ALLODD YEARLY NEWSLETTER

SEPTEMBER 2025

12 countries

13 Benficiaries

11 Partner Organisations

14 Early Stage Researchers

Why Allostery in Drug Discovery?

Most current drugs are designed to bind directly to the primary active sites (also known as orthosteric sites) of their biological targets. Allosteric modulators offer a powerful yet underexploited therapeutic approach. They can elicit a richer variety of biological responses and, since they target less conserved binding sites, higher selectivity and less adverse effects may be obtained.

ALLODD aims to train a new generation of scientists in exploiting the concept of allostery in drug design, putting together a whole array of technologies to identify and characterize allosteric modulators of protein function that will be applied to therapeutically relevant systems.

Eyes on the Future

ALLODD approach is based on a combination of experimental and simulation techniques, including fragment Screening with structural characterization (X-ray, NMR, H/D exchange), proteomics (MS/MS), ITC, DNA encoding libraries, Virtual Screening, Molecular Dynamics simulations-based methods, Synthetic Chemistry, and in vitro and cellular assays for the verification of results.

Allosteric targeting need not be achieved solely through the design of synthetic small molecules, but also can also be reached via conformationally specific allosteric antibodies, which represents an important field of future research. There are already clear examples of monoclonal antibodies that allosterically target ion channels, GPCRs, and RTKs, as well as cytokine and integrin receptors.

ALLODD website
https://www.allodd-itn.eu/

ALLODD Twitter
@ALLODD_ITN

ALLODD YouTube
Allostery in Drug Discovery

ALLODD LinkedIn
ALLODD Allostery in Drug Discovery

Dr. Zoe Cournia
ALLODD Project Coordinator
Biomedical Research Foundation,
Academy of Athens, Greece

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 956314.

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https://www.allodd-itn.eu/ ALLODD Allostery in Drug Discovery @ALLODD_ITN **Allostery in Drug Discovery**

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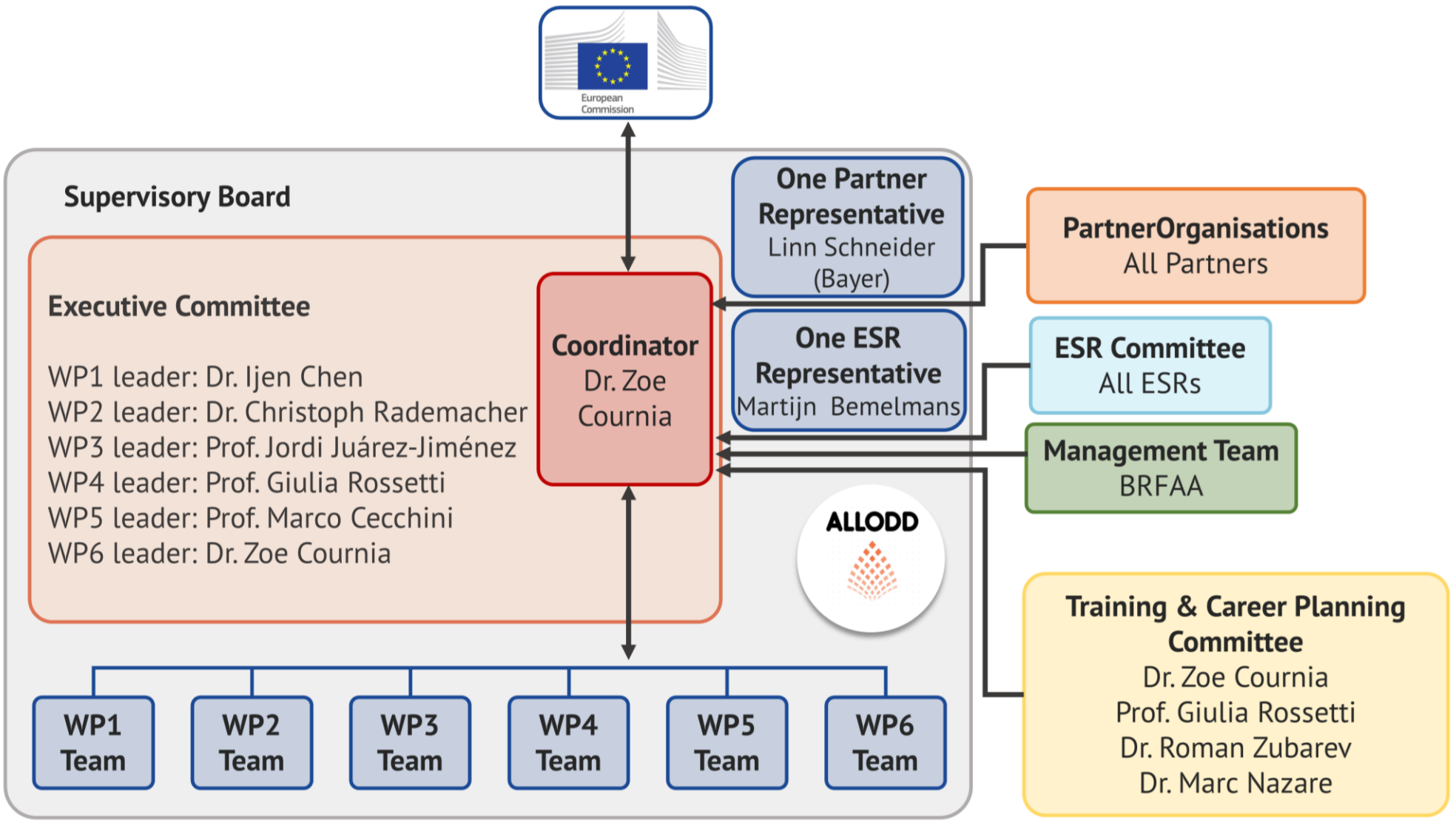
ALLODD Overview

ALLODD Governing Bodies



Dr. Zoe Cournia
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ACADEMY OF ATHENS

BRFAA
BIOMEDICAL RESEARCH FOUNDATION ACADEMY OF ATHENS

https://www.allodd-itn.eu/ ALLODD Allostery in Drug Discovery @ALLODD_ITN **Allostery in Drug Discovery**

