The BAD project: data mining, database and prediction of protein adsorption on surfaces

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Supplementary Information regarding the prediction of the thickness of adsorbed protein films
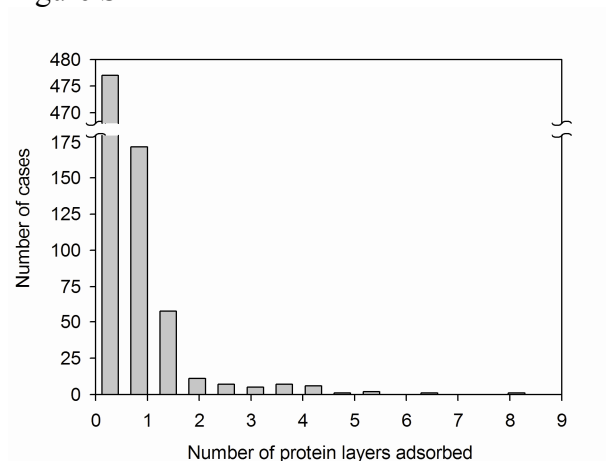
Calculation of the thickness of the adsorbed protein layer. Once the amount of the adsorbed protein has been estimated, using the neural networks prediction or experimentally, the procedure for the calculation of the protein film thickness is as follows:

1. *Protein molecule as its equivalent sphere with radius R and surface projection πR^2.* We assume that the protein partial specific volume[1] is equal to 0.73 cm^3/g and the approximate protein volume $V(nm^3) = 1.21(nm^3/Da)*M(Da)$, where M is the protein molecular weight. Thus the radius of the equivalent sphere is expressed via M as R(nm)

$$= \left(\frac{3V}{4\pi}\right)^{1/3} = 0.066\ (M)^{1/3}.$$

2. *Surface area per adsorbed protein molecule.* From the predicted or experimental protein surface density C_{surf}, the surface area per adsorbed protein molecule is calculated as A = $M/(C_{surf}\ N_A)$, where N_A is Avogadro's number.

3. *Thickness of adsorbed protein film.* If one assumes that the monolayer packing of adsorbed proteins is hexagonal, the fraction of the micro-channel covered by the protein $\pi R^2/A$ is equal to 0.907 and the thickness of the monolayer is the diameter of the equivalent sphere. If the protein adsorbs in several layers (e.g. with the hexagonal lateral packing), the average number of layers is estimated by dividing $\pi R^2/A$ by 0.907 and the thickness of the adsorbed film is taken as the product of the number of layers and 2R.

Figure SI1 shows our estimations of the number of protein layers adsorbed for the data represented in BAD. The respective proteins (cholesterol esterase was not taken into account) in more than 600 cases from 768 adsorb in sub-monolayer coverage.

APPENDIX. Estimation of the thickness of the adsorbed protein layer

Figure SI1

1.   S. B. Zimmerman and A. P. Minton, *Annual Review of Biophysics and Biomolecular Structure*, 1993, 22, 27-65.