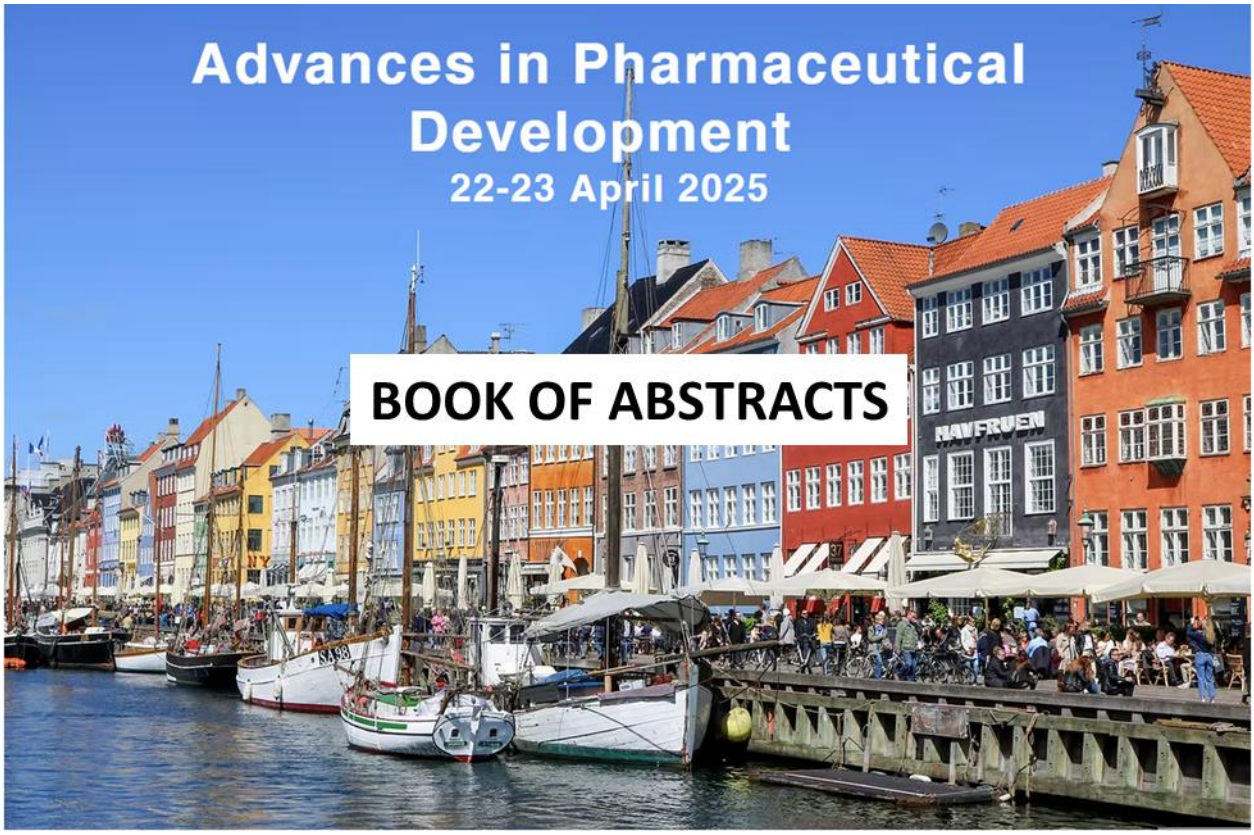
Advances in Pharmaceutical Development

22-23 April 2025



BOOK OF ABSTRACTS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Advances in the Formulation

Advances in lipid-based drug delivery

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ABSTRACT

Oral lipid-based drug delivery systems, and especially self-nanoemulsifying drug delivery systems (SNEDDS) have shown great potential for absorption of hard-to-delivery drugs, such as poorly soluble drugs and therapeutic peptides. SNEDDS are isotropic systems based on lipids and surfactants that form nanoemulsion droplets upon dispersion in aqueous media. For many small molecular BCS Class 2 or 4 drugs the solubility in SNEDDS is low, while in the case of therapeutic peptides, SNEDDS solubility is non-existing, due to the inherent hydrophilicity of these drugs. Therefore, other means are needed to enable absorption after oral drug dosing in SNEDDS. For this we have developed lipophilic complexes with the drugs, e.g. using phospholipids and anionic surfactants. These complexes are then loaded into SNEDDS and this principle have shown an increased drug absorption in rats.

However, to reduce the use of animal studies, development of in vivo predictive in vitro models are important. For BCS Class 2 and 4 molecules dissolution in the gastro-intestinal tract and permeation across barriers are the critical steps, whereas for peptides protection from gastro-intestinal enzymes and co-release of peptide and permemation enhancer to facilitate permeation are critical. By designing SNEDDS by Design of Experiment, and evaluating the above properties using in vitro models, we have been able to develop strategies for achieving a high and reproducible oral absorption of different drugs from SNEDDS.

SHORT BIO & PHOTO

Anette Müllertz is professor in oral drug delivery and industrial relations at the University of Copenhagen, Denmark (UCPH) and head of Bioneer:FARMA, a business unit of Bioneer A/S, which is a research-based, non-for-profit service provider within the area of biomedicine and pharmaceutical development. She is heading the Physiological Pharmaceutics Research Group at UCPH, focusing on developing oral lipid-based drug delivery systems and predictive biopharmaceutics tools. She has >260 publications in international, peer-reviewed journals (H-index: 75, 16229 citations, (Google Scholar 8/4-25). She is / has been supervising 12 post docs, 54 PhD students and numerous master students, primarily at the University of Copenhagen, but also at other universities. She is a Fellow at the American Association of Pharmaceutical Scientists (2022), Fellow at the Controlled Release Society (2023) and recipient of the AAPS Lipid Based Drug Delivery Award (2005) and was acknowledged by receiving the Industry Collaboration Award from the Natural Science Academy of Denmark in 2024. She is editor of Journal of Drug Delivery Science and Technology (IF2024: 4.5).

