

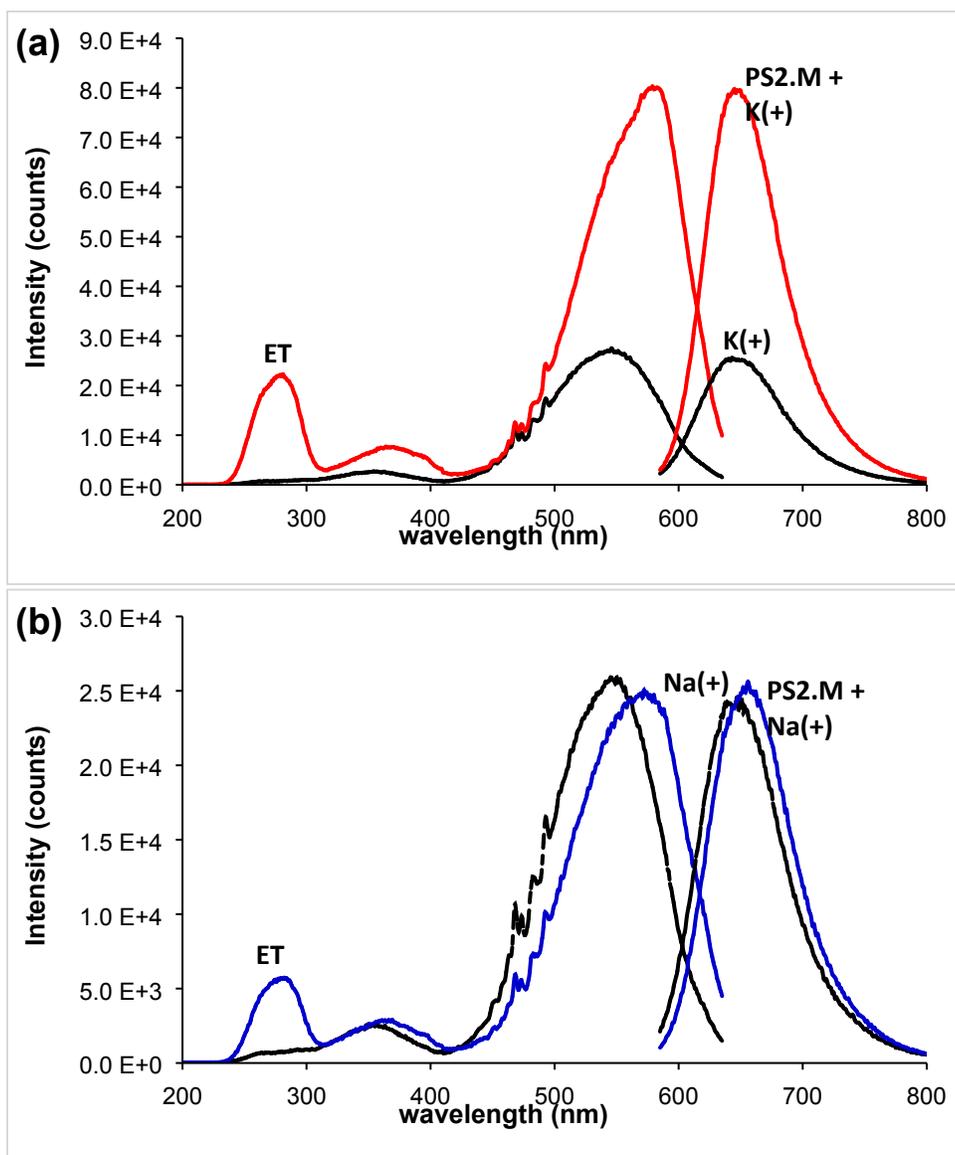
*Supporting Information for:*

## **A ratiometric fluorescent sensor of the parallel G-quadruplex produced by PS2.M: Implications for K<sup>+</sup> detection**

