

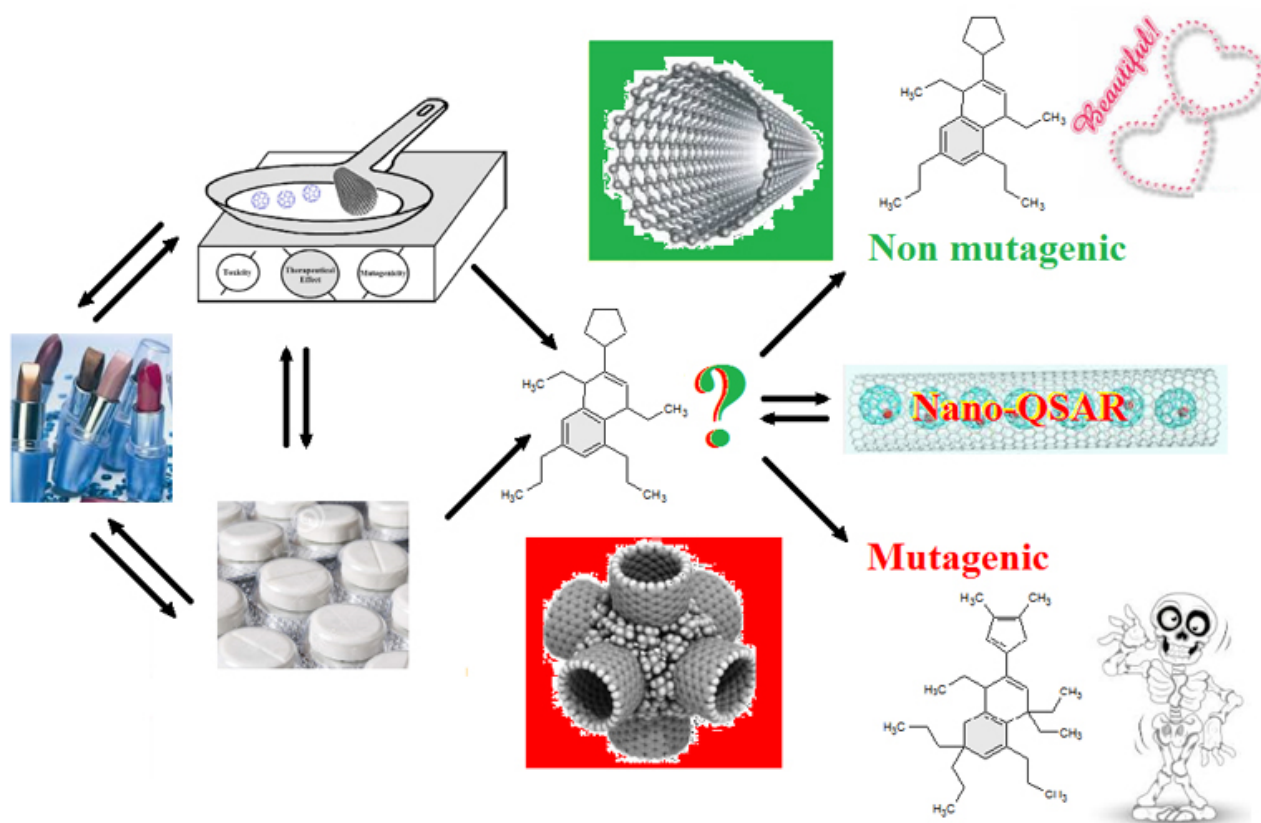
The CORAL software as spyglass to detect “coral reefs” in ocean of nanotechnologies

There are many messages about nanomaterials. There are the both bad and good facts. It is clear these substances are fastly penetrate into many fields of everyday life, such as food, cosmetics, pharmaceuticals, electronics, etc.

Therefore one should know whether these substances are useful. Moreover, one should know whether these substances are dangerous. Some toxic effect can be detected very fastly. However some other toxic effect can be detected only with using data on several generations. Mutagenicity is the kind of harm which can be detected only by means of comparison of health of several generations. Thus, exotic and magic nanomaterials can also play the role of dangerous "coral reefs" in ocean of nanotechnologies present and expected in the near future.

Nanomaterials are characterized by untypical, strange, and "inconvenient" molecular architecture. Traditional methods of prediction of physicochemical and biological behaviour as rule are not appropriate for nanomaterials, because the essence of the traditional methods is the using of data on the molecular structure for the comparison and the further prediction of the behaviour of substances.

NanoMaterials



The behavior of traditional (small) molecules is mainly defined by presence of different chemical elements and configuration of the covalent bonds between them. The behavior of nanomaterials, probably, is defined by other specific features of large clusters of chemical elements. In other words, approaches which are aimed to predict the behavior of nanomaterials need a new representation of all available factors which in principle can impact the behavior of nanomaterials.

Transition from studying of usual substances to studying of nanomaterials is similar to transition from consideration of the economic status of villages to consideration of the economic status of the cities.

A village can be weakly connected with other parts of planet. A city must be connected with other cities. The economic status of village is defined by proportion of men, women, and children: small number of workers as rule lead to decrease of economic potential of village. In the case of a city these criteria can be uninformative, but one can define special criteria of economic potential of city (uninformative for a village), e.g. the number of airports.

If to continue this analogy one can state. In the case of traditional substances the basis to predict a physicochemical and/or biological potential of substance ("village"), it is needed to compare the molecular structure of the given substance with the molecular structure of other similar substances (analogy of proportion of men, women, and children in villages), whereas, in the case of nanomaterials it is needed to compare other informative characteristics.

The conditions of synthesis and the conditions of acting of nanomaterials upon biological targets (human, animals, organs, cells, membranes) are informative characteristics, analogy of "the numbers of airports" for cities. Having a group of records related to impact of nanomaterials upon the biological targets under different conditions, one can select conditions of three categories: (i) conditions which are promoters of increase in mutagenic impact; (ii) conditions which are promoters of decrease in mutagenic impact; and (iii) conditions which have no influence upon mutagenic impact of nanomaterials.

The CORAL software (<http://www.insilico.eu/coral>) gives possibility to automatic carrying out the analysis of the above-mentioned records, related to nanomaterials. Moreover, in the future, it is possible integration of separated recommendations into united system of estimation of mutagenicity fullerene and multi walled carbon nanotubes (MWCNTs).

Publication

[Quasi-SMILES and nano-QFAR: United model for mutagenicity of fullerene and MWCNT under different conditions.](#)

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