

Supporting information for:
**Thermodynamics of the binding of lysozyme
to a dendritic polyelectrolyte: Electrostatics
vs. hydration**

Qidi Ran,^{†,‡,¶} Xiao Xu,[§] Joachim Dzubiella,^{||,‡,¶} Rainer Haag,^{*,†,¶} and Matthias
Ballauff^{*,‡,¶,⊥}

[†]Institute of Chemistry and Biochemistry, Freie Universität Berlin, Takustr. 3, 14195 Berlin,
Germany

[‡]Institute of Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin,
Hahn-Meitner-Platz 1, 14109 Berlin, Germany

[¶]Multifunctional Biomaterials for Medicine, Helmholtz Virtual Institute, Kantstr. 55, 14513
Teltow-Seehof, Germany

[§]School of Chemical Engineering, Nanjing University of Science and Technology, 200 Xiao Ling
Wei, 210094 Nanjing, P. R. China

^{||}Physikalisches Institut, Albert-Ludwigs-Universität, Hermann-Herder-Str. 3, 79104 Freiburg,
Germany

[⊥]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

E-mail: haag@chemie.fu-berlin.de; matthias.ballauff@helmholtz-berlin.de

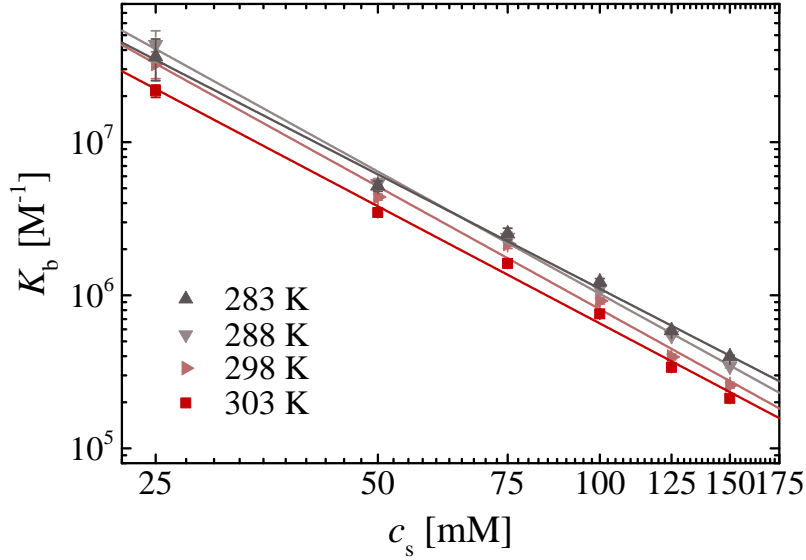


Figure S1: The salt dependence of binding constant for dPGS-Lys interaction at different temperatures. The number of released counterions ΔN_{ci} is 2.5 ± 0.1 , 2.7 ± 0.1 , 2.7 ± 0.1 , and 2.5 ± 0.1 for 283 K, 288 K, 298 K, and 303 K, respectively.

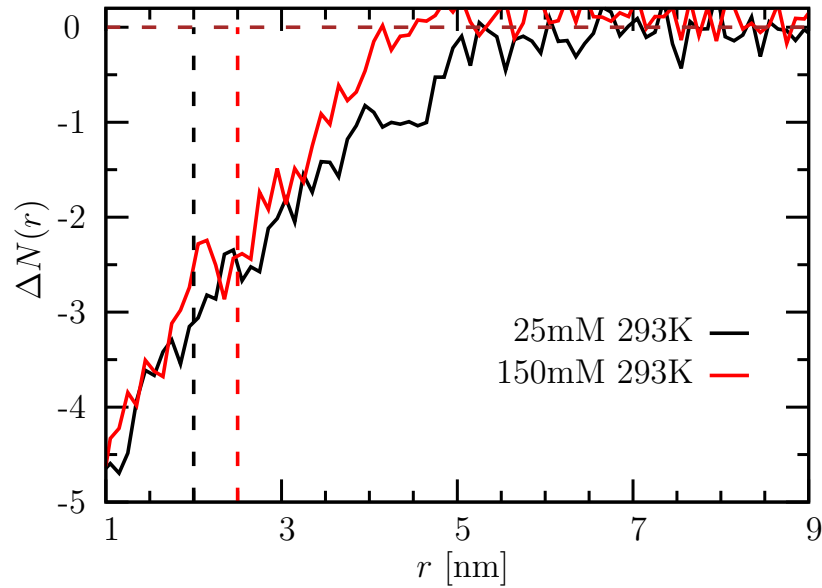


Figure S2: The decrease of condensed counterions $\Delta N(r)$ on the dPGS surface upon binding with lysozyme according to computer simulations. r denotes the center-of-mass distance between dPGS and the first bound lysozyme. The number of released counterions can be read off at the distance r_b found with the bound state (dashed lines). $\Delta N(r_b)$ is 3.0 at $r_b = 2.0$ nm, and 2.5 at $r_b = 2.5$ nm.

