

Allostery in Drug Discovery

ALLODD



2nd Training School & Networking Meeting

18-22 September 2023
Budapest, Hungary

Research Centre for Natural Sciences



<https://www.allodd-itn.eu/>



[@ALLODD_ITN](https://twitter.com/ALLODD_ITN)



[Allostery in Drug Discovery](https://www.youtube.com/watch?v=...)



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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Welcome

Welcome to the ALLODD 2nd Training School & Networking Meeting in Budapest!



Prof. György Miklós Keserű
ALLODD Budapest Meeting Organizer
Research Centre for Natural Sciences
Hungary

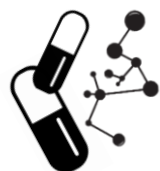


Dr. György G. Ferenczy
ALLODD Budapest Meeting Organizer
Research Centre for Natural Sciences
Hungary



ALLODD

The **ALLODD** project is a collaboration between **23 academic and industrial organizations with 14 ESRs.**



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 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.



Budapest Meeting

The **ALLODD 2nd Training School & Networking Meeting** will be held at the Research Centre for Natural Sciences (Budapest, Hungary) on September 18-22. **Days 1 and 2** include soft skill trainings for ESRs on time management and project management. **Day 3** is dedicated to progress reports by ESRs and discussions with supervisors. The two-day event of „Biophysical and computational methods in allostery – drug discovery training” starts on **Day 4** with lectures on biophysical and computational methods. The conference continues on **Day 5** with industry case studies in the morning session and a hands-on computational chemistry training on the afternoon.



All events of the meeting will take place at the lecture rooms of the Research Centre for Natural Sciences

Address: 2 Magyar tudósok krt. 1117 Budapest, Hungary

Social Event

Boat trip and dinner on the Danube (Wednesday 20.09.2023)

19:00-22:00

Embarkment: Infopark kikötő close to RCNS



Program – Day 1

<p>Day 1 18.09.2023</p>	9:00 – 9:15	<p>Welcome</p>
	<p>9:15 – 17:00 includes morning and afternoon coffee breaks and lunch</p>	<p>Time management Trainer: János Balázs KISS Mindbeat</p> <p>Focus on Priorities</p> <p>Consciousness, Principles, Practices - Who's who, agenda, personal goals</p> <ul style="list-style-type: none"> - Getting back your control - tools, habits, mindsets, focus on results (and not on activities) - Result areas, goals, tasks - goalsetting within personal key areas - Planning and keeping priorities - 'What', 'When', execution on daily, weekly, monthly basis, defining and keeping priorities every day - using the urgent/important matrix <p>Systems and habits</p> <ul style="list-style-type: none"> - When life sweeps you away... managing distractors and interruptions, no multitasking, saying no - managing stress - sources of eustress and distress, impact, control, managing your energy - task management every day - mail, comms, meetings <ul style="list-style-type: none"> - long-term tasks, (self) motivation, habits - closing: personal insights, learning, next steps



Lecture room, RCNS



Program – Day 2

Day 2 19.09.2023	9:00 – 17:00 includes morning and afternoon coffee breaks and lunch	Project management Trainer: Zbynek BRYCH Happy Training & Consulting What is project management and why it is necessary How it supports project efficiency What are the main phases of the project What its basic tools are Why projects fail or don't reach their objectives - the most common reasons Case study
	17:00-19:00	Supervisory Board and Executive Board meetings



Lecture room, RCNS



Program – Day 3

ESR Progress Reports

Day 3 20.09.2023	09:00 – 10:40	Individual research projects (10min+15min) ESR 1-4
	10:40 – 11:15	Coffee Break
	11:15 – 12:30	Individual research projects (10min+15min) ESR 5-7
	12:30 – 13:30	Lunch
	13:30 – 15:10	Individual research projects (10min+15min) ESR 8-11
	15:10 - 15:45	Coffee Break
	15:45 – 17:00	Individual research projects (10min+15min) ESR 12-14
	17:00 – 18:00	Training and Carrier Planning Committee meeting



