



GESELLSCHAFT DEUTSCHER CHEMIKER



Fachgruppe Medizinische Chemie

# Frontiers in Medicinal Chemistry

April 3 – 5, 2023 · Vienna, Austria



Deutsche  
Pharmazeutische  
Gesellschaft e.V.



[www.gdch.de/medchem2023](http://www.gdch.de/medchem2023)

P  
R  
O  
G  
R  
A  
M





Werte schaffen  
durch Innovation

*Die Gesundheit von Mensch  
und Tier zu verbessern  
– das ist unser Ziel.*

Als führendes, forschunggetriebenes biopharmazeutisches Unternehmen arbeitet Boehringer Ingelheim an bahnbrechenden Therapien in Bereichen mit hohem, ungedecktem medizinischen Bedarf. Seit seiner Gründung im Jahr 1885 ist Boehringer Ingelheim in Familienbesitz und verfolgt eine langfristige Perspektive. Mehr als 52.000 Mitarbeitende bedienen über 130 Märkte in den drei Geschäftsbereichen Humanpharma, Tiergesundheit und Biopharmazeutische Auftragsproduktion.

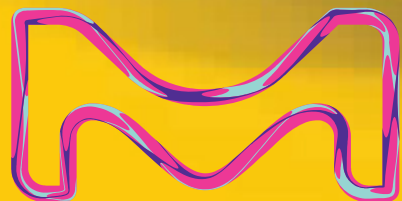
Foto: Boehringer Ingelheim

TABLE OF CONTENTS

COMMITTEES	5
SCIENTIFIC PROGRAM	7
Monday, April 3, 2023	7
Tuesday, April 4, 2023	9
Wednesday, April 5, 2023	12
LIST OF POSTERS	15
LIST OF PARTICIPANTS	26
ACKNOWLEDGEMENT	34

WHAT WE DO ALL DAY:  
**MAKE A  
DIFFERENCE.**

We are a vibrant science and technology company driving human progress. Our actions make a positive difference every day.



Would you like to learn more about us and our latest projects?



## COMMITTEES

### SCIENTIFIC COMMITTEE

<b>N. Chessum</b>	Boehringer-Ingelheim, Ingelheim/DE
<b>E. Diamanti</b>	HIPS, Saarbrücken/DE (NextGenMedChem)
<b>C. Ducho</b>	University of Saarbrücken, Saarbrücken/DE
<b>G. Hessler</b>	Sanofi-Aventis Deutschland GmbH, Frankfurt (Main)/DE (Chairman of the GDCh division)
<b>A. K. H. Hirsch</b>	University of Saarbrücken, Saarbrücken/DE
<b>T. Langer</b>	University of Vienna, Vienna/AT
<b>J. Lefranc</b>	Merck, Darmstadt/DE (NextGenMedChem)
<b>N. Schützenmeister</b>	University of Vienna, Vienna/AT
<b>F. von Nussbaum</b>	Nuvisan ICB GmbH, Berlin/DE
<b>B. Wunsch</b>	University of Münster, Münster/DE

### ORGANISATION COMMITTEE

<b>C. Birkner</b>	Frankfurt (Main)/DE
<b>M. Bundschuh</b>	Frankfurt (Main)/DE
<b>D. Krizan</b>	University of Vienna/AT
<b>T. Langer</b>	University of Vienna/AT
<b>S. Werner</b>	University of Vienna/AT



Monday, April 3, 2023

## Lecture Hall C1

10.30 a.m. **General Meeting of the GDCh Division on Medicinal Chemistry**  
**Mitgliederversammlung der GDCh-Fachgruppe Medizinische Chemie**  
 (Gäste sind herzlich Willkommen)

**Tagesordnung:**

1. Begrüßung – Tagesordnung – Protokoll der Mitgliederversammlung vom 4. November 2021
2. Der Vorstand 2023-2026 stellt sich vor
3. Bericht des Vorstands
4. NextGenMedChem
5. Veranstaltungen der Fachgruppe
6. Preise der Fachgruppe
7. Was wünscht sich die Mitgliedschaft?
8. Verschiedenes

11.15 a.m. **General Meeting of the DPhG Division of Pharmaceutical/Medicinal Chemistry**  
**Mitgliederversammlung der DPhG-Fachgruppe Pharmazeutisch-Chemische Chemie**  
 (Gäste sind herzlich Willkommen)

**Tagesordnung:**

1. Feststellung der Tagesordnung
2. Bericht und Diskussion über die Novellierung der Approbationsordnung AAppO
3. Zukünftige Tagungen „Frontiers in Medicinal Chemistry“
4. Weitere zukünftige Tagungen
5. Verschiedenes

**The leading producer. The World's Largest Stock Catalogues**

- 284,000 building blocks
- 4,000,000 screening compounds

**Original innovative design**

- Custom libraries for your compound collection enhancement
- Medicinal chemistry services with immediate access to advanced building blocks

**Integrated Discovery Services**

- High throughput screening in new chemical space
- Hit-to-lead and lead optimization, ADMET and *in-vivo* PK



www.enaminestore.com

Monday, April 3, 2023

Lecture Hall C1

1.00 p.m. **WELCOME**  
Prof. Dr. Thierry Langer (Chairman), Dr. Gerhard Hessler (Chair of the Division)

### Medicinal Chemistry Highlights & Fresh Case Studies

Chair: Darryl McConnell, Vienna

1.15 p.m. **Identification of the in vivo active KRAS G12C Inhibitor BI-0474 via Fragment Based Screening and Optimization of Reversible Binding to KRAS**  
J. Bröker, Vienna/AT

1.45 p.m. **Discovery of M4205 (IDRX-42), a highly selective inhibitor of KIT mutations**  
A. Blum, Darmstadt/DE, D. Dorsch, N. Linde, H.-P. Buchstaller, N. Glaser, U. Grädler, C. Petersson, H. Schieferstein, E. Sherbetjian, C. Esdar, Darmstadt/DE

2.15 p.m. **Discovery of the TASK-1 and TASK-3 Channel Blocker BAY 2586116 for the Treatment of Obstructive Sleep Apnea (OSA)**  
M. G. Hahn, Wuppertal/DE

2.45 p.m. COFFEE BREAK

### PhD Prize Award Ceremony

3.15 p.m. **Exploring bacterial metalloproteases as promising drug targets**  
A. Alhayek, Saarbrücken/DE

**Use of styrylbenzothiazole photoswitches in drugs for spatiotemporal control over microtubule-dependent biology**  
L. Gao, Munich/DE

