In Silico Determination of Topical Sun Protection

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Abstract

A convenient approach for the estimation of the UV screening performance of sunscreens are computational simulations. Models for the calculation of the *in silico* sun protection factor (SPF) employ the same algorithm as used with *in vitro* SPF measurements, but replace the transmission measurement by the calculation of the combined extinction of the UV filters in an irregular sunscreen film. Thus, the simulations require a database with UV spectra of the relevant UV filters as well as a mathematical description of the film irregularity. Models of film irregularity contain one or two adjustable parameters, which can be calibrated by comparison with *in vivo* results of sunscreen standards. Further refinements of the simulation algorithm imply consideration of photo instabilities of the UV filters, and their distribution in the oil and water phase of an emulsion.

Apart from the use for designing sunscreen formulations, such calculations help improving the understanding of sunscreen performance in general. For instance, it can be shown how the SPF value depends on the amount of sunscreen applied on the skin. Whether there is a linear, convex (exponential), or concave (saturation-like) relationship depends on the UVA/UVB ratio of the sunscreen absorbance profile. Another interesting example is the dependence of the SPF value on the solar irradiance spectrum, which varies in real life with time of the day and with latitude and is different in the laboratory. The SPF value of sunscreens with a UVB-biased protection profile is lower under real life conditions, since the irradiance spectrum of the solar simulator used to determine the *in vivo* SPF is also UVB biased. Sunscreens with uniform protection profile behave independent on spectral changes of the irradiation source and thus perform equally well in SPF testing and in real life.

Introduction

At the stage of development of new sun protection formulations quick and inexpensive methods for estimation of the UV screening performance are highly desirable. The most convenient approach towards this goal is computational simulation. Modern *in silico* models for the calculation of the sun protection factor (SPF) combine the algorithm used with *in vitro* SPF measurements and the approach employed with *in vivo* SPF determination. The transmission measurement is replaced by the calculation of the combined extinction of the UV filters in an irregular sunscreen film, and the *in vivo* endpoint is built in by taking the changes into account which may occur during transmission of one erythemal dose through the sunscreen film. Such simulations require the following elements:

- a database with UV spectra of the relevant UV filters
- a mathematical description of the irregularity profile of the sunscreen film on the skin
- consideration of changes in UV filter concentration due to photoinstabilities
- consideration of formulation influences like the distribution of the UV filters in the oil and water phase of an emulsion.

Models of film irregularity may contain one or two adjustable parameters, which can be determined by comparison with sunscreen standards. These parameters are the screws by which the model can be tuned to produce results as close as possible to experimental *in vivo* and *in vitro* data.

Calculation of the SPF

The sunburn protection factor (SPF) simulation makes use of the formalism first introduced by Sayre in 1979 [1]. The SPF is calculated from the average of the inverse transmission (1/T) of the respective sunscreen in the spectral range between 290 and 400 nm, including weighting with the irradiance spectrum of a UV source, $S_s(\lambda)$, and the erythemal action spectrum, $s_{er}(\lambda)$ [2]:

$$SPF = \frac{\sum_{290}^{400} s_{er}(\lambda) \cdot S_s(\lambda)}{\sum_{290}^{400} s_{er}(\lambda) \cdot S_s(\lambda) \cdot T(\lambda)} \quad (1)$$