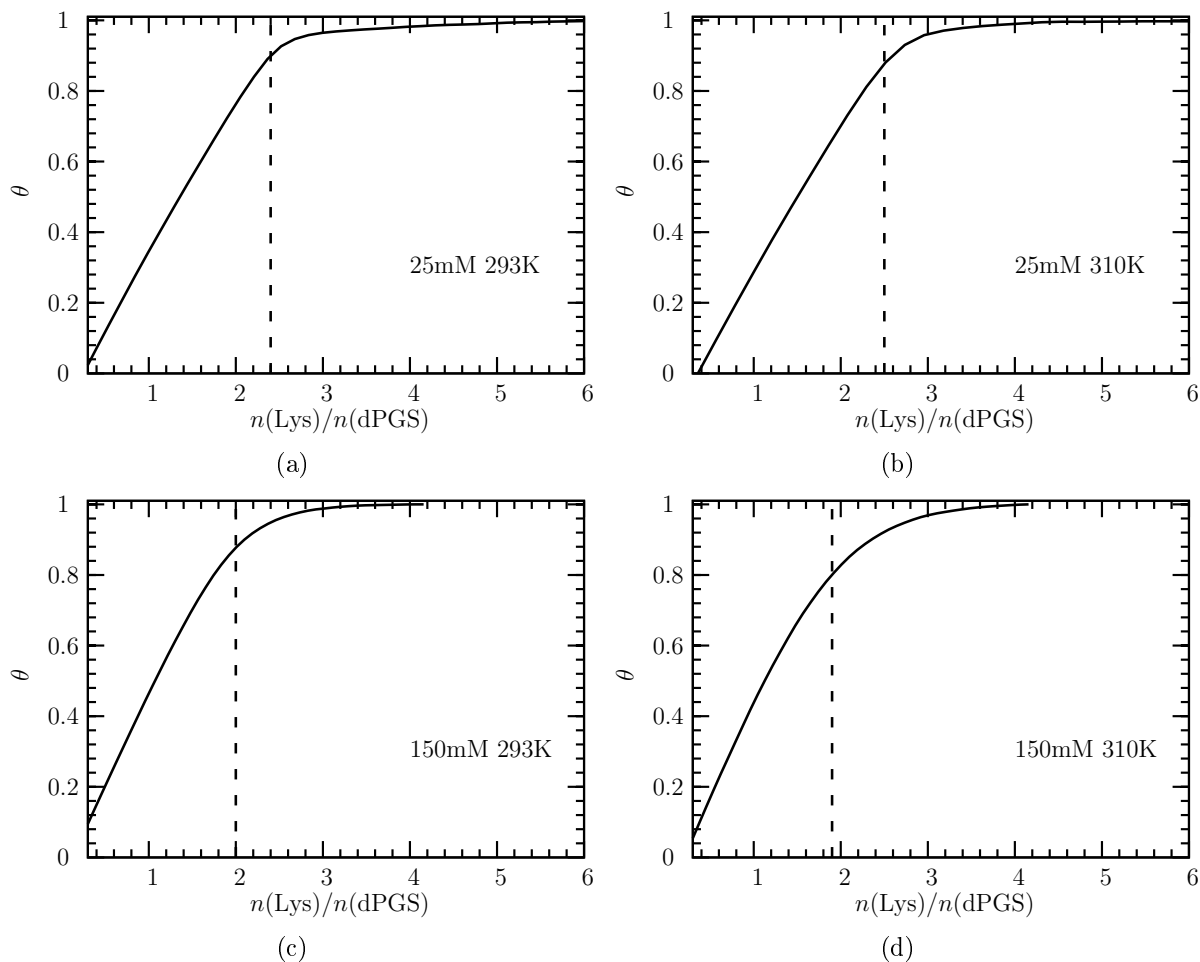


Figure S3: The protein coverage θ as a function of the molar ratio $n(\text{Lys})/n(\text{dPGS})$ in ITC measurements at different ionic strengths and temperatures. θ are plotted according to previous deviations (see the SI in ref.^{S1}). Each dashed line denotes the inflection point (binding number N) in the respective ITC isotherm. The intersection points with θ refer to the coverage θ^* at the inflection points.

References

- (S1) Xu, X.; Ran, Q.; Dey, P.; Nikam, R.; Haag, R.; Ballauff, M.; Dzubiella, J. Counterion-release entropy governs the inhibition of serum proteins by polyelectrolyte drugs. *Biomacromolecules* **2018**, *19*, 409–416.