PROGRAM

GDCh

Gesellschaft Deutscher Chemiker

GDCh MedChem

Fachgruppe Medizinische Chemie

Frontiers in Medicinal Chemistry

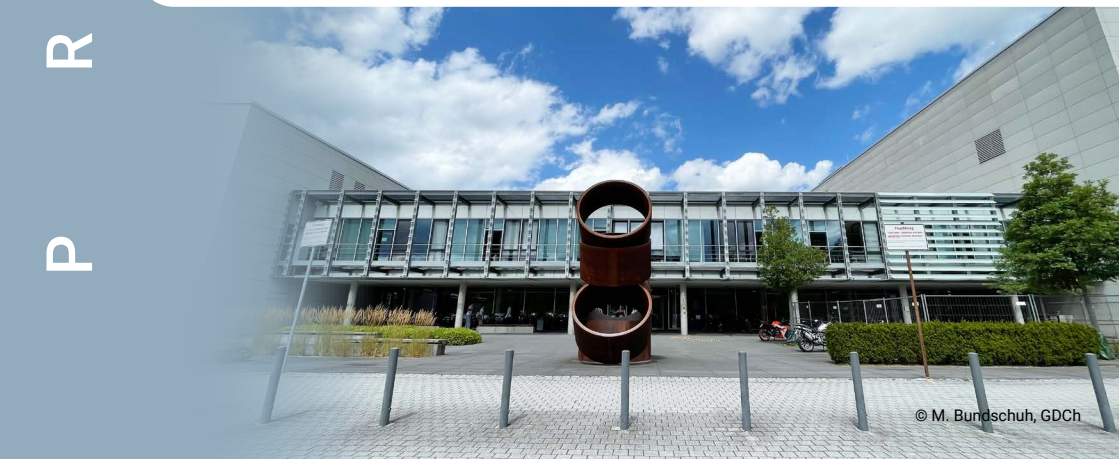
April 1 – 4, 2025 · Erlangen, Germany

FAU
Friedrich-Alexander-Universität
Erlangen-Nürnberg

DPhG
Deutsche Pharmazeutische Gesellschaft e.V.

SCS
Swiss Chemical Society
Division of Medicinal Chemistry & Chemical Biology

www.gdch.de/medchem2025



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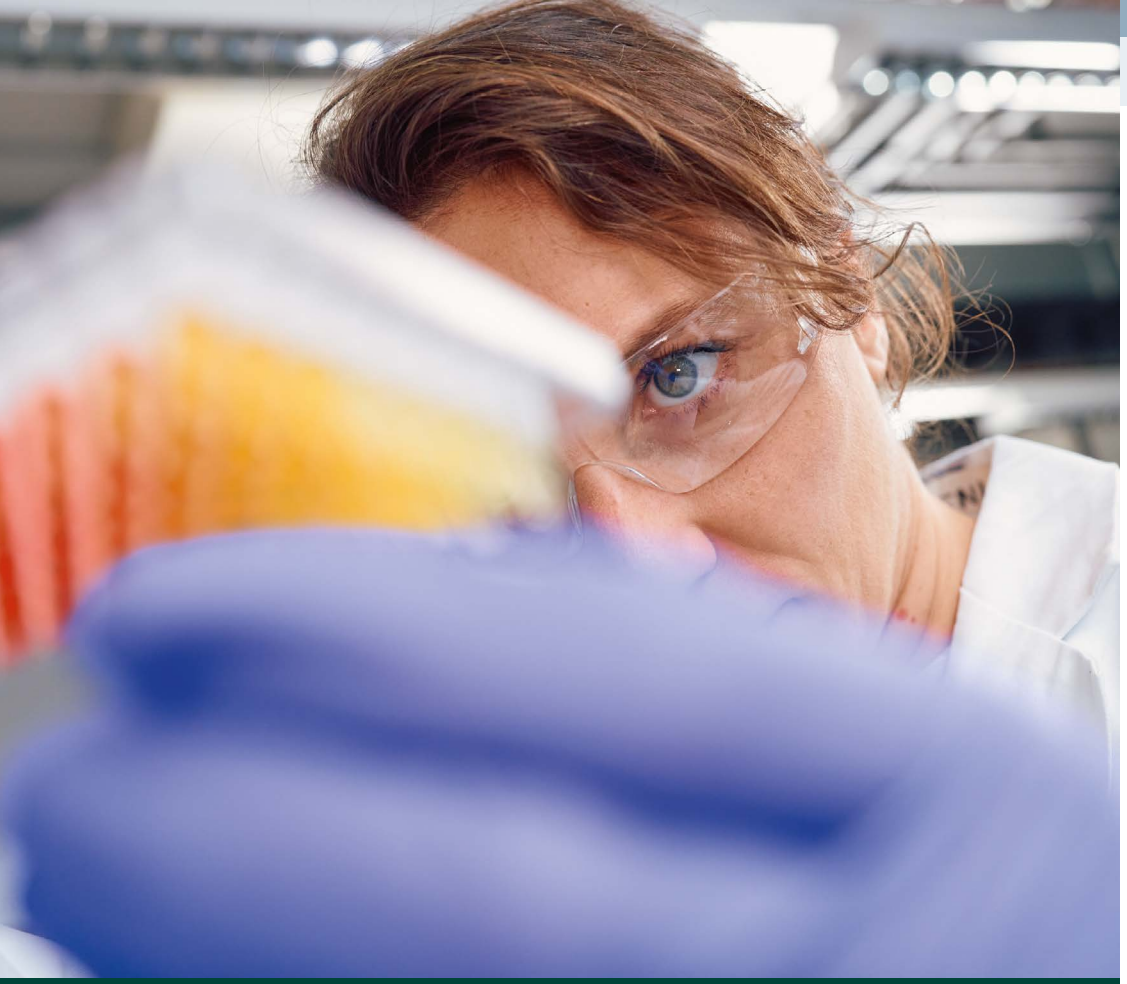

TABLE OF CONTENTS

SCIENTIFIC COMMITTEE

Y. Auberson	SCG, Basel/CH
F. Benfatti	Syngenta, Basel/CH
C. Ducho	Saarbrücken/DE
J. Eichler	Univeristy of Erlangen, Erlangen/DE
P. Gmeiner	Univeristy of Erlangen, Erlangen/DE (Chairperson)
M. Heinrich	Univeristy of Erlangen, Erlangen/DE
G. Hessler	Sanofi, Frankfurt (Main)/DE (Chairperson of the GDCh division)
S. Laufer	University of Tübingen, Tübingen/DE
M. Pinto	Abbvie, Ludwigshafen/DE
T. Ross	Merck, Darmstadt/DE
M. Schiedel	TU Braunschweig, Braunschweig/DE
B. Wünsch	University of Münster, Münster/DE

ORGANISATION COMMITTEE

C. Birkner	GDCh e.V., Frankfurt (Main)/DE
M. Bundschuh	GDCh e.V., Frankfurt (Main)/DE
H. Jäger	GDCh e.V., Frankfurt (Main)/DE
P. Gmeiner	Univeristy of Erlangen, Erlangen/DE
S. Károsi	Univeristy of Erlangen, Erlangen/DE

Tuesday, April 1, 2025

H 11

1.30 p.m. **Welcome & Opening**

H 11

Session A: Case Studies & First Disclosures

Chair: Christa Müller

1.45 p.m. **Discovery of BAY 3389934 hydrochloride, a potent and selective small molecule dual factor IIa/Xa inhibitor with short half-life for the acute treatment of sepsis-induced coagulopathy (SIC)**
H. Beck, Wuppertal/DE

2.15 p.m. **Merck's TEAD Endeavor: hit optimizations, selectivity considerations & MoA studies**
T. Heinrich, Darmstadt/DE

2.45 p.m. **BAY-9835: Discovery of the First Orally Bioavailable ADAMTS7 Inhibitor**
D. Meibom, Wuppertal/DE

3.15 p.m. COFFEE BREAK — Foyer

H 11

Session B: Theranostics

Chair: Yves Auberson

3.45 p.m. **Brain Pretargeted PET. New Horizons to Image CNS Targets with Monoclonal Antibodies**
U. M. Battisti, Copenhagen/DK

4.15 p.m. **Translational development of 68Ga-labelled siderophores for specific PET-Imaging of bacterial infections**
T. Ross, Hannover/DE

4.45 p.m. **Development of FAPI-αVβ_6-peptide conjugates as multifunctional tracers**
A. Friedel, Erlangen/DE

H 11

Young Investigators (Part I)

Chair: Yves Auberson

5.00 p.m. **First-in-Class Novel Small-Molecule ACKR3 Agonists for Modulation of Platelet Degranulation: Design, Synthesis, Biological Studies and Structure-Activity Relationship**
T. Pillaiyar, Tübingen/DE

