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

Supporting Information

Elastic Moduli of Normal and Cancer Cell Membranes Revealed by Molecular Dynamics Simulations

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To see whether the structure of membranes has relaxed to a reasonable state and is stable during the simulation timescale of 1 microsecond, we calculate the time evolution and the histogram distribution of the area per lipid (A_L) of lipids pertaining to the inner and outer leaflets. The results are shown in Figures S1 and S4 for the normal and cancer membrane

models, respectively. As seen, the area per lipid of all membrane models undergoes some fluctuations within the first 400 ns before converging to a stable value. The histogram distribution of the time evolution of area per lipid shows a Gaussian-like shape with the standard deviation of ± 1 Å^2. We note that because our membrane models have the same number of lipids in each leaflet, therefore, the area per lipid for the two leaflets are kind of forced to be the same, and this is reflected by the similar results of the two leaflets shown in Figures S1 and S4.

We also calculate the time evolution and distribution of the membrane thickness, and the results are shown in Figures S3 and S4 for the normal and cancer models, respectively. Again, the membrane thickness fluctuates within the first 400 ns and then converges to a stable value. The histogram distribution shows a Gaussian-like shape with the standard deviation of ± 0.1 nm.

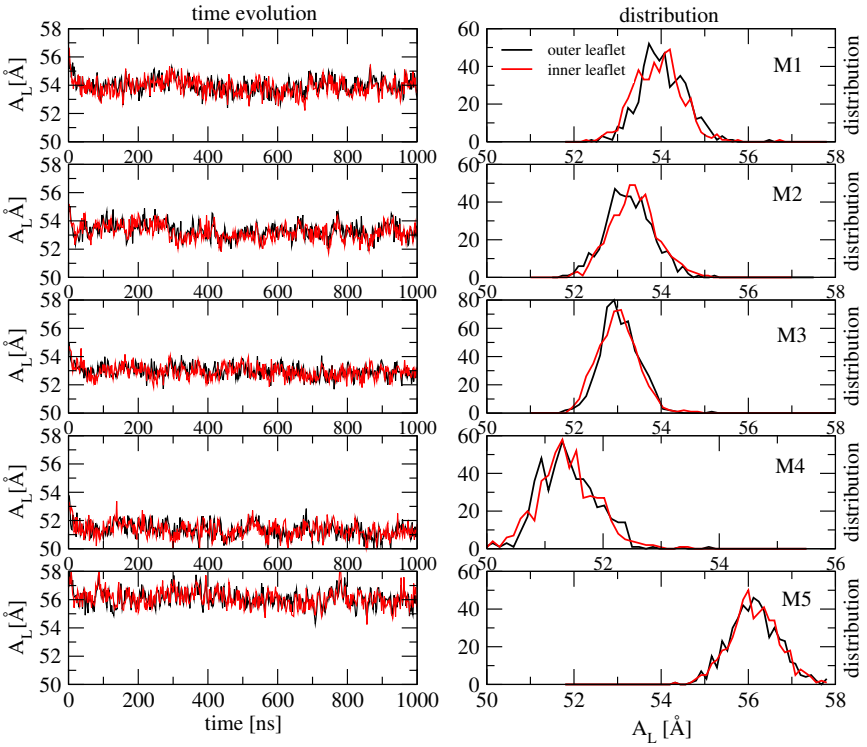

Figure S1: The time evolution (left panels) and distribution (right panels) of the area per lipid of five normal membrane models, M1$\cdots$M5. The area per lipid is shown for the outer and inner leaflets. Shown are results at 300 K.

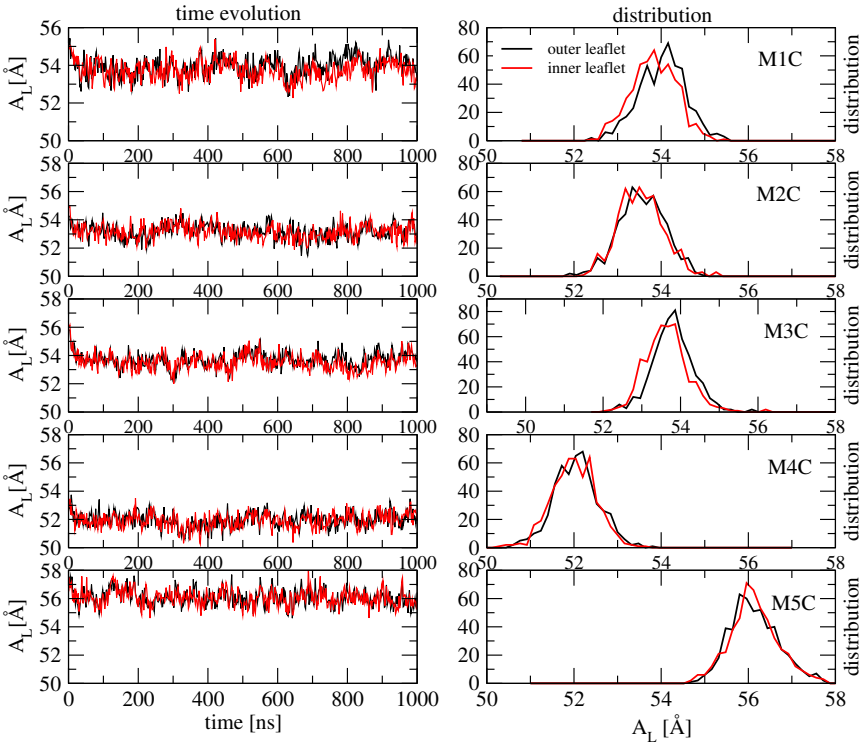

Figure S2: The time evolution (left panels) and distribution (right panels) of the area per lipid of five normal membrane models, M1*$\cdots$M5*. The area per lipid is shown for the outer and inner leaflets. Shown are results at 300 K.

