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Abstract: The inclusion of chemical ingredients in Home and Personal Care (HPC) products is based on the functionality that their individual physicochemical properties bring towards enhancing the overall performance of the product. Given the broad range of functions that HPC products provide (cleansing, moisturizing, conditioning, etc.), chemical ingredients used in these products can therefore capture a broad range of chemical classes, for instance from being extremely hydrophilic to extremely hydrophobic, neutral organics, inorganics, ionisable, and permanently charged salts. As it happens, not only do the physicochemical properties of various chemical ingredients influence the functionality of a HPC product, they also influence the behaviour and fate in test systems (in vitro, in vivo, and in silico) and in the environment. It is thus critical that the physicochemical properties be considered in both experimental design and selection of appropriate in silico tools. Using an example from industry, we examine the chemical space of a selection of HPC ingredients (>7000) and discuss implications towards assessing behaviour in vitro. We base our analysis on batch estimates of chemical properties (using SMILES strings), and discuss the validity of such estimates for the chemicals in question. We filter the chemicals using a set of basic criteria to identify groups of chemicals for which standard risk assessment procedures are not applicable. This analysis provides a comprehensive overview of the specific modelling and laboratory research challenges that risk assessors face in dealing with HPC ingredients.