

# Medicinal Chemistry & Computer Aided Drug Designing

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## Computer simulation of electrostatic micropump

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An electrostatic micro-machined pump is designed and simulated. The designed micropump has the advantages of flow rate controllability, self-priming, small chip size, and low power consumption. The designed micropump is simulated by the Runge-Kutta method. The flow rate of the designed micropump is considered 10  $\mu\text{l}/\text{min}$ , which is quite suitable for drug delivery applications such as chemotherapy. The simulation results for the first membrane deflection with different materials and at pulsed applied voltage are introduced.

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## The role of apolipoprotein E in uptake of tovaquone into the brain in murine acute and reactivated toxoplasmosis

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We investigated whether coating of Atovaquone Nanosuspensions (ANSs) with apolipoprotein E (apoE) peptides improves the uptake of atovaquone into the brain. The passage across the blood-brain barrier (BBB) of ANSs stabilized by polysorbate 80 (Tween 80), poloxamer 184 (P184), or poloxamer 338 (P338) and the same formulations coated with apoE peptides were analyzed *in vitro* and *in vivo*. Passage through a rat co-culture model of the BBB did not differ between individual atovaquone formulations, and the addition of apoE peptides did not enhance the transport. Following the induction of Toxoplasmic Encephalitis (TE) in mice, treatment with all atovaquone formulations reduced the number of parasites and inflammatory foci compared with untreated mice. Uptake of atovaquone into the brain did not depend on coating with apoE. Finally, incubation of apoE peptide-coated ANSs with brain endothelial cells for 30 min did result in the accumulation of nanoparticles on the cell surface but not in their uptake into the cells. In conclusion, ANSs coated with Tween 80 or poloxamers showed therapeutic efficacy in murine toxoplasmosis. ApoE and apoE-derived peptides do not induce the uptake of ANSs into the brain. Alternative mechanisms seem to be in operation, thereby mediating the passage of atovaquone across the BBB.

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