



Fachgruppe Medizinische Chemie

# Frontiers in Medicinal Chemistry

March 24 - 27, 2026 · Münster, Germany



[www.gdch.de/medchem2026](http://www.gdch.de/medchem2026)





## TABLE OF CONTENTS

COMMITTEES	5
SCIENTIFIC PROGRAM	7
Tuesday, March 24, 2026	7
Wednesday, March 25, 2026	9
Thursday, March 26, 2026	11
Friday, March 27, 2026	13
LIST OF POSTERS	16
ACKNOWLEDGEMENT	29
INFORMATION	30

## Making more of every life

We've learned over generations that succeeding in health innovation requires commitment, resilience, and transformative action. Decades of cutting-edge science have resulted in important breakthroughs for patients. We believe collaboration is the key to making more science. Together we can build a healthier and more sustainable future. And make more of every life.

Learn more ↓



*Life forward*

Wir erforschen die  
Wunder der **Wissenschaft**,  
damit Du Deine Träume  
leben kannst.



„Als Kind träumte ich davon, das Leben der Menschen zu verbessern. Als Wissenschaftlerin im Labor kann ich das verwirklichen.“

**Sophie, Sanofi Frankreich**

**MSAT** (Manufacturing Science, Analytics and Technology)

**sanofi**

## COMMITTEES

### ► SCIENTIFIC COMMITTEE

<b>M. Bermudez</b>	University Münster/DE
<b>C. Ducho</b>	Saarland University, Saarbrücken/DE
<b>P. Heitel</b>	University of Frankfurt (Main)/DE
<b>G. Hessler</b> (Chairperson of the GDCh division)	Sanofi, Frankfurt (Main)/DE
<b>A. K. H. Hirsch</b>	HIPS Saarbrücken/DE
<b>S. Laufer</b>	University of Tübingen/DE
<b>O. Koch</b>	University Münster/DE
<b>C. Kuttruff</b>	Biberach (Riss)/DE
<b>T. Ross</b>	Merck Healthcare KGaA, Darmstadt/DE
<b>H. Stark</b>	University of Düsseldorf/DE
<b>A. Tarasewicz</b>	Sanofi, Frankfurt (Main)/DE
<b>B. Wünsch</b> (Chairperson of the DPhG division)	University of Münster/DE

### ► ORGANISATION COMMITTEE

<b>M. Bermudez</b>	University Münster/DE
<b>C. Birkner</b>	GDCh e. V., Frankfurt (Main)/DE
<b>M. Bundschuh</b>	GDCh e. V., Frankfurt (Main)/DE
<b>J. Fabian</b>	University Münster/DE
<b>O. Koch</b>	University Münster/DE
<b>D. Schepmann</b>	University Münster/DE
<b>B. Wünsch</b>	University Münster/DE

# Driving Excellence in Contract Development & Manufacturing

Proven Quality, Tailored to your Vision



## Aenova Site Münster, Germany

- Development, production and packaging for tablets and capsules
- High potent & low dosed APIs (hormones, hormone-related substances, corticoids, narcotics)
- More than 50 years of expertise

## SCIENTIFIC PROGRAM

Tuesday, March 24, 2026

		Lecture Hall
1.30 p.m.	<b>Welcome &amp; Opening</b>	Lecture Hall
	<b>Session 1: Chemical Biology, Probes, Tool Compounds</b>	
	<i>Chair: Matthias Schiedel</i>	
2.00 p.m.	<b>Genetic code expansion for structural and dynamic studies of membrane receptors in living cells</b> <i>I. Coin, Leipzig/DE</i>	
2.30 p.m.	<b>Innovative Covalent Targeting of Glycolysis for Oncology Applications</b> <i>C. Borsari, Milan/IT</i>	
3.00 p.m.	<b>Harnessing the chemistry of plants</b> <i>S. O'Connor, Jena/DE</i>	
3.30 p.m.	<b>Tailoring Chemical Probes for the Visualization of the Endocannabinoid System</b> <i>M. Nazare, Berlin/DE</i>	
3.45 p.m.	COFFEE BREAK	Foyer Lecture Hall
	<b>Session 2: Young Investigators (Part 1)</b>	
	<i>Chair: Dennis Schade</i>	
4.15 p.m.	<b>How to optimize RNA Ligands? – Electrostatic Anchors &amp; Covalent Warheads</b> <i>C. Kersten, Mainz/DE</i>	
4.30 p.m.	<b>Molecular and functional evaluation of TREK and TRESK channel activators</b> <i>J. Schreiber, Muenster/DE</i>	
4.45 p.m.	<b>Click. Screen. Degrade. A Miniaturized D2B Workflow for Rapid PROTAC Discovery.</b> <i>K. Hiesinger, Frankfurt (Main)/DE, A. Lui, Frankfurt (Main)/DE, D. Merk, München/DE, D. Morasch, Frankfurt (Main)/DE, E. Proschak, Frankfurt (Main)/DE, E. Wolf, Kiel/DE, F. A. Greco, Frankfurt (Main)/DE, J. Schönfeld, Frankfurt (Main)/DE, L. Hoffmann, Frankfurt (Main)/DE, M. Egner, München/DE, M. Lewandowski, München/DE, M. Mitrovi, Frankfurt (Main)/DE, M. P. Schwalm, Frankfurt (Main)/DE, N. Liebisch, Frankfurt (Main)/DE, R. Chander, Frankfurt (Main)/DE, S. Knapp, Frankfurt (Main)/DE, S. Müller, Frankfurt (Main)/DE, S. A. Sivashanmugam, Frankfurt (Main)/DE, T. Hanke, Frankfurt (Main)/DE, Y. Cruz García, Kiel/DE</i>	

## Tuesday, March 24, 2026

- 5.00 p.m. **Covalent Main Protease Inhibitors as Broad-Spectrum Antivirals Against Coronaviruses**  
 T. Pillaiyar, Tübingen/DE, A. J. O'Donoghue, San Diego/US, C. E. Müller, Bonn/DE, H. Mitsuya, Tokyo/JP, J. Vishwakarma, Texas/US, K. Sylvester, Bonn/DE, M. Gütschow, Bonn/DE, N. Higashi-Kuwata, Tokyo/JP, P. Flurry, Tübingen/DE, R. Basu, Texas/US, R. S. Harris, Texas/US, S. Laufer, Tübingen/DE, S. Yang, Sichuan/CN

Lecture Hall

**Session 3: Case Studies & First Disclosures (Part 1)***Chair: Gerhard Hessler*

- 5.15 p.m. **Development of oral and inhaled Compounds for Respiratory Diseases – Case Studies**  
 W. Czechitzky, Mölndal/SE

Lecture Hall

**FRIEDRICH STOLZ-PRIZE***Chair: Franz von Nussbaum*

- 6.30 p.m. **POSTER SESSION & GET TOGETHER**

Foyer

## Wednesday, March 25, 2026

Lecture Hall

**Session 4: Ion Channels, Membrane Transport***Chair: Stefan Laufer*

- 9.00 a.m. **Experimental Potassium Channel Openers with Nanomolar Activity on Voltage-Gated Potassium Channels**  
 A. Link, Greifswald/DE, J. Lemke, Greifswald/DE
- 9.30 a.m. **Exploration of Novel Targets for Antimicrobial Compounds**  
 D. J. Slotboom, Groningen/NL, A. Cremers, Lausanne/CH, A. Hirsch, Saarbrücken/DE, A. Shams, Saarbrücken/DE, A. Speer, Amsterdam/NL, A. Tsarenko, Groningen/NL, E. Diamanti, Saarbrücken/DE, I. Exapicheidou, Saarbrücken/DE, I. Setyawati, Groningen/NL, J. Hauptenthal, Saarbrücken/DE, J. W. Veening, Lausanne/CH, K. Lubova, Groningen/NL, L. Swier, Groningen/NL, L. Yue, Groningen/NL, M. Hamed, Saarbrücken/DE, P. Gibson, Lausanne/CH, P. Hoffmann, Saarbrücken/DE, P. Souza, Lyon/FR, R. Becker, Saarbrücken/DE, R. Müller, Saarbrücken/DE, S. Bousis, Saarbrücken/DE, S. J. Marrink, Groningen/NL, V. Charitou, Amsterdam/NL, W. Bitter, Amsterdam/NL, W. Stanek, Groningen/NL
- 10.00 a.m. **Illuminating P2X7R: Fluorophore Effects and the Design of New Fluorescent Probes for Ion Channel Imaging**  
 A. Junker, Tübingen/DE, B. Weigelin, Tübingen/DE, C. A. Strassert, Münster/DE, J. Yamaguchi, Nagoya/JP, M. Höhl, Tübingen/DE, M. J. Rengel, Tübingen/DE, S. Schmidt, Tübingen/DE, V. Cappellari, Münster/DE, Z. Wang, Tübingen/DE
- 10.30 a.m. **Shining Light on Sperm Motility: Synthesis and Application of Photoactivatable CatSper Modulators for the Investigation of Male Fertility**  
 W. F. Zhu, Münster/DE, A. M. Schulte, Groningen/NL, B. Wünsch, Münster/DE, C. Brenker, Münster/DE, S. Herrmann, Münster/DE, T. Schierling, Münster/DE, T. Strücker, Münster/DE, W. Szymaski, Groningen/NL

