231
C	-4.861587	0.389951	-0.076460
O	-3.721923	0.752052	0.063130
N	-5.149131	-0.898045	-0.452252
C	-6.382250	-1.472572	-0.556118
O	-6.524898	-2.626075	-0.841506
N	-6.199260	-3.410706	2.964865
C	-6.608776	-2.097573	2.996220
N	-5.649730	-1.256048	2.929719
C	-4.512867	-2.037835	2.859295
C	-3.145096	-1.721279	2.825295
N	-2.694581	-0.471205	2.860278
N	-2.276724	-2.734665	2.782533
C	-2.738472	-3.983461	2.767043
N	-3.983320	-4.390736	2.800425
C	-4.834514	-3.370714	2.863487
H	-8.171960	5.827118	-4.448107
H	-8.388839	5.367196	-6.116903

H	-6.964234	2.402407	-3.507286
H	-8.943960	2.871512	-1.644719
H	-10.087470	5.037392	-2.807895
H	-13.990010	3.271961	-2.380694
H	-11.110086	0.325527	-3.219820
H	-12.593599	-0.028438	-2.326223
H	-11.064625	-1.857411	-1.986482
H	-8.661013	-2.227275	-0.450045
H	-8.112122	1.305768	0.091271
H	-6.699899	3.262209	0.488754
H	-5.308895	2.778052	1.447165
H	-5.098692	3.160245	-0.246452
H	-4.370234	-1.529627	-0.572162
H	-9.650232	-1.302185	1.590886
H	-11.902848	-0.389999	0.336727
H	-11.418801	-2.044609	0.161015
H	-6.766806	-4.232443	3.016252
H	-7.645915	-1.845285	3.065012
H	-1.728676	-0.283875	2.695337
H	-3.343460	0.273918	2.774843
H	-1.981815	-4.745736	2.724365
H	-9.718707	0.300398	0.894735
H	-7.953006	4.191628	-2.216077

10. Subsystem10

C	-11.539427	0.185702	-2.240278
C	-10.817292	-0.916255	-1.515289
O	-9.403670	-0.690061	-1.614943
C	-8.765170	-1.158527	-0.401891
C	-9.775156	-0.753901	0.671542
C	-11.112678	-1.033056	-0.006164
N	-7.441751	-0.621371	-0.291189
C	-7.224277	0.718522	-0.019117
C	-6.020862	1.263528	0.114639
C	-5.771205	2.701878	0.468231
C	-4.861587	0.389951	-0.076460
O	-3.721923	0.752052	0.063130
N	-5.149131	-0.898045	-0.452252
C	-6.382250	-1.472572	-0.556118
O	-6.524898	-2.626075	-0.841506



C	-3.090386	-3.747439	6.359311
H	-11.431224	1.091877	-1.681673
H	-11.110086	0.325527	-3.219820
H	-12.593599	-0.028438	-2.326223
H	-11.064625	-1.857411	-1.986482
H	-8.661013	-2.227275	-0.450045
H	-7.776689	-0.757317	-0.319206
H	-9.650232	-1.302185	1.590886
H	-11.902848	-0.389999	0.336727
H	-13.975084	-4.001114	1.264036
H	-9.960212	-4.915857	0.432791
H	-10.974945	-5.889802	1.505328
H	-8.705567	-6.532336	1.894252
H	-6.340436	-5.428063	3.000137
H	-7.645915	-1.845285	3.065012
H	-1.728676	-0.283875	2.695337
H	-3.343460	0.273918	2.774843
H	-1.981815	-4.745736	2.724365
H	-8.343964	-3.676661	4.470737
H	-7.465747	-5.046699	5.115572
H	-10.061156	-5.225263	4.117047
H	-8.969208	-6.564215	4.058772
H	-4.180127	-5.514287	6.594116
H	-6.230658	-3.963789	6.978722
H	-0.506459	-1.301566	6.042503
H	1.055902	-2.935558	5.864183
H	0.541637	-4.580162	5.876218
H	-9.718707	0.300398	0.894735

