Lessons from unsuccessful examples of chemical substitution

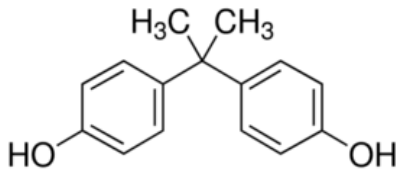
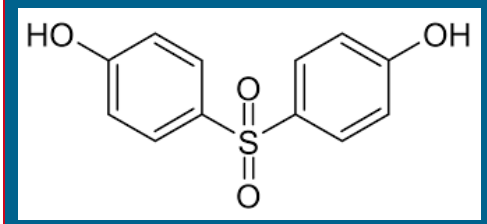
This case study aims to illustrate a chemical substitution process. It is based on publicly available information on company's experience as well as on substance hazards, alternatives to the hazardous substance and regulatory information. The case study is neither complete nor comprehensive in illustrating all substitution options of a substance but rather exemplary.

Substitution of a hazardous substance used in industrial production is a process aiming to reduce chemical hazards by finding new alternative complying with the technological needs but without such nasty properties.

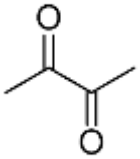
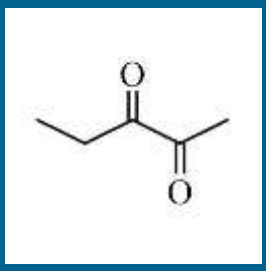
Substitution takes a lot of efforts: finding a new alternative, testing, adjusting processes. And, unfortunately, sometimes substitution fails due to lack of alternatives, or the substitute is not really less hazardous. How to overcome such problems?

In this story we look at some bad experiences and try to gain learning lessons from them: how to do better?

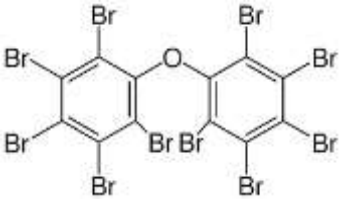
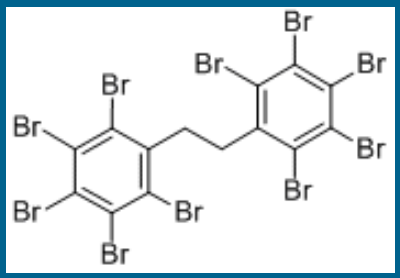
Case of Bisphenol A

Substance to be avoided	The new "alternative"
Bisphenol A 	Bisphenol S 
Why there was a need for substitution? Bisphenol A, technically good and cheap substance, with excellent chemical properties, building strong chemical bounds (see case story for Bisphenol A). However, it has endocrine disrupting properties, potentially causing harm to humans at the current exposure level.	**What is the problem with the substitute?** The chemical structure of bisphenol S to large extent mirrors bisphenol A. One the one hand, it fulfils the same functional requirements, but scientists report that it has also endocrine disrupting properties.

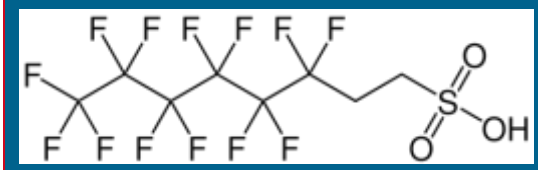
Case of diacetyl

Substance to be avoided	The new "alternative"
2,3 butanedione (diacetlyl) 	2,3 pentanedione 
Why there was a need for substitution? Aroma giving to product smell of butter. But it causes lung cell damage of workers leading to inflammation processes in bronchi.	**What is the problem with the substitute?** It provides the same aroma, and therefore was used as a replacement for diacetyl. It has similar chemical structure. However, it was found out causing the same type of damage of cells leading to inflammation of respiratory ways.

Case of brominated flame-retardants

Substance to be avoided	The new "alternative"
Commercial Deca-BDE (Decabromodiphenyl ether) 	Decabromodipheniyl ethane (DBDPE) 
Why there was a need for substitution? Deca BDE used as flame retardant in plastics. It is very stable in the environment, very bioaccumulative, for example, occuring also in human breast milk, and seems showing endocrine disrupting properties.	**What is the problem with the substitute?** Also this substance is very persistent in the environment leading to human exposure via environment.

Case of mist suppressants

Substance to be avoided	The new "alternative"
PFOS (Perfluorooctanesulfonic acid) 	H_4PFOS (1H,1H,2H,2H-Perfluorooctanesulfonicacid) 
Why there was a need for substitution? PFOS is substance used for various applications, very persistent and very bioaccumulative e.g. very hazardous for the environment. This substance is widely used for different purposes, in case discussed here as mist suppressant in metal plating, and fire – fighting foam.	**What is the problem with the substitute?** This substance was not widely used before substitution therefore little information was available about its properties. However, similar structure to PFOS possess question, is the hazardous profile (stability and bioaccumulation) the same. For example, German public authorities are monitoring occurance of this substance in the environment to get more information.

How to do better?

- Perform the "informed substitution" by assessing the alternatives and its hazardous properties carefully.
- Replacements are often carried out with less known chemicals hence the less information about their hazardous properties is available.
- In case of missing evidence, one can still assume that substance with similar chemical structure may possess similar hazardous properties and therefore it requires closer look and precaution.
- The producers of alternatives shall provide enough information about hazardous properties of the new alternatives
- Life cycle aspects shall be taken into account by assessing new alternatives to avoid switching from one adverse impact to health or environment to another.
- There is need for a wider view on the problem, giving more attention to technological changes (function-oriented design) than simple changes of substances used (selecting known substances with similar properties).

- Binding legal requirements, public funding and industry co-operation for finding best substitution options are crucial to elaborate the new alternatives.

- The information about the properties of the chemicals shall be as much as possible publicly available and all databases need to be checked.

References

From incremental to fundamental substitution in chemical alternatives assessment, Peter Fantke, Roland Weber, Martin Scheringer*, J. Sustainable Chemistry and Pharmacy*, Volume 1, 2015, pp. 1-8.

Toward substitution with no regrets, Julie B. Zimmerman, Paul T.Anastas, *J. Science*, Vol. 347, Issue 6227, pp. 1198-1199.

Leitlinien zur vorläufigen Bewertung von PFC-Verunreinigungen in Wasse und Boden, Bayerisches Landesamt für Umwelt, April 2017.

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