A Joint Workshop 2012 eu-us bridging nanoEHS research efforts
25-26 OCTOBER 2012, HELSINKI, FINLAND

Predictive Modeling for Human Health

Workshop Report

Rapporteur: Dr. Lang Tran, IOM
EU co-chair: Prof. Bengt Fadeel
US co-chair: Prof. Yoram Cohen

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- Excerpt from the scope statement:
- *"With thousands of new materials emerging, as well as thousands of variants of these materials, there is an urgent need for agreed concept of how to predict likely impacts on human health based on relationships between physico-chemical properties, properties of nanomaterials in situ under exposure conditions, and for identification of connections between those properties with impacts from studies done on previous materials."*

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- Predictive Modeling
- The session focused on approaches to predict biological responses induced by nanomaterials including quantitative structure-activity relationships (QSARs)
- Speakers: Dr. Yoram Cohen, UCLA; and Dr. Enrico Burello, TNO, The Netherlands

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Optimistic view: use of a predictive toxicological approach and high-throughput screening (HTS)

- "We define a predictive toxicological approach as the use of mechanisms-based **high-throughput screening *in vitro* to make predictions** about the physico-chemical properties of nanomaterials that may lead to the disease outcomes *in vivo*. The *in vivo* results are used to validate and improve the *in vitro* HTS and to establish structure-activity relationships that allow **hazard ranking and modeling** by an appropriate combination of *in vitro* and *in vivo* testing."
- Nel et al. Acc Chem Res. 2012 Jun 7. [Epub ahead of print].

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Main issues discussed:

- nano-SARs/QSARs; model validation; applicability domain
- Purpose of modeling? support risk assessment
- Suitability of cell models, high-throughput screening, validation of in vitro-in vivo models
- Quality of data [for modeling]: guidelines
- Barriers to progress: what can the CoR do?

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Main issues discussed:

- Inventory of modeling projects in EU, US
- Standardized reference materials, libraries of nanomaterials
- Biodurability of nanomaterials; pharmaco-kinetics
- Link to other CoRs eg. databases & ontology
- Life-span of models, keeping models current

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Scope

- Focus on nanoSARS, QSARs
- Guidelines and model validation
- Publically accessible data sets [link to CoR on databases] and a repository of models

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Membership

- Define area of interest for members
- Ensure membership with good coverage of necessary areas for modeling of adverse biological responses induced by nanomaterials

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Work modalities

- Regular webinars on topics of interest
- Sharing of documents through us-eu.org
- Link to COST action MODENA on nano-QSARs and other international events eg. International Nanotoxicology Meeting 2014

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