Electronic Supplementary Material (ESI) for Nanoscale.

pH Controlled Gating of Toxic Protein Pores by Dendrimers

Taraknath Mandal[‡a], Subbarao Kanchi[‡a,b], K. G. Ayappa[*b] and Prabal K Maiti[*a]

[a] Center for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012

[b] Department of Chemical Engineering, Center for Biosystems Science and Engineering, Indian Institute of Science, Bangalore 560012

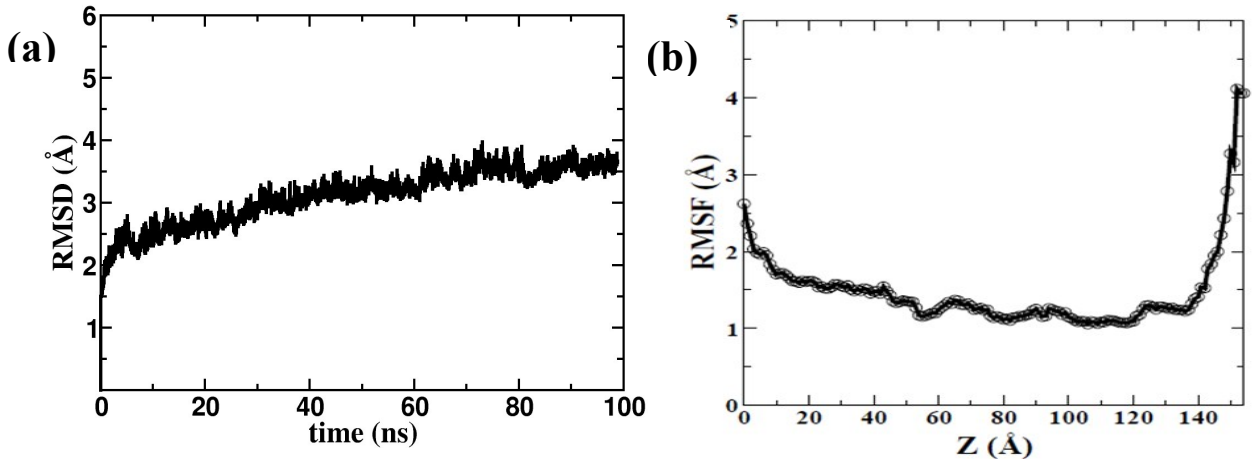

Figure S1: (a) RMSD of the protein pore as a function time. (b) RMSF of the protein pore as a function of the distance along its axis.

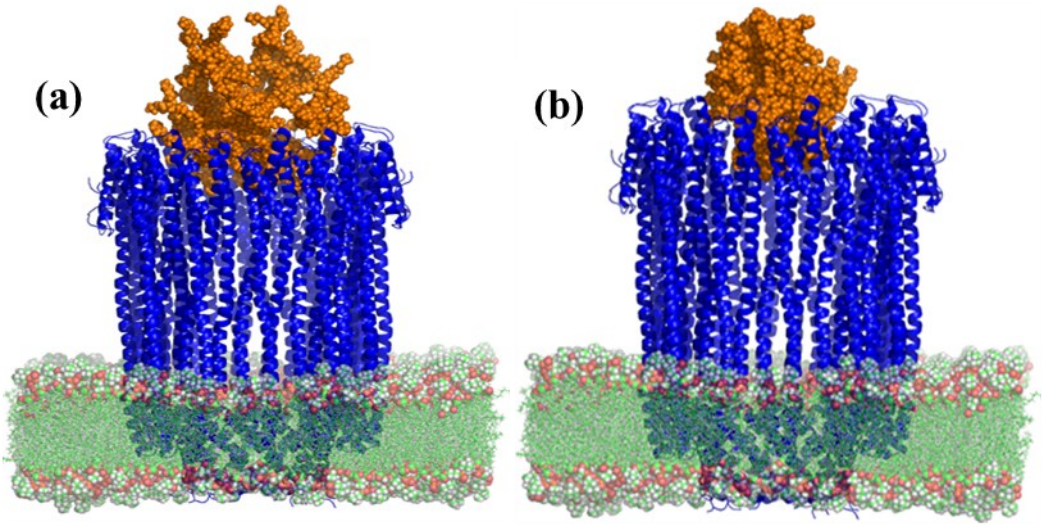

Figure S2: Initial configurations of the dendrimers which are kept near the extra cellular entrance of the pore. The dendrimers spontaneously enter into the protein lumen. We have verified the translocation of the dendrimer with several initial configurations.

