

# Alternatives to Animal Testing for Chemical Risk Assessment

A Defra LINK Project

Project no. LK0984

## DATASET DOCUMENTATION

Gerberick et al, skin sensitisation (LLNA) dataset

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## 1 Aim of this Document

This document provides supporting information relating to the Gerberick et al [1] dataset 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 Gerberick et al Dataset

The Gerberick et al dataset presents the results of skin sensitisation murine local lymph node assays on 210 chemicals that were selected from the published literature and the laboratories of Unilever and Procter and Gamble as representing the best available animal data. Data for a diverse set of relatively simple (mainly having one or two functional groups) low molecular weight chemicals is provided. Stimulation indices for individual concentrations were included in the Gerberick et al paper but only the reported potency measure (EC3 values) are given in the present table.

A corrigenda to this publication has been published on-line at <http://iccvam.niehs.nih.gov/methods/immunotox/LLNA-pot/appx/LLNAPotAppA18Jan08FD.pdf>. This required the deletion of data for one compound (3-phenyl propenal) from the Table.

The Gerberick et al 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, animal species, strain and sex, vehicle, EC3 value (%) (where specified), potency classification, source reference, original reference (used by Gerberick et al) and the Klimisch reliability score for study/data.

The Klimisch study/data reliability score was judged, for all substances, as 2 (reliable with restrictions). This was based on the test method conforming to OECD Test Guideline 429, but there being insufficient information on the purity of the individual substances tested. Klimisch et al state: "Data on the purity of a substance are necessary particularly if impurities may have a substantial influence on the toxicity. This can be assessed only on a case-to-case basis". Strongly sensitising impurities can have a marked effect on the overall test result when the main component is weakly or non-sensitising.

## 3 References

1. Gerberick GF, Ryan CA, Kern PS, Schlatter H, Dearman RJ, Kimber I, Patlewicz G and Basketter DA. Compilation of historical local lymph node assay data for the evaluation of skin sensitization alternatives. *Dermatitis* 2005: 16, 157 - 202.

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).