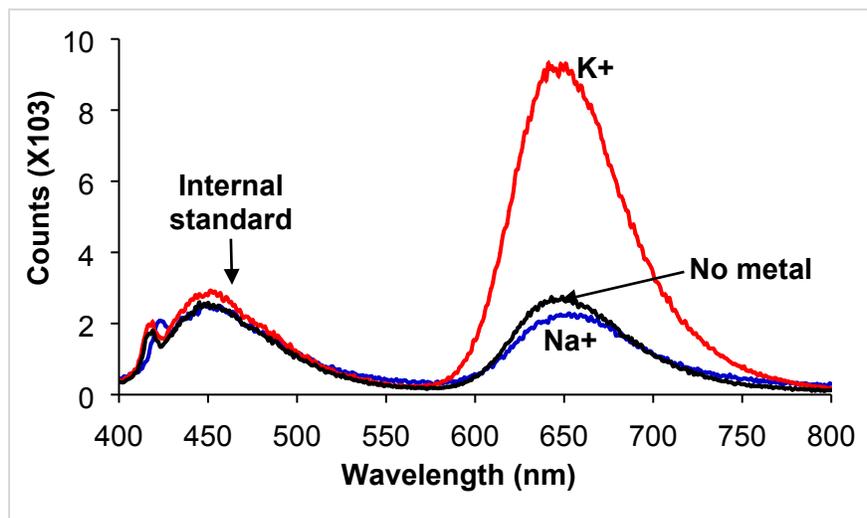
*Prashant S. Deore and Richard A. Manderville\**

### **Table of Contents:**

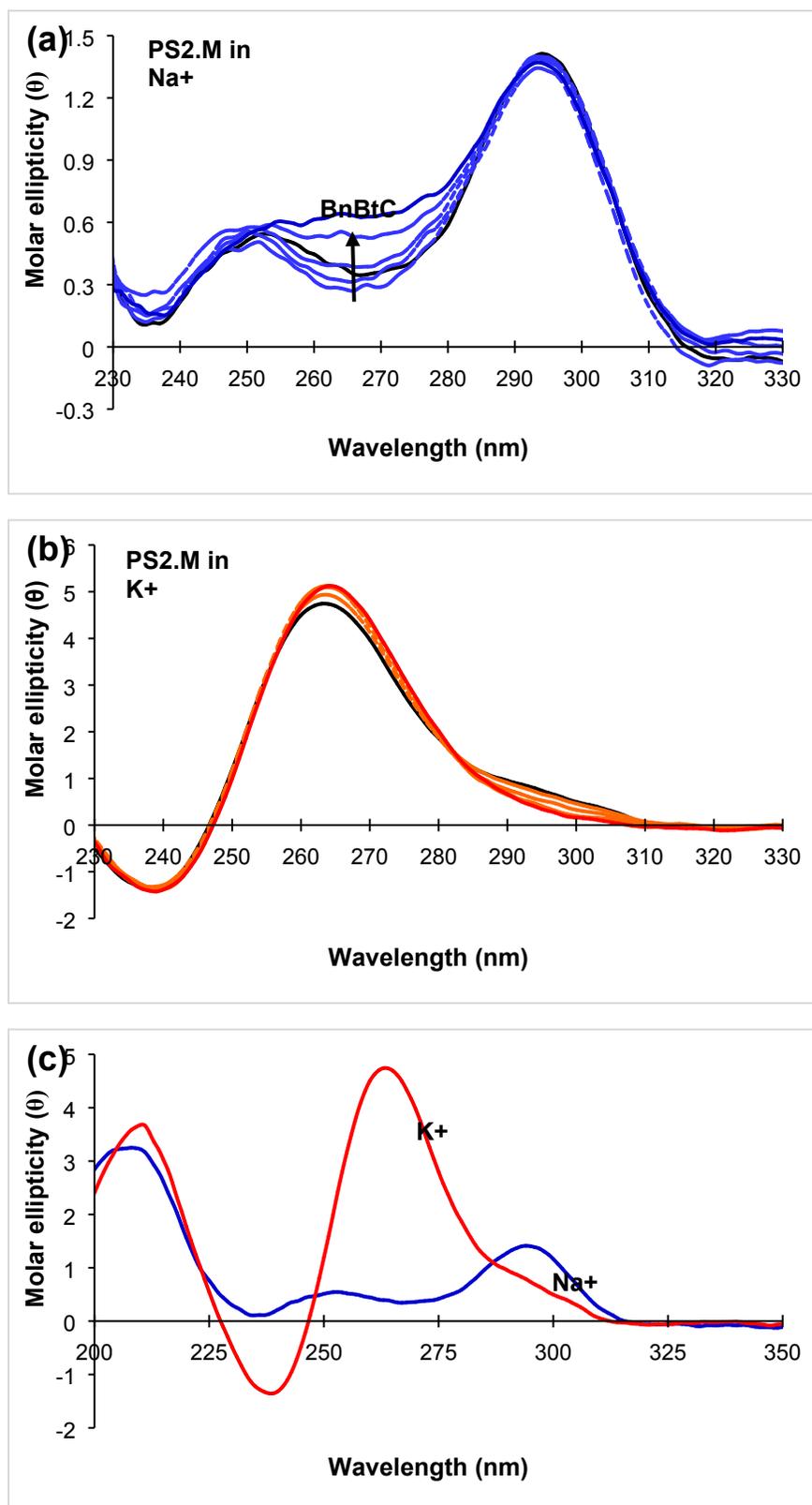
1. <b>Figure S1.</b> Fluorescence spectra of BnBtC for PS2.M folding due to Na <sup>+</sup> and K <sup>+</sup> .	<b>2</b>
2. <b>Figure S2.</b> Ratiometric fluorescence response of PS2.M–BnBtC for Na <sup>+</sup> /K <sup>+</sup> .	<b>3</b>
3. <b>Figure S3.</b> CD spectra of PS2.M GQ in Na <sup>+</sup> and K <sup>+</sup> solutions.	<b>4</b>
4. <b>Figure S4.</b> Fluorescence titration of K <sup>+</sup> into PS2.M–BnBtC.	<b>5</b>
5. <b>Figure S5.</b> LoD and LoQ determination for K <sup>+</sup> detection.	<b>5</b>
6. <b>Table S1.</b> Results of recovery experiments.	<b>6</b>



