

From Drugs to Bubbles: There and Back Again

Omar Mansour



Background

Egypt 2006-2011

BPharm/BSc Pharmaceutical Sciences

The UK 2012-present

MSc Formulation Science- UoG scholarship

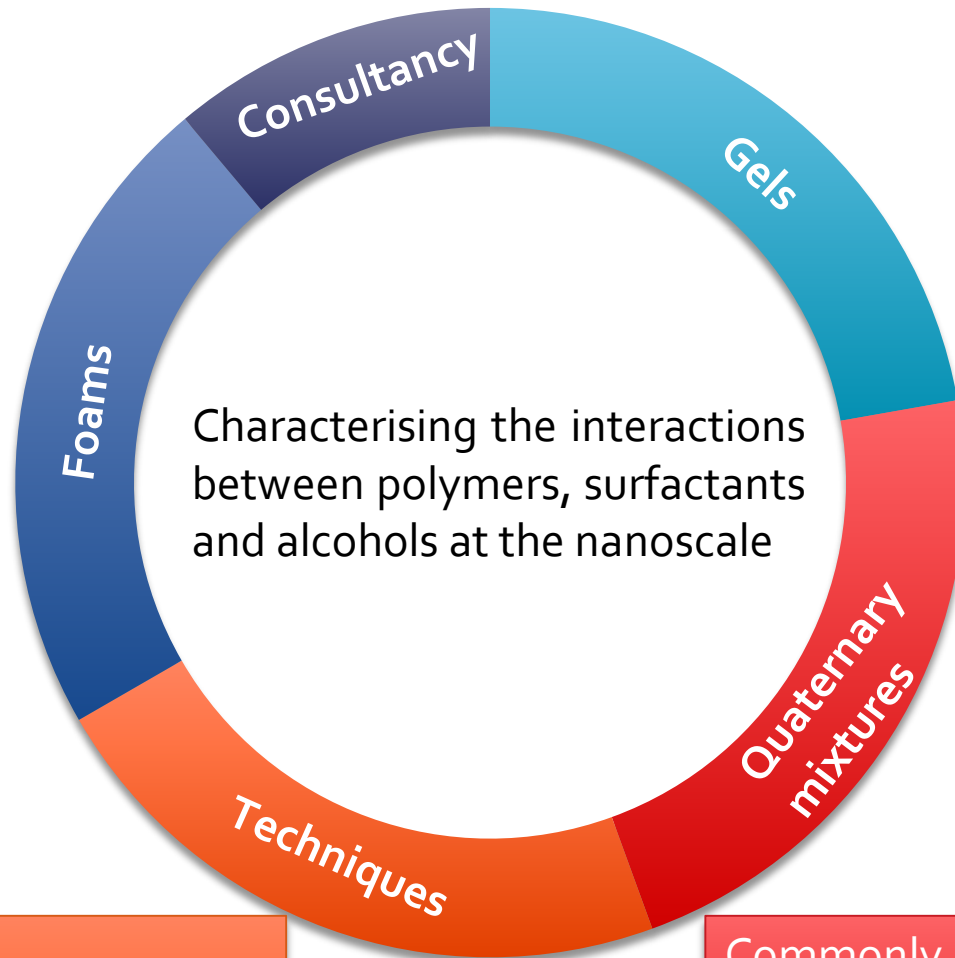
PhD in Physical Chemistry- Vice Chancellor Studentship

Post-Doctoral Research Fellow- Infineum, GSK, MSD and Unilever

Lecturer in Cosmetic Science- DMU



Background- PhD studies



Tensiometry
NMR Spectroscopy: ^1H and Diffusion
Scattering: Light and Neutrons

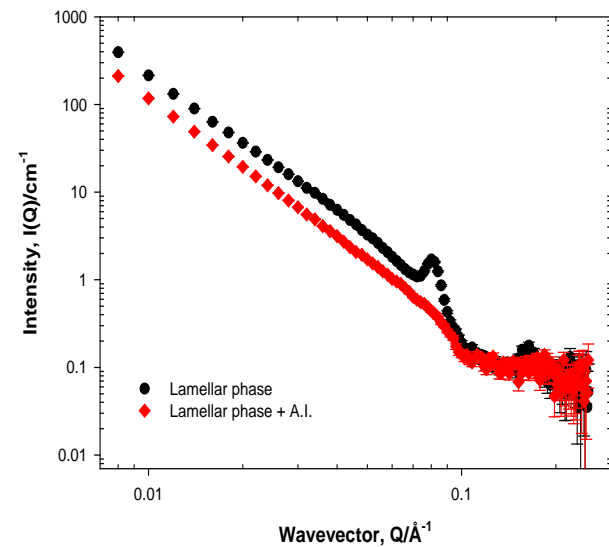
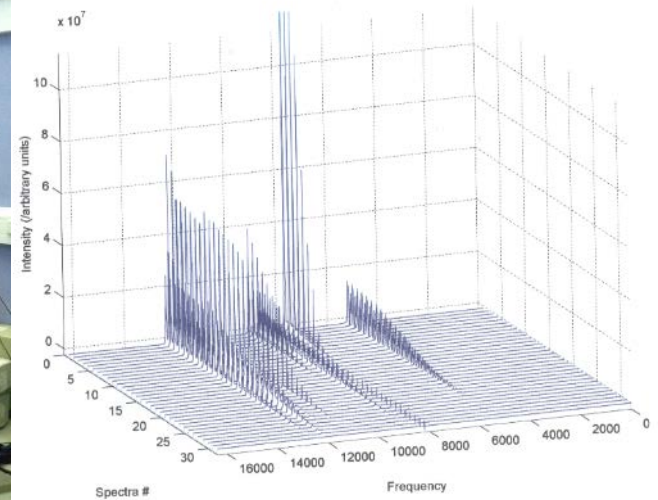
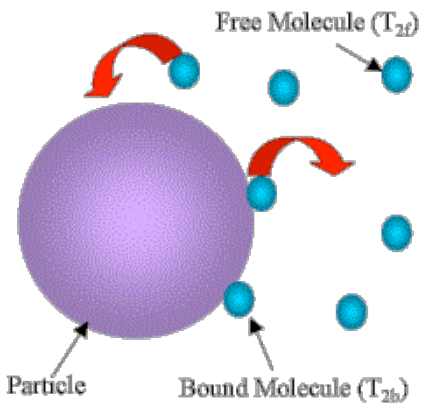
Commonly used polymers (Pluronics, PVP, PEO..), small molecule surfactants, oils and alcohols