Lecture room, RCNS

Social event Boat trip and dinner on the Danube	
19:00-22:00	Embarkment: Szent Gellért tér



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Program – Day 4

Biophysical and computational methods in allostery – drug discovery training

Day 4 21.09.2023	<i>Methods</i>	
	09:00 – 9:10	Introduction György KESERŰ, RCNS
	9:10 – 10:20	X-ray crystallography: principles and applications in drug design. Gregory VERDON, Sosei Heptares
	10:20 – 11:30	Cryo-EM in drug discovery: the basics, prospects and limitations Dóra KARANCSINÉ MENYHÁRD, Eötvös University
	11:30 – 12:00	Coffee-break
	12:00 – 13:10	NMR methods in Drug Discovery and Development. Christoph RADEMACHER, University of Vienna
	13:10-14:10	Lunch
	14:10:15:20	Label-free biophysical characterization of protein-ligand interactions Tamás MARTINEK, University of Szeged
	15:20-15:50	Coffee-break
	15:50-17:00	Which computational approach is best suited to your needs? Xavier BARRIL, University of Barcelona



Lecture room, RCNS



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Program – Day 5

Biophysical and computational methods in allostery – drug discovery training

Day 5 22.09.2022	<i>Industry case studies</i>	
	09:00 – 09:40	Development of allosteric glucokinase activators. András KOTSCHY, Servier
	09:40 – 10:20	Nucleosides in action: Discovery of JNJ-64619178 as a potent and selective PRMT5 inhibitor for the treatment of lung and hematologic cancers. Jan-Willem THURING Johnson & Johnson
	10:20 – 10:50	Coffee-break
	10:50 – 11:30	Life outside the active site. Joe COYLE, Astex
	11:30 – 12:10	Structural biology in drug discovery Linn SCHNEIDER, Bayer
	12:10 – 12:50	In silico peptide & protein design. Simone FULLE, Novo Nordisk
	13:00 – 14:00	Lunch
<i>Hands-on computational chemistry training</i>		
	14:00-17:00	Structure determination from electron density maps Gregory VERDON, Sosei Heptares Protein structure preparation for modelling Ligand docking and virtual screening György FERENCZY, RCNS Software packages to download: https://www.ccp4.ac.uk/download/#os=windows (windows version recommended) https://www.schrodinger.com/downloads/releases (node-locked licenses will be provided)



Lecture room, RCNS



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Getting to Budapest



Arriving by airplane

From the Liszt Ferenc [Airport](#), you can take a taxi, the [minibus](#) shuttle service or public transport: [RCNS is accessible](#) by taking bus 100E toward the city centre, or bus 200E toward underground M3.



Arriving by train

RCNS is easily accessible from all major train stations by public transport:
From [Déli pályaudvar](#) (Southern railway station)
From [Keleti pályaudvar](#) (Eastern railway station)
From [Nyugati pályaudvar](#) (Western railway station)



Getting to the Meeting

Location:

Research Centre for Natural Sciences

H-1117 Budapest

Magyar tudósok krt. 2.

