



# Gentle Preservatives & Innovative Emollients from LANXESS

Consumer-Friendly Chemistries to Fit Today's Customers' Needs

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September 27th, 2023

# LANXESS Segmentation

## Consumer Protection



- **Flavors & Fragrances**
- Liquid Purification Technologies
- Material Protection Products
- Saltigo

## Specialty Additives



- Lubricant Additives
- Polymer Additives
- Rhein Chemie

## Advanced Intermediates



- Advanced Industrial Intermediates
- Inorganic Pigments

**With the acquisition of Emerald Kalama Chemical, LANXESS has formed a new business unit within the Consumer Protection segment, called Flavors & Fragrances (F&F).**

# Flavors & Fragrances Global Reach

Using the highest quality standards at our facilities in the USA, Europe, and Asia

## Headquartered in Cologne, Germany

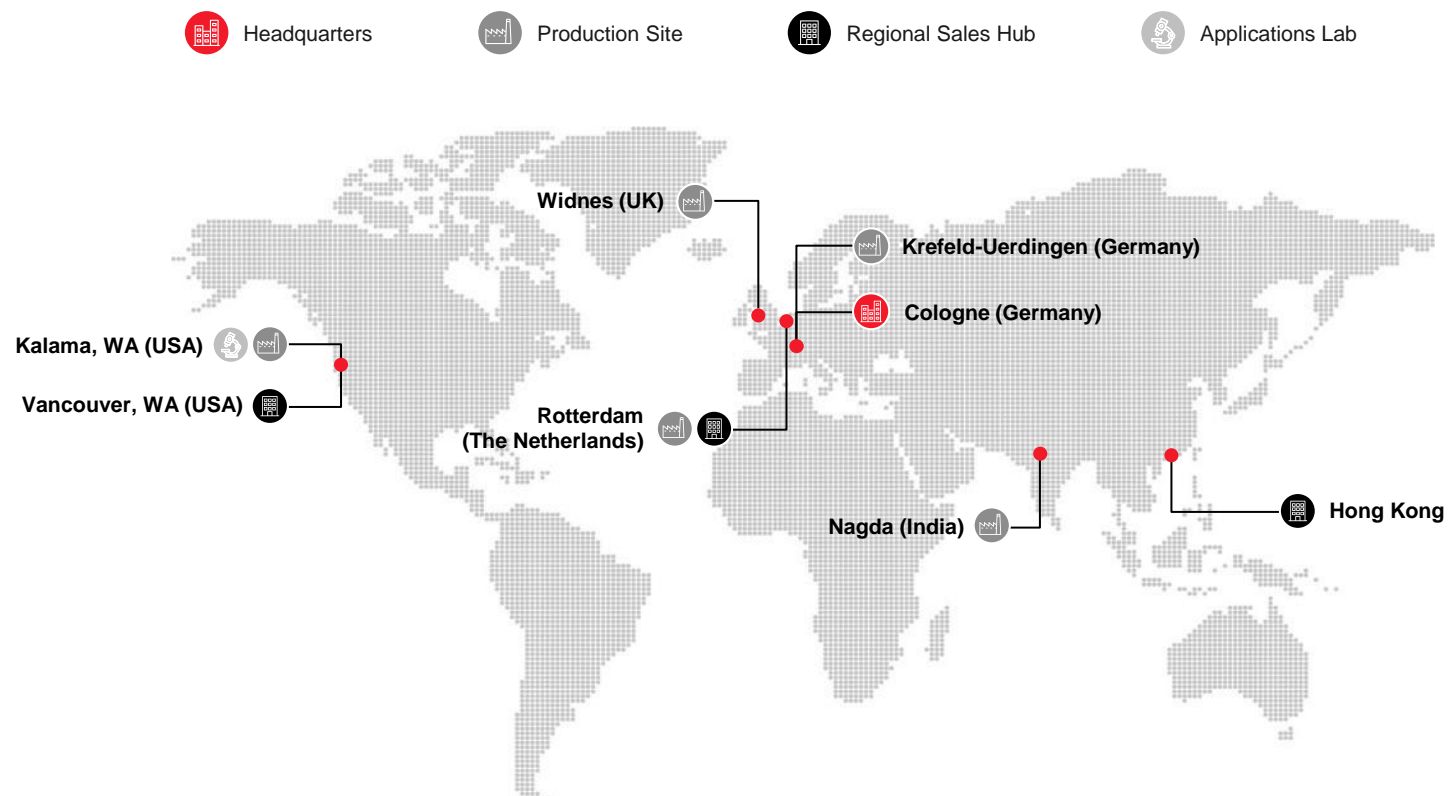
### ▪ 5 production sites

- Backward integrated in benzoic acid and benzaldehyde, offering a strategic advantage
- Multiple production locations for key products
- Certified to meet the highest industry standards for quality and HS&E

### ▪ ~50 products

### ▪ ~750 employees

### ▪ Worldwide sales and distributor network



# Sustainability Goals

LANXESS aims to play an active role in shaping a more sustainable world

## Net Zero Value Chain Initiative

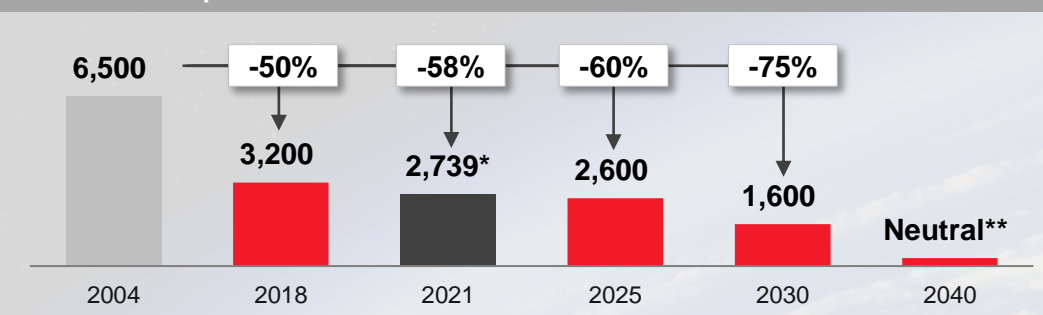
- Replacement of fossil-based feed-stock by
  - Bio-based feed-stock 🌿
  - Circular origin feed-stock ♻️
- “Net Zero Value Chain” by 2050
- Decouple emissions and growth
- Pursue technological innovations
- ISCC Plus certification is in progress



Coming soon: Certified renewable products including sodium benzoate, benzyl alcohol, and others

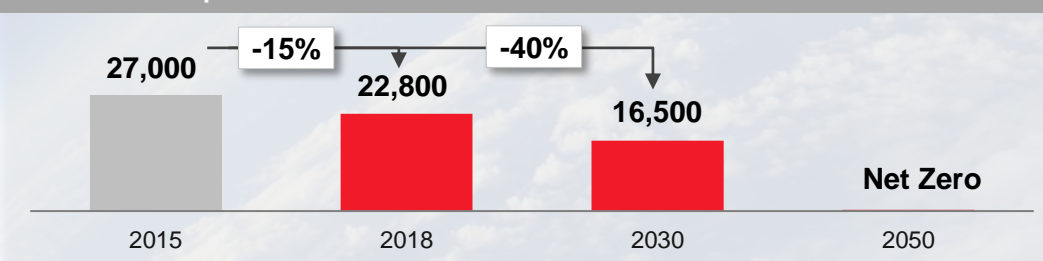
## CLIMATE NEUTRAL 2040

LANXESS Scope 1+2 emissions



## NET ZERO VALUE CHAIN

LANXESS Scope 3 emissions



\* On the basis of the current portfolio with Emerald Kalama Chemical and Theseo Group

\*\* <300kt CO<sub>2</sub>e emissions per year, reduced by compensation measures

# F&F's Trusted Family of Brands

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## Benzoates & Antimicrobials

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*Purox*<sup>®</sup>

The highest purity benzoates  
available worldwide

 **Kalaguard**<sup>®</sup>

The only BPR & EPA FIFRA  
registered sodium benzoate  
preservative

**X Solbrol**<sup>®</sup>

Effective preservatives for  
every formulation

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## Fragrance, Functionality & Freshness

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**X Purolan**<sup>®</sup>

High purity multifunctionals and  
aroma ingredients

**Kalama**<sup>®</sup>

High purity, consistent aroma  
ingredients and benzoates

## Green, Consumer Friendly, Easy-to-Use Preservative

INCI: Sodium Benzoate



### Sustainable

- Nature identical, readily biodegradable
- Listed by Nordic Swan, EU Ecolabel, others



### Gentle

- Classified as non-irritating and non-sensitizing to the skin
- Odorless, and non-discoloring



