

The second Working Group Meeting of the COST Action CA15135 has been carried out almost at the end of the second grant period in Tenerife at the Instituto Universitario de Bio-Organica “Antonio González” (IUBO-AG) of the Universidad de La Laguna from 15 to 16 March 2018. It comes basically in the middle of the COST Action life, concluding the networking tools of the first two years. Therefore, the focus of this meeting was to look at the status of the current activities among the four CA15135 working groups, intentionally joined again to keep together, as strong as possible, the MuTaLig community. Thanks to the availability of our MC substitute for Spain, José M. Padrón, the organization of the meeting was carried out in a perfect location supported by a great social activity between the first and the second day. The meeting started with the reports of the leaders, that highlighted strengths and weakness points of each Working Group.

Danijel Kikelj, WG1 leader, pointed out the good level of the collaborations already established in the first two years among the numerous components of the first Working Group. Several outcomes have been, actually, published in terms of scientific manuscripts, updated in the reference section of the www.mutalig.eu web site. Conversely, he pointed out how still preliminary is the level of implementation of the virtual Chemotheca, freely accessible at the link chemotheca.unicz.it.

Eugenio Gaudio, WG2 leader, illustrated the most used techniques adopted by the second Working Group, extrapolating them from the bibliographic references published in the first two years. Despite the good level of collaboration, he pointed out the importance of patenting in the field of multi-targeting drug discovery and basically invited all participant to always care about the protection of the intellectual property of their inventions before going on with scientific publications, even on relevant journals.

Sharon Bryant, WG3 leader, reported the activity of the third Working Group starting with the creation of the Chemotheca platform and its implementation, carried out mainly at UMG di Catanzaro by Francesco Ortuso. The two MuTaLig training schools, respectively carried out in 2017 in Vienna and Siena, were the appropriate occasions for preparing young investigators to the use of this unique tool explicitly created for our COST Action. Moreover, even if the catalogued compounds were not so many, she presented a preliminary study of virtual screening against several targets that clearly demonstrated its strong potentiality in the rapid identification of novel multi-targeting agents. Sharon concluded emphasizing the importance in the enrichment of the chemotheca catalog for the purposes of the second half of the COST Action.

Hanoch Senderowitz, WG4 leader, reported about the main analysis issues related to the fourth Working Group. Actually, the lack of many data not only in the chemical catalogue, but also in the biological list of available targets, is the problem to solve in the second period of the MuTaLig COST Action. So, again, he warmly invited all participants to potentiate the data shared within the MuTaLig community.

After the introduction reporting part, the meeting was carried out in four thematic sessions, where an invited speaker, expert in each WG field, carried out a plenary lecture, followed by several short talks performed by young and senior investigators of all participating countries. Out of 33 currently MuTaLig parties, 22 were present at the WG meeting with more than 100 attendees. Globally, 30 oral communications were presented in both days consecutive sessions. As usual, also during this meeting, a poster session was organized especially for pushing young investigators to show their results and to share them to the MuTaLig community. Forty-two posters were presented and all abstracts collected in a virtual

Report of the 2nd Working Group Meeting of COST Action CA15135 – Tenerife (Spain) March 15-16 2018

book published at the www.mutalig.eu before the meeting and always available on line. Stefano Alcaro, from the introduction to the conclusive sessions, stimulated the discussion among all participants and promised to carry out two main issues to improve the above mentioned weakness point. The former is related to put in higher evidence the chemotheca access directly from the home web page of the www.mutalig.eu site. The latter will be to start a new survey among the MuTaLig community, that now is composed by more than 400 participants. In the conclusions, some additional considerations were performed by Maria Laura Bolognesi, coordinator of the MuTaLig mobility programs, about the consistent STSM activity done in the first two years, by Alfonso Garcia-Sosa, recently nominated as Science communicator, about the network of collaborations still in progress and by Simona Rapposelli, associate editor of the first special issue promoted by MuTaLig in the qualified peer reviewed journal Frontiers in Chemistry, that will host original contributions from all the COST Action community. Then, Stefano Alcaro gave to two young investigators Gülşah Bayraktar and Tihomir Tomasic, respectively from Turkey and Slovenia, the best award certificates for their posters presented at this WG meeting. Finally, the next meeting, falling as first activity of the third grant period, was announced by the organizers, MC members from Malta Claire Shoemake and David Magri. It will be done as annual meeting in Malta on 18-19 October 2018.

