



GESELLSCHAFT DEUTSCHER CHEMIKER



Fachgruppe Medizinische Chemie

Frontiers in Medicinal Chemistry

March 17 – 20, 2024 · Munich, Germany



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COMMITTEES	5
SCIENTIFIC PROGRAM	7
Sunday, March 17, 2024	7
Monday, March 18, 2024	8
Tuesday, March 19, 2024	10
Wednesday, March 20, 2024	13
Workshops	15
LIST OF POSTERS	17
LIST OF PARTICIPANTS	26
ACKNOWLEDGEMENT	32



Bist du bereit, eine treibende Innovationskraft in der Medizinwelt zu werden?

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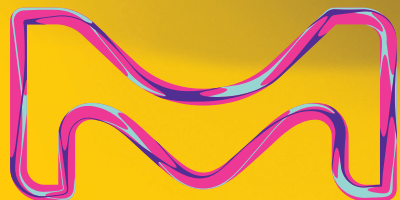


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F. Bracher	LMU, Munich/DE
C. Ducho	University of Saarbrücken, Saarbrücken/DE
G. Hessler	Sanofi, Frankfurt (Main)/DE (Chairman of the GDCh division)
A. K. H. Hirsch	University of Saarbrücken, Saarbrücken/DE
A. Hoffmann-Röder	LMU, Munich/DE
I. Huc	LMU, Munich/DE
C. Kuttruff	Boehringer-Ingelheim, Biberach/DE
S. Laufer	University of Tübingen, Tübingen/DE
C. Lamers	University of Leipzig, Leipzig/DE
M. Mendez Perez	Sanofi, Frankfurt/DE
D. Merk	LMU, Munich/DE
O. Merkel	LMU, Munich/DE
T. Ross	Merck, Darmstadt/DE
F. Paintner	LMU, Munich/DE
H. Stark	University of Düsseldorf, Düsseldorf/DE
O. Thorn-Seshold	LMU, Munich/DE
O. Trapp	LMU, Munich/DE
B. Wunsch	University of Münster, Münster/DE

► **ORGANISATION COMMITTEE**

C. Birkner	GDCh e.V., Frankfurt (Main)/DE
M. Bundschuh	GDCh e.V., Frankfurt (Main)/DE
D. Merk	LMU, Munich/DE

SCIENTIFIC PROGRAM

Sunday, March 17, 2024

Lecture Hall C1

4.45 p.m.

Welcome & Opening

Chair: D. Merk

Prof. Dr. Daniel Merk (Chairman), Dr. Gerhard Hessler (Chair of the Division)

5.00 p.m.

KEYNOTE LECTURE

De Novo Molecular Design with Machine Intelligence

G. Schneider, Zurich/CH

Foyer

6.00 p.m.

Welcome Reception & Poster Session 1

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Monday, March 18, 2024

Buchner Lecture Hall

New & Bifunctional Drug Modalities

Chair: H. Stark

- 9.00 a.m. **Reimagining Druggability using Chemoproteomic Approaches**
D. Nomura, Berkeley/US
- 9.30 a.m. **Medicinal Chemistry of MAS-related G Protein-coupled Receptors MRGPRX**
C. E. Müller, Bonn/DE
- 10.00 a.m. **Rapid PROTAC discovery platform: nanomole scale array synthesis and direct screening of reaction mixtures**
M. Plesniak, Mölndal/SE
- 10.15 a.m. **Discovery of a Potent PROTAC Enables Targeting of FKBP51's Scaffolding Functions**
F. Hausch, Darmstadt/DE, M. Walz, Darmstadt/DE, C. Meyners, Darmstadt/DE, T. M. Geiger, Darmstadt/DE
- 10.30 a.m. COFFEE BREAK

Buchner Lecture Hall

Case Studies & First Disclosures

Chair: G. Hessler

- 11.00 a.m. **From novel antimalarials to next generation Antibody-Drug Conjugate payloads**
E. W. Tate, London/GB
- 11.30 a.m. **Using PET imaging to enable neuroscience drug development.**
J. Mercier, Braine l'Alleud/BE
- 12.00 p.m. **Discovery and development of a first in class MKK-4 inhibitors to increase Liver Regeneration Tübingen Center for Academic Drug Discovery TüCAD₂**
S. Laufer, Tübingen/DE, L. Zender, Tübingen/DE

12.30 p.m. LUNCH BREAK & POSTER

Buchner Lecture Hall

Deep Learning in Drug Design

Chair: D. Merk

- 1.30 p.m. **Language Models for Molecular Design**
J. Bajorath, Bonn/DE
- 2.00 p.m. **Deep Learning in predictive modeling and generative design at Merck KGaA**
C. Schindler, Darmstadt/DE

Monday, March 18, 2024

- 2.30 p.m. **Next Generation Pharmacophore Modeling: Tools and Applications for Compound Design and Toxicity Risk Assessment**
T. Langer, Vienna/AT, T. Seidel, Vienna/AT, O. Wieder, Vienna/AT

- 2.50 p.m. **QM/AI-Approaches for Halogen Bonding**
F. M. Boeckler, Tübingen/DE, M. U. Engelhardt, Tübingen/DE, F. Mier, Tübingen/DE, M. O. Zimmermann, Tübingen/DE

3.10 p.m. COFFEE BREAK

Buchner Lecture Hall

Neglected Diseases & Orphan Targets

Chair: A. K. H. Hirsch

- 3.40 p.m. **Fragment-based drug discovery and beyond for molecular glue identification**
L. Brunsveld, Eindhoven/NL
- 4.10 p.m. **Decoding the messaging of the ubiquitin system**
M. Mulder, Leiden/NL
- 4.40 p.m. **Development of BRET-based assays and hit-to-lead optimization for the orphan GPR3 receptor in neurodegenerative diseases**
S. Pockes, Regensburg/DE

Foyer

5.00 p.m. Poster Session 2

Buchner Lecture Hall

5.00 p.m. General Meeting of the GDCh Division on Medicinal Chemistry

Tagesordnung

1. Begrüßung – Protokoll der Mitgliederversammlung vom 3. April 2023 – Tagesordnung
2. Bericht des Vorstands
3. NextGenMedChem
4. Was wünscht sich die Mitgliedschaft?
5. Verschiedenes

