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

Supporting Information

The R- and S-diastereoisomeric effects on the Guanidinohydantoin-Induced Mutations in DNA

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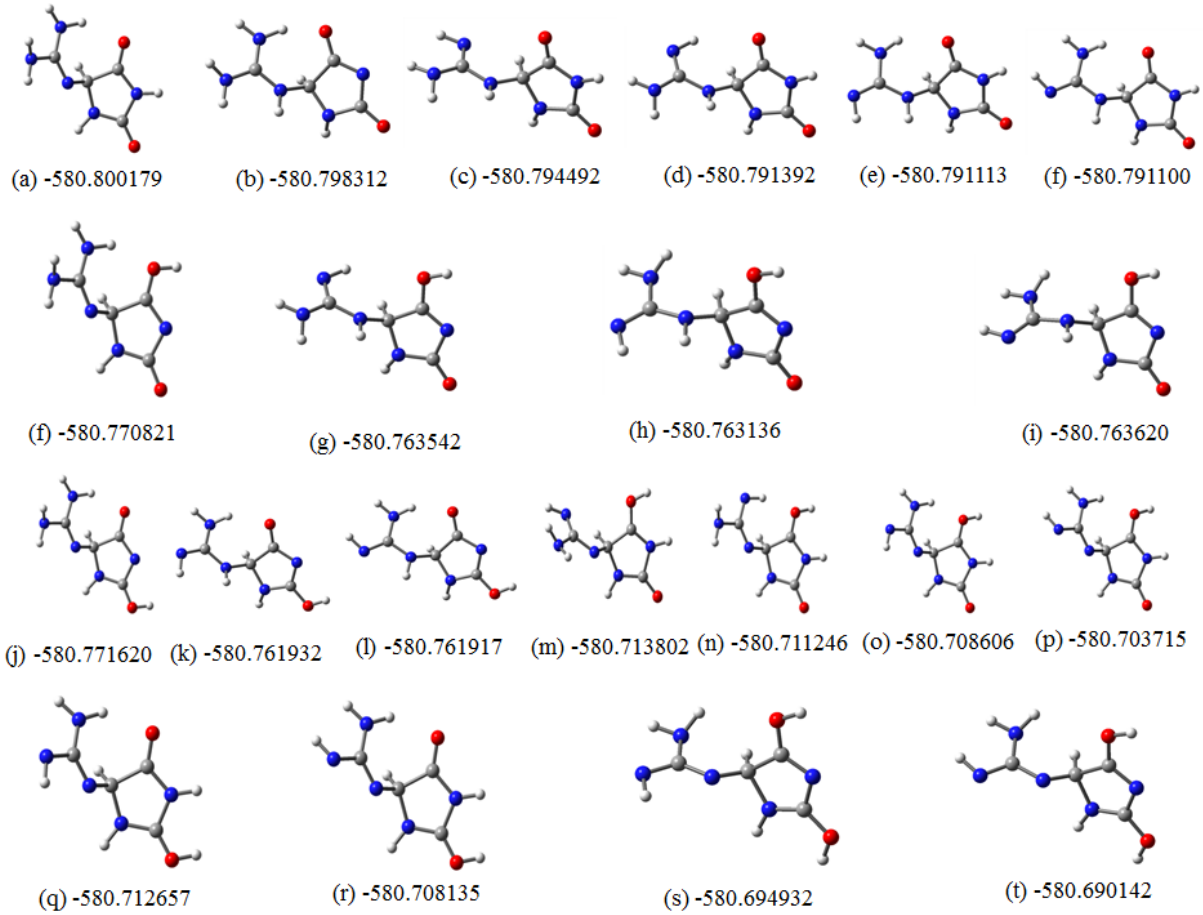

Fig. S1: Optimized structures of different tautomers of Gh1-R in aqueous medium. The ZPEC total energies (a.u.) are provided for comparison of stabilities of different tautomers. The structure presented in (a) is the most stable tautomer of Gh1-R and the structures presented in (d) and (f) were observed in the ^{1}H NMR studies [Ref 39,40]. It should be noted that the tautomers presented in lines 2-4 are about 20-70 kcal/mol less stable than the most stable tautomer shown in (a). Hence these tautomers may not be observed in DNA.

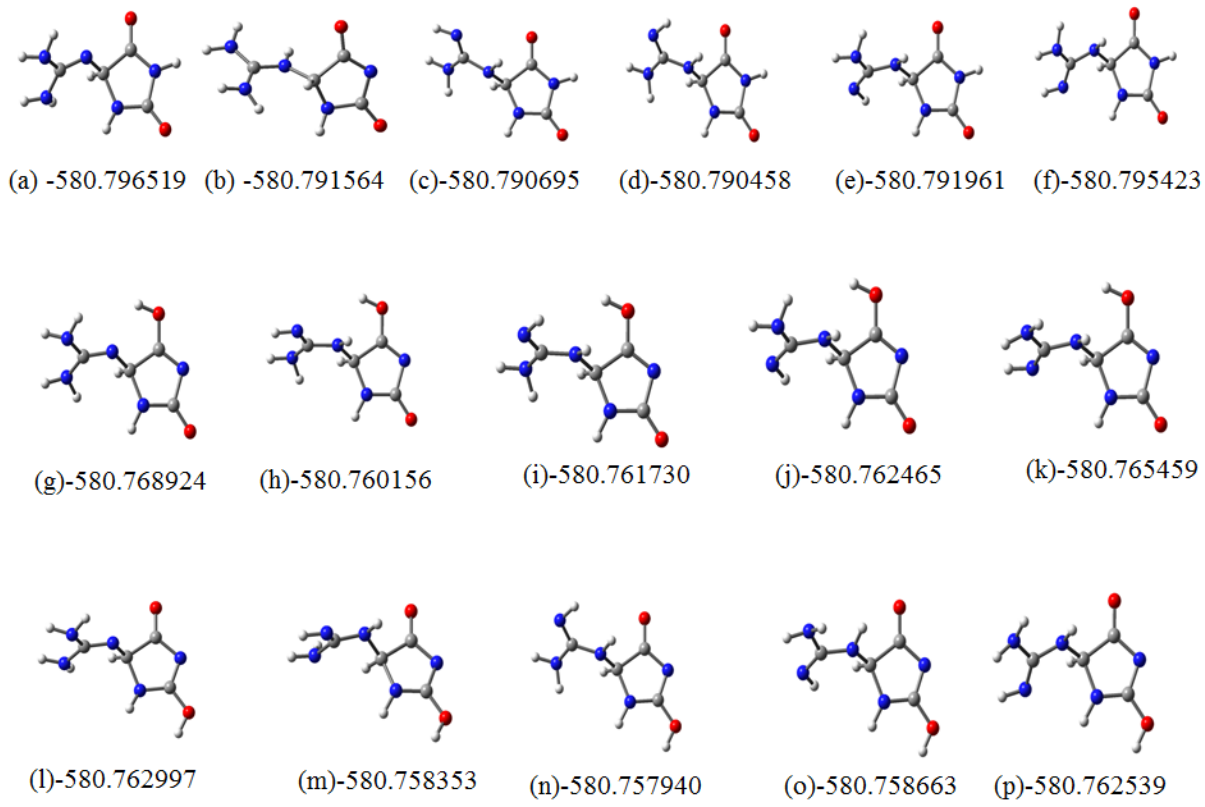

Fig. S2: Optimized structures of different tautomers of Gh2-R in aqueous medium. The ZPEC total energies (a.u.) are provided for the comparison of stabilities of different tautomers. The structure presented in (a) is the most stable tautomer of Gh2-R. It should be noted that the tautomers presented in lines 2-3 are about 17-24 kcal/mol less stable than the most stable tautomer shown in (a). Hence these tautomers may not be observed in DNA.

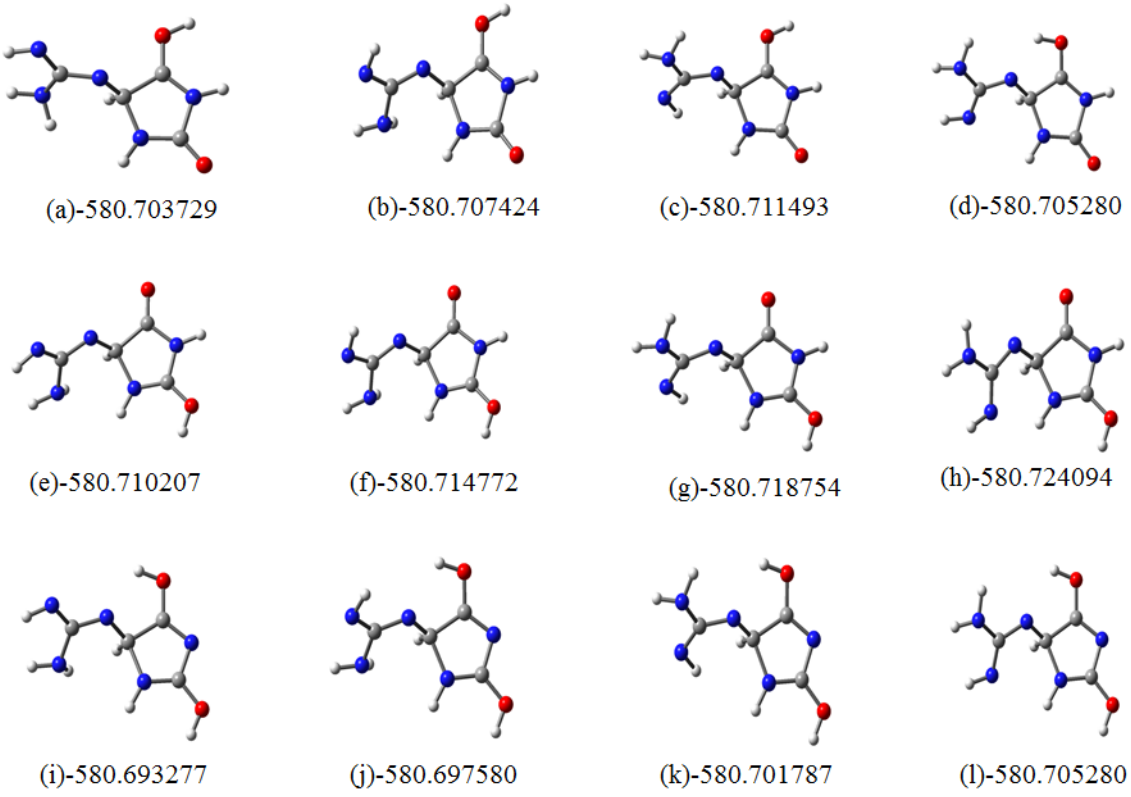

Fig. S3: Optimized structures of different tautomers of Gh2-R in aqueous medium. The ZPEC total energies (a.u.) are provided for comparison of stabilities of different tautomers. It should be noted that these tautomers are about 46-65 kcal/mol less stable than the most stable tautomer shown in Fig. S2(a). Hence these tautomers may not be observed in DNA.