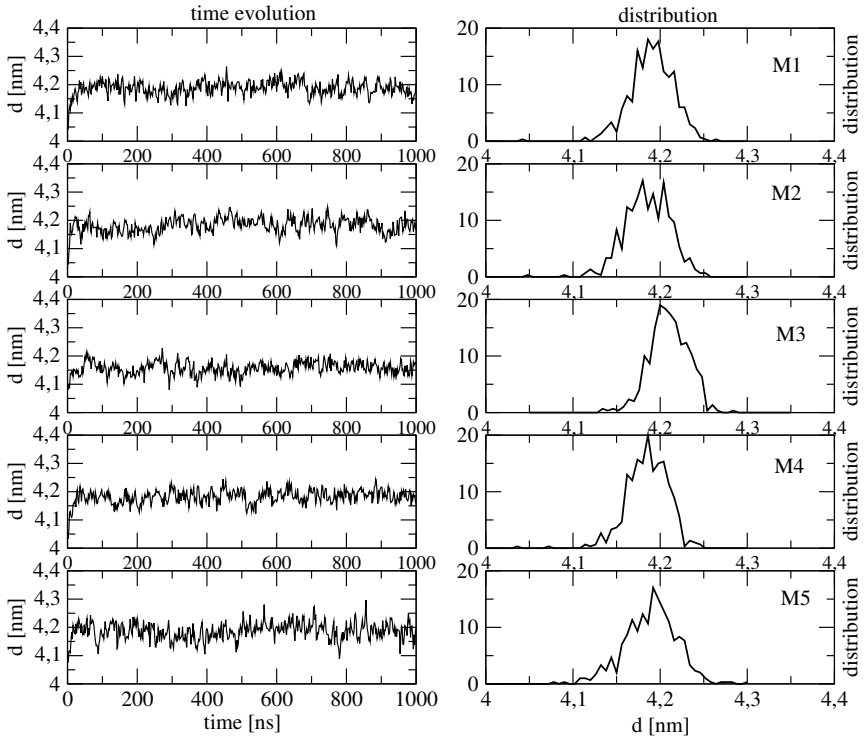

Figure S3: The time evolution (left panels) and distribution (right panels) of the thickness of five normal membrane models, M1$\cdots$M5. Shown are results at 300 K.

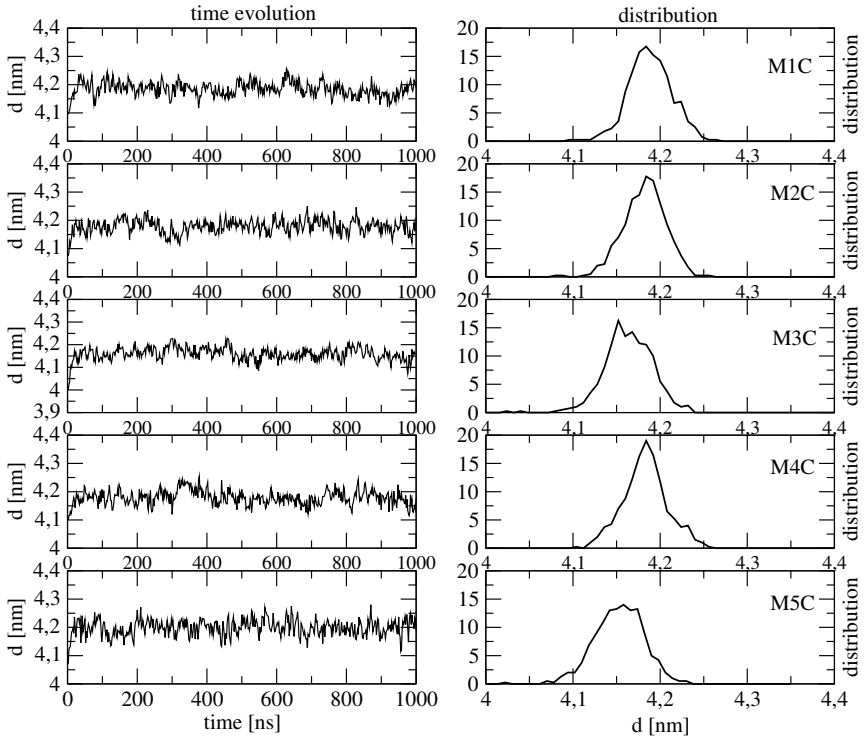

Figure S4: The time evolution (left panels) and distribution (right panels) of the thickness of five cancer membrane models, M1*$\cdots$M5*. Shown are results at 300 K.