### Effective

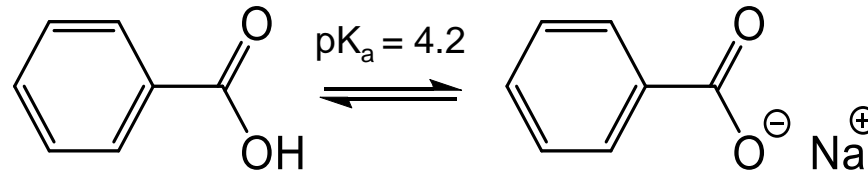
- Broad activity against bacteria, yeast, and mold
- Cost-effective preservation up to pH 6.5



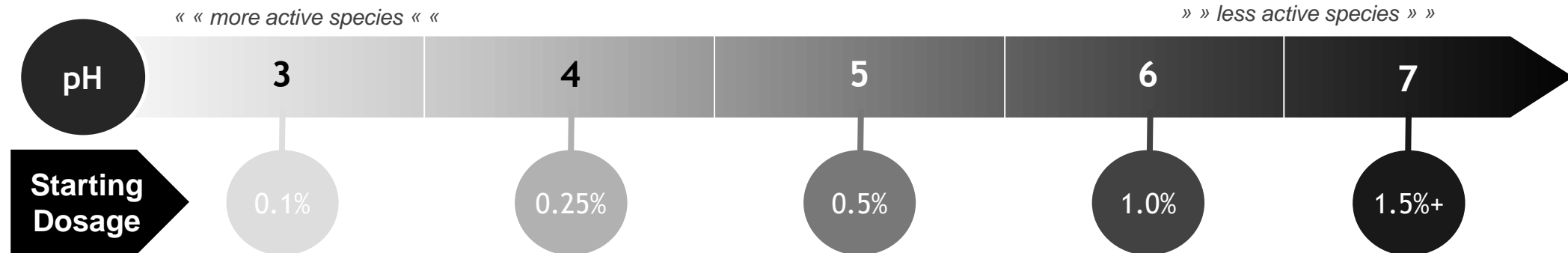
**Purox<sup>®</sup> S Sodium Benzoate is a gentle, effective, and cost-conscious preservative effective up to pH 6.5**

# Sodium Benzoate – Organic Acid Preservative

**pH must be considered when using sodium benzoate**



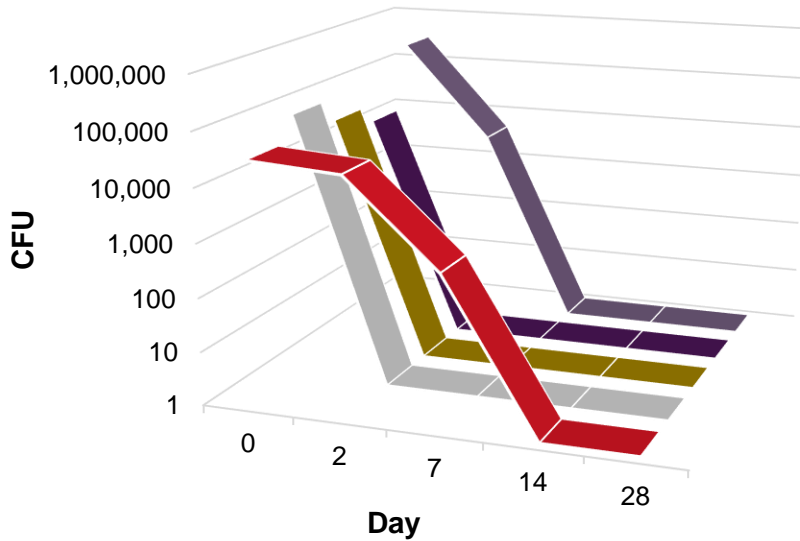
**Active Species for Preservation**



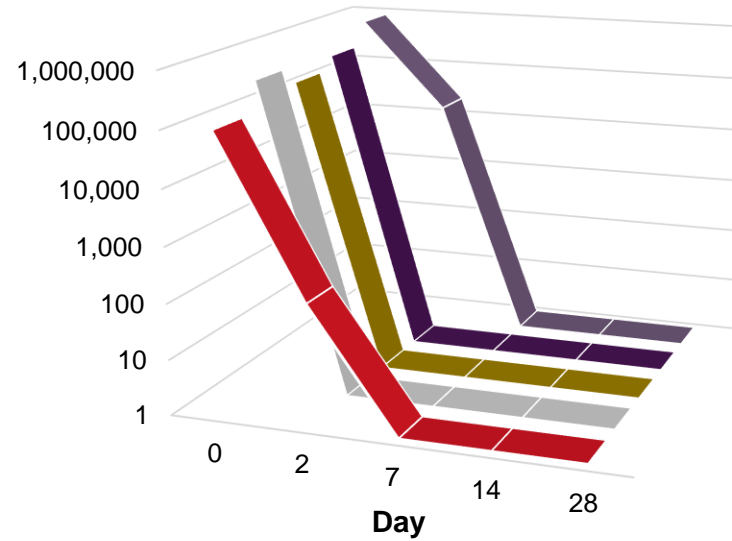
**Acidic environments favor higher activity of the acid preservative**  
**Many factors impact preservative requirements, so more or less may be required**

# Lower pH: Body wash

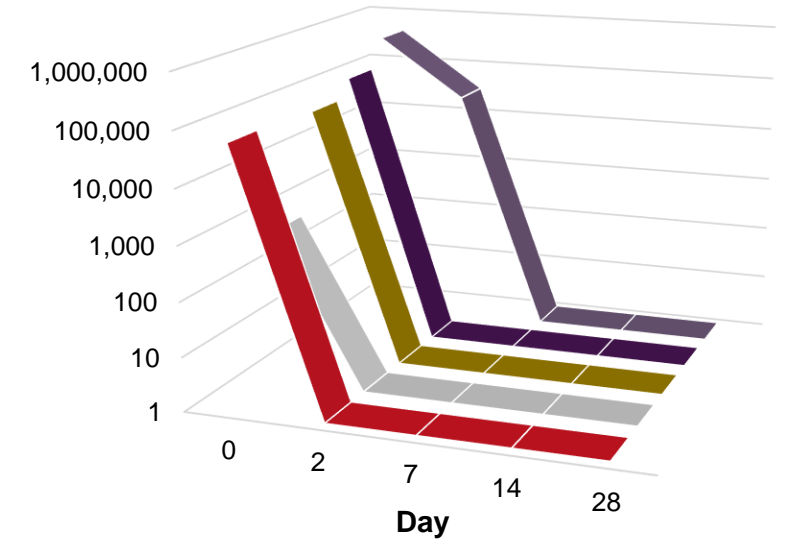
### 1.5% Purox® S, pH 6.5



### 1.0% Purox® S, pH 6.0



### 0.25% Purox® S, pH 4.5



■ *E. coli* ■ *S. aureus* ■ *P. aeruginosa* ■ *C. albicans* ■ *A. brasiliensis*

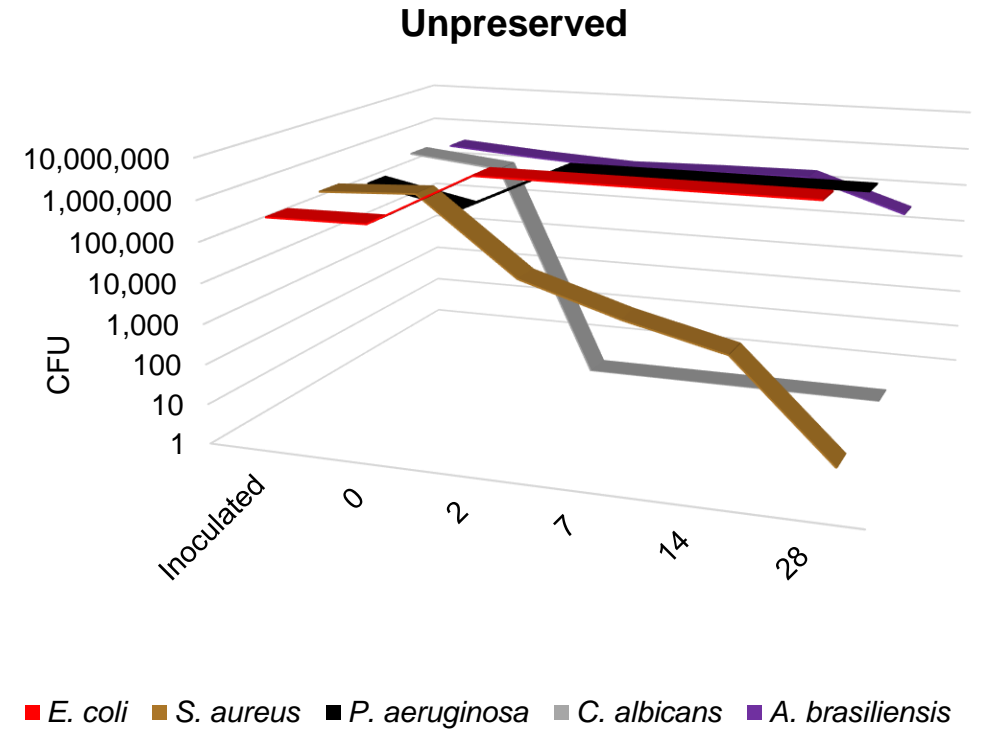
Lowering pH is a cost-effective solution to maximize the antimicrobial efficiency of Purox® S sodium benzoate.



