# Insertion free energy of PAP[5] water channels into block copolymer membranes

## Supporting information

Ritwick Kali, Scott T. Milner
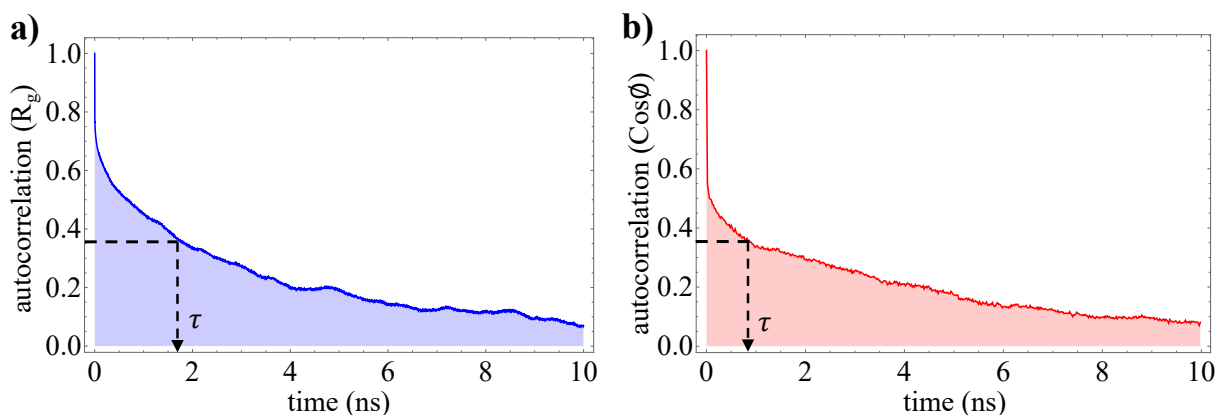
Figure SI 1: The autocorrelation function of a) radius of gyration $(R_g)$ of the hydrophobic PB blocks in PB16PEO9 membrane. b) Cosine of angular tilt of the pore collar $(\text{Cos}(\Phi))$ with respect to the membrane normal in PB16PEO9 membrane. The time in which the autocorrelation functions decay to a value of $e^{-1}$ gives a characteristic relaxation time $\tau$.

Autocorrelation function $A(k)$ of a time series $x_i = \{x_1, x_2, ....x_n\}$ is given as

$$A(k) = \frac{\Sigma_{i=1}^{n-k}(x_i - \bar{x})(x_{i+k} - \bar{x})}{\Sigma_{i=1}^{n}(x_i - \bar{x})^2} \tag{1}$$

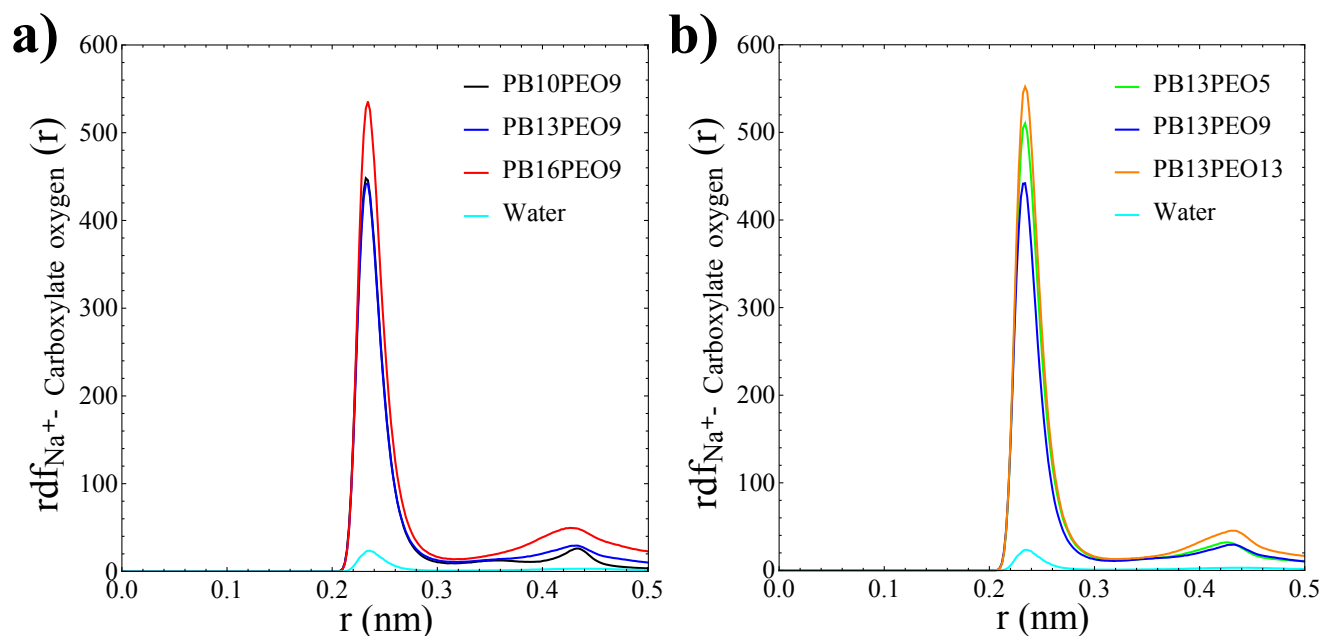where $\bar{x}$ is the mean of the time series $x_i$

