

Friday, 2nd October

16.00 – 16.30

Welcome speech & Introduction to the workshop  
**Prof. Dr. Damjana Drobne, Assist. Prof. Anita Jemec**

**TOPIC 1: ORGANISATION OF LARGE DATA SETS FOR MODELLING IN GENERAL**

*The topic will deal with the organisation of large data sets using different statistical approaches.*

16.30 – 17.00

**Assist. Prof. Ddr. David Bogataj**, The Mediterranean Institute for Advanced Studies: *The presentation title will be provided.*

17.00 – 17.30

**Assist. Prof. Dr. Cene Fišer**, Biotechnical Faculty University of Ljubljana, Slovenia:  
„Web-databases in systematics and taxonomy“

17.30 – 18.00

COFFEE BREAK

**TOPIC 2: DATA SHARING-Academia, Industry and Regulatory bodies**

*The stakeholders will present their view on the nanoscience data sharing.*

18.00 – 18.30

**Mag. Vladimir Vrečko**, Cinkarna Celje (TiO<sub>2</sub> producers), Slovenia:  
„The importance of data interpretation and dissemination for the future of nanotechnology.“

18.30 – 19.00

**Dr. Mojca Kos Durjava**, National Laboratory of Health, Environment and Food and **Mag. Karmen Kranjc**, Chemical Office of the Republic of Slovenia, Slovenia:  
„Challenges of Regulation and Risk Assessment of Nanomaterials“

Saturday, 3rd October

**TOPIC 3: QUANTITATIVE NANOSTRUCTURE-ACTIVITY (PROPERTY) RELATIONSHIPS (QNAR, QNPR) MODELLING**

*Presentation of new QNAR and QNPR models to relate intrinsic molecular (nanostructure) and physicochemical properties of nanoparticles with their adverse effects (e.g. toxicity).*

9.00 – 9.30 **Prof. Dr. Marjan Vračko**, National Institute of Chemistry, Slovenia:  
„Chemometric analysis and QSAR modelling in NANO-toxicology“

9.30 – 10.00 **Dr. Villem Aruoja**, National Institute of Chemical Physics and Biophysics, Estonia:  
„Toxicity of metal oxide nanoparticles to algae, bacteria and protozoa:  
FP7 project MODERN“

10.00 – 10.30

COFFEE BREAK and poster session

**TOPIC 4: MODELLING OF INTERACTIONS BETWEEN NANOMATERIALS AND BIOLOGICAL MODELS**

*Presentation of different databases aimed to collect information about Nanosafety related topics.*

10.30 – 11.00 **Prof. Dr. Alok Dhawan**, CSIR-Indian Institute of Toxicology Research, Lucknow, India:  
„Toxicity of Nanomaterials: The need for Novel Computational Tools and Approaches in Safety Assessment“

11.00 – 11.30 **Dr. Lokesh Baweja**, Institute of Life Sciences, Ahmedabad, Gujarat, India:  
„Computational approaches to understand the interaction of nanomaterials with biomolecules“

11.30 – 12.00 **Dr. Fabrice Carnal**, Institut F.A. Forel, University of Geneva, Switzerland:  
„Monte Carlo Modelling of Interaction Processes between Nanoparticles and Biomacromolecules of Variable Hydrophobicity“

12.00 – 12.30 **Maja Sopotnik and Prof. Dr. Kristina Sepčič**, Biotechnical Faculty, University of Ljubljana, Slovenia:  
„Interaction of carbon-based nanomaterials with cholinesterases and serum proteins“

12.30 – 13.30

LUNCH BREAK and poster session

Saturday, 3rd October

TOPIC 5: ORGANISING DATA FOR RISK ASSESSMENT/DATA QUALITY

*Presentation of databases to collect Nanosafety related information.*

- 13.30 – 14.00 **Prof. Dr. Rishi Shanker**, Institute of Life Sciences, Ahmedabad, Gujarat, India:  
„Tracking Nano-footprints in microbial food chain: Observations, Data & Challenges“
- 14.00 – 14.30 **Dr. Ashutosh Kumar**, Institute of Life Sciences, Ahmedabad, Gujarat, India:  
„Importance of *in silico* approaches in understanding the interactions of nanoparticles with biological membrane“
- 14.30 – 15.00 **Assist. Prof. Dr. Anita Jemec**, Biotechnical Faculty, University of Ljubljana, Slovenia:  
„Quality of nanotoxicity data and the importance of harmonization“
- 15.00 – 16.00 COFFEE BREAK, poster session and open discussion