All updates will be posted in the MuTaLig web www.mutalig.eu as soon as possible.

Catanzaro, April 4th 2018

Prof. Stefano Alcaro

Chair of COST Action CA15135

Photo gallery of the 2nd Working Group meeting



José Padron and Stefano Alcaro during the starting ceremony of the WG meeting.



Stefano Alcaro in the introduction session.



Hanoch Senderowitz, WG4 leader report.



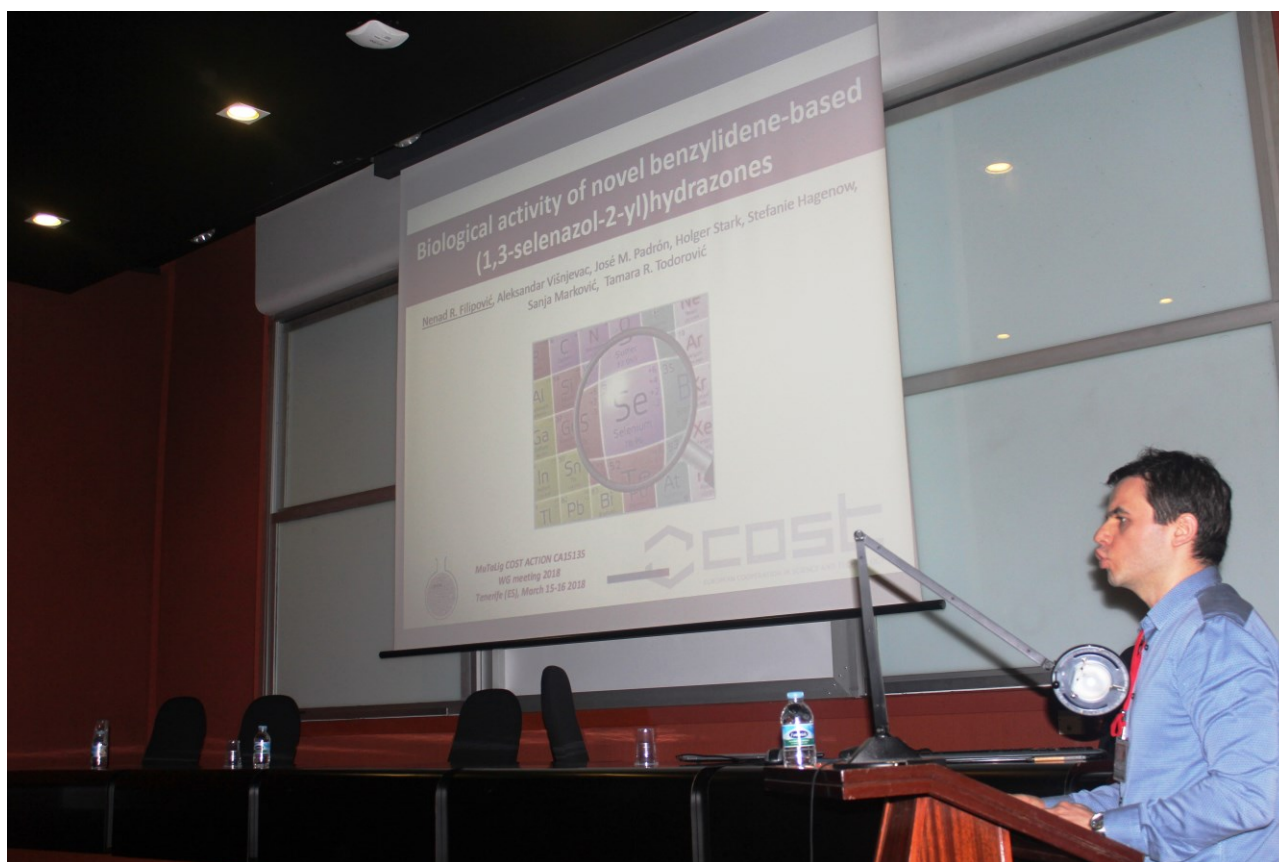
Sharon Bryant, WG3 leader report.



