



## Newsletter July-August 2023

Dear All,

I am writing to update you about our Action.

Please receive the most recent information on OneHealthdrug COST Action.

From September 2023, those who want to communicate short information/concepts, can contact me and we will include the communication in the monthly letter.

You will find below information about ongoing and forthcoming activities of the network.

- I am pleased to inform you that **STSM applications have been completed and we have used all the available grants. For those STSM that ended**, reports are being submitted and a summary will be published in the website.
- All our OneHealthdrugs grantees will prepare a summary/ movie/poster about their achievements and Elisa Uliassi will prepare an event for their presentation by this November 2023.

You can find all the abstracts in the website ([www.onehealthdrugs.com](http://www.onehealthdrugs.com)).

### 1. MANAGEMENT COMMITTEE (MC) NEWS

I am very pleased to announce two newly approved Scientists representative for Sweden who are approved for the MC:

Dr. Michael G. Bertram, PhD  
Assistant Professor  
Department of Wildlife, Fish, and Environmental Studies  
Swedish University of Agricultural Sciences (SLU, Umeå)  
[SLU Aquatic Ecology Research Group](#)  
[michaelbertram.com](http://michaelbertram.com)  
[Google Scholar](#)  
[Twitter](#)

Dr. Eli Thoré  
Postdoctoral researcher  
Swedish University of Agricultural Sciences  
Aquatic Ecology Research Group (Umeå, Sweden)  
Department of Wildlife, Fish, and Environmental Studies

### 2. ACTION CHAIR ACTIVITIES.

Routine work on the OneHealthdrugs action was enriched with the **STSM** in Theodora Calogroupoulou lab in Athens and the participation to the Paul Erlich PhD MedChem meeting in Salonicco (<https://medchem2023.com>). It was a fruitful visit and dissemination of our COST Action, thanks to the collaboration of prof. Serge Van Calenbergh who is the coordinator of the Paul Erlich PhD network (<http://www.pehrlichmedchem.eu>). We had the opportunity to attend a very interesting meeting and to present a poster and distribute a flyer, to introduce OneHealthdrugs to the meeting participants (PhD students and University Representatives from Europe). After some discussions in the meeting of the Coordinators' council, it was decided to include a session on Vector borne diseases and/or Sustainability in drug discovery in the next edition of the meeting that will take place on the next year, probably in Rome. This can be included among the OneHealthdrugs Cost action activities of the 2<sup>nd</sup> year.

I take the opportunity to inform about the network *"The intention is to promote scientific cooperation and exchange, improving Medicinal Chemistry PhD students' skills and background. Our aim is to support excellence in PhD programmes, by means of a) the creation of new knowledge through the promotion of*

research across a broad front, **b)** the development of international relationships skills, **c)** the release of internationally accepted Paul Ehrlich PhD awards. The ultimate Network goals are to influence policy in Europe toward the pivotal role of Medicinal Chemistry and to define best practice through mutual exchange of experience among the adhering Institutions.



## Paul Ehrlich MedChem

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Euro PhD Network



If your European University representative are interested, they can reach the website reported above. Great opportunity for PhD students!

### 3. ONEHEALTHDRUGS BUDGET INFORMATION

All WG leaders and Horizontal Leaders are requested to review the goals to be achieved for Year 1 of our COST Action and prepare a report by the **20<sup>th</sup> of October**.

The goals are reported below for easy reminder:

#### WG1

- 1.1 Setup of the web-platform for compounds database (FAIRDOM).
- 1.2 Definition of criteria for compounds to be included (joint goal with WG2)
2. Select proper biological targets: define criteria and collect information.
3. Identify critical issues in compounds degradability prediction.

#### WG2

- 1.1 Definition of criteria for compounds to be included (joint goal with WG1)
- 1.2 Setup a collection process for the chemical structures of compounds previously synthesized/available from different projects of the COST participants.
2. Identify which technologies are available within the COST Action and which ones are more needed (including European Research platform) for medicinal chemistry/parasitology development including One Health options. (Prepare a list) (joint goal with WG3).
3. Setup a plan for using them and include more advanced ones.

#### WG3

1. Collecting strategies for the characterization of the biological properties and environmental impact (ecotox) of the different leads (joint goal with WG2).
2. SOP coordination for standardization of animal experiments.

