Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

† Supporting Information for

Applicability of Optimal Functional Tuning in Density Functional Calculations of Ionization Potentials and Electron Affinities of Adenine-Thymine Nucleobase Pairs and Clusters

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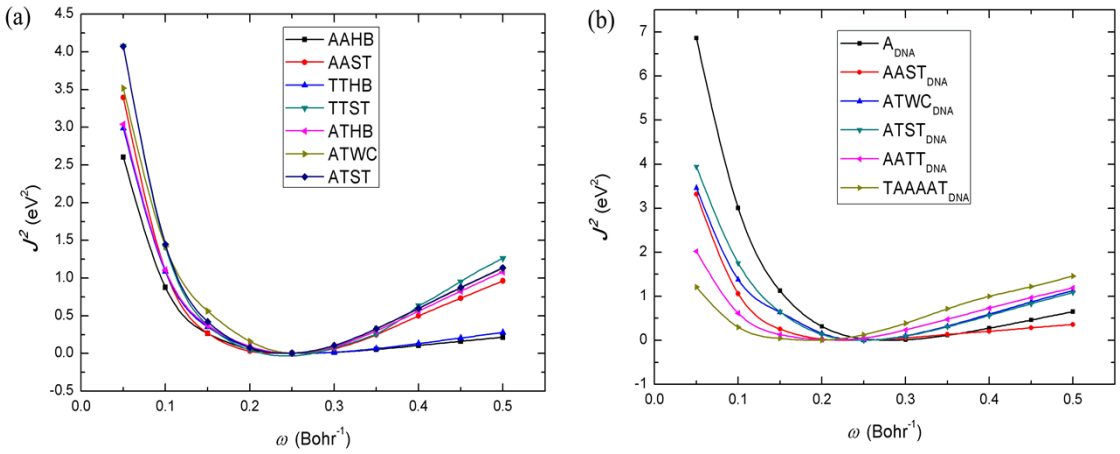

Fig. S1 J^2 as a functional of ω for various isomers of NAB pairs and clusters as determined by LC-ωPBE functional and cc-pVTZ basis set.

