

# **Solvent effect on population distribution of conformers of N-acetyl L-prolyl N'-methyleamide**

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## **ABSTRACT**

Conformational propensities of single amino acids, their contribution to the overall conformation of polypeptides, and effect of solvents on them are important domains of research. The problem is studied by statistical, experimental, and theoretical methods. A theoretical study on the conformations of N-acetyl L-prolyl N'-methyleamide (AceProNMe) as a model system has been carried out in different solvents by QM/MM method in the present work. It is observed that population distribution of conformers is correlated to the polarity function of the solvents. Moreover, the coefficients of correlation equations are correlated with the surface area and volume of the conformers of AceProNMe.

**Key words:** Proline, Conformation, Population distribution, Solvent effect, QM/MM method