



Swiss Institute of  
Bioinformatics

**bios<sup>+</sup>** Bellinzona  
Institutes  
of Science



IOR  
An institute  
affiliated to USI

# Computational platforms and nanomedicine

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COST ACTION CA 17140 – NANO2CLINIC

Working group 3 workshop

**Preclinical Development of Cancer Nanomedicines: State of the Art and Future Perspectives**

March 24-25<sup>th</sup> 2022, Institute of Oncology Research-IOR, Bellinzona, CH



COST ACTION CA 17140  
**NANO2CLINIC**  
CANCER NANOMEDICINE - FROM THE  
BENCH TO THE BEDSIDE

 **cost**  
EUROPEAN COOPERATION  
IN SCIENCE & TECHNOLOGY



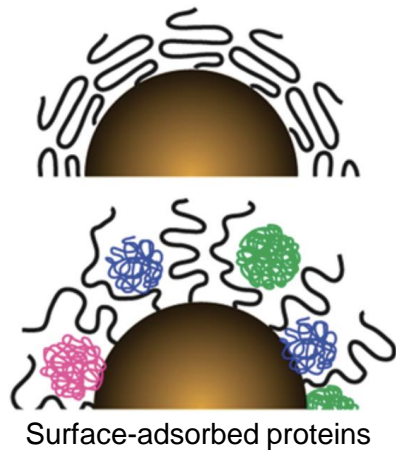
Funded by  
the European Union

# Supervised Learning and Mass Spectrometry Predicts the *in vivo* Fate of Nanomaterials

James Lazarovits, Shrey Sindhwani, Anthony J. Tavares, Yuwei Zhang, Fayi Song, Julie Audet, Jonathan R. Krieger, Abdullah Muhammad Syed, Benjamin Stordy, and Warren C. W. Chan

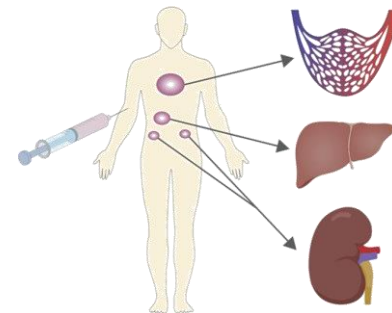
*ACS Nano* **2019** 13(7), 8023-8034

DOI: 10.1021/acsnano.9b02774



Surface of NP changes immediately after intravenous injection because blood proteins adsorb on the surface.

