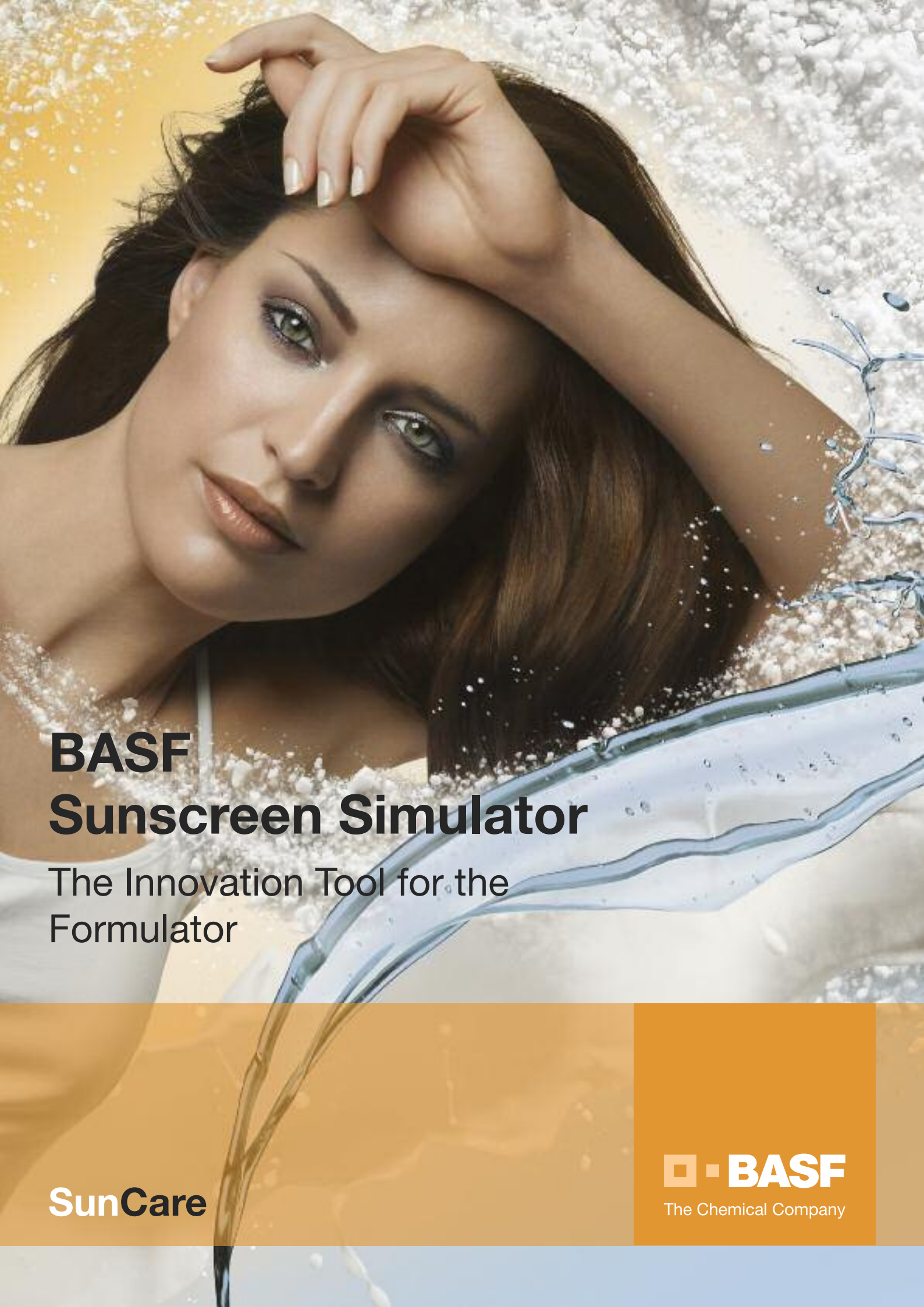


BASF Sunscreen Simulator

The Innovation Tool for the Formulator

SunCare

BASF
The Chemical Company

Scientific Background

The Sunburn 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/cm^2.

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.

