

Native electrospray mass spectrometry of DNA G-quadruplexes in potassium solution

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SUPPORTING INFORMATION

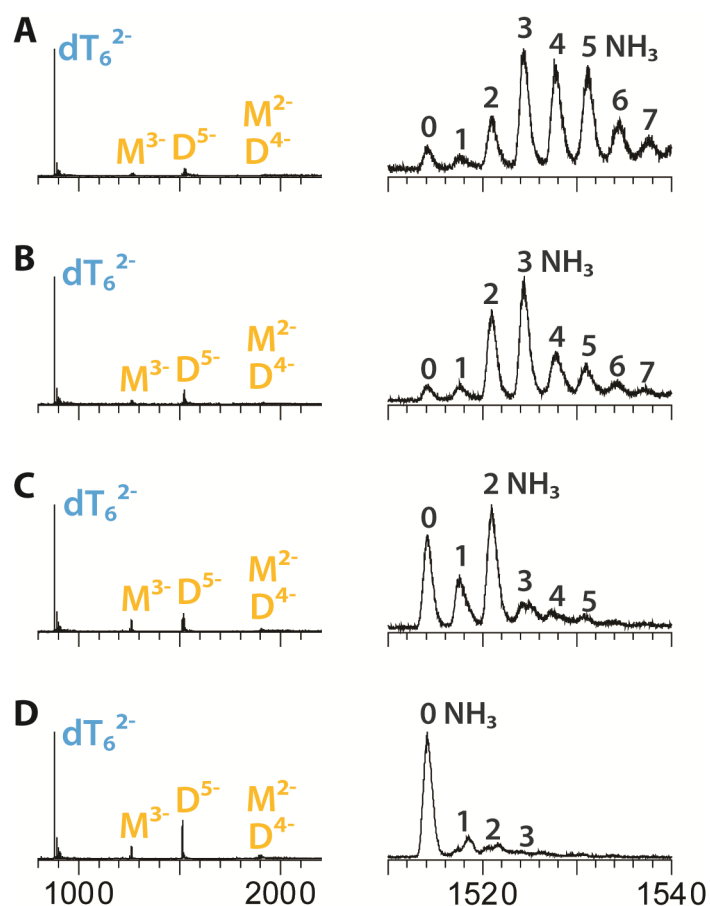


Figure S1. ESI-MS of 10 μM $\text{G}_4\text{T}_4\text{G}_4$ in 100 mM NH_4OAc . From A to D (30, 50, 70 and 90 V, respectively): the effect of the ion guide 1 voltage on the ammonium cation preservation in the gas-phase. Left is the full scale spectrum and on the right is the zoom on the dimer D^{5-} peak.

