



**Naturally derived solubilizers**  
High performance PEG-free solubilizers  
for all solubilization needs.

**TEAMWORKS 2018**

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April 11, 2018

# Cross Market trends from Personal Care to Household Care



## Naturality & Sustainability

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Natural & eco-friendly ingredients

Natural positioning helps brands build trust with consumers and grow consumer engagement



## Transparency

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Transparency presents an opportunity for companies to engage consumers by addressing ingredient safety

Corporate Social Responsibility (CSR) matters to consumers



## Performance & Safety

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Improved functionality versus not sacrificing safety

Milder formulations still require effective ingredients  
Performance & safety important to product's success



## Multifunctionality

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Less is more

Combining more than a single benefit in one product



## Health & Well-being

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Hygiene-focused product development

Aroma therapeutic products enhance sensory and support well-being

Fragrances are associated with cleanliness in beauty and similarly in home care

# Why solubilizers are needed for beauty care?

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Different kind of hydrophobic oils are used in cosmetics, need to be solubilized into water phase:

- **PERFUME OILS**

- Perfume is essential for consumers
- High variation of fragrance types

- **NATURAL OILS**

- Natural moisturization & care benefits

- **EMOLLIENTS**

- Moisturization benefits
- Solvents for other ingredients



# Why solubilizers are needed for Home Care?

Different kinds of hydrophobic oils are used in home care, like e.g.

- **ESSENTIAL OILS**

- Perfume is essential for consumers
- Naturally cleaner, antibacterial, degreaser, polish

- **NATURAL OILS**

- Natural moisturization & care benefits for leather

- **ESTER OILS**

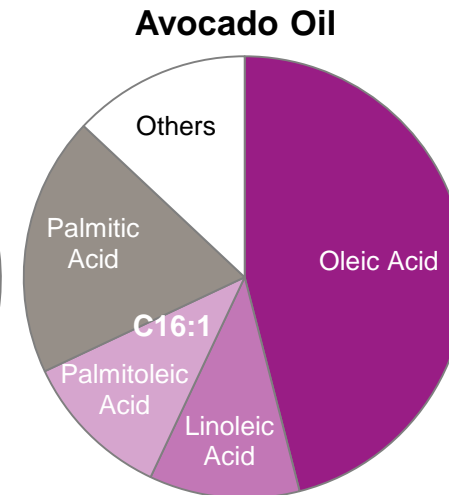
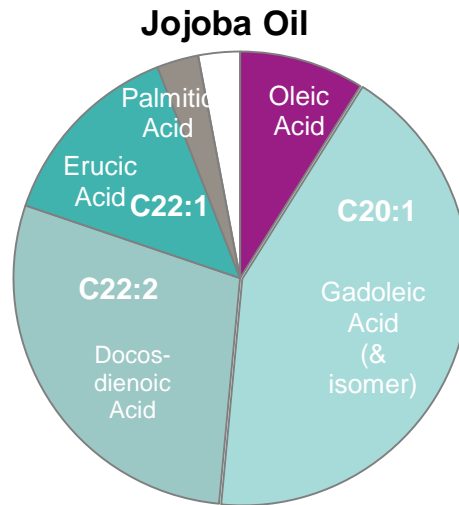
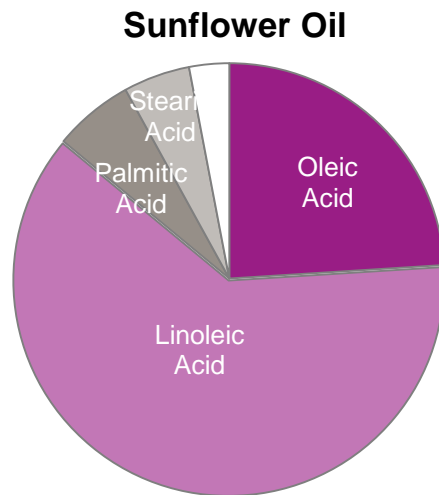
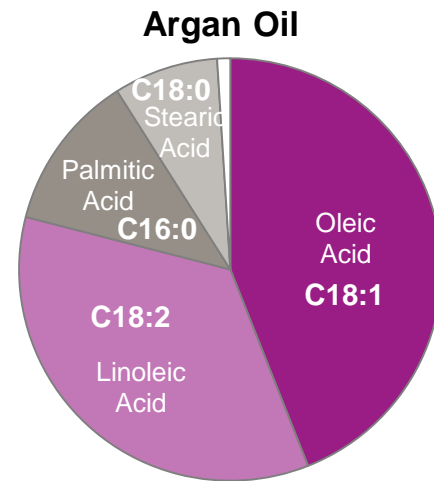
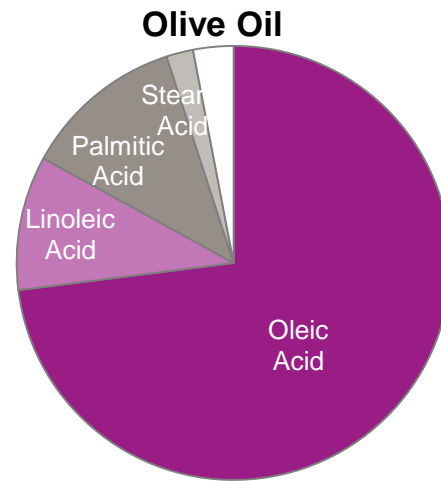
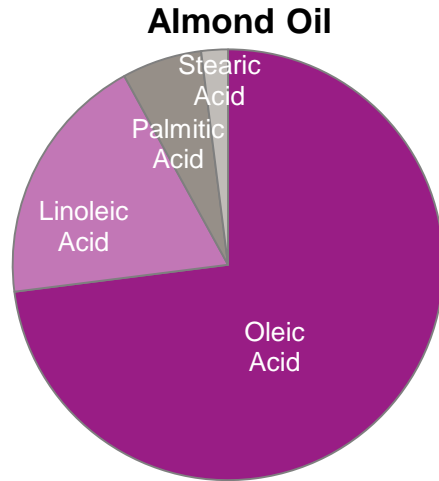
- Hydrophobizes surfaces
- Biodegradable





# What makes it challenging?

→ e.g. Complex composition of natural oils



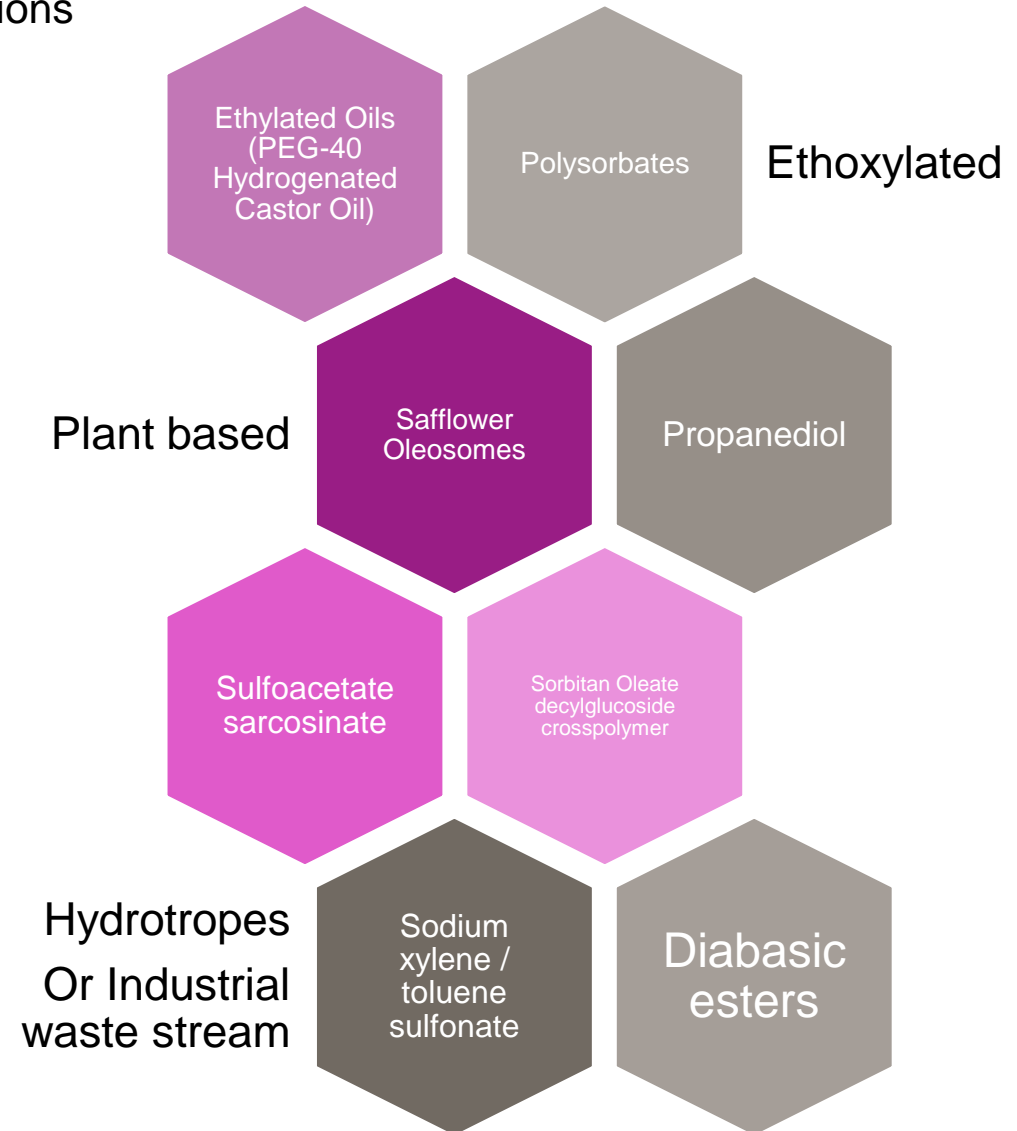
# Needs for next generation solubilizers for both Beauty and Home Care

