Committee on Environmental Improvement

Fact Sheet

DESIGNING SAFER ALTERNATIVES THROUGH GREEN CHEMISTRY AND SUSTAINABLE MOLECULAR DESIGN

The concepts of green chemistry and sustainable molecular design can support chemical innovation and alternatives assessment very early in the product development process to minimize excessive chemical and solvent use, decrease reliance on elements in limited supply, and reduce product and byproduct hazards/risks to human health and the environment. These approaches to risk/hazard reduction can involve in silico assessments of chemical activity and affinity for critical biomolecules (e.g., receptors, enzymes) associated with adverse health outcomes.

In many cases, alternatives assessment only considers chemical substitutes that have been commercialized, can be readily obtained and, typically, have known physicochemical properties or information about their effects that can be compared with the candidate for substitution. De novo design of new chemicals is a less common but important approach to finding safer alternatives to existing chemicals. While the term de novo design is used here, the concept of designing chemicals to be inherently safer is often referred to as "green chemistry." Green chemistry is a proactive approach to reducing the potential for unwanted health and environmental impacts early in chemical design or discovery. [NRC 2014]

When no alternatives exist and de novo chemical design is required, early consideration of both 1) physicochemical properties and 2) potential biological activities reduces the likelihood of new chemicals encountering issues as development and further testing proceeds. [NRC 2014] A series of qualitative structure-based or physicochemical property-based design filters can be used to assess chemical designs while they are still conceptual or have only small amounts synthesized. Then more refined tools, such as in silico modeling of mechanisms and QSAR and QSDAR, should be used to guide designs that meet environmental and health requirements as well as functional performance goals.

References

- National Research Council, 2014. A Framework to Guide Selection of Chemical Alternatives.

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