End point vs. backbone specificity governs characteristics of antibody binding to poly(ethylene glycol) brushes

Victoria M. Latza[a], Ignacio Rodriguez-Loureiro[a], Giovanna Fragneto[b], and Emanuel Schneck[a,*]

[a]Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany

[b]Institut Laue-Langevin, 71 avenue des Martyrs, 38042 Grenoble Cedex 9, France

Supporting Information

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1.) Initial parameter values of the simultaneous fits

Initial values for all parameters concerning the layered structure of the functionalized solid surface including the brush-grafting lipid monolayer were taken from the best-matching results obtained in previous studies[1, 2]. Regarding the protein volume fraction profiles, various sets of initial parameters for center position z_k^{Ab}, thickness w_k^{Ab} , and plateau volume fraction $\Phi_k^{\max}$ were tested. When they were taken from a suitable range, the parameter values during the fitting procedure converged to the values presented in the main text, for which the experimental data are well reproduced.

2.) Parameters characterizing the layer structure of the solid substrates

Sample	D_{SiO2} [Å]	D_{hc} [Å]	D_{hg} [Å]	Φ_w^{SiO2} [vol %]	$\delta_{hg,wat}$ [Å]
PEG-lipid-22, $f = 0.1$	24	40	12	12	6
PEG-lipid-114, $f = 0.01$	24	40	12	15	3
PEG-lipid-114, $f = 0.05$	19	39	14	19	2
PEG-lipid-114, $f = 0.1$	23	40	5	8	3
PEG-lipid-455, $f = 0.01$	19	40	6	5	6
Average ± stddev	22 ± 2	40 ± 1	10 ± 4	12 ± 5	4 ± 2

3.) Parameters characterizing the polymer brushes

Sample	H_0 *before ads.* [Å]	H_0 *after BB Ab ads.* [Å]
PEG-lipid-22, $f = 0.1$	35	75
PEG-lipid-114, $f = 0.01$	35	189
PEG-lipid-114, $f = 0.05$	60	57
PEG-lipid-114, $f = 0.1$	75	471
PEG-lipid-455, $f = 0.01$	215	202

4.) Full set of reflectivity data on the sequential adsorption of BB Abs and EB Abs

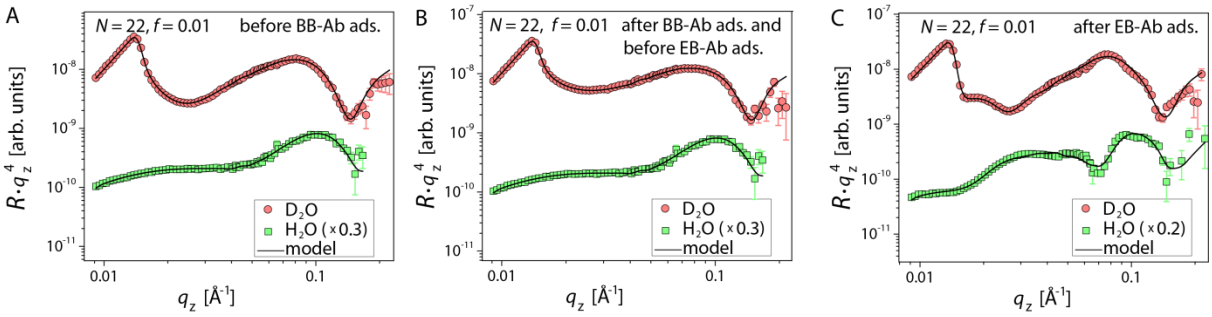

Figure S1: Reflectivity curves (PEG-lipid-22, $f = 0.01$) in two water contrasts (D_2O, and H_2O) before BB Ab adsorption (A), after BB Ab adsorption but before EB Ab adsorption (B) and after EB Ab adsorption (C). Solid lines represent the simulated intensities corresponding to the best-matching parameters in the common model.

References

1. Schneck, E.; Berts, I.; Halperin, A.; Daillant, J.; Fragneto, G., Neutron reflectometry from poly (ethylene-glycol) brushes binding anti-PEG antibodies: Evidence of ternary adsorption. *Biomaterials* **2015,** 46, 95-104.
2. Latza, V. M.; Rodriguez-Loureiro, I.; Kiesel, I.; Halperin, A.; Fragneto, G.; Schneck, E., Neutron Reflectometry Elucidates Protein Adsorption from Human Blood Serum onto PEG brushes. *Langmuir* **2017,** 33, (44), 12708-12718.