Electronic Supplementary Information for

Mechanisms of photoreactivity in hydrogen-bonded adenine-H_2O complexes

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Cartesian coordinates of the ground-state minimum-energy structures of isolated adenine (a), five conformers of the adenine-H_2O hydrogen-bonded complex (b), (c), (d), (e) and (f), the isolated N3 (adenine+H) radical (g) and the complex of the (adenine+H) radical with a water molecule (h), optimized with C_s symmetry constraint (MP2/cc-pVDZ level, standard XYZ format in Angstrom).

(a) Isolated adenine:

N	-1.113490006	1.077018165	0.000000000
C	-0.387436863	2.248753826	0.000000000
H	-0.871517873	3.223345838	0.000000000
N	0.934254744	2.053595481	0.000000000
C	1.054575447	0.671818587	0.000000000
C	2.184692075	-0.183554119	0.000000000
N	3.455631618	0.301958162	0.000000000
H	4.230481872	-0.346809582	0.000000000
H	3.616175224	1.299610908	0.000000000
N	1.990055802	-1.517713361	0.000000000
C	0.713329373	-1.985491243	0.000000000
H	0.617932576	-3.074128994	0.000000000
N	-0.440379239	-1.292284640	0.000000000
C	-0.202063984	0.035314453	0.000000000
H	-2.123425833	0.983150286	0.000000000

(b) adenine-H_2O complex

N	-1.153264430	0.997457246	0.000000000
C	-0.549824378	2.236672183	0.000000000
H	-1.129857429	3.157324789	0.000000000
N	0.785058722	2.176225529	0.000000000
C	1.043427317	0.814585104	0.000000000
C	2.255665760	0.081508389	0.000000000
N	3.467465614	0.698464284	0.000000000
H	4.312249011	0.144456847	0.000000000
H	3.516563459	1.708081685	0.000000000
N	2.191162929	-1.264986857	0.000000000
C	0.967883771	-1.867050121	0.000000000
H	0.992319147	-2.959557010	0.000000000
N	-0.245172212	-1.291236246	0.000000000
C	-0.141799860	0.054019916	0.000000000
H	-2.148652604	0.801403767	0.000000000
H	3.357181428	-2.841661243	0.000000000
O	3.603622264	-3.788043857	0.000000000
H	4.567989993	-3.793067101	0.000000000

(c) adenine-H_2O complex

N	-1.121621831	0.677091711	0.000000000
C	-0.559935651	1.932121469	0.000000000
H	-1.170173341	2.832932434	0.000000000
N	0.779224334	1.921683736	0.000000000
C	1.085719433	0.571306286	0.000000000
C	2.319615605	-0.125594460	0.000000000
N	3.513053042	0.524627418	0.000000000
H	4.368361184	-0.013782432	0.000000000
H	3.537121407	1.535055243	0.000000000
N	2.307717364	-1.475546799	0.000000000
C	1.109504636	-2.112152944	0.000000000
H	1.160067353	-3.203703211	0.000000000
N	-0.125448944	-1.576822306	0.000000000
C	-0.076539632	-0.224086252	0.000000000
H	-2.107192568	0.407972400	0.000000000
H	-2.058802572	-1.867191418	0.000000000
O	-2.930474067	-1.416240977	0.000000000
H	-3.595710903	-2.114034725	0.000000000

(d) adenine-H_2O complex

N	-1.258132915	0.972299216	0.000000000
C	-0.640793360	2.198706543	0.000000000
H	-1.202230761	3.130457779	0.000000000
N	0.692351009	2.109592182	0.000000000

C	0.942179453	0.741554616	0.000000000
C	2.140960527	-0.028171946	0.000000000
N	3.380041055	0.515880837	0.000000000
H	4.166285578	-0.120474414	0.000000000
H	3.527804421	1.523450690	0.000000000
N	2.028263251	-1.376889491	0.000000000
C	0.793098252	-1.936216032	0.000000000
H	0.777668706	-3.029114650	0.000000000
N	-0.409067604	-1.330122131	0.000000000
C	-0.262301598	0.009715703	0.000000000
H	-2.256078322	0.790308420	0.000000000
H	2.205088123	3.248365549	0.000000000
O	3.173211100	3.415256144	0.000000000
H	3.289260365	4.371761668	0.000000000