Background- PDRF



- Real life formulations have many challenges, interactions?
- Similar ingredients, different concentrations, different media = different functions
- Structured formulations are essential for good performance...

Seeing things at the nanoscale..



Seeing things at the nanoscale..

Small-Angle Neutron Scattering (SANS)

- Central facilities
- Access through a proposal/peer review process
- Several locations across Europe (ISIS in the UK, ILL in France and MLZ in Germany)



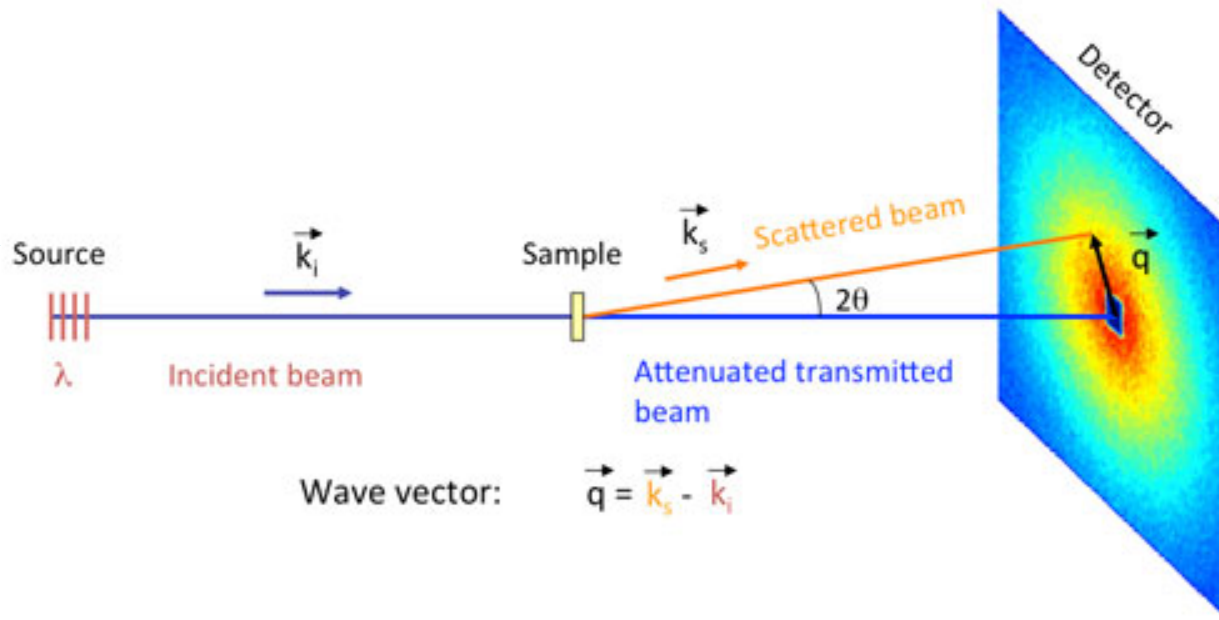
- Non-destructive
- Strong penetration in bulk (neutrons interact with nuclei)
- 0.25-300 nm
- Contrast match (H/D ratio)



Seeing things at the nanoscale..

Small-Angle Neutron Scattering (SANS)

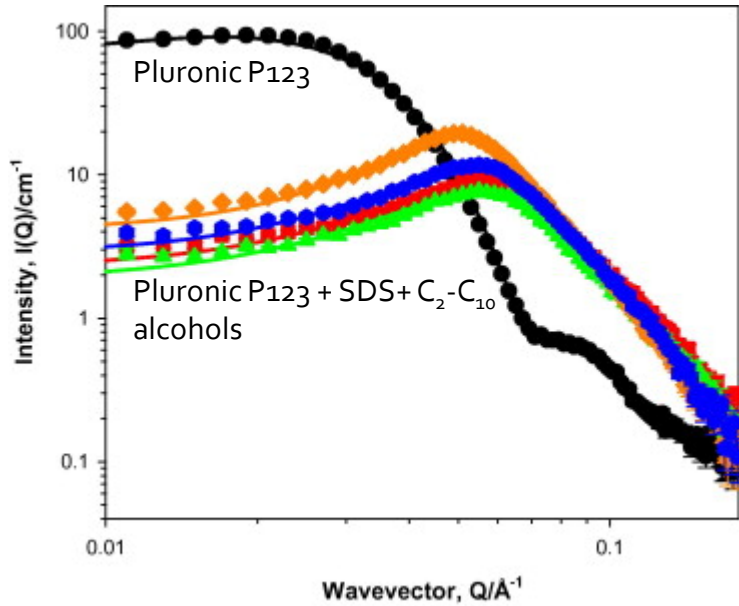
Lots of physics involved...



A simple experiment in principle. If the source is there and we are able to analyse the scattered beam on the detector!

SANS does not locate individual atoms, but rather looks at the larger structures they form, detailed info on size and shape..

