Probing protein orientation near charged nanosurfaces for simulation-assisted biosensor design

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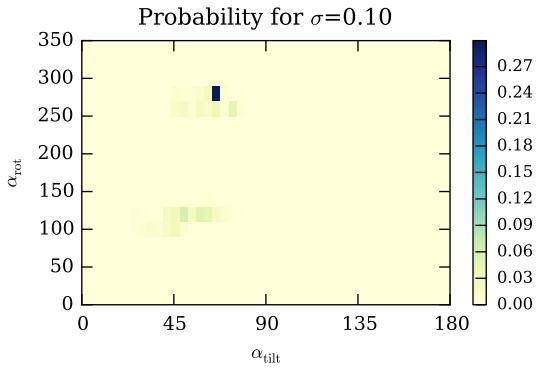
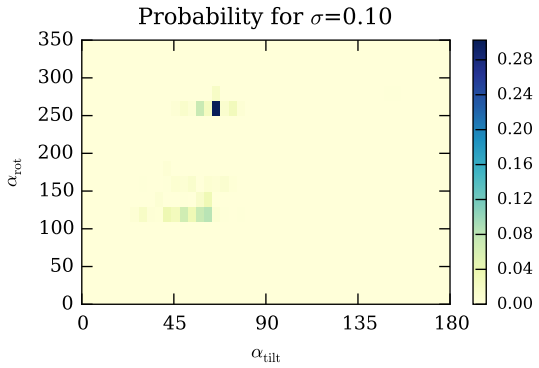
Supplementary Material

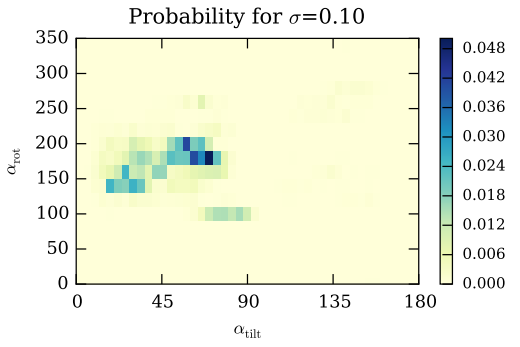
For the main result in the paper, looking at the orientation of IgG 2a near a surface with charge $\sigma = 0.1\text{C/m}^2$ immersed in a solvent with 37mM of salt, we show here the contribution of each energy component to the probability distribution. We studied the contribution of the solvation and surface energies to the orientation probability distribution to show that the orientation mechanism is guided by the solvation energy in this case. Fig. 1 shows the probability distribution computed in three ways: using the total energy (Fig. 1a), neglecting the surface energy (Fig. 1b), and neglecting the solvation energy (Fig. 1c). Both the angle combination and probability magnitude are similar in Fig. 1b and Fig. 1a, indicating that the influence of neglecting the surface energy is small. Hence, the orientation of IgG 2a under these conditions is dominated by the solvation energy.



(a) Probability distribution with the total energy



(b) Probability distribution neglecting the surface energy



(c) Probability distribution neglecting the solvation energy

FIG. 1

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