

To be used to report WG/HG meetings organised by the Action.

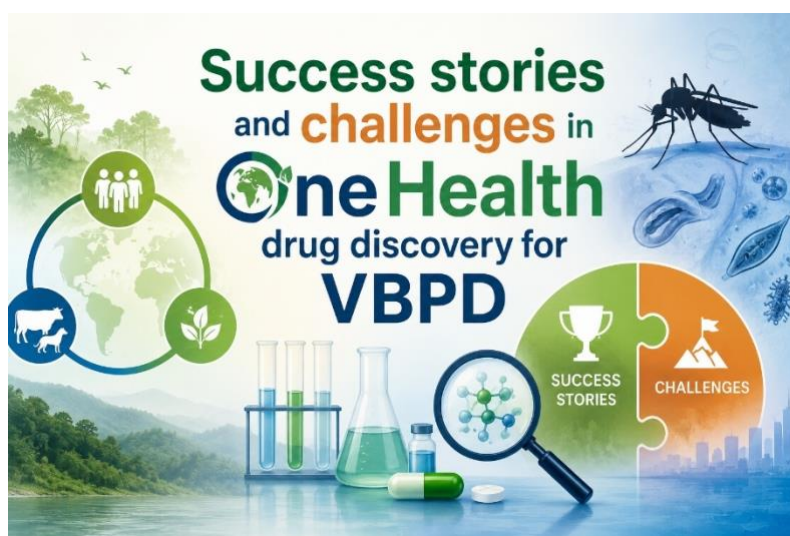
Only points 2 and 3 are mandatory, the others can be tailored to each meeting

To be sent to mariapaola.costi@unimore.it, cordeiro@ibmc.up.pt (cc piccolo@bm3s.com) within a week from the meeting

MINUTES

“Success stories and challenges in OneHealth drug discovery for VBPD” (remote HG4 + WG1–2–3–4) May 18, 2026, from 10:00 to 13:00 CET

This workshop will provide a state-of-the-art overview and help define a collaborative, multidisciplinary roadmap within COST Action CA21111 across all career stages.



This workshop will bring together senior and early-career members to highlight success stories and challenges in One Health drug discovery strategies for vector-borne parasitic diseases, encountered in both scientific and communication activities across the network.

Registration link: Here is the Google Form link to register:
<https://docs.google.com/forms/d/e/1FAIpQLScph1TMmdneLVG40cDjG04NPDGWbknM2eKL2njg-ajyA8l7Bg/viewform?usp=header>

May 18, 2026, from 10:00 to 13:00 CET

10:00 – 10:15 Welcome and introduction

10:15 – 10:35 Prof. Anabela Cordeiro Silva- I3S and Faculty of Pharmacy, University of Porto

Blended Intensive Program (BIP) on Drug Resistance in Cancer and Infectious Diseases

10:35 – 10:55 Dr Clara Lima - I3S and Faculty of Pharmacy, University of Porto

Tbd

10:55 – 11:15: Dr. Gulsah Bayraktar - Department of Pharmaceutical Chemistry, Ege University, Turkey
Development of Novel Thiazolopyrimidine Derivatives Active Against Visceral and Cutaneous Leishmania

11:15 – 11:35 Dr. Elisa Uliassi - Department of Pharmacy and Biotechnology, University of Bologna
My Journey in the OneHealthDrugs COST Action: Personal Experiences and Perspectives

10' BREAK

11:45 – 12:05: Dr Daniele Aiello - Department of Life Sciences, University of Modena and Reggio Emilia
Computational Investigation of Xanthine-Based Inhibitors Targeting Trypanosomatid Pteridine Reductase 1

12:05 – 12:20: Aurora Gaza - Department of Pharmacy and Biotechnology, University of Bologna (STSM at the School of Infection and Immunity, University of Glasgow)
Biological evaluation of small-molecule hydrophobic degraders for antiparasitic drug discovery and chemical biology applications

12:20 – 12:35: Sheraz Gul - Fraunhofer Institute, Hamburg, Germany
OHD Training School concept and outputs

12:35 – 12:50: Dr Bianca Martinengo - Department of Pharmacy and Biotechnology, University of Bologna
Unlocking Biocatalytic Oxidative Systems for the Sustainable Synthesis of Pharmaceuticals from Food Waste

12:50 Open discussion and reflections

Conclusions and way forward

Organized by Elisa Uliassi (IT, HG4 Leader), Maria Paola Costi (Action Chair), Anabela Cordeiro Silva (Action Vice-Chair)

- **CA2111 chair** mariapaola.costi <mariapaola.costi@unimore.it>
- **CA2111 vice-chair** Anabela Cordeiro Da Silva cordeiro@ibmc.up.pt

1. LIST OF ATTENDANTS

The attendance list provides the names of the participants who confirmed attendance via their personal e-COST invitation link.