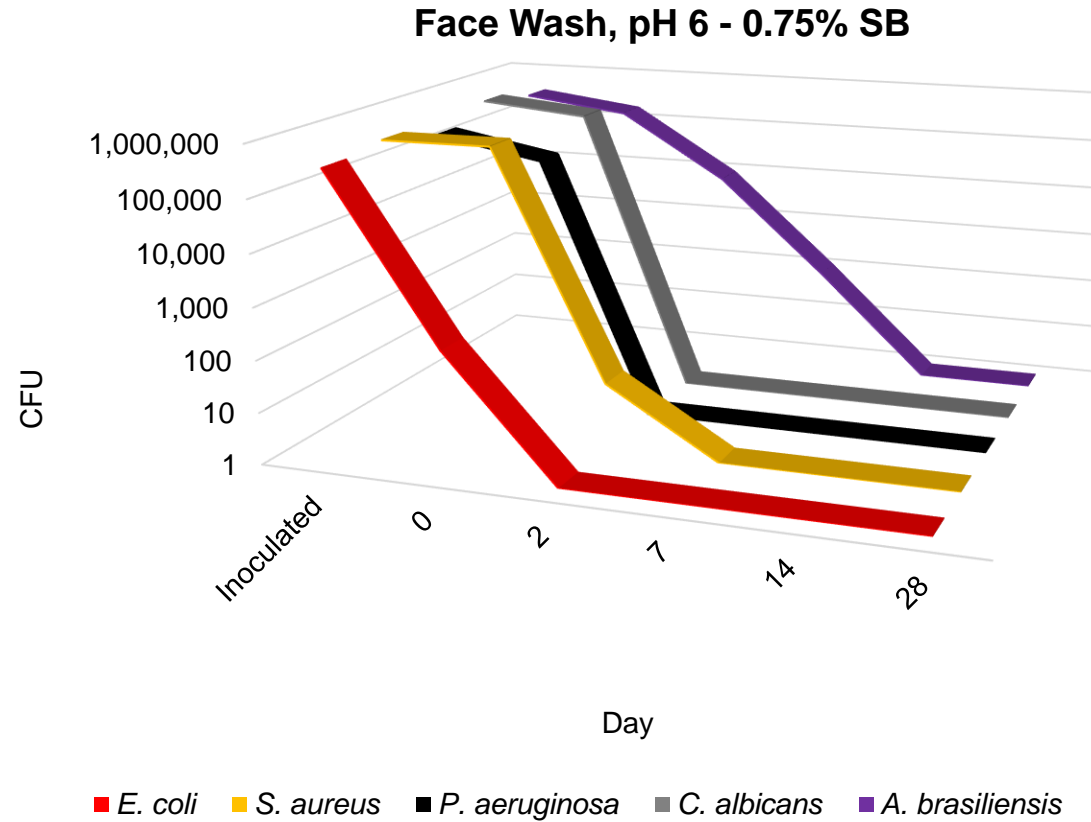
# Face Wash, pH 6.0

Stage	Ingredient Name	Function	Wt%
A	Water	Carrier	Q.S.
	PEG-150 Distearate	Rheology Modifier	0.70
	Glycerin	Humectant	0.75
B	Sodium Methyl Cocoyl Taurate	Surfactant	4.90
	Sodium Lauryol Methyl Isethionate	Surfactant	1.35
	Cocamidopropyl Betaine	Surfactant	3.60
	Baypure® CX-100	Chelating agent	0.15
	Sodium Imminodisuccinate		
C	<b>Purox® S Sodium Benzoate</b>	<b>Preservative</b>	<b>0.75</b>
	Bisabolol	Soothing agent	0.25
	Citric Acid	pH adjuster	to 6.0

Method: EP Challenge Criteria



# Purox<sup>®</sup> S – Face Wash at pH 6.0



- Bacterial control
- Fungal control

Face wash at pH 6.0 exhibits strong microbial protection with 0.75% Purox<sup>®</sup> S



# Combining Preservatives in Personal Care

Benzyl Alcohol with Sodium Benzoate

# Kalama<sup>®</sup> Benzyl Alcohol

INCI: Benzyl alcohol

## Personal Care Preservative

- Effective across broad pH range (3.0 – 8.5)
- Typical dosage 0.1 - 1.0 wt.% of total formula
- Colorless liquid, easily incorporated into formulations
- Minimal impact on viscosity and formula stability
- Broad-spectrum preservative properties
- Minimum purity of 99.9% (for FCC grade)