Requirements		Common	Challenge
Solubilization performance	Providing high clarity	x	
	Broad variety of different oils		x
Processing	Easy to handle & cold processable	x	
	Adapted foaming & thickening properties		x
Sustainability	PEG-free	x	
	Fully naturally derived		x
Aspect of formulation	High stability on olfactory needs	x	
	Colorless product with high color stability		x
Additional benefits, like	Moisturization		x
	Mildness		x



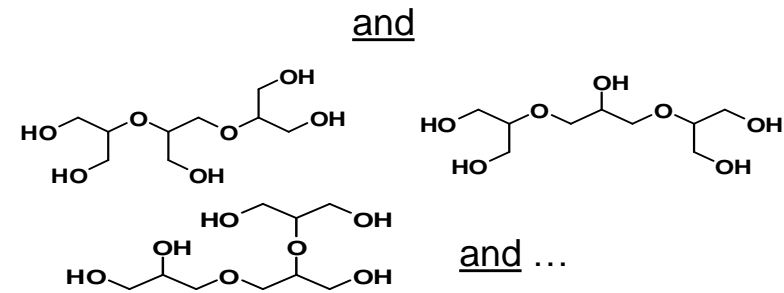
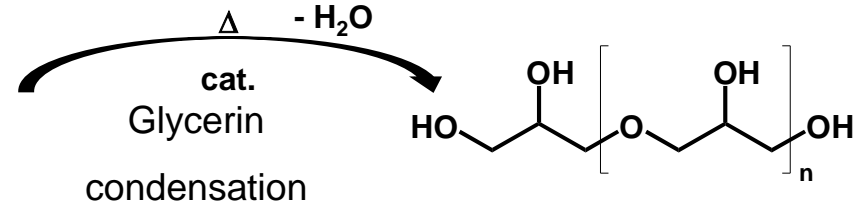
# Industrial benchmarks for Home Care and Beauty Care

- The industry keeps coming up with new solubilizer solutions
- We tend to see either:
  - Harsh chemistries
  - Milder chemistries but low solubilization power



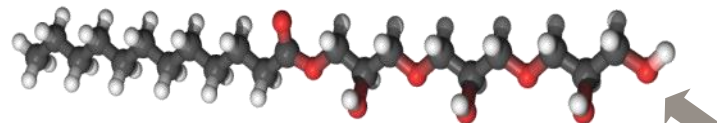
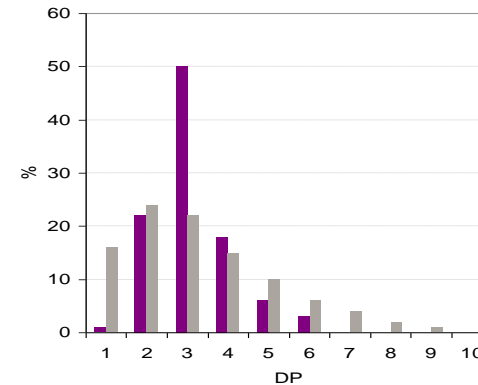
(source: <http://library.essentialwholesale.com/what-are-emulsifiers-and-solubilizers/>)

# The route to natural derived polyglycerol esters



Fatty acids

In addition: variation of degree of PG polymerisation:



Polyglycerol ester

↑ ↑ ↑  
 additional modifications possible

esterification

**By varying the condensation degree, polyglycerol esters can be tailored to specific applications.**



# Polyglycerin-based solubilization of different oils in water-based systems

## Efficient PEG-free Solubilizers

For the solubilization of

- **Essential oils** like:

Rosemary oil,      Lemon oil,  
Orange oil,        Lavender oil,  
Lemongrass oil,   Sage oil,  
Tea tree oil

- **Perfume oils**

- Benzyl Alcohol

Polyglyceryl-3 Caprate/ Caprylate/Succinate;  
Propylene Glycol (PG 55)

Polyglyceryl-6 Caprylate; Polyglyceryl-4 Caprate  
(PG 90)

For the solubilization of

- **Light and/or relatively polar emollient esters** like:

Isopropyl Myristate,  
Isopropyl Palmitate,  
Isoamyl Cocoate,  
Diethylhexyl Carbonate,  
C12-15 Alkyl Benzoate

- Short **hydrocarbons** like Isohexadecane
- Tocopherol

Polyglyceryl-4 Caprate (PG 41)

For the solubilization of

- **Fatty natural oils** like:

Sunflower oil,      Almond oil,  
Argan oil,            Olive oil,  
Soy bean oil,        Jojoba oil

- Other **triglycerides** like

Caprylic/Capric Triglyceride

- **Heavier lipophilic emollients** like

Ethylhexyl Palmitate, Decyl Cocoate,  
Cetearyl Isononanoate

Polyglyceryl-6 Caprylate; Polyglyceryl-3  
Cocoate; Polyglyceryl-4 Caprate;  
Polyglyceryl-6 Ricinoleate (PG 61)

Increasing hydrophobicity

# Polyglycerin-based solubilizers – Properties

## Efficient PEG-free Solubilizers

<ul style="list-style-type: none"> <li>• Almost colorless liquid</li> <li>• ~3000 – 5000 mPa·s</li> <li>• HLB ~15</li> <li>• Surface tension (1%): ~26 mN/m</li> <li>• ~25% Propylene Glycol</li> <li>• Bio-based 1,2-Propylene Glycol and Succinic acid</li> <li>• RSPO (MB*)</li> <li>• (Halal pending)</li> </ul>	<ul style="list-style-type: none"> <li>• Colorless to yellowish liquid</li> <li>• ~3000 - 6000 mPa·s</li> <li>• HLB ~15</li> <li>• Surface tension (0.5%): ~26 mN/m</li> <li>• ~10% Water</li> <li>• Ecocert &amp; COSMOS</li> <li>• RSPO (MB*)</li> <li>• (Halal pending)</li> </ul>	<ul style="list-style-type: none"> <li>• Almost colorless liquid</li> <li>• ~3000 – 5000 mPa·s</li> <li>• HLB ~14</li> <li>• Surface tension (0.5%): ~26 mN/m</li> <li>• ~10% Water</li> <li>• Ecocert &amp; COSMOS</li> <li>• RSPO (MB*)</li> <li>• Halal</li> </ul>	<ul style="list-style-type: none"> <li>• Slightly yellow liquid</li> <li>• ~3000 – 5000 mPa·s</li> <li>• HLB ~11</li> <li>• Surface tension (0.5%): ~30 mN/m</li> <li>• ~12% Water</li> <li>• Ecocert &amp; COSMOS</li> <li>• RSPO (MB*)</li> <li>• Halal</li> </ul>
<p>Polyglyceryl-3 Caprate/Caprylate/Succinate; Propylene Glycol (PG 55)</p>	<p>Polyglyceryl-6 Caprylate; Polyglyceryl-4 Caprate (PG 90)</p>	<p>Polyglyceryl-4 Caprate (PG 41)</p>	<p>Polyglyceryl-6 Caprylate; Polyglyceryl-3 Cocoate; Polyglyceryl-4 Caprate; Polyglyceryl-6 Ricinoleate (PG 61)</p>

