



**Solution Structure of the
Gloeobacter violaceus Ligand-Gated Ion Channel
Probed by Small-Angle Neutron Scattering**

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ESS/ILL user meeting - topical session

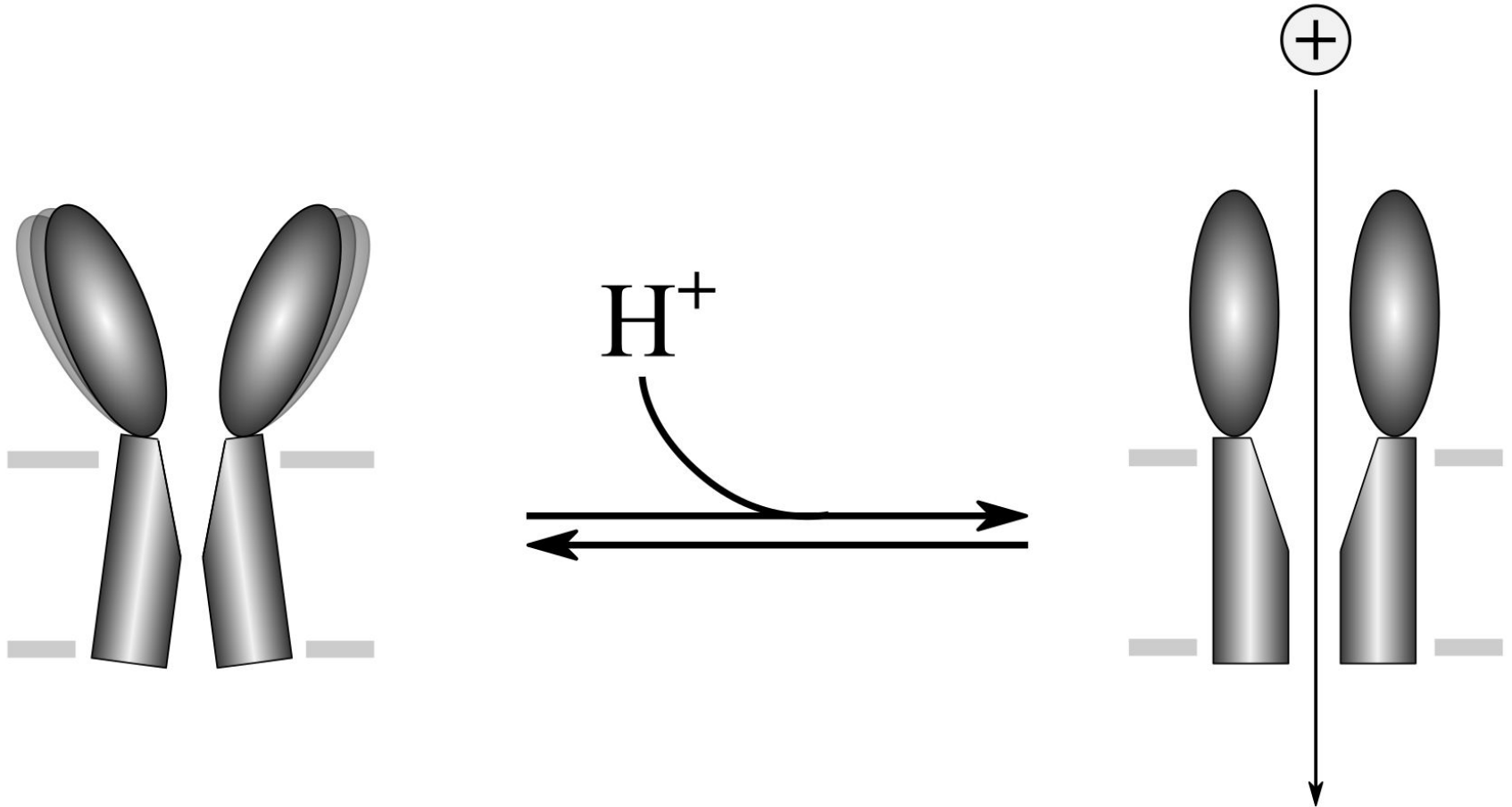
