



ECBS 2021 
EUCHEMS / EU-OPENSREEN

European Chemical Biology Symposium

26-28 MAY, 2021

VIRTUAL

CONFERENCE BOOK



European Chemical Biology Symposium

26-28 MAY, 2021 VIRTUAL

Bringing together scientists from Europe and overseas to present and discuss latest achievements in cutting edge chemical sciences

CONFERENCE BOOK

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It is our pleasure to welcome you to the European Chemical Biology Symposium (ECBS) 2021, which is jointly organised by EU-OPENSREEN and the EuChemS Division of Chemistry for Life Sciences.

WELCOME

The ECBS 2021 brings together scientists from Europe and overseas to present and discuss their latest achievements in cutting edge chemical sciences at the interface with biology and medicine, ranging from new therapeutic approaches to resistant pathogens and viral infections (special session on COVID19 research), to targeting of proteasome and protein aggregation, natural products, artificial intelligence in drug discovery, nanostructured biomaterials, synthetic biology, glycochemistry and biology. Embrace the exciting developments currently happening in chemical biology!

We also encouraged young researchers to present their work at the meeting: Oral & flash presentations were carefully selected from submitted abstracts.



Francesco Peri
University of Milano-Bicocca (Italy)

 **EuChemS**



Wolfgang Fecke
EU-OPENSREEN ERIC (Germany)

 **eu::openscreen**

Whova – virtual conference features

Even if we are currently scattered around the globe without the possibility of a physical meeting, we want to make you feel like you're attending an in-person meeting as closely as possible. This is why we chose the Whova platform to make your virtual ECBS2021 conference experience a good one!

Whova combines many features of a live meeting with remote benefits:

- + Presentations from leading experts of the research field,
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- + Live Q&A and polls
- + Live chats, group discussions, ice-breakers and attendee matchmaking for virtual networking

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Whova

European Chemical Biology Symposium
26-28 MAY, 2021 VIRTUAL

ECBS 2021
EUROPEAN CHEMICAL BIOLOGY SYMPOSIUM

European Chemical Biology Symposium 2021
May 26 - 28, 2021

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May 26 - 28, 2021

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- NAVIGATE** the event agenda and logistics, even without Wi-Fi or data. Access useful information like ridesharing and local attractions through the Community Board
- NETWORK** effectively. Plan whom to meet by exploring attendee profiles and sending out messages
- PARTICIPATE** in event activities through session likes, comments, ratings, live polling, tweeting, and

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Scientific and organisation committee

Organisation committee



Francesco Peri (Chair)

University of Milano-Bicocca, Italy



Katja Herzog

EU-OPENSREEN ERIC, Germany



Wolfgang Fecke (Chair)

EU-OPENSREEN ERIC, Germany



Bahne Stechmann

EU-OPENSREEN ERIC, Germany

Special support

We would also like to thank the following people for their support:

Nathaniel Smith (Speaker and Abstracts organization)

Holger Klimek (Content and abstracts organization, graphic- and communication design)

Scientific committee

Cristina Airoidi

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Michael Assfalg

University of Verona, Italy

Anna Bernardi

University of Milano, Italy

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MRC Laboratory of Molecular Biology, United Kingdom

Laura Cipolla

University of Milano-Bicocca, Italy

Valeria Costantino

University of Napoli, Italy

Gabriele Costantino

EFMC Representative, University of Parma, Italy

Giuliana D'ippolito

Istituto di Chimica Biomolecolare, Italy

Wolfgang Fecke (Chair)

EU-OPENSREEN ERIC, Germany

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Fraunhofer ITMP ScreeningPort, Germany

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Center for Biological Research, Spanish National Research Council, Spain

