Care Creations™

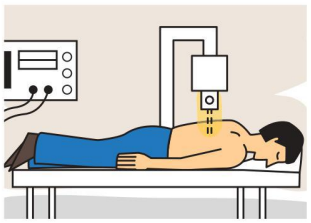
BASF Sunscreen Simulator

The Innovation Tool for Formulators

BASF
The Chemical Company

GET REAL-LIFE CALCULATIONS
www.basf.com/sunscreen-simulator

Although we do research in the real world to be inspired by life, there is nothing more practical than a good theory, just like the BASF Sunscreen Simulator, the virtual lab that makes real-life calculations to quickly test your sunscreen formulations. The BASF Sunscreen Simulator enables the estimation of the Sun Protection Factor (SPF) as well as all common UVA protection metrics. It helps the formulator to compose an optimal combination of the UV filters in a sunscreen formulation and helps to shorten the formulation work by providing realistic estimations of the final product performance. However, it does not replace actual formulary testing.



Benefits

- Explore formulation space to develop different sunscreens
- Check photostability and closeness to an ideal sunscreen
- Test *in silico* before expensive *in vitro* or *in vivo* testing
- Reduce time to market by rapid prototyping
- Get most out of the Tinosorb® and Uvinul® UV filter range

The BASF Sunscreen Simulator calculates the Sun Protection Factor (SPF) with two UV sources and at different application amounts. In addition all common UVA indices are determined:

Sun Protection Factor (SPF)

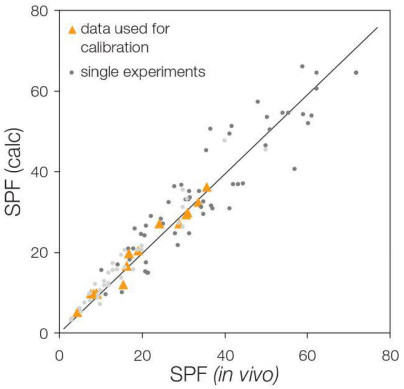
- Check sunscreen at different application amounts:
  – 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 mg/cm²
- Check sunscreen performance:
  – According to international SPF method
  – Under outdoor conditions
- Only broad-spectrum sunscreens provide realistic SPFs under clinical testing as well as outdoor conditions [1)]

UVA-Protection Indices

- UVA-PF/SPF ratio
  (EC recommendation: ≥ 1/3)
- Critical Wavelength CW
  (USA and EC recommendation: > 370 nm)
- UVA/UVB ratio (Boots 5-star-rating)
- UVA-PF (Persistent Pigment darkening PPD after JCIA, AFSSAPS, COLIPA)
- Australian UVA Standard (pass/fail)

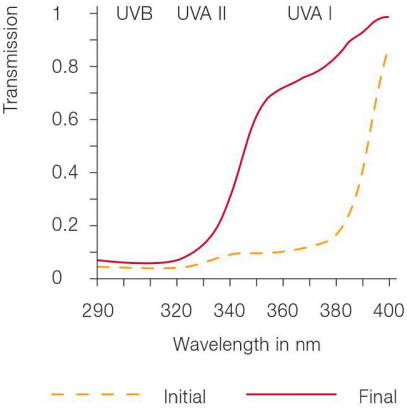
SPF *in silico* Reliability

Ten years experience in calculation of SPF and UVA metrics worldwide. The figure shows the very good correlation between SPF *in silico* (calculated) and SPF *in vivo*.



