Data Mining for characterization of nanotoxicity in mitochondrial ion channels induced by carbon nanotubes

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Single Walled Carbon Nanotubes (SWCNT) have been largely studied by the scientific community due to their great potential in several areas, ranging from industrial applications to medical uses. On nanomedicine, these SWCNT can be used to inhibit or stimulate the cells processes responsible for the production of energy required for their survival. The organelle accountable for delivering energy to cells is known as mitochondria. Ion channels found on those organelles play an important role on this process. Since the malfunctioning of these ion channels may induce some toxicity for the cells, the study of the interaction between carbon nanotubes and the ion channels is very helpful on understanding how these nanomaterials may induce toxicity on organisms. Aiming at understanding how carbon nanotubes may induce toxicity on organisms, this work proposes to perform molecular docking experiments with different carbon nanotubes and some mitochondrial ion channels proteins. After the execution of these simulations, we are going to apply a knowledge discovery in databases (KDD) process to relate carbon nanotubes characteristics with the docking results. With the results of KDD we expect to characterize the nanotoxicity that carbon nanotubes may induce on mitochondrial ion channels. To perform the molecular docking experiments we are going to use Autodock Vina and a Framework for Virtual Screening. As the target receptors we consider distinct mitochondrial ion channel proteins, found on Protein Data Bank (PDB). Some ion channel proteins do not have structure deposited on PDB and for those we are going to model the structure by homology using the sequences found on MitoProteome. As ligands, we are going to use carbon nanotubes with different geometries (armchair, chiral and zigzag), and also different functionalization, with both carboxyl and hydroxyl groups, totalizing 134 carbon nanotubes. After executing the molecular docking experiments, we will preprocess all these generated data. Then we are going to apply data mining algorithms and analyze the results aiming at characterizing the toxicity in mitochondrial ion channels induced by carbon nanotubes.