NEWSLETTR MAY_JUNE 2024

Action SiteCOST ActionLinkedInYouTubeX-Twitter

In this edition ...

Message from the Action Chair

by Maria-Paola Costi, Action Chair

Dear Valued OneHealthDrugs Members,

As we step into another vibrant period filled with crucial

Newsletter

developments and collaborative endeavours, I am thrilled to present our May 2024 Newsletter. These past months have been exceptionally busy yet fruitful, marked by significant milestones and strategic meetings that continue to propel our mission forward.

We've witnessed the successful culmination of several key events and the initiation of impactful projects. From the OHD1_Target and OHD2_Compounds database projects making substantial progress to our engaging in-person events in Porto and upcoming meetings in Rome and Oxford, our community's dedication is evident. Additionally, the continued advancement in our training programs, particularly the Naples school on natural products, underscores our commitment to education and innovation.

This edition of the newsletter will provide updates on these activities, introduce upcoming opportunities, and celebrate our collective achievements. Your active participation and contributions are vital to our success, and I look forward to seeing how we continue to evolve and make a significant impact together.

Thank you for your unwavering support and engagement.

OHD Works

Past Events

- WG3,WG4, WG6, HG4, HG5 Thematic Workshop

“Animal friendly and
environmentally relevant systems to replace or refine animal tests
during drug developmental processes for VBD” **I3S, Porto, Portugal,
14-15 May 2024**

- WG3 meeting 24th May 2024 13:00-15:00 pm CET (VIRTUAL)
- WG1 meeting 29th May 2024 15:00-16:00 pm CET (VIRTUAL)

Upcoming Events

- Core Group meeting 14th June 2024 14:30-16:00 (VIRTUAL)
- **1st Training School "Natural products in parasitic diseases". 18-20 June 2024 - 3days school. University of Naples, Naples (Italy)**
- **Workshop IN PRESENCE for YRI "Medicinal chemistry process within the OneHealth perspective for YRI 17-19th June 2024 Rome (Italy) co-organized with Paul Ehrlich MedChem2024**

WG3,WG4, WG6, HG4, HG5 Thematic Workshop

“Animal friendly and environmentally relevant systems to replace or refine animal tests during drug developmental processes for VBD”

I3S, Porto, Portugal, 14-15 May 2024

Newsletter

Summary letter from Clara Lima

Faculty of Pharmacy, University of Porto - i3S-Institute for Research and Innovation in Health

Newsletter

Porto 15th May 2024

Dear OneHealth*drugs* colleagues and friends and promising generation of young researchers and innovators,

As we draw near the conclusion of this enlightening scientific meeting, I want to take a moment to express my gratitude to all our distinguished speakers, chairs, and attendees for their invaluable contributions and active participation. It's not enough to thank the efforts of the local organizing committee, and our sincere thanks to Joana Tavares, Anabela Cordeio da Silva, Ana Tomás and the i3S events team, and all of those who supported the Scientific Commission involved in the preparation of this event. We thank Professor Paola Costi for her endless enthusiasm and dedication to OneHealth*drugs* COST Action.

Our two-day journey through the realms of science, technology, and innovation behind drug development for PVBDs has been nothing short of inspiring. We have reinforced the urgency to extend the portfolio of drugs used in the fight against PVBDs and absolute need to consider a change of the current paradigms of drug discovery and development, towards a multidisciplinary approach that takes into account innovation, drug efficiency and safety, environmental protection and safeguard of all ecosystems.

During this workshop we have learned from colleagues and experts in the field how, the current work on alternative methods to replace animal models and renew 3R principles in animal experimentation, advancements in chemistry synthesis and ecotoxicological testing, besides the proof of concept that research institutions can adopt measures to reduce their carbon footprint, have move from being utopic projects to real promising perspectives for a greener and safer future.

In this scenario, we also foresee extended career opportunities for younger generations of researchers in the fields of biomedical research and drug discovery.

