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Inolex

The Hair Science E-Summit
24 September 2023
The Eco Well (virtual)

An Update on Silicone Alternatives in Hair Care

Today's Topics

- Understanding the job(s) done by silicones
- Silicones work so well in hair care, why seek alternatives?
- Designing and implementing silicone alternative ingredients
- Developing silicone-free formulations

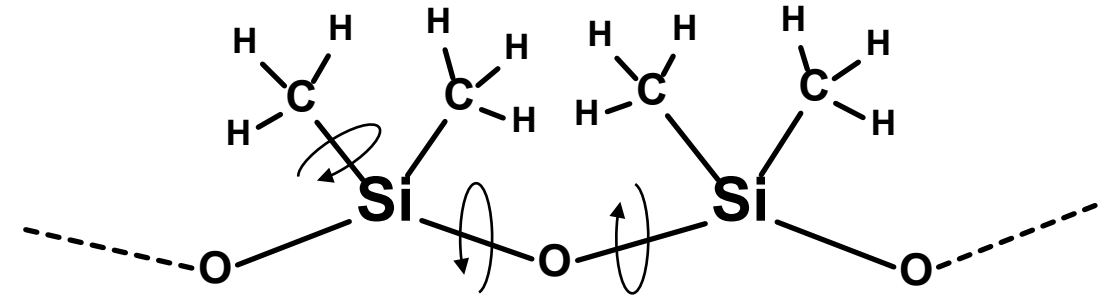


Why silicones in the first place?

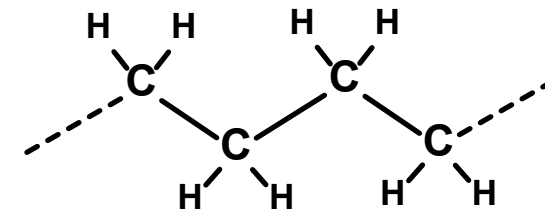
Unique chemical and physical properties deliver beneficial performance

What makes silicones so unique?

- Hybrid organic-inorganic polymers
- Si is larger and less electronegative than C
- Longer bonds with more rotational freedom and flexibility
- Non-polar, weak intermolecular forces, thus:
 - Hydrophobic, low surface energy
 - High spreadability
 - High gas diffusivity
- High thermal stability (Si–O bond very strong)



polydimethylsiloxane (dimethicone)



polyethylene

Berthiaume, M.D. Silicones in Cosmetics, Ch. 7 in *Principles of Polymer Science & Technology in Cosmetics & Personal Care*, Goddard, E. D. and Gruber, J. V., eds, Marcel Dekker Inc, New York, USA, 1999, pp 275-324.

Butts, M. et al. Silicones, in *Kirk-Othmer Encyclopedia of Chemical Technology*, John Wiley & Sons Inc, <http://onlinelibrary.wiley.com/book/10.1002/0471238961>, 20 Dec 2002, pp 1-89.

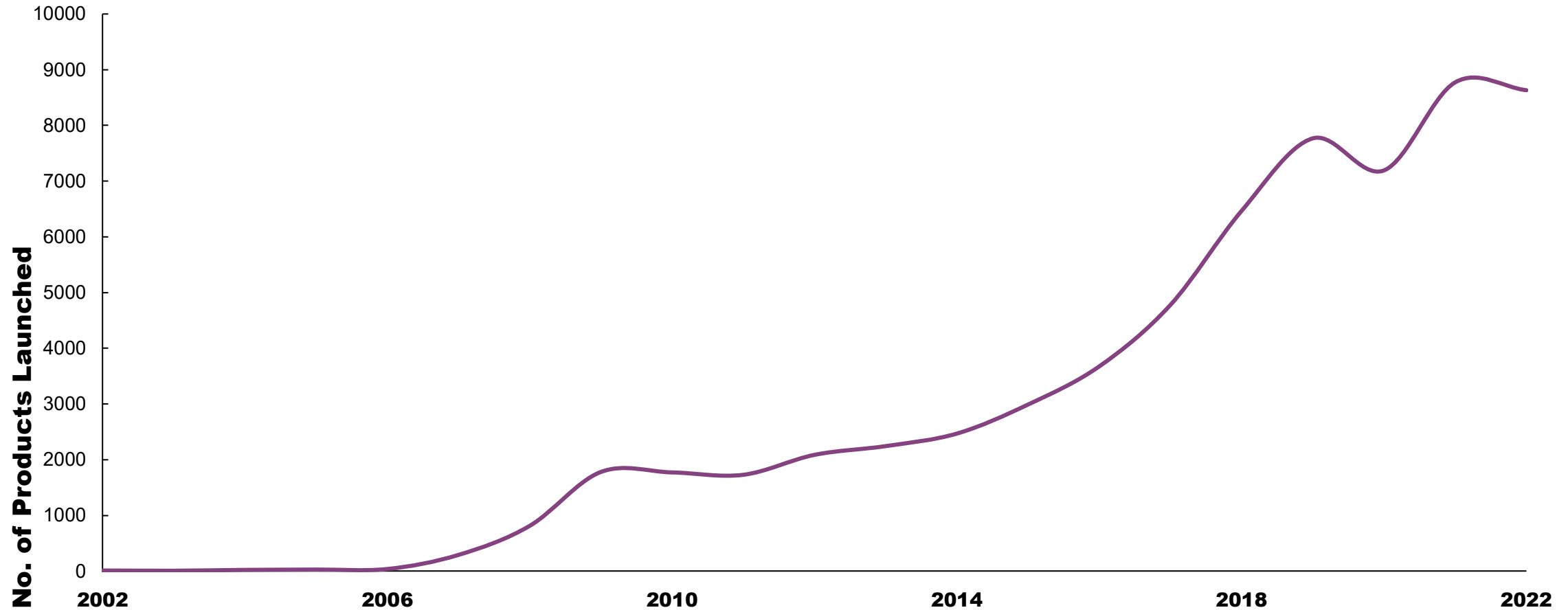
Silicone ingredients job description

Silicones and silicone derivatives improve hair care products' performance and the consumer's experience by:

- Forming thin hydrophobic films with low surface energy
- Lubricating fibers and reduce combing force
- Imparting soft feel
- Providing protective, yet breathable barrier
- Improving humidity resistance
- Enhancing shine

Berthiaume, M.D. Silicones in Cosmetics, Ch. 7 in *Principles of Polymer Science & Technology in Cosmetics & Personal Care*, Goddard, E. D. and Gruber, J. V., eds, Marcel Dekker Inc, New York, USA, 1999, pp 275-324.

