

**The intrinsic radius as a key parameter in the generalized Born
model to adjust protein-protein electrostatic interaction
(Supplementary Figure)**

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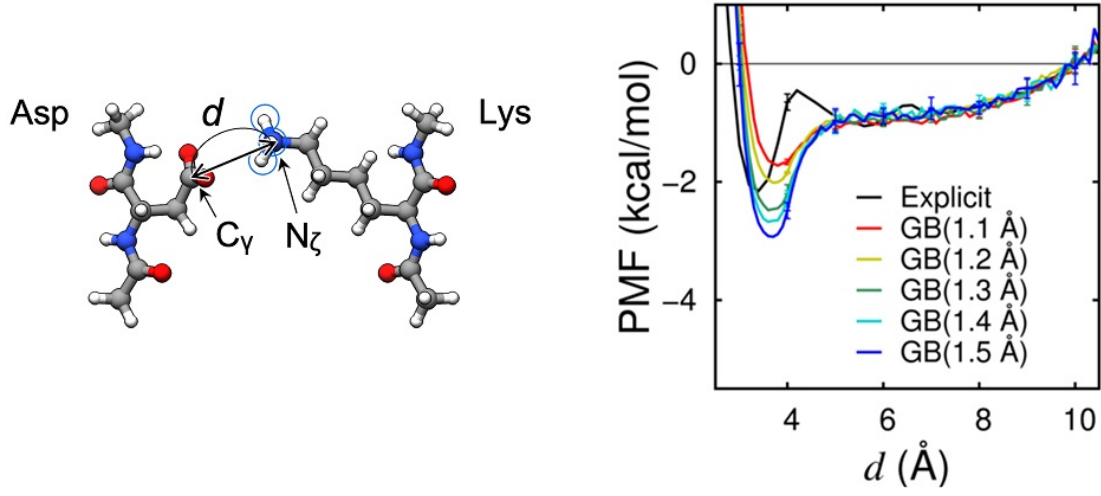


FIG. S1. Effect of ρ_H on Coulomb bond formation in Lys-Asp system. (Left) Illustration of the system. The intrinsic radii of the hydrogen atoms in the ammonium group of Lys (encircled), denoted by ρ_H , were uniformly and systematically changed from 1.1 Å to 1.5 Å. (Right) Potential of mean force (PMF) is shown as a function of d (see left) for the explicit water model (black) and for the GB solvation model at different ρ_H values (1.1 to 1.5 Å). The Lys-Asp system was prepared in the same manner as the Arg-Glu system, with the distance between C_α atoms of Lys and Asp set at 11 Å.