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Editorial

Cancer Risk Prediction and Assessment in Human Cells under Synchrotron Radiations Using Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) Studies

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Editorial

In the present editorial, Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) equations were derived using the algorithm of the partition coefficient for the cancer risk prediction and assessment in human cells under synchrotron radiations. Further mixed surfactant systems of an anionic surfactant and several non-ionic surfactant of different hydrophobic chain lengths were taken together to calculate the parameters [1-22]. Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) equations under synchrotron radiations were developed from the surface tension data to predict cancer risk assessment in human cells and compared with Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) derived values to understand probable mechanisms of action of the mixed surfactants blends for aquatic toxicity. The established Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) equations for mixed surfactants indicate the given blends of surfactant act as polar narcotic. As mentioned before, surfactants are used in personal hygiene products, laundry and dishwashing detergents which are discharged into domestic wastewater after use and thus enter the aquatic environment. Because of the increasing use of surfactants, the identification of Nano compounds with low toxicity and good surface activity properties are of great interest. Also, development Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) models provide a possible tool for this research. Quantitative Structure Activity Relationships (QSARs) relate biological, physiochemical, biochemical, pharmaceutical, clinical, medical and medicinal data such as molecular weight and solubility to biological responses. In addition, the biological, physiochemical, biochemical, pharmaceutical, clinical, medical and medicinal data describe properties such as toxicity, pharmacological effects and carcinogenicity. Using this technique only a relatively small number of experiments will be needed to construct a model which will give indications about Nano compounds that are expected to be harmful without any further biological, physiochemical, biochemical, pharmaceutical, clinical, medical and medicinal testing.

Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) studies are indubitably of great importance in modern pharmaceutical, medical and medicinal chemistry and also biochemistry. To obtain a significant correlation, it is essential that appropriate descriptors are employed, whether they are theoretical, computational, numerical, mathematical, physical and empirical or derived from readily available experimental characteristics of molecular and chemical structures. Many descriptors reflect simple molecular and chemical properties and can thus provide insight into the biological, physiochemical, biochemical, pharmaceutical, clinical, medical and medicinal nature of the activity/property under synchrotron radiations consideration. Furthermore, using combinations of topological, physiochemical, biological, biochemical, pharmaceutical, clinical, medical and medicinal parameters along with the indicator parameters, a tremendous improvement in the statistics has been observed. Activity constants can be a key parameter for understanding and quantifying chemical and physical phenomena such as reaction rates, biological uptake, biological transport and environmental fate. It has been shown that acid–base properties affect the toxicity. The research for quantitative relations between the chemical and molecular structure i.e., biological, physiochemical, biochemical, pharmaceutical, clinical, medical, medicinal, structural, molecular and conformational properties and the biological, physiochemical, biochemical, pharmaceutical, clinical, medical, medicinal, structural, molecular and conformational responses is the subject of Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) studies. These relationships will hopefully help to understand and explain the driving forces behind the Nano drugs action; ultimately supporting the development of new Nano compounds exhibiting describes biological, physiochemical, biochemical, pharmaceutical, clinical, medical, medicinal, structural, molecular and conformational properties. In modern pharmaceutical, medical and medicinal chemistry, computer – aided Nano drugs design method such as Quantitative

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Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) studies have greatly accelerated the pace of Nano drugs discovery in recent decade. The underlying assumption behind Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) analysis is that the variation of biologic activity within a group of Nano compounds can be correlated with the variation of their respective structural, molecular and chemical feature. It should be noted that many machine – learning methods have been extensively applied to the process of Nano drugs discovery for building Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Properties Relationship (QSPR) models.

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