Supporting information for the article: Ion Selectivity of α-Hemolysin with β-Cyclodextrin Adapter: II. Multi-Ion Effects Studied with Grand Canonical Monte Carlo/Brownian Dynamics Simulations. Bernhard Egwolf, Yun Luo, D. Eric Walters, and Benoît Roux.
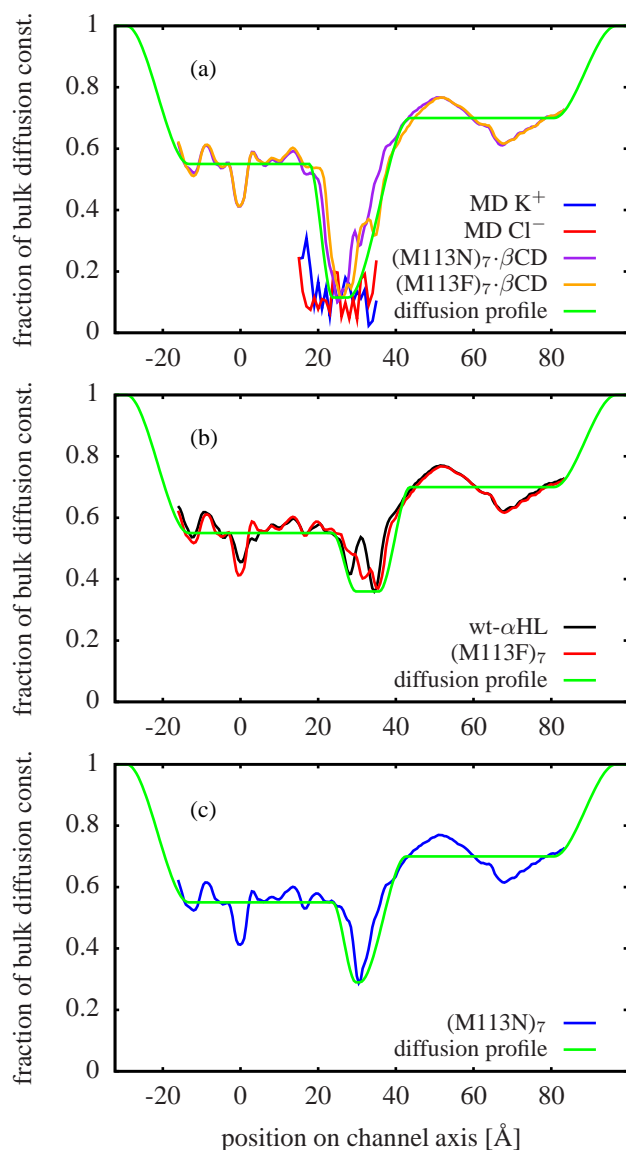

Figure S1: Fraction of the bulk diffusion constant for the different simulation systems. Green lines represent the smooth diffusion profiles used in GCMC/BD simulations. (a) MD simulation results for K^+ and Cl^- in $(M113N)_7 \cdot \beta CD$ as well as profiles for $(M113N)_7 \cdot \beta CD$ and $(M113F)_7 \cdot \beta CD$ calculated by a hydrodynamic approximation. Further diffusion profiles for (b) wt-αHL, $(M113F)_7$, and (c) $(M113N)_7$.