Supplementary Information

Understanding the Effects of PAMAM Dendrimer Size and Surface Chemistry on Serum Protein Binding with Discrete Molecular Dynamics Simulations

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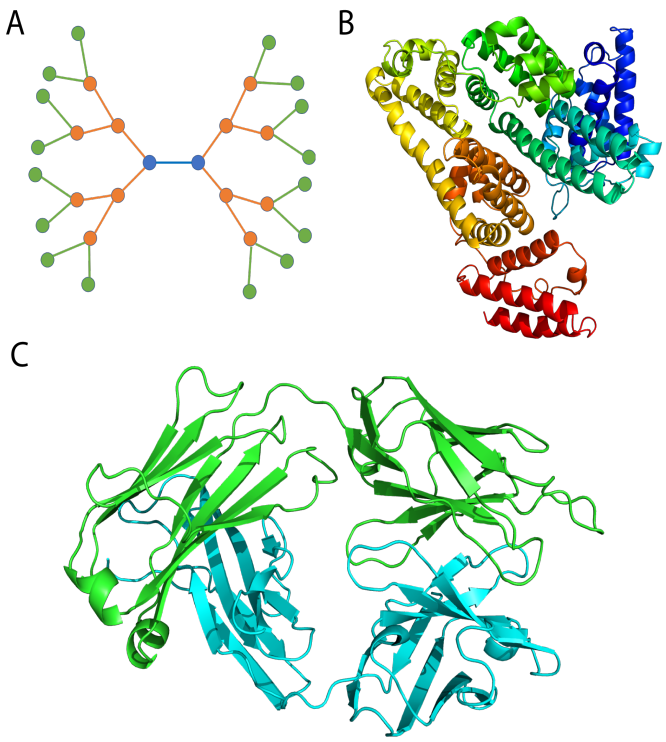

Figure S1. Molecules used in DMD simulations. (A) Schematic diagram showing the structure of a PAMAM dendrimer – blue represents the diamine core, orange denotes the branching unites, and the green shows the terminal groups. (B, C) Cartoon structures of human serum albumin (HSA) and immunoglobulin E (IgE), respectively.

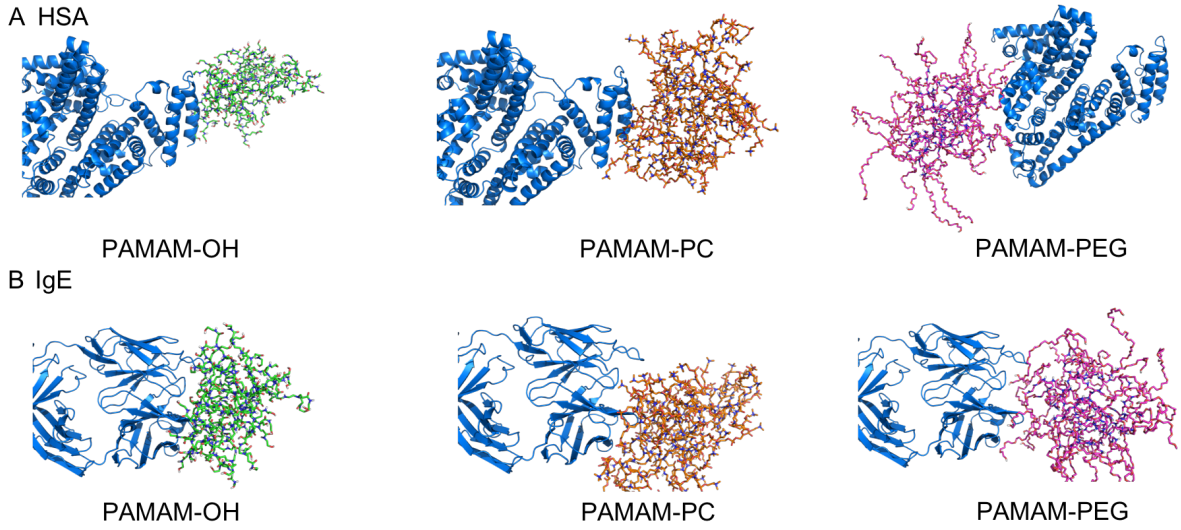

Figure S2. Snapshots of neutrally charged dendrimers binding with (A) HSA and (B) IgE.

