

## Supplementary information of

### Shape Resonance States of the Low-Energy Electron Attachments to DNA Base Tautomers

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TABLE S1. The relative energies of DNA base tautomers. (kcal/mol).

method	9H-adenine	7H-adenine		
RI-MP2/TZVPP//RI-MP2/TZVPP <sup>a</sup>	0.00	7.63		
MP2/aug-cc-pVDZ//RI-MP2/TZVPP <sup>a</sup>	0.00	7.79		
MP2/cc-pVDZ//MP2/cc-pVDZ <sup>b</sup>	0.00	7.67		
	9H-keto-guanine	7H-keto-guanine	<i>trans</i> -9H-enol-guanine	<i>cis</i> -9H-enol-guanine
RI-MP2/TZVPP//RI-MP2/TZVPP <sup>c</sup>	0.00	-0.50	0.09	0.29
MP2/aug-cc-pVDZ//RI-MP2/TZVPP <sup>c</sup>	0.00	-0.71	0.30	0.58
CCSD(T)/aug-cc-pVDZ//RI-MP2/TZVPP <sup>c</sup>	0.00	-0.59(Tian) -0.69(Hanus)	0.65(Tian) 0.22(Hanus)	1.31(Tian) 0.62(Hanus)
MP2/6-311G(d, p)//MP2/6-311G(d, p) <sup>d</sup>	0.00	0.24	0.96	1.67
MP2/cc-pVDZ//MP2/cc-pVDZ <sup>b</sup>	0.00	0.24	0.84	1.35
	Cytosine,2a	Cytosine,2b	Cytosine, 1	Cytosine, 3
RI-MP2/TZVPP//RI-MP2/TZVPP <sup>e</sup>	0.00	0.72	1.90	3.21
MP2/aug-cc-pVDZ//RI-MP2/TZVPP <sup>e</sup>	0.00	0.69	1.60	2.96
CCSD(T)/aug-cc-pVDZ//RI-MP2/TZVPP <sup>e</sup>	0.00	0.66	1.22	1.70
MP2/cc-pVDZ//MP2/cc-Pvdz <sup>e</sup>	0.00	0.67	2.57	2.96
MP2/cc-pVDZ//MP2/cc-pVDZ <sup>b</sup>	0.00	0.67	2.54	3.07

<sup>a</sup>From ref. 38.

<sup>b</sup>This work.

<sup>c</sup>From ref. 39.

<sup>d</sup>From ref. 16.

<sup>e</sup>From ref. 40.

TABLE S2. The polarizability and vertical ionization potential ( $IP_v$ ) of the DNA base tautomers used in our calculations.

	$a_{xx}(\text{a.u.})^a$	$a_{yy}(\text{a.u.})^a$	$a_{zz}(\text{a.u.})^a$	$a_{xy}(\text{a.u.})^a$	$a_{xz}(\text{a.u.})^a$	$a_{yz}(\text{a.u.})^a$	$IP_v(\text{eV})^b$
9H-adenine	113.171	94.442	34.332	1.099	0.294	-0.229	8.34
7H-adenine	109.489	96.166	35.168	4.227	-0.058	-0.659	8.70
9H-keto-guanine	124.946	95.766	36.428	4.507	0.876	0.132	7.98
7H-keto-guanine	123.597	94.730	36.539	2.335	0.967	0.249	8.11
<i>trans</i> -9H-enol-guanine	128.761	94.520	35.969	4.023	0.587	-0.254	8.02
<i>cis</i> -9H-enol-guanine	128.902	92.321	35.868	1.293	0.526	-0.250	8.06
thymine	85.499	90.262	35.053	-11.764	0.000	0.000	8.97
cytosine, 2a	89.599	71.298	27.623	-1.820	0.440	-0.112	8.78
cytosine, 2b	85.107	75.245	27.642	-0.233	0.458	-0.147	8.76
cytosine, 1	92.729	70.205	27.568	-0.222	0.409	-0.038	8.61
cytosine, 3	93.727	69.771	27.077	6.170	0.000	0.000	8.65

<sup>a</sup>The polarizability of the DNA base tautomers was calculated using B3LYP method with cc-pVDZ bases set.