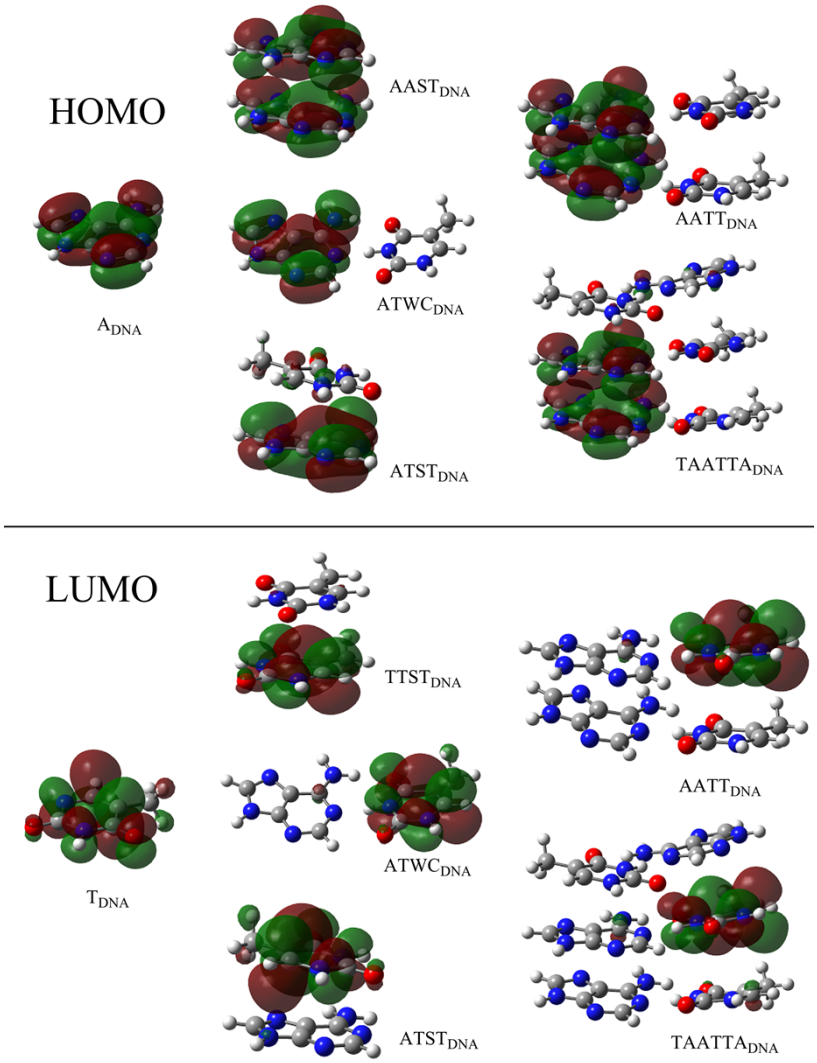

Fig. S2 Frontier molecular orbitals (HOMO and LUMO) of various NAB pairs calculated using optimally tuned LC-ωPBE*/cc-pVTZ.

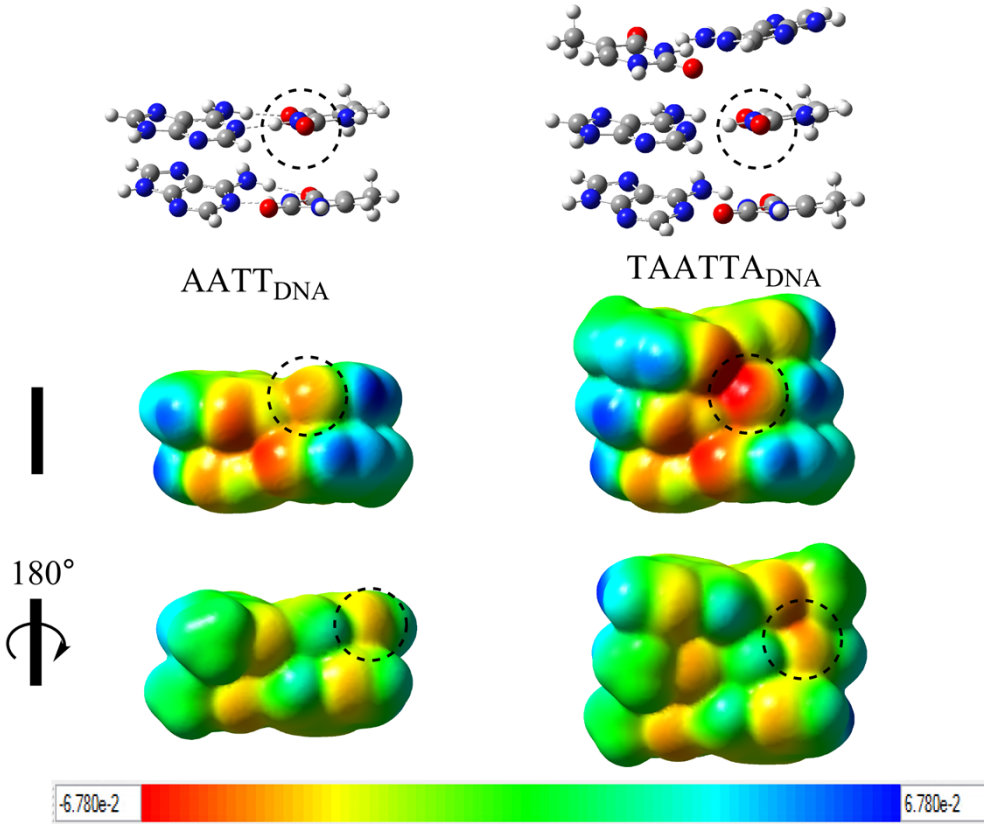

Fig. S3 3D plot of electrostatic potential (ESP) of $AATT_{DNA}$ and $TAATTA_{DNA}$. Isovalues for surface: 0.0004 au. Red color represents rich in electrons; Blue color represents poor in electrons.

