Freie Universität Berlin

Deutsche Pharmazeutische Gesellschaft

DPhG

Landesgruppe Berlin-Brandenburg

13th Scientific Symposium:

Der wissenschaftliche Nachwuchs stellt sich vor

–

Young scientists present

05 July 2024

Freie Universität Berlin
Institute of Pharmacy

The *Institute of Pharmacy of Freie Universität Berlin* and the *Deutsche Pharmazeutische Gesellschaft, Landesgruppe Berlin-Brandenburg,* warmly invite you to the 13th 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: 05 July 2024
Start: 9:00 a.m.

Venue: Freie Universität Berlin
Königin-Luise-Straße 2+4 / Königin-Luise-Straße 1-3
14195 Berlin

Oral presentation: Hörsaal Zoologie, Königin-Luise-Straße 1-3

Poster presentation: Foyer, Institut für Pharmazie, Königin-Luise-Straße 2+4

Scientific Program

09:00 – 09:05 **Welcome - Prof. Dr. Jörg Rademann**

Oral presentations - Part 1 -

Chair: ***Prof. Dr. Burkhard Kleuser***

V1 09:05 – 09:25

N. P. Doering, G. Wolber, S. De Jonghe, T. Van Loy
Modulating ORF74 – Targeting the Viral GPCR of Human Herpes Virus 8

V2 09:25 – 09:45

M. S. R. Happ, L.B.S. Aulin, M. Mondemé, M. Baldry, W. Huisinga, C. Faveeuw, J.-C. Sirard, R. Michelet, C. Kloft
How to quantify the host-drug-disease interplay: Modelling approaches to support development of new treatment strategies in resistant bacterial infections

V3 09:45 – 10:05

F. Nußhardt, C. S. Butnarasu, H. Mamkhezri, J. Thomas, I. Bayindir, D. C. Lauster
Peptide-polymer-conjugates as a new class of mucolytic therapeutics

10:05 – 10:10 **Short break**

Oral presentations - Part 2 -

Chair: ***Prof. Dr. Jörg Rademann***

V4 10:10 – 10:30

A. Sonntag, K. Gorzolka, M. Lenz, F. Herrmann, M. F. Melzig, A. Weng

A novel natural product from the leaves of a Solanum spec. (Solanaceae) shows antimicrobial activity against multiple multi-resistant pathogens

V5 10:30 – 10:50

J. Steff, M. K. Parr

Dependence of fragment ion generation in 17α-methylandrostanediols on their particular diastereomeric configuration

V6 10:50 – 11.10

L. Mahmoud, D. Wigger, F. Schumacher, B. Kleuser

Significance of IDH1R132H/+ mutation on sphingolipidoma in glioblastoma

V7 11:10 – 11:30

D. Klemczak, M. Reimann, M. Tiemann, C. Schmitt, J. Rademann

Peroxygenins – new pan-senolytic drugs selectively killing senescent cells and their potential use in tumor therapy

Closing of Oral Presentation Sessions

11:30 – 12:45 **Poster Presentation Session**

Posters

P1 A. M. Ambros, M. Tiemann, L. Dettling, J. Rademann
Pentafluorophosphates as biomimetics of phosphopeptides and phosphoproteins

P2 M. Andersson, F. Weber, L. B. S. Aulin, N. Zimmermann, F. Weinelt, R. Michelet, C. Kloft
The instantaneous minimum inhibitory concentration as promising pharmacodynamic metric to optimise dosing strategies of piperacillin/tazobactam

P3 A. Atef, U. B. A. Aziz, A. Saoud, J. Rademann
Vilsmeier-Haack and knoevenagel reactions for synthesis of new pneumolysin inhibitors

P4 U. B. A. Aziz, A. Saoud, M. Bermudez, M. Mieth, A. Atef, T. Rudolf, C. Arkona, C. Böttcher, K. Ludwig, A. Hocke, G. Wolber, Jörg Rademann
CDC-inhibitors as anti-bacterial Pathogenblockers

P5 D. A. Barrera-Adame, S. Schuster, T. H. J. Niedermeyer
On-tissue derivatization and MALDI−MS Imaging reveal hemlock alkaloid distribution in Conium maculatum

P6 C. Behnke, S. Kopylov, J. Müller, N. Mehlmer, T. Brück, J. Rademann
Development and synthesis of new bioactive Cannabinoids via synthetically and biologically designed modern platform technologies

P7 D. Bindellini, R. Michelet, J. Melin, L. B. S. Aulin, W. Huisinga, U. Neumann, O. Blankenstein, M.J. Whitaker, R. Ross, C. Kloft
Understanding the physiology of the hypothalamic-pituitary-adrenal axis to optimise cortisol replacement therapy: A quantitative modelling framework

P8 M. Breznik, Y. Chen, K. Denzinger, S. Liu, V. Talagayev, A. Pandit, K. Puls, C. A. Wolf, G. Wolber
Identification of Potential Ligands Binding to SARS-CoV-2 NSP3 Macrodomain Through 3D Pharmacophore-Based Virtual Screening, Molecular DynamicsSimulations, and High-Throughput Docking

P9 F. Buelow, T. H. J. Niedermeyer
pH-dependent membrane permeabilisation through Saponins

P10 P. Demirel, C. Arkona, J. Rademann
Self-assembly of functional peptides through templated synthesis

P11 K. Denzinger, M. Gündüz, G. Wolber
Computer-aided drug design of Cav3.2 selective modulators as novel therapeutic approach in chronic pain conditions

P12 M. Dubau, T. Tripetchr, V. Kral, B. Kleuser
iPSC-derived immunocompetent skin models as an alternative method for the in vitro identification of skin-sensitizing foreign substances

