

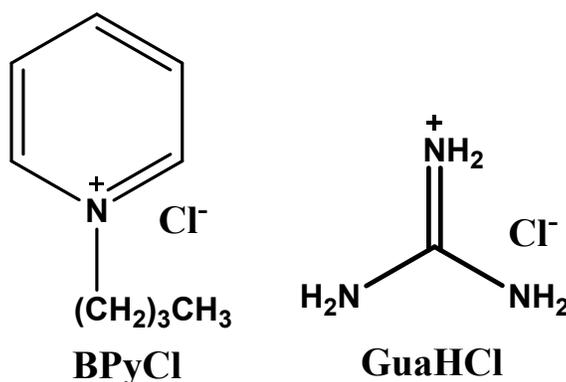
## Supporting Information

# Ionic Liquid Induced G-quadruplex Formation and Stabilization: Spectroscopic and Simulation Studies

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**Scheme S1.** Chemical structures of 1-Butylpyridinium chloride (BPyCl) and guanidine hydrochloride (GuaHCl).

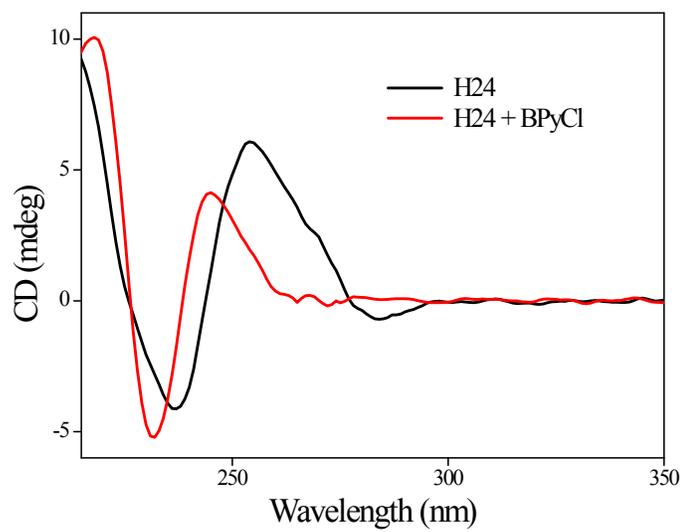
**Table S1.** Fluorescent lifetime decay parameters of fluorescent modified oligo (~ 5  $\mu\text{M}$ ) in different conditions.  $\text{K}^+$  ion and  $\text{Na}^+$  ion indicate the presence of 100 mM KCl and NaCl salt respectively; in 10 mM tris buffer solution (pH 7.2).

Sample	$\tau_{\text{avg}}$ (ns)	$\chi^2$
Mod Oligo + Gua-IL (500 $\mu\text{M}$ )	1.37	1.10
Mod Oligo + $\text{K}^+$ ion	0.98	1.11
Mod Oligo + $\text{Na}^+$	2.68	1.02

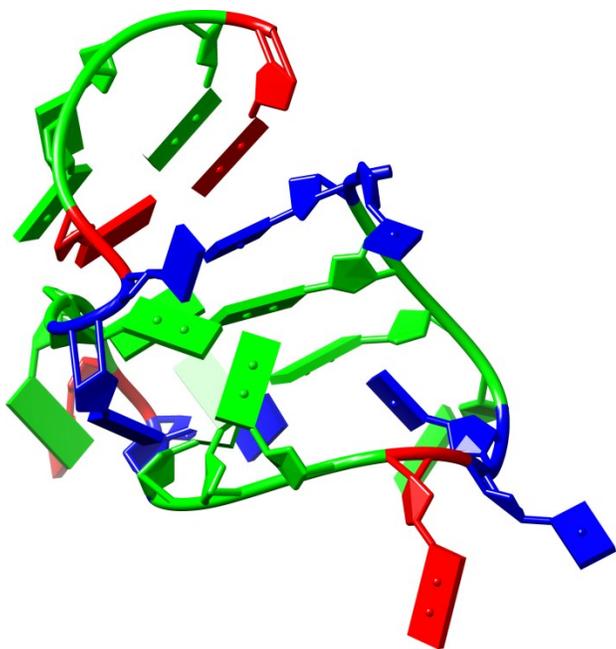
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ion