\*MB = mass balanced

PEG- & preservative free products, 100% based on renewable raw materials

# Outline:

## Benefits & application tests of polyglycerin-based solubilizers

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### 1. Solubilization performance

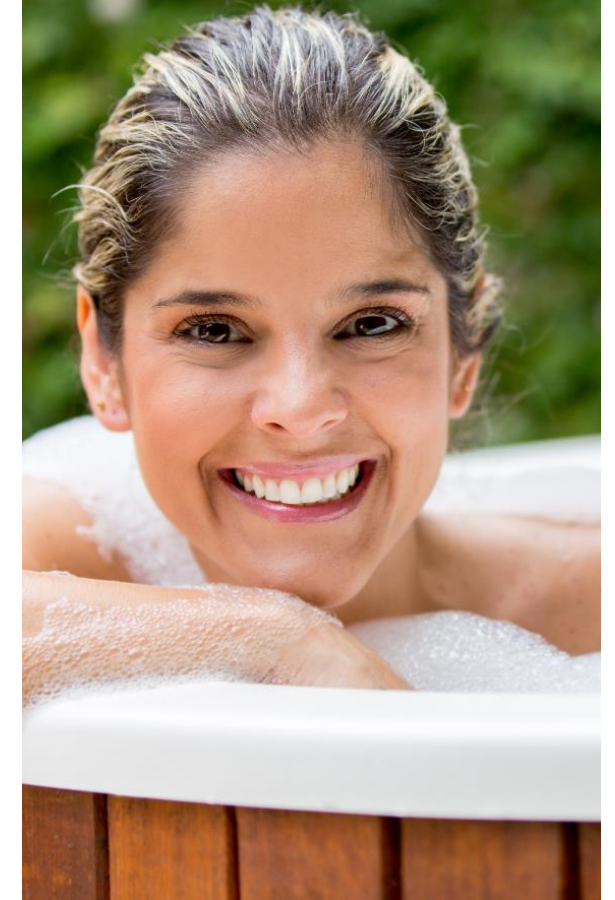
- Essential & perfume oils
- Emollients
- Fatty natural oils

### 2. Processing attributes

- Foaming
- Phase behavior during processing
- Viscosity effects in surfactant systems

### 3. Additional benefits

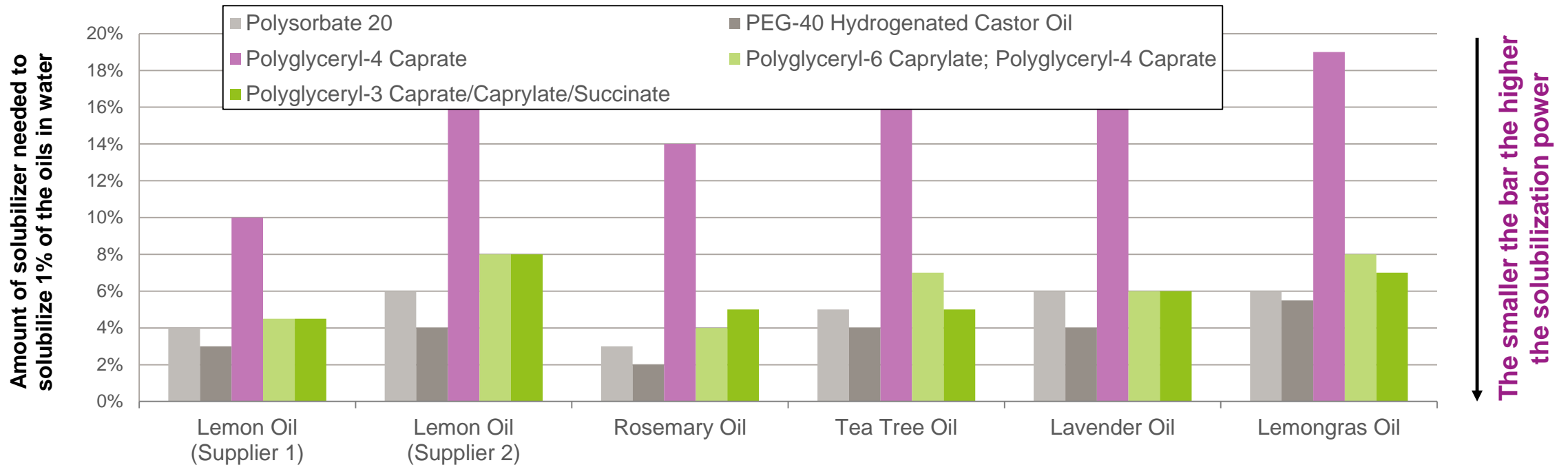
- Moisturization (Corneometer studies)
- Mildness (RBC test results)
- Make-up removing properties



# Essential oils in water – Solubilizing efficacy of Ethoxylated vs. Polyglyceryl Esters

1% essential oil + x% solubilizer + slowly add ad. 100% water.

x = necessary amount of solubilizer for a crystal clear solution (after ~30 min at r.t.).


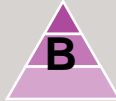







**Polyglyceryl esters show similar performance to the PEG containing market standards**

# Fragrance mapping – Tested perfume oils

A broad variety of perfume oils were tested to show the solubilizing efficacy of : Polyglyceryl-3 Caprate/Caprylate/Succinate

<b>A</b>	Aquatic / Floral (Balsamic - Powdery - Sandalwood)
<b>B</b>	Ozonic / Fruity (Citrus - Melon - Musk)
<b>C</b>	Floral / Fruity (Apple - Balsamic)
<b>D</b>	Balsamic / Floral (Fruity - Aldehyde - Musk)
<b>E</b>	Floral (Freesia - Lily Of The Valley - Rose)
<b>F</b>	Fougère / Citrus (Cassis - Lemon - Sandalwood)
<b>G</b>	Fougère / Aromatic (Green - Amber - Bergamot)

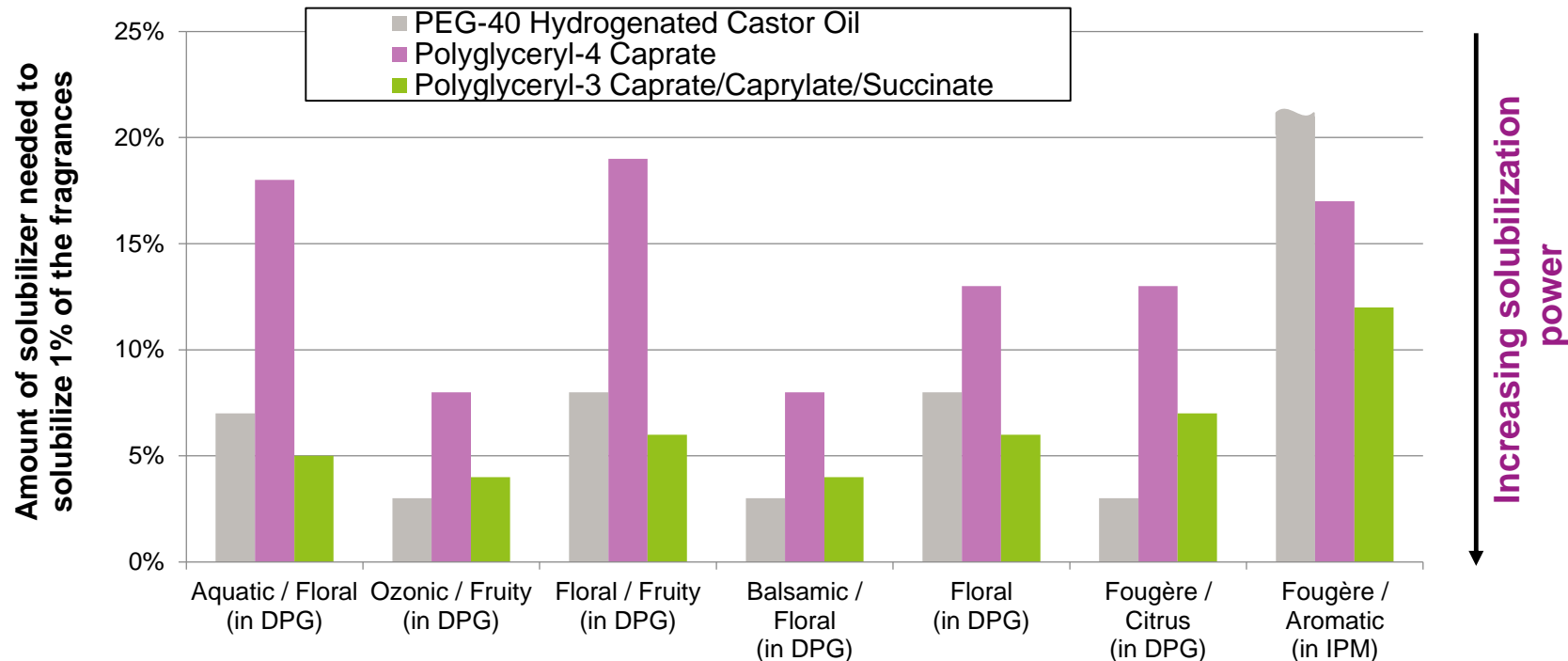
<i>Tendency</i>	Citrus	Watery	Fruity	Floral	Aromatic	Woody
<i>Basic character</i>						
Citrus						
Fruity						
Floral						
Fougère						

