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Supplementary Information For All-atom MD indicates ion-dependent behavior of therapeutic F10

Ryan L. Melvin,*[a,b] William H. Gmeiner,[c] and Freddie R. Salsbury, Jr[a]

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[a] Department of Physics, Wake Forest University, Winston Salem, NC, USA. Fax: +1 (336) 758-6142; Tel: +1 (336) 758-5337; E-mail: salsbufr@wfu.edu
[b] Department of Mathematics and Statistics, Wake Forest University, Winston Salem, NC, USA.
[c] Department of Cancer Biology, Wake Forest University School of Medicine, Winston Salem, NC, USA.

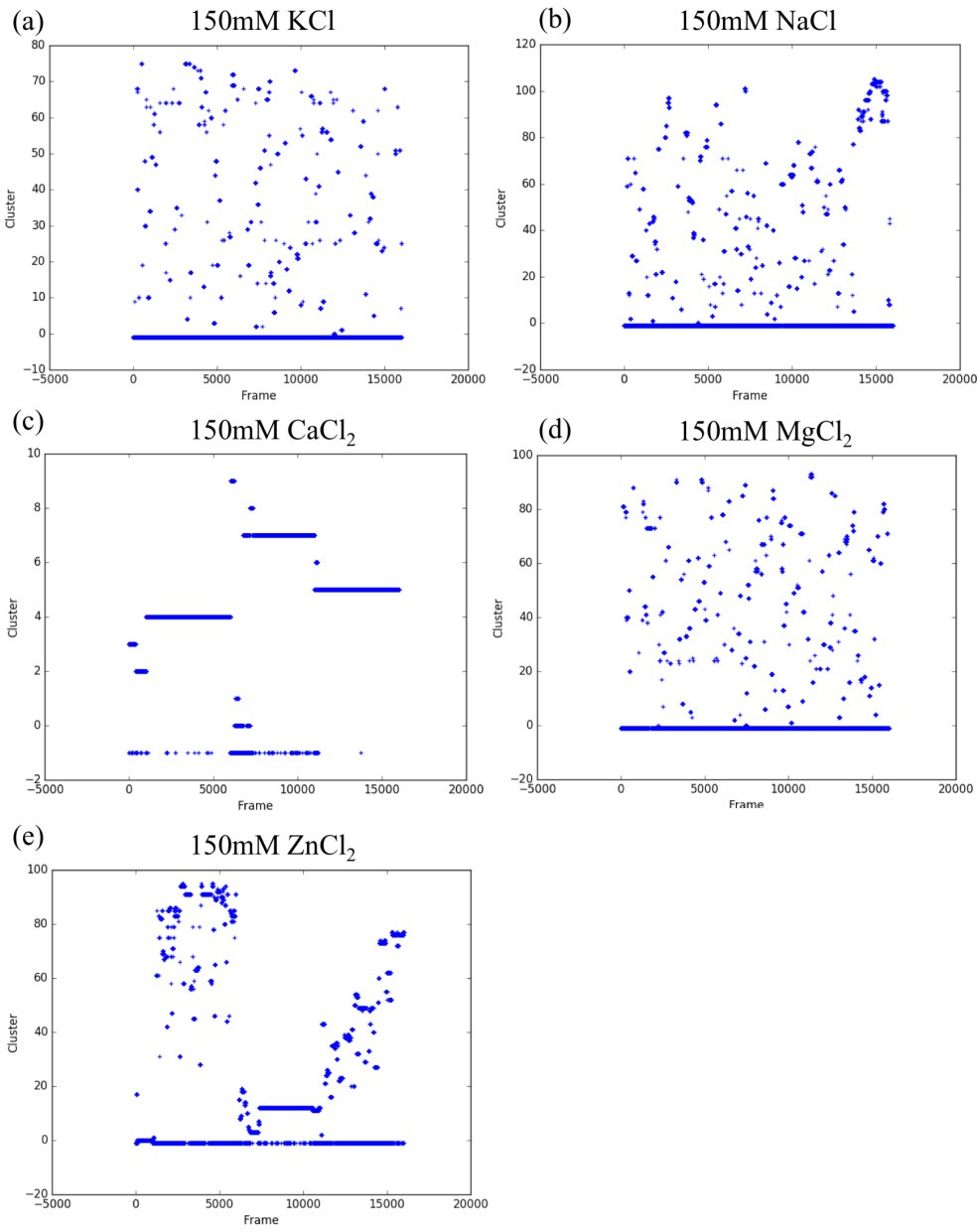

Fig. 1 Plotting HDBSCAN clustering as timeseries indicates that calcium and zinc (c, e) induce long-lived (up to microseconds at a time) states for F10 while potassium, sodium and magnesium (a, b, d) have much shorter lived states (only a few nanoseconds).