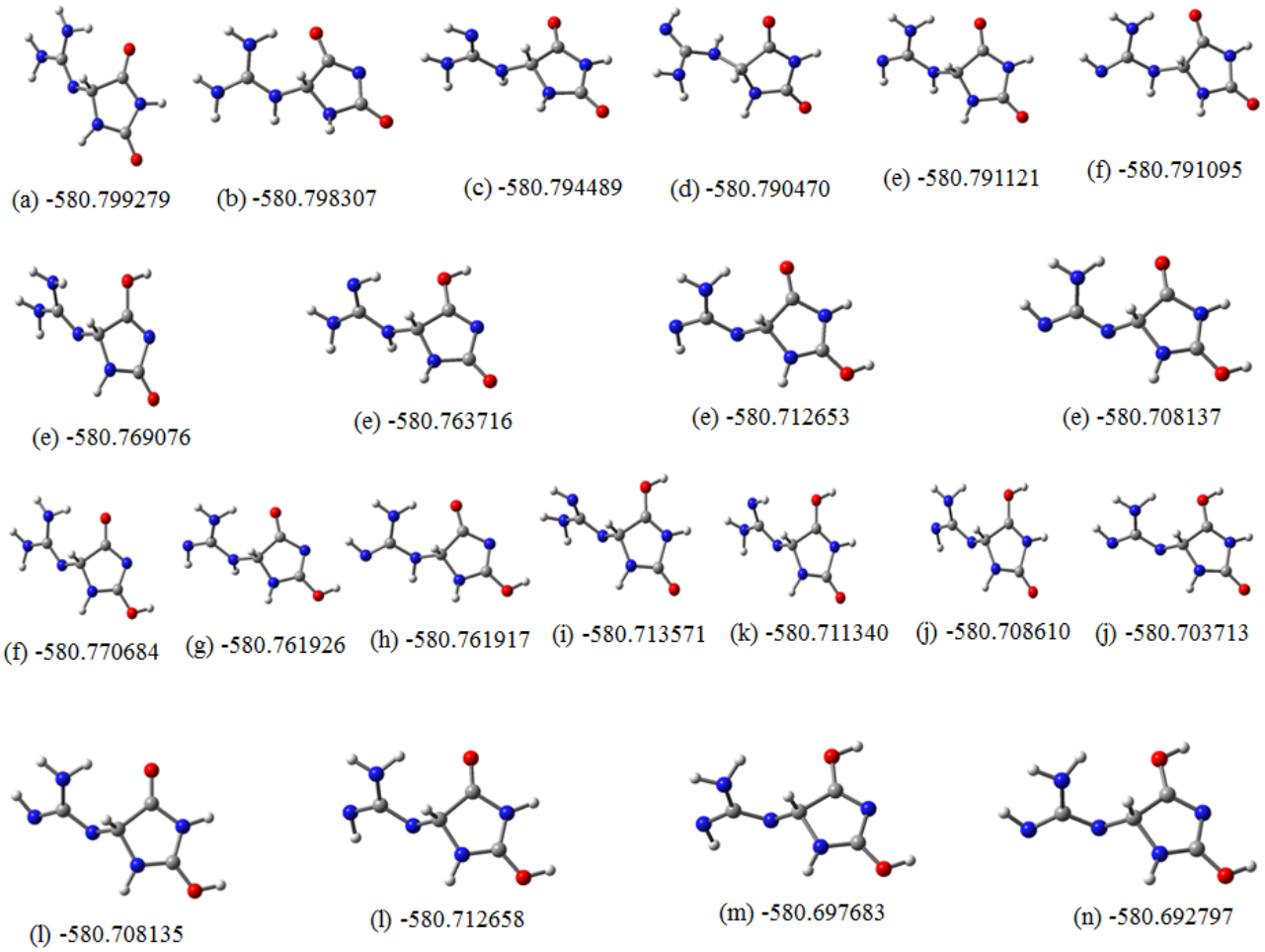

Fig. S4: Optimized structures of different tautomers of Gh1-S in aqueous medium. The ZPEC total energies (a.u.) are provided for comparison of stabilities of different tautomers. The structure presented in (a) is the most stable tautomer of Gh1-S and other tautomers are quite unstable and hence would not be observed in DNA.

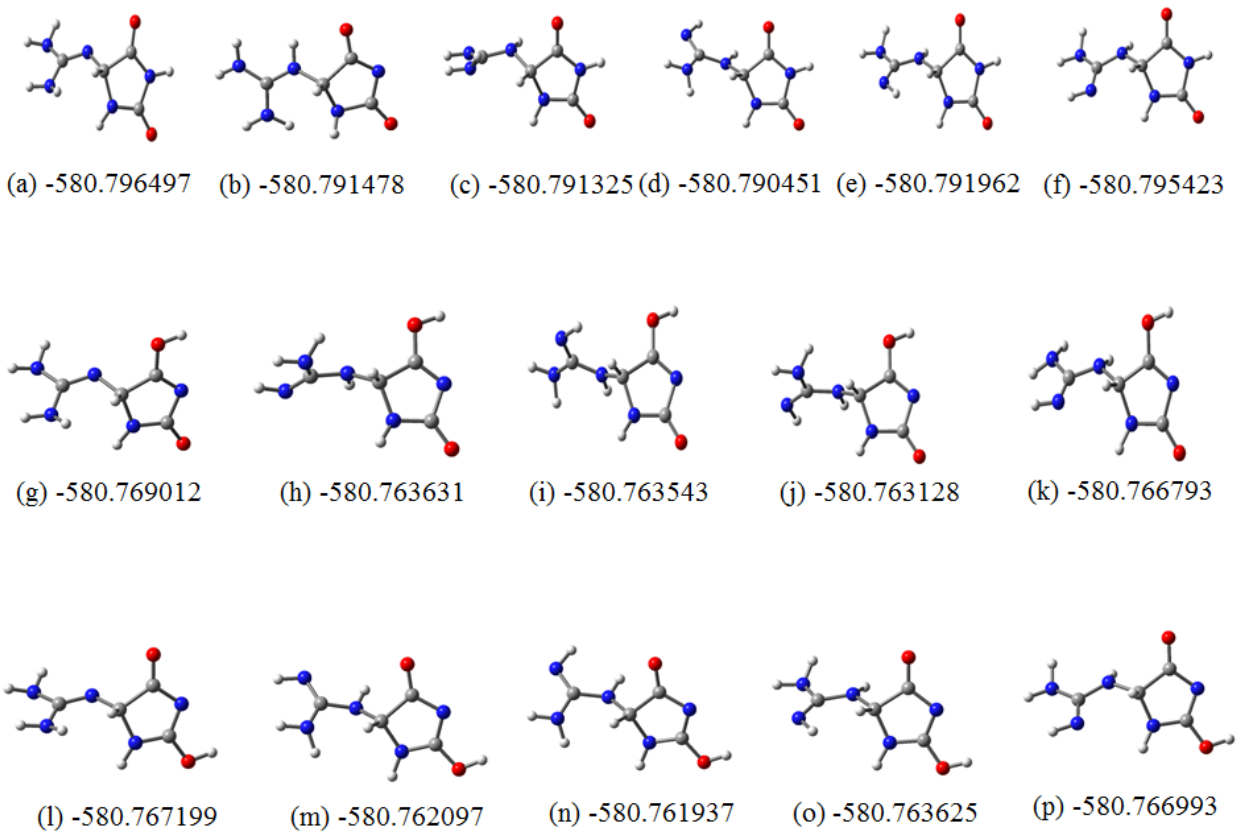

Fig.S5: Optimized structures of different tautomers of Gh2-S in aqueous medium. The ZPEC total energies (a.u.) are provided for comparison of stabilities of different tautomers. The structure presented in (a) is the most stable tautomer of Gh2-S and other tautomers are quite unstable and hence would not be observed in DNA.

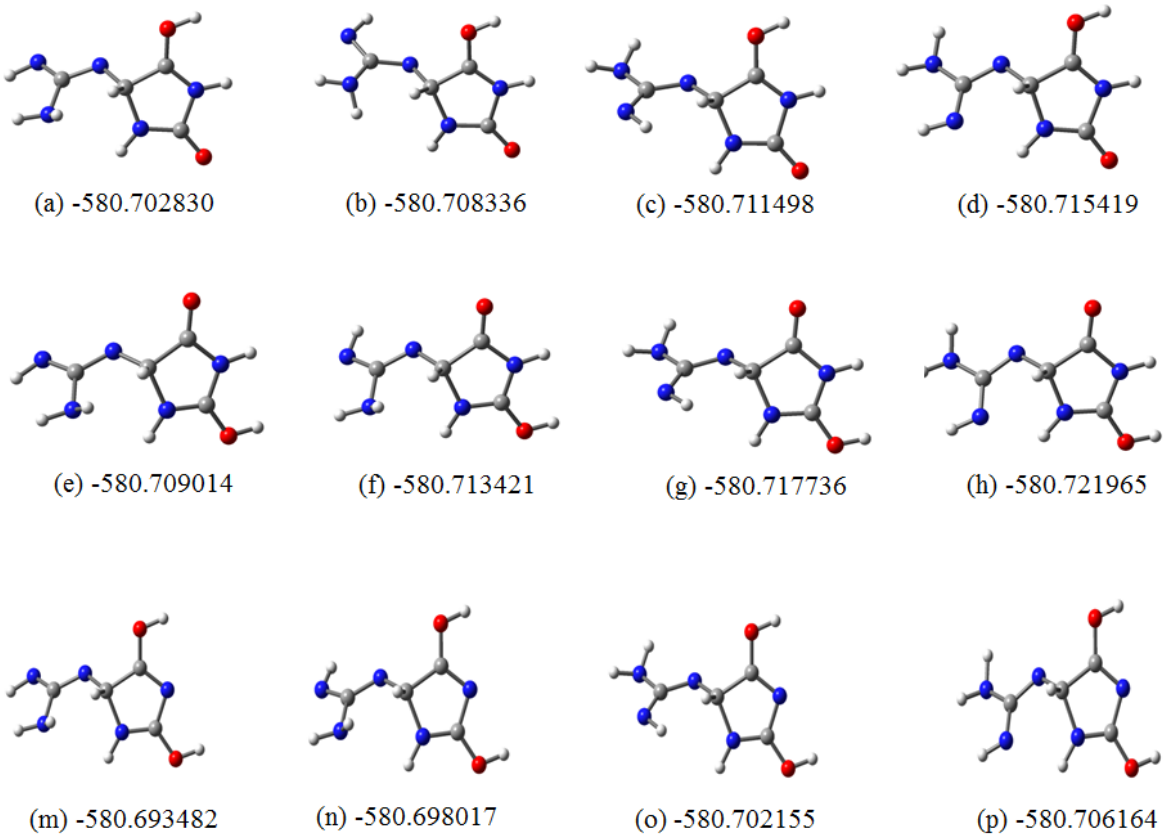

Fig.S6: Optimized structures of different tautomers of Gh2-S in aqueous medium. The ZPEC total energies (a.u.) are provided for comparison of stabilities of different tautomers. Due to relatively less stability compared to Fig. S5(a), these tautomers may not be observed in DNA.