Supported by Fragrance Resources (now IFF Fragrance GmbH)



# Perfume oils in water – Solubilizing efficacy of Polyglyceryl-3 Caprate/Caprylate/Succinate

1% perfume oil + x% solubilizer + slowly add ad. 100% water.  
x = necessary amount of solubilizer for a crystal clear solution (after ~30 min at r.t.).

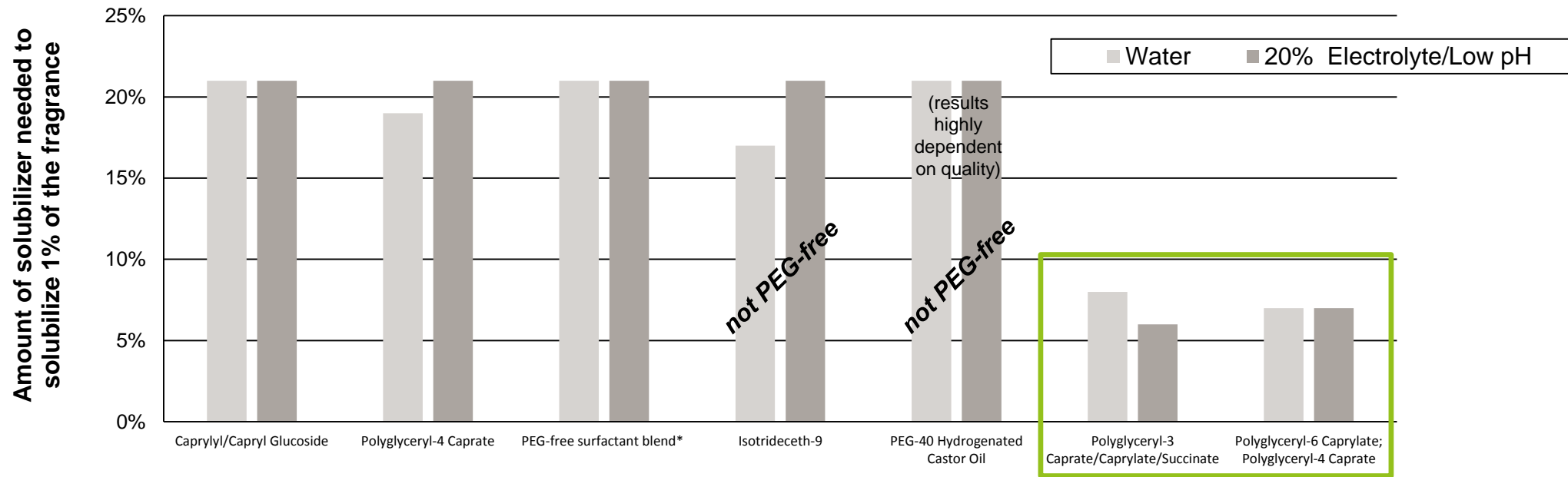


All fragrances from Fragrance Resources  
(now IFF Fragrance GmbH)

**Polyglyceryl-3 Caprate/Caprylate/Succinate in average is as effective as the PEG-based standard PEG-40 Hydrogenated Castor Oil**

# Perfume oil in water or a High Electrolyte and low pH environment – Solubilizing efficacy of standard ingredients in a corrosive environment

1% perfume oil “SPICY HERBS” (100% essential oils, BDIH quality, IFF Fragrance GmbH).  
Maximum of 21% solubilizer tested.



**Polyglyceryl esters show superior solubilizing properties in water and high electrolyte low pH systems**

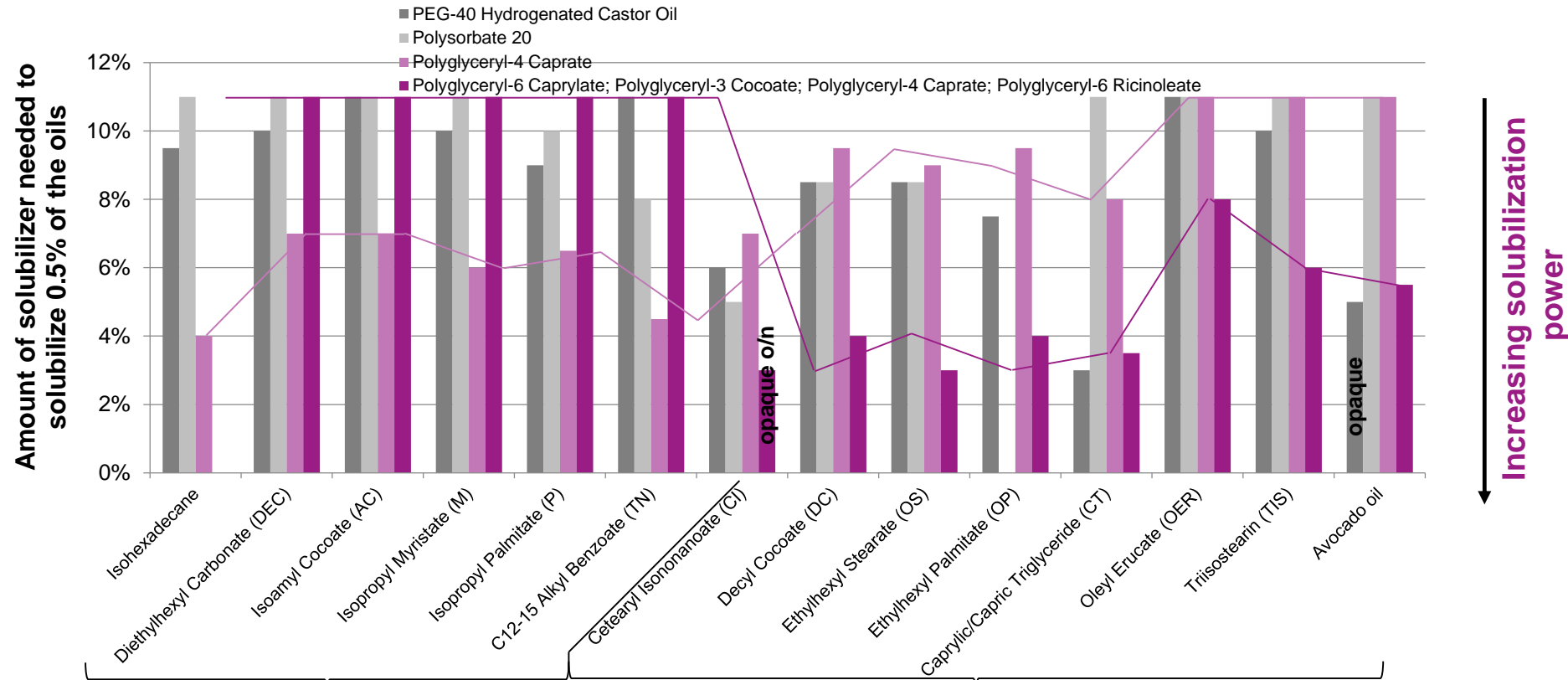
\*INCI Name: Water; Pentylene Glycol; Sodium Lauryl Sulfoacetate; Sodium Oleyl Sarcosinate; Sodium Chloride; Disodium Sulfoacetate; Sodium Oleate; Sodium Sulfate

# Emollients in water –

Solubilizing efficacy of Polyglyceryl-4 Caprate & Polyglyceryl-6 Caprylate; Polyglyceryl-3 Cocoate; Polyglyceryl-4 Caprate; Polyglyceryl-6 Ricinoleate

0.5% oil + x% solubilizer + slowly add ad. 100% water.

x = necessary amount of solubilizer for a crystal clear solution. Max. amount of solubilizer tested: 11%.



