UCLouvain

lchm2252

2018

Crystal engineering and crystallization processes

6 credits	45.0 h + 15.0 h	Q2

Teacher(s)	Leyssens Tom ;
Language :	English
Place of the course	Louvain-la-Neuve
Main themes	This course focuses on the principles of crystal engineering and the development of a crystallization process. Focusing on small organic compounds of pharmaceutical, agricultural or food industry, the student is taught about the importance of the solid state, how the solid impacts the properties of a compound, how to properly select a solid form, and how to make this form in a robust manner. The main themes are: solid form screening; modern spectroscopic and analytical methods for studying the solid form; stability studies on a solid form; basic principles of crystallization; Development of appropriate phase diagrams; Crystallization process development; Each year one of the following topics will be specifically dealt with according to the compound selected: hydrate/solvate control, co-crystallization, polymorphism control, salt crystallization, chiral resolution, purification, separation, '.
Aims	1 The aim of this course is to develop the necessary skills allowing the students selecting an appropriate solid form for a given compound, and developing a robust process to achieve this solid form. The goals of this course are to 1) familiarize students with the different notions linked to crystal engineering and the solid state of compounds of interest to pharmaceutical, agricultural or food industry; 2) allow students to select an appropriate solid form based on stability studies and industrial requirements; and 3) Develop and upscale a crystallization process for the selected form. - - - - *The contribution of this Teaching Unit to the development and command of the skills and learning outcomes of the programme(s) can be accessed at the end of this sheet, in the section entitled "Programmes/courses offering this Teaching Unit".*
Evaluation methods	The students will be evaluated on the basis of : 1. A written report on the given problematic related to the compound they were given at the start of the course (50 %) / depending on the results a report written in journal publication format will also be accepted 2. An oral exam discussing the report and the course topics (50%) -The report/publication (8-10 pages in total) will mention: Problematic related to the compound, solid form screen and its results, stability screen and form selection, crystallization development. - Any non-justified absence or non-participation in the group will be penalized in the final mark. - All work is conducted in group. The report is a group report. The oral exam is individual based.
Teaching methods	The course is developed as a hand-on training course. Students are given a specific compound with a solid state related issue at the onset of the course. The students are then expected to study the solid state of this compound, suggest a solution to the problem via a crystallization process and develop a robust process. At each step, the student will have a teacher/student discussion during which the student is familiarized with the basic notions required to proceed with this step. Furthermore an experimental plan is set up. The students then go into the lab to perform experimental work, which will be analyzed in the next teacher/student seminar session. Working this way a step-wise hand-on training course is developed in which the student learns how to select a solid form for a given compound, and how to robustly obtain this solid form through a crystallization process. The student is expected to participate actively during 10*4h sessions.
Content	1)Solid state importance and solid state properties (dissolution, stability, patentability, …) 2) Analytical techniques applied to the solid state (XRPD, DSC, TGA, IR, Raman, …) 3) Different solid forms and solid form screening 4) Thermodynamic stability studies of the solid state 5) Solvent selection and solubility 6) Developing a lab-scale crystallization process 7) Up-scaling of the crystallization process. Depending on the problematic at hand, the content will focus on • Single component system (polymorphism, amorphous state) • Multi-component system (co-crystal, salt, solvate, ….) And will treat one of following problematics: hygroscopicity, hydrate stability, enantiopurity, separation, polymorphic control, co-crystal formation, salt formation, …
Inline resources	Moodle will be used to transfer documents

Bibliography	Book, Review articles, Research papers, templates will be made available on Moodle or are available in the Science library. Non-exhaustive references: R. Hilfiker, 'Polymorphism', Wiley-VCH; ISBN: 978-3-5276-0788-4; J.W. Mullin, 'Crystallization', HB; ISBN: 978-0-7506-4833-2; A.S. Myerson, 'Handbook of Industrial Crystallization', BH; ISBN: 978-0-7506-7012-8; J. Wouters, L. Quéré, 'Pharmaceutical salts and co-crystals', RSC Publishing; ISBN: 978-1-84973-350-2; G.R. Desiraju, J.J. Vittal, A. Ramanan, 'Crystal Engineering: A textbook', Wspc/Iis; ISBN: 978-9-8143-6686-1; …
Other infos	Background: BAC or equivalent in Chemistry, Bio-engineering or Engineering;
Faculty or entity in charge	CHIM

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Aims
Master [120] in Chemistry	CHIM2M	6		