Safety assessment of cosmetic ingredients and chemicals for skin sensitization using QSAR in-silico tool.

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Skin sensitization methods are developed to protect workers and consumers from chemical exposures. These methods are well adopted in OECD 6 Test Guideline (TG) addressing 5 Key Events (KE) of the skin sensitization Adverse Outcome Pathway (AOP) such as 442C (Direct Peptide Reactivity Assay, DPRA); OECD TG 442D (KeratinoSens™) and, 7 OECD TG 442E (human Cell Line Activation Test, h-CLAT) [1]. The two biomarkers based test SENS-IS and the Genomic Allergic Detection Test 10 (GARD) are under consideration by the OECD for the development of the respective TGs [1]. Here, our study aimed to test the practicability of in-silico predictions using (Q)SAR tools i.e. Toxtree [2] and VEGA HUB [3] to evaluate their use as a time- and cost-effective alternative to relate measured and calculated physical-chemical properties of chemical compounds to their sensitization potential. The 25 compounds have been selected from literature under non-sensitizer, weak, moderate, strong and extreme category with LLNA and Sens-IS prediction [4]. These predictions are taken as benchmark for our QSAR analysis. VEGA predicted the Skin sensitization potential of these compounds with 80% accuracy. However, Toxtree predicted the Skin sensitization potential with 88% accuracy. The details QSAR data will be presented in the POSTER. The present in-silico study will help to foster discussions on in-silico alternatives to predict Skin sensitization potential of compounds.

Reference:

[1]: EURL ECVAM Recommendation on the use of non-animal approaches for skin sensitisation assessment, March 2017.
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[3]: Benfenati et al, (2013) VEGA-QSAR, ISBN 0016130073.
[4]: Ferret et al, Toxicol In Vitro. 2017 45(Pt 3):374-385