

Pressure-Induced Conformational Change of a Dipeptide. A Computational Study

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The effect of pressure on proteins' conformation has been proven many times experimentally. Relevant theoretical modelling, however, is less conclusive. To better understand the role of various parameters involved in the computations, we performed a thorough computational study on the L-alanyl-L-alanine (Ala-Ala) dipeptide.

Using molecular dynamics (MD) and weighted histogram analysis method (WHAM) we carried out a series of simulations of Ala-Ala in H₂O and water/methanol mixtures. Various conditions and force fields were tried. The effect of the pressure on conformer populations within 0–1 GPa is small, but clearly reproducible when statistical fluctuations and MD convergence are treated properly.

At higher pressure, we predict a gradual shift from conformer "A" to conformer "B" (Figure 1). The trend was reproduced with all studied water models. In the future, we plan to verify the predictions using spectroscopic methods (Raman, ROA, VCD) with diamond anvil cell.

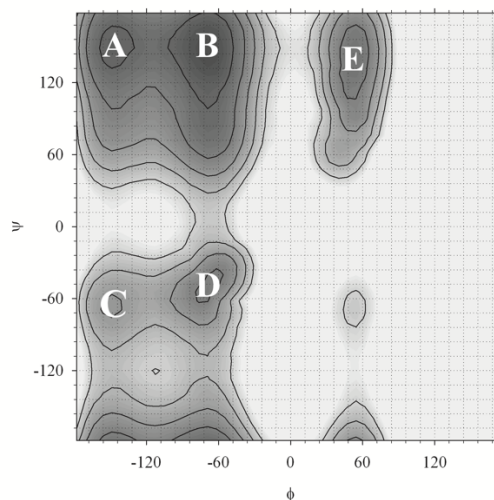


Figure 1. WHAM simulations predict conformational shift from "A" (β) to "B" (PPII).

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