Supporting Information: Competitive binding of cations to a DNA duplex revealed through molecular dynamics simulations.

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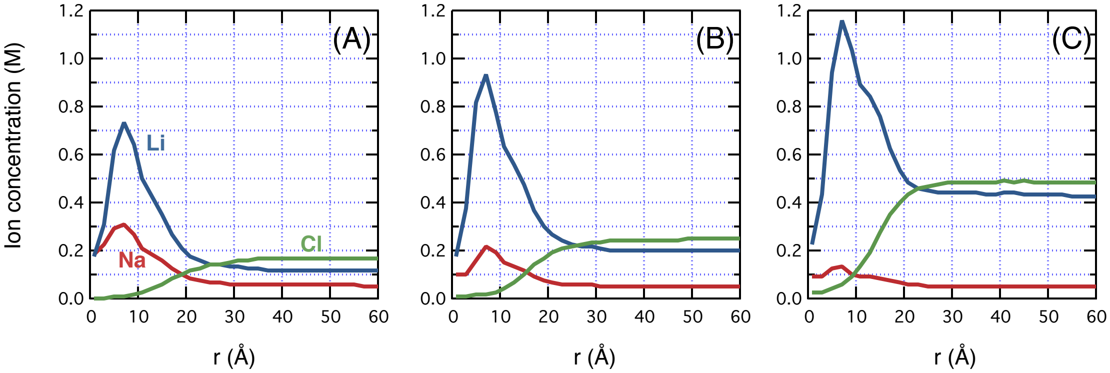

Figure S1: Radial profiles of ion concentration, $c(r)$, as a function of the distance from the DNA axis, r, in the simulations of Na50-Li110 (A), Na50-Li200 (B), and Na50-Li430 (C) systems.

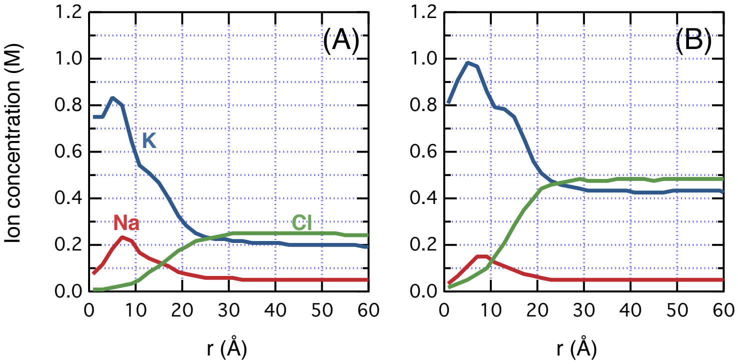

Figure S2: Radial profiles of ion concentration, $c(r)$, as a function of the distance from the DNA axis, r, in the simulations of Na50-K200 (A) and Na50-K430 (B) systems.

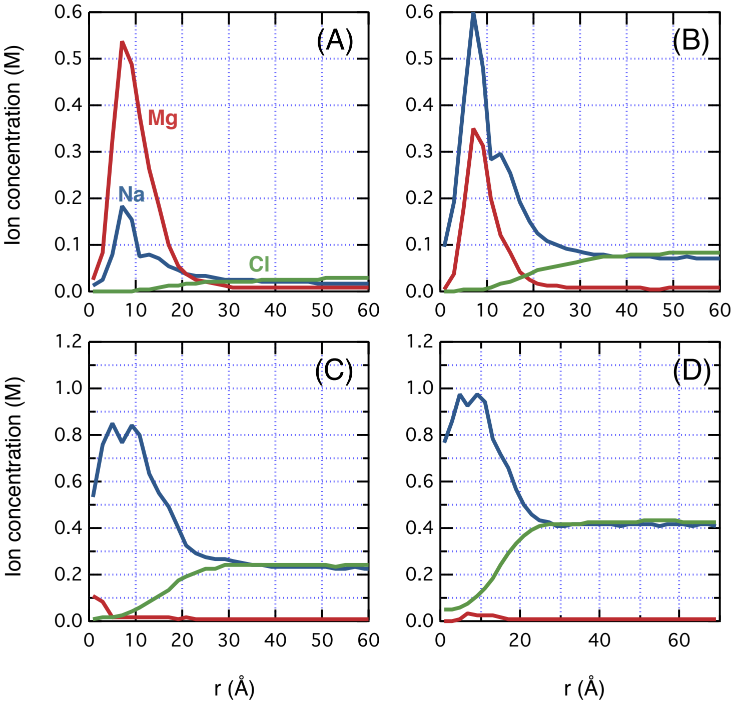

Figure S3: Radial profiles of ion concentration, $c(r)$, as a function of the distance from the DNA axis, r, in the simulations of Mg5-Na20 (A), Mg5-Na70 (B), Mg5-Na240 (C), and Mg5-Na420 (D) systems.