Buchner Lecture Hall

5.30 p.m. General Meeting of the DPhG Division of Pharmaceutical/Medicinal Chemistry

Tagesordnung

1. Feststellung der Tagesordnung
2. Bericht der Vorsitzenden
3. Zukünftige Tagungen
4. Verschiedenes

Tuesday, March 19, 2024

Buchner Lecture Hall

Young Investigators

Chair: S. Laufer/B. Wunsch

- 9.00 a.m. **Organocatalysis meets enzyme catalysis – artificial enzyme function for the treatment of disease**
M. Michel, Stockholm/SE
- 9.12 a.m. **Unlocking the Potential of Late-Stage Functionalization for Medicinal Chemistry by Integrating High-Throughput Experimentation with Geometric Deep Learning**
D. B. Konrad, München/DE, U. Grether, Basel/CH, R. Martin, Basel/CH, G. Schneider, Zürich/CH
- 9.24 a.m. **Unravelling Retinoid X Receptor mediated biology with chemogenomics in vitro**
J. A. Marschner, Munich/DE, R. Busch, Munich/DE, D. Merk, Munich/DE
- 9.36 a.m. **Synthesis and characterisation of RNA polymerase inhibitors against Mycobacterium abscessus and other mycobacteria**
A. Richter, Halle (Saale)/DE
- 9.48 a.m. **Design, Synthesis, and Biological Activity of New Inhibitors Targeting Human Blood Coagulation Factor XIIa**
D. Kalinin, Münster/DE, L. Imberg, Münster/DE, S. Platte, Münster/DE, A. Siutkina, Münster/DE, U. Karst, Münster/DE, C. Erbacher, Münster/DE, C. Dunker, Münster/DE
- 10.00 a.m. **Structure-based Design of PROTACS for the Degradation of Soluble Epoxide Hydrolase**
K. Hiesinger, Frankfurt (Main)/DE, B. S. Brunst, Frankfurt (Main)/DE, J. S. Schoenfeld, Frankfurt (Main)/DE, M. DeMeglio, Frankfurt (Main)/DE, A. Kumar, Frankfurt (Main)/DE, J. H. M. Ehrler, Frankfurt (Main)/DE, L. Weizel, Frankfurt (Main)/DE, M. Schubert-Zsilavec, Frankfurt (Main)/DE, S. Knapp, Frankfurt (Main)/DE, J. Hefendehl, Frankfurt (Main)/DE, E. Proschak, Frankfurt (Main)/DE
- 10.12 a.m. **Structure-Based Discovery of Small Molecule Inhibitors of the Immune Responsive Gene 1 (IRG1)**
W. A. M. Elgaher, Saarbrücken/DE
- 10.24 a.m. **Target Repurposing Unravels Avermectin Derivatives as Antibiotics Inhibiting the Energy-coupling Factor Transporters (ECFTs)**
S. M. Stefan, Lübeck/DE, J. Hauptenthal, Saarbrücken/DE, A. Lespine, Toulouse/FR, M. Rafehi, Augsburg/DE, K. Stefan, Lübeck/DE, A. K. H. Hirsch, Saarbrücken/DE

Tuesday, March 19, 2024

- 10.36 a.m. **Total Synthesis of Natural Products – A Tool for Drug Discovery**
N. Schützenmeister, Vienna/AT
- 10.48 a.m. **Screening of *Chelidonium Majus* Isoquinoline Alkaloids Reveals Berberine and Chelidonine as Selective Ligands for the Nuclear Receptors ROR β and HNF4 α , Respectively**
P. Heitel, Frankfurt (Main)/DE, S. Salehi, Frankfurt (Main)/DE, E. Schallmayer, Frankfurt (Main)/DE, A. Kaercher, Frankfurt (Main)/DE, N. Bandomir, Frankfurt (Main)/DE, J.-F. Gueth, Frankfurt (Main)/DE
- 11.00 a.m. COFFEE BREAK

Buchner Lecture Hall

Next Generation Drugs (NextGenMedChem session)

Chair: C. Lamers/P. Barbie

- 11.30 a.m. **Next Generation Design-Make-Test-Analysis-Cycles**
C. D. Christ, Berlin/DE, Y. Alber, Berlin/DE, H. Briem, Berlin/DE, M. Hahn, Berlin/DE, G. Hermann, Berlin/DE, F. Koelling, Berlin/DE, M. Lobell, Berlin/DE, G. Mogk, Berlin/DE, F. Mrugalla, Berlin/DE, M. Schimeczek, Berlin/DE
- 12.00 p.m. **Discovery of a novel class of brain penetrant inhibitors of KRASG12C**
M. S. Bodnarchuk, Cambridge/GB
- 12.20 p.m. **Lessons learned at GSK to identify and optimise PROTACS**
A. Miah, Stevenage/GB
- 12.40 p.m. **Ruthenium-based photoactivated chemotherapy: A promising tool in the anticancer toolbox**
S. K. Goetzfried, Leiden/NL, L. Bretin, Leiden/NL, S. Bonnet, Leiden/NL
- 1.00 p.m. LUNCH BREAK & POSTERS

Buchner Lecture Hall

Highlights in Medicinal Chemistry

Chair: S. Laufer

- 2.00 p.m. **Development of Short Oligonucleotides to Inhibit the Functions of RNA-Binding Proteins**
J. Hall, Zurich/CH, M. Vincent, Zurich/CH, C. Weller, Zurich/CH
- 2.30 p.m. **In Silico Driven Drug Discovery of a Zwitterionic $\alpha\beta 6$ Integrin Development Candidate for Fibrosis**
E. Hickey, New York/US, B. Harrison, Waltham/US, A. Gerasiyto, New York/US

Tuesday, March 19, 2024

2.50 p.m. **Kinetic Modelling of the P-Glycoprotein Mediated Efflux with a Large-Scale Matched Molecular Pair Analysis**
H. Zhao, Gothenburg/SE

11.00 a.m. COFFEE BREAK

Buchner Lecture Hall

Awards Session 1 (Ph.D. Awards)

