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On the Mechanism of Protein Unfolding by Pressure A Molecular Dynamics Simulation Study J. RAUL GRIGERA[1], ANDRES MCCARTHY , CARLOS FERRARA, IFLYSIB — Proteins are denaturized at high pressure and the mechanism of such a denaturation is still on debate. We have studied lyzozyme and apomyoglobin, under pressure up to 0.3GPa using molecular dynamics simulation. Lysozyme shows more stability, although it cannot retain the native structure. On the other hand apomyoglobin shows a continuing unfolding process during the 180 ns simulation time. The analysis of the hydrophilic and hydrophobic proteins Solvent Accessed Surface clearly shows the increment of the hydrophobic exposed area in the formation of crevices and in the appearing of hydrophobic 'spikes' around the overall surface. The observation of the final state, within the simulation time, shows a clear effect on the conformational state of the proteins. Comparing the behavior of the proteins with de aggregation state of simple non-polar solutes at different pressures we have been able to conclude that the driving force of the denaturation is the change in the hydrophobic contribution to the native folding due to the changes of water structure under pressure, which have been shown both experimental and by computer simulation.

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