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Mathematical Chemistry: An Emerging Field of Research

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Editorial

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Development of more current atoms is not a matter of chance. To minimize this lacuna of being blessed to become a professional, mathematical chemistry is the best solution. Mathematical chemistry is the exploration region visualized with novel utilizations of math and insights into science to add to a scientific model to fulfill the different wonders of science and organic components. Mathematical chemistry is an interdisciplinary subject as science gets to be more agreeable to numerically thorough study; it is likely that science will likewise turn into a ready and requesting consumer of new mathematical results. The level of intricacy of chemical problems is often very high, and modeling molecular behavior and chemical reactions does require new mathematical approaches [1]. Chemistry is witnessing an important shift in emphasis: simplistic models are no longer satisfactory, and more detailed mathematical understanding of complex chemical properties and phenomena are required. From theoretical chemistry and quantum chemistry to applied fields such as molecular modeling, drug design, molecular engineering, and the development of supra molecular structures, mathematical chemistry is an important discipline providing both explanations and predictions. Computational chemistry and effect of quantum chemistry are the two essential mainstays of mathematical chemistry. Mathematical chemistry invade into the major research areas such as chemical graph theory which deals with topochemical and topological descriptors to justify a chemical structure along with its electronic configuration, connectivity indices and the study of isomerism [2]. Major applicable area of mathematical chemistry is quantitative structure activity relationships (QSAR), quantitative structure property relationships (QSPR), quantitative structure toxicity relationships (QSTR) and many more. The quantitative structure activity relationship (QSAR) is a paradigm based on the assumption of an underlying relationship between the molecular structure and their biological activity, to predict a new molecular structure with better bioactivity. By merging the outcomes from QSAR, QSPR and QSTR experiments one can able to develop a molecule with better bioactivity, optimum physicochemical properties with very lesser amount of toxicity generation [3]. By doing so various QSAR model development methods are used (Table 1).

Table 1: Followings are various QSAR model development methods.

Categorical Dependent Variable	Continuous Dependent Variable
a) Discriminant analysis	a) Multiple Regression
b) Logistic regression	b) Principal Component Regression
c) k-Nearest Neighbor classification	c) Continuum Regression
d) Decision Trees	d) Partial Least Squares Regression
e) SIMCA	e) Canonical Correlation Analysis
	f) k-Nearest Neighbor method
	g) Artificial Neural Networks

All the outcomes are validated through r^2 coefficient of determination (>0.7), q^2 cross-validated r^2 (>0.5) ,pred_r^2 r^2 for external test set (>0.5), SEE standard error of estimate (smaller is better), F-test for statistical significance of the model (higher is better, for same set of descriptors and compounds) Alpha error probability (smaller is better), Z score randomization test (higher

is better), best_ran_q^2 highest q^2 value in the randomization test (as low as compared to q^2), best_ran_r^2 highest r^2 value in the randomization test (as low as compared to r^2) and also an external validation parameter is there known as Golbraikh and Tropsha acceptable model [4] criteria's to validate a QSAR Equation:

1. $Q^{\wedge 2}$ value is Passed (Threshold value $Q^{\wedge 2}>0.5$).
2. $r^{\wedge 2}$ value is Passed (Threshold value $r^{\wedge 2}>0.6$).
3. $|r0^{\wedge 2}-r'0^{\wedge 2}|$ value is Passed (Threshold value $|r0^{\wedge 2}-r'0^{\wedge 2}|<0.3$).

The applicability domain of the QSAR/QSPR/QSTR equation is evaluated by Manhattan's and Euclidean distance methods. Finally there is a correlation will draw in between predicted and observed values. These types of multiple linear equations are the way to develop a relation in between structural features and bioactivity. In this recent years the animal studies of the newer molecules is really impossible and there was various ethical issues with animal cruelty, in this case various mathematical chemistry software using consensus or decision tree making procedures test the bioactivity, physicochemical properties such as Log P, Log S, $CaCO_2$ cell permeability and toxicity studies such as mutagenicity, cytotoxicity, LD_{50} rat, bioconcentration factor or other aquatic and non aquatic toxicity parameters [5]. There are numerous softwares with this facility such as ADMET, TEST (Toxicity Estimation Tool by EPA) and many more. So in future in the event that we utilize the idea of mathematical chemistry, we can sublime the gap between a good and an effective molecule.

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