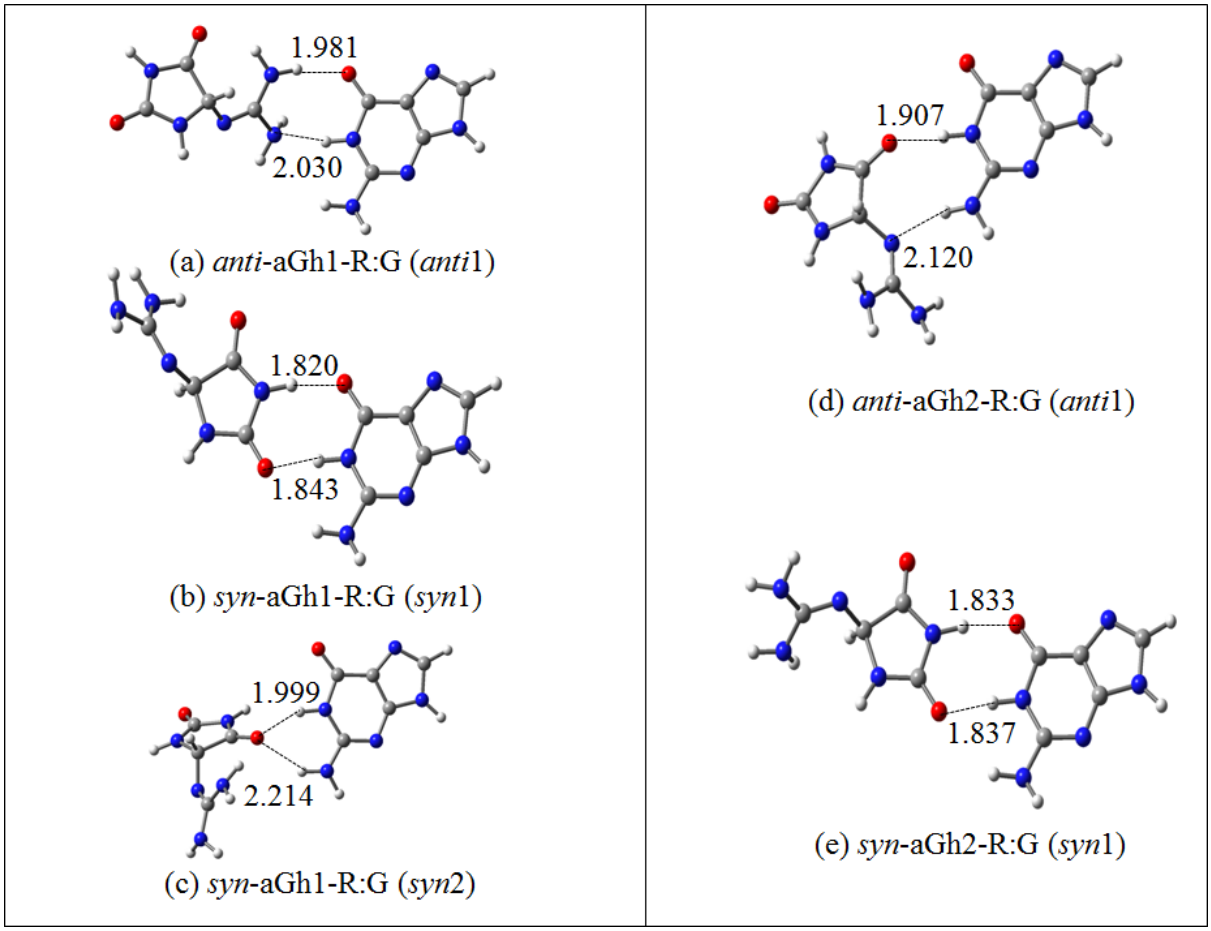

Fig. S7. Optimized structures of base pair complexes in aqueous media: (a-c) aGh1-R:G and (d,e) aGh2-R:G. Hydrogen bonds are shown by dotted lines. Here *anti*1 represents only one conformation of *anti*-aGh1-R and *anti*-aGh2-R each while *syn*1-*syn*2 represents different conformations of *syn*-aGh1-R and *syn*-aGh2-R.

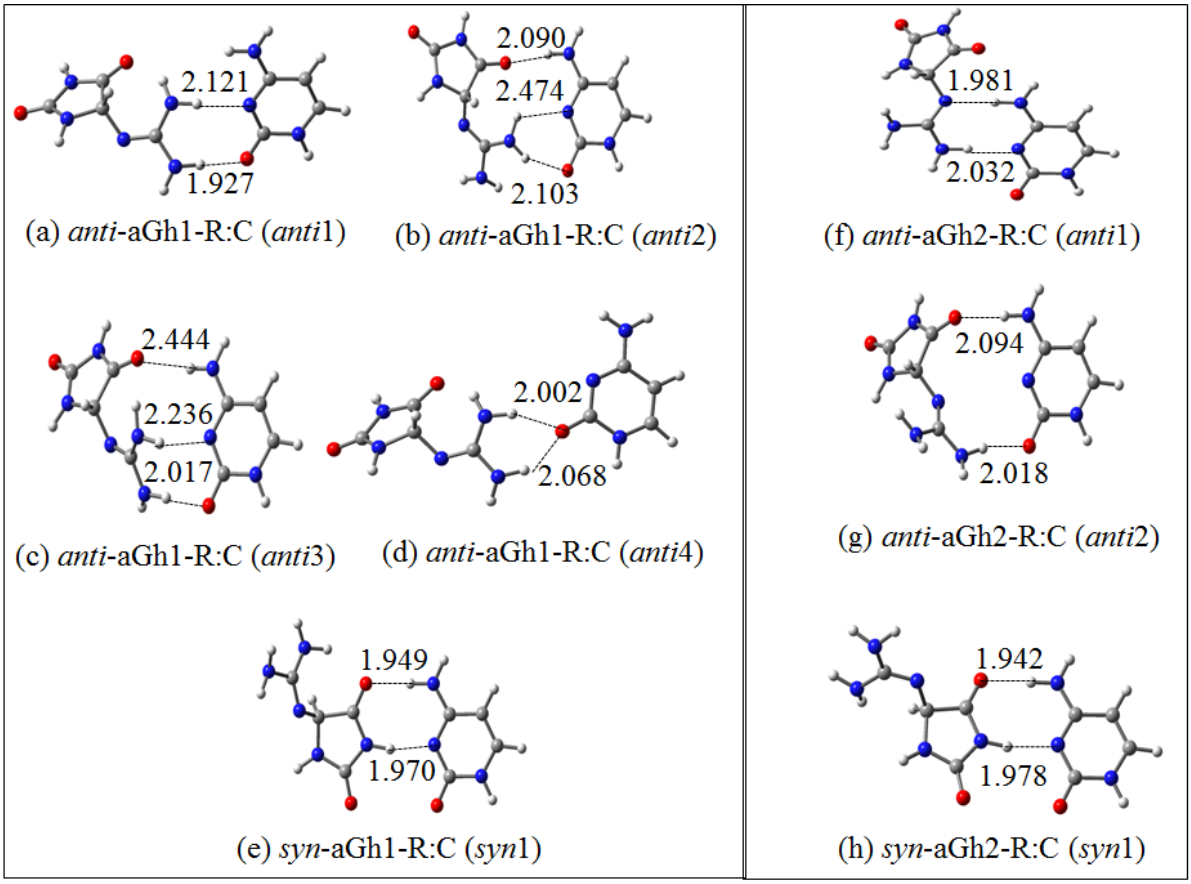

Fig. S8. Optimized structures of complexes involving cytosine in aqueous media: (a-e) aGh1-R:C and (f-h) aGh2-R:C. Hydrogen bonds are shown by dotted lines. Here *anti*1-anti4 represent different conformations of *anti*-aGh1-R and *anti*-aGh2-R while *syn*1 represents only one conformation of *syn*-aGh1-R and *syn*-aGh2-R each.

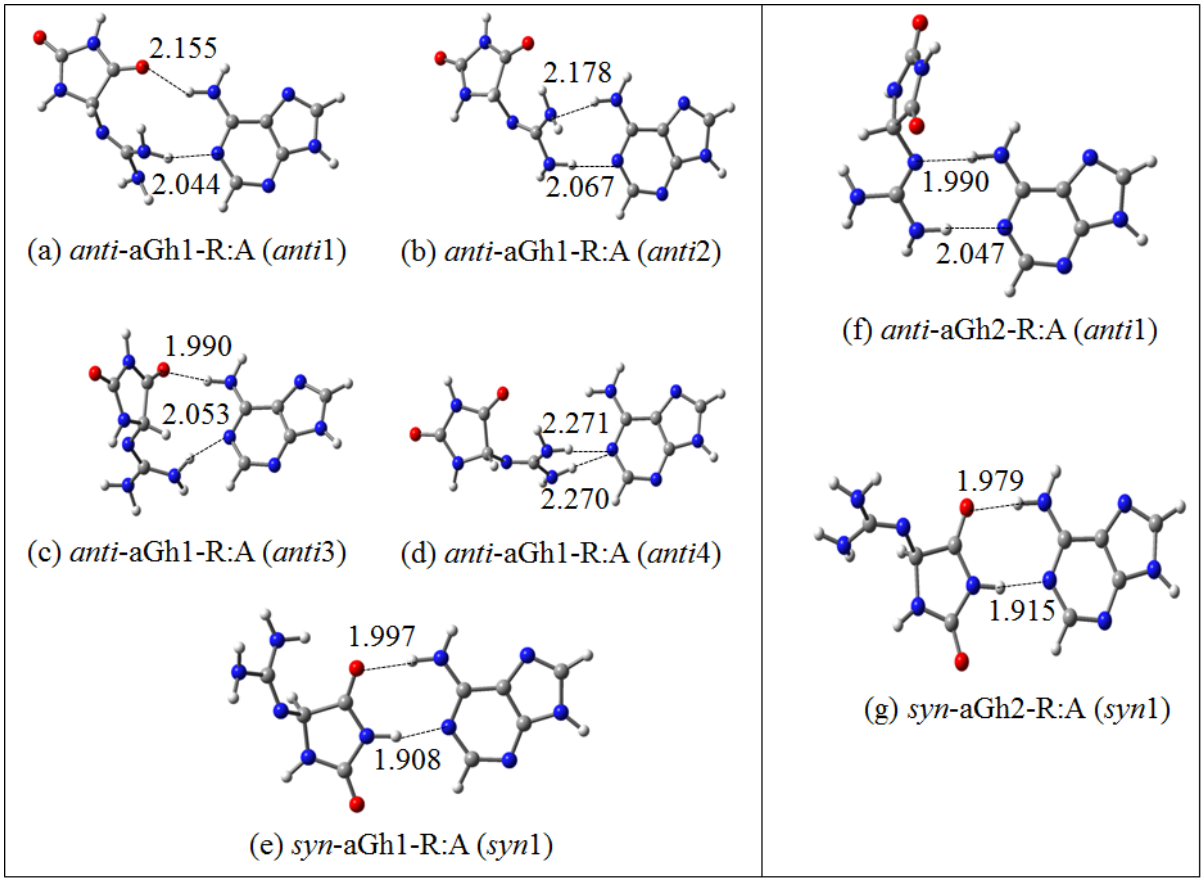

Fig. S9. Optimized structures of complexes involving adenine in aqueous media:(a-e) aGh1-R:A and (f-g) aGh2-R:A. Hydrogen bonds are shown by dotted lines. Here *anti*1-anti4 represent different conformations of *anti*-aGh1-R and *anti*-aGh2-R while *syn*1 represents only one conformation of *syn*-aGh1-R and *syn*-aGh2-R each.

