



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 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: 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 17 α -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

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

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 Dynamics Simulations, 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. Kloepfner, 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 derivatives 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. Kloppner, 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