

# B2B 5<sup>TH</sup> MEDICINAL CHEMISTRY

## STRATEGY MEETING EUROPE 2019

Crowne Plaza London Docklands  
Tuesday 19<sup>TH</sup> March, 2019



### MEDICINAL CHEMISTRY

#### COVER

#### AGENDA-AT-A GLANCE ▶

Artificial Intelligence & Machine Learning  
Design & Custom Synthesis  
Integrated Drug Discovery  
Strategic Partnership & Collaboration  
Chemical Biology & Cheminformatics

#### PAST PARTICIPANTS

#### SPONSORS

#### HOTEL & TRAVEL

HEAR ABOUT  
OUR FORMAT



## OUR UNIQUE MEETING FORMAT

### Roundtable Discussions

These interactive and informal discussion groups are the hallmark of the meeting. Small exclusive groups of Leaders who face shared challenges and strategic priorities are brought together in 60-minute sessions that enable participants to share ideas and lessons learned. Facilitated by experienced professionals, these sessions provide a valuable dialogue with peers on current challenges and topical issues. Each discussion group has limited numbers which ensures each delegate is given ample opportunity to raise questions and contribute to the discussion.

### Personalised Agenda

Each delegate receives a personalised agenda combining industry-leading keynote presentations, topical roundtable discussions, networking and business meetings. You only attend sessions and meetings that fit your challenges and interests, ensuring your time out of the office is focused and well-utilised.

### One-to-one Meetings

The most effective and time efficient way to assess potential partners at a strategic level. Compare and update your knowledge of the industry in 25-minutes informative and relaxed business meetings with solution providers of your choice.

### Networking

Strategic networking opportunities form a key benefit of participating in the meeting. Our proven format for building and strengthening alliances is underscored by a host of networking programmes, from casual networking activities such as lunches as well as formal networking opportunities that are built into your personalised agenda.

### Panel Discussion

Industry-leading professionals share their experiences in high-level strategic case study-based presentation.



*"Seniority and diversity are working good, I've seen here a quite number of people that having a high level of responsibility and level of companies and also seen people from start-ups. It's the first time I was in Proventa meeting and I think I'll comeback."*  
- Senior Vice President - Medicinal Chemistry, Merckachem

*"The one-to-one meeting are very good, this is the first time I've been here and I've been pleasantly surprised with the level of people we've been able to meet. It's the exact people I wanted to meet, we were very happy with the selection process, this two-way dating mechanism were very well frost, I respectedly would like to have more meetings."*  
- Chief Executive Officer, CommineX



## CONTRIBUTORS TO THE AGENDA



### Albert Palomer

Chief Executive Officer & Founder  
ABAC Therapeutics



### Guido Koch

Chief Operating Officer  
Topadur Pharma



### Tobias Gabriel

Global Head, External Science & Drug Discovery,  
Global Discovery Chemistry  
Novartis



### Werngard Czechtizky

Senior Director, Head Medicinal Chemistry, IMED RIA  
AstraZeneca



### Rolf Jautelat

Director Medicinal Chemistry  
Bayer Pharmaceuticals



### Anil Vasudevan

Director  
Abbvie



### Howard Riezman

Professor and Director  
University of Geneva



### Parvez Haris

Professor of Biomedical Science, and Head of  
Biomedical and Environmental Health Research  
De Montfort University