Quaternary formulations

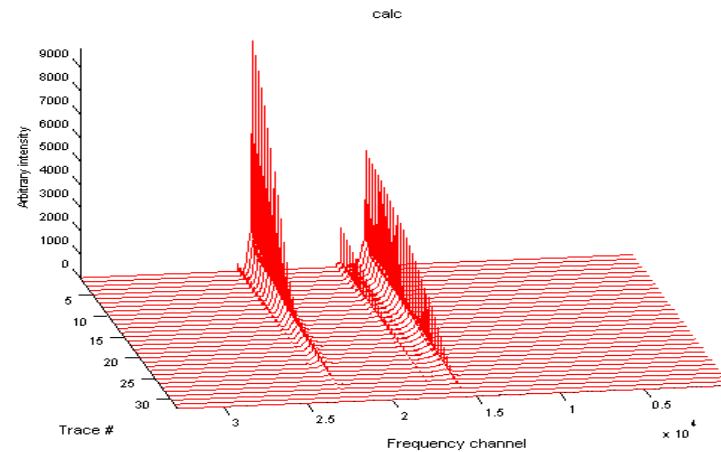
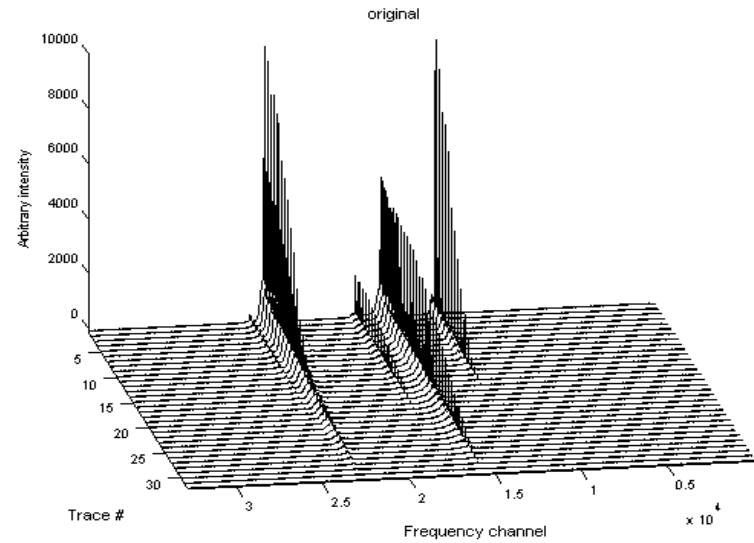


Different features in the data...

$$\overline{D}^{P123} = p_{micelle}^{P123} D_{micelle}^{P123} + (1 - p_{micelle}^{P123}) D_{monomer}^{P123}$$

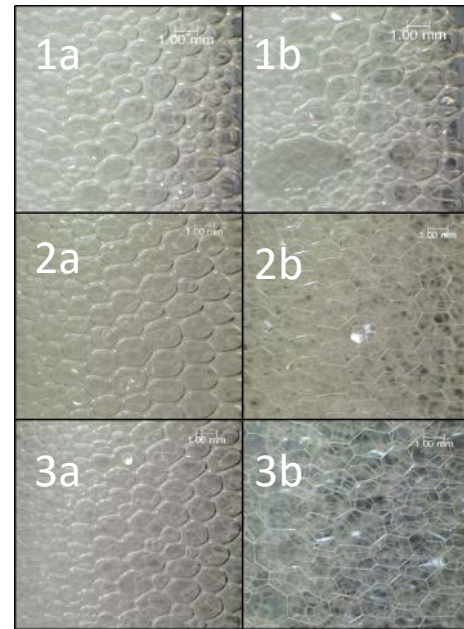
$$p_{free}^{R-OH} = \frac{D_{free}^{R-OH} - D_{micelle}^{R-OH}}{D_{free}^{R-OH} - D_{micelle}^{R-OH}}$$

Partitioning of cosmetic agents ?



Mansour et.al. *Journal of Colloids and Interface Science*, 2015, 454, 35

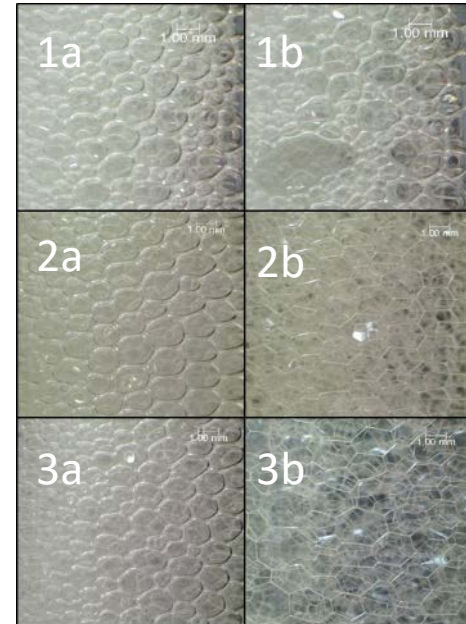
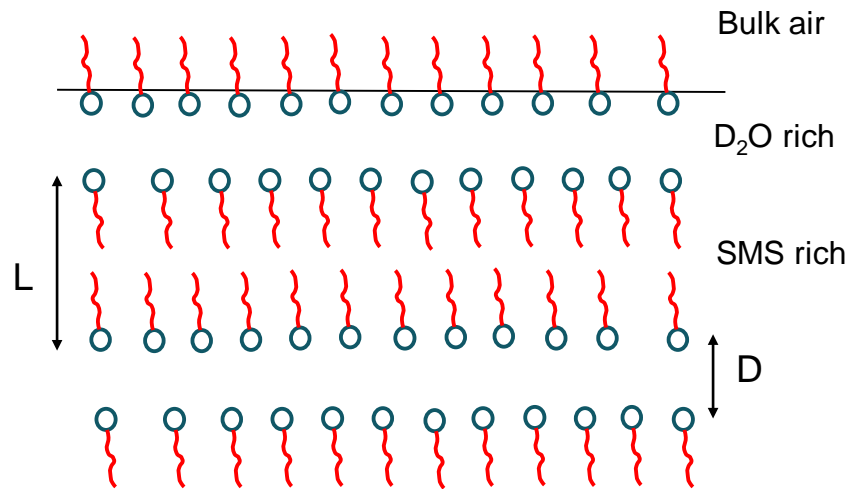
Foams stabilised by surfactants



Scattering from polymer/surfactant structures at the foam air-water interface..

