A

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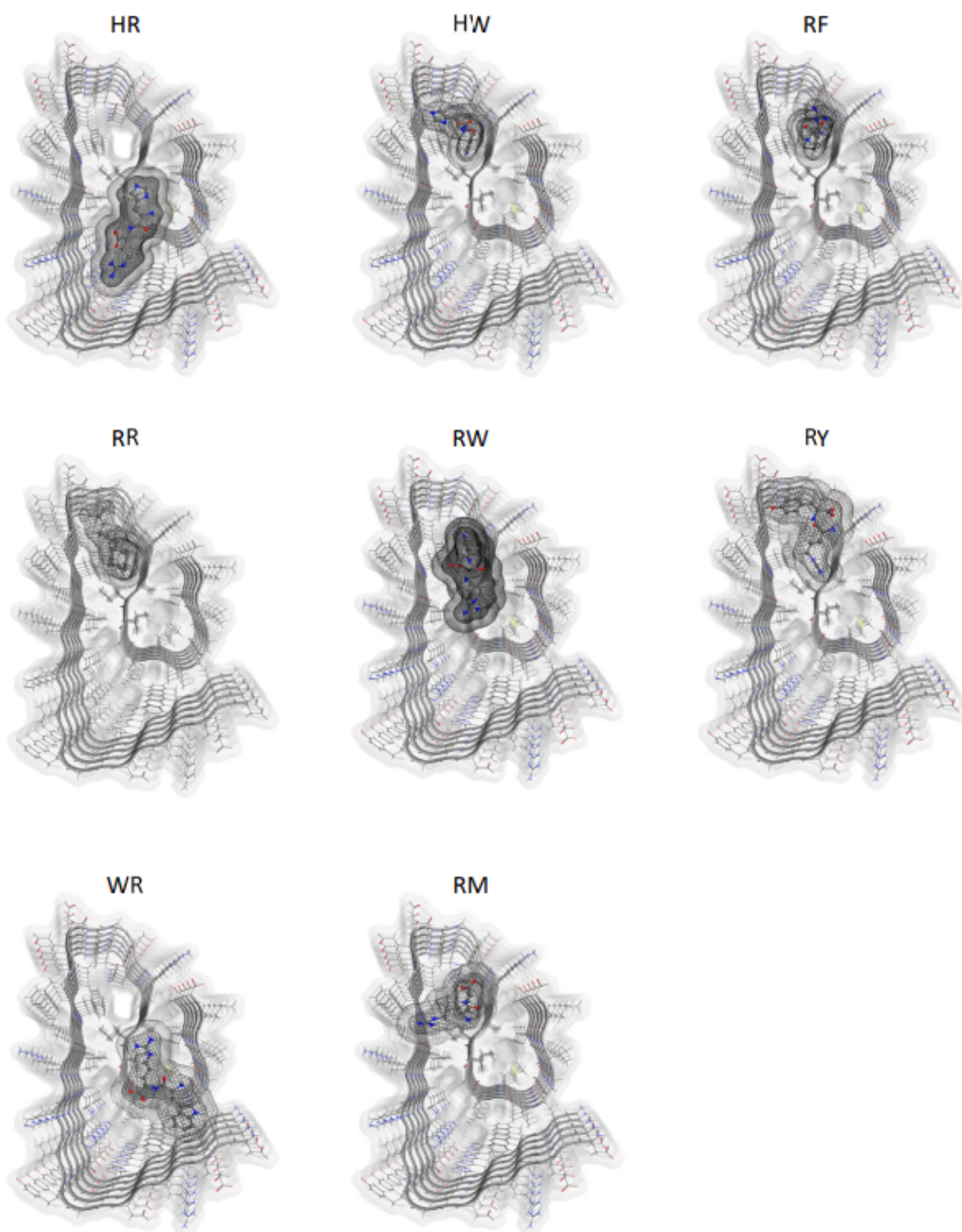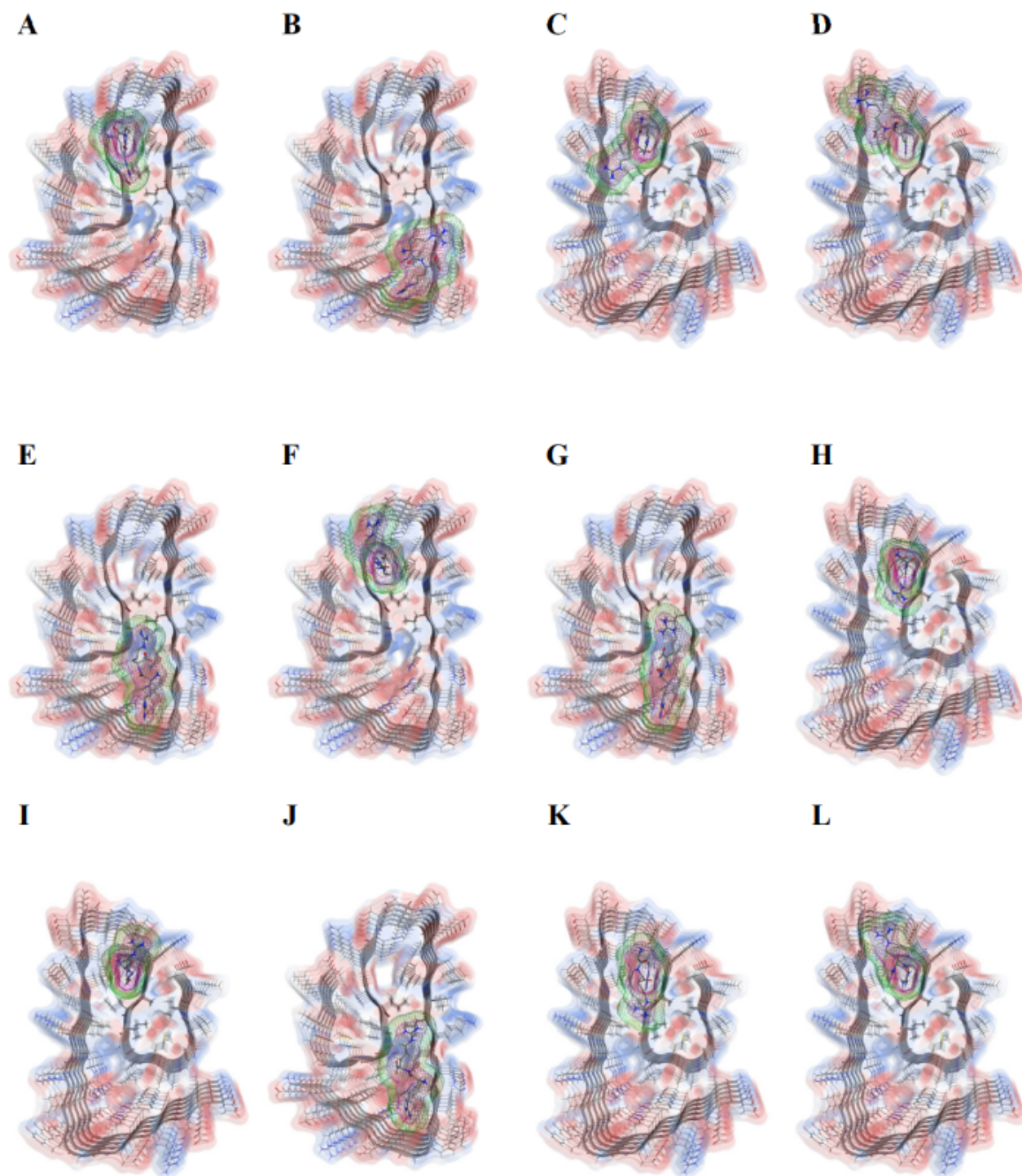
B

