

Report of the 3rd Working Group of COST Action CA15135 – Paris (France) February 23-24 2019

The third WG meeting has been performed in the beautiful context of the Faculty of Pharmacy of the University Descartes in the center of Paris in two intensive days: February 23rd-24th 2019. It started with the introduction of the local organizers Prof. Luc Demage (MC member for France) and Prof. Philippe Belmont. The dean of the faculty Prof. Jean Louis Beaudeau appreciated the initiative to dedicate the 3rd WG meeting to young investigators. The Chair of the COST Action Stefano Alcaro briefly explained the purpose of the meeting and then the first session started with two plenary lectures of French experts of Medicinal Chemistry. The first speaker was Dr. Maité Sylla Iyarreta Veitía, pharmacist working at the CNAM institute in Paris. Her talk showed some chemical modifications of the bisacodyl drug for repurposing applications. The second speaker was Prof. Hervé Galons, editor in Chief of the European Journal of Medicinal Chemistry that currently hosts the special issue on the multi-target drug discovery. He focused his attention on kinases as relevant targets in the drug discovery programs. In particular, he showed some novel CDK1, CDK2, CDK4 and CDK9 inhibitors with respect to roscovitine. The second and the third sessions were globally devoted to young investigators performed in 13 out of 18 short communication. Lou Mateo, from France, and Paloma Carrillo, from Spain, displayed their novel results in the development of anticancer agents endowed with multi-targeting mechanisms of actions. The following session was devoted to anti neurodegenerative agents. Caroline Lanthier, from France, reported interesting about an interesting international collaboration in the field of conjugated agents against Alzheimer disease. Daniel Chavarria, from Portugal, presented a medicinal chemistry program starting from the piperine natural scaffold to obtain multi-targeting agents, especially against AChE and BuChE enzymes. Gülşah Bayraktar, from Turkey, reported results of a research project related to MTDL based on the hybridization of known anti-Alzheimer drugs (tacrine and donepezil) with the aim to get novel and better bioactive chemical entities. Francesco Mesiti, from Italy, presented novel compounds developed as anti-Parkinson's agents and based on the chromone scaffold and other derivatives able to inhibit MAO targets at nanomolar concentrations. SAR and binding assay experiments completed the study. Matthias Hoffmann, from Germany, showed results of a research activity carried out in the field of inhibitors of BuChE endowed with antioxidant properties in a polypharmacology fashion. In the third session a selected number of young investigators presented their activities in different fields of multi-target drug discovery. Azzurra Stefanucci, from Italy, reported about hybridized compounds active as modulator of endocannabinoid receptors. Then Elif Alançay, from Turkey, proposed an original application of ethnobotanical bioactive compounds in pharmacology. Then, Sara Garcia, from Portugal, reported a virtual screening study carried out with different chemical databases, including the Chemotheca, against the Hexokinase 2 target. Updates in the status of the Chemotheca were presented by Raffaella Catalano, from Italy. She also announced the creation of a video tutorial to be released within the third grant period by the Net4Science academic spin-off to all MuTaLig community. Stefano Raniolo, from Switzerland, showed the progress and the features of the novel GUI based FMAP tool for analyzing sophisticated molecular metadynamic simulations. This session was closed by Gniewomir Hof, from Poland, who presented some MTDL derivatives based on xanthine and tert-amylphenoxyalkyl piperidine scaffolds. After this session a funny jazz performance was carried out by students of the Faculty of Pharmacy at the Paris Descartes University. The CORE group meeting was performed including not only the standard composition (Chair, vice-Chair, WG leaders and delegates), but also two MC members: Vittorio Limongelli (MC member for Switzerland) and Gunay Yetik Anacak (MC member for Turkey). Their presence allowed the CORE group to plan for the activities to be proposed in the last grant period of the MuTaLig COST Action (May 2019 – Apr 2020). At the end of the day social program included a special walking tour followed by an extraordinary mini-cruise on the Senna guided by the organizers.

The second day started with the session "New ideas and updates from Working Groups" where five senior participants of the MuTaLig COST Action presented some novel results in their research activities.

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Nenad Filipović, MC substitute from Serbia, showed his results with novel anticancer organometallic MTDL compounds. Magdaléna Májeková, MC member for Slovakia, focused her attention on the pyridoindole scaffold as promising chemical fragment for the development of novel multi-target agents. David Magri, MC member for Malta, reported his last news about promising naphthalimide based molecular logic gate anticancer agents. Alfonso T. García-Sosa, MC member for Estonia and MuTaLig communication manager, suggested some updates and modifications to be implemented in the Chemotheca. Finally, Antony Burke, from Portugal, reported last news about MTDL agents based on the Isatin-Triazole hybridization. It is worth noting that most of the oral communications, given by young and senior investigators, included collaborations among different parties of the COST Action that was able to catalyze them from the beginning in 2016.

