# Toward milder personal care cleansing products: Fast ex vivo screening of irritating effects of surfactants on skin using Raman microscopy

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# Overview

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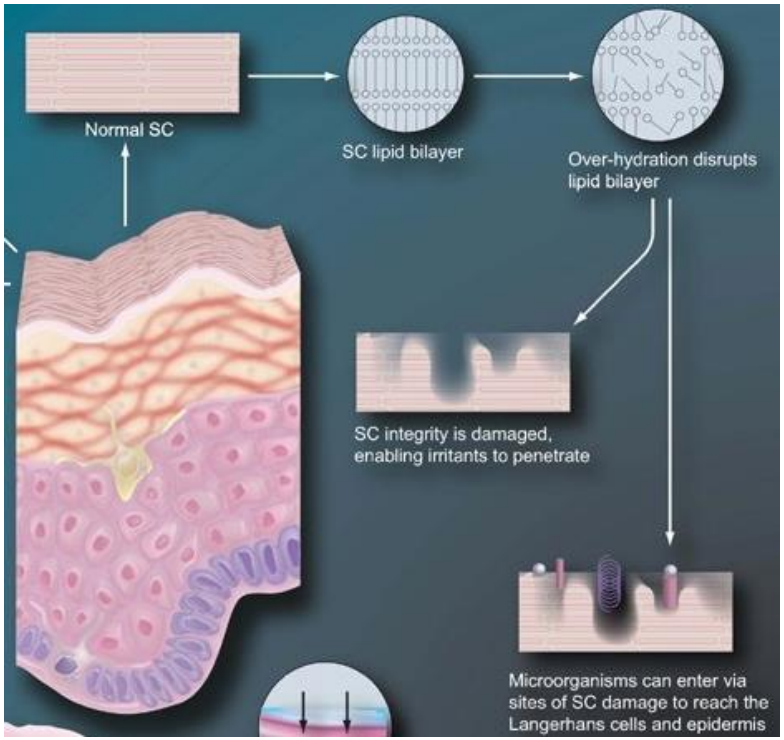
Overview: Surfactant-Skin Interactions in Industrial Formulations

**Technical Information**: Assessment and understanding of the impact of cleansing products on water retention and protein/lipid modification of skin

**Industrial Relevance**: Personal Care, Cosmetics, Pharma

# Mildness of surfactant




**Pediatr Health 2009 Future Medicine Ltd**

**Absence of skin irritation (redness, tightness, dryness, itching)**

- **integrity of the lipid barrier (dissolution and/or disorder)**
- **no denaturing of proteins (keratin)**
- **no removal of natural moisturizing factors (NMF)**
- **no biological effects (e.g., inhibition of enzymes)**

# Gap: Fast screening of surfactants mildness

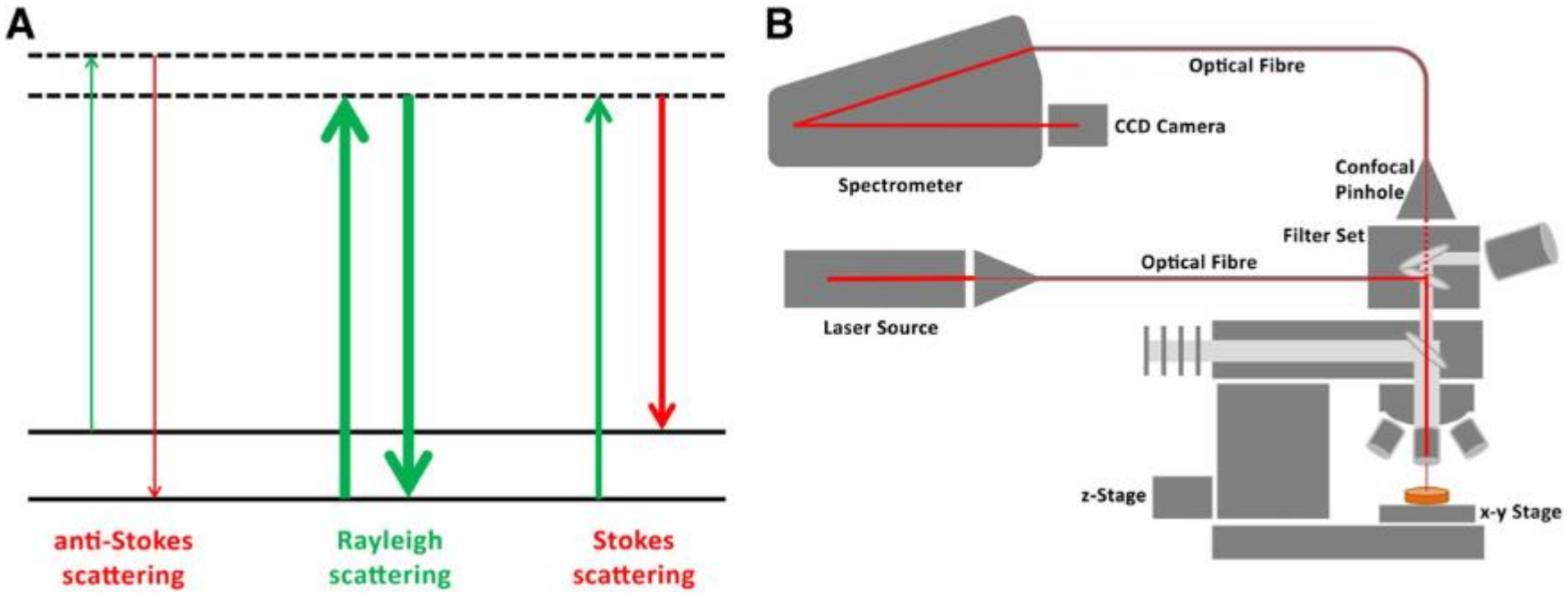
**Macroscopic methods:**

- **appearance of the skin (redness, dryness after contact with surfactant solution)**
- **staining with a dye (corneosurfametry)**
- **mechanical properties**
- **barrier properties (transepidermal water loss, transmission factor),**
- **(de)hydration/swelling of skin (conductance)**
- **protein/lipid solubility**
- **collagen swelling**