In this sense, we hope to have contributed to strengthen the foundations of YRI future careers in this field, highlighting the role of ethics and integrity in scientific production, and some insights on practical strategies that can be implemented in the process of exploring and planning a future in academia, industry and research.

In closing, let us carry forward the spirit of innovation and scientific inquiry to establish research collaborations for innovation in drug development and fuel a more sustainable future for all of those who depend on medicinal products to fight parasitic vector borne diseases.

Thank you once again to everyone who made this event possible, and we wish you all continued success in your research.
Safe travels and until we meet again.
Thank you.

OHD Action project related meetings

- Highlights from the OHD1_Target database project (Project OHD1 -Target Database 4-3-2024)
- Highlights from the OHD2_Compounds database project (Project OHD2 -Compounds Database 11-3-2024
- Grants application 1st meeting (29 February 2024)
- Paper SOP animal models - 20 March meeting
- Highlights from the OHD1_Target database project (Project OHD1 -Target Database 4-3-2024) Cecilia Pozzi and Ulrike Wittig and Marco Mazzorana

OUTCOME: Target collection for VBPD, new potential targets to be identified, new profile expected for these targets including the predictive distribution among organisms present in the environment.

- Highlights from the OHD1_Target database project (Project OHD1 - Target Database 4-3-2024)

In our recent General Assembly on May 29, 2024, chaired by Maria Paola Costi, we explored significant advancements and ongoing projects within the OneHealthdrugs initiative. Our discussion spanned from the strategic development of the BioTarget Database, aimed at promoting environmentally friendly drug targets, to substantial progress in our compound databases, which integrate ecotoxicological assessments to ensure safety and effectiveness. These efforts are pivotal as we strive to harmonize drug efficacy with environmental sustainability in our fight against parasitic vector-borne diseases.

View here the Presentation

Newsletter

- Highlights from the OHD2_Compounds database project (Project OHD2 -

This project has the double aim to develop
a **database** and
a **paper**.
We expect that the paper can be a research paper.

The title "**Antiparasitic drug discovery and emerging scaffold with predictive low environmental impact**", the paper is organized as reported below:

Section	Scientist(s) in Charge
1. Database discussion	U. Wittig (ulrike.wittig@h-its.org)
2. Collection of recent drugs	"
2.1 Leishmania	C. Borsari" (chiara.borsari@unimi.it") E. Uliassi (elisa.uliassi3@unibo.it)
2.2 HAT	M. Tonelli (michele.tonelli@unige.it)
2.3 Chagas	T. Calogeropoulou (tcalog@eie.gr)
2.4 Babesia	S. Gemma (gemma@unisi.it)
2.5 Schistosomiasis	S. Gemma (gemma@unisi.it)
2.6 Malaria	S. Blandin
Coordination of natural compounds collection	T. Schmidt
3. Scaffold retrieval	S. Gul (sheraz.gul@itmp.fraunhofer.de)
4. Ecotox evaluation of the scaffolds	M. Bertram/E. Thore/S. Gul

---

Medicinal chemists involved in the field of T.brucei, malaria, natural compounds are invited to join the project

contacts

1. Theodora Calogeropoulou at tcalog@eie.gr
2.Gemma Sandra at gemma@unisi.it

This activity is connected with the YEAR 2 goal "Upload of compound data and setup of database structure **[WG1 + WG2]"** and the In silico assessment of ecotoxicology properties of hits and leads **[WG2 + WG3+**HG6+HG7**]** because an ecotoxicology evaluation will be performed on the scaffold. And to the deliverables: D18_Report about compounds collections. M48 (WG1)

OUTCOME: the research paper is organized and the collection of the compounds in the latest 5 years started. The criteria to select the compounds is based on scaffold collections, the criteria are related to the

target product profile for HIT compounds for the different diseases. These scaffolds will be examined for a predictive ecotoxicology profile.