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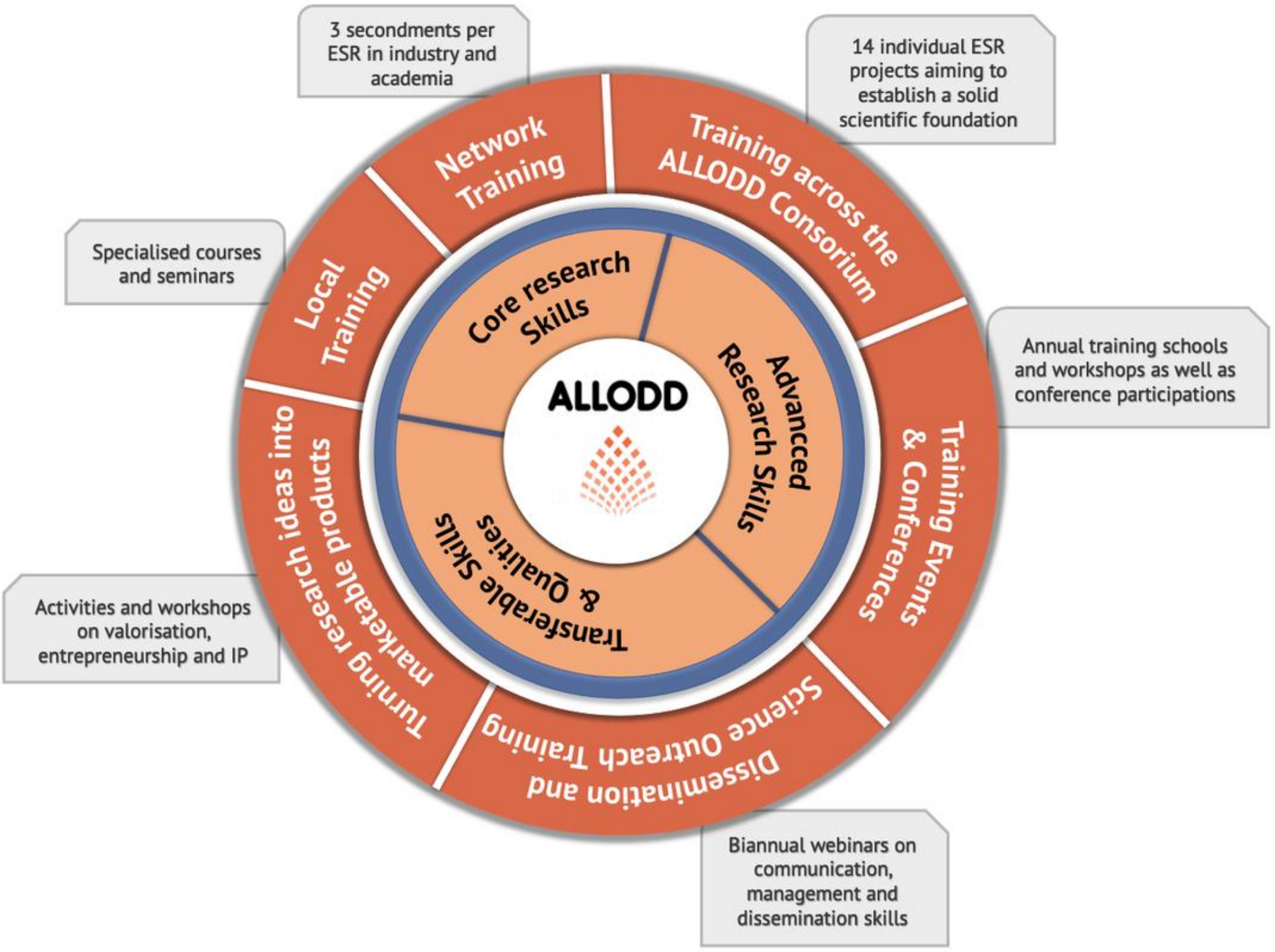
ALLODD Training

ALLODD Training Scheme



https://www.allodd-itn.eu/ ALLODD Allostery in Drug Discovery @ALLODD_ITN **Allostery in Drug Discovery**

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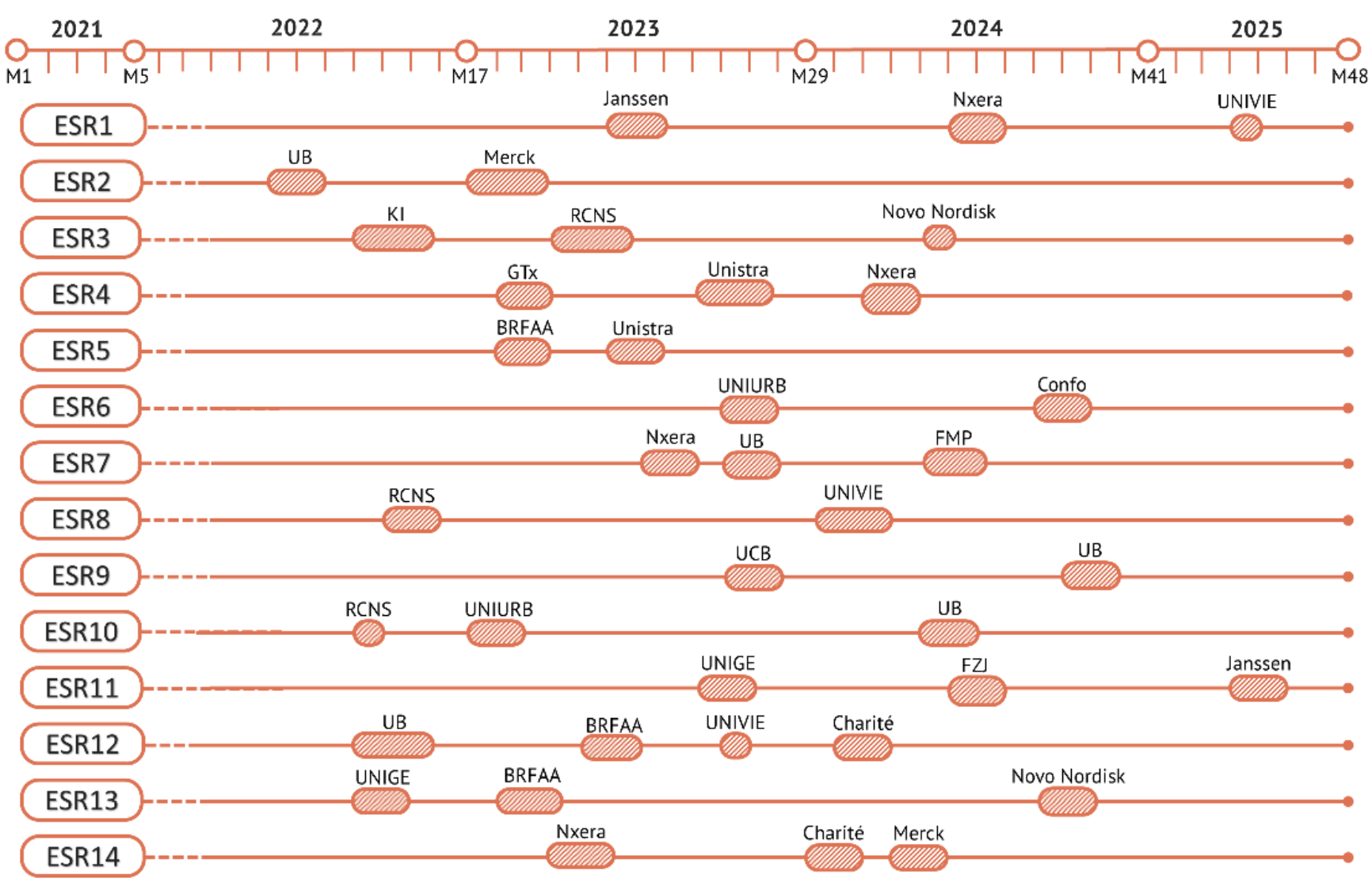
ALLODD Training