- Mansour *et.al* , Assembly of small molecule surfactants at highly dynamic air–water interfaces. *Soft Matter* **2017**, *13*, 8807–8815
- Mansour *et.al*, Segregation versus interdigitation in highly dynamic polymer/surfactant layers. *Polymers* **2019**, *11*, 109

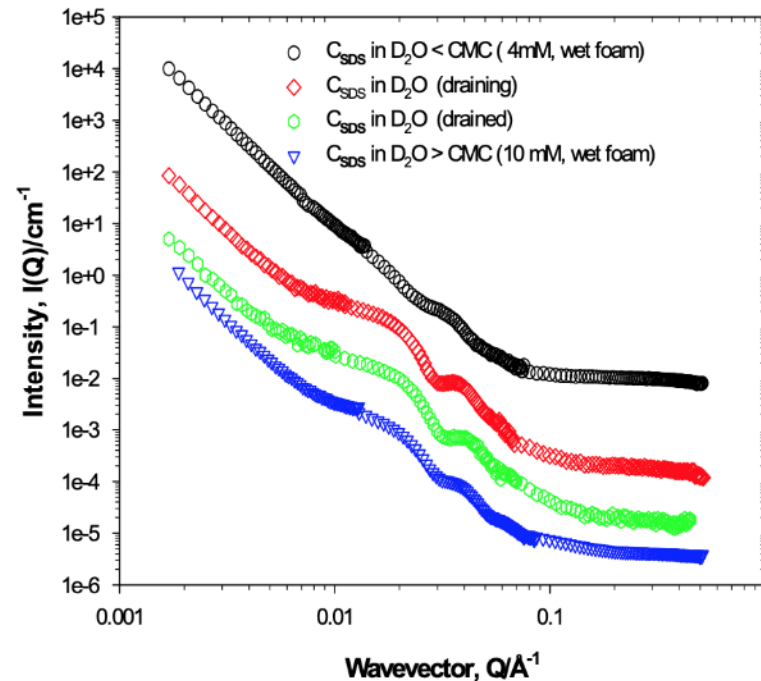
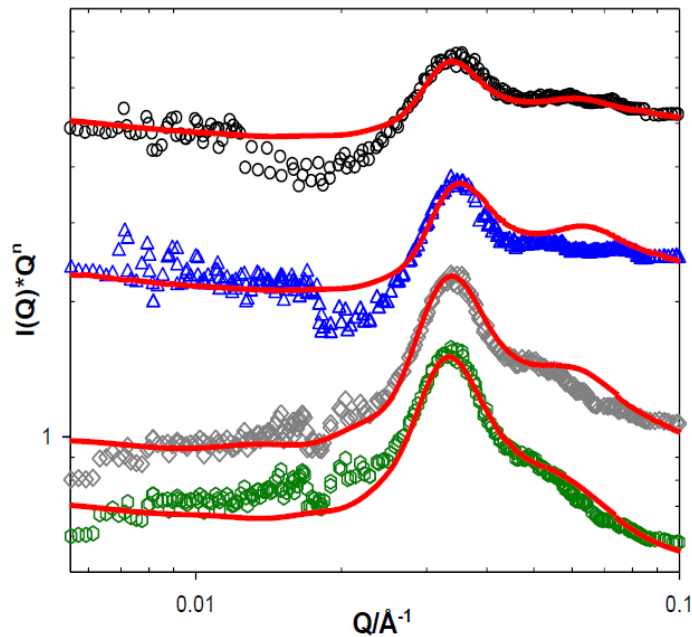
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Foams stabilised by surfactants



- Surfactant multilayers at the interface
- Sensitive to surfactant structure (chainlength...)
- Mansour *et.al* , Assembly of small molecule surfactants at highly dynamic air-water interfaces. *Soft Matter* **2017**, *13*, 8807–8815
- Surfactant multilayers at the interface
- Sensitive to surfactant concentration