**Molecular level:**

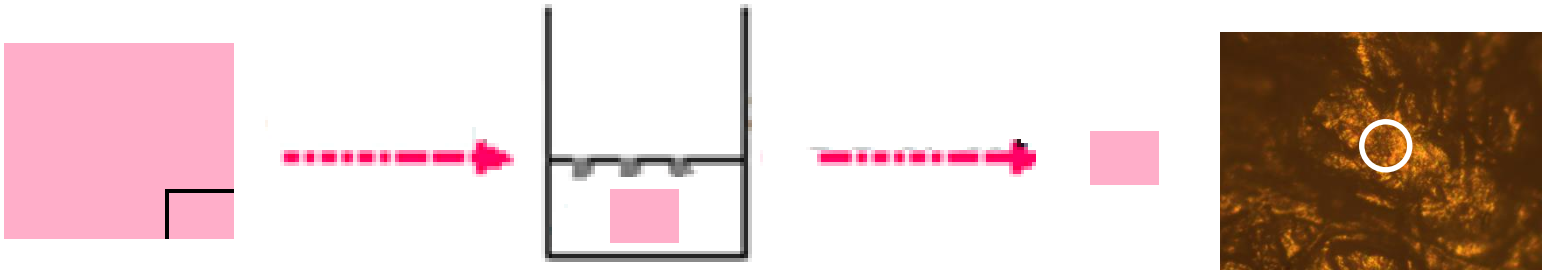
**Spectroscopies (FTIR, Raman): fast access several key properties such as water uptake and lipid/protein modification**