The rise of silicone-free claims



Note: slowed growth in 2020 is proportional to overall industry slowed growth due to the COVID-19 pandemic
Source: Mintel GNPD, Accessed Jan. 2023

Silicones' sustainability challenges

Sustainability involves issues in the following three categories: Environmental, Social, and Governance (abbreviated as ESG)

Environmental

Silicones*

- Large carbon footprint
- Non-renewable feedstock(s)
- Not biodegradable
- Biopersistence hazard

Social

Silicones*

- Consumers have a negative perception of silicones

Governance

Silicones*

- Cyclomethicones are effectively banned via restriction in the EU
- Restrictions pending on volatile linear dimethicones (L2-L6)
- Cyclomethicones are prohibited in certain retailers

*refers to the general category of silicones and silicone derivatives used as ingredients in cosmetic and personal care formulations

Silicone alternative ingredients

**By definition, if it's not silicone, then it can be an alternative.
It just may not be a good one.**

Alternatives to silicone ingredients

A wide variety of ingredients are positioned as silicone alternatives

- Naturally-occurring oils (triglycerides), e.g. Cocos Nucifera (Coconut) Oil
- Hydrocarbons, e.g. Isododecane, C13-16 Isoalkane
- Esters, e.g. Neopentyl Glycol Diheptanoate, Isoamyl Laurate
- Mixtures of the above
- (Poly)ethers, e.g. PPG-3 Isostearyl Methyl Ether, Polycitronellol
- Polyesters, e.g. Capryloyl Glycerin/Sebacic Acid Copolymer

Alternatives to silicone ingredients

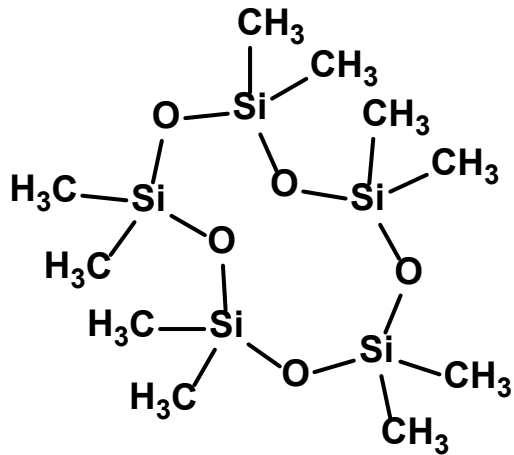
Successful alternatives are based on approximating the physical properties of silicones

Silicone Ingredient	Key Physical Properties	Alternatives
Cyclopentasiloxane	Lubricity, volatility	Hydrocarbons, Esters, and mixtures
Dimethicone	Lubricity, viscosity	Esters, Polyesters, Polyethers, and mixtures
Amodimethicone	Cationic charge , substantivity	Polyesteramines
Phenyltrimethicone	High refractive index , shine	Aromatic Esters

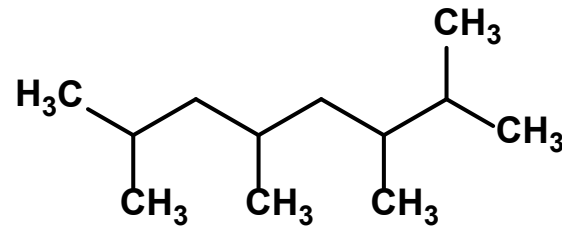
Molecular level considerations

Structural-property relationships help identify suitable alternatives, e.g. methyl (CH_3) groups, branching, unsaturation, etc.

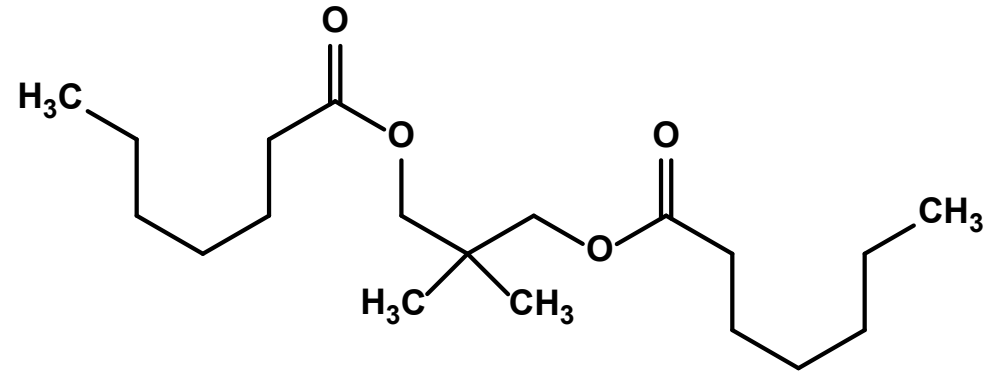
Cyclopentasiloxane



Isododecane



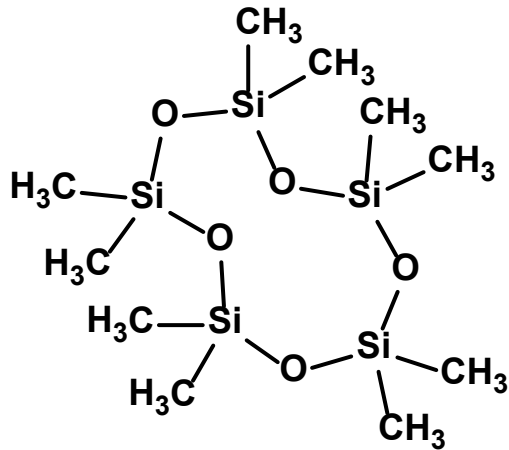
Neopentyl Glycol Diheptanoate



Molecular level considerations (con't)