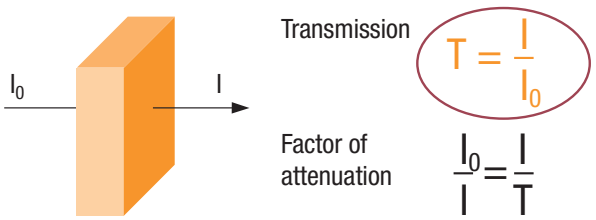
In addition the SPF is calculated for the standard UVB biased COLIPA sun spectrum and the more realistic outdoor sun spectrum. Calculation results show that broad-spectrum sunscreens provide more realistic SPF values than UVB-biased sunscreens.

(1) Definition: Sunburn Protection Factor

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

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

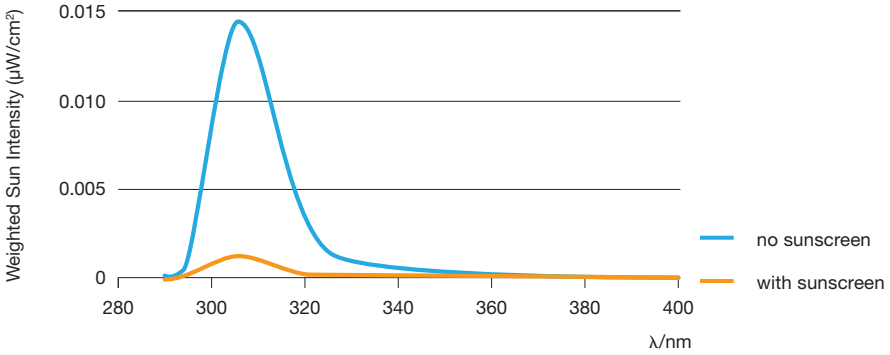
(2) Transmission Concept



(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

Sunscreen film
Skin surface

Milestone Publications

Sayre RM, Agin PP, LeVee GJ, Marlowe E: A comparison of in vivo and in vitro testing of sunscreening formulas, Photochem. Photobiol. **1979**; 29: 559 – 566

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Osterwalder and Herzog B, Sun protection factors: world wide confusion, Br. J. Dermatol., **2009**, 161, 13–24

Stanfield J, Osterwalder U, Herzog B, In Vitro Masurements of Sunscreen Protection, Photochem. Photobiol. Sci., **2009**, DOI: 10.1039/B9PP00181F

SPF Results ...
depend on type of lamp and type of sunscreen

SPF of broad-spectrum sunscreen

Example A
Broad-spectrum

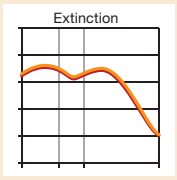
Input

Region: Europe
Application Amount: 2.0 mg/cm²

Date: 2010/03/18 14:52:00

UV Filter Composition

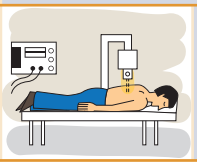
INCI Name	USAN Name	Abbreviation	Amount
Bis-Ethylhexyloxyphenol Methoxyphenyl Triazine (Tinosorb® S)	Bemotrizinol	BEMT	2.0%
Bis-Ethylhexyloxyphenol Methoxyphenyl Triazine (Tinosorb® S Aqua, active)	Bemotrizinol	BEMT	1.0%
Diethylamino Hydroxybenzoyl Hexyl Benzoate (Uvinul® A Plus)	–	DHHB	8.0%
Ethylhexyl Triazone (Uvinul® T 150)	Octyltriazone	EHT	2.5%
Phenylbenzimidazol Sulfonic Acid	Ensulizole	PBSA	3.5%
TiO_2 water phase	Titanium Dioxide	TiO_2	2.5%
		Total:	19.5%

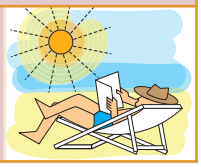


photostable

SPF

Clinical (International Method)	Outdoor Exposure
Solar Simulated Lamp	**Outdoor Sun Spectrum**
SPF (SSL): 56.0	SPF (outdoor): 50.1
Rating/LABEL: 50	**(Rating: 50)**





Clinical SPF is realistic

SPF of UVB-biased sunscreen (photo labile)