# Goal: to assess mildness/irritability under real exposure using Raman microscopy




Franzen &Windbergs. Advanced Drug Delivery Reviews 89 (2015) 91–104

# Spectroscopic (Raman) Method



Skin cut

Wash with Surfactant Formulations in $D_2O$

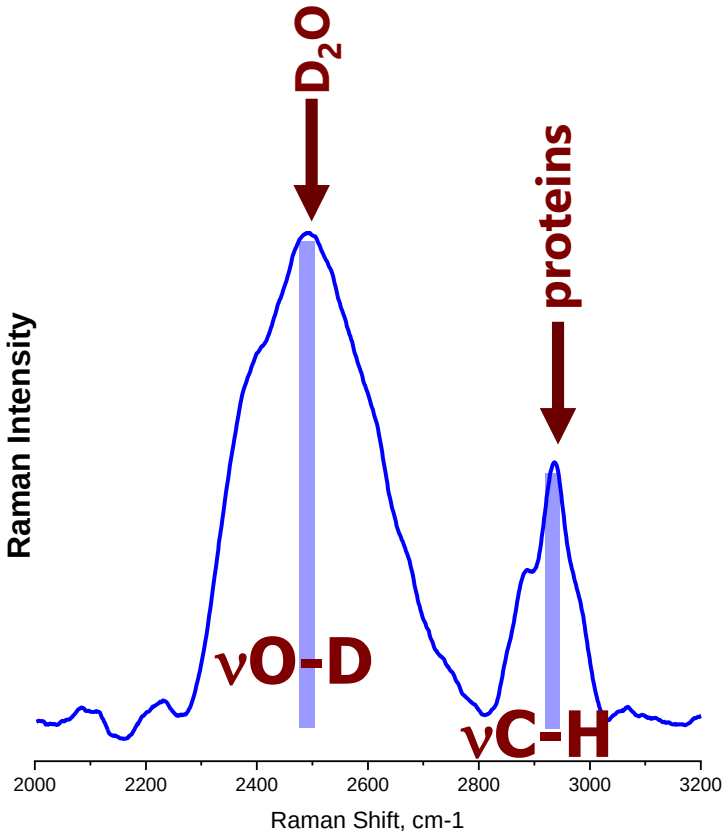


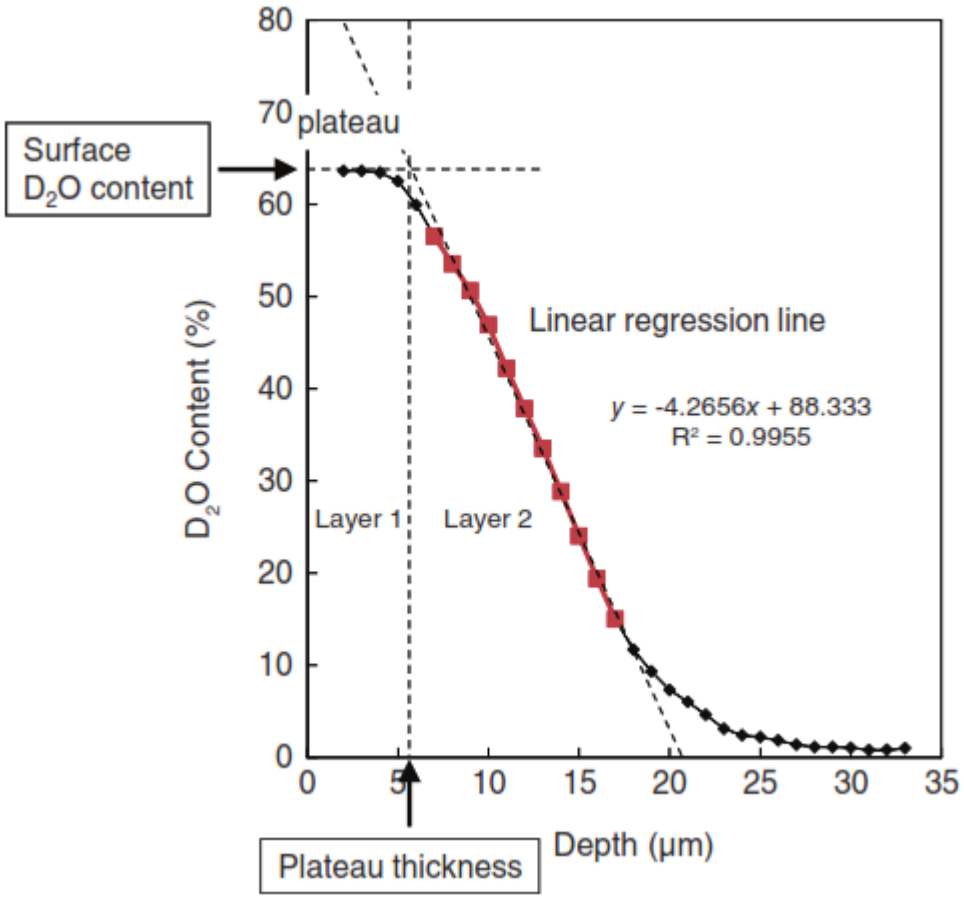
Skin isolated for Raman

- Porcine skin cut 0.2 x 0.5 $cm^2$ squares
- Conditioned for selected time with 0.05 g/mL selected surfactants in $D_2O$ and blank ($D_2O$)
- Raman measurement after treatment: 4 spectra, 1.5 min each, 1st is discarded (transient state)