Order and disorder in pharmaceutical solids – Advances in solid-state drug delivery

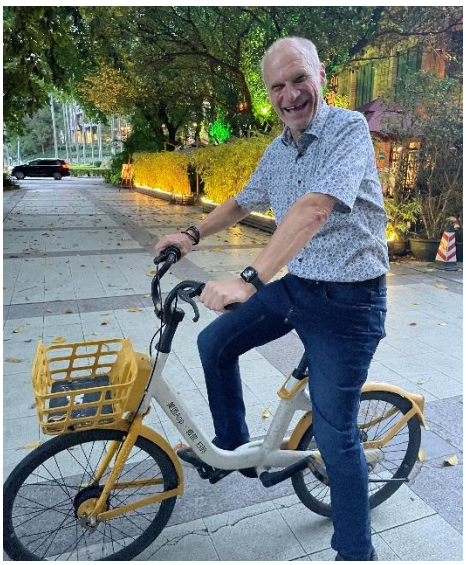
T. Rades[1]

[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark

ABSTRACT

Most drug delivery today is using solid dosage forms, especially for small molecules. However, the solid state of drugs can take many forms, and increasingly uses high energy solids, with different degrees of disorder, ranging from stable to metastable crystalline forms, to supercooled liquid crystalline forms, to amorphous forms. In this presentation we will discuss these different solid state forms and explore their usefulness for drug delivery. This overview talk will be complemented by the case studies presented by Assoc. Prof. Inês Martins, introducing the concept of amorphous engineering.

SHORT BIO & PHOTO



Since 2012 Professor **Thomas Rades** is the Research Chair in Pharmaceutical Design and Drug Delivery in the Department of Pharmacy, University of Copenhagen. Before that he has been the Chair in Pharmaceutical Sciences at the National School of Pharmacy at Otago University in New Zealand.

In 1994 he received a PhD from the University of Braunschweig, Germany for his work on thermotropic and lyotropic liquid crystalline drugs. After working as a Research Scientist in the Preclinical Development and Formulation at F. Hoffmann-La Roche in Basel, Switzerland, he became a Senior Lecturer in Pharmaceutical Sciences at Otago in 1999 and since 2003 held the Chair in Pharmaceutical Sciences in Otago. Professor Rades has developed an international reputation for his research in the physical characterization of drugs and solid dosage forms as well as in drug and vaccine delivery using nanoparticulate systems (both polymeric and lipid based). He has published more than 500 papers in international peer reviewed journals as well as 17 book chapters, 13 patents and 3 books. His current h-index (google scholar) is 95 (April. 2025).

Professor Rades is an Editor-in-Chief of the *European Journal of Pharmaceutics and Biopharmaceutics*. He holds honorary doctorates of Åbo Akademi University, and Helsinki University, Finland and an honorary professorship at the University of Otago, New Zealand. He is an Eminent Fellow of the Academy of Pharmaceutical Sciences (UK), a Fellow of the American Association of Pharmaceutical Scientists (AAPS, US), the New Zealand Institute of Chemistry (NZ) and a member of the College of Fellows of the Controlled Release Society (CRS).

Professor Rades has successfully supervised more than 85 PhD students. For his undergraduate and postgraduate teaching he was awarded the New Zealand Tertiary Teaching Excellence Award for Sustained Excellence (2005). His current research projects include: Amorphous drugs, Co-amorphous drug delivery systems, Drug solubility in polymers, Advanced lipid based drug delivery system.

Advances in Nasal Drug Delivery

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[1]Department of Pharmaceutics and Biopharmaceutics, Kiel University, Germany

ABSTRACT

Nasal delivery of drugs is known for locally acting substances such as decongestants and antiallergics, but the mucosa of the nose can also be utilised for systemic delivery including drug delivery to the CNS and the immune system. New products on the market especially make use of the rapid absorption and are used in emergency situations such as nasal naloxone (in opioid overdose), nasal glucagon (against hypoglycaemia) and nasal sumatriptan (against migraine). Further developments span from the delivery of vaccines over biologics to the nose-to-brain delivery of CNS active drugs.

This talk will give some background to the anatomy and physiology of the nose to understand the challenges in nasal drug delivery. The nose is a highly individual organ in size and geometry and serves to warm, humidify and clean inspired air. As such it has efficient clearance functions which need to be overcome if used for drug delivery.

There are three main formulation options, namely liquid solutions, liquid suspensions and nasal powders. Further options include nasal gels or local depots. They all require a device to get administered to the nose. The talk will look into these options with a focus on the excipients, their functionality and technologies used for preparation [1].

Finally, the device to administer a formulation to the nose will determine important aspects of drug delivery such as the area of delivery and distribution in the nose. The talk will look into functional characterisation of nasal products and explain existing and novel methods [2].

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SHORT BIO & PHOTO

Prof. Dr. Regina Scherließ (*1979) is a professor for Pharmaceutics and Biopharmaceutics, vice-dean for research of the Faculty of Natural Sciences at Kiel University (since 2022) and chair of the Department of Pharmaceutics at Kiel University, Germany. She is a pharmacist and received her Doctor of natural sciences in 2008 for a work on “Formulation of inhalation combination products by co-precipitation”. In 2015 she finished her “habilitation” working on “Mucosal vaccination via the respiratory tract”. She is member of the DDL scientific committee (since 2015). Her research interests include disperse systems and nanoparticles, stabilisation of biomolecules and particle engineering in spray drying, and formulations for mucosal vaccination with a focus on respiratory (nasal and pulmonary) dry powder delivery. She is a co-founder of the Nasal Research Focus Group, a research consortium from academia and industry focusing on nasal drug delivery.