Secondments

The **ALLODD network** serves as a platform for **Early-Stage Researchers (ESRs)** to complete three training secondments in ALLODD participant laboratories. Two secondments are related to the area of expertise of the ESRs, and one is in a different research area.

Secondments are a key component of the complementarity between ALLODD participants, which is required to assimilate different research methodologies, ways of thinking, and research cultures. Due to the complementarities between the teams, the recruited ESRs have the opportunity to benefit from both academic and industrial environments.



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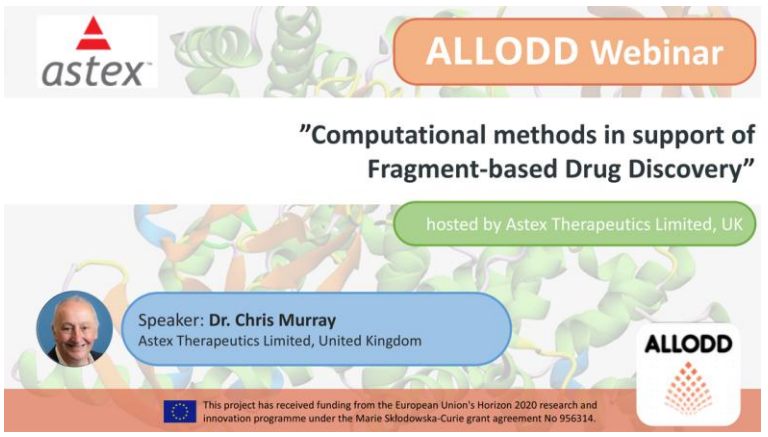
ALLODD Training

Webinars

ALLODD Webinar Prorgam

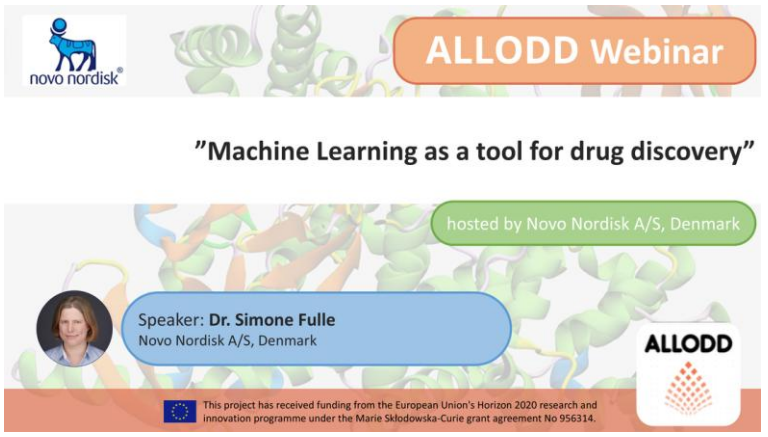
16th **Computational methods in support of Fragment-based Drug Discovery**

Speaker: **Dr. Chris Murray**
Host: Astex Therapeutics Limited, United Kingdom
Date: **06.11.2024, 3pm (CET)**



17th **Machine Learning as a tool for drug discovery**

Speaker: **Dr. Simone Fulle**
Host: Novo Nordisk A/S, Denmark
Date: **15.01.2025, 3pm (CET)**



18th **Investigating cryptic binding sites and allostery: novel methodologies**

Speaker: **Prof. Francesco L. Gervasio**
Host: University of Geneva, Switzerland
Date: **04.03.2025, 3pm (CET)**

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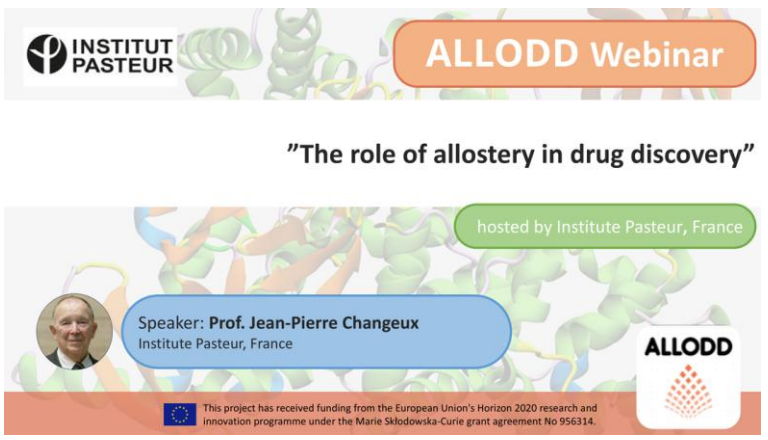
ALLODD Training

Webinars

ALLODD Webinar Prorgam

19th [The role of allostery in drug discovery]

Speaker: **Prof. Jean-Pierre Changeux**
Host: Institut Pasteur, France
Date: **07.05.2025, 3pm (CET)**



20th [Training young researchers: Soft and transferable skills]

Speaker: **Dr. Zoe Cournia**
Host: Biomedical Research Foundation, Academy of Athens, Greece
Date: **09.07.2025, 3pm (CET)**

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ESR Blog Posts

During the ALLODD project, ESRs have been writing a blog post every 6 months narrating their experiences and/or projects they are working on. ESR blogs are uploaded on the ALLODD website blog page: https://www.allodd-itn.eu/blog.