Gianluca Sbardella

University of Salerno, Italy

Bahne Stechmann

EU-OPENSREEN ERIC, Germany

Päivi Tammela

FIMM/ University of Helsinki, Finland

May 26 / Wednesday

10:00	Welcome Francesco Peri, Wolfgang Fecke
10:15	Opening Lecture Herbert Waldmann (Max-Planck Institute of Molecular Physiology) Pseudo Natural Products – Chemical Evolution of Natural Product Structure
S 1	Nanomedicine and biomaterials Chair: Claudia Bonfio
11:15	Marco Di Antonio (Imperial College London) Single-molecule visualisation of DNA G-quadruplex formation in live cells.
11:45	Oral communication: Alberto Dal Corso (University of Milan) New-generation Self-Immolative Spacers for Fast and Controlled Release of Anticancer Drugs
12:00	Oral communication: Riccardo Marin (Autonomous University of Madrid) Infrared-emitting multimodal nanostructures for controlled in vivo magnetic hyperthermia
12:15	Oral communication: Giuseppe Arrabito (University of Palermo) Printing Biology: where printing meets synthetic biology
12:30	Flash presentation: Chiara Pizzolitto (University of Trieste) Dual cross-link hydrogels with tunable viscoelasticity control stem cell differentiation
12:35	Flash presentation: Francesca Cardano (University of Milan) Squaraine NIR dyes: a structure to function study for novel bilayer membrane probes
12.45	Lunch break (75 minutes)

S 2	Targeted protein degradation Chair: Wolfgang Fecke
14:00	Alessio Ciulli (University of Dundee) How PROTAC degraders work and why the ternary complex matters
14:30	Georg Winter (Research Center for Molecular Medicine of the Austrian Academy of Sciences) Identification and Characterization of novel molecular glue degraders
14:50	Oral communication: Andrea Astolfi (University of Perugia) A novel class of small molecule degraders targeting prion protein folding intermediate
15:10	Oral Communication: Felix Hausch (University Darmstadt) De novo identification of a fully synthetic FKBP12-FRB Molecular Glue
15:30	Coffee break (15 minutes)

May 26 / Wednesday

S 3	Artificial intelligence & computational drug design Chair: Giuliana D'Ippolito, Sonsoles Martin-Santamaria
15:40	Andreas Bender (University of Cambridge) Using Artificial Intelligence and Chemical and Biological Data for Drug Discovery: Opportunities and Pitfalls
16:10	Rebecca Wade (Heidelberg Institute for Theoretical Studies) Combining molecular simulation and machine learning approaches for structure-based drug design
16:30	Oral communication: Albert Antolin (The Institute of Cancer Research, London) From probe to drug: Polypharmacology across drug discovery
16:45	Oral Communication: Katarzyna Walczewska-Szewc (Nicolaus Copernicus University) The changes in prolyl oligopeptidase structure upon inhibition modify its ability to decrease alpha-synuclein aggregation
17:00	Flash presentation: Alejandra Matamoros-Recio (Center for Biological Research (CIB) Margarita Salas / CSIC) Computational approaches to the dynamics and activation mechanism of Toll-like receptor 4
17:05	Conclusions

Ev 1	EVENING SESSION: Gender & Diversity Chair: Sonsoles Martin-Santamaria, Katja Herzog
17:45	Angela Agostiano (Past President of Società Chimica Italiana - Italian Chemical Society) Empowering diversity in science
18:05	Questions & Answers
18:30	Movie screening – "Picture a scientist" (Further information: https://www.pictureascientist.com)
20:00 approx	Interactive discussion
20:45	Conclusions

May 27 / Thursday

10:00	Welcome Francesco Peri, Wolfgang Fecke
S 4	Platforms in drug discovery Chair: Paola B. Arimondo, Gianluca Sbardella
10:05	Angelo Fontana (University of Naples "Federico II") Natural Small Molecules in Chemical Immunology
10:35	Christian Hackenberger (Leibniz Research Institute for Molecular Pharmacology) The power of chemoselectivity: Functional protein-conjugates for intra- and extracellular targeting
10:55	Stefan Laufer (Tübingen University) Covalent Inhibitors re-invented
11:15	Maria Duca (Côte d'Azur University – CNRS) Design and implementation of small-molecule RNA binders for anti-cancer and antimicrobial therapies
11:35	Annika Jenmalm-Jensen (SciLifeLab) Academic Drug Discovery capabilities at SciLifeLab, Sweden.
11:55	Päivi Tammela (University of Helsinki) EU-OPENSOURCE Academic Compound Library – Sourcing compounds from the chemistry community for new discoveries
12:10	Oral communication: Lukas Roth (University of Sydney) Immobilized Metal Affinity Chromatography as a Potential Drug Discovery Platform