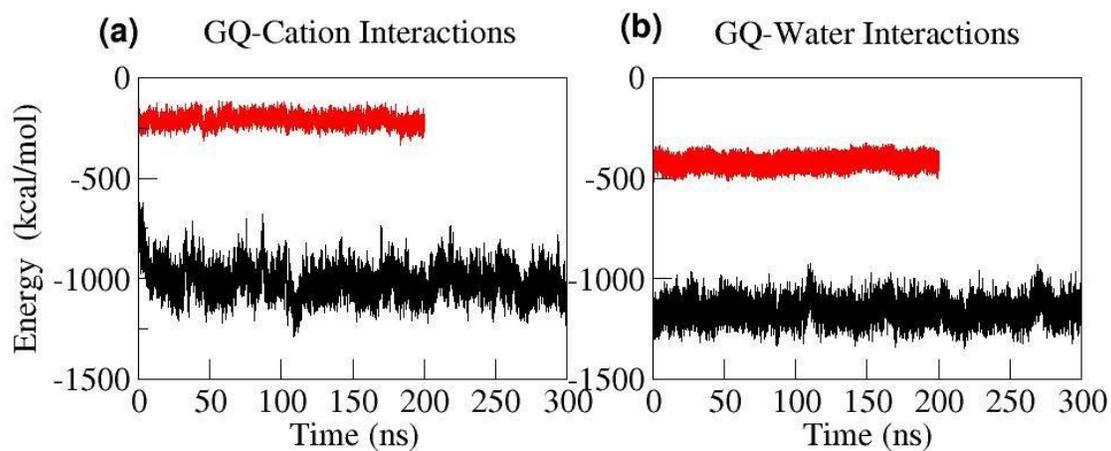
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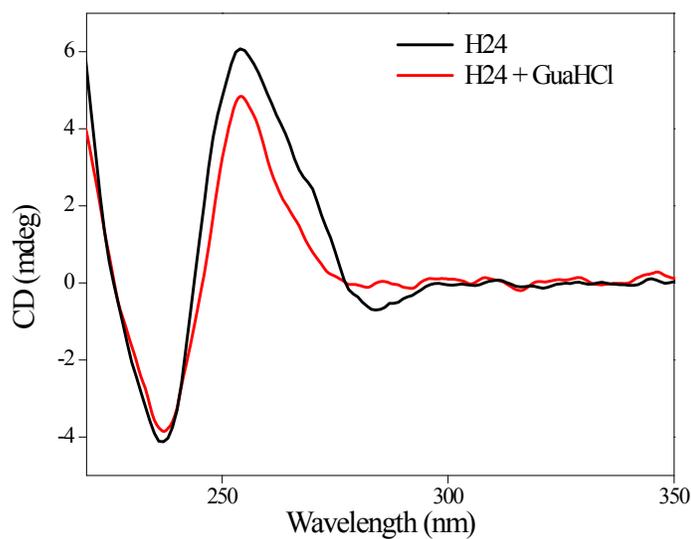
**Figure S1.** Circular dichroism spectra of H24 DNA ( $\sim 5 \mu\text{M}$ ) in deionized water in presence and absence of BPyCl (1 mM).