- **Secondments: Essential Training Tools for PhD Researchers**
  by ESR7 Vincenzo Di Lorenzo

- **My Summer Secondment at FZJ: Exploring Cation-Pi Interactions in Glycine Receptor**
  by ESR11 Hryhory Sinenka

- **EuroQSAR 2024: State of the art Drug Discovery back at home**
  by ESR14 David Sotillo Núñez

- **Nobel Prize 2024: AI Taking the Lead in Life Sciences**
  by ESR9 Bohdana Sokolova

- **Tips for navigating the maze of PhD thesis submission**
  by ESR12 Léxane Fournier

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- **Allostery: The "Second Secret of Life" & Its Growing Impact on Science**
  by ESR7 Vincenzo Di Lorenzo

- **A Scientific Gathering in Athens: Research, Careers, and Good Food**
  by ESR14 David Sotillo Núñez

- **Technology Transfer 101: How Academic Discoveries Become Real Medicines**
  by ESR9 Bohdana Sokolova

- **Connected Through Science and Beyond**
  by ESR4 Özge Ergun

- **Boltz-2: A New AI Model for Structure and Binding Affinity Prediction**
  by ESR5 Simone Mariani

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- **Becoming a Marie Curie Fellow: The Decision That Changed My Life**
  by ESR3 Varbina Ivanova

- **Secondment at Johnson & Johnson**
  by ESR11 Hryhory Sinenka

- **Wrapping up the ALLODD journey after two years**
  by ESR1 Francho Nerín Fonz

- **Protein By DesAIgn**
  by ESR13 Martijn Bemelmans

- **Industry and Academia**
  by ESR13 Martijn Bemelmans

- **A Day of Curiosity at Forschungszentrum Jülich**
  by ESR5 Simone Mariani

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ALLODD Training

ESR Science Slam Videos

ESR Science Slam Videos

During the ALLODD project, each ESR developed an ALLODD Science Slam in the form of a video on their research topic. ESR blogs are uploaded on the ALLODD website blog page: https://www.allodd-itn.eu/science-slams.html

- **Artificial Intelligence to discover new protein target sites and design better drugs**
  by ESR1 Francho Nerín Fonz

- **Investigating protein structure with cryoelectron microscopy**
  by ESR6 Sigrid Pedersen

- **Introducing G-protein-coupled Receptors and Allosteric modulation**
  by ESR10 Sonja Peter - Science Slam

- **Binding free energy calculations for synaptic receptors**
  by ESR11 Hryhory Sinenka

- **Drug Design & Förster Resonance Energy Transfer (FRET)**
  by ESR4 Özge Ergun

- **The Power of Computer-Aided Drug Discovery**
  by ESR3 Varbina Ivanova

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ESR Science Slam Videos

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- **The unsolved mystery of GPCR Dimerization**
  by ESR5 Simone Mariani

- **From cells to simulations: Studying membrane proteins**
  by ESR14 David Sotillo Núñez

- **How medicine work and covalent keys**
  by ESR7 Vincenzo Di Lorenzo

- **How sticking together a pair of protein scissors with small molecules can help to treat disease**
  by ESR8 Nina-Louisa Efrém

- **Proteomics: Decoding the city of you**
  by ESR9 Bohdana Sokolova

- **The Sound of Atoms - How NMR Spectroscopy Reveals Protein Biology**
  by ESR2 Jonathan Lefèbre

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ALLODD Training

Courses & Lectures

Courses & Lectures

ESRs attend a list of online lectures, webinars and courses that are suggested by the ALLODD consortium. These events aim to create a framework for multidisciplinary training as well as exposure of the ESRs to a wider scientific spectrum. The events have varying formats ranging from workshops, seminars to conferences. Most of them are held online enabling the participation of all ESRs regardless of their location.