10.45 a.m. COFFEE BREAK

Foyer

Lecture Hall

**Session 5: New Modalities (RipTACS)***Chair: Joachim Jose*

- 11.15 a.m. **Turning the light on: Chemical probes for Imaging with ADCs**  
 C. Deutsch, Basel/CH, L. Kueng, Basel/CH, M. Meier, Basel/CH, V. Mele, Basel/CH
- 11.45 a.m. **Development of New PROTAC Modalities for the Targeted Degradation of Histone Deacetylases**  
 F. K. Hansen, Bonn/DE
- 12.15 p.m. **Drug Discovery of Regulated Induced Proximity Targeting Chimeras (RIP-TACs): A Novel Modality for Cancer Therapy**  
 J. Zhou, Galveston/US, C. Zhang, Galveston/US, H. Chen, Galveston/US, Y. Xue, Galveston/US, Z. Ma, Galveston/US

1.00 p.m. LUNCH BREAK

Foyer

Wednesday, March 25, 2026

Lecture Hall

**Session 6: Next GenMedChem***Chairs: Anika Tarasewicz, Pascal Heitel*

2.00 p.m. **The Development of Molecular Glues that Selectively Degrade Engineered Degrons or Endogenous Zinc Fingers**

*S. J. Conway, Los Angeles/US*

2.30 p.m. **Discovery and Optimisation of Transferrin Receptor-1 Binding Bicycle Peptides for Targeted Delivery of Oligonucleotide Therapeutics**

*M. A. St. Denis, Cambridge/GB*

3.00 p.m. **Nucleases, a novel target class for DNA Damage Response (DDR): identification and optimisation to the first orally available FEN1 and EXO1 inhibitors**

*J. Lefranc, Darmstadt/DE*

3.30 p.m. COFFEE BREAK

Foyer

Lecture Hall

**Session 7: Computational Medicinal Chemistry***Chair: Oliver Koch*

4.00 p.m. **Progress on drug design on quantum computers**

*G. L. R. Anselmetti, Cologne/DE, M. Degroote, Brussels/BE, M. Streif, Freiburg/DE, N. Moll, Berlin/DE, R. Santagati, Milano/IT*

4.30 p.m. **Exploring AI-generated Trillion-Scale Virtual Screening Libraries for Drug Discovery**

*M. P. Waller, Sydney/AU*

5.00 p.m. **Large Language Models for Chemistry and Drug Discovery**

*T. Plötz, Darmstadt/DE*

5.30 p.m. **Computationally Driven Insight into Ion Channel Antagonists and Blockers**

*P. C. Biggin, Oxford/GB*

Lecture Hall

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

**Tagesordnung:**

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

Lecture Hall

6.45 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, March 26, 2026

Lecture Hall

**Session 8: New Synthetic Methods***Chair: Christian Ducho*

9.00 a.m. **P5-conjugation for generating highly efficacious antibody-conjugates for cancer therapy**

*C. Hackenberger, Berlin/DE, C. E. Stieger, Berlin/DE, M.-A. Kasper, München/DE*

9.30 a.m. **New Strategies for the Rapid, Flexible and Scalable Syntheses of Nucleoside Analogues**

*R. Britton, Burnaby/CA*

10.00 a.m. **The Synergy of Light, Organocatalysis, and Enzymes: New Radical Opportunities**

*P. Melchiorre, Bologna/IT*

10.30 a.m. COFFEE BREAK

Foyer

Lecture Hall

**Session 9: Young Investigators (Part 2)***Chair: Steffen Pockes*

11.00 a.m. **Harnessing Non-Canonical GPCR Binding Pockets for Drug Development**

*D. Weikert, Erlangen/DE*

11.15 a.m. **Targeting the Spliceosomal Protein USP39 Through Allosteric Ligands and PROTAC-Induced Degradation**

*X. Cheng, Frankfurt (Main)/DE, C. Prieto-Garcia, Frankfurt (Main)/DE, D. Schäfer, Frankfurt (Main)/DE, I. Dikic, Frankfurt (Main)/DE*

11.30 a.m. **MedChem tools and approaches to explore the sperm-specific ion channels CatSper and Slo3 as potential targets for new contraceptives**

*L. Temme, Hamburg/DE, C. Brenker, Münster/DE, J. Münchow, Münster/DE, T. Mittermair, Münster/DE, T. Strünker, Münster/DE*

Lecture Hall

11.45 a.m. **INNOVATION PRIZE**

*Chairs: Christian Ducho, Christian Kuttruff*

12.30 p.m. LUNCH BREAK

Foyer

Thursday, March 26, 2026

Lecture Hall

**Session 10: High-throughput Chemistry***Chair: Christian Kuttruff*1.45 p.m. **MicroCycle: An Integrated and Automated Platform to Accelerate Drug Discovery**C. E. Brocklehurst, Basel/CH2.15 p.m. **The Evolution of Automation for Drug Discovery at Sanofi**E. Speckmeier, Frankfurt (Main)/DE

Lecture Hall

2.45 p.m. **PhD-Prize AWARD CEREMONY***Chair: Christian Kuttruff*2.55 p.m. **55 Years Division Medicinal Chemistry***Chair: Gerhard Hessler*

3.30 p.m. POSTER SESSION AND COFFEE BREAK

Foyer

Lecture Hall

**Session 11: Case Studies & First Disclosures (Part 2)***Chair: Tatjana Ross*5.20 p.m. **Histamine H<sub>3</sub> Receptor Antagonists in Orphan Diseases**H. Stark, Düsseldorf/DE5.50 p.m. **Macrocyclic MCL-1 inhibitors for the treatment of multiple myeloma**K. Jantos, Ludwigshafen/DE

Friday, March 27, 2026

Lecture Hall

**Session 12: Highlights (Part 1)***Chair: Marcel Bermúdez*9.00 a.m. **Arene hydrogenation, photocatalysis, smart screening and data science – game changing technologies****F. Glorius, Munster/DE**9.30 a.m. **Structure-based development of functionally selective GPCR agonists****P. Gmeiner, Erlangen/DE**

Lecture Hall

**Session 13: Young Investigators (Part 3)***Chair: Marcel Bermúdez*10.00 a.m. **Cryo-EM Structure of Factor XIa and Insights into Its Allosteric Modulation**A. Siutkina, Münster/DE, A. Neuhaus, Münster/DE, C. Gatsogiannis, Münster/DE, D. Kalinin, Münster/DE10.15 a.m. **Targeting Protein Kinase Specificity through Chemical and Pharmacological Profiling**S. M. Stefan, Lübeck/DE, G. Gopakumar, Lübeck/DE, H. Busch, Lübeck/DE, J. König, Erlangen/DE, K. Stefan, Lübeck/DE, L. Prange, Lübeck/DE, M. Rafehi, Augsburg/DE, T.-N. Niehus, Lübeck/DE, V. Namasivayam, Lübeck/DE

