

Supporting Information

Custom G4 microarrays reveal selective G-quadruplex recognition of small molecule BMVC: a large-scale assessment of ligand binding selectivity

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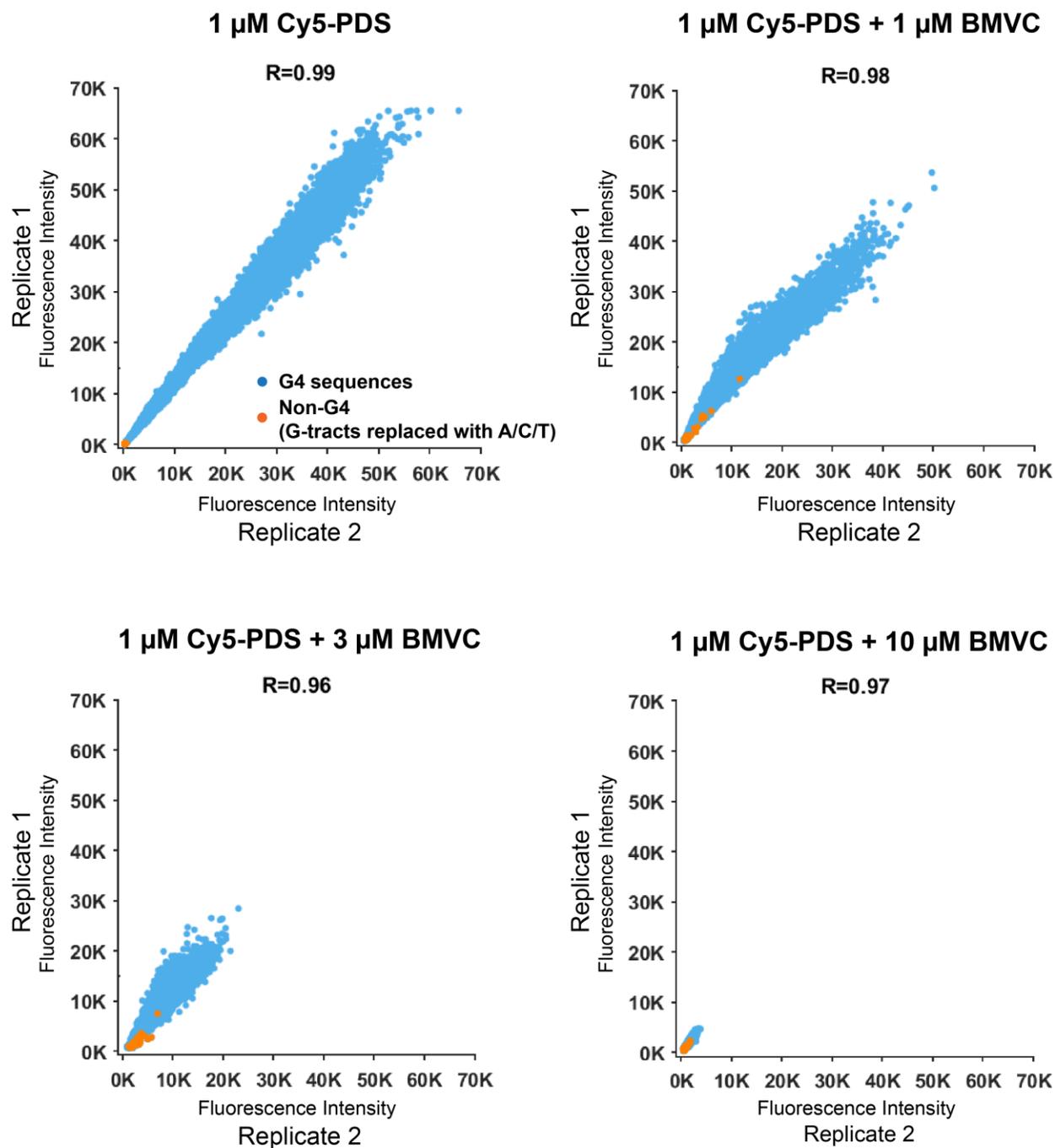


Figure S1. Comparison of replicate fluorescence intensity of Cy5-PDS in the absence and presence of 1, 3, and 10 μM of BMVC. R stands for the Pearson correlation coefficient, which measures the correlation between the X and Y values of each plot.

