

## **2nd Nordic POP Workshop on Pharmaceutical Modelling and Simulation Co-organized with the Swedish Drug Delivery Center (SweDeliver)**

**November 30-December 01, 2023  
Department of Pharmacy, Uppsala University**

### **Preliminary Schedule**

#### **Day 1:**

8.30 - 11.45: Welcome, followed by invited talks on the use of molecular modeling and simulation in different stages of drug discovery, development and delivery processes

#### **Invited Speakers:**

##### **Jens Carlsson**

Department of Cell and Molecular Biology, Uppsala University

##### **Marie Skepö**

Department of Chemistry, Lund University

##### **Vasanthanathan Poongavanam**

Department of Chemistry, Uppsala University

##### **Xuezhi Zhuo**

Department of Pharmacy, University of Copenhagen

13.00 - 16.30: Workshop on Nanoparticle – bilayer interactions

Brief Description: Here we use computer simulations to explore the aggregation of nanoparticles, specifically fullerenes, their translocation through a model lipid membrane, and the effect of nanoparticle concentration on membrane properties. We will also analyze the free energy associated with nanoparticle transport processes.

#### **Day 2:**

8.30 – 12.00: Workshop on Therapeutic peptide aggregation

Brief Description: Aggregation of peptides can hinder its therapeutic efficacy and slight changes in amino acid sequence can impact aggregation tendency. We will thoroughly explore how modeling and simulation can be used to study the aggregation of therapeutic peptides. Using a range of analysis methods, different ways to analyze molecular dynamics trajectories will be illustrated.

**Registration:** Please follow the link to register: <https://doit.medfarm.uu.se/bin/kurt3/kurt/96542>

**Deadline:** The deadline for registration is – October 31, 2023

#### **Organizing Committee:**

Shakhawath Hossain, Aleksei Kabedev, Per Larsson and Christel Bergström,  
Department of Pharmacy, Uppsala University, Sweden

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