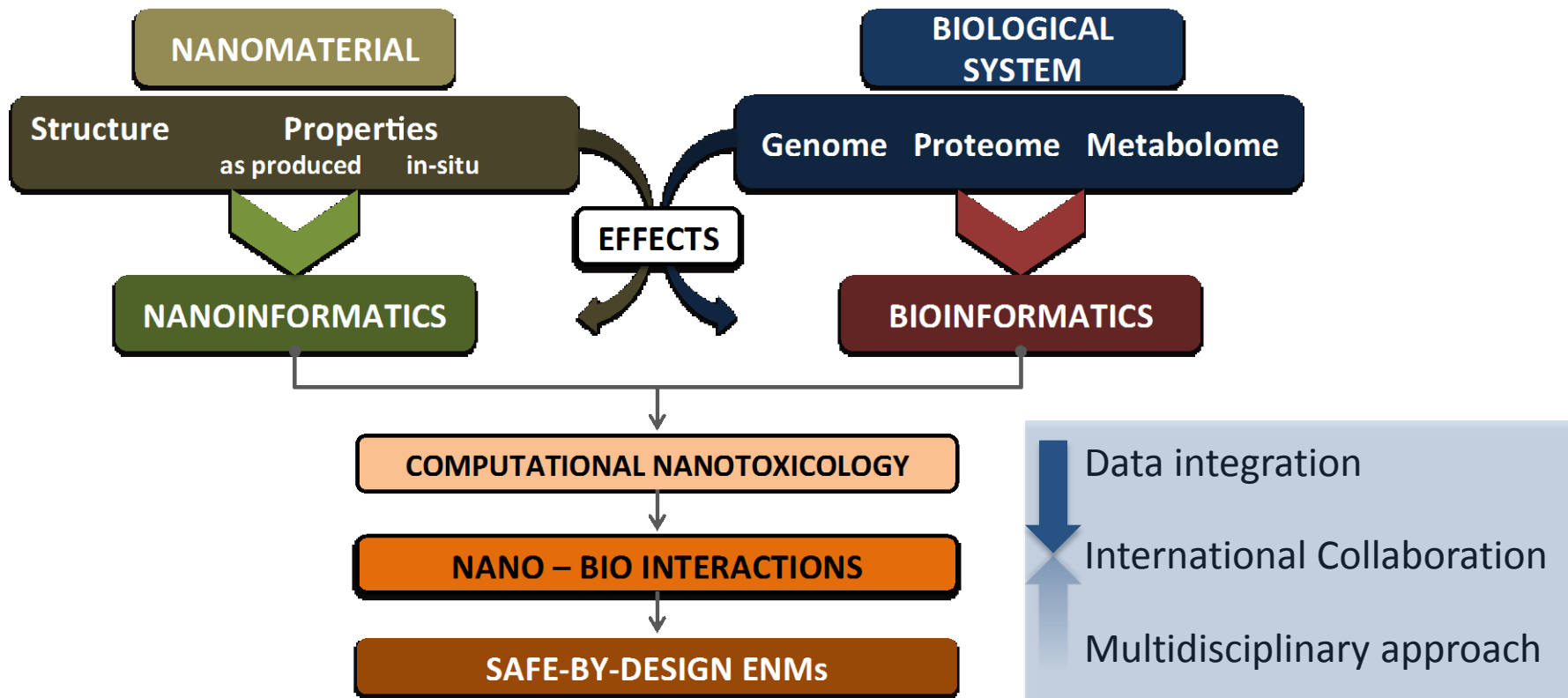


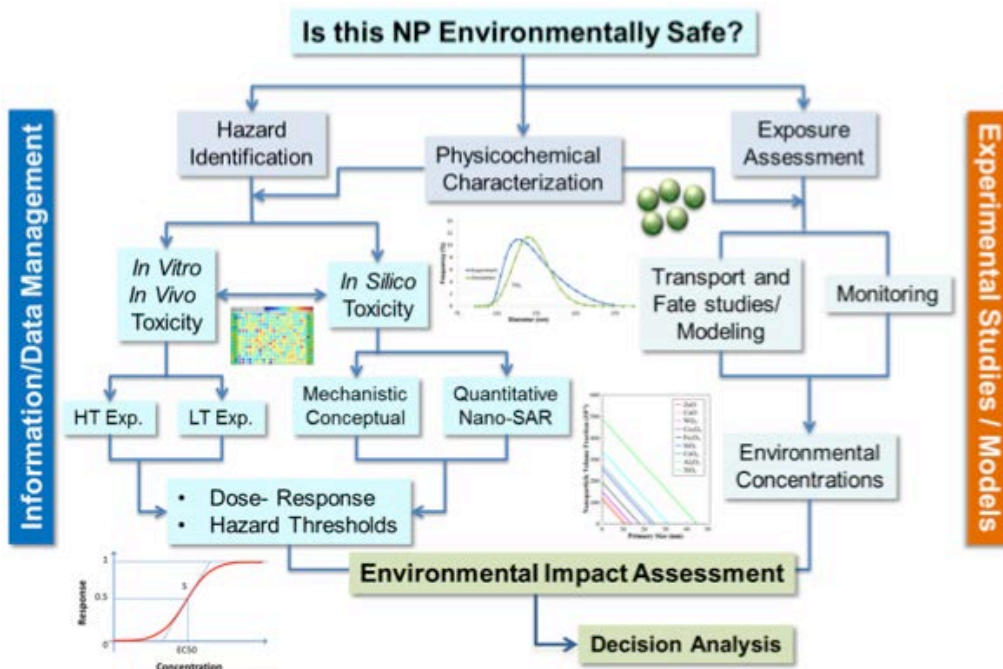
Robert Rallo, Biocentit Research Lab, Universitat Rovira i Virgili, robert.rallo@urv.cat