Example B
UVB-biased

Input

Region: Europe
Application Amount: 2.0 mg/cm²

Date: 2010/03/18 15:22:16

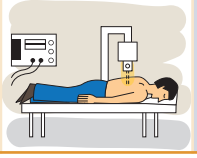
UV Filter Composition

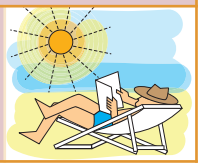
INCI Name	USAN Name	Abbreviation	Amount
Bis-Ethylhexyloxyphenol Methoxyphenyl Triazine (Tinosorb® S)	Bemotrizinol	BEMT	2%
Butyl Methoxydibenzoylmethane	Avobenzone	BMBM	5%
Ethylhexyl Methoxycinnamate (Uvinul® MC 80)	Octinoxate	EHMC	10%
Ethylhexyl Triazone (Uvinul® T 150)	Octyltriazone	EHT	3%
Octocrylene (Uvinul® N 539 T)	Octocrylene	OCR	5%
Phenylbenzimidazol Sulfonic Acid	Ensulizole	PBSA	3%
		Total:	28%

photo labile

SPF

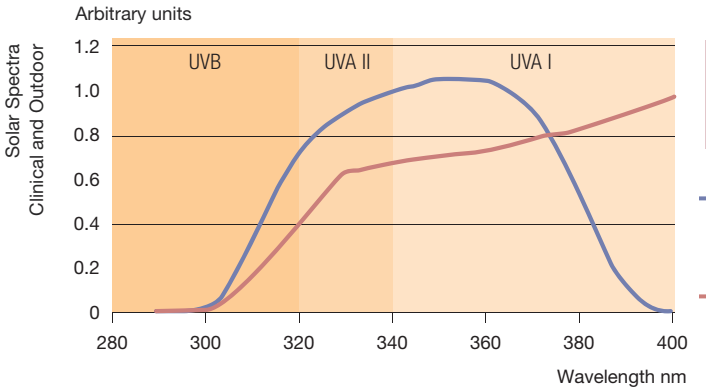
Clinical (International Method)	Outdoor Exposure
Solar Simulated Lamp	**Outdoor Sun Spectrum**
SPF (SSL): 52.9	SPF (outdoor): 40.2
Rating/LABEL: 50	**(Rating: 30)**





Clinical SPF is overestimated

More UVB in sunlight for clinical testing



More UVA I in outdoor sunlight

Sunlight for clinical testing (e.g. COLIPA)

Outdoor = midday midsummer sunlight at 40°N

UVA Indices ...
Broad-Spectrum Sunscreen

Example

A

Broad-spectrum

Input

Region: Europe
Application Amount: 2.0 mg/cm²

Date: 2010/03/18 14:52:00

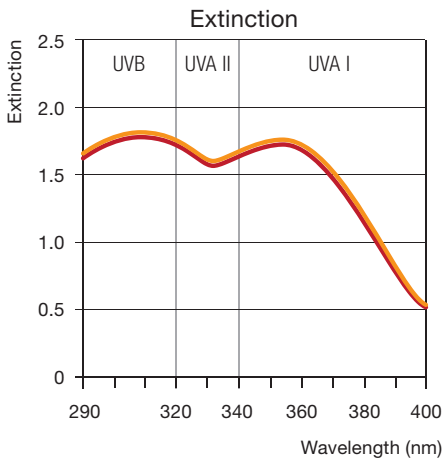
UV Filter Composition

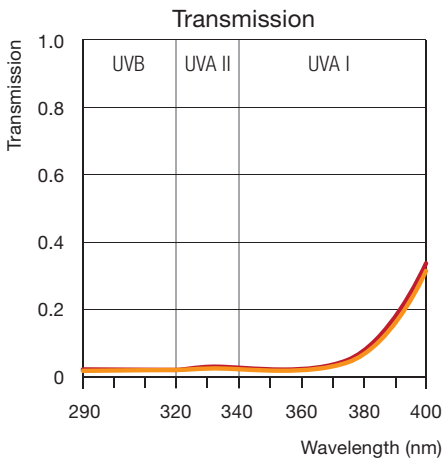
INCI Name	USAN Name	Abbreviation	Amount
Bis-Ethylhexyloxyphenol Methoxyphenyl Triazine (Tinosorb® S)	Bemotrizinol	BEMT	2.0%
Bis-Ethylhexyloxyphenol Methoxyphenyl Triazine (Tinosorb® S Aqua, active)	Bemotrizinol	BEMT	1.0%
Diethylamino Hydroxybenzoyl Hexyl Benzoate (Uvinul® A Plus)	–	DHHB	8.0%
Ethylhexyl Triazone (Uvinul® T 150)	Octyltriazone	EHT	2.5%
Phenylbenzimidazol Sulfonic Acid	Ensulizole	PBSA	3.5%
TiO_2 water phase	Titanium Dioxide	TiO_2	2.5%
		Total:	19.5%

