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Title: Stability of Liposome: Free Energy Analysis of Vesicle-to-Bicelle Transformation

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A lipid assembly composed of a finite number of lipid molecules can have multiple metastable structures. Using a series of coarse-grained molecular dynamics simulations, we evaluate the free energy barrier for the transformation of a small vesicle to a disk-like structure called a bicelle. This free energy is found to be lower than that predicted from a conventional continuum elastic theory. For small unilamellar vesicles, the relaxation of internal structure of the membrane is suggested to play an important role in lowering the free energy barrier for the vesicle-to-bicelle transformation.