Experimental and predicted aquatic ecotoxicity of suncare and rinse-off products

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CONTEXT & OBJECTIVES

The objectives of the study were to determine the toxicity of cosmetic rinse-off (RO) and sunscreen (SPF) products in order to validate an existing predictive tool, the iSafeRat WAF module to predict mixture toxicity for algae, daphnids and fish for use with multiple different categories of substances used in cosmetic product mixtures.

The WAF module has already been extensively validated for essential oils and other Natural complex Substances, but not yet for prediction of toxicity to mixtures containing substances with very different Mechanisms of toxic Action (MechoAs).

MATERIAL & METHODS

Cosmetic products are composed of dozens of ingredients (some ingredients are themselves comprised of multiple substances) and each ingredient needs to be accounted for in the toxicity tests because certain ingredients at low concentration in the formulation maybe highly toxic to aquatic organisms. The principle ingredients are outlined in tables 1 & 2. 3 Rinse-off and 4 sunscreen products were tested:

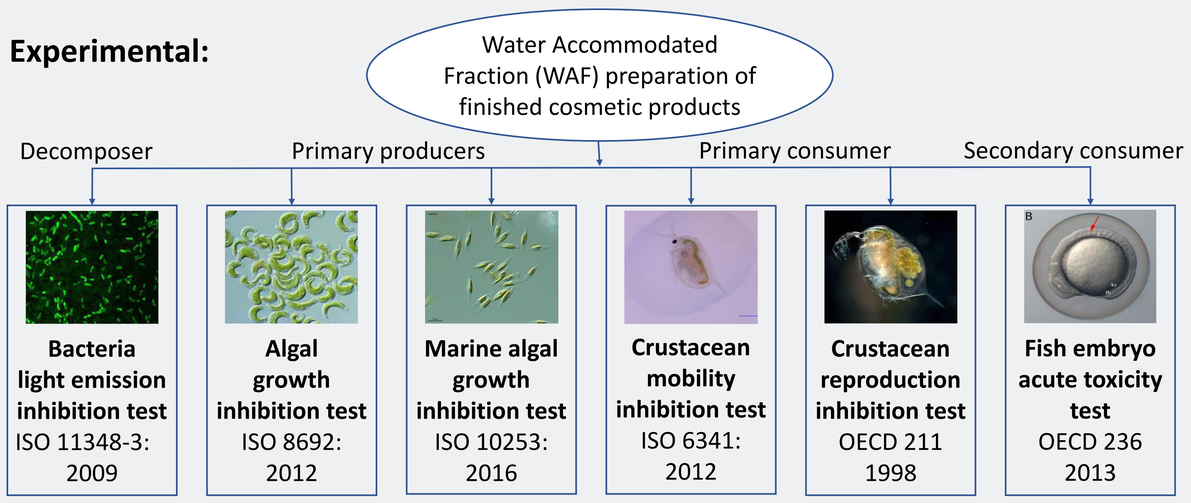
Table 1 : Summary of principal ingredients present in the tested rinse-off (RO) products

Name	Ingredient
RO#1	Sodium laureth sulfate, Cocamidopropyl betaine, decyl glucoside
RO#2	Decyl glucoside, Caprylyl/capryl glucoside, Cocamidopropyl betaine
RO#3	Sodium cocoyl isethionate, Sodium lauroyl sarcosinate

Table 2 : Summary of principal ingredients present in the tested sunscreen (SPF) products

Name	Ingredient
SPF#1-3	C12-15 alkyl benzoate, Dibutyl adipate, Butylene glycol, Ethylhexyl salicylate, Ethylhexyl triazone
SPF#4	C12-15 alkyl benzoate, Diisopropyl sebacate, Ethylhexyl salicylate, Ethylhexyl triazone

Experimental:



→ Determination of EC50 using RegTox software (version 7.07)

Calculation:

At this time the experimental ecotoxicity data are compared with CLP classification method which is based on a worst case additivity calculation as follows:

- ❑ Data source: ECOTOX database and REACH dossiers
- ❑ Data treatment: reassessment of study reliability
- ❑ Prediction model : using CLP additivity formula:

$$E(L)C_{50}(mixture) = \frac{\sum c\,(i)}{\sum i \frac{c(i)}{E(L)C_{50}(i)}}$$

Where :
- $E(L)C_{50}(i)$ is the $E(L)C_{50}$ off compound i
- $c(i)$ is the concentration of compound i in the mixture

RESULTS & DISCUSSION

The experimental data for multiple species and test types are compared in figure 1 below. Basic data for algae and daphnid acute are compared in table 3:

