



Damage intensity of Carvacrol on Prostatic cancer cells line Du145 and molecular dynamic simulation of it effect on apoptotic factors

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Abstract : Prostatic cancer is one of the most dangerous diseases in men worldwide. The apoptotic factors such as BID, BIM and APAF1 have a main role in inducing apoptotic pathways. On the other hand, some compounds can active this apoptotic factors. In this study, this notion was investigated by the use of the comet assay technique and molecular dynamics simulations. In the comet assay technique, different concentrations including 130, 230, and 360 μM of Carvacrol were selected according to IC₅₀ using MTT assay on the cell line DU145. Then, alkaline electrophoresis was performed and 100 comet pictures were analyzed using CASP software. Data were analyzed by SPSS statistical software and also using molecular dynamics simulations, wherein protein and Carvacrol were studied, thus avoiding the necessity for quantum mechanical calculations. Molecular dynamics simulations were carried out using with Carvacrol closed in a fully hydrated simulation box with a protein (Bak, Bax, Bim, Apaf1, Bid and P38). The IC₅₀ for Carvacrol was determined at 360 μM by MTT test. Rate of tail to head in alkaline electrophoresis at 130, 230, and 360 μM of Carvacrol concentrations were 13.8 \pm 0.3, 40.6 \pm 0.3, and 47.6 \pm 0.5 percent, respectively. Statistical analysis of the molecular dynamics and calculated potential energy, radius of gyration (Rg), temperature, root mean square fluctuation (RMSF) and root mean square deviation (RMSD) indicated that Carvacrol affected protein which stimulated the apoptosis cascade. Therefore, both experimental and theoretical results demonstrate carvacrol directly affects factors initiating apoptosis.

Keywords: Simulation, Carvacrol, DU145 Cells line, Prostate cancer, Comet assay.