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Structure-Activity-Relationship Development for Engineered Nanomaterials

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Refreshments served at 3:00 PM in room 51-254 CHS

ABSTRACT: Recent studies have identified that certain Engineered Nanomaterials (ENMs) possess properties that may lead to adverse biological impacts, and efforts are now mounting to map the general principles governing the toxicity potential associated with health and safety impacts of these products. In this regard, toxicity screening is critical for characterization of the potential hazard of ENMs in order to provide information that is essential for risk assessment and establishment of safe-use of ENMs. However, generation of required in vitro and in vivo toxicity characterization data, which are necessary to cope with the expected growth in number and diversity of ENMs, is a formidable task. Therefore, in addition to experimental approaches, there is a need for in silico methods (computational approaches) that enable rapid toxicity screening. In this regard, generalization of the outcome from toxicity screening studies can be accomplished using Structure-Activity Relationships (SARs) that relate biological activity (e.g., toxicity) of ENMs to their physicochemical properties. Moreover, decision-making for promoting "greener nano" also requires a thorough understanding of the relationships between the physicochemical properties and the behavior of ENMs in biological systems (i.e., nano-SAR). In this talk, I will discuss some basics about nano-SAR development that are crucial to the regulatory acceptance of nano-SARs and some of the challenging statistical/modeling issues encountered in our effort in nano-SAR development.