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# Virtual screening of OHD Compound libraries against parasitic targets: towards a One Health screening platform

13/05/2026

14:00-16:00 CET

Online

## ***Workshop of the COST Action CA21111 One Health drugs against parasitic vector borne diseases in Europe and beyond OneHealthdrugs***

The event is open to PhD, young innovators and senior scientists from both academia and pharma

### Description.

The OHD:LUB Project is the OneHealthdrugs COST Action's premier success story, showcasing how interdisciplinary synergy can fast-track drug discovery on a budget. Its workflow bridges the gap from supercomputing to sustainable therapy through three key phases:

Phase I: High-Velocity Virtual Screening – Leveraging the Vega HPC system, the team (led by Podlipnik and Jukić) has screened 36,000+ compounds against 22 targets. With 21 targets already docked, they are now using 3D interaction fingerprints to refine the most promising hits.

Phase II: The "Green" Triage – In a pioneering move, the project uses ML-driven ecotoxicity models (in collaboration with Daniele Aiello) to filter hits. This creates a "Green Drug Score," ensuring candidates are both potent and environmentally benign from the outset.

Phase III: Experimental Validation – With a deadline of October 2026, the project has launched a "call to action." While labs prepare protein purification, Sheraz Gul (Fraunhofer) provides HTS and ADMET testing infrastructure. STSM funding is prioritized for young researchers to travel and conduct the final physical assays.

## Schedule at a Glance

Time	Session	Speaker(s)
14:00 - 14:10	Introduction	MP Costi, Črtomir Podlipnik
14:10 - 14:40	Targets	Andrea Ilari, Elisa Uliassi, Cecilia Pozzi, Biljana (Rab5a), Jovana Tavares / Anabela Cordeiro (Sirtuin)
14:40 – 15:00	OHD Chemoteque & Compounds	Daniele Aiello, Sandra Gemma, Michele Tonelli, Pascal Marchand, Chiara Borsari, Maria Alice Charvalo, David Magri
15:00 - 15:15	Docking Strategy & Result Analysis	Marko Jukic
15:15 - 15:30	Presentation of Current Results	Črtomir Podlipnik
15:30 - 15:45	From Virtual Screening to Screening	Sheraz, Guy Caljon, Anabela Cordeiro
15:45 - 16:00	Future Plans and Discussion	MP Costi, Daniele Aiello, Marko Jukic, Črtomir Podlipnik

## Detailed Agenda

### 14:00 - 14:10 | Introduction

**Speakers:** MP Costi, Črtomir Podlipnik

- Welcome remarks and an overview of the workshop's goals.

### 14:10 - 14:40 | Targets

**Speakers:** Andrea Ilari, Elisa Uliassi, Cecilia Pozzi, Biljana (Rab5a), Jovana Tavares or Anabela Cordeiro (Sirtuin)

- Why specific targets are selected.
- Technical aspects and considerations to keep in mind.

- Expectations from Virtual Screening.

#### 14:40 - 14:55 | OHD Chemoteque & Compound Database

**Speakers/Contributors:** Daniele Aiello, alongside compound providers (e.g., Sandra Gemma, Michele Tonelli, Chiara Borsari, Maria Alce Charvalo, Elisa Uliassi, David Magri, MPCosti all contributors)

- Overview of current assets and the underlying strategy.
- The possible benefits and applications of the library.
- Involvement and updates from the compound database providers.

#### 14:55 - 15:10 | Docking Strategy & How to Analyze Results

**Speaker:** Marko Jukic

- Expectations from docking results and critical points of care.
- Review of methodologies: what was done and what was intentionally omitted.

#### 15:10 - 15:30 | Presentation of Current Results

**Speaker:** Ārtomir Podlipnik

- Showcasing the latest findings.
- Best practices for presenting results in accordance with FAIR principles.

#### 15:30 - 15:45 | From Virtual Screening to Screening

**Speakers:** Sheraz, Guy Caljon, Anabela Cordeiro (and others)

- Bridging the gap between in-silico predictions and physical screening.
- Evaluation of antiparasitic activity.

#### 15:45 - 16:00 | Future Plans and Discussion in OneHealthdrugs and beyond

**Panel:** MP Costi, Daniele Aiello, Marko Jukic, Ārtomir Podlipnik

- Open floor for questions, collaborative discussion, and outlining next steps.

The event registration requires two steps : 1) create an e-COST account in the [www.cost.eu](http://www.cost.eu) and 2) register here:

[https://docs.google.com/forms/d/e/1FAIpQLSc5KIJAul5siF7j2mtT9YoFzTZHPHaubsTRt\\_BsupszDCvnmA/viewform?usp=publish-editor](https://docs.google.com/forms/d/e/1FAIpQLSc5KIJAul5siF7j2mtT9YoFzTZHPHaubsTRt_BsupszDCvnmA/viewform?usp=publish-editor)

**by the 11/05/2026**