Small Angle Scattering Method applied to biological macromolecules and colloids

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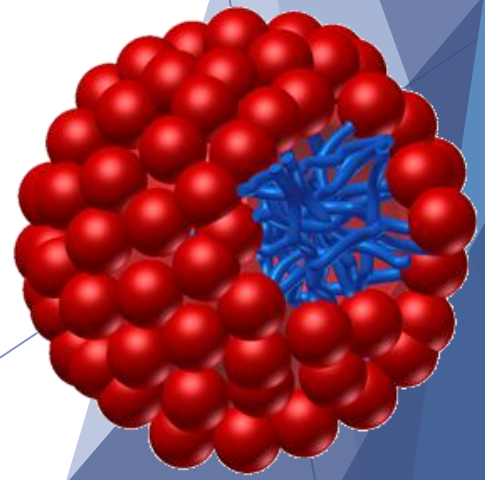
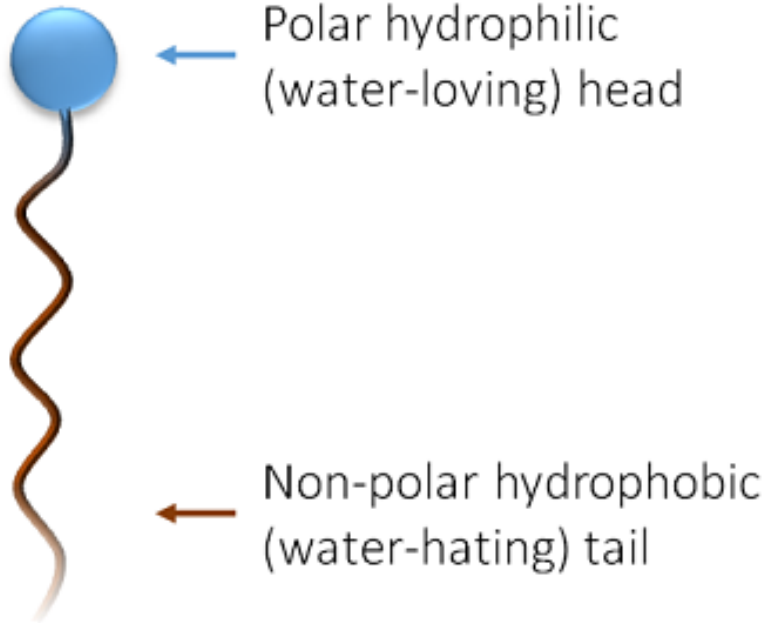
Aim of the research

- Measurement of surface tension of surfactant solution by the tensiometric method.
  - Determination of thermodynamic parameters of surfactant solutions.
- Analysis of SANS curves for surfactant solutions
  - Determination the shape of aggregates



Surfactants

Surfactants are suface active agents with hydrophilic and hydrophobic groups.



Division of surfactants:

- Anionic surfactants
- Nonionic surfactants
- Cationic surfactants

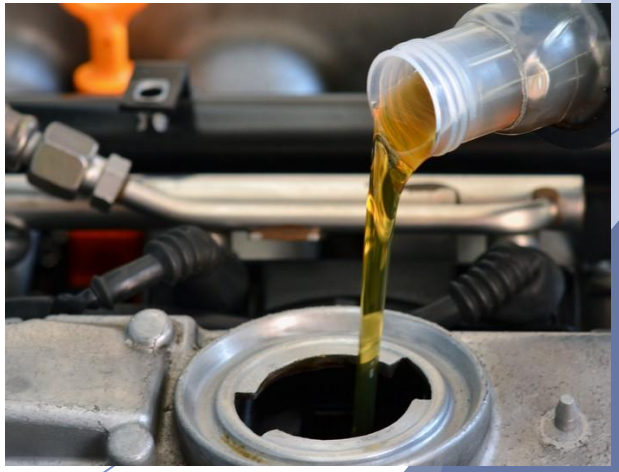
Application of surfactants

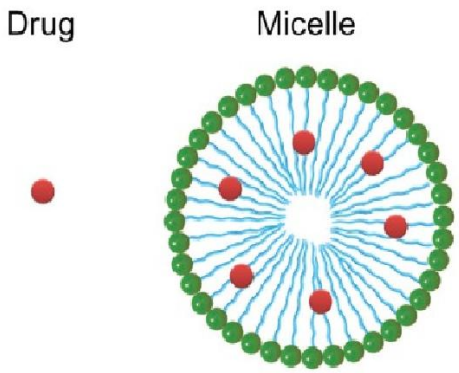
Cosmetics

Medicine

Cleaning agents

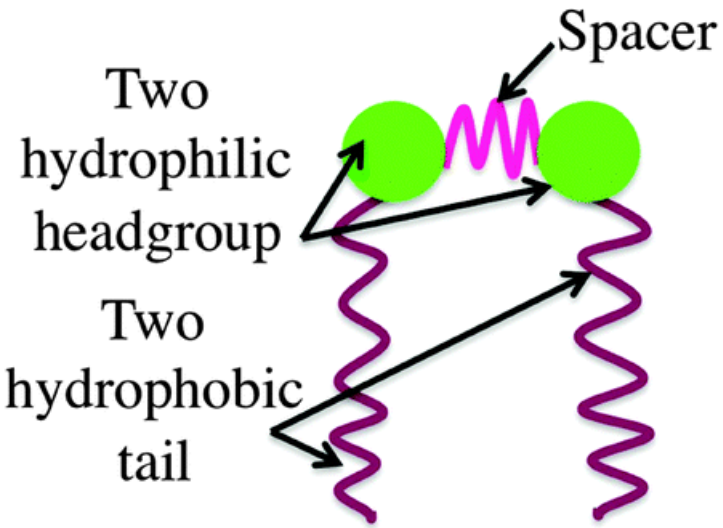
Greases



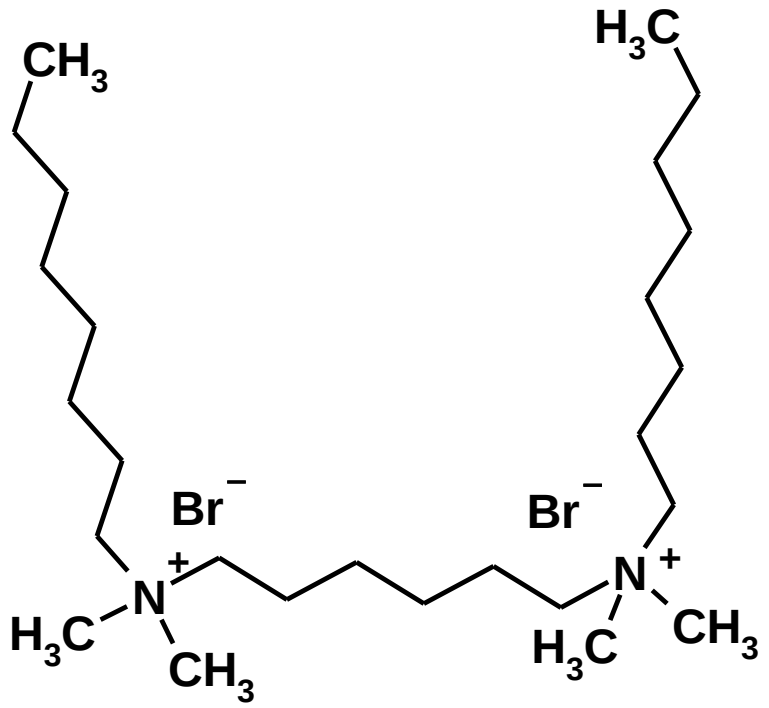


Research objects

- Cationic surfactant gemini



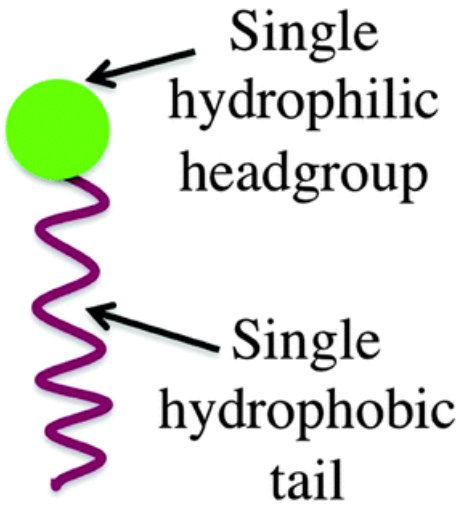
Scheme of the general structure of surfactant gemini



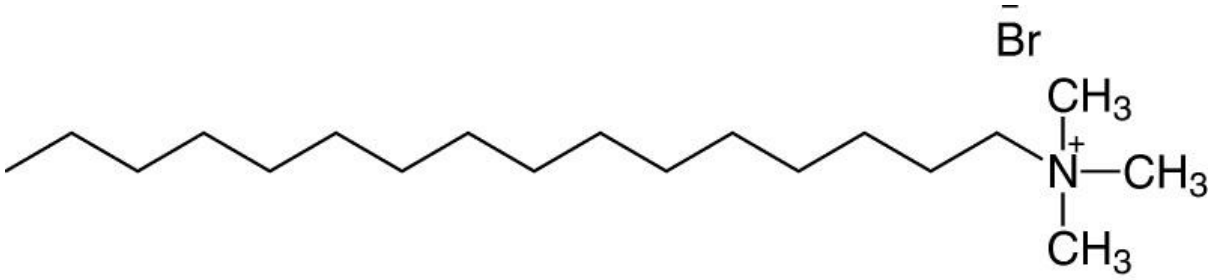
hexylene-1,6-bis (dimethyloctylammonium) bromide