Chairs: G. Hessler, T. Ross

3.10 p.m. **Entwicklung von chemischen Tools für nukleäre Rezeptoren**
S. Arifi, Frankfurt (Main)/DE

3.55 p.m. **Using iron to catch a ride – synthetic siderophores as molecular ‘Trojan Horses’ to visualize and treat MDR bacterial pathogens**
C. Peukert, San Francisco/US

4.05 p.m. **Selective Inhibitors and Targeted Degraders of Histone Deacetylase 10**
R. Steimbach, Gif sur Yvette/FR

4.10 p.m. **Innovation Prize**

Chairs: C. Ducho, C. Kuttruff,

The development of next-generation covalent azapeptide Mpro inhibitors with potent activity against SARS-CoV-2 and variants
T. Pillaiyar, Tübingen/DE

Buchner Lecture Hall

4.45 p.m. **Keynote Lecture**

Chair: D. Merk

AI and Small Molecule Drug Discovery – A Data Roadmap
A. Edwards, Toronto/CA

Wednesday, March 20, 2024

Buchner Lecture Hall

Membrane Associated Targets

Chair: F. Paintner

9.00 a.m. **Targeting Microbial Lactate Transporters – a Novel Mode of Action Against Malaria**
E. Beitz, Kiel/DE

9.30 a.m. **Discovery of Slack potassium channel activators for treatment of chronic pruritus**
E. Proschak, Frankfurt (Main)/DE, W. F. Zhu, Frankfurt (Main)/DE, A. Balzulat, Frankfurt (Main)/DE, C. Flauaus, Frankfurt (Main)/DE, V. Hernandez-Olmos, Frankfurt (Main)/DE, J. Heering, Frankfurt (Main)/DE, S. Sethumadhavan, Frankfurt (Main)/DE, M. Dubiel, Düsseldorf/DE, A. Menge, Frankfurt (Main)/DE, D. Panov, Kyiv/UA, K. Metzner, Frankfurt (Main)/DE, R. Lu, Frankfurt (Main)/DE, S. Knapp, Frankfurt (Main)/DE, S. Müller, Frankfurt (Main)/DE, D. Steinhilber, Frankfurt (Main)/DE, I. Hänelt, Frankfurt (Main)/DE, H. Stark, Düsseldorf/DE, A. Schmidtke, Frankfurt (Main)/DE

9.50 a.m. **Endogenous Nitro-Fatty Acids are a Novel Class of Novel Anti-Tumorigenic Agents for Treatment of Colorectal Cancer**
G. Manolikakes, Kaiserslautern/DE, J. Roos, Langen/DE, T. Maier, Langen/DE

10.10 a.m. **Subtype-selective agonism is driven by specific receptor dynamics at class A GPCRs**
M. Bermudez, Münster/DE, M. Kauk, Jena/DE, D. Volpato, Würzburg/DE, D. Schaller, Berlin/DE, J. Drube, Jena/DE, N. Yurdagül-Hemmrich, Würzburg/DE, N. Ziegler, Würzburg/DE, U. Zabel, Würzburg/DE, N. Lambert, Augusta/US, U. Holzgrabe, Würzburg/DE, G. Wolber, Berlin/DE, C. Hoffmann, Jena/DE

10.30 a.m. COFFEE BREAK

Wednesday, March 20, 2024

Buchner Lecture Hall

New Synthetic Methods & MedChem Technology

Chair: I. Huc

- 11.00 a.m. **Halogenations inspired by Nature: New Concepts for an Old Problem**
T. Gulder, Leipzig/DE
- 11.30 a.m. **Bind&Bite: Covalently stabilized heterodimeric coiled-coil peptides for the site-selective, cysteine-free chemical modification of proteins**
J. Eichler, Erlangen/DE, J. Beutel, Würzburg/DE, P. Tannig, Erlangen/DE, R. Di Vincenzo, Erlangen/DE, K. Überla, Erlangen/DE
- 11.50 a.m. **Automation + Miniaturization = Acceleration**
A. Dömling, Olomouc/CZ
- 12.10 p.m. **The Fruitful Interplay of Synthetic and Medicinal Chemistry – Innovative Synthetic Methods to Accelerate Drug Discovery**
S. Schiesser, Mölndal/SE

Buchner Lecture Hall

Friedrich-Stolz Award

- 12.30 p.m. **Award Session 2**
Chairs: G. Hessler, F. von Nussbaum
- 1.15 p.m. **Closing**

Sunday March 17, 2024

Buchner Lecture Hall

- 3.00 p.m. to 4.15 p.m. **Artificial Intelligence in Publishing: State of the Art and Best Practices for Researchers**
Dr. David Peralta (Chemistry Europe/Wiley-VCH)

Monday March 18, 2024

Buchner Lecture Hall

- 12.30 p.m. to 1.30 p.m. **Of Hinge Binders and Drug Candidates: Computational Design of Kinase Inhibitors**
Dr. Alexander Neumann (BioSolveIT)

Tuesday March 19, 2024

Buchner Lecture Hall

- 1.00 p.m. to 2.00 p.m. **„Career Paths in Medicinal Chemistry“ NextGenMedChem & EFMC-YSN**
Lunch session



