



Perspectives on Stakeholder Needs from a Knowledge Infrastructure: QSAR Modelling



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What would be helpful from the modelling perspective?

- Nanomaterials-related and bioassays-related **ontology**
- Nano-QSAR/QNTR/QNAR **repository**
 - models in the standardized format (e.g. PMML)
 - original data sets
 - additional data (e.g. SEM/TEM images)
- **Interface** for making predictions for new structures (based on models from the repository)
 - calculating descriptors directly
 - protocols for calculating descriptors
- **Tools** for processing data to/from ISA Tab-Nano
- Repository for system biology (-omic) analysis (?)