10.30 a.m. COFFEE BREAK

Foyer

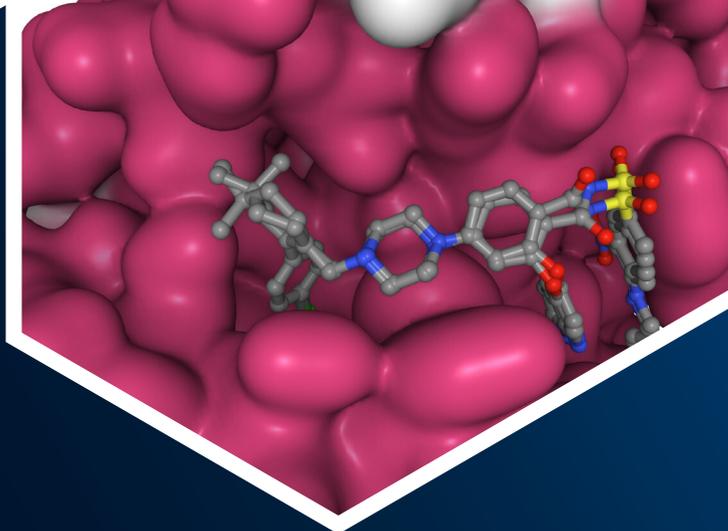
**Session 14: Highlights (Part 2)***Chair: Holger Stark*11.00 a.m. **3-Hydroxypropanamidines: A novel class of orally active antimalarials targeting Plasmodium falciparum**T. Kurz, Düsseldorf/DE, A. Moritz, Münster/DE, B. Burckhardt, Münster/DE, B. Lungerich, Düsseldorf/DE, D. Fidock, New York/US, J. Held, Tübingen/DE, J. Sandstroem, Düsseldorf/DE, J. Thibaud, Stellenbosch/ZA, K. de Villiers, Stellenbosch/ZA, L. Meyer, Düsseldorf/DE, L. Pessanha de Carvalho, Tübingen/DE, M. Rottmann, Basel/CH, S. Klein, Düsseldorf/DE, S. Wittlin, Basel/CH, T. Knaab, München/DE11.15 a.m. **Zwitterionization as a general strategy to decrease off-target retention of small molecules for diagnosis and therapy of prostate cancer**W. Maison, Hamburg/DE, J. V. Frangioni, Natick/US, L. Spickschen, Hamburg/DE

Friday, March 27, 2026

Lecture Hall

- 11.30 a.m. **Next-generation TPH inhibitor (TPHi) platform against serotonin-related diseases**  
E. Specker, Berlin/DE, D. Pleimes, Berlin/DE, M. Bader, Berlin/DE, R. Wesolowski, Berlin/DE
- 11.45 a.m. **Discovery of Remibrutinib, a highly selective, covalent BTK inhibitor for the treatment of chronic spontaneous urticaria**  
D. Angst, Basel/CH
- 12.15 p.m. **New developments in the field of nucleoside and oligonucleotide therapeutics**  
T. Carell, Munich/DE
- 12.45 p.m. **Closing Remarks**  
*Chairs: Gerhard Hessler, Manfred Jung*

Lecture Hall



CAS BIOFINDER®

# STOP DIGGING THROUGH DATA. START MAKING DISCOVERIES.

CAS BioFinder helps you connect biology and chemistry to reveal drug research insights in seconds.

Advance your research with data on biological pathways, biomarkers, antibodies and ADCs, immunotherapeutics, SAR, and more.

CAS BioFinder integrates chemistry and biology data into visualizations, predictive models, and agentic AI research support with CAS Newton<sup>SM</sup> to help you confidently identify the most promising targets and ligands.

If you can't make our hands-on CAS BioFinder Workshop, please reach out to schedule a demo and see how CAS BioFinder can advance your research projects.



**Case Studies & First Disclosures**

P001 **Optimization of Fusion Protein Inhibitors for Inhaled Therapy Against RSV**  
M. Dongock Kagho, Saarbrücken/DE, A. I. Zulu, Saarbrücken/DE, A. K. H. Hirsch, Saarbrücken/DE, A. M. Kany, Saarbrücken/DE, B. Hellwinkel, Hanover/DE, C. Karhan, Saarbrücken/DE, H. Scherer, Saarbrücken/DE, K. Wagner, Saarbrücken/DE, M. Empting, Saarbrücken/DE, S. Haid, Hanover/DE, S. Klein, Saarbrücken/DE, T. Pietschmann, Hanover/DE

P002 **Structure-Based Design of Antiviral Benzimidazoles Targeting the eIF4A–RNA Interaction**  
J. M. Saurin, Marburg/DE

P003 **Identification of WRN Helicase Purchasable Actives Enabled by Crystal Fragment Screening-Based Chemical Space Docking®**  
B. Bueschbell, St. Augustin/DE, M. Gastreich, St. Augustin/DE, R. Klein, St. Augustin/DE

**Chemical Biology, Probes, Tool Compounds**

P004 **The discovery of PI3K-C2 highly selective inhibitors targeting HBV infection**  
D. Cirillo, Berlin/DE, B. Küster, Freising/DE, G. Wolber, Berlin/DE, J. P. von Kries, Berlin/DE, K. Puls, Berlin/DE, L. Perpelittchenko, Berlin/DE, M. Albanese, Milano/IT, M. Diceglie, Berlin/DE, M. Nazaré, Berlin/DE, P. Prokofeva, Freising/DE, S. Müller, Frankfurt (Main)/DE, S. Radetzki, Berlin/DE, S. Wilhelm, Freising/DE, T. A. L. Ehret, Frankfurt (Main)/DE, V. Haucke, Berlin/DE, W.-T. Lo, Berlin/DE

P005 **Structure-based development of covalent ligands targeting the somatostatin receptor subtype 2 for radionuclide theranostics of neuroendocrine tumors**  
P. Schlitterlau, Dresden/DE, J. Pietzsch, Dresden/DE, K. Kopka, Dresden/DE, M. Laube, Dresden/DE, M. Ullrich, Dresden/DE, R. Löser, Dresden/DE, R. Wodtke, Dresden/DE, S. Stadlbauer, Dresden/DE

P006 **The FMP and EU-OPENSURE Compound Management as Integral Part of the Screening Platform of the FMP**  
E. Specker, Berlin/DE, D. Garcia, Berlin/DE, H. Sun, Berlin/DE, M. Nazaré, Berlin/DE, M. Neuenschwander, Berlin/DE, P. Gribbon, Berlin/DE

P007 **Investigation of Epigenetic Modifications in Honeysuckle derived miR2911 and synthetic approach for the incorporation of amino-terminal guanosine modifications**  
M. Frank, Munich/DE, B. Henzeler, Munich/DE, H. Hurmiz, Munich/DE, S. Schneider, Munich/DE, T. Carell, Munich/DE

**Chemical Biology, Probes, Tool Compounds**

P008 **Proteomic Analysis of HDACi treated Cancer Cells for the Identification of Potential Targets for CAR-T Cell Therapy**  
L. Bauer, Leipzig/DE, J. Meiler, Leipzig/DE, J. Schmidt, Leipzig/DE, M. Tretbar, Leipzig/DE, S. Tretbar, Leipzig/DE

P010 **Near-Infrared Fluorescent Prostate-Specific Membrane Antigen (PSMA)-targeting Probes for Optically Guided Surgery of Prostate Cancer**  
C. M. Berrou, Hannover/DE, J. Pietzsch, Dresden/DE, M. Ullrich, Dresden/DE, M. M. Weitzenberg, Hannover/DE, O. Bruns, Dresden/DE, O. Plettenburg, Hannover/DE

P011 **Silymarin Ingredients Mitigate Hepatocellular Lipogenesis by inhibiting LXR**  
N. Bandomir, Frankfurt (Main)/DE, A. Kaiser, Frankfurt (Main)/DE, F. Lillich, Frankfurt (Main)/DE, P. Heitel, Frankfurt (Main)/DE

P012 **Pharmacophore-based Design of Novel NLRP3 Inhibitors**  
E. Çevik, Frankfurt (Main)/DE, E. Proschak, Frankfurt (Main)/DE, P. Heitel, Frankfurt (Main)/DE

P013 **On-oligonucleotide Olefin Metathesis in Water**  
C. Zhang, Würzburg/DE, A. Brunschweiler, Würzburg/DE, A. Khimich, Würzburg/DE, CO. Blanco, Ottawa/CA, D. Fogg, Ottawa/CA

