Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

ASSOCIATED CONTENT

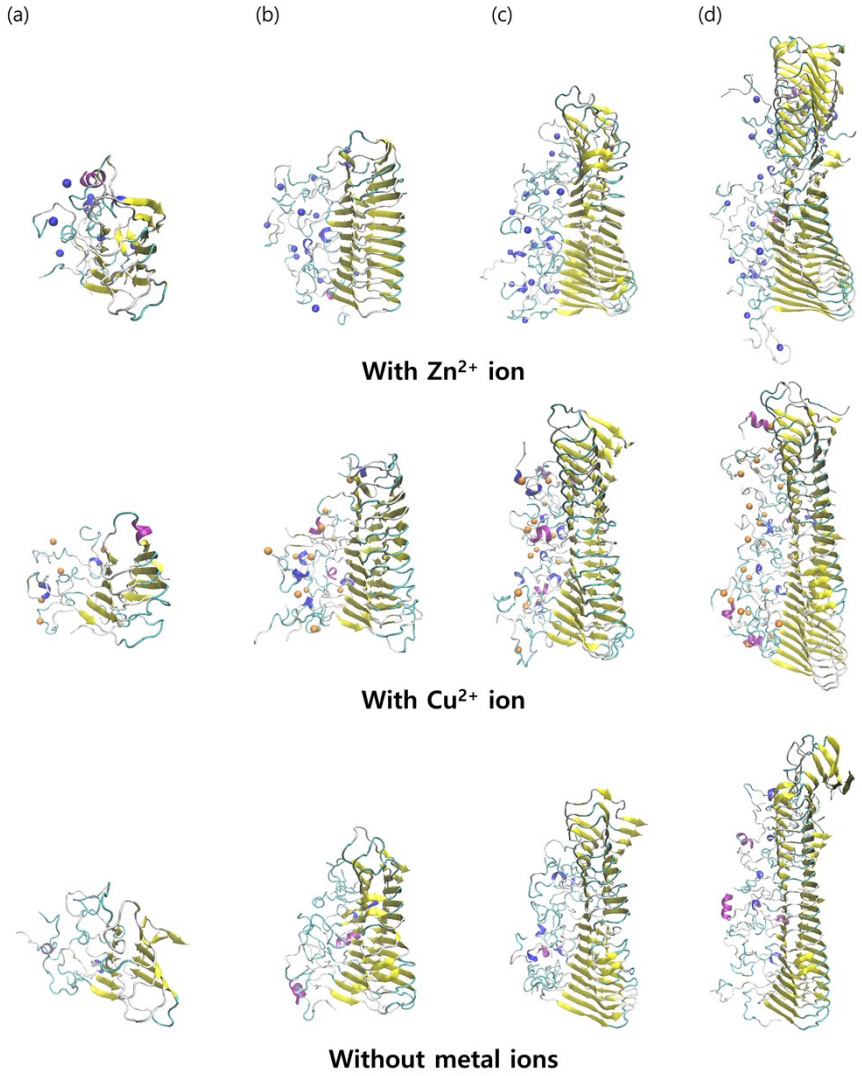


Figure S1. The molecular conformation of $A\beta_{1-42}$ amyloid aggregates with the presence and absence metal ions (i.e. copper and zinc) which are obtained after 100 ns MD simulation. (a) 6 layer of $A\beta_{1-42}$ amyloids with and without metal ion, (b) 12 layer of $A\beta_{1-42}$ amyloids with and without metal ion, (c) 18 layer of $A\beta_{1-42}$ amyloids with and without metal ion, and (d) 24 layer of $A\beta_{1-42}$ amyloids with and without metal ion.

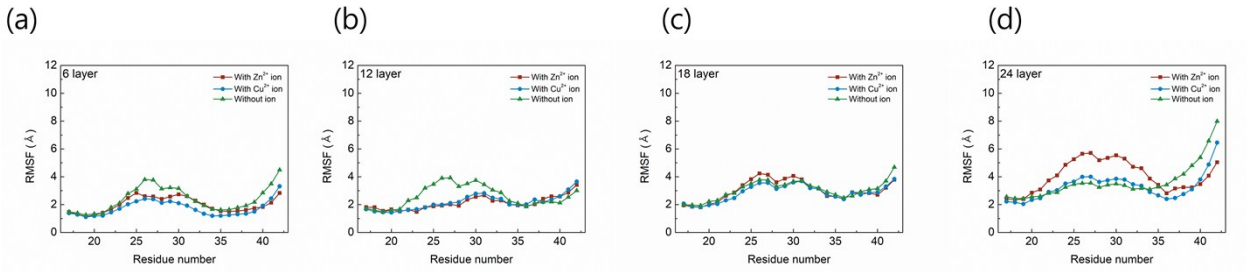


Figure S2. The RMSF analysis of crystalline region of Aβ aggregates with presence and absence of metal ions (i.e. copper and zinc). (a) 6 layer structures of crystalline Aβ aggregates, (b) 12 layer structures of crystalline region of Aβ aggregates, (c) 18 layer structures of crystalline region of Aβ aggregates, and (d) 24 layer structures of crystalline region of Aβ aggregates