### New Chemistry & modern MedChem Methods

Chair: Peter Ettmayer, Vienna

3.45 p.m. **Novel Methods in Photochemistry and Photocatalysis**  
D. Leonori, Aachen/DE

4.15 p.m. **Application of Emerging Synthetic Technologies to Fragment Based Drug Discovery**  
C. Griffiths-Jones, Cambridge/GB

4.45 p.m. **The beautiful simplicity of rearrangements: towards ideal reactions?**  
N. Maulide, Vienna/AT

5.15 p.m. **Poster Session I**

Foyer

6.15 p.m. **Get together**

Tuesday, April 4, 2023

Lecture Hall C1

### Molecular Glues & Degraders

Chair: Michael Gütschow, Bonn

8.30 a.m. **Identification and characterization of small-molecule degraders**  
G. E. Winter, Vienna/AT

9.00 a.m. **Discovery of selective and orally bioavailable VHL-recruiting SMARCA2 PROTACs**  
N. Trainor, Melbourne/AU, C. Kofink, B. Mair, H. Weinstabl, Vienna/AT, W. Farnaby, Dundee/GB

9.30 a.m. **Development of pre-loaded solid-phase resins for the synthesis of heterobifunctional histone deacetylase (HDAC) degraders**  
F. K. Hansen, Bonn/DE

10.00 a.m. COFFEE BREAK

### Young Investigators

Chair: Nina Schützenmeister, Vienna

10.30 a.m. **A new class of bioreductive prodrugs to harness dithiol-type oxidoreductases**  
O. Thorn-Seshold, Munich/DE, L. Zeisel, J. Felber, J. Thorn-Seshold, A. Kitowski, Munich/DE

10.45 a.m. **Towards a Highly Isoform-Selective Covalent Chemical Probe for the Protein Kinase S6K2**  
M. Gehringer, Tübingen/DE

11.00 a.m. **Development of cyclic peptides as inhibitors of the complement system – towards high affinity and prolonged target residence time**  
C. Lamers, Leipzig/DE, M. Smiesko, Basel/CH, P. Gros, Utrecht/NL, J. D. Lambris, Philadelphia/US, D. Ricklin, Basel/CH

11.15 a.m. **Alkyne and  $\beta$ -lactam warheads have potential for covalent inhibition of the SARS-CoV-2 main protease**  
L. Brewitz, Oxford/GB, L. Dumjahn, Y. Zhao, C. J. Schofield, Oxford/GB

11.30 a.m. **A Fragment-Based Drug Discovery Approach for the Development of Small Molecules Targeting Caspase-2**  
S. Pockes, Regensburg/DE

11.45 a.m. **Design, synthesis and biological activity of a new class of inhibitors of the virulence factor Elastase B in *Pseudomonas aeruginosa***  
G. Jézéquel, Saarbrücken/DE, J. Konstantinovic, D. Kellig, A. Kany, J. Haupenthal, A. K. H. Hirsch, Saarbrücken/DE

Tuesday, April 4, 2023

Lecture Hall C1

## Innovation Award

*Chair: Christian Ducho, Saarbrücken*12.00 p.m. **Laudatio Innovation Award Medicinal/Pharmaceutical Chemistry**12.15 p.m. **AWARD LECTURE****Targeting from the inside - New approaches for GPCR-based drug discovery**M. Schiedel, Erlangen/DE, M. E. Huber, L. Toy, M. F. Schmidt, J. Budzinski,  
M. F. N. Merten, E. Kostenis, D. Weikert, Erlangen/DE12.30 p.m. **LUNCH BREAK****LUNCH WORKSHOP**12.30 – 1.20 p.m. **BioSolveIT “In a Dialog with Your Target Complex: Interactive Compound Evolution”****In Silico Solution in MedChem***Chair: Gerhard Hessler, Frankfurt*1.30 p.m. **The NeuroDeRisk IL Profiler: DeRisking Chemical Structures for Neurotoxic Adverse Outcomes**S. D. Bryant, Vienna/AT1.50 p.m. **In silico safety model deployment at early pharmaceutical R&D stages**F. Schmidt, Frankfurt (Main)/DE2.10 p.m. **Chemical Space Docking: Novel ROCK1 Kinase Inhibitors found by Large-Scale Structure-Based Virtual Screening**F.-M. Klingler, London/GB, P. Beroza, J. J. Crawford, San Francisco/US,  
O. Ganichkin, Munich/DE, L. Gendele, S. F. Harris, San Francisco/US,  
R. Klein, Sankt Augustin/DE, A. Miu, San Francisco/US, S. Steinbacher,  
Munich/DE, C. Lemmen, Sankt Augustin/DE2.30 p.m. **COFFEE BREAK**3.00 p.m. **Poster Session II**

Tuesday, April 4, 2023

Lecture Hall C1

## Next Generation Drugs

*Chair: Eleonora Diamanti, Saarbrücken, Julien Lefranc, Darmstadt*4.00 p.m. **Discovery of LNP023, a First-in-Class, Oral Factor B Inhibitor for Treatment of Rare Alternative Complement Pathway Driven Diseases**S. Flohr, Basel/CH4.30 p.m. **Hunting for Hippo: Allosteric Inhibitors of the YAP/TEAD Protein-Protein Interaction**J. Crawford, San Francisco/US5.00 p.m. **Discovery and optimisation of potent, slow-dissociating inhaled PI4KB inhibitors**S. Bertrand, Stevenage/GB*Chair: Anna Hirsch, Saarbrücken*5.30 p.m. **PLENARY LECTURE**  
**Adventures in Neuropharmacology**D. Trauner, Philadelphia/US7.30 p.m. **Conference Dinner**

Wednesday, April 5, 2023

Lecture Hall C1

## Translational Science Case Studies

*Chair: Stefan Laufer, Tübingen*

- 8.30 a.m. **Case Studies in Professional Translational Research**  
P. Nussbaumer, Dortmund/DE
- 9.00 a.m. **Approaches towards innovative anti-infectives from microbes**  
R. Müller, Saarbrücken/DE
- 9.30 a.m. **Atomistic details of protein-drug engagement in solution**  
G. Platzer, Vienna/AT
- 9.50 a.m. **Small molecules blocking the cytolytic effects of the toxin pneumolysin generated by protein-templated aldol condensation**  
J. Rademann, Berlin/DE, U. B. A. Aziz, M. Bermudez, M. Mieth, A. Saoud, G. Wolber, A. Hocke, Berlin/DE