Chernyshova et al. *Tenside Surfactants Detergents*, 2019, in press

# $D_2O$/protein ratio as a measure of water retention in SC



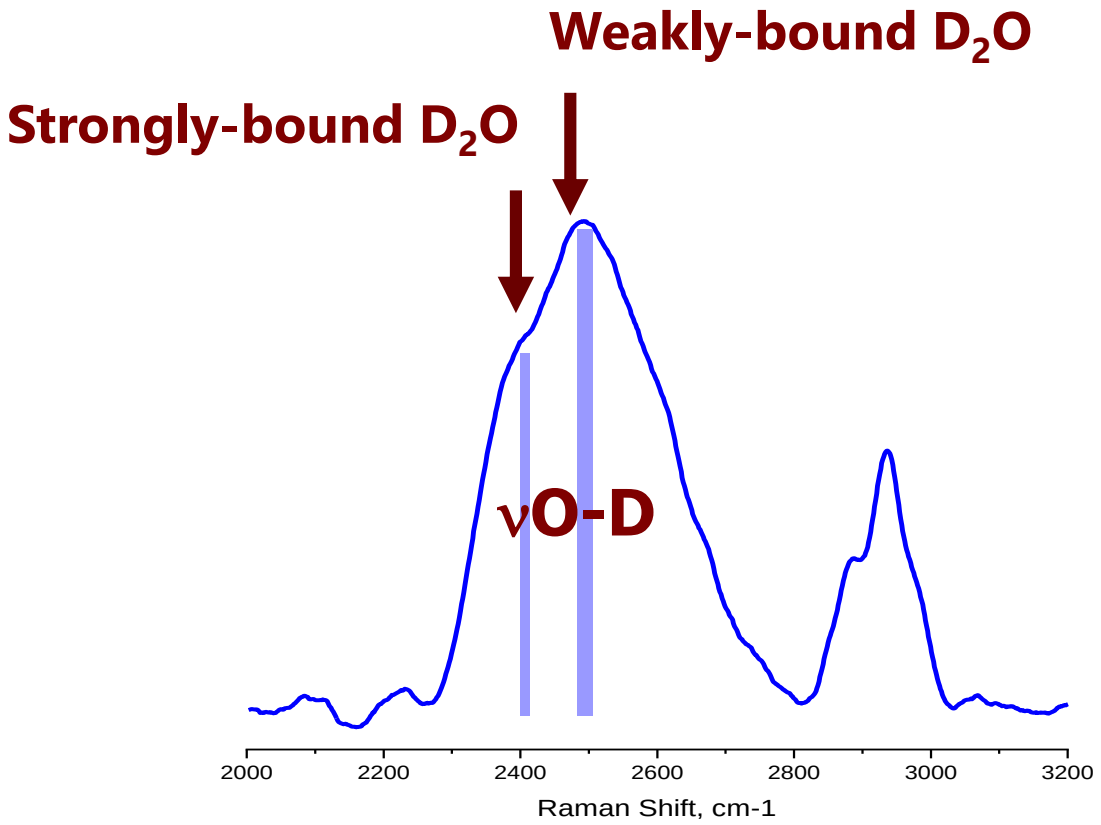




**Endo et al. *Journal of Surfactants and Detergents* 2018,** *21* (6), 777

## $D_2O$/protein peak ratio=water content

**Vyumvuhore et al. *Analyst*, 2013, 138, 4103**

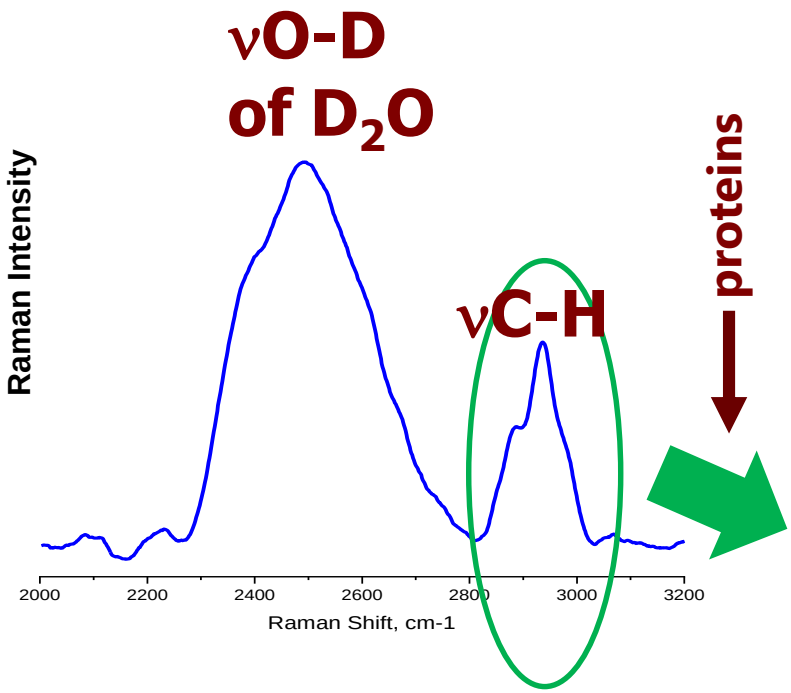
# Strongly/weakly bound heavy water $D_2O$

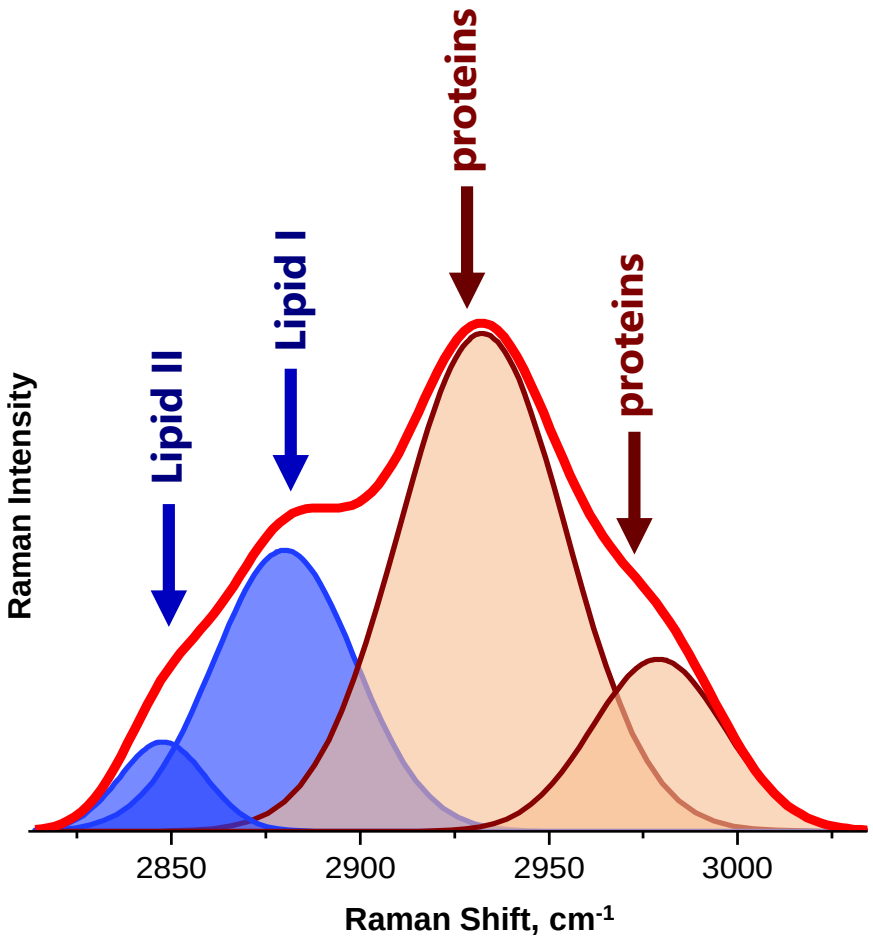



- **Strongly bound water=natural moisturizing factor (NMF)/keratin sites**
- **Weakly bound water increases greatly when all sites for strongly bound water are saturated**

