

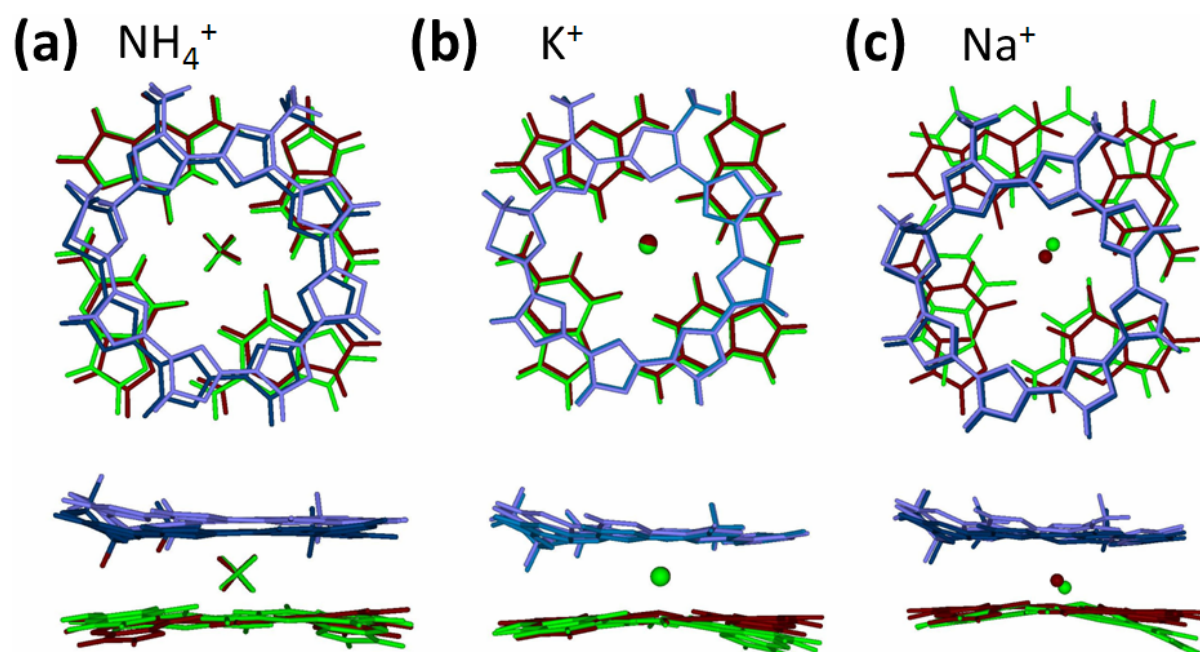
Cation Involvement in Telomestatin Binding to G-Quadruplex DNA

Valérie Gabelica^{1,2*}, Frédéric Rosu^{1,2*}, Nicolas Smargiasso^{1,2}, Gabriel Mazzucchelli^{1,2}, Kazuo Shinya³, Edwin De Pauw^{1,2}

1. Mass Spectrometry Laboratory, Department of Chemistry, University of Liège, Belgium
2. GIGA-Systems Biology and Chemical Biology, University of Liège, Belgium
3. Biomedical Information Research Center, National Institute of Advanced Industrial Science and Technology, Biological Systems Control Team, Tokyo, Japan.

* Joint first authors.

Supporting information



Supporting Information Figure S1: Manual superimposition of optimized geometry of the ternary complex telomestatin - cation - G-quartet obtained using B3LYP and MPWB1K functionals (top view and side view). (a) NH_4^+ , (b) K^+ , (c) Na^+ . The B3LYP optimized structures are in green (G-quartet) and purple (telomestatin). The MPWB1K optimized structures are in red (G-tetrad) and blue (telomestatin).

Supporting Information Table S1: Comparison of the geometries optimized with the different hybrid functional: root mean square distances (RMSD) of two-by-two comparisons (in Å).

	Cation + telomestatin complex	Cation + telomestatin + G-quartet complex
B3LYP vs BHHLYP		
NH₄⁺	0.045	0.265
K⁺	0.045	0.131
Na⁺	0.000	0.856
B3LYP vs MPWB1K		
NH₄⁺	0.085	0.350
K⁺	0.083	0.276
Na⁺	0.069	0.726
MPWB1K vs BHHLYP		
NH₄⁺	0.054	0.302
K⁺	0.055	0.188
Na⁺	0.069	0.573

Supporting Information Table S2: Interaction energies of NH_4^+ , K^+ and Na^+ with telomestatin alone, telomestatin + one G-quartet, computed with DFT, 6-31G(d,p) basis set, and three different hybrid functionals: B3LYP, BHandHLYP, and MPWB1K. The calculation of the interaction energy of the cation in the complex (BSSE corrected) has been calculated using the following equations:

$$\Delta E_{\text{int}} = E_{(\text{telomestatin}+\text{cation})} - E_{(\text{telomestatin})} - E_{(\text{cation})} - E_{(\text{BSSE})}$$

$$\Delta E_{\text{int}} = E_{(\text{G4}+\text{telomestatin}+\text{cation})} - E_{(\text{G4}+\text{telomestatin})} - E_{(\text{cation})} - E_{(\text{BSSE})}$$

	Cation interaction energy with telomestatin alone (kcal/mol)	Cation interaction energy with telomestatin + G-quartet (kcal/mol)
B3LYP		
NH_4^+	-84.9	-115.8
K^+	-82.7	-119.9
Na^+	-93.8	-141.2
BHandHLYP		
NH_4^+	-87.4	-120.7
K^+	-86.0	-117.9
Na^+	-95.4	-147.0
MPWB1K		
NH_4^+	-88.1	-121.6
K^+	-86.1	-124.3
Na^+	-95.6	-145.6