5.15 p.m. **RNA-Binding Small Molecules: Structure-Based Hit Identification and Optimization Strategies**
C. Kersten, Mainz/DE

5.30 p.m. **FRIEDRICH STOLZ-PRIZE**
Chair: Gerhard Hessler, Bernhard Wünsch

6.15 p.m. POSTER SESSION & GET TOGETHER — Foyer

Wednesday, April 2, 2025

H 11

Session D: GPCRs and other Membrane Proteins (Part I)

Chair: Peter Gmeiner

9.00 a.m. **Structure-based Discovery of GPCR Ligands Using Artificial Intelligence**
J. Carlsson, Uppsala/SE

9.30 a.m. **A curious find in OX2R drug discovery**
P. Claes, Ghent/BE

10.00 a.m. **New insights from the inside – Novel approaches for the discovery of intracellular GPCR modulators**
M. Schiedel, Braunschweig/DE

10.30 a.m. **From hit finding to Ph1 with AZD5462, the first oral RXFP1 agonist in clinical development**
K. L. Granberg, Gothenburg/SE

11.00 a.m. COFFEE BREAK — Foyer

H 11

Session E: GPCRs and other Membrane Proteins (Part II)

Chair: Peter Kolb

11.30 a.m. **PG Protein-coupled Peptide Receptors: Structure, Function and Innovative Therapeutic Concepts**
A. Beck-Sickinger, Leipzig/DE

12.00 p.m. **Molecular basis of GPR3 signaling regulated by orthosteric and allosteric ligands**
J. Xu, Shenzhen/CN

12.30 p.m. **Functionally selective GPCR ligands**
M. Casiraghi, Milan/IT

1.00 p.m. **Focused fragment-based approach identifies subnanomolar antagonists for the MAS-related G protein-coupled receptor MRGPRX2 and its putative mouse ortholog MRGPRB2 showing efficacy in human mast cells and mouse models**
C. E. Müller, Bonn/DE

1.15 p.m. LUNCH BREAK — Foyer

H 11

1.15 p.m. **LUNCH SESSION**
“Careers in Medicinal Chemistry”
organized by NextGenMedChem and EFMC-YSN

Wednesday, April 2, 2025

H 11

Session F: Computational Technologies in Medicinal Chemistry

Chair: Daniel Merk

2.15 p.m. **Revolutionizing Cryo-EM with AI: Unveiling Atomic Structures with Precision**
A. Rak, Paris/FR

2.45 p.m. **More pockets for (allosteric) GPCR ligands**
P. Kolb, Marburg/DE

3.15 p.m. **Computational approaches empower novel avenues in target-based anti-infective drug discovery**
A. K. H. Hirsch, Saarbrücken/DE

3.45 p.m. COFFEE BREAK — Foyer

H 11

Session G: New Modalities

Chair: Jutta Eichler

4.30 p.m. **Cell-permeable cyclic peptides for addressing intracellular targets and oral delivery**
C. Heinis, Lausanne/CH

5.00 p.m. **Targeted PROTAC Delivery - Principles of crafting PROTAC-ADCs and self-assembling PROxAb shuttles**
S. Schlesiger, Darmstadt/DE

5.30 p.m. **Chemical Neuroscience in Alzheimer’s Disease: Hybrid Molecules and Photopharmacology at Enzymes and GPCRs**
M. Decker, Würzburg/DE

6.00 p.m. **Scientific Publishing – Behind the Scenes of Angewandte Chemie**
C. Gers-Panther, Wiley-VCH, Weinheim/DE

H 11

6.15 p.m. **GENERAL MEETING OF THE GDCH DIVISION ON MEDICINAL CHEMISTRY**

Tagesordnung
1. Begrüßung
2. Bericht des Vorstands
3. NextGenMedChem
4. Verschiedenes

H 11

6.35 p.m. **GENERAL MEETING OF THE DPHG DIVISION OF PHARMACEUTICAL / MEDICINAL CHEMISTRY**

Tagesordnung
1. Feststellung der Tagesordnung
2. Bericht der Vorsitzenden
3. Novellierung der Approbationsordnung AAppO
4. Zukünftige Tagungen
5. Verschiedenes

Thursday, April 3, 2025

H 11

Session H: Young Investigators (Part I/ PhD-Prize Award Ceremony)

Chair: Christian Ducho

9.00 a.m. **The insect-derived serine protease inhibitor ISPI-2 blocks influenza virus replication**
K. Hardes, Giessen/DE

9.15 a.m. **Barcode-free hit discovery from massive libraries enabled by automated small molecule structure annotation**
S. Pomplun, Leiden/NL

9.30 a.m. **Structural Basis for Lipid-mediated Activation of G Protein-coupled Receptor GPR55**
T. Claff, Biberach (Riß)/DE

9.45 a.m. **Elucidation of non-canonical GPCR binding pockets employing nanoBRET**
D. Weikert, Erlangen/DE

PhD-Prize AWARD CEREMONY

10.00 a.m. **tba**
F. Brandt, Pirna/DE

10.15 a.m. **Discovery of Small Molecule Activators of Slack Potassium Channels for the Treatment of Histamine-independent Itch**
W. F. Zhu, Münster/DE

10.30 a.m. COFFEE BREAK — Foyer

H 11

Session I: Young Investigators (Part II/ Innovation Prize)

Chair: Christian Kuttruff

11.00 a.m. **Ultralarge Tailored Library of Amino Acid Derivatives Designed to Target Peptide GPCRs**
S. Pach, Uppsala/SE

11.15 a.m. **Discovery and evolution of functionally selective serotonin 5-HT$_{1A}$ receptor agonists for the treatment of pain**
E. Neu, Erlangen/DE

11.30 a.m. INNOVATION PRIZE
Microscale Parallel Synthesis for Targeting Human Blood Coagulation Factors
D. V. Kalinin, Münster/DE

12.00 p.m. LUNCH BREAK — Foyer

Thursday, April 3, 2025

H 11

12.15 p.m. WORKSHOP (during Lunch break)
Bioisosteres in Motion: Structure-Guided Design for Lead Optimization
Dr. Beatriz Büschbell, Dr. Marcus Gastreich, BioSolveIT

H 11

Session J: Next Generation Drugs

Chairs: Marta Pinto, Matthias Schiedel

1.30 p.m. **Insurmountable antagonists for chemokine receptor CCR2 – from allosteric antagonists to PROTACs**
L. Heitman, Leiden/NL

2.00 p.m. **Discovery of NVP-DFF332 as a selective inhibitor of the transcription factor hypoxia-inducible factor-2alpha**
R. A. Fairhurst, Basel/CH

2.30 p.m. **A Covalent-First Chemoproteomic Approach to the Identification of KEAP1 Modulators**
D. Weinstein, San Diego/US

3.00 p.m. COFFEE BREAK — Foyer

H 11

Session K: Inflammation

Chair: Stefan Laufer

3.30 p.m. **Allosteric activation of lipoxygenases for promoting inflammation resolution**
O. Werz, Jena/DE

4.00 p.m. **Discovery and optimization of a new class of RIPK1 inhibitors enabled by late stage photoredox catalysis**
M. Mendez Perez, Frankfurt (Main)/DE

4.30 p.m. **Novel Macrocyclic NLRP3 inhibitors**
S. Mesch, Basel/CH

H 11

Plenary Lecture (Keynote)

Chair: Tatjana Ross

5.00 p.m. **Synthesis of Macrocyclic Natural Products and Their Functional Exploration**
K.-H. Altmann, Zurich/CH

Friday, April 4, 2025

H 11

Session L: Young Investigators (Part III)

Chair: Dorothee Weikert

9.00 a.m. **Development of clinically used HIF-1α prolyl hydroxylase inhibitors into potent and selective γ-butyrobetaine hydroxylase inhibitors**
L. Brewitz, Oxford/GB

9.15 a.m. **Medicinal Chemistry Efforts Toward the Development of Pyridine- and Dihydropteridinone-based Inhibitors for the Underexplored Human Vaccinia-Related Kinases 1 and 2**
R. A. M. Serafim, Barcelona/ES

9.30 a.m. **Assaying the protein-protein interaction sites of receptor tyrosine kinases as drug targets**
L. Temme, Hamburg/DE

9.45 a.m. **1-(2-((4-Chlorophenyl)amino)-2-oxoethyl)-N-(pyridin-3-yl)-1H-indazole-3-carboxamide ('SN-8.1') – A Synthetically Optimized Chemical Probe to Target Conserved Binding Motifs amongst Membrane Transporters**
S. M. Stefan, Lübeck/DE

H 11

Session M: Highlights in Medicinal Chemistry

Chair: Bernhard Wünsch

10.00 a.m. **Novel drug discovery strategies for neurodegenerative disorders**
M. Ishikawa, Miyagi/JP

10.30 a.m. COFFEE BREAK — Foyer

H 11

Session M: Highlights in Medicinal Chemistry

Chair: Bernhard Wünsch

11.00 a.m. **Disrupting the YAP-TEAD Protein-Protein Interaction with Small Molecules - Discovery of NVP-IAG933**
N. Soldermann, Basel/CH

11.30 a.m. **Advancing Clinical Candidate Development through Chemical Biology**
U. Grether, Basel/CH

12.00 p.m. **Probing the Protein Kinases' Cysteinome by Covalent Fragments**
M. Gehringer, Tübingen/DE

Friday, April 4, 2025

H 11

12.15 p.m. **Photoactivated chemotherapy prodrugs for skin, brain, and eye cancer treatment**
S. Bonnet, Leiden/NL

12.30 p.m. **Closing Remarks**

Wednesday April 2, 2025

H 11

1.15 p.m. to 2.15 p.m. (during lunch break)

Lunch session:
"Careers in Medicinal Chemistry"
organized by NextGenMedChem and EFMC-YSN

Thursday April 3, 2025

H 11

12.15 p.m. to 1.30 p.m.