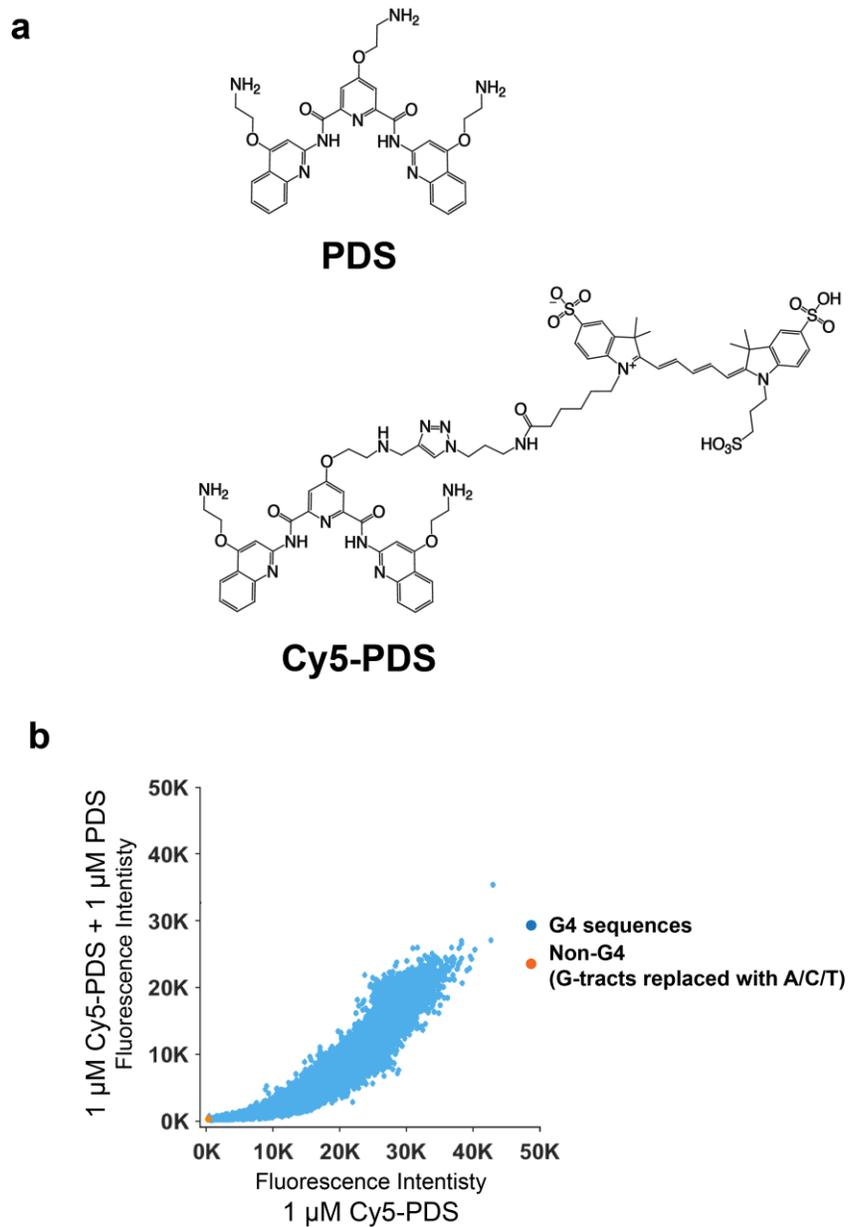


Figure S2. (a) Chemical structures of PDS and Cy5-PDS. (b) The competition microarray experiments of 1 μ M Cy5-PDS with 1 μ M unlabeled PDS. The scatterplot showing the fluorescence of 1 μ M Cy5-PDS in the presence of 1 μ M unlabeled PDS vs. the fluorescence of 1 μ M Cy5-PDS in the absence of PDS.