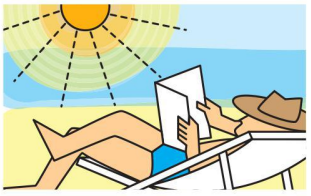
UV Transmission

Example: Profile of a photo-unstable sunscreen (before/after irradiation)



More *in silico* Results

- UVA protection metrics *(in vitro)*
- Protection profile: 290-400nm
- SPF with real-life sun
- UV dose transmitted @ 1MED [2)]



[1)] **Explanation:** The SPF *in vivo* method (Int. method, 2006) uses as irradiation source a solar simulator with a cut-off of radiation >400 nm, thus emitting also far less UVA radiation than the sun. In contrast, the Real-Life SPF is calculated using a standard solar spectrum with full UVA content. Since sunscreens are commonly UVB biased, the Real-Life SPF is smaller than the SPF obtained with the solar simulator. The two SPFs are only the same in the case of the "ideal sunscreen" with spectral homeostasis (Compare with example)

[2)] **Explanation:** The irradiance of the sun is stronger in the UVA range than in the UVB range. Therefore, the total Transmitted UV Dose (from 290 to 400 nm) after having received 1 MED depends strongly on the spectral properties of the applied sunscreen. See text in example.

SUNSCREEN SIMULATOR IN ACTION (Example)

SPF, UVA-Metrics, Protection Profile, Real-Life Calculations etc.

Input

Region: Europe
Application amount: 2.0 mg/cm²

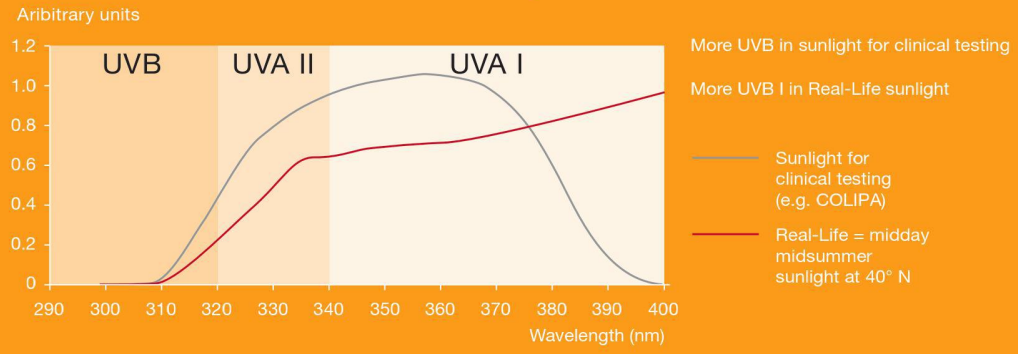
Date: 2013/02/22 12:12:37

UV Filter composition INCI name	USAN name	Abbreviation	Amount
Bis-Ethylhexyloxyphenol Methoxyphenyl Triazine (Tinosorb® S)	Bemotrizinol	BEMT	1 %
Bis-Ethylhexyloxyphenol Methoxyphenyl Triazine (Tinosorb® S Aqua, active)	Bemotrizinol	BEMT	2 %
Diethylamino Hydroxybenzoyl Hexyl Benzoate (Uvinul® A Plus)	–	DHHB	4 %
Methylene Bis-Benzotriazolyl Tetramethylbutylphenol (nano) (Tinosorb® M, active)	Bisoctrizole	MBBT	3 %
Ethylhexyl Methoxycinnamate (Uvinul® MC80)	Octinoxate	EHMC	4 %
		Total:	14 %

SPF

SPF (international method): **32.3** Rating: 30	Simulation of the sun protection factor *in vivo* (SPF, int. method 2006) is performed. A description of the calculations is given in: "*In silico* Determination of Topical Sun Protection", Bernd Herzog and Uli Osterwalder, Cosmetic Science Technology 2011, 62 - 70
Filter efficiency: **2.3** (SPF/% UV Filter)	The UV Filter efficiency is the ratio of SPF and total UV Filter concentration (in %). The higher this value, the less Filter is required to achieve a certain SPF. This means a higher degree of freedom in the choice of other ingredients in a sunscreen formulation.