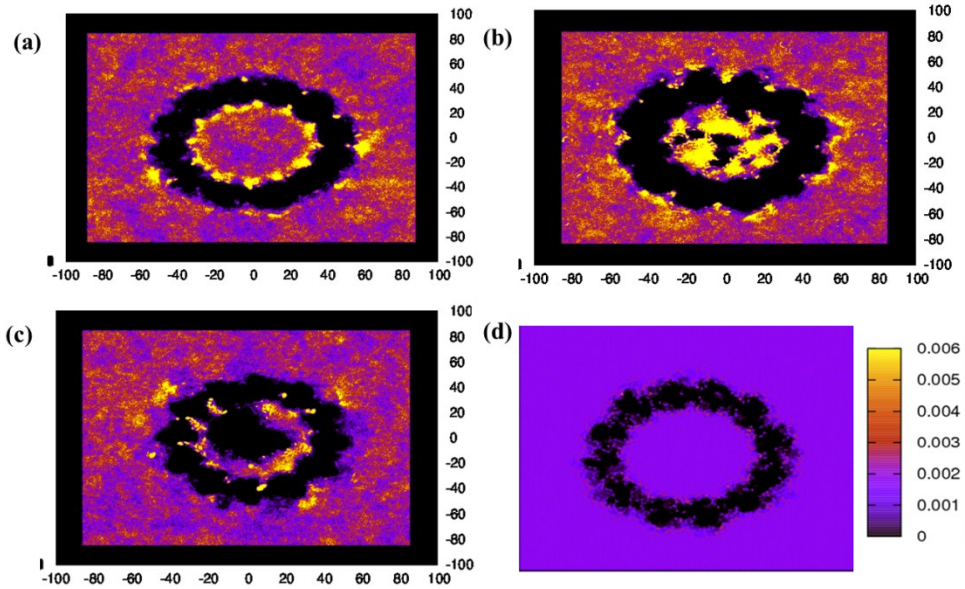

Figure S3: Total ions density distributions in x-y plane under electric field for (a) free protein channel (b) channel modified by P dendrimer (c) channel modified by NP dendrimer and (d) water density distribution in x-y plane under constant force for the free protein channel.

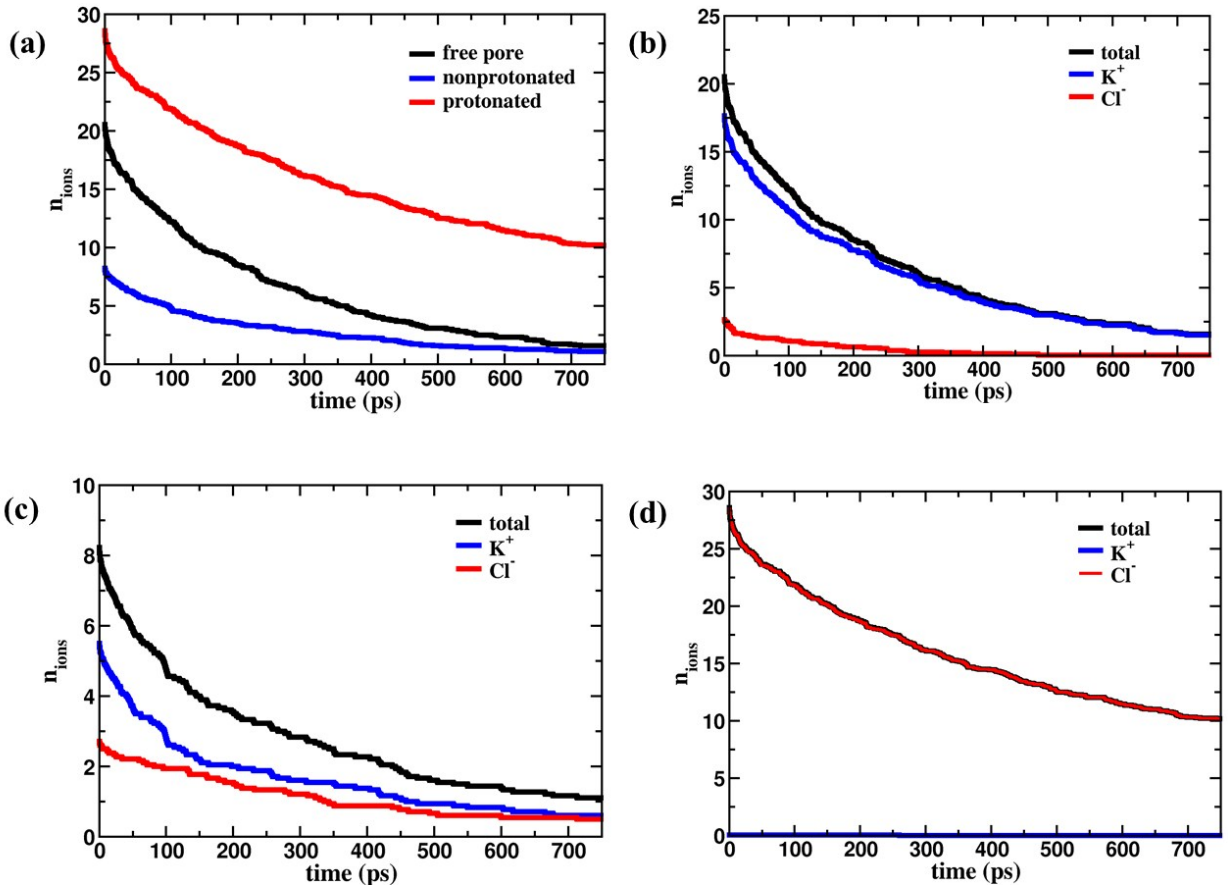

Figure S4: Number of resident ions (a) all three cases (b) partial ion contributions in free pore (c) partial ion contributions in the vicinity of NP dendrimer inside the ClyA pore and (d) partial ion contributions in the vicinity of P dendrimer inside the ClyA pore.

Corresponding Authors:

* Prabal K Maiti, Center for condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore. Phone: (091)80-2293-2865. E-mail: maiti@physics.iisc.ernet.in.

*K G. Ayappa, Department of Chemical Engineering, Center for Biosystems Science and Engineering, Indian Institute of Science, Bangalore. Phone: (091)80-2293-2769. Email: ayappa@chemeng.iisc.ernet.in

Author Contributions

The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript. ‡These authors contributed equally.