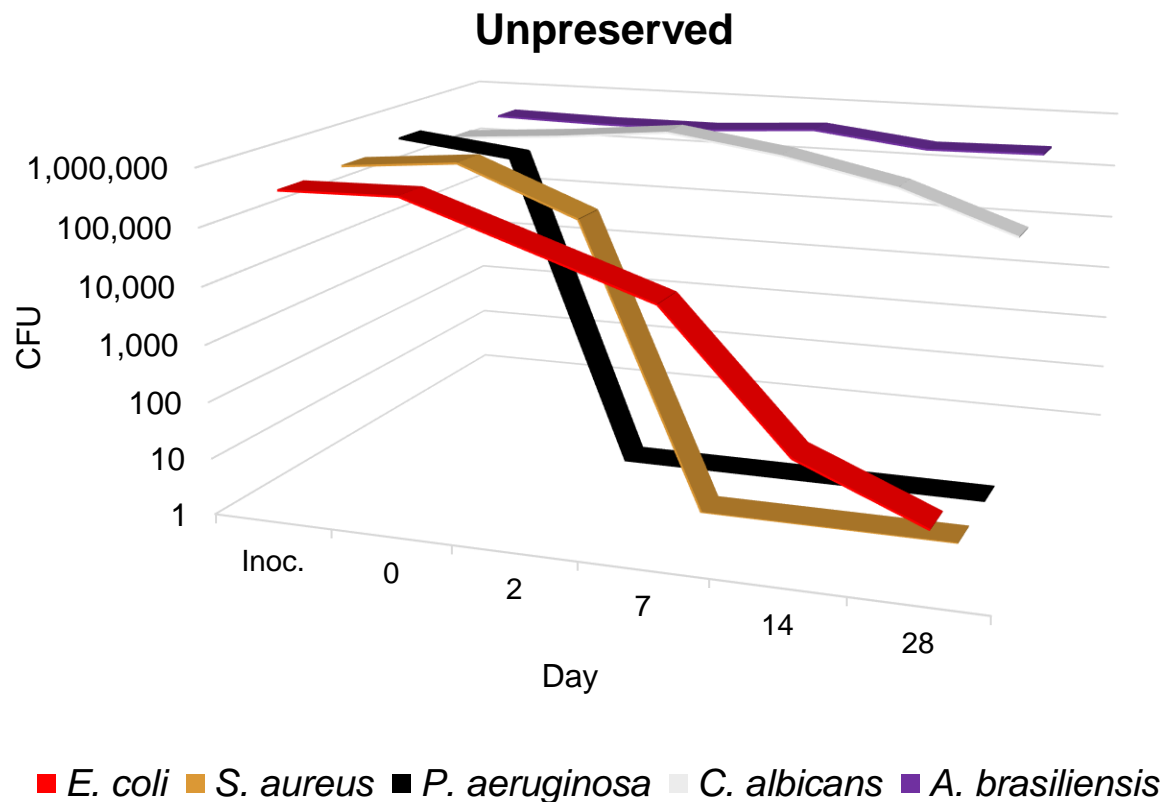


**Broad-spectrum preservative with great applications in hair care**

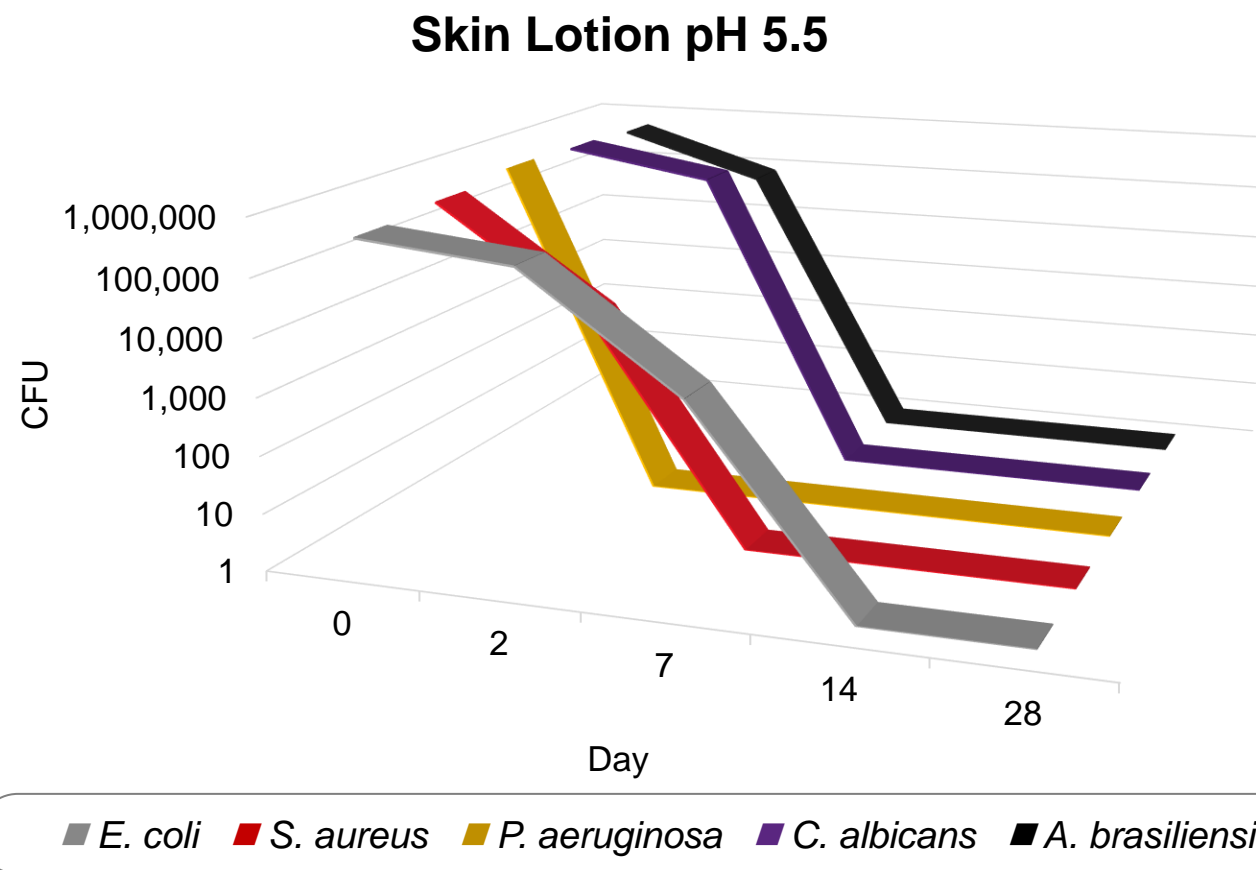
# Kalama® Benzyl Alcohol – Skin Lotion

Stage	Ingredient Name	Function	Wt%
A	Water	Carrier	Q.S.
	Glycerin	Humectant	5.0
	Xanthan Gum	Rheology Modifier	0.1
B	Cetearyl Alcohol	Rheology Modifier	3.0
	Steareth-21	Emulsifier	2.0
	Steareth-2	Emulsifier	2.0
	Paraffinum Liquidum	Emollient	5.0
	Petrolatum	Emollient	2.0
C	<b>Purox® S Sodium Benzoate</b>	<b>Preservative</b>	<b>0.5</b>
	<b>Kalama® Benzyl Alcohol</b>	<b>Preservative</b>	<b>0.5</b>
	Citric Acid/Sodium Hydroxide	pH adjuster	to 5.5

Method: EP Challenge Criteria



# Skin Lotion with Purox<sup>®</sup> S & Kalama<sup>®</sup> Benzyl Alcohol



**0.5% Purox<sup>®</sup> S Sodium Benzoate, 0.5% Kalama<sup>®</sup> Benzyl Alcohol work together to preserve skin lotion at pH 5.5.**



**LANXESS**  
Energizing Chemistry

# Multifunctional Ingredients for Personal Care & Cosmetics

# Kalama<sup>®</sup> 3PP Multifunctional

INCI: 3-Phenylpropanol

## Personal Care Solvent & Synergist

- Odor masking, intrinsic light fragrance
- Typical dosage 0.1 - 0.5 wt.% of total formula
- Desirable HSE profile
  - **Readily biodegradable**
  - **Non-sensitizing**, low toxicity, nature identical
- FCC grade, Generally Recognized As Safe (FDA GRAS)
- TSCA Approved, REACH registered



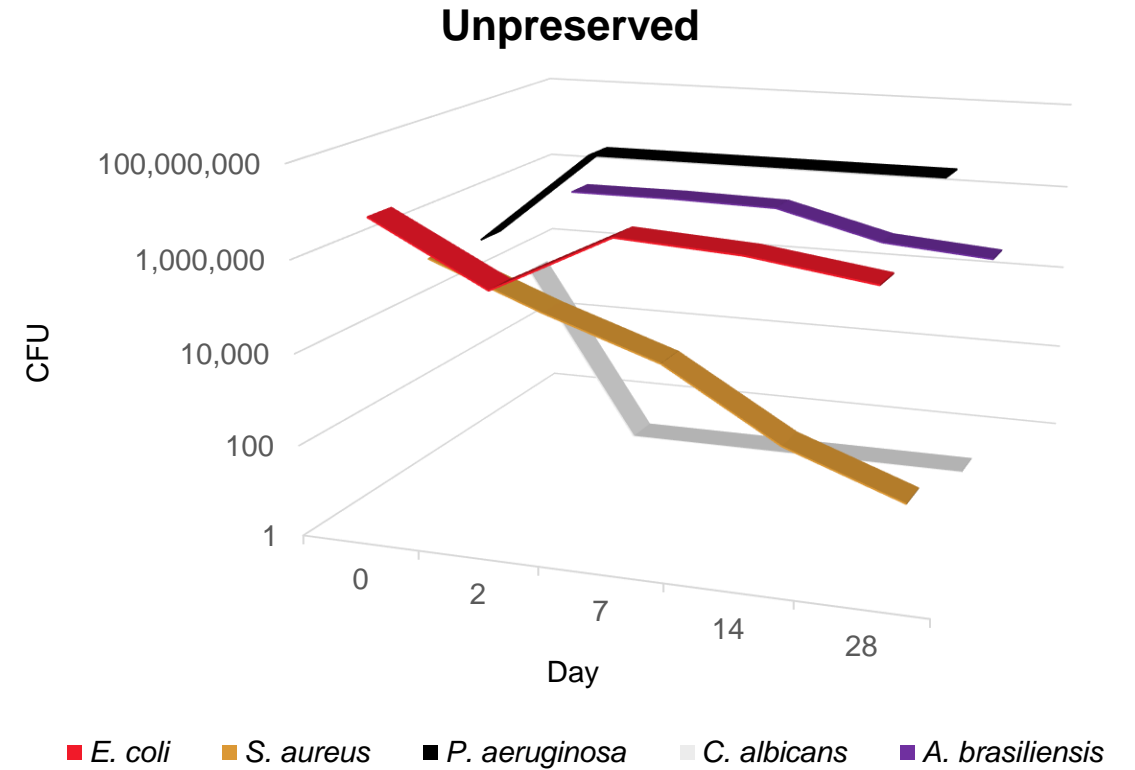
Effective across broad pH range 2.0 – 10.0





# Body Wash Base, pH 6.5

Stage	Ingredient Name	Function	Wt%
A	Water	Carrier	Q.S.
	Sodium Laureth Sulfate	Surfactant	12.0
	Lauryl / Myristyl Glucoside	Surfactant	4.0
	Sodium Coco Fatty Alcohol Sulfate	Surfactant	3.0
B	<b>Purox® S Sodium Benzoate</b>	Preservative	1.0
	<b>Kalama® 3PP</b>	Multifunctional	0.2
	Sodium Chloride	Viscosity Builder	1.0
C	Citric Acid	pH adjuster	to 6.5

