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### Conformational Modeling of PEVK-TITIN

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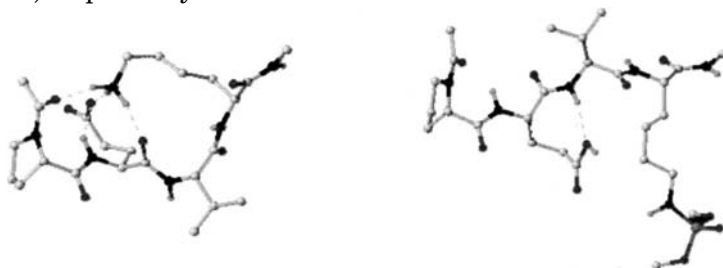
## CONFORMATIONAL MODELING OF PEVK-TITIN

Ming Sun,<sup>a,b</sup> Yan-Mei Li,<sup>a</sup> Bo Tan,<sup>a</sup> Yang Jiang,<sup>a</sup>  
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Titin is a class of elastic protein with a flexible elastic segment of PEVK, proline, glutamate, valine, and lysine.<sup>1</sup> The extension of this PEVK segment is a key event in the elastic response of striated muscle to passive stretch.<sup>2</sup>

The conformational modeling on designed template molecules PEVK and phosphorylated PEVK (PEVK-P) was carried out with the purpose of understanding how the conformation of the peptide was controlled by phosphorylation and de-phosphorylation. Conformational searches were performed with MacroModel<sup>3</sup> version 7.0 on SGI O2 R12000 workstation. MacroModel implementation of AMBER\* force field and GB/SA solvate continuum model were used. The study revealed that the phosphorylation may destroy some hydrogen bonds in PEVK molecule, which could result in the extension of PEVK molecule. Figure 1 shows the molecular structures of typical low energy conformers of PEVK and PEVK-P, respectively.



**FIGURE 1** Molecular structures of typical low energy conformer of PEVK and PEVK-P.

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