Research objects

- Cationic surfactants CTAB



Scheme of the general structure of surfactant CTAB

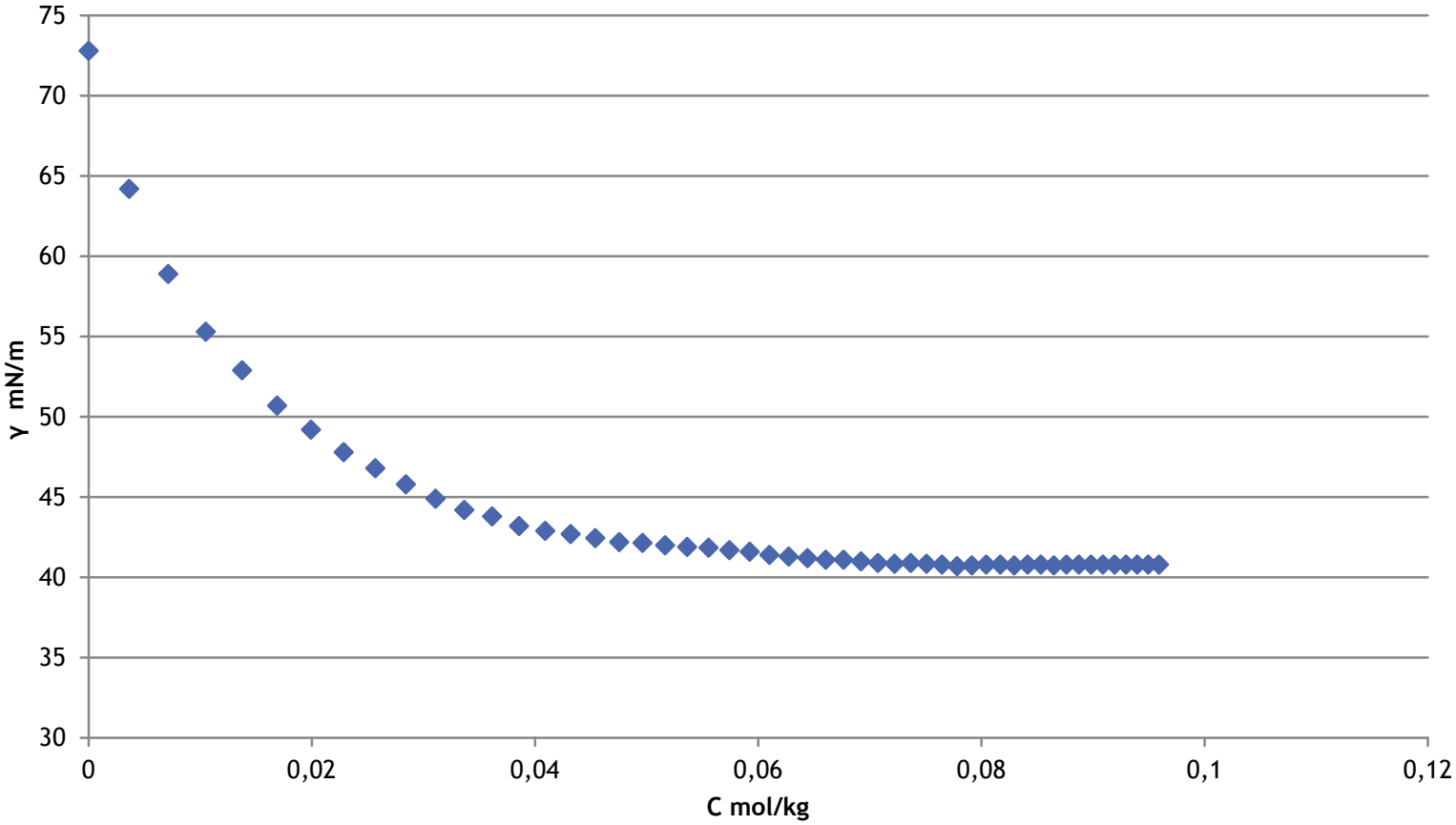


Cetyltrimethylammonium bromide

The process of micelles creating

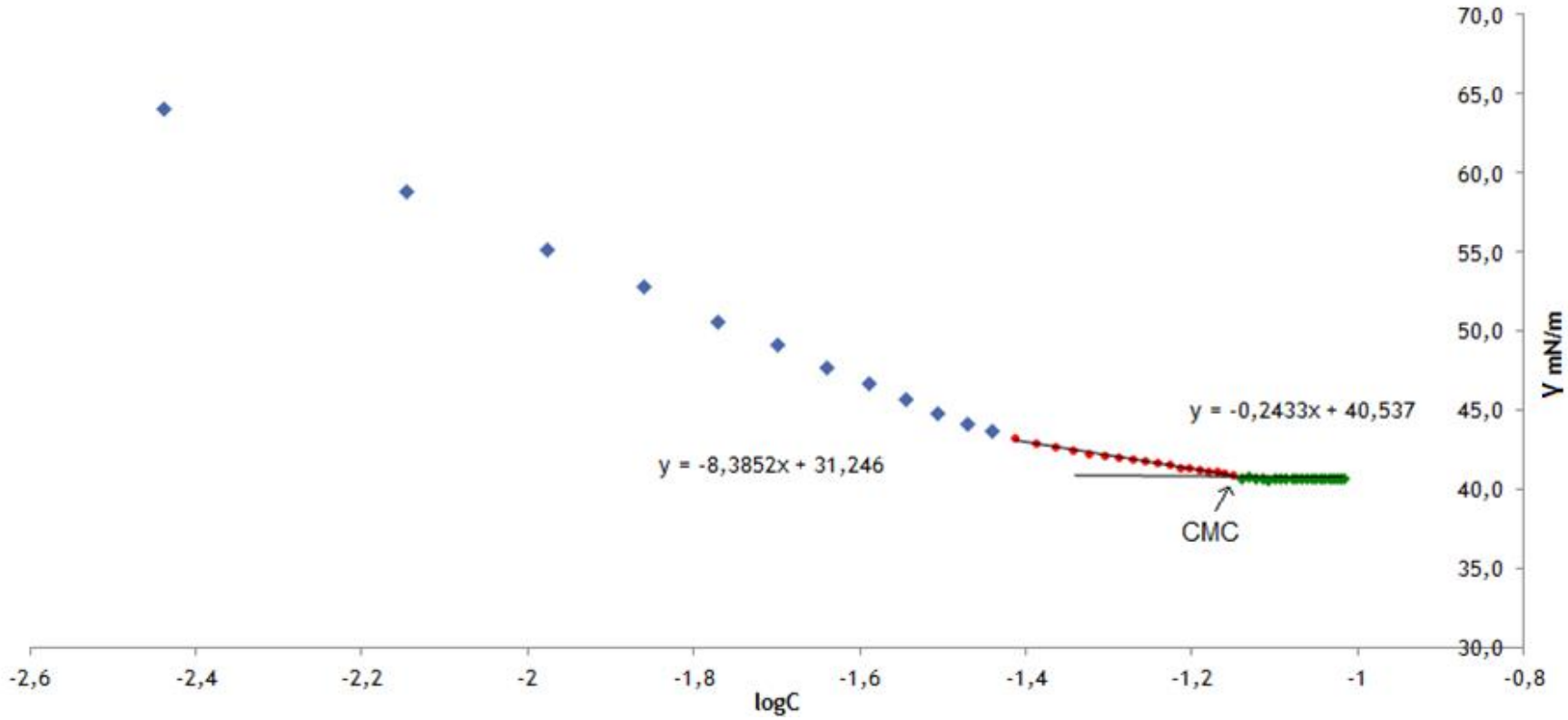
Experiment of surface tension measurment

Experiment results



Surface tension as a function of surfactant concentration

Experiment results



Surface tension as a function of logarithm surfactant concentration

Determination of thermodynamic parameters

Thermodynamic parameter	Π_{CMC} [mN/m]	Γ_{max} [mol/m]	a_x [nm^2]
	32,0	1,12 * 10^{-6}	1,47

$$\Pi_{c.m.c} = \gamma_0 - \gamma_{c.m.c}$$

Effectiveness of the surface tension reduction

$$\Gamma_{max} = \left(\frac{-1}{nRT}\right)\left(\frac{d\gamma}{d\ln\frac{c}{c^o}}\right)_{p,T}$$