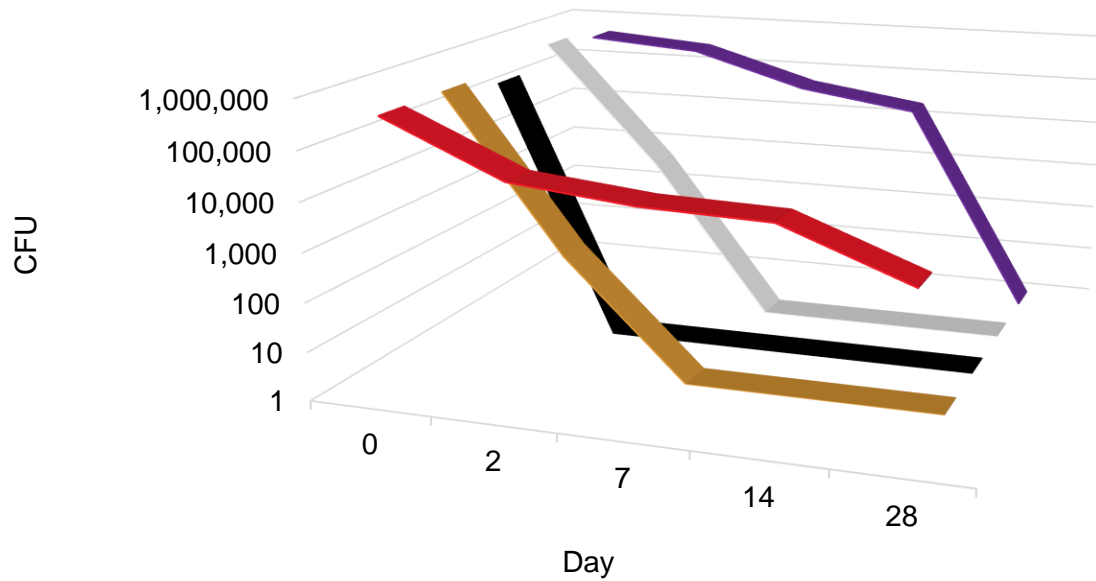


Method: EP Challenge Criteria

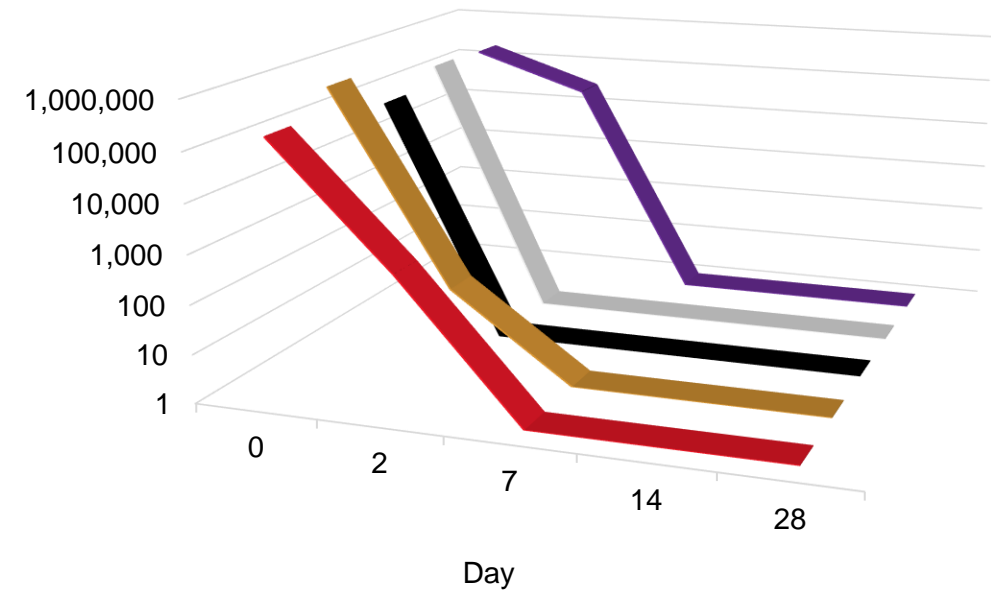


# Body Wash Base, pH 6.5

### 1.0% Purox® S



### 1.0% Purox® S + 0.2% Kalama® 3PP



■ *E. coli* ■ *S. aureus* ■ *P. aeruginosa* ■ *C. albicans* ■ *A. brasiliensis*

Combination of Kalama® 3PP and Purox® S sodium benzoate results in control against all microbes at day 7

# **PUROLAN® Isoparaffins as Silicone Replacements**

Characterization and Analysis of Critical Personal Care Properties

Cyclomethicones and dimethicones face de-selection and regulation due to bio-persistence.

## PUROLAN® IDD – *Isododecane (C12)*

- Solvent
- Fast drying, superb spreadability
- Excellent for color cosmetics, deodorants, hair care
- Alternative for cyclopentasiloxane (D5)

## PUROLAN® IHD – *Isohexadecane (C16)*

- Solvent, emollient
- Silky, lightweight on skin & hair
- Great for hair, skin, & sun care
- Alternative for polydimethylsiloxane/dimethicone

PUROLAN® Isoparaffins are a cost-competitive alternative without compromising performance.

# Challenges Against Silicones

- EU restrictions

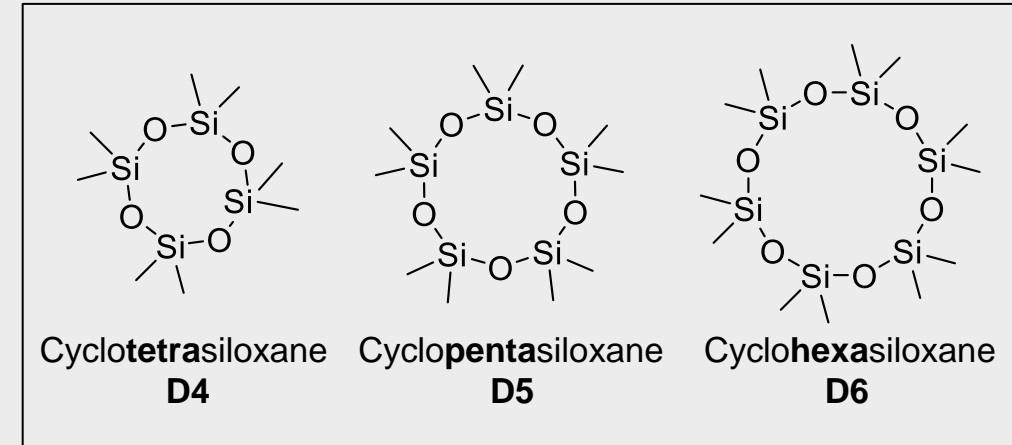
- The two most common siloxanes (D4 and D5) are currently limited to 0.1% in rinse-off applications

- Bioaccumulation

- All 3 cyclic siloxanes are listed as “Persistent, Bioaccumulative, and Toxic” by EU, and are *Substances of Very High Concern*

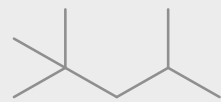
- Increasing price of US-manufactured silicones

- Consumer stigma against silicones in hair care, as some high molecular weight silicones can build up in hair

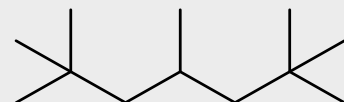


# Overview of Isoparaffins

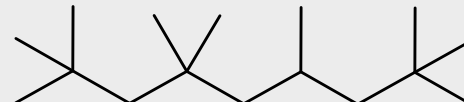
- Isododecane (IDD) and isohexadecane (IHD) are highly branched, lipophilic, alkanes derived from petroleum
- Highly branched structure mimics silicones due to numerous methyl groups on the outer surface of the molecule
- Generally, have a similar or better safety, toxicity, and flammability profile when compared to equivalent silicones
- Other waxy ester replacements can have similar skin feel and emollience, but lack volatility, low surface tension, and high spreadability



**Isooctane**  
PUROLAN® IOC



**Isododecane**  
PUROLAN® IDD



**Isohexadecane**  
PUROLAN® IHD

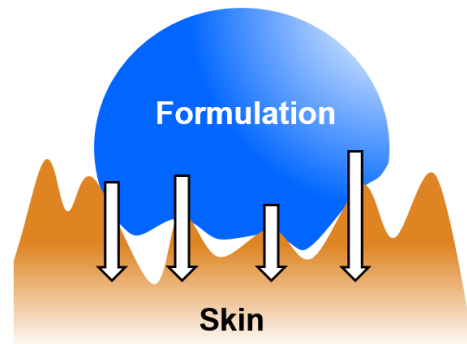


**Isoeicosane**  
PUROLAN® IEC

# Low Viscosity + Low Surface Tension = High Spreadability

## High viscosity, high surface tension

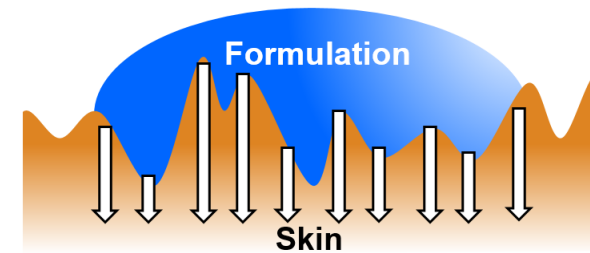
example: castor oil



- poor spreadability
- small contact area
- limited skin penetration

## Low viscosity, low surface tension

example: isoparaffins



- good spreadability
- large contact area
- excellent skin penetration

**Isoparaffins allow for easily applied and fast-absorbing formulations**

# Spreadability in Personal Care

- Spreadability is a highly desirable trait for hair and skin care products
- Liquid ingredients with very low viscosity and low surface tension can easily disperse throughout the hair, carrying natural oils and other emollients at lower levels to produce an evenly distributed, lightweight, non-greasy after-feel.
- Non-polar ingredients (silicones, isoparaffins, waxy esters, etc) with high spreadability tend to impart a luxurious feel to lotions and creams when used at moderate levels (1-5%).