NP-blood interface changes during circulation and impacts on NP distribution

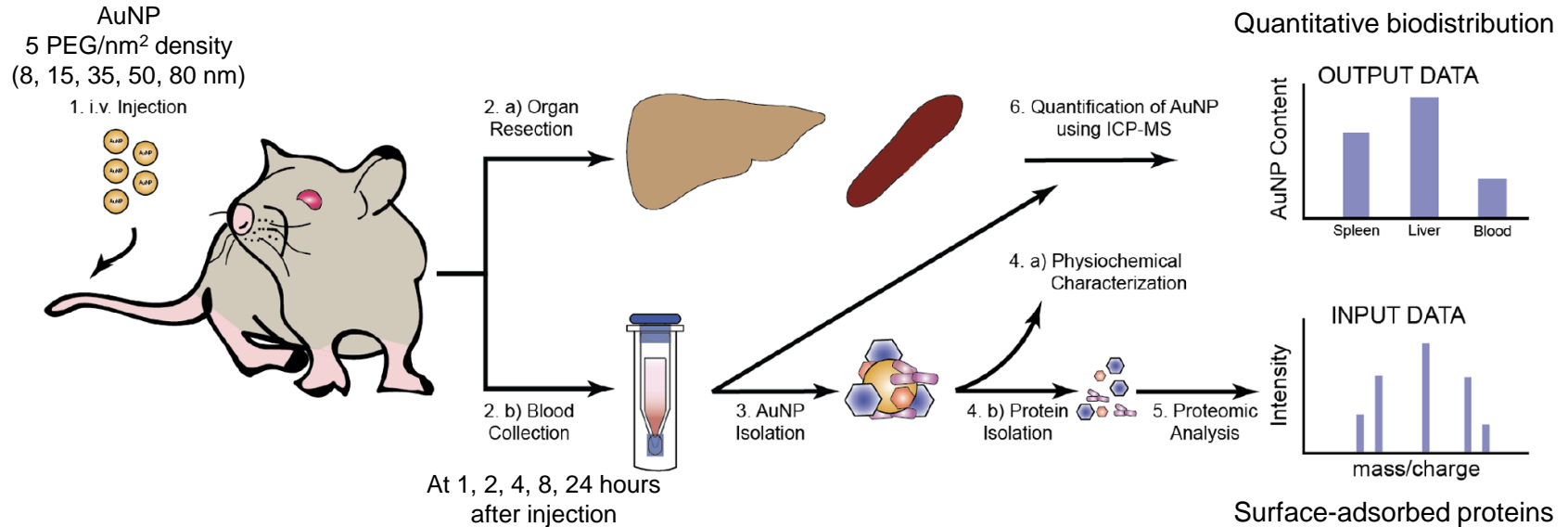


Quantitative biodistribution

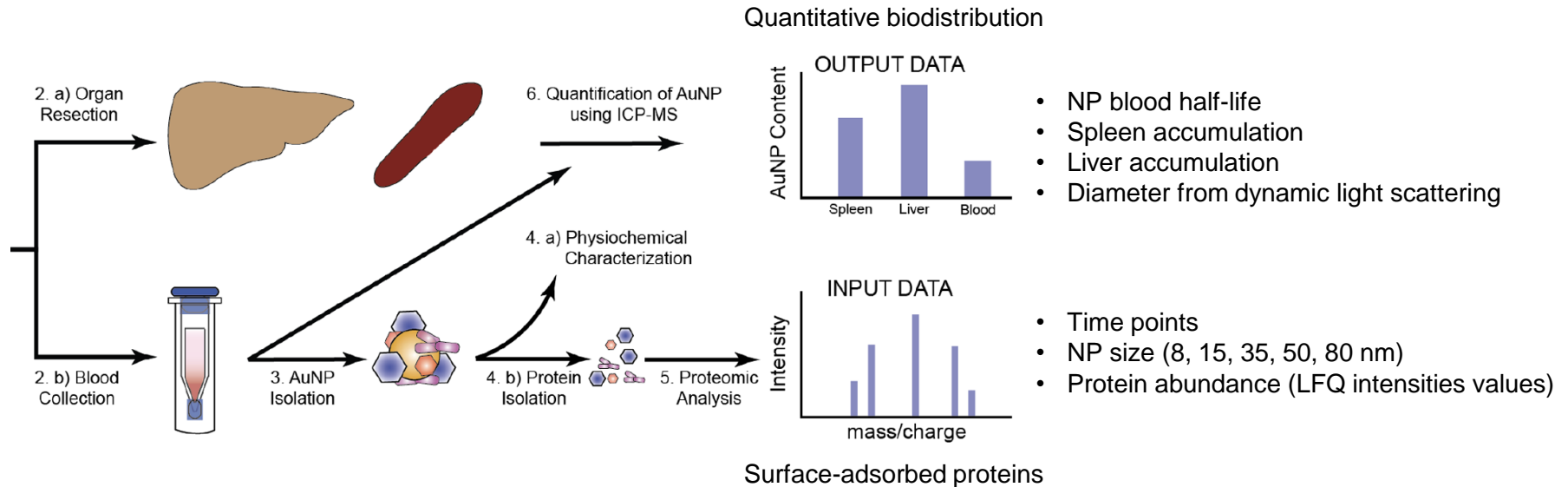
Aim

Discover the relationship between NP adsorption and biodistribution

# Experimental design

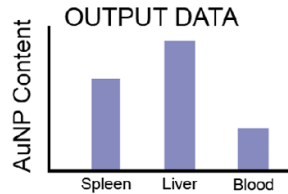


# Machine learning model

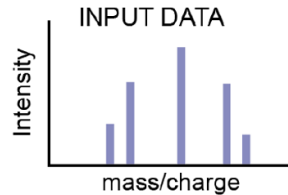


# Machine learning model

## Quantitative biodistribution

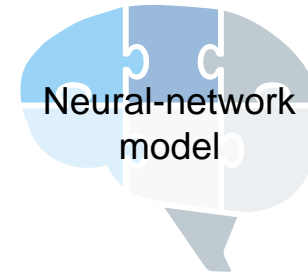


- NP blood half-life
- Spleen accumulation
- Liver accumulation
- Diameter from dynamic light scattering

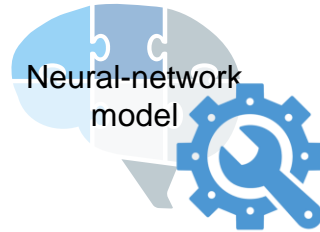


- Time points
- NP size (8, 15, 35, 50, 80 nm)
- Protein abundance (LFQ intensities values)