12:25	Oral communication: Sebastian Pomplun (Massachusetts Institute of Technology) Combinatorial discovery of synthetic biohybrid ligands for RNA-hairpins and for the SARS-CoV-2-spike protein
12:40	Flash presentation: Elva Morretta (University of Salerno) Label-free functional proteomics links the anti-angiogenic properties of the pyrazolyl-urea GeGe-3 to Calreticulin binding
12:45	Flash presentation: Evgeny Kuleskiy (University of Helsinki) Development of small molecule inhibitors of the endocytic cytoskeleton
12:50	Flash presentation: Callum Rosser (University of Sydney) The synthesis and activity of analogues of the HDAC inhibitor panobinostat with added hydrogen bonding capacity
12:55	Flash presentation: Cosmin Butnarusu (University of Turin) Understanding the mechanisms governing the interaction of drugs with mucus using a novel biosimilar mucus model
13:00	Lunch Break (30 minutes)

May 27 / Thursday

S 5	Fighting resistant pathogens; new antiviral therapies Chair: Cristina Airoidi, Francesco Peri
13:30	Mark Brönstrup (Helmholtz Centre for Infectious Research) Assault, Siege or Trojan Horse Strategy: Use of Natural Products to Fight Bacterial Infections
14:00	Vito Ferro (University of Queensland) Synthetic Heparan Sulfate Mimetics Potently Inhibit SARS-CoV-2 by Disrupting the Spike-ACE2 Interaction
14:20	Sara Sattin (University of Milano) Interfering with bacterial survival strategies
14:35	Boris Vauzeilles (Paris-Sud University) Detecting pathogens and Reactive Oxygen Species using Chemical Biology
14:50	Oral communication: Anna Hirsch (Helmholtz Institute for Pharmaceutical Research Saarland) Discovery of antibacterial agents inhibiting the energy-coupling factor (ECF) transporters by structure-based virtual screening
15:05	Coffee break (5 minutes)

S 6	Natural compound chemistry and biology Chair: Valeria Costantino, Giuliana D'Ippolito
15:10	Laura Steindler (University of Haifa) Defining host-microbe interactions in a basal metazoan: the sponge.
15:40	Jeanette H. Andersen (University of Tromsø) Arctic marine biodiversity as a source for novel compounds
16:00	Pedro Leao (University of Porto) Incorporation and modification of fatty acids in cyanobacterial secondary metabolism
16:20	Oral communication: Slava Ziegler (Max Planck Institute of Molecular Physiology) Morphological Profiling of Small Molecules for Mode-of-Action Prediction
16:35	Oral Communication: Francisco Castillo (MEDINA Foundation) Target-based screening strategies for the identification of novel natural products as protein-protein interaction inhibitors
16:50	Oral Communication: Deniz Tasdemir (GEOMAR Centre for Marine Biotechnology) Metabolomics-Assisted Discovery of Bioactive Marine Natural Products
17:05	Flash presentation: Angela Casillo (University of Naples Federico II) Bacterial mannan polysaccharide: chemical structure and conformational studies
17:10	Conclusions