Table S1. Calculated Negative HOMO energy $-\varepsilon_{HOMO}$, LUMO energy $-\varepsilon_{LUMO}$, IP, EA, Orbital Energy Gap $\Delta\varepsilon$ and Fundamental Gap ΔE_F for various isomers of NAB pairs.[a] All units are in eVs.

	PBE	B3LYP	M06-2X	LC-ωPBE	LC-ωPBE*	EOM-IP-CCSD/CCSD[c]
				TTHB		
$-\varepsilon_{HOMO}$	5.93	6.83	8.22	9.52	8.83	
IP	7.87	8.29	8.94	9.25	8.83	8.88
$-\varepsilon_{LUMO}$	2.11	1.43	0.39	-0.99	-0.58	
EA	0.19	-0.01	-0.34	-0.74	-0.58	-0.62
$\Delta\varepsilon$	3.82	5.4	7.83	10.51	9.41	
ΔE_F	7.68	8.3	9.28	9.99	9.41	
				TTST		
$-\varepsilon_{HOMO}$	5.98	6.91	8.31	9.60	8.77	
IP	8.15	8.55	9.08	9.07	8.79	8.91
$-\varepsilon_{LUMO}$	2.25	1.61	0.59	-0.80	-0.31	
EA	0.06	-0.08	-0.24	-0.20	-0.31	-0.13
$\Delta\varepsilon$	3.73	5.3	7.72	10.4	9.08	
ΔE_F	8.09	8.63	9.32	9.27	9.10	
				AAHB		
$-\varepsilon_{HOMO}$	5.45	6.24	7.57	8.88	8.26	
IP	7.31	7.67	8.28	8.67	8.29	8.23
$-\varepsilon_{LUMO}$	1.62	0.94	-0.03	-1.31	-0.91	
EA	-0.21	-0.45	-0.76	-1.06	-0.89	-1.02
$\Delta\varepsilon$	3.83	5.3	7.6	10.19	9.17	
ΔE_F	7.52	8.12	9.04	9.73	9.18	
				AAST		
$-\varepsilon_{HOMO}$	5.44	6.24	7.56	8.85	8.09	
IP	7.52	7.81	8.31	8.36	8.07	8.16
$-\varepsilon_{LUMO}$	1.65	0.98	0.02	-1.27	-0.77	
EA	-0.35	-0.54	-0.75	-0.97	-0.75	-0.37
$\Delta\varepsilon$	3.79	5.26	7.54	10.12	8.8	
ΔE_F	7.87	8.35	9.06	9.33	8.82	
				ATHB		
$-\varepsilon_{HOMO}$	5.59	6.38	7.70	9.01	8.33	
IP	7.59	7.69	8.53	8.52	8.36	8.36
$-\varepsilon_{LUMO}$	1.97	1.31	0.28	-1.09	-0.62	
EA	-0.01	-0.22	-0.50	-0.50	-0.59	-0.64

$\Delta\varepsilon$	3.62	5.07	7.42	10.1	8.95	
ΔE_F	7.6	7.91	9.03	9.02	8.95	
				$AAST_{DNA}$		
$-\varepsilon_{HOMO}$	5.13	5.92	7.20	8.51	7.73	
IP	7.20	7.48	7.95	8.19	7.75	7.81
$-\varepsilon_{LUMO}$	1.46	0.79	-0.16	-1.47	-0.94	
EA	-0.52	-0.71	-0.93	-1.16	-0.94	-
$\Delta\varepsilon$	3.67	5.13	7.36	9.98	8.67	
ΔE_F	7.72	8.19	8.88	9.35	8.69	
				$ATWC_{DNA}$		
$-\varepsilon_{HOMO}$	5.29	6.08	7.41	8.72	8.10	
IP	7.43	7.78	8.26	8.24	8.08	8.01
$-\varepsilon_{LUMO}$	1.88	1.21	0.17	-1.21	-0.77	
EA	-0.22	-0.43	-0.65	-0.58	-0.73	-
$\Delta\varepsilon$	3.41	4.87	7.24	9.93	8.87	
ΔE_F	7.65	8.21	8.91	8.82	8.81	

