Additional file 7

Equilibration of solvent boxes by molecular dynamics simulations

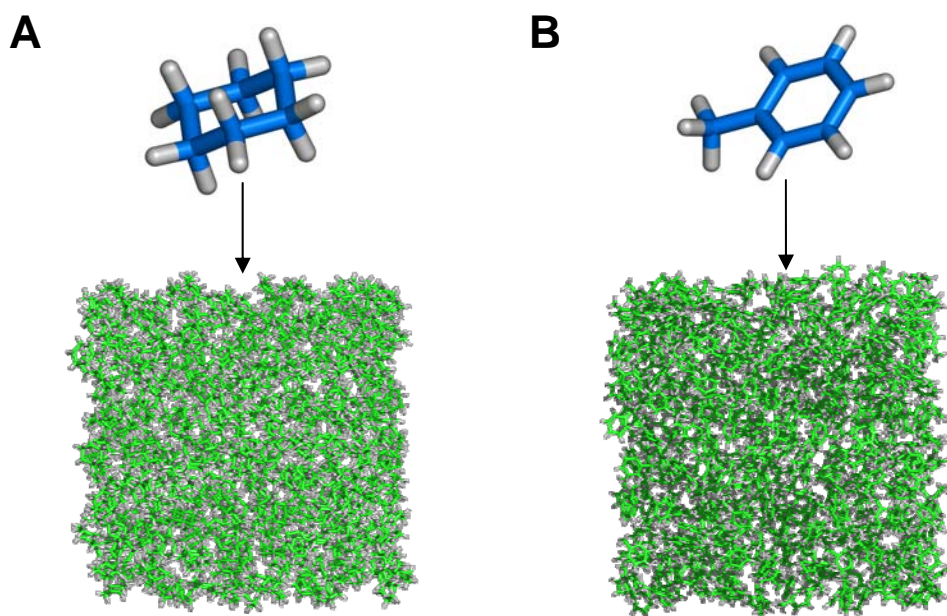**A**   **B**

Figure Solvent molecules (blue) and equilibrated solvent boxes by molecular dynamics simulations (green) of cyclohexane (A) and toluene (B)

Table: Number of solvent molecules in simulated solvent boxes

Solvent	Number of solvent molecules in the box	Edge length of the box after simulation [Å]
Cyclohexane	379	41.1
Isopentane	351	40.7
Toluene	436	46.4

Table: Comparison of the experimental density and the density of parametrized solvent models after simulation. Experimental densities were taken from the product properties at www.sigmaaldrich.com.

Solvent	Density after simulation [g/cm^3]	Experimental density [g/cm^3]
Cyclohexane	0.76	0.78
Isopentane	0.63	0.63
Toluene	0.84	0.86