

MINUTES HG7/WG2 Workshop

Green and bioinformatic approaches including biodegradability prediction in antiparasitic drug discovery

Tuesday, 18th March 2025

Teams platform and Cloudpharm P.C Cana Laboratories, Athens, Greece

Prepared by Sandra Gemma (HG7 Leader), Marina Roussaki (Local organizer) and Theodora Calogeropoulou (WG2 leader)

1. MEETING LINK

2. https://teams.microsoft.com/l/meetup-join/19%3ameeting_NGY2MWNkNjktNWJhNC00ODQyLTk1MDAtZjY5YWRiNmNINzhm%40thread.v2/0?context=%7b%22id%22%3a%2289c77242-811d-4184-a23b-c980834ae8cb%22%2c%22Oid%22%3a%22e2b3d427-848f-4da3-9974-b8c2ee28b288%22%7d

3. LIST OF ATTENDANTS

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For a complete list, check the COST platform

2. PROOF OF ATTENDANCE

Teams attendance report and screen shots of participants; Signed attendance list

3. DESCRIPTION OF THE ACTIVITIES

E-COST invitations were sent to all working groups members. The workshop was attended by 27 participants in presence and 10 participants from remote.

The workshop began with opening remarks from **Sandra Gemma** (HG7 leader), **Theodora Calogeropoulou** (WG2 leader), and **Marina Roussaki** (Cloudpharm P.C., Local organizer), who welcomed participants and introduced the key themes of the workshop. Following this, **Maria Paola Costi**, the Action Chair, provided an update on the **OneHealthdrugs Action**, highlighting recent developments and ongoing research efforts. The first session, **Opening and Environmental Impact of Pharmaceuticals** was chaired by **Prof. Anabela Cordeiro Silva** and consisted of three lectures. **Panagiotis Zoumpoulakis** (Cloudpharm P.C) and **Dimitris Moraitis** (Cosmos Health Inc.) presented an overview of Cloudpharm P.C. and CANA Laboratories, detailing their contributions to the pharmaceutical sector and environmental research. **Marina Roussaki** (Cloudpharm P.C) introduced the **EU-funded project "ENVIROMED"**, discussing its objectives in assessing pharmaceutical environmental impact. **Eleni Chontzopoulou** (Cloudpharm P.C) explored the biodegradability and pharmaceutical metabolites in environmental toxicology, emphasizing challenges in sustainable drug

