The Influence of the Membrane Potential on the Protonation of Bacteriorhodopsin: Insights from Electrostatic Calculations into the Regulation of Proton Pumping.

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Supporting Information

Reference 44.

MacKerell, A. D.; Bashford, D.; Bellott, M.; Dunbrack, R. L.; Jr.; Evanseck, J. D.; Field, M. J.; Fischer, S.; Gao, J.; Guo, H.; Ha, S.; Joseph-McCarthy, D.; Kuchnir, L.; Kuczera, K.; Lau, F. T. K.; Mattos, C.; Michnick, S.; Ngo, T.; Nguyen, D. T.; Prodhom, B.; Reiher, W. E.; Roux, B.; Schlenkrich, M.; Smith, J. C.; Stote, R.; Straub, J.; Watanabe, M.; Wiorkiewicz-Kuczera, J.; Yin, D.; Karplus, M. *J. Phys. Chem. B*, **1998**, *102*, 3586–3616.

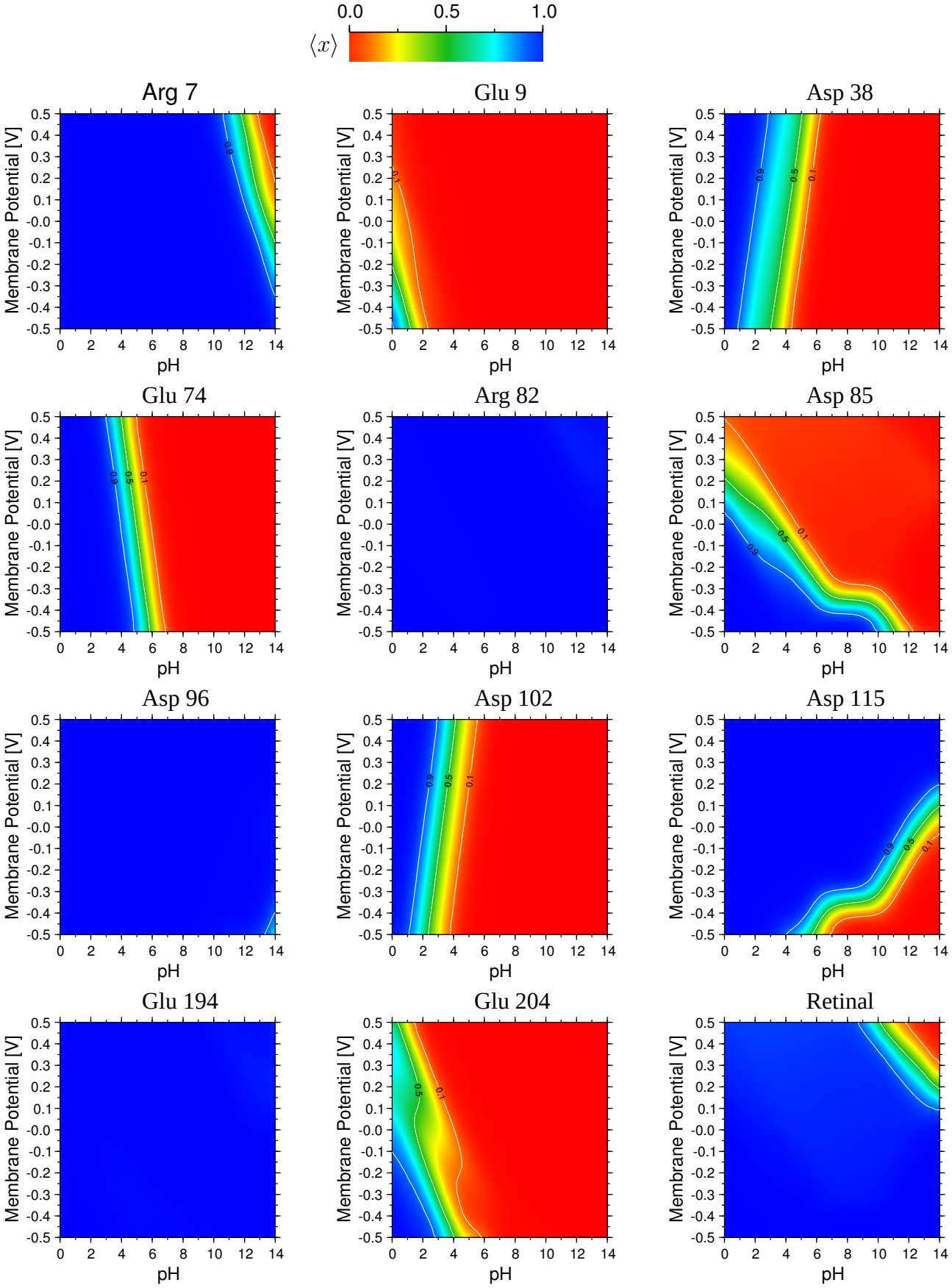

Figure S 1: Protonation probabilities of functionally important sites of bacteriorhopsin in dependence on the pH and the membrane potential Ψ. The protonation probability $\langle x \rangle$ is given by a color scale.

