

NEWSLETTER JUNE 2023

Dear All,

I know this is holidays period for some of us, however I will not stop updating you about our Action! Please receive the most recent information on our OneHealth*drug* COST Action. From September 2023, those who want to communicate short information/concepts, can contact me and

we will include the communication in this 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 almost used all the available grants (list of the grantee enclosed). I remind you that these are open to all researchers. The research visiting period can be performed up to the end of August. Be ready for the next period application starting by the end of the year! All our OneHealth*drugs* grantees will prepare a summary/ movie/poster about their achievements and I will propose an event for their presentation by this November 2023.

You will find their abstract in the website shortly.

 $\sqrt{}$ Grant awarding for ITC conference have been assigned to:

1. Clara Lima to attend the following conference: "Comparative study on a multi-parametric serological approach to feline *Leishmania* infection "

2. Essia Sebai who will present a communication entitled:

"Phytochemical profile and anthelmintic effects of *Laurus nobilis* essential oil against the ovine nematode *Haemonchus contortus* and the murine helminth model *Heligmosomoides polygyrus*"

Clara and Essia will participate to the same conference.

Conference Details. Conference title: 29th conference of the World Association for the Advancement of Veterinary Parasitology

Conference web-page: https://waavp2023.com

Conference venue: in-person participation; The Leela Palace, Chennai, India Conference start and end date: 20/08/2023 to 24/08/2023

Congratulations to both of you!

See below the list of our GRANT award recipients

applicantName	title	accountHolderCountry	applicantPrimaryInstitution
Kayhan Ilbeigi	PhD Student	Belgium	University of Antwerp
Bianca Martinengo	Sustainable biocatalytic derivatization of antiparasitic natural lipids and CNSL derivatives using UPO enzymes	Italy	University of Bologna
Essia Sebai	29th International Conference of the World Association for the Advancement of Veterinary Parasitology	Tunisia	National Veterinary School of Sidi Thabet, Tunisia
Gülşah Bayraktar	Design, Synthesis and Biological Evaluation of Antileishmanial Azaheterocyclic Compounds as Inhibitors of the Parasitic Exokinas	Turkey	Ege University
Sara Luelmo Moya	ADMET studies on novel thiazolidinone derivatives with promising in vitro anti- Leishmanial activity.	Spain	I3S-Instituto de Investigação e Inovação em Saúde da Universidade do Porto
Federica Piccolo	Supporting the OneHealthdrugs network in virtual and hybrid settings	Italy	Federica Piccolo
Vittoria Monaco	Activity-based Protein Profiling to investigate the interactome of the antimalarial early lead Plasmodione	Italy	University of Naples "Federico II"
Sophia Girgis	Malaria Integrative Analysis to Discover Biomarkers of Infection Outcome (MADBIO)	France	University of Montpellier
Clara Lima	DVM, MsC	Portugal	i3S-Institute for Research and Innovation in Health, University of Porto

COST_Action_AGA-CA21111-1_applications_export_01-07-2023

Federica Piccolo is our Action assistant. Thank you, Federica for your everyday support!

TRAINING SCHOOLS

- √ Our first training school One Health Drug discovery against parasitic vector borne diseases in Europe and beyond. 8-10/05/2023 - 3 days school, Hamburg-Germany, was concluded. Please find the Report by Elton Ragozi about the Training School at the following link: https://www.onehealthdrugs.com/events/training-schools/fraunhofer-itmp-hamburg-germany/
- $\sqrt{}$ Our next Training school will be in Siena organized by Sandra Gemma and Cecilia Pozzi: "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. Calls will be opened soon and will be closed by the 15th of July. Please stay in touch with the website where you will find the call invitation.

<u>Description</u>. 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.



Action Chair activities.

Routine work on the OneHealth*drugs* action was enriched with the COST Academy activities.

