Computing osmotic permeabilities of aquaporins AQP4, AQP5, and GlpF from near-equilibrium simulations\textsuperscript{1} THIERRY WAMBO, ROBERTO RODRIGUEZ, LIAO CHEN, The University of Texas at San Antonio — Measuring or computing the single-channel permeability of aquaporins/aquaglyceroporins (AQPs) has long been a challenge. We report large scale simulations of osmotic current under sub M gradient through three AQPs (water channels AQP4 and AQP5 and glycerol-water channel GlpF). These simulations were implemented with hybrid periodic boundary conditions devised to avoid the artifactitious mixing across the membrane in a regular PME simulation. The computed single-channel permeabilities at 5°C and 25°C are in agreement with recently refined experiments on GlpF. The Arrhenius activation energies extracted from our simulations for all the three AQPs agree with the \textit{in vitro} measurements. We observe that AQP4, that is particularly rich in the central nervous system, is more efficient in water conduction and more temperature-sensitive than other water-only channels (excluding glycerol channels that also conduct water when not inhibited by glycerol).

\textsuperscript{1}The authors acknowledge support from the NIH (GM 084834 and GM 060655) and the computing resources provided by the Texas Advanced Computing Center at University of Texas at Austin.