

## عنوان مقاله:

A Study on The Effect of Temperature on Human Prion Protein Structure through Molecular Dynamic Simulation

## محل انتشار:

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## خلاصه مقاله:

**Background & Aims:** The normal form of the prion protein is called PrP<sup>C</sup> and its infectious form is called PrP<sup>Sc</sup>. This protein functions like a crystallized core for the transformation of PrP<sup>C</sup> into an abnormal PrP<sup>Sc</sup>. The aim of the present study was to investigate the effect of temperature on human prion protein structure through molecular dynamic simulation. **Methods:** In this research, the GROMACS software was used in Linux operating system for simulation. After performing molecular dynamic simulation, the parameters were extracted from the trajectory and data analysis was performed. The results were entered into an Excel spreadsheet and figures and tables were designed in this software. **Results:** In this study, the effect of temperature and density of sodium chloride on human prion protein stability was studied by molecular dynamics simulation during 10 nanoseconds. The results of this study show that, with 0.1 molar sodium chloride (natural density in tissues), a change in the temperature of environment from 37 (natural temperature of the body) to 27 or 47 leads to structural changes. This can be studied using root mean squared deviation (RMSD) of protein root and structure, radius of gyration of hydrophobic accessible surface, and distances between ionic groups of protein. **Conclusion:** The results of this study show that in 0.1 molar sodium chloride and 37, protein regains its natural structure and an increase or decrease in temperature causes protein to change to an abnormal structure. This can be the cause of the abnormal structure of this protein observed in some illness like mad cow diseases. It is noteworthy that an increase in temperature is more effective in causing this anomaly than a decrease.

## کلمات کلیدی:

Prion protein, Molecular dynamic, GROMACS, RMSD

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