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- P001 **Towards the Ab Initio Design of Foldamer Ligands for Protein Surface**
L. Wang, Munich/DE, J. Sigl, Munich/DE, Y. Zhang, New York/US, Z. Liu, New Jersey/US
- P002 **Investigation of the Structure-Activity Relationship of Liver X Receptor (LXR) Antagonists for Conversion to Agonists**
A. Kaercher, Frankfurt (Main)/DE, P. Heitel, Frankfurt (Main)/DE
- P003 **Development of synthetic modulators of the nuclear receptor LHR-1**
A. Lang, Frankfurt (Main)/DE, M. Schubert-Zsilavec, Frankfurt (Main)/DE, D. Merk, Frankfurt (Main)/DE
- P004 **Development of Cysteine-Selective Probes for Native Reactivity Profiling**
C. M. Nuber, Munich/DE, A. V. Milton, Munich/DE, M. C. Isaza Alvarez, Munich/DE, D. B. Konrad, Munich/DE
- P005 **Design and Crystallographic Screening of a Diverse and Highly Sociable Fragment Library**
P. Janssen, Münster/DE, F. Becker, Münster/DE, F. Füsser, Münster/DE, T. Matviyuk, Kyiv/UA, I. Kondratov, Kyiv/UA, D. Kümmel, Münster/DE, M. Weiss, Berlin/DE, O. Koch, Münster/DE
- P006 **Spiro[3.3]heptane as a Saturated Benzene Bioisostere**
O. Kolodiazhna, Kyiv/UA, I. Pishel, Kyiv/UA, V. Kubyshkin, Kyiv/UA, P. Mykhailiuk, Kyiv/UA, K. Prysiazhniuk, Kyiv/UA, O. Datsenko, Kyiv/UA, O. Polishchuk, Kyiv/UA, S. Shulha, Kyiv/UA, O. Shablykin, Kyiv/UA, Y. Nikandrova, Kyiv/UA, K. Horbatok, Kyiv/UA, I. Bodenchuk, Kyiv/UA, P. Borysko, Kyiv/UA, D. Shepilov, Kyiv/UA
- P007 **Borylated cyclobutanes via thermal [2+2]-cycloaddition**
O. Kolodiazhna, Kyiv/UA, K. Prysiazhniuk, Kyiv/UA, O. Datsenko, Kyiv/UA, O. Polishchuk, Kyiv/UA, S. Shulha, Kyiv/UA, K. Gudzikeych, Kyiv/UA, V. Kubyshkin, Kyiv/UA, P. Mykhailiuk, Kyiv/UA
- P008 **LXR Modulators as Tools to Decipher Anti-atherosclerotic and Lipogenic Effects**
N. Bandomir, Frankfurt (Main)/DE, P. Heitel, Frankfurt (Main)/DE
- P009 **The Activity of Benzocaine Benzene Ring Bioisosteres**
Y. Holota, Kyiv/UA, I. Pishel, Kyiv/UA, P. Mykhailiuk, Kyiv/UA, V. Ripenko, Kyiv/UA, D. Lesyk, Kyiv/UA, A. Anisiforova, Kyiv/UA, K. Prysiazhniuk, Kyiv/UA, O. Datsenko, Kyiv/UA, O. Polishchuk, Kyiv/UA, S. Shulha, Kyiv/UA, O. Shablykin, Kyiv/UA, P. Borysko, Kyiv/UA, D. Shepilov, Kyiv/UA
- P010 **2-Oxabicyclo[2.2.2]Octane Bioisostere of Vorinostat: Synthesis and Biological Activity**
Y. Holota, Kyiv/UA, D. Lesyk, Kyiv/UA, Y. Bas, Kyiv/UA, D. Dudenko, Kyiv/UA, P. Mykhailiuk, Kyiv/UA, V. Levterov, Kyiv/UA, Y. Panasiuk, Kyiv/UA, K. Sahun, Kyiv/UA, O. Stashkeych, Kyiv/UA, V. Badlo, Kyiv/UA, O. Shablykin, Kyiv/UA, I. Sadkova, Kyiv/UA, P. Borysko, Kyiv/UA, K. Horbatok, Kyiv/UA, I. Bodenchuk, Kyiv/UA

- P011 **DNA Mimic Foldamers in Biological Systems**
M. Loos, Munich/DE, J. Wu, Munich/DE, V. Corvaglia, Munich/DE, D. Deepak, Munich/DE, F. Xu, Munich/DE, T. Carell, Munich/DE, I. Huc, Munich/DE
- P012 **A novel class of antimalarials targeting the parasite's lactate/H⁺ symporter**
C. Nerlich, Kiel/DE, E. Beitz, Kiel/DE
- P013 **Turning old into new - converting known Pim-1 kinase inhibitors into new actives by FTrees**
D. Hubach, Marburg/DE, P. M. M. Hochban, Marburg/DE, G. Bach, Marburg/DE, C. Wegscheid-Gerlach, Marburg/DE, W. E. Diederich, Marburg/DE
- P014 **Development of Antiviral PROTACs based on the Kinase Inhibitor Pelitinib for the SARS-CoV-2 Main Protease**
L. D. Laube, Marburg/DE, C. Veeck, Marburg/DE, W. E. Diederich, Marburg/DE, S. Becker, Marburg/DE
- P015 **Enhancing the features of DNA mimic foldamers for structural investigations**
J. Wu, Munich/DE, V. Corvaglia, Munich/DE, M. Loos, Munich/DE, D. Deepak, Munich/DE, I. Huc, Munich/DE
- P016 **Development of First-in-Class Dual Sirt2/HDAC6 Inhibitors as Molecular Tools for Dual Inhibition of Tubulin Deacetylation**
M. Schiedel, Braunschweig/DE, L. Sinatra, Leipzig/DE, A. Vogelmann, Freiburg/DE, F. Friedrich, Freiburg/DE, M. A. Tararina, Philadelphia/US, E. Neuwirt, Freiburg/DE, A. Colcerasa, Freiburg/DE, P. König, Bonn/DE, L. Toy, Erlangen/DE, T. Z. Yesiloglu, Halle/DE, W. Sippl, Halle/DE, O. Groß, Freiburg/DE, G. Bendas, Bonn/DE, D. W. Christianson, Philadelphia/US, F. K. Hansen, Bonn/DE, M. Jung, Freiburg/DE
- P017 **Designing potent TLX agonists by combinatorial chemistry**
T. Stiller, Munich/DE, D. Merk, Munich/DE
- P018 **Automated Design of Multi-target Ligands by Generative Deep Learning**
L. Isigkeit, Frankfurt (Main)/DE, T. Hörmann, Munich/DE, E. Schallmayer, Frankfurt (Main)/DE, K. Scholz, Munich/DE, F. F. Lillich, Frankfurt (Main)/DE, J. H. M. Ehrler, Frankfurt (Main)/DE, B. Hufnagel, Frankfurt (Main)/DE, J. Büchner, Frankfurt (Main)/DE, J. A. Marschner, Munich/DE, J. Pabel, Munich/DE, E. Proschak, Frankfurt (Main)/DE, D. Merk, Munich/DE
- P019 **Tetrazine-derived histamine H3 receptor ligands for Click chemistry**
H. Stark, Düsseldorf/DE, M. Stark, Düsseldorf/DE, L. Leitzbach, Düsseldorf/DE
- P020 **Leveraging Chemical Language Models with Iterative Fine-Tuning for Ligand Optimization**
T. I. Hörmann, Munich/DE, A. C. Hunklinger, Munich/DE, M. Lewandowski, Munich/DE, D. Merk, Munich/DE
- P021 **Targeting Proteins with Peptide-Foldamer-Hybrid Macrocycles**
C. Rivière, Munich/DE, R. T. Howard, Munich/DE, V. Morozov, Munich/DE, C. Tsiamantas, Tokyo/JP, D. Deepak, Munich/DE, C. Douat, Munich/DE, H. Suga, Tokyo/JP, I. Huc, Munich/DE