Vyumvuhore et al. *Analyst*, 2013, 138, 4103

# νC-H Lipid peak ratio as a measure of lipid order

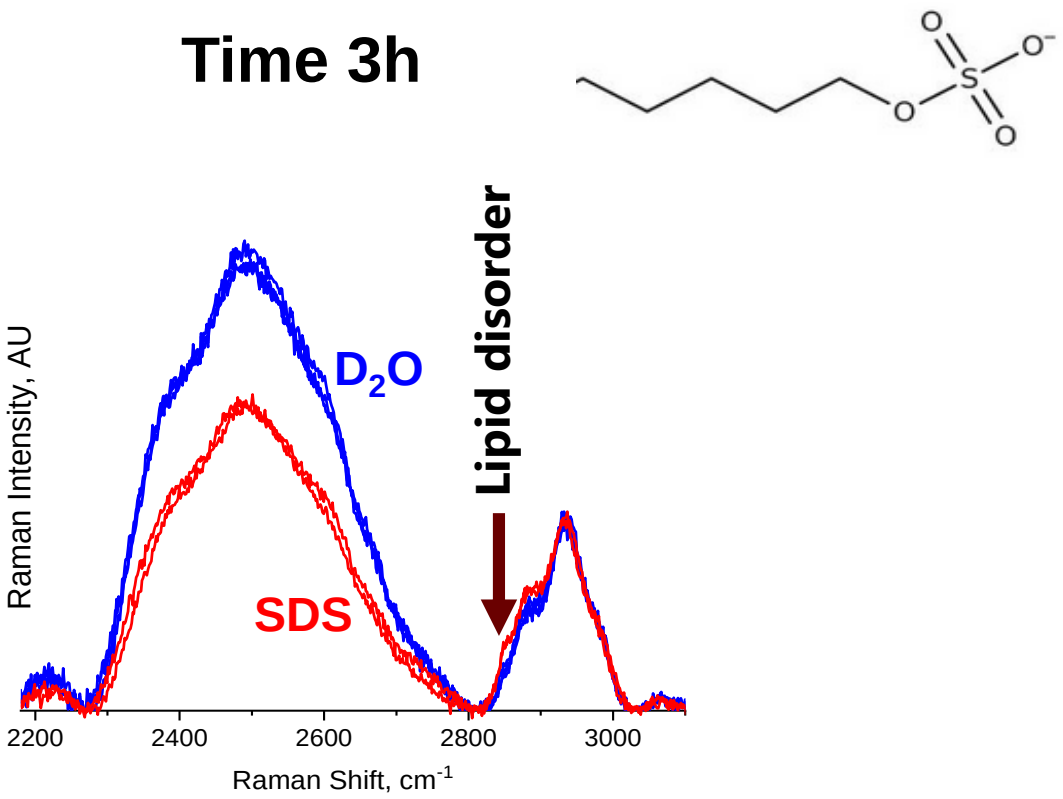



**"Lipid I"/"Lipid II" peak ratio ↑ = lipid order ↑**

# Preliminary tests of single surfactants: SDS

## Harsh at long exposure: weakens the skin barrier and increases lipid disorder

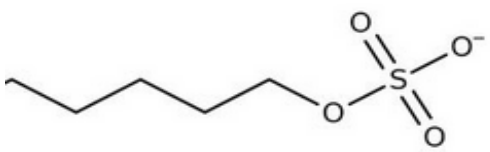


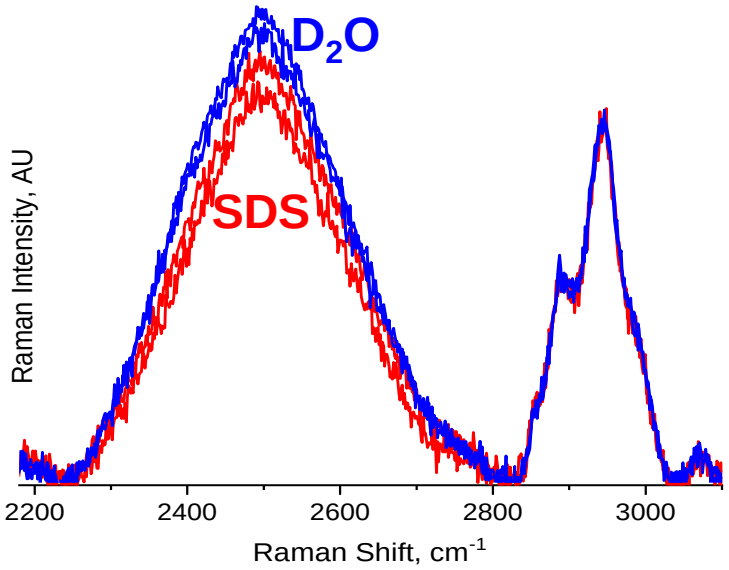

**In agreement with lit. data** [**Walters et al.** ***Dermatology Research and Practice*** **2012,** 2012, 9; **Yanase& Hatta.** ***International Journal of Cosmetic Science*** **2018**, 40 (1), 44-49]