[a] The orbital energies are calculated with cc-pVTZ basis set. [b] EOM-IP-CCSD values are calculated with 6-311+G(d,p) basis set, taken from references [1, 2]. The CCSD values are calculated with aug-cc-pVDZ basis set in this work.

Table S2. Calculated reactivity descriptors of electrophilicity ω and global hardness η of ATWC as a function of electric field strength along the *x* axe at different DFT levels with cc-pVTZ basis set. 1 au = 51.4 V/Å = 51.4 × 10^{10} V/m.

Electric Filed	PBE	B3LYP	M06-2X	LC-ωPBE	LC-ωPBE*	CCSD/aug-cc-pVDZ
				Electrophilicity ω		
0	3.892317	2.790302	2.011455	1.431144	1.532574	1.55556
0.002	3.372748	2.503159	1.875767	1.389231	1.477171	
0.004	3.83608	2.73505	2.035813	1.511649	1.592138	
0.006	4.606101	3.086746	2.198064	1.596676	1.696216	
0.008	5.801584	3.561146	2.399354	1.698015	1.821521	
0.01	7.880507	4.22706	2.651969	1.819649	1.973575	
-0.002	4.668612	3.17799	2.201012	1.532253	1.652959	
-0.004	5.806465	3.682323	2.428199	1.648354	1.79229	
-0.006	7.627083	4.36355	2.703329	1.781508	1.954758	
-0.008	10.98543	5.329134	3.042326	1.935574	2.145654	
-0.01	19.07806	6.800683	3.469375	2.115468	2.373003	
				Global hardness η		
0	1.64388	2.367855	3.544633	4.884415	4.31623	4.3333
0.002	1.879125	2.61562	3.787911	5.09681	4.524814	

0.004	1.64837	2.448535	3.646275	4.943605	4.325894
0.006	1.369445	2.162945	3.358776	4.655019	4.042617
0.008	1.087255	1.87355	3.067198	4.362084	3.75539
0.01	0.80221	1.58075	2.772085	4.065608	3.465041
-0.002	1.39094	2.10757	3.280816	4.620736	4.058671
-0.004	1.13515	1.844565	3.013592	4.353241	3.797571
-0.006	0.87745	1.578975	2.743785	4.083023	3.533751
-0.008	0.618665	1.31162	2.471935	3.810497	3.267617
-0.01	0.36178	1.0429	2.198185	3.535792	2.999172

Geometry Details

For $TTST_{DNA}$, $AAST_{DNA}$, $ATWC_{DNA}$, $ATST_{DNA}$, $AATT_{DNA}$ and $TAATTA_{DNA}$ initial geometries are extracted from the original structure of the DNA 18-mer duplex from the X-ray DNA structure (PDB ID: 3BSE).[3] All the geometries are documented below. NABs from dA8, dA9, dT10, dA29, dT30, and dT31 were used for the hexmer model. The C1′ sugar atoms covalently bound to the bases were replaced by hydrogens. The hydrogen atoms were added using the Gaussview software[4] and their positions were optimized at the ωB97X-D/6-31+G(d,p) level. For ATWC and ATST, geometries are optimized at the RI-MP2/cc-pVTZ level, taken from reference [5]. For others, optimized geometries are obtained by the hybrid B3LYP-D[6-8] dispersion-corrected functional and the 6-31+G(d,p) basis set, taken from reference [2].

