

The last event of the first grant period of the COST Action CA15135 was performed in Vienna with the Training School (TS) “Computational Approaches to Polypharmacology” from February 8 to 10 2017. The Pharmaziezentrum at the University of Vienna was the location of this event organized by Sharon Bryan, MC member for Austria, WG3 leader and CEO of Inte:Ligand Company co-proposer of the MuTaLig COST Action. The purpose of the TS was focusing and training on computational techniques to speed up the process of identification of bioactive compounds endowed with multi-targeting properties and potentially useful for the prevention and the synergistic cure of high-impact diseases.

The TS activity structure was very professional, due to the experience, the competence and the great efforts of the local organizer and staff, in particular Thierry Langer, professor of Medicinal Chemistry at the University of Vienna and MC substitute for Austria. After the introduction, done by the local organizer Sharon Bryant and the Chair of CA15135 Stefano Alcaro, the TS activities were carried out by trainers by regular lectures in the morning and practical sessions in two groups in the afternoon. More than 60 participants, mostly young researchers with a good gender balance, were registered in the TS from 10 different countries (Austria, Bulgaria, Czech Republic, Greece, Israel, Italy, Morocco, Poland, Serbia, Slovenia e Turkey) on the e-cost platform. The lecturers were performed by experts in the field of computational chemistry coming from academia (Thierry Langer and Gerard Ecker from University of Vienna, Hanoch Senderowitz Bar Ilan University, Andrea Danani from Andrea Danani, IDSIA of Lugano, Rita Guedes from University of Lisboa) and industrial institutions (Peter Ertl and Richard Lewis from Novartis, Peter Ettmayer from Boehringer-Ingelheim, Marie-Louise Jung from Prestwick Chemicals e Stefan Kubicek from the austrian CeMM spinoff). Two working groups were respectively divided into computer rooms. In the first afternoon the former was trained on the use of pharmacophore models, docking and molecular dynamics and the latter on data mining, machine learning tools and in silico chemical libraries. In the second afternoon the groups were exchanged in order to cover all trainees with the available software and exercises. During the last day an interactive session for all participant was performed in order to officially present the Chemotheca, the web-based cheminformatics tool developed by Francesco Ortuso, associate professor at the CCLab (Computational Chemistry lab) of the Università Magna Græcia di Catanzaro. This tool, accessible at the link [chemotheca.unicz.it](http://chemotheca.unicz.it), allows any participant to register and to insert his/her set of compounds in order to create and enrich a common molecular database, useful to speed up the identification of multi-targeting compounds within the MuTaLig scientific community of COST Action CA15135.

The TS activities ended with the summary and the conclusions of Stefano Alcaro and Fernanda Borges, respectively Chair and Vice-Chair of the COST Action CA15135. The first TS resulted very useful for all attendees, trainees and trainers. The atmosphere was friendly and appropriate for exchanging ideas and information about all TS topics. The presence of industrial and academic trainers represented an essential issue of the MuTaLig COST Action, that has in its mission the integration of knowledge of multi-targeting among the two scientific domains. The COST Action Chair concluded the meeting acknowledging the organizing staff and giving some preliminary announcements about the next CA15135 appointments for the next grant period (May 2017 – April 2018) along with the recommendation to periodically browse the MuTaLig web [www.mutalig.eu](http://www.mutalig.eu) for additional information.

Catanzaro, February 20<sup>th</sup> 2017

Prof. Stefano Alcaro

Chair of COST Action CA15135



Prof. Sharon Byant – Inte:Ligand CEO & University of Vienna, WG3 leader CA15135 and local organizer of the Vienna Training School



Training School classroom



Prof. Thierry Langer, University of Vienna, CA15135 MC substitute and Dr. Peter Ettmayer, Boehringer-Ingelheim, Austria



Prof. Thierry Langer, University of Vienna, CA15135 MC substitute and Prof. Andrea Danani, IDSIA, MC substitute Switzerland