Comparison of Solar Simulator and Real-Life Sunlight



Real-Life Calculations

Real-Life Sunburn Protection Factor (calculated with midday midsummer sunlight at 40°N) SPF (Real-Life): **30.9** Rating: 30	The SPF *in vivo* method (Int. method, 2006) uses as irradiation source a solar simulator with a cut-off of radiation > 400 nm, thus emitting also far less UVA I radiation than the sun. In contrast, the real-life SPF is calculated using a standard solar spectrum with full UVA content. Since sunscreens are commonly UVB biased, the Real-Life SPF is smaller than the SPF obtained with the solar simulator. The two SPFs are only the same in the case of the "ideal sunscreen" with spectral homeostasis.
Transmitted UV Dose at 1 MED: **15.6 J/cm²** Normalized Transmitted UV Dose at 1 MED: **2.0**	The irradiance of the sun is stronger in the UVA range than in the UVB range. Therefore, the total Transmitted UV Dose (from 290 to 400 nm) after having received 1 MED depends strongly on the spectral properties of the applied sunscreen. The Transmitted UV Dose at 1 MED is calculated in J/cm² using the same standard solar spectrum as for the Real-Life SPF. An "ideal sunscreen" would perform like a neutral density filter with the same protection at any wavelength. In such a case the Transmitted UV Dose at 1 MED has a value of 7.9 J/cm². This value is used to normalize the Transmitted UV Dose at 1 MED. The closer the normalized value comes to 1, the more ideal is the spectral profile of the respective sunscreen.

UVA-Metrics

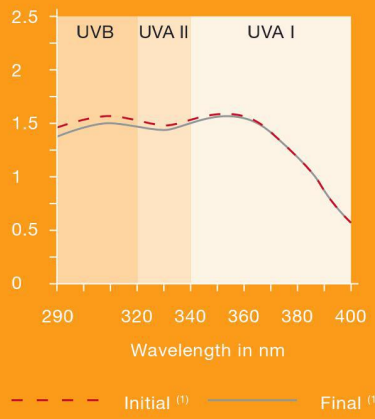
Country	*in vivo*	*in vitro*	Rating
EU/CH	Simulated PPD UVA: 18.0 Critical wavelength: 382.0 nm	EC Recommendation (UVA-PF/SPF > 0.33) UVA-PF 24.4 UVA-PF/SPF: 0.8	UVA
	Labeled SPF: -	UVA-PF UVA-PF/SPF: -	
USA		FDA Final Rule Critical wavelength: 379.0 nm	Broad Spectrum
GB		Boots Star-Rating UVA/UVB ratio w/o irradiation: 0.87 with irradiation: 0.87	UVA ****
JP	JCIA Rating UVA-PF (PPD): 18.0		PA ++++
AUS/ MERCOSUR	Simulated PPD UVA: 18.0 Critical wavelength: 382.0 nm	EC Recommendation (UVA-PF/SPF > 0.33) UVA-PF 24.4 UVA-PF/SPF: 0.8	UVA
	Labeled SPF: -	UVA-PF UVA-PF/SPF: -	
Global	No global standard has been defined, yet.		

Normalized Transmitted UV Dose at 1MED

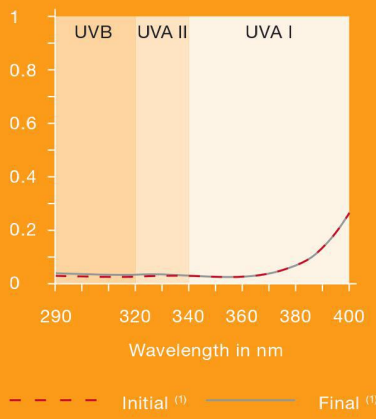
An "ideal sunscreen" would perform like a neutral density filter with the same protection at any wavelength. In such a case the Transmitted UV Dose at 1 MED has a value of 7.9 J/cm². This value is used to normalize the Transmitted UV Dose at 1 MED. The closer the normalized value comes to 1, the more ideal is the spectral profile of the respective sunscreen.