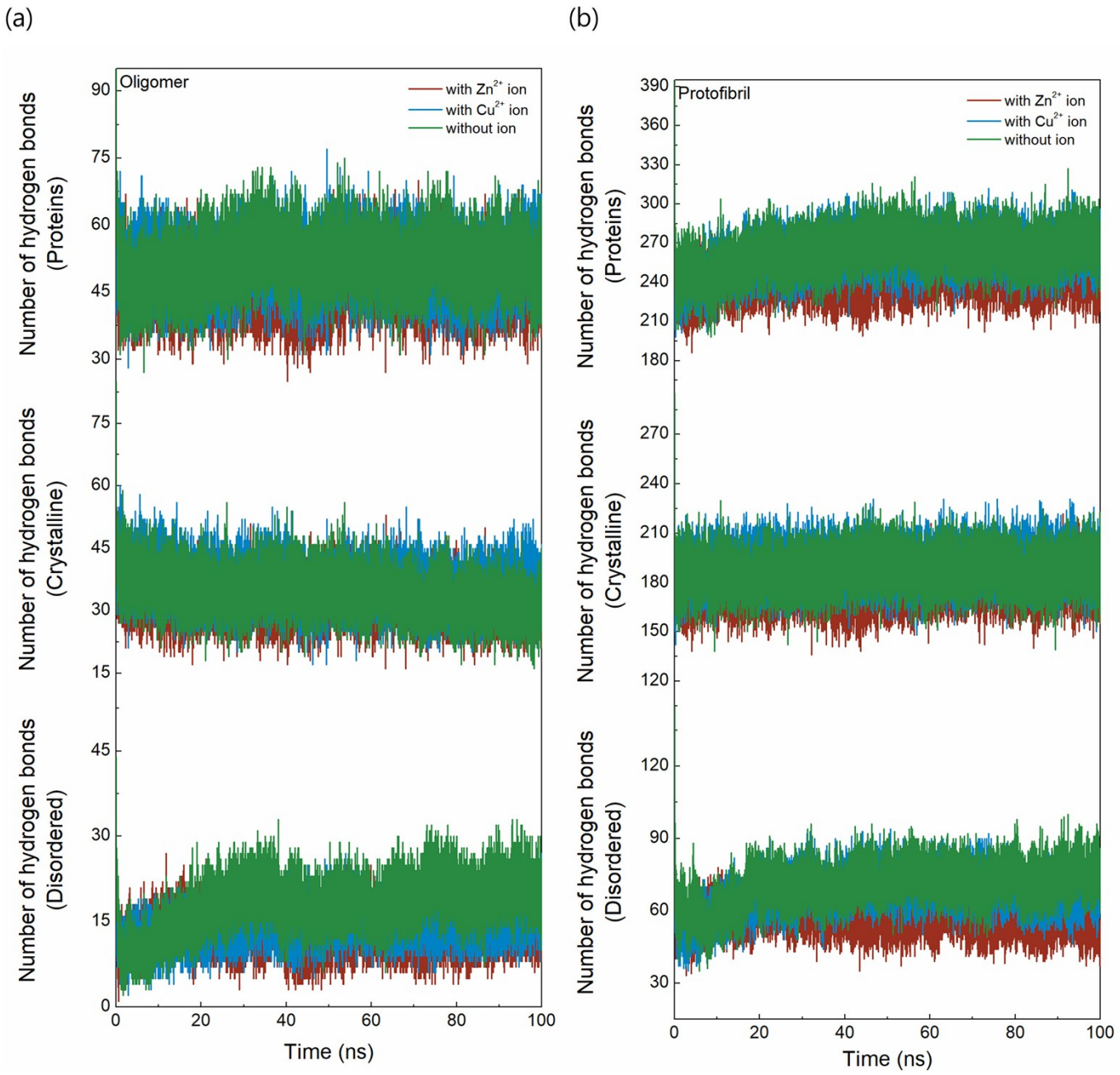


Figure S3. The number of hydrogen bonds of $A\beta_{1-42}$ oligomers with the presence and absence of zinc ions, and (b) the number of hydrogen bonds of $A\beta_{1-42}$ protofibrils with the presence and absence of zinc ions.