Bioisosteres in Motion:
Structure-Guided Design for Lead Optimization
Dr. Beatriz Büschbell, Dr. Marcus Gastreich, BioSolveIT GmbH

P001 **Live-Cell Identification of Inhibitors of the Lipid Transfer Protein CERT Using Nanoluciferase Bioluminescence Resonance Energy Transfer (NanoBRET)**
C. Arenz, Berlin/DE, M. A. Kirmpaki, Berlin/DE, E. M. Saied, Berlin/DE

P002 **Design, Synthesis, and Evaluation of Novel Elastase (LasB) Inhibitors: A Promising Strategy to Combat Pseudomonas aeruginosa Virulence and Antibiotic Resistance**
A. Amin, Saarbrücken/DE, G. Jézéquel, Saarbrücken/DE, D. Kolling, Saarbrücken/DE, C. Schütz, Saarbrücken/DE, A. M. Kany, Saarbrücken/DE, J. Koehnke, Hannover/DE, J. Haupenthal, Saarbrücken/DE, A. K. H. Hirsch, Saarbrücken/DE

P003 **Generative AI for Drug Design: A Powerful Tool to Support Medicinal Chemists**
R. Cedeno, Strasbourg/FR, Y. Fischer, Strasbourg/FR, D. Triki, Strasbourg/FR, P. Schambel, Strasbourg/FR

P004 **Evaluating the Diversity and Target Addressability of DELs using Scaffold Analysis and Machine Learning**
R. Cedeno, Strasbourg/FR, Y. Fischer, Strasbourg/FR, D. Triki, Strasbourg/FR, B. Vivet, Strasbourg/FR, P. Schambel, Strasbourg/FR

P005 **Molecular Insights into the Transmembrane Proline Transporter (PROT, SLC6A7): Structure and Ligand Interaction Analysis**
D. Stary, Cracow/PL, M. Bajda, Cracow/PL

P006 **Generation of 3D Diverse DNA-Encoded Libraries**
R. G. Petersen, Copenhagen/DK, A. B. Christensen, Copenhagen/DK, A. Taranta, Copenhagen/DK, C. Andersen, Copenhagen/DK, F. A. Sløk, Copenhagen/DK, L. K. Larsen, Copenhagen/DK, L. K. Petersen, Copenhagen/DK, O. Kristensen, Copenhagen/DK, P. Blakskjær, Copenhagen/DK, T. N. Hansen, Copenhagen/DK, N. J. V. Hansen, Copenhagen/DK

P007 **Neglected Cage Compounds – Transitioning From Rare Molecules to Casual MedChem Tools**
S. Ryabukhin, Kyiv/UA, O. Pashenko, Kyiv/UA, O. Smyrnov, Kyiv/UA, A. Gaidai, Kyiv/UA, D. Volochnyuk, Kyiv/UA

P008 **Creating cocktails for ^{19}F NMR-assisted FBDD approach based on Enamine's in-stock collection**
S. Ryabukhin, Kyiv/UA, K. Melnykov, Kyiv/UA, Y. Filatov, Kyiv/UA, S. Tyukhtenko, Kyiv/UA, D. Volochnyuk, Kyiv/UA

P009 **A Leap Toward Incorporating Oxetane Core into MedChem Relevant Compounds**
D. O. Leha, Kyiv/UA, E. Litskan, Kyiv/UA, D. Granat, Kyiv/UA, S. Ryabukhin, Kyiv/UA, D. Volochnyuk, Kyiv/UA

P010 **Up-Scale Diazomethane Generation in Flow: Safe Handling and Broad Use in Organic Synthesis**
D. O. Leha, Kyiv/UA, V. Pendiukh, Kyiv/UA, O. Pashenko, Kyiv/UA, O. Rozhenko, Kyiv/UA, D. Volochnyuk, Kyiv/UA

P011 **From Photocontrol to Chromocontrol: Efficacy Switches for TRPC4/5**
M. Müller, Dresden/DE, K. Niemeyer, Leipzig/DE, N. K. Ojha, Saarbrücken/DE, S. A. Porav, Leeds/GB, D. Vinayagam, Dortmund/DE, N. Urban, Leipzig/DE, F. Büchau, Leipzig/DE, K. Oleinikov, Saarbrücken/DE, M. Makke, Saarbrücken/DE, C. C. Bauer, Leeds/GB, A. V. Johnson, Leeds/GB, S. P: Muench, Leeds/GB, F. Zufall, Saarbrücken/DE, D. Bruns, Saarbrücken/DE, Y. Schwarz, Saarbrücken/DE, S. Raunser, Dortmund/DE, T. Leinders-Zufall, Saarbrücken/DE, R. S. Bon, Leeds/GB, M. Schaefer, Leipzig/DE, O. Thorn-Seshold, Munich/DE

P012 **Synthesis and pharmacological characterization of M_5 Receptor ligands based on a Tetrahydropyridine scaffold**
S. Groß, Regensburg/DE, A. Straßer, Regensburg/DE, P. Koch, Regensburg/DE

P013 **Photochemical conversion of indazoles into benzimidazoles**
C. S. Buettner, Aachen/DE, T. dos Santos, Aachen/DE, D. Berna Yildiz, Aachen/DE, M. Mamone, Aachen/DE, A. Ruffoni, Aachen/DE, D. Leonori, Aachen/DE

P014 **Derivatization and (bio)chemical profiling of 1-TbAd – a lysosomotropic terpene nucleoside from Mycobacterium tuberculosis**
P. Wienecke, Groningen/NL, A.-L. E. Lawrence, Boston/US, R. Liu, Leiden/NL, S. L. Stellnberger, Vienna/AT, N. Gasaly, Groningen/NL, S. Render, Groningen/NL, O. Stavrinou, Groningen/NL, J. Buter, Groningen/NL, P. de Vos, Groningen/NL, V. Pichler, Vienna/AT, D. van der Es, Leiden/NL, L. H. Heitman, Leiden/NL, S. Tan, Boston/US, D. B. Moody, Boston/US, A. J. Minnaard, Groningen/NL

P015 **Development of a NanoBRET Assay Platform to Detect Intracellular Ligands for the Chemokine Receptors CCR6 and CXCR1**
M. Schiedel, Braunschweig/DE, M. E. Huber, Erlangen/DE, S. L. Wurnig, Bonn/DE, A. F. A. Moumbock, Freiburg/DE, L. Toy, Erlangen/DE, E. Kostenis, Bonn/DE, A. Alonso Bartolomé, Esch-sur-Alzette/LU, M. Szpakowska, Esch-sur-Alzette/LU, A. Chevigné, Esch-sur-Alzette/LU, S. Günther, Freiburg/DE, F. K. Hansen, Bonn/DE

P016 **Structure-Guided Development of MAD22 as a Next-Generation RXR Agonist**
M. Lewandowski, Munich/DE, M. Granger-Rivière, Munich/DE, D. Mayer, Munich/DE, J. A. Marschner, Munich/DE, D. Merk, Munich/DE

P017 **Synthon-based ultra-large Library virtual Screening meets RNA to find novel Ligands for the SAM-I Riboswitch**
L. Almena Rodriguez, Mainz/DE, E. Kallert, Mainz/DE, S. Hoba, Mainz/DE, M. Schwickert, Mainz/DE, C. Kersten, Mainz/DE

P018 **Development of TLX Agonist Chemical Tools**
E. C. Hank, Munich/DE, M. Sai, Munich/DE, T. Kasch, Munich/DE, I. Meijer, Munich/DE, J. A. Marschner, Munich/DE, D. Merk, Munich/DE