<sup>b</sup>The  $IP_v$  of the DNA base tautomers was calculated using P3 method (J. V. Ortiz, *J. Chem. Phys.* 1996, **104**, 7599) with cc-pVDZ bases set.

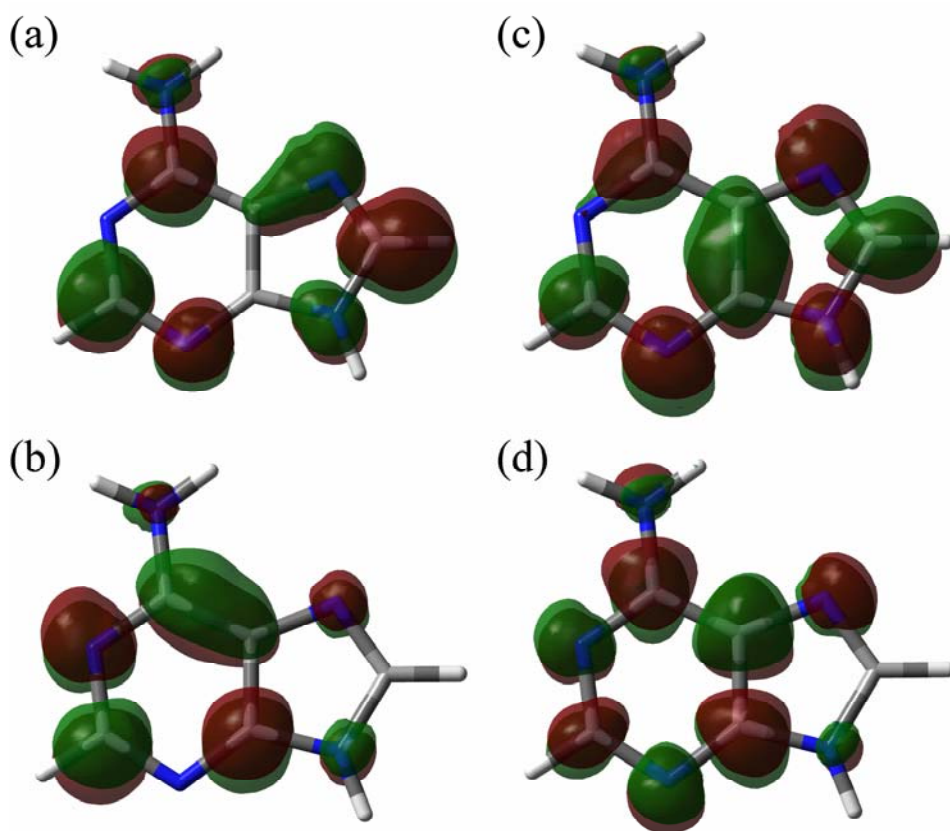


Figure S1. Wave function plots of four  $\pi^*$  resonance states (a:  $\pi_1^*$ , b:  $\pi_2^*$ , c:  $\pi_3^*$ , d:  $\pi_4^*$ ) for 9H-adenine.