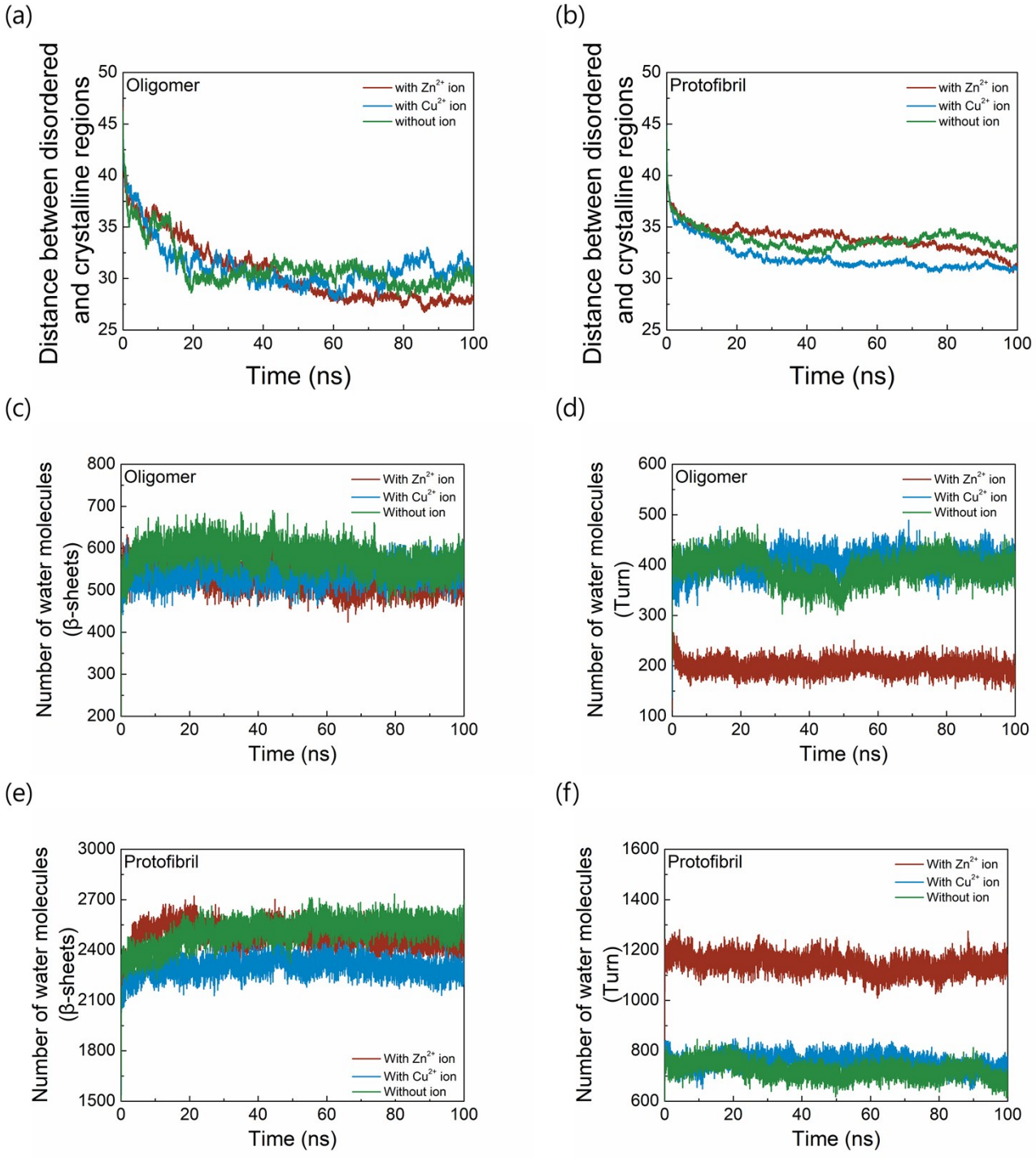


Figure S4. (a) The distance between crystalline and disordered region of Aβ oligomers with presence and absence of metal ions (i.e. zinc and copper) and (b) The distance between crystalline and disordered region of Aβ fibrils with presence and absence of

metal ions. (c) The number of water molecules near turn region at Aβ oligomer with presence and absence of metal ions. (d) The number of water molecules near turn region at Aβ fibrils with presence and absence of metal ions. (e) The number of water molecules near β-sheets region at Aβ oligomer with presence and absence of metal ions. (f) The number of water molecules near β-sheets region at Aβ fibrils with presence and absence of metal ions.

