Biology at Work

...a journey through applied life sciences

Symposium Handbook

7th International EMBL PhD Students Symposium
Heidelberg, Germany, 1-3 December 2005

EMBL

P67 - Design of a nanosyninge for the targeted delivery of molecules

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Methods of molecular dynamics were applied to the study of a molecular device able to selectively inject molecules through the cell membrane. This nanosyringe is a nanotube which carries not too big molecules to the membrane. At the next step the nanotube interacts with a receptor site on the membrane in accordance with the molecular tuning of the free end of the nanosyringe. Then the active agent can be shot from the nanosyringe through the membrane structure due to a chemical reaction of the working medium which increases its volume. As a model of the microexplosive agent a set of Van der Waals spheres was taken. The spheres' volumes were growing at a certain rate.
The changes of dynamic properties of the polyalanine appeared to depend on the local environment of the polypeptide chain's ends to a great extent. The uptake of the peptide to the nanotube proved to be energetically favorable and can take place spontaneously. The preceding adsorption on the external side of the nanotube insignificantly destabilized the alpha helix which increased the mobility of alanine residues. The time of self-assembly was estimated as 40 microseconds. Under the shock action the polyalanine's alpha helix greatly changed the conformation and partially denaturated. In the model system the delivery of a compound to the membrane under the action of a nanoexplosion turned out to be possible. The future biomedical implementation of the nanodevice promises a new milestone in molecular therapy.