10.10 a.m. COFFEE BREAK

## RNA Modifying Enzyme

*Chair: Yann Foricher, Paris*

- 10.40 a.m. **Development of anti-viral inhibitors against SARS-CoV-2 using NNR-supported drug discovery**  
H. Schwalbe, Frankfurt (Main)/DE
- 11.10 a.m. **Optical Control of mRNA Translation**  
A. Rentmeister, Münster/DE
- 11.40 a.m. **Targeting RNA Methyltransferases with small molecules**  
M. Helm, Mainz/DE
- Chair: Franz von Nussbaum, Berlin*
- 12.10 a.m. **FRIEDRICH STOLZ-AWARD**  
**Recent Progress in the Discovery of Selective Inhibitors of Steroid Hormone Biosynthesis**  
R. Hartmann, Saarbrücken/DE

12.35 p.m. LUNCH BREAK

Wednesday, April 5, 2023

Lecture Hall C1

## Medicinal Chemistry Case Studies

*Chair: Bernhard Wunsch, Münster*

- 1.30 p.m. **Insight into the Axial Chirality in Drugs**  
H. Takahashi, Tokyo/JP
- 2.00 p.m. **Discovery of RMC-5552, a selective bi-steric inhibitor of mTORC1 that suppresses 4EBP1 phosphorylation, for the treatment of mTORC1-activated tumors including RAS pathway escape**  
G. L. Burnett, Redwood City/US, M. Gliedt, C. M. Semko, J. Jiang, Y. C. Yang, C. J. Schulze, A. Marquez, J. W. Evans, S. L. Wilson, T. Hsieh, Z. C. Wang, B. J. Lee, T. J. Choi, D. F. Reyes, Y. Zhao, D. Wildes, Z. P. Wang, M. Singh, J. A. M. Smith, A. L. Gill, Redwood City/US

2.30 p.m. COFFEE BREAK

## Medicinal Chemistry Case Studies

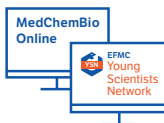
*Chair: Thierry Langer, Vienna*

- 3.00 p.m. **Development of a chemical toolbox for the neuroprotective transcription factor Nurr1**  
D. Merk, Munich/DE
- 3.20 p.m. **Novel METTL3 Inhibitors as Potential Cancer Therapies**  
M. Fyfe, Cambridge/GB, N. Webster, B. Andrews, R. Fosbeary, P. Guest, D. Hardick, B. Thomas, N. Irigoyen, M. Eleftheriou, M. Gozdecka, J. Dias, E. Yankova, W. Blackaby, M. Albertella, J. Rak, E. De Braekeleer, G. Tsagkogeorga, D. Aspris, D. Leggate, A. Hendrick, A. Bannister, G. Vassiliou, O. Rausch, K. Tzelepis, T. Kouzarides, Cambridge/GB
- 3.40 p.m. **Redirecting the Peptide Cleavage: Ultrapotent Cathepsin B Inhibitors with Inversely Oriented Warheads**  
M. Gütschow, Bonn/DE
- 4.00 p.m. **BAY-7081 – A cyanopyridone-based PDE9A inhibitor**  
D. Meibom, Wuppertal/DE
- 4.30 p.m. **Closing**



Upcoming Events

**EFMC-YSN MedChemBioOnline**  
Webinars mixing science, soft-skills training  
& round table discussions  
[www.efmc.info/efmc-ysn-medchembioonline](http://www.efmc.info/efmc-ysn-medchembioonline)



**17th EFMC Short Course on Medicinal Chemistry**  
Oegstgeest, The Netherlands | April 23-26, 2023



**EFMC-ASMC'25**  
**IX International Symposium on Advances in Synthetic and Medicinal Chemistry**  
Zagreb, Croatia | September 3-7, 2023



**EFMC-YMCS 2023**  
**10th EFMC Young Medicinal Chemists' Symposium**  
Zagreb, Croatia | September 7-8, 2023



**EFMC-ISCB 2023**  
**International Symposium on Chemical Biology**  
Basel, Switzerland | November 16-18, 2023



Awards

- The Nauta Pharmacology Award for Medicinal Chemistry and Chemical Biology
- The "UCB-Ehrlich Award for Excellence in Medicinal Chemistry"
- Prous Institute - Overton and Meyer Award for New Technologies in Drug Discovery
- The "EFMC-WuXi AppTec Award for Excellence in Chemical Biology"

Visit [www.efmc.info/awards](http://www.efmc.info/awards) for more information

Prizes

- EFMC Prizes for Young Medicinal Chemists in Industry & Academia
- EFMC-YSN PhD Prize
- Symeres PhD Prize for Excellence in Chemistry in Life Sciences Research

Visit [www.efmc.info/prizes](http://www.efmc.info/prizes) for more information

EFMC-YSN

**The Young Scientists Network**  
Building a strong network at an early stage in your career is crucial!  
The aim of the EFMC-YSN is to **inspire, connect and provide opportunities** to medicinal chemists and chemical biologists in their Early Career.  
Visit [www.efmc.info/ysn](http://www.efmc.info/ysn) for more information

- P001 **Greenpharma-Prestwick Chemical: Complementary Tools to support Drug Discovery**  
M. L. Jung, Orléans/FR, B. Didier, Illkirch/FR, Q. T. Do, Orléans/FR
- P002 **Benchmarking successive virtual screening**  
M. Modest von Korff, Allschwil/CH, T. Sander, Allschwil/CH, J. Wahl, Allschwil/CH
- P003 **A Biomolecular Sensor Based on Chemically Functionalized Polymeric Ion Conducting Nanopores for Medical Diagnostics**  
W. Ensinger, Darmstadt/DE
- P004 **Synthesis, Structure-Activity Relationships and Biological Evaluation of 2-Phenoxybenzimidazoles as Antiplasmodial Agents**  
T. Hermann, Graz/AT, R. Weis, Graz/AT
- P005 **Beneficial modulation of inflammatory mediators by inhibition of GSK3 $\beta$  and CDKs with indirubin derivatives in human monocytes**  
V. Bachmann, Jena/DE, P. Schädel, Jena/DE, F. Schömborg, Jena/DE, M. Peric, Jena/DE, I. Vilotijevic, Jena/DE, O. Werz, Jena/DE
- P006 **Addressing the Energy Coupling Factor Transporters as Novel Anti-Infective Target**  
E. Diamanti, Saarbrücken/DE, M. Hamed, Saarbrücken/DE, I. Exapicheidou, Saarbrücken/DE, A. Shams, Saarbrücken/DE, P. Souza, Lyon/FR, D. Slotboom, Groningen/NL
- P007 **Raloxifene as PhzB inhibitor: aryl replacement and its effect on pyocyanin inhibition in *Pseudomonas aeruginosa***  
M. Zimmermann, Braunschweig/DE, M. Thiemann, Braunschweig/DE, J. Baumgarten, Braunschweig/DE, W. Blankenfeldt, Braunschweig/DE, C. Kunick, Braunschweig/DE
- P008 **Structure based development of pyocyanin inhibitors as pathoblockers against *Pseudomonas aeruginosa***  
M. Thiemann, Braunschweig/DE, M. Zimmermann, Braunschweig/DE, J. Baumgarten, Braunschweig/DE, W. Blankenfeldt, Braunschweig/DE, C. Kunick, Braunschweig/DE
- P010 **Controlling cell membrane permeability: from membrane damage probes to intracellularly retained enzyme imaging probes**  
P. Mauker, Munich/DE, D. Beckmann, Munich/DE, N. A. Veprek, Munich/DE, O. Thorn-Seshold, Munich/DE
- P011 **A consensus compound/bioactivity dataset for chemogenomics and application to the nuclear receptor subfamily NR1**  
L. Isigkeit, Frankfurt (Main)/DE, E. Schallmayer, Frankfurt (Main)/DE, A. Chaikuad, Frankfurt (Main)/DE, D. Merk, Munich/DE
- P012 **Discovery and structure-activity relationship studies of fatty acid mimetic Nurr1 ligands**  
T. Stiller, Munich/DE, D. Merk, Munich/DE



