## Estimating the Thermal Transition Temperature of the Collagen-Like Peptide By Molecular Dynamic Simulation

Shangzhi Pu<sup>1</sup>, Wenhua Zhang<sup>2\*</sup>

<sup>1</sup>College of Chemistry, Sichuan University, Chengdu 610064 China <sup>2</sup>National Engineering Laboratory for Clean Technology of Leather Manufacture, Sichuan University, 610064 China \*Corresponding author: zhangwh@scu.edu.cn

**Abstract:** Molecular dynamics simulations were carried out to investigate the effect of temperature on the state parameters of a collagen-like peptide with 79 amino acid residues in water. All the simulations were performed using the Consistent Valence Force Field (CVFF) molecular mechanical force field and isothermal-isobaric ensemble (NPT). The temperature dependence of thermodynamic quantities, such as heat capacity ( $C_p$ ), density ( $\rho$ ) and specific volume ( $V_{\text{specific}}$ ), may be obtained by NPT-MD in the temperature range of 280–360 K. These parameters showed a discontinuity at a special temperature in the plot of state parameter versus temperature. The special temperature obtained by MD simulation agrees well with the DSC results (310–314 K) and other theoretical calculated results (312.6 K). The results illustrate the power of current molecular simulation force fields and techniques in establishing the link between thermodynamic quantities and conformational distributions. **Key words:** collagen-like peptide; molecular dynamics simulation; thermal transition