Development of Anti-Inflammatory Electrospun Dressings for Treating Inflammatory Skin Diseases

A.-L. Gürtler[1], Jonathan P. Sirois[1], Julia C. Lang[2,3], Keira Melican[2,3], Thomas Rades[1], and Andrea Heinz[1]

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[2] Center for the Advancement of Integrated Medical and Engineering Sciences (AIMES), Karolinska Institutet and KTH Royal Institute of Technology, Stockholm, Sweden.

[3] Department of Neuroscience Karolinska Institutet, Stockholm, Sweden

ABSTRACT

Topical treatments for inflammatory skin conditions often result in poor patient adherence due to greasiness and the need for frequent applications[1]. In recent years, electrospun dressings have shown potential for the treatment of inflammatory skin diseases[2]. In this presentation, our recently developed electrospun fiber dressing combining salicylic acid and hydrocortisone will be introduced. The polycaprolactone-based dressing features a dual release system, with a burst release of salicylic acid and sustained release of hydrocortisone, allowing for a once-daily use, aiming to improve patient comfort. While electrospun dressings are well-studied for drug release, limited research has been conducted on their skin permeation. Hence, we investigated both drug release and skin permeation data. Rapid release of salicylic acid and delayed release of hydrocortisone were observed, with hydrocortisone successfully penetrating skin layers despite lower release levels in permeation studies. Anti-inflammatory effects of the dressing were confirmed in human skin models, with enhanced hydrocortisone penetration compared to standard formulations. This presentation will highlight the potential of combining multiple drugs in a single electrospun system and emphasizes the importance of correlating release and permeation data for effective drug delivery evaluation.

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SHORT BIO & PHOTO

Andrea Heinz works as an Associate Professor in at the LEO Foundation Center for Cutaneous Drug Delivery, Department of Pharmacy of the University of Copenhagen in Denmark. She studied Pharmacy at the Martin Luther University Halle-Wittenberg, Germany and received her PhD at the University of Otago, New Zealand in 2008 for her work on solid-state characterization of amorphous drugs. Her current research focuses on the development of cutaneous drug delivery systems for the treatment of wounds and impaired skin that occurs as a result of skin pathologies. Her group develops for instance protein-based biomaterials for the use as wound dressings prepared by electrospinning and stimuli-responsive hydrogels and cubosomes.

ASD and implant development made easy

Daniel Treffer[1]

[1]MeltPrep GmbH, Graz, Austria

ABSTRACT

In the early stages of development, efficient tools are essential when APIs are rare and valuable. Vacuum compression molding (VCM) emerges as a solution, enabling formulation testing with just 1 mg of material. Initially introduced for perfect sample preparation for characterization, VCM has evolved into a powerful formulation screening tool due to its lossless nature. It melts thermoplastics using heat, vacuum, and compression, effectively preventing sticking and bubble formation. The principle behind VCM is its ability to convert small quantities of thermoplastic material into solid specimens with defined geometries. The smaller the geometry, the less material is required. Various sizes are also tailored to prototype rod-shaped implants or formulation prototypes for different analytical methods.

However, drug delivery often requires more complex geometries than cylinders or bars, and VCM has been further developed to prototype virtually any complex three-dimensional shape. This new method is called free-d molding, as researchers' ideas are freed from stuck processing equipment. The advancement is based on the benefits of conventional 3D printing. 3D printing is facilitated to shape molds out of non-stick material with negative cavities in the desired dosage form. The molds are inserted in the VCM chamber, and the polymer melt is squeezed into the cavity. Arbitrary shapes can be obtained with minimum process development, as only processing temperature and time are necessary.

Only after narrowing the wide range of formulation possibilities to a few promising ones will process development be necessary. Having the formulation prototypes before the process development provides material properties for process simulations and in-silico approaches. Additionally, rheological measurements provide insights into material properties needed for process optimization. The application of these principles for development will be demonstrated in case studies published in peer-reviewed articles by leading researchers.

SHORT BIO & PHOTO

Daniel burned his hands while working on hot melt extrusion during his Ph.D. This experience fueled his drive to reinvent how ASDs and implants are developed. He founded MeltPrep to provide tools to labs around the globe, enabling individual researchers to develop their ASDs and implants.

Advances in the Characterization

Introduction to Brillouin and low-frequency Raman spectroscopy for pharmaceutical applications

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[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark

ABSTRACT

This presentation will delve into the theoretical foundations and historical evolution of Brillouin and low-frequency Raman spectroscopy, highlighting how modern technical interpretations and advanced data analysis approaches can drive pharmaceutical and biomedical applications. Drawing on examples from both literature and personal experience, I will showcase current trends and emerging use cases, including their potential for in-line manufacturing control.[1,2] The goal is to inspire the audience to explore how these powerful tools can enhance research and innovation in both academic and industrial settings.

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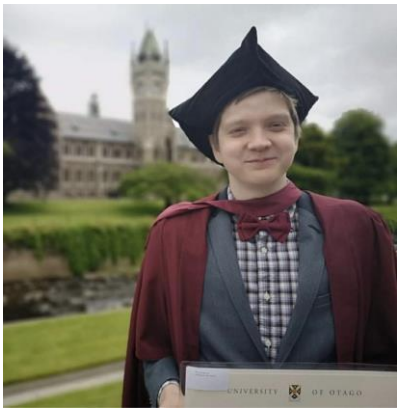
2. Palombo F, Fioretto D. Brillouin light scattering: applications in biomedical sciences. *Chemical Reviews*. 2019, 119, 7833-7847. doi:10.1021/acs.chemrev.9b00019.

