## Report of the fourth Training School of COST Action CA15135 - Lugano 5-12 October 2019

The "BioInformatics meets BioSimulations in protein and DNA studies: from theory to practice" (BImBS 2019) training school was organized by COST Action CA15135 in collaboration with CECAM. The event was held from October 5 to October 12th, 2019, at the Università della Svizzera italiana (USI) in Lugano (Switzerland). The BImBS training school aimed at introducing young scientists to the theory and practice of the state-of-the-art bioinformatics and biosimulations techniques. This school was organized by the WG4, thanks to the effort of Prof. Vittorio Limongelli, which is an outstanding scientist with more than ten years of experience in the field of advanced calculations applied to pharmacologically relevant systems.

At the deadline of August 20th 2019, we have collected 45 participation requests that were more than the available slots. The COST action has supported 30 selected applicants to partially cover their travel and accommodation expenses. The selection of the COST supported trainees was carried out by a Scientific Commission composed by four members of the COST Action, involved in computational research activities.

In-silico approaches cover an increasing important role in drug discovery. In particular, theoretical studies embrace bioinformatics and biosimulations, which are apparently two separated communities in which researchers work on thematically related topics but do not communicate each to the other. The final goal of the school was to unveil potential interaction and synergies between the two communities, which is fundamental especially in the education of young scientists like PhD students and postdocts. Indeed, the BImBS school provided an holistic picture of the possible applications of the state-of-the-art techniques in bioinformatics and biosimulations contributing to the formation of young researchers in the resolution of problems that might require cross-disciplinary preparation. The BImBS school was a unique event in which apparently different expertise were combined, however preserving a deep analysis of the techniques presented and also paying attention to bridge the gap between computations and experiments.

The school program was organized in 8 days, each day was divided in a morning theoretical session covering 2 different topics, followed by a noon practical session in which the participants could reproduce part of the studies presented in the morning. World-leading scientists, having an average H-index of 84, held the morning lectures.

Particular attention was paid to the practical sessions as they represented a unique opportunity for the attendees to i) get a deep understanding of each presented technique, ii) acquire basic skills to use the methodology, and iii) solve technical issues that are typically encountered.

In order to give voice to the young participants and favour their interaction with the senior speakers, a poster session was organised on school day 6 with a competition for the best presentation. In addition, an oral session of 90 minutes composed by 6 mini-talks of 15 min each, was dedicated to the best abstracts submitted by the attendees and selected by an internal committee.

The required infrastructure, in terms of computers and software, was provided by the host Institution USI Lugano and the organisers.

Different types of activities were organized during the school, aimed at establishing a collaborative environment and strenghtening the interaction among the young participants and the senior scientists.

At the end of the school all the participants expressed a highly positive evaluation on: 1) the topics treated during the 8 days courses; 2) the scientific level of the invited speakers; and, particularly, 3) the general organization of the event, wishing the possibility that the school will be promoted again in the following years.

A special thank goes to Prof. Vittorio Limongelli and his team for the perfect organization.

Catanzaro, November 11<sup>th</sup> 2019

Prof. Stefano Alcaro

Chair of COST Action CA15135



## Photo gallery of the 4<sup>th</sup> Training School of COST Action CA15135 and CECAM (BImBS)

Lugano, 5-12 October 2019



The students in the USI's "Aula Magna" during one of the morning theoretical sessions.



The students in the USI's "Computer room" during one of the afternoon practical sessions.



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The BImBS group photo in front of the USI's main building



The BImBS group photo in the "Room Machines" of the Swiss National Supercomputing Centre - CSCS  $\,$ 



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Professor Limongelli with speakers and students during the BImBS social dinner.

Mu.Ta.Lig. COST Action speeds up the European Drug Discovery process

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