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| TRACKS      | ARTIFICIAL INTELLIGENCE & MACHINE LEARNING                                                                             | DESIGN & CUSTOM SYNTHESIS                                                                                                             | INTEGRATED DRUG DISCOVERY                                                                                              | STRATEGIC PARTNERSHIP & COLLABORATION                                                                                               | CHEMICAL BIOLOGY & CHEMINFORMATICS                                                                                   |
|-------------|------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|
| 08:00-08:30 | REGISTRATION & BREAKFAST NETWORKING                                                                                    |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |
| 08:30-09:00 | WELCOME SPEECH & KEYNOTE PRESENTATION                                                                                  |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |
| 09:00-10:00 | Employing AI for medicinal chemistry & small molecule drug discovery<br><b>Rolf Jautelat,</b><br>Bayer Pharmaceuticals | How 'robotic drug discovery' - an automated design and synthesis system stimulates SAR investigations<br><b>Confirmed for Sponsor</b> | Pioneering novel targets with High Throughput RNAi Screening<br><b>Confirmed for Sponsor</b>                           | Translational research advancement for drug discovery through strategic partnerships<br><b>Albert Palomer,</b><br>ABAC Therapeutics | Novel chemical biology approaches for diagnostics and therapeutics<br><b>Howard Riezman,</b><br>University of Geneva |
| 10:00-10:05 | MORNING BREAK                                                                                                          |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |
| 10:05-10:30 | 1-1 MEETINGS / NETWORKING                                                                                              |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |
| 10:30-10:35 | BREAK                                                                                                                  |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |
| 10:35-11:00 | 1-1 MEETINGS / NETWORKING                                                                                              |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |
| 11:00-12:00 | Artificial intelligence in big data and clinical research development<br><b>Confirmed for Sponsor</b>                  | Advancing complex molecule expansion by cumulating chemical synthesis and formulation<br><b>Guido Koch,</b><br>Topadur Pharma         | Expanding the chemical space of DNA encoded libraries <b>Title TBC</b><br><b>Sarma BVNBS,</b><br>SAI Life Sciences Ltd | Strategies to de-risk precompetitive initiatives in collaborative drug discovery<br><b>Confirmed for Sponsor</b>                    | Integration of Chemogenomics data for applications in chemical biology<br><b>Confirmed for Sponsor</b>               |
| 12:00-12:05 | BREAK                                                                                                                  |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |
| 12:05-12:30 | 1-1 MEETINGS / NETWORKING                                                                                              |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |
| 12:30-12:35 | BREAK                                                                                                                  |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |
| 12:30-13:00 | 1-1 MEETINGS / NETWORKING                                                                                              |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |
| 13:00-14:00 | LUNCH                                                                                                                  |                                                                                                                                       |                                                                                                                        |                                                                                                                                     |                                                                                                                      |



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| TRACKS      | ARTIFICIAL INTELLIGENCE & MACHINE LEARNING                                                                                                     | DESIGN & CUSTOM SYNTHESIS                                                                                            | INTEGRATED DRUG DISCOVERY                                                                                                                                               | STRATEGIC PARTNERSHIP & COLLABORATION                                                                                                                                        | CHEMICAL BIOLOGY & CHEMINFORMATICS                                                                                                               |
|-------------|------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| 14:00-14:30 | KEYNOTE PRESENTATION                                                                                                                           |                                                                                                                      |                                                                                                                                                                         |                                                                                                                                                                              |                                                                                                                                                  |
| 14:30-15:30 | In silico prognosis of chemical toxicity for drug design utilizing machine learning methods and structural alerts<br><br>Confirmed for Sponsor | Chemistry observation throughout a particular scaffold for library synthesis validation<br><br>Confirmed for Sponsor | Harnessing the power of phenotypic screening to uncover novel biology and to identify new targets and new modalities for drug discovery<br><br>Tobias Gabriel, Novartis | Assessing and utilizing strategic deliberations for external delivery technologies<br><br>Confirmed for Sponsor                                                              | Molecular descriptors in chemoinformatics, computational combinatorial chemistry, and virtual screening<br><br>Confirmed for Sponsor             |
| 15:30-15:35 | AFTERNOON BREAK                                                                                                                                |                                                                                                                      |                                                                                                                                                                         |                                                                                                                                                                              |                                                                                                                                                  |
| 15:35-16:00 | 1-1 MEETINGS / NETWORKING                                                                                                                      |                                                                                                                      |                                                                                                                                                                         |                                                                                                                                                                              |                                                                                                                                                  |
| 16:00-17:00 | The involvement of machine learning in biological data sets<br><br>Facilitator to be Announced                                                 | Composition of target molecules of any structural or stereochemical complexity<br><br>Anil Vasudevan, Abbvie         | Resolving the challenges in peptide discovery with the use of nanosystems<br><br>Werngard Czechtizky, AstraZeneca                                                       | Understanding the FDA regulations for new drug applications, legal framework and intellectual property laws encompassing drug repurposing<br><br>Facilitator to be Announced | Controlling the potential of natural products in drug discovery from a cheminformatics vantage point<br><br>Parvez Haris, De Montfort University |
| 17:00-18:00 | DRINKS & CONVERSATION                                                                                                                          |                                                                                                                      |                                                                                                                                                                         |                                                                                                                                                                              |                                                                                                                                                  |

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## ARTIFICIAL INTELLIGENCE & MACHINE LEARNING



### Rolf Jautelat

Director Medicinal Chemistry  
Bayer Pharmaceuticals

09:00-10:00

Employing AI for medicinal chemistry & small molecule drug discovery

- ▶ Paradigm changes enabling "AI for medicinal chemistry": Past - present - future?
- ▶ Key areas where "AI/machine learning/data science" may truly improve medicinal chemistry & small molecule drug discovery in the next five years
- ▶ The hype cycle for "AI in life science": Which current claims are vastly exaggerated?
- ▶ What are good ways to mingle and grow scientist and AI specialists in a productive setting
- ▶ Will AI restrict the creativity of scientists or hinder serendipity?