https://www.allodd-itn.eu/courses--lectures.html

CCPBioSim

EFMC²

EFMC² Tandem Talks

Tandem Talks

MŰEGYETEM 1782

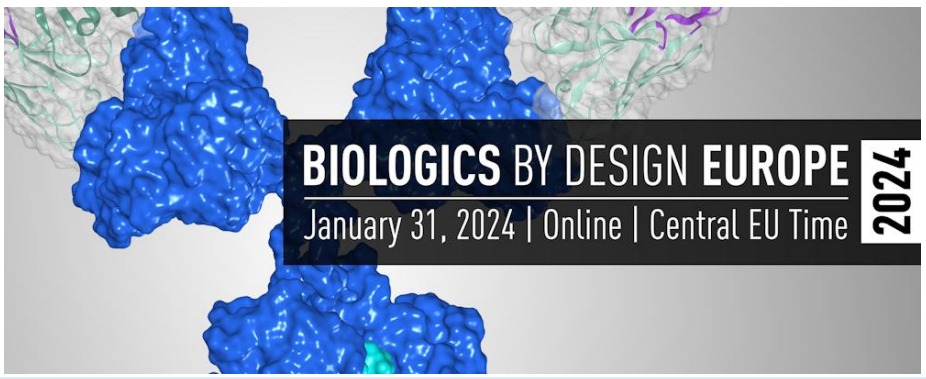
#MedChemCASES webinars

GDCh MedChem

Courses offered by Jülich Forschungszentrum

JÜLICH Forschungszentrum

Google DeepMind



Bristol Myers Squibb

EFMC Young Scientists Network

EFMC-YSN MedChemBioOnline

MedChemBio Online

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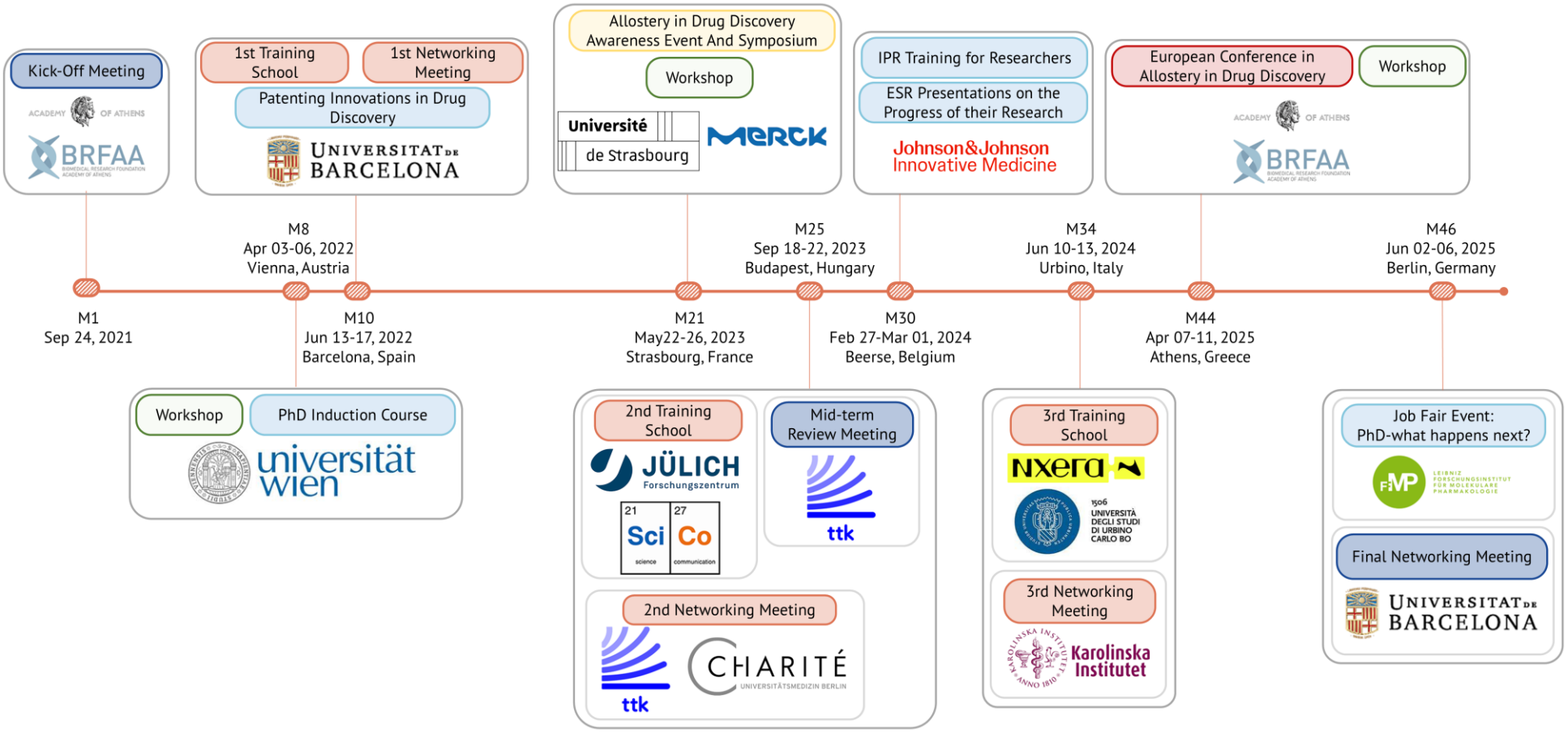
ALLODD Events

Overview

ALLODD trains the new generation of scientists to learn how they can exploit the concept of allostery in drug discovery. We offer a multidisciplinary training program that employs a variety of scientific methodologies based on the complementarity of the academic and industry ALLODD partners.

Through the ALLODD events program, the 14 ESRs gain core and advanced research skills, as well as transferable skills and qualities.
https://www.allodd-itn.eu/allodd-events.html



https://www.allodd-itn.eu/ ALLODD Allostery in Drug Discovery @ALLODD_ITN **Allostery in Drug Discovery**

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ALLODD Events

European Conference on Allostery in Drug Discovery

European Conference on Allostery in Drug Discovery

Host Organization: Biomedical Research Foundation, Academy of Athens, Greece

Scientist-in-charge: Dr. Zoe Cournia

Dates: 7-8 April 2025 ALLODD ESR Workshop
9-11 April 2025 European Conference on Allostery in Drug Discovery

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Watch conference videos!

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ACADEMY OF ATHENS

https://www.allodd-itn.eu/ ALLODD Allostery in Drug Discovery @ALLODD_ITN **Allostery in Drug Discovery**

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ALLODD Events

Final Networking Meeting

Final Networking Meeting

Host Organization: LEIBNIZ-RESEARCH INSTITUTE FOR MOLECULAR PHARMACOLOGY (FMP) in FORSCHUNGSVERBUND BERLIN EV (FVB) and Charité - Universitätsmedizin Berlin, Germany

Scientists-in-charge:
Prof. Marc Nazaré
Dr. Patrick Scheerer

Dates: 3-6 June, 2025

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ALLODD Events

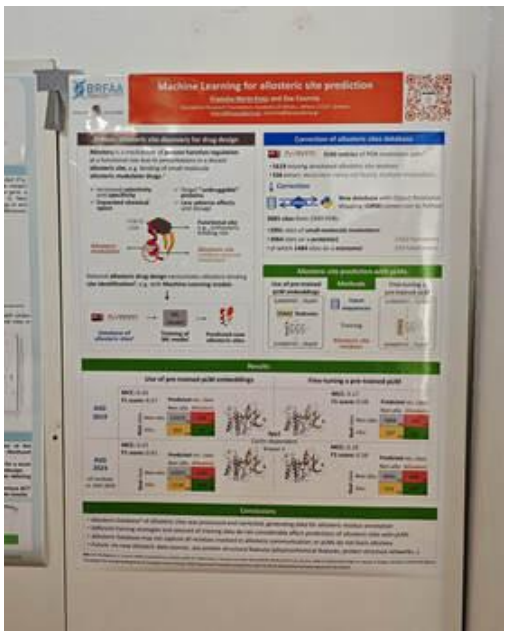
Communication Events

Bio3 2024: Biomedicine, Bioinformatics & Biotechnology Forum: Fostering Collaboration in Industry & Academia

Date: 1-5 September 2024
Location: Technopolis City of Athens

ALLODD participated in the Bio3 2024: Biomedicine, Bioinformatics & Biotechnology Forum: Fostering Collaboration in Industry & Academia in Technopolis City of Athens. The Bio3 2024 unlocks the limitless potential of AI in biotech, pharma, human health, and microbiome research, where groundbreaking discoveries, industry insights, and collaborative opportunities will converge to accelerate innovation and foster commercial success.

This year top experts, biotech innovators, and investors from across the globe gathered for engaging discussions, groundbreaking innovation showcases, and unparalleled networking opportunities. **The Cournia lab including Francho Nerín Fonz (ESR1)** through their speeches and poster presentations presented ALLODD to scientists and undergraduate and graduate students.



Find out more about this event here.

