Deutsche Pharmazeutische Gesellschaft

DPhG

Landesgruppe Berlin-Brandenburg

Freie Universität Berlin

12th Scientific Symposium:

Der wissenschaftliche Nachwuchs stellt sich vor

–

Young scientists present

08 July 2022

Freie Universität Berlin
Institute of Pharmacy

The *Deutsche Pharmazeutische Gesellschaft, Landesgruppe Berlin-Brandenburg* and the *Institute of Pharmacy, Freie Universität Berlin,* warmly invite you to the 12th Scientific Symposium on:

"Der wissenschaftliche Nachwuchs stellt sich vor
–
Young scientists present"

Young Scientists of our Institute at Freie Universität Berlin will present their research as oral or poster presentations.

Date: 08 July 2022
Start: 9:00 a.m.

Venue: Freie Universität Berlin
Pflanzenphysiologie
Königin-Luise-Straße 12-16
14195 Berlin

Oral presentation: Haberlandt-Hörsaal (Pflanzenphysiologie)

Poster presentation: Foyer (Pflanzenphysiologie)

Scientific Program

09:00 – 09:05 **Welcome - Prof. Dr. Charlotte Kloft**

Oral presentations - Part 1 -

Chair: ***Prof. Dr. Jörg Rademann***

V1 09:05 – 09:20

M. Dubau, T. Tripetchr, B. Kleuser
Autologous approach to develop an immunocompetent skin model using iPSC-generated fibroblast, keratinocytes, and immune cells

V2 09:20 – 09:35

Y. Jia, C. Arkona, Y. Pfeifer, L. Deng, B. Kuropka, C. Fröhlich, K. Ataka, S. Bergemann, G. Wolber, H.-K. S. Leiros, M. Mielke, G. Werner, J. Rademann
Fragment-based development of inhibitors of New Delhi metallo- β-lactamase-1 (NDM-1) and validation of their mode-of-action against multiresistant bacteria

V3 09:35 – 09:50

F. Klima, A. Mc Laughlin, E. Schmulenson, O. Teplytska, S. Zimmermann, P. Opitz, S. Groenland, A. Huitema, N. Steeghs, S. Fuxius, M. Joerger, F. Mayer, U. Fuhr, S. Holdenrieder, G. Hempel, O. Scherf-Clavel, G. Mikus, U. Jaehde, C. Kloft
Feasibility of Therapeutic Drug Monitoring for targeted oral anticancer drugs in clinical routine: The ON-TARGET study

V4 09:50 – 10:05

T. M. P. Neumann-Tran, D. Klinger
Turning the defense mechanism of antibiotic resistant bacteria against themselves: New Polymer-Drug-Conjugates

10:05 – 10:10 Short break

Oral presentations - Part 2 -

Chair: ***Prof. Dr. Charlotte Kloft***

V5 10:10 – 10:25

T. Noonan, D. Schaller, R. Nikolay, C. Spahn, M. Bermudez, G. Wolber

A novel antibiotic target: Identifying bacterial ribosomal assembly inhibitors via 3D pharmacophore-based virtual screening

V6 10:25 – 10:40

K. Pail, R. Bodmeier

Effect of glycerine on the conformation of Poloxamer P407 and its implication on the nano-milling of a poorly water-soluble drug

V7 10:40 – 10:55

M. K. Parr, Y. Sun, L. Harps, M. Bureik

Human sulfotransferase assay with PAPS production in situ

10:55 – 11:00 **Closing of Oral Presentation Sessions**

11:00 – 12:30 **Poster Presentation Session**

Posters

P1 M. N. Alam, A. Dashevskiy, R. Bodmeier
Pulsatile drug release from compression-coated tablets

P2 A. M. Ambros, P. Hailer, C. Arkona, G. Wolber, J. Rademann
Molecular modeling and chemical optimization of fragment-based inhibitors of STAT5 as a novel anti-leukemia strategy

P3 L. B. S. Aulin, R. Michelet, M. Ursino, S. Boulet, J. C. Sirard, E. Comets, S. Zohar, C. Kloft
The FAIR approach: Utilising a modelling and simulation workflow leveraging multisource data to support preclinical development and clinical trials