- P022 **Development of Anticancer Agents based on the 1,1'-Binaphthyl-2,2'-diamine (BINAM) Structure**
P. J. Bednarski, Greifswald/DE, M. Eichelbaum, Greifswald/DE
- P023 **Merged molecular switches excel as optoacoustic dyes: azobenzene-cyanines are loud and photostable NIR imaging agents**
M. Müller, Munich/DE, N. Liu, Munich/DE, V. Gujrati, Munich/DE, A. Valavalkar, Jena/DE, S. Hartmann, Munich/DE, A. Telek, Munich/DE, D. Dietzek-Ivanšić, Jena/DE, A. Hartschuh, Munich/DE, B. Ntziachristos, Munich/DE, O. Thorn-Seshold, Munich/DE
- P024 **Preparation of Nano Magnesium Oxide Loaded with Syrian Inula Plant Extract and Study of antibacterial activity Against Vibrio cholera**
A. Hammal, Aleppo/SY
- P025 **Fluorescently Labeled Pyrrolones Targeting the Intracellular Allosteric Binding Site of Chemokine Receptor CCR1**
L. Toy, Erlangen/DE, M. E. Huber, Erlangen/DE, M. Szpakowska, Esch-sur-Alzette/LU, A. Chevigné, Esch-sur-Alzette/LU, M. Schiedel, Braunschweig/DE
- P026 **Novel dual inhibitors of the amine oxidases VAP-1 and MAO B for the treatment of inflammatory diseases**
J. Kampschulze, Münster/DE, T. Pöstges, Münster/DE, W. Hanekamp, Münster/DE, M. Bermúdez, Münster/DE, M. Lehr, Münster/DE
- P027 **Establishing structure-activity relationships of a TLX lead agonist**
E. C. Hank, Munich/DE, D. Merk, Munich/DE
- P028 **Development of an LC-ESI-MS/MS based screening system for allosteric ligands of PPAR γ using ultrafiltration**
L. Obeser, Munich/DE, G. Höfner, Munich/DE, D. Merk, Munich/DE
- P029 **Elucidating Nurr1 Ligand Binding Sites and Activation Mechanisms by Modeling and Mutagenesis**
U. López-García, Munich/DE, T. Wein, Munich/DE, D. Merk, Munich/DE
- P030 **Covalent Inhibitors for Kallikrein-Related Peptidase 6**
H. Rebmann, Heidelberg/DE, A. Baumann, Heidelberg/DE, P. K. A. Jagtap, Bayreuth/DE, J. Hennig, Bayreuth/DE, A. K. Miller, Heidelberg/DE
- P031 **Development of cytosolic phospholipase A2 α -inhibiting indole-substituted 5-tetrazolypentanoic acids with increased metabolic stability**
J. Einerhand, Münster/DE, I. Meyer zu Vilsendorf, Münster/DE, W. Hanekamp, Münster/DE, M. Lehr, Münster/DE
- P032 **Tailored Phenyl Esters Inhibit ClpXP and Attenuate Staphylococcus aureus α -Hemolysin Secretion**
M. Schwarz, Munich/DE, I. Hübner, Munich/DE, S. A. Sieber, Munich/DE
- P033 **Can a lucky hit be further optimised? Systematic synthesis and biological evaluation of novel steroidal DHCR24 inhibitors**
M. Hollweck, Munich/DE, L. Spieth, Munich/DE, S. A. Berghoff, Munich/DE, F. Bracher, Munich/DE, C. Müller, Munich/DE