Meeting Attendance list

2. PROOF OF ATTENDANCE

One Health drugs against parasitic vector borne diseases in Europe and beyond **OneHealthdrugs** **Cost Action CA21111**

Blended Intensive Program (BIP)

Drug Resistance in Cancer and Infectious Diseases
European Collaboration within **COST Action CA21111**

Anabela Cordeiro da Silva
cordeiro@ff.up.pt/cordeiro@3s.up.pt

Participating Countries:
Portugal - Italy - Greece
Representatives:
Anabela Cordeiro da Silva - Maria Paola Costi - Ioannis Papanastasiou

Added Value of the Tri-Country Collaboration

- Portugal, Italy, and Greece share:
 - Comparable health challenges
 - Complementary expertise
- The BIP:
 - Reinforced South-European scientific leadership
 - Enhanced COST Action visibility
 - Built sustainable research connections

Partecipanti

In questa riunione (16)

- EU Elisa Uliassi
- AM Ana Mikelic
- AS Anabela Silva
- BM Bianca Martinengo
- CL Clara Lima
- DA DANIELE AIELLO
- GB Gulzah Bayraktar
- GC Guy Caljon
- HD Harry de-Koning
- IB Ibukun Busari
- MQ Maria Joao Ribeiro Peixoto Queiroz
- MA Maria Laura Bolognesi
- MC Maria Paola COSTI
- MC Organizzatore
- RA Rokaya Ahmad
- ZS Zvota Selakovc

One Health drugs against parasitic vector borne diseases in Europe and beyond **OneHealthdrugs**

Cost Action CA21111

The screenshot displays a Zoom meeting interface. The top bar shows the time as 57:12. The main grid contains 16 video feeds. Some feeds show participants, while others show a large colored circle with a letter (e.g., OK, GC, AM, ZS, RA, MQ, IB, AG). The right sidebar lists 23 participants with their names and initials. The bottom bar shows the time as 01:02:56. The interface is in Italian, with the title bar reading 'In questa riunione: (23)'.

Participants (from top to bottom in list):

- MC: Maria Paola COSTI (Organizzatore)
- EU: Elisa Uliassi
- AM: Ana Mikelic
- AS: Anabela Silva
- AG: Aurora Gaze
- BD: Bianca Martinengo
- CL: Clara Lima
- CN: Corinne Ngameko
- DA: DANIELE AIELLO
- DD: Darline DIZE
- DM: Dolores Mullaliu
- GB: Gulshah Bayraktar
- GC: Guy Caljon
- HD: Harry de-Koning
- IB: Ibukun Busari
- JP: János Dr. Pálhalmi
- MQ: Maria João Ribeiro Peixoto Queirós
- MS: MURAT SENTURK

One Health drugs against parasitic vector borne diseases in Europe and beyond **OneHealthdrugs**

Cost Action CA21111

The screenshot displays a Zoom meeting interface. The top bar shows the time as 01:03:11 and various controls like Chat, DSR, Participants, and Video. The main area is a grid of 16 video feeds. The first row shows four participants: Elia Ulissi, DANIELE AIELLO, Anabela Silva, and Clara Lima. The second row shows Gulnash Bayraktar, a placeholder with 'OK', Maria Paula COSTA, and Guy Cajon. The third row shows Ana Mikolic, a placeholder with 'ZS', Rokaya Ahmad, and Maria João Ribeiro Peixoto Queiróz. The fourth row shows Harry de Koning, a placeholder with 'IB', Bianca Martinengo, and Aurora Gatta. The right sidebar lists 24 participants with their names and status icons. The bottom of the screen shows a Windows taskbar with the search bar and system clock at 10:53 on 18/01/2025.

One Health drugs against parasitic vector borne diseases in Europe and beyond OneHealthdrugs

Cost Action CA21111

Workshop - Success stories and challenges in One-Health drug discovery for VBDs* 18/05/2026 10:00 to 13:00 CET

01:04:04

Alma Mater Studiorum Università di Bologna

In questa riunione, (25)

Disattiva l'audio di t...