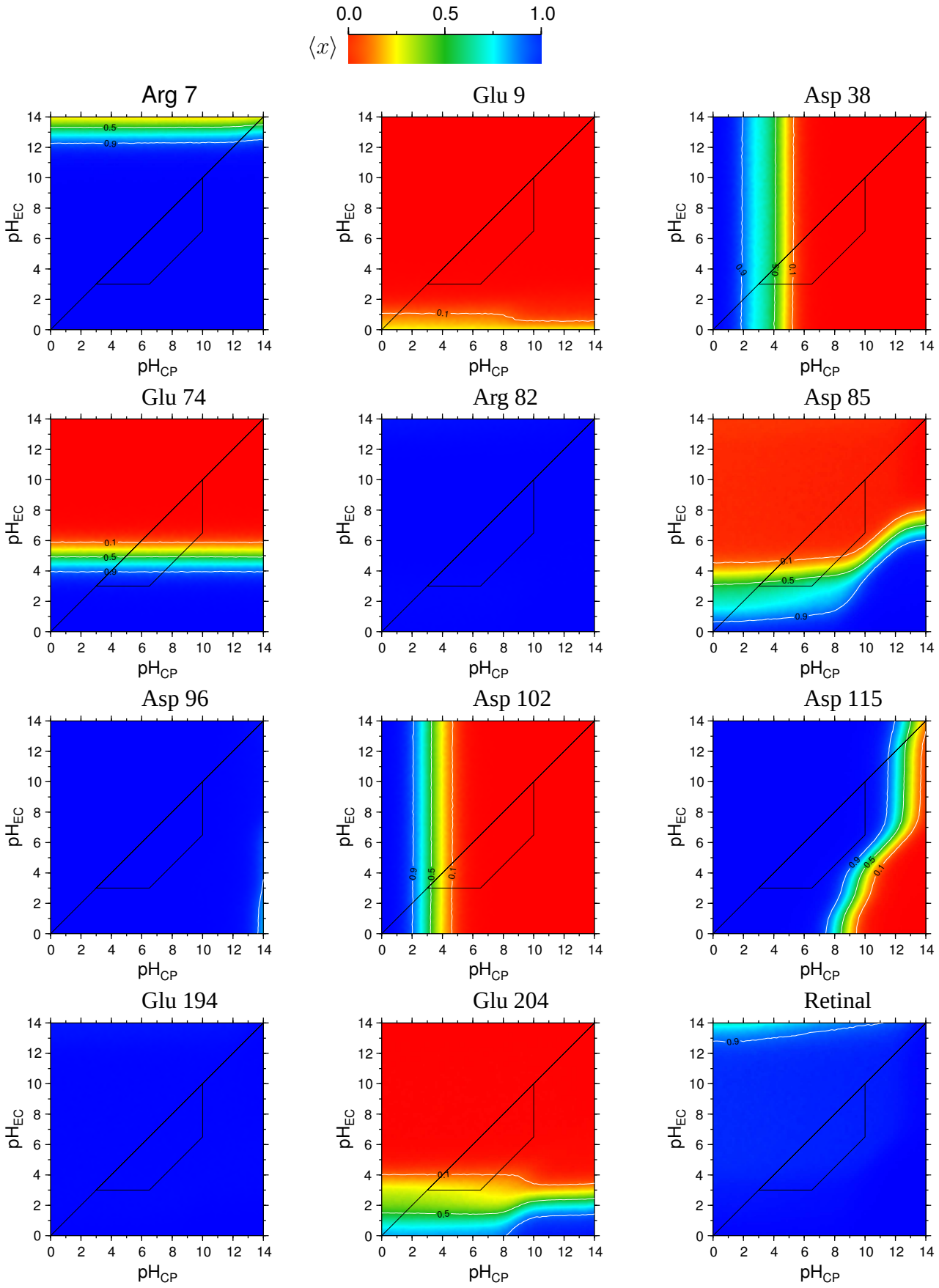

Figure S 2: Protonation probabilities of functionally important sites of bacteriorhopsin in dependence on pH_{EC} and pH_{CP}. The effect of the pH gradient on the membrane potential is compensated by other ions and thus the membrane potential is zero. The protonation probability $\langle x \rangle$ is given by a color scale.

