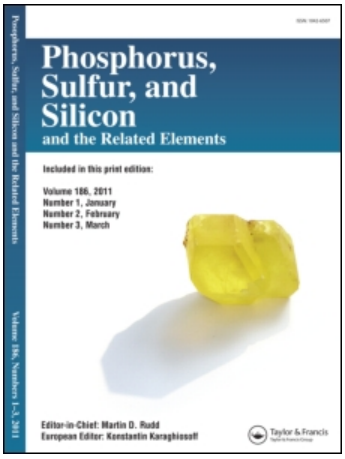

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Conformational Modeling of PEVK-TITIN

Ming Sun[ab]; Yan-Mei Li[a]; Bo Tan[a]; Yang Jiang[a]; Yu-Fen Zhao[a]
[a] Tsinghua University, China [b] Tianjin Normal University, China

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CONFORMATIONAL MODELING OF PEVK-TITIN

Ming Sun,[a,b] *Yan-Mei Li,*[a] *Bo Tan,*[a] *Yang Jiang,*[a] *and Yu-Fen Zhao,*[a]
Tsinghua University, China[a] *and Tianjin Normal University, China*[b]

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Titin is a class of elastic protein with a flexible elastic segment of PEVK, proline, glutamate, valine, and lysine.[1] The extension of this PEVK segment is a key event in the elastic response of striated muscle to passive stretch.[2]

The conformational modeling on designed template molecules PEVK and phosphorylized 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 was performed with MacroModel[3] version 7.0 on SGI O2 R12000 workstation. MacroModeimplementation of AMBER* force filed 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.

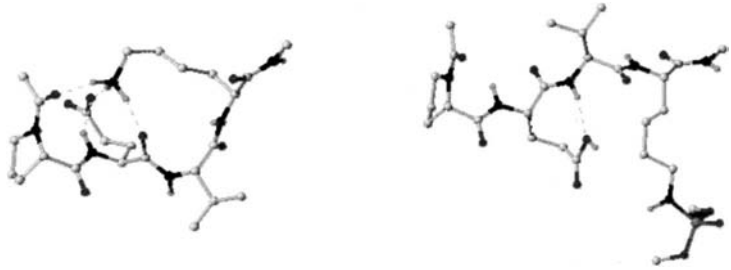

FIGURE 1 Molecular structures of typical low energy conformer of PEVK and PEVK-P.

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Address correspondence to Yu-Fen Zhao, Bioorganic Phosphorus Chemistry Laboratory, Department of Chemistry, School of Life Science and Engineering, Tsinghua University, Beijing 100084, China.

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