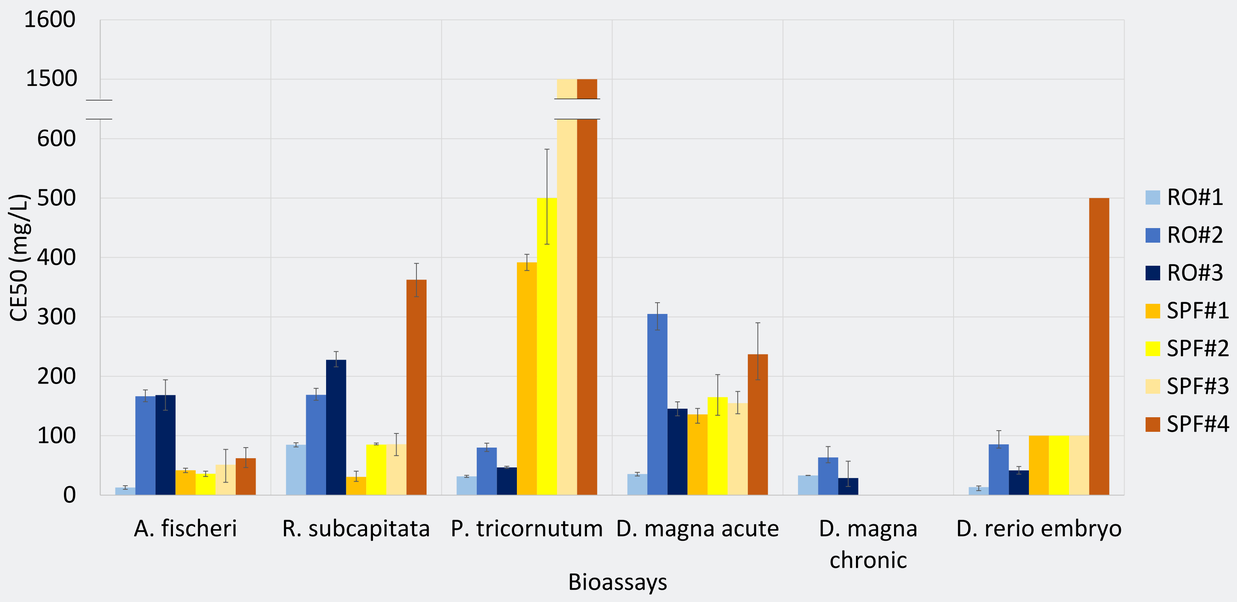


Figure 1 : EC50 (mg/L) of the different tested cosmetic products (RO: rinse-off products ; SPF: sunscreen products) for the 6 normalized bioassays

Table 3 : Summary of experimental and predicted EC50 (mg/L) with their confidence interval obtained for freshwater algae and acute daphnia bioassays for the tested products (RO: rinse-off products ; SPF: sunscreen products)

Product	Assay	Experimental EC_{50} (mg/L)	Calculated EC_{50} (mg/L)
RO#1	Freshwater algae	84,7 [81,1 ; 88,1]	87,1
	Acute daphnia	35,5 [32,2 ; 38,3]	29
RO#2	Freshwater algae	168,7 [159,6 ; 179,7]	147,6
	Acute daphnia	304,9 [285 ; 326,8]	171,7
RO#3	Freshwater algae	227,6 [215,9 ; 241,6]	215,9
	Acute daphnia	145,5 [133,4 ; 157,1]	134,8
SPF#1	Freshwater algae	30,7 [23,1 ; 40,3]	>solubility limit
	Acute daphnia	135,9 [121,2 ; 145,8]	>solubility limit
SPF#2	Freshwater algae	84,9 [85,2 ; 87,7]	>solubility limit
	Acute daphnia	164,9 [134,4 ; 202,9]	>solubility limit
SPF#3	Freshwater algae	85,7 [66,5 ; 103,7]	>solubility limit
	Acute daphnia	154,9 [136,9 ; 174,5]	>solubility limit
SPF#4	Freshwater algae	362,5 [333,9 ; 390]	>solubility limit
	Acute daphnia	237,1 [194 ; 290,1]	>solubility limit

- ❑ EC_{50} above 10mg/L and NOECs above 1mg/L were observed → tested products are not classified according to CLP regulation (n° 1272/2008)
- ❑ RO#1 is more toxic than RO#2 and RO#3. This was expected as the surfactant in RO#1 is sodium lauryl ether sulfate which is more toxic than other surfactants tested
- ❑ SPF#4 is less toxic than others SPF products. The solubilizing agent in SPF#4 is diisopropyl sebacate which is less toxic than dibutyl adipate used in other SPF products
- ❑ For RO#1, RO#2, and RO#3 experimental data and those calculated by the concentration addition method are similar (Table 3), so the toxicity of these mixtures are additive and well predicted by CLP however, this does not seem to be the case for the SPF products

PERSPECTIVES

Since CLP prediction method is a straightforward approach, and can be used for certain mixtures (*i.e.* rinse-off products) but is limited for more complex ones (*e.g.* Suncreams). In the next steps, the experimental data will be further compared to the *in silico* method : *in silico* WAF iSafeRat® (KREATiS). This method takes into consideration the modification of bioavailability of the ingredients present in the mixture during the WAF preparation.

REFERENCES

KREATiS. QSAR Model Reporting Format (QMRF) for iSafeRat® High Accuracy QSAR for Water Solubility: iSafeRat® WatSol – version 2.0 - (KTS/QMRF/HOL/09). 27 March 2023

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