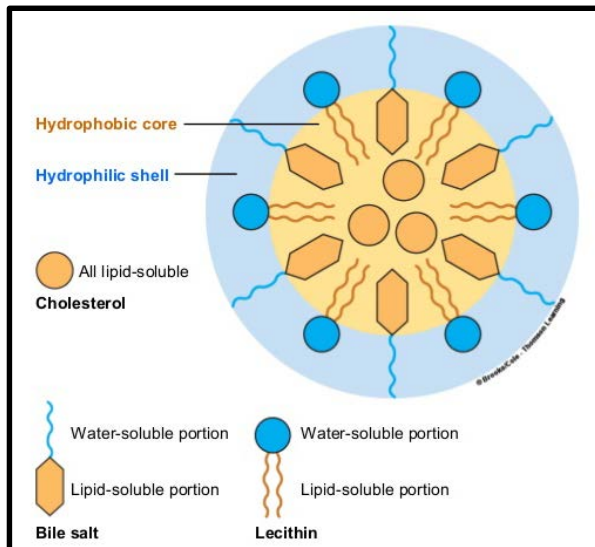
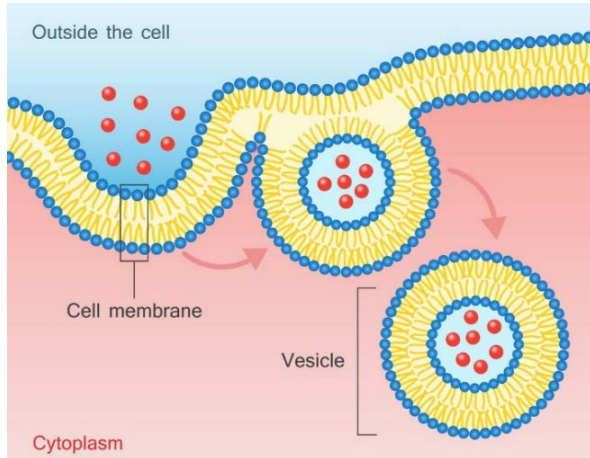




UPPSALA
UNIVERSITET

MOLECULAR PHYSICAL PHARMACY 7.5 HP



Course Content:

- Self-assembly of amphiphilic molecules in pharmaceutical and biological systems (3 Lectures)
- Macromolecules, biopolymers and gels in pharmaceutical and biological systems (2 Lectures)
- Transport and release of drug molecules (2 Lectures)
- Classical molecular simulations for relevant systems in pharmaceuticals (2 Lectures)
- Introduction to scattering techniques for structural characterization of pharmaceutical and biological systems (2 Lectures)



MOLECULAR PHYSICAL PHARMACY

LEARNING OUTCOMES

On completion of the course, the student should be able to:

- apply knowledge dealing with thermodynamic principles and models for the self-assembly of amphiphilic molecules
- apply knowledge dealing with models based on bending elasticity and spontaneous curvature to understand the formation of micelles, membranes and microemulsions
- account for assumptions and restrictions in different theories for macromolecules
- apply knowledge dealing with the thermodynamic driving forces that underlies swelling of polymer coils and gels, phase separation in polymer solutions and formation of complexes in systems of oppositely charged polyelectrolytes
- apply knowledge dealing with different transport mechanisms and their relevance for the release of drugs from different pharmaceutical formulations
- account for how the structure of materials influence the effective transport properties, in particular with respect to diffusion
- use molecular dynamics simulations as a tool for simulations of pharmaceutically relevant molecules, for example peptides
- analyze structural and dynamic properties of the simulated systems
- apply knowledge how different levels of coarse-graining are applicable in different circumstances.
- apply knowledge dealing with basic principles of the experimental techniques static and dynamic light scattering, small-angle x-ray and neutron scattering
- perform simple analysis of experimental light scattering and small-angle scattering data
- apply analytic methods to solve quantitative problems



UPPSALA
UNIVERSITET

MOLECULAR PHYSICAL PHARMACY

Schedule

L = Lecture
S = Supervision
E = Exercise

TEACHERS

Magnus Bergström magnus.bergstrom@ilk.uu.se
Per Hansson per.hansson@ilk.uu.se
Göran Frenning goran.frenning@farmbio.uu.se
Per Larsson per.r.larsson@farmaci.uu.se

| | Content | Date | Teacher |
|-----|--|---------------|---------------------------------|
| I | Course introduction | 30/8, 9-10 | Magnus Bergström |
| L1 | Introduction to self-assembly of surfactants and phospholipids | 30/8, 10-12 | Magnus Bergström |
| L2 | Thermodynamics of self-assembly | 31/9, 10-12 | Magnus Bergström |
| L3 | Curvature properties of micelles, bilayers and microemulsions. Surfactants as solubilization agents. | 1/9, 10-12 | Magnus Bergström |
| L4 | Macromolecules and biopolymers 1 | 2/9, 10-12 | Per Hansson |
| S1 | Self-assembly of surfactants and phospholipids | 3/9, 10-12 | Magnus Bergström |
| L5 | Macromolecules and biopolymers 2 | 6/9, 10-12 | Per Hansson |
| S2 | Macromolecules and biopolymers | 8/9, 10-12 | Per Hansson |
| L6 | Introduction to transport properties and drug release processes | 9/9, 10-12 | Göran Frenning |
| L7 | Mathematical modelling of drug release | 10/9, 10-12 | Göran Frenning |
| S3 | Transport properties and drug release | 14/9, 10-12 | Göran Frenning |
| L8 | Molecular dynamics 1 | 15/9, 10-12 | Per Larsson |
| L9 | Molecular dynamics 2 | 16/9, 10-12 | Per Larsson |
| L10 | Introduction to scattering techniques | 17/9, 10-12 | Magnus Bergström |
| L11 | SLS, SAXS, SANS | 17/9, 13-15 | Magnus Bergström |
| S4 | Molecular dynamics | 20/9, 10-12 | Per Larsson |
| E1 | Molecular dynamics computer exercise | 21-22/9, 8-17 | Per Larsson |
| E2 | SLS and SAXS experimental exercise | 21-22/9, 8-17 | Magnus Bergström Per Hansson |