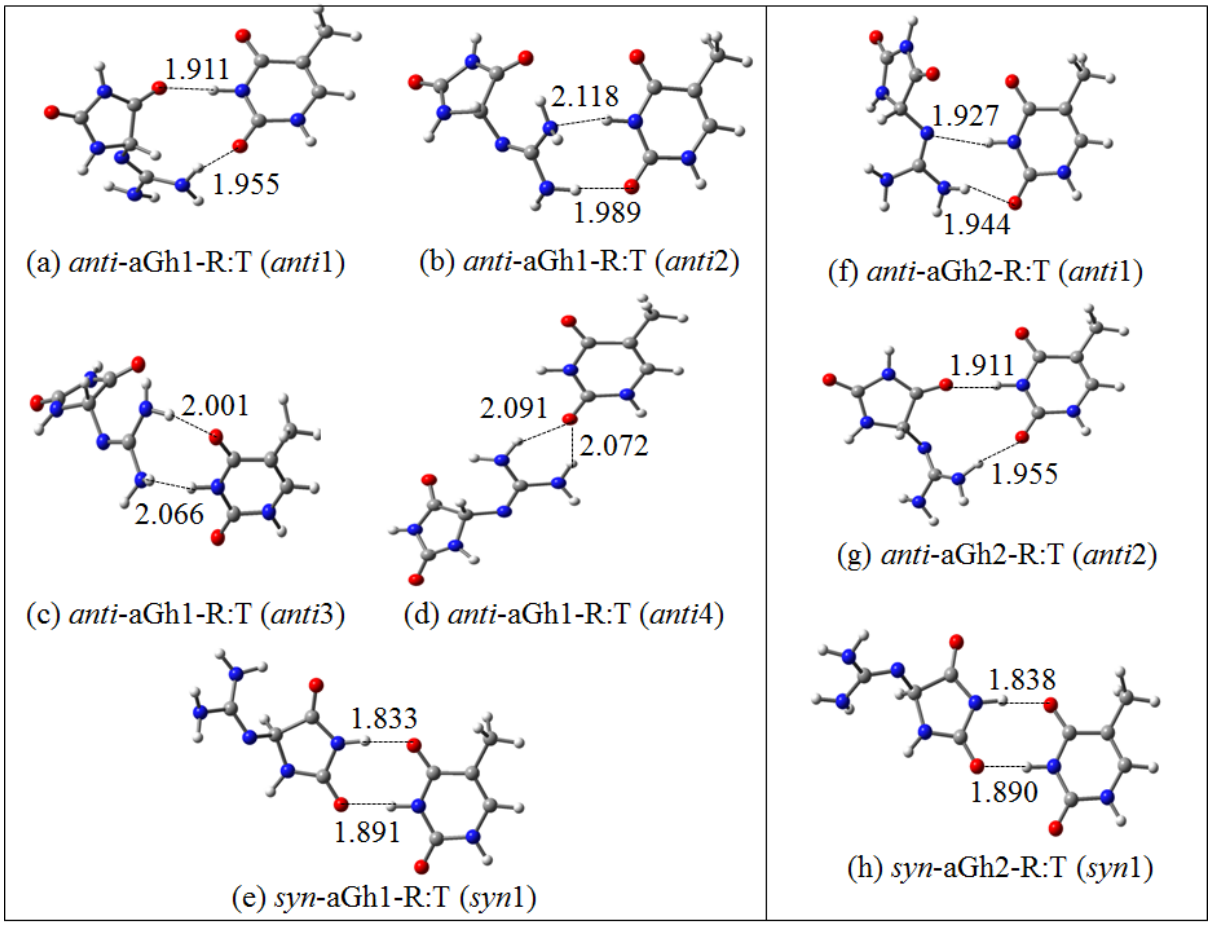

Fig. S10. Optimized structures of complexes involving thymine in aqueous media: (a-e) aGh1-R:T complex and (f-h) aGh2-R:T complex. Hydrogen bonds are shown by dotted lines. Here *anti*1-anti4 represent different conformations of *anti*-aGh1-R and *anti*-aGh2-R while *syn*1 represents only one conformation of *syn*-aGh1-R and *syn*-aGh2-R each.

Table S1. Zero-point energy-corrected binding energies (kcal/mol) of different base pair complexes involving aGh1-Rand aGh2-R in aqueous medium. For comparison, the ZPE-corrected binding energies of T:G, G:C, and A:T base pair complexes in aqueous medium are given in parentheses. Absence of entry shows that the corresponding structure does not exist. Here *anti*1 to *anti*4 represent different possible conformations of *anti*-aGh1-R and *anti*-aGh2-R while *syn*1 to *syn*2 represent different possible conformations of *syn*-aGh1-R and *syn*-aGh2-R (Figs 2-5).

Base Pair	Method	aGh1-R						aGh2-R		
		*anti*1	*anti*2	*anti*3	*anti*4	*syn*1	*syn*2	*anti*1	*anti*2	*syn*1
Gh:G **(T:G)**	B3LYP	-4.21 **(-7.41)**				-8.01	-3.74	-5.27		-7.79
	ωB97XD	-7.41 **(-10.82)**				-11.26	-5.97	-9.18		-11.05
Gh:C **(G:C)** [a]	B3LYP	-5.49 **(-11.63)**	-3.32	-2.95	-4.20	-5.94		-5.81	-3.21	-6.15
	ωB97XD	-8.31 **(-16.26)**	-6.39	-7.01	1.74	-9.20		-10.24	-5.32	-9.34
Gh:A **(A:T)**[a]	B3LYP	-2.74 **(-6.57)**	-2.25	-1.64	-3.00	-6.30		-5.93		-6.48
	ωB97XD	-6.27 **(-10.30)**	-5.39	-5.33	-6.18	-9.61		-9.87		-9.71
Gh:T	B3LYP	-4.37	-5.47	-2.87	-2.94	-6.83		-6.04	-2.47	-6.89
	ωB97XD	-7.16	-5.59	-5.93	-4.29	-9.59		-11.17	-4.33	-9.71

[a] Ref [51,54].

Table S2. Zero-point energy-corrected (ZPEC) binding energies (kcal/mol) of different base pair complexes involving aGh1-R and aGh2-R in the gas phase. Absence of entry shows that the corresponding structure does not exist. Here *anti*1-*anti*4 represent different conformations of *anti*-aGh1-R and *anti*-aGh2-R while *syn*1-*syn*4 represent different conformations of *syn*-aGh1-R and *syn*-aGh2-R.

Base Pair	Method	aGh1-R						aGh2-R		
		*anti*1	*anti*2	*anti*3	*anti*4	*syn*1	*syn*2	*anti*1	*anti*2	*syn*1
Gh:G	B3LYP	-10.43				-16.28				
	ωB97XD	-23.62				-27.81				
Gh:C	B3LYP	-10.65	-8.61	-12.04	-10.66	-10.05				
	ωB97XD	-22.51	-20.87	-21.83	1.29	-23.20				
Gh:A	B3LYP	-6.15	-5.44	-6.12	-6.09	-10.34				
	ωB97XD	2.44	-14.30	-3.46	-15.34	-18.52				
Gh:T	B3LYP	-6.97	-6.59	-6.50	-5.90	-10.98				
	ωB97XD	-15.99	-14.80	-15.63	-15.25	-19.44				

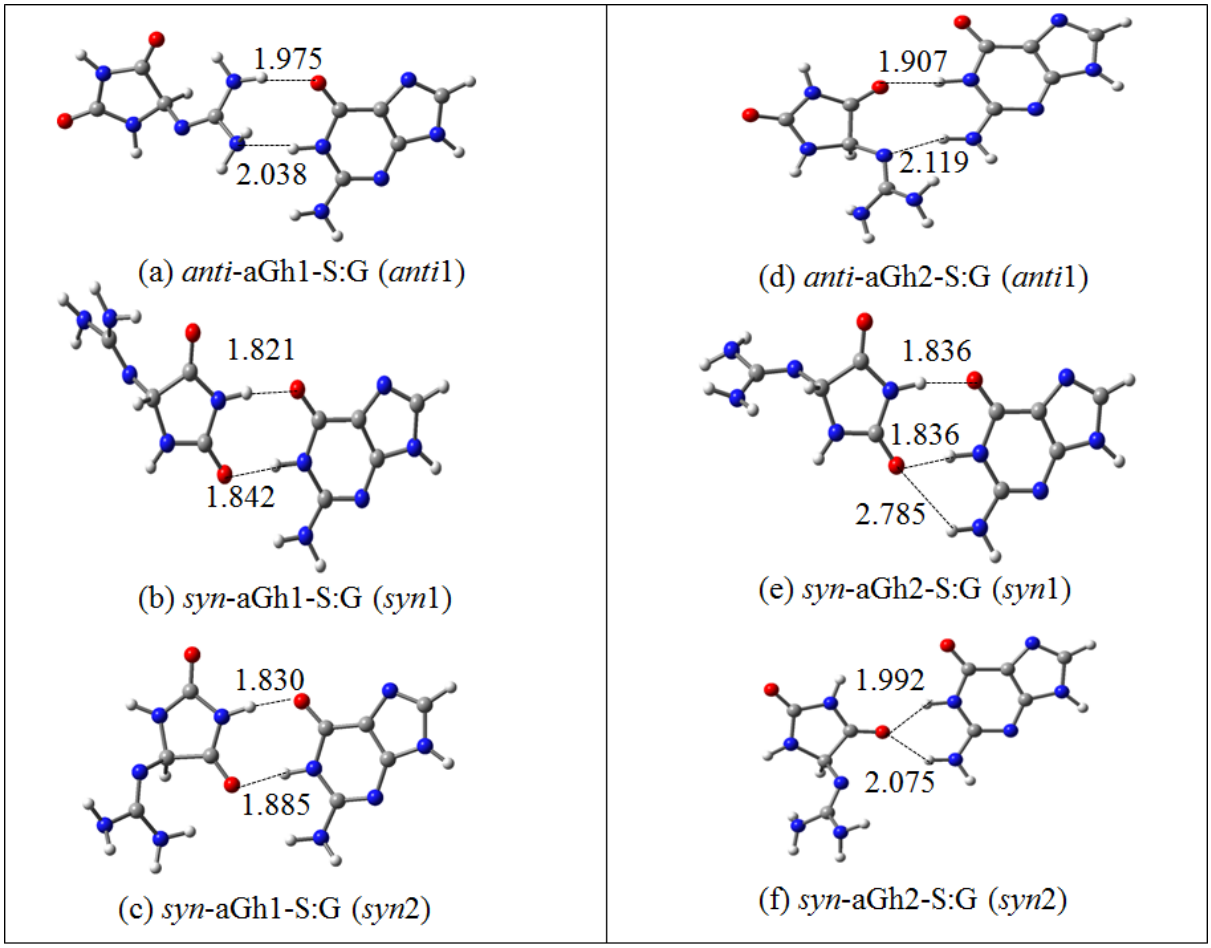

Fig. S11.Optimized structures of complexes of aGh1-S and aGh2-S with guanine in aqueous media: (a-c) aGh1-S:G and (d-f) aGh2-S:G. Hydrogen bonds are shown by dotted lines. Here *anti*1 represents only one conformation of *anti*-aGh1-R and *anti*-aGh2-R each while *syn*1-*syn*2 represent two different possible conformations of *syn*-aGh1-R and *syn*-aGh2-R.