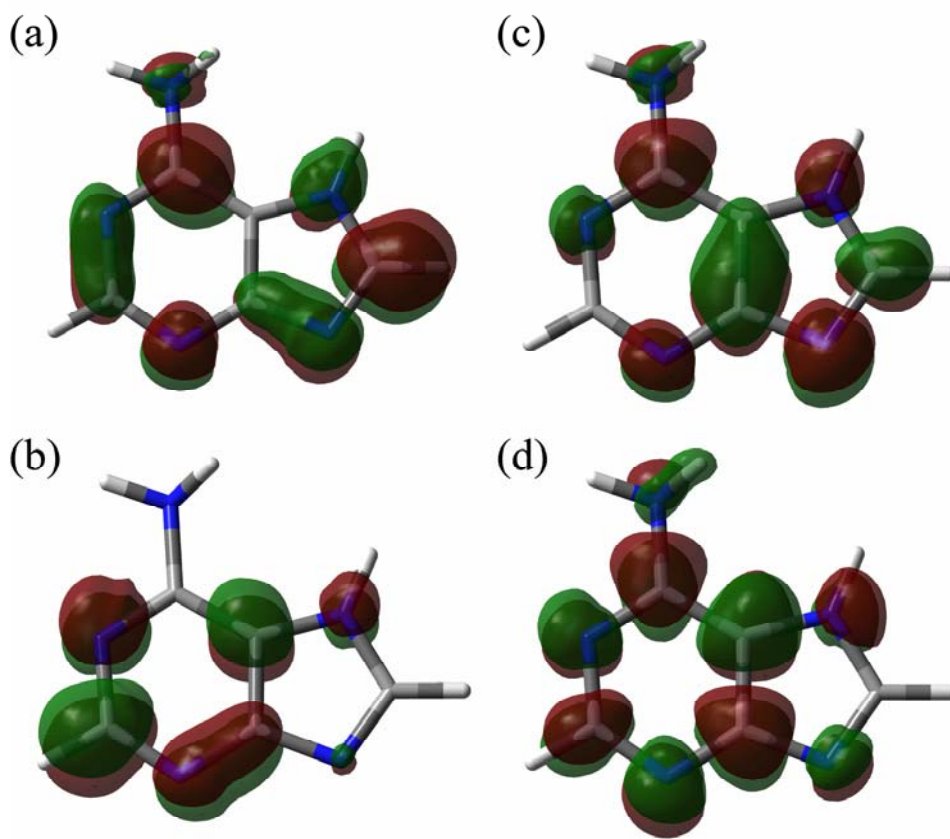


Figure S2. Wave function plots of four  $\pi^*$  resonance states (a:  $\pi_1^*$ , b:  $\pi_2^*$ , c:  $\pi_3^*$ , d:  $\pi_4^*$ ) for 7H-adenine.

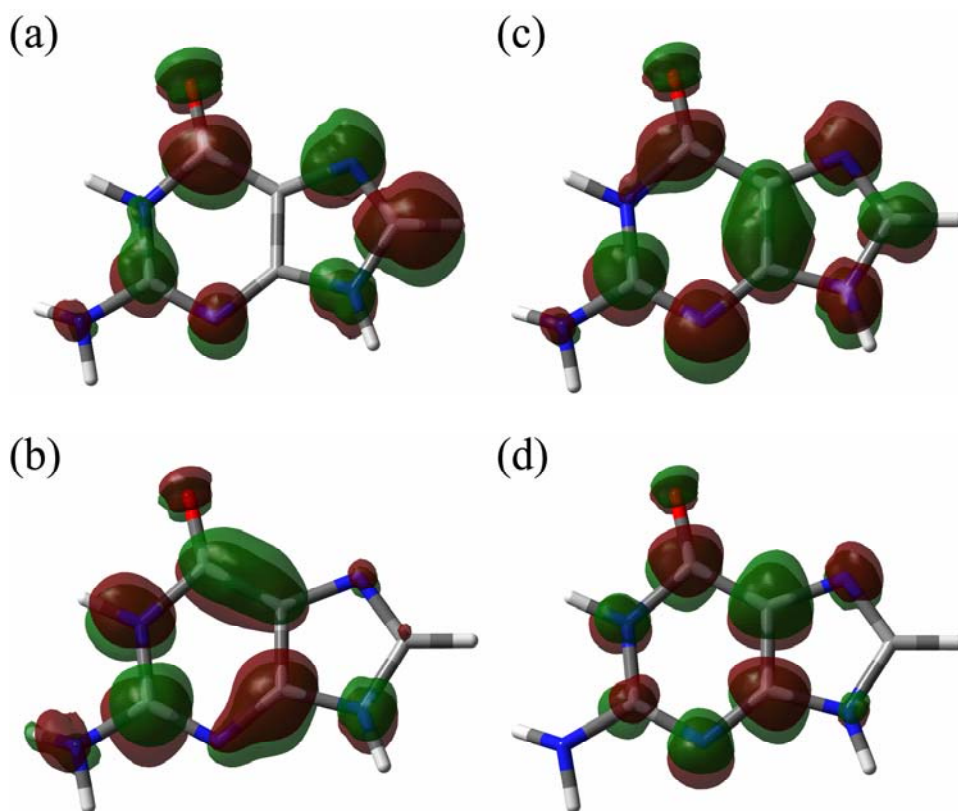


Figure S3. Wave function plots of four  $\pi^*$  resonance states (a:  $\pi_1^*$ , b:  $\pi_2^*$ , c:  $\pi_3^*$ , d:  $\pi_4^*$ ) for 9H-keto-guanine.

