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# Supporting Information

## Interaction between Charged Nanoparticle and Vesicle: Coarse-Grained Molecular Dynamics Simulations

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### Potential of mean force (PMF) calculations via umbrella sampling MD simulations

The PMF of CNP translocation through the vesicle membrane was studied using a combination of the umbrella sampling and weighted-histogram analysis method (WHAM). All the simulation parameters and conditions were identical as for the unbiased simulations. The distance between the CNP and the center of the vesicle was increased from 0 to 11 nm with 0.1 nm increments. Each simulation was 10 ns long, for a total simulation time of 1100 ns for each PMF. A force constant of 1000 kJ $mol^{-1}$ $nm^{-2}$ was used for the biasing potential in the vesicular radial direction. Actually, this force constant influences the width of the umbrella histogram[1]. If the umbrella histograms have significant overlapping, there will be sufficient information to determine a meaningful PMF. Application of this constant force and a window spacing distance of 0.1 nm results in the production of multiple overlaps of umbrella histogram (Fig. S1 and Fig. S2).

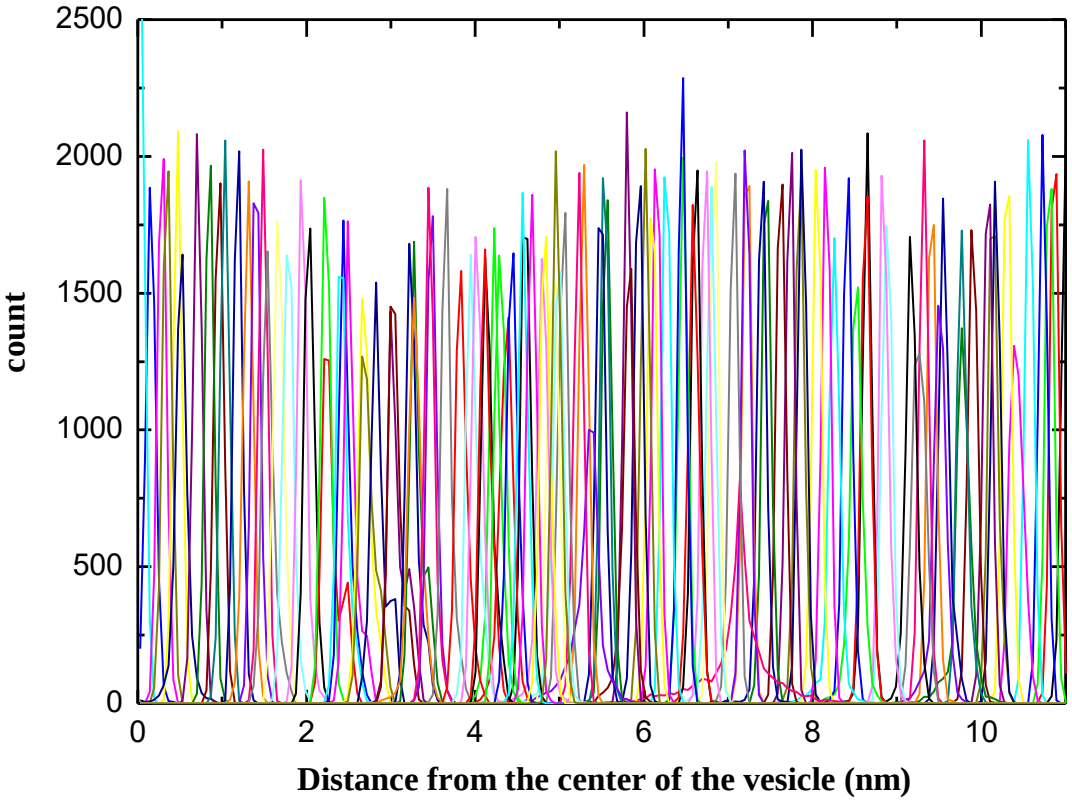


Fig. S1 The umbrella histogram for the case of of the neutral NP.

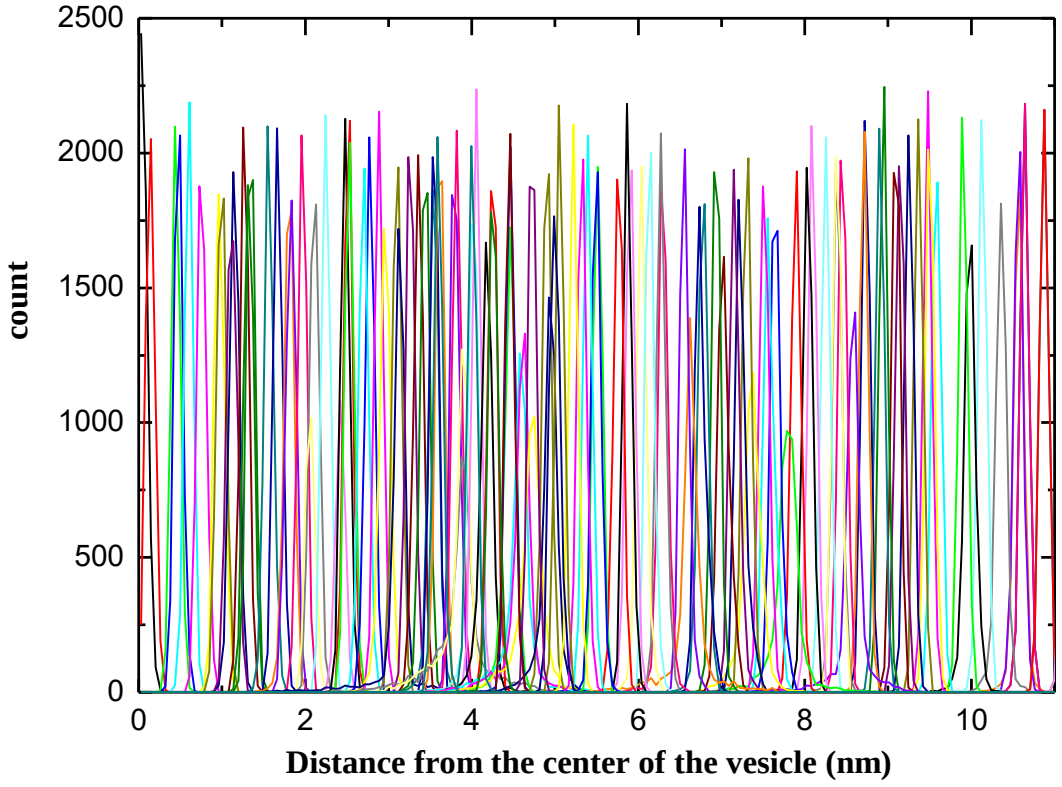


Fig. S2 The umbrella histogram for the case of the q-135-2-minus CNP.

## Reference:

[1] J. S. Hub, B. L. de Groot, and D. van der Spoel, “g_wham-A Free Weighted Histogram Analysis Implementation Including Robust Error and Autocorrelation Estimates,” *Journal Of Chemical Theory And Computation*, vol. 6, no. 12, pp. 3713-3720, Dec, 2010.