Center for Environmental Implications of Nanotechnology, UCLA

MODERN FP7-NMP, *Deputy coordinator*

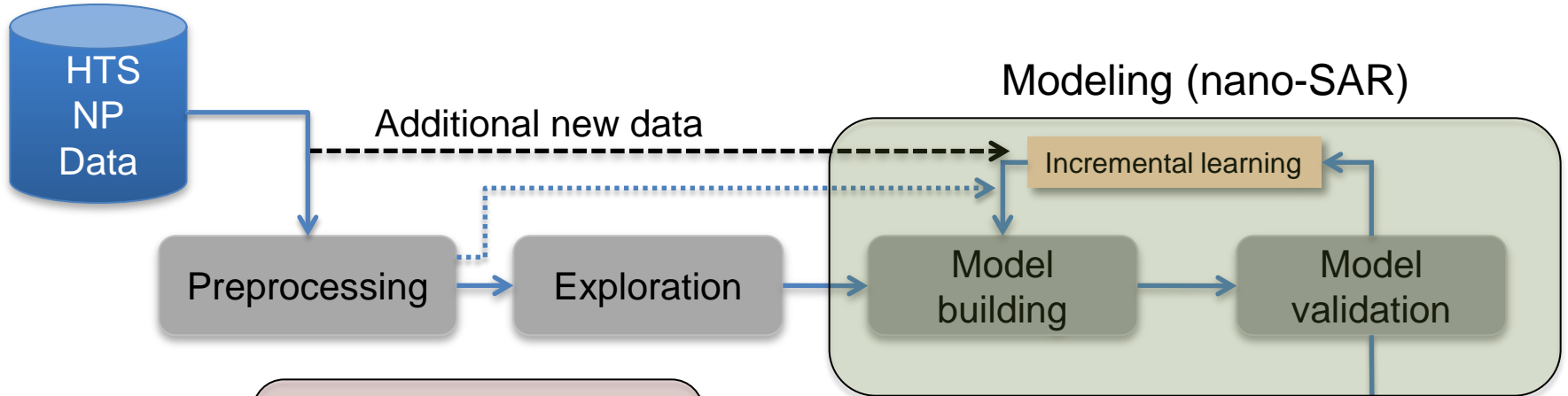
EU Nanosafety Cluster - Modeling WG, *Chair*