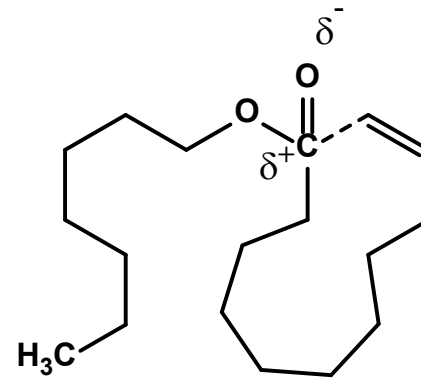
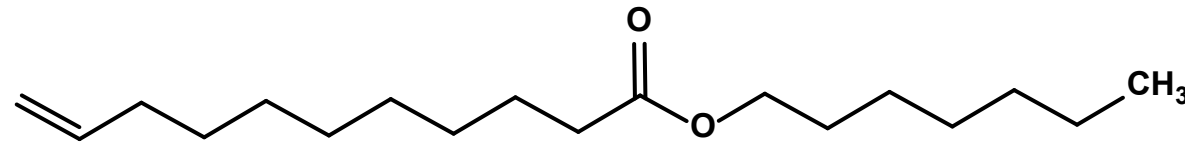
Structural-property relationships help identify suitable alternatives, e.g. methyl (CH₃) groups, branching, unsaturation, etc.

Cyclopentasiloxane



Heptyl Undecylenate

(LexFeel™ Natural)



Sensory Fluid Alternatives

Ingredient (INCI)	Chemical Class	Surface Tension @ 25 °C (mN/m)	Interfacial Tension with H ₂ O @ 25 °C (mN/m)
LexFeel™ 7 (Neopentyl Glycol Diheptanoate)	ester	29.0	10.2
Isododecane	hydrocarbon	22.2	28.9
LexFeel™ D5 (Neopentyl Glycol Diheptanoate (and) Isododecane)	ester + hydrocarbon	24.0	20.9
SustOleo™ MCT (Triheptanoin)	ester	29.4	8.4
Neossance Hemisqualane (C13-16 Isoalkane)	hydrocarbon	24.8	25.2
LexFeel™ WOW (Triheptanoin (and) C13-16 Isoalkane)	ester + hydrocarbon	26.6	13.2

Polar esters combine with nonpolar hydrocarbons for **synergistic improvement**

Ester

- Lowers interfacial tension with water
- Improves wetting
- Enhances emulsion stability

Hydrocarbon

- Lowers surface tension
- Improves spreading
- Provides partial volatility

Personal Care Products That Do Not Contain Tetramer or Pentamer Cyclomethicones, [US20040241200A1](#), 2004, assigned to INOLEX Investment Corp.

Natural Hydrocarbon/Ester Compositions with Improved Sensory Properties, Formulations and Related Methods, [US11229589B2](#), 2022, assigned to INOLEX Investment Corp.

LexFeel™ WOW

INCI

Triheptanoin (and) C13-16 Isoalkane

Made from

Sugarcane | Coconut | Castor

100% Plant-Based Cyclomethicone Replacement

- Fast spreading with powdery, non-greasy afterfeel
- Functional benefits in skincare, hair care, sun care, color cosmetics
- Equivalent to cyclopentasiloxane (D5) in sensory and functional performance
- Globally compliant