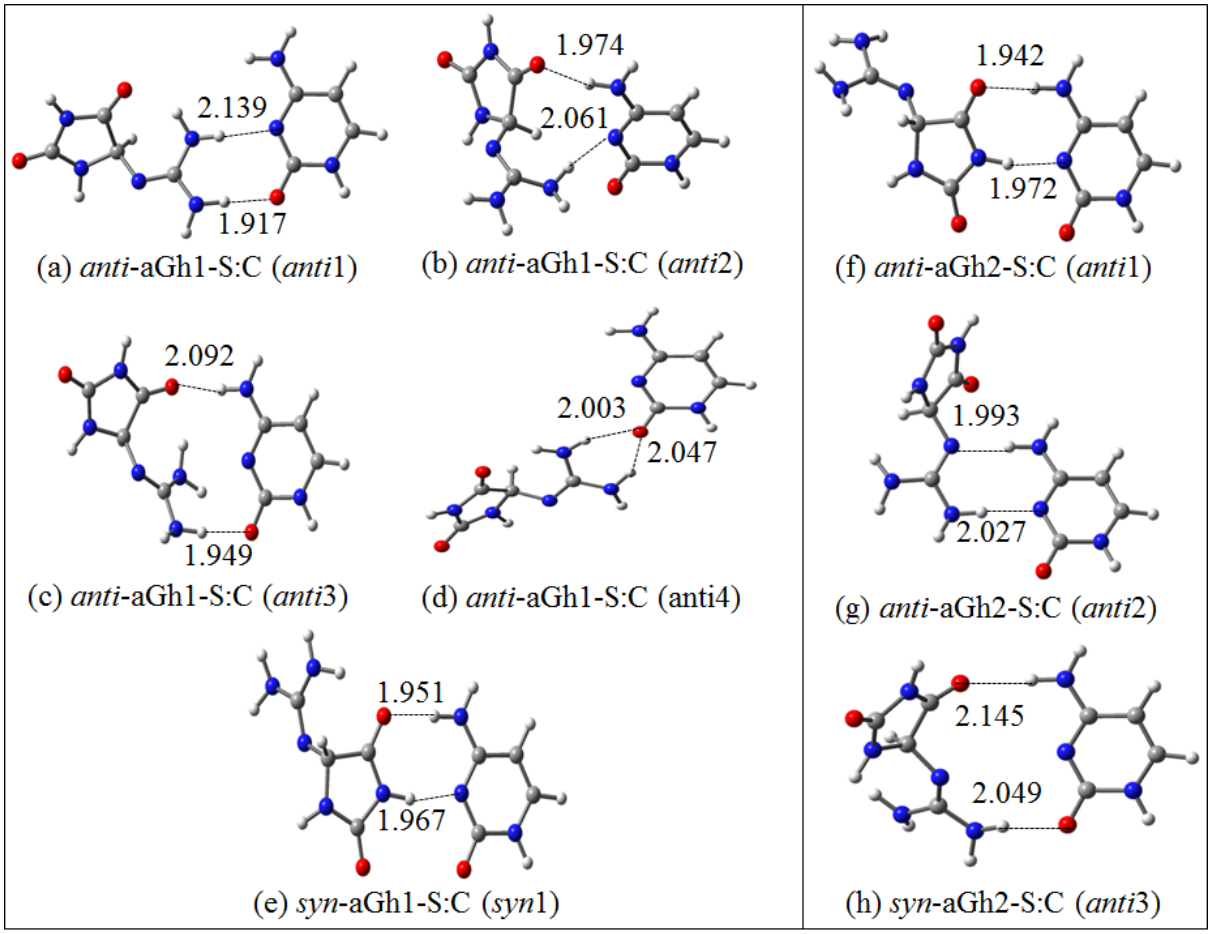

Fig. S12.Optimized structures of complexes of aGh1 and aGh2 with cytosine in aqueous meda: (a-e) aGh1-S:C and (f-h) aGh2-S:C. Hydrogen bonds are shown by dotted lines. Here *anti*1-*anti*4 represent different possible conformations of *anti*-aGh1-R and *anti*-aGh2-R while *syn*1 represents only one conformation of *syn*-aGh1-R and *syn*-aGh2-R each.

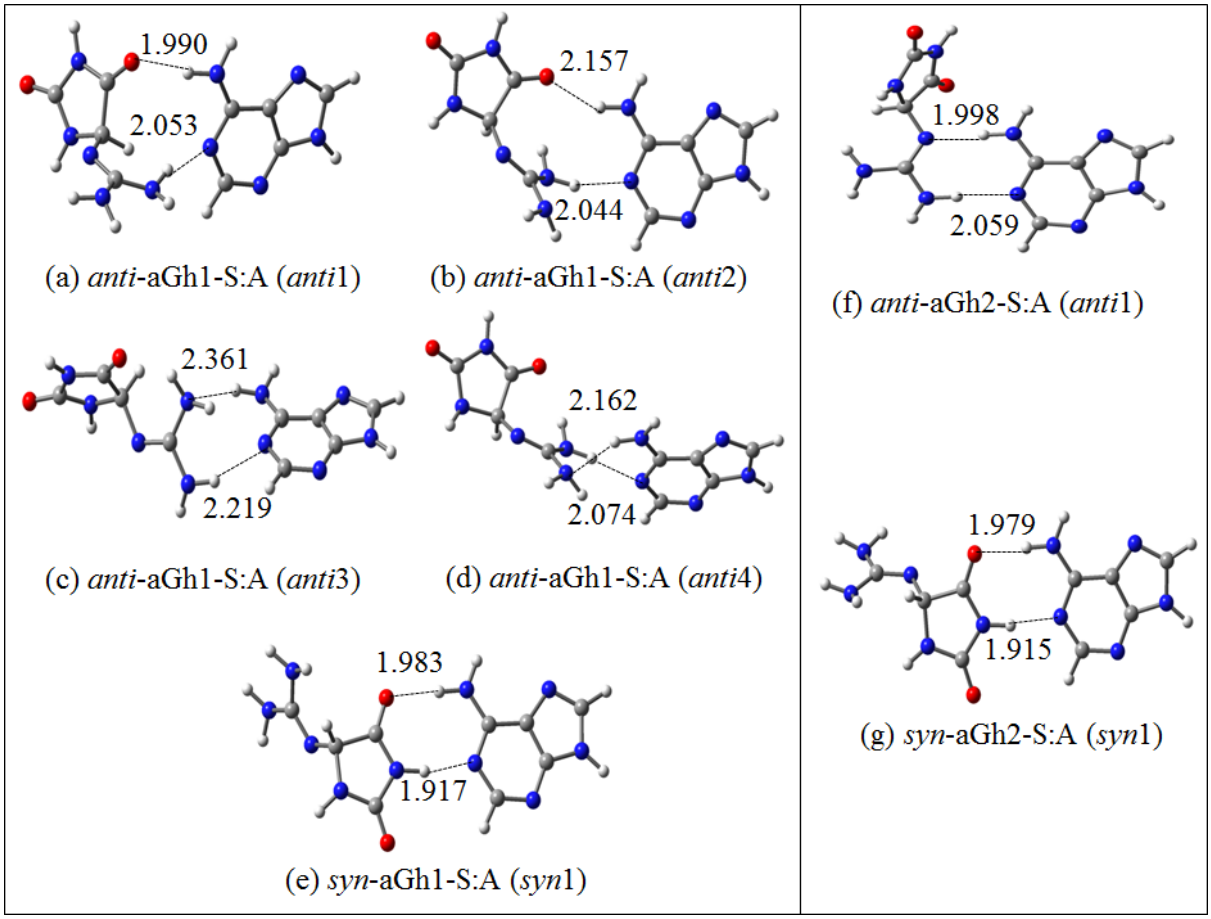

Fig. S13.Optimized structures of complexes of aGh1-S and aGh2-S with adenine in aqueous media: (a-e) aGh1-S:A and (f-h) aGh2-S:A. Hydrogen bonds are shown by dotted lines. Here *anti*1-*anti*4 represent different possible conformations of *anti*-aGh1-R and *anti*-aGh2-R while *syn*1 represents only one conformation of *syn*-aGh1-R and *syn*-aGh2-R each.

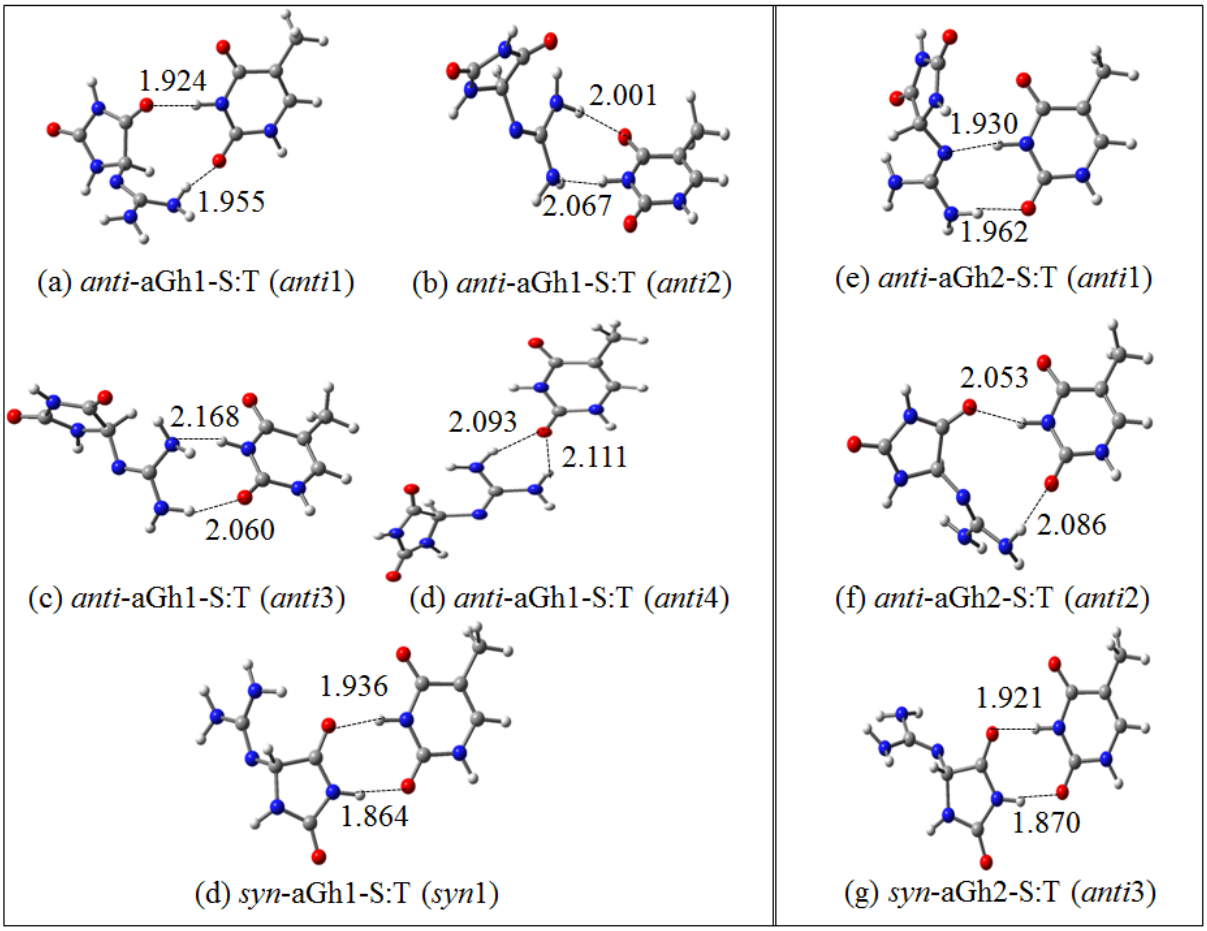

Fig. S14.Optimized structures of complexes of aGh1-S and aGh2-S with thymine in aqueous media: (a-d) aGh1-S:T and (e-g) aGh2-S:T complexes. Hydrogen bonds are shown as dotted lines. Here *anti*1-*anti*4 represent different possible conformations of *anti*-aGh1-R and *anti*-aGh2-R while *syn*1 represents only one conformation of *syn*-aGh1-R and *syn*-aGh2-R each.