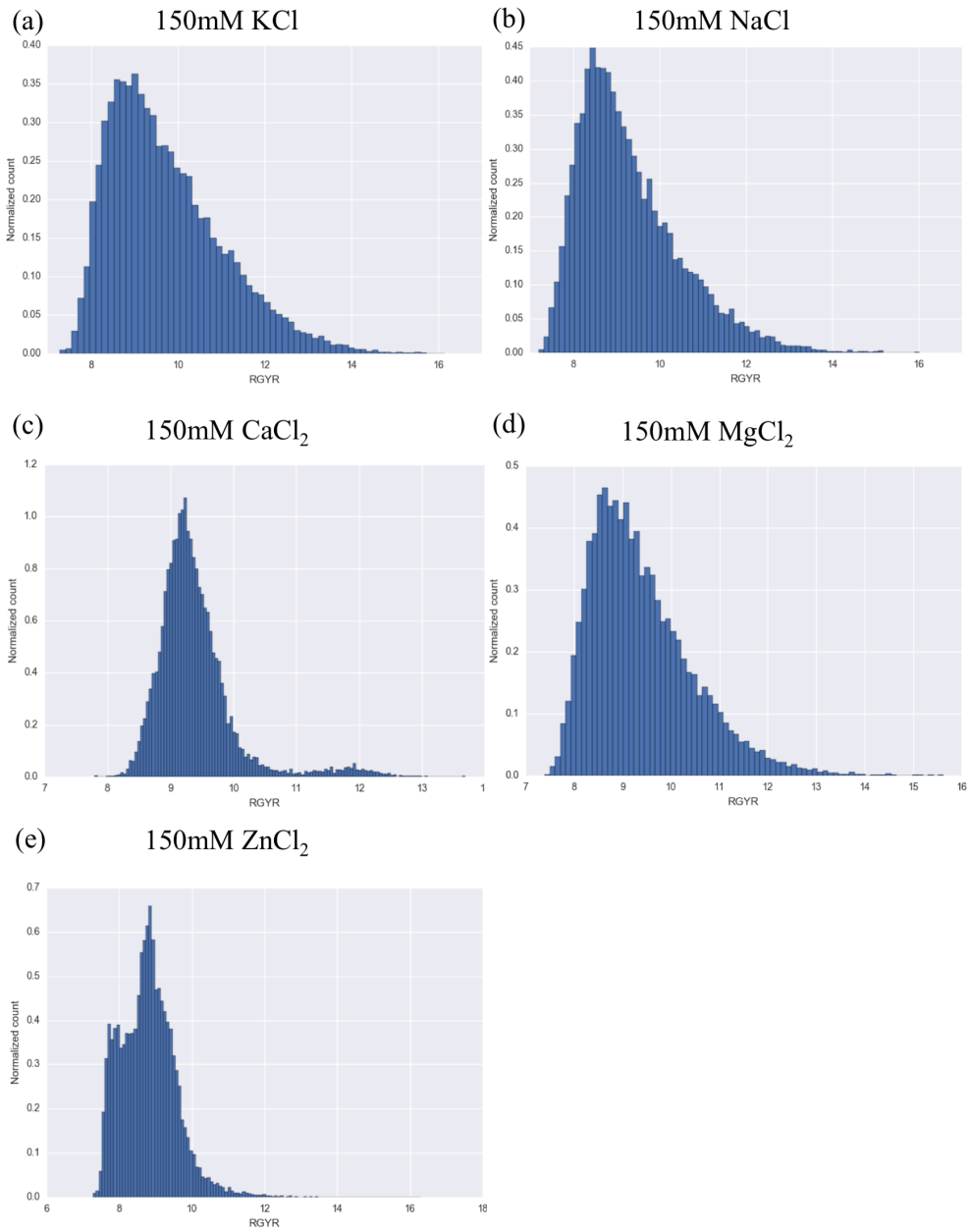

Fig. 2 The largest observed persistence length occurs in simulations of F10 solvated in 150mM KCl. We see a similar pattern of compactness in terms of distributions of RGYR values.

