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

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Supplementary Information regarding the prediction of the surface tension

Calculation of the surface tension of the protein-covered surface. The calculation of the fraction of the surface covered by the protein allows estimation of the surface tension of the combined surface:

1. *Surface tension of the bare surface*. The calculation of the solid-vapour surface tension, γ_{SV}, from the contact angle θ requires fitting the equation of state proposed by Neumann et al[1]

$$\cos\theta = -1 + 2\sqrt{\frac{\gamma_{sv}}{\gamma_{lv}}}\, e^{-\beta(\gamma_{lv}-\gamma_{sv})^2}$$

where β is a constant equal to 1.247 10^{-4} $(m^2\ mJ^{-1})^2$.

The online Java applet (implemented in the BAD website) performs the non-linear regression for the equation of state, which allows the calculation of γ_{SL}, requiring as input the contact angle, θ, and the liquid-vapour surface tension, γ_{LV}. In BAD, the reported contact angle data are obtained with water and we assume that γ_{LV} is equal to 72.8 mJ/m^2.
The solid-liquid surface tension γ_{SL} can be calculated from the Young equation:

$$\gamma_{SL} = \gamma_{SV} - \gamma_{LV}\cos\theta$$

2. *Calculation of the surface tension of the protein*. Assuming that the protein can form a continuous layer, similar to a bulk material, the solid-vapour surface tension of the protein, γ_{PV}, can be calculated from the amino acid contributions, according to the formula:

$$\gamma_{PV} = \sum_{i=1}^{20} x_i \cdot \gamma_{aa,i}$$

where x_i is the fraction of the i^{th} amino acid (i=1 to 20); and $\gamma_{aa,i}$ is the solid-vapour surface tension of the i^{th} amino acid. The solid-vapour tension of the amino acids has been calculated from atomic contributions, by an algorithm implemented in SciPolymer software. The surface tension of the 20 natural amino acids is presented at the end of this Supplementary Information section.

Calculation of the surface fraction covered by proteins. The fraction of the surface covered by adsorbed proteins is calculated as $\pi R^2/A$ (see Supplementary Information regarding the prediction of the thickness of adsorbed protein films) and shows how the surface coverage is far away from the monolayer one. For instance, it will be close to 0.907 for monolayer hexagonal packing of the proteins.

3. *Calculation of the surface tension for the surface with the adsorbed protein.*
    a. If monolayer coverage is reached or the protein adsorbs in more than a monolayer (taking into account particular model for the surface packing) the surface tension of the protein-covered surface, γ_{CV} is that of the adsorbed protein:

        $\gamma_{CV} = \gamma_{PV}$

    b. Otherwise, the surface tension of the partially covered surface, γ_{CV}, is calculated from the relative contributions of the protein-free surface, γ_{SV}, and the protein, γ_{PV}, as follows:

        $\gamma_{CV} = A_P \cdot \gamma_{PV} + (1-A_P) \cdot \gamma_{SV}$,

where A_P is the fraction of the surface covered by the adsorbed proteins.

APPENDIX. Estimation of the surface tension of the protein

A. Surface tension of the 20 natural amino acids

Table SI 1. Estimated surface tension of amino acids

Amino acid residue	Surface tension, γ_{aaV} (mJ/m^2)
ALA	58.2
GLY	79.3
SER	71.7
THR	59.5
LEU	45.1
ILE	46.3
VAL	47.5
ASN	66
GLN	59.9
ARG	46.2
HIS	59.3
TRP	52.5
PHE	56.2
TYR	59.6
GLU	55.8
ASP	61
LYS	47.8
PRO	51.4
CYS	55.4
MET	53.4

Note: values calculated from atomic contributions of respective amino acids using SciPolymer.

B. Validation of the calculation of the surface tension of the protein

To validate the estimation of the protein surface tension, we calculated the surface tension of three proteins (human serum albumin, mouse immunoglobulin G, and human fibrinogen) using their amino acid primary structures. We compared out results with the surface tension of these proteins, as reported in the literature[2, 3]. The comparative results are presented in Table SI 2.

Table SI 2. Comparison of the calculated and experimental protein surface tension

Protein	Molecular weight, kDa	Surface tension, mJ/m^2	
		calculated	experimental
human serum albumin	66.5	56.93	70.2
immunoglobulin G (2)	145.25*	55.77*	67.2
fibrinogen	353.9	56.5	63.2

Notes: 1. Molecular weight calculated from FASTA; 2. mouse IgG

References

1. D. Y. Kwok and A. W. Neumann, *Advances in Colloid and Interface Science*, 1999, **81**, 167-249.

2. D. R. Absolom and A. W. Neumann, *Colloids and surfaces*, 1987, **30**, 25-45.
3. C. J. Van Oss, D. R. Absolom, A. W. Neumann and W. Zingg, *Biochimica et biophysica acta*, 1981, **670**, 64-73.