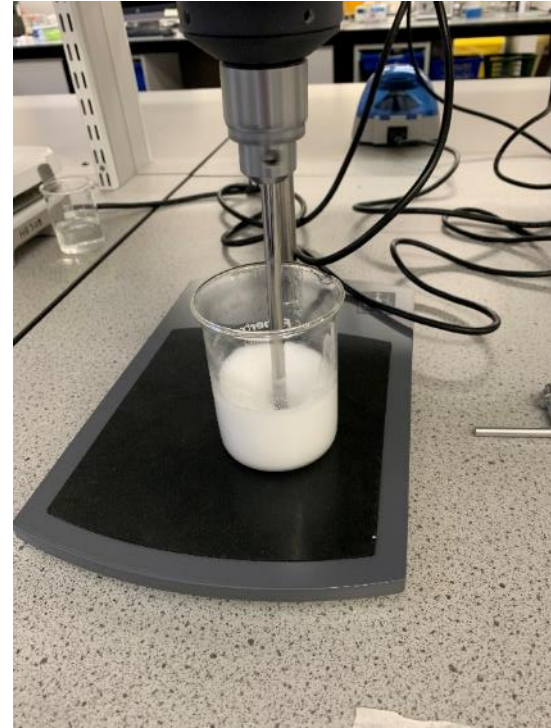
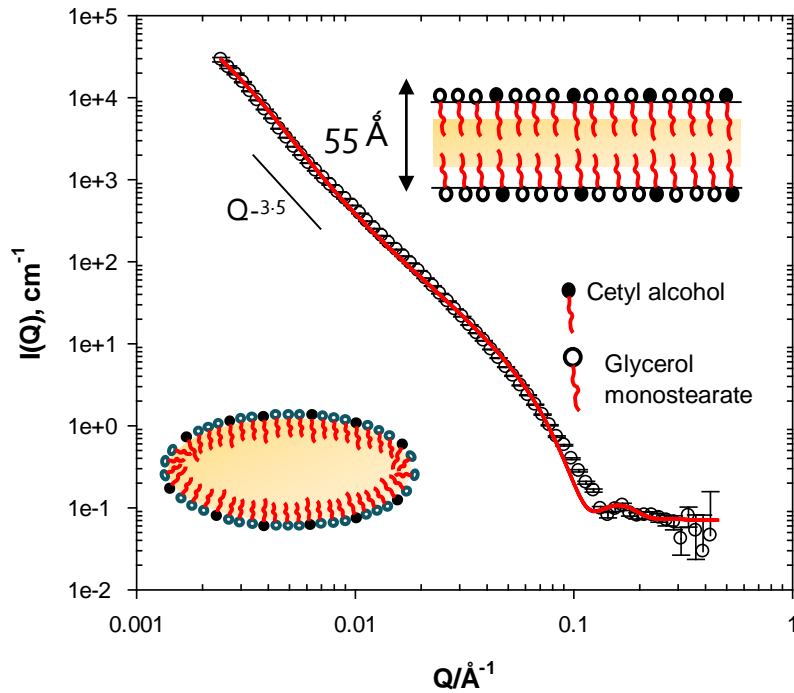
Sunscreen lotions: what's inside the bottle?

Aqua, Homosalate, Octocrylene, Glycerin, Butyl Methoxydibenzoylmethane, Ethylhexyl Salicylate, Bis-Ethylhexyloxyphenol Methoxyphenyl Triazine, Alcohol Denat., Butylene Glycol Dicaprylate/Dicaprate, Sodium Phenylbenzimidazole Sulfonate, Panthenol, Ceteareth-20, VP/Hexadecene Copolymer, C18-36 Acid Triglyceride, Tocopheryl Acetate, Sodium Acrylates/C10-30 Alkyl Acrylate Crosspolymer, Trisodium EDTA, Phenoxyethanol, Methylparaben, Ethylparaben, Linalool, Limonene, Butylphenyl Methylpropional, Benzyl Alcohol, Alpha-Isomethyl Ionone, Citronellol, Eugenol, Coumarin, Parfum



- Many ingredients = complex structure
- Interactions between the ingredients?
- Could this affect the performance ?

Sunscreen lotions: what's inside the bottle?



- Simpler formulation: Mineral oil, cetyl alcohol, glycerol, glycerol monostearate and water
- Large oil droplets coexisting with lamellar phases
- Mansour *et al*, Insights into sunscreen lotions: A small-angle neutron scattering study. *RSC Advances* **2021**, submitted

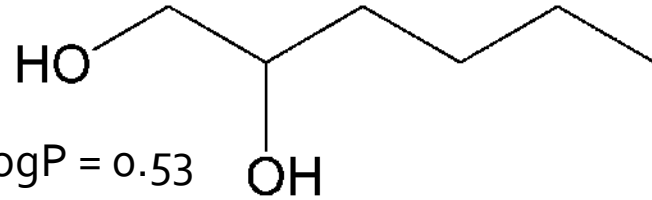
Sunscreen lotions: what's inside the bottle?

Adding water soluble preservatives



$\log P = 0.14$

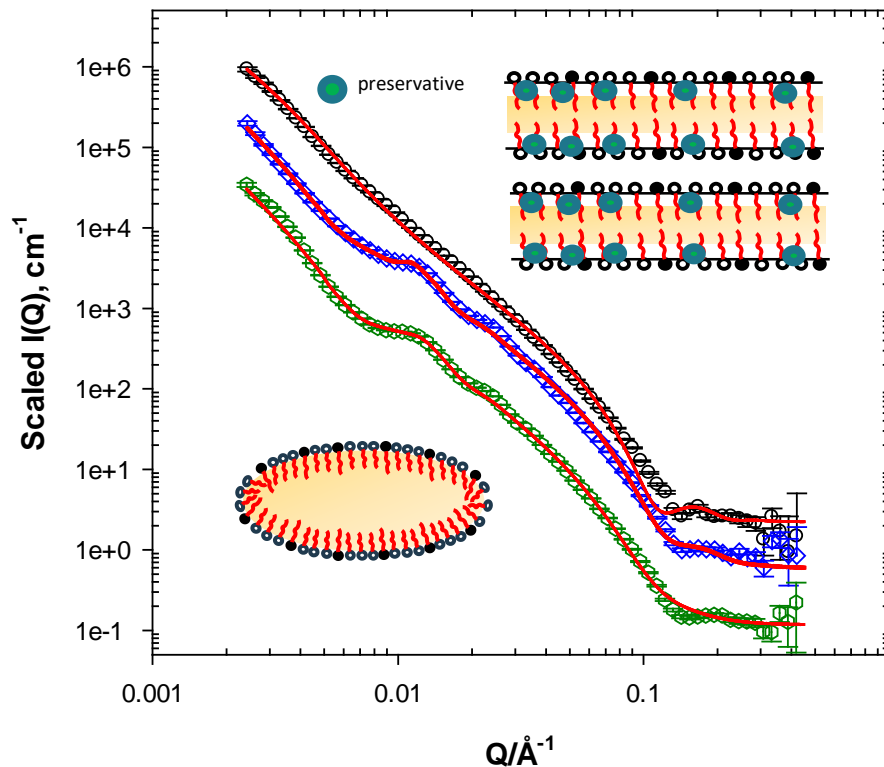
1,5-pentanediol (PD)