Standards & Certifications



100% Natural



100% USDA
certified
biobased
content



Natural
Origin Index:
1.0



Biodegradable



NSF/ANSI
305 Approved



China IECIC
Listed*



Non-palm
Derived



Kosher
Compliant



Vegan &
Cruelty Free



Halal
Certified

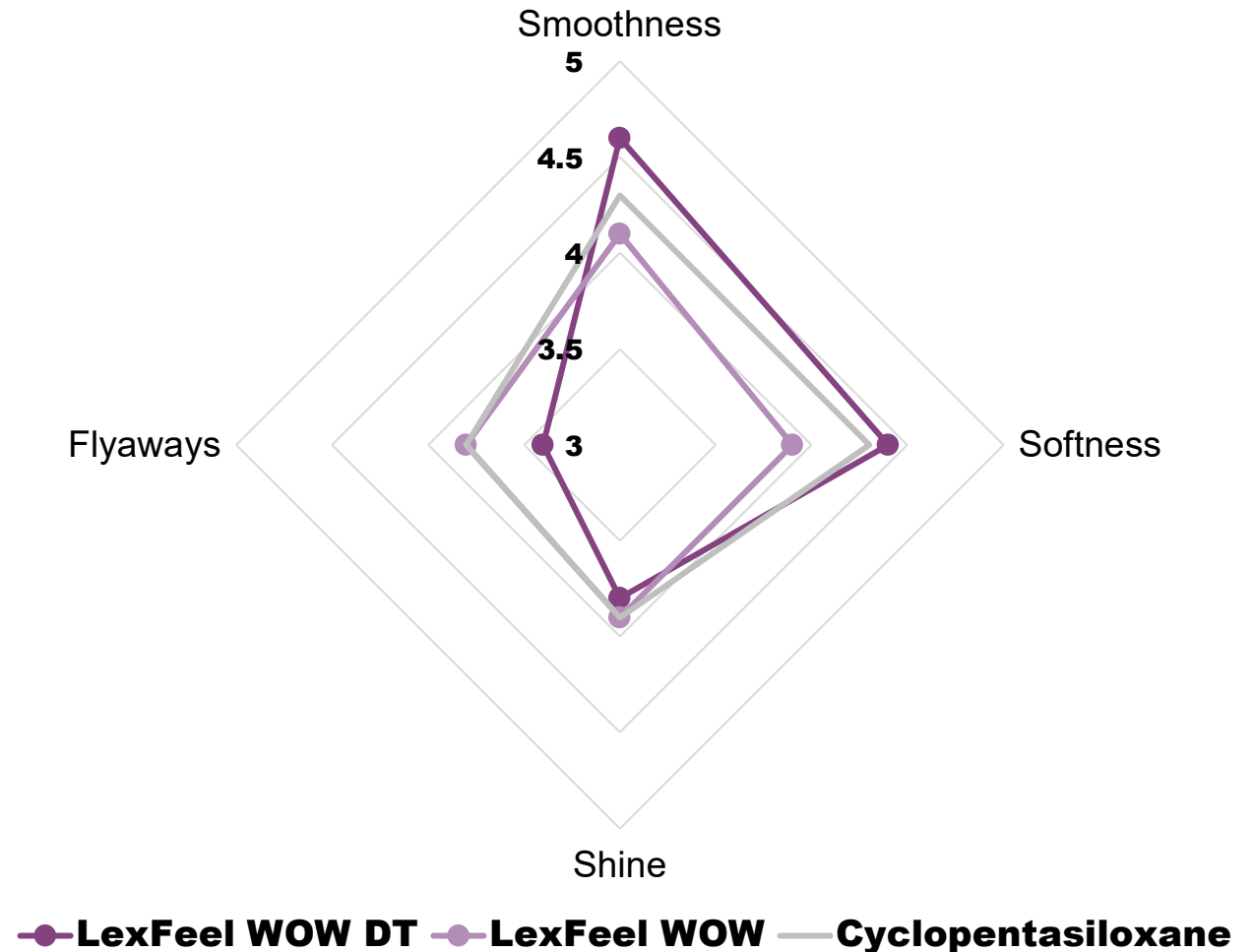


Clean Beauty
Preferred

*China IECIC Listed INCI name is C13-15 Alkane

Sensory profile in hair serum

LexFeel™ WOW and
LexFeel™ WOW DT perform
equivalent to
cyclopentasiloxane (D5)



Test Method

Test Formulation: 25% tested emollient; 20% C13-16 Isoalkane, 33% Natural oil blend, 20% CCT (quantitative formulation available upon request, 659-058)

Panelist half-head application of Hair Serum formulation post-wash to wet hair.

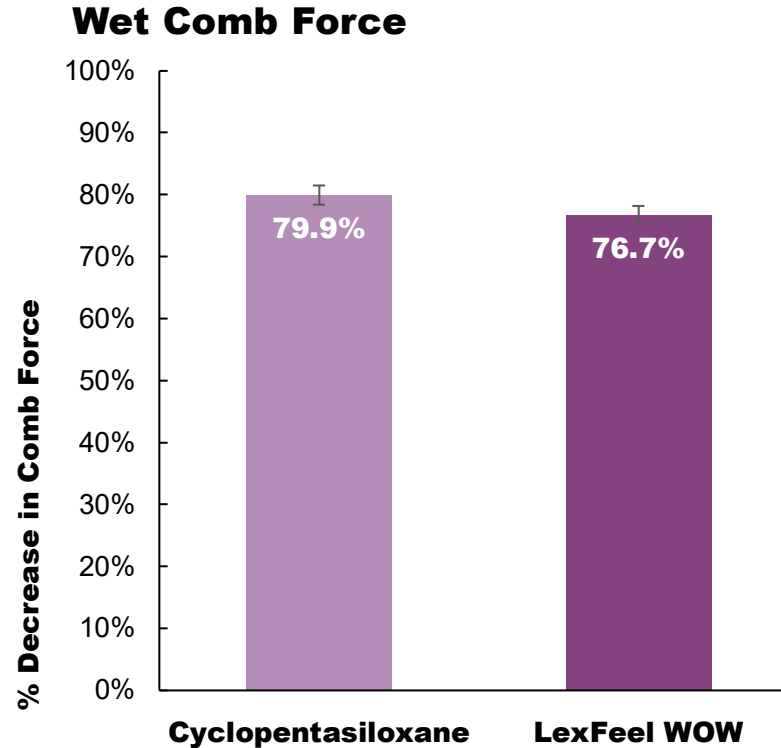
Blow dry & style. Expert grader evaluation. Scale: 1 to 5, n=20.

Full study report available upon request.

Conditioning performance

Conditioners with **LexFeel™**
WOW perform
comparably to
 conditioners with
cyclopentasiloxane (D5)
 on wet hair

Amidoamine-based formulation



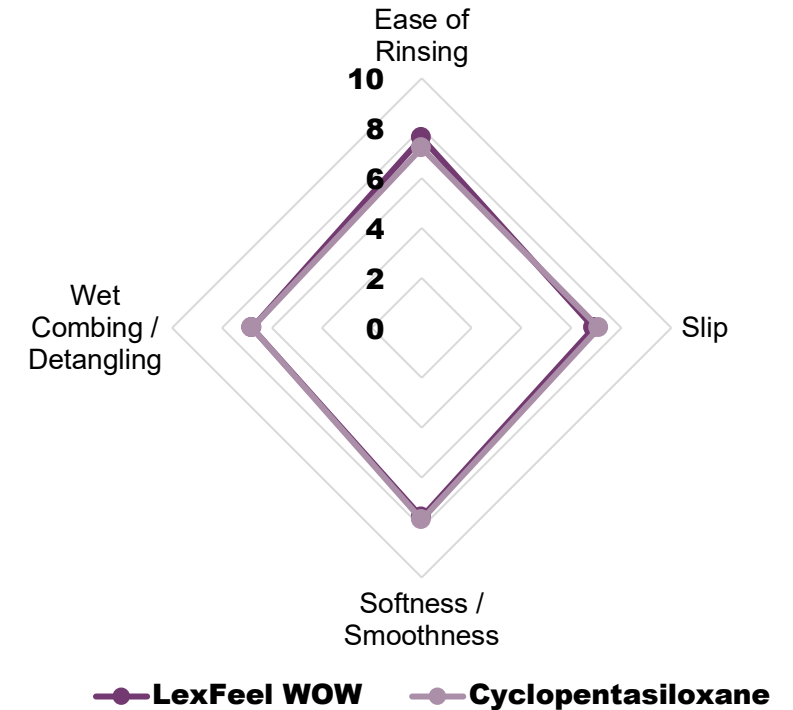
Test Method

2% conditioning agent (ProCondition™ 22), 6% fatty alcohol, 2.5% tested emollient (660-67C, 660-67D)

