

**Supporting Information for: Potential of mean  
force calculations of solute permeation across  
UT-B and AQP1: A comparison between  
molecular dynamics and 3D-RISM**

Igor Ariz-Extreme and Jochen S. Hub\*

*Institute for Microbiology and Genetics, Georg-August-Universität, Göttingen*

E-mail: [jhub@gwdg.de](mailto:jhub@gwdg.de)

Phone: +49-551-39-14189. Fax: +49-551-39-14082

---

\*To whom correspondence should be addressed

# Additional details on DRISM and 3D-RISM calculations.

**Table S1:** Different closure relations and residual errors (tolerances) used to converge DRISM calculations for different solvents (KH, Kovalenko-Hirata; PSE<sub>n</sub>, partial series expansion of order-n; HNC, hypernetted-chain equation).

DRISM		
Solvent	Closure	Tolerance
water 55.5M	KH, PSE <sub>2</sub> , PSE <sub>3</sub> , HNC	1e-12
water 55.5M + NH <sub>3</sub> 0.5M	KH	1e-12
water 55.5M + urea 0.5M	KH, PSE <sub>2</sub> , PSE <sub>3</sub> , HNC	1e-12, 1e-03, 1e-03, 1e-03
water 55.5M + O <sub>2</sub> 0.5M	KH	1e-12
water 55.5M + Methanol 0.5M	KH	1e-12

**Table S2:** Different closure relations and residual errors (tolerances) used to converge 3D-RISM calculations for all solvent systems.

3D-RISM		
Solvent	Closure	Tolerance
water 55.5M	KH, PSE <sub>2</sub> , PSE <sub>1</sub> /PSE <sub>2</sub> /PSE <sub>3</sub>	1e-05
water 55.5M + NH <sub>3</sub> 0.5M	KH, PSE <sub>1</sub> /PSE <sub>2</sub> , PSE <sub>1</sub> /PSE <sub>2</sub> /PSE <sub>3</sub>	1e-05, 1e-05/6e-03, 1e-05/6e-03/1e-02
water 55.5M + urea 0.5M	KH, PSE <sub>1</sub> /PSE <sub>2</sub>	5e-03, 5e-03/5e-02
water 55.5M + O <sub>2</sub> 0.5M	KH, PSE <sub>1</sub> /PSE <sub>2</sub> , PSE <sub>1</sub> /PSE <sub>2</sub> /PSE <sub>3</sub>	1e-05, 1e-05/1e-05, 1e-05/1e-05/1e-04
water 55.5M + Methanol 0.5M	KH, PSE <sub>1</sub> /PSE <sub>2</sub>	5e-03, 3e-03/1e-02