Polyglyceryl-4 Caprate best for light and polar emollients

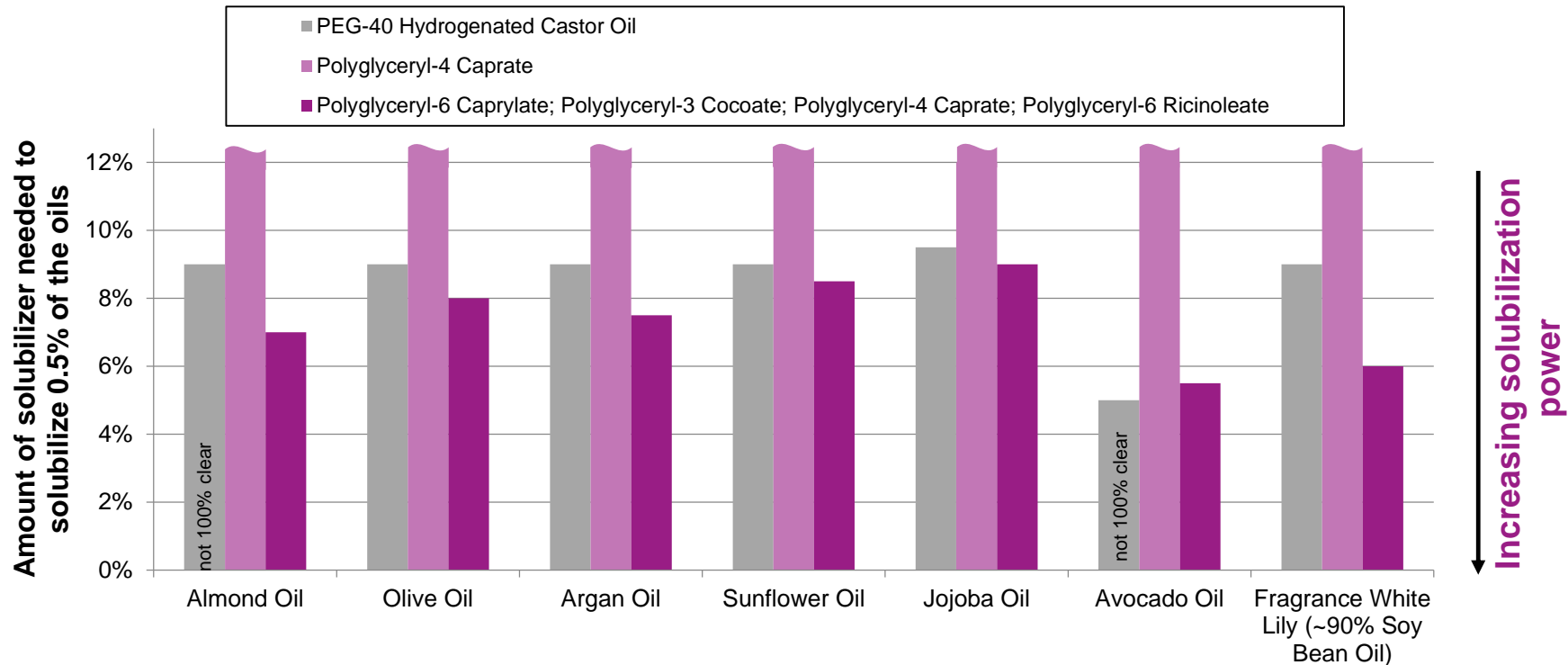
Polyglyceryl-6 Caprylate; Polyglyceryl-3 Cocoate; Polyglyceryl-4 Caprate; Polyglyceryl-6 Ricinoleate best for highly lipophilic emollients

# Natural oils in water –

Solubilizing efficacy of Polyglyceryl-6 Caprylate; Polyglyceryl-3 Cocoate; Polyglyceryl-4 Caprate; Polyglyceryl-6 Ricinoleate

0.5% oil + x% solubilizer + slowly add water ad. 100%.

x = necessary amount of solubilizer for a crystal clear solution. Max. amount of solubilizer tested: 12%.



**Polyglyceryl-6 Caprylate; Polyglyceryl-3 Cocoate; Polyglyceryl-4 Caprate; Polyglyceryl-6 Ricinoleate is more efficient (~15 – 20%) than the PEG-based market standard (PEG-40 Hydrogenated Castor Oil)**

# Outline:

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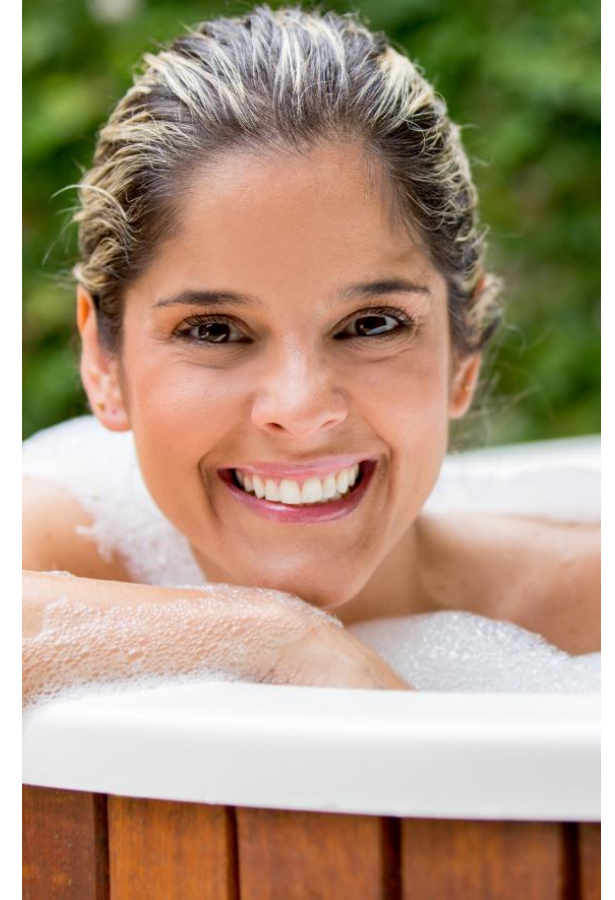
- Essential & perfume oils
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### 2. Processing attributes

- **Foaming**
- **Phase behavior during processing**
- **Viscosity effects in surfactant systems**