<http://www.ttk.hu/en>

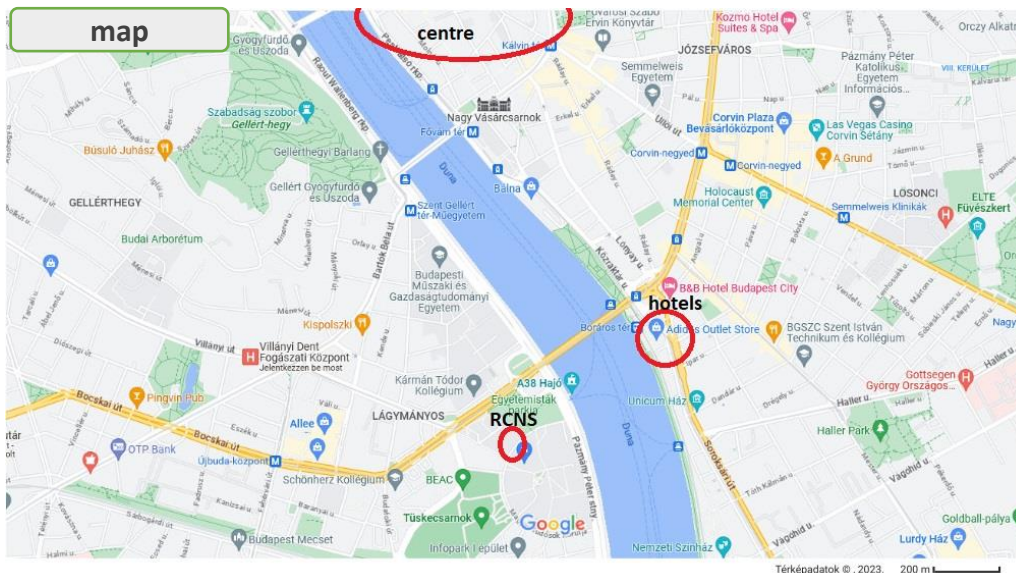
GPS: 47.47415, 19.06019



streetview



map



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Hotels

The hotels below are within walking distance from RCNS and are along tram lines 4 and 6.

[B&B HOTEL Budapest City](#)

Angyal u. 1-3, 1094 Budapest
1.2 km from RCNS

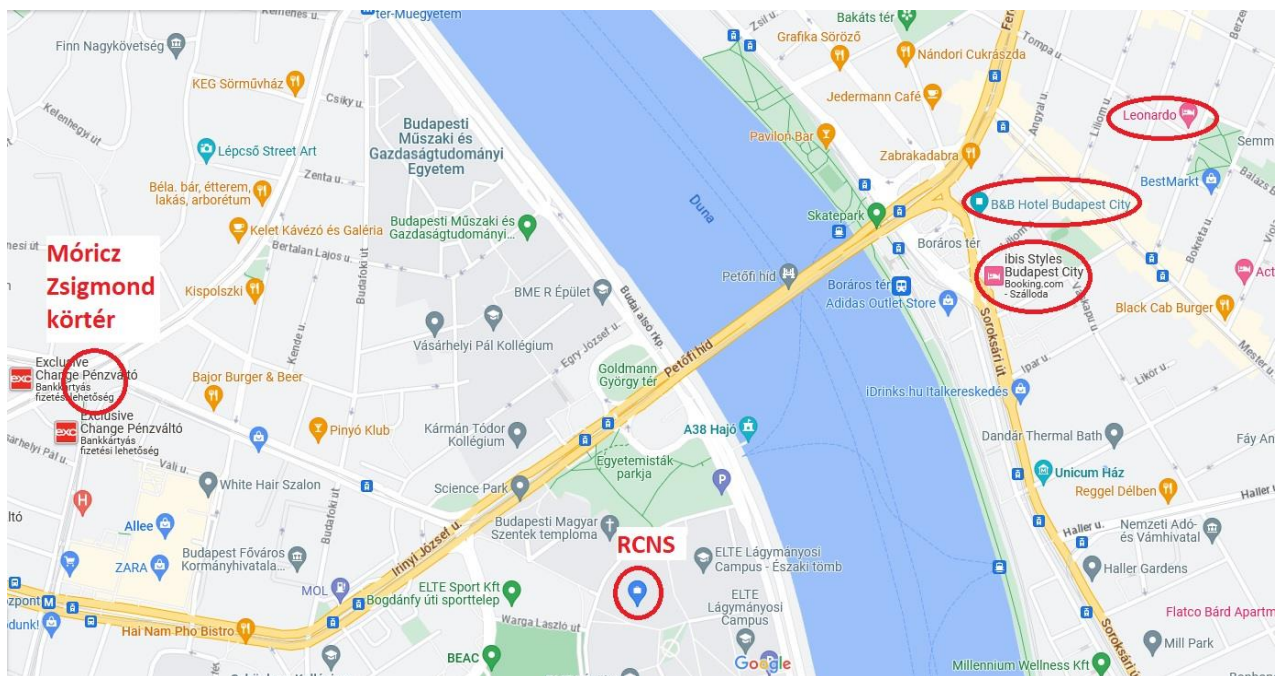
[ibis Styles Budapest City](#)