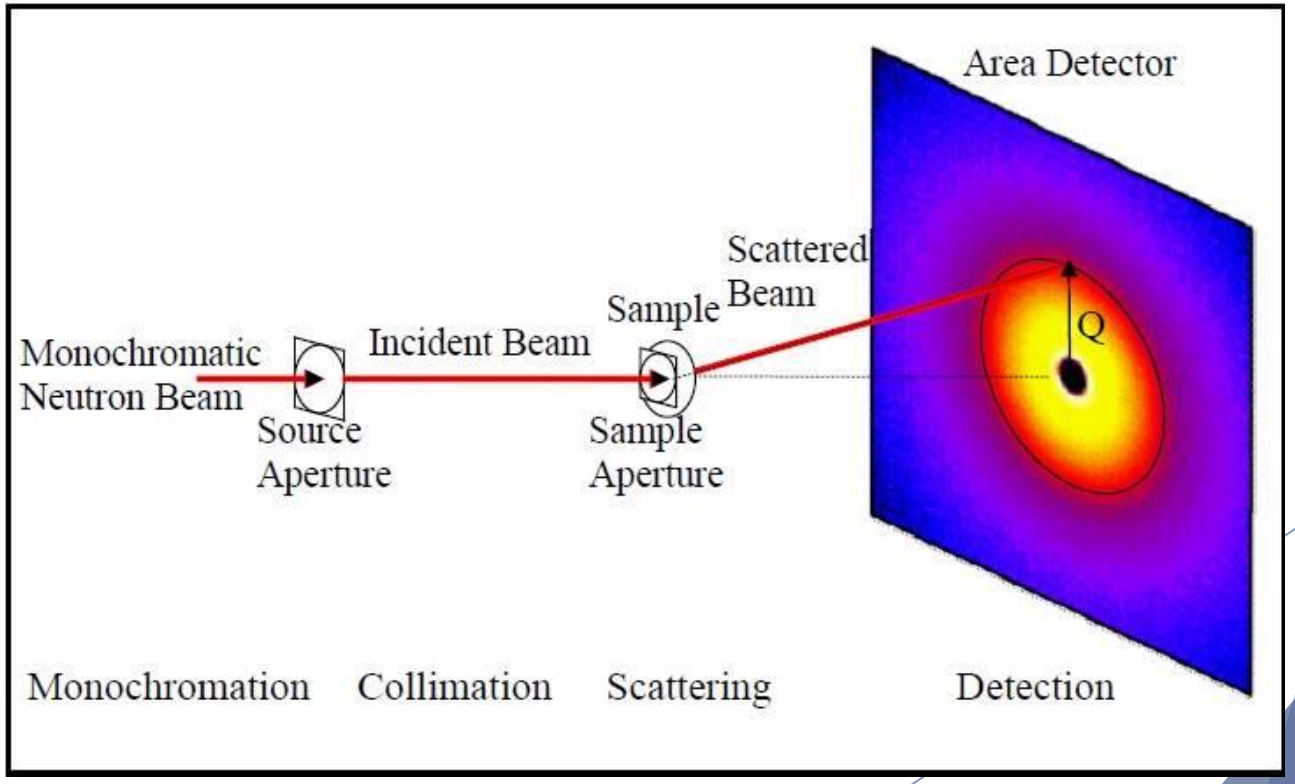
Maximum surface excess concentration

$$a_x = \left(\frac{1}{\Gamma_{max} N_A}\right)$$

The cross-section surface area per molecule of surfactant at the air/solution interface adsorbed

SANS method

- SANS – **S**mall-**A**ngle **N**eutron **S**cattering is a technique for the characterization of structures in the nanoscale size range
- SANS can measure density fluctuations and composition (or concentration) fluctuations



SANS principle

- A typical SANS result is a graphic of the scattering intensity function of a wavevector **Q**
- **Q** is defined as

$$Q = 4\pi \frac{\sin\left(\frac{\theta}{2}\right)}{\lambda}$$

where:

Q = wavevector
Theta = scattering angle
Lambda = Wavelength of incident beam

The scattering intensity is defined as:

$$I(Q) = \phi P(Q) S(Q)$$

where:

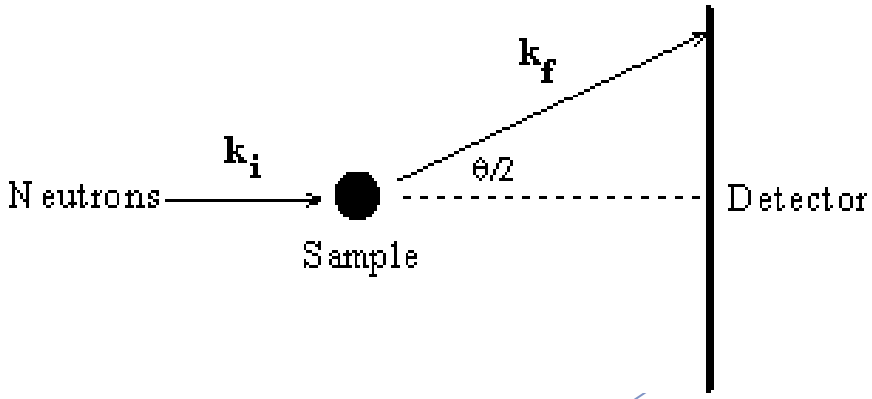
I(Q) = scattering intensity
Phi = density of particles in volume
P(Q) = form factor
S(Q) = structure factor