Figure SI 2: The radial distribution function of Na$^+$ and carboxylate oxygens for a) different PB block lengths and b) different PEO block lengths, plotted out to the second counterion shell boundary (0.5 nm).
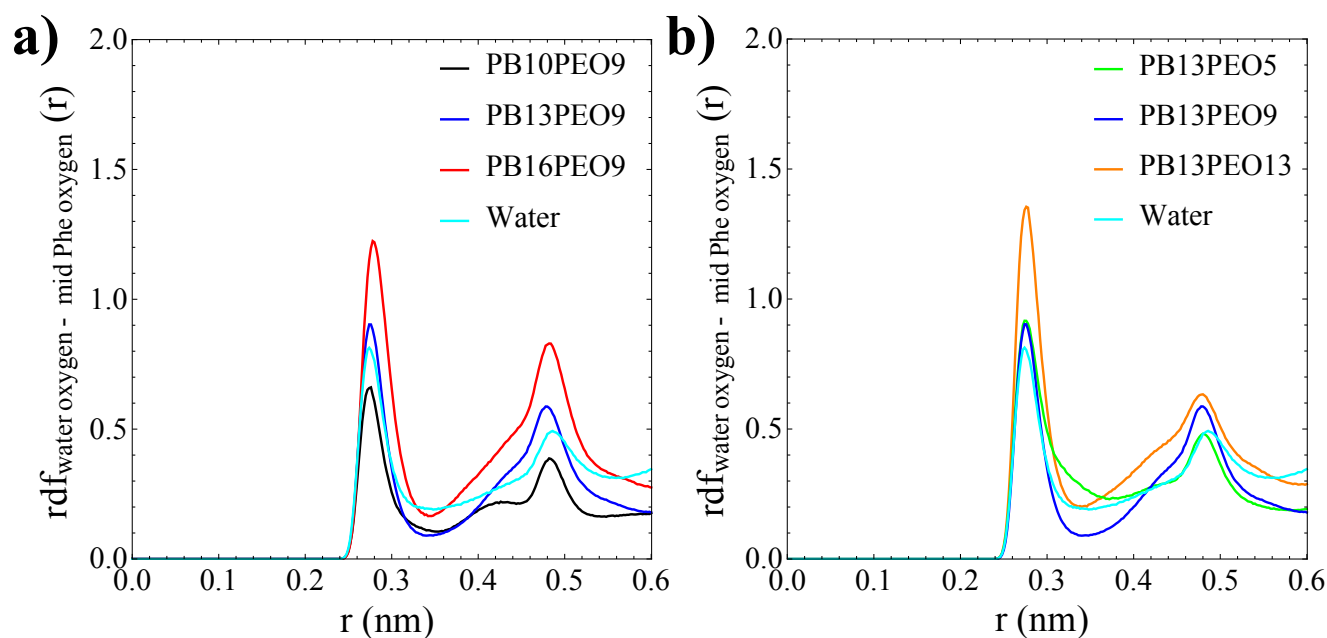


Figure SI 3: The radial distribution function of water oxygens and mid-phenylalanine carbonyl oxygen for a) different PB block lengths and b) different PEO block lengths, plotted out to the second hydration shell boundary (0.6 nm)