

## Supplementary Materials

### Binding of protofibrillar A $\beta$ trimers to lipid bilayer surface enhances A $\beta$ structural stability and causes membrane thinning

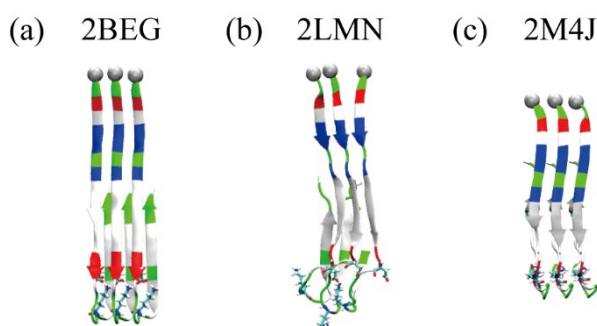
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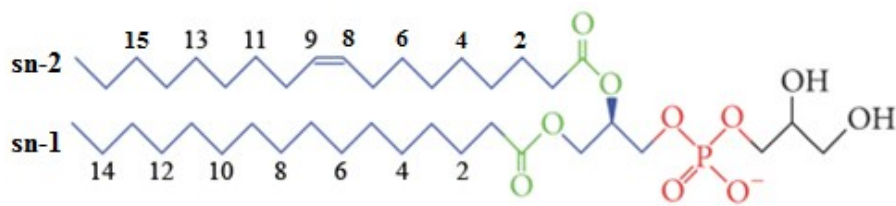
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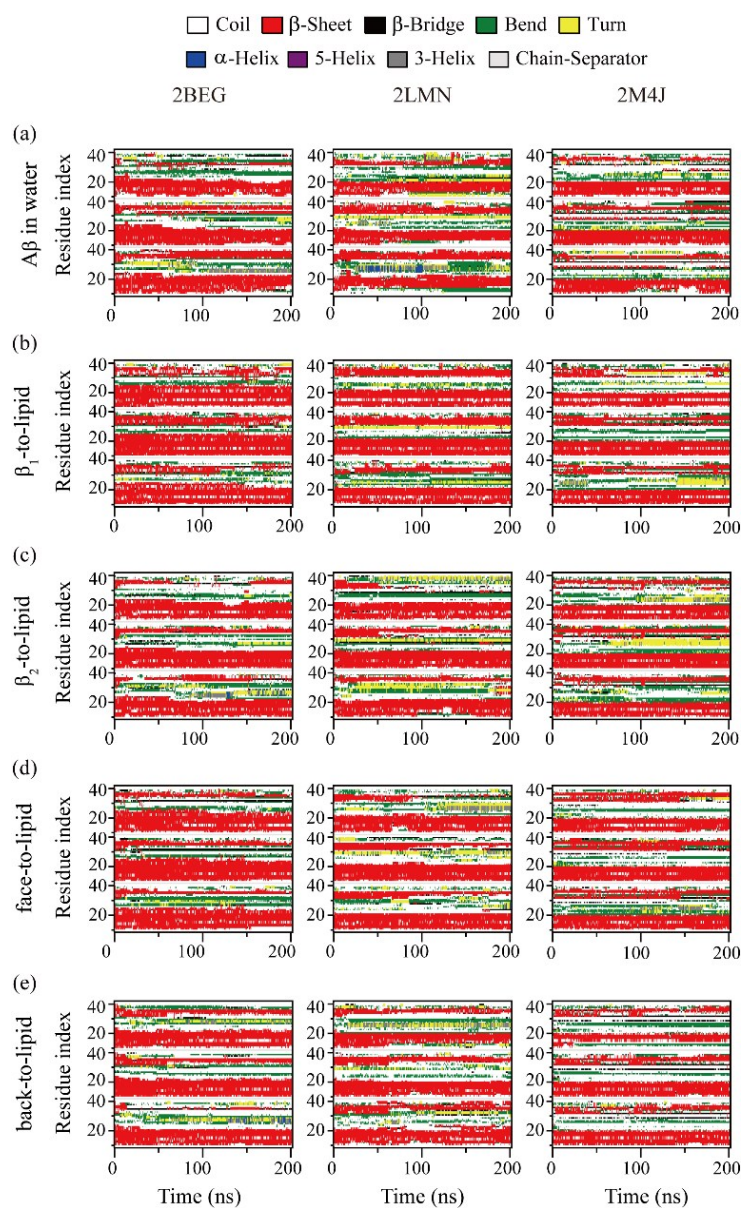
**This material contains five supplementary figures.**