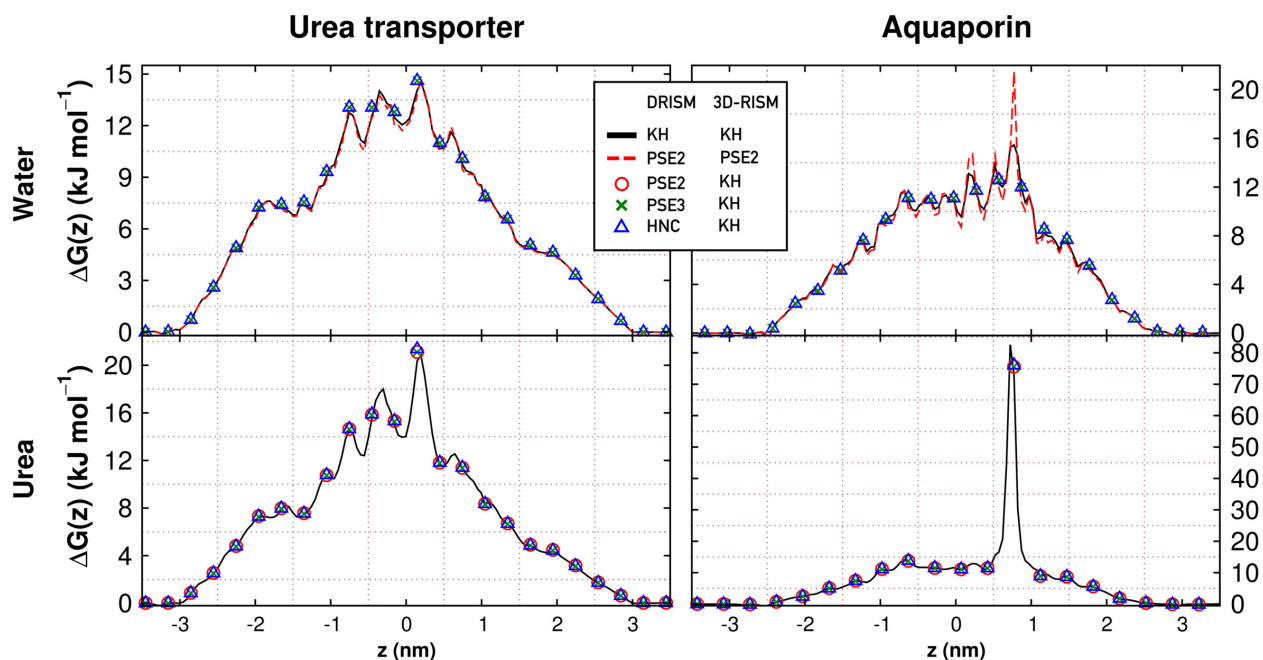


Figure S1: PMFs  $\Delta G(z)$  for water (top row) and urea (bottom row), using various combinations of closure relations during DRISM and 3D-RISM, as indicated in the legend. The closure relation has only a small influence on the PMFs. An exception is the water PMFs in aquaporin based on the PSE<sub>2</sub> closure, exhibiting a spuriously high peak at the ar/R region (top right, red dashed line at  $z \approx 0.7$  nm).

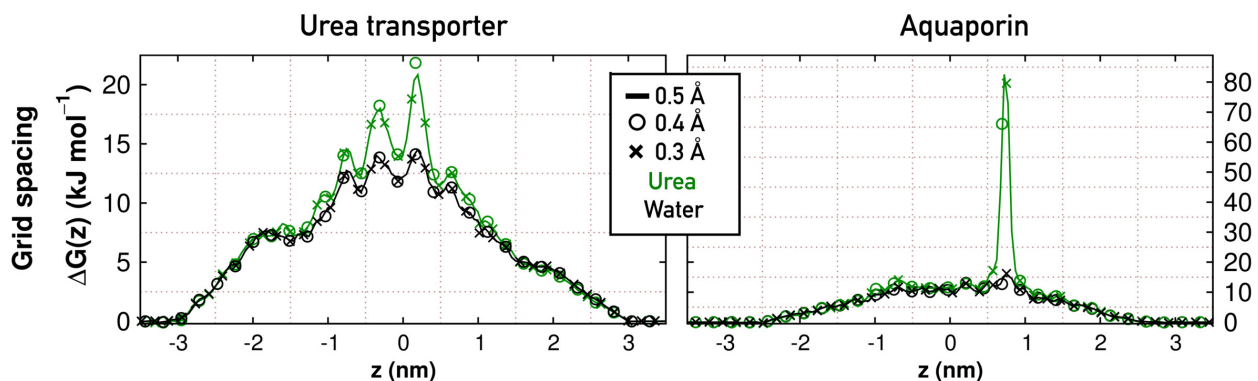


Figure S2: Water and urea PMFs  $\Delta G(z)$  for water (green) and urea (black) calculated with 3D-RISM across UT-B channel (left) and AQP1 (right) using different grid spacings. The grid spacing of 0.5 Å (line), 0.4 Å (circles), and 0.3 Å (crosses) were tested. The PMFs suggest that changing the grid spacing in the range of 0.2 Å to 0.5 Å has only a small effect on the PMFs.