P014 **Development of fluorogenic sEH substrates based on PHOME**  
C. Kolmer, Frankfurt (Main)/DE, E. Proschak, Frankfurt (Main)/DE, J. Schönfeld, Frankfurt (Main)/DE, K. Hiesinger, Frankfurt (Main)/DE, R. Damm, Frankfurt (Main)/DE

P015 **Amide-Based Slow Substrates as Potent SIRT2 Inhibitors**  
F. Kollmer, Freiburg/DE, C. Barinka, Vestec/CZ, C. Schiene-Fischer, Halle (Saale)/DE, D. Kalbas, Halle (Saale)/DE, F. Friedrich, Freiburg /DE, J. Ruprecht, Freiburg/DE, J. Ruprecht, Freiburg/DE, L. Zhang, Freiburg/DE, M. Jung, Freiburg/DE, M. Meleshin, Halle (Saale)/DE, M. Schutkowski, Halle (Saale)/DE, M. Zessin, Halle (Saale)/DE, O. Einsle, Freiburg/DE, S. Hilscher, Halle (Saale)/DE, W. Sippl, Halle (Saale)/DE

P016 **Investigating the BamA-BamD interaction: a target for novel antibiotics?**  
S. Schreiber, Münster/DE, J. Jose, Münster/DE

P017 **Indolizine-derived tubulin inhibitors with selective antiproliferative activity**  
V. H. Catricala-Fernandes, Ribeirão Preto/BR, A. Junker, Tübingen/DE, A. M. Leopoldino, Ribeirão Preto/BR, F. J. Caires, Ribeirão Preto/BR, G. Silva, Ribeirão Preto/BR, G. C. Clososki, Ribeirão Preto/BR, G. P. Bueno, Ribeirão Preto/BR, M. B. Giometti, Ribeirão Preto/BR

**Chemical Biology, Probes, Tool Compounds**

P018 **Prodrug design, synthesis and evaluation of a very potent NMDA receptor subtype-specific agonist**  
N. Spent, Münster/DE, B. Wünsch, Münster/DE

P019 **Development of Pathoblockers Targeting EclA, A Novel Lectin from Enterobacter cloacae**  
B. Tawfik, Saarbrücken/DE, A. Titz, Saarbrücken/DE, J. Köhnke, Hannover/DE, K. Patel, Hannover/DE, M. Bischoff, Homburg/DE, M. Fares, Saarbrücken/DE

- P020 **Dual Nurr1/RXR Agonism Enables Dimer-Selective Nurr1 Modulation**  
K. Scholz, Munich/DE, D. Merk, Munich/DE, J. Marschner, Munich/DE, R. Busch, Munich/DE, Ú. López-García, Munich/DE
- P021 **Biochemical Determinants of Disease in Okur-Chung Neurodevelopmental Syndrome Variants**  
J. M. Fellhölder, Münster/DE, A. Gast, Münster/DE, C. Werner, Cologne/DE, J. Jose, Münster/DE, K. Niefind, Cologne/DE
- P022 **A Cell-based Screening Approach for C-terminal Inhibitors of Hsp90**  
L. van Impel, Münster/DE, J. Jose, Münster/DE, K. Jürgens, Münster/DE
- P023 **Surface display of heterologous antigens in Salmonella Typhi Ty21a for oral vaccine development**  
C. Trugge, Münster/DE, F. Lenz, Münster/DE, H. Tian, Münster/DE, J. Jose, Münster/DE, K. Mukherjee, Münster/DE, M. Umlauf, Münster/DE, Y. Börgeling, Münster/DE
- P024 **Phenyl-alkylidene linked 9(10H)-Anthracenones as Inhibitors of Protein Kinase CK2**  
T. Bödeker, Münster/DE, A. Gast, Münster/DE, C. Werner, Cologne/DE, H. Prinz, Münster/DE, J. Jelschen, Münster/DE, J. Jose, Münster/DE, K. Niefind, Münster/DE
- P025 **Quantitative uptake studies of CK2-targeting inhibitors in eukaryotic cells and qualitative metabolomic analysis using HPLC-MS**  
J. Riße, Münster/DE, J. Jose, Münster/DE, M. Le Borgne, Lyon/FR, R. Birus, Münster/DE
- Computational Medicinal Chemistry**
- P026 **AI Driven Fragment Growing for the Design of Thioredoxin Reductase Inhibitors**  
O. Brouwer, Münster/DE, F. Becker, Münster/DE, J. Massa, Münster/DE, M. Yücel, Münster/DE, O. Koch, Münster/DE, P. Janssen, Münster/DE
- P027 **ChI-SOM: Performant Self-Organizing Maps for Drug Discovery**  
J. Kaminski, Münster/DE, O. Koch, Münster/DE
- P029 **Computational Approaches for Fragment Pose Prediction**  
P. Kempanna, Münster/DE, C. Lemmen, Sankt Augustin/DE, J. Massa, Münster/DE, M. Gastreich, Sankt Augustin/DE, O. Koch, Münster/DE
- P030 **Machine Learning-Driven Discovery and Experimental Validation of Novel Tankyrase 1 Inhibitors**  
M. Bilotta, Catanzaro/IT, A. Gargano, Catanzaro/IT, R. Rocca, Catanzaro/IT, S. Alcaro, Catanzaro/IT
- P031 **Unraveling The Allosteric Mechanism of FtsZ in Detail**  
A. O. Fernandes, Münster/DE, M. Bermudez, Münster/DE
- P032 **Fragment-Based Design and Synthesis of New Inhibitors targeting Mycobacterial Thioredoxin Reductase**  
R. Baumann, Münster/DE, F. Becker, Münster/DE, O. Koch, Münster/DE, P. Janssen, Münster/DE

- P033 **Context Matters in Generative Chemistry: Redefining Druglikeness with Target-Family Specific Scoring**  
M. A. Yucel, Münster/DE, O. Koch, Münster/DE
- P034 **Improving Neural Fingerprints for Virtual Screening**  
S. K. R. Homberg, Münster/DE, B. Risse, Münster/DE, M. L. Modlich, Münster/DE, O. Koch, Münster/DE
- P035 **Fragment-Based Drug Design Towards New Antituberculosic Drugs: Learnings from Crystallographic Fragment Screenings**  
F. Becker, Münster/DE, D. Kümmel, Münster/DE, F. T. Füsser, Münster/DE, M. S. Weiss, Berlin/DE, O. Koch, Münster/DE, P. Janssen, Münster/DE
- P036 **Receptor-Specific Allosteric Architectures Underlie GPCR Coupling Specificity Despite Conserved Activation Mechanisms**  
M. Tattera, Münster/DE, M. Bermúdez, Münster/DE
- P037 **Stabilizing Plasmodium falciparum Proteins for Small Molecule Drug Discovery**  
S. Günther, Freiburg/DE, M. Amann, Freiburg/DE, O. Einsle, Freiburg/DE, T. Sträßler, Freiburg/DE
- P038 **Analysis of Biased Ligand Data for Pharmaceutical Applications**  
B. Khashin, Münster/DE, M. Bermudez, Münster/DE
- P039 **Protons and Water: A Coupled Case Study for Endothiapepsin**  
L. Johannknecht, Mainz/DE, P. Czodrowski<sup>1</sup>, Mainz/DE
- P040 **Dynamic pharmacophores unveil binding mode ensembles for classical partial agonists at the M2 receptor**  
F. Wunsch, Münster/DE, C. Hoffmann, Jena/DE, G. Wolber, Berlin/DE, J. Filor, Jena/DE, M. Bermudez, Münster/DE, M. Kauk, Jena/DE, U. Holzgrabe, Würzburg/DE
- P041 **The fragment-based strategy: an effective approach for designing new small molecules that act as GLS1 inhibitors**  
S. Allahi, Genova/IT, A. Carbone, Genova/IT, C. Vagaggini, Siena/IT, E. Dreassi, Siena/IT, F. Poggialini, Siena/IT, G. A. Trombetti, Milan/IT, M. Tonelli, Genova/IT, P. D'Ursi, Milan/IT, P. Fossa, Genova/IT, S. Schenone, Genova/IT
- P042 **Integrative Analysis of Metabolic Stability and Biotransformation Pathways of Muscarinic Receptor Antagonists by LC HRMS**  
M. Spreitzer, Vienna/AT, I. Süreitzer, Vienna/AT, J. Kilian, Vienna/AT, J. Kirchmair, Vienna/AT, J. Wackerlig, Vienna/AT, L. Kogler, Vienna/AT, M. Ozenil, Vienna/AT, M. Starovoit, Králové/CZ, T. Langer, Vienna/AT, V. Pichler, Vienna/AT
- P043 **Bioactivity prediction with chemical language models trained on labeled molecules**  
T. Hörmann, Munich/DE, D. Merk, Munich/DE, E. Proschak, Frankfurt (Main)/DE, F. Grisoni, Eindhoven/NL, J. H. M. Ehrler, Frankfurt (Main)/DE, L. Isigkeit, Frankfurt/DE, V. Lembo, Genoa/IT