P019 **Accelerating Hit Discovery Through Combination of In Silico Screening with Semi-Automated Synthesis**
S. McKenna, Leiden/NL, M. Sicho, Prague/CZ, W. Jesper, Leiden/NL, A. Bernatavicius, Leiden/NL, E. van der Nol, Leiden/NL, C. van der Horst, Leiden/NL, L. Heitman, Leiden/NL, G. van Westen, Leiden/NL, S. Pomplun, Leiden/NL

P020 **The More the Merrier — Application of Chemical Space Docking to Hunt Novel Covalent Inhibitors**
B. Büschbell, St. Augustin/DE, M. Gastreich, St. Augustin/DE

P021 **Cholic Acid-3-Chloropiperidine Conjugates as Selective Drugs**
J. Semmler, Giessen/DE, R. Göttlich, Giessen/DE

P022 **Synthesis of 3-NBD Bile Acid Conjugates as Surrogate Molecules in Transport Studies**
C. Drossel, Giessen/DE, R. Göttlich, Giessen/DE

P023 **Optimization of the celluar uptake assay for gram-negative bacteria**
M. Nitsch, Saarbrücken/DE, S. C. Weck, Saarbrücken/DE, C. Ducho, Saarbrücken/DE

P024 **Pathoblockers as Inhibitors of Clostridoides histolyticum virulence factor ColH and Pseudomonas aeruginosa virulence factor LasB**
S. B. Dahmen, Saarbrücken/DE, K. Sprenger, Saarbrücken/DE, M. Engel, Saarbrücken/DE, C. Ducho, Saarbrücken/DE

P025 **Towards Lipophilic Prodrugs of Antisense Oligonucleotides**
A. Heib, Saarbrücken/DE, V. Böttner-Schäfer, Saarbrücken/DE, C. Ducho, Saarbrücken/DE

P026 **Small Molecule-Oligonucleotide Conjugates with Therapeutic Potential Against Breast Cancer**
F. Marschall, Saarbrücken/DE, M. Hawner, Saarbrücken/DE, C. Dahlem, Saarbrücken/DE, A. K. Kiemer, Saarbrücken/DE, G. Wenz, Saarbrücken/DE, C. Ducho, Saarbrücken/DE

P027 **Prodrugs of Muraymycin-Nucleoside-Antibiotics**
L. S. Thilmont, Saarbrücken/DE, D. Wiegmann, Saarbrücken/DE, C. Ducho, Saarbrücken/DE

P028 **Fully reversible control over DNA-intercalation with visible light**
D. E. Grantz, Groningen/NL, C. Lachance-Brais, Groningen/NL, G. Giangreco, Bologna/IT, E. J. Mattioli, Bologna/IT, M. Calvaresi, Bologna/IT, W. Szymanski, Groningen/NL, B. L. Feringa, Groningen/NL

P029 **P. aeruginosa-targeting Antibiotics with Infection-triggered Release**
J. Knigge, Saarbrücken/DE, S. Hilker, Braunschweig/DE, K. Rox, Braunschweig/DE, E. Gillon, Grenoble/FR, A. Imberty, Grenoble/FR, M. Brönstrup, Braunschweig/DE, A. Titz, Saarbrücken/DE

P030 **Structure optimization of a CLM-designed dual PPARδ/sEH modulator scaffold for designed polypharmacology**
X. Ge, Munich/DE, D. Merk, Munich/DE

P031 **Targeting the Dengue Virus 5'-Untranslated Region Stem-Loop A by Fragment-Based Drug Design**
K. Meisel, Mainz/DE, S. Sreeramulu, Frankfurt (Main)/DE, C. Richter, Frankfurt (Main)/DE, A. Baumann, Bergen/NO, V. N. Panchal, Bergen/NO, R. Brenk, Bergen/NO, H. Schwalbe, Frankfurt (Main)/DE, C. Kersten, Mainz/DE

P032 **LXR Modulators as Tools to Decipher Anti-atherosclerotic and Lipogenic Effects**
N. Bandomir, Frankfurt (Main)/DE, P. Heitel, Frankfurt (Main)/DE

P033 **Characterizing the effects of NR4A modulation in neuroinflammation in vitro**
R. Busch, Munich/DE, J. A. Marschner, Munich/DE, D. Merk, Munich/DE

P034 **Structure-based design of antibody mimetic peptides: HIV-1 antibody PG16**
S. Leukel, Erlangen/DE, L. Weißenborn, Erlangen/DE, M. Deubler, Erlangen/DE, H. Sticht, Erlangen/DE, J. Eichler, Erlangen/DE

P035 **Site-selective Fusion of Synthetic Antiviral Peptides to the Fc Protein Using Chemo-selective Ligation**
H. Lepper, Erlangen/DE, L. Weißenborn, Erlangen/DE, J. Beutel, Erlangen/DE, J. Eichler, Erlangen/DE

P036 **Peptide Inhibitors of the human Cytomegalovirus core nuclear egress Complex**
F. Braun, Erlangen/DE, S. Alkhashrom, Erlangen/DE, J. Schweininger, Erlangen/DE, J. Kicuntod, Erlangen/DE, M. Marschall, Erlangen/DE, Y. Muller, Erlangen/DE, J. Eichler, Erlangen/DE

P037 **Benzimidazole derivatives as antimalarial agents: Design, Synthesis and Structure-Activity relationship studies**
S. Eisa, Saarbrücken/DE, G. Cernicchi, Saarbrücken/DE, F. Boerman, Saarbrücken/DE, A. Lacour, Saarbrücken/DE, P. Bravo, Allschwill/CH, D. Taylor, Cape Town/ZA, S. Ghorpade, Cape Town/ZA, K. Wicht, Cape Town/ZA, M. Rottmann, Allschwill/ZA, M. Hamed, Saarbrücken/DE, A. Hirsch, Saarbrücken/DE

P038 **Development of selective RNA-targeted covalent ligands (RNA TCLs) to boost affinity and therapeutic potential**
D. Tarasek, Mainz/DE, C. Kersten, Mainz/DE

P039 **Novel peptide inhibitors of SARS-CoV-2 infection**
N. Raasch, Erlangen/DE, L. Weißenborn, Oslo/NO, E. Richel, Erlangen/DE, S. Schäfer, Erlangen/DE, H. Sticht, Erlangen/DE, K. Überla, Erlangen/DE, J. Eichler, Erlangen/DE

P040 **A Scaffold Hopping Method for Subtype-selective Liver X Receptor β Agonists**
A. Kaercher, Frankfurt (Main)/DE, F. Motel, Frankfurt (Main)/DE, E. Proschak, Frankfurt (Main)/DE, P. Heitel, Frankfurt (Main)/DE

P041 **Design and Synthesis of Novel UBA1 Inhibitors for Targeting the Ubiquitin-Proteasome System (UPS)**
M. Mroczkiewicz, Kazun Nowy/PL, D. Kozłowska, Kazun Nowy/PL, A. Gornicka, Kazun Nowy/PL, J. Hucz-Kalitowska, Kazun Nowy/PL, A. Stanczak, Kazun Nowy/PL, J. Pieczykolan, Kazun Nowy/PL, M. Wieczorek, Kazun Nowy/PL, B. Stypik, Kazun Nowy/PL, K. Szymczak, Kazun Nowy/PL, A. Moroz, Kazun Nowy/PL, A. Blocka, Kazun Nowy/PL, D. Smuga, Kazun Nowy/PL, K. Mulewski, Kazun Nowy/PL, K. Dubiel, Kazun Nowy/PL, F. Mituła, Kazun Nowy/PL, D. Popiel, Kazun Nowy/PL, A. Mikołajczyk, Kazun Nowy/PL

P042 **Elucidating the structural-activity and selectivity relationships of RNA methyltransferase inhibitors by SAM-binding-site targeting and focused chemical space exploration**
S. N. Hoba, Mainz/DE, M. Schwickert, Mainz/DE, Z. Nidoieva, Mainz/DE, L. Kammerer, Mainz/DE, M. Sabin, Mainz/DE, A. Weldert, Mainz/DE, S. Schmidt, Mainz/DE, J. L. Meidner, Mainz/DE, F. Barthels, Mainz/DE, C. Kersten, Mainz/DE, T. Schirmeister, Mainz/DE

P043 **Synthesis of Potential Pseudokinase Modulators**
T. Betzholz, Saarbrücken/DE, M. Engel, Saarbrücken/DE, C. Ducho, Saarbrücken/DE, S. Knapp, Frankfurt (Main)/DE, S. Mathea, Frankfurt (Main)/DE

P044 **[^{3}H]UR-FS094: A Nonpeptidic Radioligand for the Neuropeptide Y Y_5 Receptor**
F. Schettler, Regensburg/DE, M. Keller, Regensburg/DE

