

# Neutron reflectometry elucidates density profiles of deuterated proteins adsorbed onto surfaces displaying poly(ethylene glycol) brushes: evidence for primary adsorption

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## Supporting Material

### 1.) Exchange between hydrogenated and deuterated myoglobin

The initial adsorption of deuterated myoglobin (D-Mb) onto the polymer-decorated surfaces was carried out as described in the main text. The samples were then incubated in aqueous solutions of hydrogenated myoglobin (H-Mb) for 72 h. The reflectivity curves measured before and after incubation with H-Mb are not significantly different (Fig. S1). Importantly, the reflectivity curve measured after incubation is still well represented by the model that assumes that the interfacial protein layers remain constituted by D-Mb (solid red line), while a model that assumes exchange between D-Mb and H-Mb (solid green line) fails to represent the measured curve. This result also suggests that immersion in a neat solvent has negligible effect on measurements involving short immersion in a pure contrast fluid.

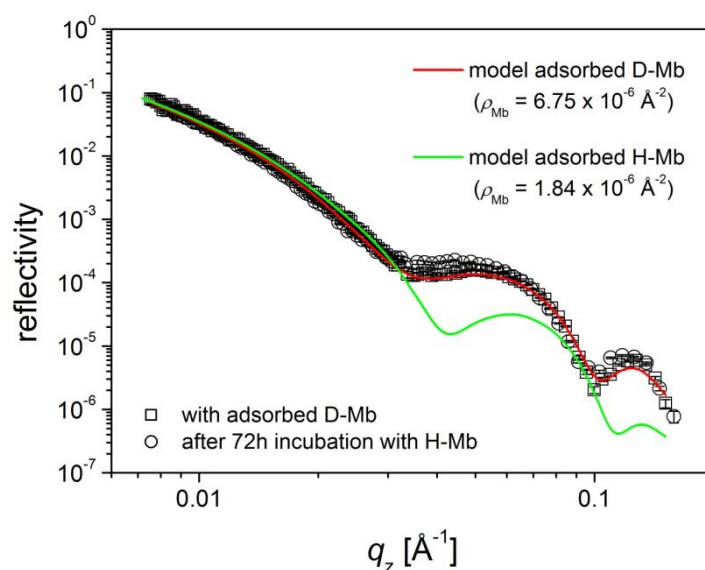


Figure S1: Reflectivity of  $N = 770$  brushes at  $\sigma = 5.2 \pm 0.9 \times 10^{16} \text{ m}^{-2}$  with adsorbed deuterated myoglobin (D-Mb) in  $\text{H}_2\text{O}$  before and after 72 h incubation with a solution of hydrogenated myoglobin (H-Mb). Solid lines are model reflectivity curves assuming that there is no exchange (red) and complete exchange (green) between H-Mb and D-Mb in the interfacial layers.

## 2.) Scattering length densities of the contrast fluids as obtained from the reflectivity fits

Table S1 summarizes the scattering length densities of the contrast fluids as determined by the simultaneous fits to the reflectivity data for all samples identified by  $N$  and  $\sigma$ . Deviations from the nominal values ( $D_2O$ :  $6.36 \times 10^{-6} \text{ \AA}^{-2}$ , 4-matched water:  $4 \times 10^{-6} \text{ \AA}^{-2}$ , silicon matched water:  $2.07 \times 10^{-6} \text{ \AA}^{-2}$ ,  $H_2O$ :  $-0.56 \times 10^{-6} \text{ \AA}^{-2}$ ) are due to incomplete liquid exchange in the measurement cells.

$N$	$\sigma$ [ $10^{16} \text{ m}^{-2}$ ]	$D_2O$	silicon matched water	$H_2O$	4-matched water after Mb adsorption	silicon matched water after Mb adsorption	$H_2O$ after Mb adsorption
770	1.1±0.8	6.36	2.4	-0.5	4.1	1.8	-0.56
770	1.2±0.8	6.36	2.8	-0.1	-	1.5	-0.56
770	1.9±1.0	6.36	2.1	-0.56	-	2.0	-0.56
770	3.8±0.9	6.36	2.0	-0.56	-	1.8	-0.3
770	5.2±0.9	6.36	2.3	-0.56	-	1.9	-0.56
146	2 (<5)	6.36	2.5	-0.56	-	1.8	-0.4
146	5±3	6.2	-	0.1	-	2.5	-0.2

Table S1: Scattering length densities of the contrast fluids as obtained from the reflectivity fits. Numbers are given in units of  $10^{-6} \text{ \AA}^{-2}$ .