- P044 **A Genetic Algorithm for Multi-Objective Unconstrained Virtual Screening of Chemical Space**  
M. Grieswelle, Münster/DE, D. Pallez, Nice/FR, O. Koch, Münster/DE
- P045 **Applying structure- and ligand-based methods to identify and design novel selective HDAC11 inhibitors**  
F. Baseliou, Halle (Saale)/DE, C. Barinka, Vestec/CZ, D. Robaa, Halle (Saale)/DE, L. Handke, Halle (Saale)/DE, M Schutkowski, Halle (Saale)/DE, S. Hagemann, Halle (Saale)/DE, S. Hilscher, Halle (Saale)/DE, S. Hüttelmaier, Halle (Saale)/DE, S. Tripathee, Halle (Saale)/DE, W. Sippl, Halle (Saale)/DE
- P046 **Development of Dual PTR1/DHFR Inhibitors for Trypanosomatid Parasites Through Dynamic Pharmacophore-Based Virtual Screening**  
F. Oyatsi, Münster/DE, M. Bermudez, Münster/DE, T. J. Schmidt, Münster/DE
- P047 **A new benchmark for deep-learning-based affinity prediction: Solving the interprotein scoring noise problem**  
O. Koch, Münster/DE, A.-K. Prinz, Münster/DE, J. Kaminski, Münster/DE, J. Massa, Münster/DE, M. Grieswelle, Münster/DE, P. Janssen, Münster/DE, S. Georgiev, Münster/DE, S. K. R. Homberg, Münster/DE
- P048 **Computational Design and Experimental Validation of Peptides and Peptidomimetics Targeting C5aR1**  
M. Sorokina, Leipzig/DE, C. Lamers, Leipzig/DE, J. Meiler, Leipzig/DE
- P049 **Discovery of Gut Microbiota Metabolite Mimicking Drugs for Autoimmune/ Infectious Diseases Using Heuristic Search Algorithm**  
S. El-Atawneh, Münster/DE, O. Koch, Münster/DE
- P050 **Highlighting molecular similarity using explainable AI**  
S. Georgiev, Münster/DE, B. Risse, Münster/DE, M. Grieswelle, Münster/DE, M. Modlich, Münster/DE, O. Koch, Münster/DE, S. K. R. Homberg, Münster/DE
- P051 **Gyroscopic-Like Stabilization: Deciphering the Pharmacophore of SARS-CoV M Protein Inhibitors**  
O. I. Alwassil, Riyadh/SA
- P052 **Analysis of Compound Libraries and Combinatorial Chemical Spaces with a Novel Benchmark Set of Bioactive Molecules**  
A. Neumann, Sankt Augustin/DE, R. Klein, Sankt Augustin/DE
- P053 **Towards a Comprehensive De Novo Design Approach: the Discovery of p38:MK2 Molecular Glues**  
G. D'Arrigo, Mannheim/DE
- Highlights in Medicinal Chemistry**
- P054 **Design, Synthesis, and Biochemical Evaluation of Triazapentalene-Based Modulators Targeting Glycogen Synthase Kinase 3**  
R. Köhne, Darmstadt/DE, B. Schmidt, Darmstadt/DE

- P055 **Chlorotonil Optimization: Semi-Synthetic Modifications and Dehalogenil Discovery**  
C. Guimard, Saarbrücken/DE, A. K. H. Hirsch, Saarbrücken/DE, A. M. Kany, Saarbrücken/DE, F. Deschner, Saarbrücken/DE, G. Han, Saarbrücken/DE, G. Jézéquel, Saarbrücken/DE, J. Held, Tübingen/DE, J. Herrmann, Saarbrücken/DE, L. Pessanha de Carvalho, Tübingen/DE, M. Bischoff, Homburg/DE, M. Große, Braunschweig/DE, M. Stadler, Braunschweig/DE, R. Müller, Saarbrücken/DE, W. Hofer, Saarbrücken/DE
- P056 **Discovery of Immune-responsvie Gene 1 (IRG1) Modulators as Potential Host-directed Anti-infective Agents**  
G. Bianchi, Saarbrücken/DE, A. Kany, Saarbrücken/DE, F. Pessler, Hannover/DE, F. Waqas, Hannover/DE, K. Büssow, Braunschweig/DE, M. Zhao, Braunschweig/DE, R. Müller, Saarbrücken/DE, S. Rasheed, Saarbrücken/DE, U. Hapko, Saarbrücken/DE, W. Elgaher, Saarbrücken/DE
- P057 **Chemically Stable Diazo Peptides as Cysteine Protease Inhibitors and Precursors for Diazomethyl Ketone Petides with increased Activity**  
J. Wahl, Berlin/DE, J. Rademann, Berlin/DE
- P058 **Illuminating the Dark Kinome: Integrating Artificial Intelligence with Large-Scale Medicinal Chemistry Data for Academic Drug Discovery**  
J. Kundrat, Tübingen/DE, F. W. Hacker, Tübingen/DE, G. S. Businger, Tübingen/DE, J. Bajorath, Bonn/DE, S. A. Laufer, Tübingen/DE
- P059 **Design, Synthesis, and Biochemical Evaluation of Novel MLK3 Inhibitors: A Target Hopping Example**  
T. Feyerabend, Tübingen/DE, A. Krämer, Frankfurt/DE, A. Rasch, Tübingen/DE, A. Sievers-Engler, Tübingen/DE, B. Masberg, Tübingen/DE, M. Lämmerhofer, Tübingen/DE, M.P. Schwalm, Frankfurt/DE, P. Sander, Tübingen/DE, R. Selig, Tübingen/DE, S. Knapp, Frankfurt/DE, S. Müller, Frankfurt/DE, S.A. Laufer, Tübingen/DE, W. Albrecht, Tübingen/DE
- P060 **Development of tetrahydroisoquinoline-based PET tracers to image  $\sigma_2$  receptors in the brain**  
N. S. Jakobus, Münster/DE, B. Wünsch, Münster/DE
- P061 **Fragment-based drug discovery and optimization of covalent Caspase-2 small molecule inhibitors with CNS drug-like properties**  
J. Daschner, Regensburg/DE, A. Hubmann, Regensburg/DE, B. Vallaster, Regensburg/DE, K. H. Ashe, Minneapolis/US, L. Forster, Regensburg/DE, L. Wirth, Regensburg/DE, M. A. Walters, Minneapolis/US, M. E. Cuellar, Minneapolis/US, S. Pockes, Regensburg/DE, S. Scheuerer, Regensburg/DE
- P062 **Combining a rational drug design approach with reactivity assessment of covalent reactive small molecule Casp2 inhibitors**  
B. Vallaster, Regensburg/DE, A. Hubmann, Regensburg/DE, K. Ashe, Minneapolis/US, L. Forster, Regensburg/DE, L. Wirth, Regensburg/DE, M. Walters, Minneapolis/US, S. Pockes, Regensburg/DE, S. Scheuerer, Regensburg/DE