- P013 **Establishing structure-activity relationships of a TLX lead agonist**  
E. C. Hank, Munich/DE, D. Merk, Munich/DE
- P014 **5-Lipoxygenase-activating protein (FLAP) antagonists differentially modulate leukotriene and specialized pro-resolving lipid mediator (SPM) biosynthesis**  
P. Dahlke, Jena/DE, P. M. Jordan, Jena/DE, O. Werz, Jena/DE
- P015 **A Domino 10-Step Total Synthesis of FR252921 and Its Analogues, Complex Macrocyclic Immunosuppressants**  
T. Leischner, Vienna/AT, M. Schupp, Vienna/AT, I. Saridakis, Vienna/AT, H. Zhang, Vienna /AT, N. Maulide, Vienna/AT
- P016 **A Practical Guide to FAIR Research Data Management in Medicinal Chemistry**  
B. Golub, Braunschweig/DE, C. Draheim, Braunschweig/DE, S. Wulle, Braunschweig/DE
- P017 **Towards modulation of polymicrobial communities in chronic lung diseases through targeting the Carbon Storage regulator A (CsrA)**  
B. G. E. Zoller, Saarbrücken/DE, Y Wu, Saarbrücken/DE, V. Jakob, Saarbrücken/DE, M. Hust, Saarbrücken/DE, M. Empting, Saarbrücken/DE
- P018 **Design, Synthesis and Evaluation of First-In-Class Covalent KRas<sup>G13C</sup> Inhibitors**  
T. Kirschner, Dortmund/DE, J. D. Warmuth, Dortmund/DE, J. N. Wiese, Dortmund/DE, M. Beerbaum, Dortmund/DE, M. P. Müller, Dortmund/DE, D. Rauh, Dortmund/DE
- P019 **Targeting the fatty acid binding pocket of SARS- CoV-2 Spike Protein Receptor-Binding Domain (RBD)**  
E. Kosche, Saarbrücken/DE, R. Creutzmacher, Lübeck/DE, T. Maass, Lübeck/DE, T. Krey, Lübeck/DE, T. Peters, Lübeck/DE, M. Empting, Saarbrücken/DE
- P020 **Synthesis and biological evaluation of inhibitors of the lysine methyltransferase KMT9**  
V. Hazai, Freiburg/DE, S. Klein, Freiburg/DE, G. Rennar, Freiburg/DE, N. Barthes, Freiburg/DE, M. Staudt, Freiburg/DE, J. Bacher, Freiburg/DE, S. Wang, Freiburg/DE, E. Metzger, Freiburg/DE, R. Schüle, Freiburg/DE, M. Jung, Freiburg/DE
- P021 **Evaluation of machine learning models for the de novo design of dual ligands**  
K. Scholz, Munich/DE, T. Hörmann, Munich/DE, L. Isigkeit, Frankfurt (Main)/DE, D. Merk, Munich/DE
- P022 **Mechanistic Insights on Molecular Glue Degradation Gained from SAR Studies**  
F. Forster, Vienna/AT, G. Zenkeviciute, Vienna/AT, X. Farge, Vienna/AT, D. Gassner, Vienna/AT, A. Donald, Vienna/AT, D. Thomson, Vienna/AT, M. Brand, Vienna/AT
- P023 **Structural optimization of oxaprozin for selective inverse Nurr1 agonism**  
S. Willems, Munich/DE, S. Schierle, Frankfurt/DE, L. Rüger, Frankfurt/DE, M. Ballarotto, Munich/DE, J. Pabel, Munich/DE, F. Nawa, Munich/DE, J. Ohrndorf, Frankfurt/DE, S. Arifi, Frankfurt/DE, D. Zaienne, Frankfurt/DE, D. Merk, Munich/DE

