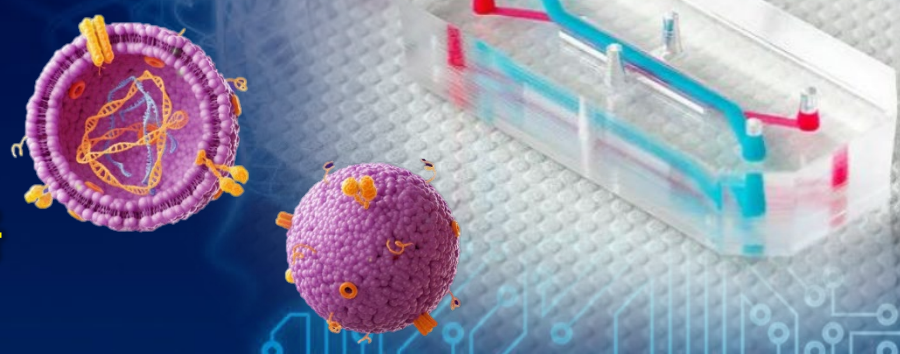
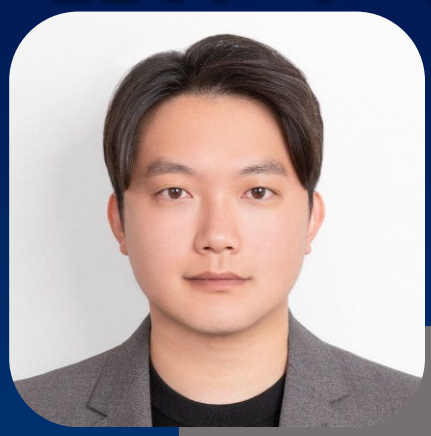
한림대학교

제 136회
ORGAN ON A CHIP
기술교류회

2026. 11. 5 목 오후 4시 30분

한림대학교 의료·바이오융합연구원 포스터홀





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약물 약동학 예측을 위한 AI-디지털트윈-미세생리시스템 개발

AI-Digital Twin Meets MPS: Leveraging Hybrid Approaches for Advanced Drug PK Prediction

Predicting systemic pharmacokinetics (PK) of subcutaneously (SC) administered biologics remains challenging because local drug disposition—matrix binding, cellular uptake, degradation, and lymphatic/vascular absorption—are difficult to capture with existing in vitro models. Here, we present an integrated framework combining a finite-element-based digital twin (DT), an AI surrogate model, and microphysiological systems (MPS) to address this gap. A DT model was computationally built from an anatomically minimal functional unit of the SC space (arteriole, venule, capillary bed, blind-ended lymphatic, and matrix), incorporating reversible matrix binding, first-order decay, and transendothelial flux. To enable rapid parameter exploration, a coefficient-based neural network surrogate was trained on 500 FEM simulations, reproducing four-compartment concentration profiles with high accuracy. Global sensitivity analysis using this surrogate identified degradation rate, vascular permeability, and hydraulic conductivity at the local injection site as the dominant determinants of systemic PK readouts—bioavailability, absorption rate, and half-life, respectively. These predictions were cross-checked against independent on-chip experiments: a Lymphatic Chip confirmed that drainage rate depends on pressure gradient rather than molecular size, consistent with the low sensitivity of lymphatic permeability; a tri-culture SC Matrix Chip showed that cell-mediated matrix remodeling minimally affects binding and diffusion for most tested molecules, consistent with the low sensitivity of binding kinetics; and a Vascularized SC Chip provided experimental vascular permeability values for a subset of therapeutics. Furthermore, when experimental decay rates reported in the literature for small peptides (<10 kDa) and monoclonal antibodies (~150 kDa) were applied to our model in conjunction with the aforementioned values, the predicted bioavailability successfully aligned with human clinical ranges for most of the therapeutic agents. In conclusion, by bridging in vitro MPS with in silico approaches, this hybrid framework could offer a scalable roadmap to transform current paradigms for a broad spectrum of biologic drugs.

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