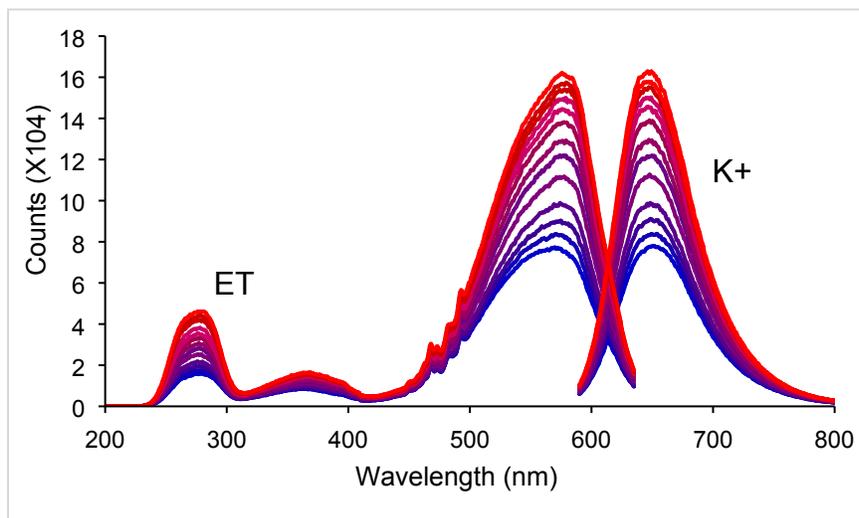
**Figure S1.** Fluorescence excitation and emission spectra of 5  $\mu\text{M}$  of BnBtC in the presence of (a) 100 mM of KCl and (b) 100 mM of NaCl, which were recorded the absence of PS2.M (dotted green traces) and in presence of PS2.M with metal ions ( $\text{Na}^+$ , dashed blue traces) and with  $\text{K}^+$ , solid red traces). The spectra were recorded in tris-acetate buffer (pH = 6.7) at ambient temperature (25  $^{\circ}\text{C}$ ).