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ALLODD Events

Communication Events

Mednight – Nuit Mediterranéenne des Chercheuses 2024 (European Researcher's Night 2024)

Date: 27 September 2024
Location: Lycee Joffre in Montpellier

Sigrid Pedersen (ESR 6) took part in Montpellier's version of the **European Researcher's Night,** organised by Genopolys and partners of the **Mednight consortium**. The event, open to the public from five years and up, saw almost 150 researchers from different fields gather to share their passion for science through interactive workshops, conferences, games and debates.

Sigrid Pedersen participated as part of the **EU corner** ("Coin de l'UE"), which was focused on teaching about EU-actions, especially Marie Sklodowska-Curie actions, European women researchers and science through a wheel of fortune game and the distribution of learning material.

More information can be found here.

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ALLODD Events

Communication Events

Nit de la Recerca 2024 (European Researcher´s Night 2024)

Date: 27 September 2024
Location: Museu de la Ciència Cosmo Caixa, Barcelona, Spain

ALLODD members **Varbina Ivanova (ESR 3), Özge Ergün (ESR 4), David Sotillo (ESR 14), Prof. Jordi Juarez** and **Prof. Carles Curutchet** participated in **Researcher´s Night** activities held in Museu de la Ciència Cosmo Caixa (Science Museum) in Barcelona.

They organized a science fair with the title “A visual trip to binding of a drug to a receptor” targeting the general public from kids to adults. They demonstrated different protein structures and ligands by using VR glasses and also enlightened people about the ALLODD program. Attendees also got the chance to try on the glasses and get hands-on experience in the virtual protein world.

More information can be found here.

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Life is Science (European Researcher´s Night 2024)

Date: 27 September 2024
Location: University of Graz, Graz, Austria

ALLODD member **Jonathan Lefèbre (ESR2)** participated in the **European Researcher's Night**, held at the University of Graz. Organized by the acib GmbH, the University of Graz, and the University of Applied Sciences St. Pölten, the event allowed participants of all ages and backgrounds to explore and engage with science, technology, and scientific collaboration through a variety of exhibitions, workshops, and shows.

At a hands-on station, Jonathan presented the **goals of the ALLODD project**, explaining how it aims to facilitate the **discovery of drugs** for difficult-to-treat diseases. Attendees explored the complexities and opportunities of **allosteric drug discovery** by building models of approved allosteric drugs and learning about their protein targets.

More information can be found here.

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 956314.

ALLODD Events

Communication Events

Matí de la Recerca 2024 (European Researcher's Night 2024)

Date: 30 September
Location: Jesuïtes de Sarrià – Sant Ignasi

The ALLODD member **David Sotillo Núñez (ESR14)** participated in the activity "Matí de la Recerca" in the framework of 2024 **Researcher's Night** in the school Jesuïtes de Sarrià – Sant Ignasi.

There, he organized a talk for students on their last high school year. The talk focused on bringing the process and techniques used in Drug Discovery to the students. Computational techniques such as **Docking** and **Molecular Dynamics** were discussed and demonstrated. Lastly, the ALLODD project was showcased, as well as the ESR work within it to serve as a practical example to what was explained.

More information can be found here.

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Utställningen Unga Forskare 2025 (The Young Scientists Exhibition)

Date: February 10-14, 2025
Location: Online

ESR9 Bohdana Sokolova participated as an **expert scientific juror** in **Utställningen Unga Forskare 2025**, **Sweden's largest youth science competition**, where she engaged directly with Swedish high school students. In this role, she actively interacted with students' research projects during February 10-14, 2025, providing detailed scientific feedback and guidance to **help them develop their research skills and scientific thinking**. The event involved over **720 participants** from across Sweden, and she personally worked with and mentored **6 high school students**.


Tilldelas:

Bohdana Sokolova

Stort tack för ditt värdefulla medverkande som juryledamot!
Detta är ett certifikat för ditt ideella engagemang som:

Digitaljuryledamot

UTSTÄLLNINGEN UNGA FORSKARE

Hälsningar: Albert Isaksson

Digitaljuryansvarig, Utställningen Unga Forskare 2025

Through this digital mentorship, Bohdana engaged in constructive dialogue about their work, shared insights from her field, and **helped nurture the next generation of Swedish researchers**. This outreach activity was conducted as part of **her work with ALLODD**, allowing her to translate her research expertise into meaningful educational impact.

More information can be found here.

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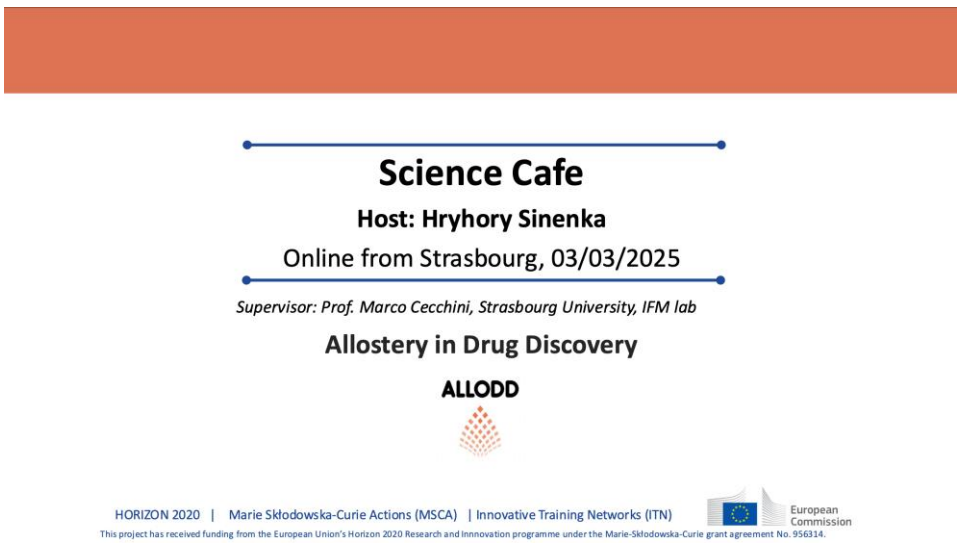
ALLODD Events

Communication Events

ALLODD Science Cafe with ESR 11 Hryhory Sinenka

Date: March 3, 2025
Location: Online

ESR11 Hryhory Sinenka has hosted an **online Science Café** devoted to his PhD research done under the ALLODD initiative. The Science Café was accessible to the general public and focused on an easy-to-comprehend discussion of the science of **synaptic receptors' modulation** and relevant **computational chemistry** techniques. Additionally, the ALLODD Network was presented and explained, as well as the **concept of allostery**. In the end, listeners' questions were addressed, establishing a direct connection with the general public. This initiative brought better awareness of the ESR11 work to the wider audience outside of the academic setting.