January 20th 2021



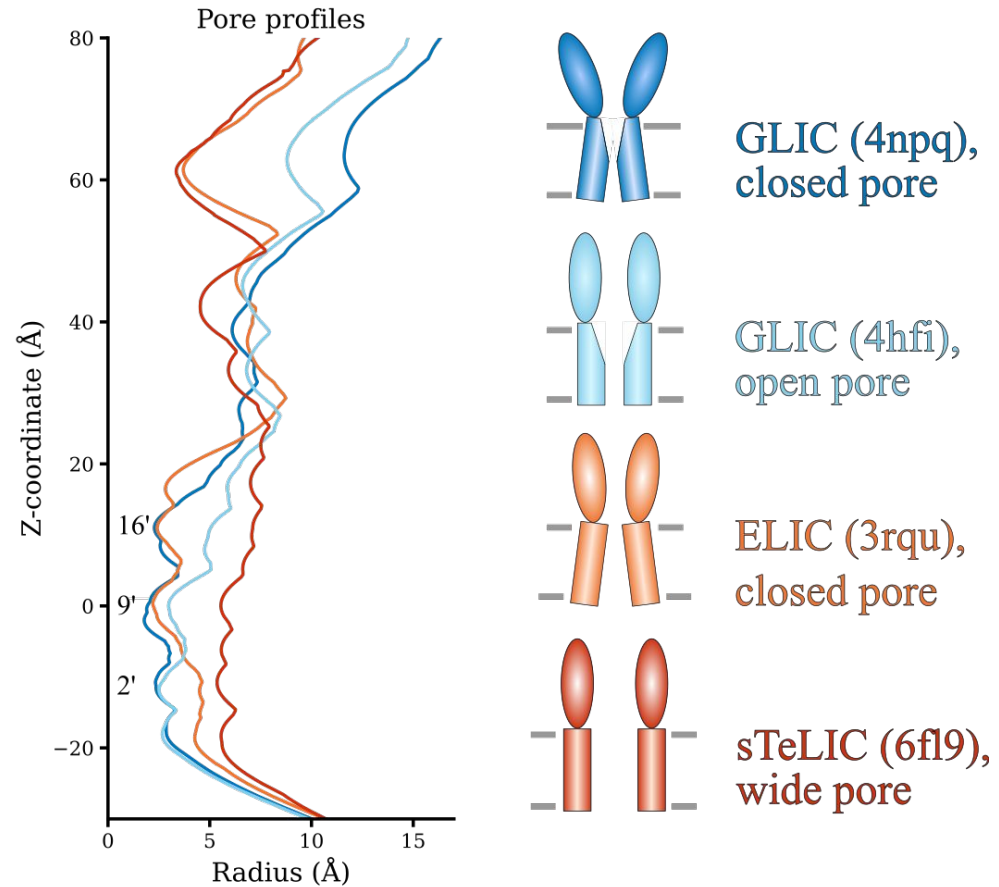
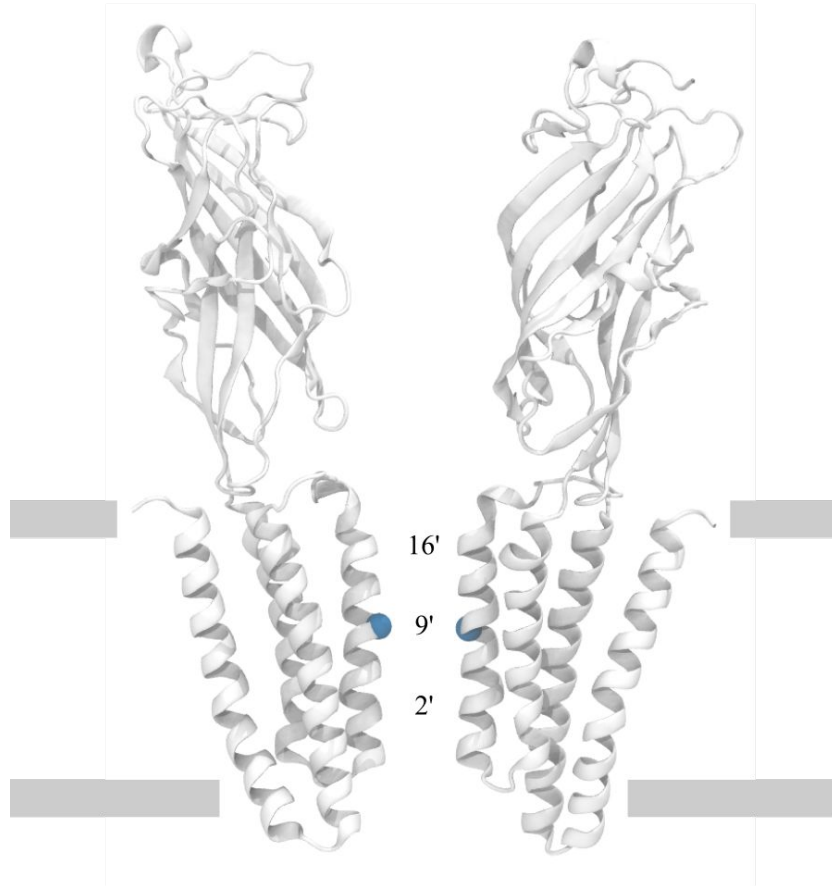
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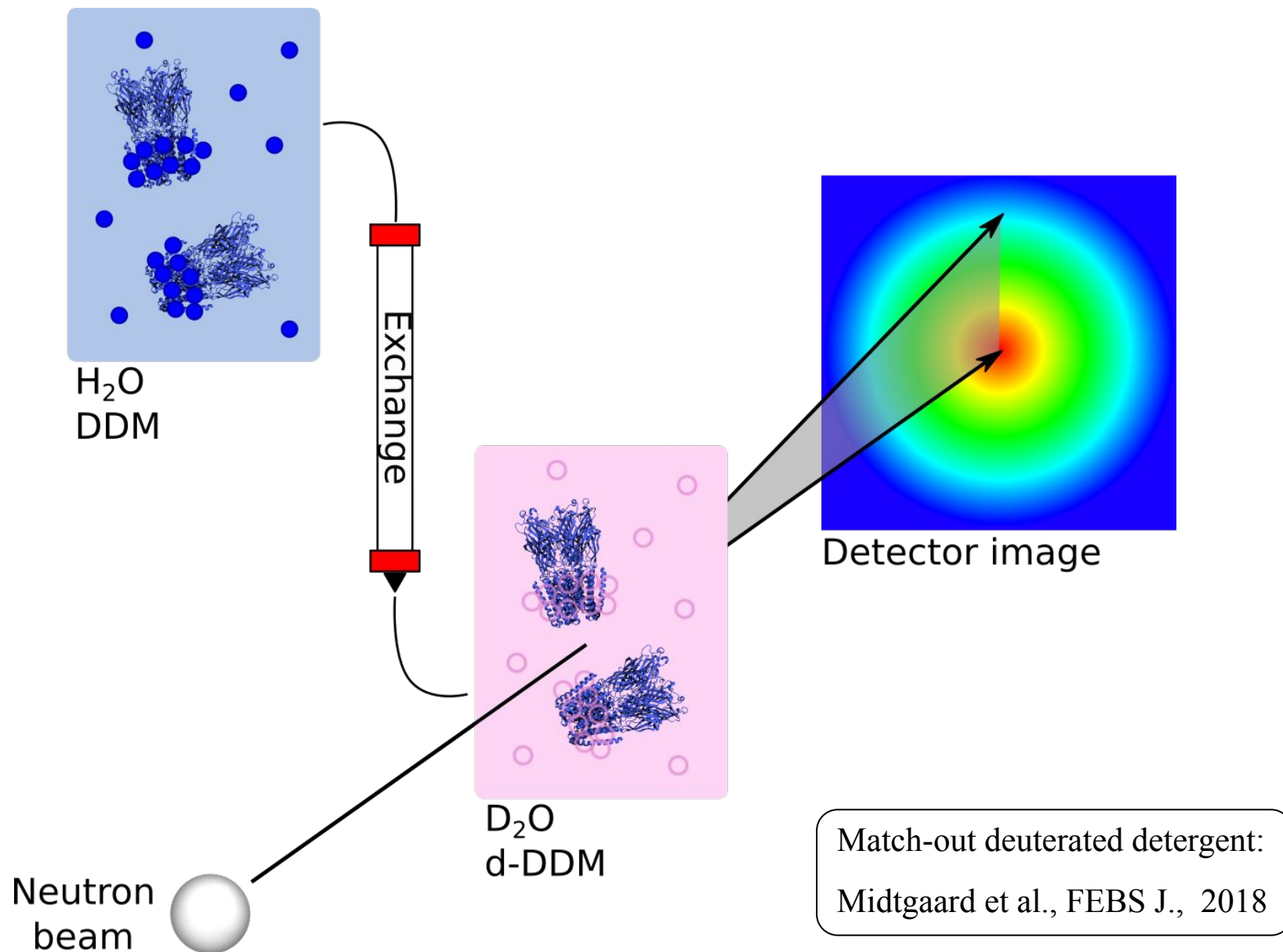
GLIC - a model system for pentameric ligand-gated ion channels