- P024 **Structure-based design and synthesis of HDAC10 epigenetic inhibitors**  
F. Mahmoudi, Halle (Saale)/DE, P. Zeyen, Halle (Saale)/DE, Y. Zeyn, Mainz/DE, M. Zessin, Halle (Saale)/DE, M. Schutkowski, Halle (Saale)/DE, O. H. Krämer, Mainz/DE, W. Sippl, Halle (Saale)/DE
- P025 **Design and synthesis of novel inhibitors targeting the RNA binding protein IGF2BP2/IMP2 for cancer therapy**  
K. Wagner, Saarbrücken/DE, Y. Wu, Saarbrücken/DE, B. Zoller, Saarbrücken/DE, C. Dahlem, Saarbrücken/DE, A. K. Kiemer, Saarbrücken/DE, S. Both, Saarbrücken/DE, M. Empting, Saarbrücken/DE
- P026 **Development of potent and selective inhibitor of the carnitine biosynthesis enzyme  $\gamma$ -butyrobetaine hydroxylase (BBOX)**  
S. Basak, Oxford/GB, E. Salah, Oxford/GB, A. Tumber, Oxford/GB, M. Jabbary, Oxford/GB, S. Sharma, Oxford/GB, C. Schofield, Oxford/GB
- P027 **Development of a pH-acetonitrile double gradient HPLC method for physico-chemical characterisation of small bioactive compounds**  
N. Neitzke, Halle (Saale)/DE, L. Müller, Halle (Saale)/DE, P. Froberg, Halle (Saale)/DE
- P028 **Structure-activity relationship study of novel antimalarial targeting IspD in the methylerythritol phosphate pathway**  
D. Willocx, Saarbrücken/DE, P. Bravo, Basel/CH, E. Diamanti, Saarbrücken/DE, M. Hamed, Saarbrücken/DE, B. Illarionov, Hamburg/DE, M. Witschel, Ludwigshafen/DE, A. K. H. Hirsch, Saarbrücken/DE
- P030 **Thiazolidinedione HDAC inhibitors**  
F.-J. Meyer-Almes, Darmstadt/DE, C. S. Ramaa, Mumbai/IN
- P031 **Novel BODIPY-Based Photothermal Agents for Cancer Treatment**  
L. Schneider, Zürich/CH, M. Kalt, Zürich/CH, B. Spingler, Zürich/CH
- P032 **Maskwiomin: Investigation of Medicinal Properties of a Canadian Indigenous Topical Skin Remedy made from Birch Bark**  
M. Bierenstiel, Sydney/CA, R. Kaliaperumal, Sydney/CA, T. Young, Sydney/CA
- P033 **Organocatalysis meets enzyme catalysis – controlling DNA repair at will**  
M. Michel, Stockholm/SE
- P034 **Structure-based virtual screening yields first-in-class inhibitors of the anti-infective target 1-deoxy-D-xylulose-5-phosphate synthase (DXPS)**  
A. Lacour, Saarbrücken/DE, E. Diamanti, Saarbrücken/DE, Z. Hamid, Saarbrücken/DE, S. Eisa, Saarbrücken/DE, A. H. K. Hirsch, Saarbrücken/DE
- P035 **Unveiling the complete profile and syntheses of active molecules with Reaxys Academic Edition, a tool for every chemist**  
G. Monceli, Amsterdam/NL

- P036 **Development of Bioactive Compounds Suppressing the Activation of Pathogenic Fibroblastss**  
V. Mavrikaki, Vari/GR, D. Papadopoulou, Vari/GR, F. Charalampous, Vari/GR, D. Georgiadis, Athens/GR, G. Kollias, Vari/GR, A. Matralis, Vari/GR
- P037 **Stereoselectivity in drug membrane transport**  
 M. Rafehi, Göttingen/DE, S. M. Stefan, Lübeck/DE, L. Gebauer, Göttingen/DE, O. Jensen, Göttingen/DE, J. Brockmüller, Göttingen/DE
- P039 **Medicinal Polypharmacology and Its High Potential to Explore Undruggable Targets of the Future**  
 S. M. Stefan, Lübeck/DE, K. Stefan, Oslo/NO, M. Rafehi, Göttingen/DE, J. Pahnke, Oslo/NO, V. Namasivayam, Lübeck/DE
- P040 **Photoactivated chemotherapy - a novel strategy for caging chemotherapeutics**  
 S. K. Goetzfried, Leiden/NL, A. Busemann, Leiden/NL, S. Bonnet, Leiden/NL
- P041 **Automated Nano Synthesis-based Drug Discovery**  
 A. Dömling, Olomouc/CZ
- P042 **Induction of specialized pro-resolving mediator formation and inhibition of eicosanoid biosynthesis, a novel anti-inflammatory class-effect of cannabinoids**  
 L. K. Peltner, Jena/DE, L. Gluthmann, Jena/DE, F. Börner, Jena/DE, S. Pace, Jena/DE, C. Kretzer, Jena/DE, R. Bilancia, Naples/IT, F. Pollastro, Novara/IT, A. Koeberle, Innsbruck/AT, G. Appendino, Novara/IT, A. Rossi, Naples/IT, M. E. Newcomer, Baton Rouge/US, N. C. Gilbert, Baton Rouge/US, P. M. Jordan, Jena/DE, O. Werz, Jena/DE
- P043 **Discovery of Submicromolar Inhibitors of the Virulence Factor LasB from *Pseudomonas aeruginosa* using Rational Design**  
 C. Schütz, Saarbrücken/DE, S. Speicher, Saarbrücken/DE, D. Kolling, Saarbrücken/DE, K. Rox, Braunschweig/DE, A. F. Kiefer, Saarbrücken/DE, A. M. Kany, Saarbrücken/DE, J. Konstantinovic, Saarbrücken/DE, A. Sikandar, Saarbrücken/DE, R. P. Jumde, Saarbrücken/DE, A. Klein, Saarbrücken/
- P044 **2-Aryl Indole Derivatives as Activators of DNA Glycosylase OGG1**  
 F. Ortis, Stockholm/SE, M. Varga, St. Andrews/GB, O. Wallner, Stockholm/SE, E. Homan, Stockholm/SE, T. Helleday, Stockholm/SE, P. Andersson, Stockholm/SE, M. Michel, Stockholm/SE
- P045 **Mining Novel and Relevant Chemistry from Billion-Sized Chemical Spaces**  
 A. Neumann, Sankt Augustin/DE, M. Gastreich, Sankt Augustin/DE
- P046 **Learning to block bacterial pathogenicity – how to exploit this new anti-infective modality on the example of quorum sensing inhibitors**  
 M. Empting, Saarbrücken/DE

