Derek Nexus - Achieving High Accuracy with High Coverage

The recently published paper 'Evaluation of the Global Performance of Eight *in silico* Skin Sensitization Models Using Human Data', available at this **website**, evaluates the accuracy of eight *in silico* skin sensitization models against two human data sets: one data set highly curated and reviewed by experts, taken from the literature (Basketter *et al.* 2014) and one screening level data set compiled from the Hazardous Substances Data Bank (HSDB).

Lhasa's expert, knowledge-based toxicology software Derek Nexus performs very well for both Basketter and HSDB data sets, combining high coverage (98% and 90% respectively) with high accuracy (86% and 70% respectively) when using base settings.

When comparing all the models against the Basketter data set, all models predict skin sensitization hazard fairly well (>60% accuracy) when using their optimal sensitization model settings (see paper for more information). However, when the coverage is also taken into account the overall accuracy for each model tends to drop significantly. Due to Derek's high coverage (90%) the accuracy of its predictions remains high at 77% (Figure 1).

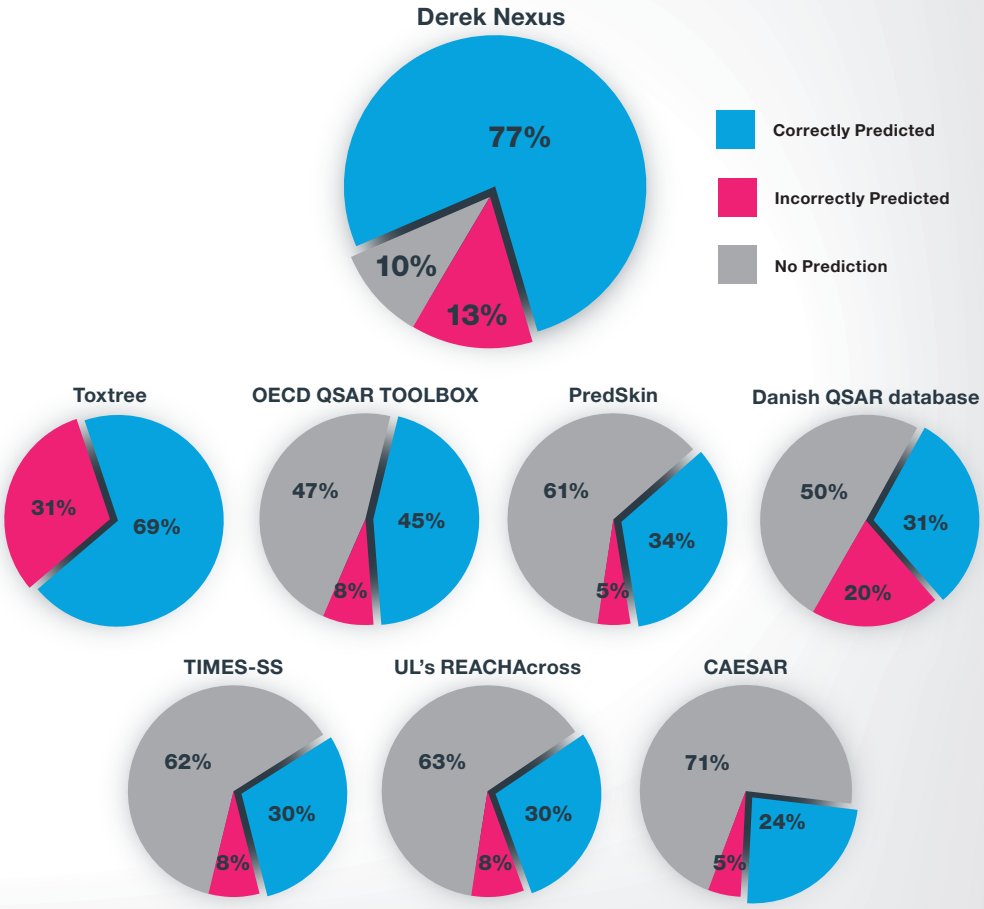

Figure 1. Percentage of correctly predicted compounds (blue), incorrectly predicted compounds (red) and compounds where no prediction was possible (grey) for each skin sensitization model assessed in Golden *et al.*, 2020 using optimal settings against the Basketter data set. 'No Prediction' refers to compounds with no SMILES string, no CAS® number or compounds out of domain of the model. This can be used to indicate coverage.

References:

Golden *et al*,. (2020). Evaluation of the global performance of eight *in silico* skin sensitization models using human data. ALTEX - Alternatives to animal experimentation, pre-print. **https://doi.org/10.14573/altex.1911261**

Basketter *et al*,. (2014). Categorization of chemicals according to their relative human skin sensitizing potency, 25, 11–21. **https://doi.org/10.1097/der.0000000000000003**

HSDB - **https://pubchem.ncbi.nlm.nih.gov/source/11933**

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