$\log P = 0.53$

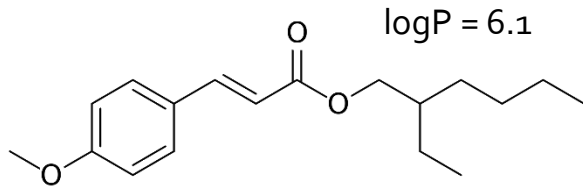
1,2-hexanediol (HD)

Multilamellar +
oil droplet
model

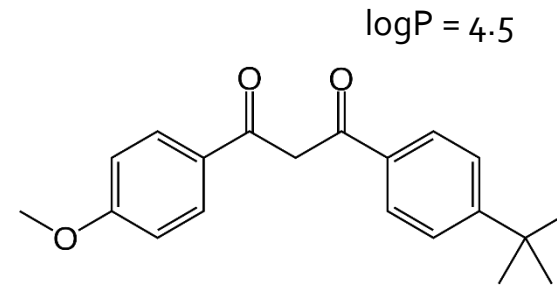
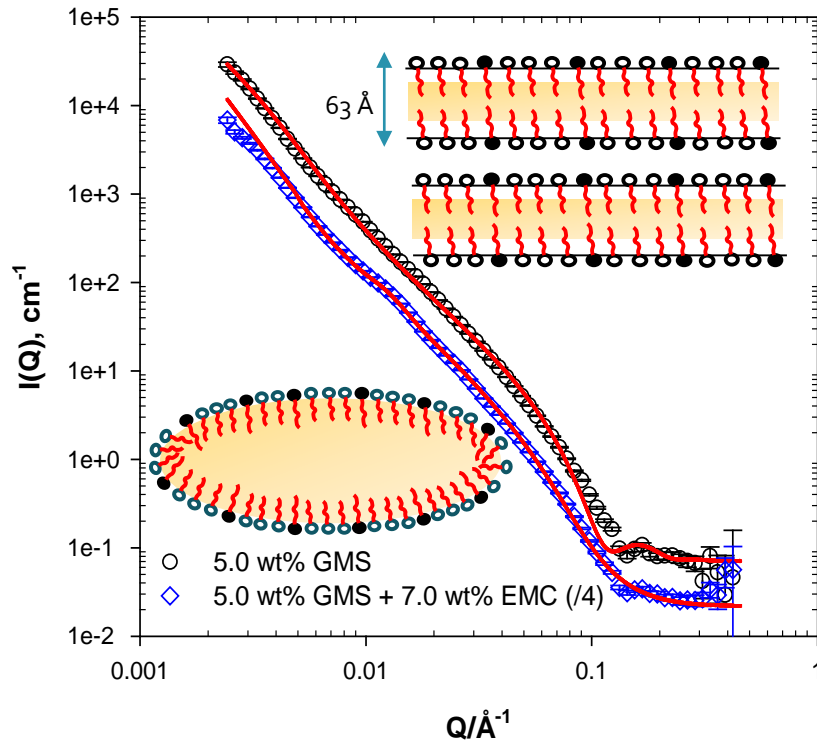


Sunscreen lotions: what's inside the bottle?

