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Molecular Dynamics Modeling of Actin Network Formation

RONALD PANDOLFI, PETER BECICH, UC Merced, LAM NGUYEN, FSU, LINDA HIRST, UC Merced — Actin filaments are ubiquitous and critical in cellular functions. The polymer protein F-actin is a semi-flexible filament that forms networks in the presence of binding proteins (i.e. α -actinin, filamin, fascin). Molecular dynamics modeling and simulation of the formation of these networks has revealed the dependence of network structure on the ratio of G-actin monomers to cross-linkers, cross-linker shape, and filament length. In this study we focus on the effects of filament length on the assembled system. Comparative experimental work informs the accuracy of the modeled systems. Fourier analysis of the simulated networks allows quantitative characterization of the network structure.

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