C

Supplementary Figure S1. Molecular dynamics analysis of the conformation of $A\beta_{42}$ monomer in dilute sodium chloride solution. **A.** The conformation of $A\beta_{42}$ in 0.1 M sodium chloride solution after 1000 ns simulation by GROMACS using the AMBER99SB force field and TIP3P explicit water model. **B.** Ramachandran plot of dihedral angles of the $A\beta_{42}$ monomer. **C.** Electrostatic distribution on the surface of $A\beta_{42}$ monomer.

Supplementary Figure S2. Docking position of eight dipeptides on Aβ$_{42}$ pentamer. The eight dipeptides bound to Aβ$_{42}$ was screened out by molecular docking. HR: Histidine-arginine; HW: Histidine-tryptophan; RF: Arginine-phenylalanine; RR: Arginine dipeptide; RW: Arginine-tryptophan; RY: Arginine-tyrosine; WR: Tryptophan-Arginine; RM: Arginine-methionine. The molecular surface of dipeptides and the boundary of van der Waal's force were indicated by dark and light grey mesh diagrams.

Supplementary Figure S3. Docking position of arginine dipeptide (RR) on Aβ$_{42}$ pentamer. The conformation of Aβ$_{42}$ pentamer was adapted from the structure (PDB #5oqv) determined by cryo-electron microscopy. **A–L.** Binding sites and conformation of RR on Aβ$_{42}$. The magenta mesh represents molecular surface of RR, and the green mesh represents the boundary of van der Waal's force.