References

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$TAATTA_{DNA}$

N	-4.66638436	-2.92799422	-2.04684916
C	-4.24297532	-2.41853218	-3.25562225
N	-2.93612022	-2.37077318	-3.38435726
C	-2.46540919	-2.87328722	-2.17570517
C	-1.16874409	-3.08996624	-1.67548113
N	-0.05078300	-2.83018622	-2.35878018
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$AATT_{DNA}$

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C	1.43037000	0.49916800	-1.88876600
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N	4.35491500	-1.74365700	0.89267400
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N	1.47708500	-2.41216200	-0.06348200
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N	2.31505400	0.59784600	2.68232600
C	3.28749400	-0.15934600	2.14541000
N	-4.11986500	-1.17512200	1.66880600
C	-2.78898100	-0.85207900	1.84501300
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N	-1.93784500	-1.40098200	0.91673100
C	-2.27558200	-2.20519600	-0.15744400
O	-1.38920300	-2.64481700	-0.89967100
C	-3.69182400	-2.47007900	-0.30935000
C	-4.15614000	-3.29099500	-1.47558100
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C	-1.78928400	2.71104100	0.63031600
O	-0.84048300	3.16806200	1.24356300
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C	-2.63698000	1.33634700	-1.22564700
O	-2.34614400	0.64597700	-2.19558200
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C	-5.13791500	0.99543700	-1.51116200
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H	0.74651400	-1.08215200	-2.95974200
H	-0.50193400	0.00278700	-2.39161200
H	1.60821600	3.15529900	0.00439300
H	6.29145500	-1.20703700	1.58625600
H	2.21667200	-2.88123400	-0.56188300
H	0.51924300	-2.48570700	-0.40627500
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$ATWC_{DNA}$

N	-4.94483308	0.52486182	-0.04366884
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C	-1.66500124	-0.75298465	0.04110328
N	-1.01042280	-1.90997997	-0.08958039
N	-0.95186792	0.36380260	0.30629913
C	-1.60469237	1.52778157	0.44274013
N	-2.90492336	1.77746814	0.36132102
C	-3.58555319	0.65074243	0.09984419
N	3.71243232	1.64652532	-0.27304850
C	2.34290128	1.59210783	-0.16282705
O	1.63553900	2.58007757	-0.25619411
N	1.83135955	0.33925205	0.05009791
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C	4.82363270	-1.94778945	0.07728493
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H	5.55053598	0.67382923	-0.31908386
H	-5.61884732	1.27114249	-0.00277834
H	4.10661602	2.54735088	-0.49528994

$AAST_{DNA}$

N	4.93337200	-0.65240100	1.56796300
C	4.78240000	0.48276100	2.33511800
N	3.53138400	0.77455300	2.61280400
C	2.80818700	-0.23000500	1.97837500
C	1.43037100	-0.49899700	1.88862500
N	0.48445400	0.24201200	2.47200800
N	1.05047300	-1.57732500	1.16821700
C	1.99665200	-2.32748000	0.58370400
N	3.31501400	-2.18183300	0.60047900
C	3.66096300	-1.10587200	1.32419500
N	4.64895400	0.06223700	-2.37004600
C	5.22266100	1.04416100	-1.59512400
N	4.35489400	1.74385600	-0.89281500
C	3.12438200	1.19164100	-1.23469100
C	1.79653800	1.47371000	-0.82005300
N	1.47705800	2.41233400	0.06334100
N	0.80269000	0.73058000	-1.34751700
C	1.11889700	-0.23368300	-2.22237290
N	2.31505600	-0.59766600	-2.68246700
C	3.28748900	0.15953500	-2.14555100
H	5.63406300	1.06461700	2.65710100
H	0.74650000	1.08231700	2.95960100
H	-0.50193800	-0.00263400	2.39147100
H	1.60824200	-3.15512600	-0.00453400
H	6.29144000	1.20725500	-1.58639700
H	2.21664100	2.88141300	0.56174200
H	0.51921500	2.48587000	0.40613400
H	0.26972000	-0.79608700	-2.60133100
H	5.78541900	-1.04996200	1.20898800
H	5.10105300	-0.60127300	-2.97811100

