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 µM) in different conditions. K+ ion and Na+ ion indicate the presence of 100 mM KCl and NaCl salt respectively; in 10 mM tris buffer solution (pH 7.2).

<table>
<thead>
<tr>
<th>Sample</th>
<th>τ_{avg} (ns)</th>
<th>χ²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mod Oligo + Gua-IL</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(500 µM)</td>
<td>1.37</td>
<td>1.10</td>
</tr>
<tr>
<td>Mod Oligo + K+ ion</td>
<td>0.98</td>
<td>1.11</td>
</tr>
<tr>
<td>Mod Oligo + Na+ ion</td>
<td>2.68</td>
<td>1.02</td>
</tr>
</tbody>
</table>
**Figure S1.** Circular dichroism spectra of H24 DNA (~ 5 μM) 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.

![Graph of GQ-Cation Interactions and GQ-Water Interactions](image)

**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 (~ 5 μM) 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. Gua⁺ ions; (b) anions i.e. FEP⁻ for Gua-IL and 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 μM) in deionized water in absence and presence of Gua-IL (500 μM).

**Figure S9.** UV melting profile of H24 DNA (~ 5 μM) in deionized water in presence of Gua-IL (500 μM) and K⁺ ion containing buffer. K⁺ 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 (~ 5 μM) 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. K⁺ ion and 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 Gua⁺ (carbon atom of 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$^+$ (Green) and FEP$^-$ (dark red) in case of Gua-IL; (b) BP$y^+$ (light pink) and Cl$^-$ (yellow) in case of BP$y$Cl and (c) Gua$^+$ (Green) and Cl$^-$ (yellow) in case of GuaHCl.

![Figure showing spatial distribution function](image)

**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 showing 3 closest Guanidinium residues](image)
**Figure S14** The figure showing distance between closest Gua\(^+\) residues such as Gua-1 (Gua\(^+\) 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\(^+\) (CZ) and CoM of quadruplex quartet is considered for calculations.