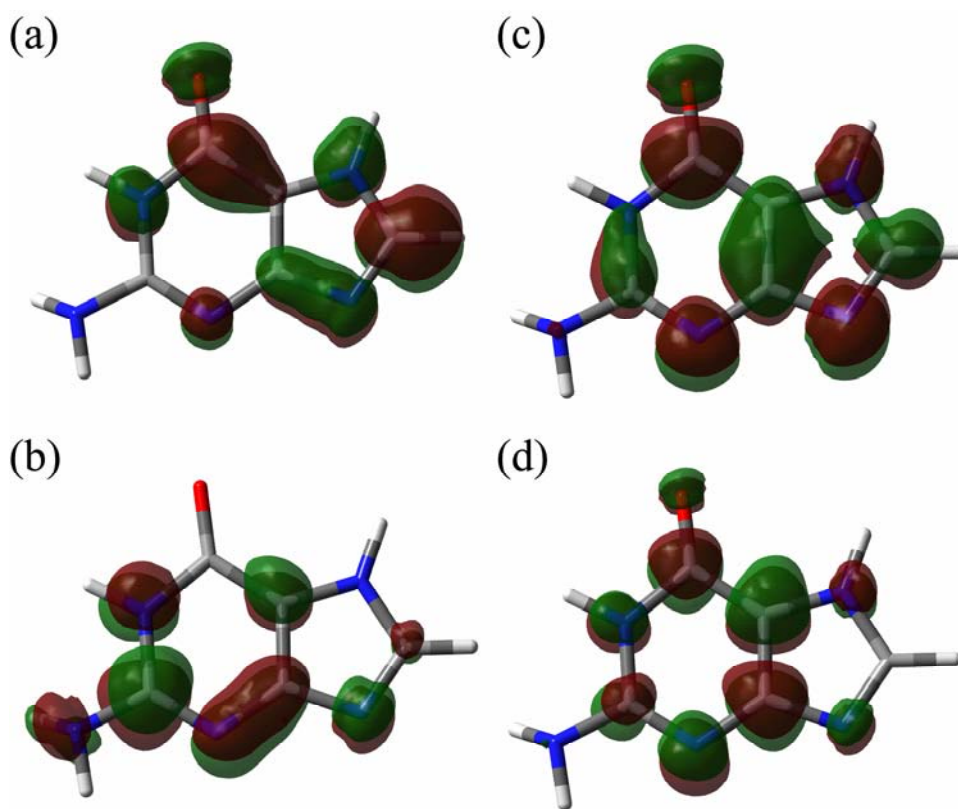


Figure S4. Wave function plots of four  $\pi^*$  resonance states (a:  $\pi_1^*$ , b:  $\pi_2^*$ , c:  $\pi_3^*$ , d:  $\pi_4^*$ ) for 7H-keto-guanine.