### 3. Additional benefits

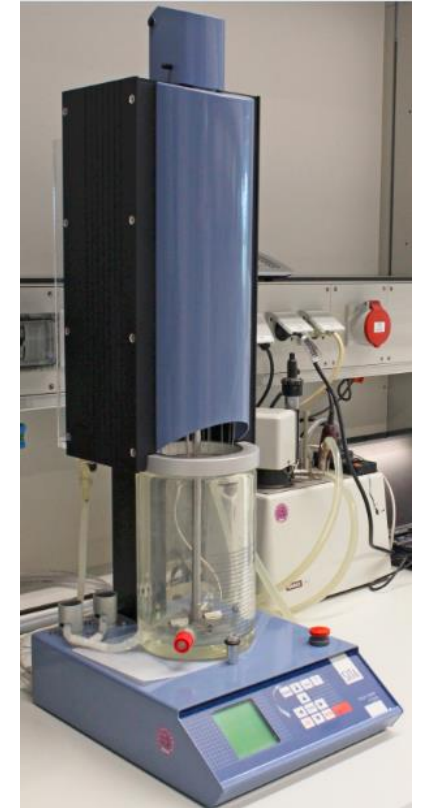
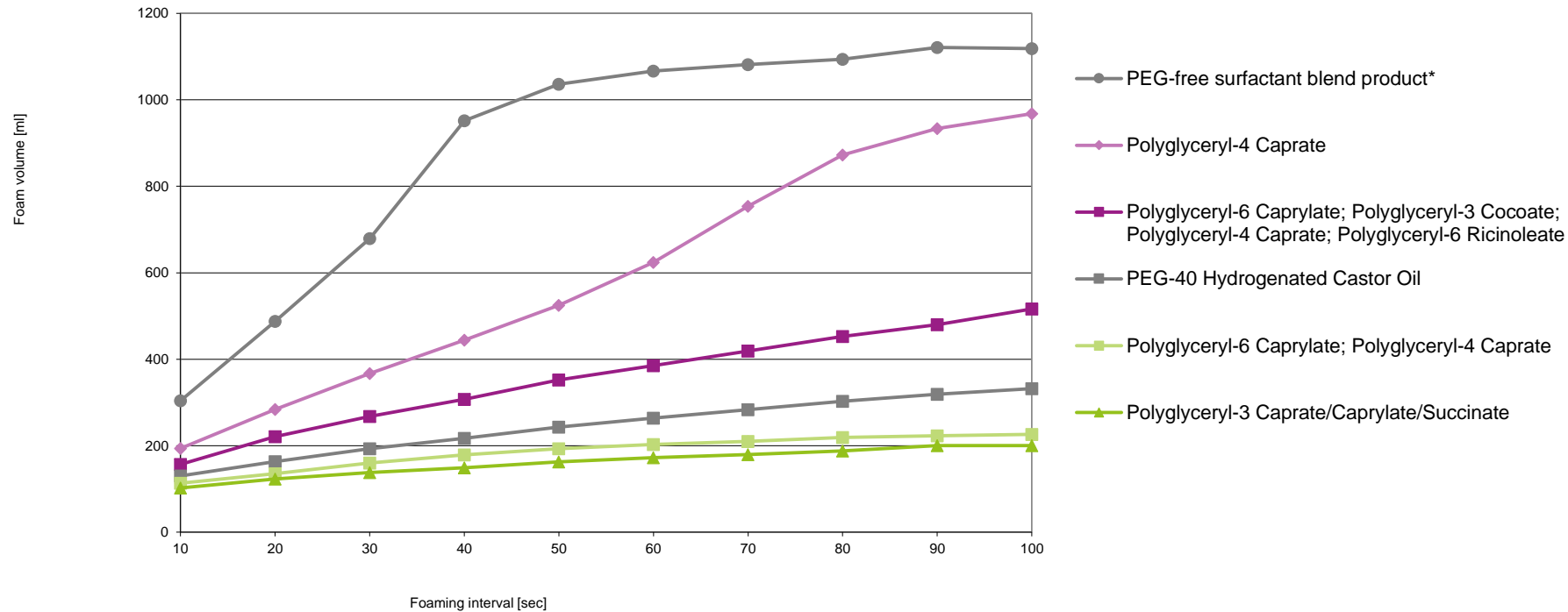
- Moisturization (Corneometer studies)
- Mildness (RBC test results)
- Make-up removing properties





# Foaming during processing

Foam kinetics / Flash foam in water – SITA method,  
c=0.5% in water (~10 °dH), T= 30 °C, pH ~6, 1500 rpm



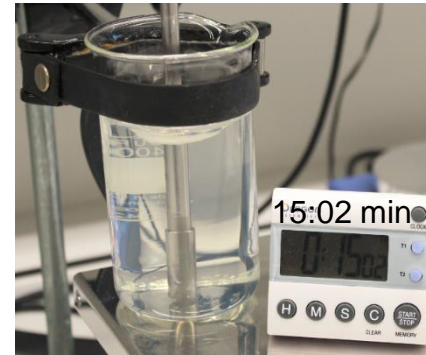
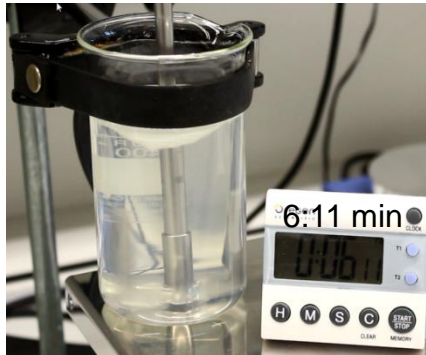
**Polyglycerin-based solubilizers are low foaming in water, thus enabling easy processing**

\*INCI Name: Water; Pentylene Glycol; Sodium Lauryl Sulfoacetate; Sodium Oleyl Sarcosinate; Sodium Chloride; Disodium Sulfoacetate; Sodium Oleate; Sodium Sulfate

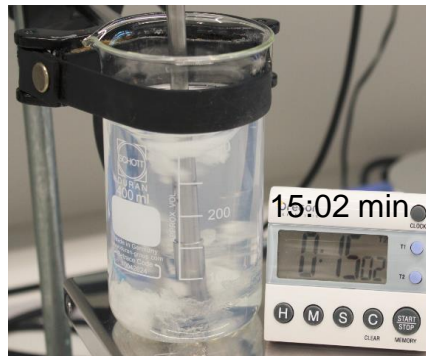
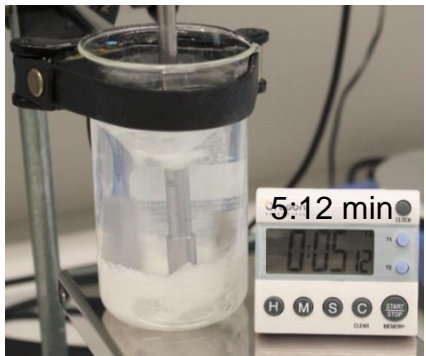
# Processing versus PEG-40 Hydrogenated Castor Oil

Test for processing of Almond oil in water: 0.5% Almond oil + 9% solubilizer at r.t., slowly add water ad 100%