May 27 / Thursday

Ev 2	EVENING SESSION: Covid19 research Chair: Gabriele Costantino (EFMC representative)
19:00	Welcome by Rui Moreira (EFMC, iMED Lisboa)
19:10	Philip Gribbon (Fraunhofer ITMP Screening Port Hamburg) Compound repurposing by target based and phenotypic approaches to identify in-vitro inhibitors of SARS-CoV2 viral entry and replication
19:30	Oral communication: Kamyar Hadian Acriflavine, a clinically approved drug, inhibits SARS-CoV-2 and other betacoronaviruses
19:45	Flash presentation: Miguel Santos (NOVA University Lisbon) *potentially pre-recorded Enhanced formulations of Hydroxychloroquine as Organic Salts and Ionic Liquids to fight COVID-19
19:50	Flash presentation: Wieslaw Nowak (Nicolaus Copernicus University) Nanomechanics of nanobodies-protein S SARS-CoV-2 virus complexes revealed by a Virtual Atomic Force Microscope
19:55	Panel discussion: Covid19 – challenges and next steps
20:30	Conclusions

May 28 / Friday

10:00	Welcome Francesco Peri, Wolfgang Fecke
S 7	Protein aggregation and self-assembly in disease Chair: Cristina Airoidi, Michael Assfalg
10:05	Laura Steindler (University of Haifa) Defining host-microbe interactions in a basal metazoan: the sponge.
10:35	Jeanette H. Andersen (University of Tromsø) Arctic marine biodiversity as a source for novel compounds
10:55	Pedro Leao (University of Porto) Incorporation and modification of fatty acids in cyanobacterial secondary metabolism
11:15	Oral communication: Slava Ziegler (Max Planck Institute of Molecular Physiology) Morphological Profiling of Small Molecules for Mode-of-Action Prediction
11:30	Oral Communication: Francisco Castillo (MEDINA Foundation) Target-based screening strategies for the identification of novel natural products as protein-protein interaction inhibitors
11:35	Lunch Break (55 minutes)

May 28 / Friday

S 8	Glycochemistry & -biology Chair: Anna Bernardi
12:30	Christoph Rademacher (University of Vienna) Carbohydrate receptor ligands enable targeted delivery to immune cells
13:00	Jeroen Codee (Leiden University) Of sugars and phosphates: synthesis and application of well-defined bacterial oligosaccharide structures
13:30	Carme Rovira (University of Barcelona) Using computers to understand how carbohydrates are processed in nature
13:50	Oral Communication: Gavin Miller (Keele University) Chemoenzymatic synthesis of sugar nucleotide chemical biology tools to explore the GDP-D-mannose dehydrogenase from <i>Pseudomonas aeruginosa</i>
14:05	Flash Presentation: Maria Isabel Garcia-Moreno (University of Seville) GalNAc-related sp2-iminosugars as mutant lysosomal β -hexosaminidase A activity enhancers in late-onset Tay-Sachs disease patients' fibroblasts
14:10	Coffee Break (20 minutes)

S 9	Origin of Life & synthetic biology Chair: Claudia Bonfio
14:30	Matthew Powner (University College London) On the unified chemical origins of peptides and nucleic acids
15:00	Dora Tang (Max Planck Institute of Molecular Cell Biology and Genetics) Coacervates as protocellular models?
15:20	Kamila Muchowska (University of Strasbourg) Non-enzymatic metabolic reactions and life's origins
15:40	Oral Communication: Roger Rubio-Sánchez (University of Cambridge) A Modular, Dynamic, DNA-based Platform for Regulating Cargo Distribution and Transport between Lipid Domains
15:55	Flash presentation: Karina Nakashima (Radboud University) Active coacervate droplets: protocells that grow and survive
16:00	Prize ceremony Chair: Katja Herzog, Sonsoles Martin-Santamaria, Francesco Peri
16:15	Conclusions

Presentation prizes

We are pleased to offer several prizes for the for the 9 best presentations (200€ each) and 12 best posters (100€ each)



The Italian Chemical Society (Divisions of Organic Chemistry, Medicinal Chemistry and Chemistry in Life Sciences) sponsors prizes in the categories

- + Organic chemistry interfacing biology
- + Innovative hit compounds and biomaterials for drug discovery and development
- + Innovative approaches in life science



The Spanish Royal Society of Chemistry (Divisions of Chemical Biology, Carbohydrates and Natural Products) sponsors prizes in the categories

- + Chemical tools in biology
- + Chemical glycobiology
- + Natural products in chemical biology



HOST ORGANISATION PROFILE

A COMPETENCE NETWORK FOR DRUG RESEARCH AND BASIC SCIENCE

EU-OPENSREEN

EU-OPENSREEN is a not-for-profit European Research Infrastructure Consortium (ERIC) for chemical biology and early drug discovery with more than 20 affiliated high-throughput screening and chemistry partner sites in eight member countries. EU-OPENSREEN operates an openaccess database and a central compound management facility which stores, quality-controls and manages the EU-OPENSREEN compound collection.