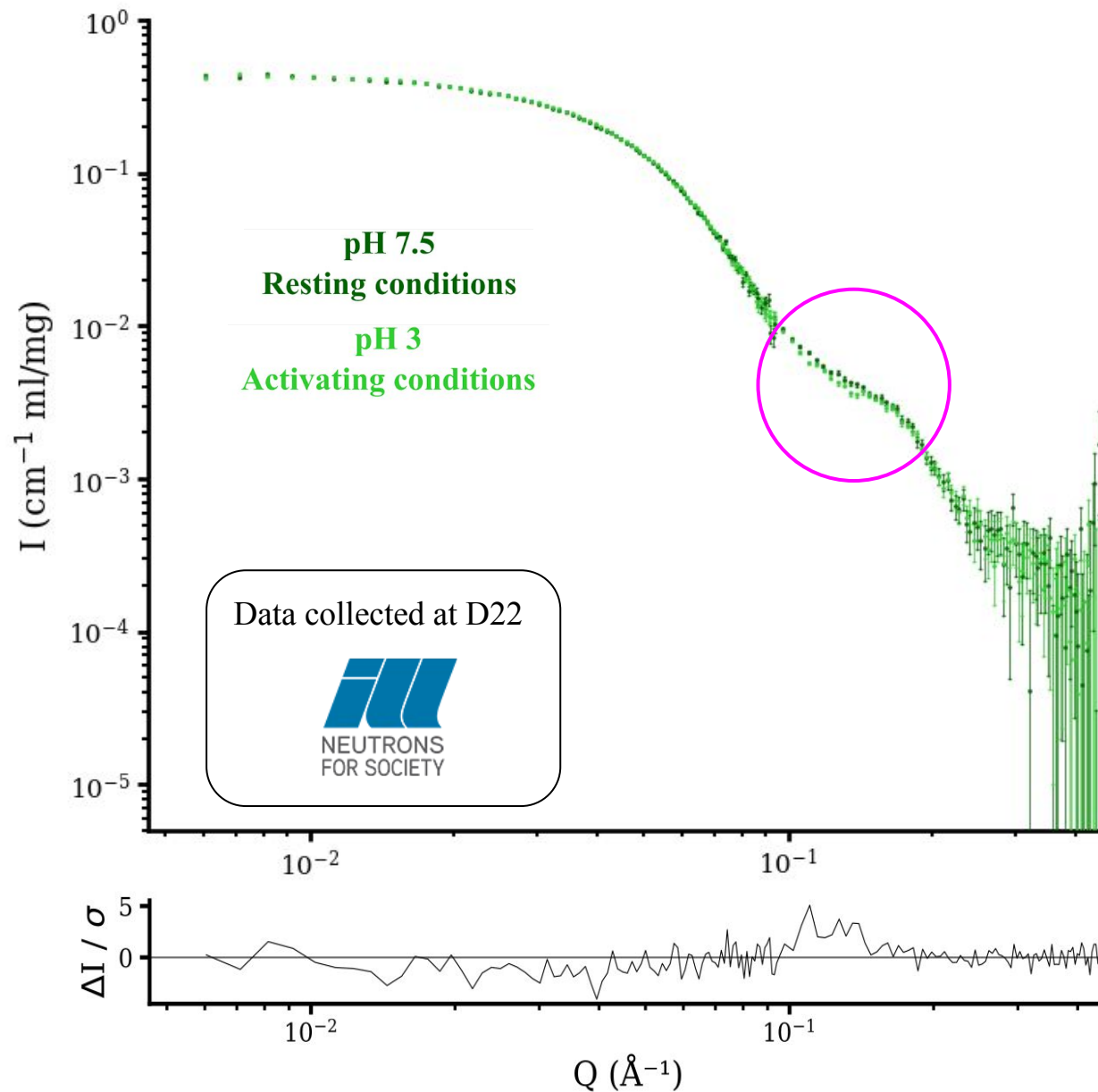
Multiple conformations are known from crystal structures