#### WG4

1. Identification of assays for ecotoxicology studies and markers in the different projects.
2. Roadmaps planning for assessing the environmental impact of leads WG5

#### WG5

1. Website composed and published.
2. Identification of the main problems of the environmental impact of drugs to focus on for dissemination activity.
3. 1 original research papers published 📄 (we will select one paper as open access among the published papers within COST Action)
4. 1 review on the OneHealthdrugs topic.
5. Integration of the activities from the Science dissemination plan.

#### WG6

1. Coordination of the transfer of knowledge activities.
2. Coordinating the exploitation plan from different projects.

The new activities will be decided in a dedicated meeting. More information will be sent to WG leaders and HG leaders.

#### Good news!

The general annual meeting will be held in Oxford (UK) organized by Marco Mazzorana on the next June-July (dates and details to be announced). Thank you, Marco for your proposal!

Congratulations for this important achievement.

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#### 4. MEDIA ACTIVITIES

- Our **website updates** ([www.onehealthdrugs.com](http://www.onehealthdrugs.com)). The website is continuously updated. We hope and trust your collaboration for implementing it at best. We are looking for interested collaborators who want to help with the website activity and Action promotion.

All participants are invited to contribute with items like: -

- publications information in which you have acknowledged our OneHealthdrugs COST Action
- Nice/your preferred pictures from your lab work,
- scientific news about discoveries with comments
- other news useful for increasing interests in our Action
- picture should be 1000x1000 pixel

you can send it to [mariapaola.costi@unimore.it](mailto:mariapaola.costi@unimore.it) for now while we are looking for someone who is interested in keeping the website updated.

If you are interested, please let me know!

#### 5. DISSEMINATION ACTIVITY

Clara lima and Essia Sebai are organizing their congress participation as grantees of the COST Action dissemination grants.

If anyone else have done some additional work in the dissemination of OneHealthdrugs Action, please let me know.

#### 6. EVENTS Calendar for July-September 2023

Finally, please stay connected with the events organized in June. Sometimes technical reasons the real events hours are different from those of the invitations sent through the COST web platform:

1. **WG leaders meetings** (WG) are invited to plan 1 hr meeting with their WG participant to monitor the achievements of year 1 and to plan their next activity by defining the goals achievements for year 2. WG meetings have been organized by Ulrike (WG1 meeting), Theodora Calogeropoulou (WG2 meeting) and Guy Cajon (WG3 meeting), another one WG6 is being organized by Clara Lima.
2. **September-October workshops**
  - **WG3 workshop2 “Animal models for lead selection against vector borne parasitic diseases within the One Health concept”**

**Date 8 September 2023 online**

Organizers: Guy Caljon and Mirco Bunduschuh

#### Description

Within OneHealthdrugs we strive to discover new drugs against vector borne diseases with a minimal environmental impact. Animal infection models in combination with a thorough in vitro characterization of potency and selectivity represent indispensable tools for drug discovery.

In the transition from *in vitro* to *in vivo* evaluation we adhere to and advocate for the 3R principles (Replacement, Reduction and Refinement). This workshop will therefore cover several aspects of preclinical research in animal models, including principles of 3R and reporting according to the ARRIVE guidelines. As part of the refinement and reduction of animal research, several new imaging technologies have found their introduction in drug discovery for infectious diseases. The workshop also aims to cover some limitations of animal models and to offer a broader perspective beyond mouse models.

The workshop will consist of invited presentations and communications based on abstract selection. Given the upcoming online WG3 workshop we are launching a call for abstracts within this theme. The deadline for abstract submission was **6th August**.

Please find the abstract template in attachment and send it to: [Guy.Caljon@uantwerpen.be](mailto:Guy.Caljon@uantwerpen.be)

If you want to register to the meeting, please fill the form at the below reported link:

<https://docs.google.com/forms/d/e/1FAIpQLScKZMglluY63O9CgYX37-jjeFemeFFUPi86W7ufMEVIZa7x2Q/viewform?usp=sharing>

- **WG4- workshop 2 in presence “Biomarkers, screening, standardized and non-standardized ecotoxicological testing in One Health drug discovery and development”**

Date 20-21 September 2023, Giessen University. Germany. Organizer Rolf-Alexander Düring  
Second workshop WG4, Gießen. In presence.