Soroksári út 12, 1095 Budapest
1.3 km from RCNS

[Leonardo Hotel Budapest](#)

Tompa utca 30-34, 1094 Budapest
1.8 km from RCNS

Many other options are available. Hotels along tram lines 4 and 6 provide easy access to RCNS. Other convenient locations are those with direct access to Móricz Zsigmond körtér (metro line 4, trams 17, 19, 41, 47, 49, 56, 61, bus 7) from where RCNS is accessible with tram 6 or with a 15-minute walk.



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Further information

Childcare arrangements will be provided upon request. If you are interested in this service, please, contact the event organisers:

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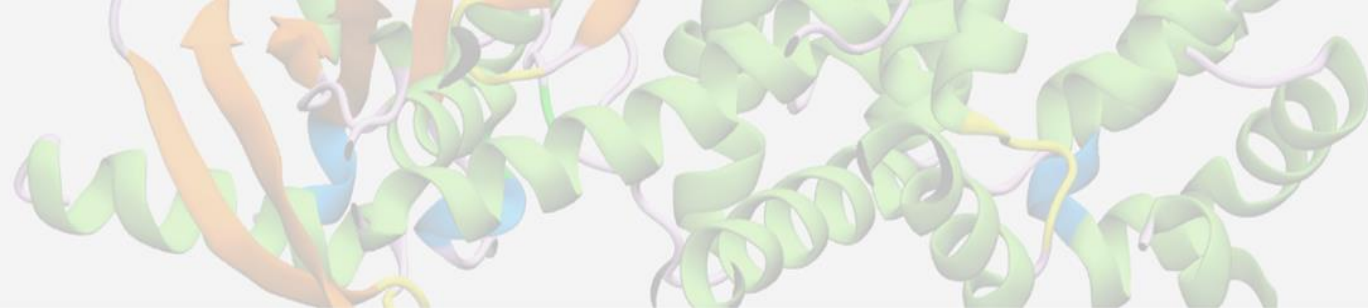
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Biomedical Research Foundation, Academy of Athens, Greece



Meeting Organizers

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RCNS, Budapest, Hungary



<https://www.allodd-itn.eu/>



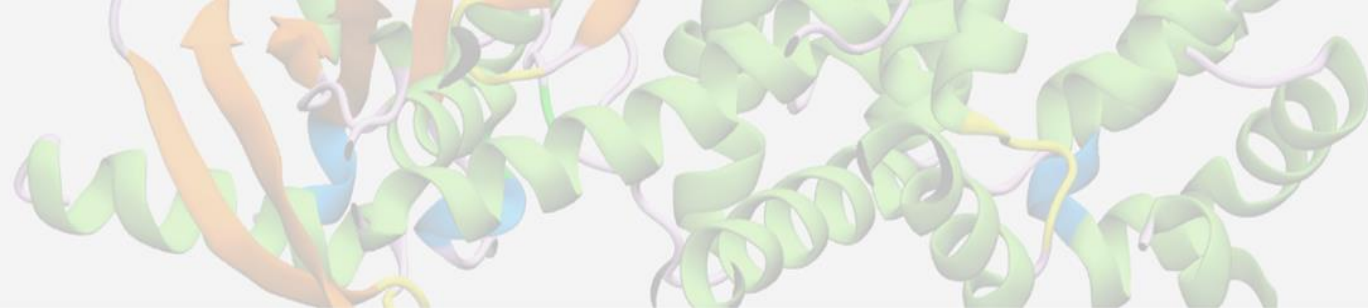
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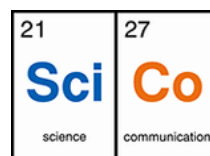
ALLODD Beneficiaries



Karolinska
Institutet



ALLODD Partner Organizations



<https://www.allodd-itn.eu/>



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