Information processing needs and challenges in the context of Nanomedicine

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Nanomedicine, defined "*as the application of nanotechnology in view of making a medical diagnosis or treating or preventing diseases*"[1], opens new research avenues which increasingly demand sound methods and tools for data and knowledge management. For this reason, a new sub-discipline of Biomedical Informatics named "Nanoinformatics" [2] has been proposed as a way to facilitate the access of researchers, clinicians and other health professionals to the relevant information that is needed for the advancement of nanomedicine.

The main contributions of nanoinformatics that can support the effective processing of information in this field are summarized in Figure 1. They include: -nanomaterial characterization databases, -standardization and controlled vocabularies and taxonomies for nanomedicine, -data and image analysis techniques and -modelling and simulation (and even prediction) of biological behaviour of nanomaterial. Here follows a succint description of each of them:

- Nanomaterial characterization databases. Nanoinformatics is contributing to the development of data repositories in the context of nanomedicine [3]. Nanolibraries and databases with information about physical-chemical, biological and toxicological properties of nanoparticles are already available. However, important challenges remain in integrating and providing a unified interface for these resources. This represents a key aspect in order to study the biocompatibility of nanomaterials. There is a clear need of new tools to define and store the minimum information associated with the characterization of nanoparticles. Again, nanomedicine poses new challenging issues for informatics in terms of integrating nanomaterial data with biological and clinical information that is already available in biomedical databases.

- Standardization and controlled vocabularies and taxonomies for nanomedicine. The large amount of experimental and bibliographic data that is being produced on a daily basis requires the setting up of information-based models and tools that allow for the sharing of all these data. Taxonomies, ontologies and controlled vocabularies are central issues in this regard [4]. To facilitate data interoperability in all areas of nanomedicine, from atomic and molecular level to the clinical level, there is a need to develop nano-ontologies to achieve a conceptual (semantic) consensus of terminology, for the development of nanotechnology applications in Health.

- Data and image analysis techniques. Once those data were available, it would be possible to use advanced informatics techniques (such as data and text mining) in order to extract new knowledge based on previous results [5]. Advances in nanomedicine are expected to produce less invasive and more precise imaging modalities, however due to the size and properties of nanoparticles, image processing methods will require considerable computational power in order to efficiently manage the huge amount of data about nanoparticles that will be generated along the process and new image analysis tecniques will be needed in order to correlate theoretical discoveries with experimental results.

- Modelling and simulation (and even prediction) of biological behaviour of nanomaterials. The analysis of positive and negative effects of nanoparticles based on "in vitro" or "in vivo" studies is expected to be complemented with "in silico" modeling and simulation techniques that will be used to predict nanoscale biomedical systems behaviour.

In summary, the term nanoinformatics encompasses the application of computer technologies, information science and molecular simulations, arising as a key methodology in the short-term development of nanomedicine.

References:

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Figure 1. The four main areas of research in Nanoinformatics are supported by integration of biomedical resources and knowledge management processes.