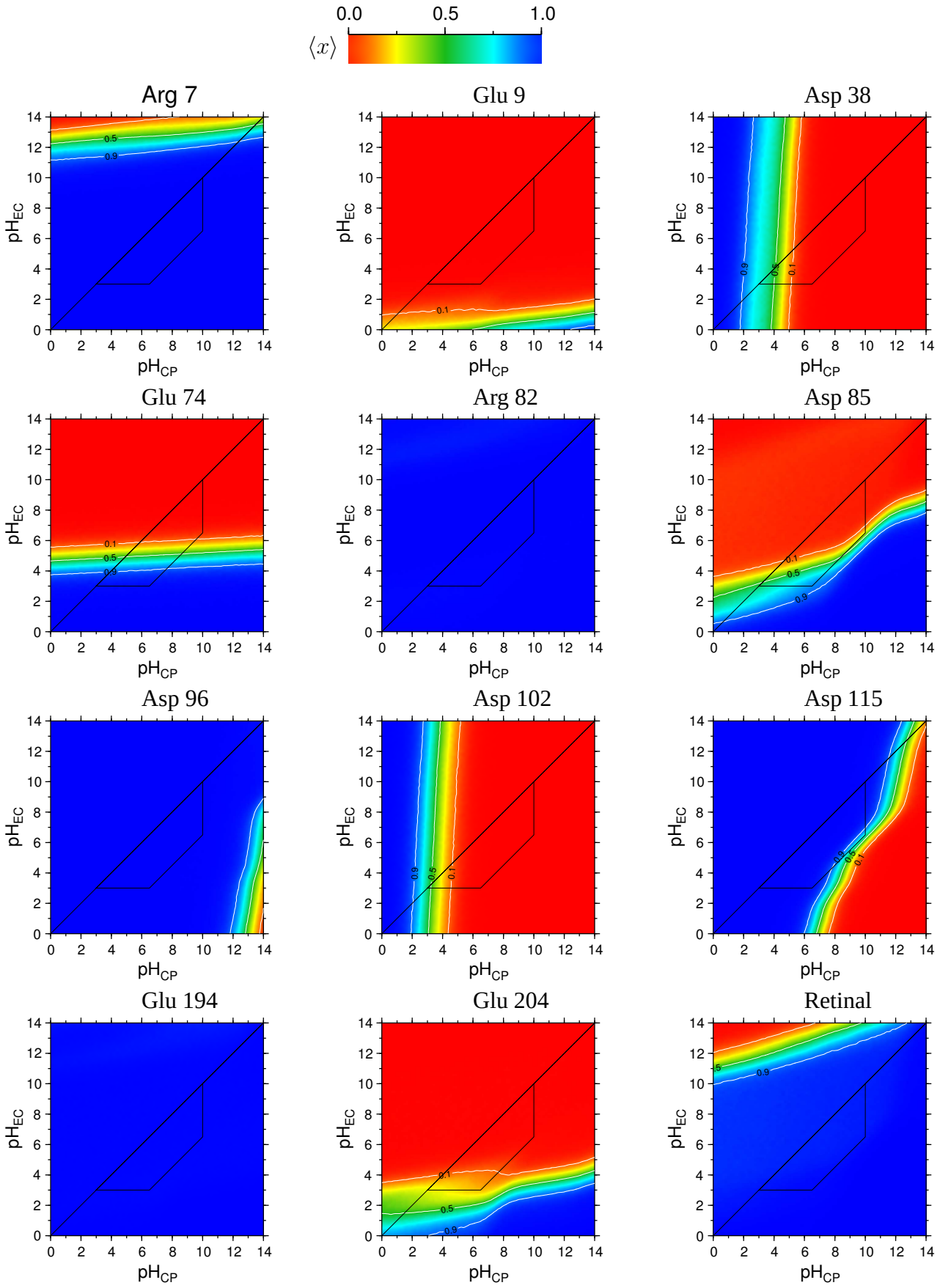

Figure S 3: Protonation probabilities of functionally important sites of bacteriorhopsin in dependence on pH_{EC} and pH_{CP}. The pH gradient between the two sides of the membrane gives rise to a membrane potential which is proportial to ΔpH. The proportionality factor *a* is assumed to be 0.5. The protonation probability $\langle x \rangle$ is given by a color scale.