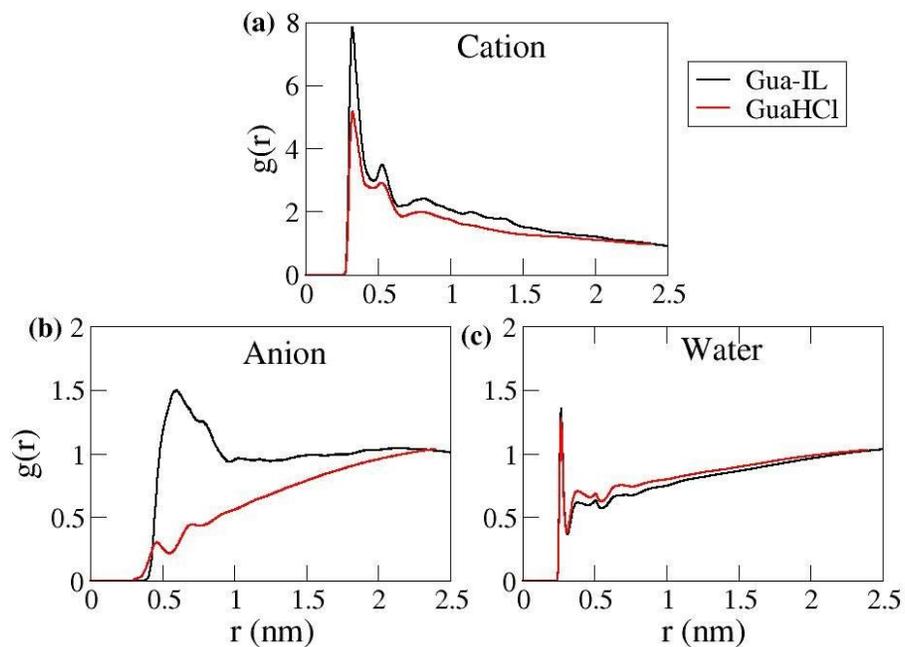
**Figure S2.** The disrupted structure of GQ in presence of BPyCl after 200 ns.



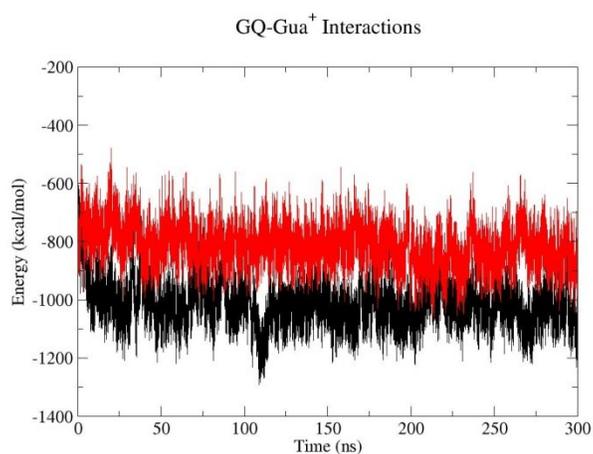
**Figure S3.** The figure showing interactions energy between (a) G-quadruplex and first solvation shell cation molecule and (b) G-quadruplex and first solvation shell water molecules in case of Gua-IL (black line) and BPyCl (red line).



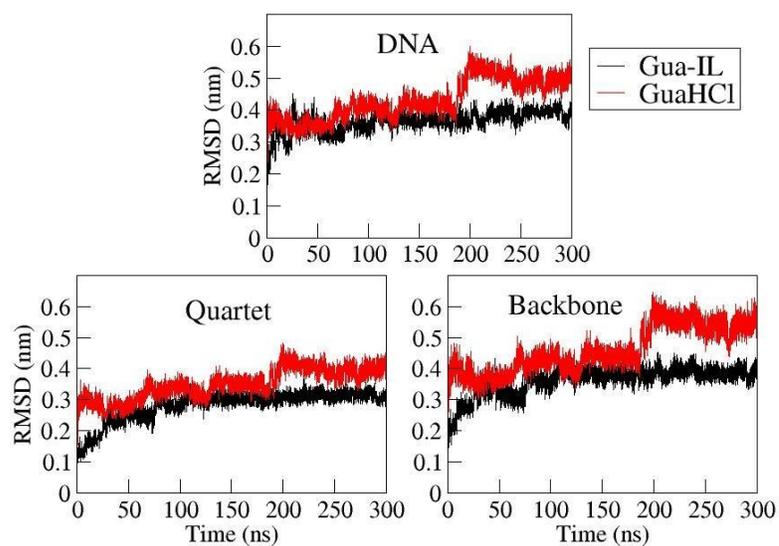
**Figure S4.** Circular dichroism spectra of H24 DNA ( $\sim 5 \mu\text{M}$ ) in deionized water in presence and absence of GuaHCl (5 mM).