P045 **Mechanistic profiling of natural product mimetic dual Nurr1/RXR modulators**
K. Scholz, Munich/DE, D. Merk, Munich/DE

P046 **Fluorescent neurotensin NTS_1R ligands with subnanomolar binding affinity**
F. J. Ertl, Regensburg/DE, M. Keller, Regensburg/DE

P047 **Synthesis of novel α_{2A} agonists for the treatment of pain**
T. Pfeiffer, Erlangen/DE, P. Seemann, Erlangen/DE, H. Hübner, Erlangen/DE, P. Gmeiner, Erlangen/DE

P048 **Development of fluorescent Probes for novel Methyltransferase Targets**
J. Meidner, Mainz/DE, R. Zimmermann, Mainz/DE, M. Schwickert, Mainz/DE, M. Sabin, Mainz/DE, Z. Nidoieva, Mainz/DE, T. Dewald, Mainz/DE, A. Weldert, Mainz/DE, F. Barthels, Mainz/DE, T. Schirmeister, Mainz/DE

P049 **Synthesis and characterization of a ^{18}F-labelled nonpeptidic neuropeptide Y Y_1 receptor PET ligand with subnanomolar binding affinity**
M. Keller, Regensburg/DE, C. Müller, Regensburg/DE, S. Maschauer, Erlangen/DE, O. Prante, Erlangen/DE

P050 **Fragment-based discovery of dual ligand pharmacophores for lipid-sensing transcription factors for designed polypharmacology**
T. Stiller, Munich/DE, D. Merk, Munich/DE

P051 **Light-enabled scalable synthesis of bicyclo[1.1.1]pentane halides and their functionalizations**
O. Kolodiazhna, Kyiv/UA, V. Tolmachev, Kyiv/UA, I. Sadkova, Kyiv/UA, I. Pishel, Kyiv/UA, K. Horbatok, Kyiv/UA, V. Kosach, Kyiv/UA, Y. Nikandrova, Kyiv/UA, P. K. Mykhailiuk, Kyiv/UA, V. Ripenko, Kyiv/UA, V. Sham, Kyiv/UA, V. Levchenko, Kyiv/UA, S. Holovchuk, Kyiv/UA, D. Vysochyn, Kyiv/UA, I. Klymov, Kyiv/UA, D. Kyslyi, Kyiv/UA, S. Veselovych, Kyiv/UA, S. Zhersh, Kyiv/UA, Y. Dmytriv, Kyiv/UA

P052 **2-Oxabicyclo[2.2.2]octane as a new bioisostere of the phenyl ring**
V. Levterov, Kyiv/UA, D. Borysko, Kyiv/UA, K. Horbatok, Kyiv/UA, I. Bodenchuk, Kyiv/UA, Y. Bas, Kyiv/UA, D. Dudenko, Kyiv/UA, P. Mykhailiuk, Kyiv/UA, Y. Panasiuk, Kyiv/UA, K. Sahun, Kyiv/UA, O. Stashkevych, Kyiv/UA, V. Badlo, Kyiv/UA, O. Shablykin, Kyiv/UA, I. Sadkova, Kyiv/UA, L. Bortnichuk, Kyiv/UA, O. Klymenko-Ulianov, Kyiv/UA, Y. Holota, Kyiv/UA, L. Lachmann, Kyiv/UA

P053 **P2X1 Receptor Antagonists:A Promising Avenue for Thrombosis Prevention and Beyond**
J. Chudziak, Münster/DE, D. Kalinin, Münster/DE

P054 **A fluorescent probe enables the discovery of improved monovalent and membrane-anchored antagonists targeting the intracellular allosteric site of the chemokine receptor CCR7**
T. B. El-Jourani, Braunschweig/DE, S. L. Wurnig, Bonn/DE, M. E. Huber, Erlangen/DE, C. Weiler, Bonn/DE, N. Merten, Bonn/DE, P. Kolb, Marburg/DE, E. Kostenis, Bonn/DE, F. K. Hansen, Bonn/DE, M. Schiedel, Braunschweig/DE

P055 **Development of new anti-infectives targeting the pyocyanin biosynthesis enzyme PhzB in Pseudomonas aeruginosa**
M. Handke, Braunschweig/DE, M. Thiemann , Braunschweig/DE, M. Zimmermann , Braunschweig/DE, C. Kunick, Braunschweig/DE, W. Blankenfeldt , Braunschweig/DE, M. Schiedel , Braunschweig/DE

P056 **Targeting Mitochondrial Ion Channels: Synthesis and Evaluation of mitoK_{Ca}3.1 Inhibitors**
C. Kick, Münster/DE, H. Noguera Hurtado, Münster/DE, J. Massa, Münster/DE, O. Koch, Münster/DE, A. Schwab, Münster/DE, B. Wünsch, Münster/DE

P057 **Discovery and evolution of functionally selective serotonin 5-HT1A receptor agonists for the treatment of pain - structural studies**
J. Schneider, Erlangen/DE, A. Ullrich, Erlangen/DE, H. Hübner, Erlangen/DE, M. Stanek, Erlangen/DE, L. Mühlberg, Erlangen/DE, D. Pappas, Erlangen/DE, B. Böttcher, Würzburg/DE, D. Weikert, Erlangen/DE, P. Gmeiner, Erlangen/DE

P058 **Discovery and evolution of functionally selective serotonin 5-HT_{1A} receptor agonists for the treatment of pain – computational studies**
E. Neu, Erlangen/DE, J. Schneider, Erlangen/DE, N. Staffen, Erlangen/DE, J. Bláhová, Erlangen/DE, D. Pappas, Erlangen/DE, A. Ullrich, Erlangen/DE, D. Weikert, Erlangen/DE, H. Hübner, Erlangen/DE, P. Gmeiner, Erlangen/DE

P059 **Functional investigation of ST171, a novel 5-HT_{1A} receptor agonist for the treatment of pain**
J. Bláhová, Erlangen/DE, M. Stanek, Erlangen/DE, P. Seemann, Erlangen/DE, H. Hübner, Erlangen/DE, D. Weikert, Erlangen/DE, P. Gmeiner, Erlangen/DE

P060 **Enantiopure Synthesis of β1 Adrenergic Antagonists with Location Bias**
T. Braun, Erlangen/DE, T. Pröll, Erlangen/DE, H. Hübner, Erlangen/DE, P. Gmeiner, Erlangen/DE

P061 **Hit Identification and Optimization of Energy-Coupling Factor (ECF) Transporter Inhibitors to Combat Antimicrobial Resistance**
M. Hamed, Saarbrücken/DE, E. Diamanti, Saarbrücken/DE, I. A. Exapicheidou, Saarbrücken/DE, A. Tsarenko, Groningen/NL, C. Baumann, Saarbrücken/DE, A. Shams, Saarbrücken/DE, J. Haupenthal, Saarbrücken/DE, J. Herrmann, Saarbrücken/DE, R. Müller, Saarbrücken/DE, D. J. Slotboom, Groningen/NL, A. K. H. Hirsch, Saarbrücken/DE, A. K. H. Hirsch, Saarbrücken/DE

P062 **Structural and computational investigation of a sub-pocket in the M3 muscarinic acetylcholine receptor enables selective antagonist development**
N. Staffen, Erlangen/DE, B. Schaake, Erlangen/DE, X. Zhang, Beijing/CN, X. Liu, Beijing/CN, B. Kobilka, Stanford/US, P. Gmeiner, Erlangen/DE

P063 **Structural and computational investigation of a sub-pocket in the M3 muscarinic acetylcholine receptor enables selective antagonist development**
N. Staffen, Erlangen/DE, B. Schaake, Erlangen/DE, X. Zhang, Beijing/CN, X. Liu, Beijing/CN, B. Kobilka, Stanford/US, P. Gmeiner, Erlangen/DE

P064 **From Monomers to Dendrimers: Engineering Highly Branched Peptide Nanostructures for Next-Generation Drug Delivery**
T. Götze-Ebert, Leipzig/DE, C. Lamers, Leipzig/DE

P065 **Structure-guided discovery of orexin receptor-binding PET ligands**
K. Distler, Erlangen/DE, S. Maschauer, Erlangen/DE, E. Neu, Erlangen/DE, H. Hübner, Erlangen/DE, J. Einsiedel, Erlangen/DE, O. Prante, Erlangen/DE, P. Gmeiner, Erlangen/DE

P066 **Synthesis and antibacterial properties of C-glycosidic LpxC inhibitors based on D-Ribose**
J. von Rönn, Hamburg/DE, F. Wichter, Hamburg/DE, R. Holl, Hamburg/DE

