Supporting Information for:

Ligand-Induced G-Quadruplex Polymorphism: A DNA Nanodevice for Label-Free Aptasensor Platforms

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Figure S1. Fluorescence titration of H-Telo22 (1 µM) with BtC (0–10 µM) showing displacement of NMM (5 µM) in 50 mM potassium phosphate buffer containing 100 mM KCl at 25 °C. Inset: Binding isotherm obtained by plotting fluorescence excitation at 580 nm ($\lambda_{Em} = 609$ nm) and $K_d = 1.0 \pm 0.1$ µM measured using sigma plot software – simple ligand binding model.

Figure S2. CD spectra of H-Telo22 (3 µM) with (a) BtC (15 µM, solid green trace) and (b) 4Ql (15 µM, solid red trace) ligands and their corresponding displacement (dashed purple traces) by NMM ligand (30 µM) in 50 mM potassium phosphate buffer containing 100 mM KCl at 15 °C.
**Figure S3.** Fluorescence titrations of (a) BtC (0.5 µM, dotted green traces) and (b) 4QI (0.5 µM, dotted red traces) with H-Telo22 (0–1.5 µM). Inset: Binding isotherm obtained by plotting corresponding fluorescence emission at 645 nm (λ<sub>Ex</sub> = 580 nm) and 595 nm (λ<sub>Ex</sub> = 533 nm) to provide binding constants as $K_d = 2.9 \pm 0.8$ µM and $K_d = 2.8 \pm 0.2$ µM for BtC and 4QI binding to H-Telo22 in 50 mM Tris buffer containing 50 mM NaCl at 25 °C.
Figure S4. Respective (a) CD and (b) fluorescence titrations demonstrating changes in GQ topology of H-Telo22 (3 and 1 µM) with displacement of (a) 4QI (30 and 5 µM) by BtC (240 and 20 µM) ligand in 50 mM Tris buffer containing 50 mM NaCl at 15 and 25 °C. Fluorescence emission was monitored for 4QI at 595 nm (λ_{Ex} = 533 nm) and binding isotherm was plotted against the ratio of BtC to 4QI to obtain $K_d = 7.9 \pm 1.4$ µM using sigma plot software – simple ligand binding model.
Figure S5. Fluorescence spectra for 5 µM of (a) NMM (purple), (b) BtC (green) and (c) 4QI (red) fluorescent ligands in the absence (solid blue lines) and in presence of H-Telo22 (1 µM, dashed lines), acquired in 50 mM potassium phosphate buffer containing 100 mM KCl at 25 °C.
**Figure S6.** Binding isotherm obtained and $K_d$ value determined using sigma plot software – simple ligand binding model for OTABA (0–12 µM) binding to ThT (6 µM, blue trace), 4QI (6 µM, red trace) and BtC (6 µM, green trace). Fluorescence titrations were performed in OTA binding buffer (pH = 8) and at 25 °C. Inset: Color of 10 µM of ThT, 4QI and BtC probes in absence and in presence of 5 µM of OTABA, respectively.

**Figure S7.** Determination of Limits of Detection (LoD) and quantification (LoQ) for OTA binding to OTABA and displacing ThT (blue markers), 4QI (red markers) and BtC (green markers).
Figure S8. Fluorescence emission spectra of 1 µM of ThT (solid blue), 4QI (dotted red) and BtC (dashed green) in the presence of 0.5 µM OTABA recorded at 25 °C in the OTA binding buffer.

Figure S9. Selectivity and anti-interference response of BtC–OTABA system towards OTA. Fluorescence response BtC–OTABA probe (1:0.5 µM) in terms of % drop for presence of individual mycotoxins (4 µM) and also in co-existence with OTA (4 µM). %D_{Analyte} is the % intensity drop measured for different analytes, individually or in co-existence of OTA, as indicated.
Table S1. Results of recovery experiments from the analysis of spiked red wine samples using OTABA–BtC system.

<table>
<thead>
<tr>
<th>spiked OTA (µM)</th>
<th>recovered OTA (µM)</th>
<th>% recovery</th>
<th>RSD (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.13</td>
<td>0.15</td>
<td>115 ± 2.3</td>
<td>1.06</td>
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<tr>
<td>0.27</td>
<td>0.24</td>
<td>89 ± 3.8</td>
<td>1.83</td>
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<tr>
<td>0.53</td>
<td>0.49</td>
<td>93 ± 3.9</td>
<td>2.12</td>
</tr>
<tr>
<td>1.00</td>
<td>0.95</td>
<td>95 ± 4.3</td>
<td>2.50</td>
</tr>
</tbody>
</table>

Figure S10. $^1$H NMR spectra of 4QI.

Figure S11. $^{13}$C-jmod NMR spectra of 4QI.
Figure S12. HRMS spectra of 4QI.

Figure S13. $^1$H NMR spectra of BtC.