## Surface-adsorbed proteins

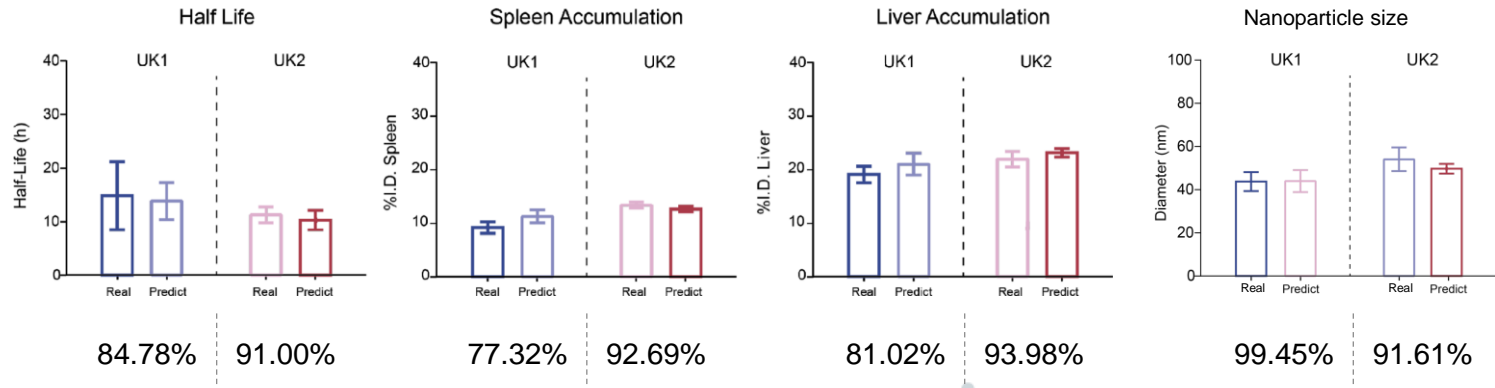


# Machine learning model performance



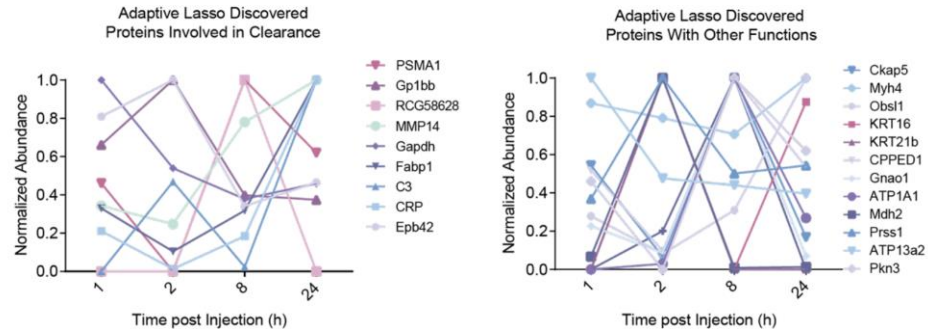
TESTING

UK1, UK2  
2 test nanoparticle formulations



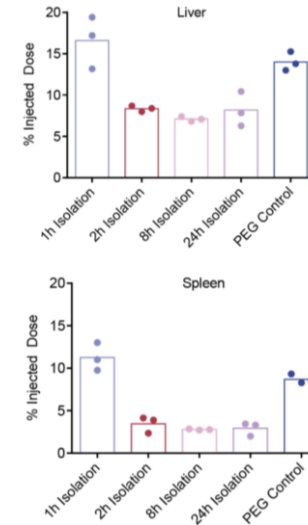
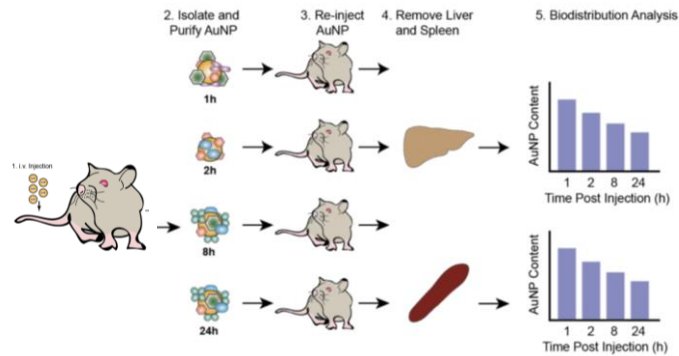
# Set of proteins associated with biodistribution

**Adaptive lasso model**  
identifies a subset of 21 proteins



Clearance is dictated by combinations of protein that form patterns on the nanoparticle surface.

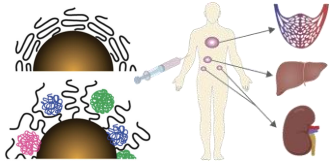
# SIMBA - Serial Injection of Materials for Biodistribution Analysis



SIMBA enables to both evaluate the mechanism of NP uptake and use the body as bioreactor to controllably build surface chemistries that avoid liver and spleen uptake



# Conclusions



Discover the relationship between NP adsorption and biodistribution

Biodistribution is dictated by combinations of NP-adsorbed protein



Artificial learning systems should be a key component in the future design of therapeutic and diagnostic agents



**Thanks!**

**Any questions?**