- P047 **Cyclic disulfides extend the reach of bioreductive prodrugs: applications to seco-duocarmycins targeting the thioredoxin system**  
 J. G. Felber, Munich/DE, L. Zeisel, Munich/DE, A. Kitowski, Munich/DE, J. Thorn-Seshold, Munich/DE, O. Thorn-Seshold, Munich/DE
- P048 **Designing Selective Drug-like Molecular Glues of the Glucocorticoid Receptor/14-3-3 Protein-Protein Interaction**  
 J. S. Pallesen, Gothenburg/SE, C. C. Munier, Gothenburg/SE, F. Bosica, Gothenburg/SE, S. A. Andrei, Eindhoven/NL, K. Edman, Gothenburg/SE, A. Gunnarsson, Gothenburg/SE, G. La Sala, Gothenburg/SE, O. D. Putra, Gothenburg/SE, S. Srdanovic, Leeds/GB, A. Wilson, Leeds/GB, L. Wissler, Gothenburg/SE, C. Ottmann, Eindhoven/NL, M. W. D. Perry, Gothenburg/SE, G. O'Mahony, Gothenburg/SE
- P049 **Computer-aided search for multi-target-directed ligands blocking PDE4B, PDE8A and TRPA1 with potential application in the pharmacotherapy of asthma and COPD**  
 A. Gawalska, Cracow/PL, N. Czub, Cracow/PL, A. Mendyk, Cracow/PL, A. Bucki, Cracow/PL, M. Kołaczkowski, Cracow/PL
- P050 **Machine Learning-Based Scoring Function for Virtual Screening of New 5-HT<sub>6</sub>R Ligand Candidates**  
 M. Sapa, Cracow/PL, A. Gawalska, Cracow/PL, M. Kołaczkowski, Cracow/PL, A. Bucki, Cracow/PL
- P052 **A novel class of antimalarials targeting the parasite's lactate/H<sup>+</sup> symporter**  
 C. Nerlich, Kiel/DE, E. Beitz, Kiel/DE
- P053 **Novel Dimerized Peptides Bind VEGF with High Affinity and Display Anti-Angiogenesis Activity**  
 X. Ye, Paris/FR, J. François-Gaucher, Paris/FR, L. Wang, Hangzhou/CN, H. Hu, Hangzhou/CN, M. Vidal, Paris/FR, F. Broussy, Paris/FR
- P054 **Functional characterization of the intracellular catalytic complex from *Plasmodium falciparum* cation ATPase 4**  
 T. Beyer, Kiel/DE, J. Caliebe, Kiel/DE, E. Beitz, Kiel/DE
- P055 **On-The-Fly Small Molecule Docking with JAMDA on ProteinsPlus**  
 C. Ehrh, Hamburg/DE, F. Flachsenberg, Hamburg/DE, T. Gutermuth, Hamburg/DE, M. Rarey, Hamburg/DE
- P056 **Fluorescent ligands targeting the intracellular allosteric binding site of the chemokine receptor CCR2**  
 L. Toy, Erlangen/DE, M. E. Huber, Erlangen/DE, M. F. Schmidt, Erlangen/DE, D. Weikert, Erlangen/DE, M. Schiedel, Erlangen/DE

- P057 **Photocaging of Pyridinylimidazole Based Covalent JNK3 Inhibitors Affords Spatiotemporal Control of the Binding Affinity in Live Cells**  
B. S. Hoffelner, Regensburg/DE, S. Andreev, Regensburg/DE, N. Plank, Regensburg/DE, P. Koch, Regensburg/DE
- P058 **Fighting chronic inflammation via dual sEH/FLAP inhibition: Synthesis of difl-apolin derivatives containing a naphthyridine or quinoline core**  
T. Hasenoehrl, Innsbruck/AT, B. Matuszczak, Innsbruck/AT, D. Schuster, Salzburg/AT, A. Koeberle, Innsbruck/AT, V. Temml, Salzburg/AT, L. Walzl, Innsbruck/AT, L. Aulinger, Innsbruck/AT, A. Lutz, Innsbruck/AT
- P059 **Pentafluorophosphato-phenylalanines are novel, amphiphilic biomimetics of phosphotyrosine**  
M. Tiemann, Berlin/DE, M. Accorsi, Berlin/DE, L. Wehrhan, Berlin/DE, L. M. Finn, Berlin/DE, R. Cruz, Berlin/DE, M. Rautenberg, Berlin/DE, F. Emmerling, Berlin/DE, J. Heberle, Berlin/DE, B. G. Keller, Berlin/DE, J. Rademann, Berlin/DE
- P060 **Synthesis and biological evaluation of major metabolites of highly active 1,3,5-triazine ligands of the serotonin 5-HT<sub>6</sub> receptor as therapeutic prospects for Alzheimer's disease**  
K. Czarnota-Lydkka, Kraków/PL, S. Sudoł-Tałaj, Kraków/PL, K. Kucwaj-Brysz, Kraków/PL, M. Głuch-Lutwin, Kraków/PL, B. Mordyl, Kraków/PL, G. Latacz, Kraków/PL, J. Handzlik, Kraków/PL
- P061 **Development of synthetic modulators of the nuclear receptor LHR-1**  
A. Lang, Frankfurt (Main)/DE, M. Schubert-Zsilavec, Frankfurt (Main)/DE, D. Merk, Munich/DE
- P062 **New inhibitors of aldo-keto reductase 1C3 (AKR1C3) and carbonyl reductase 1 (CBR1) with the potential to support anticancer activity and protect from cardiotoxicity of anthracycline antibiotics**  
M. Jamrozik, Cracow/PL, K. Piska, Cracow/PL, A. Bucki, Cracow/PL, P. Koczurkiewicz-Adamczyk, Cracow/PL, E. Pękała, Cracow/PL, M. Kołaczkowski, Cracow/PL
- P063 **Indazole Isomers as GluN2B-Selective NMDA Receptor Antagonists: Synthesis without Protective Groups**  
J. Lüken, Münster/DE, B. Wunsch, Münster/DE
- P064 **Molecular modeling and chemical optimization of fragment-based inhibitors of STAT5b as a novel anti-leukemia strategy**  
A. M. Ambros, Berlin/DE, C. Arkona, Berlin/DE, G. Wolber, Berlin/DE, J. Rademann, Berlin/DE
- P065 **Structure-based design of covalent ligands for the p97 N-domain**  
S. Böhler, Würzburg/DE, S. Bothe, Würzburg/DE, P. Hänzelmann, Würzburg/DE, H. Schindelin, Würzburg/DE, C. Sotriffer, Würzburg/DE