SHORT BIO & PHOTO



Kārlis Bērziņš is a postdoctoral researcher in the Structured Biointerfaces group, led by Professor Ben Boyd. He earned his PhD from the University of Otago in 2021 under the supervision of Professor Keith C. Gordon and Dr. Sara J. Fraser-Miller, focusing on low-frequency Raman spectroscopy for pharmaceutical applications. Before his PhD, he spent a year as a visiting research fellow at the University of Minnesota under the guidance of Professor Raj Suryanarayanan.

His research interests lie in the material science of pharmaceutical solids, including innovative drug delivery platforms, with a strong focus on novel characterization and dynamic analysis techniques, as well as the application of machine learning toolsets. He has expertise in solid-state characterization methods such as SAXS/WAXS, thermal analysis, and Raman/IR spectroscopy, along with advanced statistical modeling for data interpretation and periodic boundary DFT simulations.

Elucidating structural heterogeneities of pharmaceuticals with stimulated Raman scattering microscopy

T. Tomberg[1,2], A. Arbiol[1], E. Harju[1], L. Wurr[1], B. van Veen, C. J. Strachan[1]

[1]Drug Research Program, Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki, Helsinki, Finland
[2]Department of Chemistry, Faculty of Science, University of Helsinki, Helsinki, Finland
[3]Orion Corporation, Espoo, Finland

ABSTRACT

The quality and safety of pharmaceuticals are profoundly affected by complex microscale chemical and physical structures within drugs and dosage forms. Unfortunately, analysing and fully understanding these structures and their changes during production, storage and patient administration can be difficult or impossible with established analytical methods. Stimulated Raman microscopy is a relatively new analytical technology to address this analytical gap – it offers rapid, non-destructive, label-free, chemically and solid-state specific imaging of drugs and dosage forms with (sub)micron spatial resolution. It can reveal, for example, microscale (changes in) crystallinity, drug and excipient distributions in dosage forms, and drug release behaviour. Furthermore, the technique can be augmented with additional correlative imaging modalities, including sum-frequency generation and two-photon fluorescence, for even greater analytical power. Through the use of analytical case studies, this talk will highlight collaborative work between pharmaceutical industry and academia, in which a newly established in-house built coherent Raman microscope with fast spectral focusing[1] at the University of Helsinki is employed to enhance pharmaceutical research and development.

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SHORT BIO & PHOTO

Clare Strachan's research primarily advances pharmaceutical analysis with vibrational spectroscopy and imaging. She has a particular interest in Raman, coherent Raman and other forms of non-linear optical methods to better understand drug and dosage form behaviour. She is currently the recipient of a Finnish Research Impact Foundation Tandem Industry-Academia Professorial Fellowship, during which she is based at Orion Corporation, Finland's largest pharmaceutical company, and investigates multimodal nonlinear optical imaging to enlighten the often complex solid-state behaviour of pharmaceuticals during drug development.

Clare Strachan completed a PhD in 2005 on the spectroscopic characterisation of solid state drugs at the University of Otago, New Zealand. During this time she was also based at TeraView Ltd and the Cavendish Laboratory, University of Cambridge, UK, where she employed terahertz spectroscopy for solid-state analysis. She is now Professor of Pharmaceutical Analysis at the University of Helsinki where she leads the Pharmaceutical Spectroscopy and Imaging research group, as well as the Helsinki Institute of Life Sciences (HiLIFE) Molecular Spectroscopy for Life Sciences (LifeSpec) infrastructure. She has published approximately 130 articles in international scientific journals as well as several book chapters.

From crystalline to amorphous solid forms: which tools can we use for their structural characterization?

Inês C. B. Martins[1]

[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark

ABSTRACT

Around 90% of all drug candidates in the pipeline of pharmaceutical companies exhibit poor aqueous solubility, which results in a low and variable oral absorption, and therefore an insufficient bioavailability and therapeutic effect. This is considered one of the most pressing issues in drug development, as even the most promising and active drug candidates fail during the discovery stage, resulting in their discontinuation in the next development phase. To overcome this issue, several strategies have been used, including the preparation of single and multicomponent pharmaceutical systems (e.g., polymorphs, co-crystals, salts, amorphous forms and co-amorphous systems). In this presentation we will discuss, not only the importance of these solid-state forms, but also the methods used for their characterization. In particular, I will draw your attention to the experimental and computational methods used to characterize amorphous forms of drugs, with a focus on a controversial and highly debated solid-state phenomenon termed poly*A*morphism (i.e., existence of more than one amorphous form of a drug presenting distinct physicochemical properties).[1]

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SHORT BIO & PHOTO

Inês C. B. Martins is an Associate Professor at the Department of Pharmacy, University of Copenhagen, Denmark. She has obtained her PhD in Chemistry in 2018 at University of Lisbon, Portugal. Her thesis was focused on using combined solid-state structural characterization techniques with computational methods to solve the structure of complex crystalline multicomponent pharmaceutical systems. After completing her PhD, she was enrolled as an Adolf Martens Fellow, for 2-years at the Federal Institute for Materials Research and Testing (BAM), Berlin, Germany. From 2021 to 2023, Inês was enrolled as a Postdoctoral Researcher of Prof. Thomas Rades at the Department of Pharmacy, University of Copenhagen, to investigate a controversial and highly debated solid-state phenomenon termed poly*A*morphism using both solid-state experimental methods and computational modelling. Her current research activities are focused on investigating the formation of poly*A*morphism and on elucidating its molecular-level organization in pharmaceutical systems. To further investigate this solid state phenomenon and thus to establish a new research area called “amorphous engineering”, Inês was recently awarded a prestigious “Inge Lehmann grant”.