As usual, the meeting was concluded by a brief round table, where all MuTaLig participants were invited to discuss with WG leaders and delegates about the activities currently running. Also in this occasion an awarding ceremony, cared by the organizing committee, was performed. This time the awarding certificates were reserved for four young investigators: two oral communications, respectively performed by Elif Alançay (gold medal) and Lou Mateo (silver medal); and two for posters of Martina Durcik (#6 from Slovenia) and Pedro Soares (#20 from Portugal).

The meeting was then concluded wishing to all participant to meet again for the next appointment that will be held in Catanzaro in conjunction the Paul Ehrlich Euro-PhD Network as already posted at the link <http://medchem2019.unicz.it>.

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

Catanzaro, March 4th 2019


Prof. Stefano Alcaro

Chair of COST Action CA15135

Photo gallery of the 3rd WG meeting



Meeting venue at the Faculty of Pharmacy of the University Descartes (Paris).



Meeting venue at the Faculty of Pharmacy of the University Descartes (Paris).



The local organizers Luc Demage (MC member for France) and Philippe Belmont.



Aula Magna at the Faculty of Pharmacy of the University Descartes (Paris).



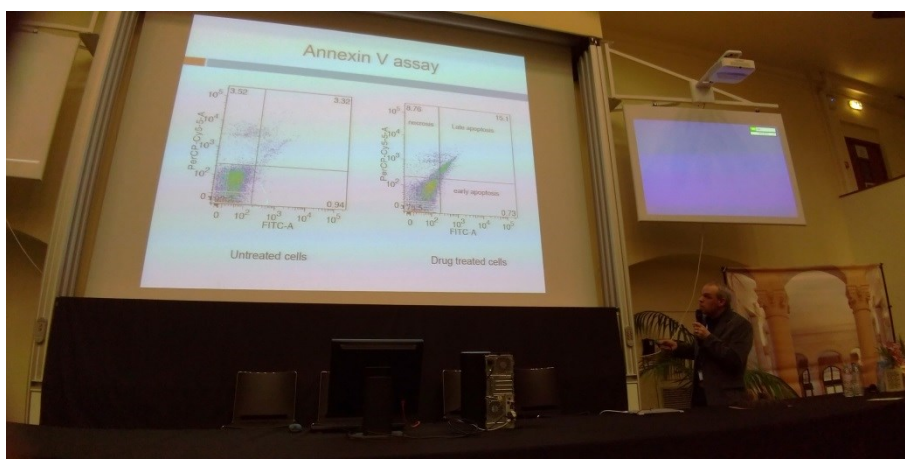
Jean Louis Beaudoux, Dean of the Faculty of Pharmacy of the University Descartes (Paris).



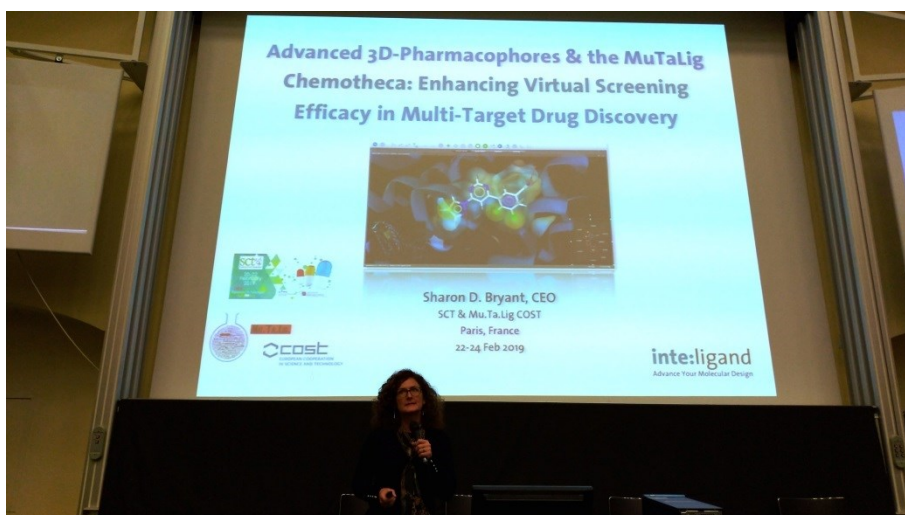
Introduction of the MuTaLig COST Action Chair Stefano Alcaro.