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Open Day (Tag der Neugier) 2025 at Forschungszentrum Jülich

Date: September 7, 2025
Location: Jülich, Germany

ESR5 (Simone Mariani) actively contributed to the highly successful **Open Day (Tag der Neugier) 2025 at Forschungszentrum Jülich**, which welcomed **over 22,000 visitors** to the campus. Throughout the day, he supported a variety of engaging activities both inside and outside the building. These included a puzzle-based computer game illustrating the complexity of protein folding, creative activities for children such as coloring biomolecule and cell structure printouts, assembling three-dimensional virus models from paper and tape, and an interactive computer game that allowed visitors to guide AI in generating imaginative images blending proteins with animals. He also introduced a software tool that translated visitors' names or short sentences into unique protein sequences, making the experience both educational and entertaining for participants of all ages.

More information can be found here.

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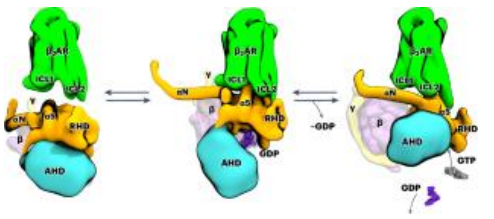
ALLODD Results

Publications 2024-2025

Batebi H., Pérez-Hernández G., Rahman S.N., Lan B., Kamprad A., Shi M., Speck D., Tiemann J.K.S., Guixà-González R., Reinhardt F., Stadler P.F., Papasergi-Scott M.M., Skiniotis G., Scheerer P., Kobilka B.K., Mathiesen J.M., Liu X., Hildebrand P.W., 2024
Mechanistic insights into G-protein coupling with an agonist-bound G-protein-coupled receptor.
Nat. Struct. Mol. Biol.
https://doi.org/10.1038/s41594-024-01334-2



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Mapping protein binding sites by photoreactive fragment pharmacophores.
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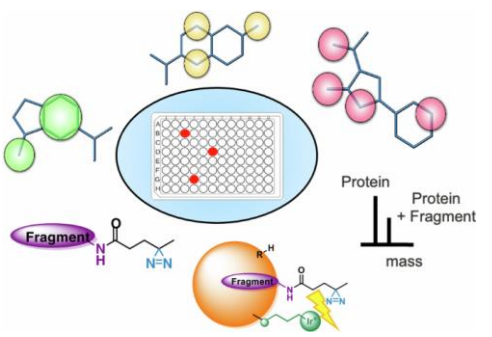

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Discovery of potent allosteric antibodies inhibiting EGFR.
mAbs
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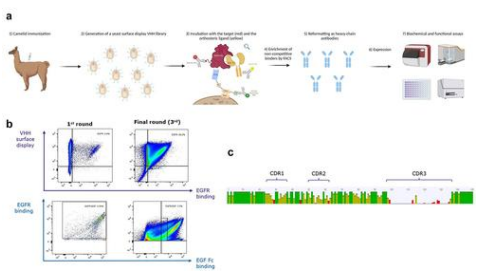
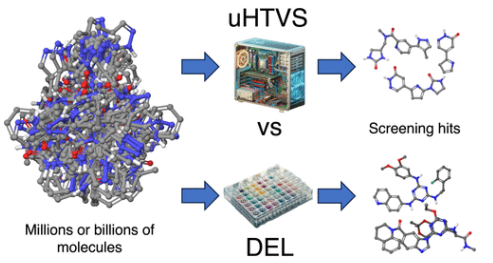


Mihalovits, L.M., Szalai, T.V., Bajusz, D., Keserű, G.M., 2024
Exploring Chemical Spaces in the Billion Range: Is Docking a Computational Alternative to DNA-Encoded Libraries?
J. Chem. Inf. Model.
https://doi.org/10.1021/acs.jcim.4c00803



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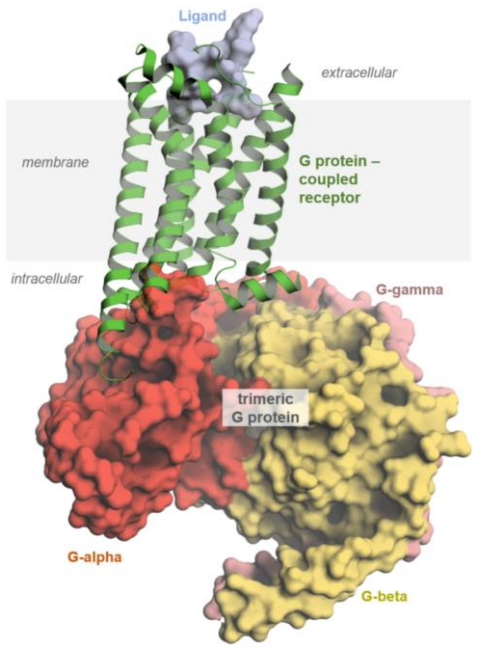

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 956314.

ALLODD Results

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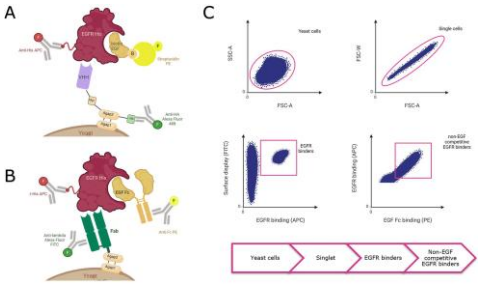

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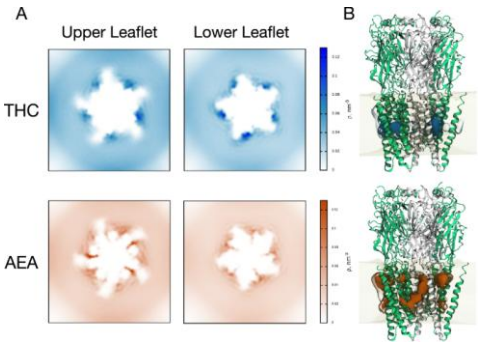

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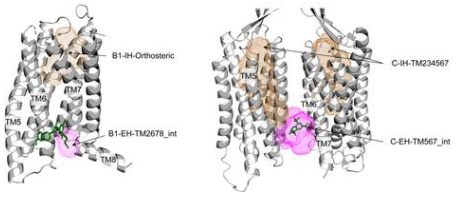

