

Table S1. The electron density (e/au^3), the values of H-bond energy (kJ mol^{-1}) evaluated using EML formula and the donor-acceptor interaction energies (kJ mol^{-1}) in the quaternary systems having guanine–thymine mispair and guanine–cytosine base pair. ^a

	ρ	$E_{\text{EML,HB}}$	$E_{\text{HB}}^{(2)}$
G [*] –T in	0.0407 (0.0349) <i>0.0210</i>	-50.90 (-35.99) <i>-20.15</i>	106.02 (97.70) <i>35.56</i>
G [*] –T G–C			
G–C in	0.0356 (0.0310) <i>0.0163</i>	-41.53 (-31.00) <i>-14.31</i>	91.67 (78.99) <i>17.03</i>
G [*] –T G–C			
G [*] –T in	0.0409 (0.0352) <i>0.0177</i>	-51.56 (-36.28) <i>-16.04</i>	108.53 (103.47) <i>26.53</i>
T–G [*] G–C			
G–C in	0.0280 (0.0320) <i>0.0290</i>	-30.12 (-32.04) <i>-31.68</i>	63.85 (87.28) <i>63.93</i>
T–G [*] G–C			
G–T [*] in	0.0637 (0.0393) <i>0.0216</i>	-90.57 (-43.75) <i>-20.95</i>	226.19 (112.93) <i>39.92</i>
G–T [*] G–C			
G–C in	0.0383 (0.0296) <i>0.0211</i>	-46.42 (-28.95) <i>-20.27</i>	104.73 (75.52) <i>37.36</i>
G–T [*] G–C			
G–T [*] in	0.0556 (0.0387) <i>0.0227</i>	-76.47 (-42.56) <i>-22.42</i>	180.79 (111.63) <i>44.60</i>
T [*] –G G–C			
G–C in	0.0275 (0.0328) <i>0.0288</i>	-29.36 (-33.28) <i>-31.39</i>	60.88 (90.37) <i>63.18</i>
T [*] –G G–C			

^a The normal data, data in the parentheses and italicized data correspond to HB1, HB2 and HB3, respectively.