- Grants application 1st meeting (29 February 2024)

The meeting was participated by 63 participants interested in contributing to the grant applications. Unfortunately, the calls are very close and there is no sufficient time to plan the Grant. The topic is on virus borne diseases and it is peripheral with respect to the OHD topic.

Theodora Calogeropoulou and Maria Laura Bolognesi proposed to develop a MSCA application within the OHD project.

OUTCOME: there will be initiatives on the development of MSCA applications.

- Paper SOP animal models - 20 March meeting

This activity relates to the WG3 goal of YEAR 1 entitled “SOP coordination for animal experiment standardization [WG3] and Roadmap toward a position paper on animal experiment standardization [WG3]. Moreover, it is linked to the deliverable: D14_Report on SOP coordination on standardization of animal experiments. M42 (WG3).

Background: The development of drugs against neglected tropical diseases caused by kinetoplastids, such as Leishmania, Trypanosoma brucei spp. and Trypanosoma cruzi, is not only challenging because of the lack of available funding, but is especially complicated by the use of various procedures in different labs. Besides obscuring the comparison of obtained research results, the application of different experimental methodologies, both in vitro and in vivo, might strongly influence decisions made during the drug development pipeline.

Objectives: This review aims to summarise and compare all current available research approaches used in the development of drugs against visceral and cutaneous leishmaniasis, African trypanosomiasis and Chagas disease, and to develop a series of well-considered standard operating procedures that should facilitate and homogenise future drug development.

Conclusions: This review not only provides a list of standard operating procedures for the evaluation of novel drug candidates with a special focus on in vivo animal models, but also provides a tool that can be used for decision making during the translation from in vitro to in vivo research, hereby supporting the development high quality drug leads.

OUTCOME: SOP standardization and stakeholder communication

- OHD4 Veterinary drugs and environmental impact

Review of veterinary pharmaceuticals against Parasitic Vector-Borne Diseases and their environmental impacts.
From 20240426 Operational meeting 2. –
Review approaches by section
Section I. Veterinary Medicinal Products applied to the prevention and treatment of PVBD of animals
Section II. Chemical structure and pharmacological properties of antiparasitic drugs of veterinary application
Section III. Biodegradability and environmental fate of the drugs
Section IV. Ecotoxicological assessment of the most important veterinary parasiticidal drugs – evidence of environmental harm

---

OHD Works

Events in progress and Upcoming events

Naples Training school on Natural products and antiparasitic drugs

Title: Natural products in antiparasitic drug discovery: experimental and computational approaches
Date: 18 June – 20 June 2024
Department of Pharmacy- University of Naples “Federico”, Naples, Italy

Newsletter

Organizers: Concetta Imperatore, Marco Persico, Marcello Casertano, Carmina Sirignano

Description:
Natural products and their (semi)synthetic derivatives have played a significant role in the discovery of antiparasitic drugs. Plants and marine organisms have been identified to be sources for the isolation and identification of natural products with very high degree of chemical diversity, making them a generous source of hit structures for drug discovery. The identification of new hits as well as the subsequent hit to lead optimization process rely on both computational and experimental approaches. The focus of this training school will be to explore the principles underlying i) methods for isolation and structural characterization of antiparasitic metabolites from plants and marine organisms, ii) in silico methods for hit identification and optimization, and iii) green synthetic approaches for structural optimization. A combination of lectures and practical work sessions will provide an engaging experience and help the participants to prepare for playing a leading role in the future research efforts in this field.

