Optimizing the structure and performance of biomimetic water channels

Supporting information

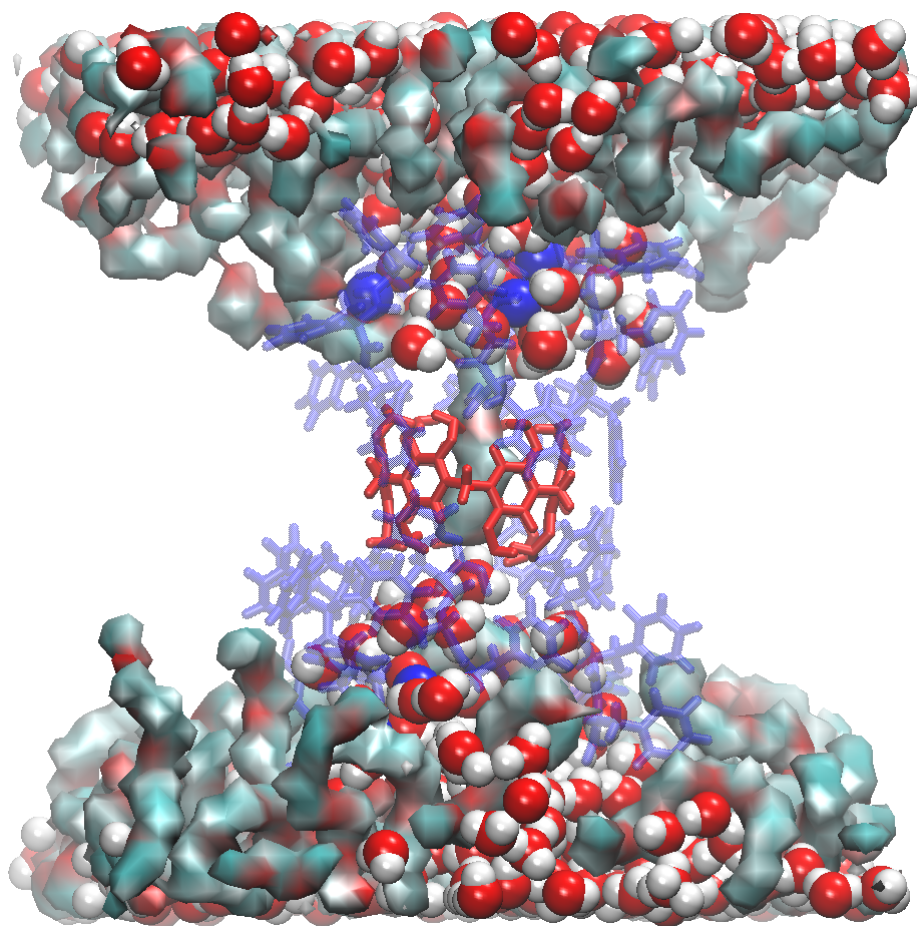Ritwick Kali, Wezi D. Mkandawire, Scott T. Milner