- P034 **Total Synthesis of Microketide A and Elucidation of its Antibiotic Mode of Action in Gram-Negative Bacteria**
M. F. Köllen, Munich/DE, S. A. Sieber, Munich/DE
- P035 **Repurposing Proton Pump Inhibitors (PPIs) for Targeted Degradation of Zinc-Finger Proteins**
N. Richert, Heidelberg/DE, J. Lohbeck, Heidelberg/DE, T. Marker, Heidelberg/DE, T. Dick, Heidelberg/DE, A. K. Miller, Heidelberg/DE
- P036 **Optimization of dual-target carboxylic acid fragments modulating Nurr1/RXR activity**
K. Scholz, Munich/DE, D. Merk, Munich/DE
- P037 **Designed polypharmacology in MASH: Development and profiling of dual PPAR δ /sEH modulators**
X. Ge, Munich/DE, D. Merk, Munich/DE
- P038 **FKBP12-assisted Molecular Glues Targeting BRD4^{BD2}**
J. K. Dreizler, Darmstadt/DE, C. Meyners, Darmstadt/DE, W. O. Sugiarto, Darmstadt/DE, T. M. Geiger, Darmstadt/DE, F. Hausch, Darmstadt/DE
- P039 **Characterisation of Dual Nurr1 Activator/DHODH Inhibitor Vidofludimus Calcium and Development Towards a Nurr1 Selective Tool Compound**
C. Gege, Gräfelfing/DE, H. Wu, Duarte/US, J. Vietor, Munich/DE, T. Wulff, Gräfelfing/DE, M. Jafari, Gräfelfing/DE, E. Peelen, Gräfelfing/DE, T. Stiller, Munich/DE, R. Busch, Munich/DE, J. Marschner, Munich/DE, D. Merk, Munich/DE, Z. Sun, Duarte/US, H. Kohlhof, Gräfelfing/DE, D. Vitt, Gräfelfing/DE
- P040 **Development of Small-Molecule Plasma Kallikrein Inhibitor via Microscale Parallel Synthesis and Screening**
H. Lin, Münster/DE, J. Ren, Münster/DE, D. V. Kalinin, Münster/DE
- P041 **Overcoming Promiscuity: Small Molecule Screening Strategies to Target Activin A**
L. Quambusch, Cambridge/GB, M. Hyvönen, Cambridge/GB
- P042 **Synthesis and Characterization of dually labelled neuropeptide NTS₁R ligands**
F. J. Ertl, Regensburg/DE, S. Kopanchuk, Tartu/EE, N. C. Dijon, Nottingham/GB, J. Köckenberger, Erlangen/DE, M. R. Heinrich, Erlangen/DE, N. D. Holliday, Nottingham/GB, A. Rinken, Tartu/EE, M. Keller, Regensburg/DE
- P043 **UR-JG114 - a novel fluorescent tool compound for luminescence-based neuropeptide Y Y₄R binding studies**
J. Gleixner, Regensburg/DE, L. Grätz, Regensburg/DE, J. Köckenberger, Erlangen/DE, M. R. Heinrich, Erlangen/DE, M. Keller, Regensburg/DE
- P044 **Enantioselective approach to 1-benzyltetrahydroisoquinolines and their five- and seven-membered homologues**
C. Zenger, Munich/DE, M. Kintzel, London/GB, F. Bracher, Munich/DE
- P045 **Unveiling Hidden Treasures: Exploring Large Chemical Spaces with Machine Learning Models Trained on DNA-Encoded Libraries Selection Results**
A. Kapeliukha, Kyiv/UA, O. Strapak, Kyiv/UA, O. Tarkhanova, Kyiv/UA, S. Zozulya, Kyiv/UA, Y. Moroz, Kyiv/UA

- P046 **Estradiol derivatives and analogs as blockers of TRPML1 cation channels**
P. Rühl, Munich/DE, F. Bracher, Munich/DE
- P047 **Development of highly redshifted azobenzenes**
K. Lützel, Munich/DE, D. B. Konrad, Munich/DE, H. Laqua, Munich/DE, J. K. Szántó, Munich/DE, G. Savasci, Munich/DE, L. Allmendinger, Munich/DE, B. Kicin, Munich/DE, V. Ruf, Munich/DE, K. Karaghiosoff, Munich/DE, A. M. Ali, Assiut/EG, C. Ochsenfeld, Munich/DE, T. Fehrentz, Heidelberg/DE
- P048 **Searching with new algorithms for drug like molecules in large combinatorial spaces**
M. von Korff, Dornach/CH, T. Sander, Reinach/CH
- P049 **Indole Derivatives as Activators of 8-Oxo-Guanine DNA Glycosylase**
F. Ortis, Klosterneuburg/AT, M. Varga, St. Andrews/GB, E. R. Scaletti, Stockholm/SE, O. Wallner, Stockholm/SE, K. Mamonov, Copenhagen/DK, E. Homan, Stockholm/SE, A. Watson, St. Andrews/GB, P. Stenmark, Stockholm/SE, M. Michel, Stockholm/SE
- P050 **Synthesis and Biological Evaluation of LpxC Inhibitors Addressing the UDP Binding Pocket**
S. Wimmer, Hamburg/DE, F. Wichter, Hamburg/DE, R. Holl, Hamburg/DE
- P051 **Sirtuin 6 inhibitors – first structure variations of a potential new antiprotozoal target**
F. Breu, Munich/DE, C. Leser, Munich/DE, F. Bracher, Munich/DE
- P052 **Fluorogenic chemical probes for wash-free imaging of cell membrane damage in ferroptosis and necrosis**
P. Mauker, Munich/DE, D. Beckmann, Munich/DE, A. J. Davidson, Glasgow/GB, T. Misgeld, Munich/DE, M. Kerschensteiner, Munich/DE, O. Thorn-Seshold, Munich/DE
- P053 **Light-controlled inhibition of the circadian regulator ROR γ**
M. Reynders, Munich/DE, S. Willems, Munich/DE, J. A. Marschner, Munich/DE, T. Wein, Munich/DE, D. Merk, Munich/DE, O. Thorn-Seshold, Munich/DE
- P054 **Photocaged Epithilone allows Spatiotemporal Control over the Cytoskeleton**
C. Schmitt, Munich/DE, N. Veprek, Munich/DE, J. Meiring, Utrecht/NL, P. Mauker, Munich/DE, A. Akhmanova, Utrecht/NL, O. Thorn-Seshold, Munich/DE
- P055 **Covalent inhibitors and covalent fragments in drug discovery programs**
B. Carbain, Basel/CH, S. Blanc, Basel/CH, C. Bournez, Basel/CH, G. Müller, Basel/CH, Q. Lefebvre, Basel/CH
- P056 **Developing a multi-compound based BBB model system using HBEC-5i cells**
T. Kasch, Munich/DE, J. Marschner, Munich/DE, D. Merk, Munich/DE