HD Harry de-Koning
AS Anabela Silva
EU Elisa Uliassi
A Agah
AM Ana Mikelić
AG Aurora Gaza
Bianca Martinengo
CL Clara Lima
CN Corinne Ngnamkoko
DA DANIELE AIELLO
DO Darline DIZE
DM Doloreza Mullaliu
Filippo Piazza
GB Gulshah Bayraktar
GC Guy Caljon
IB Ibukun Busari
JP János Dr. Pálhalmi
MQ Maria João Ribeiro Peixoto Queiróz

Workshop - Success stories and challenges in One-Health drug discovery for VBDs* 18/05/2026 10:00 to 13:00 CET

01:20:02

Alma Mater Studiorum Università di Bologna

In questa riunione, (27)

Disattiva l'audio di t...

EU Elisa Uliassi
A Agah
AM Ana Mikelić
AS Anabela Silva
AG Aurora Gaza
Bianca Martinengo
CL Clara Lima
CN Corinne Ngnamkoko
DA DANIELE AIELLO
DO Darline DIZE
DM Doloreza Mullaliu
SG Gul, Sheraz
GB Gulshah Bayraktar
GC Guy Caljon
HD Harry de-Koning
JP János Dr. Pálhalmi
MQ Maria João Ribeiro Peixoto Queiróz
MC Maria Paola COSTI
Organizzatore

Synthesis

Archiv der Pharmazie, 353(8), 1900325

One Health drugs against parasitic vector borne diseases in Europe and beyond OneHealthdrugs

Cost Action CA21111

Workshop - Success stories and challenges in One-Health drug discovery for VBCs* 15/05/2025 10:00 to 13:00 CET

01:20:34

Alma Mater Studiorum Università di Bologna

Contenti Chat D&R Partecipanti Menu Reazioni Vista Altro Webcam Microfono Condividi Abbandona

In questa riunione, (27)

Disattiva l'audio di t...

HD Anabela Silva CL Clara Lima OK Gulshah Bayraktar MC Maria Paola COSTI GC Guy Caljon

Bioactivity Studies

Gulshah Bayraktar

25°C

Workshop - Success stories and challenges in One-Health drug discovery for VBCs* 15/05/2025 10:00 to 13:00 CET

Cerca

ITA

13:10

02:15:54

Contenti Chat D&R Partecipanti Menu Reazioni Vista Altro Webcam Microfono Condividi Abbandona

In questa riunione, (22)

Disattiva l'audio di t...

HD Anabela Silva CL Clara Lima OK DANIELE AIELLO RA Rokaya Ahmad

TbPTR1 versus LmPTR1 Structural comparison between the complexes TbPTR1-DHB and LmPTR1-DHB

TbPTR1-DHB (chain A)

LmPTR1-DHB

Structural comparison between the complexes TbPTR1-DHB (chain A) and LmPTR1-DHB

TbPTR1

- Compact aromatic/hydrophobic region
- Phe97 aromatic floor
- Trp221 and Tyr174 reinforce the aromatic/hydrophobic pocket
- Ser95 and Arg14 provide polar or charged anchoring points

PTR1 kinetic data versus DHB

	TbPTR1	LmPTR1
$K_{M,DHB}$ (μ M)	6.0 ($\pm$ 0.7)	5.3 ($\pm$ 0.8)
$k_{cat,DHB}$ (s^{-1})	0.7 ($\pm$ 0.2)	6.8 ($\pm$ 0.7)

LmPTR1

- More distributed interaction landscape
- Phe113 as the main aromatic residue
- His241 and Leu188/Leu226/Leu229 contribute additional polar/hydrophobic features
- Binding-site hydration strongly reshapes accessible contact patterns

Substrate-binding loop

DANIELE AIELLO

One Health drugs against parasitic vector borne diseases in Europe and beyond OneHealthdrugs

Cost Action CA21111

02:16:18

Controllo Conferenza Chat DLR Participanti Mappa Reazioni Vista Altro Webcam Microfono Condividi Abbandona

In questa riunione: (22) Disattiva l'audio di L...