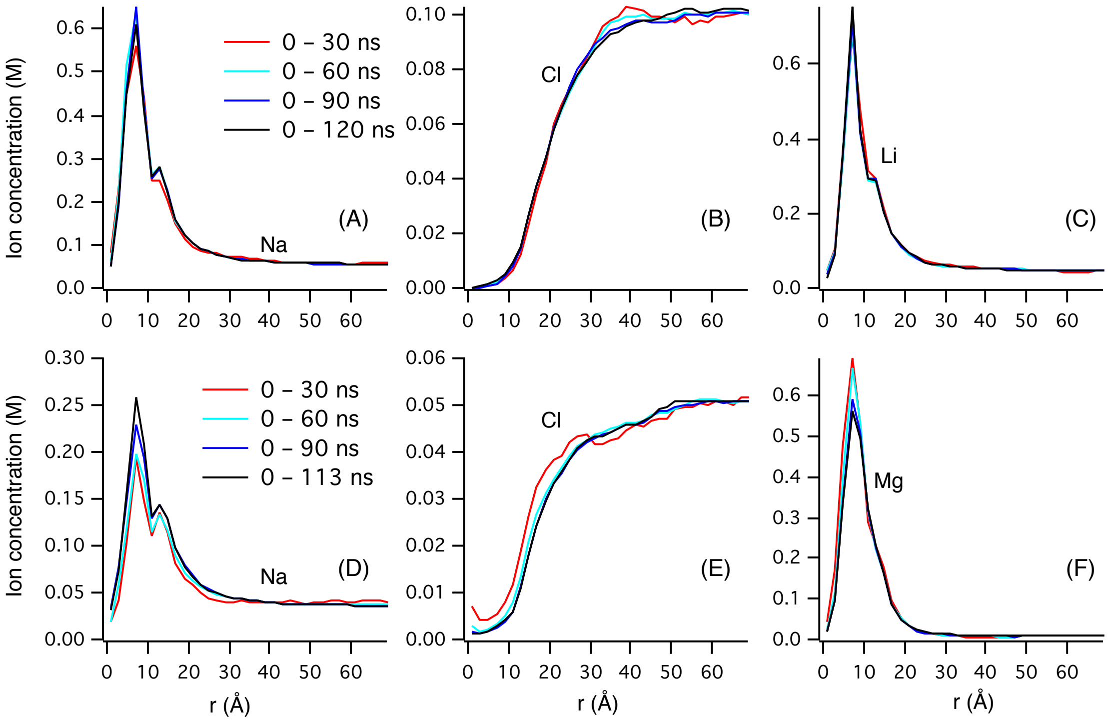

Figure S4: Radial profiles of ion concentration as a function of sampling time for the Na50-Li50 (A-C) and Mg5-Na40 (D-F) systems.

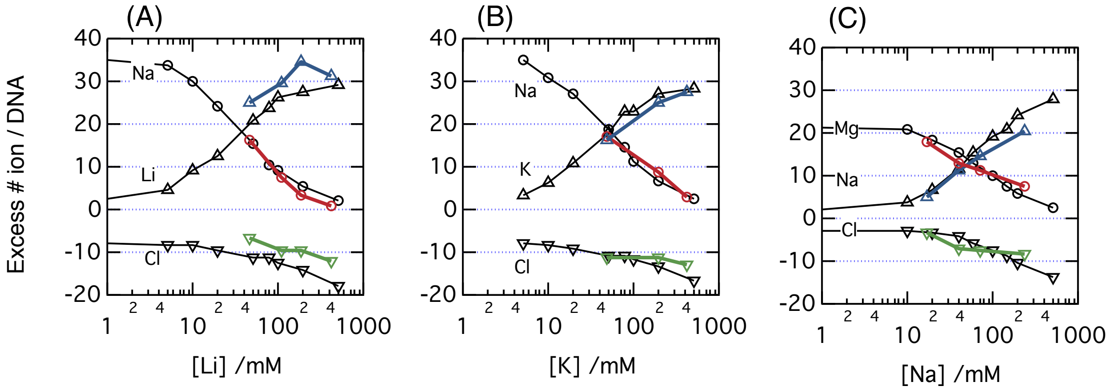

Figure S5: Comparisons between simulated and experimentally measured[1] number of excess ions in ion atmosphere of a DNA duplex. The simulation data shown in this plot were obtained using standard parametrization of cation–phosphate interactions,[2,3] without using NBFIX corrections.[4] Li^+ (CC) or K^+ (CC) were titrated into a background of 50 mM Na^+ (BC) in (A) and (B), respectively. In (C), Na^+ (CC) was titrated into a background of 5 mM Mg^{2+} (BC). In all panels, ◯, △, and ▽ denote the ion counts for BC, CC, and anion. The simulated ion counts are colored in red (BC), blue (CC), and green (anion). All experimental results are shown in black.