# Preliminary tests of single surfactants: SDS

**The negative effects are much less pronounced at 10 min exposure**

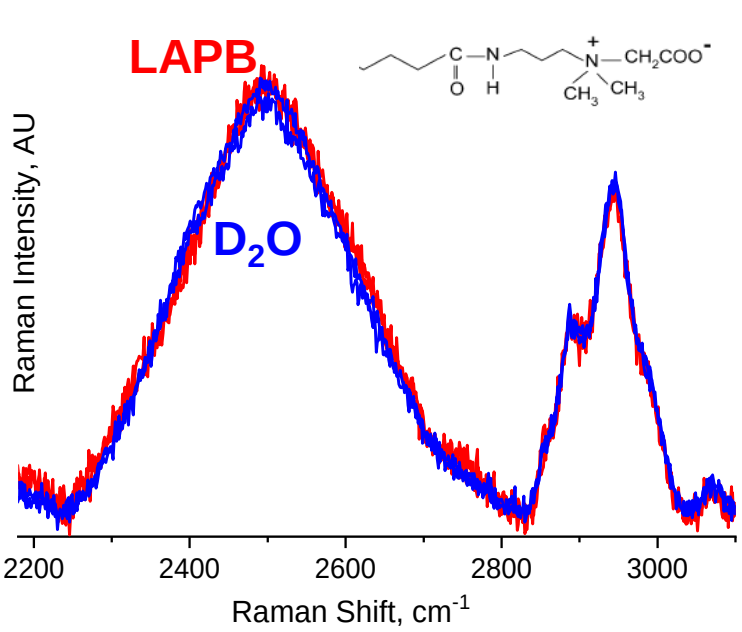
## Time 10min

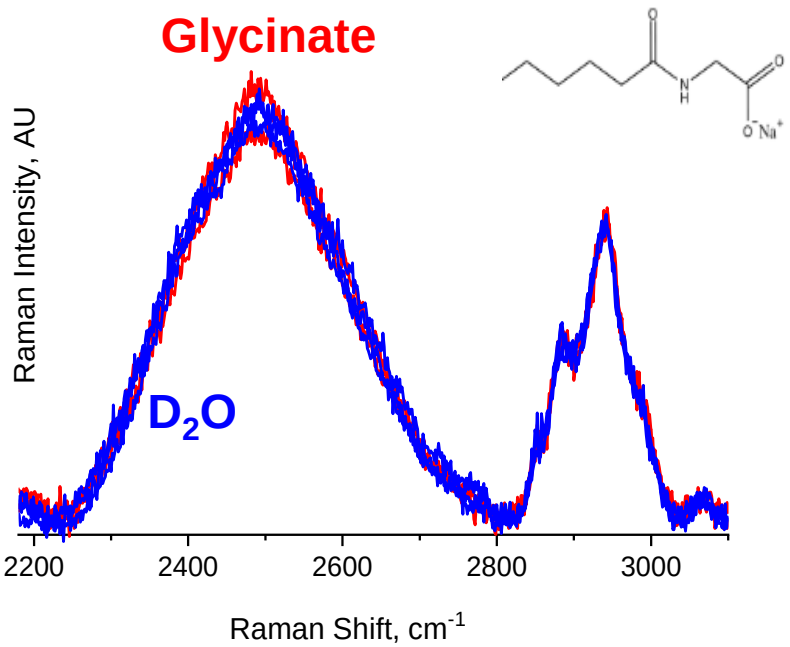




# Preliminary tests of single surfactants

## No impact of amino-acid based anionic and zwitter-ionic surfactants

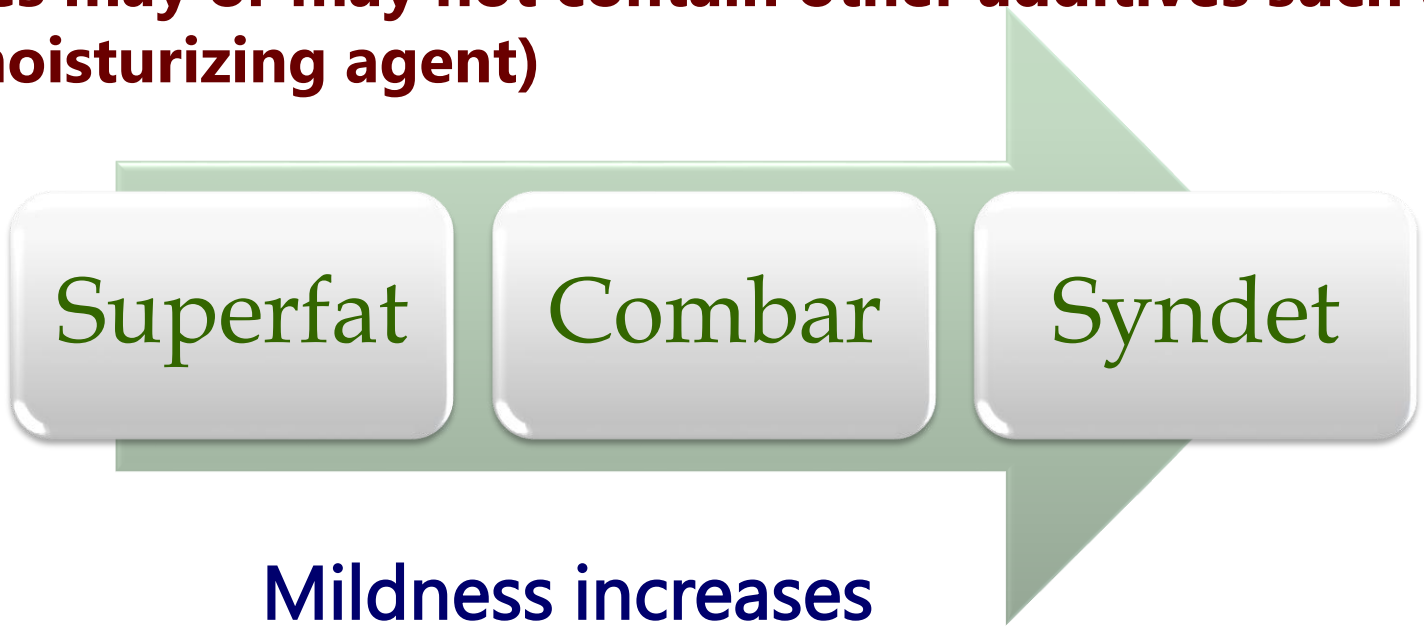