EU Elisa Ullasi
A Agish
AM Ana Mikić
AS Anabela Silva
AG Aurora Gaza
B Bianca Martino
CL Clara Lima
CN Corinne Ngameko
DA DANIELE AIELLO
EP Edmond Pua
SG Gul Sheraz
HD Harry de-Koning
MQ Maria João Ribeiro Peixoto Queirós
MC Maria Paola COSTI
M Induarte
MS MURAT SENTURK
RS Relja Surucic
RA Rokaya Ahmad

Computational results **From screening hit to optimized xanthine analogues**

UNIMORE UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

Fraunhofer ITMP

3s INSTITUTO DE INVESTIGAÇÃO E INOVAÇÃO EM SAÚDE UNIVERSIDADE DO PORTO

TYDOCK PHARMA chemical library

Target **Screening and data analysis** **HIT compounds**

LmPTR1/TbPTR1

NMT-TY0177

1-22

To explore structure-activity relationships, we designed and synthesized a xanthine-based focused library 1-22.

% inhibition TbPTR1 @50 µM: 70%
% inhibition LmPTR1 @50 µM: 89%
% inhibition T. brucei @10 µM: 47%

Comparison of inhibitor activity against LmPTR1 and TbPTR1 at 50 µM

% inhibition (mean ± SD)

Compound

% inhibition (mean ± SD)

Primary inhibition screening at 50 µM. Several optimized analogues show stronger inhibition of TbPTR1 than LmPTR1.

DANIELE AIELLO

CLASSICAL EARLY DRUG DISCOVERY WORK-FLOW

	Reagent validation	Assay development	Screening	Hit-to-Lead	Lead-to-Candidate
TYPICAL TIME (M)	<3	<6	<6	12-24	12-24
BIOLOGY SUPPORT	Protein construct generation & purification/detection tags	Functional, binding, cell-based & selectivity assays	Hit confirmation, MvA studies, cytotoxicity, selectivity & ADMET	SAR (potency & selectivity), MvA & ADMET/DMX	SAR (potency & selectivity), MvA & ADMET/DMX
MILESTONES	High quality reagents	Fit-for-purpose assays	Validated hits	Lead Declaration	Candidate Declaration

Physico-chemical properties

In vitro safety profiling

Assay miniaturization and validation

Hit qualification and expansion

DMPK

Toxicology

Reagent generation and scale-up

Compound profiling (cellular/biochemical/biophysical)

Primary screen and triage

Medicinal chemistry

Chemistry scale-up

Formulation

AM Ana Mikić

RS Relja Surucic

IP Ismael Papanastasiou

< 2/2 >

Gul Sheraz

One Health drugs against parasitic vector borne diseases in Europe and beyond OneHealthdrugs

Cost Action CA21111

Workshop - Success stories and challenges in One-Health drug discovery for VBDs 16/05/2026 1000 to 1300 CET

02:34:57

CLASSICAL EARLY DRUG DISCOVERY WORK-FLOW

	Reagent validation	Assay development	Screening	Hit to Lead	Lead to Candidate
TYPICAL TIMELINE (M)	< 3	< 6	< 6	12-24	12-24
BIOLOGY SUPPORT	Protein construct generation & purification/selection tags	Functional, binding, cell-based & selectivity assays	Hit confirmation, Mock studies, open-sourcing, selectivity & ADMET	SAR (potency & selectivity), Mock & ADMET/TOXPK	SAR (potency & selectivity), Mock & ADMET/TOXPK
MILESTONES	High quality reagents	Fit-for-purpose assays	Validated Hit	Lead Declaration	Candidate Declaration