**Polyglyceryl-6 Caprylate;  
Polyglyceryl-3 Cocoate;  
Polyglyceryl-4 Caprate;  
Polyglyceryl-6 Ricinoleate**



**PEG-40  
Hydrogenated  
Castor Oil**

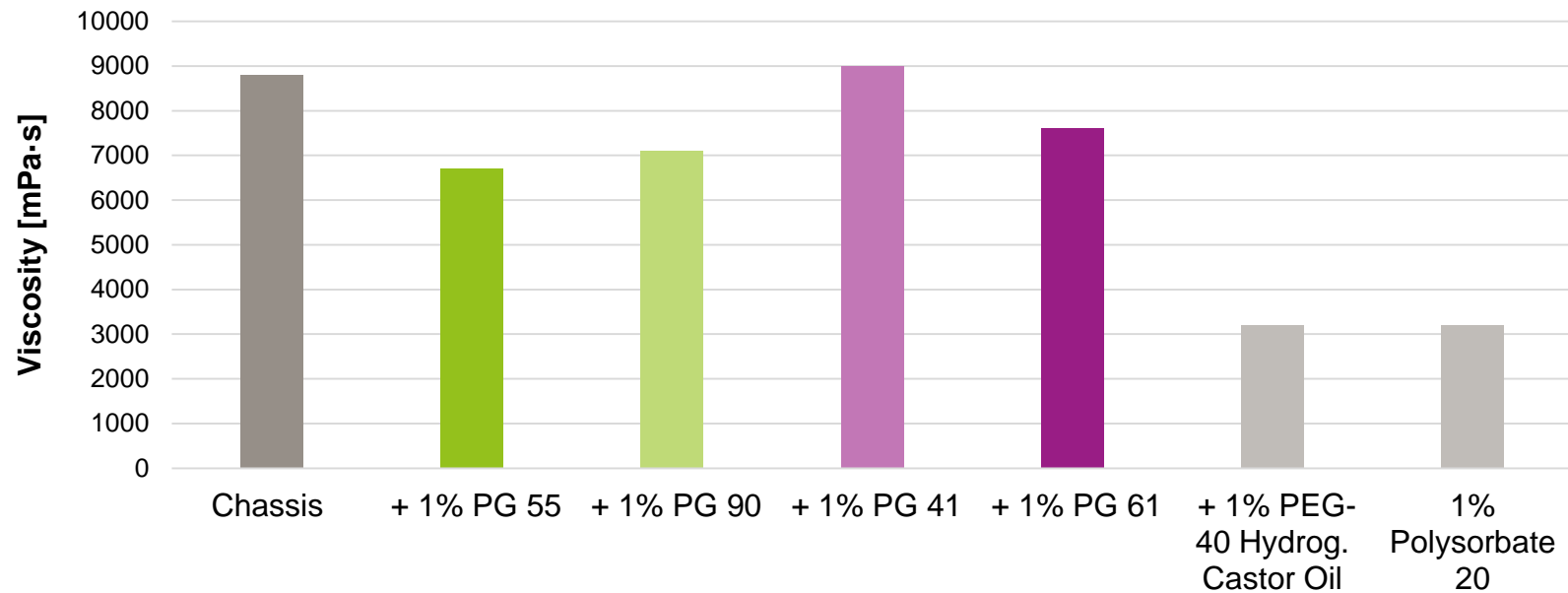


**Polyglycerin-based solubilizers are cold processable and do not form a gel phase in contrast to some PEG-containing solubilizers in high concentrations**

# Viscosity effects (I) – Comparison to PEG-40 Hydrogenated Castor Oil & Polysorbate 20

Influence of solubilizers on the viscosity:

Chassis: 9% SLES, 3% CAPB, 0.2% PQ-10, 0.5% NaCl,  
2.5% PEG-18 Glyceryl Oleate/Cocotate; pH 5.5



**Polyglycerin-based solubilizers show significantly lower viscosity reduction than PEG-40 Hydrogenated Castor Oil or Polysorbate 20**

# Outline:

## benefits & application tests of polyglycerin-based solubilizers

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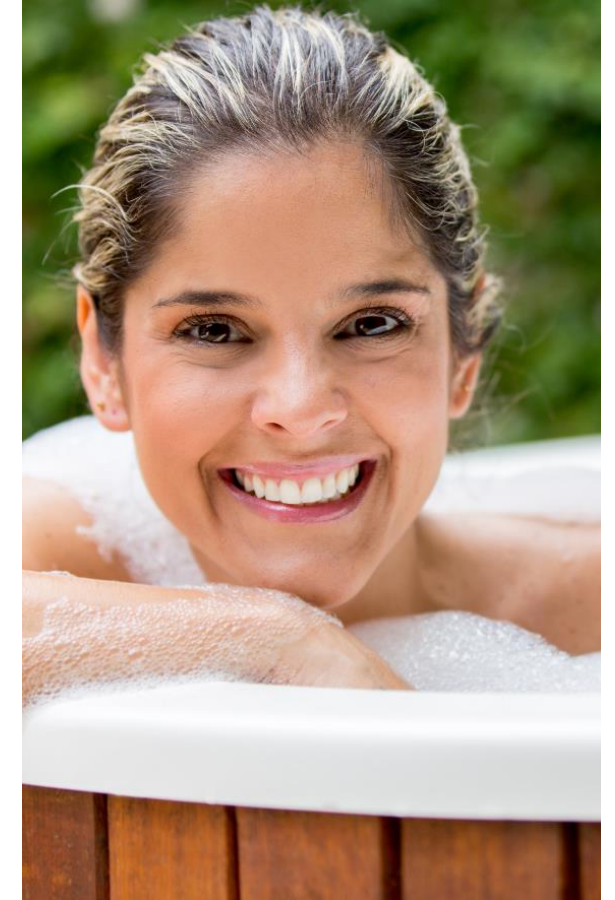
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- **Moisturization (Corneometer studies)**
- **Mildness (RBC test results)**
- **Make-up removing properties**



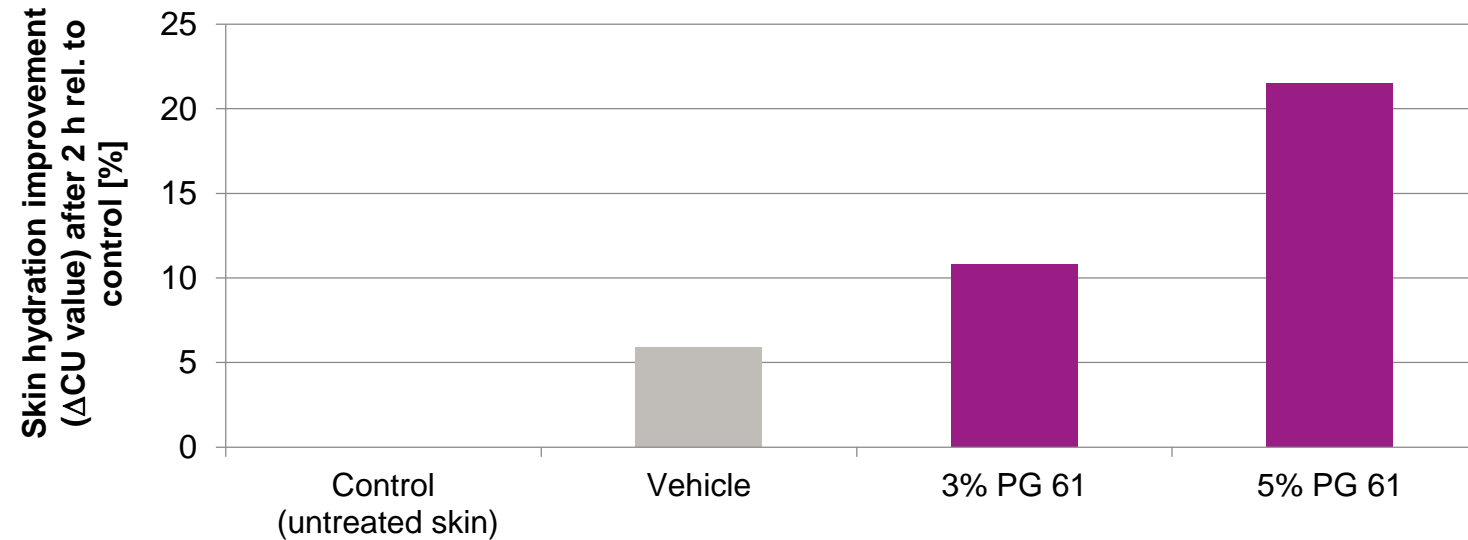
# Moisturizing properties – *In vivo* Corneometer test results

*In vivo* short-term moisturization test with a leave-on O/W treatment.

Test area: 5 cm<sup>2</sup> (inner forearm); 20 µg test formulation;

Time points: Start & 2 h after application;

14 test persons (Nov. 2013), 22-23 measurements / formula



**Polyglycerin-based solubilizers act as a humectant and provides moisturization benefits**



# In-vitro Mildness Assessment – Red Blood Cell Test

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- Lipids and proteins of the skin surface are comparable with cell membranes of erythrocytes
- Influence of irritating surfactants:
  - Damage of the erythrocyte-membrane:
    - Haemolysis (release of hemoglobin)
    - Damage of the protein (denaturation of hemoglobin)

## RBC-Test

- Substrate: animal blood (pig, cow, calf, guinea pig)
- Measurement of:
  - Cell membrane destruction
  - Protein denaturation
- Reference: Sodium Dodecyl Sulfate