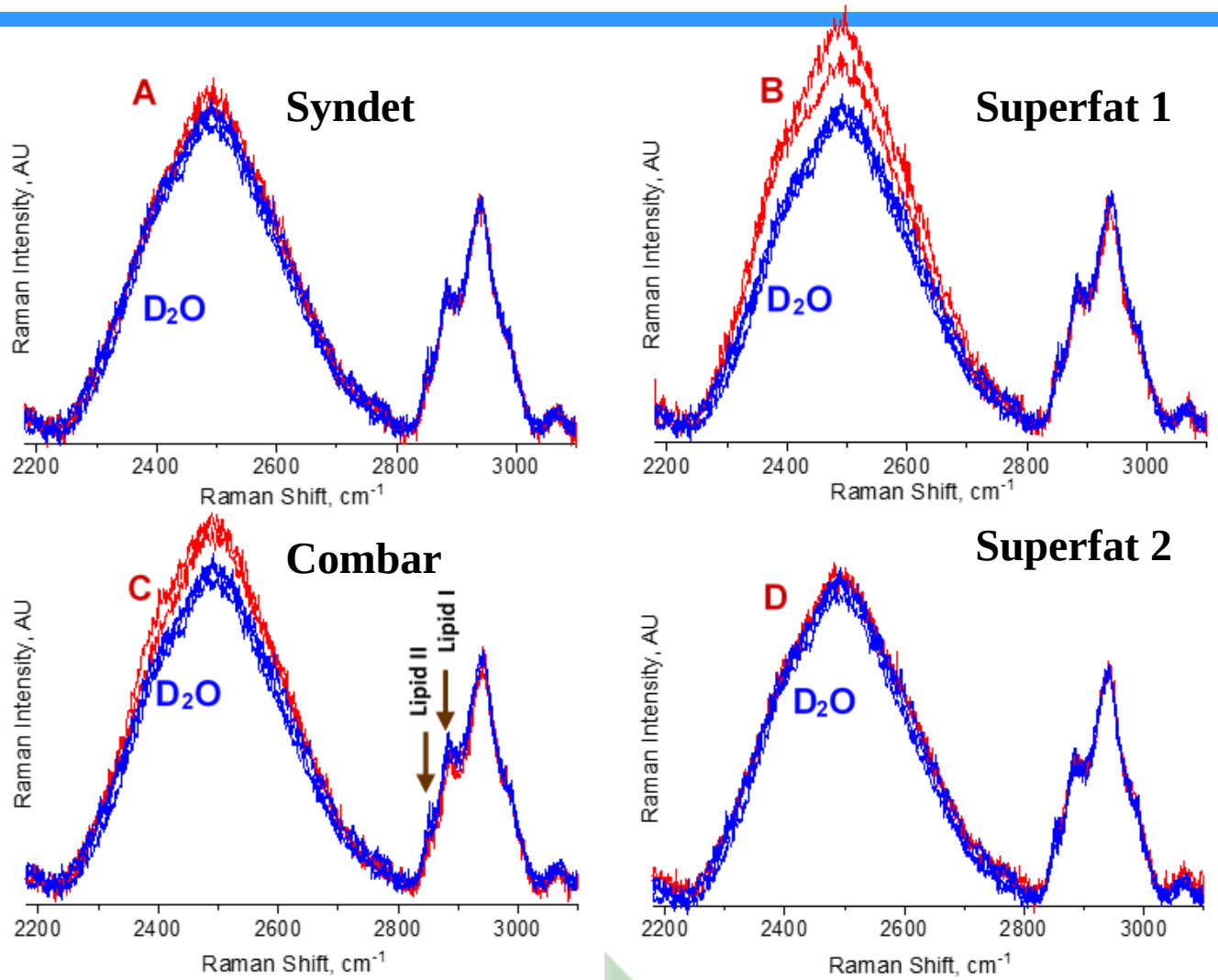
# Test of three typical types of bar soaps

1 "Superfat": fatty acid soap
2 "Combar": combination of 90% fatty acid soap and non-soap-based surfactants, e.g. betaine
3 "Syndet": non-soap-based surfactants such as lauroyl isethionate and betaine

All types may or may not contain other additives such as stearic acid (moisturizing agent)



