OHD:LUB project

Guidelines for Structure-Based Simulation Project Collaborations

Project Background: Scientists from the University of Ljubljana and the University of Modena and Reggio Emilia (the Simulation Team) have conducted structure-based simulation research on 22 drug targets for trypanosomatidic parasites, at the moment.

Methodology: The research involves protein preparation, docking studies, and virtual screening against a predefined compound database. From these studies, initial compound shortlists have been generated and filtered based on ecotoxicity properties. The final selection is fully profiled for ADME-TOX and ECOTOX characteristics.

Collaboration Opportunity: Interested researchers are invited to initiate a formal collaboration with the Simulation Team.

Initiating Projects: Researchers should contact the Simulation Team directly to propose a new medicinal chemistry project based on these targets.

Requirement for Access: Before receiving the shortlisted compound data, researchers must formally agree to these collaborative guidelines.

Collaborative Guidelines:

1. **Active Participation:** The Simulation Team must be actively involved as contributors to the medicinal chemistry project developed by the researcher.
2. **Communication:** The Simulation Team must be kept updated on the project's progression and results.
3. **Authorship:** Members of the Simulation Team must be included as co-authors on any manuscript resulting from the medicinal chemistry project.
4. **Acknowledgement:** All publications resulting from this collaboration must include an acknowledgement of the OneHealthdrugs COST Action (CA21111) (see the exact wording in the COST Action website, www.cost.eu)
5. **Notification:** The Chair and Vice-Chair of the COST Action must be notified when a new medicinal chemistry project commences.

Note on Future Platform Integration: As part of COST Action CA21111, we are exploring the establishment of a permanent OHD Simulation Platform. If such a platform is formalized as a technical tool of the Action, active medicinal chemistry projects may be listed as "ongoing projects" based on input from the lead researcher. Please note that the specific mechanisms for this integration are currently under discussion and subject to change.