Additive Manufacturing in Drug Formulation Characterization

L. Siebert[1,2]

[1]KU Leuven, Center for Membrane Separations, Adsorption, Catalysis, and Spectroscopy (cMACS), Leuven, Belgium
[2]Kiel University, Department of Materials Science, Kiel, Germany

ABSTRACT

Additive manufacturing (AM), commonly referred to as 3D printing, is emerging as a transformative tool in pharmaceutical research and development. While its applications in personalized medicine and drug delivery are well established, its growing role in drug characterization presents new opportunities for innovation. This talk explores how AM technologies can enhance key characterization processes, particularly dissolution profiling and stability testing. By enabling the precise control of dosage form geometry and internal structure, AM facilitates the design of tailored drug release profiles, improving in vitro dissolution studies. Additionally, 3D printing supports the rapid prototyping of custom testing apparatuses and the development of formulations for accelerated stability assessment. Recent case studies highlight the integration of AM in producing patient-specific dosage forms and innovative testing platforms, demonstrating its potential to streamline pharmaceutical workflows. The talk will also address current challenges and regulatory considerations, offering a forward-looking perspective on the role of additive manufacturing in the future of drug development.

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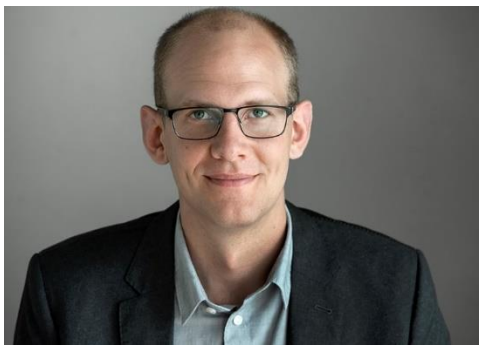
SHORT BIO & PHOTO



Dr.-Ing. Leonard Siebert is a postdoctoral researcher at KU Leuven's Center for Membrane Separations, Adsorption, Catalysis, and Spectroscopy (cMACS) in Leuven, Belgium. Having studied materials science and engineering at Kiel University, Germany, he specializes in additive manufacturing techniques and their applications. His current research integrates novel 3D-printing approaches and self-organization principles to create advanced materials for drug delivery and healthcare.

Prior to joining KU Leuven, Dr. Siebert completed his PhD in Materials Science and Engineering at Kiel University in Germany. In 2021, he was honored with the MaterialVital Award by the Federal Ministery for Research and Education, Germany, for his developments of 3D-printed smart band aids. More recently, Dr. Siebert earned a prestigious Marie Skłodowska-Curie Postdoctoral Fellowship, and in 2026 he will continue his research at the University of Copenhagen working with Assoc. Prof. Inês Martins and Prof. Thomas Rades.

Characterisation in Early Product Development

P. Tajarobi[1]

[1]Early Product Development and Manufacture, Pharmaceutical Sciences, R&D, AstraZeneca Gothenburg, Sweden

ABSTRACT

Tablet development is challenging during early clinical phases due to the dose uncertainty, limited drug substance availability and short lead times. Pharmaceutical industry is aiming to minimize the use of drug substance in development also for sustainability reasons. Established modelling and simulation tools together with risk assessments are important players to succeed with this goal.
Drug substance properties are needed both for *in silico* tools and risk assessments to ensure the selection of a robust formulation and manufacturing process, hence making the drug substance characterization an essential part of early development. In this presentation the most common characterization methods for drug substance and intermediates will be discussed.

SHORT BIO & PHOTO

Pirjo Tajarobi (née Luukkonen) is a pharmacist by training and received her Ph.D. in the pharmaceutical technology from the University of Helsinki (Finland) in 2001. She joined AstraZeneca Mölndal, Sweden 2001 and she has worked in the area of Product Development, Material Science and Manufacturability for nearly 24 years. Currently Dr. Tajarobi is working as a Principal Scientist in the Early Product Development and Manufacture at AstraZeneca Gothenburg. She is an Associate Professor both at the University of Helsinki and Åbo Akademi University in Finland and is regularly supervising both Master's thesis and PhD students. She is an expert in the areas of high-shear wet granulation, continuous wet granulation, roller compaction, continuous direct compression, material characterization and product development. She has published > 35 peer-reviewed papers in these areas.

Advances in the Pharmaceutical Manufacturing

Tailor-Made Doses of Pharmaceuticals by Tunable Modular Design

[1]N. Genina

[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark

ABSTRACT

Additive manufacturing (AM), comprising 2D and 3D printing techniques, has emerged in the pharmaceutical field as a new digitally controlled way to fabricate personalized drug delivery systems, in terms of dose, drug release profile, and customized functionality. Two or more printing and non-printing techniques can be combined to enhance the potential of AM and overcome the limitations of a particular technique. A new approach, so-called tunable modular design (TMD) was proposed to produce a wide range of accurate and tailored doses of biopharmaceutics classification system (BCS) class I and II drugs. The main idea of TMD is to use the combination of two techniques, namely (1) freeze-drying of cellulose ether-based gels to produce porous sturdy solid foams with fixed doses (step size of 3 mg) of an active pharmaceutical ingredient (API) (modules) and (2) inkjet printing to fine-tune the desired dose of an API with the step size of 0.1 mg (Fig. 1). The produced TMD drug products with submicron precision were bench-marked with commercially available tablets that were manually divided. Self-manipulation of doses was proven inaccurate and highlighted the need for new approaches, such as TMD, to produce accurate and personalized doses.

