# A U S H A N G

---

# FREIE UNIVERSITÄT BERLIN
**Fachbereich Mathematik und Informatik**

Promotionsbüro, Arnimallee 14, 14195 Berlin

# D I S P U T A T I O N

---

## Dienstag, 9. Juli 2024, 10:00 Uhr

### Ort: Seminarraum 120
**(Fachbereich Mathematik und Informatik, Arnimallee 3, 14195 Berlin)**

**Disputation über die Doktorarbeit von**

## Jan-Louis Mönning

**Thema der Dissertation:**
## Physiologically-based toxicokinetic modelling of lipophilic contaminants and plant secondary metabolites in dairy cows, calves and pigs

**Thema der Disputation:**
## In silico prediction of volume of distribution using machine learning approaches

Die Arbeit wurde unter der Betreuung von **Prof. Dr. M. von Kleist** durchgeführt.

---

Abstract: Accurately predicting the tissue distribution of substances is essential to understanding their behaviour in biological systems. This knowledge is critical in fields like drug development, where it informs decisions about pharmacokinetics, therapeutic efficacy and potential toxicity; in the field of food safety, where it helps understand the accumulation of contaminants in edible tissues and excreta; and in environmental science, where it aids in understanding bioaccumulation in ecosystems. One commonly used parameter to describe the distribution of substances within an organism is the volume of distribution, which describes the theoretical amount of blood plasma needed to account for the total amount of substance in the rest of the body given its concentration in plasma. Besides several in vivo and in vitro methods developed over the years, some in silico methods have also been developed to predict such parameters. These in silico methods require only limited and more easily derivable experimental data for their prediction by extrapolating from existing data or using mechanistic equations describing mass transfer processes. This can reduce the need for in vitro and, especially, in vivo studies, thus saving time, money and reducing animal suffering. In recent years, much effort has been spent into the development of machine learning approaches for predicting the volume of distribution; machine learning is a more data-driven approach that does not require as much knowledge of the mechanistic behaviour as traditional in silico methods. Machine learning approaches utilize a range of algorithms, ranging from well-known ones such as random forest or support vector machine approaches to more novel algorithm based on a neural network architecture. In the presentation, an overview of the recent advancements in these machine learning approaches for predicting the volume of distribution will be provided.

---

Die Disputation besteht aus dem o. g. Vortrag, danach der Vorstellung der Dissertation einschließlich jeweils anschließenden Aussprachen.

## Interessierte werden hiermit herzlich eingeladen

Der Vorsitzende der Promotionskommission
Prof. Dr. M. von Kleist