We support scientists from academia and industry from countries inside and outside of the European Union, in the development of chemical tool compounds and early therapeutic candidate molecules.

Our collaborators work with peerreviewed and experienced biological and chemical institutes by combining biological screening assays with medicinal chemistry expertise.

Our partner sites provide chemical biology related services including assay development, assay adaptation, screening, and medicinal chemistry (including compound design, synthesis, analytics and SAR generation).

These services are carried out in the member countries. The partner sites are organisationally independent of the EU-OPENSREEN ERIC and remain embedded in their host institutions

HOST ORGANISATION PROFILE

THE EUROPEAN
NETWORK THAT
REPRESENTS MORE
THAN 160,000
CHEMISTS FROM 50
MEMBER SOCIETIES



EuChemS

EuChemS, the European Chemical Society (www.euchems.eu), is an umbrella organisation representing national Chemical Societies and other chemistry-related organisations in Europe. EuChemS aims to nurture a platform for scientific discussion and to provide a single, unbiased European voice on key policy issues in chemistry and related fields.

EuChemS has been active since 1970, initially under the name of FECS (Federation of European Chemical Sciences). Representing more than 160,000 chemists from 50 Member Societies and other chemistry related organisations, EuChemS relies on a unique network of active researchers involved in all the fields of chemistry. Through this network, EuChemS organises several specialised academic conferences as well as the biannual EuChemS Chemistry Congress, the European congress of chemical sciences.

EuChemS also promotes the role and image of the chemical sciences among the general public and policy-makers through social media, newsletters and through the organisation of conferences and workshops open to the society.

Through the promotion of chemistry and by providing expert and scientific advice, EuChemS aims to take part in the solution to today's major societal challenges.

The EuChemS Division of Chemistry in Life Sciences aims to promote, inspire and support science in Europe at the frontier of the chemistry with biology and biomedicine. At this intersection, organic & biological chemistry, biotechnology, computational biology, machine learning, drug discovery, synthetic biology, biomedical materials and chemical glycobiology nicely meet.

HOST ORGANISATION PROFILE

TO PROMOTE AND SUPPORT THE DEVELOPMENT OF CHEMISTRY AND SCIENTIFIC RESEARCH



Società Chimica Italiana

Italian Chemical Society

The Italian Chemical Society (Italian: Società Chimica Italiana) is the national association in Italy representing the chemical sciences. Its main aim is to promote and support the development of chemistry and scientific research, spreading the knowledge of chemistry and its applications in order to improve the welfare of the country, establishing and maintaining relations with organizations from other countries with similar purposes and promoting the study of this subject at school and university.

Fundamental objective of the SCI is the spreading of chemical science and its applications to evidence the importance that it covers in the modern society.

Divisions group the associates who follow a same scientific address in their research.

The SCI organizes a wide number of conventions, workshop, courses and seminars both to a national and international level.

In order to spread the principles of chemical science in advanced secondary school it organizes the national selection for the "Chemistry Olympic Games", a competition in which students from all over the world put to the test their own acquaintances in this field. The publishing activity of the Society concerns the issuing of scientific periodicals of high international level

Sponsoring

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3 DAYS

892

REGISTRATIONS

169

SUBMITTED
ABSTRACTS

60

SPEAKERS

30

SELECTED
ABSTRACTS

ECBS 2023

May 2023, 3 days

Oral presentations

Poster sessions

Networking opportunities

www.ecbs2023.eu