List of awarded participants

Surname	First name		Email
Aiello	Daniele	università di Modena e Reggio Emilia	daaiello@unimore.it
Gattringer	Jasmin	Medical University of Vienna	jasmin.gattringer@meduniwien.ac.at
Surucic	Relja	University of Banja Luka	relja.surucic@med.unibl.org
Ahmed	Shahira	Faculty of Medicine (FOM), Suez Canal University	shahira_ahmed@med.suez.edu.eg
Francesconi	Valeria	UNIVERSITA' DI GENOVA	valeria.francesconi@edu.unige.it
MARIMUTHU	PARTHIBAN	Åbo Akademi University	parthiban.marimuthu@abo.fi
Lesanavičius	Mindaugas	Vilnius University	mindaugas.lesanavicius@gmc.vu.lt
Sergeeva	Alisa	FU Berlin	alisa.sergeeva@fu-berlin.de
Ouni	Samiha	Faculty of Sciences of Tunis	ouni_samiha@yahoo.fr
Granith	Philip	Åbo Akademi University	philip.granith@abo.fi
Doko	Iori	Università Telematica eCampus	dokolori6@gmail.com
HafizMuhammad	Safwan	University of Catalunia	HafizMuhammad.Safwan@autonoma.ca

Newsletter

In summary

1st Training School

Learn more here

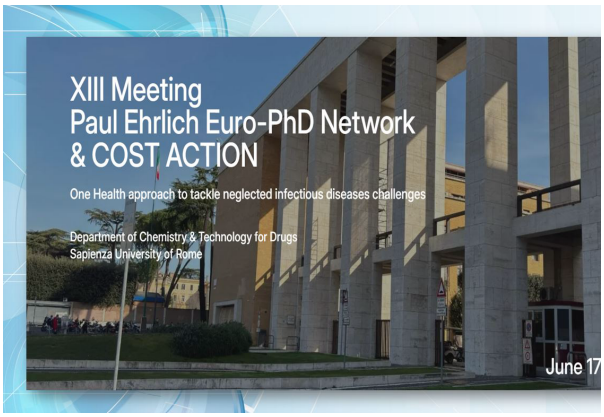
Natural Products Training School

Learn more here

Paul Ehrlich & OneHealthdrugs Meeting for YRIs

OneHealthDrugs Annual Conference

Newsletter



Learn more here

Learn more here

Conference grants application is over

Available spots: 2 applicants. The first one is granted to Eli Torè for the Conference organized by the European Tracking Network (ETN Symposium 2024) which will be held in Mallorca (Spain) from October 15-20.
Title: **Meds and motions: Understanding fish behavior in medicated habitats**

The conference is about conservation and sustainable management of aquatic ecosystems through acoustic tracking, and I would like to present (oral or poster) our upcoming project in which we will use acoustic tracking to study how mixtures of pharmaceuticals affect the behavior and migration of European eels in the wild. Immediately after the conference, I also plan to attend the Mallorca Science School from October 20-26. I will receive relevant training about tracking fish in the wild, and all attendees will present a poster about their research. I plan to use this moment to

spread the word about the behavioural impacts of pharmaceutical pollutants on aquatic wildlife, and the need for including such information (for example in the drug development process) towards a more sustainable future.

Update on the OHD1_Target Database Initiative (Project OHD1 -Target Database 4-3-2024) Cecilia Pozzi and Ulrike Wittig and Marco Mazzorana

Highlights from the OHD1_Target database project (Project OHD1 -Target Database 4-3-2024)

Objective: Target collection for VBPD, new potential targets to be identified, new profile expected for these targets including the predictive distribution among organisms present in the environment.

The OHD1_Target database is progressing well, aligning with the objectives for WG1 – YEAR 2: to define the biological target criteria and commence the collection of target data. This ongoing effort also contributes to the deliverable:
D7_Report on target selection and structural biology. M36 (WG1)

This initiative is linked to the events scheduled for the 17th of April, titled “Structural and functional aspects of targets involved in vector borne diseases."
On March 4th at 15:38, we had a productive meeting where we introduced the project and began creating a template to gather information on the targets within the CA21111. We've started drafting a document to compile this data and have outlined the main sections and some parameters.

We've shared a folder for the BioTarget Database which can be accessed here: BioTarget Database Folder. Within this folder, you'll find the "BioTarget DB template CA21111.docx" file here: BioTarget DB Template.

Please feel free to add new sections or parameters, and suggest any modifications to the existing content.