P067 **Development Of Novel Neurokinin-1 Antagonists Targeting The Receptor in Endosomes**
B. Loew, Erlangen/DE, D. D. Jensen, New York/US, A. R. B. Thomsen, New York/US, B. L. Schmidt, New York/US, W. L. Imlach, Parkville/AU, N. W. Bunnett, New York/US, P. Gmeiner, Erlangen/DE, A. Hegron, New York/US, C. J. Peach, New York/US, R. Tonello, New York/US, P. Seemann, Erlangen/DE, S. Teng, New York/US, R. Latorre, New York/US, H. Huebner, Erlangen/DE, D. Weikert, Erlangen/DE, J. Rientjes, Clayton/AU, N. A. Veldhuis, Parkville/AU

P068 **Structure-Based Discovery of Novel Non-Peptide NK_1 Receptor Agonists**
S. Gleich, Erlangen/DE, H. Hübner, Erlangen/DE, J. Carlsson, Uppsala/SE, P. Gmeiner, Erlangen/DE

P069 **Comparative Analysis of Machine Learning Model Architectures for Predicting ADME Endpoints**
L. Tesmer, Frankfurt (Main)/DE, M. Baltruschat, Frankfurt (Main)/DE, C. Grebner, Frankfurt (Main)/DE, H. Matter, Frankfurt (Main)/DE, G. Hessler, Frankfurt (Main)/DE

P070 **Novel KEAP1-recruiting Ligands for PROTAC Development**
T. Muffel, Bonn/DE, S. Zhai, Bonn/DE, F. K. Hansen, Bonn/DE, I. Sosič, Ljubljana/SI, M. Gütschow, Bonn/DE, C. Steinebach, Bonn/DE

P071 **Snake Venom Protease Detection and Inhibition for Diagnosis and Therapy**
M. Riedel, Mainz/DE, C. Kersten, Mainz/DE

P073 **Conformational Control and Property Enhancement by Linker Derivatization in Macrocycles**
F. Hausch, Darmstadt/DE

P074 **Evaluation of Cu-labeled NTSR1 PET ligands for imaging of pancreatic cancer**
M. Müller, Erlangen/DE, S. Maschauer, Erlangen/DE, R. Potemkin, Erlangen/DE, G. Reischl, Tübingen/DE, P. Gmeiner, Erlangen/DE, O Prante, Erlangen/DE

P075 **Design, Synthesis, Molecular Dynamic and Quantum Chemical Parameter (DFT) Analysis of New Benzothiazole Based Derivatives: Targeting DPP-4 for Antidiabetic Activity Against Diabetes Mellitus**
V. Mathur, Delhi/IN, O. Alam, Delhi/IN

P077 **Novel Indium Phthalocyanine-Based Sono-Photosensitizers: Synthesis and Sonophotophysical Investigation for Sonophotodynamic Therapy**
S. N. Alegöz, Istanbul/TR, A. Erdoğmuş, Istanbul/TR

P078 **Ligand-bases desing of indolyl acrylamides as antibacterial agents against multidrug-resistant Acinetobacter baumannii strains.**
V. Dominguez, Ciudad de Mexico/MX, R.M. Chávez , Ciudad de Mexico/MX, K. Carrillo, Ciudad de Mexico/MX, A. Santoyo, Ciudad de Mexico/MX, S. Ramírez, Ciudad de Mexico/MX, A. Hernandez, Ciudad de Mexico/MX, C. D. Ceapa, Ciudad de Mexico/MX, J. Rivera, Ciudad de Mexico/MX, R. Martinez, Ciudad de Mexico/MX, R. Aguayo, Ciudad de Mexico/MX

P079 **Peptides as Competitive Inhibitors of EphA2-ephrin-A1 Protein-Protein Interaction**
M. Knobloch, Hamburg/DE, J. Schick, Münster/DE, M. Erdélyi, Uppsala/SE, L. Temme, Hamburg/DE

P080 **Structure-based design of bitopic and covalent ligands inducing biased signaling at the β_2-adrenoceptor**
T. Gehrig, Würzburg/DE, T. Braun, Erlangen/DE, H. Hübner, Erlangen/DE, P. Gmeiner, Erlangen/DE, C. Sotriffer, Würzburg/DE

P081 **Computational development of PET radioligands for imaging of mutant isocitrate dehydrogenase in brain tumours**
M. Diwaker, Leipzig/DE, R. P. Moldovan, Leipzig/DE, W. Deuther-Conrad, Leipzig/DE, B. Wenzel, Leipzig/DE, A. Maurer, Leipzig/DE

P082 **The FAU Expired Drug Initiative (FAU EDI) – recovery of APIs and scientific applications**
L. Lochschmidt, Erlangen/DE, M. Kuschow, Erlangen/DE, L. Drees, Erlangen/DE, L. Zähnle, Erlangen/DE, F. Lenart, Erlangen/DE, A. Roggenhofer, Erlangen/DE, M. R. Heinrich, Erlangen/DE

P083 **Development of novel bitopic ligands to study adenosine A_1 receptors**
M. Flaßhoff, Bern/CH, T. Sarvanathan, Bern/CH, A. Pearce, Cambridge/GB, G. Ladds, Cambridge/GB, M. Lochner, Bern/CH

P084 **Targeting the MYC interacting protein RuvBL1/2 by virtual screening for ATP-competitive inhibitors**
R. Würz, Würzburg/DE, M. Diebold, Würzburg/DE, K. Schneider, Kiel/DE, E. Wolf, Kiel/DE, C. Sotriffer, Würzburg/DE

P085 **Fragment-Based Design of Cofactor-Specific Inhibitors of p97**
R. Toshe, Würzburg/DE, S. Böhler, Würzburg/DE, S. Kolle, Würzburg/DE, N. Nilparuk, Würzburg/DE, S. Bothe, Würzburg/DE, H. Schindelin, Würzburg/DE, C. Sotriffer, Würzburg/DE

P086 **Fluorogenic Chemical Probes for Wash-free Imaging of Cell Membrane Damage in Ferroptosis, Necrosis, and Axon Injury**
P. Mauker, Munich/DE, D. Beckmann, Munich/DE, A. Davidson, Glasgow/GB, T. Misgeld, Munich/DE, M. Kerschensteiner, Munich/DE, O. Thorn-Seshold, Dresden/DE

P087 **4-Trifluoromethoxy Proline: Synthesis of Stereoisomers and Lipophilicity Study**
I. Kondratov, Frankfurt (Main)/DE, I. Logvinenko, Kyiv/UA

P088 **Breaking the Code: DNAzyme-Mediated Cleavage of HIV-1 Gag RNA**
T. Hoang Duc, Erlangen/DE, I. Span, Erlangen/DE, M. Hebeis, Erlangen/DE, N. Kirchgässler, Düsseldorf/DE

P089 **Investigation of Male Fertility: Photoactivatable Tool Compounds for CatSper Modulation with Spatiotemporal Control**
W. F. Zhu, Münster/DE, T. Schierling, Münster/DE, A. Schulte, Groningen/NL, J. Münchow, Groningen/NL, C. Brenker, Münster/DE, W. Szymanski, Groningen/NL, T. Strünker, Münster/DE, B. Wünsch, Münster/DE

P090 **Development of New Anticoagulants Targeting Thrombin and Blood Coagulation Factor XIIa**
D. V. Kalinin, Münster/DE, L. Imberg, Münster/DE, A. I. Siutkina, Münster/DE, C. Erbacher, Münster/DE, C. Daniliuc, Münster/DE, U. Karst, Münster/DE

P091 **Correlating Structure-Activity Relationship analysis with BRET assays in living cells to design dualsteric ligands as pharmacological tools to study mAChR1**
C.A. Lombo, Würzburg/DE, J.C. Filor, Jena/DE, C. Große, Jena/DE, C. Hoffmann, Jena/DE, U. Holzgrabe, Würzburg/DE