Classroom discussion



Classroom discussion

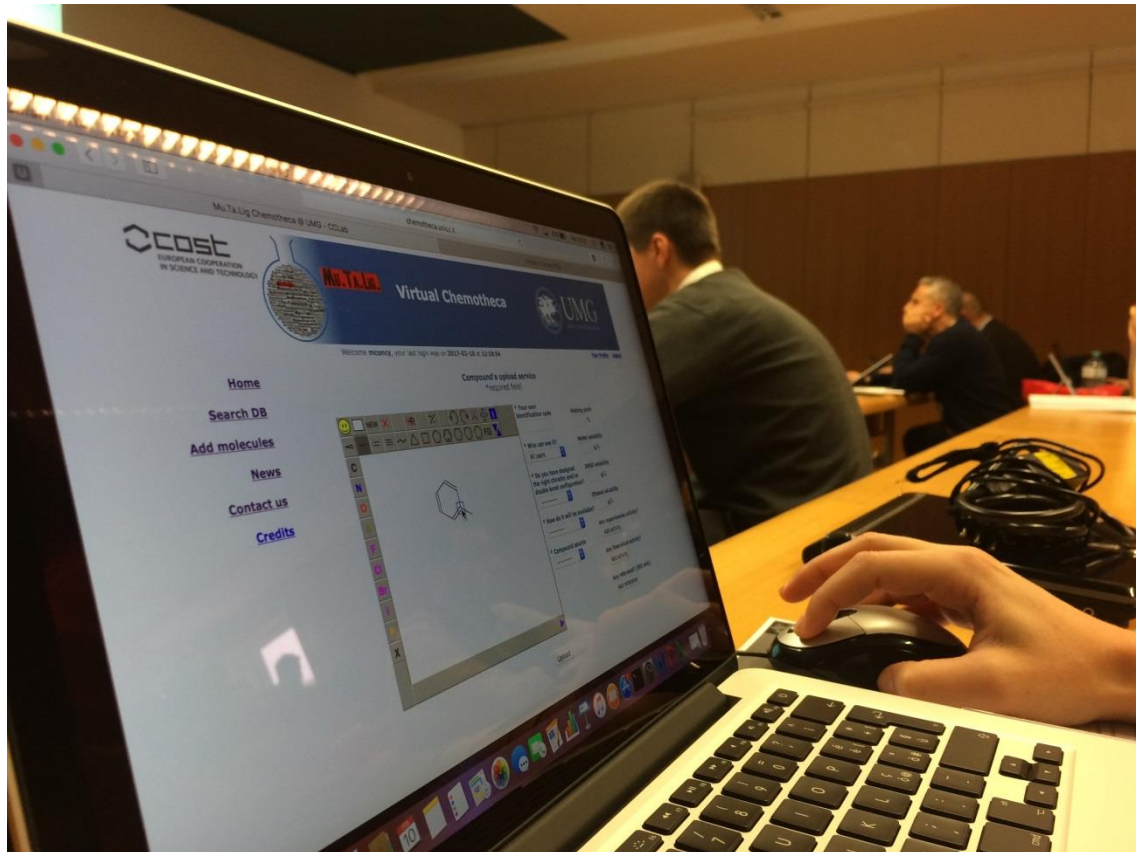


Prof. Thierry Langer, University of Vienna, CA15135 MC substitute and Dr. Rita Guedes, University of Lisbon, MC member Portugal

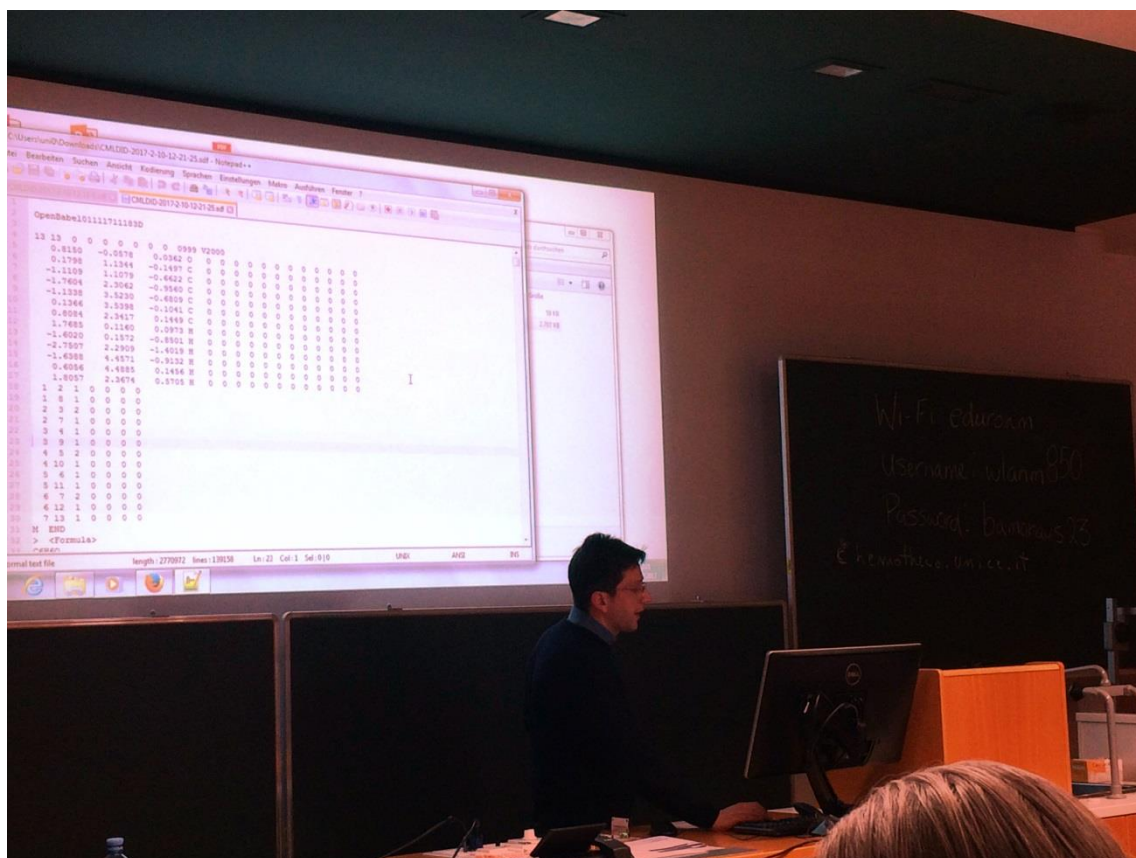


Classroom discussion





Chemotheca interactive practice session



Prof. Francesco Ortuso, University "Magna Græcia" of Catanzaro, developer of the CA15135 Chemotheca



Chemotheca presentation



Conclusions by Hanoch Senderowitz, WG4 leader, Fernanda Borges, Vice-Chair and Stefano Alcaro, Chair of CA15135





Social activity



Social activity





Group Photo



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