Table S3. Zero-point energy-corrected binding energies (kcal/mol) of different base pair complexes involving aGh1-S and aGh2-S in aqueous medium. Absence of entry shows that the corresponding structure does not exist. Here *anti*1-*anti*4 and *syn*1-*syn*4 represent different possible conformations of *anti*-aGh-R and *syn*-aGh-R respectively (Figs.6-8,10).

Base Pair	Method	aGh1-S						aGh2-S		
		*anti*1	*anti*2	*anti*3	*anti*4	*syn*1	*syn2*	*anti*1	*anti*2	*syn*1
Gh:G	B3LYP	-4.78				-7.95	-7.64	-5.28	-4.52	-8.17
	ωB97XD	-7.91				-11.27	-10.87	-9.19	-6.47	-11.22
Gh:C	B3LYP	-5.78	-3.14	-3.89	-4.62	-6.02		-5.96	-3.26	-6.46
	ωB97XD	-8.57	-6.82	-7.84	-6.13	-9.32		-10.78	-4.74	-9.45
Gh:A	B3LYP	-3.30	-2.21	**-3.07**	-3.17	-4.86		-6.12		-6.37
	ωB97XD	-6.80	-5.85	-6.58	-6.56	-8.04		-10.12		-9.73
Gh:T	B3LYP	-3.58	-3.44	-2.85	-3.49	-5.99		-8.37	-2.47	-6.47
	ωB97XD	-6.22	-5.03	-5.93	-4.74	-8.71		-13.20	-5.05	-8.88

Table S4. Zero-point energy-corrected (ZPEC) binding energies (kcal/mol) of different base pair complexes involving aGh1-S and aGh2-S in the gas phase. Absence of entry shows that the corresponding structure does not exist. Here *anti*1-*anti*4 represent different conformations of *anti*-aGh1-S and *anti*-aGh2-S while *syn*1-*syn*4 represent different conformations of *syn*-aGh1-S and *syn*-aGh2-S.

Base Pair	Method	aGh1-S						aGh2-S		
		*anti*1	*anti*2	*anti*3	*anti*4	*syn*1	*syn*2	*anti*1	*anti*2	*syn*1
Gh:G	B3LYP	-11.27				-16.26				
(G:C)	ωB97XD	-24.39				-27.78				
Gh:C	B3LYP	-11.16	-11.71	-13.07	-11.20	-10.11				
	ωB97XD	-22.95	-21.30	-22.58	4.66	-23.20				
Gh:A	B3LYP	-7.83	-6.66	-6.46	-7.83	-11.37				
(A:T)	ωB97XD	-15.52	-15.72	-15.02	-16.02	-19.24				
Gh:T	B3LYP	-8.03	-7.63	-7.53	-6.47	-9.86				
	ωB97XD	-16.73	-15.54	1.43	-15.02	-18.54				

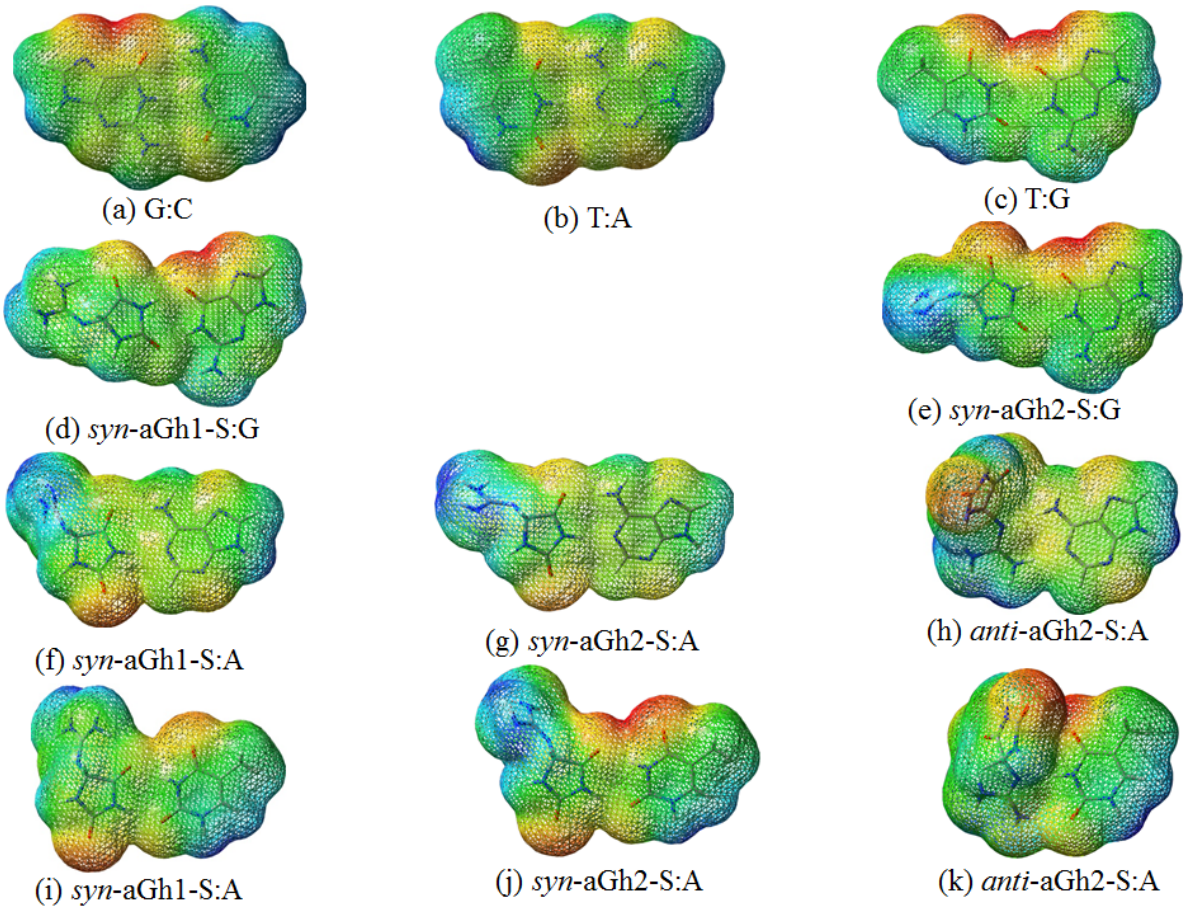

Fig. S15: Electrostatic potentials mapped onto the electronic densities (0.0004 e/Bohr^3) of different vital base pair complexes involving aGh-S as obtained at the B3LYP/6-31+G* level in aqueous medium.

Table S5: XYZ-coordinates of *syn*-aGh1-R_1:G

C	5.52878	-0.3122	0.55922
N	4.48653	0.46905	0.56068
C	3.60488	0.42322	-0.57794
C	2.58453	-0.74236	-0.55162
O	2.8613	-1.93498	-0.6067
N	1.34225	-0.18534	-0.44638
C	1.40132	1.21505	-0.42775
O	0.41954	1.95509	-0.30655
N	2.69768	1.56899	-0.58535
N	5.7721	-1.31112	-0.35769
N	6.53959	-0.07754	1.47103
N	-5.80309	-0.78491	0.35706
C	-5.47416	-2.12221	0.2702
N	-4.18769	-2.32016	0.09856
C	-3.64266	-1.04543	0.07023
C	-2.29399	-0.60875	-0.08399
N	-2.1963	0.79171	-0.053
C	-3.24873	1.66099	0.1081
N	-4.50263	1.26903	0.25973
C	-4.6389	-0.07522	0.23054
H	4.1584	0.37087	-1.52924
H	6.60273	-1.87661	-0.22703
H	7.00293	-0.8885	1.86573
H	-6.22809	-2.89431	0.34142
H	0.44104	-0.68865	-0.37822
H	4.95697	-1.83242	-0.67095
H	6.30926	0.62432	2.16485
O	-1.26668	-1.30204	-0.23229
H	-1.24792	1.18332	-0.15959
N	-2.95448	2.99001	0.05378
H	-3.67392	3.62048	0.38432
H	-2.00152	3.29393	0.21131
H	-6.73056	-0.39922	0.48804
H	3.01297	2.51569	-0.41717

Table S6: XYZ-coordinates of *syn*-aGh2-R_1:G

C	5.64014	0.04104	0.51907
N	4.47593	-0.54317	0.55087
C	3.58178	-0.35009	-0.55461
C	2.42229	-1.37457	-0.48674
O	2.53214	-2.58938	-0.50248
N	1.25958	-0.65328	-0.40901
C	1.4924	0.72616	-0.40817
O	0.60923	1.58757	-0.31938
N	2.82516	0.91249	-0.53188
N	6.12371	0.84725	-0.48805
N	6.43975	-0.03626	1.64015
N	-5.91474	-0.30845	0.33473
C	-5.76523	-1.67906	0.27897
N	-4.51463	-2.04918	0.12787
C	-3.80507	-0.85867	0.08111
C	-2.40873	-0.60745	-0.06485
N	-2.12737	0.76823	-0.06118
C	-3.05683	1.77212	0.06878
N	-4.35305	1.55292	0.21274
C	-4.66551	0.23802	0.20881
H	4.06027	-0.47216	-1.54037
H	7.10784	1.08693	-0.47423
H	7.44396	-0.01152	1.50621
H	-6.61578	-2.34263	0.35535
H	0.3039	-1.03891	-0.33532
H	5.76578	0.70847	-1.42441
H	6.14032	-0.73746	2.30736
O	-1.48019	-1.43253	-0.18583
H	-1.13504	1.0302	-0.16864
N	-2.58737	3.04869	-0.00905
H	-3.21826	3.77657	0.30156
H	-1.60342	3.22453	0.15318
H	-6.78414	0.19931	0.44629
H	3.24482	1.83183	-0.49000