Fig. 1 Examples of drug products by tunable modular design.
Reference to https://doi.org/10.1002/adma.202403852

SHORT BIO & PHOTO

Natalja Genina is an associate professor at the Department of Pharmacy, University of Copenhagen. She obtained her PhD from the University of Helsinki (Finland). Dr. Genina is a pharmacist by training. Her main scientific focus areas are

- Advanced drug delivery systems
- Additive manufacturing
- Personalized medicine
- Implementation of spectroscopic methods for non-destructive quantitative analysis of personalized drug product
- Patient-centric formulations
- Data-enriched edible pharmaceuticals
- Digital health

Technological Challenges for the Adoption of FDM 3D Printing in Pharmaceutical Practice

M. Kurek[1]

[1] Department of Pharmaceutical Technology and Biopharmaceutics, Jagiellonian University Medical College, Kraków, Poland

ABSTRACT

Fused deposition modeling (FDM) has emerged as a prominent additive manufacturing technique within pharmaceutical research, offering unparalleled flexibility in dosage form design and tailored API dissolution profiles (1). Despite its potential, FDM's translation into routine pharmaceutical practice lags behind semisolid extrusion, which has already achieved successful implementation in hospital settings (2). This presentation will address critical technological aspects influencing FDM adoption in pharmaceutical practice. A primary challenge lies in producing filaments with consistent diameter, robust mechanical properties, and long-term stability. Consequently, the presentation will focus on filament-related topics, including material selection, preparation methodologies, quality control procedures, and critical quality attributes. Furthermore, current knowledge gaps surrounding FDM will be highlighted and future research directions will be discussed. The presentation draws on both personal experience and literature.

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SHORT BIO & PHOTO

Dr. Mateusz Kurek, is a pharmacist by training and researcher at Jagiellonian University Medical College in Kraków, Poland, from which he also graduated. His expertise lies in pharmaceutical technology, specifically the development of drug formulations designed to improve the dissolution of poorly water-soluble active pharmaceutical ingredients. His doctoral studies centered on utilizing liquisolid tablet technology to enhance furosemide dissolution. His research interests have expanded over the past ten years to include the application of 3D printing technologies in personalized medicine. Among various 3D printing methods, fused deposition modeling (FDM) is of particular interest due to its integration of hot-melt extrusion processing. This technique is also used for API amorphization, effectively combining two of current Dr. Kurek's primary research areas.

Make poorly soluble drugs great again

K. Löbmann[1]

[1]Zerion Pharma, Copenhagen, Denmark

ABSTRACT

The Dispersome technology is a new drug formulation platform that is based on using the protein beta-lactoglobulin (BLG) as novel pharmaceutical excipient. By mixing a drug compound with BLG, the technology dramatically increases solubility and bioavailability of poorly soluble drugs. The Dispersome® technology makes it possible to develop drugs that would otherwise never reach the market and thereby enables the development of new medication and treatment options for patients. In addition, the technology can be used for innovation in the reformulation of marketed drug products, e.g. by decreasing the drug dose, reducing the dosing regimen and/or dosing frequency, or improved side effect profile. The presentation will give a comprehensive overview on the science behind the Dispersome® technology as well as showcase different case studies.

SHORT BIO & PHOTO

Korbinian Löbmann has a PhD in pharmaceutical sciences and a strong track record in pharmaceutical formulation and drug delivery with more than 10 years of experience in solid formulation and dosage form development. This includes in particular the development of new enabling formulation strategies for poorly soluble drugs using amorphous drug delivery systems. He is co-founder and CSO of the pharmaceutical company ZERION, a spinout from the University of Copenhagen, which is based on the proprietary solubility enhancing Dispersome® technology. He has authored more than 120 peer-reviewed papers and patents.

Enhancing Solubility of Small and Large Molecules with Polyvinyl Alcohol

Dr. Markus Lubda[1]

[1] Strategic Product Manager for Excipients, Merck Life Science KGaA, Darmstadt, Germany

ABSTRACT

During the formulation development of oral solid dosage forms, complex formulation challenges like API instability and low solubility are on the rise. Due to its various functionalities the multi-talent polyvinyl alcohol (PVA) offers effective solutions to these challenges. PVA is suitable for spray drying applications[1] and enhances thereby solubility of small and emerging larger molecule APIs such as PROTACs[2]. Additionally, this polymer can be used for hot-melt extrusion, vacuum compression molding, 3D printing and thin film applications to formulate versatile APIs. Get technical insights on how PVA can be used and that it has even potential to outperform marketed drug formulations. Multiple case studies will show case the flexibility of this polymer and its ability to enhance the solubility and stability of the most challenging small and large molecules.

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SHORT BIO & PHOTO

Markus is a strategic product manager in the field of excipients within Merck Life Science KGaA, Darmstadt Germany. Thereby his focus is to enhance solubility and bioavailability of the most challenging small and large APIs with specifically engineered excipients for oral solid applications. He holds a PhD in Bio/Chemistry on topical penetration of actives and a Master in Biomolecular Engineering from the Technical University of Darmstadt. He is responsible for the strategic development and positioning of an excipient portfolio for oral solid and parental liquid dosage form applications. His ambition is to identify the perfect solution for your solubility problem, by using a broad solubility enhancement toolbox approach.

Latest advancements in additive manufacturing for solubility enhancement

Dr. Thomas Kipping[1]

[1]Associate Director, Head of 3D Printing & Solubility Enhancement, Merck Life Science KGaA, Darmstadt, Germany

ABSTRACT

Many pharmaceutical compounds face poor solubility, impacting their bioavailability and ultimately challenging their successful development. The combination of 3D printing technology with solubility enhancement concepts has the potential to transform the classical manufacturing approaches. By combining the flexibility of additive manufacturing with classical solubility enhancement techniques like solid dispersions and silica loading a versatile on-demand production of personalized medications can be enabled. 3D printing offers advantages such as the ability to create complex geometries that optimize drug release profiles. Techniques like advanced melt drop deposition enable precise formulation control, enhancing the solubility of poorly soluble compounds while ensuring consistent quality and reducing manufacturing costs [1]. For powder-based 3D printing the incorporation of solubility-enhancing excipients directly into the printed matrix can improve drug stability and create effective, patient-friendly formulations. These innovative approaches drive a shift in pharmaceutical manufacturing, paving the way for personalized medicine that enhance drug bioavailability and improve patient outcomes.