P13 L. Gerlach, J. Preira, M. Bureik, M. K. Parr
Construction of new fission yeast strains expressing human AKRs

P14 A. L. Jendretzki, L. C. Harps, Y. Sun, F. Bredendiek, M. Bureik, U. Girreser, X. de la Torre, F. M. Botrè, M. K. Parr
Biosynthesis of Salbutamol-4'-O-sulfate as Reference for Identification of Intake Routes and Enantiopure Salbutamol Administration by Achiral UHPLC-MS/MS

P15 S. Kanwal, D. Klinger
Sulfonium-Based Polymers for Antimicrobial Use: Influence of Structure and Composition

P16 F. Klima, T. Helland, R. Michelet, W. Huisinga, D. Hertz, C. Kloft
Quantifying the impact of CYP2D6 allele activity on Z-endoxifen formation leveraging the multi-study CEPAM database: Towards treatment optimisation of tamoxifen

P17 L. Kloeppner, L. C. Harps, M. K. Parr
Sample Preparation Techniques for Growth-Promoting Agents in Various Mammalian Specimen Preceding MS-Analytics

P18 M. Klose, F. Thoma, L. Kovar, W. Huisinga, R. Michelet, C. Kloft
Machine learning-driven flattening of model priors: A comparative simulation study across multiple compounds

P19 L. Koch, S. Tragust, T. H. J. Niedermeyer
Formicine Ant Venoms Put to the Acid Test

P20 A. P. Konrad, A. Saleh, J. Schulz, L. B. S. Aulin, F. Kluwe, R. Michelet, G. Mikus, C. Kloft
Mechanistic investigations to understand the complex metabolism of voriconazole by cross-linking in silico and in vitro methods

P21 D. Krueger, A. Weng
EKO-YAM - Investigating Dioscorea for a sustainable future

P22 K. Lam, E. K. Aslan, C. Dengiz, K. Denzinger, I. Y. D. Erdamar, S. Huang, G. W. Zamponi, M. G. Gündüz, G. Wolber
Molecular modelling studies of novel 1,4-dihydropyridine derivates in T-type calcium channel

P23 L. Lassak, J. Rademann
Establishing biological activity of hyperfluorinated pentafluorophosphato bisphosphonates

P24 S. Liu, J. Kirchmair, G. Wolber
Predicting aromatase (CYP19A1) inhibitors with machine learning (ML) models

P25 F. Mueller, E. Hermans, D. Bindellini, L. B. S. Aulin, R. Michelet, P. De Paepe, P. De Cock, M. Devreese, M, C. Kloft
Understanding variability in microdialysis measurements: introducing a combined calibration approach for piperacillin and tazobactam in LPS-induced septic piglets

P26 T. Noonan, D. Schaller, R. Nikolay, C. Spahn, M. Bermudez, G. Wolber
Interfering with Bacterial Ribosomal Assembly as a Novel Antibiotic Approach

P27 V. Rebhahn, T.H.J. Niedermeyer
Investigation into the mode of action of Aetokthonotoxin

P28 S. Reger, M. K. Parr, M. Bureik
Optimization of a fluorescence microplate assay to investigate the influence of various substances on human UDP-glucuronosyltransferase activity

P29 W. Rohland, D. Klinger
Turning the Defense Mechanism of Antibiotic Resistant Bacteria against Themselves: New Polymer-Drug-Conjugates

P30 G. F. Salchert, J. Rademann
CO2-mediated synthesis of functional peptides

P31 F. Schanbacher, T. H. J. Niedermeyer
Fantastic Compounds and How to find them: Mass Spectrometry´s Role in Uncovering New Natural Products

P32 W. Song, J. Rademann
Development of Orthosteric Inhibitors of SHP2 Derived from GS493

P33 B. Stattelmann, J. Rademann
Validation of peroxygenins as potential senolytic agents in cellular models

P34 L. L. Stock, C. A. Wolf, S. Schuster, H. Enke, D. Enke, T. H. J. Niedermeyer
Derivatization of microcystins can increase target inhibition while reducing cellular uptake

P35 V. Talagayev, Y. Chen, N. P. Doering, L. Obendorf, K. Denzinger, K. Puls, K. Lam, S. Liu, C. A. Wolf, T. Noonan, M. Breznik, G. Wolber
OpenMMDL: Streamlined Workflow for Protein-Ligand MD Simulations

P36 S. A. Tuerschmann, L. Kloeppner, M. K. Parr
Development of a LC-MS/MS method for the quantitation of Ecdysterone and its metabolites in different biological specimens

P37 J. Wahl, A. Ahsanullah, H. Zupan, F. Gottschalk, A. Nerlich, C. Arkona, A. Hocke, B. Keller, J. Rademann
Chemically Stable Diazo Peptides as Protease Inhibitors Active in Living Cells

P38 F. E. Weber, F. A. Weinelt, C. Nyhoegen, F. Pfäfflin, A. Theloe, U. Trost, P. Kießling, W. Huisinga, S. G. Wicha, R. Michelet, S. Hennig, M. S. Stegemann, C. Kloft
Successful validation of a model-informed precision dosing instrument for meropenem in critically ill patients, the DoseCalculator, against NONMEM®

P39 C. A. Wolf, M. Bureik, G. Wolber
Dynamic pharmacophore-based screening for novel CYP4A11 inhibitors

P40 X. Zhang, J. Rademann
Fragment-based inhibitors of SARS-CoV-2 main protease via protein-templated reactions involving in-situ Strecker couplings

P41 N. Zimmermann, R. Michelet, C. Kloft
Fosfomycin and amikacin show a highly synergistic interaction against resistant Escherichia coli – a promising antibiotic combination therapy