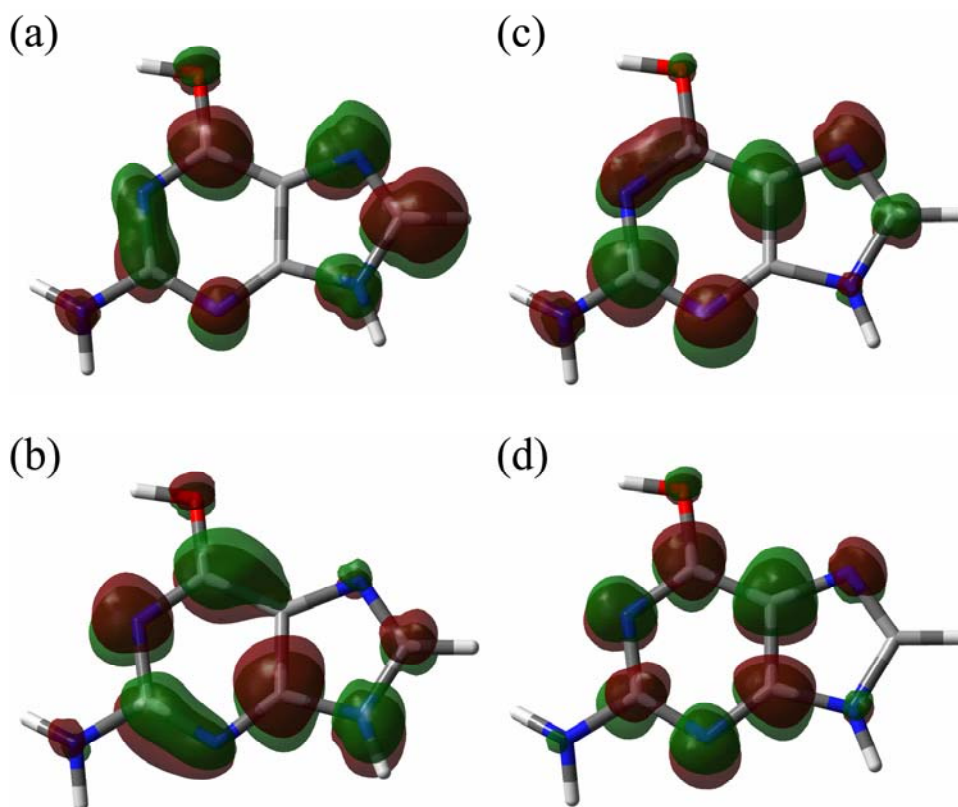


Figure S5. Wave function plots of four  $\pi^*$  resonance states (a:  $\pi_1^*$ , b:  $\pi_2^*$ , c:  $\pi_3^*$ , d:  $\pi_4^*$ ) for trans-9H-enol-guanine.