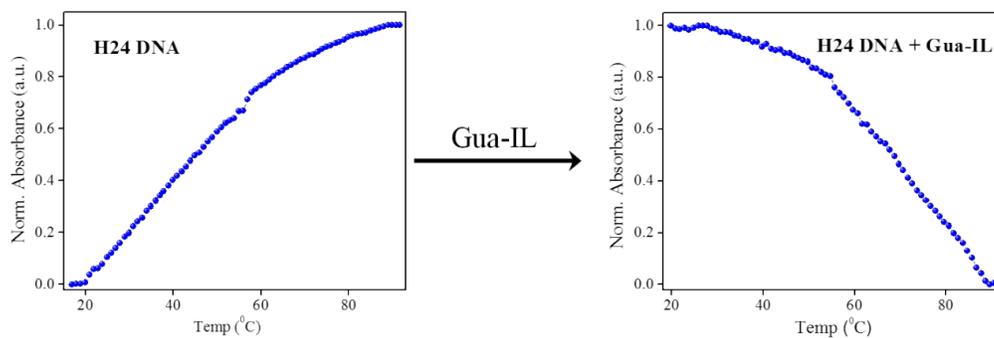
**Figure S5.** The RDF of various atoms around surface of G-quadruplex in case of Gua-IL (black line) and GuaHCl (red line) for (a) cations i.e.  $\text{Gua}^+$  ions ; (b) anions i.e.  $\text{FEP}^-$  for Gua-IL and  $\text{Cl}^-$  for GuaHCl and (c) water oxygen (OW) atoms.



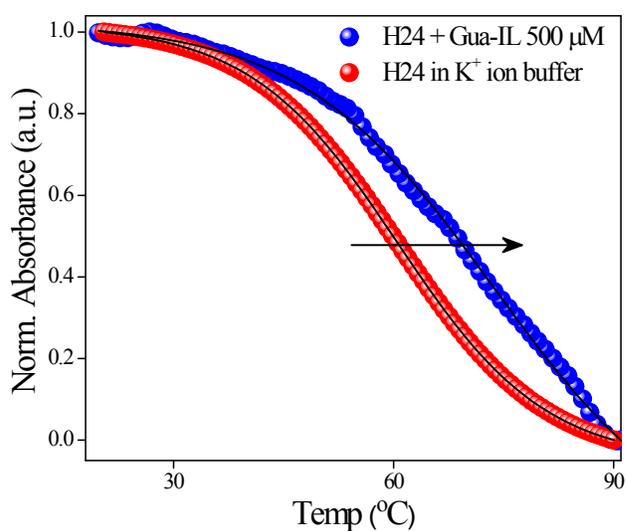
**Figure S6.** The interaction energy between G-quadruplex and cations present in the first solvation shell for two ILs - Gua-IL (black line) and GuaHCl (red line).



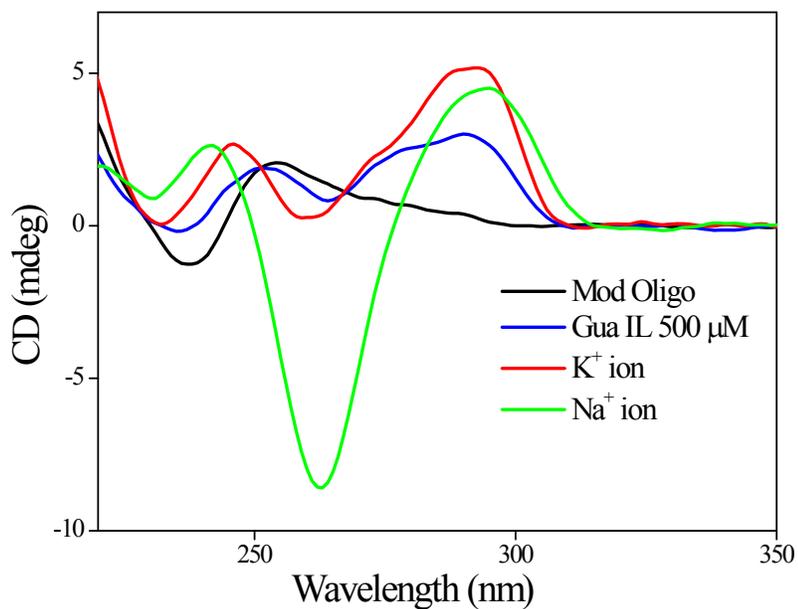
**Figure S7.** The RMSD of heavy atoms of G-quadruplex, heavy atoms of Quartet and heavy atoms of backbone in case of Gua-IL (black line) and GuaHCl (red line).