UPPSALA
UNIVERSITET

MOLECULAR PHYSICAL PHARMACY

Electronic Examination on Inspira:

4 exercises, 15 p each

1. Self-assembly of amphiphilic molecules
2. Macromolecules
3. Transport and release
4. Molecular simulations

36 p required for passing the exam with the grade approved (G)
48 p required for the grade well approved (VG)



UPPSALA
UNIVERSITET

MOLECULAR PHYSICAL PHARMACY

Home Tasks and Bonus:

Exercises will be handed out for each subject. Approved home tasks will each give maximum 5 points that is added to each exercise on the examine.



UPPSALA
UNIVERSITET

MOLECULAR PHYSICAL PHARMACY

Laboratory exercises:

1. Molecular Dynamics

21-22 Sep

2. Scattering Techniques (SLS and SAXS)

21-22 Sep at D3:4, BMC



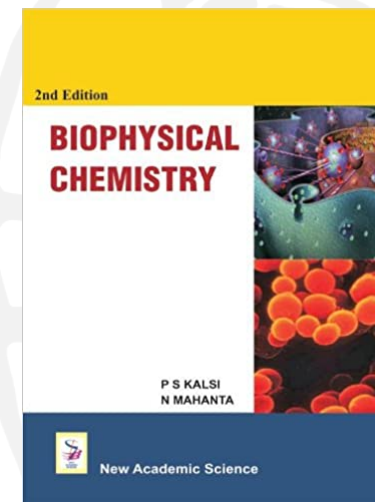
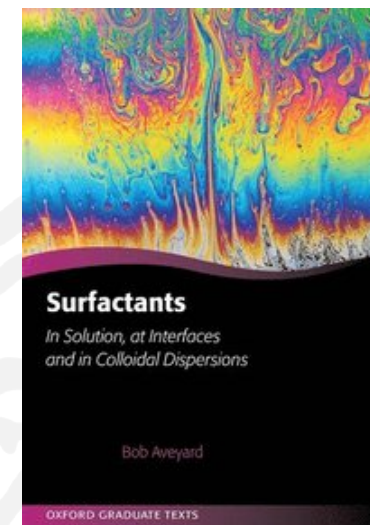
UPPSALA
UNIVERSITET

MOLECULAR PHYSICAL PHARMACY

Course literature:

Recommended Literature

- *Surfactants – In Solution, at Interfaces and Colloidal Dispersions* (Aveyard), Oxford Graduate Texts, 2019, ISBN 978-0-19-882860-0
- *Biophysical Chemistry* (Kalsi and Mahanta), New Academic Science, 2014, ISBN 978-1-78-183003-1

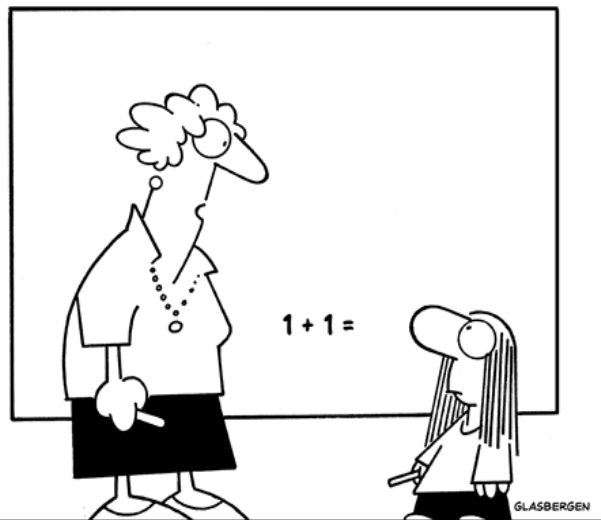




UPPSALA
UNIVERSITET

MOLECULAR PHYSICAL PHARMACY

Why mathematics?



"Yes, this will be useful to you later in life."

The book of nature is written in
the language of mathematics.

Galileo Galilei

To not know math is a
severe limitation to
understanding the world.

Richard P. Feynman

Math is the only place
where truth and beauty
mean the same thing.

Danica McKellar

A mathematician is a device for turning
coffee into theorems.

-Paul Erdos



UPPSALA
UNIVERSITET

MOLECULAR PHYSICAL PHARMACY

Course administration located at A5:3

Course administrators:

Sandra Bratt

William Lozancic

E-mail: kursadmin@ilk.uu.se



UPPSALA
UNIVERSITET

MOLECULAR PHYSICAL PHARMACY

*Don't forget to fill in the
course evaluation!*

BMC planned actions due to the pandemic

Access card required to enter BMC, A11 entrance open 08:00-15:00 during the start of the semester

Follow the recommendations issued by the Public Health Agency of Sweden, Folkhälsomyndigheten

Dual info desks with access card handling active during start of the semester

Information screens showing recommendations regarding handwash, physical distance etc.

Floor markers reminding about keeping 2 metres distance

Limitations in central dish facility, info desk and goods reception

Divided corridor next to the restaurant to grant easy passage

Maps showing the closest entrance to minimize the risk of crowds inside BMC