$ATST_{DNA}$

N	0.88073981	1.53141505	-1.89001719
C	1.02746884	2.51306250	-0.93678599

N	1.48501423	2.07133484	0.21709095
C	1.64239914	0.70386279	0.01368529
C	2.11178487	-0.34349651	0.84850682
N	2.52742622	-0.16916359	2.09771550
N	2.14941209	-1.58888401	0.33273759
C	1.75288987	-1.76959539	-0.93428966
N	1.30262457	-0.87612203	-1.81406713
C	1.27069968	0.35512608	-1.27539202
N	-2.10349667	-1.10505884	-1.08747144
C	-1.54253007	-1.85507549	-0.08355568
O	-1.33542164	-3.05002171	-0.19102383
N	-1.23458644	-1.15562402	1.05573657
C	-1.43041136	0.19197695	1.28420167
O	-1.08093028	0.68953378	2.35597040
C	-2.04684199	0.92048852	0.18835702
C	-2.32731343	2.38055991	0.35350439
C	-2.34331284	0.24232190	-0.92854920
H	0.78018387	3.54523283	-1.14398724
H	1.80564525	-2.79801584	-1.27989578
H	-2.69158511	2.82007104	-0.57927195
H	-1.42092283	2.90658503	0.66685194
H	-3.07745546	2.54875958	1.13279111
H	-2.79377365	0.72993733	-1.78710463
H	0.59495122	1.62981525	-2.85033340
H	2.92463900	-0.94880913	2.62304861
H	2.57284482	0.76463095	2.47256684
H	-0.84403480	-1.72700591	1.82934748
H	-2.25860980	-1.57796698	-1.96375508

ATWC

N	-4.1463095	0.0276066	0.4989510
C	-4.1783269	0.0241149	1.8693855
C	-3.0503934	0.0075345	2.6143561
C	-1.7764463	-0.0075165	1.9134149
N	-1.8409343	-0.0044729	0.5342848
C	-2.9776615	0.0158134	-0.2412098
C	-3.0337782	0.0039661	4.1067561
O	-0.6903188	-0.0223257	2.4988523
O	-2.9710806	0.0231200	-1.4594154
N	0.6342733	-0.0396251	-0.8445604
C	1.8085815	-0.0725030	-0.1925510
C	2.9816390	-0.0450617	-0.9713088
C	2.8096988	0.0150597	-2.3538115
N	1.6523629	0.0464189	-3.0268028
C	0.6173449	0.0155645	-2.1932329
N	4.3110053	-0.0631092	-0.6210230
C	4.9362856	-0.0138224	-1.7844380
N	4.0874208	0.0345553	-2.8553711
N	1.8292763	-0.1390909	1.1445440
H	-0.3707005	0.0368460	-2.6349270
H	6.0061912	-0.0105896	-1.9082208
H	4.3375082	0.0791089	-3.8297046
H	0.9607282	-0.0976204	1.6743842
H	2.7192948	-0.1141775	1.6075837
H	-4.9945252	0.0435817	-0.0428232
H	-0.9349425	-0.0189830	0.0123682
H	-5.1632478	0.0355348	2.3150232
H	-2.5162678	-0.8784794	4.4795452
H	-2.4928573	0.8705738	4.4831417
H	-4.0449522	0.0166200	4.5078085

ATST

N	0.2793014	2.4068393	-0.6057517
C	-1.0848570	2.4457461	-0.5511608
H	-1.6594403	3.0230294	-1.2560905
N	-1.5977117	1.7179877	0.4287543
C	-0.4897255	1.1714358	1.0301910
C	-0.3461366	0.2914710	2.1172343
N	-1.4187090	-0.1677767	2.8101441