### Confirmed for Sponsor

11:00-12:00

Artificial intelligence in big data and clinical research development



### Confirmed for Sponsor

14:30-15:30

In silico prognosis of chemical toxicity for drug design utilizing machine learning methods and structural alerts



### Facilitator to be Announced

16:00-17:00

The involvement of machine learning in biological data sets

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## DESIGN & CUSTOM SYNTHESIS



### Confirmed for Sponsor

09:00-10:00

How 'robotic drug discovery' - an automated design and synthesis system stimulates SAR investigations



### Guido Koch

Chief Operating Officer  
Topadur Pharma

11:00-12:00

Advancing complex molecule expansion by cumulating chemical synthesis and formulation

- ▶ Opportunities by investing in the discovery and development of complex drug candidates
- ▶ Strategies for addressing challenges in synthesis
- ▶ Opportunities by investing in formulation development
- ▶ Established and approved formulation concepts vs. new and innovative formulation strategies
- ▶ Timing and resourcing



### Confirmed for Sponsor

14:30-15:30

Chemistry observation throughout a particular scaffold for library synthesis validation



### Anil Vasudevan

Director  
Abbvie

16:00-17:00

Composition of target molecules of any structural or stereochemical complexity

- ▶ Do we need specialist synthesis groups in the discovery area?
- ▶ Value of academic collaborations on development of new synthetic methods
- ▶ What robust reaction chemistries are we missing for parallel synthesis groups?
- ▶ Value of proprietary building blocks or fragments?

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## INTEGRATED DRUG DISCOVERY



### Confirmed for Sponsor

09:00-10:00

Pioneering novel targets with High Throughput RNAi Screening



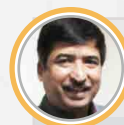
### Tobias Gabriel

Global Head, External Science & Drug Discovery, Global Discovery Chemistry, **Novartis**

14:30-15:30

Harnessing the power of phenotypic screening to uncover novel biology and to identify new targets and new modalities for drug discovery

- ▶ What are the learnings from successful phenotypic screening?
- ▶ How can we envision phenotypic screening coupled with proteomics analysis to uncover the biology of unknown or lesser-characterized ligases to identify novel scaffolds of degradation and targets?
- ▶ How can we design screening libraries for phenotypic screening to accelerate the discovery of novel targets and medicines?
- ▶ How are novel screening technologies expected to accelerate phenotypic drug discovery?
- ▶ How can high-content screening, image recognition and machine learning help accelerate drug discovery?



### Sarma BVNBS

Senior Vice President of Discovery Sciences  
**Sai Life Sciences**



11:00-12:00

Expanding the chemical space of DNA encoded libraries  
**Title TBC**



### Werngard Czechtizky

Senior Director, Head Medicinal Chemistry, IMED RIA  
**AstraZeneca**

16:00-17:00

Resolving the challenges in peptide discovery with the use of nanosystems

- ▶ Peptides and nano formulations – what are the preferred systems and why?
- ▶ When is the moment to go for nano formulation instead of or in parallel to chemical modification?
- ▶ How to characterize the properties of nano formulations? How to assess the immunogenicity of nano formulations?
- ▶ Sc, oral and inhaled – what are the experiences depending on administration route?



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## STRATEGIC PARTNERSHIP & COLLABORATION



### Albert Palomer

Chief Executive Officer & Founder  
ABAC Therapeutics

09:00-10:00

Translational research advancement for drug discovery  
through strategic partnerships

- ▶ Narrow spectrum antibiotics
- ▶ Resistant pathogens
- ▶ Promoting alliances in true-sharing mode
- ▶ Discovering new innovative medicines



### Confirmed for Sponsor

11:00-12:00

Strategies to de-risk precompetitive initiatives in  
collaborative drug discovery



### Confirmed for Sponsor

14:30-15:30

Assessing and utilizing strategic deliberations for external  
delivery technologies