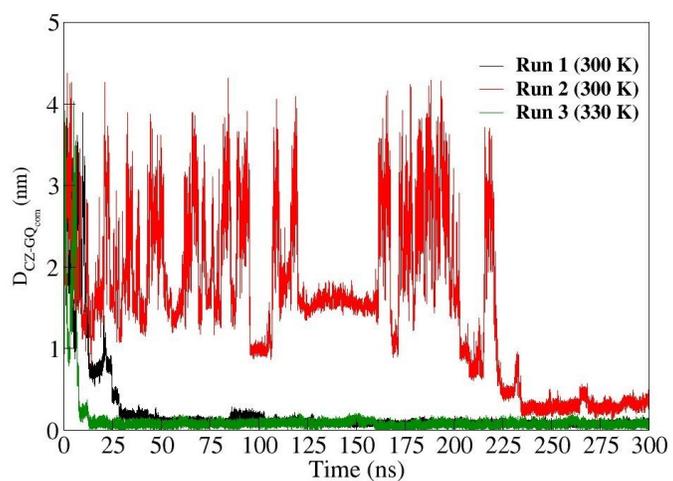
**Figure S8.** UV melting profile of H24 DNA (~ 5  $\mu\text{M}$ ) in deionized water in absence and presence of Gua-IL (500  $\mu\text{M}$ ).



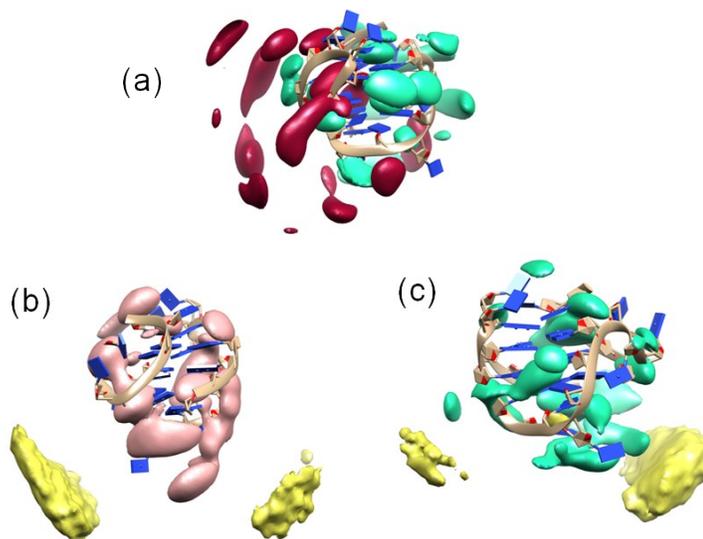
**Figure S9.** UV melting profile of H24 DNA (~ 5  $\mu\text{M}$ ) in deionized water in presence of Gua-IL (500  $\mu\text{M}$ ) and K<sup>+</sup> ion containing buffer. K<sup>+</sup> ion legend indicates the presence of 100 mM KCl salt in 10 mM tris buffer (pH 7.2) solution.



