OECD Quantitative Structure-Activity Relationships Project [(Q)SARs]

The use of alternative methods to predict the toxicity of chemicals

Objective

Regulatory toxicology has traditionally relied on studies in laboratory animals to characterise the hazards of chemicals. Given the growth of legislative mandates worldwide, traditional approaches are unlikely to be sufficient to address the increase in chemical assessments required. Alternative approaches such as (Quantitative) Structure Activity Relationships ((Q)SAR) are a cost effective solution and have the potential to save time, money and minimise animal testing. The OECD is actively working towards the development of alternative non-testing approaches such as chemical categories and read-across as well as (Q)SAR to predict chemical behaviour and activity of chemicals.

Outcome

The OECD has developed extensive technical guidance as well as a QSAR Toolbox to facilitate the practical application and uptake of (Q)SAR approaches for regulatory purposes by governments and industry. Guidance includes development of the OECD principles for the validation of (Q)SAR models and their interpretation, technical guidance for the grouping of chemicals into chemical categories for read-across as well as the manuals to exploit the functionality of the QSAR Toolbox itself. The OECD QSAR Toolbox is a software application intended to be used in filling data gaps concerning (eco)toxicity and other data related to potentially hazardous properties needed for assessing chemicals. The Toolbox incorporates information and tools from various sources in a logical workflow.

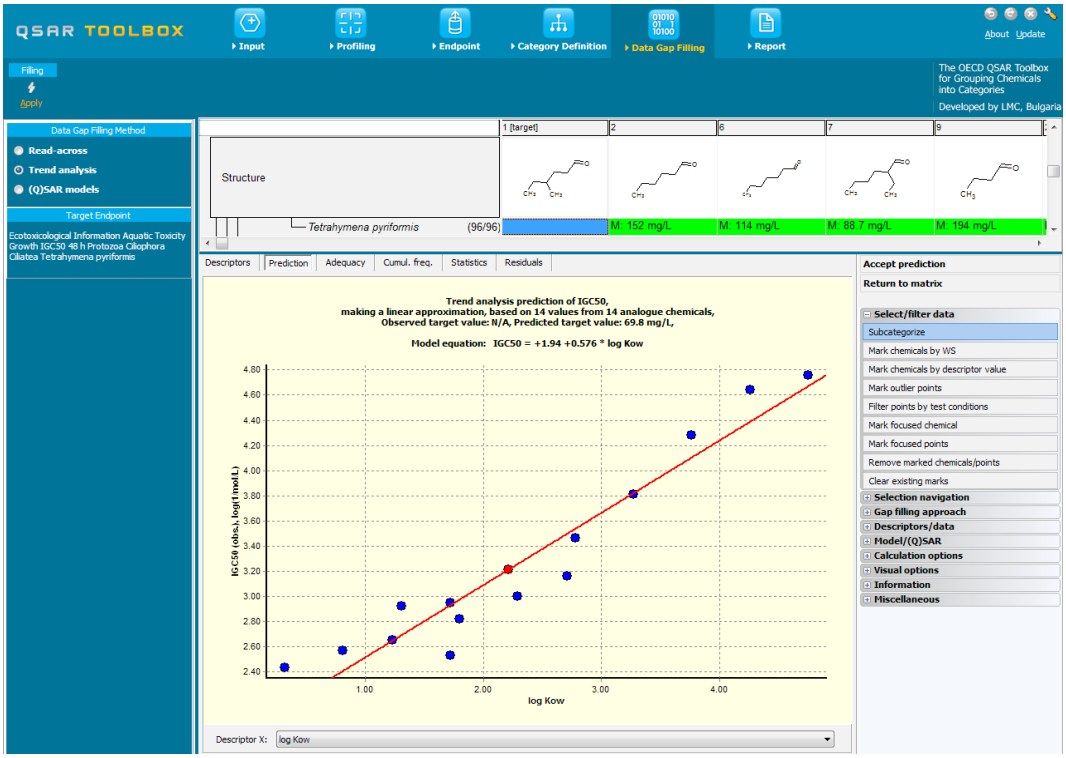
Benefits for countries & industry

Governments and the chemical industry spend millions of dollars every year testing chemicals to characterise their hazard profiles. The QSAR Toolbox software enables regulators and industry to save time and money and minimise animal testing by providing the capability to predict the potential hazard properties of chemicals. The QSAR Toolbox's key strengths are for screening environmental fate endpoints, acute ecotoxicity endpoints and toxicity endpoints such as skin/eye irritation, sensitisation and mutagenicity. The Toolbox can also be used to screen potential novel chemicals early on in the R&D process to identify those chemicals that are most likely to possess a favourable hazard profile. In the future, the Toolbox may be used to predict the properties of manufactured nanomaterials.

QSAR Toolbox

The QSAR Toolbox is a software application intended to be used by governments, chemical industry and other stakeholders to predict the hazards of chemicals. The QSAR Toolbox incorporates information and tools from various sources into a logical workflow. The workflow outlines the steps involved in grouping chemicals into chemical categories for read-across. Chemical categories are groups of chemicals whose physicochemical and human health and/or ecotoxicological properties and/or environmental fate properties are likely to be similar or follow a regular pattern, usually as a result of structural similarity. As a result of these similarities, data gap filling within a chemical category may be carried out by: read-across, trend analysis or external (Q)SAR.

In the read-across approach, endpoint information for one chemical is used to predict the same endpoint for another chemical, which is considered to be “similar” usually on the basis of structural similarity and/or on the basis of a similar mode or mechanism of action. In principle, read-across (whether qualitative or quantitative) can be used to assess physicochemical properties, toxicity, environmental fate and ecotoxicity endpoints. Within a chemical category, members are often related by a trend in an effect for a given endpoint, and a trend analysis may be carried out based on the data for the category members themselves. Additional evidence to substantiate the category rationale and justify the data gap filling approach may be obtained through conducting bridging studies e.g. in vitro tests, in chemico assays or reliable predictions from validated (Q)SAR models.



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