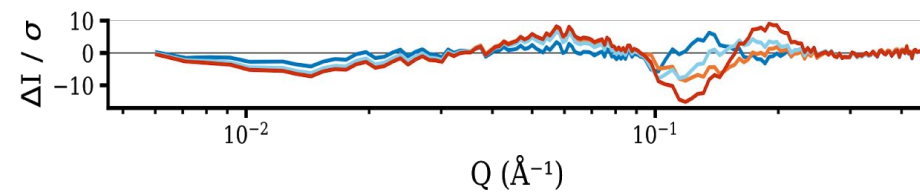
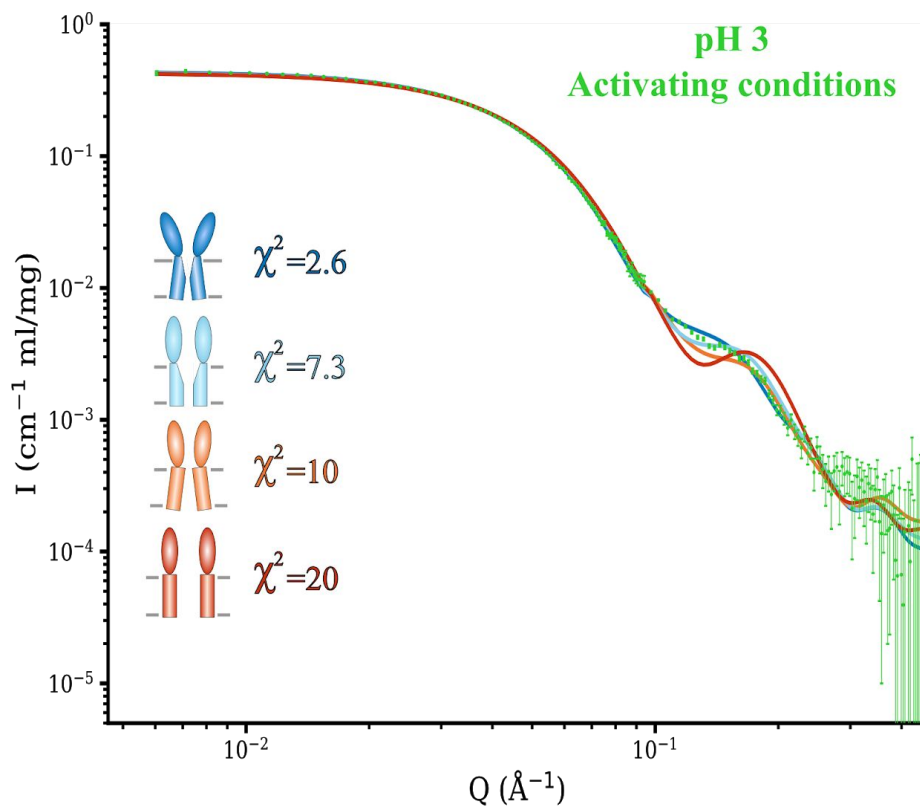
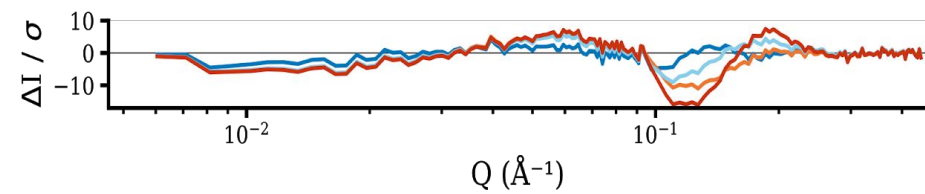
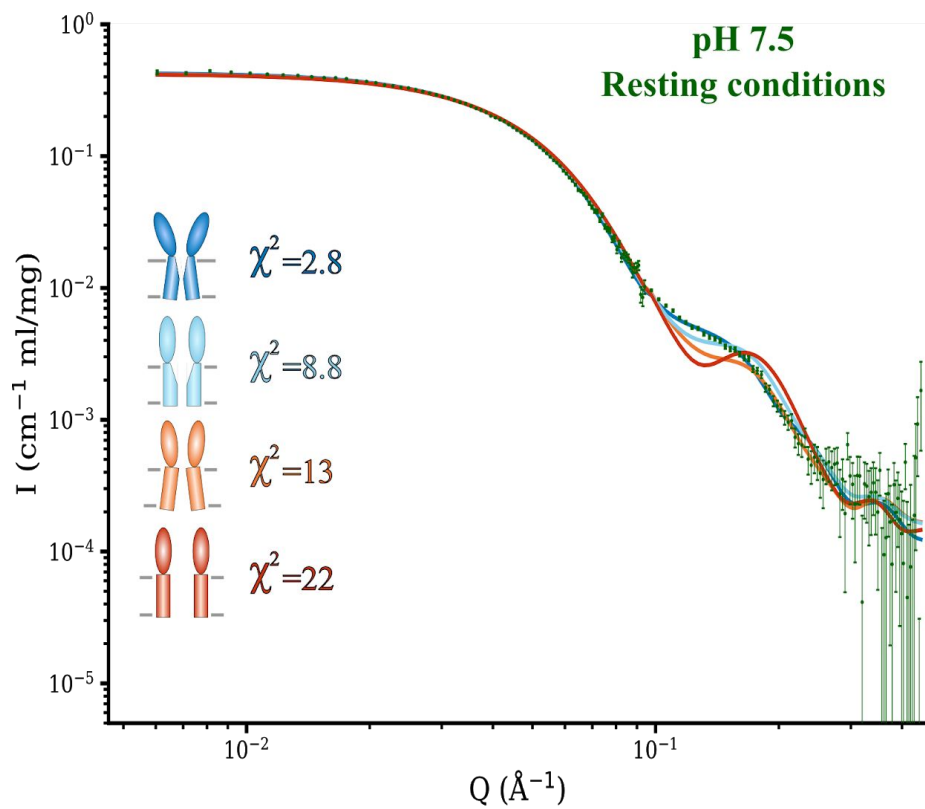
SEC-SANS & match-out deuterated detergent