#### Description

In the development of new active substances, consideration of possible effects on non-target organisms is becoming increasingly important. What is already well established in pesticide development, namely the assessment of environmental effects, is still in its infancy in drug development. Here, the **One Health approach** often still falls short, as environmental health is an integral part of this concept, in addition to animal and human health. Efficient, innovative but also standardizable test methods and assays are needed to assess the behavior and effects of active ingredients released into the natural environment. The second workshop of WG4 will provide a platform to present and discuss different assays and test methods. Initial results of WG1-3 will be summarized and evaluated in an integrative manner with the goal of proposing a guideline paper to address ecotoxicological concerns in drug discovery and development in the anti-parasitic field. Visits to two research facilities focusing on drug discovery from bioresources or on risk assessment up to the mesocosm or field scale will round out the workshop.

For questions, contact the meeting organizer: **Rolf-Alexander Düring**,  
[Rolf.alexander.duering@umwelt.uni-giessen.de](mailto:Rolf.alexander.duering@umwelt.uni-giessen.de)

If interested in participating in presence, please register at the following link:

[https://docs.google.com/forms/d/e/1FAIpQLSeuamqceQhC4PU3uGigEljD1eOUgjR81mXamuQtJWNsTg\\_zLw/viewform?usp=sharin](https://docs.google.com/forms/d/e/1FAIpQLSeuamqceQhC4PU3uGigEljD1eOUgjR81mXamuQtJWNsTg_zLw/viewform?usp=sharin)

- **WG1-Workshop 2 online\_ Chemoinformatic Tools, Compound Databases and Data Management Platforms**

Date 9 October 2023 - 2pm-4pm - online

Organizer: Ulrike Wittig and Cecilia Pozzi

#### Description

High quality data on compound properties and activities form the backbone of the daily work for many members of the COST Action OneHealthdrugs. Chemoinformatics tools, compound repositories and data management platforms play an essential role in providing access to vital compound information and facilitating the analysis of compound properties for modelling of drug targets and developing compounds as potential drug candidates against parasitic diseases. The aim of this workshop is to introduce knowledge



in using various cheminformatics tools, accessing and navigating compound databases, and efficiently managing chemical data through data management platforms.

You are invited to **submit your abstract by the 04/09/2023** and send it to [ulrike.wittig@h-its.org](mailto:ulrike.wittig@h-its.org) using the provided template. The workshop will consist of presentations from invited speakers and selected abstracts.

The event registration requires two steps:

- 1) create an e-COST account in the [www.cost.eu](http://www.cost.eu) and
- 2) register **by the 06/10/2023**

online <https://docs.google.com/forms/d/e/1FAIpQLScKZMglluY63O9CgYX37-jjeFemeFFUPi86W7ufMEVIZa7x2Q/viewform?usp=sharing>

2nd Training School "MedChem and structural biology: tools and strategies for hit and lead optimization in the One Health perspective. 27-29/09/2023 - 3days school. Siena-Italy. Organizers Sandra Gemma and Cecilia Pozzi.

**Description.** Drug discovery is a complex process aiming to develop compounds with appropriate safety and efficacy profiles allowing to proceed to their clinical evaluation. On this purpose structural biology, medicinal chemistry and computational chemistry provide key information to guide the rational design of effective drugs. The first focus of this Training School will be to explore how drugs are designed and synthesized, with a particular focus on the green aspects that should be considered both in the design, synthetic approaches, and in the prediction of their environmental fate. The second focus of the Training School will be the structural characterization of macromolecular targets and of their interactions with substrates and compounds for drug development purposes. The main topics that will be part of the Training School scientific program are in silico methods for the toxicity prediction applications related to environmental issues, green medchem/synthetic approaches, integrative structural biology approaches for investigating macromolecular targets, structural characterization of enzyme-inhibitor and enzyme-substrate complexes through X-ray crystallography. At the end of the training school, the participants will work together to create a report that summarizes the main topics and subjects covered during the training.

The Training School within *OneHealthdrugs* will cover the cost of travel and allowance (for accommodation, catering, and short-distance travel) for 10 trainees (additional 2 trainees will be accepted based on funding availability). The selection of trainees has been completed and the list of selected participants is reported below:

<b>Surname</b>	<b>First name</b>	<b>Country</b>
1. Corfu	Ioana Alexandra	Italy
2. Carvalho	Maria Alice	Portugal
3. Valiauga	Benjaminas	Lithuania
4. Aliyeva	Gunel	Azerbaijan
5. Santamaría	Aguirre Javier	Spain
6. Stojanovski	Stojmir	North Macedonia
7. Haziri	Imer	Kosovo
8. Mahmutovic	Vranic Sabina	Bosnia and Herzegovina
9. Ebiloma	Godwin	UK
10. Cintesun	Sener	Turkey

Congratulations for this achievement!