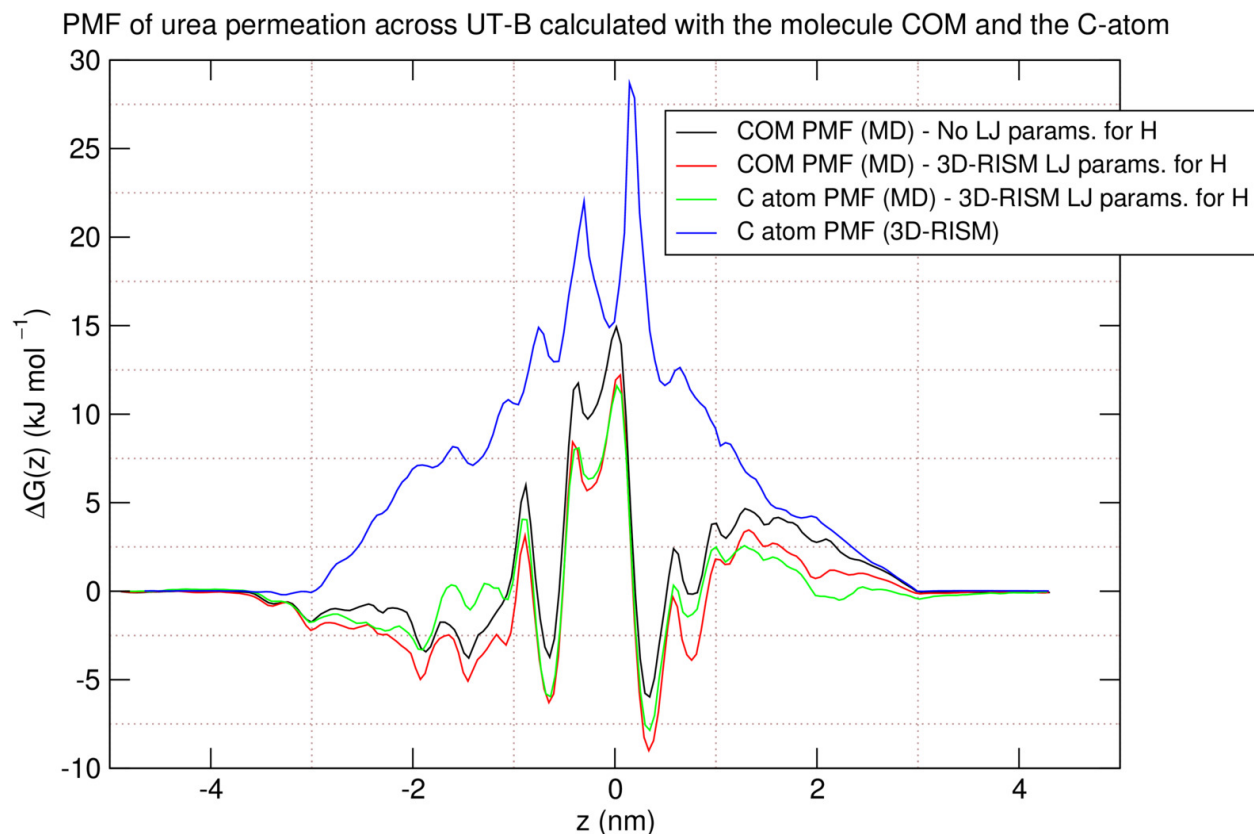


Figure S3: PMFs  $\Delta G(z)$  for urea permeation across UT-B, testing the influence of (i) the Lennard-Jones (LJ) parameters of the urea hydrogen atoms (H-atoms), and (ii) the definition of the reaction coordinate. PMFs were computed from MD simulations without LJ interactions on H-atoms (black curve), or using finite LJ interactions of H-atoms (red curve), as used during 3D-RISM. The similarity between the black and red curves suggests that slightly different topologies (with or without LJ interactions of H-atoms) do not account for the large discrepancies between MD and 3D-RISM (compare 3D-RISM PMF, blue curve). In addition, to exclude that the details of the reaction coordinate would explain the differences between MD and 3D-RISM, the PMF was computed with MD based on the center of mass (COM) of urea (red curve) or based on the position of the urea carbon atom (green curve), as used for 3D-RISM. The similarity between the red and green curves suggest that the different reaction coordinates (urea carbon atom vs. urea COM) do not account for the discrepancies between MD and 3D-RISM.