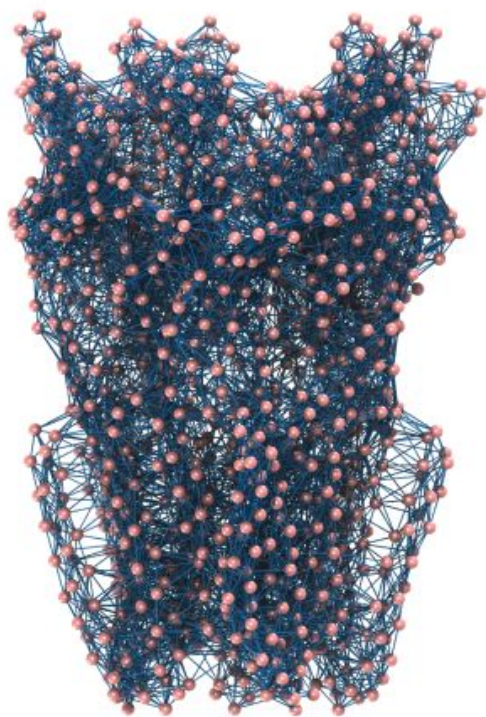
SANS data collected under resting and activating conditions



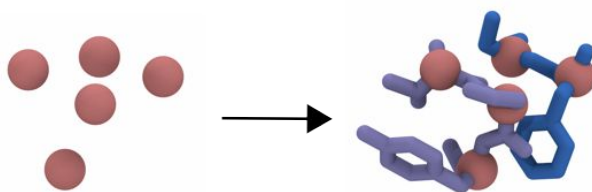
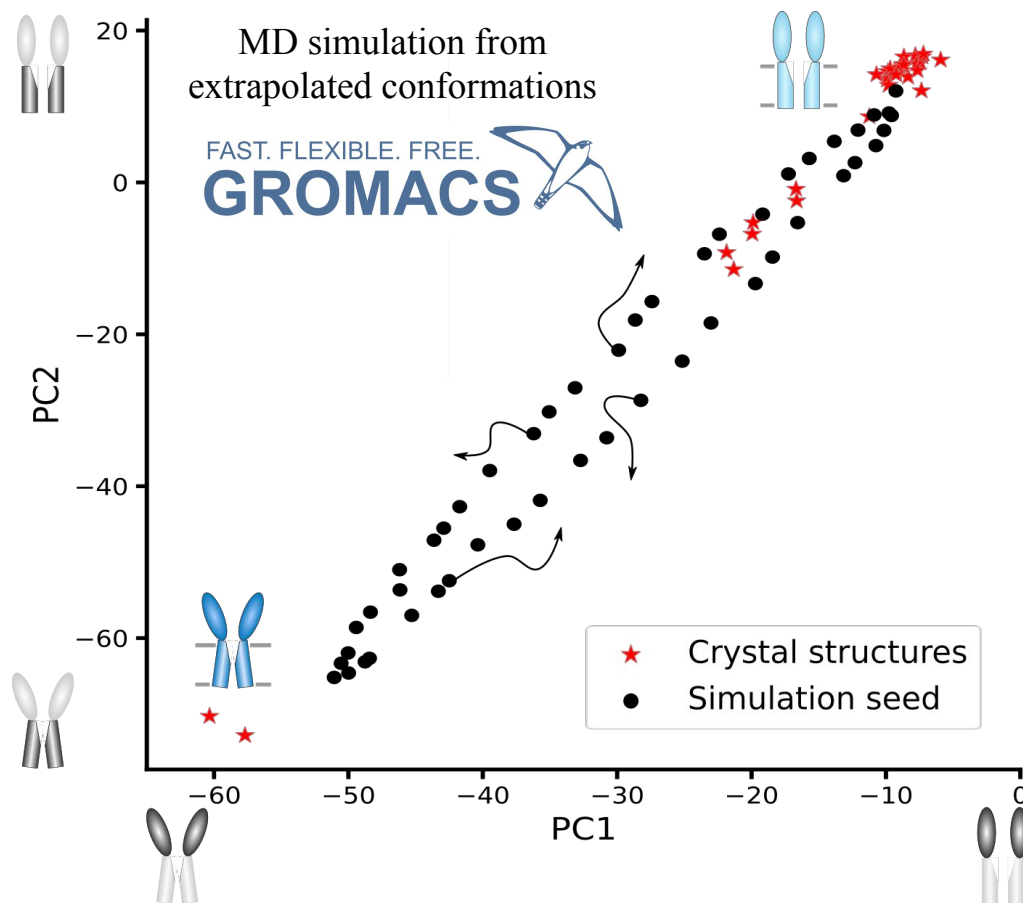
Fits of crystal structures - Resting state gives best fit



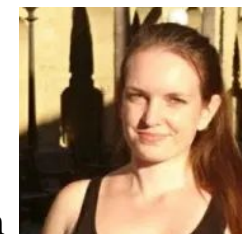
Coarse grained extrapolation & all-atom Molecular Dynamics simulations