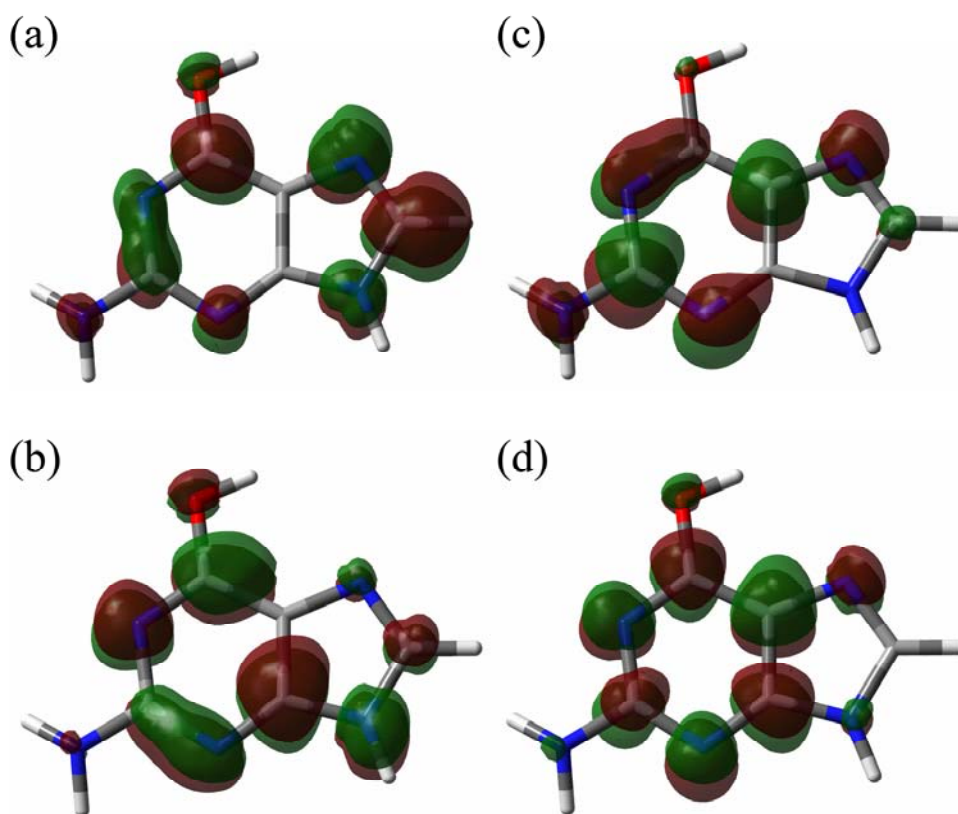


Figure S6. Wave function plots of four  $\pi^*$  resonance states (a:  $\pi_1^*$ , b:  $\pi_2^*$ , c:  $\pi_3^*$ , d:  $\pi_4^*$ ) for cis-9H-enol-guanine.



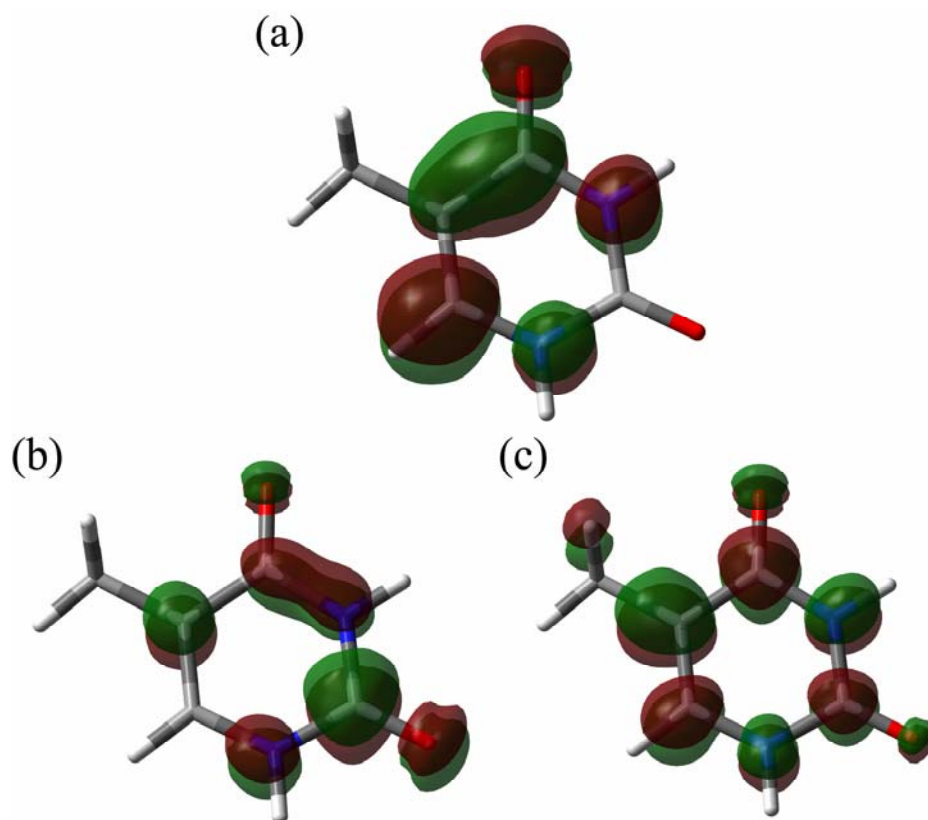


Figure S7. Wave function plots of three  $\pi^*$  resonance states (a:  $\pi_1^*$ , b:  $\pi_2^*$ , c:  $\pi_3^*$ ) for thymine