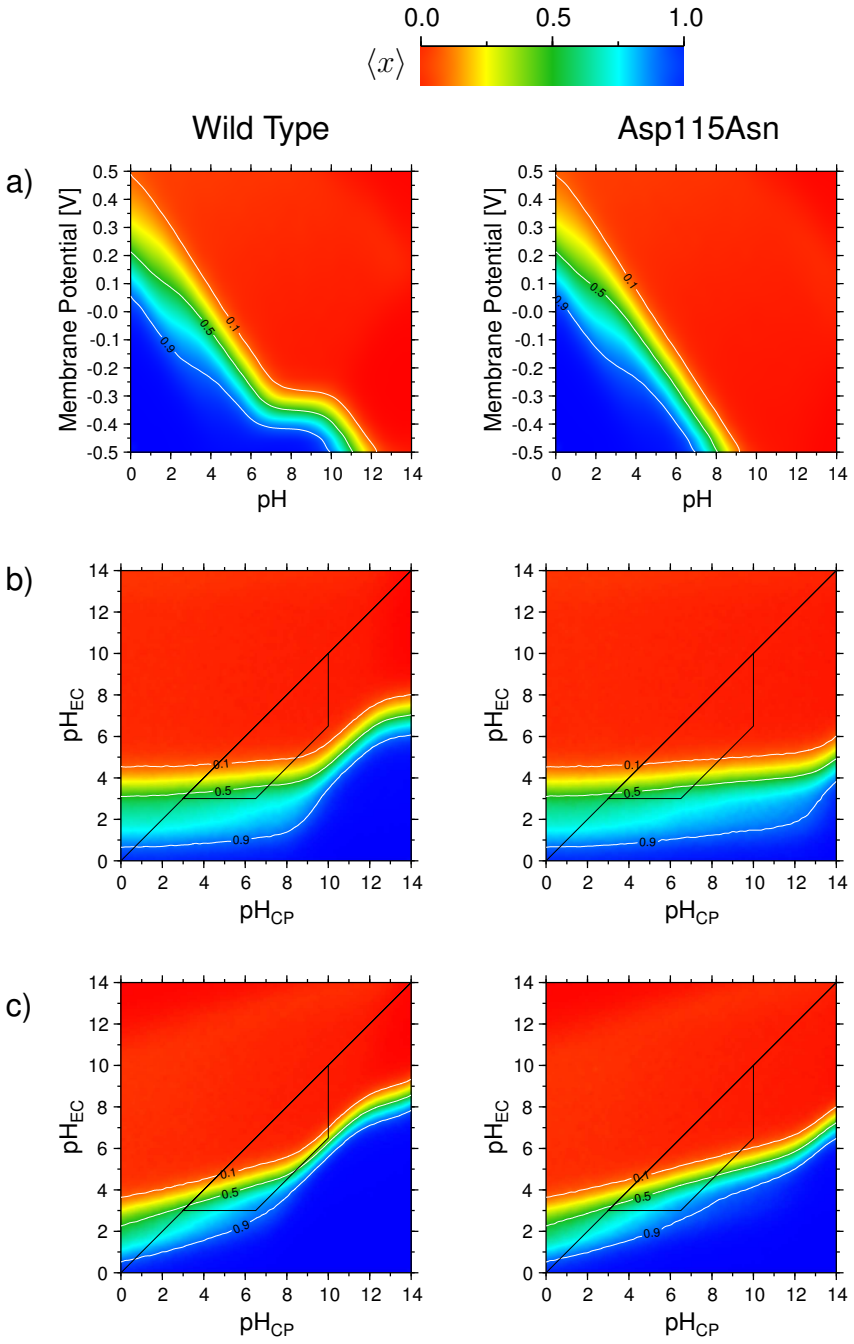

Figure S 4: Protonation probabilities of Asp85 in the wild type protein (left) and in the Asp115Asn mutation (right) under different conditions. It can be seen that the mutation strongly influences the titration behavior. A regulation of the photocycle in the mutant protein seems not to be possible. a) Protonation probability in dependence on the pH and the membrane potential Ψ b) Protonation probability in dependence on $\mathrm{pH_{EC}}$ and $\mathrm{pH_{CP}}$. The effect of the pH gradient on the membrane potential is compensated by other ions and thus the membrane potential is zero. c) Protonation probability in dependence on $\mathrm{pH_{EC}}$ and $\mathrm{pH_{CP}}$. The pH gradient between the two sides of the membrane gives rise to a membrane potential which is proportial to ΔpH. The proportionality factor a is assumed to be 0.5. The protonation probability $\langle x \rangle$ is given by a color scale.