<u>Description</u>, Drug discovery is a complete process aiming to develop compounds with appropriate safety and differy profiles allowing to process to their clinical restation. On this purpose attructural isology, medicinal chemistry and computational chemistry provide key information to guide the resional design of reflective drugs. The first focus of the Training School will be to explore the ovirge of edges de and proteinates 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 late. The accord focus of the Training School will be the structural characterisation of macromolecular targets and of their interactions with substrates and compounds for darge therebas for the turbuly prediction approaches. For investigating macromolecular targets, structural approaches, integrative structural biology approaches for investigating macromolecular targets, structural interacterisation or example: how the interactions with approaches provides approaches, integrative structural biology approaches for investigating macromolecular targets, structural accessed and approaches provides approaches for investigating macromolecular targets, structural accessed approaches.

I was in Brussels on the 1th of June at a COST Academy event on "How to coordinate international research networks on 1 June 2023 Agenda and Practicalities". https://www.cost.eu/cost-events/cost-academy-how-to-coordinate-intl-research-networks/ A second COST Academy training was hold on the 27 and 28th June on the topic:

'SCIENCE FOR POLICY' WORKSHOP FOR COST ACTIONS-27 June 2023 "SCIENCE DIPLOMACY" WORKSHOP FOR COST ACTIONS-278June 2023 Anabela Cordeiro, as vice chair, and I attended this second appointment. Lucky to be there together. Difficult, but so interesting!

You can find a few slides in short on the event, enclosed.

After the Academy meeting in Brussels, I visited Guy's labs in Antwerp on the 29th June and we had interesting discussion about our Action.

 $\sqrt{}$ Our **website** has been published (www.onehealthdrugs.com). The website is not completed yet and we miss information and pictures. We hope and trust your collaboration for implementing it at best.

All participants are invited to contribute with items like:

- Nice/your preferred pictures from your lab work,
 - publications information in which you have acknowledged our OneHealthdrugs COST Action
 - · 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 <u>mariapaola.costi@unimore.it</u> for now while we are looking for someone who is interested in keeping the website updated.

If you are interested, please let me know!

SURVEYS

SURVEY 1 status: 60% completed You have received the *entry SURVEY* entitled "WG6 - Survey on research perspectives for drug development targeting vector-borne diseases and environmental impact" by Clara Lima.

This data collection (or survey) was prepared by Clara and some Collaborators. We are expecting to achieve the 95% coverage of the network participants.

This data collection represents the entry ID for all new OneHealth*drugs* applicants. Description.

This questionnaire is being conducted under COST Action 21111 on "One Health drugs for Vector-Borne Diseases", aiming to survey the current trends and status of the research and drug development for the treatment of Vector-Borne Diseases. In addition, we intend to assess the level of awareness about the sustainability and environmental impact of the process of developing drugs for parasitic Vector-Borne Diseases (PVBDs). To answer each question, please select one or more options to reply to each question. The questionnaire is composed of 33 questions and shouldn't take more than 20 min to reply. The answers will be summarized and analyzed. From the results of this survey, we aim to develop training opportunities and guidelines to help researchers and their institutes produce more sustainable and environmentally safe compounds for the treatment of Parasitic Vector-Borne diseases.

This survey has to be filled by each COST participant as an entry document, all those registering to the Action are requested to fill the data collection. *Thank you for your help and time!*

SURVEY 2

Survey on compounds database (WG1)

Description

This survey is organized by WG1, Ulrike Witting, (*Compound libraries coordination and integration of compound design*) of COST Action CA21111 "OneHealth*drugs*" and collects information from COST Action members about the handling of chemical compound information and the usage of compound databases/repositories. The results will help to coordinate and integrate compound data from different resources for searching and screening purposes by the COST Action participants. The survey is finished for this first year.

To this aim, I will visit NHRF in Athens in one week from now to plan the manuscript about **HITS, LEADS** and **Database in the field of vector borne diseases.**

Interested chemists are invited to contribute.

Our website report the database selected by the network participants, under the following field WORKING AREA-> Database collections, open sources and vendors.