H	-1.2388750	-0.9594802	3.4047578
H	-2.2918734	-0.1788223	2.3073619
N	0.8857630	-0.0700763	2.4919494
C	1.9352348	0.4072878	1.7968022
H	2.9060330	0.0788414	2.1458181
N	1.9409775	1.2242019	0.7402202
C	0.6952186	1.5779858	0.4063984
H	0.8610073	2.8298045	-1.3104502
N	1.2754606	-0.6478993	-1.9779104
C	1.4130533	-1.5536850	-0.9550667
H	2.4258769	-1.8670780	-0.7468778
C	0.3575976	-2.0239499	-0.2530575
C	0.4821292	-3.0179494	0.8521221
H	0.1757705	-2.5756065	1.7986281
H	-0.1601691	-3.8770412	0.6639498
H	1.5112443	-3.3572767	0.9513659
C	-0.9684711	-1.5298112	-0.5939792
O	-2.0029280	-1.8396957	-0.0199453
N	-0.9956916	-0.6383870	-1.6720420
H	-1.9014057	-0.2501720	-1.8985760
C	0.0684702	-0.1191762	-2.3763759
O	-0.0397875	0.7227006	-3.2531083
H	2.0853289	-0.2760176	-2.4454577

ATHB

H	5.990680	0.261936	0.007501
H	5.818471	2.006005	0.007529
N	5.408496	1.085033	0.009942
C	4.063858	0.957723	0.006878
N	3.916164	-1.595541	0.005675
N	3.302013	2.071889	0.005763
C	3.430653	-0.302343	0.005408
C	2.827886	-2.337474	0.003632
H	2.815707	-3.419133	0.003179
C	1.969674	1.936226	0.003504
C	2.031727	-0.293949	0.003158
H	1.402969	2.864153	0.002647
N	1.658956	-1.610112	0.002120
N	1.250614	0.805001	0.002169
H	0.680973	-1.938493	-0.000302
H	-0.528210	0.451838	0.000450
O	-1.091749	-2.045098	-0.004659
N	-1.543977	0.213925	0.004308
C	-1.902639	-1.109138	0.002315
H	-2.051103	2.230064	0.012779
C	-2.474534	1.230957	0.012025
H	-5.480364	2.043824	0.907311
N	-3.263880	-1.330159	0.008941
H	-3.558801	-2.300286	0.007696
C	-3.814118	1.020988	0.018347
C	-4.290346	-0.362473	0.017006
H	-4.344720	3.103667	0.029706
C	-4.832907	2.123496	0.026392
O	-5.464084	-0.713025	0.022360
H	-5.485207	2.052483	-0.851747

AAHB

H	6.306448	0.877476	0.000000
H	2.349822	3.024994	0.000000
N	3.925667	1.700061	0.000000
C	2.613107	1.970068	0.000000
N	5.636908	0.123873	0.000000
H	5.942501	-0.836834	0.000000
C	4.316045	0.408860	0.000000
H	-1.820123	3.393478	0.000000
N	1.588242	1.107244	0.000000
C	-2.152511	2.363801	0.000000
H	-0.208865	1.373792	0.000000
C	3.333710	-0.602690	0.000000

C	2.000326	-0.177295	0.000000
N	-1.250714	1.323859	0.000000
N	-3.413164	1.981441	0.000000
N	3.413164	-1.981441	0.000000
C	-2.000326	0.177295	0.000000
N	1.250714	-1.323859	0.000000
C	-3.333710	0.602690	0.000000
C	2.152511	-2.363801	0.000000
H	-5.942501	0.836834	0.000000
H	0.208865	-1.373792	0.000000
N	-1.588242	-1.107244	0.000000
C	-4.316045	-0.408860	0.000000
H	1.820123	-3.393478	0.000000
N	-5.636908	-0.123873	0.000000
C	-2.613107	-1.970068	0.000000
H	-6.306448	-0.877476	0.000000
N	-3.925667	-1.700061	0.000000
H	-2.349822	-3.024994	0.000000