Measurement of Wet Combing Forces using Instron tensile tester, TRI/Princeton European medium brown hair tresses, bleached; 8 replicate tresses

Treatment procedure: (1) SLES wash, (2) 3 minute conditioner application, (3) 30s rinse
 Combing experiments performed in the wet state, 6 comb strokes per tress

Wet Conditioning Profile



Test Method

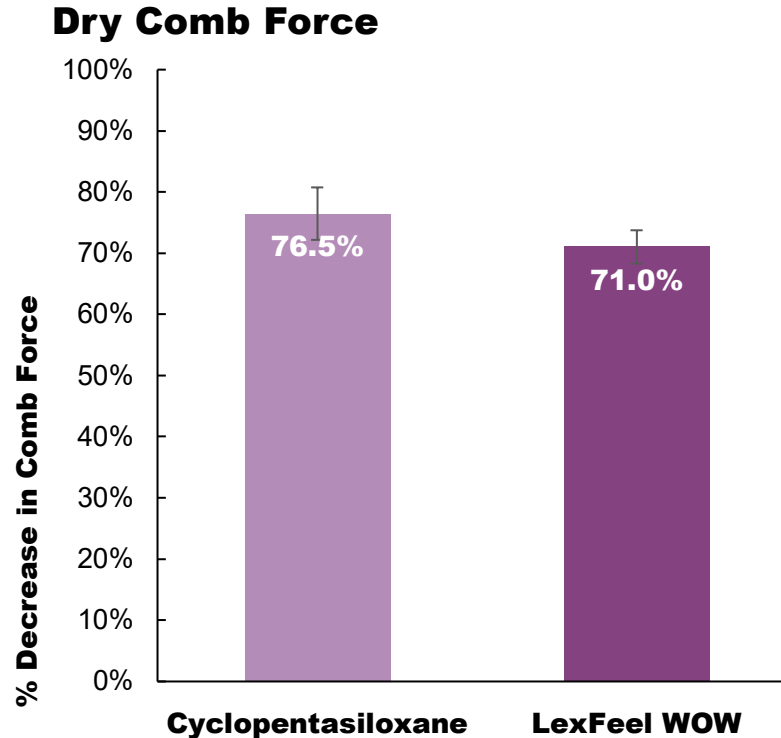
Test formula: 90% water, 7% conditioning base (Kerabase™ LC MB), 2% tested emollient, 1% preservation system (Phenostat™)

Panel half-head application of two conditioners post-wash to wet hair.
 Grader evaluation scale 1-10, n=9.

Conditioning performance

Conditioners with **LexFeel™**
WOW perform comparably to
 conditioners with
cyclopentasiloxane (D5)
 on dry hair

Amidoamine-based formulation



Test Method

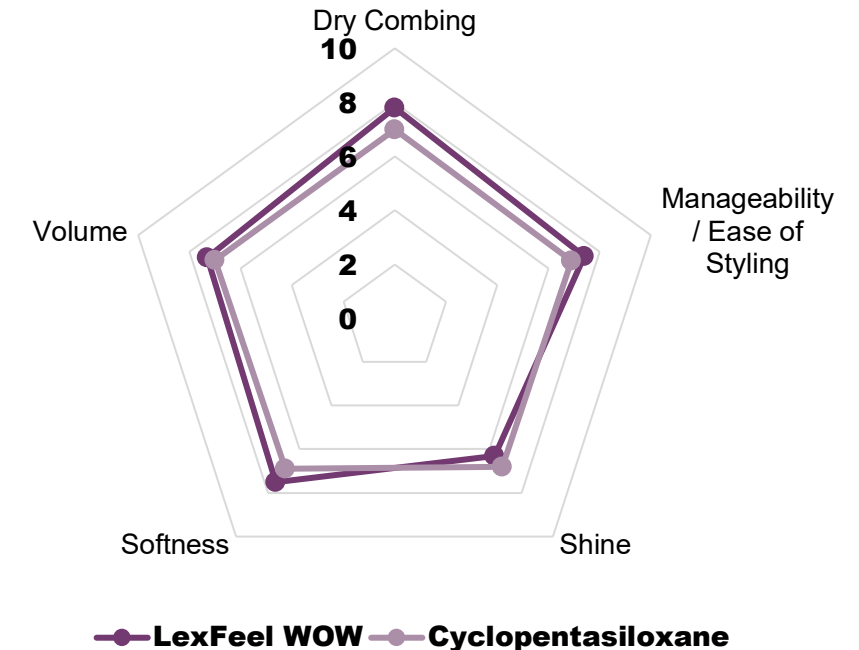
2% conditioning agent (ProCondition™ 22), 6% fatty alcohol, 2.5% tested emollient (660-67C-D)

Measurement of Wet Combing Forces using Instron tensile tester, TRI/Princeton European medium brown hair tresses, bleached; 8 replicate tresses

Treatment procedure: (1) SLES wash, (2) 3 minute conditioner application, (3) 30s rinse, (4) tresses dried overnight in controlled temperature and humidity (60% RH)

Combing experiments performed in the dry state, 6 comb strokes per tress

Dry Conditioning Profile



Test Method

Test formula: 90% water, 7% conditioning base (Kerabase™ LC MB), 2% tested emollient, 1% preservation system (Phenostat™)

Panel half-head application of two conditioners post-wash to wet hair.

Grader evaluation scale 1-10, n=9.

