The Applications of 3D Printing Atomic Structures

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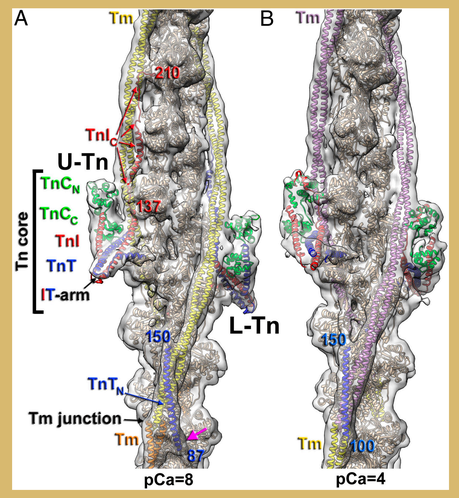
Introduction

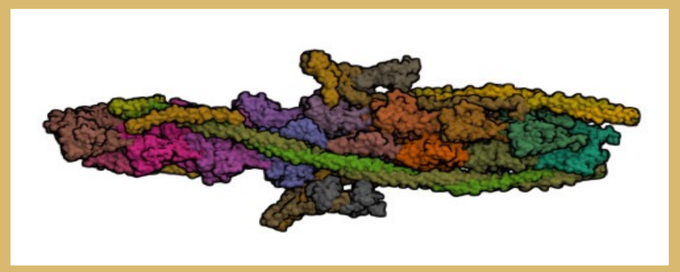
3D printing is a form of manufacturing physical objects from a three-dimensional digital model. ChimeraX is a software used to manipulate and analyze atomic structures and their molecular components. This program allows for the modification of 7KO4, a structure of calcium free cardiac thin filament, 7KO5, calcium bound thin filament, and other high-resolution structures such as 8UWW (troponin), to prepare for 3D printing. Through the EMDB website, these structures were downloaded, modified, and through many iterations, successfully printed. The physical structure of 7K04 can now be used to clarify findings in muscle mechanic laboratories among researchers in the Biology Department

Immediate Goals

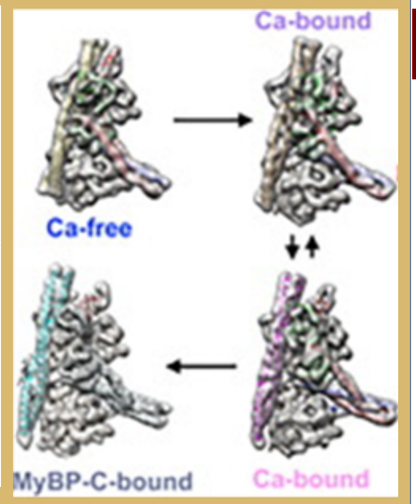
The goal of this project is to bring awareness to the benefits of visual model usage in educational settings as well as for future research purposes through the use of 3D printing.



Figures A and B: The structure of the cardiac native TF at low (pCa = 8) and high (pCa = 4) Ca^{2+} levels. (A) The model of the Ca^{2+}-free TF at pCa = 8 A total of 12 actin subunits (tan) are shown with a pair of Tm cables (yellow) and a pair of Tn complexes composed of TnC N- and C-lobes (green), TnI (red) spanning up from the Tn core over three actin subunits (red arrows), and TnT (blue) with its N terminus (blue arrow) extended to the Tm junction region (black arrow) to make a contact with actin (magenta arrow). The two Tn complexes are not equivalent and are therefore marked as upper (U-Tn) and lower (L-Tn). (B) The model of the Ca^{2+}-bound at pCa = 4. In contrast to A, the TnIC is not locked (6) on the surface of the TF, and TnTN does not make a contact with actin.



7KO4: Structure of cardiac native thin filament at pCa=5.8 having upper and lower troponins in Ca^{2+} free state



Discussion

The 3D prints of 7KO4 and 7KO5 recapitulate the molecular level changes when calcium binds. For instance, Troponin (Tn) shifts Tropomyosin (Tm) away from myosin-binding sites on actin at elevated Ca^{2+} levels to allow formation of force-producing actomyosin cross-bridges. Recently, we have printed cryo-EM of native cTFs converted to PDB files to show that cTF Tn core adopts multiple structural conformations at high and low Ca^{2+} levels and that the two strands are structurally distinct. At high Ca^{2+} levels, cTF is not entirely activated by Ca^{2+} but exists in either partially or fully activated state. Overall, suggestive that allosteric coupling between Tn subunits and Tm is required to control actomyosin interactions. The 3D printing of these structures allowed the hypothesis of TnT-1 crossing all the way over and interacting with the troponin and contributes to future research in this subject.

References