Alépée et al.: Off to a Good Start? Review of the Predictivity of Reactivity Methods Modelling the Molecular Initiating Event of Skin Sensitization

Supplementary Data

Fig. S1: Distribution of molecular weight (MW), water solubility (in M), logKOW, and the volatility classes of all substances (n = 255; no data for 5 substances) (see Tab. S1), the 91 substances with data for all test methods (core) and the non-core substances
Fig. S2: Distribution of physicochemical properties for LLNA grouped by UN GHS categories
Fig. S3: Correlation of physicochemical properties with LLNA EC3 values
Fig. S4: ROC-curves of the DPRA and ADRA for predicting UN GHS No Cat. vs UN GHS Cat. 1A and 1B (A: No vs 1A/1B) and for predicting UN GHS No Cat. and Cat. 1B vs UN GHS Cat. 1A (A: No/1B vs 1A)
Fig. S5: Predictivity of the four test methods depending on the molecular weight (MW) and water solubility (WS) of all available substances

A) The left-hand side dot plots show the MW distributions of false positives (FP) as circles, false negatives (FN) in grey, and correct classification (TP and TN) in black. The right-hand side shows the dependence of the predictivity parameters accuracy (black dots), specificity (white dots), and sensitivity (grey dots) on the MW, calculated for all substances (left side) up to those substances with a MW > 500. B) The left-hand side dot plots show the WS distributions of FP as circles, FN in grey, and correct classification (TP and TN) in black. The right-hand side shows the dependence of the predictivity parameters accuracy (black dots), specificity (white dots) and sensitivity (grey dots) on the WS, calculated for all substances (right side) up to those substances with a WS < 0.0001. (Asterisks indicate the result of Kruskal-Wallis test (**: p-value < 0.01; ***: p-value < 0.001))