The survey results is enclosed in this e-mail and is deposited in FairdomHub with the following DOI

https://doi.org/10.15490/fairdomhub.1.document.4187.1

SURVEY 3 about HITS and LEADS profile

SURVEY 3 is conducted by WG2 and WG3 with the aim of collecting information from the network about the most important compounds existing among the network members that can respect the HITS or LEAD profile. The use of the structural-chemical information will be useful for further medicinal chemistry application in the field. This activity is in line with WG1 activity on compound database collection. The excel files containing the HITS and LEADS profile have been distributed among WG2 and WG3 for now, and will be corrected and updated. Finally, it will be distributed to the whole network for inclusion of all available compounds.

DISSEMINATION ACTIVITY

✓ The presentation prepared by Annette Ivette is available on the website. This can be then used for every presentation on the topic by the network participants. Please let me know when you use it.

We have started the communication with One Health Commission (OHC) the US organization **One Health Commission (OHC)** A U.S. based non-profit organization working globally to 'connect' One Health Stakeholders, to 'create' teams and networks that work together across disciplines to 'educate' about One Health and One Health issues. https://www.onehealthcommission.org/

OneHealth*drugs* has established a connection with OHC and we will exchange news and initiatives for disseminating about One Health principles and guidelines in the respective field. Globally and within drug development in vector borne parasitic diseases



please visit our website at:

https://www.onehealthdrugs.com/news/other-news/ and the OHC website at https://www.onehealthcommission.org/

 $\sqrt{}$ If interested in 3R principle in biological evaluation of drugs and responsible and alternative use of research animal models, you can consider to participate to the congress organized in Bruxelles in September 2023 (communication Guy Caljon).

Within Onehealth*drugs* we strive to make optimal selection of new drug candidates against vector borne diseases to ensure potency with a minimal environmental impact. In the transition from *in vitro* to *in vivo* evaluation we adhere to and advocate for the 3R principle (Replacement, Reduction and Refinement). This joint symposium of the Innovation Centre 3Rs (IC-3Rs), together with RE-Place and the European Horizon 2020 funded TWINALT consortium, will be an opportunity to obtain latest insights into the most advanced 3R-alternative models. This is a strong added value for anyone working with laboratory animals.

https://joint3rsymposium.org/



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:

$\sqrt{}$ Core group meeting will take place on the 12th of July 2023

 $\sqrt{}$ WG leaders (WG1, WG4, WG5 and WG6) are invited to plan for 1 hr meeting with their WG participant to plan their next activity and define the goals achievements.

September meetings

5th MC meeting +WGs Meeting entitled "Biomarker and indicators for ecotoxicology's studies in the drug R&D process" (in presence and VIRTUAL) (20-21 September 2023), Giessen University. Germany. Organizer Rolf-Alexander Düring

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.

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

The special issue invitation was submitted to ACS Infectious disease and edited by the Editor Dr. Felix Calderon with the following title:

One Health and Vector Borne Parasitic Diseases

The issue is in the context of the OneHealth*drugs* 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.

The issue will be dedicated to the OneHealth*drugs* topics but it will be extended to Scientists external to OneHealth*drugs* Action. This was asked/suggested by the Editor.

Deadline for submission: 31st December 2023 Title: One Health and Vector Borne Parasitic Diseases Editorial submission deadline: 31st January 2024 VSI in the web: February 2024 VSI editorial included in the March 2024 ACS ID issue

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, CAxxxx >, supported by COST (European Cooperation in Science and Technology) If a book, all references should appear. Details: follow this link. <u>https://www.cost.eu/uploads/2022/11/COST-Action-Visual-Branding-Guidelines-071122.pdf</u>

News from our members

We congratulate with <u>Philippe Loiseau</u>: he is the recipient of the Medal of Honor from the French Society of Parasitology in Marrakech during the congress from May 24 to 27, 2023. Well deserved Philippe!



If you are interested in some specific aspects, please let me know. I would like to remember 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 <mark>#OneHealthdrugs</mark> This is from us and please use it in your communications!

https://twitter.com/1Healthdrugs_ca https://www.linkedin.com/company/86838804/