P4 D. Bindellini, D. Busse, P. Simon, R. Michelet, D. Petroff, L. B. S. Aulin, C. Dorn, M. Zeitlinger, H. Wrigge, W. Huisinga, C. Kloft
Semi-mechanistic model-based analysis to evaluate differences in plasma and target site cefazolin pharmacokinetics and protein binding in obese and nonobese patients

P5 M. Breznik, S. Pach, S. Gobec, G. Wolber
Retrosynthesis-driven *in silico* optimization of antiviral agents targeting 3C and 3C-like proteases

P6 Y. Chen, Q. T. Wang
The application oft he MM/GBSA method in the binding pose prediction of FGFR inhibitors

P7 A. Démaris, E. L. Plan, W. Huisinga, L. B. S. Aulin, S. H. Lee, J. H. Lee, W. Reinisch, R. Michelet, C. Kloft
Characterising and predicting the risk of immunogenicity in Crohn's disease patients receiving infliximab therapy

P8 P. Demirel, C. Arkona, J. Rademann
Pre-biotic evolution of functional peptides through templated synthesis

P9 K. Denzinger, M. Dündüz, G. Wolber
Probing the binding pockets of L-type and T-type calcium channels using dynamic pharmacophores – a new approach for pain medication

P10 Y. Dyck, D. Rehm, K. Winkler, V. Sandig, W. Jabs, M. K. Parr
Identification of susceptible residues in a monoclonal antibody after forced degradation by peptide mapping

P11 Y. Fan, M. K. Parr
Complete reaction phenotyping of propranolol and 4-hydroxypropranolol with the 19 enzymes of the human UGT1 and UGT2 families

P12 L. Gerlach
Establishment of a method to determine the cell number of Schizosaccharomyces pombe for the standardisation of biotransformation assays

P13 G. Giacomello, C. Boettcher, M. K. Parr
Development and validation of a method to trace ^{13}C through glucose metabolism

P14 T. Heinrich, A. Dashevskiy, R. Bodmeier
Effect of ethanol on the release mechanism from hydrophilic matrix tablets

P15 S. Kanwal, T. M. P. Neumann-Tran, D. Klinger
New antimicrobial polymers to fight against resistant bacteria

P16 F. Kias, R. Bodmeier
Diafiltration-assisted solvent extraction for achieving rapid organic solvent removal during the preparation of biodegradable poly(lactide-co-glycolide) (PLGA) microparticles

P17 D. Klemczak, A. Horatscheck, R. Raz, J. P. Kries, S. Bergemann, A. V. Rudnev, P. Broekmann, J. Rademann
Peroxygenins (POG) are redox-activated inhibitors of protein tyrosine phosphatases and target cells with high reduction potential

P18 A. P. Konrad, F. Bredendieck, F. Schumacher, C. Kloft
Bioanalytical method development for the determination of target-site concentrations of posaconazole

P19 L. Lassak, J. Rademann
Pentafluorophosphato-phosphonates: biomimetics of organic pyrophosphates?

P20 L. Y. Liu, L. Hobohm, F. Bredendieck, A. Froschauer, O. Zierau, M. K. Parr, A. M. Keiler
Medaka embryos as a model for metabolism of anabolic steroids

P21 S. Liu, F. Yang, M. K. Parr, G. Wolber
Comparative modelling of human Uridine 5'-diphosphoglucuronosyltransferase guided by molecular dynamics (MD) simulations

P22 C. López-Iglesias, R. Cui, A. Markovina, A. Gruber, D. Klinger
Synthesis, characterization, and applications of amphiphilic nanogels based on polymethacrylates and polycarbonates

P23 S. Märker, M. Körber, R. Bodmeier
Mechanical properties of biodegradable poly(lactide-co-glycolide) (PLGA) implants determined by a three-point bending test

P24 H. Mitdank, M. Tröger, A. Sonntag, N. A. Shirazi, E. Woith, H. Fuchs, D. Kobelt, W. Walther, A. Weng
Suicide nanoplasmids coding for ribosome-inactivating proteins

P25 F. L. Mueller, L. Ilia, K. Foerster, J. Burhenne, R. Michelet, C. Kloft
Variability in protein binding determination: A comparison of microdialysis, ultrafiltration and rapid equilibrium dialysis

P26 S. Pach, D. Schaller, G. Wolber
Extracting 3D pharmacophores from molecular dynamics simulations: A case study