UVA Indices

Country	in vivo	in vitro	Rating
EU/CH	**Simulated PPD** UVA: 20.3 Critical wavelength: 379.0 nm	**EC Recommendation (UVA-PF/SPF > 0.33)** UVA-PF: 20.4 UVA-PF/SPF: 0.6	UVA
	Labeled SPF: 50.0	UVA-PF: 26.8 (re-calculated) UVA-PF/SPF: 0.54	UVA
USA	**FDA Proposed Rule** UVA-PF (PPD): 20.3	**FDA Proposed Rule** UVA-I/UV ratio: 0.89	★★★☆ **High**
GBR		**Boots Star-Rating: UVA/UVB ratio** w/o irradiation: 0.82 with irradiation: 0.82	UVA ★★★ SUPERIOR
		Spectral Uniformity Index SUI: 15.3	**Very High**
JAP	**JCIA Rating** UVA-PF (PPD): 20.3		**PA+++**
AUS		**Australian UVA Standard**	**PASS**

UV Protection Profile





1) Profiles before (Initial) and after (Final) irradiation dose of SPF x MED (1 Minimal Erythema Dose passes trough sunscreen)

® = Registered trademark of BASF group

BASF Sunscreen Simulator

The innovation tool for formulators reduces time to market by rapid prototyping:

- **Explore formulation space**
- **Check photostability**
- **Test *in silico* before expensive *in vitro* or *in vivo* testing**

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

Sunburn Protection Factor (SPF)

- Check sunscreen at different application amounts:
  – 0.5, 1.0, 1.5, **2.0**, 2.5 and 3.0 mg/cm^2
- Check sunscreen performance:
  – According to international SPF method
  – Under outdoor conditions
- Only broad-spectrum sunscreens provide realistic SPFs under clinical testing and outdoor conditions.

UVA-Protection Indices

- UVA-PF/SPF ratio (EC recommendation: ≥ 1/3)
- Critical Wavelength (EC recommendation: > 370 nm)
- UVAI/UV (US proposed rule, 4-star-rating)
- UVA/UVB ratio (Boots 5-star-rating)
- Spectral Uniformity Index (SUI)
- UVA-PF (PPD after JCIA, AFSAPS, COLIPA)
- Australian UVA Standard (pass/fail)

The BASF Sunscreen Simulator assists in the exploration of the formulation space thus helping in the optimization of the active ingredients in a sunscreen formulation. However, it does not replace actual formulary testing.

www.basf.com/sunscreen-simulator

Europe, Africa, West Asia

BASF SE
Personal Care Ingredients Europe
67056 Ludwigshafen, Germany
personal-care-eu@basf.com
Phone: +800 2273 4444
Fax: +49 621 60 76992

BASF ChemTrade GmbH
Industriestraße 20
91593 Burgbernheim, Germany
info-chemtrade@basf.com
Phone: +49 9843 98 28 0
Fax: +49 9843 98 28 900
www.basf-chemtrade.de

North America

BASF Corporation
Personal Care Ingredients
100 Campus Drive
Florham Park, NJ 07932, USA
personal-care-na@basf.com

U.S. and Canada

Phone: +1 800 880 5768
Fax: +1 973 245 6764

Mexico

Phone: +1 800 723 3000
Phone: +1 800 552 4288

South and Central America

BASF S.A.
Personal Care Ingredients
Av. Brigadeiro Faria Lima, 3600
04538-132 São Paulo, Brazil
personal-care-sa@basf.com
Phone: +55 11 3043 2284
Fax: +55 11 3043 2255

Asia Pacific

BASF East Asia
Regional Headquarters Ltd.
Personal Care Ingredients
45/F Jardine House
No.1 Connaught Place
Central, Hong Kong
personal-care-hk@basf.com
Phone: +852 2731 0190
Fax: +852 2731 5639

Personal Care Ingredients

BASF offers one of the most comprehensive ingredients portfolio in the personal care industry. It is designed to meet the customers' needs in the HairCare, SunCare, SkinCare, ColorCare, BodyCare and OralCare markets. The high quality product range includes e. g. polymers, UV filters, effect pigments, actives, hair dyes and surfactants. BASF constantly strives to anticipate the requirements of the personal care market and creates innovative products for the sustainable development of the industry.

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Labeling
Details about the classification and labeling of our products and further advice on safe handling are contained in the current safety data sheets.

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