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Editorial OMICS International

Computer Aided Molecular Design (CAMD)

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Editorial

The exceptionally efficient and effective use of computer technology for various humane practices is the greatest and the most epic of the revolutions since the advent of human civilization. Perhaps computer has transformed the way we perceive, think and execute our works today.

Hitherto, there were many enemies of humanity; poverty, illiteracy, women demeaning to name a few but in the coming years these will probably be eradicated from their roots. From my viewpoint, diseases and terrorism will be the only ones surviving. I foresee a future in which all countries will forget their sore internal ties for some time and hold hands together on a common platform, to exterminate these two enemies from their very roots.

Computer Aided Molecular Design (CAMD), together with computational chemistry, is a relatively a very efficient discipline of chemistry with outstanding projection. The possibility to virtually design new useful compounds with well-defined properties reducing high costs of experimental synthesis has recently promoted investment in theoretical research. The effective design of chemical structure and the desirable therapeutic properties is directed towards Computer-Aided Drug Design (CADD) a well-established area of CAMD among others.

These techniques comprise of a methodologies such as molecular modeling and the rationalized and systematized discipline of Quantitative Structure Activity Relationship (QSAR). QSAR methodology is a successful means for describing the relation of biological activity of drugs to structure information and model based on structure and to structure interpretation. These models can be used to suggest effective compounds whose activity can be predicted by the Model. The QSAR have been shown to be a reliable methodology for activity prediction of organic compounds.

Mathematical characterization of molecules has been used in the present computer-based experimentation because it leads to hundreds of molecular descriptors and their number continues to grow and also they play an important role in structure-property relationships (QSPR) as well as QSAR. Significant models for monitoring, modeling, estimating and generating QSAR and QSPR models of twelve organic compounds series acting as drugs have been given in the study.

The QSAR technique is used in the research of relevant drugs for various type of diseases. It is, therefore known as Drug Design technique. As a result, the Drug Design technique is a very useful for genetic medicine also. To find the root cause of diseases is a pretty daunting task for our scientists at present. Therefore, genetic medicine, the way to cure genetic diseases is the key to a better tomorrow. In near future, more researches on genetic disorders and their effective cures are being made so that our future generations are not affected and we head into a healthier community life. Furthermore, the most efficient key to our aforementioned vision is the Computer Aided Molecular Design (CAMD) that is environment friendly as it doesn't hamper it and designs drugs in order to synthesize them.

The predicted compounds by using the molecular modeling technique greatly help to design new compounds before synthesis. Using in Thus, attempts have been made to design and develop new drugs against various type disease on a rational basis so as to decreases the trial and error factor and predict the biological activity before synthesis.

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