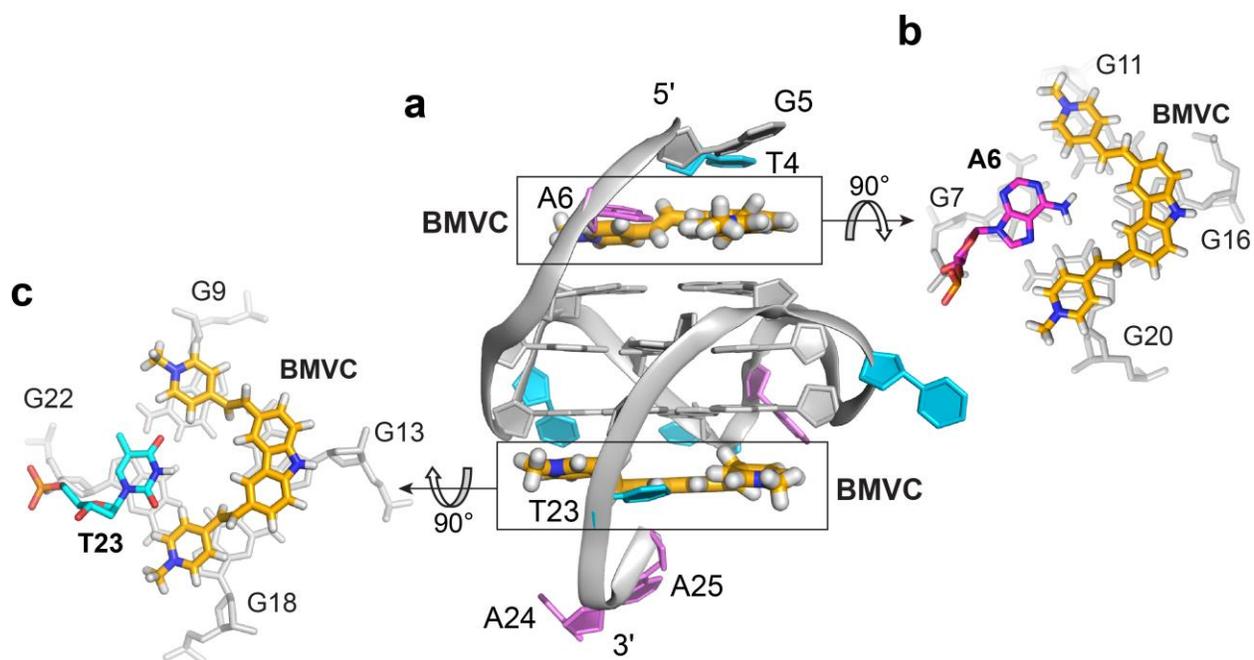


Figure S3. The NMR solution structure of a 2:1 complex of BMVC and MYC_14/23T G4 (PDB ID: 6O2L). (a) BMVC (stick model) binds at both the 5'-end and 3'-end of MYC_14/23T G4 (cartoon representation). (b-c) For the specific binding, BMVC recruits a flanking base to form a ligand-base pair at both of the 5'-end binding site (b) and the 3'-end binding site (c). BMVC = orange, Thymine = cyan, Adenine = magenta, Guanine = gray.