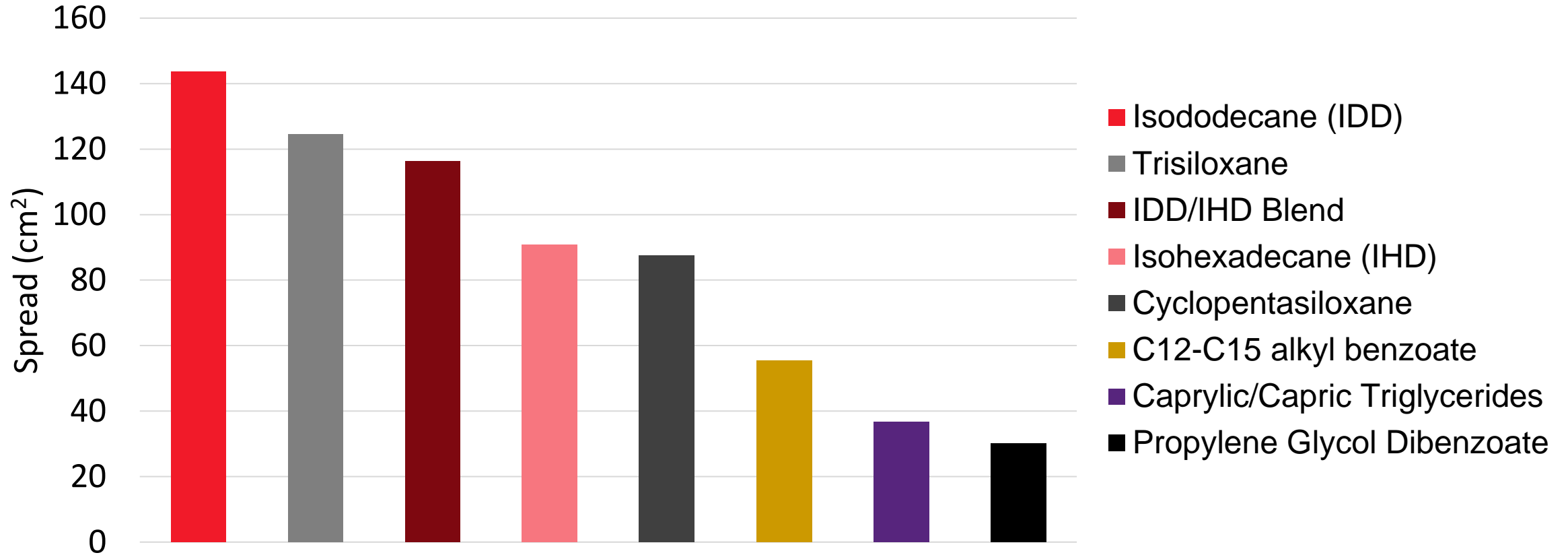


**High spreadability is closely associated with more desirable sensory profiles**



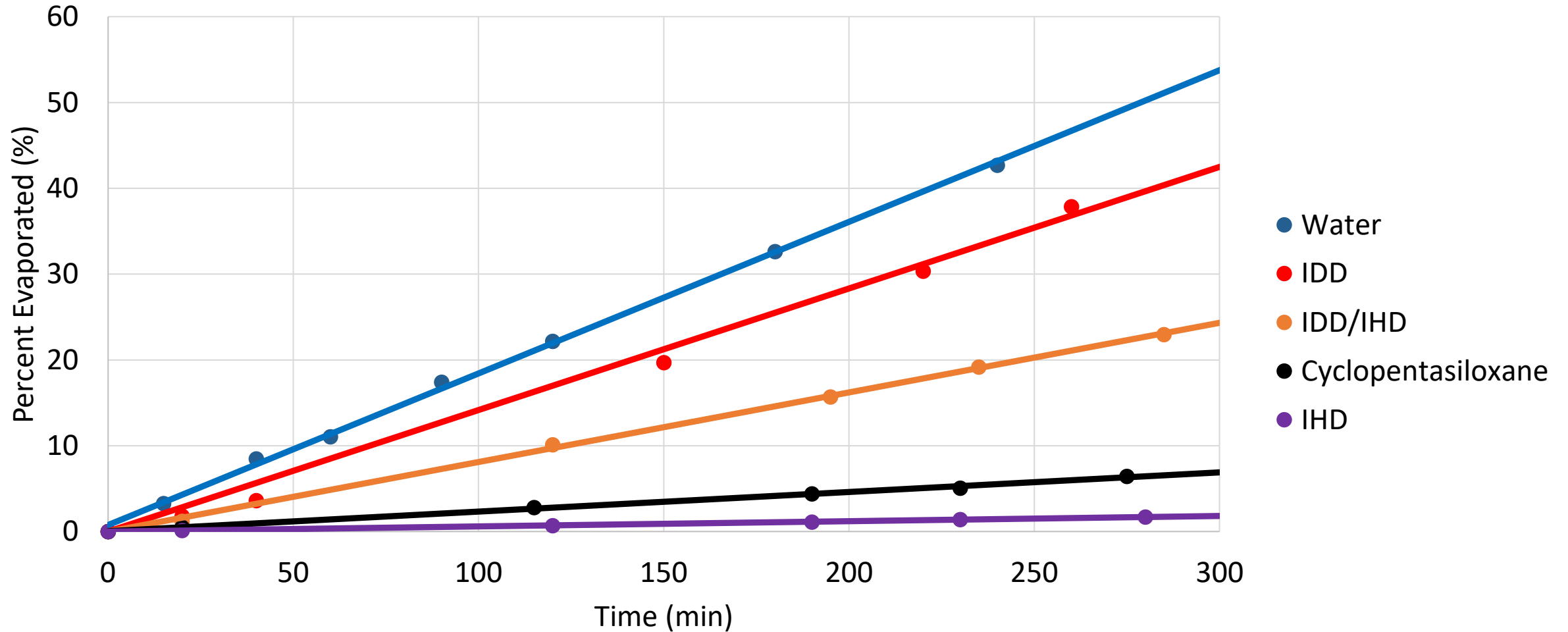
# Spreadability of Various Emollients

Parallel plate method



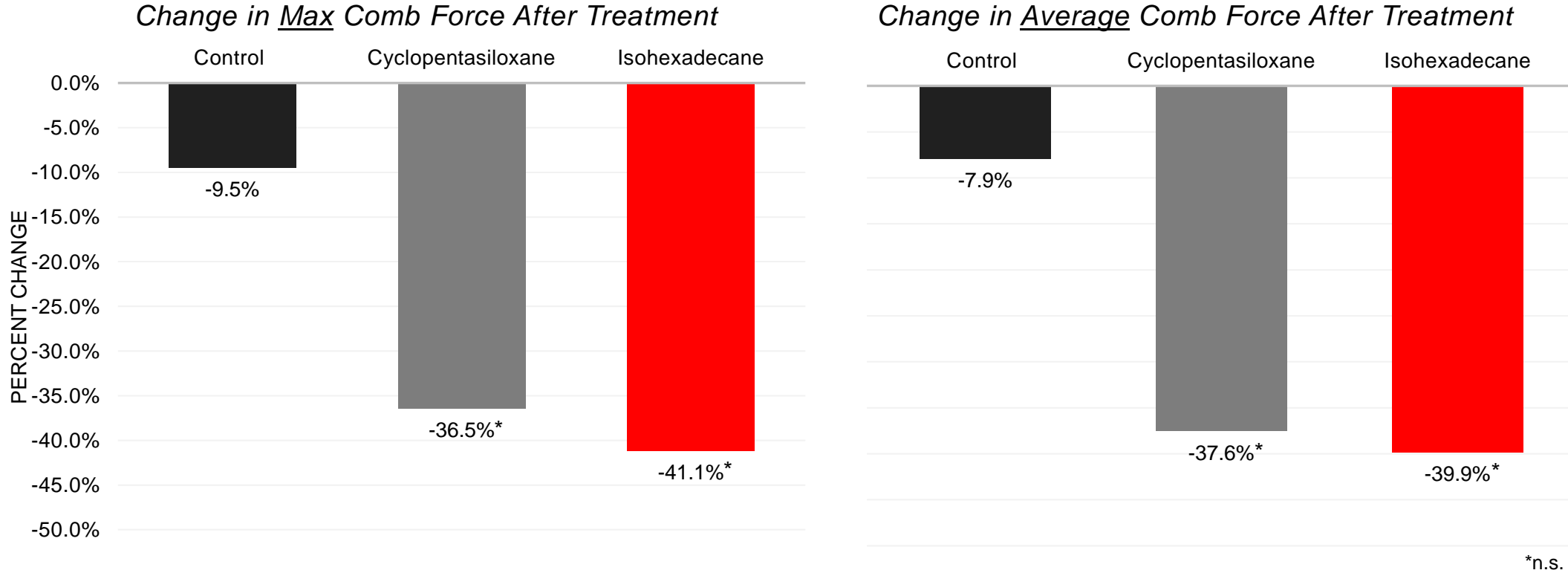
**Isoparaffins demonstrate superior spreadability when compared to analogous silicones**