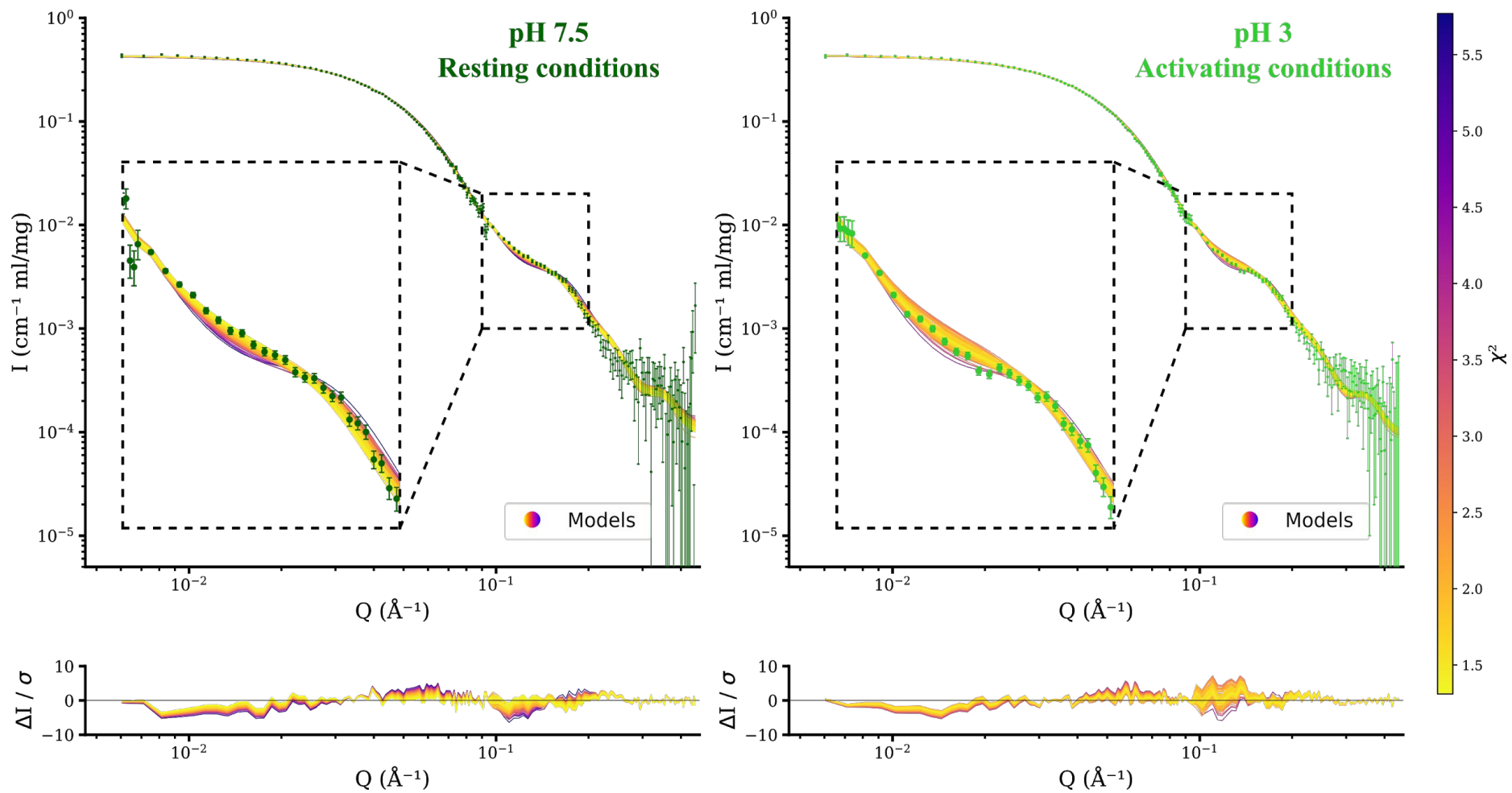
Coarse grained extrapolation using eBDIMS
<https://ebdims.biophysics.se/>



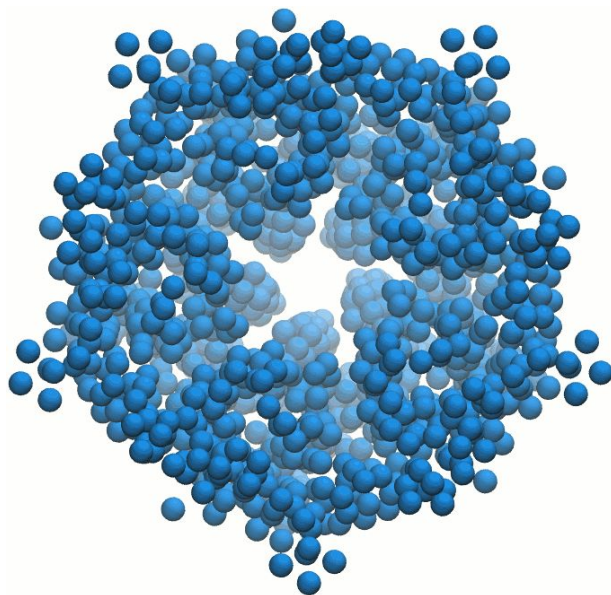
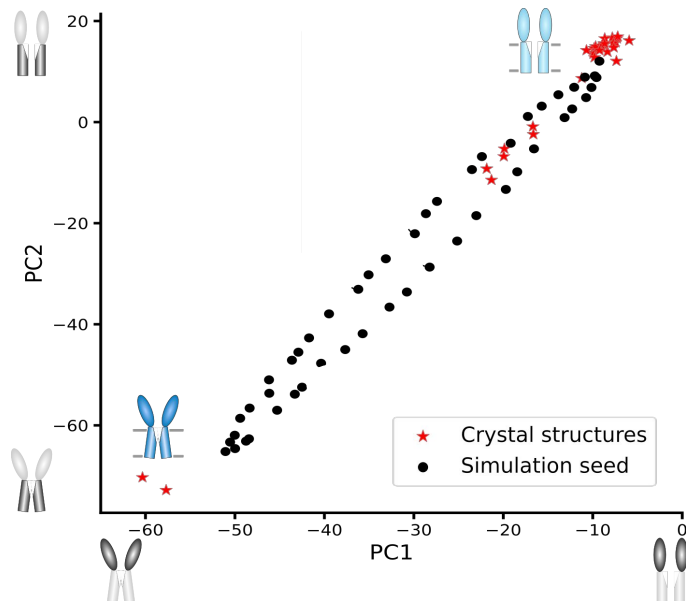
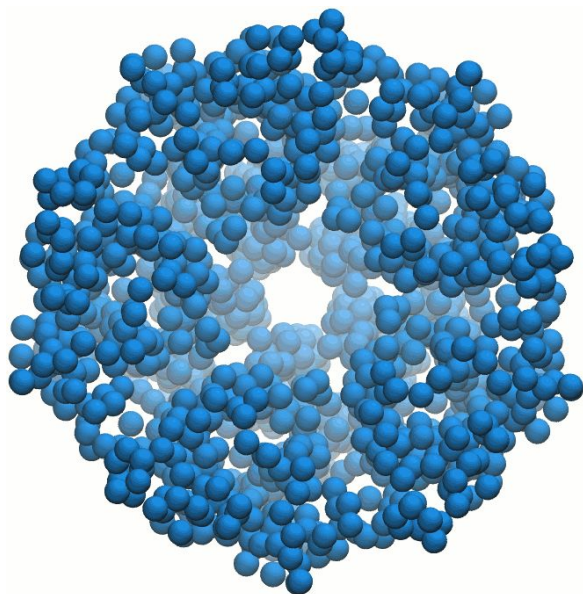
Cathrine Bergh