A		
Adams, Christopher M. Dr.	Novartis Pharma AG	US-02139 Cambridge, MA
Arifi, Silvia Dr.		DE-60326 Frankfurt (Main)
B		
Bajorath, Jürgen Prof. Dr.	University of Bonn	DE-53115 Bonn
Balabon, Olga Dr.	Life Chemicals Europe GmbH	DE-82008 Unterhaching
Baltrukevich, Hanna	University of Marburg	DE-35037 Marburg
Bandomir, Nils Christiaan	University of Frankfurt	DE-60438 Frankfurt (Main)
Barbie, Philipp Dr.	Bayer AG	DE-13353 Berlin
Barna, Bence	Mcule	HU-1115 Budapest
Batsios, Petros Dr.	Merck KGaA	DE-82024 Taufkirchen
Bayrak, Alp	University of Tübingen	DE-72076 Tübingen
Bednarski, Patrick Prof. Dr.	University of Greifswald	DE-17489 Greifswald
Beena Sathian, Manjima	University of Munich	DE-81377 Munich
Beitz, Eric Prof. Dr.	Universität zu Kiel	DE-24118 Kiel
Bermudez, Marcel Prof. Dr.		DE-48149 Münster
Bodnarchuk, Michael Dr.	AstraZeneca	GB-CB2 0AA Cambridge
Boeckler, Frank Prof. Dr.	University of Tübingen	DE-72076 Tübingen
Bossert, Michael	Enamine Ltd.	UA-02094 Kyiv
Bracher, Franz Prof. Dr.	University of Munich	DE-81377 Munich
Braun, Josef	Technical University of Munich	DE-81371 München
Breu, Ferdinand		DE-81377 Munich
Brewitz, Lennart Dr.		GB-OX13TA Oxford
Brunschweiger, Andreas Prof. Dr.		DE-97074 Würzburg
Brunsveld, Luc Prof. Dr.	Technical University Eindhoven	NL-5600 MB Eindhoven
Busch, Romy	University of Munich	DE-81377 Munich
Büschbell, Beatriz Dr.	BioSolveIT	DE-53757 Sankt Augustin
C		
Carbain, Benoit Dr.	SpiroChem AG	CH-4058 Basel
Cedeno, Ruel Dr.	Novalix	FR-67000 Strasbourg
Christ, Clara Dr.	Bayer AG	DE-13342 Berlin
Cid Echevarria, Irene		DE-81377 Munich
Cirillo, Davide Dr.		DE-101789 Berlin
D		
Dayrem, Rémy	nevoLAB GmbH	DE-88167 Maierhöfen
Diederich, Wibke Prof. Dr.	University of Marburg	DE-35043 Marburg
Dimitrov, Teodor Dr.	Beiersdorf AG	DE-20245 Hamburg
Dömling, Alexander Prof. Dr.	Palacký University in Olomouc	CZ-77900 Olomouc
Dreizler, Johannes	Technical University Darmstadt	DE-64287 Darmstadt
Ducho, Christian Prof. Dr.	Saarland University	DE-66123 Saarbrücken
E		
Edwards, Aled Prof. Dr.	University of Toronto	CA-ON M5G 1L7 Toronto
Egner, Markus	University of Munich	DE-81377 Munich
Eichler, Jutta Prof. Dr.	Universität Erlangen-Nürnberg	DE-91058 Erlangen
Einerhand, Judith		DE-48149 Münster
Elgaher, Walid A. M. Dr.	Helmholtz Institute for Pharmaceutical Research Saarland	DE-66123 Saarbrücken
Ertl, Fabian	University of Regensburg	DE-93053 Regensburg
F		
Felber, Jan Dr.		DE-80337 Munich

Fleck, Martin Dr.	Proteros	DE-82152 Martinsried
Flohr, Stefanie Dr.	Novartis Pharma AG	CH-4001 Basel
Flury, Philipp	Universität of Tübingen	DE-72076 Tübingen
Foley, Anne Dr.	UCB	GB-SL1 3WE Slough
Freund, Robert Dr.	Nuvisan ICB GmbH	DE-13353 Berlin
Fürst, Rebekka		DE-72076 Tübingen
G		
Ge, Xiu	University of Munich	DE-81377 Munich
Gege, Christian Dr.	Immunic AG	DE-82166 Gräfelfing
Gehringer, Matthias Prof. Dr.	University of Tübingen	DE-72076 Tübingen
Gleixner, Jakob		DE-92648 Vohenstrauss
Goetzfried, Sina Katharina Dr.	Leiden Institute of Chemistry	NL-2333 CC Leiden
Groß, Ulrike Dr.	Boehringer Ingelheim Pharma GmbH & Co. KG	DE-88397 Biberach (Riss)
Gulder, Tanja Prof. Dr.	University of Leipzig	DE-04103 Leipzig
H		
Hagel, Marcel Dr.	ChemPUR Feinchemikalien und Forschungsbedarf GmbH	DE-76137 Karlsruhe
Hahne, Hannes Dr.	OmicScouts GmbH	DE-85354 Freising
Hall, Jonathan Prof. Dr.	ETH Zürich	CH-8093 Zürich
Hank, Emily	University of Munich	DE-81377 Munich
Happ, Bobby Dr.		DE-63128 Dietzenbach
Harvey, Freya Dr.		CH-1595 Faoug
Hausch, Felix Prof.	Technical University Darmstadt	DE-64287 Darmstadt
He, Guoli Dr.	AbbVie Deutschland	DE-67061 Ludwigshafen
Heimhalt, Maren Dr.	Ludwig-Maximilians-Universität	DE-82152 Planegg
Heinrich, Markus Prof. Dr.	University Erlangen-Nürnberg	DE-91058 Erlangen
Heitel, Pascal Dr.	University of Frankfurt	DE-60438 Frankfurt (Main)
Hentsch, Axel	FMP Berlin	DE-13125 Berlin
Hernandez Olmos, Victor Dr.	Fraunhofer ITMP	DE-60438 Frankfurt (Main)
Hessler, Gerhard Dr.	Sanofi-Aventis Deutschland GmbH	DE-65926 Frankfurt (Main)
Heuer, Hubert Dr.		DE-55270 Schwabenheim
Hickey, Eugene Dr.	Schrödinger	US-10036 New York
Hiesinger, Kerstin Dr.		DE-60438 Frankfurt (Main)
Hirsch, Anna K. H. Prof. Dr.	HIPS Saarbrücken	DE-66123 Saarbrücken
Höfner, Georg Dr.	University of Munich	DE-81377 Munich
Holl, Ralph Prof. Dr.		DE-20146 Hamburg
Hollweck, Miriam		DE-81377 Munich
Holota, Yuliia Dr.	Enamine Ltd.	UA-02094 Kyiv
Hörmann, Tim Ingmar	University of Munich	DE-81377 Munich
Hubach, Dominik		DE-35043 Marburg
Huc, Ivan Prof. Dr.	University of Munich	DE-81377 Munich
I		
Isigkeit, Laura	University of Frankfurt	DE-60438 Frankfurt (Main)
J		
Jagtap, Anil Dr.	Tubulis Gmbh	DE-82152 Munich
Janssen, Philipp	University of Münster	DE-48149 Münster
K		
Kachkovskyi, Georgiy Dr.	Selvita S. A.	PL-30-394 Krakow
Kaercher, Annette	University of Frankfurt	DE-60438 Frankfurt (Main)
Kalinin, Dmitrii Dr.	University of Münster	DE-48149 Münster

Kampschulze, Jan	Universität Münster	DE-48143 Münster
Kapeliukha, Anna	Chemspace	UA-02094 Kyiv
Karges, Johannes Dr.		DE-44780 Bochum
Kasch, Till	University of Munich	DE-81377 Munich
Keydel, Tobias		DE-17489 Greifswald
Khan, Ashiq Dr.	Schrödinger	DE-80538 München
Knuemann, Loris	University of Munich	DE-81377 Munich
Koch, Pierre Prof. Dr.	University of Regensburg	DE-93053 Regensburg
Koch, Jeannette		DE-69120 Heidelberg
Koch, Oliver Prof. Dr.	University of Münster	DE-48149 Münster
Köllen, Martin	Technical University of Munich	DE-85774 Unterföhring
Kolodiazhna, Olha Dr.	Enamine Ltd.	UA-02094 Kyiv
Kondratov, Ivan Dr.	Enamine Germany GmbH	DE-65926 Frankfurt (Main)
Konrad, David Dr.	University of Munich	DE-81377 Munich
Köstler, Roland Dr.	Origenis GmbH	DE-82152 Planegg
Kottrayil, Jafarkhan		US-CA 92618 Irvine
Kumar, Anupriya Dr.	OpenEye Scientific Software, Cadence Molecular Sciences	DE-50668 Cologne
Kuttruff, Christian Dr.	Boehringer Ingelheim Pharma GmbH & Co. KG	DE-78166 Donaueschingen
L		
Lacour, Antoine	Helmholtz Institute for Pharmaceutical Research	DE-66123 Saarbrücken
Lamers, Christina Prof. Dr.	University of Leipzig	DE-04103 Leipzig
Lang, Alisa	University of Frankfurt	DE-60438 Frankfurt (Main)
Langer, Thierry Prof. Dr.	University of Vienna	AT-1090 Wien
Laube, Lennart		DE-35043 Marburg
Laufer, Stefan Prof. Dr.	University of Tübingen	DE-72076 Tübingen
Lemke, Jana	Universität Greifswald	DE-17489 Greifswald
Lewandowski, Max	University of Munich	DE-81377 Munich
Liang, Xiaojun Julia	University of Tübingen	DE-72076 Tübingen
Lin, Hengbo	Univeristy of Münster	DE-48149 Münster
Link, Andreas Prof. Dr.	University of Greifswald	DE-17489 Greifswald
Loos, Manuel	University of Munich	DE-81377 Munich
López García, Úrsula	University of Munich	DE-81377 Munich
Lorenz, Manfred	nevoLAB GmbH	DE-88167 Maierhöfen
Lützel, Kyra		DE-81377 Munich
M		
Mach, Leonard	FMP Berlin	DE-13125 Berlin
Maier, Martin Dr.	AbbVie Deutschland GmbH & Co. KG	DE-67061 Ludwigshafen
Manolikakes, Georg Prof. Dr.	RPTU Kaiserslautern-Landau	DE-67663 Kaiserslautern
Marschner, Julian Dr.	University of Munich	DE-81377 Munich
Mauker, Philipp	University of Munich	DE-81377 Munich
Mercier, Joel Dr.	UCB SA	BE-1420 Braine l'Alleud
Merk, Daniel Prof. Dr.	University of Munich	DE-81377 Munich
Messinger, Josef	Orion Corporation Orion Pharma	FI-02100 Espoo
Meyer, Stephanie Dr.	Deutsches Krebsforschungszentrum	DE-69120 Heidelberg
Miah, Afjal Dr.	GSK	GB-SG12NY Stevenage
Michel, Maurice Dr.		SE-17165 Solna
Miller, Aubry Dr.	German Cancer Research Center	DE-69120 Heidelberg
Milton, Anna	University of Munich	DE-81377 Munich