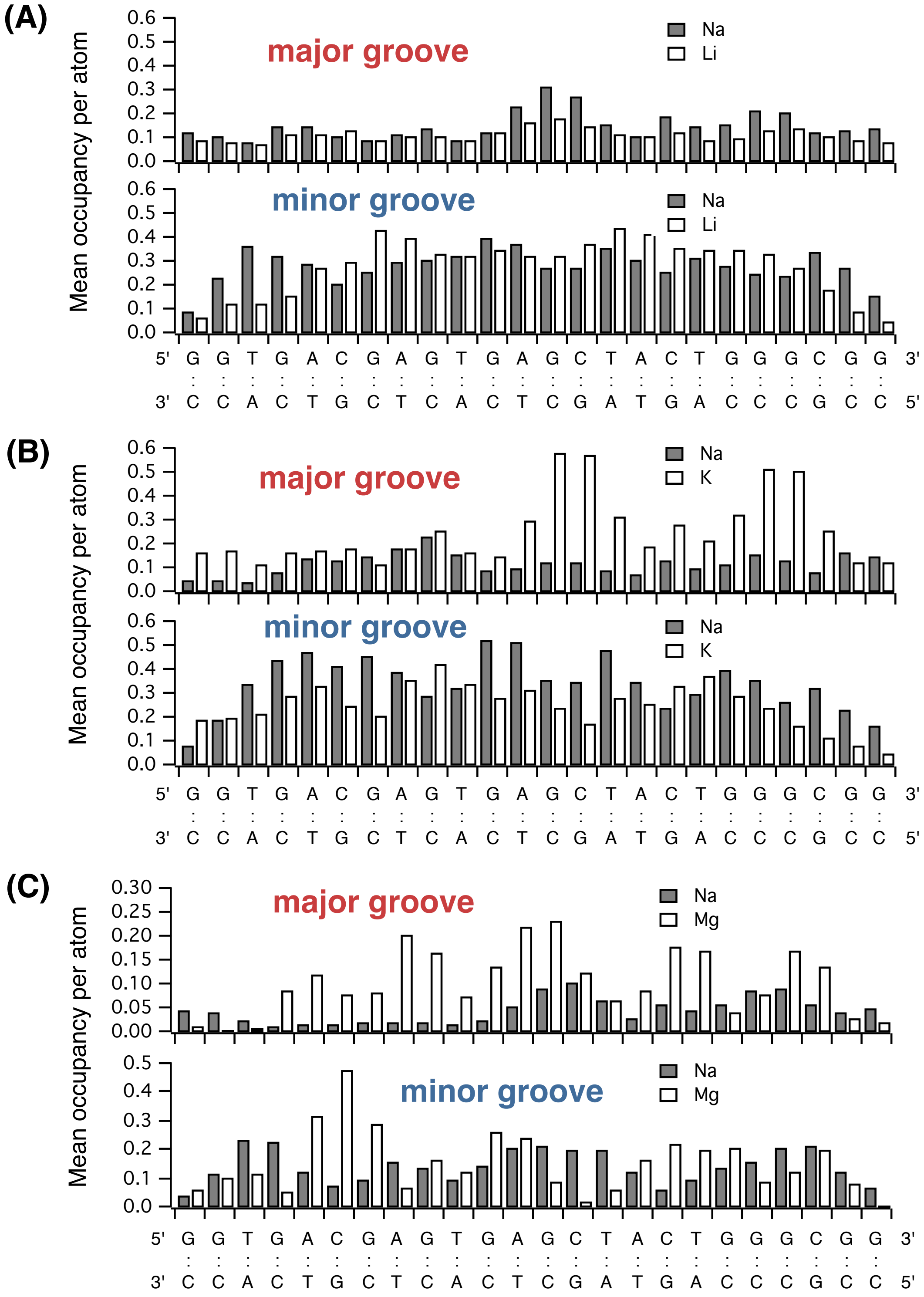

Figure S6: Mean occupancy of electronegative atoms of each DNA base pair in the major (top) or minor (bottom) grooves of duplex DNA. The mean occupancy was computed by taking arithmetic mean of occupancies of all electronegative atoms of a base pair in either major or minor groove. See Fig. 5A for our definition of the electronegative atoms and their assignment to the minor and major grooves.

