

Poster presentation

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An online-system for the evaluation of hazardous substances

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More than 50 million compounds with molecular structures are known today. Reliable hazard information is available for only a few thousand of them. Nevertheless, laws and regulations can (and have to) be applied to all chemical substances used in a laboratory. For this purpose, a new web-based system [1] has been developed for the online evaluation of hazardous substances.

Using a web form which offers a structure editor, any given structure can be submitted to a SciDex-driven backend [2]. In the first step of evaluation, the backend runs a database query to a CLAKS-Database [3] with more than 140 000 known substances. If the substance is already known to the database, the backend returns the applicable danger symbols, R- and S-Phrases. If it is not found in the database, a substructure analysis according to several regulations will be done. Furthermore, relevant degradation compounds are calculated and analysed.

Relevant laws and regulations are e.g. European Hazard Law [4], the Chemical Weapons Convention [5], German law about narcotics [6], regulations about explosives [7] and lists of known poisons.

References

1. [<http://www.chemie.uni-hamburg.de/claks/obw.html>].
2. **Scientific Data Explorer** [<http://www.lci-publisher.com/scidex.html>]
3. **Chemikalien-Lager- und Kataster-System** [<http://www.chemie.uni-hamburg.de/claks/index.html>]
4. 67/548/EEC, *Amtsblatt der Europäischen Union* Nr. 196 1967. S. 1–98 and Updates
5. **Chemical Weapons Convention** [<http://www.opcw.org/chemical-weapons-convention/>]
6. Betäubungsmittelgesetz, *Bundesgesetzblatt I*: 2007. S. 154
7. Sprengstoffgesetz, *Bundesgesetzblatt I*: 2006. S. 2407