Maria Josè Camarasa, invited speaker WG1.



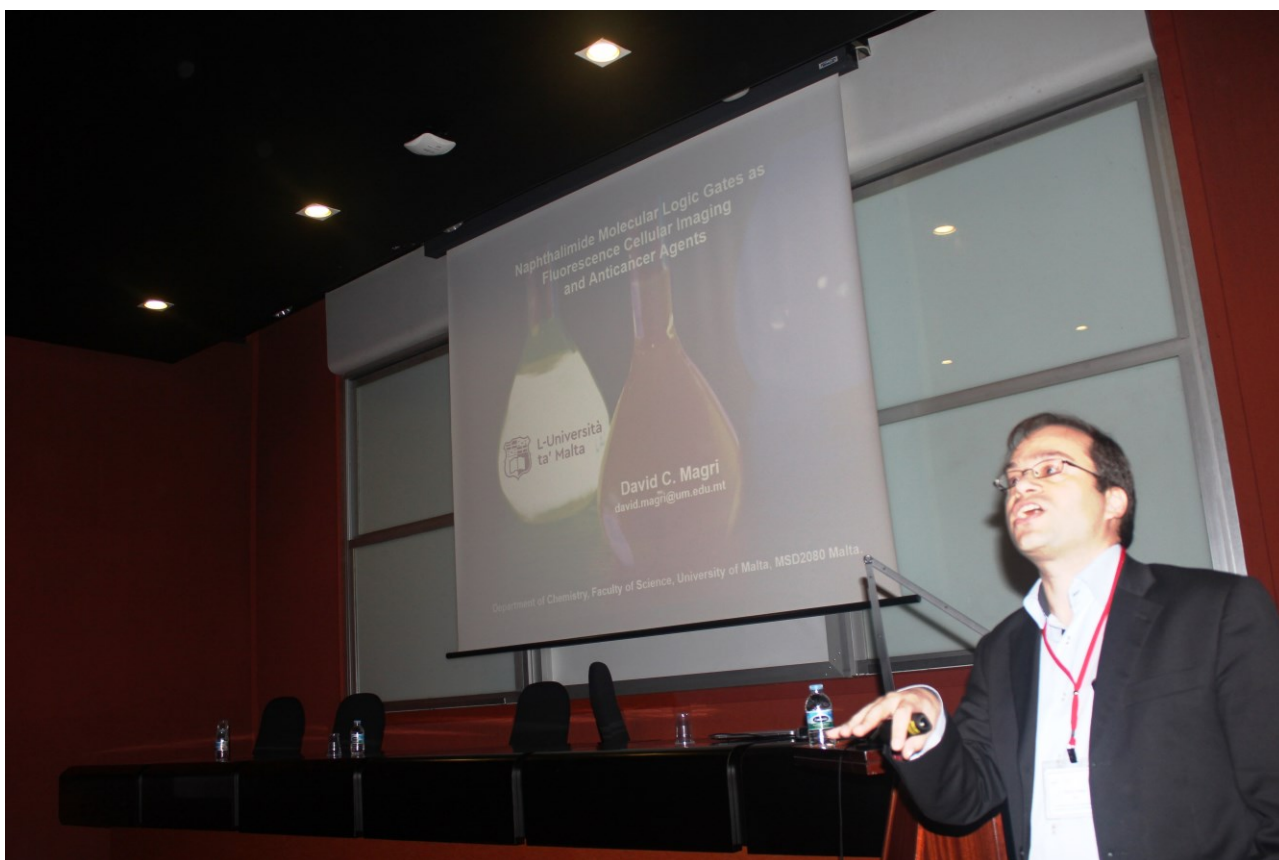
Holger Stark (MC member DE).



Nenad Filipović, WG1 speaker.



Oscar López, WG1 speaker.



David Magri (MC member ML), WG1 speaker.



Christian Muller, WG1 speaker.



Michael Gütschow, WG1 speaker.