OUTCOME: Target collection for VBPD, new potential targets to be identified, new profile expected for these targets including the predictive distribution among organisms present in the environment.

Highlights from the OHD2_Compounds database project

(Project OHD2- Compounds Database 11-3-2024)

This project is designed with dual objectives: to develop both a database and a scholarly article. The anticipated research paper, titled "Antiparasitic Drug Discovery and Emerging Scaffold with Predictive Low Environmental Impact," aligns with our Year 2 goal to "Upload of compound data and set up database structure [WG1 + WG2]." This initiative also ties into the in silico assessment of ecotoxicology properties of hits and leads [WG2 + WG3 + HG6 + HG7], as it includes an ecotoxicological evaluation of the scaffolds. Additionally, this effort contributes to deliverable D18_Report about compound collections, due in Month 48 (WG1).
Outcome: The research paper is structured, and the compilation of compound data over the past five years has commenced. The selection criteria for these compounds are based on scaffold collections, which are pertinent to the target product profile for hit compounds across various diseases. These scaffolds are also being analysed for their predictive ecotoxicology profiles, ensuring a comprehensive assessment of their environmental impact.

Non-exhaustive list of paper published from the OHD Participants

Acknowledgement: This work draws upon research from COST Action CA21111 - One Health drugs against parasitic vector-borne diseases in Europe and beyond (OneHealthdrugs), which is supported by COST (European Cooperation in Science and Technology). While not directly funded by COST Action, this research benefits from the concepts developed and collaborations within the Action, including contributions from its members.

Paper published end of May 2024 in the ACS Infectious diseases special issue.

Publication in the ACS Infectious and other publications

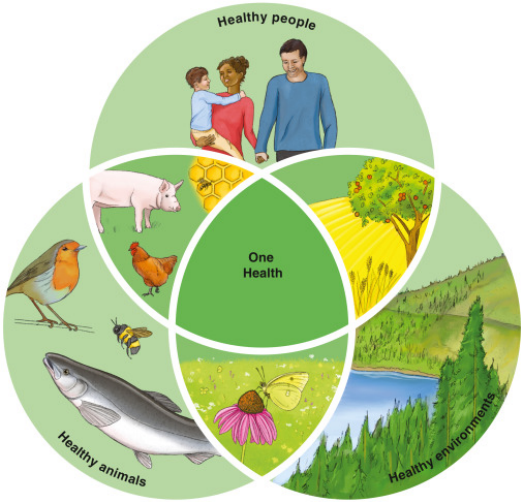
TITLE	TYPE	CORRESPONDING AUTHOR
Assessing environmental risks during the drug development process for parasitic vector-borne diseases: a critical reflection	Perspective	Bundschuh, Mirco
Synthesis and anti-Chagas activity profile of a novel redox-active lead 3-benzylmenadione revealed by high-content imaging	Article	Davioud-Charvet, Elisabeth
Metallo-enzyme inhibitors against zoonotic infections: focus on Leishmania and Schistosoma	Review	Gemma, Sandra
Harnessing the 12 Green Chemistry principles for sustainable antiparasitic drugs: towards the One Health approach	Perspective	Martinengo, Bianca
Discovery of Novel 1,3,4-Oxadiazole Derivatives as Broad-Spectrum Antiparasitic Agents	Article	Borsari, Chiara

1. Stijlemans, B., De Baetselier, P., Van Molle, I. *et al.* Guy Caljon. Q586B2 is a crucial virulence factor during the early stages of *Trypanosoma brucei* infection that is conserved amongst trypanosomatids. *Nat Commun* 15, 1779 (2024). https://doi.org/10.1038/s41467-024-46067-4

2. Gendron T., Lanfranchi D. A., Wenzel N. I., Kessedjian H., Jannack B., **Maes L.**, Cojean S., Müller T. J. J., **Loiseau P. M., Davioud-Charvet E.** Chemoselective synthesis and anti-kinetoplastidal properties of 2,6-diaryl-4H-tetrahydro-thiopyran-4-one S-oxides: their interplay in a cascade of redox reactions from diarylideneacetones. *Molecules* 2024 (Manuscript ID: molecules-2848648). Accepted 01-04-2024.