12. Subsystem12

C	-10.215405	-5.124814	1.459531
C	-8.984230	-5.538475	2.218078
O	-7.921244	-4.625417	1.919288
C	-7.009053	-4.583188	3.038186
C	-7.956463	-4.658608	4.239286
C	-9.101519	-5.546740	3.755227
N	-6.199260	-3.410706	2.964865
C	-6.608776	-2.097573	2.996220
N	-5.649730	-1.256048	2.929719
C	-4.512867	-2.037835	2.859295
C	-3.145096	-1.721279	2.825295
N	-2.694581	-0.471205	2.860278
N	-2.276724	-2.734665	2.782533

C	-2.738472	-3.983461	2.767043
N	-3.983320	-4.390736	2.800425
C	-4.834514	-3.370714	2.863487
O	-8.920122	-6.941682	4.171382
P	-8.990508	-7.512187	5.641260
O	-9.521232	-8.988604	5.428494
O	-9.758206	-6.703610	6.575249
O	-7.492393	-7.740930	6.038909
C	-6.439847	-8.374427	5.269074
C	-5.110710	-7.920564	5.803927
O	-4.933628	-6.524890	5.517740
C	-4.172711	-5.934365	6.606785
C	-4.807680	-6.614284	7.816605
C	-4.926725	-8.051772	7.330366
N	-4.197769	-4.514897	6.563975
C	-5.236054	-3.623259	6.779237
N	-4.870036	-2.404435	6.713488
C	-3.512401	-2.449088	6.453425
C	-2.526364	-1.419258	6.340021
O	-2.653402	-0.217840	6.401208
N	-1.257805	-1.964703	6.128798
C	-0.958817	-3.289038	6.055973
N	0.320927	-3.611902	5.883188
N	-1.858276	-4.228891	6.152007
C	-3.090386	-3.747439	6.359311
H	-10.616151	-4.238055	1.904460
H	-9.960212	-4.915857	0.432791
H	-10.974945	-5.889802	1.505328
H	-8.705567	-6.532336	1.894252
H	-6.340436	-5.428063	3.000137
H	-7.645915	-1.845285	3.065012
H	-1.728676	-0.283875	2.695337
H	-3.343460	0.273918	2.774843
H	-1.981815	-4.745736	2.724365
H	-8.343964	-3.676661	4.470737
H	-7.465747	-5.046699	5.115572
H	-10.061156	-5.225263	4.117047
H	-10.407582	-9.250304	5.652978
H	-6.537708	-8.089284	4.233974
H	-6.554911	-9.443702	5.367536
H	-4.333390	-8.489942	5.313900
H	-3.139416	-6.219791	6.496566
H	-6.230658	-3.963789	6.978722

H	-0.506459	-1.301566	6.042503	N	2.214561	-1.505159	12.752537
H	1.055902	-2.935558	5.864183	C	3.484535	-1.862279	12.409611
H	0.541637	-4.580162	5.876218	O	4.360481	-1.060146	12.266048
H	-5.800551	-6.220421	7.986220	H	-1.198438	-8.735866	8.343784
H	-4.239516	-6.518292	8.726561	H	-0.927269	-8.431487	6.645845
H	-5.694840	-8.621768	7.821827	H	-0.297608	-9.898891	7.415270
H	-3.997384	-8.566931	7.456217	H	1.539833	-8.356837	7.211228

### 13. Subsystem13

C	-0.496702	-8.844560	7.543376
C	0.760134	-8.092501	7.909292
O	0.515493	-6.678163	7.819374
C	0.841857	-5.998210	9.058568
C	0.755533	-7.110417	10.103529
C	1.242057	-8.331660	9.346193
N	-0.028053	-4.891716	9.282360
C	-1.387958	-4.889138	9.534627
N	-1.857352	-3.721171	9.737363
C	-0.772472	-2.872245	9.610594
C	-0.652581	-1.450208	9.740183
O	-1.499036	-0.624221	9.977050
N	0.672585	-1.044465	9.549165
C	1.726776	-1.858086	9.276123
N	2.921749	-1.280054	9.147162
N	1.616590	-3.151850	9.151712
C	0.359650	-3.586135	9.323712
O	2.712902	-8.341162	9.284822
P	3.724332	-8.464503	10.486491
O	4.877198	-9.388481	9.917753
O	3.119424	-8.915521	11.732157
O	4.435753	-7.073369	10.577802
C	5.310777	-6.397709	9.630488
C	5.939441	-5.214952	10.321294
O	4.937410	-4.209025	10.523809
C	4.984846	-3.679812	11.870430
C	5.566244	-4.837209	12.685695
C	6.521466	-5.514583	11.712456
N	3.681310	-3.227302	12.266202
C	2.634703	-4.121559	12.417659
C	1.407415	-3.766759	12.783058
C	0.267828	-4.718513	13.011315
C	1.136061	-2.335400	12.943572
O	0.054842	-1.893297	13.219819