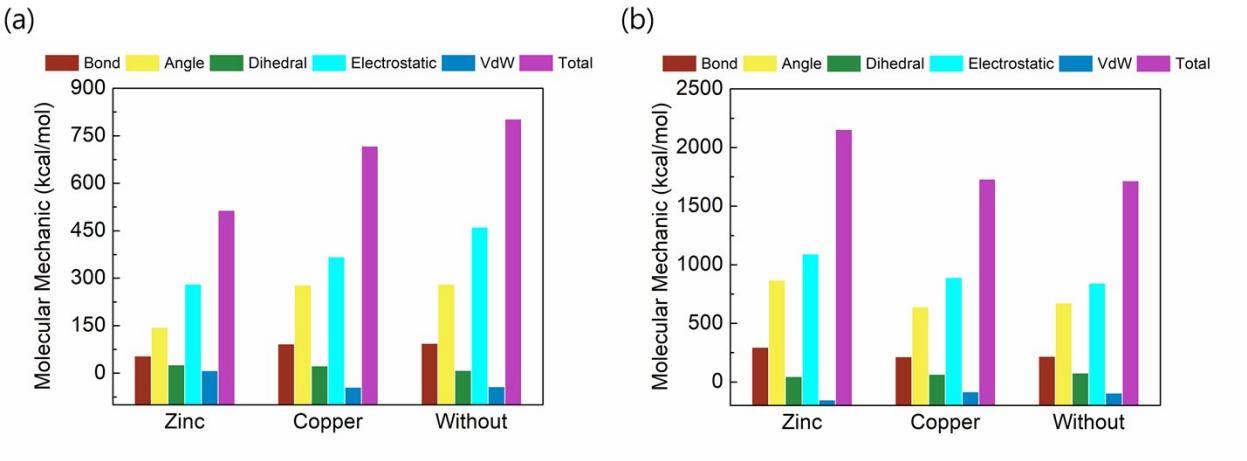
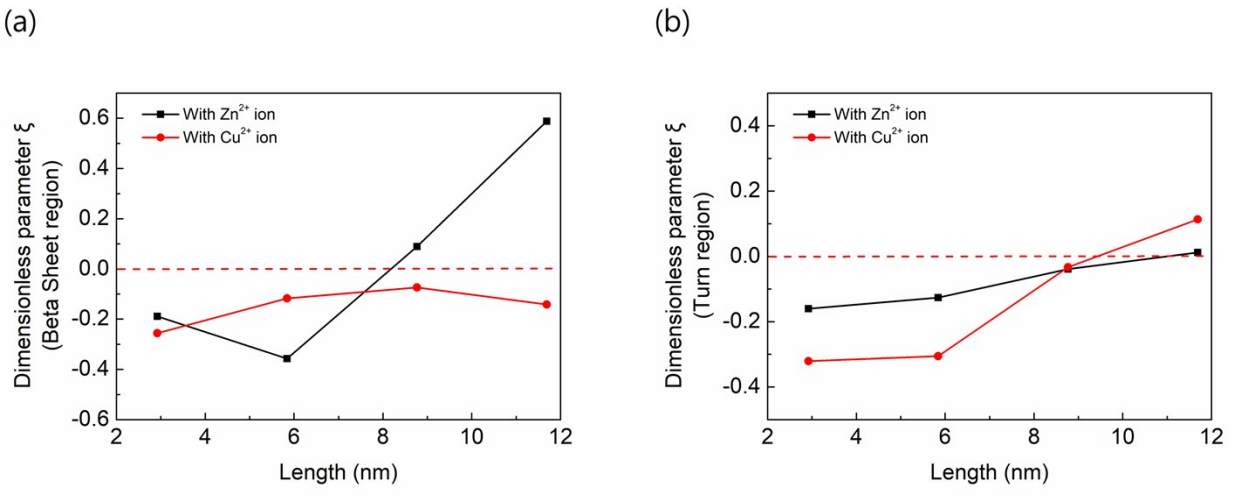


Figure S5. Potential energy analyses near turn regions (including the salt-bridge region) of Aβ aggregates. (a) Components of potential energy for the turn region of Aβ oligomer and (b) Potential energy components for the turn region of Aβ fibril.



Figures S6. Dimensionless parameter of Aβ amyloids based on normalized RMSF. (a) Dimensionless parameter of β-sheet region of the Aβ amyloids with consideration of zinc and copper ions, and (b) dimensionless parameter of turn region of the Aβ amyloids with consideration of zinc and copper ions.