- P066 **Structure-based screening for inhibitors of the Vaccinia virus RNA polymerase complex**  
C. Herbst, Würzburg/DE, J. Bartuli, Würzburg/DE, C. Grimm, Würzburg/DE, U. Fischer, Würzburg/DE, C. Sotriffer, Würzburg/DE
- P067 **Nucleobase-inspired catalysts for the enzymatic activation of 8-oxo Guanine DNA Glycosylase 1**  
N. D'Arcy-Evans, St. Andrews/GB, E. Hank, Munich/DE, O. Wallner, Stockholm/SE, L. Meng, Stockholm/SE, P. Calvo, Madrid/ES, E. Scaletti, Stockholm/SE, F. Ortis, Stockholm/SE, S. Kosnenina, Stockholm/SE, E. Holman, Stockholm/SE, E. Wiita, Stockholm/SE, A. Jemth, Stockholm/SE, C. Benitez-Buelga, Stockholm/SE, O. Mortusewicz, Stockholm/SE, K. Sanjiv, Stockholm/SE, M. Scobie, Stockholm/SE, T. Helleday, Stockholm/SE, P. Stenmark, Stockholm/SE, M. de Vega, Madrid/ES, M. Michel, Stockholm/SE
- P068 **Design and Synthesis of Tyrosine-Targeting Covalent Inhibitors for the Janus Kinase 3**  
L. Hillebrand, Tübingen/DE, A. Rasch, Tübingen/DE, M. Gehringer, Tübingen/DE
- P069 **Development of a Highly Isoform-Selective and Potent S6K2 Kinase Inhibitor**  
L. Haarer, Tübingen/DE, S. Gerstenecker, Tübingen/DE, M. Gehringer, Tübingen/DE
- P070 **Altered Substrate Specificity in Okur-Chung Neurodevelopmental Syndrome Mutant CK2 $\alpha^{Lys198Arg}$ ; structural and enzymological evidence**  
A. Gast, Münster/DE, C. Werner, Cologne/DE, D. Lindenblatt, Cologne/DE, A. Nickelsen, Münster/DE, K. Niefind, Cologne/DE, J. Hochscherf, Cologne/DE, J. Jose, Münster/DE
- P071 **Palladium-labile prodrugs for the prevention of implant-associated bacterial biofilms**  
J. Braun, Munich/DE, M. C. Ortega Liebana, Granada/ES, M. Bauer, Munich/DE, O. Lieleg, Munich/DE, V. Sebastian, Zaragoza/ES, A. Unciti-Broceta, Edinburgh/GB, S. Sieber, Munich/DE
- P072 **The histamine H3 receptor antagonist E169 counteracts memory impairments induced by dizocilpine and modulates overexpression of PI3K, Akt and GSK-3 $\beta$  proteins in mice**  
B. Sadek, Abu Dhabi/AE
- P073 **Synthesis of novel harmine and dihydroartemisinin hybrid compounds**  
L. Bilandzija, Zagreb/HR, G. Poje, Zagreb/HR, Z. Rajic, Zagreb/HR
- P074 **Synthesis of novel amide-type harmisinins, hybrids based on beta-carboline and artesunate scaffolds**  
G. Poje, Zagreb/HR, R. Klaric-Kukuz, Zagreb/HR, Z. Rajic, Zagreb/HR

- P075 **Synthesis of cystobactamid analogs as antibiotics**  
M. Stappert, Braunschweig/DE, D. Kohnhäuser, Braunschweig/DE, G. Testolin, Braunschweig/DE, K. Cirnski, Saarbrücken/DE, J. Krull, Braunschweig/DE, J. Herrmann, Saarbrücken/DE, A. Kirschning, Hannover/DE, R. Müller, Saarbrücken/DE, M. Brönstrup, Braunschweig/DE
- P076 **Unlocking Gram-negative Activity through the Addition of a Positive Charge to an Antimalarial Compound**  
M. Braun-Cornejo, Zoetermeer/NL, A. K. H. Hirsch, Saarbrücken/DE, M. Platteschorre, Zoetermeer/NL, V. de Vries, Zoetermeer/NL, D. Piet, Zoetermeer/NL, E. Diamanti, Saarbrücken/DE, J. Haupenthal, Saarbrücken/DE, P. Bravo, Basel/CH, V. Sonawane, Borstel/DE, N. Reiling, Borstel/DE, M. Rottmann, Basel/CH, P. Maas, Zoetermeer/NL
- P077 **Synthesis and characterization of modulators of the inflammatory cascade with a 1,2,4-triazole scaffold**  
L. Müller, Halle (Saale)/DE, N. Neitzke, Halle (Saale)/DE, R. Goddard, Mülheim (Ruhr)/DE, R. Seidel, Halle (Saale)/DE, L. Tietze, Leipzig/DE, P. Froberg, Halle (Saale)/DE
- P078 **Biological Evaluation of Halogenated Rubrolide Analogues**  
J. de Vries, Vienna/AT, M. Assmann, Hamburg/DE, N. Schützenmeister, Vienna/AT
- P079 **Novel  $\kappa$ -Opioid Receptor Agonists for the treatment and understanding of Neuroinflammation**  
L. Flämig, Münster/DE, B. Wunsch, Münster/DE, M. Bermúdez, Münster/DE
- P080 **Discovery of Hedgehog Acyltransferase (HHAT) Inhibitors to Target Hedgehog Signalling in Cancer**  
E. S. Gavriil, London/GB, Z. Xiao, London/GB, S. Andrei, London/GB, L. Senatla, London/GB, C. E. Coupland, Oxford/GB, P. Kumar, Oxford/GB, L. Carrique, Oxford/GB, T. Lanyon-Hogg, Oxford/GB, C. Siebold, Oxford/GB, E. W. Tate, London/GB
- P081 **Chemical probes to study the role of the lysine demethylase LSD1 in Leishmania infection**  
A. Baniahmad, Freiburg/DE, J. Seitz, Freiburg/DE, J. Schulz-Fincke, Freiburg/DE, M. Jung, Freiburg/DE, G. Spaeth, Paris/FR
- P082 **Total synthesis of the 3R,9R,14R,17R diastereomer of depsipeptide PM181110, *in vitro* kinase activity, *in vivo* toxicology in wild-type zebra fish embryos *Danio rerio* and *in silico* docking**  
A. Kenfack Sipoho, Darmstadt/DE, B. Schmidt, Darmstadt/DE
- P083 **Synthesis and structure-activity relationships of novel P2Y<sub>2</sub> receptor antagonists**  
K. Schlegel, Münster/DE, A. Junker, Münster/DE
- P084 **Fragment-based design of mycobacterial thioredoxin reductase inhibitors: socializing a fragment by combining AI-based synthesis predictions with chemical space exploration.**  
P. Otten, Münster/DE, F. Füsser, Münster/DE, A. Junker, Münster/DE, O. Koch, Münster/DE