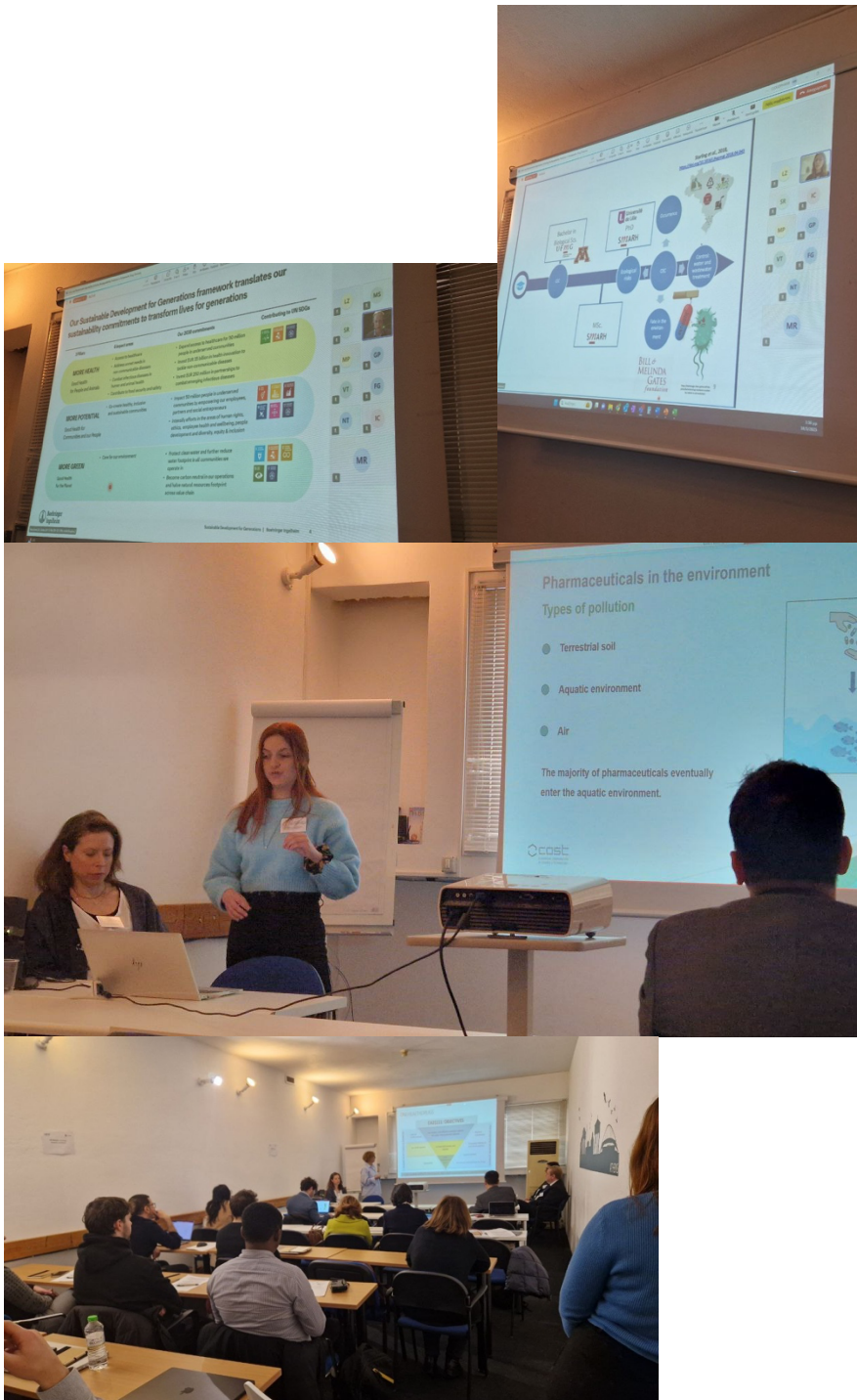
development. The second section, “**Computational Approaches in Ecotoxicology & Drug Discovery**” was chaired by Prof. **Theodora Calogeropoulou** and consisted of two lectures. The first was presented by **Vagelis Tsoukas** (Cloudpharm P.C) who described the use of machine learning-based predictive models for ecotoxicity assessment, focusing on LC50 and bioconcentration factors. In the second lecture, **Antreas Afantitis** (NovaMechanics MIKE), introduced **Isalos Analytics Platform**, a zero-code machine learning solution for cheminformatics, offering insights into its applications in drug discovery and ecotoxicology. After lunch break, **Sandra Gemma** and **Maria Paola Costi** chaired the third session titled “**Advanced Research in One Health and Drug Development**”. Two lectures were presented by speakers presenting from remote: **Tobias Harschneck** (Boehringer Ingelheim Vetmedica GmbH) provided a cross-industry perspective on biodegradation of active pharmaceutical ingredients (APIs); while Prof. **Maria Clara Starling** (Universidade Federal de Minas Gerais) discussed emerging contaminants in the environment, their One Health implications and approaches for their removal from water. The last speaker of the session, Prof. **Sandra Gemma** (University of Siena), presented an integrated in silico and experimental approach for targeting leishmaniasis within the One Health framework. A short break followed afterward the workshop activities continued with the last section comprising **the selected Young Researchers' Contributions**. The section was chaired by Dr **Marina Roussaki** and the two trainees presented their work: **Daniele Aiello** (University of Modena and Reggio Emilia) explored an antiparasitic drug discovery approach, integrating structural analysis and ecotoxicological profiling; **Ludovica Marotta** (University of Siena) introduced a Design of Experiment (DoE) methodology for a sustainable synthesis of chalcones with antimicrobial potential.

4. SCIENTIFIC PLANNING/STRATEGIES/WHO DOES WHAT

N/A

5. CONCLUSIONS

The workshop successfully fostered discussions on the environmental impact of pharmaceuticals, computational ecotoxicology, and sustainable drug development. The presentations exposed, each one followed by several questions from the audience highlighting key aspects and takeaways, facilitated knowledge exchange across disciplines. The talks and discussion highlighted the need to take further steps toward a thorough assessment of environmental impact of drugs. These steps include expanding computational methodologies, acquire new experimental data, and developing new technologies for reinforcing experimental and bioinformatic approaches to biodegradability prediction and assessment useful for implementing benign-by-design strategies in drug development.





ΕΘΝΙΚΟ ΙΔΡΥΜΑ ΕΡΕΥΝΩΝ
National Hellenic Research Foundation

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

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OF

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LABORATORIES

LIST
ANNEXES