SAR- and analogue-based safety assessments of cosmetic ingredients

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The new EU Cosmetics Regulation (EC) 1223/2009 has replaced the former EU Cosmetics Directive 76/768/EEC and outlines the requirement for cosmetic product manufacturer to keep a product information file (PIF). An important aspect of the PIF is the availability of a detailed cosmetic safety report supporting the safe use of the cosmetic product and its ingredients. However, not for all ingredients present in today's cosmetic products there will be sufficient ingredient-specific data to address each toxicological endpoint individually and the animal testing ban for cosmetic product ingredients which came into force in March 2013 precludes the generation of new toxicology data in experimental animals. Nevertheless, our current understanding of structure activity relationships paired with the high number of regulatory databases containing quality toxicology information allow the SAR- and analogue- or grouping based safety assessment of many cosmetic ingredients for most, if not all toxicological endpoints even in the absence of substance-specific toxicology data. This poster presentation will discuss on the basis of case studies structured approaches and frameworks how the safety of cosmetic ingredients can be assessed on the basis of available toxicological data on structural analogues. This includes our strategies for identification of suitable analogues and chemical similarity assessment using IT tools (e.g., through determination of molecular similarity indices such as Tanimoto score), followed by assessment of the physico-chemical properties, structure reactivity and metabolism of the identified analogues and expert judgement on final chemical-specific assessment approach.

Keywords: safety; cosmetic ingredient; animal testing; SAR