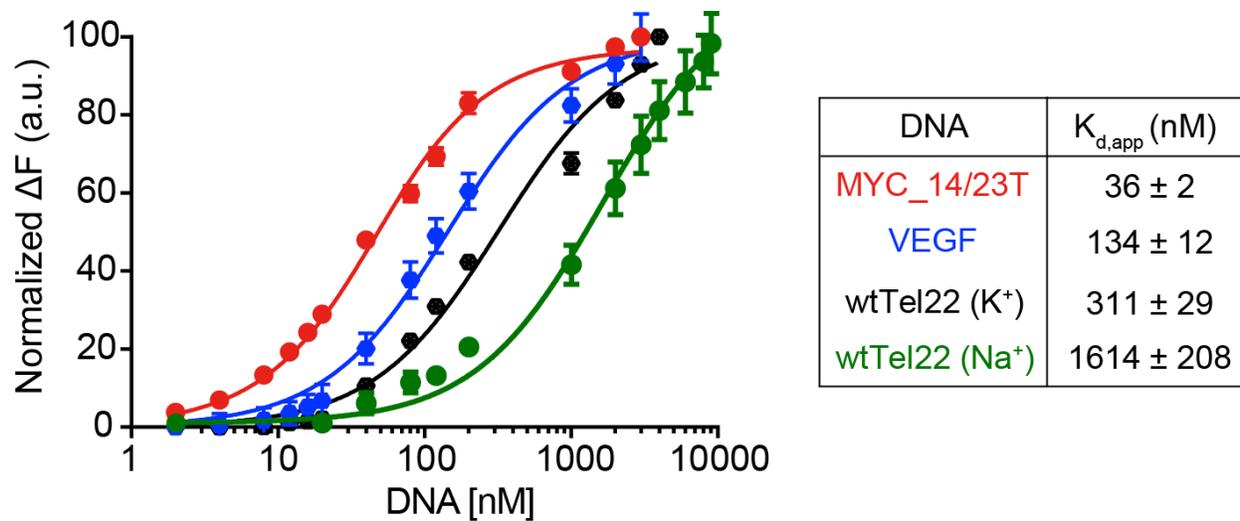


Figure S4. Apparent dissociation constant ($K_{d,app}$) of BMVC binding to various G4 structures determined by BMVC fluorescence. Conditions: 20 nM BMVC, 25 °C, pH 7, 100 mM K⁺ (100 mM Na⁺ for wtTel22).

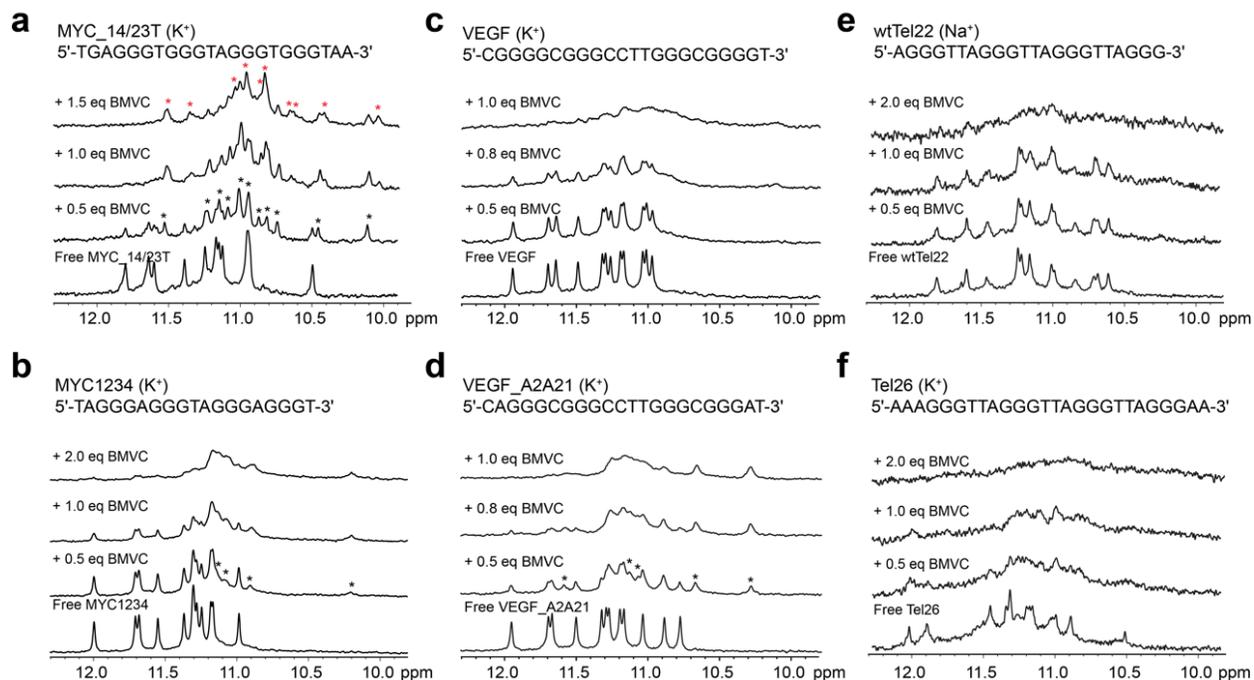


Figure S5. Imino proton regions of the 1D ^1H NMR titration spectra of BMVC with various G4 sequences. **(a)** MYC_14/23T, the major parallel G4 formed from the MYC promoter NHE III₁. **(b)** MYC1234, a parallel G4 formed from the 5'-end runs of guanines of the MYC promoter NHE III₁. **(c)** VEGF, a parallel G4 formed in the VEGF promoter. **(d)** VEGF_A2A21, the major parallel G4 formed from the VEGF promoter. **(e)** wtTel22 human telomeric sequence forms a basket-type G4 in Na^+ solution. **(f)** Tel26, the hybrid-1 human telomeric G4. Imino protons arising from the 1:1 or 2:1 complex formation are marked with asterisks in black or red, respectively. All spectra were collected at 25 °C, pH=7.