Table S7: XYZ-coordinates of *syn*-aGh1-R_1:A

C	4.70803	-1.17504	0.417
N	4.19914	0.01906	0.52439
C	3.3554	0.4925	-0.54548
C	1.8932	0.00006	-0.46736
O	1.52423	-1.17062	-0.58243
N	1.10682	1.08239	-0.24045
C	1.85885	2.27437	-0.17912
O	1.39688	3.38415	0.05929
N	3.14903	1.93561	-0.45731
N	4.37014	-2.0991	-0.54773
N	5.74601	-1.53696	1.25362
N	-5.73261	-0.08415	0.32207
C	-5.71225	-1.43992	0.09254
N	-4.50076	-1.9122	-0.11353
C	-3.68262	-0.79854	-0.01321
C	-2.28277	-0.63327	-0.13282
N	-1.44749	-1.65547	-0.39419
N	-1.782	0.61757	0.02383
C	-2.62562	1.63537	0.28359
N	-3.95139	1.59919	0.4172
C	-4.4312	0.35165	0.25828
H	3.75553	0.2225	-1.53599
H	4.8119	-3.0097	-0.49901
H	5.75982	-2.49573	1.58347
H	-6.62196	-2.02501	0.09014
H	-0.4388	-1.51745	-0.46007
H	-2.15567	2.60938	0.39756
H	-1.8181	-2.58977	-0.49884
H	0.07511	1.02963	-0.12628
H	3.38827	-2.12578	-0.81055
H	5.93493	-0.86255	1.98614
H	-6.55238	0.48248	0.5036
H	3.90794	2.56915	-0.24102

Table S8: XYZ-coordinates of *syn*-aGh2-R_1:A

C	5.195	-0.80783	0.43805
N	3.8947	-0.73809	0.48723
C	3.20363	-0.03344	-0.55626
C	1.70049	-0.38726	-0.52272
O	1.21832	-1.50461	-0.68134
N	1.01635	0.76513	-0.28413
C	1.87096	1.87541	-0.147
O	1.5064	3.01641	0.11737
N	3.13378	1.42549	-0.3841
N	6.00918	-0.25812	-0.52768
N	5.85756	-1.37543	1.5062
N	-5.89286	0.16027	0.3722
C	-5.98566	-1.1915	0.13691
N	-4.82133	-1.75611	-0.10515
C	-3.9154	-0.71084	-0.02285
C	-2.5103	-0.65561	-0.17845
N	-1.76473	-1.73782	-0.46748
N	-1.9087	0.55118	-0.02982
C	-2.66229	1.63043	0.25639
N	-3.98304	1.69783	0.4254
C	-4.56332	0.49283	0.27417
H	3.5688	-0.26875	-1.56959
H	6.97401	-0.56423	-0.56855
H	6.75041	-1.81993	1.32804
H	-6.93859	-1.70291	0.15742
H	-0.74827	-1.6804	-0.54654
H	-2.11416	2.56371	0.36222
H	-2.20902	-2.64126	-0.55488
H	-0.01634	0.80441	-0.18523
H	5.61275	-0.08232	-1.44187
H	5.25735	-1.90905	2.12359
H	-6.66012	0.78805	0.57983
H	3.94032	2.00469	-0.19072

Table S9: XYZ-coordinates of *anti*-aGh1-R_1:A

C	1.87864	2.25735	-0.25659
N	1.87286	0.97001	-0.00672
C	3.1245	0.29203	0.17419
C	3.0202	-0.7653	1.30299
O	2.74949	-0.55085	2.47245
N	3.29433	-1.97901	0.7282
C	3.55565	-1.88455	-0.65406
O	3.77794	-2.83691	-1.39297
N	3.52325	-0.56067	-0.95712
N	0.69806	2.94192	-0.2039
N	3.00297	3.02475	-0.4802
N	-5.28702	-0.85694	0.01044
C	-4.72488	-2.1013	-0.15313
N	-3.41083	-2.07006	-0.22635
C	-3.09643	-0.72538	-0.10378
C	-1.86296	-0.03051	-0.10301
N	-0.672	-0.63785	-0.24801
N	-1.89966	1.31826	0.03988
C	-3.08973	1.92986	0.17463
N	-4.30872	1.38504	0.18915
C	-4.25271	0.04805	0.04486
H	0.60176	3.77972	-0.76407
H	2.86482	3.99387	-0.73864
H	-5.33508	-2.99256	-0.21114
H	0.20484	-0.10423	-0.16503
H	-3.04644	3.01109	0.28572
H	-0.63158	-1.64635	-0.30218
H	3.2886	-2.86545	1.21978
H	-0.16004	2.39024	-0.0939
H	3.78927	2.59921	-0.95253
H	-6.27515	-0.64912	0.08861
H	3.52113	-0.24863	-1.91937
H	3.95195	0.96455	0.44266

Table S10: XYZ-coordinates of *syn*-aGh1-R_1:T

C	-5.08207	0.08959	0.52465
N	-4.00299	-0.63953	0.50398
C	-3.10938	-0.49338	-0.61736
N	-2.14677	0.71621	-0.51512
O	-2.48011	1.8959	-0.51526
N	-0.88208	0.21311	-0.41675
C	-0.87211	-1.1887	-0.46938
O	0.14169	-1.88355	-0.36633
N	-2.14918	-1.59369	-0.67036
N	-5.36177	1.12008	-0.34577
N	-6.09253	-0.23883	1.40758
N	5.04213	-0.79762	0.33099
C	5.14434	0.57316	0.34313
C	3.85001	-1.47242	0.16566
H	-3.65312	-0.41627	-1.57269
H	-6.22167	1.63633	-0.20112
H	-6.59884	0.52865	1.83516
H	-0.00563	0.74772	-0.31435
H	-4.5692	1.69621	-0.61811
H	-5.83747	-0.96304	2.06906
O	3.76928	-2.70045	0.15693
N	2.75834	-0.63943	0.01082
C	2.76855	0.75317	0.01332
C	4.06662	1.38595	0.19204
H	6.14909	0.95637	0.48204
O	1.70474	1.38162	-0.13272
H	1.84792	-1.10652	-0.11738
C	4.15574	2.88623	0.20237
H	5.19048	3.21216	0.34337
H	3.78637	3.31046	-0.73875
H	3.54724	3.3128	1.0085
H	-2.42257	-2.56008	-0.54651
H	5.86955	-1.37054	0.45057

Table S11: XYZ-coordinates of *syn*-aGh2-R_1:T

C	-5.16879	-0.18025	0.47893
N	-4.01585	0.42325	0.54039
C	-3.10981	0.28523	-0.56417
C	-1.97806	1.33712	-0.45648
O	-2.11954	2.5491	-0.44283
N	-0.79961	0.6437	-0.38244
C	-0.99438	-0.74208	-0.42045
O	-0.08994	-1.57874	-0.33896
N	-2.32166	-0.95784	-0.57322
N	-5.63	-0.96078	-0.55855
N	-5.97943	-0.15536	1.59467
N	4.92391	-1.21519	0.27659
C	5.22431	0.12591	0.30787
C	3.6442	-1.70719	0.12187
H	-3.58538	0.42435	-1.54903
H	-6.61086	-1.21394	-0.56263
H	-6.98157	-0.19508	1.44955
H	0.14505	1.04466	-0.28557
H	-5.26432	-0.78681	-1.48595
H	-5.7004	0.52986	2.28683
O	3.38642	-2.91045	0.09551
N	2.68257	-0.72253	-0.00041
C	2.89541	0.65381	0.01954
C	4.27395	1.08872	0.18697
H	6.27594	0.35673	0.43645
O	1.93243	1.43185	-0.10205
H	1.71171	-1.05061	-0.1184
C	4.58057	2.5598	0.21817
H	5.65315	2.72877	0.35172
H	4.26766	3.04842	-0.71214
H	4.04855	3.05732	1.03765
H	-2.72014	-1.88697	-0.54152
H	5.66178	-1.90405	0.36697

Table S12: XYZ-coordinates of *syn*-aGh2-R_1:T

C	1.82658	2.29427	-0.3502
N	1.42042	1.10745	0.03689
C	2.39005	0.0942	0.32396
C	1.85777	-0.92319	1.36499
O	1.37008	-0.66178	2.45132
N	2.07171	-2.16735	0.83352
C	2.57916	-2.12292	-0.47881
O	2.83804	-3.10474	-1.16568
N	2.70888	-0.80713	-0.79417
N	3.12678	2.66144	-0.6084
N	0.88311	3.2416	-0.63001
N	-3.62871	1.2452	0.19823
C	-4.13277	-0.02042	-0.00784
C	-2.28401	1.5343	0.18528
H	3.32672	0.48932	0.75151
H	3.35065	3.64906	-0.61376
H	1.16986	4.20793	-0.71254
H	1.78507	-3.03448	1.27283
H	3.87681	2.08879	-0.24657
H	-0.05384	3.08912	-0.25242
O	-1.85136	2.68138	0.3654
N	-1.47198	0.45073	-0.0449
C	-1.88834	-0.86595	-0.27115
C	-3.33232	-1.09007	-0.24281
H	-5.21407	-0.09279	0.03121
O	-1.04522	-1.74653	-0.47451
H	-0.44597	0.63603	-0.0359
C	-3.85752	-2.47927	-0.47183
H	-4.95015	-2.49616	-0.4181
H	-3.55466	-2.85888	-1.45502
H	-3.46449	-3.17791	0.27643
H	3.21466	-0.51939	-1.62168
H	-4.25602	2.02336	0.36405

Table S13: XYZ-coordinates of syn-aGh1-S_1:G

C	-5.44567	-0.28118	0.61094
N	-4.48712	0.56807	0.42014
C	-3.60202	0.40513	-0.7037
C	-2.59815	-0.77401	-0.6108
O	-2.89037	-1.95922	-0.64235
N	-1.34775	-0.22537	-0.49544
C	-1.3936	1.1702	-0.52538
O	-0.42615	1.91745	-0.36508
N	-2.68099	1.53936	-0.78604
N	-5.69811	-1.41595	-0.13767
N	-6.32592	-0.05124	1.65884
N	5.79272	-0.72653	0.31909
C	5.48866	-2.07653	0.22709
N	4.20784	-2.29985	0.08911
C	3.63199	-1.04154	0.09078
C	2.26488	-0.63224	-0.03477
N	2.15123	0.77518	0.02657
C	3.18753	1.65966	0.16959
N	4.45099	1.29805	0.27375
C	4.60595	-0.04624	0.23287
H	-4.15896	0.30106	-1.64929
H	-6.32877	-2.08928	0.28197
H	-7.26829	-0.4055	1.54854
H	6.25893	-2.83524	0.26949
H	-0.45513	-0.74237	-0.38143
H	-4.86331	-1.86319	-0.51908
H	-6.29281	0.89955	2.00631
O	1.24605	-1.32038	-0.18245
H	1.19622	1.15016	-0.06869
N	2.84779	2.9829	0.2474
H	3.60905	3.63873	0.1389
H	1.94087	3.27831	-0.09125
H	6.70525	-0.30584	0.43195
H	-2.99159	2.45895	-0.49832