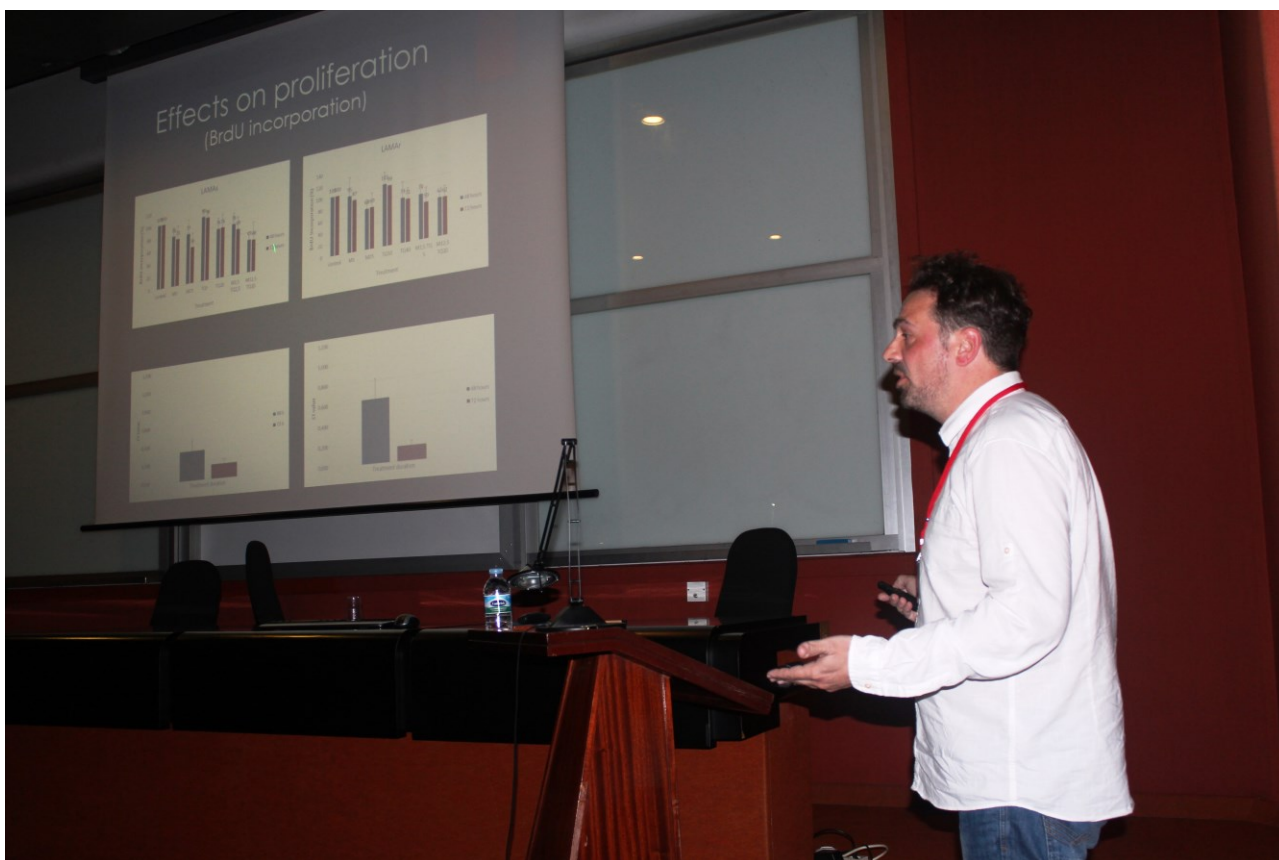
José Padron, organizer of the WG meeting.



Rami Aqeilan invited speaker WG2.



Gunay Yetik Anacak (MC member TK) , WG2 speaker.



Mirza Suljagic (MC member BA) WG2 speaker.



Susana Cristobal (MC member SE), WG2 speaker.



Wieslawa Agnieszka Fogel (MC member PL), WG2 speaker.

2 best pose compared to 4EY7 PDB model

Compound 2 binding mode

4EY7 PDB model

Stacking interaction could play a key role

11



Annachiara Gandini, WG3 speaker.



Christelle André (MC member LU), WG3 speaker.



Francesco Orofino, WG3 speaker.