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SHORT BIO & PHOTO

Dr. Thomas Kipping is a distinguished expert in the field of pharmaceutical technology and formulation development. Thomas is currently the Head of 3D Printing & Solubility Enhancement at Merck Life Science KGaA. With more than 12 years of industrial experience spanning across various sectors within the pharmaceutical industry including drug product development and CDMO services, he has consistently demonstrated a strong commitment to advancing pharmaceutical sciences and enhancing drug development processes. His areas of expertise include formulation development, solubility enhancement, advanced manufacturing, regulatory compliance, quality assurance, and research and development.

Advances in the Computational Methods

Advanced approaches for structural characterization by synchrotron X-ray radiation

Philipp Hans[1]

[1]Department for Pharmacy, University of Copenhagen, Copenhagen, Demark

ABSTRACT

Structure-property relationships are what we study when we study how a substance's structure at the microscopic level determines, for example, its electrical, magnetic, optical, or thermal properties, but also its solubility or melting point. Widely used tools for the structural characterization of a specimen and the elucidation of structure-property relationships are structural probes such as electron, neutron, or X-ray scattering. They lie at the heart of many crystallographic investigations and give information about the average arrangement of atoms in a specimen. The aim of this article is to present examples of applications of hard X-rays for structural investigations and to introduce the term "synchrotron", as synchrotrons are becoming increasingly important in science. Synchrotrons are a type of particle accelerator in which high-intensity photons (gamma and X-rays, but also lower energies) are generated by the interaction of charged particles with strong magnetic fields. Modern synchrotrons not only deliver photons with high intensity, but often also with high brilliance, i.e. with high coherence and spatial concentration, depending on the size of the source, which enables time- and spatially resolved experiments. We will take a tour through structural investigations related to atomic order and disorder studied in situ, such as mapping experiments or laser-induced amorphisation/crystallisation in inorganic thin films or phase transitions in drugs under non-ambient conditions, which could be inspiring for pharmacists.

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SHORT BIO & PHOTO

Philipp Hans studied technical chemistry and crystallography at the Vienna University of Technology (TU Wien). After working in Germany, Italy, France, the USA and Jordan both as a researcher and as a beamline scientist (X-ray diffraction and X-ray computed tomography), he now works at the Institute of Pharmacy at the University of Copenhagen, where he develops AI methods for the interpretation of electron diffraction data.

Additive Manufacturing in Drug Formulation Characterization

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[2]Molecular Quantum Solutions, Copenhagen, Denmark

ABSTRACT

This work aims to systematically investigate ILs' potential as next-generation CDD by correlating their physicochemical properties with biological performance, utilizing formulation development, quantum chemistry, and the COSMO model. Emphasis will be placed on the biophysical characterization of drug solubility linked to computer simulation models and structural understanding of our formulation, and how these factors affect skin barrier interaction and biological readout. Advanced scattering techniques will be employed to ensure effective local drug delivery while maintaining skin barrier integrity.

ABSTRACT

Stine Rønholt is an Assistant Professor at the LEO Foundation Center for Cutaneous Drug Delivery, University of Copenhagen. She holds a PhD in food biophysics and an MSc in pharmaceutical science. Her research focuses on barrier interactions between biological membranes and advanced drug delivery systems (DDS), using techniques like synchrotron X-ray and neutron scattering, rheology, and advanced microscopy. Stine aims to understand how diseases affect drug uptake and barrier interaction, developing a multimodal research platform to explore these interactions with deep eutectics and ionic liquids.

Effect of simulation box size and shear on the structure of amorphous hydrochlorothiazide

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[1]CMAC, University of Strathclyde, Glasgow, UK
[2]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark
[3]Cambridge Crystallographic Data Cente, Cambridge, UK

ABSTRACT

Molecular dynamics simulations have been used to study the effect of box size and shear on the structure of amorphous hydrochlorothiazide (HCTZ). Box size was crucial in obtaining consistent simulation results, in terms of the local structure of amorphous HCTZ, with 250 molecules being the minimum to consistently represent intermediate-range order, as found by comparison to experimental pair distribution function (PDF) data. Additionally, it was found that the distribution of short-range intermolecular interactions was also influenced by the number of molecules in the simulation cell. Subsequently, shear simulations were used to replicate the effect of ball milling on the structure of amorphous HCTZ, to understand preparation method-dependent properties of the amorphous form as reported previously[1]. It was found that ball-milled HCTZ undergoes conformational changes similar to those previously observed in simulations of the melt-quenched form, which exhibits similar properties such as glass transition temperature. Additionally, changes in the distribution of intermolecular contacts are also observed. These structural changes are retained once the shear force is removed, giving a structural explanation for the different properties arising from different preparation routes. This work reinforces the value of molecular dynamics simulations in developing understanding of structure-property relationships in amorphous solids, and demonstrates its importance in the context of small-molecule pharmaceuticals.

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SHORT BIO & PHOTO

Michael is a research associate working on structure and physical stability prediction in amorphous solids. Michael has experience in structural modelling of pharmaceuticals, with a focus on the solid-state structure of amorphous solids, and is also working on database development to support data-driven modelling for prediction of pharmaceutical solid properties. Michael has a PhD focussed on understanding structure in amorphous materials, and has also worked as a project scientist in pharmaceutical formulation (continuous direct compression) with MMIC before rejoining CMAC as a researcher in 2022.

Artificial Intelligence based Co-crystal Prediction Tool

Mitali Bhagwat[1]

[1]Strategic Product Manager at Merck KGaA, Darmstadt, Germany

ABSTRACT

In recent years several approaches have been developed to screen for cocrystals computationally to tackle increasing solubility challenges. But screening for co-formers can be time and resource intensive.
Merck has developed mPredict™, a co-crystal prediction tool using the combination of quantum chemistry and statistical thermodynamics. By calculating excess enthalpies and several other parameters, it can predict cocrystal formation. Hence, it is able to predict the optimum co-former for a particular API and rank it according to likelihood of co-crystal formation. mPredict™ shows strong improvement over physical modelling and is three times more effective than random digital screening.
We will examine key technical considerations we have utilized to build mPredict™ – a co-former screening tool. During this session, you will learn how AI-based computational screening can be used to predict optimum co-formers to co-crystallize your API.