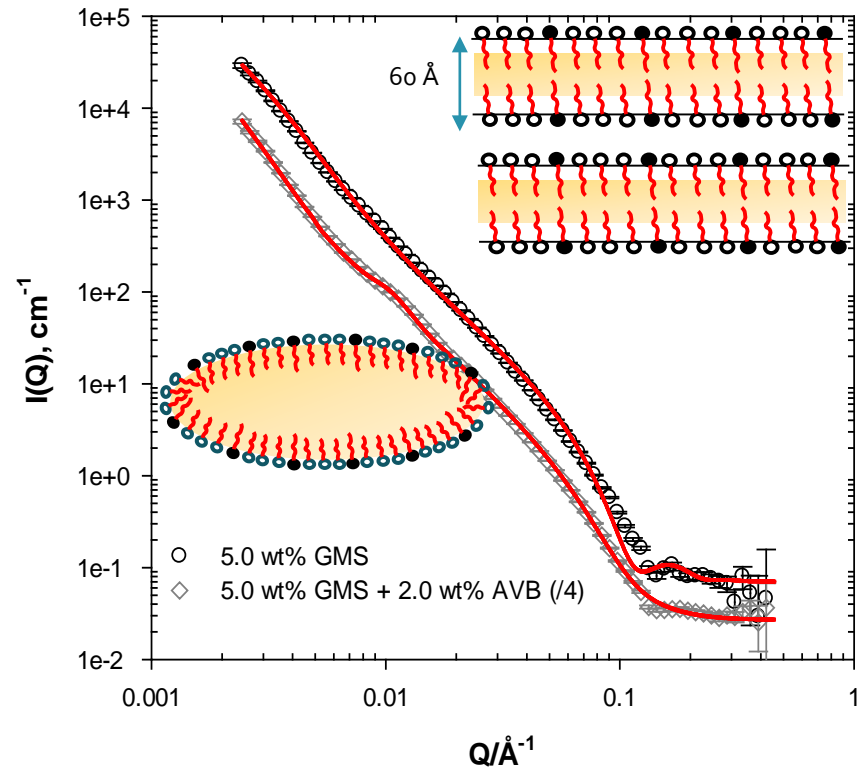
Adding organic UV filters



UVB: Ethylhexyl methoxycinnamate (EMC), 7 wt%

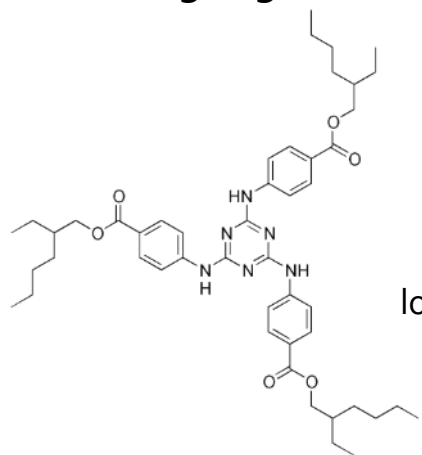


UVA: Avobenzone (AVB), 2 wt%



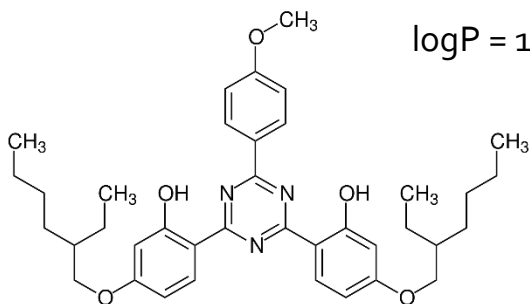
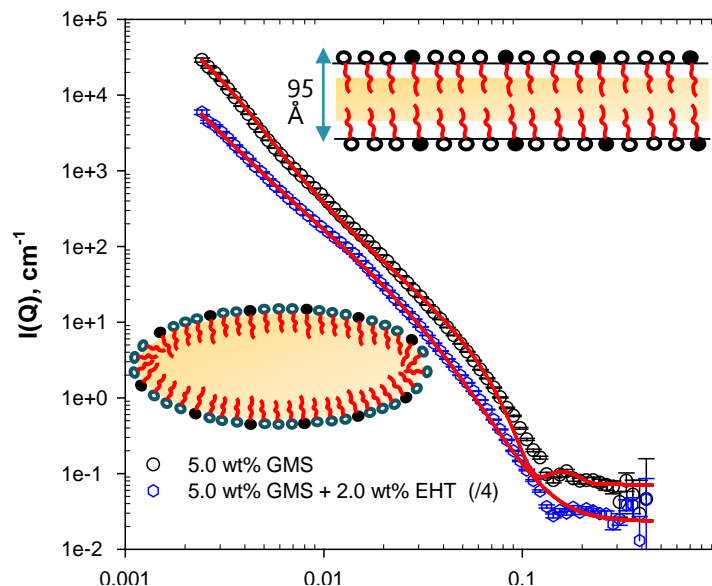
Sunscreen lotions: what's inside the bottle?

Adding organic UV filters



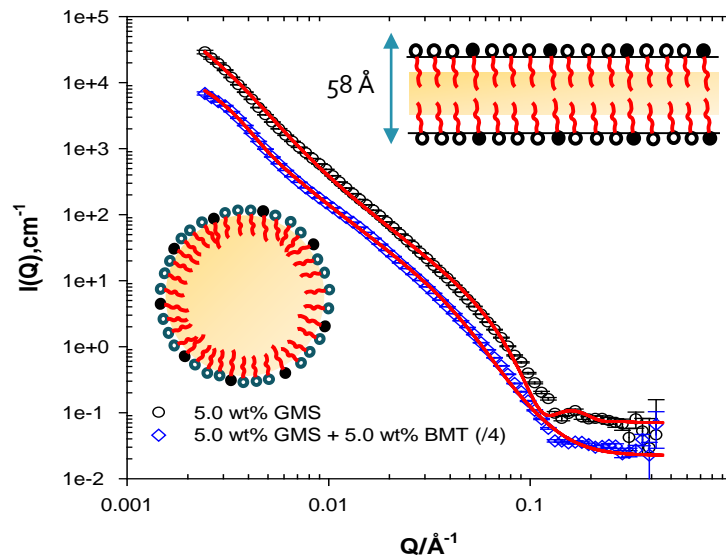
logP = 7.0

UVB: Ethylhexyl triazone (EHT), 2 wt%



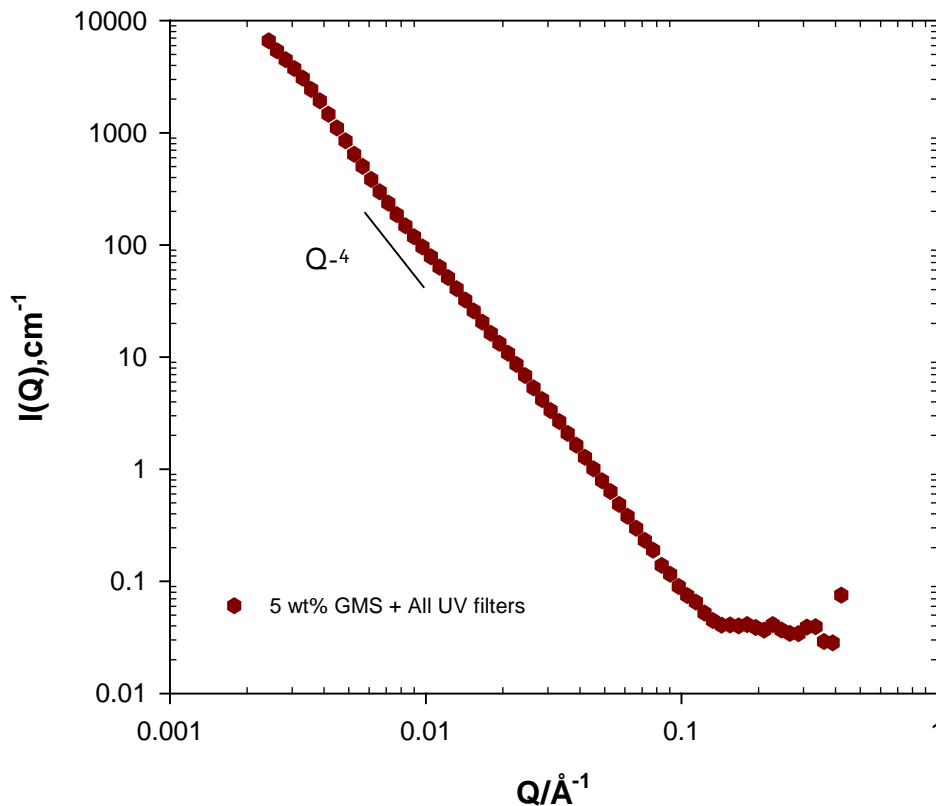
logP = 12.6

UVA/B: Bemotrizinol (BMT), 5 wt%



Sunscreen lotions: what's inside the bottle?