UV Protection Profile

Extinction



Transmission



Initial [1] Final [1]

1) Profiles before (Initial) and after (Final) Irradiation dose of SPF x MED (1 Minimal Erthema Dose passes through sunscreen onto skin)

HOW IT WORKS: THE SCIENTIFIC BACKGROUND

The Sun Protection Factor (SPF) is defined as the ratio of the Minimal Erythema Dose of protected skin and unprotected skin **(1).**

The transmission of UV radiation through a film of sunscreen is defined as the inverse ratio of the intensity before and after passing through the sunscreen film **(2).** UV filters in the sunscreen film lower the transmission based on their extinction spectrum.

Sayre's formula describing the SPF in terms of Sun Spectrum, Erythema Action Spectrum and UV Transmission is the core of the Sunscreen Simulator **(3)**. The ratio can be visualized by the ratio of areas between erythemally weighted sun intensity with and without sunscreen.

Sunscreen on skin does not form a film of regular thickness. Irregularities are taken into account in the Sunscreen Simulator **(4).** SPF and the UVA indices can be calculated for application amounts lower or higher than the standard 2mg/cm².

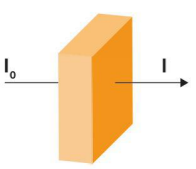
Furthermore the photoinstability of certain UV filter combinations as well as the synergistic effect arising from having UV filters in the oil and in the water phase, are also considered. The results of any calculated combination of UV Filters is presented as extinction and transmission of UV radiation from 290 to 400 nm. In addition the SPF is calculated for the standard UVB biased COLIPA sun spectrum and the more realistic outdoor sun spectrum. Calculation results show that broad-spectrum sunscreens provide more realistic SPF values than UVB-biased sunscreens.

(1) Definition: Sun Protection Factor

$$SPF = \frac{MED_P}{MED_U}$$

MED_U= minimal erythemal dose with unprotected skin
MED_P= minimal erythemal dose with protected skin

(2) Transmission Concept



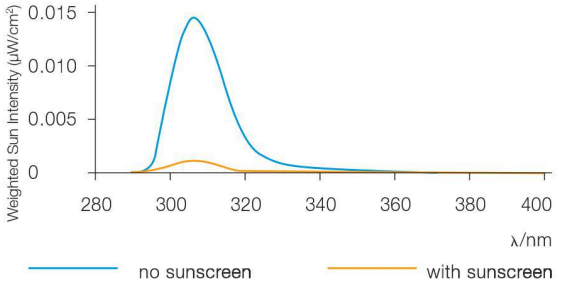
Transmission $T = \frac{I}{I_0}$

Protection Factor $\frac{I_0}{I} = \frac{I}{T}$

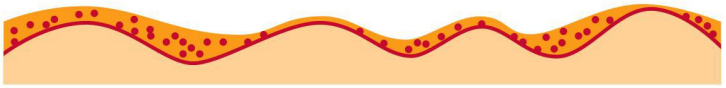
(3) SPF Formula (Sayre 1979)

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

$S_S(\lambda)$...Spectrum of UV source,
$s_{er}(\lambda)$...Erythema Action Spectrum



(4) Sunscreen film on skin



Milestone Publications

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PERSONAL CARE INGREDIENTS

BASF Personal Care is the world's leading supplier of high performance ingredients for the personal care industry. As part of BASF's Care Chemicals division, the unit provides all the resources of a global industry leader combined with consumer insights and innovation-driven solutions.

BASF Personal Care strives to anticipate market demands for new personal care products and concepts for all applications in the personal care market. Its wide product range includes, beside others, surfactants and emulsifiers, polymers, emollients, specialty actives, pigments and UV filters. With production and development sites as well as sales and marketing offices all over the world, the business unit offers its customers the winning combination of global reach, technological excellence and formulation expertise. Its focus on consumer trends, specific industry requirements, and ability to innovate and bring new products rapidly to market contribute strongly to the success of customers – making BASF Personal Care a valued partner for the personal care industry.

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