**Ecotoxicological investigations on poorly soluble cosmetic compounds – methods for a reliable environmental risk assessment**

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Cosmetics (also: personal care products) include a broad range of highly hydrophobic compounds that are poorly soluble in water (log KOW > 6, water solubility << 1 mg/L). Due to the high production volume and their typical ‘rinse off’ application, substantial amounts of these chemicals end up in the waste-water and may subsequently enter aquatic systems. This causes the need for a reliable assessment of their environmental behavior and toxicity, as requested for example by the European REACH-Regulation. Additionally, these substances might be considered as potential PBT-candidates due to their intrinsic properties. Due to their high lipophilicity, and extensive adsorption to surfaces like test vessels and organisms, standard ecotoxicity tests are often not suitable. In addition, lack of consistent, reliable results due to the difficulties in maintaining constant test concentrations may lead to improper assessment of possible environmental risks.

One approach addressing this problem is the “poorly solubles approach” proposed by Tolls et al. (2009). It is based upon the ETNCaqua concept (de Wolf et al. 2005) reflecting the results of a statistical analysis of validated ecotoxicological literature data of chemicals. The hypothesis is that substances with a narcotic mode of action and a water solubility below a toxicity threshold (ETNCaqua) of 1.9 µg/l do not exhibit any acute or chronic aquatic toxicity (hydrophobicity cutoff). The aim of this project was to develop ecotoxicological methods and suitable analytics for highly hydrophobic substances, and to compare the results with the “poorly solubles approach” in reference to acute and chronic aquatic ecotoxicity.

Dodecylbenzene (DDB) has been selected as a model compound exhibiting substance properties suitable for testing the poorly soluble approach. It is liquid under standard conditions and with a log Kow of 8.65 its hydrophobicity is exceedingly high. Reliable aquatic toxicity data were not available. A method for chemical analysis of DDB using gas chromatography / mass spectrometry (GC/MS) has been successfully developed and allows concentration measurements of DDB in all tested media, e.g. for solubility studies, exposure confirmations and mass balance determination in ecotoxicological tests.

Different passive dosing techniques have been successfully developed and utilized as delivery tools for highly hydrophobic compounds in aquatic ecotoxicity test systems (Smith et al. 2010). The advantage of these techniques is the possible controlled release of the test substance from an inert reservoir (i.e. silicone O-rings), compensating losses by sorption, dilution, degradation, and volatilization, and the provision of stable concentrations of freely dissolved test substance up to its maximum solubility, i.e. in range of the ETNCaqua.

Different solubility studies of DDB were conducted and different acute and chronic ecotoxicological tests have been performed as proposed by OECD guidelines adapted to passive dosing techniques (acute: Microtox® assay, *Daphnia magna* immobilization assay, fish embryo acute toxicity test; chronic: algal growth inhibition assay, *Daphnia magna* reproduction assay). The validation of the results is in progress. Finally it will be discussed whether the “poorly solubles approach” according to the ETNCaqua hypothesis might be applicable for this model substance.

Tolls J., Müller M., Willing A., Steber J., 2009, A New Concept for the Environmental Risk Assessment of Poorly Water Soluble Compounds and Its Application to Consumer Products, Integrated Environmental Assessment and Management (5) 274-378.

De Wolf W, Siebel-Sauer A, Lecloux A, Koch V, Holt M, Feijtel T, Comber M, Boeije G. 2005. Mode of action and aquatic exposure threshold of no concern. Environmental Toxicology and Chemistry 24 (479 - 485).

Smith K.E.C., Oostingh G.J., Mayer P., 2010, Passive Dosing for Producing Defined and Constant Exposure of Hydrophobic Organic Compounds during in Vitro Toxicity Tests, Chemical Research in Toxicology (23), 55-65.