# Evaporation Rate



Through blending, isoparaffins exhibit tunable volatility to achieve a range of evaporation rates

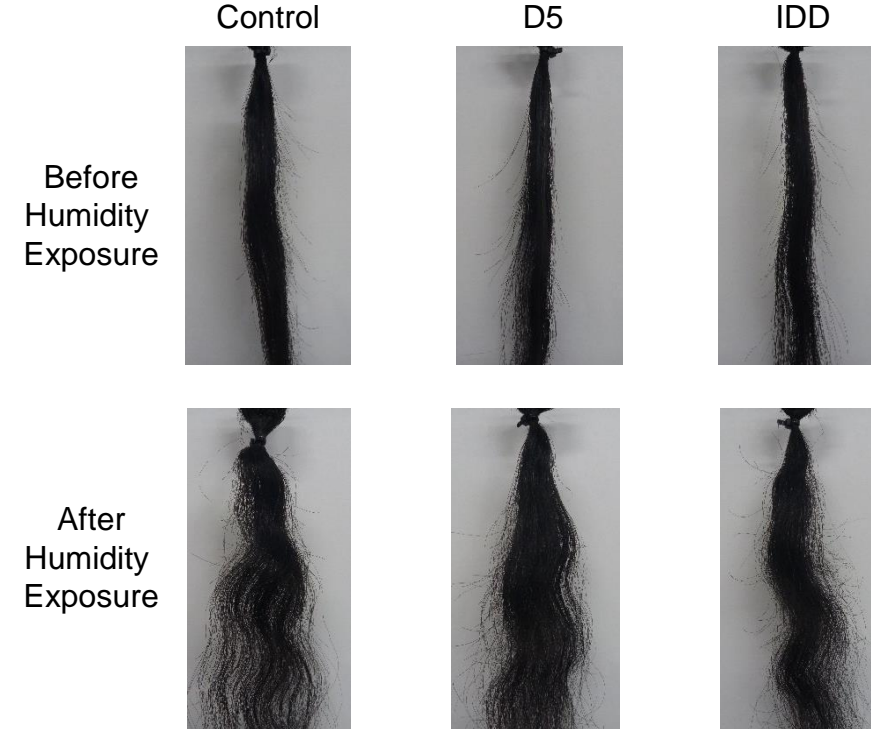
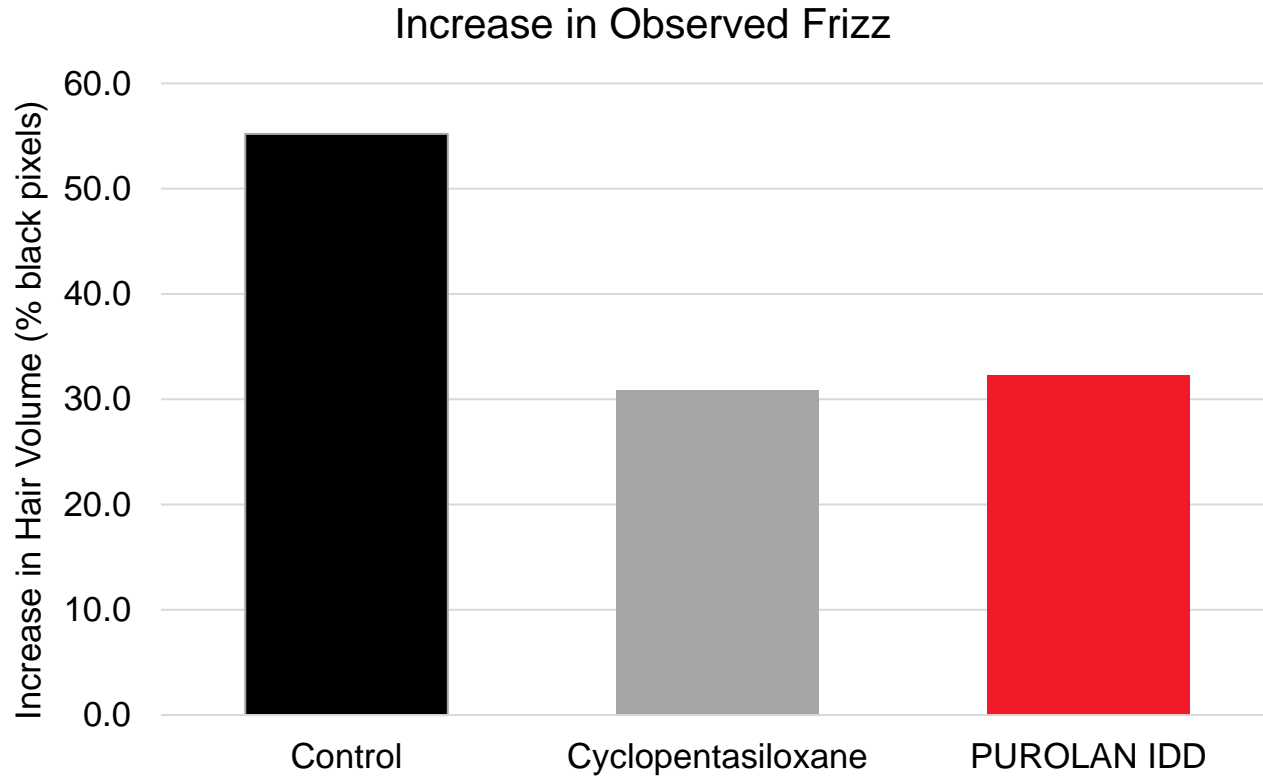
# IHD Performs Well in a Hair Combability Test



***When blended into a conditioner at 3%, isohexadecane (IHD) shows equal performance to cyclopentasiloxane (D5) at reducing maximum and average combing forces***

**IHD matches the performance of D5 at reducing combing forces in wet hair**

# IDD Reduces Humidity-Induced Frizz

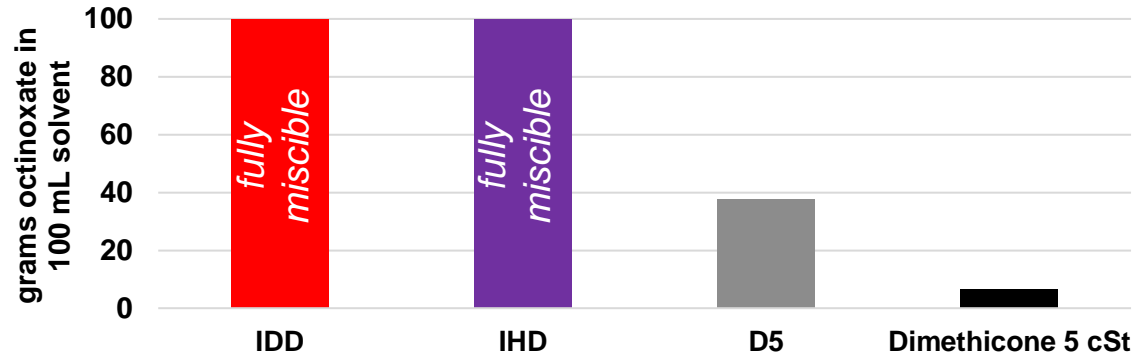


***When applied to dry hair prior to very high temperature (410 °F, 10 x) straightening, PUROLAN® IDD reduces the frizz effect when exposed to 3 h of 95% humidity as much as cyclopentasiloxane***

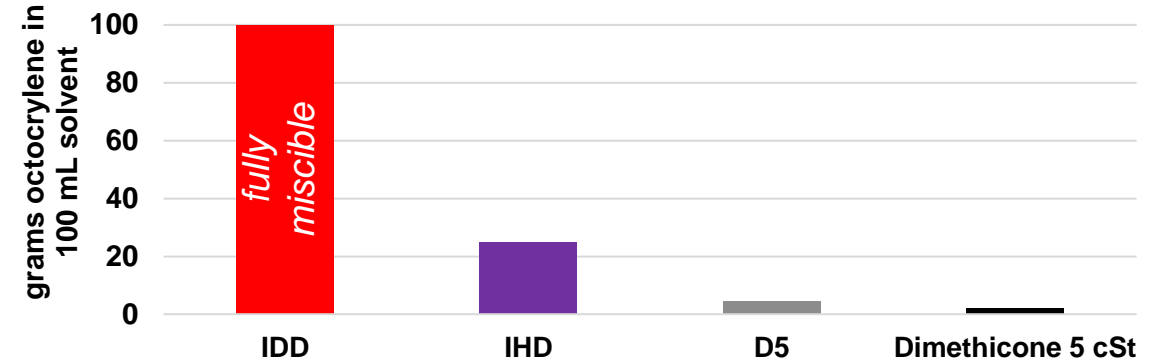
**ID matches the performance of D5 at reducing humidity-induced frizz**