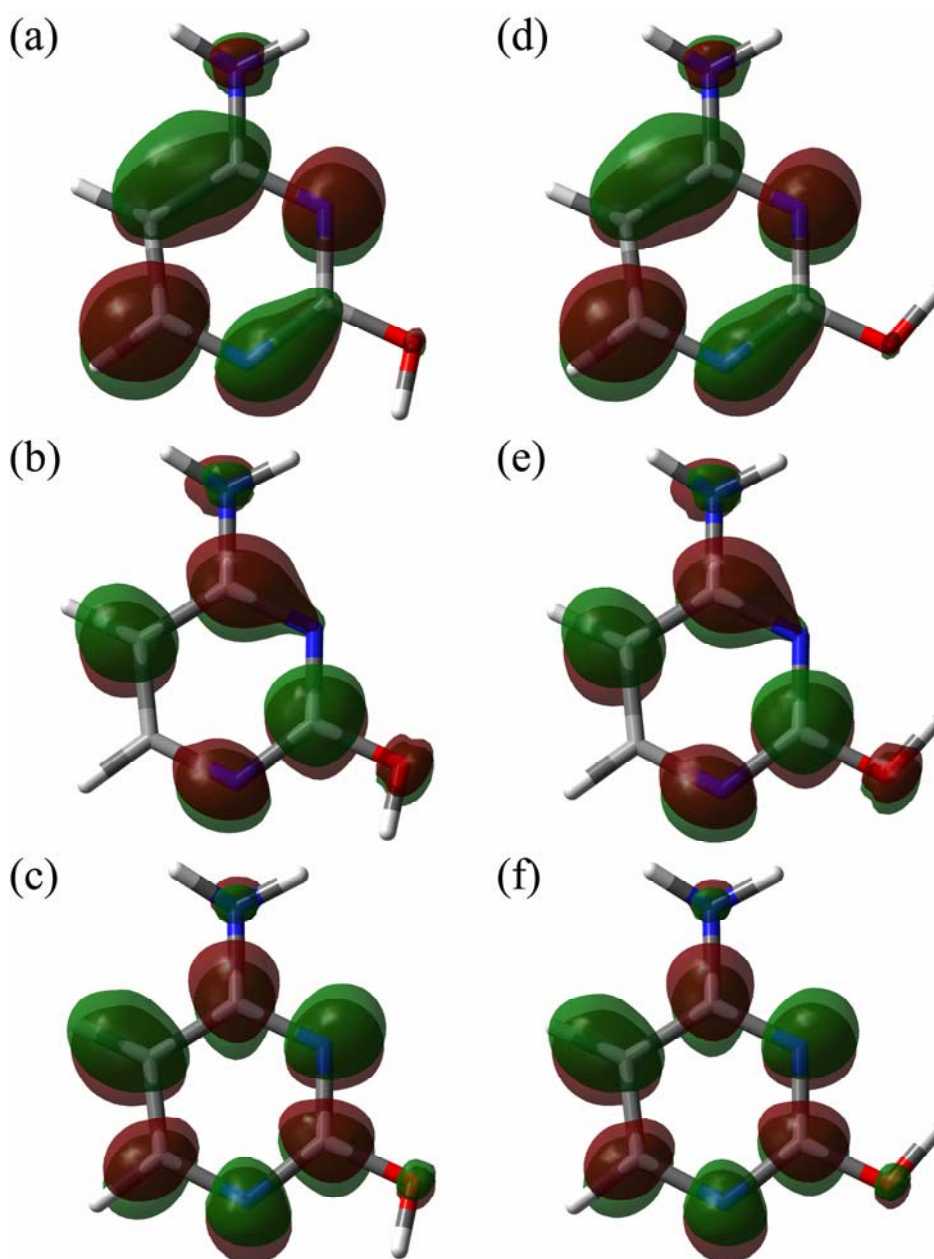


Figure S8. Wave function plots of three  $\pi^*$  resonance states for tautomers 2a (a:  $\pi_1^*$ , b:  $\pi_2^*$ , c:  $\pi_3^*$ ) and 2b (d:  $\pi_1^*$ , e:  $\pi_2^*$ , f:  $\pi_3^*$ ) of cytosine.

