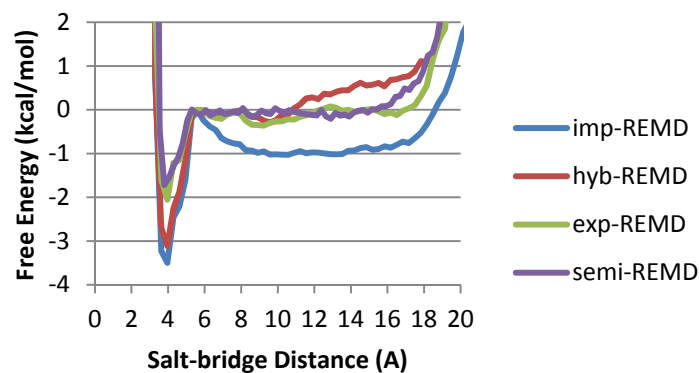
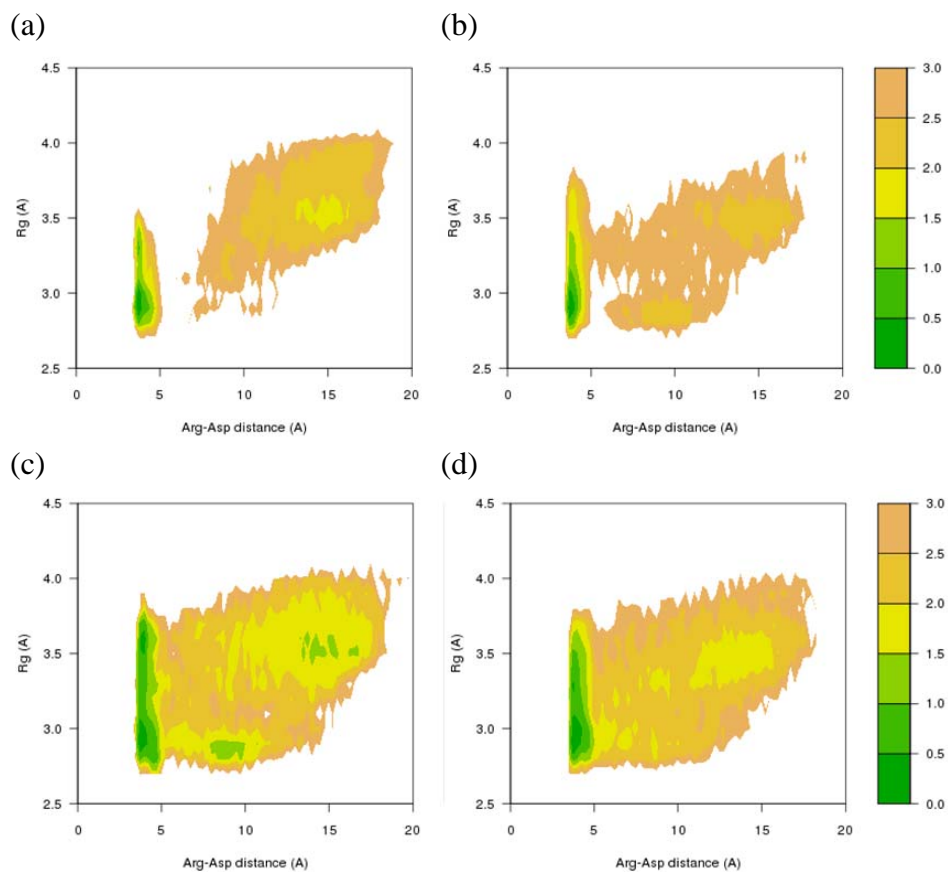


SUPPLEMENTAL FIGURES



Supplemental Figure 1. PMF at 298 K with respect to salt-bridge distance for the implicit, hybrid, explicit methods compared with a ‘semi-hybrid’ approach that includes the 200 nearest water molecules during replica exchanges.



Supplemental Figure 2. 2D PMF at 298 K with respect to salt-bridge distance and radius of gyration for the (a) implicit, (b) hybrid, (c) explicit methods compared with a (d) ‘semi-hybrid’ approach that includes the 200 nearest water molecules during replica exchanges.