Inconherent scattering cross section

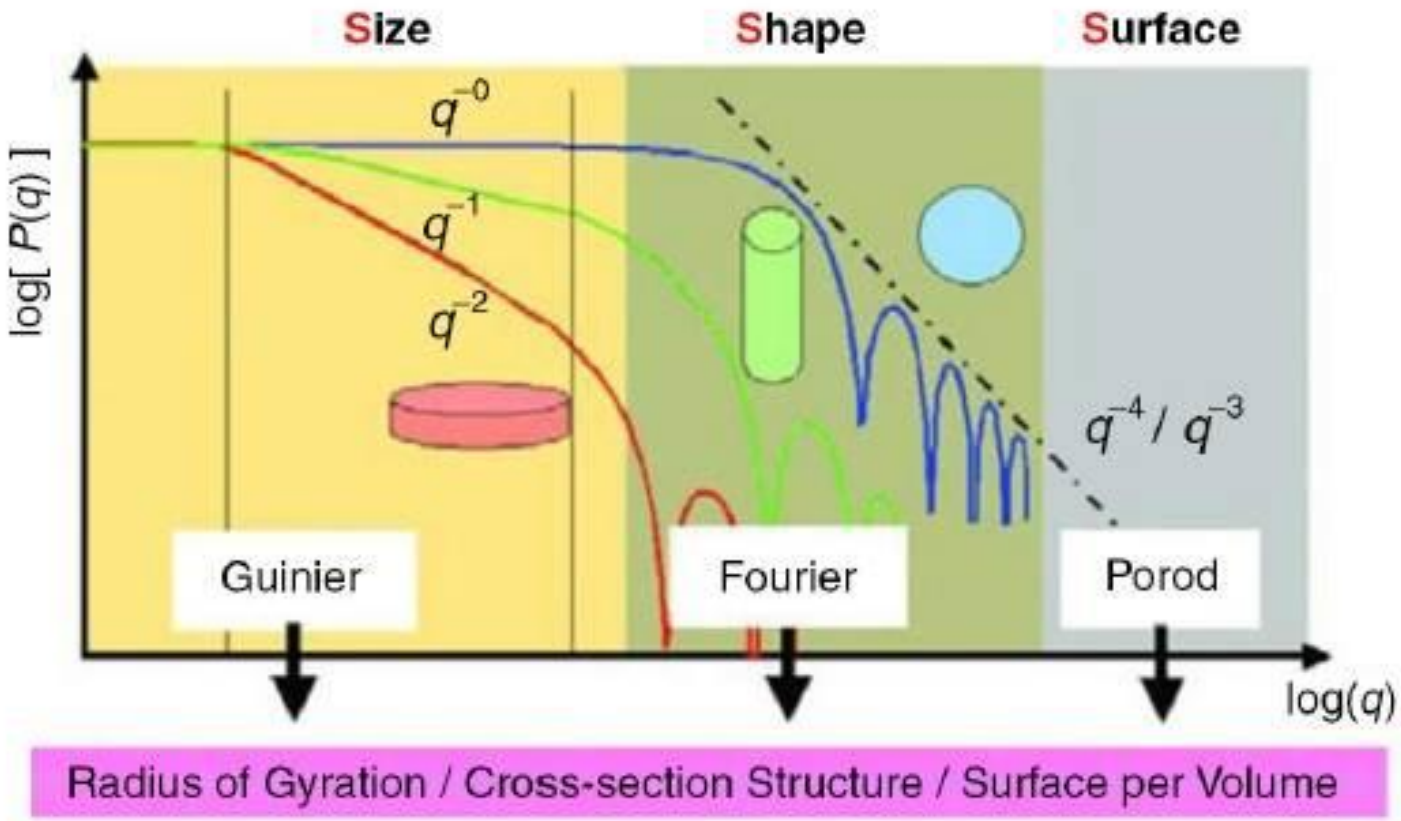
$$\frac{d\sum_c(Q)}{d\Omega} = \left(\frac{N}{V}\right) V_p^2 \Delta\rho^2 P(Q) S_I(Q)$$

where:

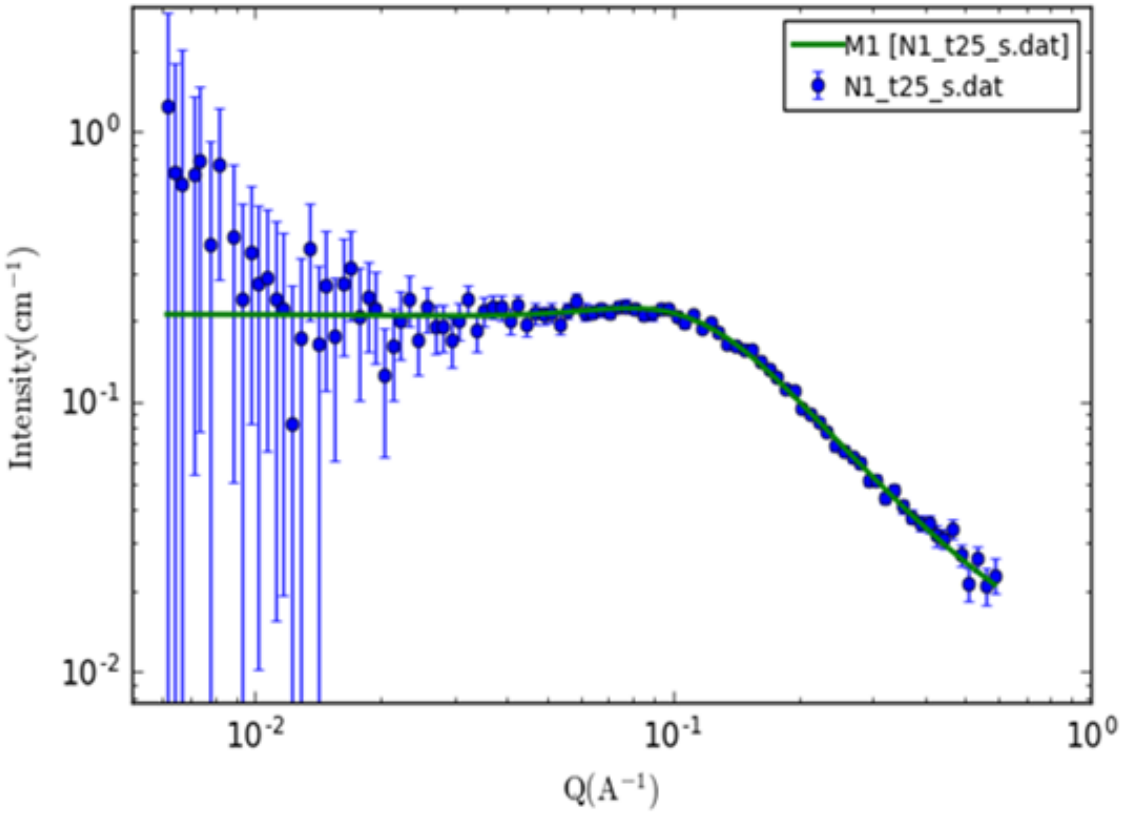
$\frac{N}{V}$ - numer dencity of particles
Vp - particle volume
$\Delta\rho^2$ - contrast factor
P(Q) - single particle form factor
$S_I(Q)$ - inter-particle structure factor