AAST

H	-2.834372	-2.827774	-0.095099
C	-2.421533	-1.857494	0.171482
H	0.442668	-2.516571	-2.043933
N	-1.323100	-1.891033	0.943320
N	-3.065728	-0.790733	-0.316879
H	-0.928707	-0.561356	-2.960494
N	0.614423	-1.544828	-1.830351
C	-0.107607	-0.452301	-2.265103
C	-0.761276	-0.726192	1.321946
H	0.839972	-1.641867	2.144645
C	-2.482886	0.349426	0.075717
N	2.475946	-1.759533	-0.259924
C	1.554458	-1.071273	-0.946647
N	0.344779	-0.761835	2.105687
C	-1.354948	0.480375	0.893590
H	-3.595994	1.913570	-0.847909
N	-2.829181	1.640046	-0.251020
N	0.295696	0.680578	-1.739903
C	1.338274	0.311867	-0.906540
H	0.898484	0.078440	2.187841
C	3.209461	-0.955007	0.515907
H	3.992645	-1.434327	1.098545
N	-1.009173	1.811920	1.058031
C	-1.910075	2.463900	0.360341
N	3.094086	0.374890	0.687700
C	2.152899	1.037196	-0.012626
H	-1.960350	3.539627	0.255504
H	1.089813	2.746140	-0.001399
N	2.018292	2.379496	0.164606
H	2.508140	2.761539	0.962679

TTHB

H	3.130831	2.438223	0.000000
H	-2.708747	2.322662	0.000000
H	-5.148886	2.638728	0.000000
H	-6.009205	1.347009	0.879542
O	5.350666	1.332647	0.000000
N	3.067800	1.426206	0.000000
O	0.784875	1.608956	0.000000
C	-5.394886	1.572015	0.000000
C	-2.893721	1.253796	0.000000
H	-0.818910	0.915296	0.000000
C	4.290942	0.719485	0.000000
C	1.798611	0.893983	0.000000
H	-6.009205	1.347009	-0.879542
C	-4.147361	0.737321	0.000000
N	-1.755734	0.474501	0.000000
N	1.755734	-0.474501	0.000000
C	4.147361	-0.737321	0.000000

H	6.009205	-1.347009	-0.879542
C	-1.798611	-0.893983	0.000000
C	-4.290942	-0.719485	0.000000
H	0.818910	-0.915296	0.000000
C	2.893721	-1.253796	0.000000
C	5.394886	-1.572015	0.000000
O	-0.784875	-1.608956	0.000000
N	-3.067800	-1.426206	0.000000
O	-5.350666	-1.332647	0.000000
H	6.009205	-1.347009	0.879542
H	5.148886	-2.638728	0.000000
H	2.708747	-2.322662	0.000000
H	-3.130831	-2.438223	0.000000

TTST

C	-0.680221	1.774938	-0.220433
C	-0.909771	1.428567	1.185427
C	-1.687305	0.354917	1.461178
N	-2.291157	-0.398883	0.477311
C	-2.078218	-0.187653	-0.876689
H	-2.686138	-1.300805	0.710897
N	-1.350902	0.958864	-1.147564
O	0.041940	2.687894	-0.606706
O	-2.477344	-0.959153	-1.737834
H	-1.093075	1.085521	-2.121737
H	-1.874649	0.019738	2.475335
C	-0.226996	2.251180	2.237770
H	-0.513311	1.917253	3.240710
H	-0.481919	3.311161	2.128313
H	0.862999	2.178698	2.134214
H	3.557202	0.755276	-1.768558
C	2.178382	-0.009343	-0.312703
C	1.229646	-0.683299	-1.206033
C	2.209109	-0.389927	0.985345
C	3.015807	1.097282	-0.879976
C	0.383529	-1.991315	0.751868
N	1.368320	-1.362854	1.496083
N	0.421519	-1.660194	-0.588812
O	1.090837	-0.439030	-2.397053
O	-0.440978	-2.752638	1.244920
H	1.379151	-1.592362	2.479478
H	2.885548	0.060402	1.703687
H	-0.295345	-2.081241	-1.174661
H	3.732447	1.462516	-0.136944
H	2.366338	1.926515	-1.185291