LexFeel™ N Series

INCI

Diheptyl Succinate (and)
Capryloyl Glycerin/Sebacic Acid
Copolymer

Made from

Coconut | Palm | Castor | Corn

100% Plant-based Dimethicone Alternatives

- Match spreading speed of comparable dimethicones
- Disperse color pigments and inorganic UV filters
- Functional benefits of comparable dimethicones
- Range of dimethicone alternatives: 5 cSt, 20 cSt, 50 cSt, 100 cSt, 200 cSt, 350 cSt

Standards & Certifications



100% Natural



100% USDA
certified
biobased
content



Natural
Origin Index:
1.0



Biodegradable



RSPO Mass
Balance
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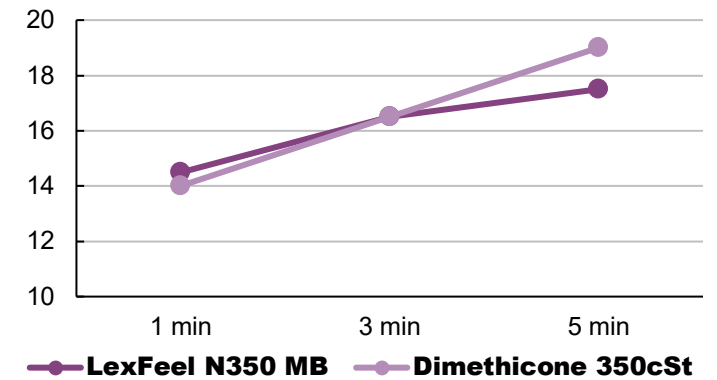
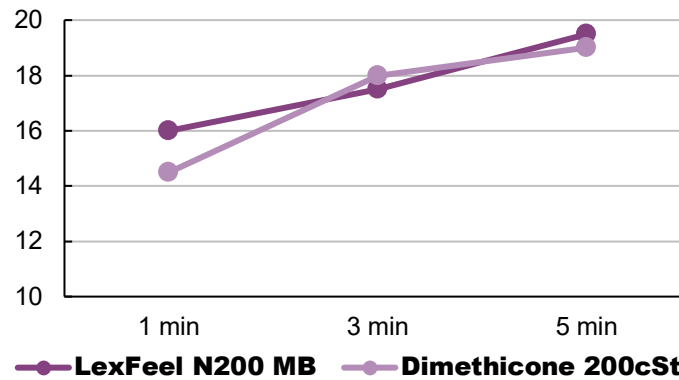
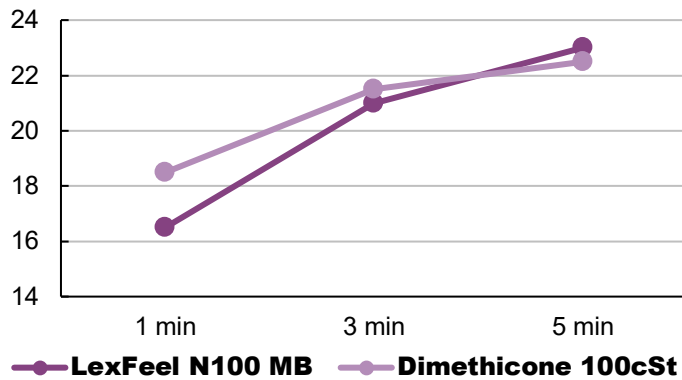
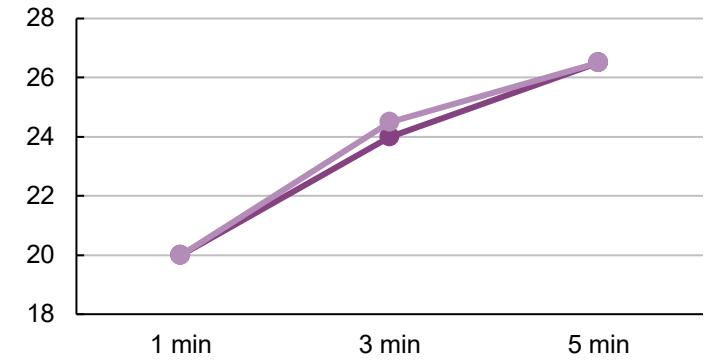
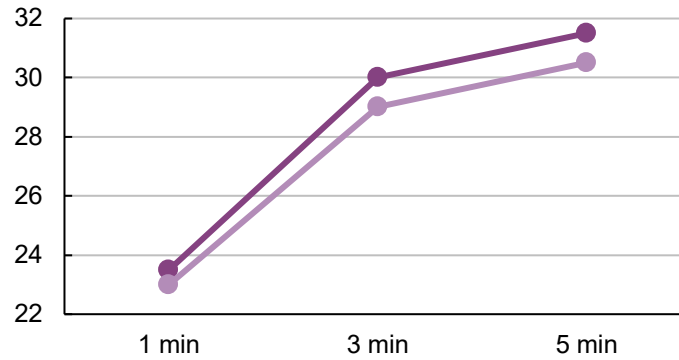
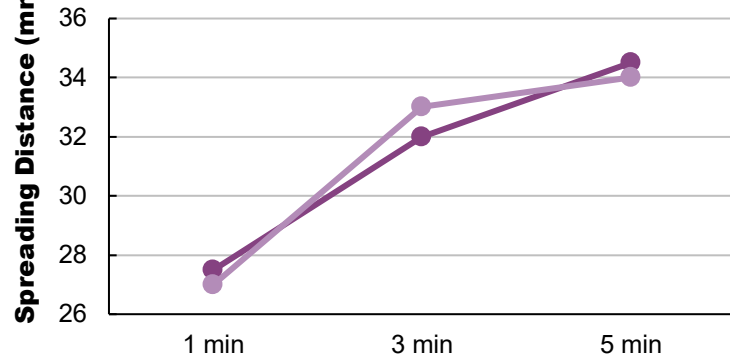
Halal
Certified



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Spreadability

Spreading Speed



Test Method
 A piece of filter paper was placed over Petri dish using 50 μ L of sample was applied to the approximate center. After 1 minute, 3 minutes, and 5 minutes, the diameter of the circle created was measured. Two measurements were taken of each circle.