P27 A. Prell, ,F. Schumacher, D. Wigger, B. Kleuser
Target and off-target effects of sphingosine kinase inhibitors on the sphingolipidome in different cell lines

P28 K. Puls, H. Schmidhammer, G. Wolber, M. Spetea
Enlightment through dynamics: How the peripheral analgesic HS-731 discriminates between opioid receptors

P29 A. Saoud, J. Rademann
Pore-blockers: Small-molecule inhibitors of cholesterol-dependent cytolysins

P30 L. Schlaak, C. Weise, B. Kuropka, A. Weng
Sapovaccarin-S1 and -S2, two type I ribosome-inactivating protein isoforms from the seeds of *Saponaria vaccaria* L.

P31 K. Schreck, M. F. Melzig
The expression of selected intestinal glucose, fructose and long chain fatty acid transporters investigated in Caco-2 cells

P32 W. Song, J. Rademann
Development of orthosteric inhibitors of SHP2

P33 A. Sonntag, H. Mitdank, A. Weng
Construction of Minicircle suicide genes coding for ribosome-inactivating proteins

P34 J. Steff, X. de la Torre, F. Botrè, M. K. Parr
Stereoselective chemosynthetic approach to obtain metabolites of metandienone with a fully reduced
A-ring as reference material

P35 V. Talagayev, A. Dolsak, D. Sribar, G. Wolber, M. Sova, G. Weindl
An innovative approach fo Toll-like receptor dynamics exploitation for structure optimization through
3D pharmacophore analysis

P36 M. Tiemann, M. Accorsi, L. Wehrhan, L. M. Finn, R. Cruz, M. Rautenberg, F. Emmerling, J. Heberle, B. G. Keller, J. Rademann
Pentafluorphosphato-phenyl-alanines as amphiphilic mimetics of phosphotyrosine

P37 T. Tripetchr, M. Dubau, B. Kleuser
Development of a skin sensitization assay using *in vitro* immunocompetent skin models

P38 R. Wamser, S. Pach, C. Arkona, M. Baumgardt, U. B. A. Aziz, A. Hocke, G. Wolber, R. Rademann
Covalent inhibitors of SARS-CoV-2 main protease targeting the S1-site with pyridine fragments

P39 T. Wang, S. Staufenbiel, R. Bodmeier
Preparation and characterization of a stabilizer-free dexamethasone oily nanosuspension

P40 F. E. Weber, F. A. Weinelt, M. Stegemann, A. Theloe, F. Pfäfflin, L. Aulin, U. Trost, W. Huisinga, S. Hennig, C. Kloft
Optimising meropenem dosing in the intensive care unit with a model-informed precision dosing tool: The TIAS study

P41 E. Widigson, D. Busse, D. Bindellini, D. Petroff, C. Dorn, L. B. Aulin, R. Michelet, M. Zeitlinger, W. Huisinga, H. Wrigge, P. Simon, C. Kloft
A pharmacometric evaluation of atypical plasma protein binding and probability of target attainment of tigecycline in obese and nonobese patients

P42 E. Woith, A. Jendretzki, A. von zur Gathen, M. F. Melzig
Plant extracellular vesicle lipids and secondary metabolites

P43 C. A. Wolf, S. Liu, D. Machalz, J. Zhao, M. K. Parr, M. Bureik, G. Wolber
Observing subtle changes in conformational dynamics caused by mutation P340A in orphan cytochrome
P450 3A43 for drug design

P44 W. Xie, M. F. Melzig
The stability of medicinal plant microRNAs in herb preparation process

P45 G. Ambrosio, T. Yuliandra, K. Touvleliou, B. Wuest, M. Mazzarino, X. de la Torre, F. Botrè, P. Diel, E. Isenmann, M. K. Parr
Excretion study of ecdysterone following a single-dose administration in humans

P46 C. Zhang, R. Bodmeier
Encapsulating dexamethasone nanocrystals into PLGA microparticles by a simplified solvent evaporation process

P47 X. Zhang, J. Rademann
Development and evaluation of fragment-based inhibitors of SARS-CoV-2 main protease

P48 N. Zimmermann, B. Pourshacheraghi, S. Wolf, T. Semmler, C. Kloft
Integrated *in vitro* approach to understand the exposure-effect relationship of fosfomycin against *Escherichia coli*