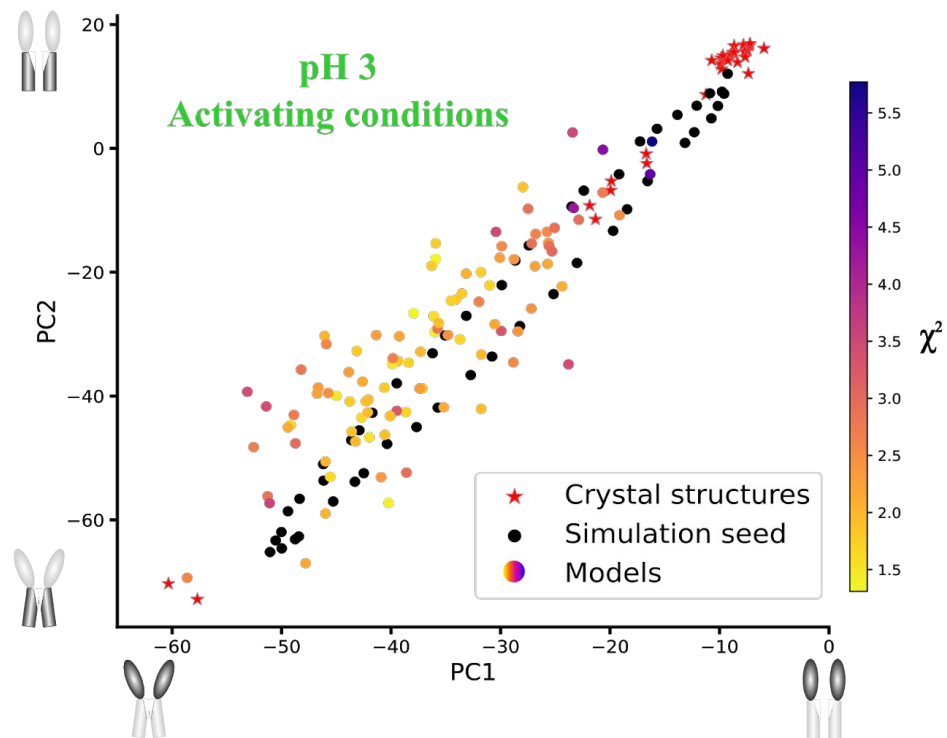
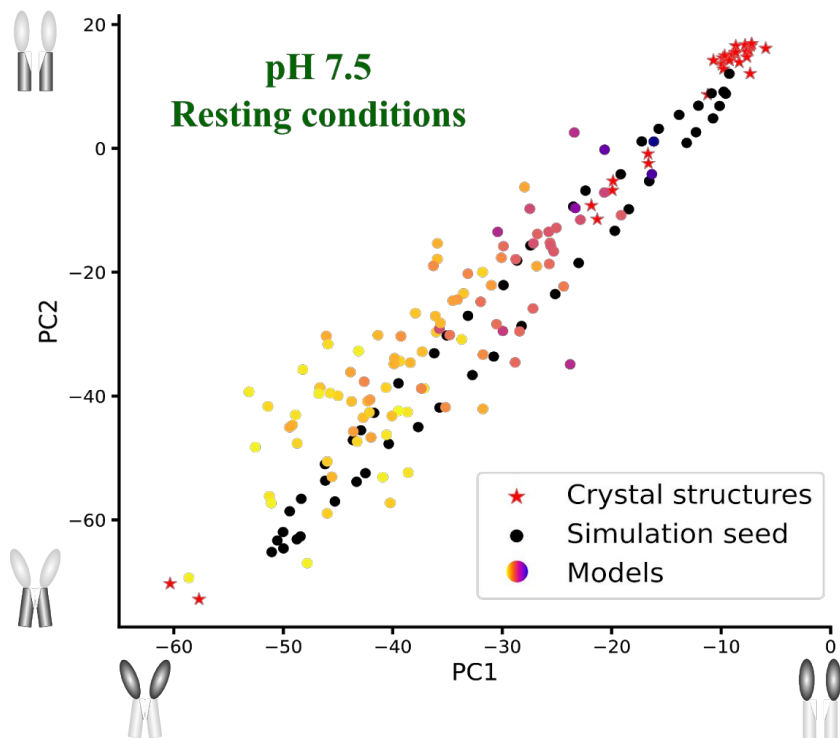
Improved fit using models from MD simulations