3. Iacobucci I., **Monaco V.**, Dupouy B., Hovasse A., Keumoe R., Cichocki B., Elhabiri M., **Blandin S. A.**, Meunier B., Strub J.-M., Monti M., Cianférani S., Schaeffer-Reiss C., **Davioud-Charvet E.** Proteomic profiling of antimalarial plasmodione using 3-benz(o)ylmenadione activity-based probes. *ChemBioChem* 2024, submitted on 29/02/2024, cbic.202300505. Accepted with revisions-26-03-2024. Revisions are in progress. Monaco Vittoria is the STSM grantee of the CA21111

Newsletter



Newly received papers on the COST Action topics from the Participant of the Action (no acknowledgement, very interesting):

1. Michael G. Bertram, Maria Paola Costi, Eli S.J. Thoré, Tara Sabo-Attwood, Bryan W. Brooks, One Health, Current Biology, Volume 34, Issue 11, 2024, Pages R517-R519, ISSN 0960-9822, https://doi.org/10.1016/j.cub.2024.04.025.

2. https://doi.org/10.1038/s41893-024-01374-y
The urgent need for designing greener drugs Tomas Brodin, Michael G. Bertram, Kathryn E. Arnold, Alistair B. A. Boxall, Bryan W. Brooks, Daniel Cerveny, Manuela Jörg, Karen A. Kidd, Unax Lertxundi, Jake M. Martin, Lauren T. May, Erin S. McCallum, Marcus Michelangeli, Charles R. Tyler, Bob B. M. Wong, Klaus Kümmerer & Gorka Orive
The pervasive contamination of ecosystems with active pharmaceutical ingredients poses a serious threat to biodiversity,
ecosystem services and public health. Urgent action is needed to design greener drugs that maintain efficacy but also minimize
environmental impact.

3. Heinrich, A.P., Pooda, S.H., Porciani, A. *et al.* Rolf During. An ecotoxicological view on malaria vector control with ivermectin-treated cattle. *Nat Sustain* (2024). https://doi.org/10.1038/s41893-024-01332
Environmental implications (soil sorption and dissipation) of excreted ivermectin and potential ecotoxicological risks to non-target dung organisms in West Africa are discussed, in addition to actionable, locally inspired risk mitigation measures to protect sub-Saharan soils and agroecosystems from chemical pollution. We highlight how ecotoxicology and environmental chemistry improve livestock-based vector control with ivermectin for effective and more sustainable malaria management.