Figure SI 1: Hydrophilic PEO chain (cyan) clogging a PAP[6] pore. The PAP[6] collar is colored red and the petals are transparent and blue. The hydrophobic core of the membrane has been hidden for clarity. The red and white spheres are water molecules and the blue spheres are Na^+ ions.
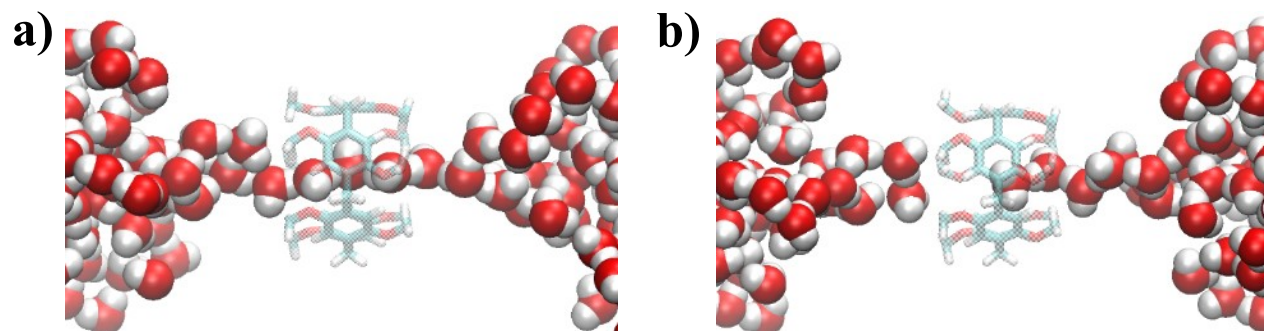
Figure SI 2: a) A continuous water string containing five water molecules. b) A broken water string containing three water molecules. The PAP[5] petals have been hidden and the collar is shown as a transparent imprint for clarity.
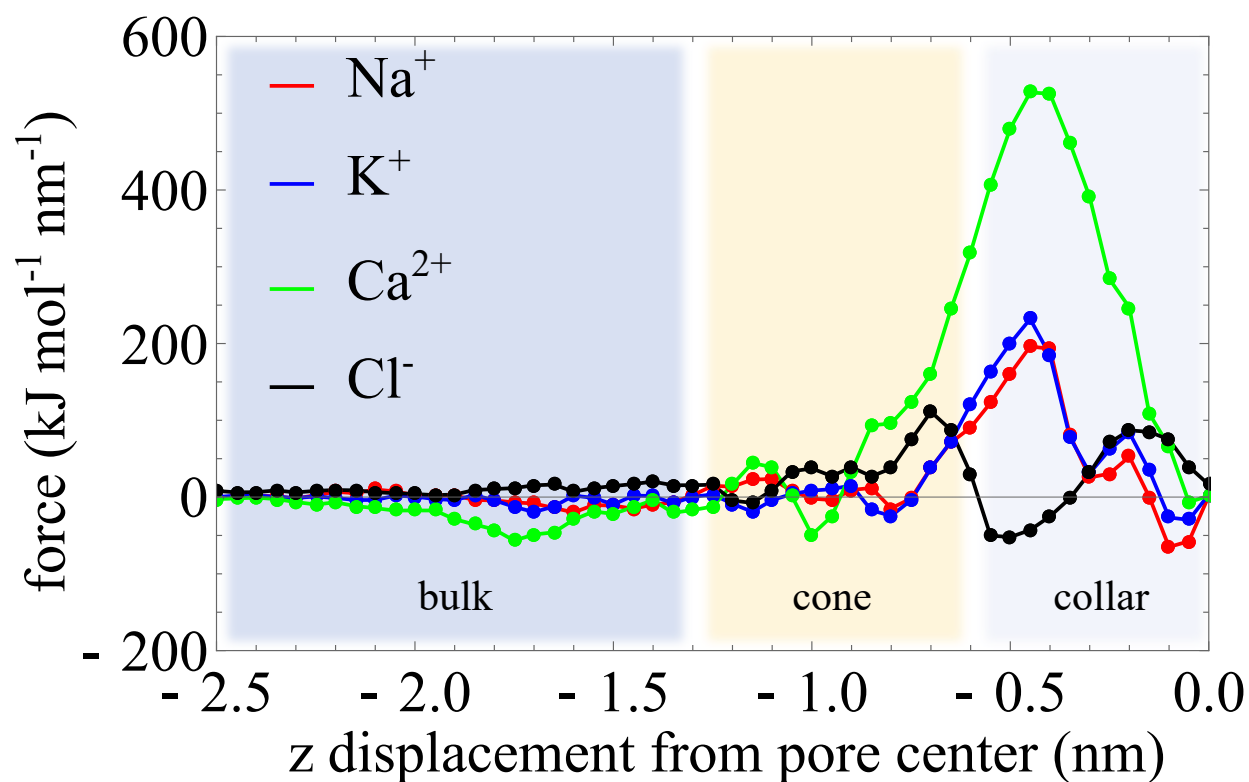