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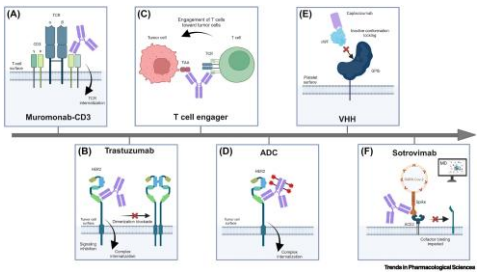

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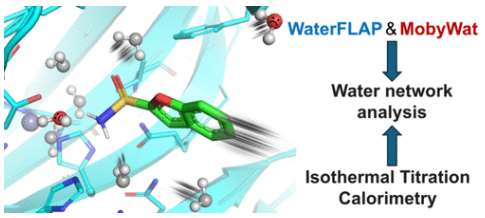

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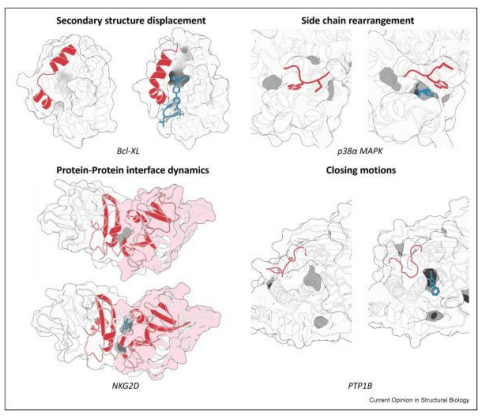

https://www.allodd-itn.eu/ ALLODD Allostery in Drug Discovery @ALLODD_ITN **Allostery in Drug Discovery**

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ALLODD Results

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Syntheses of differentially fluorinated triazole-based 1-deoxysphingosine analogues en route to SphK inhibitors.
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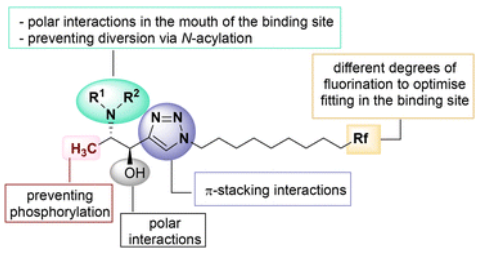

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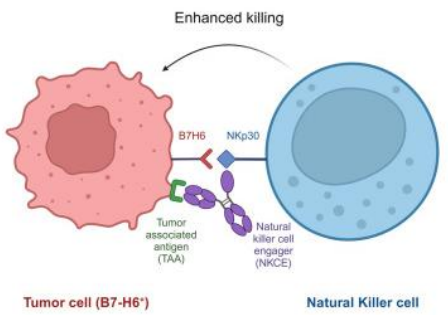

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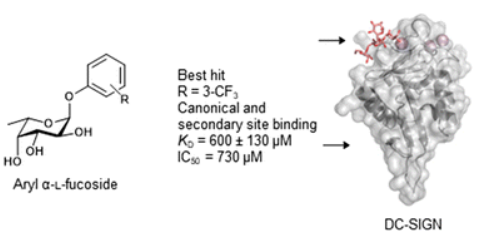

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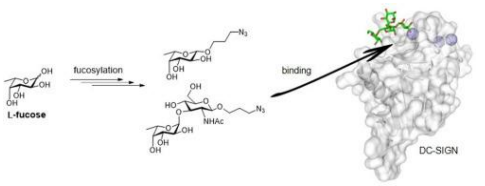

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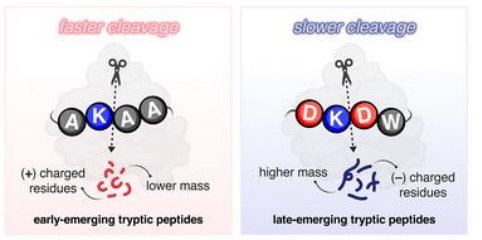

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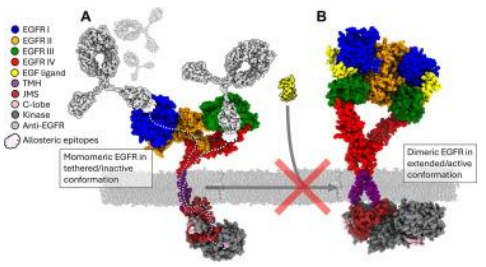

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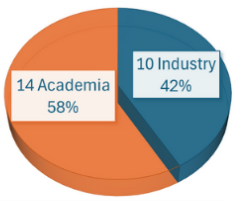
ALLODD Infographic

ALLODD Infographic

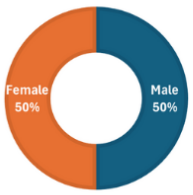
8 FACTS ABOUT ALLODD

01.
13 Beneficiaries &
11 Partner
Organisations



02.
12 Countries

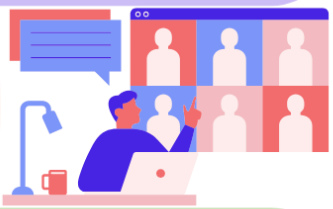
03.
14 Early Stage
Researchers



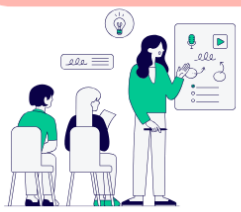
04.
60 YouTube
videos

05.
41 Publications &
54 Conference
Presentations

06.
38 Secondments



07.
20 Webinars



08.
8 Training Events

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ALLOSTERY IN DRUG DISCOVERY

ALLODD Beneficiaries

- Academy of Athens BRFAA
- Universität Wien
- Universitat de Barcelona
- ttk
- Jülich Forschungszentrum
- Karolinska Institutet
- Charité Universitätsmedizin Berlin
- 1506 Università degli Studi di Urbino Carlo Bo
- FMP Leibniz Forschungsinstitut für Molekulare Pharmakologie
- Nxera
- Université de Strasbourg
- Merck
- Johnson & Johnson Innovative Medicine

ALLODD Partner Organizations

- Bayer
- 21 Sci 27 Co science communication
- ucb
- Semmelweis Egyetem 1782
- GAIN Therapeutics
- novo nordisk
- confo therapeutics
- Université de Genève
- Institut Pasteur
- astex

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