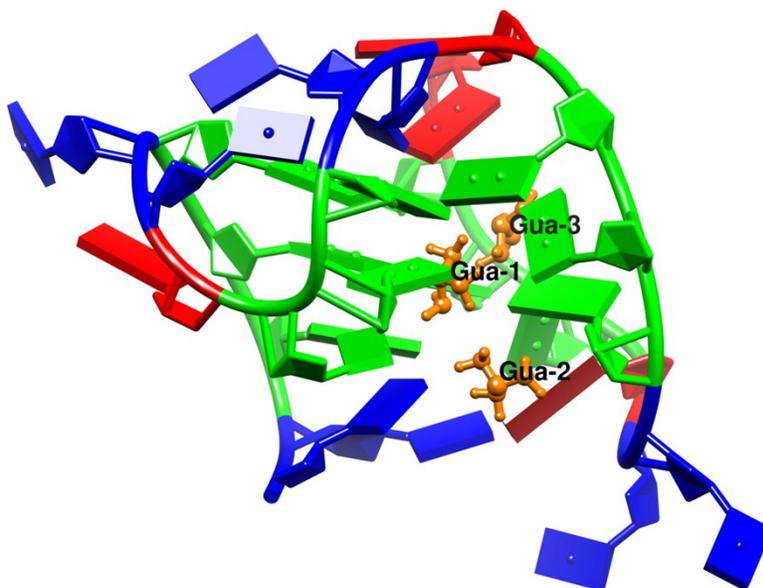
**Figure S10.** Circular dichroism spectra of fluorescent modified oligomer ( $\sim 5 \mu\text{M}$ ) in different conditions. “Mod Oligo” legend in the figure corresponds to the CD spectra of fluorescent modified oligomer in absence of any ion i.e. in deionised water.  $\text{K}^+$  ion and  $\text{Na}^+$  ion legends indicate the presence of 100 mM KCl and 100 mM NaCl respectively, in 10 mM tris buffer (pH 7.2) solution.



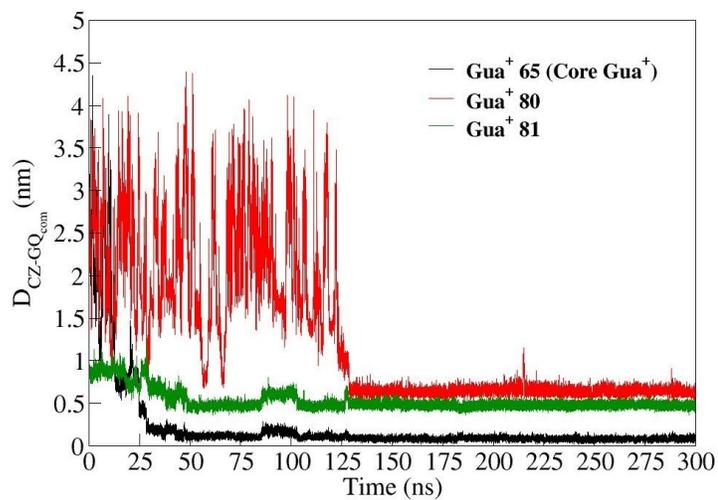
**Figure S11.** Distance between central  $\text{Gua}^+$  (carbon atom of  $\text{Gua}^+$  (CZ)) and CoM of G-quadruplex quartet region along time for Run 1 (black line) and Run 2 (red line) at 300K as well as for Run 3 (green line) performed at 330 K.



**Figure S12.** The Figure showing spatial distribution function of cations and anions around G-quadruplex as shown in (a) side view presentation of Gua<sup>+</sup> (Green) and FEP<sup>-</sup> (dark red) in case of Gua-IL; (b) BPy<sup>+</sup> (light pink) and Cl<sup>-</sup> (yellow) in case of BPyCl and (c) Gua<sup>+</sup> (Green) and Cl<sup>-</sup> (yellow) in case of GuaHCl.



**Figure S13.** The figure showing 3 closest Guanidinium residues Gua-1, Gua-2 and Gua-3 in case of Gua-IL simulation-1 performed at 300 K.



**Figure S14** The figure showing distance between closest Gua<sup>+</sup> residues such as Gua-1 (Gua<sup>+</sup> present in the GQ core, black line), Gua-2 and Gua-3 (strongly bound from outer side, red and green line) along time. The carbon atom of Gua<sup>+</sup> (CZ) and CoM of quadruplex quartet is considered for calculations.