# PUROLAN Isoparaffins Demonstrate Superior UV Filter Solubility

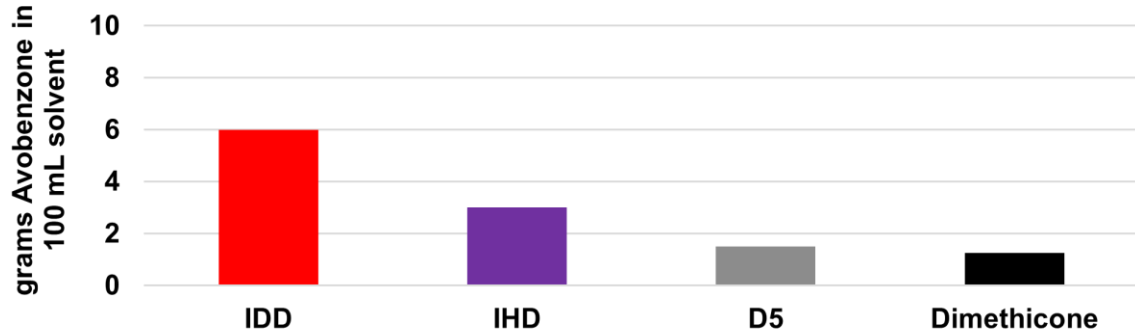
### Octinoxate Solubility



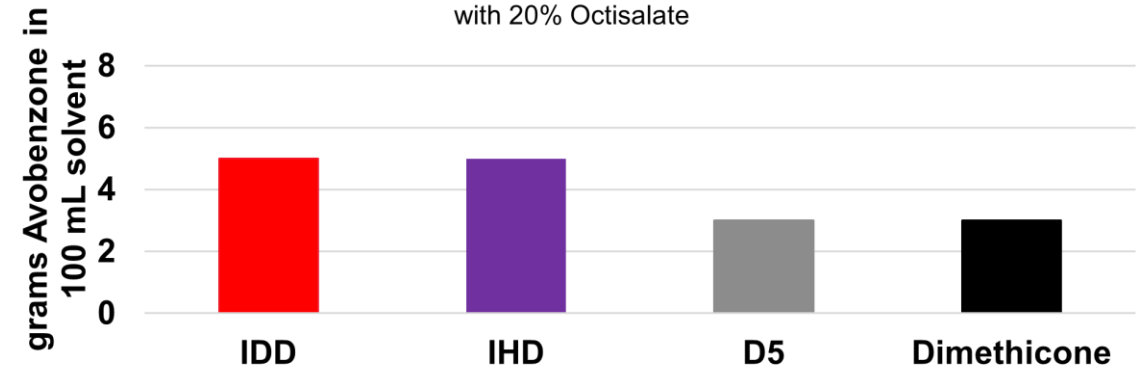
### Octocrylene Solubility



### Avobenzone Solubility with 15% C12-C15 Alkyl Benzoate



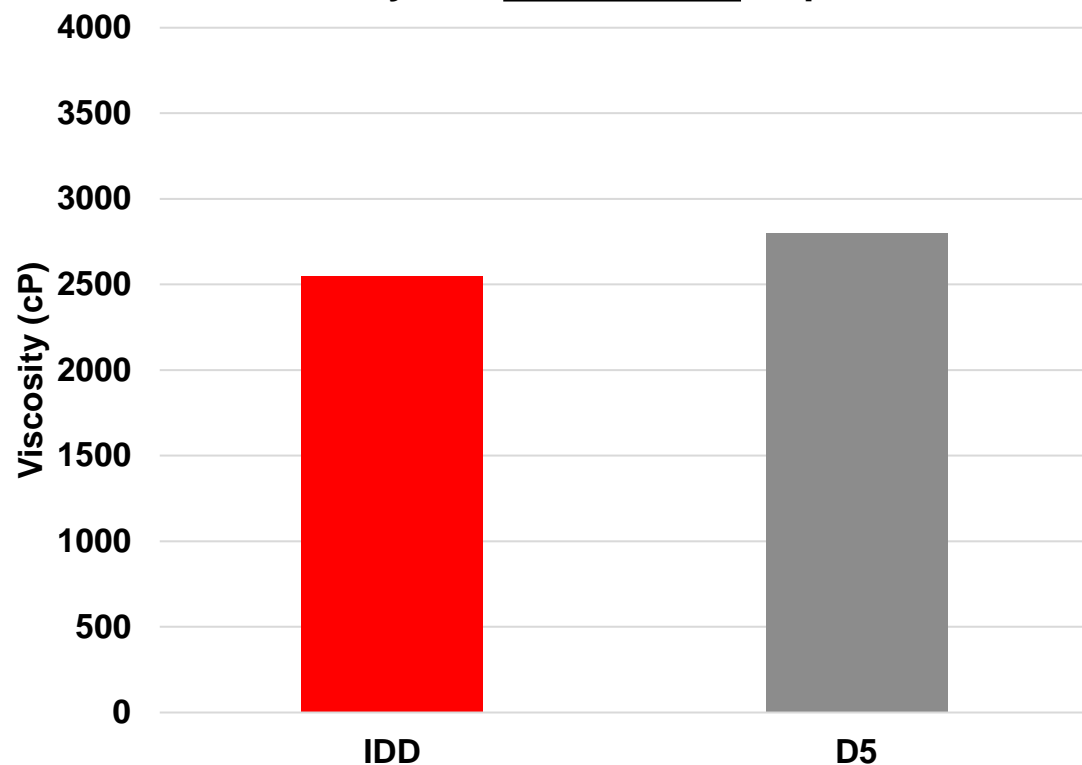
### Oxybenzone Solubility with 20% Octisalate



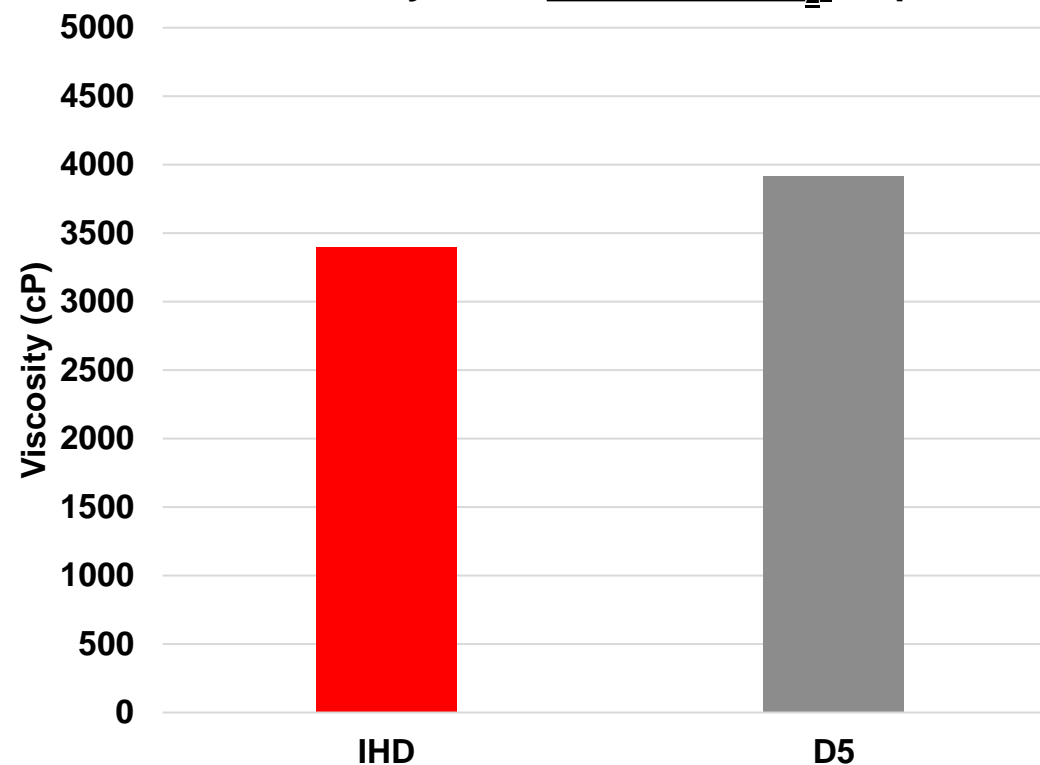
**Both IDD and IHD are superior at solubilizing UV filters than silicones**

# Dispersion of Mineral UV Filters

### Viscosity of a Coated ZnO Dispersion



### Viscosity of an Uncoated TiO<sub>2</sub> Dispersion



**Isoparaffins can generate mineral dispersions at equal or lower viscosities**

*Sunscreens are inherently challenging formulas in part due to large proportions of the formulation being chemical or mineral UV filters*

- Stabilization and solubilization of liquid UV filters can help sensorial properties of the final formulation
- Greater solubility of crystalline filters will help boost and retain SPF<sup>†</sup> throughout storage
- Lower viscosity dispersion of mineral filters aids in processing and provides an improved skin feel

<sup>†</sup> Vallejo, Jhon; Mesa, Monica; Gallardo, Cecilia. (2011). Vitae. 18. 63-71.



**Thank you**

**LANXESS Flavors & Fragrances**

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Energizing Chemistry