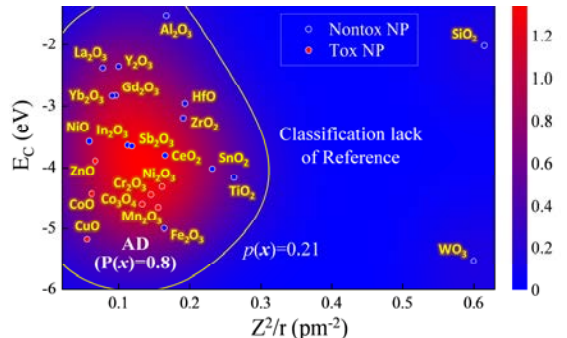
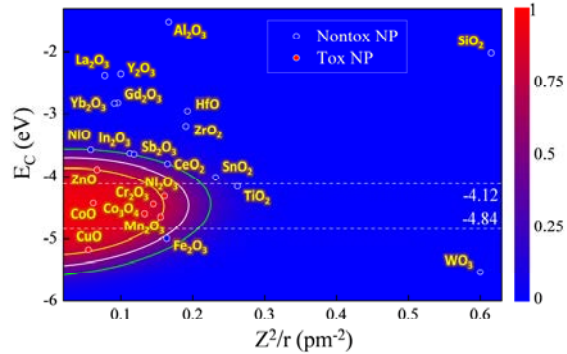
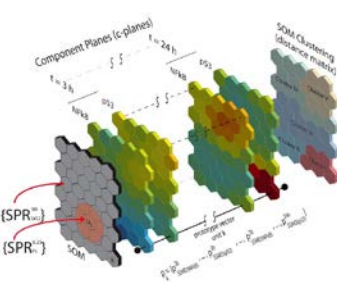
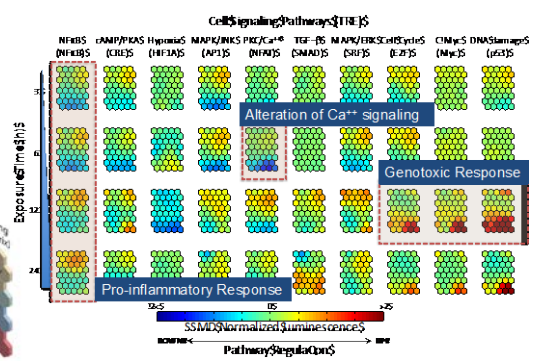
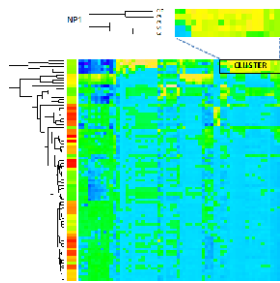


- *In vitro* and *in vivo* HTS/HCS platforms facilitate the **rapid screening of nanomaterial toxicity** and provide the amount of information required to develop data-driven models
- Reliable (and validated) ***in silico* models are necessary** to implement hazard ranking and risk assessment of nanomaterials

Reliable models require abundant and high quality data



Data Mining & Knowledge Extraction



Application Domain Performance Interpretability

Virtual Screening of New NPs

- **Strategies for data generation (experimental, extracted from literature, ...)**

- Dialogue across disciplines (experimentalists vs modelers)
- Minimum information standards
- Well-defined and validated experimental protocols
- Quality Control
- Data curation

- **Access to data**

- Open data -> involvement of publishing companies
- Development of a set of benchmark datasets
- Repositories accessible by modeling tools

- **Protocols for information exchange**

- Data and model sharing
- Common vocabularies, ontologies
- Data analysis pipelines, modeling workflow

- **Specialized tools for data analysis**