- P057 **Assessing the activity of anilines, anilides, benzodioxols, phenols, and aryl ureas as radical trapping antioxidants that inhibit ferroptosis**
H. Zahran, Munich/DE, H. Schricker, Munich/DE, M. M. Mouzayek, Munich/DE, J. Wanninger, Munich/DE, K. Lützel, Munich/DE, A. V. Milton, Munich/DE, E. Mishima, Munich/DE, B. Proneth, Munich/DE, M. Conrad, Munich/DE, D. Konrad, Munich/DE
- P058 **Synthesis and Characterization of a Novel Photochemical Probe to Unravel the Role of Truncated Phospholipid in Membrane Permeability: Insights into the Mechanism of Ferroptosis**
M. Sathian, Munich/DE, D. Konrad, Munich/DE
- P059 **Development of a photoswitchable fatty acid mimetic based on a cinalukast derived PPAR α -Modulator**
N. G. L. van Herwijnen, Munich/DE, M. Sai, Munich/DE, D. Merk, Munich/DE
- P060 **Engineering novel electrophilic fragments as small molecules targeting caspase-2 deriving from a fragment-based drug discovery approach**
S. Pockes, Regensburg/DE, L. Wirth, Regensburg/DE, M. Ködel, Regensburg/DE, M. Cuellar, Minneapolis/US, L. Forster, Regensburg/DE, M. Hall, Rockville/US, S. Patnaik, Rockville/US, K. Ashe, Minneapolis/US, M. Walters, Minneapolis/US
- P061 **Fluorescent AF64394 analogues enables real-time binding studies for the orphan class A GPCR GPR3**
S. Pockes, Regensburg/DE, M. Bresinsky, Regensburg/DE, A. Shahraki, Marburg/DE, P. Kolb, Marburg/DE, H. Schihada, Marburg/DE
- P062 **The tritiated radioligand [3 H]UR-MN259 shows high-affinity and selectivity for the histamine H₃ receptor**
S. Pockes, Regensburg/DE, D. Mönnich, Regensburg/DE, M. Nagl, Regensburg/DE, L. Forster, Regensburg/DE, N. Rosier, Regensburg/DE, P. Igel, Regensburg/DE
- P063 **Development of specific chemical probes targeting the protein kinase BMX**
X. J. Liang, Tübingen/DE, C. Albertini, Bologna/IT, M. Forster, Tübingen/DE, M. Schröder, Frankfurt (Main)/DE, S. Gerstenecker, Tübingen/DE, A. Chaikuad, Frankfurt (Main)/DE, S. Knapp, Frankfurt (Main)/DE, S. Laufer, Tübingen/DE, M. Gehringer, Tübingen/DE
- P064 **Characterization of cancer progression mechanisms in non-small cell lung cancer cell lines**
A. V. Milton, Munich/DE, H. Schricker, Munich/DE, B. Bissinger, Munich/DE, K. Lützel, Munich/DE, P. Kielkowski, Munich/DE, D. B. Konrad, Munich/DE
- P065 **Synthesis of new alpha2A agonists fo the treatment of pain**
T. Pfeiffer, Erlangen/DE, P. Seemann, Erlangen/DE, H. Hübner, Erlangen/DE, P. Gmeiner, Erlangen/DE

- P066 **Interpreting Graph Neural Networks with Myerson Values for Cheminformatics Approaches**
S. K. R. Homberg, Münster/DE, M. L. Modlich, Münster/DE, J. Menke, Gothenborg/SE, G. M. Morris, Oxford/GB, B. Risse, Münster/DE, O. Koch, Münster/DE
- P067 **Photocaged GPX4 Inhibitors for the Spatiotemporal Control of the Induction of Ferroptosis as a Foundation for Mechanistic Investigations**
B. Nißl, Munich/DE, D. Cheff, Stockholm/SE, K. Lützel, Munich/DE, E. Arnér, Stockholm/DE, D. B. Konrad, Munich/DE
- P068 **Computational Investigation of GPR3: An orphan receptor with high pharmaceutical relevance**
N. Staffen, Erlangen/DE, G Chen, Shenzhen/CN, Z. Wu, Shenzhen/CN, X. Xu, Beijing/CN, J. Pan, Beijing/CN, A. Inoue, Sendai/JP, T. Shi, Shenzhen/CN, Y. Du, Shenzhen/CN, J. Xu, Shenzhen/CN, P. Gmeiner, Erlangen/DE
- P069 **Investigating the Binding Kinetics of Novel Photoswitchable Covalent Ligands for the β_2 -Adrenergic Receptor using Markov State Models**
E. Neu, Erlangen/DE, U. Wirth, Regensburg/DE, D. Provasi, New York/US, H. Hübner, Erlangen/DE, M. Filizola, New York/US, B. König, Regensburg/DE, P. Gmeiner, Erlangen/DE
- P070 **Comparison of old and new methods for the synthesis of acylals as prodrugs motifs**
T. Keydel, Greifswald/DE, A. Link, Greifswald/DE
- P071 **Searching for a small molecule ligand for the GPR182 receptor**
H. Baltrukevich, Marburg/DE, R. Bonnavion, Bad Nauheim/DE, S. Offermanns, Bad Nauheim/DE, P. Kolb, Marburg/DE
- P072 **Characterizing the Effects of NR4A Agonism in Neuroinflammation *In Vitro***
R. Busch, Munich/DE, J. A. Marschner, Munich/DE, C. Gege, Gräfelfing/DE, H. Kohlhof, Gräfelfing/DE, D. Merk, Munich/DE
- P073 **Drug design of positive allosteric modulators of potassium channels between lipophilicity and solubility: Maintaining the balance to achieve optimal function**
J. Lemke, Greifswald/DE, K. W. Wurm, Greifswald/DE, F.-M. Bartz, Greifswald/DE, N. Assenheimer, Greifswald/DE, L. Schulig, Greifswald/DE, P. J. Bednarski, Greifswald/DE, A. Link, Greifswald/DE
- P074 **Pyrazole-Based Small-Molecule Inhibitors of Thrombin**
A. Siutkina, Münster/DE, C. Dunker, Münster/DE, L. Imberg, Münster/DE, D. Kalinin, Münster/DE
- P075 **Development of oxPTM-targeting chemical probes to address advanced lung cancers**
L. L. Seidl, Munich/DE, C. Pignot, Munich/DE, I. Cid, Munich/DE, D. Konrad, Munich/DE

