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Pharmacokinetics-Pharmadynamics Model for Nanomedicine Targeted Drug Delivery

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Nanomedicines are the next generation of medicines based on pharmaceutical nanoparticles (NPs). Nanomedicines are used for medical purposes such as diagnosis, monitoring, medical treatment, etc. For better clinical results, they are designed to modify the pharmacokinetics (PK) and pharmacodynamics (PD) of their associated drugs. We present a new graph-based model for PK-PD of NPs-based drugs. The model is based on a population of NPs performing a directed walk on a graph describing the blood vessels and organs, taking into consideration the interactions between the NPs and themselves and with the environment. We define a mechanism to perform different prediction (forward) queries on the proposed model by using analyzed two in vivo experiments with eight different NPs, done on mice. The accuracy and robustness of the proposed model were obtained by comparing the biodistribution of two types of particles (one type consists of six particles distinct from each other by their outer shell, shape, and size in five organs. The second type contains two particles that differ from each other by their core material) in five organs 24 hours after the injection. We obtain a fitting of 0.862±0.01and 0.659±0.12 (mean±SEM), respectively, between the in vivo values and the in-silico results.

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