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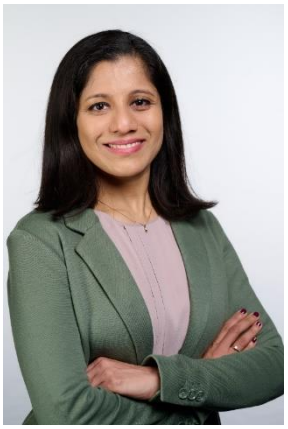
SHORT BIO & PHOTO

Mitali works at Merck KGaA, Darmstadt, Germany as a Strategic Product Manager in the field of excipients used for solid formulation drug development and is leading the group's digital strategy with its flagship product mPredict™. She has a Master's degree in Pharmaceutical Sciences and 10 years of work experience in the industry around product development and IP strategies. After completing her MBA in International Management from Hochschule Pforzheim, Germany and working as a management consultant in the industry, her ambition now is to bring drug formulation closer to digital / AI technologies.



Computationally assisted design (CAD) for lipid and polymer based drug delivery systems

Alex Bunker[1]

[1]Faculty of Pharmacy, University of Helsinki, Helsinki, Finland

ABSTRACT

Lipid and polymer based systems have become the dominant form of delivery vehicles for a wide range of therapies. This involves many nanoparticle forms, including liposomes, polymeric micelles and lipid nanoparticles. The formulation space is extremely broad: there are near limitless modifications that can be made to polymer structures and lipid compositions; a design approach based on mechanistic understanding of the link between structure and function is needed. While there are many experimental techniques capable of getting results for different aspects of nanoparticle structure and behavior, different experimental results measure different aspects of the system and gaps remain, precluding a complete picture. Molecular dynamics (MD) simulation provides a unique window that can fill in the gaps between experimental methodologies and thus enable a design approach. We argue that it has the promise to play a role analogous to computationally assisted design (CAD) in mechanical and civil engineering. From our initial work using all atom molecular dynamics (MD) simulation of the surface of a poly(ethylene-glycol) (PEG) coated (PEGylated) lipid membrane to elucidate properties of drug delivery liposomes that we published in 2011 [1] to then studying targeting ligands, alternatives to PEG, and other aspects of liposome design to poly(2-oxazoline) and poly(2-oxazine) based ABA triblock co-polymer micelles[2], and ultimately lipid nanoparticles, developing MD simulation as a design tool for polymer and lipid based drug delivery systems represents 15 years of research. While I will give an overview of the broad arc of the research, I will mostly discuss our most recent work simulating lipid nanoparticles and polymeric micelles.

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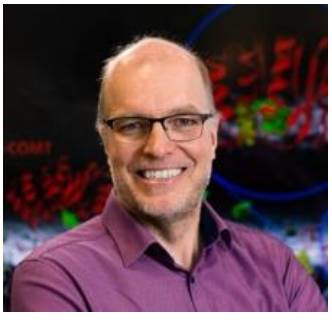
SHORT BIO & PHOTO



I am a senior researcher (Adj. Prof.) at the Faculty of Pharmacy of the University of Helsinki. Originally a computational physicist by training (PhD, Physics, University of Georgia, 1998) I completed a post-doctoral fellowship at the Max Planck Institute for Polymer Research and had a stint in industry before starting my current position where I have pursued the application of the conceptual toolkit of computational biophysics to pharmaceutical research. For more than 15 years I have pioneered use of large-scale molecular dynamics as a design tool for drug delivery systems and obtaining mechanistic insight relevant to drug selection factors for targeting weakly membrane associated proteins.

Solving crystal structures using a neural network

Anders Støttrup Larsen[1], Toms Rekis[2], Anders Østergaard Madsen[1]

[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark
[2]Department of Chemistry, Goethe University Frankfurt, Frankfurt, Germany

ABSTRACT

Solving the crystallographic phase problem remains a central challenge in determining three-dimensional crystal structures solely from measured diffraction data. Classical *ab initio* approaches—such as direct methods and charge-flipping algorithms—typically require atomic-resolution data and can struggle with lower-resolution or incomplete datasets. To address these limitations, we introduce PhAI, a deep-learning–based framework that predicts phases from measured amplitudes alone. Trained on millions of synthetic organic and metal–organic crystal structures, PhAI learns relationships between structure factors and electron densities that bypass the need for atomic-resolution diffraction data. In tests on thousands of real crystal structures—covering common space groups and small unit-cell dimensions—PhAI successfully retrieves accurate electron density maps at resolutions as low as 2.0 Å, using only 10–20% of the reflections typically required by classical methods. Remarkably, it also achieves phase extension, predicting phase information for reflections beyond those provided at the start. Applied to experimental single-crystal and powder diffraction data, PhAI proves robust and outperforms classical approaches in low-resolution regimes, enabling more efficient and accurate structural solutions. These findings demonstrate that deep-learning architectures can fundamentally reshape the boundaries of *ab initio* phasing, opening avenues for structure determinations under challenging conditions such as weak scattering, limited resolution, and low completeness.

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SHORT BIO & PHOTO

Anders is a postdoctoral researcher at the Department of Pharmacy, University of Copenhagen, and completed his PhD there in 2018. He has a background in molecular dynamics, machine learning, and computational chemistry. He has used molecular dynamics to simulate phase changes in hydrate crystals and is currently working on neural network–based methods to improve the determination of crystal structures from X-ray and electron diffraction.