03:00:15

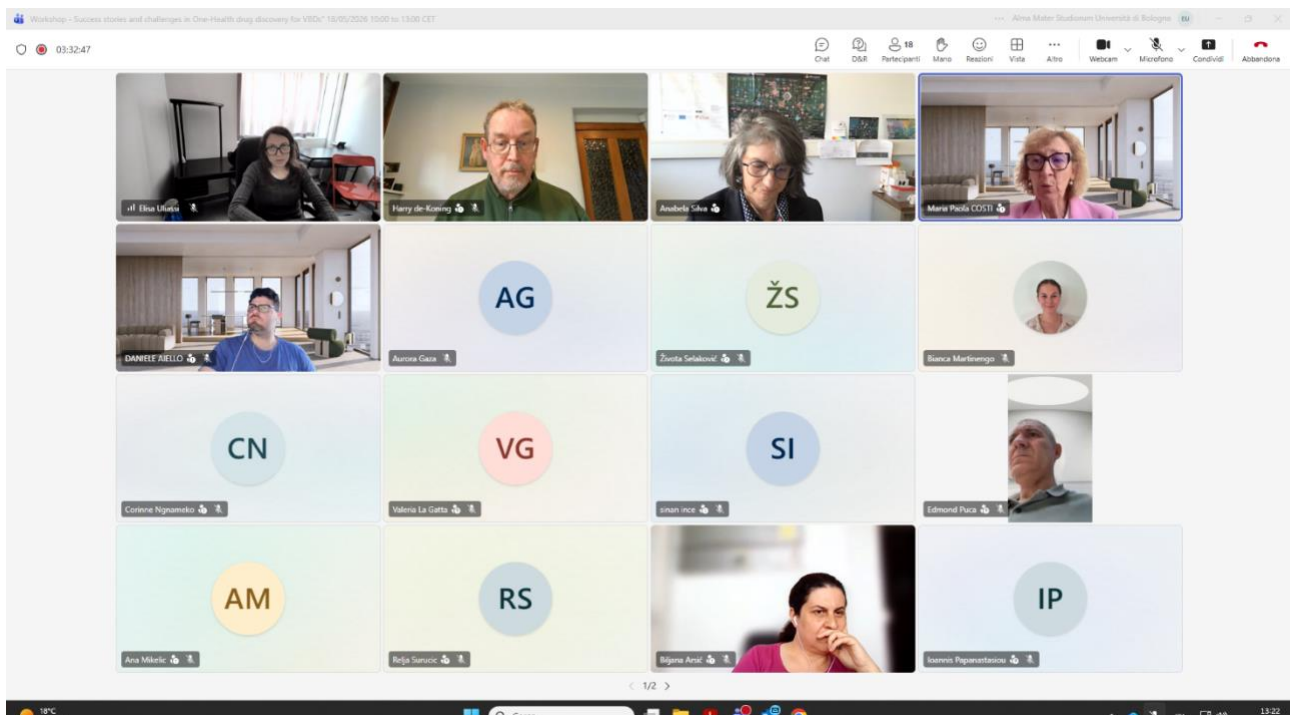
Method

CRISPR-Cas9 Gene Editing Method - Tagging

Beneke T, Madden R, Makin L, Valli J, Sunter J, Guenz E. A CRISPR Cas9 high-throughput genome editing toolkit for kinetoplastids. *R Soc Open Sci*. 2017 3;4(5):170095.
Beneke T, Guenz E. LeishGEdit: A Method for Rapid Gene Knockout and Tagging Using CRISPR-Cas9. *Methods Mol Biol*. 2019;121:189-220

11

One Health drugs against parasitic vector borne diseases in Europe and beyond
OneHealthdrugs
Cost Action CA21111



3. DESCRIPTION OF THE ACTIVITIES

Opening Remarks

The workshop was opened by **Elisa Uliassi**, who emphasized the objective of fostering collaboration across all career stages within the COST Action. She highlighted the importance of sharing success stories, addressing challenges, and promoting new ideas for research, education, and communication activities. As leader of **Horizontal Group 4 (Young Research Innovators)**, she underlined the role of the workshop in stimulating future initiatives and interdisciplinary projects. Participants were welcomed and invited to engage in presentations and discussions.

1. Blended Intensive Program (BIP) on Drug Resistance

Presenter: Anabela Silva

- Introduced a Blended Intensive Program (BIP) addressing drug resistance in cancer and infectious diseases.
- Program structure combines **online webinars and in-person training**, promoting multidisciplinary and international learning.
- Supported by COST Action framework, targeting PhD students and postdoctoral researchers.

Key contributions:

- Portugal: Scientific leadership and coordination
- Italy: Experimental models and network integration
- Greece: Translational collaboration support

Impact:

- Strengthened scientific mobility and visibility of COST Action
- Built sustainable collaborations across Southern Europe

Future activity:

- Upcoming training in Porto focusing on personalized cancer therapy, antibiotics, and antiparasitic drugs, followed by networking and evaluation activities

Discussion:

Opportunities for broader participation were discussed. Although current enrollment is closed, future editions will remain open and evolving.

