Insect multimeric G-quadruplexes fold into antiparallel structures of different compactness and stability in K⁺ and Na⁺ solutions

Chao Gao,^{a,†} Jixin Chen,^{a†} Naureen Anwar,^b Jieya Deng,^{a,} Zhangqian Wang,^{a,*} Muhammad Umer^{c*}, and Yi He^{a,*}

^{a.} National R&D Center for Se-rich Agricultural Products Processing, Hubei Engineering Research Center for Deep Processing of Green Se-rich Agricultural Products, School of Modern Industry for Selenium Science and Engineering, Wuhan Polytechnic University, Wuhan 430023, China.

^{b.} Department of Biology, Faculty of Science and Technology, Virtual University of Pakistan, Punjab, 54000, Pakistan.

^{c.} Institute for Forest Resources and Environment of Guizhou and Forestry College, Research Center of Forest Ecology, Guizhou University, Guiyang, 550025, China.

[†] The authors wish it to be known that, in their opinion, the first two authors should be regarded as Joint First Authors.

*To whom correspondence should be addressed. Email: wzqsnu@whpu.edu.cn, umer@gzu.edu.cn, yi.he@whpu.edu.cn.

| Supplementary tables and figures2 |
|---|
| Table S1. Oligonucleotide sequences used in the experiment |
| Figure S1. Fluorescence spectra of a modified (A) Bom17 and (B) Bom 37 with |
| 5'-FAM and 3'-TAMRA in 10 mM Tris-HCl (pH 7.5) buffer containing 100 mM |
| KCl/NaCl4 |
| Figure S2. CD spectra of <i>c-MYC</i> G-quadruplex in 10 mM Tris-HCl (pH 7.50) and |
| 100 mM KCl/NaCl solutions |
| Figure S3. Determination of FRET efficiency of c-MYC G-quadruplexes in |
| KCl/NaCl |
| solutions6 |
| Figure S4. Native polyacrylamide gel electrophoresis analysis of Bom17 and Bom37 in K ⁺ /Na ⁺ solutions |
| Figure S5. Fluorescence spectra of 3.0 µM BMPQ-1 with/withou 10.0 µM Bom17 G-quadruplex in 10 mM Tris-HCl (pH 7.5) buffer containing 100 mM KCl or NaCl |
| Figure S6. The dissociation constant (K_D) values of BMPQ-1 and Bom17, Bom37 |

| Table S1 | Ongonucleonde sequences used in the experiment |
|------------|--|
| Name | Sequence(5'→3') |
| Bom17 | GG(TTAGG) ₃ |
| Bom37 | GG(TTAGG)7 |
| Bom57 | GG(TTAGG)11 |
| Bom77 | GG(TTAGG)15 |
| Bom97 | GG(TTAGG)19 |
| c-MYC | TGGGGAGGGTGGGGAGGGTGGGGAAGG |
| Bom39-Ap1 | (2-AP)GG(TTAGG)7A |
| Bom39-AP21 | AGG(TTAGG)3TT(2-AP)GG(TTAGG)3A |
| Bom39-AP39 | (2-AP)GG(TTAGG)7(2-AP) |

 Table S1
 Oligonucleotide sequences used in the experiment



Figure S1. Fluorescence spectra of a modified (A) Bom17 and (B) Bom 37 with 5'-FAM and 3'-TAMRA in 10 mM Tris-HCl (pH 7.5) buffer containing 100 mM KCl/NaCl. $\lambda ex = 488$ nm.



Figure S2. CD spectra of *c-MYC* G-quadruplex in 10 mM Tris-HCl (pH 7.50) and 100 mM KCl/NaCl solutions. The concentration of oligonucleotides was 10 μ M.



Figure S3. Determination of FRET efficiency of *c-MYC* G-quadruplexes in KCl/NaCl solutions. (A) Fluorescence spectra of a modified *c-MYC* with 5'-FAM and 3'-TAMRA in 10 mM Tris-HCl (pH 7.50) buffer containing 100 mM KCl/NaCl. $\lambda ex =$ 488 nm. (B) FRET efficiency of *c-MYC* G-quadruplex in KCl/NaCl solutions. Fluorescence intensities were measured at $\lambda em = 525$ nm (FAM) and 585 nm (TAMRA).



Figure S4. Native polyacrylamide gel electrophoresis analysis of Bom17 and Bom37 in 100 mM (A) K⁺ and (B) solution. Native gel electrophoresis was run on 20% polyacrylamide gel. The concentration of oligonucleotides was 6.0 μ M.



Figure S5. Fluorescence spectra of BMPQ-1 with/withou Bom17 G-quadruplex in 10 mM Tris-HCl (pH 7.5) buffer containing 100 mM (A) KCl or (B) NaCl. The concentration of Bom17 was 10.0 μ M, and BMPQ-1 was 3.0 μ M. λ ex = 395 nm.



Figure S6. Benesi-Hildebrand plot of 1/(F-F0) versus 1/[DNA]. The dissociation constant (K_D) value of BMPQ-1 and (A) Bom17 and (B) Bom37 G-quadruplexes in 100 mM KCl solution was calculated as 12.72 ± 2.52 µM and 1.46 ± 0.16 µM, respectively. The dissociation constant (K_D) value of BMPQ-1 and (C) Bom17 and (D) Bom37 G-quadruplexes in 100 mM NaCl solution was calculated as 34.49 ± 6.55 µM and 5.15 ± 1.09 µM, respectively.



Figure S7. The survival rate of SF9 cells after 48 hours of treatment with different concentrations of BMPQ-1.