(e) adenine-H_2O complex

N	-1.464077341	0.856957430	0.000000000
C	-0.891473497	2.107384849	0.000000000
H	-1.493547731	3.013784553	0.000000000
N	0.447286050	2.084707228	0.000000000
C	0.742127858	0.731209233	0.000000000
C	1.970620888	0.025162632	0.000000000
N	3.169730116	0.666126139	0.000000000
H	4.020610910	0.120800993	0.000000000
H	3.202088595	1.676260758	0.000000000
N	1.946803362	-1.324090042	0.000000000
C	0.741174709	-1.949472324	0.000000000
H	0.784985056	-3.041586357	0.000000000
N	-0.492223719	-1.408057668	0.000000000
C	-0.426916139	-0.055842924	0.000000000
H	-2.451500518	0.587850671	0.000000000
H	-3.119443753	-1.505811827	0.747044604
H	-3.119443753	-1.505811827	-0.747044604
O	-3.566801092	-1.079571517	0.000000000

(f) adenine-H_2O complex

N	-1.121200058	0.926579329	0.000000000
C	-0.550248627	2.181494278	0.000000000
H	-1.154294433	3.086602002	0.000000000
N	0.785480747	2.155184081	0.000000000
C	1.080346569	0.800349093	0.000000000
C	2.315924111	0.102389402	0.000000000
N	3.508115825	0.748415713	0.000000000
H	4.369751544	0.204945161	0.000000000

H	3.517972269	1.759324076	0.000000000
N	2.287797946	-1.252129178	0.000000000
C	1.078592049	-1.876972049	0.000000000
H	1.121766827	-2.969282191	0.000000000
N	-0.153001028	-1.338209054	0.000000000
C	-0.084684638	0.010178966	0.000000000
H	-2.110966327	0.704605864	0.000000000
O	5.349982717	-1.584729420	0.000000000
H	4.800374072	-1.870031889	-0.745514177
H	4.800374072	-1.870031889	0.745514177

(g) (adenine+H) radical

N	-0.095409000	1.921969900	0.000000000
C	0.183404000	0.563888200	0.000000000
N	-0.996185100	-1.555520800	0.000000000
C	0.298789200	-2.183371200	0.000000000
N	1.459360800	-1.457498300	0.000000000
C	-0.987157000	-0.186586400	0.000000000
N	-2.005161800	0.738691000	0.000000000
C	-1.408715400	1.993564300	0.000000000
C	1.445216500	-0.154638600	0.000000000
N	2.597921500	0.569391600	0.000000000
H	-2.003214800	2.903734900	0.000000000
H	3.484773700	0.085419300	0.000000000
H	2.557346700	1.578575000	0.000000000
H	0.315155400	-3.266688600	0.000000000
H	-3.002052800	0.554454600	0.000000000
H	-1.844072100	-2.105384900	0.000000000

(h) (adenine+H)-H_2O radical

N	-1.091579200	0.332466300	0.000000000
C	0.033575300	-0.455487800	0.000000000
C	1.103776500	0.431214300	0.000000000
N	0.657422000	1.745024600	0.000000000
C	-0.655567900	1.648066200	0.000000000
N	0.182318500	-1.814950600	0.000000000
C	1.537696400	-2.286099600	0.000000000
N	2.608261400	-1.427480100	0.000000000
C	2.440165500	-0.134876300	0.000000000
N	3.502465800	0.718784200	0.000000000
O	-2.933885300	-1.966746900	0.000000000
H	-1.356295600	2.479431600	0.000000000
H	4.439275900	0.340879700	0.000000000
H	3.344232500	1.716195200	0.000000000

H	1.685933400	-3.359457300	0.000000000
H	-2.045645100	-0.018046300	0.000000000
H	-0.617641100	-2.434203000	0.000000000
H	-3.424431400	-2.302169600	-0.762890800
H	-3.424431400	-2.302169600	0.762890800