2. Career Development & OneHealthDrugs Integration

Presenter: Dr. Clara Lima

- PhD research focused on **Leishmania surveillance in Portugal (cats and dogs)**.
- Improved diagnostic approaches using a One Health framework.

COST Action contribution:

- Leadership role in WG6
- Development of international collaborations (including Morocco)
- Active engagement as **OneHealthDrugs Ambassador**

Additional initiatives:

- Founding member of NGO establishing a system for redistribution of unused veterinary medicines
- Outreach activities promoting sustainability in veterinary practice

Discussion:

- Regulatory and liability challenges of drug redistribution were highlighted.
- Suggestions included consulting established systems (e.g., ValorMed).
- Proposal to develop a standardized educational module on pharmaceutical environmental impact was agreed as a potential output.

3. Development of Pyrimidine Derivatives for leishmaniasis

Presenter: Gulsah Bayraktar

- Research focused on **pyrimidine-based compounds for leishmaniasis treatment**.
- Transitioned from PTR1 enzyme targeting to kinase inhibition studies.
- Identified promising structural leads with in vivo activity.

COST Action impact:

- STSM at University of Nantes enabled computational modeling collaboration
- Strengthened project development and international networking

Future work:

- New grant in Turkey to expand chemical space (thiazolopyrimidines, oxazole, imidazole analogues)

Outcome:

- Significant professional growth and recognition of career progression within COST network

Technical discussion:

- Recommendation to test selectivity against human kinases
- Suggestion to use primary cells for improved biological relevance
- Proposal to integrate kinase targets into COST Action database

4. Personal Journey within COST Action OneHealthDrugs

Presenter: Elisa Uliassi

- Described progression from working group member to Core Group leader and Ambassador.
- Research focus: **green chemistry and sustainable drug design for vector-borne diseases**.

Key contributions:

- Coordination of >100 young researchers
- Organization of workshops, training schools, and “One Health Drug Marathon”
- Survey design and database development on sustainability practices in drug discovery

Discussion:

- Strong emphasis on publishing survey results (“Brooks Project”)
- Recognition of COST Action-related publications
- Importance of policy impact and regulatory translation highlighted

5. Computational Studies on PTR1-Based Inhibitors

Presenter: Daniele Aiello

- Work on **Trypanosoma brucei** and **Leishmania** **PTR1 inhibitors** using computational approaches.
- Identified role of conserved water molecules influencing binding affinity differences.

Key insight:

- Water-mediated interactions contribute to reduced binding efficiency in Leishmania PTR1

Future direction:

- Development of independent QSAR platform (“ChemML Studio”)
- Aim to reduce dependency on external computational tools

6. Training School Overview

Presenter: Sheraz Gul

- Overview of training school program across **7 locations** and **>100 researchers trained**.
- Structured application and review system ensures fairness and inclusivity.

Impact:

- Strong pipeline from training schools to STSMs and publications
- Example of participant progression leading to collaborative research output

Future perspective:

- Proposal to explore commercialization of training modules for external scientific and industrial use

7. Hydrophobic Degraders & Gene Editing tools to study degradation in parasites

Presenter: Aurora Gadza

- Research on **protein degradation strategies in Trypanosoma and Leishmania**.

Key results:

- Selective activity observed against intracellular amastigote stage
- Use of CRISPR-Cas9 for generation of engineered Leishmania cell lines

Future work:

- Testing degraders in engineered models to confirm mechanism of action

8. Biocatalysis & Food Waste Valorization

Presenter: Bianca Martinengo

- STSM at University College London focusing on **cashew nut shell liquid (CNSL) valorization**.

Scientific approach:

- Use of peroxxygenases and lipase-based systems for oxidation reactions
- Production of epoxides as intermediates for antiparasitic drug development

Impact:

- Integration of circular economy principles into drug discovery
- Strengthening collaboration with producing countries for sustainable resource use

4. Conclusion

The workshop highlighted the **multidisciplinary strength of the OneHealthDrugs COST Action**, showcasing contributions across medicinal chemistry, computational biology, sustainability, and public engagement.

Key overarching themes included:

- Strong integration of early-career researchers
- Importance of training, mobility, and STSMs
- Expansion of One Health and sustainability principles
- Need for continued dissemination, publication, and policy translation

The organizers emphasized the value of these activities in shaping future collaborative research and strengthening the impact of the COST Action beyond its duration.

6. LIST OF ANNEXES

No annexes used at the meeting