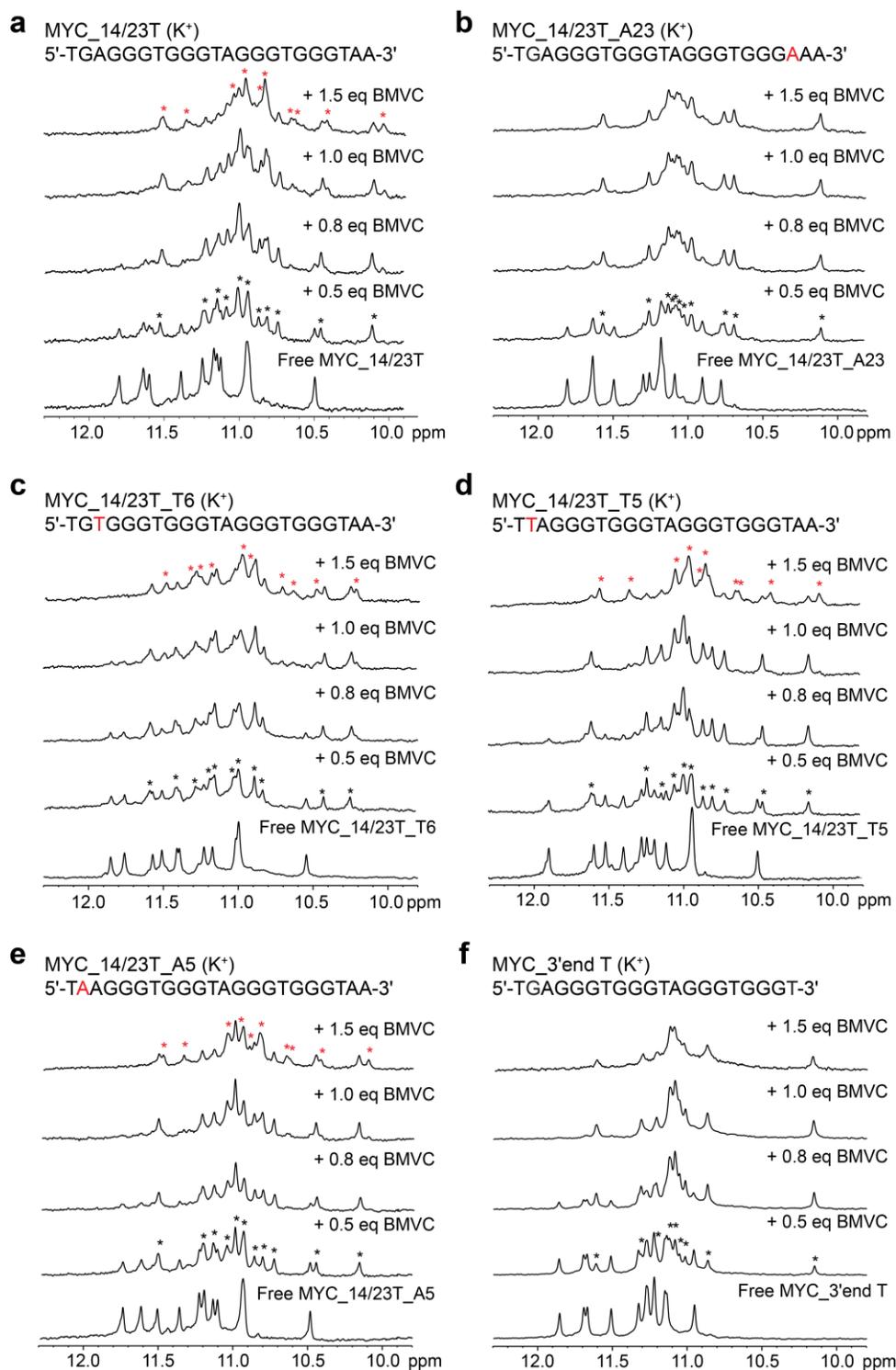


Figure S6. Imino proton regions of the 1D ^1H NMR titration spectra of BMVC with MYC_{1423T} G4 (**a**), its 3'-end modified (**b, f**) and 5'-end modified (**c-e**) sequences. Imino protons arising from the 1:1 or 2:1 complex formation are marked with asterisks in black or red, respectively. All spectra were collected in 95 mM K^+ , pH=7 solution, at 25 °C.