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Modeling and Simulation for Drug Development

Computational modeling can be used to reveal insights into the mechanisms and potential side effects of a new drug. Here we will focus on two major diseases: diabetes, which affects 1 in 10 people in North America, and hypertension, which affects 1 in 3 adults. For diabetes, we are interested in a class of relatively novel drug treatment, the SGLT2 inhibitors (sodium-glucose co-transporter 2 inhibitors). E.g., Dapagliflozin, Canagliflozin, and Empagliflozin. We conduct simulations to better understand any side effect these drugs may have on our kidneys (which are the targets of SGLT2 inhibitors). Interestingly, these drugs may have both positive and negative side effects. For hypertension, we want to better understand the sex differences in the efficacy of some of the drug treatments. Women generally respond better to ARBs (angiotensin receptor blockers) than ACE inhibitors (angiotensin converting enzyme inhibitors), whereas the opposite is true for men. We have developed the first sex-specific computational model of blood pressure regulation, and applied that model to assess whether the "one-size-fits-all" approach to blood pressure control is appropriate with regards to sex.