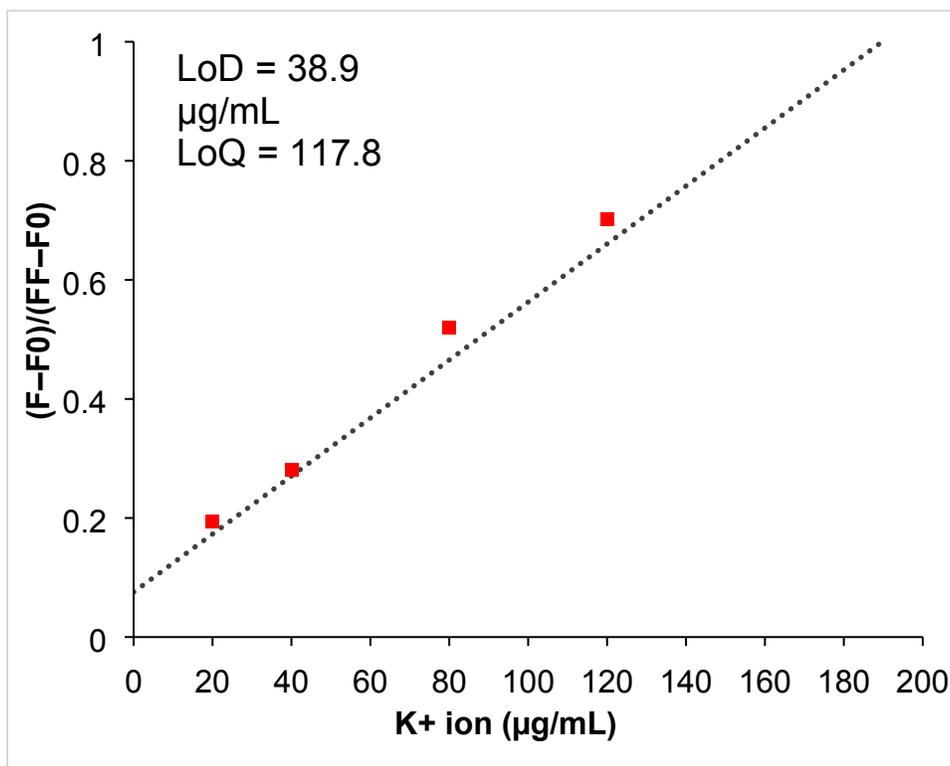
**Figure S2.** Ratiometric fluorescence emission response of 1  $\mu\text{M}$  of PS2.M-BnBtC (1:1,  $\lambda_{\text{Ex}}$  = 367 nm) in the presence of 100 mM of KCl (solid red trace), 100 mM of NaCl (dashed blue trace) and in absence of metal cation (dotted black trace) in 20 mM tris-acetate buffer (pH = 6.7) at 25  $^{\circ}\text{C}$ .



**Figure S3.** Effect of BnBtC probe on GQ of PS2.M stabilized by (a) Na<sup>+</sup> and (b) K<sup>+</sup>, respectively. Dashed black traces denotes initial CD profile of PS2.M DNA (5  $\mu$ M) with Na<sup>+</sup>/K<sup>+</sup> (100 mM). The dashed blue and red traces are the effective CD spectra of PS2.M GQ upon addition of BnBtC probe (upto 25  $\mu$ M, 5 equivalents to DNA) in Na<sup>+</sup> and K<sup>+</sup> solutions, respectively. (c) CD profile of PS2.M GQ in Na<sup>+</sup> (solid blue trace) and K<sup>+</sup> (dotted red trace) solutions without added ligands.



**Figure S4.** Fluorescence titration of  $K^+$  (0→200 mM) into PS2.M–BnBtC system (1:5  $\mu$ M) performed in 20 mM tris-acetate buffer (pH = 6.7) containing 100 mM of NaCl at 25 °C. An increase in energy transfer intensity at ~ 256 nm is observed with increased binding efficiency of the probe to DNA with increasing  $K^+$  concentration.



**Figure S5.** Determination of Limits of Detection (LoD) and quantification (LoQ) for  $K^+$  induced GQ folding in PS2.M DNA (1  $\mu$ M) monitored by fluorescence of BnBtC probe (5  $\mu$ M,  $\lambda_{Ex}/\lambda_{Em}$  = 550/645 nm). Where,  $F^0$ ,  $F$  and  $F^F$  are the fluorescence intensities in the absence, varying and maximum (200  $\mu$ g/mL)  $K^+$  concentration, respectively.

**Table S1.** Results of recovery experiments from the analysis of real-water samples. <sup>a,b</sup>

water sample	added K <sup>+</sup> (mM)	found K <sup>+</sup> (mM)	% error	% recovery	avg % recovery	avg % RSD
mineral	1	0.96	4	96	106	11.78
	2	2.04	2	102		
tap	1	1.02	2	102	101.5	8.63
	2	1.85	8	92.5		
speed river	1	0.92	8	92	99.3	8.14
	2	2.16	8	108		

<sup>a</sup>All the samples were analyzed as collected, without any treatment. <sup>b</sup>The measurements were performed using Spectramax i3 instrument using 384 well plate, while the reported values for each measurements were averaged from an independent triplicate measurement for each addition for that data.