Molitor, Maximilian	University of Frankfurt	DE-60438 Frankfurt (Main)
Mulder, Monique Dr.	Leiden University Medical Center	NL-2333 Leiden
Müller, Christa Prof. Dr.	University of Bonn	DE-53121 Bonn
Müller, Markus		DE-80469 Munich
N		
Naiken, Naomie	NovAliX	FR-67000 Strasbourg
Narine, Arun Dr.	Nuvisan ICB GmbH	DE-13353 Berlin
Nawa, Felix	University of Munich	DE-81377 Munich
Nerlich, Cornelius		DE-24118 Kiel
Neu, Eduard		DE-91058 Erlangen
Neumann, Alexander Dr.	BioSolveIT	DE-53757 Sankt Augustin
Nißl, Benedikt		DE-81377 Munich
Nomura, Dan Prof. Dr.	University of California, Berkeley	US-CA 94710 Berkeley
Nuber, Constantin	University of Munich	DE-81377 Munich
O		
Obeser, Lennart	University of Munich	DE-81377 Munich
Ortis, Florian	ISTA - Institute of Science and Technology Austria	AT-3400 Klosterneuburg
P		
Pabel, Jörg Dr.	University of Munich	DE-81377 Munich
Paessens, Lutz Christian Dr.	Novalix	FR-67080 Strasbourg
Paintner, Franz Prof. Dr.	University of Munich	DE-81377 Munich
Pape, Felix Dr.	Nuvisan Innovation Campus Berlin	DE-13353 Berlin
Peralta, David Dr.	Chemistry Europe / Wiley-VCH	DE-69469 Weinheim
Petry, Stefan Matthias Dr.	Sanofi-Aventis Deutschalnd GmbH	DE-65926 Frankfurt (Main)
Peukert, Carsten Dr.		US-CA 94109 San Francisco
Pfeiffer, Tara		DE-91058 Erlangen
Pillaiyar, Thanigaimalai Dr.	University of Tübingen	DE-72076 Tübingen
Pinto, Marta	AbbVie Deutschland GmbH & Co. KG	DE-67061 Ludwigshafen
Plesniak, Mateusz Dr.	AstraZeneca	SE-431 83 Mölndal
Pockes, Steffen Dr.	University of Regensburg	DE-93053 Regensburg
Prikler, Greg	Mcule	HU-1115 Budapest
Prömmer, Anna	Life Chemicals Europe GmbH	DE-82008 Unterhaching
Proschak, Eugen Prof. Dr.	University of Frankfurt	DE-60438 Frankfurt (Main)
Q		
Quambusch, Lena Dr.	University of Cambridge	GB-CB2 1GA Cambridge
R		
Rebmann, Heiko Dr.		DE-69121 Heidelberg
Reynders, Martin Dr.	University of Munich	DE-81377 Munich
Richert, Nick		DE-69120 Heidelberg
Richter, Adrian Dr.	Universität Halle-Wittenberg	DE-06120 Halle (Saale)
Ritter, Kurt Dr.		DE-60594 Frankfurt (Main)
Rivière, Cyrille	University of Munich	DE-81377 Munich
Ross, Tatjana Dr.	Merck Healthcare KGaA	DE-64293 Darmstadt
Rühl, Philipp		DE-81377 Munich
Rupiani, Sebastiano Dr.	Merck KGaA	DE-64293 Darmstadt
S		
Sai, Minh	University of Munich	DE-81377 Munich
Sander, Thomas Dr.	Alipheron AG	CH-4143 Dornach

Scarano, Naomi	University of Genoa	IT-13048 Vercelli
Schadt, Oliver Dr.	Merck Healthcare KGaA	DE-64293 Darmstadt
Schiedel, Matthias Prof. Dr.	Technical University Braunschweig	DE-38106 Braunschweig
Schiesser, Stefan Dr.	AstraZeneca	SE-43183 Mölndal
Schindler, Christina Dr.	Merck KGaA	DE-64293 Darmstadt
Schinzer, Dieter Prof. Dr.	Universität Magdeburg	DE-39106 Magdeburg
Schmitt, Carina		DE-81377 Munich
Schneider, Gisbert Prof. Dr.	ETH Zürich	CH-8093 Zürich
Scholz, Katharina	University of Munich	DE-81377 Munich
Schützenmeister, Nina Prof. Dr.	University of Vienna	AT-1090 Vienna
Schwarz, Markus		DE-80539 Munich
Seidl, Leonardo		DE-80799 Munich
Sikora, Katarzyna	Selvita S. A.	PL-30-394 Krakow
Siutkina, Alena	University of Münster	DE-48149 Münster
Spiske, Moritz	Technical University Darmstadt	DE-64287 Darmstadt
Staffen, Nico		DE-91058 Erlangen
Stahl, Gunther Dr.	OpenEye, Cadence Molecular Sciences	DE-50668 Cologne
Stark, Holger Prof. Dr.	University of Düsseldorf	DE-40225 Düsseldorf
Stefan, Sven Marcel Dr.	University of Lübeck	DE-23538 Lübeck
Steimbach, Raphael Dr.	Servier	FR-91190 Gif sur Yvette
Steinbrunn, Dominik	OmicScouts GmbH	DE-85354 Freising
Stieber, Frank Dr.	Merck Electronics KGaA	DE-64293 Darmstadt
Stiller, Tanja	University of Munich	DE-81377 Munich
Strapak, Olena	Chemspace	UA-02094 Kyiv
Stypka, Ewa	Concept Life Sciences	GB-SK23 0PG Chapel-en-le-frith
T		
Tate, Ed Prof.	Imperial College London	GB-SW7 2AZ London
Tiedjens, Finn		DE-24118 Kiel
Toy, Lara		DE-91058 Erlangen
V		
van Herwijnen, Niels	University of Munich	DE-80687 Munich
Vietor, Jan	University of Munich	DE-81377 Munich
von Korff, Modest Dr.	Alipheron AG	CH-4143 Dornach
Von Nussbaum, Franz Dr.	Nuvisan ICB GmbH	DE-13353 Berlin
W		
Walz, Carlo	Technical University Darmstadt	DE-64287 Darmstadt
Wang, Lingfei	University of Munich	DE-81377 Munich
Wanner, Klaus Prof. Dr.		DE-81377 Munich
Wehner, Volkmar Dr.	Sanofi-Aventis Deutschland GmbH	DE-65926 Frankfurt (Main)
Wein, Thomas Dr.	University of Munich	DE-81377 Munich
Wilhelmi, Erik		DE-35039 Marburg
Wilkes, Robin Dr.	SYNthesis med chem	GB-Cheshire SK10 4TG
Wimmer, Stefan		DE-20146 Hamburg
Wippich, Julian Dr.	Boehringer Ingelheim Pharma GmbH & Co. KG	DE-88397 Biberach (Riss)
Wollenhaupt, Jan Dr.	Proteros Biostructures GmbH	DE-82152 Planegg
Wu, Jiaojiao	University of Munich	DE-81375 Munich
Z		
Zahran, Hala	University of Munich	DE-81377 Munich

Zaręba, Przemysław Dr.	Politechnika Krakowska im.Tadeusza Kościuszki	PL-31-155 Cracow
Zeidan, Nicolas Dr.	F. Hoffmann-La Roche AG	CH-4070 Basel
Zeisel, Lukas	University of Munich	DE-81373 Munich
Zenger, Can		DE-81377 Munich
Zhao, Hongtao Dr.	AstraZeneca	SE-43183 Mölndal

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