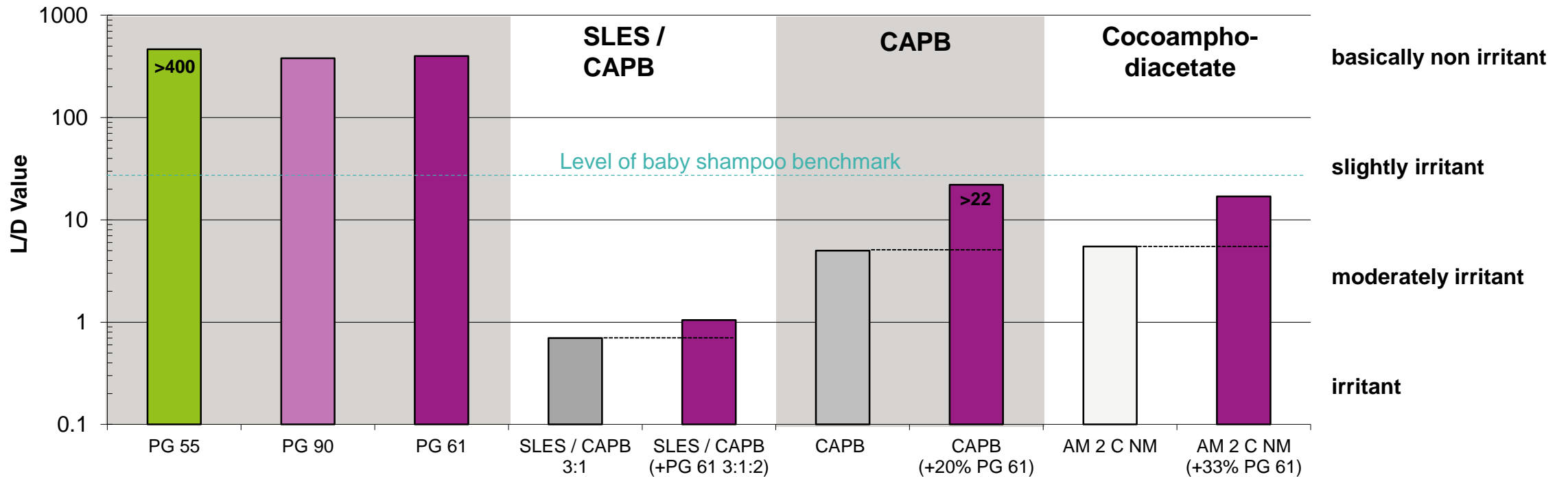
W.J.W. Pape, U. Hoppe, *Drug Res.* [40](#) (I), 4, 498-502 (1990)



# Mildness – Red Blood Cell (RBC) test results of surfactant mixtures

RBC test results of different surfactants with PG 61.

PG 61 is added on top (as an additive) and not calculated into the surfactant active matter.



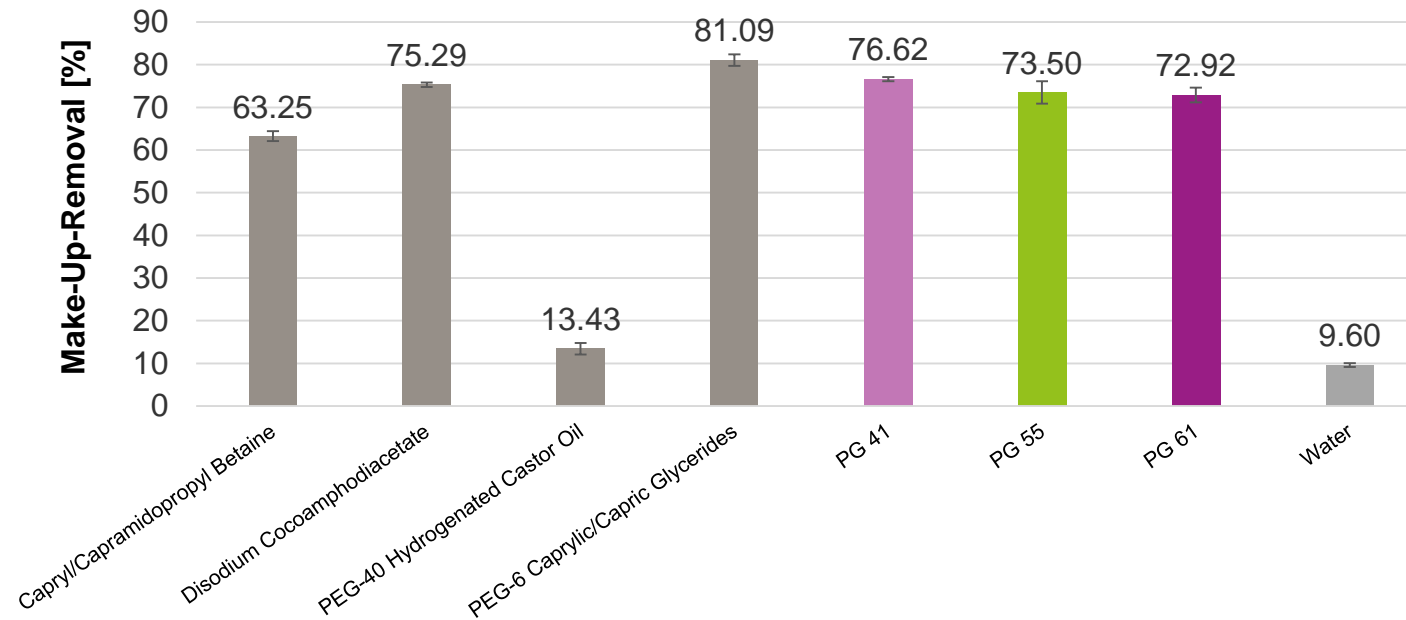
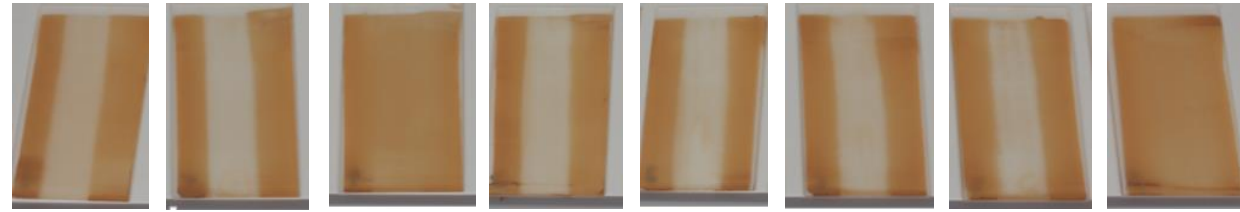
**The Polyglycerin-based solubilizers are basically non irritant and improve the mildness of surfactant mixtures**

# Make-up removal – Test results with aqueous solutions

Removal of make-up applied on PMMA-plates. Aqueous solution (3% a.m. surfactants) was put on a cotton pad attached to a sled.



long lasting make-up (L'Oréal)



**Polyglycerin-based solubilizers efficiently remove make-up in a very mild way**

# Polyglycerin-based solubilizers – Benefits at a glance

## Essential & Perfume oils

- Polyglyceryl-3 Caprate/Caprylate/Succinate
- Polyglyceryl-6 Caprylate; Polyglyceryl-4 Caprate

## Light and/or relatively polar emollients

- Polyglyceryl-4 Caprate

## Fatty natural oils

### Heavier lipophilic emollients

- Polyglyceryl-6 Caprylate; Polyglyceryl-3 Cocoate; Polyglyceryl-4 Caprate; Polyglyceryl-6 Ricinoleate

- **Crystal clear** formulations possible
- **Low foaming during processing**
- Easy to handle, **cold processable** (no gel phase)
- **Low influence on viscosity** in surfactant solutions
- Additional benefits:
  - **Moisturizing** benefits
  - **Ultra-mild cleansing** properties
- PEG- and preservative-free
- 100% based on **renewable raw materials**, suitable for natural beauty and home care formulations





**EVONIK**

**POWER TO CREATE**



# RBC-Test – in-vitro mildness assessment

## Values

- H 50 (Hemolysis)
  - Concentration of surfactant at which 50% of the erythrocytes are destroyed [ppm]
  - Release of haemoglobin due to cellular damage (UV/VIS at 560 or 530 nm)
- DI (Denaturation-Index)
  - Denaturation of haemoglobin compared to SDS [%] (UV/VIS at 575 and 540 nm)
- L/D – value ( $L/D = H50 \text{ [ppm]} / DI \text{ [%]}$ )
  - quotient lysis/denaturation (H50/DI)
  - correlates with mean index of ocular irritation (Draize)

**Classification:  $L/D > 100$  basically non irritant**

Very mild formulas  
(e. g. baby shampoos)

$L/D > 10$	slightly irritant
$L/D > 1$	moderately irritant
$L/D > 0.1$	irritant
$L/D < 0.1$	very irritant