- P085 **Optimization of Covalent Inhibitors Targeting the Protein Kinase BMX**  
X. J. Liang, Tübingen/DE, C. Albertini, Bologna/IT, M. Gehringer, Tübingen/DE, 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
- P086 **Decoding the Mystery of Avapritinib's Binding Characteristics: A Study on its Interactions with PDGFRA and c-KIT in GIST-relevant Mutants**  
A. Teuber, Dortmund/DE, T. Schulz, Dortmund/DE, I. Landel, Dortmund/DE, R. Gontla, Dortmund/DE, S. B. Kleinbölting, Dortmund/DE, J. Niggenaber, Dortmund/DE, M. P. Müller, Dortmund/DE, D. Rauh, Dortmund/DE
- P087 **Targeting the nuclear receptor Nurr1 with potent statin derived fragments**  
J. P. Vietor, Munich/DE, S. Willems, Munich/DE, D. Merk, Munich/DE
- P088 **Developing an Orthogonal Assay Platform to Screen for Inhibitors of the Protein Methyltransferase METTL21A**  
M. Staudt, Freiburg/DE, L. Peng, Freiburg/DE, S. Wang, Freiburg/DE, E. Metzger, Freiburg/DE, R. Schüle, Freiburg/DE, M. Jung, Freiburg/DE
- P089 **Benzodiazepindione-based P2X<sub>4</sub>R antagonists – a structure-activity relationships study**  
K. S. Erlitz, Münster/DE, A. Junker, Münster/DE
- P090 **Development of novel retinoid X receptor modulators based on a tetrahydroquinoline scaffold**  
F. Nawa, Munich/DE, G. Faudone, Frankfurt (Main)/DE, D. Merk, Munich/DE
- P091 **Stereoselective synthesis of  $\beta$ -amino alcohols as novel GluN2B-selective NMDA receptor antagonists**  
M. Korff, Münster/DE, B. Wunsch, Münster/DE
- P092 **Total Synthesis of Prostaglandin A<sub>2</sub>**  
J. Lackner, Vienna/AT, N. Schützenmeister, Vienna/AT
- P093 **Synthesis of 4-Aminopiperidine-based Peptidomimetics as potential Human Blood Coagulation Factor FXIIa inhibitors**  
S. Platte, Münster/DE, D. Kalinin, Münster/DE
- P094 **Development and structural optimization of potent hepatic nuclear factor 4 $\alpha$  ligands**  
E. Schallmayer, Frankfurt (Main)/DE, I. Meijer, Frankfurt (Main)/DE, S. Willems, Munich/DE, D. Merk, Munich/DE
- P095 **Mechanistic profiling of chemical tools for the retinoid X receptor**  
R. Busch, Munich/DE, J. A. Marschner, Munich/DE, D. Merk, Munich/DE
- P096 **Synthesis of Cyclic  $\beta$ -Amino Alcohols**  
L. Supe, Riga/LV, I. Mutule, Riga/LV, T. Bengtsson, Stockholm/SE, B. Pelcman, Stockholm/SE



- P097 **X-Ray crystallography of inhibitor complexes of the human NAD<sup>+</sup>-dependent lysine deacylase Sirtuin 2**  
F. Friedrich, Freiburg/DE, A. Vogelmann, Freiburg/DE, M. Schiedel, Erlangen/DE, S. Hammelmann, Freiburg/DE, L. Zhang, Freiburg/DE, O. Einsle, Freiburg/DE, M. Jung, Freiburg/DE
- P098 **Photochemical transformations for the expedient synthesis of sp<sup>3</sup>-rich molecules in the field of medicinal chemistry**  
D. Elliott, Basel/CH, Q. Lefebvre, Basel/CH, H. Grab, Basel/CH, T. Fessard, Basel/CH, C. Salomé, Basel/CH
- P099 **Development of lactam-based inhibitors of SARS-CoV-2 M<sup>pro</sup>**  
L. Kinena, Riga/LV, E. Suna, Riga/LV, D. Jelisejevs, Riga/LV
- P100 **Synthesis and biological evaluation of novel RU1968-derived CatSper inhibitors with simplified structure and improved properties**  
T. Schierling, Münster/DE, T. Strünker, Münster/DE, B. Wünsch, Münster/DE
- P101 **A Chemical Biology Toolbox Targeting the Intracellular Binding Site of CCR9: Fluorescent Ligands, New Drug Leads and PROTACs**  
M. E. Huber, Erlangen/DE, L. Toy, Erlangen/DE, M. Schmidt, Erlangen/DE, H. Vogt, Erlangen/DE, J. Budzinski, Erlangen/DE, M. Wiefhoff, Bonn/DE, N. Merten, Bonn/DE, E. Kostenis, Bonn/DE, D. Weikert, Erlangen/DE, M. Schiedel, Erlangen/DE
- P102 **Isotope labelling to fine-tune protein NMR characterization**  
G. Toscano, Vienna/AT, R. Lichtenecker, Vienna/AT
- P103 **Modelling-supported exploration towards an innovative molecule with potential action on Alzheimer's Disease through dual inhibition of 5-HT<sub>6</sub> receptor and CDK5 kinase**  
S. Sudoł-Tałaj, Kraków/PL, K. Czarnota-Łydka, Kraków/PL, S. Podlewska, Kraków/PL, G. Satała, Kraków/PL, B. Mordyl, Kraków/PL, M. Głuch-Lutwin, Kraków/PL, K. Kucwaj-Brysz, Kraków/PL, J. Handzlik, Kraków/PL
- P104 **Do it right the first time: predicting optimal conditions for chemical reactions using HTE and ML**  
F. Ulatowski, Warsaw/PL, P. Wach, Warsaw/PL, A. Chołuj, Warsaw/PL, Ł. Szczupak, Warsaw/PL, J. Rzymkowski, Warsaw/PL, P. Dąbrowski-Tumański, Warsaw/PL, S. Jastrzębski, Warsaw/PL, P. Włodarczyk-Pruszyński, Warsaw/PL, P. Byrski, Warsaw/PL
- P106 **Design, Synthesis, and Optimization of Dual Inhibitors of Cathepsin L and SARS-CoV-2 Main Protease**  
T. Pillaiyar, Tübingen/DE, P. Flury, Tübingen/DE, J. Breidenbach, Bonn/DE, L. Schäkel, Bonn/DE, N. Krüger, Göttingen /DE, S. Laufer, Tübingen/DE, C.E. Müller, Bonn/DE, M. Gütschow, Bonn/DE

- P107 **Covalent inhibitors of thrombin and blood coagulation factor XIIa: synthesis and anticoagulant properties**  
D. V. Kalinin, Münster/DE, L. Imberg, Münster/DE, S. Platte, Münster/DE, A. I. Siutkina, Münster/DE, C. Dunker, Münster/DE, C. Erbacher, Münster/DE, U. Karst, Münster/DE
- P108 **Yes, you should use AI for medicinal chemistry**  
C. Housseman, Paris/FR, Q. Perron, Paris/FR
- P109 **Novel podophyllotoxin analogues as potent anticancer agents**  
S. Nerella, Warangal/IN, V. Allam, Warangal/IN

## ACKNOWLEDGEMENTS

### ▶ PLATINUM SPONSORS



sanofi

### ▶ GOLD SPONSORS



inte:ligand

MERCK



### ▶ SILVER SPONSORS



idorsia



Selvita

### ▶ BRONZE SPONSORS



PFEIFFER VACUUM

### ▶ OTHER SPONSORS



Date: March 3, 2023



Durch den *Fortschritt* wachsen wir zusammen, lernen und überwinden die Grenzen unserer Möglichkeiten.

Wir erforschen die *Wunder* der Wissenschaft, um das Leben der Menschen zu verbessern.

**sanofi**

[www.sanofi.de](http://www.sanofi.de)