Two QSAR Paradigms- Congenericity Principle versus Diversity Begets Diversity Principle- analyzed using computed mathematical chemodescriptors of homogeneous and diverse sets of chemical mutagens

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QSAR development

The basic idea underlying QSAR development can be conveniently expressed by the following equation:

$P = f(S)$ …….. Eq. 1

where P is any physical, biological, medicinal or toxicological property of interest and S represents the relevant aspect of the structure that determines the property.

Congenericity principle

QSARs are usually developed on congeneric sets of chemicals based on the structure- property similarity principle.

Diversity begets diversity principle

From QSARs of various congeneric and diverse data sets we observed that for good QSAR of diverse sets we need a diverse collection of descriptors– the diversity begets diversity principle

Results

Starting with the same collection of molecular descriptors, QSARs for a congeneric set of 95 amine mutagens and diverse set of 508 mutagens were developed

While the amines had only 7 significant descriptors, the diverse set had 42 significant descriptors

Conclusion

The results supports the “Diversity begets diversity” hypothesis. Further comparative studies using congeneric and diverse data sets are needed to test the validity of this hypothesis.