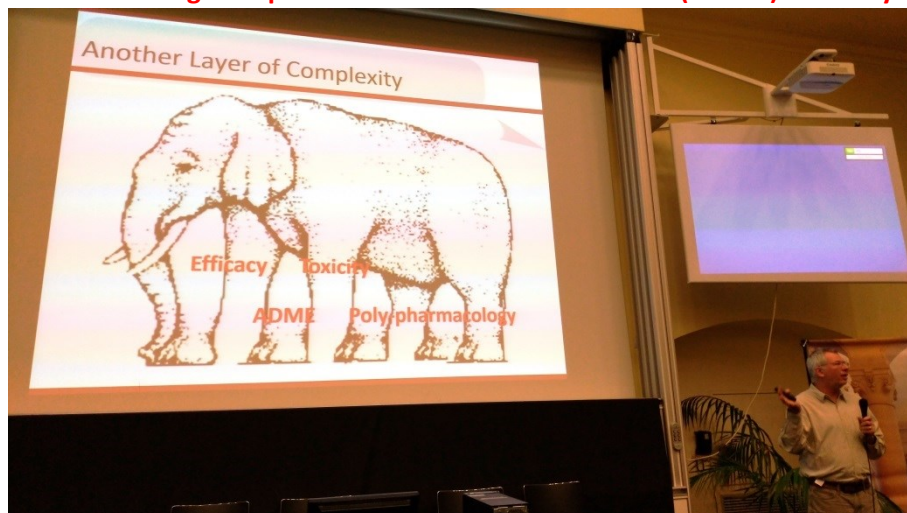
Vice-Chair of the MuTaLig COST Action Fernanda Borges.



The WG2 leader of the MuTaLig COST Action Eugenio Gaudio.



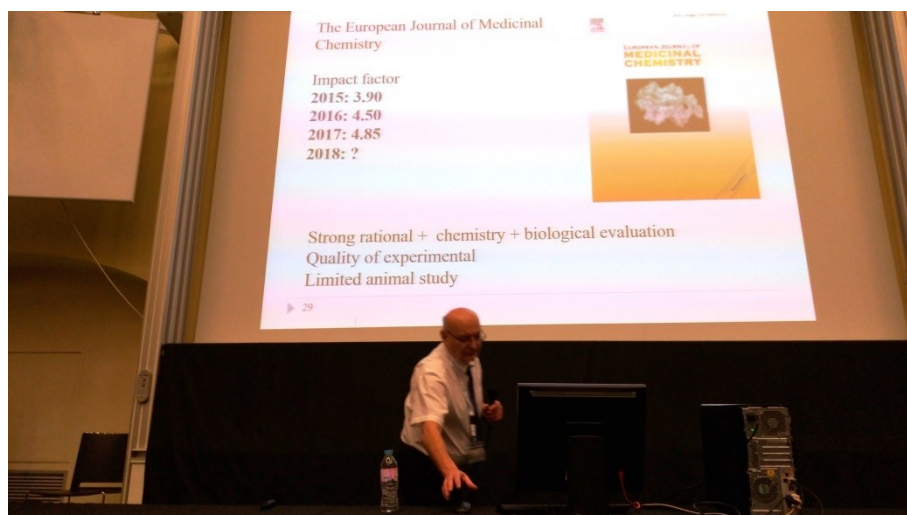
The WG3 leader of the MuTaLig COST Action Sharon Bryant.



The WG4 leader of the MuTaLig COST Action Hanoch Senderowitz.



The plenary speaker Maité Sylla Iyarreta Veitia.



The plenary speaker Hervé Galons.



The short communication of Daniel Chavarria.



The short communication of Raffaella Catalano.



The short communication of Caroline Lanthier



The short communication of Francesco Mesiti.



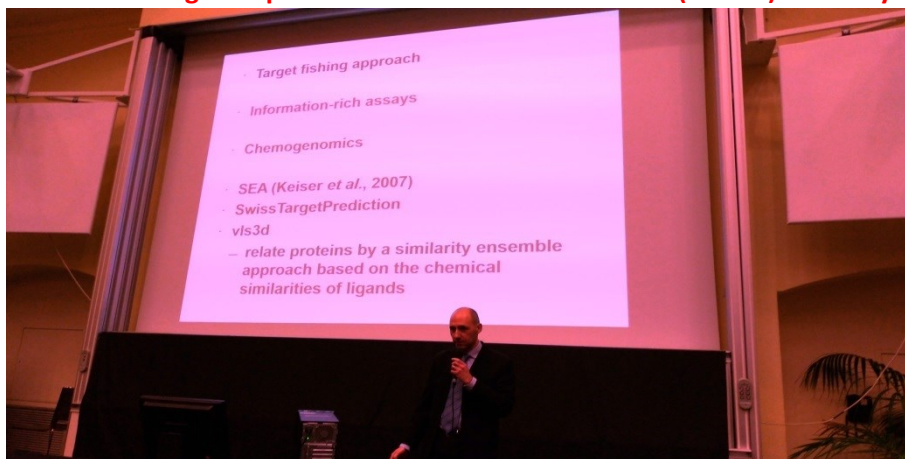
The short communication of Nenad Filipović.



The short communication of David Magri.



The short communication of Magdaléna Májeková.



The short communication of Alfonso García-Sosa.



Conclusions of the WG meeting coordinated by Danijel Kikelj (WG1 leader).



The organizers, the vice-Chair and the awarded young investigators.



Jazz performance by the students of the Faculty of Pharmacy at the Paris Descartes University.



The organizers visiting the Musée François Tillequin.



The organizers at the social program.



Social activity at the Faculty of Pharmacy of the Paris Descartes University.



Dinner with the speakers.



Group photo at the social tour.



The social tour symbol.