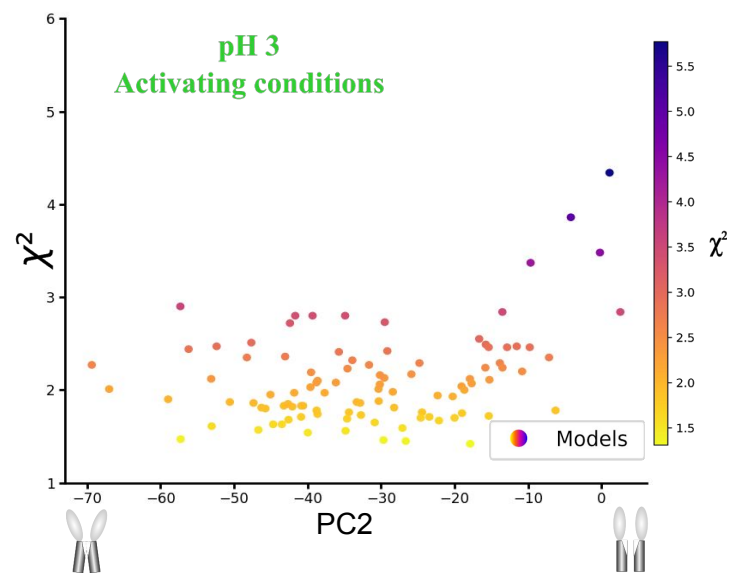
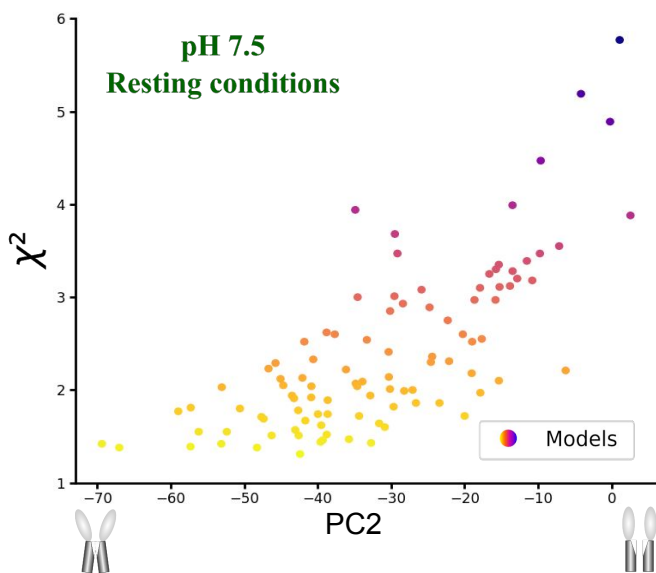
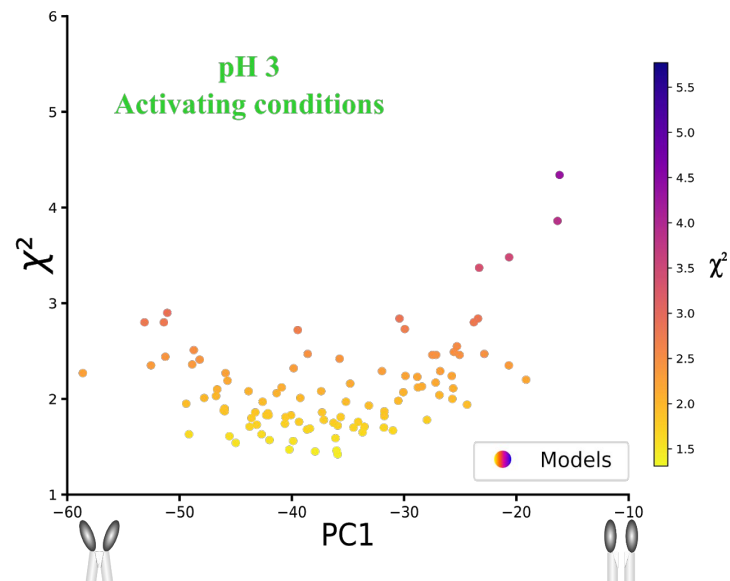
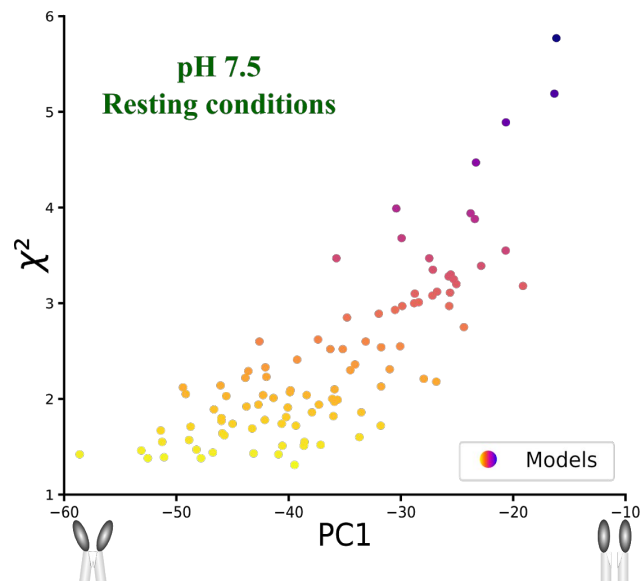
Conformational landscape as described by principal components



Best fitting population shifts between the experimental conditions

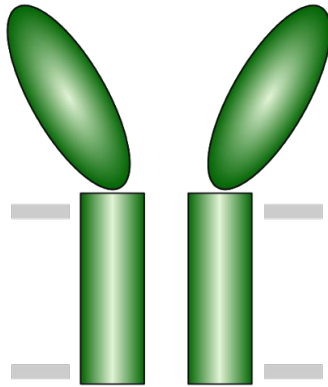


Goodness of fit at pH 3 is mainly impacted by the extracellular domain



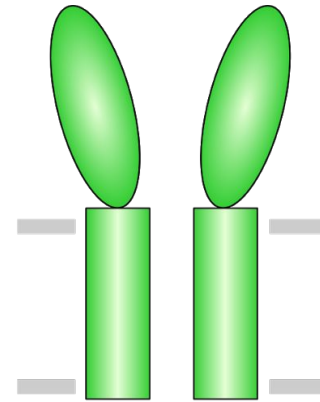
The average solution structure of GLIC

pH 7.5
Resting conditions



Extracellular domain is expanded

pH 3
Activating conditions



**Intermediate expansion of
extracellular domain**



MOLECULAR BIOPHYSICS STOCKHOLM

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Rebecca J Howard
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Cathrine Bergh

and the entire group



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SWEDISH FOUNDATION for
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