Figure SI 3: Force profiles for different ions in PAP[6]. The profiles have been segmented into regions based on the position of the ion on the water string.
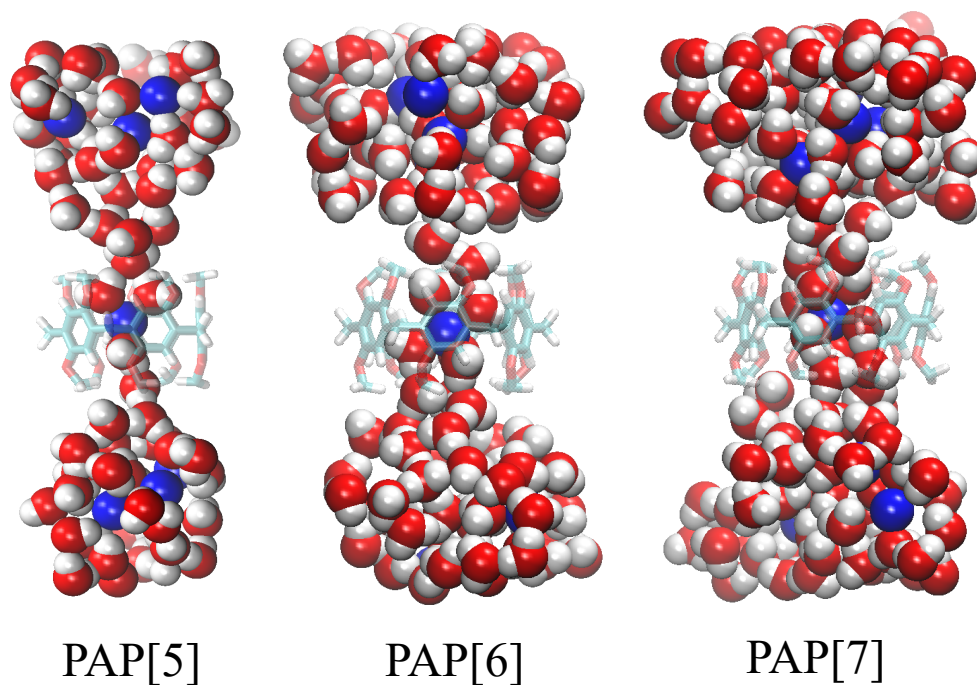
Figure SI 4: PAP[5], PAP[6] and PAP[7] water channels with a NA$^+$ ion at the center. The number of solvating water molecules around the ion increases as the pore diameter broadens from PAP[5] to PAP[6] to PAP[7]. The cyan transparent imprint is the channel collar. The membrane and the channel petals have been hidden for clarity.
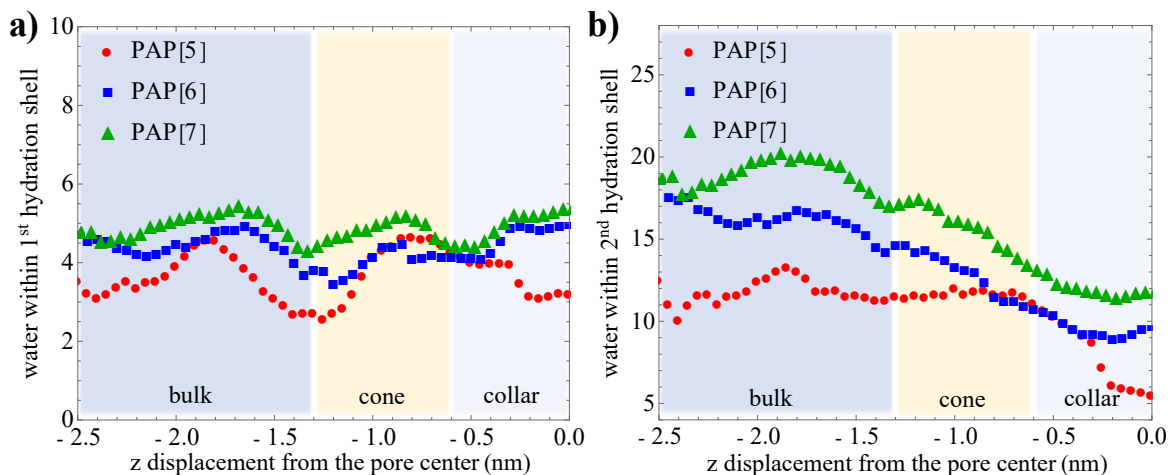

Figure SI 5: The variation of number of water molecules within the a) primary hydration shell b) secondary hydration shell of Na$^+$ ion along the axis of a PAP[n] pore. The profiles have been segmented into regions based on the position of the ion on the water string.
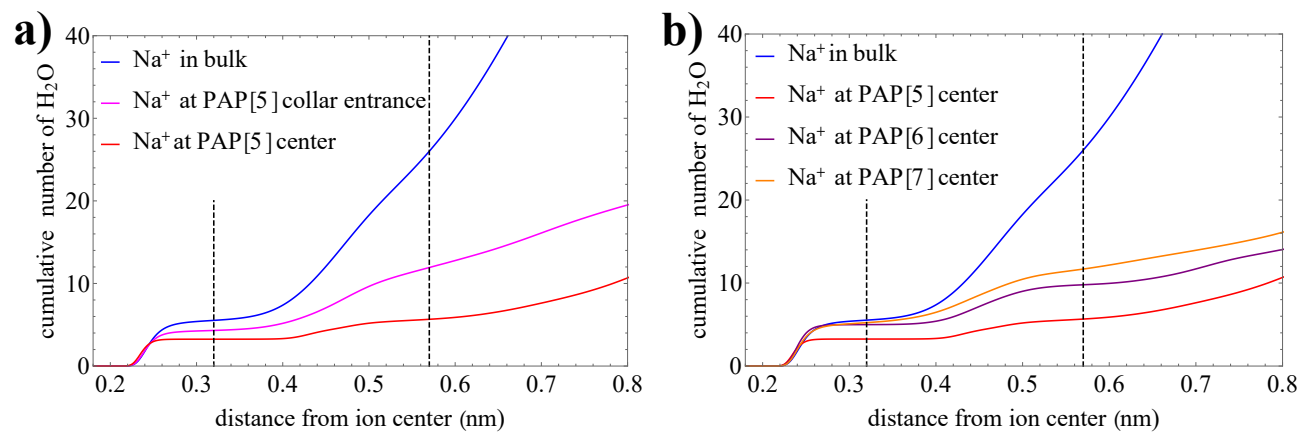
Figure SI 6: Cumulative number of water molecules versus distance from ion center a) in PAP[5] channel and b) at center of all PAP channels. The dashed vertical lines indicates the position of the valleys of the first and second hydration shells.