Structural insight into the UNC-45–myosin complex

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9/12/2014 Micar21

Structural insight into the UNC-45–myosin complex

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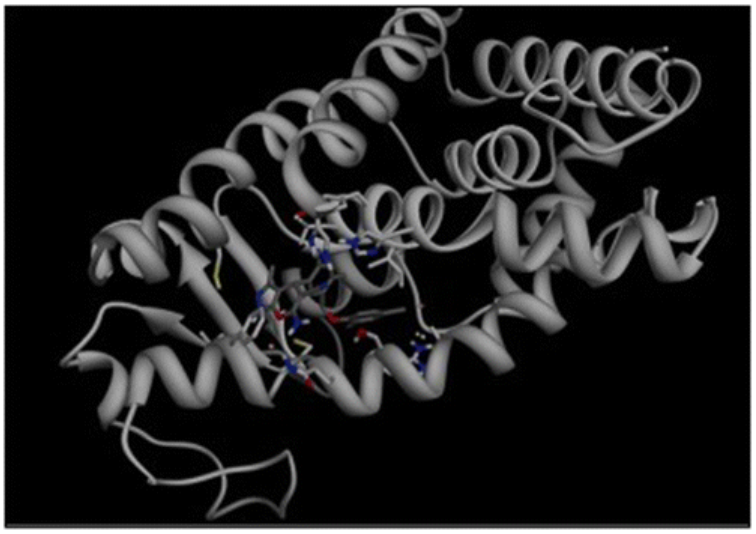
Article first published online: 10 APR 2013
DOI: 10.1002/prot.24270

Abstract



Keywords:
UNC-45;myosin;molecular dynamics;docking;HCM

The UNC-45 chaperone protein interacts with and affects the folding, stability, and the ATPase activity of myosins. It plays a critical role in the cardiomyopathy development and in the breast cancer tumor growth. Here we propose the first structural model of the UNC-45–myosin complex using various in silico methods. Initially, the human UNC-45B binding epitope was identified and the protein was docked to the cardiac myosin (MYH7) motor domain. The final UNC45B–MYH7 structure was obtained by performing of total 630 ns molecular dynamics simulations. The results indicate a complex formation, which is mainly stabilized by electrostatic interactions. Remarkably, the contact surface area is similar to that of the myosin-actin complex. A significant interspecies difference in the myosin binding epitope is observed. Our results reveal the structural basis of MYH7 exons 15–16 hypertrophic cardiomyopathy mutations and provide directions for drug targeting.
Proteins 2013; 81:1212–1221.

Proteins: Structure, Function, and Bioinformatics (Full version)
(http://onlinelibrary.wiley.com/doi/10.1002/prot.24270/abstract;jsessionid=E6E6602579FC1A520437C90E57780756.f04t03)

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