

Alternatives to Animal Testing for Chemical Risk Assessment

A Defra LINK Project

Project no. LK0984

DATASET DOCUMENTATION

Cronin and Basketter Skin Sensitisation (GPMT/MSIAT) Dataset

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1 Aim of this Document

This document provides supporting information relating to the Cronin and Basketter dataset [1] reported in the framework of the Defra LINK LK0984 project. The dataset described in this document is available on <http://www.inchemicotox.org/>.

2 The Cronin and Basketter Dataset

The Cronin and Basketter dataset contains the results of guinea pig skin sensitisation tests on 260 chemicals (245 guinea pig maximisation tests and 15 modified single injection adjuvant tests), published in 1994 [1]. The results were generated by a single laboratory (Unilever Environmental Safety Laboratory) using well recognised standard published procedures. Details of the test conditions such as vehicles, induction and challenge concentrations are absent.

The Cronin and Basketter dataset is available on the inchemicotox web-site in Excel .xls format. It was created and contributed to the project for publication by Lhasa Limited. Care has been taken in its preparation but Lhasa Limited does not warrant that the information contained in it is wholly accurate and any use of it is entirely at the user's risk.

The following information is provided for each chemical: name, 2D structure, SMILES, CAS number, molecular formula, molecular weight, assay type and test method followed, species, vehicle, classification (strong, medium, weak or non-sensitiser), and our Klimisch reliability score for the study/data. The classification is derived from the percentage of animals sensitised in the test: non-sensitiser = 0-9%, weak sensitiser = 10-29%, moderate sensitiser = 30-79%, strong sensitiser = 80-100%.

A significant limitation of this dataset is the frequently trivial names given for the compounds in the published paper which makes definitive assignment of the molecular structure impracticable in many cases. A substantial ambiguity of the molecular structure has been found to be present for at least 30 chemicals; in these cases the most likely structure has been given. Information on the purity of the substances and any impurities present is also absent throughout. However, given that standard experimental procedures were employed, for those test results on compounds with well established structures a Klimisch reliability score of 2 (reliable with restrictions) has been assigned, reflecting the absence of information on impurities and individual test parameters. For test results on chemicals with uncertain chemical identity, a reliability score of 4 has been given (reliability "not assignable" [2]).

3 References

1. Cronin MTD and Basketter DA. Multivariate QSAR analysis of a skin sensitization database. SAR and QSAR in Environmental Research, 2, 159-179 (1994).
2. Klimisch HJ, Andreae M and Tillmann U. A systematic approach for evaluating the quality of experimental and ecotoxicological data. Regul. Toxicol. Pharmacol. 25, 1-5 (1997).