H	1.837174	-5.596216	8.976967
H	-1.947859	-5.800233	9.547320
H	0.832164	-0.053490	9.628048
H	3.079205	-0.308621	9.328666
H	3.696485	-1.887239	9.019825
H	-0.268806	-7.272932	10.401799
H	1.338565	-6.905207	10.984847
H	0.924090	-9.267194	9.771179
H	4.977959	-10.302782	10.158649
H	4.715859	-6.065269	8.795719
H	6.059258	-7.103330	9.303087
H	6.719887	-4.818547	9.688079
H	5.628610	-2.821476	11.889873
H	2.888178	-5.143124	12.218606
H	0.600759	-5.747583	12.946053
H	-0.159818	-4.562085	13.995461
H	-0.529090	-4.553851	12.296678
H	2.056029	-0.513289	12.886015
H	4.804406	-5.546144	12.971402
H	6.063037	-4.484565	13.574759
H	6.662093	-6.562614	11.910317
H	7.482603	-5.045694	11.747934

### 14. Subsystem14

C	8.856764	-2.353513	13.519342
C	8.274806	-1.522498	14.628525
O	6.841245	-1.602967	14.583700
C	6.359438	-1.348040	15.925676
C	7.316485	-2.209478	16.750763
C	8.654391	-1.947272	16.063277
N	4.952411	-1.634109	16.023899
C	4.479648	-2.909061	16.000472
C	3.181195	-3.197829	16.134637
C	2.279393	-2.086777	16.292405
N	0.978974	-2.287290	16.438150
N	2.736992	-0.843837	16.278251

C	4.053402	-0.561346	16.147278	H	9.916290	-2.178085	13.416153
O	4.481770	0.600855	16.148702	H	8.579671	-0.494891	14.487049
O	9.331557	-0.789377	16.655073	H	6.471493	-0.302697	16.149554
P	10.118465	-0.789276	18.111291	H	5.209438	-3.679507	15.865417
O	11.715656	-0.619708	17.661879	H	2.826434	-4.208615	16.114641
O	9.825545	-2.013827	19.036607	H	0.343385	-1.510866	16.495711
O	9.727976	0.672040	18.746116	H	0.595870	-3.200277	16.455356
C	9.865812	2.006738	18.182404	H	7.086050	-3.259659	16.640529
C	9.108982	2.942989	19.091664	H	7.317519	-1.979556	17.801248
O	7.704917	2.713223	18.917969	H	9.322053	-2.789947	16.100029
C	7.028078	2.417799	20.158882	H	12.393647	-1.148742	18.074218
C	8.154824	2.030178	21.124901	H	9.435350	2.018180	17.194507
C	9.387216	2.740464	20.586265	H	10.918037	2.245874	18.143154
N	6.065184	1.380378	19.952049	H	9.336167	3.962381	18.818150
C	6.319436	0.057000	19.634293	H	6.485423	3.286855	20.482715
N	5.239997	-0.644209	19.513430	H	7.309720	-0.309023	19.516349
C	4.200752	0.242180	19.770521	H	1.234532	-1.208348	19.705470
C	2.815718	0.060674	19.858270	H	2.785361	-1.945103	19.653230
N	2.228753	-1.128033	19.719164	H	2.008992	3.167669	20.488668
N	2.071390	1.151064	20.124360	H	8.329511	0.965720	21.101915
C	2.663580	2.345615	20.298799	H	7.913696	2.313012	22.136445
N	3.962193	2.589016	20.275371	H	10.304128	2.215493	20.791778
C	4.700543	1.502245	20.015798	H	9.472907	3.724059	20.998696
H	8.718674	-3.387804	13.756140				
H	8.353859	-2.133510	12.591111				(End)