Transfer of arginine into lipid bilayers is non-additive

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Running Title: Transfer of arginine is non-additive

Online Supporting information

We determined a PMF for arginine partitioning from water into a cyclohexane slab using the CHARMM27 force field (41). We ran the simulations using GROMACS 4 (64). Umbrella sampling was used to determine the PMF with parameters similar to the DOPC PMFs in the main text. Smooth particle mesh Ewald (35) was used for electrostatics with a real space cut-off of 1.2 nm, a sixth order spline and a 0.16 grid spacing. Lennard-Jones interactions were shifted from 1 nm to 1.2 nm. Temperature was maintained using the weak-coupling algorithm at 298 K (31). The x and y box dimensions were kept constant, while the pressure in the z dimension was kept at 1 bar using a weak-coupling algorithm (31).

The PMF using CHARMM and OPLS are nearly identical from water through the interface. The free energy minima at the interface are -12.9 and -12.7 kJ/mol for the OPLS and CHARMM force fields.
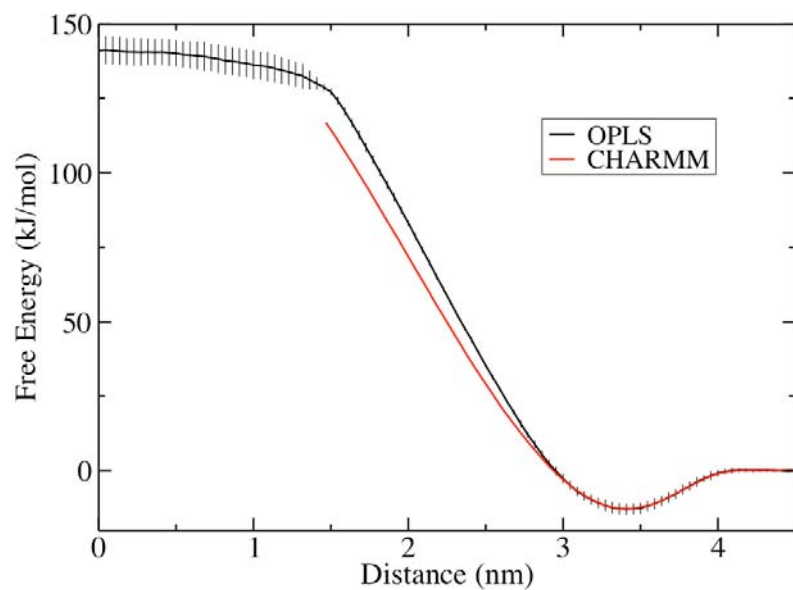
Figure S1: PMFs for moving an arginine side chain from water (x > 4.2) into a cyclohexane slab using the CHARMM and OPLS force field. The two PMFs were set equal to zero at bulk water. For ease of comparison, the CHARMM PMF was shifted so that the minimum was at the same distance as the OPLS PMF (3.4 nm).