Conditioning Performance

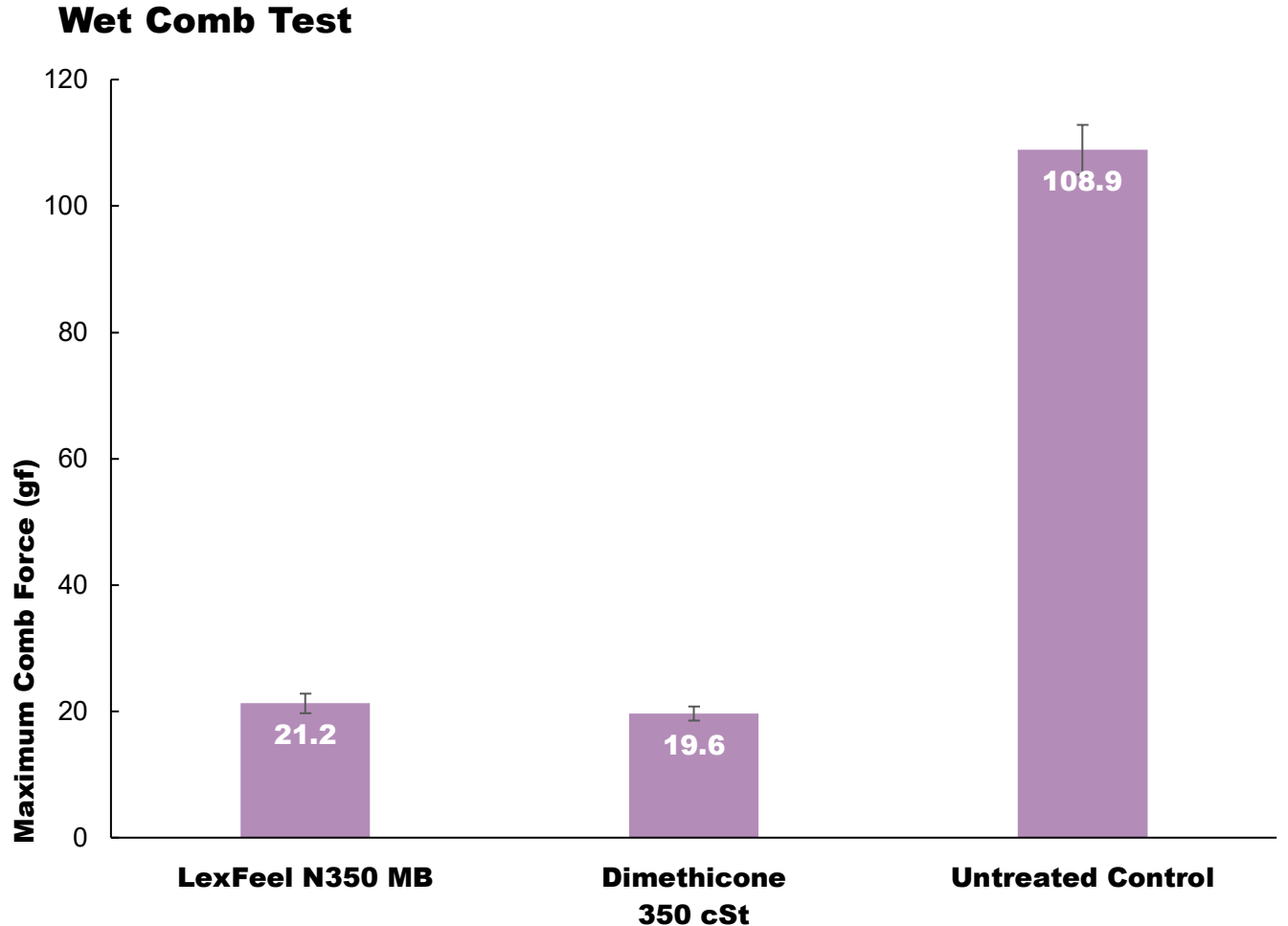
LexFeel™ N350 MB provides equivalent conditioning to **Dimethicone**

Significant reduction in wet comb force from rinse-off conditioners

Test Method

- Measurement using Instron tensile tester, Study performed by TRI/Princeton
- European medium brown hair tresses, bleached
- Test Formulation (660-066E-F): 2% w/w BTAC; 2.5% conditioning in water; pH ~4.0