Adding the 4 organic UV filters

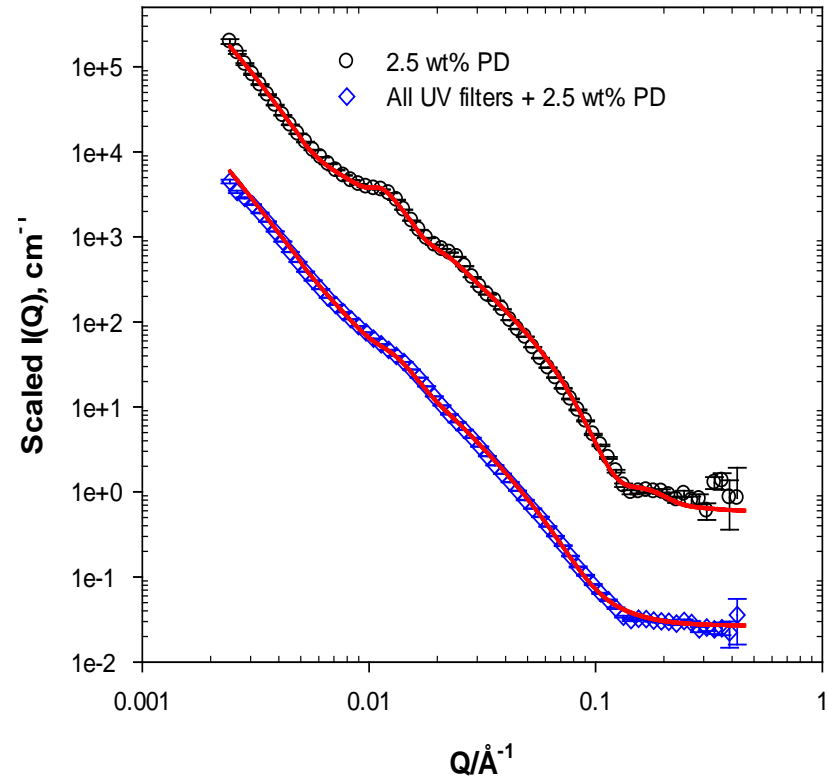
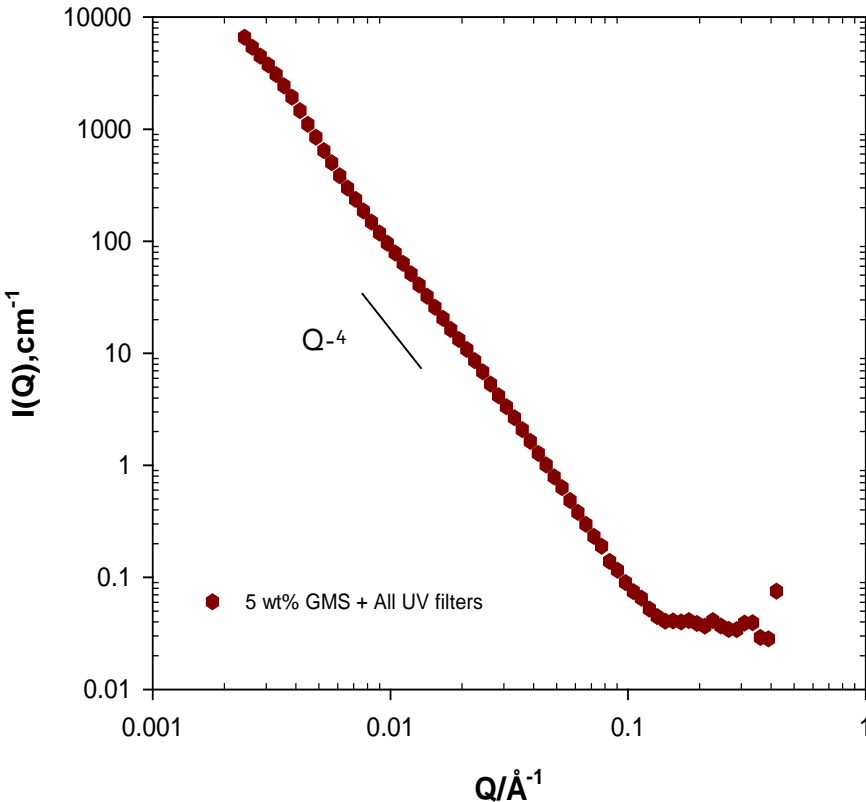


- Strong Q^{-4} dependence
- Large smooth/spherical surface
- Strongly suggesting that all UV filters have partitioned in the oil droplet...

- Mansour *et al*, Insights into sunscreen lotions: A small-angle neutron scattering study. *RSC Advances* 2021, submitted

Sunscreen lotions: what's inside the bottle?

Adding the 4 organic UV filters



Accessibility variations, and lotions' traditional structure could be actually compromised

- Mansour *et al*, Insights into sunscreen lotions: A small-angle neutron scattering study. *RSC Advances* **2021**, submitted

Conclusions

- It is not dark art
- Cosmetic formulations are far more complex than widely understood..
- Unknown complexities affect the performance of the formulation (sunscreens, lotions)
- NMR and SANS data analysis from lotions/foams offers valuable new information to our understanding of the microstructure

Acknowledgements



Thank you