- P076 **In silico exploration of LANCL2-ABA binding mode towards the identification of novel LANCL2 agonists**
N. Scarano, Genoa/IT, F. Di Palma, Genoa/IT, S. Spinelli, Genoa/IT, L. Sturla, Genoa/IT, A. Cavalli, Genoa/IT, F. Musumeci, Genoa/IT, S. Schenone, Genoa/IT, E. Cichero, Genoa/IT
- P077 **3-Polyfluoroalkyl Prolines: Synthesis and Study of 3-Polyfluoroalkyl Group Impact on Peptide Proteolytic Stability**
I. Kondratov, Frankfurt (Main)/DE, A. Chernykh, Kyiv/UA, O. Grygorenko, Kyiv/UA
- P078 **Anthelmintic activity of Ethanol and Aqueous Extracts of *Khaya grandifoliola* Stem Bark against *Heligmosomoides polygyrus*: In vitro and in silico approach**
M. Yagoobi, Leuven/BE, Y. Cedric, Bambili/CM, N. C. Nadia, Dschang/CM, M. Besati, Valencia/ES
- P079 **Proteome-wide Monitoring of Drug Action in Living Cells using a novel label-free Solvent-based Shift Assay**
D. Steinbrunn, Freising/DE, H. Hahne, Freising/DE
- P080 **Cell-based Reactive Cysteine Profiling of an Electrophile Fragment Library to Explore Novel Target Opportunities**
H. Hahne, Freising/DE, M. Holzner, Freising/DE, S. Poser, Freising/DE, M. I. Faria, Freising/DE, P. Weber, Freising/DE, C. Zasada, Freising/DE, K. Cassidy, Watertown/US, R. Agafonov, Watertown/US, B. Appleton, Watertown/US, J. Schülke, Freising/US, J. Muntel, Freising/DE
- P082 **Chem-CRISPR/dCas9^{FCPF} - A platform for chemically induced single-gene epigenome editing**
X. Cheng, Frankfurt (Main)/DE
- P083 **Introducing DockM8 : An All-in-One Open-Source Platform for Consensus Virtual Screening in Drug Design**
A. M. L. Lacour, Saarbrücken/DE, H. Ibrahim, Saarbrücken/DE, A. Volkamer, Saarbrücken/DE, A. H. K. Hirsch, Saarbrücken/DE
- P084 **Sulfonamide derivatives of 1,4-dihydroquinazolin-2-amine as a new scaffold for selective 5-HT₆R ligand design**
P. Zareba, Cracow/PL, A. K. Drabczyk, Cracow/PL, J. Kuliś, Cracow/PL, N. Kozień, Cracow/PL, G. Bieda, Cracow/PL, G. Satała, Cracow/PL, G. Latacz, Cracow/PL
- P085 **Rational Chemical Design of RX1, a Modular 1,2 Thiaselenane Redox Probe That Selectively Reports on Cellular Thioredoxin Reductase Activity**
L. Zeisel, Munich/DE, J. G. Felber, Munich/DE, K. C. Stolzen, Stockholm/SE, E. S. J. Arnér, Stockholm/SE, O. Thorn-Seshold, Munich/DE
- P086 **Old Drugs Lead to Leads for Novel Drugs – Evidence from historical reality**
H. Heuer, Schwabenheim/DE
- P087 **Lightning Up Platinum Complexes for Tumor-Targeted Anticancer Therapy**
J. Karges, Bochum/DE

- P089 **Miniaturized Fluorescent MAGL Probes with Drug-Like Properties**
A. Hentsch, Berlin/DE, M. Guberman, Berlin/DE, S. Radetzki, Berlin/DE, M. Schippers, Basel/CH, J. Blaising, Basel/CH, Y. He, Zürich/CH, J. Paul, Berlin/DE, J. Benz, Basel/CH, B. Kuhn, Basel/CH, L. Mu, Zürich/CH, U. Grether, Basel/CH, M. Nazare, Berlin/DE
- P090 **Ligand directed labeling of CB₁R enables the construction of a biosensor for orthosteric and allosteric cannabinoid ligands**
L. Mach, Berlin/DE, D. Sykes, Nottingham/GB, R. M. Vitale, Pozzuoli/IT, J. Frank, Portland/US, E. Koers, Nottingham/GB, J. Bouma, Leiden/NL, C. van der Horst, Leiden/NL, W. Guba, Basel/CH, L. H. Heitman, Leiden/NL, U. Grether, Basel/CH, D. Veprintsev, Nottingham/GB, M. Nazare, Berlin/DE
- P091 **Highly selective probes for Phosphoinositide 3-Kinase Class II β : the Discovery of a Selectivity Switch**
D. Cirillo, Berlin/DE, W. T. Lo, Berlin/DE, M. Diceglie, Berlin/DE, L. Perepelittchenko, Berlin/DE, T. A. L. Ehret, Frankfurt/DE, S. Radetzki, Berlin/DE, S. Wilhelm, Freising/DE, J. P. von Kries, Berlin/DE, S. Müller, Frankfurt/DE, V. Haucke, Berlin/DE, M. Nazaré, Berlin/DE
- P092 **Macrocyclization as a Strategy for Solubility Improvement - A Systematic Analysis of Matched Molecular Pairs**
C. Walz, Darmstadt/DE, M. Spiske, Darmstadt/DE, M. Walter, Darmstadt/DE, C. Hoft, Darmstadt/DE, M. Mezler, Darmstadt/DE, F. Pohlki, Darmstadt/DE, S. Vukelić, Darmstadt/DE, F. Hausch, Darmstadt/DE
- P093 **Targeting ACKR3 – Novel Small Molecule Platelet Modulators**
A. Bayrak, Tübingen/DE, F. Mohr, Tübingen/DE, K. Kolb, Tübingen/DE, M. Szpakowska, Luxembourg/LU, E. Shevchenko, Tübingen/DE, V. Dicenta, Tübingen/DE, A.-K. Rohlfing, Tübingen/DE, R. Ditzinger, Tübingen/DE, A. Rasch, Tübingen/DE, T. Pansar, Tübingen/DE, M. Günther, Tübingen/DE, A. A. Kaczor, Lubin/PL, A. Chevigné, Luxemburg/LU, T. Pillaiyar, Tübingen/DE, M. Gawaz, Tübingen/DE, S. A. Laufer, Tübingen/DE
- P094 **The development of novel azapeptide Mpro inhibitors with potent activity against SARS-CoV-2 and variants**
P. Flury, Tübingen/DE, K. Sylvester, Bonn/DE, M. Gütschow, Bonn/DE, H. C. Hong, Hong Kong/CN, S. Yang, Sichuan/CN, S. A. Laufer, Tübingen/DE, C. E. Müller, Bonn/DE, T. Pillaiyar, Tübingen/DE

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