

1.	Field of study	Biophysics
2.	Faculty	Faculty of Science and Technology
3.	Academic year of entry	2022/2023 (winter term), 2023/2024 (winter term), 2024/2025 (winter term), 2025/2026 (winter term)
4.	Level of qualifications/degree	second-cycle studies
5.	Degree profile	general academic
6.	Mode of study	full-time

Module: Materials Science of Drugs

Module code: W4-2BF-MB-21-13

1. Number of the ECTS credits: 4

2. Learning outcomes of the module			
code	description	learning outcomes of the programme	level of competence (scale 1-5)
MB_13_1	students will be able to discuss the equilibrium conditions for a phase or phase coexistence, draw multiphase and/or binary phase diagrams, and distinguish between different equilibrium, metastable, and unstable states, and their relevance for drug formulations	KBF_K06	3
		KBF_U01	4
		KBF_U02	4
		KBF_U11	3
		KBF_W02	4

3. Module description	
Description	<p>The purpose of this unit is to provide an overview of the thermodynamics of phase equilibrium and phase transitions, with application to the polymorphism of drugs, and to introduce binary phase diagrams and the non-equilibrium glass state, with applications in the field of amorphous drugs.</p> <p>Course syllabus:</p> <p>(1) Basic concepts of crystallography: translational order, unit cell, Bravais lattices. Point groups, space groups, crystal systems. Crystallographic planes, reciprocal lattice, Miller indices. From crystal system to molecular structure and geometry: crystals with a base and molecular crystals. Calculation and modeling of diffraction patterns from atomic and structure scattering factors. Solid-state polymorphism of drugs and other organic molecules.</p> <p>(2) Phase Equilibrium and phase transitions (Thermodynamic Potentials for hydrostatic pV-T systems; Maxwell relations; TdS equations; General conditions for equilibrium; Fluctuations; Le Châtelier principle)</p> <p>(3) Phase transitions and topological pressure-temperature phase diagram (Equilibrium conditions for hydrostatic pV-T systems; First-order phase transitions: Clausius-Clapeyron equation. Stability and metastability domains; High-order phase transitions. Group-subgroup phase transitions. Second-harmonic generation; Critical and triple points; Topological P-T phase diagram.</p> <p>(4) Landau's theory for phase transitions. Ferroelastic phase transitions. Long-range anisotropic interactions. Self-accommodation. Structural phase transitions. Mechanistic and kinetic classification of phase transitions.</p>

	(5) Phases out of equilibrium (Glass state and glass transition; dynamics and structural relationships in the glass state; pressure dependence of the glass transition temperature; non-equilibrium phases and mesophases of drugs) (6) Binary systems (thermodynamics of mixing, thermodynamic potential; types of binary phase diagrams: eutectic, metatectic, and peritectic; solubility and miscibility; metastable and unstable states; nucleation vs spinoidal decomposition. The course will include laboratory sessions.
Prerequisites	

4. Assessment of the learning outcomes of the module			
code	type	description	learning outcomes of the module
MB_13_w_1	credit	the basis for obtaining credit will be the grades from homework and laboratory reports	MB_13_1

5. Forms of teaching						
code	form of teaching			required hours of student's own work		assessment of the learning outcomes of the module
	type	description (including teaching methods)	number of hours	description	number of hours	
MB_13_fs_1	lecture	Detailed discussion by the lecturer of the issues listed in the table "module description" using the table and/or multimedia presentations	30	Supplementary reading, working with the textbook, doing homework	45	MB_13_w_1
MB_13_fs_2	laboratory classes	Performance of exercises on the subject consistent with the issues listed in the table "module description"	6	Acquiring knowledge in the scope of the exercise, preparation of the final report on a given exercise	19	MB_13_w_1