* p < 0.05



Color Protection

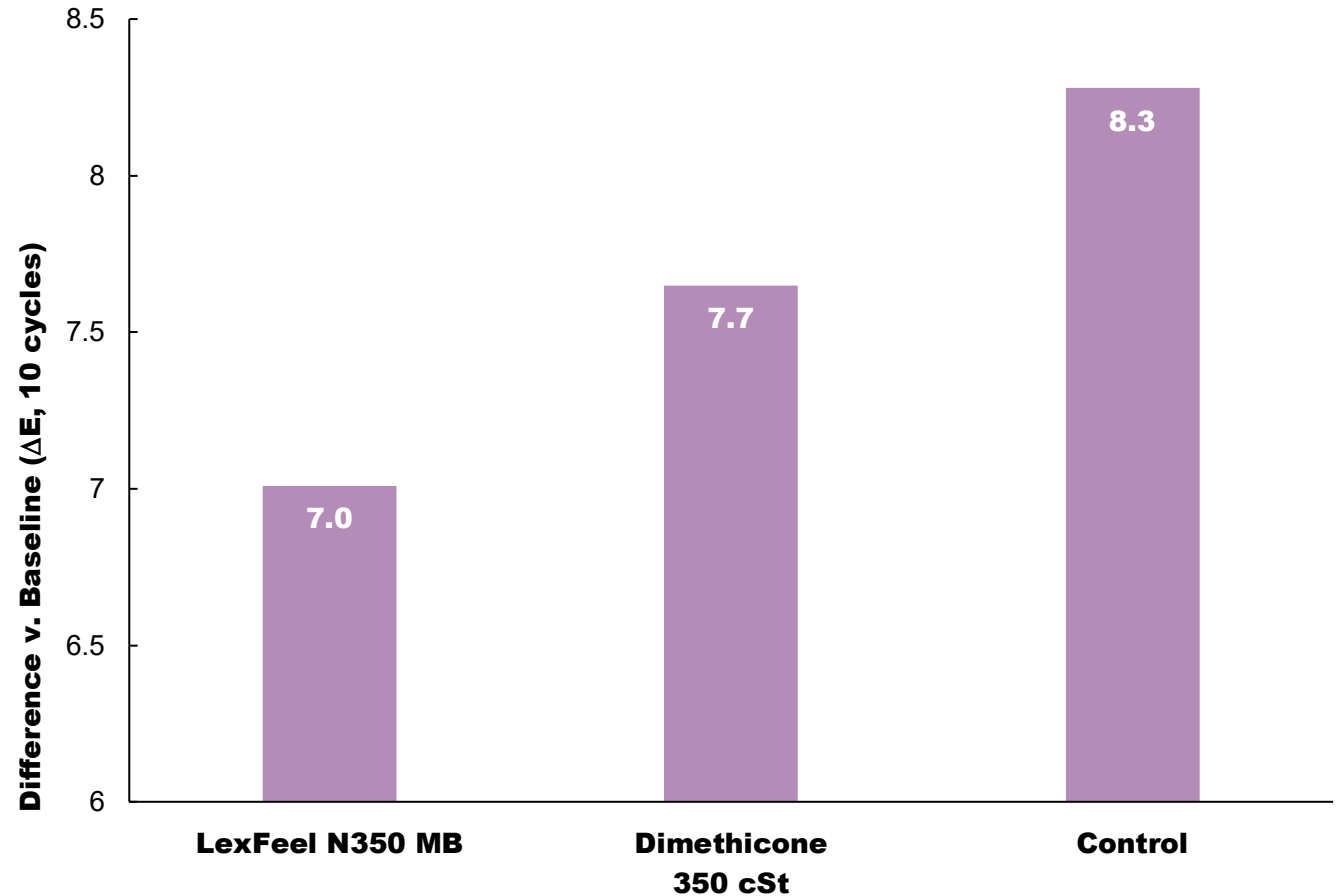
LexFeel™ N350 MB visibly maintains hair color

- Visible color retention improvement after 10 wash/condition cycles compared to control ($\Delta E > 1$)
- Color retention equivalent to Dimethicone 350 cSt

Test Method:

- Measurement using Konica Minolta CR-300 Chroma Meter
- Study performed by Inolex R&D
- European medium brown hair tresses, bleached
- Test formula conditioning package: 10% LexFeel N350 MB (610-179A) or Dimethicone (610-179B); Control: No conditioning agent
- L'Oréal Paris Permanent Color in Medium Auburn
- $\Delta E > 1$ results in visible color difference

Color Retention Test



Silicone-free formulations



Formulating without silicones

Functional analysis is required at the ingredient and formulation level

Reformulating existing products

- What is the job of the formula?
- What role was the silicone playing?
- What ingredient(s) would perform the same job?
- How will removing the silicone affect the system?

Developing new products

- What is the job of the formula?
- What mechanism(s) are at work?
- What ingredient(s) will deliver the benefit?

Detangling sprays



AUSSIE Total Miracle Detangling Spray

Ingredients:

Water, Prunus Armeniaca (Apricot) Kernel Oil, Macadamia Ternifolia Seed Oil, Fragrance, Phenoxyethanol, Trisodium Ethylenediamine Disuccinate, **Amodimethicone**, PEG-40 Hydrogenated Castor Oil, Benzyl Alcohol, Polyquaternium-11, Citric Acid, Ethylhexylglycerin, Trideceth-12, Cetrimonium Chloride



JOHNSON'S® No More Tangles® Detangling Spray

Ingredients:

Water, **Amodimethicone**, Glycerin, Sodium Benzoate, Polysorbate 20, Distearyltrimonium Chloride, Behentrimonium Chloride, Citric Acid, Fragrance, Trideceth-12, Cetrimonium Chloride

Polyesteramines such as Polyester-11 (Kerazyme™ MB) are ideal candidates to replace Amodimethicone

Conditioning benefit

	Mean % Reduction in Dry Comb Force
0.5% Kerazyme™ MB + 2% SAPDMA	45%
0.5% Amodimethicone + 2% SAPDMA	15%

Kerazyme™ MB offers superior dry combability in rinse-off conditioner formulations **compared to amodimethicone**

Test Method:

Mass Market Type Formula with 2.5% total actives evaluated. Kerazyme™ MB and Amodimethicone (DC 2-8566cps) evaluated as additives to SAPDMA

Amino Lipid Detangler (HC-1180)

Trade Name	Ingredient (INCI)	%(w/w)
Deionized Water	Water	97.01
Gluconal® CAM ¹	Calcium Gluconate	0.14
Jaguar® HP 105 ²	Hydroxypropyl Guar	0.35
AminoSensyl™ SC*	Brassica Alcohol (and) Brassicyl Valinate Esylate (and) Brassica Glycerides	1.00
Spectrastat™ PHL*	Caprylhydroxamic Acid (and) 1,2-Hexanediol (and) Propanediol	1.5

*Inolex, ¹Corbion, ²Solvay Novecare

Silicone-free detangling spray formulation

Lubricity and wet/dry comb force reduction provided by combination of:

- Cationic liquid crystal dispersion (AminoSensyl™ SC)
- High molecular weight water-soluble polymer (Hydroxypropyl Guar)

Conclusion

Key takeaways

- Real (sustainability) and perceived (safety) concerns about silicones continues to drive their replacement with alternatives.
- Functional analysis (what is the job to be done?) is critical for successful implementation of silicone alternatives at the ingredient (reformulation) and formula (new product development) levels.
- The broad offering of silicone alternatives in the market coupled with new formulation approaches makes silicone-free formulation easier than ever; however, some gaps still remain, e.g. extreme heat protection.
- As newer generations of consumers with less experience of silicone-based products continue to enter the market, consumer expectations will gradually evolve toward greater acceptance of silicone-free products.

Thank You

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