- P063 **Development of anti-leukemic HDAC inhibitors**  
J. Kremeyer, Düsseldorf/DE, J.-W. Tu, Düsseldorf/DE, M. Kassack, Düsseldorf/DE, S. Bhatia, Düsseldorf/DE, S. Buntrock, Düsseldorf/DE, T. Kurz, Düsseldorf/DE
- P064 **Synthesis and structure-activity-relationships of potent antagonists for the MAS-related G protein-coupled receptor MRGPRX2**  
J. Dörner, Bonn/DE, C. E. Müller, Bonn/DE, D. Thimm, Bonn/DE, G. Al Hamwi, Bonn/DE
- P065 **Optimization of Psychedelic-Assisted Therapy via Medicinal Chemistry**  
J. Stirn, Heidelberg/DE, C. Schmidt, Göttingen/DE, C. D. Klein, Heidelberg/DE, D. Mytzka, Heidelberg/DE, F. Wiedmann, Göttingen/DE, H. Hübner, Erlangen-Nuremberg/DE, L. Fiege, Heidelberg/DE, P. Gmeiner, Erlangen-Nuremberg/DE, T. R. Sundermann, Heidelberg/DE
- P066 **Synthesis and Structure-Activity Relationships of Novel Proline-Based LpxC Inhibitors**  
J. Bartenbach, Hamburg/DE, F. Wichter, Hamburg/DE, R. Holl, Hamburg/DE
- P067 **Synthesis and SAR of dual inhibitors of LpxA and LpxD**  
J. Jäger, Hamburg/DE, F. Wichter, Hamburg/DE, R. Holl, Hamburg/DE, T. Krüger, Hamburg/DE
- P068 **Pathoblockers as Inhibitors of Clostridoides histolyticum virulence factor ColH and Pseudomonas aeruginosa virulence factor LasB**  
S. Dahmen, Saarbrücken/DE
- P069 **Prodrugs of Muraymycin Nucleoside Antibiotics**  
L. S. Thilmont, Saarbrücken/DE, C. Ducho, Saarbrücken/DE, D. Wiegmann, Saarbrücken/DE
- P070 **Discovery of the First Highly Selective 1,4-Dihydropyrido[3,4-b]pyrazin-3(2H)-one MKK4 Inhibitor**  
E. Eberlein, Tübingen/DE, A. Rasch, Tübingen/DE, L. Katzengruber, Tübingen/DE, L. Zender, Tübingen/DE, P. Sander, Tübingen/DE, R. Selig, Tübingen/DE, S. Zwirner, Tübingen/DE, S. A. Laufer, Tübingen/DE, W. Albrecht, Tübingen/DE
- P071 **Type I½ p38 MAP Kinase Inhibitors with Ultralong Target Residence Time – A Promising Treatment for Colorectal Cancer**  
E. Hermann, Tübingen/DE, D. Dauch, Tübingen/DE, H.K. Wentsch-Teltschik, Tübingen/DE, J. Harbig, Tübingen/DE, L. Zender, Tübingen/DE, M. Forster, Tübingen/DE, M. Kudolo, Tübingen/DE, N.M. Tormählen, Tübingen/DE, R. Rudalska, Tübingen/DE, R.B. Ditzinger, Tübingen/DE, S.A. Laufer, Tübingen/DE
- P072 **Development of new anti-infectives targeting the pyocyanin biosynthesis enzyme PhzB in Pseudomonas aeruginosa**  
A. F. A. Moumbock, Braunschweig/DE, C. Kunick, Braunschweig/DE, M. Handke, Braunschweig/DE, M. Schiedel, Münster/DE, M. Thiemann, Braunschweig/DE, M. Zimmermann, Braunschweig/DE, W. Blankenfeldt, Braunschweig/DE

- P073 **Sequential Structure-Guided Optimization to Identify Potent Azapeptide-Derived SARS-CoV-2 Main Protease Inhibitors**  
N. Gone, Tübingen/DE, C. E. Müller, Bonn/DE, K. Sylvester, Bonn/DE, N. Krüger, Göttingen/DE, P. Flury, Tübingen/DE, S. A. Laufer, Tübingen/DE, T. Pillaiyar, Tübingen/DE
- P074 **Development of Small-Molecule Plasma Kallikrein Inhibitor via Multicomponent Microscale Parallel Synthesis and Screening**  
H. Lin, Münster/DE, D. V. Kalinin, Galway/IE
- P075 **Ring-Closing Metathesis Expands DNA-Encoded Macrocyclic Library Design**  
C. Zhang, Würzburg/DE, A. Brunschweiler, Würzburg/DE
- P076 **Design, Synthesis, and Docking Analysis of a Novel Series of Methylene Disalicylic Acid/thiazole Hybrids as DNA Gyrase and Topoisomerase IV Inhibitors with Antibacterial Properties**  
B. Alyami, Najran/SA, B. Youssif, Assiut/EG, Y. Alqahtani, Najran/SA
- P077 **Development of Sulfonamides as eIF4A inhibitors as potential broad spectrum antiviral drugs**  
L. M. Kemena, Marburg/DE, A. Grünweller, Marburg/DE, C. Müller-Ruttloff, Gießen/DE, E. Raso, Gießen/DE, F. Magari, Marburg/DE, H. Messner, Marburg/DE, J. Ziebuhr, Gießen/DE, K. A. Mentchen, Marburg/DE, M. Schlitzer, Marburg/DE, N. Biedenkopf, Marburg/DE, P. Pham, Marburg/DE
- P078 **A Scaffold Hopping Method Yields-selective Liver X Receptor Agonists**  
A. Kaercher, Frankfurt (Main)/DE, E. Proschak, Frankfurt (Main)/DE, F. Lillich, Frankfurt (Main)/DE, F. Motel, Frankfurt (Main)/DE, P. Heitel, Frankfurt (Main)/DE
- P079 **Agonists for a Super-Conserved Orphan GPCR Receptor GPR85**  
R. Cristofalo, Tuebingen/DE, J. Hanson, Liège/BE, M. Stoffel, Liège/BE, M. Wozniak, Liège/BE, S. A. Laufer, Tuebingen/DE, T. Pillaiyar, Tuebingen/DE
- P080 **Design Synthesis and Pharmacological Evaluation of Azaindole-Based Meriolin Analogues as Multitarget Kinase Inhibitors**  
E. Chatziorfanou, Athens/GR, A. D. Kalampaliki, Athens/GR, B. Baratte, Roscoff/FR, I. K. Kostakis, Athens/GR, S. Bach, Roscoff/FR
- P081 **Design and Synthesis of Novel Phloreszin-Based Compounds**  
I. Kostakis, Athens/GR, A. Papapetropoulos, Athens/GR, A. L. Skaltsounis, Athens/GR, E. Chatziorfanou, Athens/GR, E. M. Spailari, Athens/GR, P. Zampas, Athens/GR
- P082 **Chemoproteomic Discovery of CEM198 as the First Small-Molecule Ligand of Tubulin-Tyrosine Ligase**  
I. Kostakis, Athens/GR, A. Tsigara, Athens/GR, B. Kuster, Munich/DE, D. Makarov, Munich/DE, E. A. Georgiou, Athens/GR, G. Médard, Munich/DE, I. K. Kostakis, Athens/GR, L. Persoons, Munich/DE, P. Kielkowski, Munich/DE, R. R. Abanti, Munich/DE, S. Lechner, Munich/DE, S. D. Jonghe, Leuven/BE