### Facilitator to be Announced

16:00-17:00

Understanding the FDA regulations for new drug  
applications, legal framework and intellectual property laws  
encompassing drug repurposing

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## CHEMICAL BIOLOGY & CHEMINFORMATICS



### Howard Riezman

Professor and Director  
University of Geneva

09:00-10:00

Novel chemical biology approaches for diagnostics and therapeutics

- ▶ Novel chemical biology tools to study membrane properties
- ▶ Membranes and lipids as therapeutic targets
- ▶ Chemical biology methods to target protein-lipid interactions
- ▶ Chemical biology tools to increase cellular entry



### Confirmed for Sponsor

11:00-12:00

Integration of Chemogenomics data for applications in chemical biology



### Confirmed for Sponsor

14:30-15:30

Molecular descriptors in chemoinformatics, computational combinatorial chemistry, and virtual screening



### Parvez Haris

Professor of Biomedical Science, and Head of Biomedical and Environmental Health Research, **De Montfort University**

16:00-17:00

Controlling the potential of natural products in drug discovery from a cheminformatics vantage point

- ▶ What are the key achievements and challenges of cheminformatics as applied to discovery of drugs derived from natural products?
- ▶ Progress in the integration of cheminformatics with genomics, bioinformatics, structural biology, molecular pharmacology, and medicinal chemistry
- ▶ Latest advances in the development of cheminformatics tools
- ▶ Chemoinformatics in the era of big data



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## 2018 PARTICIPANTS

**AB Science** - Head of Computational Chemistry  
**ABAC Therapeutics** - CEO  
**Allegra therapeutics** - CMC director  
**Arrowhead Pharma (US)** - Vice President, Head of Chemistry and Manufacturing  
**AstraZeneca** - Senior Director, Head Medicinal Chemistry, IMED RIA  
**AstraZeneca** - Senior Medicinal Chemist  
**Axanton Technology** - Founder  
**Bayer AG** - Director, Medicinal Chemistry  
**Bioversys** - Chief Scientific Officer  
**Boehringer Ingelheim** - Director Cancer Cell Signalling  
**Boehringer Ingelheim** - Director, Medicinal Chemistry  
**Boehringer Ingelheim** - Global Head BD&L Technologies  
**e Therapeutics** - Programme Manager  
**Eli Lilly and Company** - Chief Scientific Officer, Head of Chemistry  
**F. Hoffmann-La Roche AG** - Head Medicinal Chemistry  
**F. Hoffmann-La Roche AG** - Section Head CADD Team  
**Forendo Pharma** - Head of Drug Discovery  
**Galapagos** - Team Leader  
**Heptares Therapeutics** - Medicinal Chemistry Director  
**Heptares Therapeutics Ltd** - Senior Research Fellow / Head CADD  
**Hoffmann-La Roche** - Principal Scientist  
**Idorsia Pharma** - Director  
**InterAx Biotech** - CEO  
**InterAx Biotech** - CTO  
**Inventiva Pharma** - Head of Chemistry  
**Ipsen** - SVP, Peptides Development, Head of Pharmaceutical Development Site (Dreux, France) General Manager, Octreopharm Sciences GmbH (Berlin, Germany)  
**Jansenn** - Senior Principal Scientist  
**Leo Pharma** - Vice President  
**Lifearc** - Head of Chemistry

**Medivir** - Director Medicinal Chemistry  
**Merck** - Vice President, Global Head of Medicinal Chemistry  
**Merck KGaA** - Associate Director Medicinal Chemistry  
**Merck KGaA** - Director Discovery DMPK  
**MMV** - Associate Director  
**MMV** - Discovery Scientist  
**MSD Research GmbH** - Scientific Associate VicePresident, European Chemistry Lead  
**Nerviano Medical Sciences** - Director  
**Netris Pharma** - CBO  
**Neurocycle Therapeutics** - CEO  
**NMD Pharma Aps** - Director of Chemistry  
**Novartis** - Basel Head Chemical Biology and Therapeutics  
**Novartis** - Director, Computer-aided Drug design  
**Novartis** - Executive Director, Medicinal Chemistry  
**Novartis** - Global Head, External Science & Drug Discovery, Global Discovery Chemistry  
**Novartis** - Head GDC Discovery Technologies  
**Novartis** - Project Leader/Principal Scientist  
**Novartis** - Research Investigator III  
**Novartis** - Senior Investigator  
**Novartis** - Senior Investigator I  
**Novartis Pharma AG** - Director  
**Orion Pharma** - Director of Medicine Design  
**Polyphor** - Head Medicinal Chemistry  
**Roche** - Head Small Molecule Discovery Workflows  
**Sanofi** - Department Head  
**Sanofi** - Head of Structural Design & Informatics  
**Sprint Bioscience** - Director Protein Science and Drug Design  
**Topadur Pharma** - COO  
**Universität Tübingen** - Chair Pharmaceutical/Medicinal Chemistry  
**University of Bonn** - University Professor  
**University of Glaslow** - Professor of Chemical Biology  
**University of Hamburg** - Professor  
**University of Zurich** - Senior Scientist

