

Grouping of the SIN List chemicals

How many chemicals are being manufactured in the world? Nobody knows. About 150 000 chemicals were pre-registered under REACH and more than 13 000 have been registered so far. The SIN List contains more than 800 individual CAS numbers. To facilitate for companies and other users of the SIN List, ChemSec wants to make the SIN List even more user-friendly and we have therefore grouped the substances on the SIN List.

GROUPING OF THE SIN LIST

Chemicals can be divided into groups based on their structure, which in turn can be linked to their toxicological effects. A group may be justified on more than one basis, for example overall structure, a common functional group, common precursors or the likelihood of common breakdown products.

The justification of groups has traditionally been made in a manual way by careful examination of chemical structures and their effects. For larger data sets, computational methods can facilitate this procedure much. Most known are quantitative structure-activity relationship models (QSAR).

The SIN List has been grouped with the aim to make it more user-friendly and to create the basics for the SINilarity tool. Since the substances have been put on the SIN List because of their hazardous properties, this is also what we chose to base the grouping on. The SIN List chemicals were manually divided into groups to get the most accurate division. For each chemical, the structural elements responsible for the hazardous properties were identified. This was done by consulting scientific literature and experts (from the Department of Chemistry and



Molecular Biology, University of Gothenburg and The Swedish Environmental Institute (IVL)). Finally, the substances were divided into 31 groups. All substances but about 60 were assigned to one or more groups. Since many compounds contain several of these group specific structural elements, one chemical can belong to multiple groups.

Structural element

A structural element is a part of a molecular structure that is important for a certain property. The element can be a well defined functional group or consist of smaller parts of the molecule connected or placed in a specific way. In the context of the SIN List, these structural elements are thought to be responsible for the hazardous properties.

THE GROUPS OF THE SIN LIST ARE:

- Alkylphenols
- Amino carbonyl compounds
- Antimony compounds
- Aromatic amines
- Arsenic compounds
- Azo compounds
- Beryllium compounds
- Bisphenols
- Boron compounds
- Cadmium compounds
- Chromium compounds
- Cobalt compounds
- Electrophiles
- Glycol ethers
- Hydrazines
- Lead compounds
- Mercury compounds
- Mineral fibres
- Nickel compounds
- Nitro compounds
- Nitrosamines
- Organotin compounds
- Parabens
- Perfluorinated compounds
- Petroleum
- Phthalates
- Polyaromatics
- Polyhalogenated aromatics
- Polyhalogenated alkanes
- Polyhalogenated alkenes
- Thioamino carbonyl compounds

The SINimilarity tool – to avoid regrettable substitution

Lack of toxicological data is a constant problem in the world of chemicals. The SINimilarity tool has been set up to give a first indication whether a substance has similar structure and/or contain specific structural elements as substances on the SIN List. For such substances we would recommend further investigations before use. This is a tool to help mainly non-chemists to easily identify substances that are similar to SIN List substances. The aim is to help avoiding regrettable substitution – so that you do not invest in substitution efforts without really improving the safety of the products.

With the SINimilarity tool you can compare more than 480,000 substances with the substances on the SIN List. It compares the structural similarity and identifies common pre-defined structural elements. The tool is simple to use. Just specify the chemical that you want information about and the search gives information on structural similarity to SIN substances. You can compare the overall structure and also find out if the substance you searched for also contains any pre-defined structural

elements from the SIN groups. You do not have to be a chemical expert to do this, as is the case for many other tools. Please note however that compounds that are similar and/or contain the same structural elements does not always have similar toxicities, the SINimilarity tool will only give a first indication. To further evaluate the substances you will need expertise in assessing chemicals.

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