Table S14: XYZ-coordinates of syn-aGh1-S_1:G

C	-5.70649	-0.01077	0.4683
N	-4.45932	-0.3653	0.59423
C	-3.57206	-0.22419	-0.52234
C	-2.43543	-1.27578	-0.44272
O	-2.57471	-2.48758	-0.45071
N	-1.25641	-0.5816	-0.36369
C	-1.458	0.80235	-0.37374
O	-0.55759	1.64435	-0.27488
N	-2.78444	1.0192	-0.52285
N	-6.28647	0.64926	-0.59103
N	-6.57706	-0.30175	1.49929
N	5.93763	-0.37804	0.24515
C	5.76265	-1.74519	0.17915
N	4.50102	-2.09236	0.07121
C	3.81072	-0.88979	0.06642
C	2.41517	-0.61323	-0.03351
N	2.15782	0.7668	0.00016
C	3.10803	1.75324	0.11167
N	4.40513	1.51073	0.19942
C	4.69407	0.19072	0.17397
H	-4.05767	-0.35198	-1.50301
H	-7.28414	0.53238	-0.72401
H	-7.34193	0.34556	1.65367
H	6.60398	-2.42372	0.21588
H	-0.31009	-0.98838	-0.28409
H	-5.77474	0.71401	-1.46077
H	-6.11516	-0.58658	2.355
O	1.46933	-1.42035	-0.14085
H	1.1674	1.04666	-0.07411
N	2.64951	3.03435	0.18323
H	3.33847	3.76283	0.0453
H	1.71774	3.24584	-0.15238
H	6.81909	0.11377	0.33021
H	-3.18292	1.94525	-0.43909

Table S15: XYZ-coordinates of syn-aGh1-S_1:A

C	-4.82765	-1.1108	0.43484
N	-4.0983	-0.041	0.57211
C	-3.32227	0.45265	-0.52967
C	-1.85149	-0.0319	-0.48826
O	-1.46801	-1.19183	-0.61235
N	-1.07212	1.06289	-0.26904
C	-1.83153	2.2438	-0.17413
O	-1.37745	3.35548	0.0733
N	-3.12552	1.8994	-0.43347
N	-4.89482	-1.94125	-0.65889
N	-5.54755	-1.54408	1.5328
N	5.77213	-0.1012	0.34049
C	5.75037	-1.45936	0.12526
N	4.5403	-1.9299	-0.09238
C	3.72439	-0.81272	-0.01462
C	2.32656	-0.64457	-0.15364
N	1.49157	-1.66629	-0.41742
N	1.82762	0.60929	-0.01571
C	2.67108	1.62701	0.24397
N	3.99516	1.58848	0.39448
C	4.47298	0.33792	0.25473
H	-5.71623	-2.52134	-0.7774
H	-6.35526	-2.13211	1.36471
H	6.65807	-2.04735	0.14148
H	0.48258	-1.52707	-0.48692
H	2.20285	2.60356	0.3424
H	1.85981	-2.60391	-0.49819
H	-0.04002	1.01779	-0.16551
H	-4.48023	-1.63826	-1.5289
H	-5.71023	-0.82627	2.22852
H	6.59111	0.46487	0.52712
H	-3.88282	2.51956	-0.17605
H	-3.73992	0.21488	-1.52073

Table S16: XYZ-coordinates of syn-aGh2-S_1:A

C	-5.19541	-0.80751	0.43768
N	-3.89513	-0.73801	0.48731
C	-3.20357	-0.03385	-0.55619
C	-1.70043	-0.38766	-0.52178
O	-1.21816	-1.50508	-0.67957
N	-1.01642	0.76489	-0.28356
C	-1.8711	1.87524	-0.14747
O	-1.50668	3.01642	0.11633
N	-3.13381	1.42514	-0.38477
N	-6.0091	-0.25801	-0.52861
N	-5.85852	-1.37452	1.50576
N	5.89315	0.16074	0.3713
C	5.98615	-1.19096	0.13572
N	4.82183	-1.7558	-0.10587
C	3.9157	-0.71076	-0.02293
C	2.51051	-0.65581	-0.17783
N	1.76502	-1.73813	-0.46666
N	1.9087	0.55081	-0.02868
C	2.66219	1.63017	0.25737
N	3.983	1.69786	0.42573
C	4.56349	0.49301	0.27399
H	-6.97407	-0.56367	-0.56952
H	-6.75131	-1.81906	1.32747
H	6.93921	-1.70215	0.15567
H	0.74854	-1.68082	-0.5454
H	2.11389	2.56331	0.36365
H	2.20944	-2.64144	-0.55465
H	0.01622	0.80431	-0.1844
H	-5.61236	-0.0829	-1.44279
H	-5.25865	-1.90764	2.12391
H	6.66038	0.78864	0.5787
H	-3.94046	2.00445	-0.1922
H	-3.56827	-0.26969	-1.56957

Table S17: XYZ-coordinates of *anti*-aGh2-S_1:A

C	1.81712	2.0652	-0.44367
N	1.80012	0.76566	-0.37953
C	3.01787	0.0505	-0.63495
C	2.72859	-1.46754	-0.74863
O	1.98146	-2.0042	-1.54037
N	3.48334	-2.07393	0.22814
C	4.18255	-1.15911	1.04244
O	4.81235	-1.44	2.04248
N	4.01301	0.07535	0.45477
N	2.95895	2.84712	-0.61088
N	0.65438	2.77109	-0.32353
N	-5.40663	-0.7012	0.33191
C	-4.97559	-1.89861	-0.20566
N	-3.6929	-1.90914	-0.47963
C	-3.25493	-0.65032	-0.10294
C	-1.9779	-0.03759	-0.1401
N	-0.8822	-0.65862	-0.60019
N	-1.88159	1.23918	0.31179
C	-2.98585	1.85243	0.77589
N	-4.22987	1.38077	0.86363
C	-4.30356	0.12029	0.40573
H	3.7735	2.38086	-0.99153
H	0.71251	3.70989	0.04904
H	-5.65594	-2.72395	-0.37034
H	0.03692	-0.20721	-0.56644
H	-2.83903	2.87263	1.12505
H	-0.94814	-1.60308	-0.95306
H	3.46191	-3.06537	0.43181
H	2.80853	3.7529	-1.04067
H	-0.18742	2.24339	-0.05033
H	4.12619	0.89069	1.04467
H	-6.34488	-0.46028	0.62171
H	3.49932	0.35756	-1.58075

Table S18: XYZ-coordinates of syn-aGh1-S_1:T

C	3.82444	-1.03051	-2.12652
N	3.80817	0.20563	-1.71539
C	3.32505	0.47892	-0.38527
C	1.7865	0.52423	-0.26249
O	1.02643	-0.43478	-0.41395
N	1.43694	1.80273	0.02661
C	2.56469	2.64233	0.15875
O	2.51944	3.8464	0.377
N	3.65863	1.84223	0.02244
N	3.30039	-2.10685	-1.43982
N	4.40868	-1.3088	-3.34378
N	-3.57829	1.51964	0.25903
C	-4.5221	0.52215	0.14249
C	-2.22787	1.30031	0.13787
H	3.7083	-0.24295	0.35364
H	3.27172	-2.99542	-1.92681
H	4.66165	-2.26891	-3.54206
H	0.46171	2.11196	0.13689
H	2.44504	-1.9164	-0.92337
H	5.09769	-0.63341	-3.6516
O	-1.3968	2.21321	0.24651
N	-1.89013	-0.00869	-0.11187
C	-2.7718	-1.091	-0.24553
C	-4.18886	-0.76992	-0.10177
H	-5.54847	0.85042	0.26198
O	-2.32187	-2.21862	-0.47046
H	-0.88706	-0.21176	-0.2176
C	-5.20043	-1.87338	-0.23131
H	-6.21602	-1.48748	-0.10336
H	-5.03033	-2.65373	0.51997
H	-5.13492	-2.35442	-1.21446
H	-3.86583	2.47373	0.44442
H	4.57024	2.24188	-0.16078

Table S19: XYZ-coordinates of syn-aGh2-S_1:T

C	-4.43391	-1.50405	0.31485
N	-3.38686	-0.76567	0.54922
C	-2.85538	0.06414	-0.49269
C	-1.32214	0.18586	-0.34231
O	-0.51463	-0.73539	-0.41987
N	-1.04083	1.49579	-0.10527
C	-2.19918	2.29824	-0.08261
O	-2.21668	3.50007	0.15693
N	-3.24129	1.47989	-0.39519
N	-5.2365	-1.49431	-0.8034
N	-4.82624	-2.40739	1.28258
N	3.96695	1.421	0.37807
C	4.95502	0.46401	0.29393
C	2.63288	1.14791	0.19742
H	-3.05158	-0.30293	-1.51212
H	-5.74833	-2.34268	-1.01568
H	-5.81981	-2.59334	1.36203
H	-0.08724	1.84619	0.05345
H	-4.91038	-1.00993	-1.62884
H	-4.37307	-2.26717	2.17799
O	1.76132	2.02525	0.27813
N	2.35964	-0.1711	-0.07713
C	3.29037	-1.21432	-0.18499
C	4.68593	-0.83724	0.02131
H	5.96101	0.8321	0.46136
O	2.89789	-2.35722	-0.43908
H	1.36846	-0.41566	-0.21287
C	5.74699	-1.8966	-0.07626
H	6.73852	-1.47233	0.10704
H	5.74886	-2.36218	-1.06903
H	5.57319	-2.69655	0.65319
H	4.20692	2.38439	0.58189
H	-4.19726	1.78327	-0.26115

Table S20: XYZ-coordinates of *anti*-aGh2-S_1:T

C	1.81127	2.1914	-0.12147
N	1.39468	1.02527	0.30953
C	2.38832	0.01344	0.57145
C	2.82884	-0.80273	-0.6688
O	3.34672	-0.34467	-1.67977
N	2.53	-2.10833	-0.40731
C	1.93493	-2.28446	0.86338
O	1.58452	-3.362	1.328
N	1.86473	-1.05002	1.41954
N	3.09288	2.44	-0.55798
N	0.97031	3.26846	-0.0543
N	-3.63385	1.31097	0.38084
C	-4.18841	0.12544	-0.04876
C	-2.27727	1.52661	0.459
H	3.2972	0.44734	1.01975
H	3.29903	3.37299	-0.8951
H	1.05657	3.98593	-0.76362
H	2.68657	-2.88075	-1.0452
H	3.53084	1.69573	-1.09476
H	0.01764	3.08165	0.26379
O	-1.79991	2.60721	0.83169
N	-1.50835	0.44963	0.08773
C	-1.97777	-0.78597	-0.37364
C	-3.43075	-0.93248	-0.4312
H	-5.27255	0.10597	-0.0593
O	-1.17258	-1.66514	-0.69947
H	-0.47704	0.57846	0.15873
C	-4.01276	-2.23289	-0.90885
H	-5.10626	-2.19835	-0.89459
H	-3.68529	-3.06769	-0.27776
H	-3.68831	-2.45811	-1.93183
H	-4.23006	2.08621	0.64574
H	1.47043	-0.8946	2.33746