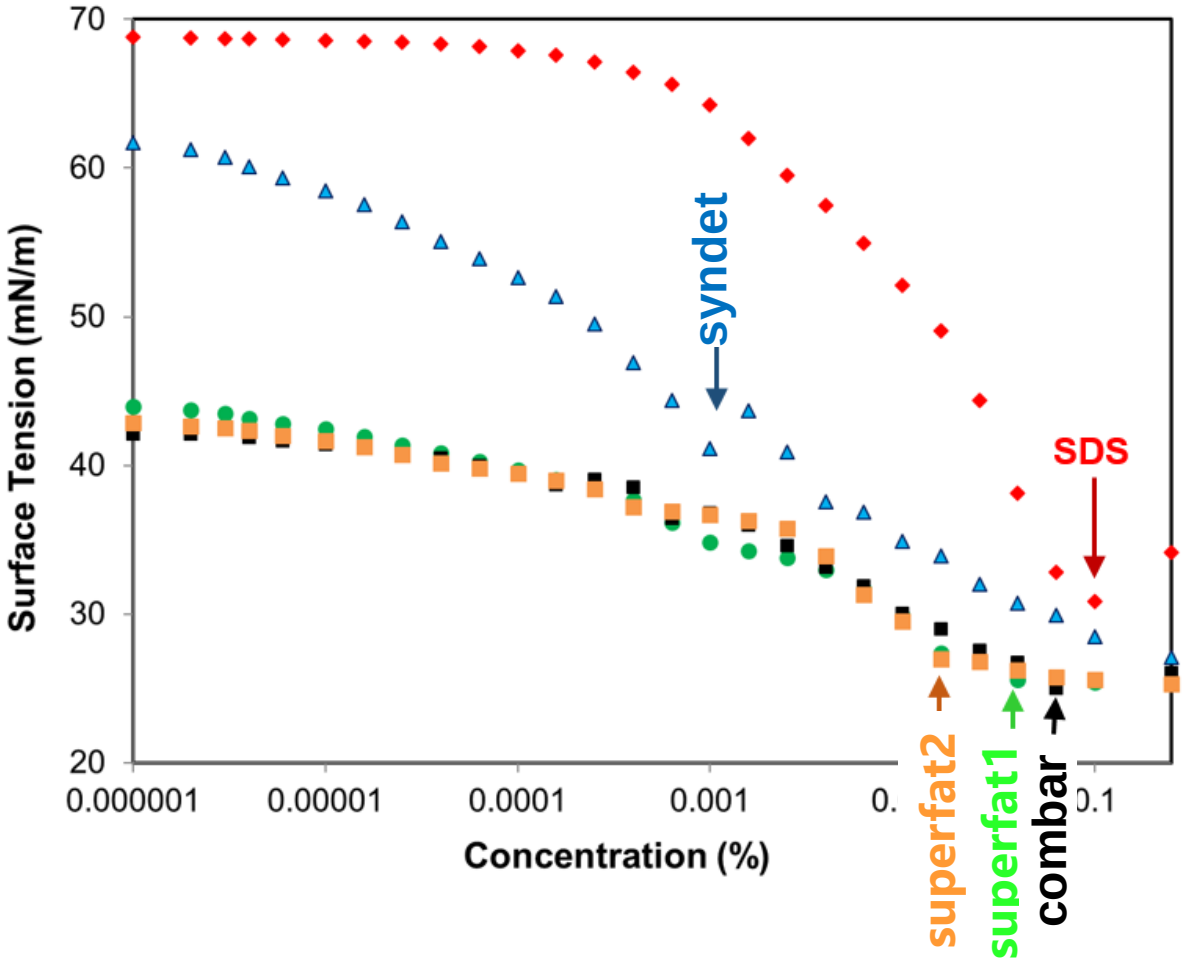
# Raman Test of Bar Soaps




Superfat 1 → Combar → Syndet → Superfat 2

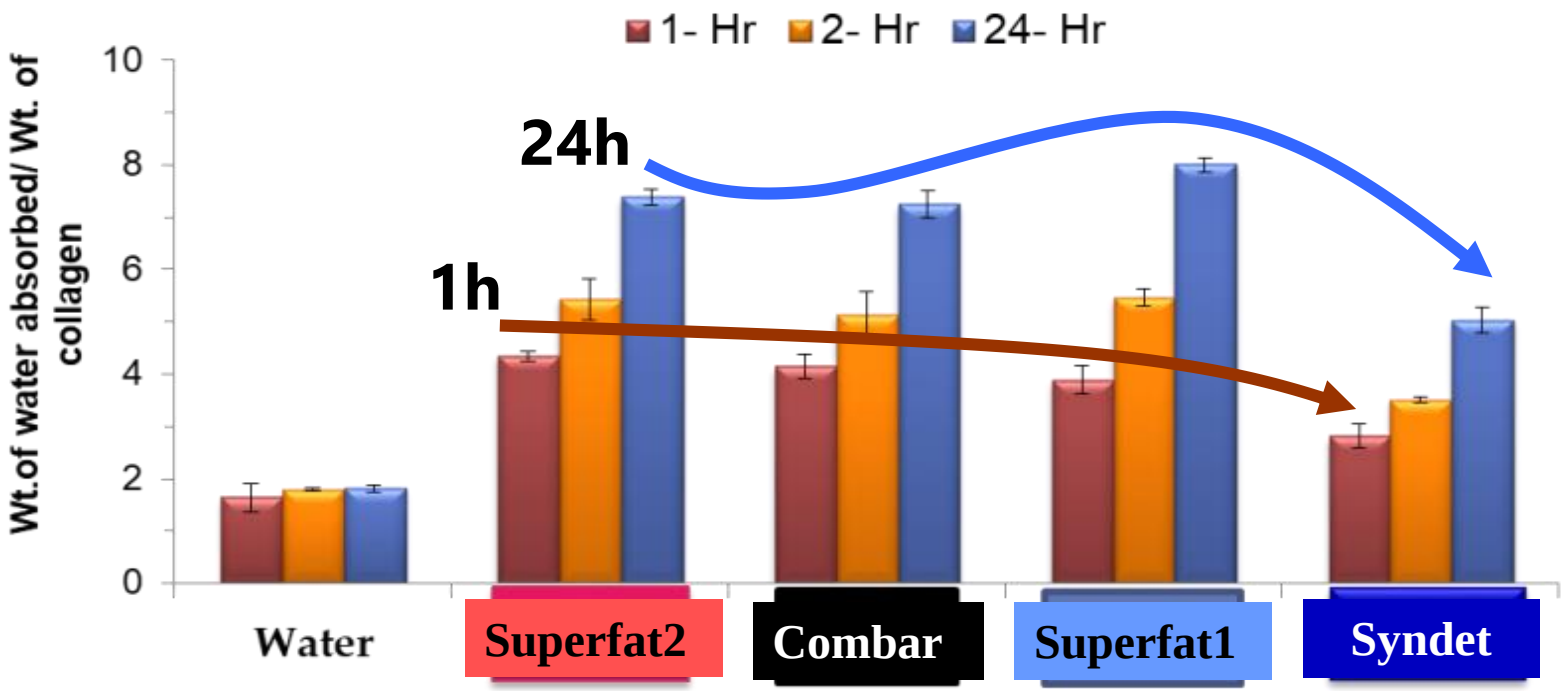
Mildness increases

# No correlation with CMC




**CMC decreases in the row SDS > combar > superfat1 > superfat2 >> syndet**

# No correlation with collagen swelling




**Swelling/ranking depends on time: It decreases**

**At 1h: superfat2 > combar ≈ superfat1 > syndet**

**At 24h: superfat1 > combar ≈ superfat2 > syndet**

# Conclusions

- **Developed a novel *ex vivo* Raman technique for real exposure**
- **At brief exposure times the ranking of surfactant formulations based on the molecular-level response of the SC and model macroscopic tests such as collagen swelling and CMC can significantly be different**

# Further Work

**More systematic study to develop molecular-level descriptors of the SC response to the exposure.**

**Develop a spectroscopic probe of the electric charge density/local electric field of micelles and diffusivity of surfactants to verify the current models of the surfactant mildness**

# Acknowledgements






## Disclaimer

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