I would like to remind that the criteria for the selection have been approved by the MC and Core group. First, we need to follow the requirements of the COST Action rules and then we will not give multiple grants to the same Applicant, to allow equal distribution of resources.

**CRITERIA FOR COST EXCELLENCE AND INCLUSIVENESS, AND GENDER POLICIES (COST Actions rules)**



- Career stage. (Is the applicant Young Researcher and Innovator at time of the Application)?
- Gender
- Country of affiliation (COST member country, NNC and low-income country)

#### CA2111 INTERNAL SELECTION CRITERIA

- Coherence of research activities with School thematic
- Quality of the motivation letter
- Quality of CV

Thank you, Sandra and Cecilia for the organization!

One important note: we want to encourage female scientist applications from ITC Countries and NNC!

For those not selected: you are encouraged to apply again. Please, try to fit as much as possible with the listed criteria! The selection process is sustained by the Organizers, Sheraz Gul (HG leader for the Training Schools) and Anabela Cordeiro/myself if needed, as substitutes. All documents are available for transparency of the process.

### 7. PUBLICATIONS

#### Publications: ACS Infectious disease Issue associated with the Modena meeting January 2023.

The special issue is now approved, ACS Infectious disease has published the Call for paper by the Editor Dr. Felix Calderon with the following title:

*One Health and Vector Borne Parasitic Diseases*

The screenshot shows the ACS Publications website page for the call for papers. The title is "Call for Papers: One Health and Vector-Borne Parasitic Diseases" edited by Maria P. Costi and Anabela Cordero-da-Silva. The article has 151 views and 1 altmetric. The page includes a PDF download button (895 Kb) and a references section with three entries: 1. Banler, R. H., Constat, A., Krueger, K. Arthropod Innate Immune Systems and Vector-Borne Diseases. *Biochemistry* 2017, 56 (7), 907-918. DOI: 10.1021/acs.biochem.6b00870 [ACS Full Text w/]. [CAS] [Google Scholar] 2. Centers for Disease Control and Prevention (CDC), www.cdc.gov. 3. Larsson, J. D. G., Flach, C. Antibiotic resistance in the environment.

The issue is in the context of the OneHealthdrugs COST Action focused on the topic of the discovery of antiparasitic drugs against vector borne parasitic diseases with low environmental impact. The Issue will include articles on the medicinal chemistry methods, new drugs and environmental impact of the same other than some aspects of ecotoxicology. Both human and veterinary medicine fall within our interest. With this issue we would like to raise the interest of those experts researching in the field of parasitic infectious disease, who want to

integrate their knowledge in closely related fields of high interest by considering the sustainability aspects of their research. We will also include a few manuscripts on the OneHealth concept.

I received about 18-20 publication titles that allowed the approval of the Issue by ACS.

The issue is dedicated to the OneHealthdrugs topics and extended to Scientists external to OneHealthdrugs Action.

Deadline for submission: 31st December 2023

Title: One Health and Vector Borne Parasitic Diseases

Editorial submission deadline: 31st January 2024

Virtual Special Issue (VSI) in the web: February 2024

VSI editorial included in the March 2024 ACS ID issue

You can visit <https://doi.org/10.1021/acsinfectdis.3c00304>

We are All encouraged to publish papers together and acknowledge OneHealthdrugs Action. The rule is that the Authors should belong to at least 3 different COST countries.

For those who wants to publish with the COST acknowledgement, please follow the instructions:



Here is the link where you'll find all the info related to your question. Check the box according to the type of support. Publication if article: (c): This article/publication is based upon work from COST Action < insert name of Action or initials, CA21111, supported by COST (European Cooperation in Science and Technology). If a book, all references should appear. Details: follow this link. <https://www.cost.eu/uploads/2022/11/COST-Action-Visual-Branding-Guidelines-071122.pdf>

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If you are interested in some specific aspects, please let me know.

It is worth noticing that **active participation** to the COST Actions corresponds to the 35% of participation to successfully granted EU project.

Take this participation as an extraordinary opportunity for you and your research.

Have a good day!

Paola

PS

*Note that in our media LinkedIn and twitter we have now the following hashtag*

**[#OneHealthdrugs](#)**

*This is from us and please use it in your communications!*

[https://twitter.com/1Healthdrugs\\_ca](https://twitter.com/1Healthdrugs_ca)

<https://www.linkedin.com/company/86838804/>