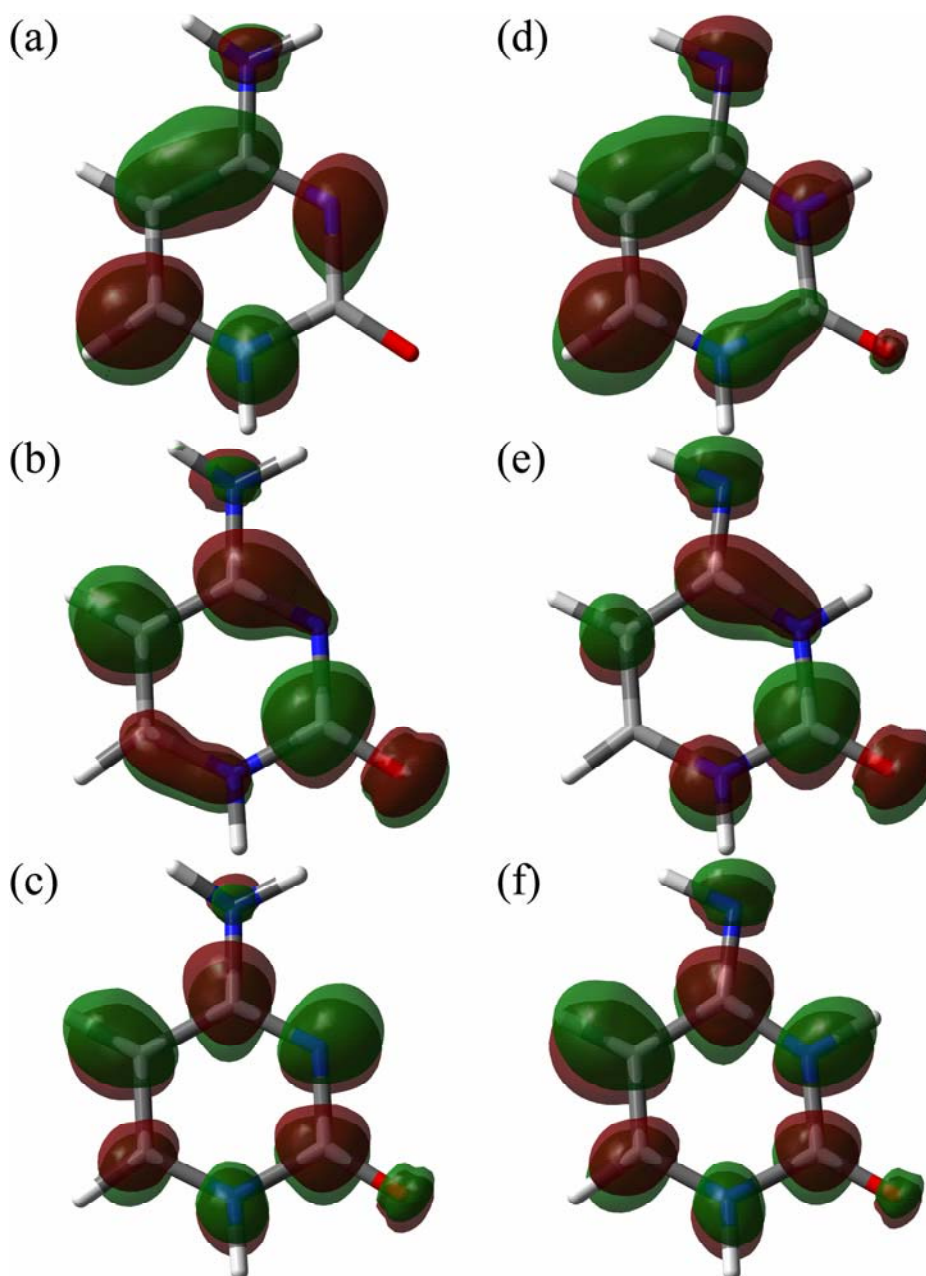


Figure S9. Wave function plots of three  $\pi^*$  resonance states for tautomers 1 (a:  $\pi_1^*$ , b:  $\pi_2^*$ , c:  $\pi_3^*$ ) and 3 (d:  $\pi_1^*$ , e:  $\pi_2^*$ , f:  $\pi_3^*$ ) of cytosine.