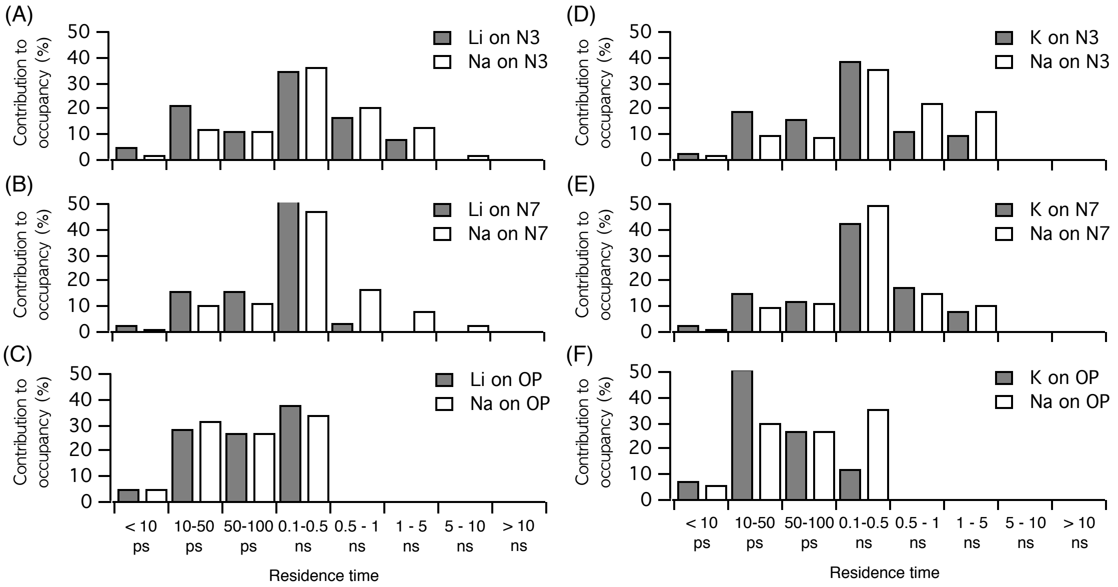

Figure S7: Contribution to DNA atoms' occupancies by contacts from a specific range of ion residence time. Each panel displays data for either Li^+ and Na^+ (A–C) or $K^+$and Na^+ (D–F) binding for minor-groove atom N3 of purine (A,D), major-groove atom N7 of purine (B,E), and backbone atom OP (C,F). The data were obtained from trajectories of Li50-Na50 (A–C) and K50-Na50 (D–E) systems.

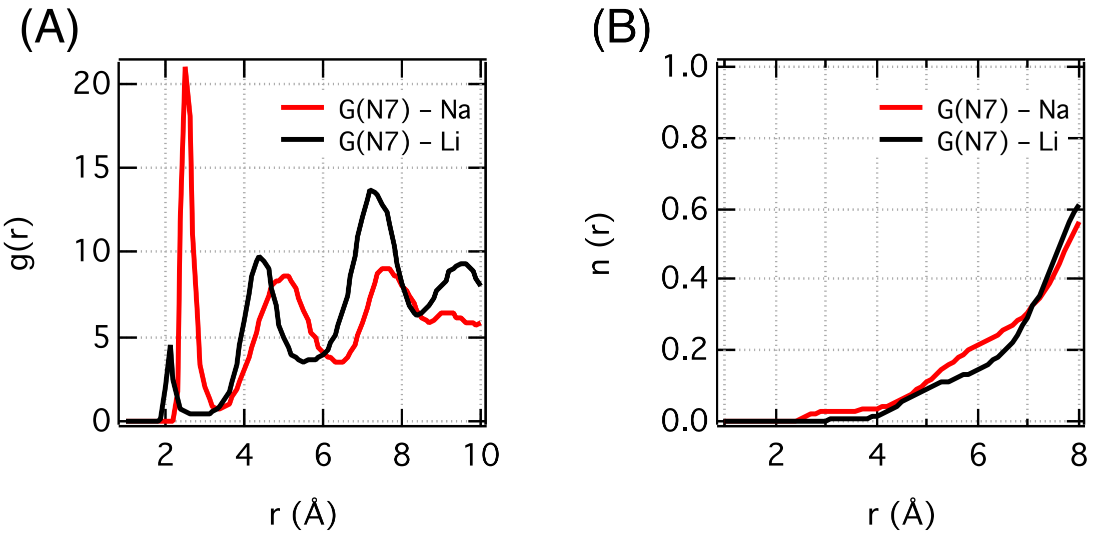

Figure S8: (A) Radial distribution functions, $g(r)$, of Na$^+$ (red) and Li$^+$ (black) around the N7 atom of guanine in the Na50-Li50 simulation. (B) The average number of ion within r, $n(r)$, obtained by integrating $g(r)$ shown in (A).

References

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