- P083 **Synthesis of new triazole-based sirtuin rearranging ligands (SirReals) as Sirt2 inhibitors**  
J. Schneider, Münster/DE, F. Friedrich, Freiburg/DE, F. B. Kollmer, Freiburg/DE, M. Jung, Freiburg/DE, M. Schiedel, Münster/DE
- P084 **Benzophenone derivatives as a new class of anti-infectives against Acanthamoeba spp.**  
H. Geisler, Braunschweig/DE, A. F. A. Moumbock, Münster/DE, M. Schiedel, Münster/DE, S. Reichl, Braunschweig/DE, T. Rimkus, Braunschweig/DE, T. B. El-Jourani, Braunschweig/DE
- P085 **Development of Novel Functionally Selective 5-HT1A Receptor Agonists for the Treatment of Pain**  
B. Löw, Erlangen/DE, C. Sotriffer, Würzburg/DE, H. Hübner, Erlangen/DE, P. Gmeiner, Erlangen/DE, T. Gehrig, Würzburg/DE
- P086 **Spiro3.3heptane as a Saturated Benzene Bioisostere for 3D Drug Design**  
A. Khutorianskyi, Kyiv/UA, A. Kysil, Kyiv/UA, D. Shepilov, Kyiv/UA, I. Bodenchuk, Kyiv/UA, I. Pishel, Kyiv/UA, K. Horbatok, Kyiv/UA, K. Prysiazniuk, Kyiv/UA, O. Datsenko, Kyiv/UA, O. Kolodiazhna, Kyiv/UA, O. Polishchuk, Kyiv/UA, O. Shablykin, Kyiv/UA, P. Borysko, Kyiv/UA, P. Mykhailiuk, Kyiv/UA, S. Shulha, Kyiv/UA, T. Yegorova, Kyiv/UA, V. Kubyshkin, Kyiv/UA, Y. Nikandrova, Kyiv/UA
- P087 **Fluorescence polarization-based screening for new small molecule inhibitors directed against the Insulin-Like Growth Factor 2 mRNA Binding Protein 2 (IGF2BP2/IMP2) KH34 domains**  
K. Mazlom, Saarbrücken/DE, A. Bewanger, Saarbrücken /DE, A. Kiemer, Saarbrücken/DE, A. K. H. Hirsch, Saarbrücken/DE, A. M. Kany, Saarbrücken/DE, K. Wagner, Saarbrücken/DE, M. Empting, Saarbrücken/DE, S. Both, Saarbrücken/DE, S. Klein, Saarbrücken/DE
- P088 **Target Identification and Lead-Optimization of a Broad-Spectrum Antiviral Inhibitor**  
M. Calvin-Brown, Saarbrücken/DE, A. Berwanger, Saarbrücken/DE, C. Münz, Zurich/CH, E. Schönborn, Saarbrücken/DE, J. Zischke, Hannover/DE, M. Böni, Zurich/CH, M. Empting, Saarbrücken/DE, T. Schulz, Hannover/DE
- P089 **From Tetrazole to Isoquinolinone: Structure-Based Optimization and Late-Stage Diversification of AR-C118925-Derived P2Y Receptor Antagonists**  
R. A. M. Abdalrahman, Tübingen/DE, A. Dotz, Tübingen/DE, A. Junker, Tübingen/DE, G. C. Clososki, Ribeirão Preto/BR, K. Schlegel, Münster/DE, M. Bermúdez, Münster/DE, V. H. C. Fernandes, Tübingen/DE
- P090 **Structural Insights into Polypharmacological Targeting of the  $\alpha$ 2A-Adrenergic Receptor and the 5-HT1A Receptor for Pain Treatment**  
L. Mühlberg, Erlangen/DE, G. Chen, Shenzhen/CN, H. Hübner, Erlangen/DE, J. Schneider, Erlangen/DE, J. Xu, Shenzhen/CN, P. Gmeiner, Erlangen/DE, T. Pfeiffer, Erlangen/DE

- P091 **Quorum sensing Inhibition impacts polymicrobial environments of Pseudomonas aeruginosa Infections**  
H. Zhan, Saarbrücken/DE, A. K. H. Hirsch, Saarbrücken/DE, A. M. Kany, Saarbrücken/DE, D. Unterweger, Munich/DE, E. Kosche, Saarbrücken/DE, K. Rox, Braunschweig/DE, M. Empting, Saarbrücken/DE, O. Kelting, Kiel/DE
- P092 **Structure Activity Relationships of Inactive-State EGFR Inhibitors Bridging the ATP and Allosteric Sites**  
F. Wittlinger, Tübingen/DE, D. E. Heppner, Buffalo/US, M. Günther, Tübingen/DE, M. Möllers, Tübingen/DE, M. J. Eck, Boston/US, S. A. Laufer, Tübingen/DE, S. P. Chitnis, Buffalo/US, T. S. Beyett, Atlanta/US
- P093 **Reliable Guide for Development of Sustainable HPLC Methods in Pharmaceutical Analytics and Preparative Drug Synthesis**  
T. B. El-Jourani, Braunschweig/DE, F. Pögel, Braunschweig/DE, H. Wätzig, Braunschweig/DE, M. Schiedel, Münster/DE
- P094 **Targeting the Open Conformation of PhzF to Inhibit Pyocyanin Biosynthesis in Pseudomonas aeruginosa**  
J. Baumgarten, Braunschweig/DE, A. F. A. Moumbock, Münster/DE, C. Kunick, Braunschweig/DE, M. Handke, Braunschweig/DE, M. Schiedel, Münster/DE, M. Thiemann, Braunschweig/DE, M. Zimmermann, Braunschweig/DE, W. Blankenfeldt, Braunschweig/DE
- High-throughput Chemistry**
- P095 **Discovery and Optimization of a Potent and Selective METTL1 Inhibitor**  
V. Kadenbach, Mainz/DE, A. Hübner, Mainz/DE, A. Weldert, Mainz/DE, F. Barthels, Mainz/DE, F. Krähe, Mainz/DE, M. Sabin, Mainz/DE, R. Zimmermann, Mainz/DE, S. Hoba, Mainz/DE, T. Dewald, Mainz/DE, Z. Nidoieva, Mainz/DE
- P096 **Plate-based Chemistry/Direct-to-Biology Approach for Accelerated Drug Discovery**  
F. Pape, Berlin/DE, A. Schneider, Berlin/DE, D. Schaller, Berlin/DE, F. von Nussbaum, Berlin/DE, J. Kramer, Berlin/DE, M. Fürst, Berlin/DE, M. Koy, Berlin/DE, N. Schmees, Berlin/DE, O. Knittelfelder, Berlin/DE, S. Werner, Berlin/DE
- Ion Channels, Membrane Transport**
- P097 **First Total Synthesis and Biological Evaluation of ( $\pm$ )-Rhynchone A reveals its effects on human CatSper and sperm function**  
J. Münchow, Münster/DE, A. Malkov, Loughborough/GB, L. Temme, Hamburg/DE, T. Strünker, Münster/DE
- P098 **Computational Investigation of PIEZO1 Channel Activation and Deactivation**  
J. Massa, Münster/DE, B. Frieg, Gothenburg/SE, C. Tyrchan, Gothenburg/SE, O. Koch, Münster/DE

- P099 **Computational Studies of KCa3.1 and KCa2.2 Channel Modulators**  
M. Gozzi, Münster/DE, J. Massa, Münster/DE, O. Koch, Münster/DE
- P100 **Development of an Autodisplay-based Screening Assay for the Identification of cAMP-competitive Ligands of HCN2**  
H. Kuss, Münster/DE, J. Jose, Münster/DE
- P101 **DELS in Cells – Screening of Integral Membrane Proteins**  
R. G. Petersen, Copenhagen/DK, A. Taranta, Copenhagen/DK, A. B. Christensen, Copenhagen/DK, C. Andersen, Copenhagen/DK, F. A. Sløk, Copenhagen/DK, L. K. Larsen, Copenhagen/DK, L. K. Petersen, Copenhagen/DK, N. J. V. Hansen, Copenhagen/DK, O. Kristensen, Copenhagen/DK, P. Blakskjær, Copenhagen/DK, T. N. Hansen, Copenhagen/DK
- P102 **Steroidal NMDA Receptor Modulators with Inverse Effects on GluN2A and GluN2B**  
A. Dombovski, Münster/DE, A. Labbaf, Münster/DE, B. Sikora, Münster/DE, C. Heusel, Münster/DE, F. Glorius, Münster/DE, G. Goerges, Münster/DE, G. Seebohm, Münster/DE, J. Jose, Münster/DE, J. Osthuus, Münster/DE, J. A. Schreiber, Münster/DE, L. Vyklicky, Prague/CZ, M. Düfer, Münster/DE, \*M. Korinek, Prague/CZ, M. Pierau, Münster/DE, T. Budde, Münster/DE
- P103 **Unraveling the Role of mitoKCa3.1 Channels in Cancer: Synthesis and Evaluation of mitoKCa3.1 Selective Inhibitors**  
C. Kick, Münster/DE, A. Schwab, Münster/DE, B. Wünsch, Münster/DE, H. Noguera Hurtado, Münster/DE, J. Massa, Münster/DE, O. Koch, Münster/DE
- P104 **Synthesis of bridged quinoline systems as potential NMDA receptor ligands**  
N. Spieker, Münster/DE, B. Wünsch, Münster/DE
- P105 **Structure-activity relationship study on ligands activating the voltage-gated potassium channel Kv7.1**  
F. Roßner, Münster/DE, B. Wünsch, Münster/DE, G. Seebohm, Münster/DE