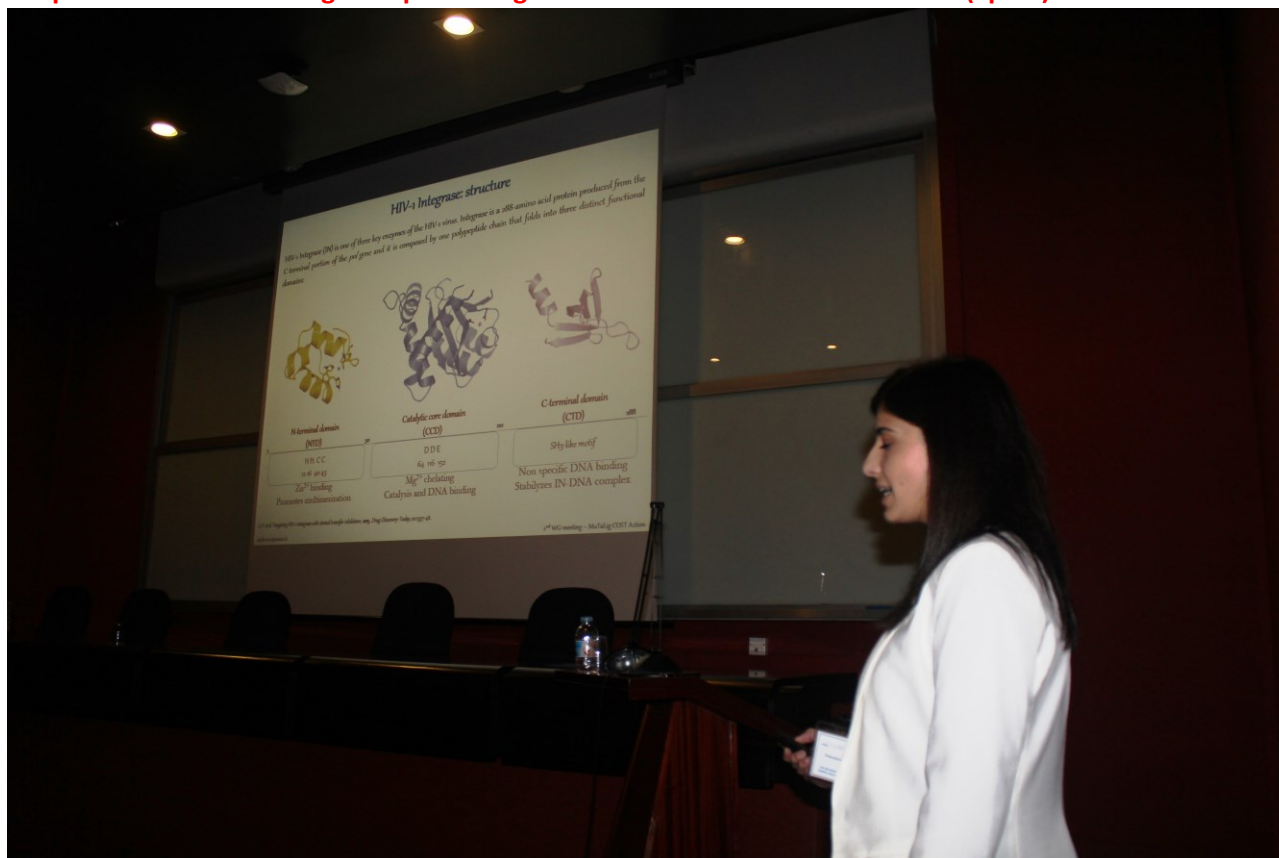
Thierry Langer (MC substitute A), invited speaker WG4.



Olli Pentikäinen (new MC member FI), WG4 speaker.



Andrea Danani (MC substitute CH) , WG4 speaker.



Francesca Alessandra Ambrosio, WG4 speaker.



Sanja Zivanovic, WG4 speaker.



Alfonso Garcia-Sosa (MC member EE, communication manager CA15135).



Poster session.



Poster session.



Simona Rapposelli (Associate Editor Frontiers in Chemistry).



Round table with Eugenio Gaudio, Fernanda Borges, Hanoch Senderowitz, Sharon Bryant and Danijel Kikelj.



Round table with Fernanda Borges Alfonso Garcia-Sosa and Stefano Alcaro.



Best poster award to Gülşah Bayraktar.



Best poster award to Tihomir Tomasic.



Group photo with all MuTaLig participants to the Tenerife WG meeting.



MuTaLig. COST Action speeds up the European Drug Discovery process