Newsletter

NEW! Grants applications

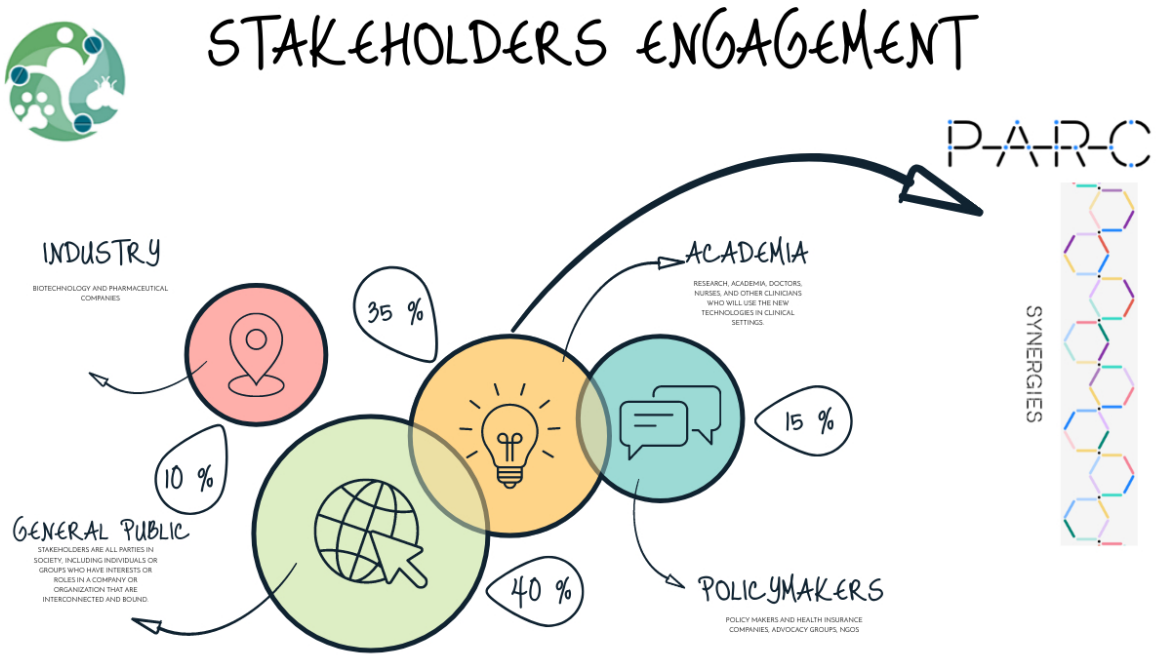
List of currently identified open applications of potential interest.
This is not intended as an exhaustive list of open calls, but a selection of the chair. Those who are interested, can alert about other calls.
We are all encouraged to participate/lead projects involving our network participants, (not exclusively OHD participants)
If you apply (inside or outside the OHD Action) please inform the Chair, it is important to list the activities stemming from and thanks to the OneHealthdrugs action

9.1. HORIZON EUROPE projects - OHD contact: Anabela Cordeiro and Maria Paola Costi

Surveys status - SURVEY 4 on available Technologies will be delivered in June.

Newsletter

Stakeholder engagement



In response to the pressing need for consensus on the **environmental impact of pharmaceuticals**, we are launching a crucial initiative in **stakeholder engagement**, set to be discussed at our Annual Meeting in Oxford this July. This endeavour will focus on harmonising diverse perspectives from key stakeholders, including environmental groups, public health advocates, veterinary associations, pharmaceutical industries, and intergovernmental agencies. Our goal is to facilitate informed discussions and knowledge exchange, thereby fostering a unified approach to assessing and addressing the ecological consequences of pharmaceuticals used in treating parasitic diseases.

Central to this initiative will be the design and deployment of a framework that encourages robust participation from all members of the COST Action network. By July, we aim to establish a dynamic platform for **identifying**, **attracting**, **engaging**, and **retaining** stakeholders critical to our mission. This platform will not only integrate the latest regulatory measures, such as the EMA's updated environmental vigilance for veterinary medicinal products but also promote the adoption of sustainable drug delivery methods. Through this collaborative effort, we strive to advance our understanding and management of the environmental footprint of antiparasitic drugs, ensuring that our strategies align with the highest standards of environmental and public health.

Newsletter

Help us shape the OHD Network: Identify Key Stakeholders

This survey is designed to gather insights from OHD members on identifyin key stakeholders for the One Health Drugs Dissemination & Exploitation. Yo valuable input will help us understand our network better and facilitate mo effective collaborations.

