

Integrative Prediction Approaches in Genotoxicity / Carcinogenicity Structure-Activity Relationships. Part I

Among structure-activity relationship approaches, which are more fine tuned:
Structural Alerts or QSARs?

What are the Structural Alerts? Please, give an example.

What are the Modulating factors?

Which are the theoretical and chemical principles underlying the Structural Alerts for genotoxic carcinogenicity?

Structural Alerts are meant to be applied to congeneric and/or non congeneric class of chemicals?
Please discuss briefly this issue.

Which kind of data can be modeled with Structural Alerts, continuous and/or dichotomic?

Are there available public or commercial softwares for the application of Structural Alerts concepts?

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What is a QSAR?

Are QSARs meant to be applied to congeneric and/or non congeneric classes of chemicals? Please discuss briefly this issue.

Which are the key elements of the “Hansch approach” to QSAR?

Is it possible to link the result of a QSAR with mechanisms of action?

Which kind of data are modeled by QSARs, continuous and/or dichotomic?

What is a QSAR applicability domain?

How a QSAR external predictivity analysis should be performed?

Are there available public or commercial softwares for the application of QSAR concepts?

Are alternative methods foreseen at regulatory level for chemical risk assesment?

The OECD (Q)SAR Toolbox

Is the OECD (Q)SAR Toolbox available in the public domain?

Which are the possible applications of the OECD (Q)SAR Toolbox?

Which is the main purpose of the OECD (Q)SAR Toolbox?

What is the final goal of creating a Chemical Category?

Explain the “read-across” approach.

Which are the criteria available in the OECD (Q)SAR Toolbox to group substances into a chemical category?

If you are intended to investigate a chemical with the OECD (Q)SAR Toolbox, which initial information do you need?

What kind of information on a chemical you can obtain with the OECD (Q)SAR Toolbox?

Exploratory Data Analysis: Methods and Results

Which are the main theories for chemical carcinogenicity?

In what nongenotoxic carcinogens are different from genotoxic ones?

What are the Mutagenicity Short-Term Tests to predict Carcinogenicity? Please give some examples.

Are Mutagenicity Short-Term Tests for Carcinogenicity in general able to predict nongenotoxic carcinogenic chemicals?

What is Multivariate Data Analysis, and where/when can it be applied?