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**WuXi AppTec** is a leading pharmaceutical, biopharmaceutical, and medical device open-access platform global company. As an innovation-driven and customer-focused company, WuXi AppTec provides a broad and integrated portfolio of services that enables drug and medical device R&D through cost-effective and efficient solutions. WuXi's Oncology Unit possesses world leading oncology and immuno-oncology platforms providing a comprehensive panel of tumor model systems, including human cancer cell line-derived xenograft models, murine syngeneic tumor models, humanized animal models and patient-derived xenograft (PDX) models with in-depth genomic characterization. Our proprietary database - OncoWuXi - has over 1,200 tumor models with full annotation. WuXi Oncology also has strong expertise in CRISPR and specialized tumor cell biology assays.

#### CO-HOST SPONSORS



**Dotmatics** delivers a ready-to-use platform to capture, register, share, collaborate, query, visualise and analyse all the information and knowledge generated in the modern, highly collaborative scientific industries. Dotmatics has significant expertise in scientific informatics, including database management for chemistry and biologics, electronic laboratory notebooks, chemical and biological registration, screening data management, SAR analysis, reporting, and visualisation.



**MercachemSyncom** has a 30 year track record in assisting leading pharma and biotechnology companies with medicinal chemistry programs. Starting as a chemistry service provider, MercachemSyncom has transformed into an integrated drug discovery CRO offering chemistry services, in vitro screening, ADME studies, pharmacokinetics and in vivo pharmacology. Primary chemistry activities include medicinal chemistry services, hit-to-lead optimization programs, synthesis of key building blocks, library synthesis, route scouting services, process research activities, scale up, and cGMP manufacturing. On custom basis, we also synthesize metabolites, impurities, reference standards and stable labelled compounds. Our services are backed by state-of-the-art analytical technologies such as SFC, HPLC, GC, LC-MS, GC-MS and NMR. MercachemSyncom is based in Europe (The Netherlands and Czech Republic) and employs around 300 chemists (>50% PhDs).



**Sai Life Sciences** provides services to our pharma innovator partners, which accelerate the discovery, development and manufacture of complex small molecule therapeutics. Our clients gain clear competitive advantages through shorter time to market and risk minimization using our integrated and high-quality scientific services. Established in 1999, Sai has >2,000 employees located at 4 R&D and manufacturing sites in India. Sai has focused on building expert core capabilities in all areas of chemistry from hit discovery to GMP manufacturing. Sai also provides high-value integrated services in pharmacology, DMPK, toxicology and formulation development to better support the increasing needs of our customers.



**Sygnature Discovery** is the UK's largest independent provider of integrated drug discovery resource. We accelerate the search for new medicines by providing flexible scientific resource and advanced drug discovery knowledge and expertise. Core capabilities include medicinal chemistry, in vitro bioscience, computational chemistry, DMPK, physical sciences and informatics; all co-located in our superb technologically advanced facility. Our experienced and highly qualified PhD scientists utilize novel technologies and innovative ways of working to ensure that we successfully deliver on your most complex integrated research programmes.



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### KEY OPINION LEADER



**NovAliX**



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### VENUE

**Crowne Plaza London Docklands**  
Royal Victoria Dock, Western Gateway,  
London E16 1AL, UK

*To make an individual room reservation,  
please do contact Crowne Plaza Reservation  
Department under.*

**PHONE:** +44 20 7055 2101

**EMAIL:** [group@cpdocklands.co.uk](mailto:group@cpdocklands.co.uk)

### DISCOUNT ROOM RATES

Single Occupancy: \$ 219  
Double Occupancy: \$ 229

### DISCOUNT ROOM RATE CUT OFF

18<sup>TH</sup> February, 2019

**Proventa Code: PI4**

**CLICK  
HERE**  
for more details

**MAP & DIRECTIONS**