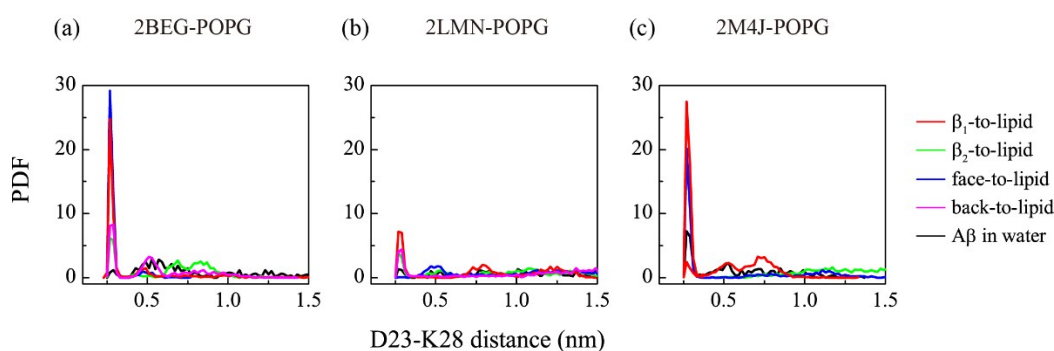
**Fig. S1** Snapshots showing the four surfaces of the three protofibrillar A $\beta$  trimers derived from solid-state NMR fibrils<sup>1-3</sup>: 2BEG (a), 2LMN (b) and 2M4J (c). The surface in the outside of the trimer is  $\beta_1$  surface and the surface in the back represents  $\beta_2$  surface. The surfaces in the right and left of the protofibrillar A $\beta$  trimer represent the face and back surfaces, respectively. It is noted that  $\beta_1$  region and  $\beta_2$  region are staggered. Thus the face surface and the back surface are not symmetric. The A $\beta$  trimer is shown in cartoon representation, with basic residues in blue, acidic residues in red, polar residues in green and non-polar residues in white. The C $\alpha$  atom of each G9 residue is denoted by a silver sphere. D23 and K28 residues are represented in licorice.



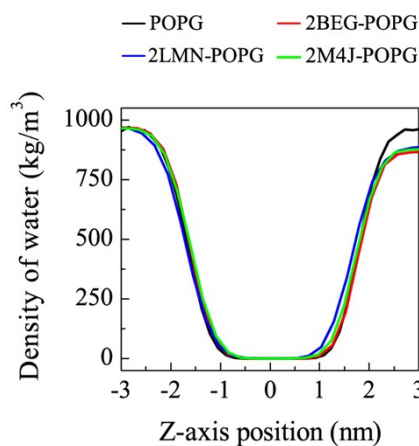
**Fig. S2** Molecular structure of a POPG lipid molecule. Different lipid groups are colored differently: glycerol in black, phosphate group in red, ester group in green, and other carbon atoms in blue. The carbon atoms in the acyl chains (*sn*-1 and *sn*-2) are labelled by numbers.



**Fig. S3** Secondary structure of each residue for  $A\beta_{9-40}$  trimer with and without the POPG bilayer as a function of simulation time.



**Fig. S4** Probability density distribution of the D23 to K28 distance in each MD run for each A $\beta$  and A $\beta$ -POPG systems. The PDF was calculated using the last 50 ns data of each MD run.



**Fig. S5** Density distribution of water molecules in each A $\beta$ -POPG system. For comparison, the water density distribution in a pure POPG bilayer is also given. The z-position of the membrane center is at z=0 nm. The protofibrillar A $\beta$  trimer binds on the upper surface (z = ~1.7 nm) of the POPG bilayer.

## References

1. T. Luhrs, C. Ritter, M. Adrian, D. Riek-Loher, B. Bohrmann, H. Dobeli, D. Schubert and R. Riek, *Proceedings of the National Academy of Sciences of the United States of America*, 2005, **102**, 17342-17347.
2. A. K. Paravastu, R. D. Leapman, W. M. Yau and R. Tycko, *Proceedings of the National Academy of Sciences of the United States of America*, 2008, **105**, 18349-18354.
3. J. X. Lu, W. Qiang, W. M. Yau, C. D. Schwieters, S. C. Meredith and R. Tycko, *Cell*, 2013, **154**, 1257-1268.