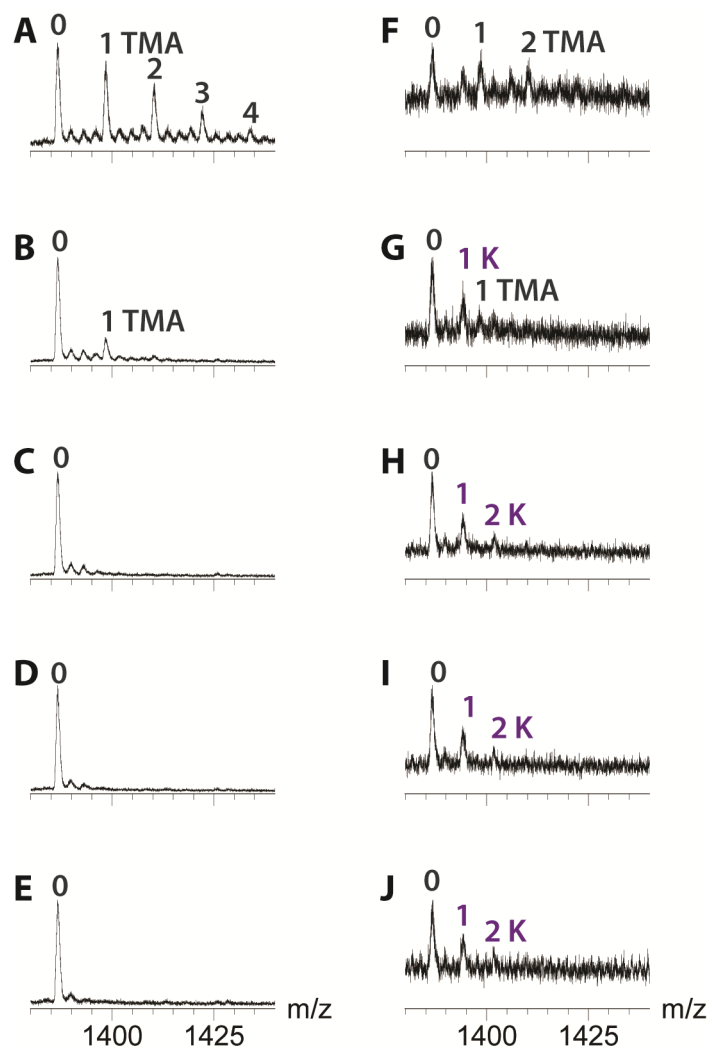


Figure S2. ESI-MS of 5 μ M 22non-G4 sequence d(GGG-ATG-CGA-CAG-AGA-GGA-CGG-G). From A to E and from F to J the ion guide 1 voltage is increased to 30, 50, 70, 90 and 110 V, respectively. (A-E): 22non-G4 in 100 mM TMAA and (F-J): 22non-G4 in 100 mM TMA + 1 mM KCl. The predominant stoichiometry is the oligonucleotide without any adducts.

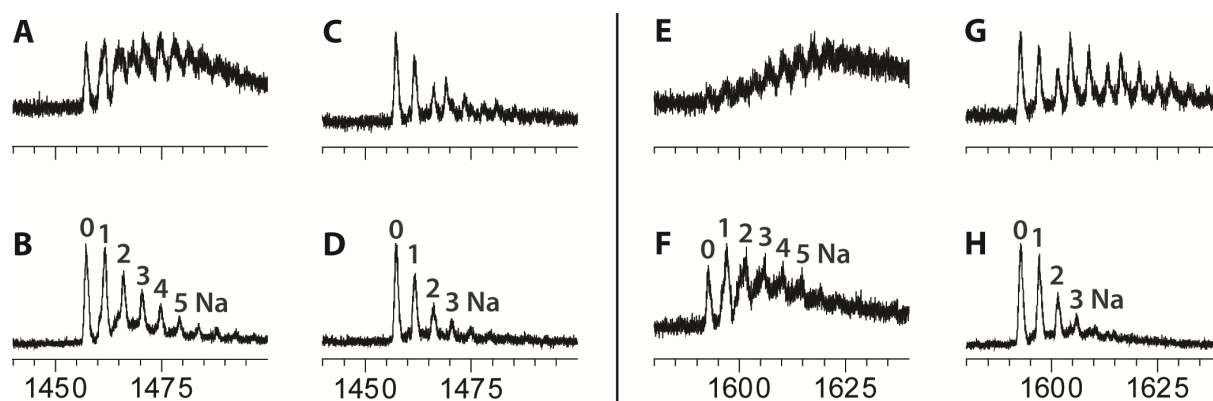


Figure S3. ESI-MS of 5 μM duplex DNA made by two d(CGC-GAA-TTC-GCG) strands = DK66 (A-D) and 5 μM hairpin DNA d(CAA-TCG-GAT-CGA-ATT-CGA-TCC-GAT-TG) hp26 (E-H) in 100 mM NH_4OAc + 1mM NaCl (A-B and E-F) or 100 mM TMAA + 1 mM NaCl (C-D and G-H). (A, C, E and G) Ion guide 1 voltage is 50 V and (B, D, F and H) 70 V. Zoom on the 5- charge state. It appears clearly that TMAA is more efficient to decrease the amount of nonspecific adducts.

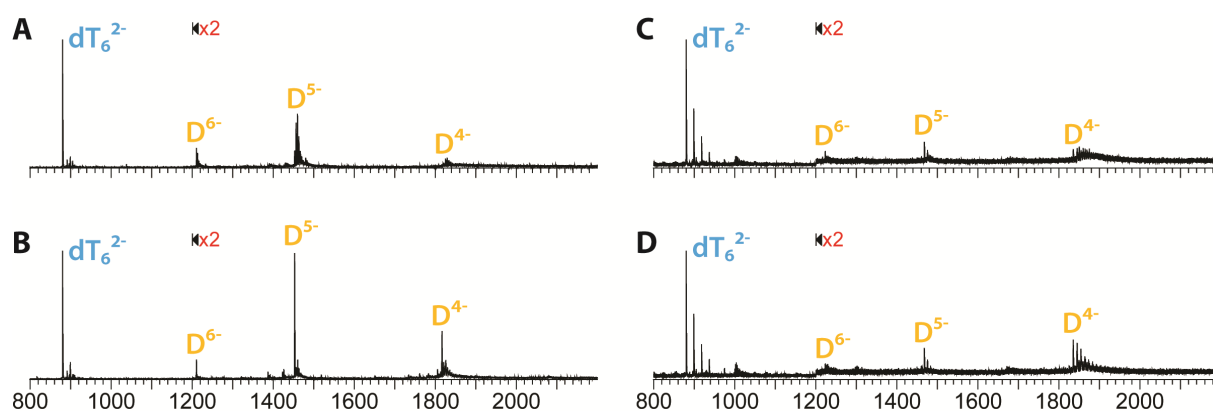


Figure S4. ESI-MS of 5 μM 23TAG; (A) and (B): electrosprayed in 100 mM NH_4OAc with ion guide 1 of 50 and 70 V, respectively; (C) and (D) in 100 mM TMAA + 1 mM KCl with ion guide 1 of 50 and 70 V, respectively. Note the 2 $\times$ zoom in the 1200 – 2200 m/z region. In NH_4OAc , charge states are clearly centered on the 5- form. In TMAA + KCl at 70 V the 4- becomes the predominant charge state.

