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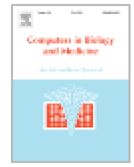

Investigation of the effects of porosity and volume fraction on the atomic behavior of cancer cells and microvascular cells of 3DN5 and 5OTF macromolecular structures during hematogenous metastasis using the molecular dynamics method

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Abstract

Background and objective

The molecular dynamics (MD) simulation is a powerful tool for researching how cancer patients are treated. The efficiency of many factors may be predicted using this approach in great detail and with atomic accuracy.

Methods

The MD simulation method was used to investigate the impact of porosity and the number of cancer cells on the atomic behavior of cancer cells during the hematogenous spread. In order to examine the stability of simulated structures, temperature and potential energy (PE) values are used. To evaluate how cell structure has changed, physical parameters such as gyration radius, interaction force, and interaction energy are also used.

Results

The findings demonstrate that the samples' gyration radius, interaction energy, and interaction force rose from 41.33Å, −551.38kcal/mol, and −207.10kcal/mol Å to 49.49, −535.94kcal/mol, and −190.05kcal/mol Å, respectively, when the porosity grew from 0% to 5%. Also, the interaction energy and force in the samples fell from −551.38kcal/mol and −207.10kcal/mol to −588.03kcal/mol and −237.81kcal/mol Å, and the amount of gyration radius reduced from 41.33 to 37.14Å as the number of cancer cells rose from 1 to 5 molecules. The strength and stability of the simulated samples will improve when the radius of gyration is decreased.

Conclusions

Therefore, high accumulation of cancer cells will make them resistant to atomic collapse. It is expected that the results of this simulation should be used to optimize cancer treatment processes further.