Electronic Supplementary Material (ESI) for Chemical Communications

Electric field induced DNA damage: an open door for selective mutations

(Supporting Information)

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(i) Computational Details

The well-known polarisable continuum model (PCM)[1] is included through single point energy calculations performed on the gas phase geometries. These single-point calculations have been performed with larger basis sets (including diffuse functions) aiming to provide the most accurate results. The used level of theory is: PCM-(M06-2X/6-311++G(d,p):M06-2X/6-31+G(d):PM6)//M06-2X/6-311G(d,p):M06-2X/6-31G(d):PM6.

(ii) Relatives energies

Table S-1: Relative total electronic energies for all located minima and transition states (in kcal/mol). The canonical GC base pair is taken as reference for computing energies.

	Negative strengths				Positive strengths			
$\|\|E_{ext}\|\|$	GC1ts	GC1	GC21ts	GC21	GC1ts	GC1	GC21ts	GC21
0			19.54	11.42				
10			19.56	10.48			18.28	10.73
20			19.75	10.30			17.52	10.78
40			8.99	9.97			16.48	11.25
60			–	9.75	–	4.46	15.33	11.26
80	4.81	-3.80	–	9.61	–	-0.71	13.90	11.52
100	2.81	-9.29	–	8.52	–	-1.37	14.64	13.76

The energies listed in Table S-2 confirm the larger impact of electric fields in the stability of GC1 and GC2 rare tautomeres compared to the effect on the GC21 form. Indeed, at -100 and -100×10^{-4} au, GC1 and GC2 become ca. 20 and 15 kcal mol^{-1} more stable than GC21. Consequently, in our paper we only discuss the effects of the most stable mutated forms at each field strength.

[1] J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.*, 2005, **105**, 2999–3093.

(iii) Rare tautomer structures

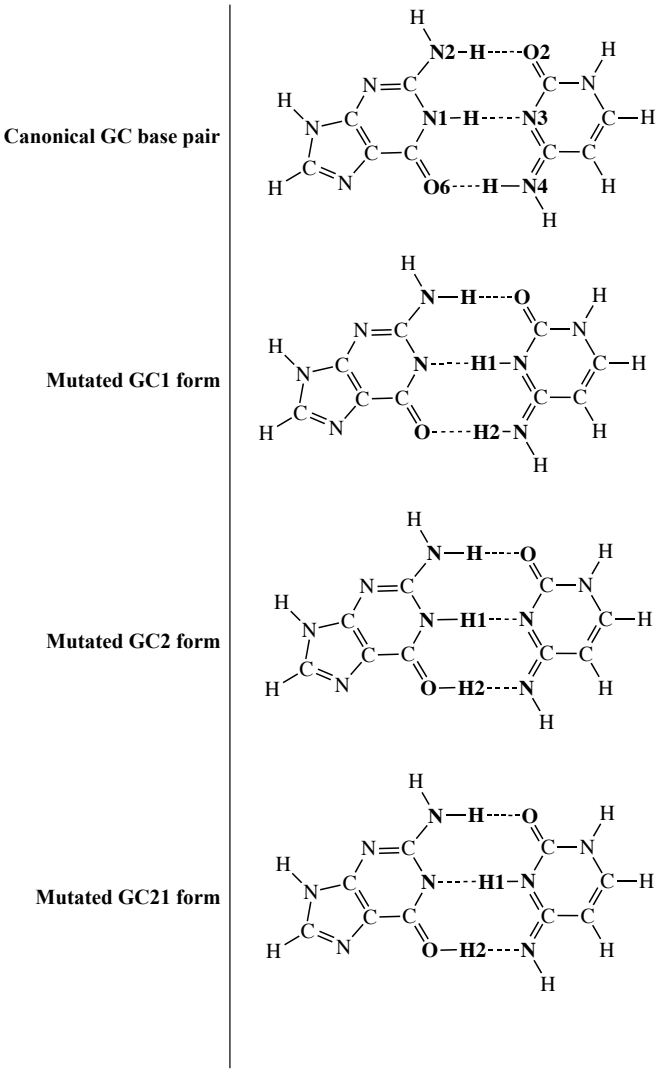

Figure S-1: Chemical structures and atomic numbering for the canonical and rare tautomeric forms of the GC base pairs.

Table S-2: Stacking effect on the GC H-bond distances (Å) under several external electric fields (au/10^{-4}).

E_{ext}	O_6–N_4	N_1–N_3	N_2–O_2
Single GC pair[a]			
0	2.80	2.94	2.92
−10	2.83	2.94	2.90
−20	2.85	2.93	2.88
−40	2.89	2.93	2.84
−60	2.93	2.92	2.79
−80	2.97	2.92	2.75
−100	3.01	2.92	2.71
DNA-embedded GC pair			
0	2.74	2.96	2.99
−10	2.76	2.96	2.97
−20	2.78	2.96	2.97
−40	2.80	2.97	2.95
−60	2.83	2.97	2.94
−80	2.86	2.97	2.92
−100	2.90	2.97	2.88

[a] Data from Ref. 12 (see main text).