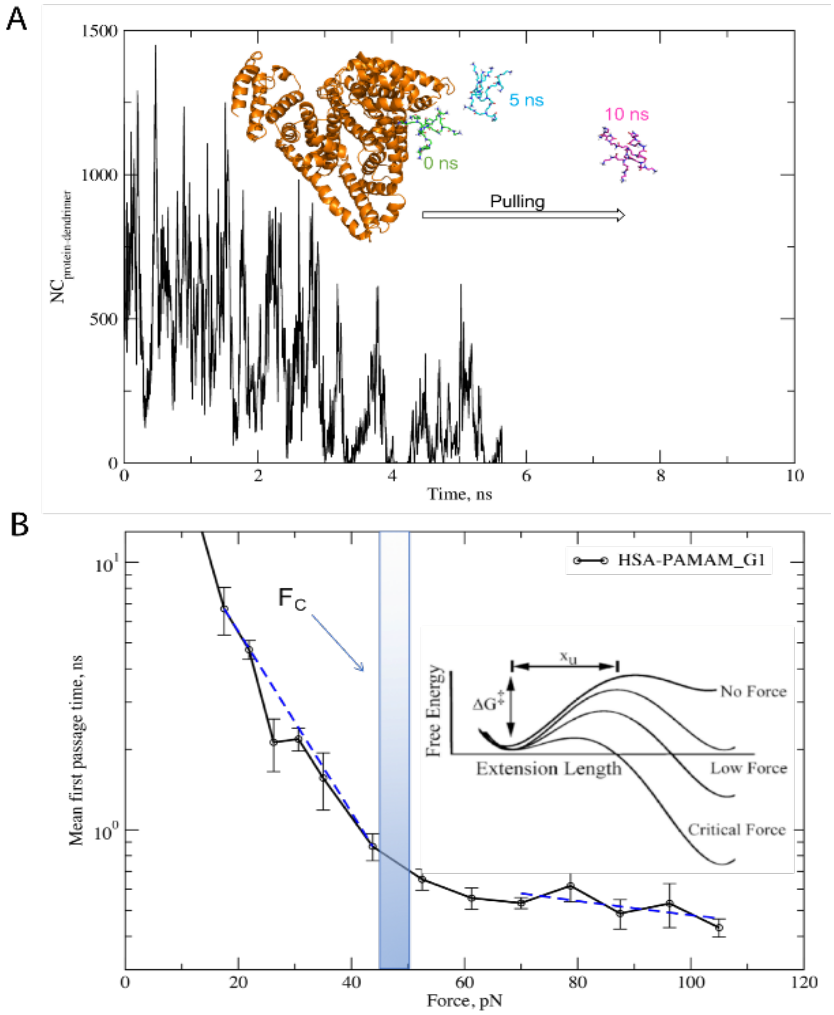

Figure S3. Pulling simulations with SDMD. (A) Time evolution of inter-molecular contact numbers between dendrimer and HSA. Snapshots at different times are shown in the inset, where HSA is shown as cartoon and PAMAM-G1 in stick. (B) Schematic illustrating how to estimate the critical force by linear fitting of both the barrier-ed and barrier-less regimes (see Methods).

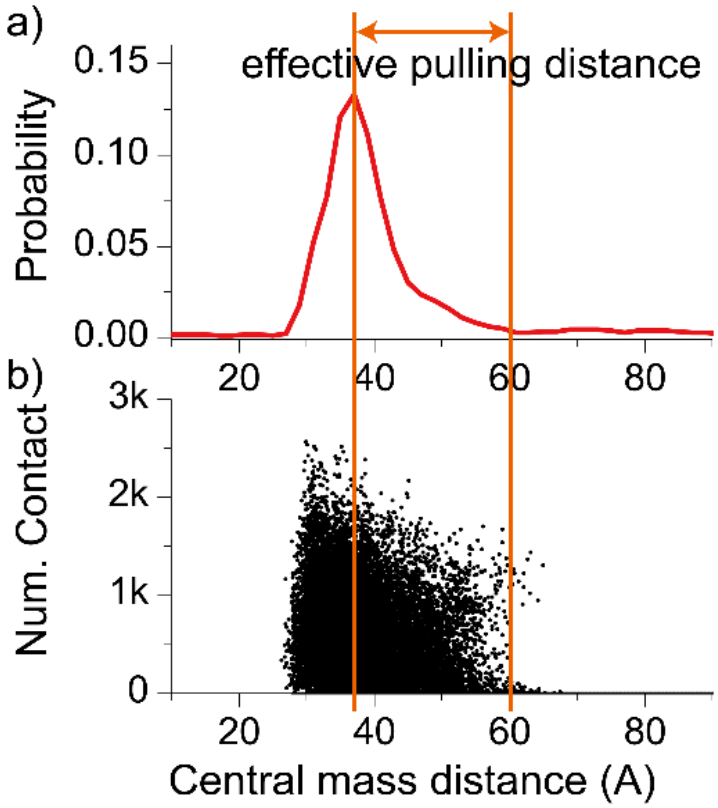

Figure S4. Estimation of the pulling distance used for calculating the binding free energy. (a) Histogram of inter-molecular distance from the SDMD simulations. (b) Scatter plot of the inter-molecular contact numbers versus inter-molecular distances. Equilibrium distance, d^{eq}, was estimated as the first peak, and the dissociation distance, d^{*}, was estimated where the number of contacts approached zero (see Methods).