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Dr. Kaushik Chakravarty, PhD, is the Head of Translational Sciences, and works specifically in the areas of preclinical data translatability, relevant endpoints, and exhaustive review of preclinical models. His research and development experience encompasses metabolic disease, physiology, *in vivo* pharmacology and translational science. He has extensive experience working with small molecule and antisense compounds. He has been in the drug discovery space for 15+ years with one of his antisense compounds completing Phase II clinical trials recently. Prior to VeriSIM Life, Chakravarty lead teams at Pfizer, Roshe, and NASA.

Co-Authored Publications:

Maksim Khotimchenko, Victor Antontsev, Kaushik Chakravarty, Hypatia Hou, Jyotika Varshney (2021). In silico simulation of the systemic drug exposure following 2 the topical application of opioid analgesics in patients with cutaneous lesions (2021). Pharmaceutics.

Kaushik Chakravarty, Victor Antontsev, Yogesh Bunday, Jyotika Varshney. Driving success in personalized medicine through AI-enabled computational modeling. (2021). Drug Discovery Today.

Chakravarty, Kaushik and Antontsev, Victor G. and Khotimchenko, Maksim and Gupta, Nilesh and Jagarpu, Aditya and Bunday, Yogesh and Hou, Hypatia and Maharao, Neha and Varshney, Jyotika (2021). Accelerated Repurposing and Drug Development of Pulmonary Hypertension Therapies for COVID-19 Treatment Using an AI-Integrated Biosimulation Platform (2021). iScience.

Daniel M. Walden, Yogesh Bunday, Aditya Jagarapu, Victor Antontsev, Kaushik Chakravarty and Jyotika Varshney. Molecular Simulation and Statistical Learning Methods to-wards Predicting Drug–Polymer Amorphous Solid Dispersion Miscibility, Stability, and Formulation Design. (2021). *Molecules* 2021, 26, 182.

San-Huei Lai Polo, Amanda M. Saravia-Butler, Valery Boyko, Marie T. Dinh, Yi-Chun Chen, Homer Fogle, Sigrid S. Reinsch, Shayoni Ray, Kaushik Chakravarty, Oana Marcu, Rick B. Chen, Sylvain V. Costes, Jonathan M. Galazka (2020). RNAseq analysis of rodent spaceflight experiments is confounded by sample collection techniques (2020). *iScience*. 23: 12, 101733

Behesti Afshin*, Chakravarty Kaushik*, Fogle Homer, et al. Multi-omics analysis of multiple missions to space reveal a theme of lipid dysregulation in mouse liver. *Nature Scientific Reports*, 9, 19195 (2019) (* indicates equal contribution)

ABSTRACT

“A novel AI/ML-driven In silico simulation of the opioid drug transdermal absorption in normal skin and cutaneous lesions”

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Transdermal drug delivery is gaining popularity in the healthcare industry, as an alternative to traditional routes of administration because of its painless and noninvasive nature and reduced systemic exposure to drug compounds. Clinical investigations of transdermal drug formulations, especially in patients with skin lesions, are often hindered due to the patient intolerance, high cost of the studies, and ethical aspects. In the present work, we used the “BIOiSIM” model, an artificial intelligence (AI)-integrated biosimulation platform, to generate a “digital skin” approach, for prediction of the transdermal disposition of opioid analgesics. Opioids are commonly used in treating severe pain and it is frequently associated with putative adverse effects. Topical applications of opioids were shown to have high efficacy with a favorable safety profile in clinical settings. With the use of the “BIOiSIM” model, we successfully predicted systemic exposure and drug skin accumulation following the topical application of central opioid agonist buprenorphine and peripheral agonist oxycodone in healthy human subjects with simulation of intra-skin exposure in subjects with skin lesions. Predicted skin concentrations and plasma levels of analgesics were used to evaluate the safety of the therapeutic pain control in patients with the dermal structural impairments caused by acute or chronic cutaneous lesions with topical opioid analgesics.