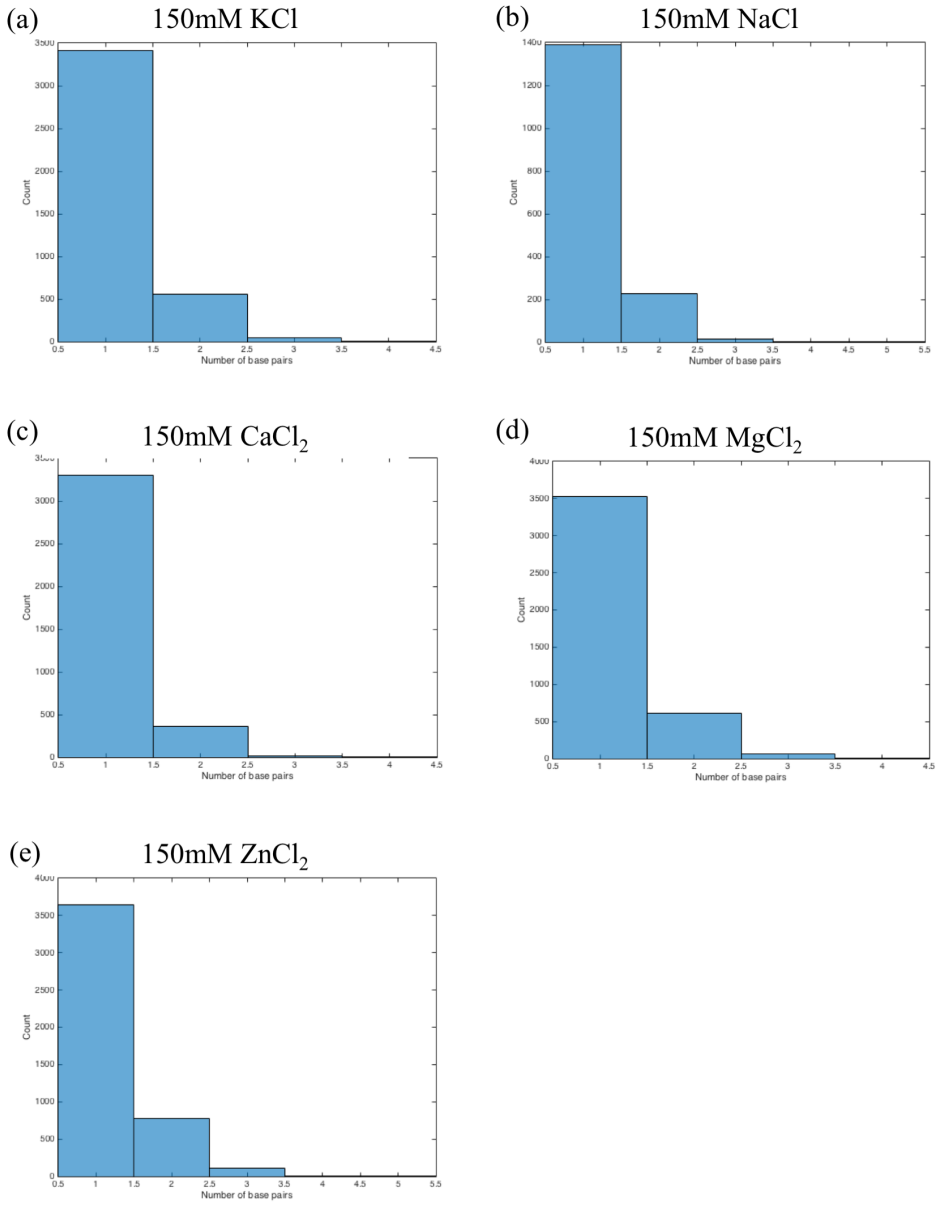

Fig. 3 Histogram counts of base-base interactions in each trajectory frame reveals that F10 prefers single base-base interactions.