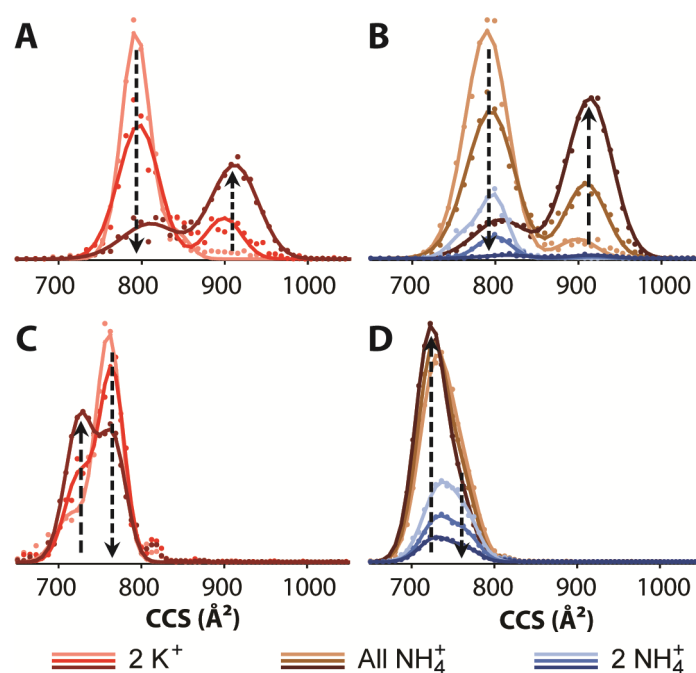


Figure S5. Collision cross section distribution of 5 μM 23TAG in 100 mM TMAA + 1mM KCl (red) or 100 mM NH_4OAc (brown and blue). Bias voltage increase from light to dark colors (respectively 18, 25 and 30 V). Brown colors represent the collision cross section reconstructed from the sum of the G-quadruplexes with zero, one and two ammonium cations and blue ones are the collision cross section of the G-quadruplexes with two ammonium ions exclusively. Red colors are the G-quadruplexes with two potassium ions.

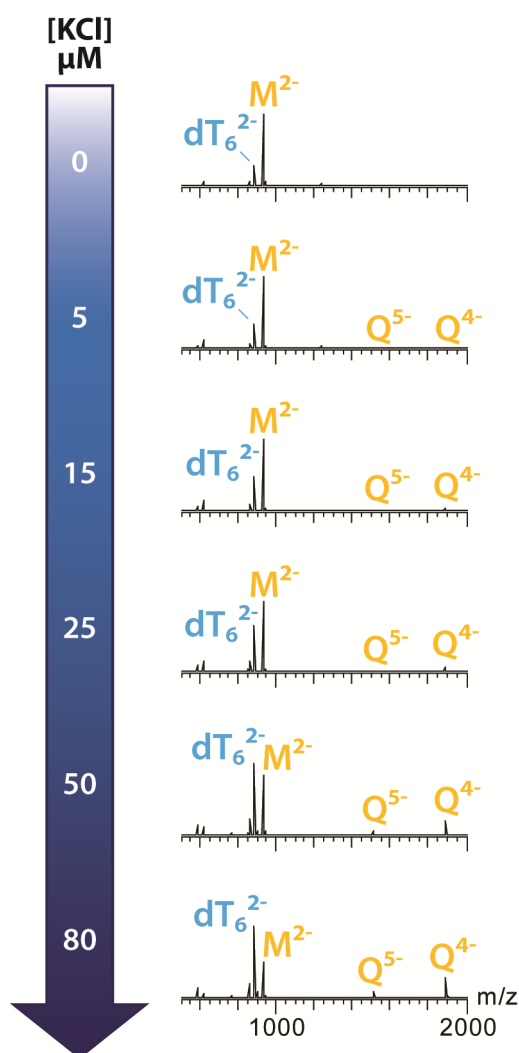


Figure S6. Mass spectrometry titration of 20 μM TG_4T into 100 mM TMAA doped by KCl. Full scale ESI-MS are showed. M and Q represent the monomer and quadruplex species, respectively. The solutions were prepared with 100 μM in TG_4T single strand for 24 hours before being diluted to 20 μM .