What we can extract from the SANS curve?



SANS experiment results – gemini surfactant



SANS curve for gemini surfactant

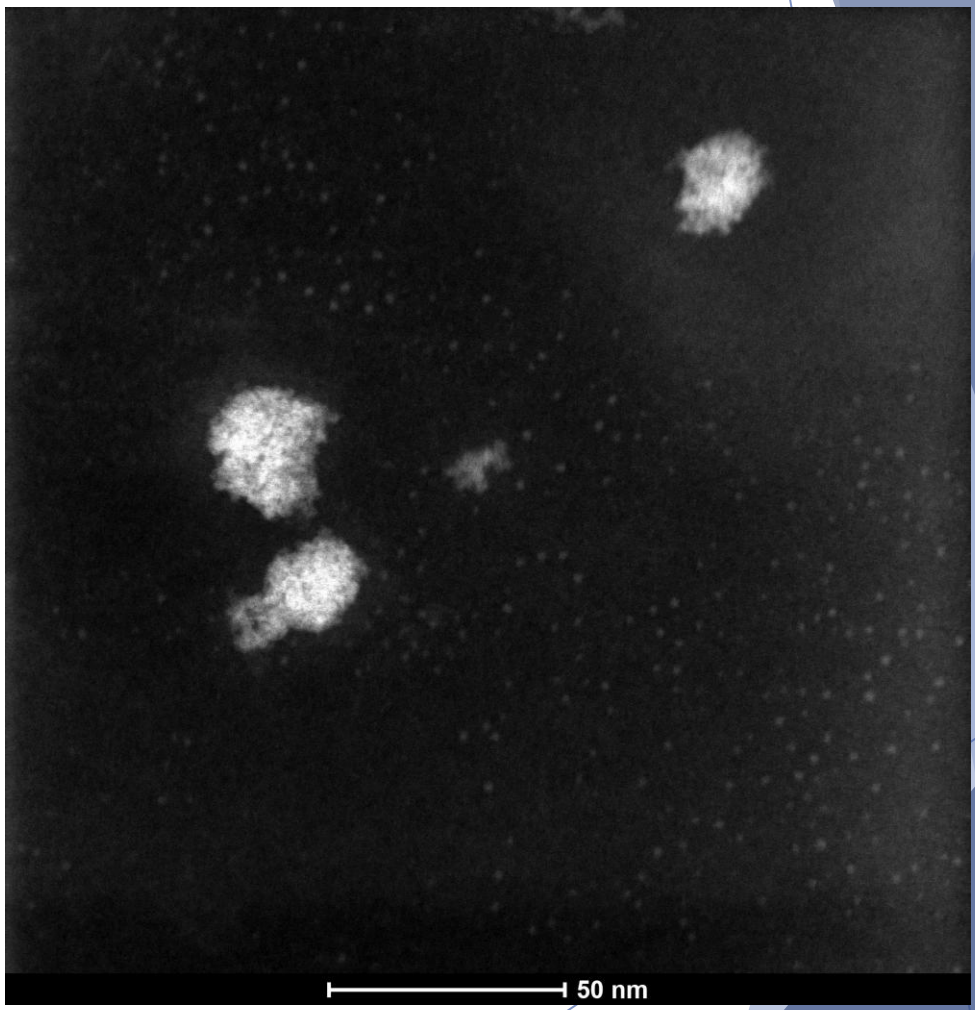
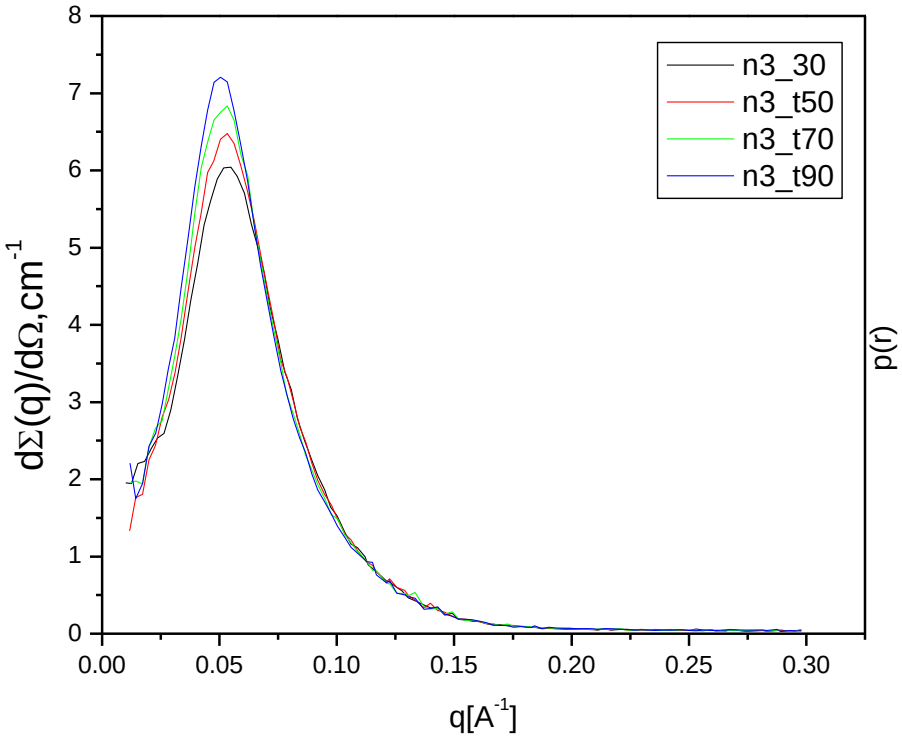
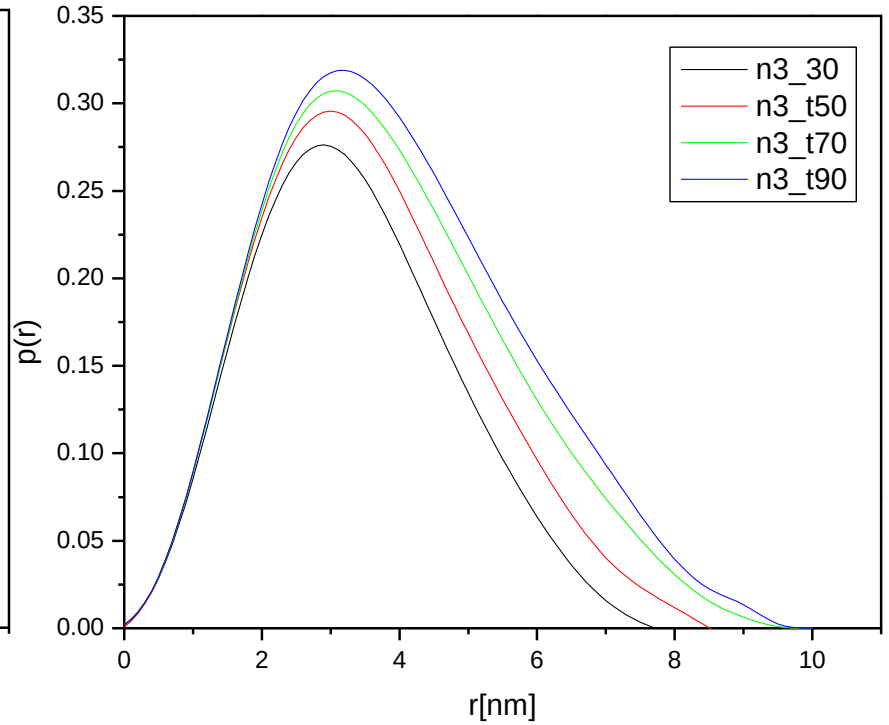


Figure from TEM

SANS experiment results – CTAB surfactant





SANS curves for CTAB surfactant

Conclusion

- Quite low value of a_x of gemini surfactants indicates that molecules at the interface are tightly packed.
- The graphs show that the micelles of CTAB surfactants are spherical, which is consistent with the simple structure of surfactants.
- In the case of gemini surfactants micelles, the SANS curve shows that their shape differs from spherical. This is the result of their construction, because they consist of two structures connected by spacer.