**Reading across Skin Sensitization With a New large-scale Data Base**

Marcus Hillebrand1,2, Ralph Kühne1, Ralf-Uwe Ebert1, Gerrit Schüürmann1,2

1 UFZ Department of Ecological Chemistry, Helmholtz Centre for Environmental Research, Permoserstr. 15, 04318 Leipzig, Germany.

2 Institute for Organic Chemistry, Technical University Bergakademie Freiberg, Leipziger Str. 29, 09596 Freiberg, Germany.

The European REACH regulation requires for all industrial chemicals with market volumes of at least 1 t/a information about their skin sensitzation potential. In this context, the experimental gold standard is given by the local lymph node assay (LLNA) and thus an animal test. At the same time, REACH encourages the use of non-animal and non-test information, the latter of which includes read-across as well as qualitative and quantitative structure-activity relationships (QSARs) as outlined in its Annex XI.

Up to now, most currently available QSARs for predicting the skin sensitization potential of organic com­pounds rely on subsets of LLNA data published some time ago [i.e. 1, 2], sometimes augmented by data from the guinea pig maximization test (GPMT). The accordingly limited chemical space makes confident QSAR predictions in the regulatory context difficult [3]. In order to improve this situation, an extensive literature search has been conducted, resulting in a significantly larger experimental data base that includes LLNA, GPMT and Buehler (guinea pig) test results. Careful data quality analyses led to a new data base covering 1867 compounds with a molecular weight range from 30 to 2285 Dalton that are built from atom types C, H, N, O, P, S, F, Cl, Br, I, Si, and Sn, and contain 932 aromatics, 935 non-aromatics, 40 hydrocarbons, 1446 compounds with N or O or both as additional atom type, 280 compounds including P or S or both, and 101 compounds with other or further atom types. Following a methodological approach introduced earlier [4, 5], a first read-across model based on atom-centered fragments [6] has been developed and computerized in our ChemProp software package [7]. Employing structural similarity as trigger, the model enables identification of compounds for which reasonable to good prediction performances are obtained.

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