**New Modalities (RipTACS)**

- P106 **Mitochondrial Complex I as a Hidden Liability in Targeted Protein Degradation**  
N. Richert, Heidelberg/DE, A. K. Miller, Heidelberg/DE, B. S. Ivanov, Cambridge/GB, F. Deis, Heidelberg/DE, H. Nsková, Heidelberg/DE, J. Hirst, Cambridge/GB, J. Samarin, Heidelberg/DE, N. de Vries, Heidelberg/DE, N. Gunkel, Heidelberg/DE, S. Ziegler, Dortmund/DE
- P107 **Development of RNA-based PROTACs for targeting RNA-modifying enzymes**  
T. Dewald, Mainz/DE, A. Weldert, Mainz/DE, F. Barthels, Mainz/DE, L. Kammerer, Mainz/DE, M. Helm, Mainz/DE, V. Kadenbach, Mainz/DE, Z. Nidoieva, Mainz/DE
- P108 **Heterobifunctional Protein Binders Enable Cell Type-Specific Killing Through In-cell Enrichment**  
F. Hausch, Darmstadt/DE, A. BUlldan, Darmstadt/DE, A. Löwer, Darmstadt/DE, C. Meyners, Darmstadt/DE

**New Synthetic Methods**

- P109 **Saturated benzene bioisosteres**  
P. K. Mykhailiuk, Kyiv/UA
- P110 **5-Trifluoromethyl-Substituted Saturated O- and S-Heterocycles: Synthesis and Physicochemical Characterization**  
I. Kondratov, Frankfurt (Main)/DE, M. Redka, Kyiv/UA, O. Grygorenko, Kyiv/UA, O. Liashuk, Kyiv/UA
- P111 **Synthesis and Physicochemical Characterization of 6-Trifluoromethyl Spiro[3.3]heptane Building Blocks**  
I. Kondratov, Frankfurt (Main)/DE, A. Chernykh, Kyiv/UA, O. Grygorenko, Kyiv/UA, O. Olifir, Kyiv/UA
- P113 **Toward Synthetic Access to (+)-Neosorangin A, a Structurally Distinct RNA Polymerase Inhibitor**  
M. Wenninger, Magdeburg/DE, D. Schinzer, Magdeburg/DE, L. Chang, Magdeburg/DE, M. Munt, Magdeburg/DE, O. Spieß, Magdeburg/DE
- P114 **A Divergent Synthetic Approach to Novel  $\kappa$ -Opioid Receptor Agonists: Exploiting Bicyclic Scaffolds for Enhanced SAR Studies**  
N. Pöttgen, Münster/DE, B. Wünsch, Münster/DE
- P115 **Synthesis of Anti-MRSA Active Diorcinol Derivatives**  
F. Aichinger, Marburg/DE, N. Schützenmeister, Marburg/DE
- P116 **Optimization, Upscaling, and Automatization of Pyrrolone Synthesis**  
M. Lee, Münster/DE, A.-M. Heidrich, Braunschweig/DE, L. Jäger, Braunschweig/DE, M. Schiedel, Münster/DE, S. Gutperl, Braunschweig/DE, S. Scholl, Braunschweig/DE

**Next GenMedChem**

- P117 **From Unsociable to Sociable: Fragment Space Analysis and the Development of a Sociable Fragment Library**  
P. Janssen, Münster/DE, D. Kümmel, Münster/DE, F. Becker, Münster/DE, I. Kondratov, Kiev/UA, L. S. Benz, Berlin/DE, M.S. Weiss, Berlin/DE, O. Koch, Münster/DE, T. Matviyuk, Kiev/UA
- P118 **Functionalised arene ruthenium complexes for photodynamic therapy**  
C. Papadimou, Neuchatel/CH, B. Therrien, Neuchatel/CH

**Young Investigators**

- P119 **Pentafluoro-Phosphates: New Amphiphilic Chemical Entities with Remarkable Biochemical and Biophysical Properties**  
A. M. Ambros, Berlin/DE, J. Rademann, Berlin/DE

- P120 **Natural Product-Like Fragments Unlock Novel Chemotypes for a Kinase Target –Exploring Options beyond the Flatland**  
 A. Santura, Mainz/DE, A. Metz, Marburg/DE, A. Sandner, Marburg/DE, G. Klebe, Marburg/DE, I.-C. Tutzschky, Mainz/DE, J. Müller, Hamburg/DE, M. Ruf, Marburg/DE, M. Wolter, Hamburg/DE, P. Czodrowski, Mainz/DE, S. Glinca, Hamburg/DE, S. Merkl, Marburg/DE
- P121 **High-Throughput Synthesis and Direct Biological Screening of a Large Library of Streptomycin Derivatives Against Clinically Relevant Bacterial Pathogens**  
 K. Salama, Olomouc/CZ, A. Domling, Olomouc/CZ, L. Gyr, Jena/DE, O. Aehlig, Jena/DE, T. Leistner, Jena/DE
- P122 **Bidirectional optical control of osteogenesis with a light activated vitamin D mimetic (photo-vitD)**  
 X. Ge, Munich/DE, D. Merk, Munich/DE, D. Trauner, New York/US, F. Melfi, Chieti/IT, F. Melfi, Munich/DE, G. Sbriccoli, Munich/DE, J. Artzy, Philadelphia/US, J. Morstein, New York/US, J. Pabel, Munich/DE, J. A. Marschner, Munich/DE, L. Knümann, Munich/DE, S. Willems, Munich/DE, T. Mukhopadhyay, New York/US
- P123 **Covalent Inhibitors Targeting the Drug-Resistant Solvent-Front Mutation G680R in PDGFRA-driven GIST**  
 M. Beerbaum, Dortmund/DE, A. Scrima, Dortmund/DE, D. Rauh, Dortmund/DE, M. P. Müller, Dortmund/DE, S. Bauer, Dortmund/DE, S. Sievers, Dortmund/DE, T. Mühlenberg, Essen/DE, T. Schulz, Dortmund/DE
- P124 **Searching Ultra Large Combinatorial Spaces with Pharmacophores for Covalent Binders**  
 M. von Korff, Basel/CH, C. Loeffeld, Basel/CH, T. Sander, Basel/CH
- P125 **Reshaping Natural Products: New Fidaxomicin Antibiotics and Darobactin-Like Peptides**  
 E. Jung, Berlin/DE
- P126 **Medicinal Chemistry Division of GDCh**  
 GDCh, Fachgruppe Medizinische Chemie, NextGenMedChem

▶ PLATINUM SPONSORS



▶ GOLD SPONSORS



▶ SILVER SPONSORS



▶ BRONZE SPONSORS



▶ OTHER SPONSORS





# VAST Chemical Space

Virtual. Automated. Swift. Tailored.

To navigate the actionable, yet unexplored chemical space - powered by automation and proprietary data

## ✿ VAST contains

Novel, synthetically accessible compounds with quick delivery and competitive pricing



- **85%+** success rate
- 1-2 synthetic steps



- **300+** automated workstations with autonomous AI agents
- Streamlined workflow for high-volume compound delivery



- Average lead time: **2-4 weeks**
- Based on **58,000** in-stock unique building blocks including chiral BBs

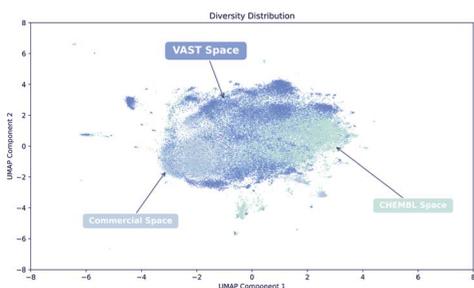


- Favorable physiochemical property profile
- Project-specific subsets available
- **4.66B** unique compounds ready for download

## ✿ Access here

- Go to:  
<https://www.aifchem.com/vast>
- Click download
- Request the Code

## ✿Unlocking the Vast Novel Chemical Space



In total of **4.66 billion** unique compounds

- Diversity subset (1, 10, 100 million) ready for quick start
- Ro5 subset (3.4 B) and Beyond-Ro5 subset for flexible choices

XtalPi Inc.

Shenzhen, China · Beijing, China · Shanghai, China · Liverpool, UK · Boston, USA

Email: [VAST@xtalpi.com](mailto:VAST@xtalpi.com)

Website: [www.en.xtalpi.com](http://www.en.xtalpi.com)

Follow us on LinkedIn: <https://www.linkedin.com/company/xtalpi/>