Start

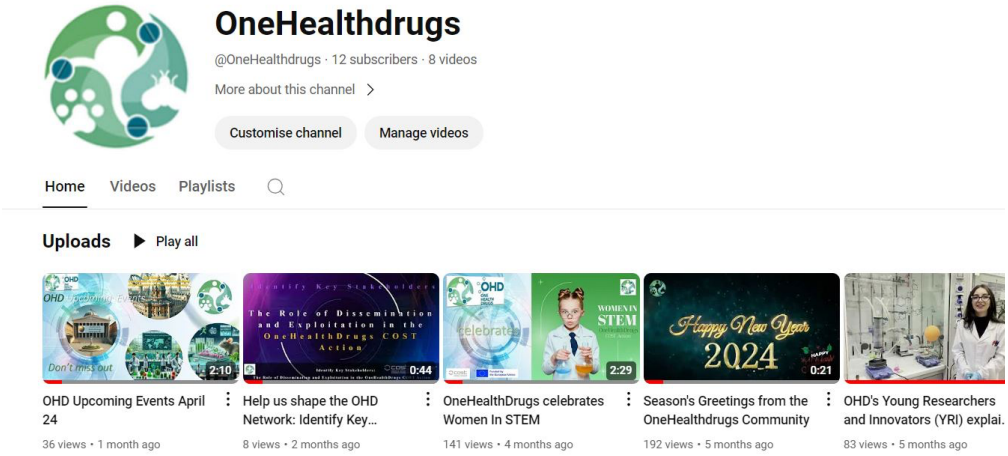
OHD SciComm activity

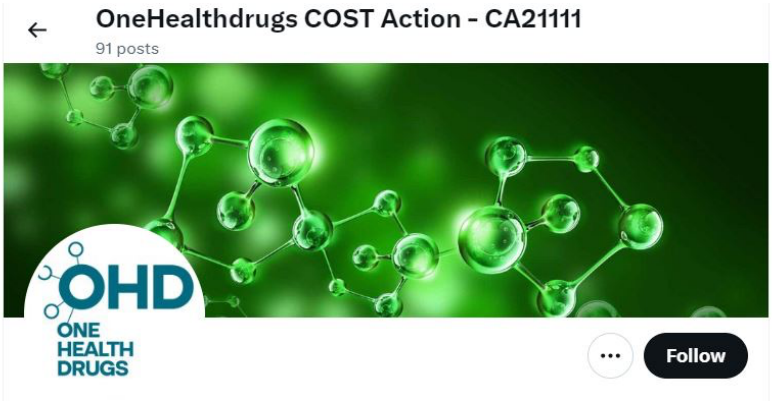
We invite you to actively support our Action's SciComm plan, which is crucial for amplifying our collective impact and enhancing your visibility within the scientific community. Join our LinkedIn group and subscribe to our YouTube channel to post your work, engage in discussions, and share our content. Your participation is vital in expanding our reach and elevating your professional presence in the field.

Newsletter

Join the OneHealthdrugs LinkedIn Group!

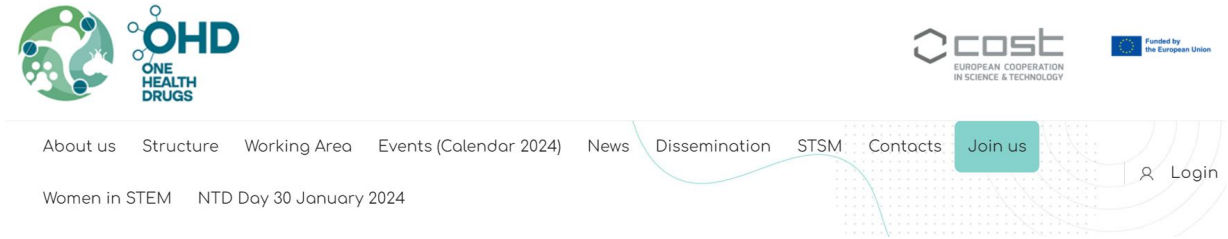
Subscribe to our YouTube channel





Follow us on X (Twitter)

visit our website



and don't forget to complete our survey, if you haven't done it so far.

OHD available positions

- WG6 Leadership
- WG4-Vice leader
- Young Researcher and Innovators

I wish to share with the OHD Community

Give us your valuable feedback

We will be pleased to answer any questions you may have or consider suggestions for improving our Community.

Please email us at onehealthdrugs.events@gmail.com

Contact us if you have any questions, suggestions or you wish to share your news